The interpretation of nuclear observables in the laboratory frame in terms of the intrinsic deformation parameters $\beta$ and $\gamma$ is a classical theme in nuclear structure. Here we use the quadrupole invariants (Kumar [1]) to clarify the meaning and limitations of assigning definite values to these intrinsic parameters. In particular, we find that the parameter $\beta$ often has a non-negligible degree of softness, and that the angle $\gamma$ is usually characterized by large fluctuations, rendering its effective value not meaningful.

**Introduction.** The description of collectivity in nuclear structure has its roots in the unified model of Bohr and Mottelson [2]. The treatment of the dominant quadrupole correlations and the description of nuclear deformation have been often carried out in the intrinsic frame, and quadrupole shapes have been characterized by the intrinsic deformation parameters $\beta$ and $\gamma$. We commonly characterize a nucleus as prolate when $\gamma=0^\circ$, oblate when $\gamma=60^\circ$, fully triaxial when $\gamma=30^\circ$, prolate triaxial when $0^\circ < \gamma < 30^\circ$, and oblate triaxial when $30^\circ < \gamma < 60^\circ$. Quite often the same nucleus exhibits signatures of intrinsic structures with different values of $\beta$ and $\gamma$, a phenomenon known as shape coexistence [3]. The values of these deformation parameters can change along isotopic or isotonic chains, which we refer to as shape evolution or shape transition.

The intrinsic shape parameters are usually inferred from laboratory frame experimental values of observables such as excitation energies, $E2$ transitions, and spectroscopic quadrupole and magnetic moments. They can also be extracted from calculations performed in the laboratory frame. In both cases it is necessary to agree on a set of rules of transforming from the laboratory frame to an intrinsic frame. These existed since long ago; see for example in the work of Davidov and Filipov [4] and many others. However, the only rigorous method to relate the intrinsic parameters to laboratory-frame observables is provided by the so-called quadrupole invariants $Q^i$ of the second-rank quadrupole operator $\hat{Q}$ introduced by Kumar [1] (see also Ref. [2]). The calculation of $\beta$ and $\gamma$ requires the knowledge of the expectation values of the second- and third-order invariants defined, respectively, by $\hat{Q}^2 = \hat{Q} \cdot \hat{Q}$ and $\hat{Q}^3 = (\hat{Q} \times \hat{Q}) \cdot \hat{Q}$ (where $\hat{Q} \times \hat{Q}$ is the coupling of $\hat{Q}$ with itself to a second-rank operator). These invariants were recently applied to study the evolution of collectivity in cadmium isotopes [5].

However, it is not very meaningful to assign effective values to $\beta$ and $\gamma$ without also studying their fluctuations. Our goal is to go beyond the extraction of effective values of these intrinsic parameters and calculate their variances. To this end, we will calculate the variances $\sigma^2$ of $\hat{Q}^2$ and $\hat{Q}^3$ defined by

$$\sigma(\hat{Q}^2) = \langle (\hat{Q}^2)^2 \rangle - \langle \hat{Q}^2 \rangle^2$$

and

$$\sigma(\hat{Q}^3) = \langle (\hat{Q}^3)^2 \rangle - \langle \hat{Q}^3 \rangle^2 .$$

**Higher-order invariants.** The choice of the fourth-order invariant $\hat{Q}^4$ is unique [2] and we take it as $\hat{Q}^4 = (\hat{Q}^2)^2 = (\hat{Q} \cdot \hat{Q})^2$. This invariant was used in Refs. [2,5] to estimate the fluctuations in $\beta$ in heavy rare-earth nuclei. The fifth-order invariant is also unique and we take it as $\hat{Q}^5 = \hat{Q}^2 \hat{Q}^3 = (\hat{Q} \cdot \hat{Q})(\hat{Q} \times \hat{Q}) \cdot \hat{Q}$. The sixth order invariant is not unique. There are two choices but the adequate one to use in Eq. [2] is $\hat{Q}^6 = (\hat{Q}^3)^2 = (\hat{Q} \times \hat{Q})^2$.

To compute the expectation values of these invariants, we take advantage of the fact that our shell model codes incorporate naturally the projected Lanczos strength function method [10]. To make our analysis as simple as possible we confine our study to the ground states of even-even nuclei and to certain excited $0^+$ states which are of particular interest. The method we implement follows several steps:

(i) We perform a shell model calculation to obtain the wave function of the $|0^+\rangle$ state of interest.

(ii) We apply the axial quadrupole operator $\hat{Q}_{20}$ to this state to obtain

$$\hat{Q}_{20}|0^+\rangle = \text{SR}1(2^+)\frac{1}{2\sqrt{2}}|2^+(1)\rangle ,$$

where the constant SR1(2+) is defined such that the state $|2^+(1)\rangle$ is normalized. This state is not an eigenstate of the Hamiltonian but can be considered a “doorway” or a “sum rule” state (hence the notation SR).

(iii) Using (3) we have

$$\langle \hat{Q}^2 \rangle = 5\text{SR}1(2^+) .$$


(iv) We compute the reduced matrix element of $\hat{Q}$ in the
doorway state $|2^+(1)\rangle$ and define
\[ \langle \hat{Q} \rangle = \frac{1}{\sqrt{5}} |2^+(1)\rangle \langle \hat{Q} |2^+(1)\rangle . \] (5)

(v) Using $\langle \hat{Q}^3 \rangle = -5\sqrt{7/2} \langle \hat{Q}^3_2 \rangle$ together with $\Pi$ and $\Box$, we obtain
\[ \langle \hat{Q}^3 \rangle = \langle \hat{Q}^2 \rangle \langle \hat{Q} \rangle . \] (6)

(vi) Making a second iteration with $\hat{Q}_{20}$ on the doorway state in $\Box$, we produce three new normalized doorway states, $|0^+(2)\rangle$, $|2^+(2)\rangle$, and $|4^+(2)\rangle$, along with their corresponding projected sum rules $SR_2(0^+)$, $SR_2(2^+)$, and $SR_2(4^+)$. 

(vii) The expectation value of the fourth-order invariant is then calculated from
\[ \langle \hat{Q}^4 \rangle = 5 \langle \hat{Q}^2 \rangle SR_2(0^+) . \] (7)

(viii) Iterating again with $\hat{Q}_{20}$ on the doorway state $|2^+(2)\rangle$, we obtain new doorway states, $|0^+(3)\rangle$, $|2^+(3)\rangle$, and $|4^+(3)\rangle$, and their corresponding projected sum rules $SR_3(0^+)$, $SR_3(2^+)$, and $SR_3(4^+)$. 

(ix) Using the doorway states in (viii), we calculate the expectation value of the sixth-order invariant from
\[ \langle \hat{Q}^6 \rangle = 5 \langle \hat{Q}^2 \rangle SR_2(2^+) SR_3(0^+) . \] (8)

(x) The expectation value of the fifth-order invariant can also be calculated using
\[ \langle \hat{Q}^5 \rangle = 5 \langle \hat{Q}^2 \rangle SR_2(0^+)^{1/2} SR_2(2^+)^{1/2} SR_3(0^+)^{1/2} \times |0^+(2)\rangle |0^+(3)\rangle \langle \hat{Q}^3 \rangle . \] (9)

In Fig. $\Pi$ we present a schematic diagram of how we produce all the doorway states that are needed to compute the expectation values of the quadrupole invariants up to sixth order.

(xi) The final expressions for the width-to-average ratios for $\hat{Q}^2$ and $\hat{Q}^3$ are given by
\[ \frac{\sigma(\hat{Q}^2)}{\langle \hat{Q}^2 \rangle} = \left( \frac{5 SR_2(0^+)}{\langle \hat{Q}^2 \rangle} - 1 \right)^{1/2} , \] (10)
and
\[ \frac{\sigma(\hat{Q}^3)}{\langle \hat{Q}^3 \rangle} = \left( \frac{5 SR_2(2^+) SR_3(0^+)}{\langle \hat{Q}^2 \rangle \langle \hat{Q} \rangle^2} - 1 \right)^{1/2} . \] (11)

The intrinsic quadrupole moment $Q_0$ and effective values of the Bohr-Mottelson shape parameters $\beta$ and $\gamma$ can be calculated from the expectation values of the second- and third-order invariants using
\[ Q_0 = \sqrt{\frac{16\pi}{5} \langle \hat{Q}^2 \rangle^{1/2}} , \] (12)
\[ \beta = \frac{4\pi}{3\hbar^2} \langle \hat{Q}^2 \rangle^{1/2} A^{5/3} , \] (13)
with $r_0=1.2$ fm, and
\[ \cos 3\gamma = -\sqrt{\frac{7}{2}} \frac{\langle \hat{Q}^3 \rangle}{\langle \hat{Q}^2 \rangle^{3/2}} = -\sqrt{\frac{7}{2}} \frac{\langle \hat{Q} \rangle}{\langle \hat{Q}^2 \rangle^{1/2}} . \] (14)

To gain insight into how well defined are these effective shape parameters, we also calculate their variances in the framework of the shell model. These variances, as we will show below, tell us to what extent the intrinsic shapes are blurred in the laboratory frame, and whether and when the very notion of shape makes sense at all.

**Fluctuations of $\beta$.** The standard deviation $\Delta\beta$ of the effective $\beta$ parameter is easily determined from the standard deviation of $\hat{Q}^2$
\[ \frac{\Delta\beta}{\beta} = \frac{1}{2} \frac{\sigma(\hat{Q}^2)}{\langle \hat{Q}^2 \rangle} . \] (15)

The fluctuations of $\beta$ have been studied in Refs. [1.12] for the ground state and the deformed excited band of $^{42}$Ca using large-scale shell-model calculations, and in Ref. [12] for a series of neodymium and samarium isotopes, using the auxiliary-field quantum Monte Carlo (AFMC) approach. Before discussing these and our results, we note that there is a limit in which the quadrupole shape parameters are sharply defined; this limit corresponds to

**FIG. 1.** Schematic diagram demonstrating the computation of the quadrupole invariants up to sixth order. Except for the initial $0^+$ states, all states are sum rule or doorway states, which are not eigenstates of the Hamiltonian but have good spin and parity. Each arrow represents the action of the axial quadrupole $\hat{Q}_{20}$ operator between the two states which it connects. The red wiggly line denotes the overlap between the two different $0^+$ doorway states.
Elliott’s $SU(3)$ model [13], when the variances of $\langle Q^2 \rangle$ and $(Q^3)$ are strictly zero, as are the variances of $\beta$ and $\gamma$. This $SU(3)$ limit can be used to test our calculation of the variances, which indeed vanish up to numerical accuracy. Shell model calculations of $\sigma(Q^2)/(Q^2)$ for the ground state and the first excited $0^+$ of $^{42}$Ca were reported in Ref. [12], with values of 1.96 and 0.40, respectively. It is thus obvious that it is not meaningful to specify a value for the $\beta$ parameter in the ground state. In contrast, the effective value of $\beta$ for the excited state has only a 20% uncertainty, and we can interpret this state as a $\beta$-soft state. In the AFMC calculation of Ref. [3], values of $\sigma(Q^2)/(Q^2)$ ranging from 0.57 to 0.27 were obtained for $\beta$ values ranging from 0.106 to 0.230. The effective value of $\beta$ and its variance were found to be anti-correlated, with larger values of $\beta$ associated with smaller fluctuations.

**TABLE I. Effective deformation parameters $\beta$, $\gamma$, and their fluctuations for the nuclei discussed in the text.**

| Nucleus | $\Delta \beta$ | $\sigma(Q^2)/(Q^2)$ | $\gamma$ | $\sigma(Q^3)/(Q^3)$ | $\delta_{\text{sv}}$ | $\sigma(\cos 3\gamma)$ | $\gamma$ range |
|---------|----------------|----------------------|--------|----------------------|----------------|------------------------|--------------|
| $^{20}$Ne | 0.02 | 0.07 | 0.24 | 3$^\circ$ | 0.44 | 0.10 | 0.09 | 0$^\circ$ - 9$^\circ$ |
| $^{22}$Ne | 0.59 | 0.08 | 0.27 | 13$^\circ$ | 0.53 | 0.12 | 0.21 | 2$^\circ$ - 18$^\circ$ |
| $^{24}$Mg | 0.60 | 0.07 | 0.25 | 18$^\circ$ | 0.42 | 0.07 | 0.21 | 12$^\circ$ - 22$^\circ$ |
| $^{28}$Si | 0.46 | 0.09 | 0.41 | 50$^\circ$ | 0.91 | 0.32 | 0.42 | 38$^\circ$ - 60$^\circ$ |
| $^{30}$Cr | 0.31 | 0.06 | 0.41 | 13$^\circ$ | 0.84 | 0.32 | 0.30 | 0$^\circ$ - 20$^\circ$ |
| $^{34}$Si | 0.18 | 0.10 | 1.07 | 40$^\circ$ | 3.61 | 1.72 | 1.52 | 0$^\circ$ - 60$^\circ$ |
| $^{36}$Sr | 0.42 | 0.08 | 0.37 | 40$^\circ$ | 1.14 | 0.17 | 0.53 | 30$^\circ$ - 60$^\circ$ |
| $^{38}$Sr | 0.30 | 0.07 | 0.43 | 27$^\circ$ | 5.46 | 0.46 | 0.87 | 0$^\circ$ - 45$^\circ$ |
| $^{40}$K | 0.31 | 0.07 | 0.43 | 21$^\circ$ | 1.63 | 0.36 | 0.67 | 0$^\circ$ - 34$^\circ$ |
| $^{68}$Ni | 0.11 | 0.06 | 1.10 | 36$^\circ$ | 5.70 | 1.96 | 1.58 | 0$^\circ$ - 60$^\circ$ |
| $^{69}$Zn | 0.19 | 0.05 | 0.55 | 38$^\circ$ | 1.96 | 0.28 | 0.78 | 23$^\circ$ - 60$^\circ$ |
| $^{64}$Cr | 0.29 | 0.05 | 0.36 | 16$^\circ$ | 0.94 | 0.28 | 0.39 | 0$^\circ$ - 24$^\circ$ |
| $^{70}$Zn | 0.23 | 0.06 | 0.50 | 29$^\circ$ | 13.57 | 2.45 | 0.77 | 12$^\circ$ - 45$^\circ$ |
| $^{76}$Ge | 0.25 | 0.03 | 0.27 | 28$^\circ$ | 3.59 | 1.0 | 0.45 | 18$^\circ$ - 36$^\circ$ |

In the upper-right part of Table I we show our results for the parameter $\beta$ and its fluctuations for several nuclei in the $sd$ shell with the interaction USD-A [14], in the $pf$-shell with KB3 [13], and in the $sd-pf$ shell with the interactions SDPFU-MIX [16] and SDPFU [17]. In all cases we compute the mass quadrupole with a Dufour-Zuker isoscalar effective factor of 1.77 [18]. The results pertaining to the charge distribution are very similar. In almost all cases we find values of $\Delta \beta$ around 20% or less, and the reference to an intrinsic structure is justified.

Two rows of Table I are devoted to $^{34}$Si. This neutron-rich isotope is doubly magic [19], and its first excited state is a $0^+$ state [20]. The states shown in Table I confirm that the ground state is indeed spherical, and with a value of $\frac{\sigma(Q^2)}{(Q^2)} = 1.07$, the notion of a well-defined intrinsic state is meaningless. In contrast, the excited $0^+$ state can clearly be interpreted as deformed. The isotope $^{44}$S belongs to the $N = 28$ Island of Inversion (IoI) and its collective character has been much debated [21]. Here we find that the ground state and the first excited $0^+$ state in $^{44}$S are both deformed with similar effective values of $\beta$.

Fluctuations of $\gamma$. Next we calculate and interpret the uncertainties in the $\gamma$ angle which arise from the non-vanishing variances of $(Q^2)$ and $(Q^3)$. In particular, we compute the variance of $\cos 3\gamma$ using

$$\sigma^2(\cos 3\gamma) = \frac{\sigma^2(Q^3)}{(Q^3)^2} + \frac{9\sigma^2(Q^2)}{(Q^2)^2} - \frac{3(\langle Q^5 \rangle - \langle Q^3 \rangle \langle Q^2 \rangle)}{(Q^5) \langle Q^2 \rangle}.$$  

Eq. (16) requires the knowledge of all the moments up to the sixth order, including the fifth-order invariant that appears in the covariance term of $\hat{Q}^3$ and $\hat{Q}^4$, which we denote by $-3\hat{Q}^3\hat{Q}^4$. Eq. (16) becomes singular for $\gamma = 30^\circ$ (i.e., $(Q^3) = 0$), in which case the relevant formula is

$$\sigma(\cos 3\gamma) = \sqrt{\frac{7}{2} \left( \frac{Q^6}{(Q^3)^{3/2}} \right)}.$$  

In upper-left part of Table I we list the results for the effective values of $\gamma$ and its fluctuations. We compute the standard deviation $\sigma(\cos \gamma)$ using Eq. (16), in which the value of $(Q^3)$ is calculated from Eq. (9). We then compute the values of $\cos^{-1}(\cos 3\gamma \pm \sigma(\cos 3\gamma))$ and determine the corresponding range of the values of $\gamma$. We often find values which are outside the allowed cosine range, in which case we set $\gamma = 0^\circ$ or $\gamma = 60^\circ$. The ranges of $\gamma$ values in the table are surprising; in most cases they span the complete prolate or oblate sectors, in which case it is at least meaningful to characterize the nucleus as prolate or oblate. Overall, the $\gamma$ degree of freedom is so soft that it is no longer meaningful to assign to it an effective value. We have found only one axial nucleus, $^{20}$Ne, and a mildly triaxial nucleus, $^{24}$Mg, in which the fluctuations of $\gamma$ do not blur its effective value. Both nuclei are close to Elliott’s $SU(3)$ limit.

Shape coexistence in $^{68}$Ni revisited. With $N = 40$ neutrons and $Z = 28$ protons, $^{68}$Ni is an example of a nucleus far from stability that displays shape coexistence. Its ground state is spherical, and it has two excited $0^+$ states, one that is considered to be a weakly deformed oblate and a second that is a strongly deformed prolate. These states have been the object of several recent experimental studies [22, 23].

We explore the nature of these three $0^+$ states using the quadrupole invariants. The results using the shell model wavefunctions computed with the LNPS valence space and effective interaction [24] are summarized in Table I and in Fig. 2. With $\sigma(Q^2) \sim (Q^2)$ and $\gamma$ completely undefined, the ground state of $^{68}$Ni is clearly spherical. The first excited $0^+$ is very soft in the $\beta$ parameter, but
we can perhaps still call it deformed, even though its underlying intrinsic structure is fragile. One could call it oblate, although the $\gamma$ values cover a non-negligible fraction of the prolate sector. The second excited $0^+$ has a larger and relatively more well-defined value of $\beta$. The spread in $\gamma$ is very large ($24^\circ$), but at least it remains confined into the prolate sector.

We also include in Table I results for $^{64}$Cr, a nucleus at the center of the $N = 40$ IoI, to confirm that they are nearly identical to those of the well-deformed excited $0^+$ band-head of $^{68}$Ni. This provides another evidence of the role of shape coexistence in doubly magic nuclei as the role of shape coexistence in doubly magic nuclei as the

**Shape fluctuations in $^{76}$Se.** In a very recent article entitled “Triaxiality in $^{76}$Se” [20], Kumar’s invariants were extracted from the experimental data and from shell model calculations. This article states “from the CI calculations higher-order invariants can be constructed to assess the degree of rigidity in $\langle Q^2 \rangle$ and cos3$\gamma$. It is found that the jj44b calculations correspond to a very $\gamma$-soft structure, whereas the JUN45 calculations result in a more rigid configuration,” without providing more details. We calculated the dispersions in $\langle Q^2 \rangle$ and $\gamma$ to be, respectively, 27(36)% and 36(35)° for both interactions.

**Hybrids.** There are even more peculiar manifestations of intrinsic shapes when inferred from laboratory frame observables. We focus on $^{32}$Mg, which is known to have a very low excited $0^+$ state, recently found at Isolde [27]. Ref. 16 concluded that the ground state is mainly a mixture of a deformed $(2p - 2h$ across $N = 20$) and a superdeformed $(4p - 4h$ configurations, whereas the excited $0^+$ state is mainly a mixture of a superdeformed and a spherical $(0p - 0h$) configurations. It is interesting to find out how these complex wavefunctions are viewed through the lens of Kumar’s invariants. The pure $2p - 2h$ band has $\beta = 0.48 \pm 0.06$ and $\gamma = (20^{+19}_{-13})^\circ$; a well deformed prolate shape which is $\gamma$-soft. The pure $4p - 4h$ band has in turn $\beta = 0.66 \pm 0.07$ and $\gamma = (15^{+5}_{-8})^\circ$ a mildly triaxial superdeformed structure with a narrow $\gamma$ dispersion, suggesting that the $4p - 4h$ state is near the quasi-$SU(3)$ limit. What eventually matters is the behavior of the physical mixed state. We find that the ground state has $\beta = 0.48 \pm 0.13$ and $\gamma = (17^{+10}_{-14})^\circ$, thus its deformed character survives even though $\beta$ has a significant spread and $\gamma$ explores the complete prolate sector. The real hybrid is the excited $0^+$ state, which has $\beta = 0.50 \pm 0.20$ and $\gamma = (10^{+11}_{-10})^\circ$, and is thus very soft in both parameters. This is not so surprising considering the exotic mixture of spherical and superdeformed structures.

**Conclusion.** It may well happen that the angle $\gamma$ has well-defined values in heavier strongly deformed nuclei, or when $SU(3)$ is approximately a good symmetry. However, in the mass regions we explored, we found only two such examples, $^{20}$Ne and $^{24}$Mg. In general, it is more meaningful to describe the state in terms of a probability distribution of intrinsic shapes [29] rather than assigning particular values to $\beta$ and $\gamma$. Our analysis has direct consequences regarding the interpretation of laboratory frame results (experimental or theoretical) in the $(\beta, \gamma)$ plane of intrinsic shapes, as is often done in mean-field (and beyond) approaches [29]. We find that it is particularly important to estimate the dispersion in $\gamma$ before assigning to it a well-defined value. This brings us back to Proposition 7 of the Tractatus: Whereof one cannot speak, thereof one must be silent [30].
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