On prolate shape predominance in nuclear deformation

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Abstract. We use the volume-conserving deformed liquid drop model to perform a quantitative study of the experimentally observed strong predominance of prolate over oblate shapes of nuclei. Except for very light nuclei, the binding energy difference between both types of quadrupole deformation is given by almost equal contributions from the Coulomb and surface terms. We perform an analysis using up-to-date experimental data for electric quadrupole moments and \(B(E2)\) transition probabilities and show that, for a significant number of well-deformed nuclei, the prolate-oblate difference in binding energy reaches values of the order of 500-800 keV, which are considerably higher than typical low-lying excitation energies for these nuclei.

1. Introduction

Why do the majority of deformed nuclei have an elongated, cigar-like prolate shape, while there are only few flattened, oblate nuclei? This insistent question has attracted the attention of nuclear physicists for more than half a century. A definitive explanation for the origin of this preponderance is still a matter of discussion and represents a fundamental challenge in nuclear structure physics [1, 2]. The fact that prolate shapes are predominant is evident from a detailed analysis of intrinsic electric quadrupole moments obtained by experiment [3] as displayed in Figure 1, where the sign of the quadrupole deformation parameter \(\beta\), extracted from measured electric quadrupole moments, determines the nuclear shape: \(\beta > 0\) corresponds to prolate, \(\beta = 0\) to spherical, and \(\beta < 0\) to oblate deformation. It is obvious from the Figure that most of the nuclei lie in the half-plane \(\beta > 0\), while oblate shapes are quite exceptional.

Due to the fundamental nature of this phenomenon, a large number of attempts have been made over the years to uncover its physical origin. The microscopic onset of deformation is accounted for by the Federman-Pittel mechanism, as due to the attractive interaction between protons and neutrons occupying orbitals which are spin-orbit partners and have a large radial overlap [4]. This mechanism, however, does not in itself distinguish between prolate and oblate configurations. Most of the models that propose explanations for the prolate-oblate shape assymetry are based on single-particle Nilsson-type shell models with a deformed harmonic oscillator potential.

Ref. [5] presents a qualitative illustration relying on the fact that in the Nilsson scheme, downward (upward) sloping orbits of a given spin \(I\) have low (high) values of the projection \(K\) onto the symmetry axis on the prolate side, while the opposite is true on the oblate side. In a major shell with many different \(I\)-shells there are more orbits with low \(K\), whose mutual
interaction forces the lowest prolate orbits even deeper in energy. The related gain in binding energy allows to obtain a prolate preference in the beginning of a shell and leads towards oblate shapes later. However, this bulk effect is sensitive to the choice of a potential and strength of spin-spin and spin-orbit couplings [6].

Concerning quantitative studies, the simplest version of the model, without any residual interaction and without the spin-orbit, $l^2$ and pairing terms, gives an equal number of prolate (until a valence shell is half-filled with nucleons) and oblate shapes (from half-filled to filled shells), although the deformation is slightly larger on the prolate side [1, 7, 8]. Assuming a sharply defined nuclear surface in single-particle models, in order to approach the more realistic Wood-Saxon potential, leads to (i) a shell model with an isotropic quartic correction [7], and (ii) a model of particles bound in an infinite-well ellipsoidal cavity [1]. Both models show (for numbers of particles relevant for nuclear physics) that a prolate shape is energetically favorable, with its energy usually a few MeV lower than a corresponding oblate shape. However, these models predict that oblate states prevail mainly at the beginning of shells and prolate at the end, which

Figure 1. Deformation parameter $\beta_Q$ calculated from the electric quadrupole moments $Q$. Most nuclei have prolate shape. (a) Isotopes of each element are connected by lines. Nuclei with significantly high oblate deformation are labeled by their chemical symbols. (b) A detail of the rare-earth region nuclei. The deformation size is coded in shades of gray, and the sign is expressed by squares (prolate shape) and diamonds (oblate shape). It is obvious that a majority of oblate nuclei appears mostly near shell closures.
is at odds with the experimental observation (see Figure 1). Prolate shape preponderance in the infinite-well ellipsoidal cavity has also been examined from a semiclassical point of view by means of an analysis of classical periodic orbits [9].

Recently, Horoi and Zelevinsky [2] carried out a statistical study of the shell model with a random two-body interaction, with angular momentum, parity and isospin conservation. Their analysis shows that for a subset of realizations of nuclei exhibiting collective features carefully selected from the whole ensemble of all possible realizations, the ratio of prolate shapes can reach 80%, depending drastically, however, on the choice and order of interacting levels; for other subsets oblate forms can predominate.

Explanations in terms of shell effects in Nilson-type models or schematic non-interacting particle models are seemingly in conflict with the robustness of the predominance of prolate over oblate nuclei and the fact that deformation is a collective phenomenon, rather than a single-particle effect. Although compelling, most of them are of a qualitative nature, are model dependent, or they need some fine-tuning to achieve the required result.

In contrast to the single-particle methods, explanations based on collective approaches have also been put forward. Zickendraht [10] demonstrates that the volume element measuring available configuration space is larger for the prolate shape than for the oblate. Moments of inertia for prolate and oblate deformations have been shown to differ [11]. Collective models with single-particle (Strutinsky) corrections have been studied in applications to nuclear masses [12], giving predominance of prolate shapes. In addition, it has been pointed out that the prolate-oblate energy difference is relevant in determining the low-lying structure of even-even nuclei [11, 13].

Incorporating the spin-orbit, \( l^2 \) and pairing interactions in the shell model with deformed harmonic oscillator potential, and applying the Nilsson-Strutinsky method (containing a macroscopic collective part) to determine the shape, analyses the problem from both the macroscopic and microscopic points of view. Results of the calculation give the ratio of prolate to all nuclei varying from 40% to 89% [14] depending on the interaction strengths, which are usually separately fixed by experiment for individual shells [12]. This is in agreement with experimental observations, but being an emergent property of the model coupling the microscopic and collective parts, it impedes a transparent discussion of the physical origin of the phenomenon of the prolate shapes preponderance. Similar conclusions can be extracted from other sophisticated numerical models such as Hartree-Fock self-consistent calculations [15]. As Wigner famously quipped: “I am very glad that the computer understands the problem, but I would like to understand it too” [16].

In this paper we aim to demonstrate that a simple form of the collective model of nuclear masses, the deformed Liquid Drop Model (LDM), gives rise to a significant energy difference between prolate and oblate shapes, originating from a sum of surface and Coulomb energy contributions, and thus offers a robust explanation for the observed preponderance of prolate over oblate nuclei. Although the contribution from Coulomb repulsion, which favors an elongated shape, is mentioned in the literature [1, 9], it is usually dismissed as being too small to be a significant effect and relevant only for heavy nuclei. We stress the importance of the surface term which, to the best of our knowledge, has been overlooked in earlier studies, but which gives a crucial contribution to the prolate-oblate energy difference, especially for lighter nuclei. It is known that the Bohr-Mottelson \( \beta \) deformation variable takes values close to 0.3 for well-deformed nuclei, which is sufficient to evaluate the order of magnitude of prolate-oblate collective energy difference. However, for the sake of completeness, we carry out a careful analysis of available experimental data on quadrupole moments [3] and \( B(E2) \) transition probabilities [17] to determine the prolate-oblate preponderance in detail. We show that for a significant number of nuclei, the collective part predicts the prolate configuration to be 500-800 keV lower in energy than the oblate one.
2. Deformed Liquid Drop Model

The deformed liquid drop model was first formulated by Von Weizsäcker and Bethe [18]. It treats the atomic nucleus as an incompressible charged fluid of nuclear matter with uniform density and a sharp surface. Its total energy is given by the difference of the mass of \( N \) neutrons and \( Z \) protons and the binding energy:

\[
B_{\text{LQM}} = a_V A - a_S A^\frac{2}{3} f_S(\alpha) - a_C \frac{Z(Z - 1)}{A} f_C(\alpha) - a_A \frac{(A - 2Z)^2}{A} + \delta,
\]

where \( A = N + Z \) is the mass number. The volume term \( (a_V) \) expresses the saturation of short-range nuclear interaction. It is corrected by the surface term \( (a_S) \), reflecting the absence of interaction between surface nucleons and the exterior of the nucleus. Electrostatic repulsion between protons further diminishes the bond via the Coulomb term \( (a_C) \). An imbalance between protons and neutrons gives rise to the asymmetry term \( (a_A) \), and spin-coupling to a pairing term \( (\delta) \). All the parameters \( a_i \) of the model are positive [18, 19, 20].

Since its original publication, this model has been improved by including new degrees of freedom, such as a compressibility and polarizability of the nuclear fluid, a diffuse surface layer, various higher multipole deformations and additional effects related to the deformation (higher order curvature terms), as well as terms augmenting the original macroscopic model with features that come from the microscopic theory, such as shell corrections and an improved pairing contribution. At present, this so-called droplet model and its further extensions are commonly used as a starting point for fitting and predicting nuclear masses and studying nuclear fission [12, 20].

In our work, we shall deal with a simple version of the model of Eq. (1), extended with a shape dependence, and discuss briefly the effect of shell corrections. The shape dependence of the binding energy comes through the functions \( f_S, f_C(\alpha) \), where \( \alpha \) are an arbitrary set of deformation parameters. We use a common expansion into spherical harmonics, restricting ourselves to the leading quadrupole term and axial shapes: \( R(\theta) = R_0 [1 + \alpha_0 + \alpha_2 P_2(\cos \theta)] \). The monopole factor \( \alpha_0 \) is restricted by the requirement of volume conservation, and dipole oscillations are identically zero in the center-of-mass coordinate system. The sign of the quadrupole parameter \( \alpha_2 = \beta/\sqrt{4\pi/5} \) is crucial to distinguish an elongated (prolate) shape \( (\alpha_2 > 0) \) from a squeezed (oblate) shape \( (\alpha_2 < 0) \).

The corrections to the surface and Coulomb terms up to the 4th order in the quadrupole deformation parameter \( \alpha_2 \) (with the volume conservation already included) are [21]

\[
\begin{align*}
    f_S(\alpha_2) &= 1 + \frac{2}{5} \alpha_2^2 - \frac{4}{105} \alpha_2^3 - \frac{38}{175} \alpha_2^4, \\
    f_C(\alpha_2) &= 1 - \frac{1}{5} \alpha_2^2 - \frac{4}{105} \alpha_2^3 + \frac{157}{1225} \alpha_2^4.
\end{align*}
\]

The leading quadratic term shows no difference between prolate and oblate shapes with the same deformation sizes (it demonstrates instead a competition between the surface energy, which clearly prefers a spherical shape, and the Coulomb repulsion decreasing the total energy by stretching the charged nuclear medium). Quartic terms, that are also symmetric with respect to the prolate-oblate deformation, lightly reduce the effect of quadratic terms due to their opposite signs.

It is the cubic correction that plays the crucial role in the analysis of the prolate shape predominance, since it distinguishes between prolate and oblate deformations. As follows from Eqs. (1) and (2), the prolate-oblate binding energy difference \( \Delta B = B(A, Z, |\alpha_2|) - B(A, Z, -|\alpha_2|) \) takes the value

\[
\Delta B = \frac{8}{105} \left[ a_S A^\frac{2}{3} + a_C \frac{Z(Z - 1)}{A^{\frac{2}{3}}} \right] |\alpha_2|^3.
\]
Figure 2. (a) Surface and (b) Coulomb contributions to the total prolate-oblate binding energy difference $\Delta B$ calculated from the electric quadrupole moments $Q$. Both contributions have very similar values, especially in the rare-earth region. Surface energy is higher for lighter nuclei, Coulomb energy becomes important with increasing charge of nuclei. Thus, the effects of surface and Coulomb forces sum and diminish the total energy of the prolate shape, which is therefore always favored energetically over the oblate shape.

We now qualitatively discuss the effect of the shell corrections that induce shape stabilization. Numerical values of the LDM parameters $a_S$ and $a_C$ [see Eq. (7) below] imply that the global minimum of nuclei around the valley of stability always occurs at $\alpha_2 = 0$, i.e. for a spherical shape. In order to describe the ground state deformation, shell effects must be taken into account. Under the assumption of a bunched Fermi-gas spectrum of levels, Myers and Świątecki derived an explicit formula for the shell corrections [19] with the following properties: (i) the energy of the shell corrections is deeply negative at shell closures, exceeding a value of 10 MeV (ii) it is slightly positive in mid-shell regions, reaching values of a few MeV, and (iii) it decreases rapidly with an attenuating factor $\exp(-\alpha_2^2/c^2)$ when the shape is deformed ($c$ is an adjustable parameter). Thus, at closed shells the spherical shape is perfectly stable. In the intermediate region, however, the fast exponential decay of positive shell correction energy competes with the rise in the collective part of the binding energy due to the quadratic terms in Eq. (2). The spherical shape is not stable anymore. Two local minima appear instead, one on the prolate side and the other on the oblate. Since the attenuating fraction is symmetric with respect to deformation, it does not contribute to the binding energy difference of (3), and therefore the prolate minimum always lies deeper in energy. Note that the appearance of few oblate nuclei can be explained by more sophisticated Strutinsky’s shell corrections, as presented, for example, in [14]. However, the robustness of the Strutinsky’s method can be called into question [12].

3. Results
The question can now be raised: is the difference in binding energy between prolate and oblate deformation given by the liquid drop model large enough to explain the observed predominance of deformed nuclei with prolate shapes? In order to answer this, we calculate the values of $\Delta B$ employing two distinct sets of experimental data from which the quadrupole deformation parameter $\beta$ of axially symmetric nuclei can be extracted: (i) the electric quadrupole moment $Q$ (reflecting the deviation of the charge distribution of the protons from the spherical shape), and (ii) the transition probability $B(E2 : 0^+ \rightarrow 2^+)$ of the first excited $2^+$ state in even-even
nuclei [8]:

\[ \beta_Q = 0.95 \frac{5}{4} \frac{Q_0}{ZR^2}, \]  

(4)

and

\[ |\beta_{B(E2)}| = \frac{4\pi}{3ZR^2} \sqrt{B(E2)}. \]  

(5)

Here \( R = R_0 A^{1/3} \) is the nuclear radius (\( R_0 = 1.20 \text{ fm} \)) and \( Q_0 \) the body-fixed (intrinsic) electric quadrupole moment which is related to the space-fixed (spectroscopic) quadrupole moment \( Q \) of a state with spin \( I \) and projection onto the symmetry axis \( K \):

\[ Q = \frac{3K^2 - I(I+1)}{(I+1)(2I+3)}Q_0. \]  

(6)

Note that \( Q \) can supply information of both magnitude and sign of deformation, whereas \( B(E2) \) values give only magnitude [see Eqs. (4), (5)].

Numerical values of the LDM coefficients \( a_{S,C} \) for the binding energies are usually determined in studies of nuclear masses and exhibit very little variation in the empirical values among different fits [12, 19, 20]. Since our model highly resembles the model used in Ref. [19], we use the values listed there:

\[ a_S^{(0)} = 18.56 \text{ MeV}, \quad a_C = 0.72 \text{ MeV}, \quad \kappa = 1.79, \]  

(7)

where \( a_S = a_S^{(0)} (1 - \kappa I^2) \) is the surface parameter corrected to the neutron excess through an additional parameter \( \kappa \).

Figure 1 shows the values of deformation parameter \( \beta \) that were determined from a compilation of experimental quadrupole moments [3], picking up states with \( I = 2 \) and \( K = 0 \) from the yrast band for even nuclei and \( I = K \neq 1/2 \) states for odd nuclei. In cases of more than one listed value of \( Q \) for a given nuclide, we selected the most recent value or that with the smallest relative error; for the sake of clarity the error is not shown. In the region of very light nuclei the value of the deformation parameter seems to be scattered with no apparent order, but from the shell closure \( N = 50 \) on, the figure exhibits a clear pattern: the deformation \( \beta \) is well pronounced inside the shells, while it tends to be much smaller for closed shells. This effect is even more obvious from panel (b), where the rare-earth nuclei are displayed in detail. This region exhibits a high correlation in the size of the deformation between isotones, and inside the shell the deformation is nearly constant with a well-known average of \( \approx 0.3 \). A few oblate nuclei appear near shell closures, but a value \( \beta < -0.2 \) is rather exceptional.

The distribution of the total prolate-oblate binding energy difference between the spherical and the Coulomb part calculated with \( \beta_Q \) of the electric quadrupole moments is depicted in Figure 2. The ratio of both contributions, \( (a_S/a_C)A/[Z(Z-1)] \), is larger than one for very light nuclei and it decreases with rising proton number. In the region of rare-earth nuclei it is \( \approx 1 \), so that both contributions have almost the same magnitude of the order of 300-400 keV each except for nuclei near shell closures.

Figure 3 shows the combined effect of the surface and Coulomb deformation energy. It compares values of \( \Delta B \) obtained (a) from known \( B(E2) \) values of even-even nuclei in the whole nuclear chart [17], and (b) from electric quadrupole moments \( Q \) in the region of rare-earth nuclei. The binding energy difference between the prolate and oblate shapes reaches values up to 800 keV for a few nuclei at mid-shell, which is a significant amount, especially in comparison with typical excitation energies of the first excited state in deformed nuclei (in the rare-earth region this is typically of the order of 100-200 keV, for even-even nuclei lower than 100 keV).

Finally, Figure 4 shows the distribution of prolate-oblate energy difference values for all nuclei determined from the compilation of the \( Q \) moments. For a major part of nuclei \( \Delta B \) is lower
than 100 keV (see the first bin), which correspond to slightly deformed shapes. On the other hand, about a third of all nuclei show a difference $\Delta B$ that exceeds 100 keV, and there is even a significant amount of nuclei that have this energy difference in the range 500-1000 keV. This demonstrates that nuclei with significantly high value of $\delta B$ are not an exception. Their presence in different areas of the nuclear chart give strong evidence in favor of the simple collective explanation of predominant prolate shapes.

4. Concluding remarks
In this paper we have shown that surface and Coulomb collective effects are strong enough to induce the propensities of nuclei to acquire prolate shapes. We employed the deformed liquid drop model in which the effects of quadrupole deformation are taken into account up to quartic order. It was shown that the cubic corrections to the surface and Coulomb terms contribute approximately equally to the prolate-oblate binding energy difference with the exception of very light nuclei. An analysis of the data based on compilations of experimental values of...
Figure 4. A histogram showing the distribution of the total prolate-oblate binding energy difference $\Delta B$ calculated from the electric quadrupole moments $Q$. A significant number of nuclei with $\Delta B$ of the order of several hundreds keV's is observed.

quadrupole moments and $B(E2)$ transitions yield energy differences of the order of 500-800 keV for a significant number of nuclei. These energies are comparable with typical excitation energies in deformed nuclei, and also with respect to shell corrections to the deformed LDM. The results suggest that the observed predominance of prolate nuclear shapes can be essentially explained as a collective effect with a transparent physical picture. A more detailed analysis will be presented in [6].

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