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Comparison of the confined β -soft Rotor Model and a microscopic collective Hamiltonian based on the relativistic mean field model in $^{150,152}\text{Nd}$

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Abstract. A comparison between the analytical wavefunction of the Confined β -soft Rotor Model and a collective Hamiltonian based on the relativistic mean field model has been performed for the low lying states in the ground state band and β -band of the nuclei $^{150,152}\text{Nd}$. A remarkable similarity of the two models in energies, intra- and interband $B(E2)$ -values and centrifugal stretching has been observed. In the transitional nucleus ^{150}Nd the relative stretching is about $0.025/\hbar$ whereas the rotational nucleus ^{152}Nd with a much stiffer potential in the quadrupole deformation parameter β stretches with approximately $0.01/\hbar$. The centroids of the wave functions almost exactly coincide in the two models for the ground state band and also for the β -band. The Ansatz in the CBS model of an outer potential wall that stays almost constant with increasing number of valence neutrons and an inner wall that shifts to higher deformations has been successfully justified microscopically.

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1. Introduction

The understanding of transitional nuclei has considerably deepened during the last decade. Inspired by the formulation of the E(5) and X(5) solution of the geometrical Bohr Hamiltonian [1, 2, 3] a great deal of experimental and theoretical work has been spent on the investigation of nuclei at the shape phase transitional points [4, 5, 6, 7]. The remarkable quantitative success of a geometrical nuclear structure model using a square well potential has been demonstrated to microscopically originate from the fact that near the shape phase transitional point quite flat and soft potentials can develop [8, 9].

Beyond the transitional point X(5) with an $R_{4/2}$ ratio of 2.9 deformed nuclei rapidly evolve into almost rigidly rotating bodies with $R_{4/2}$ values close to 3.33. The rigid rotor limit is, however, hardly reached exactly. Deformed nuclei typically exhibit $R_{4/2}$ values between 3.2 and 3.32 while very few deformed nuclei have $R_{4/2}$ values between 2.9 and 3.2. Inspired by the success of the X(5) model that was based on the phenomenon of intrinsic excitations and centrifugal stretching in a soft potential, the X(5) model has been generalized in terms of the Confined β -Soft (CBS) rotor model [10, 11]. Similar to the X(5) model, the CBS rotor model considers a square-well potential, however, with the inner potential boundary shifted away from $\beta=0$ (see section 2.2). Alike X(5) the CBS rotor model is analytically solvable in terms of Bessel functions. It has been demonstrated to have a remarkable capability for quantitatively describing the evolution of excitation energies of rotational bands in deformed nuclei [12, 13]. It is interesting to study whether and to what extent microscopic calculations justify or contradict the choice of simplistic potentials and resulting nuclear wave functions of the CBS rotor model.

Within this article we compare the results for the transitional and deformed neighbouring even-even isotopes ^{150}Nd and ^{152}Nd for which microscopic calculations based on the Relativistic Mean Field approach are available [8, 9]. Fig. 1 displays the effective potentials as a function of the quadrupole deformation parameter β for the description of $^{150,152}\text{Nd}$. The square-well potentials of the CBS rotor model have been obtained from a fit to the $R_{4/2}$ ratios and the $B(E2; 2_1^+ \rightarrow 0_1^+)$ values, while the potential curves have been calculated microscopically from Relativistic Mean Field potentials. For a better comparison, the RMF curves are actually projections on the β -axis of a full triaxial calculation in the $\beta - \gamma$ -plane. One obvious observation is that the inner potential boundary shifts much more as a function of neutron number than the outer boundary according to both models. The outer boundary seems to be almost insensitive to the transition from spherical to axially prolate nuclei. The purpose of this paper is to study the impact on the evolution of nuclear structure originating in the shift of the inner potential wall and to what extent the use of square well potentials for the description of transitional nuclei is microscopically justified.

In the next section we will shortly summarize the basic concepts of the models before we discuss their application to the nuclei $^{150,152}\text{Nd}$ and the comparison of their results

in section III.

Figure 1. Relativistic Mean field Potentials compared to the CBS square well potentials that make an analytical solution of the Bohr Hamiltonian possible.

2. Model definition

2.1. The Collective Hamiltonian

The collective Hamiltonian

$$\hat{H} = \hat{T}_{\text{vib}} + \hat{T}_{\text{rot}} + V_{\text{coll}} \quad (1)$$

in a very general form [14] describes the collective motion of a nucleus with the vibrational kinetic energy

$$\begin{aligned} \hat{T}_{\text{vib}} = & -\frac{\hbar^2}{2\sqrt{wr}} \left\{ \frac{1}{\beta^4} \left[\frac{\partial}{\partial \beta} \sqrt{\frac{r}{w}} \beta^4 B_{\gamma\gamma} \frac{\partial}{\partial \beta} - \frac{\partial}{\partial \beta} \sqrt{\frac{r}{w}} \beta^3 B_{\beta\gamma} \frac{\partial}{\partial \gamma} \right] \right. \\ & \left. + \frac{1}{\beta \sin 3\gamma} \left[-\frac{\partial}{\partial \gamma} \sqrt{\frac{r}{w}} \sin 3\gamma B_{\beta\gamma} \frac{\partial}{\partial \beta} + \frac{1}{\beta} \frac{\partial}{\partial \gamma} \sqrt{\frac{r}{w}} \sin 3\gamma B_{\beta\beta} \frac{\partial}{\partial \gamma} \right] \right\} \end{aligned} \quad (2)$$

and the rotational kinetic energy

$$\hat{T}_{\text{rot}} = \frac{1}{2} \sum_{k=1}^3 \frac{\hat{J}_k^2}{\mathcal{I}_k}. \quad (3)$$

V_{coll} is the collective potential. For this potential there are different ansatzes, and we'll discuss two of them in this paper.

$\hat{J}_k$ denotes the components of the angular momentum in the body-fixed frame of a nucleus, and the mass parameters $B_{\beta\beta}$, $B_{\beta\gamma}$, $B_{\gamma\gamma}$ [15], as well as the moments of inertia $\mathcal{I}_k$, depend on the quadrupole deformation variables β and γ :

$$\mathcal{I}_k = 4B_k\beta^2 \sin^2(\gamma - 2k\pi/3). \quad (4)$$

Two additional quantities that appear in the expression for the vibrational energy: $r = B_1 B_2 B_3$, and $w = B_{\beta\beta} B_{\gamma\gamma} - B_{\beta\gamma}^2$, determine the volume element in the collective space. In the next two chapters some assumptions for the CBS model and the Relativistic Mean Field approach will be made and the collective potentials will be specified in order to solve the Schrödinger Equation.

2.2. The Confined β -soft Rotor Model

The CBS rotor model represents an approximate analytical solution to the collective Hamiltonian in equation (1) as it was proposed by Bohr and Mottelson [14] in the quadrupole shape parameters β and γ . Taking the Hamiltonian in equation (1) and (2) and assuming that $B_k = B_{\gamma\gamma} = B_{\beta\beta} = B$ and $B_{\beta\gamma} = 0$, the Hamiltonian simplifies to

$$H = -\frac{\hbar^2}{2B} \left[\frac{1}{\beta^4} \frac{\partial}{\partial \beta} \beta^4 \frac{\partial}{\partial \beta} + \frac{1}{\beta^2 \sin 3\gamma} \frac{\partial}{\partial \gamma} \sin 3\gamma \frac{\partial}{\partial \gamma} - \frac{1}{4\beta^2} \sum_k \frac{\hat{J}_k^2}{\sin^2(\gamma - \frac{2}{3}\pi k)} \right] + V(\beta, \gamma). \quad (5)$$

Assuming a separable potential $V(\beta, \gamma) = u(\beta) + v(\gamma)$ the wave functions approximately separate into

$$\Psi(\phi, \theta, \psi, \beta, \gamma) = \xi_L(\beta) \eta_K(\gamma) \Phi_{MK}^I(\Omega). \quad (6)$$

The angular part corresponds to linear combinations of the Wigner functions

$$\Phi_{MK}^I(\Omega) = \sqrt{\frac{2I+1}{16\pi^2(1+\delta_{K0})}} [D_{MK}^{I*}(\Omega) + (-1)^I D_{M-K}^{I*}(\Omega)] \quad (7)$$

and η_K denotes the appropriate wave function in γ . For sufficiently axially symmetric prolate nuclei one might consider a steep harmonic oscillator in γ [2]. $\xi_L(\beta)$ describes the part of the wave function depending on the deformation variable β . The approximate separation of variables [2] leads to the differential equation

$$-\frac{\hbar^2}{2B} \left[\frac{1}{\beta^4} \frac{\partial}{\partial \beta} \beta^4 \frac{\partial}{\partial \beta} - \frac{1}{3\beta^2} L(L+1) + u(\beta) \right] \xi_L(\beta) = E \xi_L(\beta) \quad (8)$$

for $\xi_L(\beta)$. It can be considered as the 'radial' equation in the space of quadrupole deformation parameters. It contains the angular momentum dependence through the centrifugal term. The CBS rotor model assumes for prolate axially symmetric nuclei an infinite square well potential $u(\beta)$, with boundaries at $\beta_M > \beta_m \geq 0$. For this potential the differential equation (8) is analytically solvable. The ratio $r_\beta = \beta_m/\beta_M$ parameterizes the width of this potential, that is the stiffness of the nucleus in the β degree of freedom. For $r_\beta = 0$ the X(5) limit is obtained with large fluctuations in β . The

Rigid Rotor Limit without fluctuations in β corresponds to $r_\beta \rightarrow 1$. The quantization condition of the CBS rotor model is

$$Q_{\nu(L)}^{r_\beta}(z) = J_{\nu(L)}(z) Y_{\nu(L)}(r_\beta z) - J_{\nu(L)}(r_\beta z) Y_{\nu(L)}(z) = 0 \quad (9)$$

with J_ν and Y_ν being Bessel functions of first and second kind of irrational order $\nu = \sqrt{[L(L+1) - K^2]/3 + 9/4}$. For a given structural parameter r_β and any spin value L the s th zero of equation (9) is denoted by $z_{L,s}^{r_\beta}$. The full solution of equation(8) with the aforementioned choice of the CBS square-well potential is then given as

$$\xi_{L,s}(\beta) = c_{L,s} \beta^{-\frac{3}{2}} \left[J_\nu \left(z_{L,s}^{r_\beta} \frac{\beta}{\beta_M} \right) + \frac{J_\nu(r_\beta z_{L,s}^{r_\beta})}{Y_\nu(r_\beta z_{L,s}^{r_\beta})} Y_\nu \left(z_{L,s}^{r_\beta} \frac{\beta}{\beta_M} \right) \right]. \quad (10)$$

The normalization constant $c_{L,s}$ of the wave function (10) is given by the normalization condition

$$1 = \int_{\beta_m}^{\beta_M} \beta^4 [\xi_{L,s}(\beta)]^2 d\beta. \quad (11)$$

The eigenvalues of equation (8) are obtained as

$$E_{L,s} = \frac{\hbar^2}{2B\beta_M^2} (z_{L,s}^{r_\beta})^2. \quad (12)$$

The CBS rotor model well describes the evolution of low-energy 0^+ bands [10], ground bands of strongly deformed nuclei [12], and the dependence of relative moments of inertia as a function of spin in deformed transitional nuclei [13]. The CBS rotor model has also been successfully used for studying relative as well as absolute E0 transitions in the region of the X(5) nuclei up to the rigid rotor limit [16].

2.3. Microscopic Relativistic Mean Field Approach

In this work a microscopic collective Hamiltonian based on the relativistic mean field model is used [8, 9]. The kinetic energy part of the Hamiltonian is in the general form as already seen in equations (1) - (3). The seven functions, i.e. the three moments of inertia $\mathcal{I}_k$, the three mass parameters $B_{\beta\beta}$, $B_{\beta\gamma}$, $B_{\gamma\gamma}$, and the collective potential V_{coll} , are determined by the choice of a particular microscopic nuclear energy-density functional or effective interaction. In the particle-hole channel we use the relativistic functional PC-F1 (point-coupling Lagrangian) [17], as we did in our previous studies of shape transitions in the Nd-chain [9]. Also a density-independent δ force in the particle-particle channel treated by the BCS approximation was used. The moments of inertia are calculated microscopically from the Inglis-Belyaev formula:

$$\mathcal{I}_k = \sum_{i,j} \frac{(u_i v_j - v_i u_j)^2}{E_i + E_j} \langle i | \hat{J}_k | j \rangle^2 \quad k = 1, 2, 3, \quad (13)$$

where the summation runs over the proton and neutron quasiparticle states, and k denotes the axis of rotation. The quasiparticle energies E_i , occupation probabilities v_i ,

and single-nucleon wave functions ψ_i are determined by solutions of the constrained RMF+BCS equations. The mass parameters associated with the two quadrupole collective coordinates $q_0 = \langle \hat{Q}_{20} \rangle$ and $q_2 = \langle \hat{Q}_{22} \rangle$ are also calculated in the cranking approximation

$$B_{\mu\nu}(q_0, q_2) = \frac{\hbar^2}{2} \left[\mathcal{M}_{(1)}^{-1} \mathcal{M}_{(3)} \mathcal{M}_{(1)}^{-1} \right]_{\mu\nu} , \quad (14)$$

with

$$\mathcal{M}_{(n),\mu\nu}(q_0, q_2) = \sum_{i,j} \frac{\langle i | \hat{Q}_{2\mu} | j \rangle \langle j | \hat{Q}_{2\nu} | i \rangle}{(E_i + E_j)^n} (u_i v_j + v_i u_j)^2 . \quad (15)$$

In contrast to the CBS Model, the potential V_{coll} in the collective Hamiltonian Equation (1) is obtained by subtracting the zero-point energy corrections from the total energy that corresponds to the solution of constrained RMF+BCS equations, at each point on the triaxial deformation plane.

The Hamiltonian (1) describes quadrupole vibrations, rotations, and the coupling of these collective modes. The corresponding eigenvalue problem is solved using an expansion of eigenfunctions in terms of a complete set of basis functions that depend on the deformation variables β and γ , and the Euler angles ϕ , θ and ψ . The diagonalization of the Hamiltonian yields the excitation energies and collective wave functions

$$\Psi_{\alpha}^{IM}(\beta, \gamma, \Omega) = \sum_{K \in \Delta I} \psi_{\alpha K}^I(\beta, \gamma) \Phi_{MK}^I(\Omega), \quad (16)$$

that are used to calculate observables. The angular part corresponds to linear combinations of the Wigner functions [see equation (7)] and the summation in equation (16) is over the allowed set of K values:

$$\Delta I = \begin{cases} 0, 2, \dots, I & \text{for } I \bmod 2 = 0 \\ 2, 4, \dots, I-1 & \text{for } I \bmod 2 = 1 . \end{cases} \quad (17)$$

For a given collective state in equation (16), the probability density distribution in the $\beta - \gamma$ -plane is defined by

$$\rho_{I\alpha}(\beta, \gamma) = \sum_{K \in \Delta I} |\psi_{\alpha K}^I(\beta, \gamma)|^2 \beta^3 |\sin 3\gamma| . \quad (18)$$

The normalization reads

$$\int_0^\infty \beta d\beta \int_0^{2\pi} d\gamma \rho_{I\alpha}(\beta, \gamma) = 1 . \quad (19)$$

If we integrate the wave function (16) along γ , we obtain the projection

$$\rho'_{I\alpha}(\beta) = \sum_{K \in \Delta I} \int_0^{2\pi} |\psi_{\alpha K}^I(\beta, \gamma)|^2 \beta^4 |\sin 3\gamma| d\gamma . \quad (20)$$

of the density distribution as a function of β for the desired comparison with the results from the CBS model. Its normalization reads:

$$\int_0^\infty \rho'_{I\alpha}(\beta) d\beta = 1 . \quad (21)$$

3. Comparison of the CBS and RMF for the transitional nuclei $^{150,152}\text{Nd}$

3.1. Description of $K=0$ bands and their centrifugal stretching

Figure 2 shows the low lying excitation spectrum of the nucleus ^{150}Nd [18] in comparison to the two models. For the CBS rotor model we have fitted the structural parameter r_β to the $4_1^+/2_1^+$ -energy ratio $R_{4/2}$. For ^{150}Nd we used $r_\beta = 0.078$ and for ^{152}Nd $r_\beta = 0.35$. The energy-scale parameter $\frac{\hbar^2}{2B\beta_M^2}$ [see equation (12)] has been fitted to the excitation energies of the 2_1^+ states and takes the values of 37.9 keV for ^{150}Nd and 30.7 keV for ^{152}Nd . The effective E2 charges of the first order ($\Delta k = 0$)-part of the transition operator $T(E2) = \frac{3}{4\pi}ZeR^2\beta_M(\beta/\beta_M)D_{\mu 0}^2$ [10] have been scaled to the experimental $B(E2; 2_1^+ \rightarrow 0_1^+)$ values. For the calculations we used $\beta_M = 0.451$ for ^{150}Nd and $\beta_M = 0.471$ for ^{152}Nd .

For the RMF model we have multiplied the Inglis-Belyaev moments of inertia in equation (13) with a common factor $(1 + \alpha)$ determined in such a way that the calculated energy of the 2_1^+ state coincides with the experimental value. This is because the well-known fact that the Inglis-Belyaev formula predicts effective moments of inertia that are considerably smaller than empirical values. For ^{150}Nd we used $\alpha = 0.40$ and for ^{152}Nd $\alpha = 0.57$. The transition rates are calculated in the full configuration space using bare charges [8, 9].

The $s=1$ ground state band is very well reproduced by the two models. In the microscopic RMF approach the energies differ only by a few percent compared to the experimental energies. In the CBS rotor model the deviation is even less than 0.3 % [12]. In the $s=2$ band, which is the collective β -band for this nucleus, the rotational structure is very well reproduced in the two models and the deviations in energy primarily result from a mismatch of the rotational moment of inertia by up to 25 %. The $B(E2)$ intra- and interband transition strengths show a satisfactory agreement in both models. Note, that both, energies and $B(E2)$ values for the excited $k=0$ band in the CBS model, represent model predictions without any further parameter adjustment.

Figure 3 shows the same spectra for the nucleus ^{152}Nd [19]. In this case, only few data is available. Here, the two models show again a nice agreement in the excitation energies and $B(E2)$ values for the ground state band, as well as for the β -band.

One underlying mechanism at work in the CBS model is the centrifugal stretching of the nucleus which can be classically understood as an increase in the moment of inertia (MoI) as a function of the rotational angular momentum. In the upper graph in figure 4 the evolution of the MoI with spin, here plotted as the relative dynamical moment of inertia (see also [12])

$$\frac{\theta(J)}{\theta(2)} = \left[\frac{J(J+1)}{6} \right] \frac{E(J=2)}{E(J)} \quad (22)$$

is compared to the CBS and microscopic RMF predictions. Both models well agree with the data on the ground state bands of $^{150,152}\text{Nd}$.

The stretching for the two models has been calculated for the ground state rotational

Figure 2. Low lying energy levels in ^{150}Nd for the relativistic mean field Hamiltonian (left), the CBS model (middle) and experimental values (right). Energies and $B(E2)$ values for Exp. and RMF were taken from reference [9].

Figure 3. Low lying energy levels in ^{152}Nd for the relativistic mean field Hamiltonian (left), the CBS model (middle) and experimental values (right). Energies and $B(E2)$ -values for Exp. were taken from reference [19].

bands in the nuclei $^{150,152}\text{Nd}$. Defining a dimensionless stretching parameter

$$S(J) = \frac{\langle \beta \rangle_{J_i} - \langle \beta \rangle_{0_1^+}}{\langle \beta \rangle_{0_1^+}}, \quad (23)$$

one can quantitatively see in the lower graph of figure 4, that the two models show a very good agreement on the predicted centrifugal stretching. In this figure the centrifugal stretching goes more or less linearly with the spin, and an increasing potential stiffness means a decrease in centrifugal stretching. It is remarkable how well the experimental

Figure 4. Upper graph: Experimental Moments of Inertia and theoretical predictions for the ground state band in the nuclei $^{150,152}\text{Nd}$.

lower graph: Comparison of the centrifugal stretching parameter $S(J)$ in $^{150,152}\text{Nd}$ for the two models as a function of spin.

MoI graph in the upper part of the figure correlates with the theoretically calculated stretching parameters in the lower part. The slope for the centrifugal stretching in ^{150}Nd is for both models approximately $0.025/\hbar$. The much stiffer potential in β for ^{152}Nd creates only a slope of approximately $0.01/\hbar$. Looking at the evolution as a function of valence nucleons, the centrifugal stretching decreases approximately by a factor of 2.5, going from the X(5) nucleus ^{150}Nd to the well deformed rotor ^{152}Nd . The agreement of both models in figure 4 appears to be worse for ^{150}Nd than for ^{152}Nd . However, the disagreement between the models simply scales with the size of the effect. In ^{150}Nd the dynamical MoI for the 10_1^+ state is 49 % larger than the one for the 2_1^+

state. The RMF model predicts an increase of 40 %, only, i.e., underestimates this increase by about one fifth of its size. In ^{152}Nd the dynamical MoI for the 10_1^+ state is 11 % larger than the one for the 2_1^+ state. Here, the RMF model predicts an increase of 14 %, i.e., again, at slight variance to the data.

3.2. Comparison of the collective wave functions

Figure 5 shows wave functions of the ground state bands in ^{150}Nd and ^{152}Nd as a function of β . The vertical bold lines in the first and third subfigure represent the potential boundaries of the square-well CBS potential. The vertical lines inside the wave functions represent the centroid of each wave function. Comparing these nuclides, one can easily see the similar amount of centrifugal stretching in the two models. The fact, that the potential stiffens with increasing neutron number can also be seen by comparing the upper and the lower two subfigures. The wavefunctions of the rotational nucleus ^{152}Nd are more compressed and shifted towards a larger average deformation.

Figure 5 and 6 indicate that just a very small fraction of the wave functions computed microscopically in the relativistic mean field model turns out to lie outside of the CBS square well potential walls. In fact, the wave functions of the two models are very similar. They almost exactly show the same amplitude as well as the same centroid for the ground state band in ^{150}Nd and ^{152}Nd , respectively.

Figure 6 shows the wave functions of the β -band heads. They have one node in the deformation coordinate β . One can clearly see the large overlap of the wave functions between the two models. The centroids of the two peaks in the wave functions of the β -band head almost exactly coincide in the case of ^{152}Nd . However, the shapes of the wave functions in the β -band differ slightly for both models. Here, the CBS model shows two peaks in the β -band that have almost the same amplitude whereas the microscopic RMF model produces a smaller peak for the waist of the wave function at larger deformation than for the waist at smaller deformation.

For the case of ^{150}Nd the difference between the prediction of the models for the 0_2^+ wave function is slightly larger than for the more rotational nucleus ^{152}Nd . The top of figure 6 shows, that the amplitudes of the two waists of the wave functions are very similar, and the centroids of the second waist are close, but here, the first maxima of the wave functions occur at different deformations. For this example the RMF potential is more repulsive for small deformations than the CBS potential, see figure 1, and hence, the RMF wave function is reduced for lower β in comparison to the CBS model.

4. Summary

In conclusion, a comparison between the analytical wave functions of the CBS rotor model and a microscopic Hamiltonian based on the relativistic mean field model has been performed for the low lying states in the ground state band and β -band of the nuclei $^{150,152}\text{Nd}$. The energy levels of these states and the relative evolution of their

Figure 5. Wave functions of the groundstate band in $^{150,152}\text{Nd}$ for the CBS rotor model and the relativistic mean field model. The black borders show the potential walls in case of the CBS potential.

MoIs agree satisfactorily with data.

A remarkable similarity of the two models in energies, intra- and interband $B(E2)$ -

Figure 6. Wave functions of the band heads of the β -band in $^{150,152}\text{Nd}$. The black borders show the potential walls in case of the CBS potential.

values and centrifugal stretching has been observed. In the transitional nucleus ^{150}Nd the stretching is about $0.025/\hbar$ whereas the rotational nucleus ^{152}Nd with a much stiffer potential in β stretches with approximately $0.01/\hbar$. The centroids of the wave functions almost exactly coincide in the two models for the ground state band and also for the β -band. The wave functions, especially for the ground state band in $^{150,152}\text{Nd}$, are very similar in the two models, although the two models base on completely different ansatzes.

In particular, the Ansatz in the CBS model of an outer potential wall that stays almost constant with a varying number of valence neutrons and an inner wall that shifts to higher deformations has been microscopically justified for the given example of the isotopes $^{150,152}\text{Nd}$ near the shape phase transitional point. In both compared models, the position of the outer potential wall seems to be almost independent of a transition from a spherical to an axially symmetric shape of the nucleus while the change in structure as a function of nucleon number is dominated by the change of the potential at small deformation.

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