Global Calculations of Ground-State Axial Shape Asymmetry of Nuclei

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Important insight into the symmetry properties of the nuclear ground-state (gs) shape is obtained from the characteristics of low-lying collective energy-level spectra. In the 1950s, experimental and theoretical studies showed that in the gs many nuclei are spheroidal in shape rather than spherical. Later, a hexadecapole component of the gs shape was identified. In the 1970–1995 time frame, a consensus that reflection symmetry of the gs shape was broken for some nuclei emerged. Here we present the first calculation across the nuclear chart of axial symmetry breaking in the nuclear gs. We show that we fulfill a necessary condition: Where we calculate axial symmetry breaking, characteristic gamma bands are observed experimentally. Moreover, we find that, for those nuclei where axial asymmetry is found, a systematic deviation between calculated and measured masses is removed.

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Much about nuclear properties at excitation energies up to a few MeV is learned by calculating the nuclear ground-state shape and the low-lying energy levels and other properties corresponding to this shape. There are innumerable theoretical nuclear-structure studies in limited regions of nuclei that locally describe known properties well. However, for many important applications, such as modeling the properties of the hundreds of different fission-fragment nuclei in a nuclear reactor or the properties of the thousands of nuclei involved in stellar nucleosynthesis processes, for example the rapid-neutron capture process, models that have predictive power and are global, unified, and universal are required. By global and unified we mean that the model describes nuclei from very light (normally ^{16}O) to the heaviest nuclei with a consistent set of parameters for all studied properties and all nuclei. By universal we mean that several nuclear properties such as nuclear ground-state masses, shapes, low-lying energy levels, β-decay transition rates, and fission barriers are well described by the model. At present, there are only two models on record that are global, unified, and universal, namely the Hartree-Fock-Bogoliubov model as implemented by the Pearson-Goriely collaboration [1,2] and the macroscopic-microscopic finite-range droplet model (FRDM) or finite-range liquid-drop model (FRLDM) [3–6]. As shown in the literature, the FRDM and FRLDM have been more universally applied [4,6]. In terms of nuclear masses, all three approaches extrapolate to previously unknown regions of nuclei with encouraging stability [2,4].

Although axial asymmetry of rapidly rotating nuclei has been studied for a long time, less attention has been given to axial asymmetry in the nuclear ground state, and previous results are very sparse. Several different calculations, for example Refs. [7–9], predict that some neutron-deficient rare-earth nuclei with $N = 76$ are triaxially deformed in the ground state. However, very different results are obtained for the magnitude of the effect. For ^{138}Sm, it is found that axial asymmetry lowers the ground-state energy by 0.7 MeV in Ref. [9] but only by about 0.2 MeV in Refs. [7,8]. Furthermore, the models were not applied globally throughout the chart of the nuclides. Therefore, no specific general conclusions could be drawn. This is

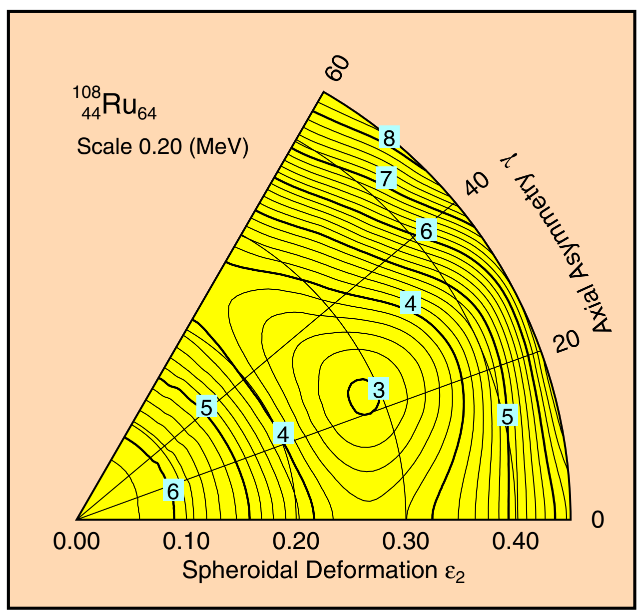

FIG. 1 (color online). Calculated potential-energy surface versus ε_2 and γ for ^{108}Ru. Each combination of the radial coordinate (ϵ_2) and angle (γ) corresponds to a specific nuclear shape. The tip of the sector corresponds to a spherical shape. Along the horizontal line at $\gamma = 0$, the shapes grow increasingly prolate with increasing ϵ_2, and, along the line at $\gamma = 60$, the shapes grow increasingly oblate with distance from the tip.

also hinted at by the comment: "one can therefore conclude that triaxial shapes for medium-mass and heavy nuclei are rather rare—if they exist at all" in a comprehensive review article on nuclear shapes [10].

Here we present somewhat different and more conclusive results obtained in our unified, universal FRLDM, which has very well-tested properties and excellent extrapolatability. We perform the first global calculation of axial asymmetry of the static nuclear ground-state shape and are, therefore, able to draw specific conclusions on this asymmetry. A complete description of the model and extensive discussions of its previous accomplishments can be found in Refs. [3,4,11–14]. More recently, an improved, very detailed description of the fission barrier was obtained within the model [6,15]. For consistency, we use here the parameter set obtained in this latest study. However, the effect of the new parameters on the results presented here is minute; the main effect is on fission barrier heights. We also revisit our previous results on reflection asymmetry [3]. By analyzing the effect of reflection asymmetry on the nuclear ground-state mass in the same format as applied here to axial asymmetry, we better understand the significance of the earlier and current results on symmetry breaking.

We calculate three-dimensional nuclear potential-energy surfaces for 7206 nuclei from the proton drip line to the neutron drip line for nuclei from nucleon number $A = 31$ (below which the effect of axial asymmetry is negligible) to $A = 290$. For compatibility with previous studies, we use the so-called Nilsson perturbed-spheroid shape parametrization or ε parametrization. We use the deformation grid $\varepsilon_2 = (0.0, 0.025, \ldots, 0.45)$, $\gamma = (0.0, 2.5, \ldots 60.0)$, and $\varepsilon_4 = (-0.12, -0.10, \ldots, 0.12)$, altogether 6175 grid points. When $\varepsilon_4 = 0$, the shape is exactly ellipsoidal, that is, the nuclear surface is described by the equation:

$$\frac{x^2}{a^2} + \frac{y^2}{b^2} + \frac{z^2}{c^2} = 1. \tag{1}$$

For $\gamma = 0$, the shape is rotationally symmetric around the z axis, that is, $a = b$, and for $\gamma = 60°$ it is rotationally symmetric around the x axis, that is, $b = c$. For intermediate values of γ, the shape is axially asymmetric, or triaxial, with $a < b < c$. When $\varepsilon_4 \neq 0$, a hexadecapole component is superimposed on the shape described by Eq. (1). The definition of the shape given in Ref. [3] assures that the hexadecapole component transforms like a tensor. We find that some nuclear ground states are neither oblate nor

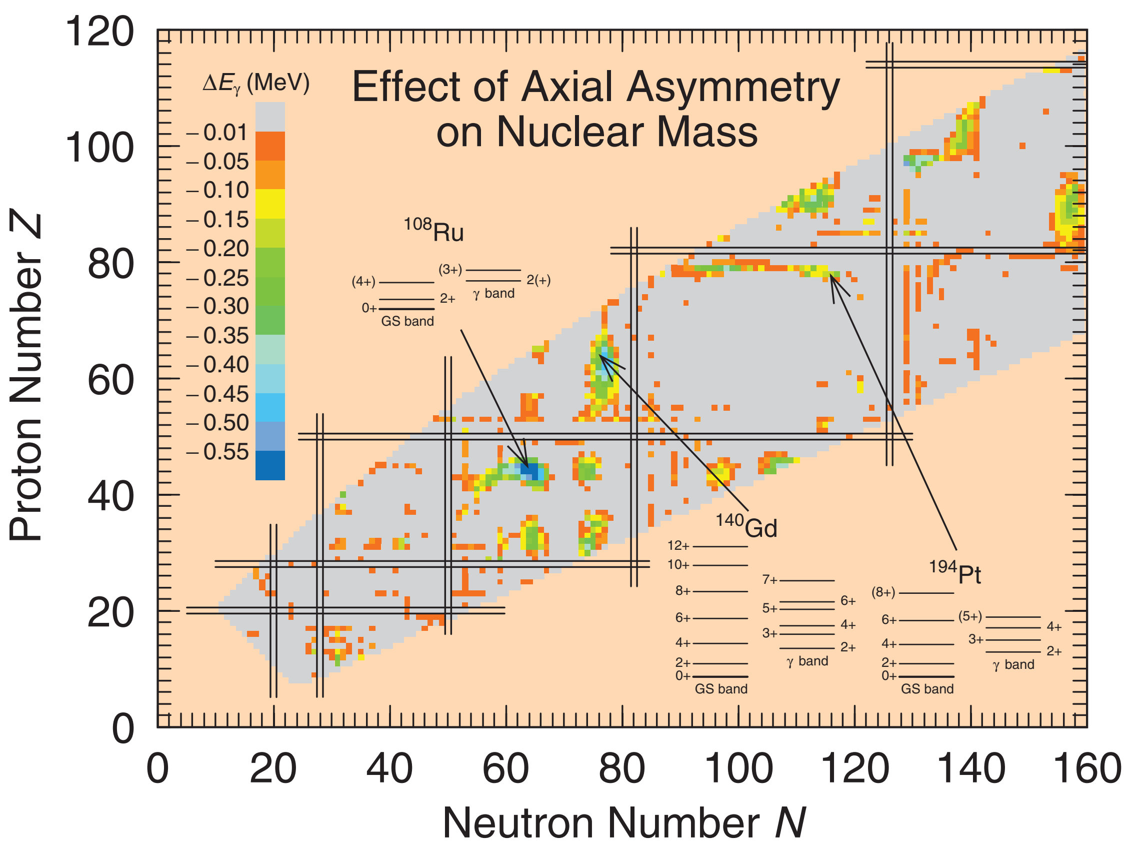

FIG. 2 (color). Calculated lowering of the nuclear ground-state energy when axial symmetry is broken, relative to calculations limited to axially symmetric shapes only. Near the center of each of the three regions of axially asymmetric nuclei accessible to experiment, we show a measured spectrum [16]. All three spectra exhibit characteristic γ bands. This can be thought of as a necessary condition: γ bands should be present when the shapes are axially asymmetric.

prolate. Instead, the ground-state minimum is axially asymmetric in shape as shown in Fig. 1 for ^{108}Ru. The energy is relative to the spherical macroscopic FRLDM.

In Fig. 2, we plot the effect of axial asymmetry on the ground-state mass for 5900 nuclei from $A = 31$ to $N = 160$. We have studied an additional 1306 nuclei above $N = 160$. These are not included in Fig. 2, since triaxial ground states of nuclei with $N > 160$ are found only at such a large neutron excess that such nuclei are of marginal interest. Specifically, Fig. 2 shows how much lower the axially asymmetric ground state is relative to the lowest minimum obtained in a calculation restricted to axial symmetry. Colder, bluer colors indicate a stronger effect and a more well-established axial asymmetry. The effect of axial asymmetry on the zero-point energy is not modeled.

The magnitude of γ deformation of nuclei in their ground states is not very directly measurable in experiments. However, we would expect (in fact, it is *necessary*) that γ bands are present in nuclei for regions of the nuclear chart where the ground-state shape is axially asymmetric. Second, if our results are realistic, we would also expect that calculated masses are improved when we account for axial asymmetry.

In Fig. 2, the two regions where we obtain the largest effects lie close to stable nuclei. These regions are centered around $Z = 44$, $N = 64$ and $Z = 62$, $N = 76$, and experimental level spectra are available for some of these nuclei [16]. We show in Fig. 2 one representative level spectrum for each of these two regions. Both exhibit typical γ bands, which are related to axial shape asymmetry. Many other nearby nuclei also exhibit γ bands [16]. Another experimentally accessible region where γ bands are observed, but for which the effect of axial asymmetry on the calculated ground-state mass is smaller, is the Pt region, around $Z = 78$ and $N = 116$.

To investigate how axial asymmetry affects calculated nuclear masses for the nuclei where we calculate a non-negligible effect, we take our published global nuclear mass table [3], which did not consider axially asymmetric shapes, and add the correction displayed in Fig. 2 to the previously calculated ground-state masses. There are 159 nuclei with $N \leq 160$ for which the mass is lowered

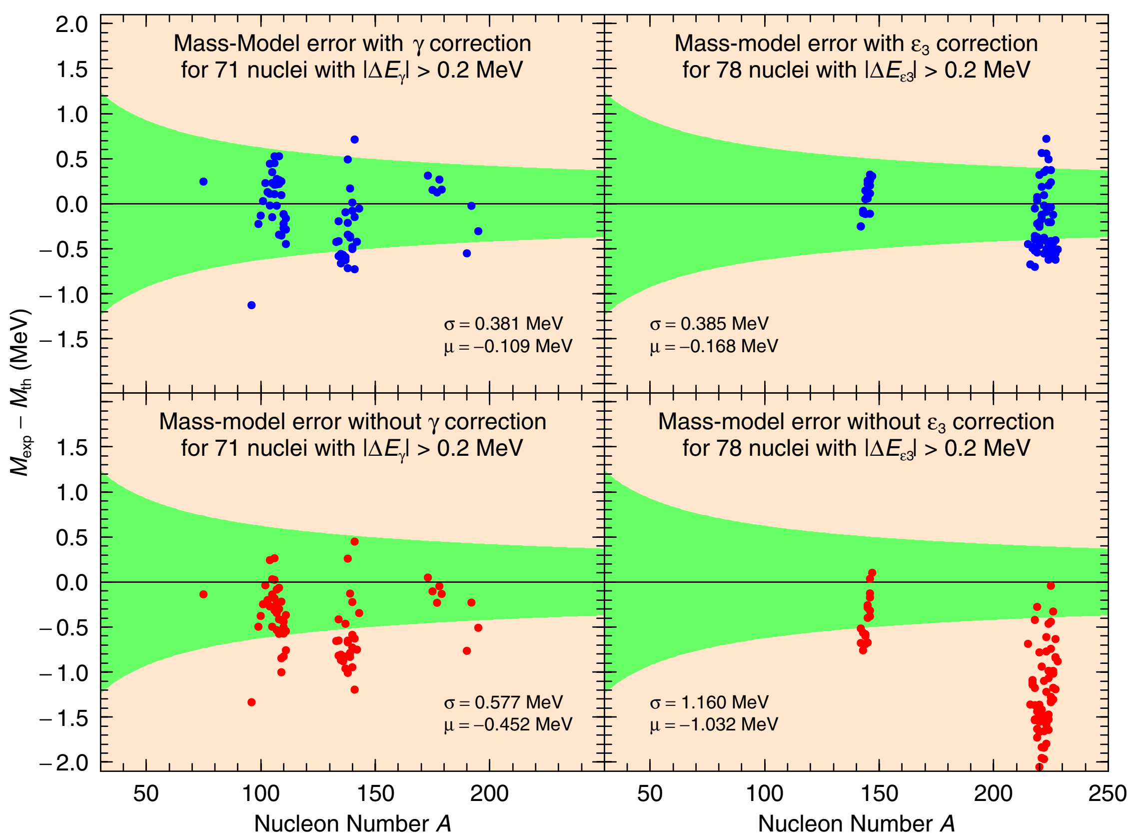

FIG. 3 (color online). Difference between experimental masses and calculated masses, where the calculations (i) do not consider asymmetric shapes (bottom two panels) or (ii) do consider asymmetric shapes (top two panels) versus the number of nucleons in the nucleus. The plots include only nuclei where we find that axial or reflection asymmetries lower the ground-state mass by more than 0.2 MeV. The left two panels are for axial asymmetry; the right two panels are for reflection asymmetry. The dark gray (green) regions indicate the FRDM 1σ deviation, which depends on A; see Ref. [3] for precise definitions. The systematic deviations present in the lower two panels disappear when axial and reflection asymmetries are included. Because axial and reflection asymmetry mix different single-particle states, we do not think that a simultaneous variation of both shape types would change the above results.

by at least 0.2 MeV, which is equal to the separation between the contour lines in Fig. 1 and which we selected as the cutoff for a non-negligible effect. We also checked cutoffs of 0.1 and 0.3 MeV and find that our results are stable with respect to the exact cutoff choice. For a cutoff of 0.2 MeV, experimental masses are available for 71 nuclei [17]. For these, we present in the left part of Fig. 3 the differences between experimental masses and masses calculated without considering axial shape asymmetry (bottom panel) and with consideration of axially asymmetric shapes (top panel). Also given in the figure are results of a statistical determination of the model error σ and mean deviation μ between experimental and calculated masses for these nuclei. Roughly, $\sigma_{\mathrm{th},\mu=0}$ is similar to a root-mean-square (rms) error but is determined in such a way that experimental errors do not contribute to this quantity; see Ref. [3] for precise definitions of μ, σ, and $\sigma_{\mathrm{th},\mu=0}$. The inclusion of axial asymmetry has an impressive effect on the 71 affected calculated masses: Without axial asymmetry, they are systematically too high by 0.45 MeV; with axial asymmetry included, the systematic deviation μ is reduced by 76.5% and the rms-type error is also significantly reduced.

A global theoretical picture of reflection asymmetry of the ground states of nuclei emerged gradually during the years 1981–1995 [3,12,18,19]. The models used in those studies were very similar predecessors to the model used here. It was shown that calculated masses agreed better with experimental data when the potential energy was minimized also with respect to reflection-asymmetric shapes in mass calculations. However, we can better understand our current results on axial asymmetry and better understand to what degree our model gives a realistic description of ground-state shape asymmetries if we present the reflection asymmetry effect on masses in the same format as we used for the calculated axial-asymmetry effects. This type of statistical analysis has not been performed before. For nuclei for which experimental masses are available, we calculate that reflection asymmetry lowers the ground-state mass by more than 0.2 MeV for 78 nuclei. In the right part of Fig. 3, we show the deviation between experimental and calculated masses without and with the effect of reflection asymmetry for these 78 nuclei. Also here the results are striking. Without reflection asymmetry, the calculated masses are systematically too high by 1.032 MeV on the average ($\mu = -1.032$ MeV); with reflection asymmetry included, the systematic deviation has almost disappeared ($\mu = -0.168$ MeV) and the model error is reduced by about two-thirds.

In summary, we have conducted the first global, systematic study of the last major shape asymmetry of nuclei, namely axial asymmetry. We have verified that, for those regions where we calculate that nuclei are axially asymmetric, characteristic γ bands are observed experimentally for many nuclei. Also, when we take into account the calculated effect of axial asymmetry on nuclear masses, a previously present systematic deviation between experimental and calculated masses is removed. We have also shown that previously calculated reflection-asymmetric effects on masses remove a similar, large systematic deviation between experimental and calculated masses.

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