Equilibrium ground-state deformation of medium and heavy nuclei calculated on the basis of deformed Woods–Saxon potential with variable surface diffuseness

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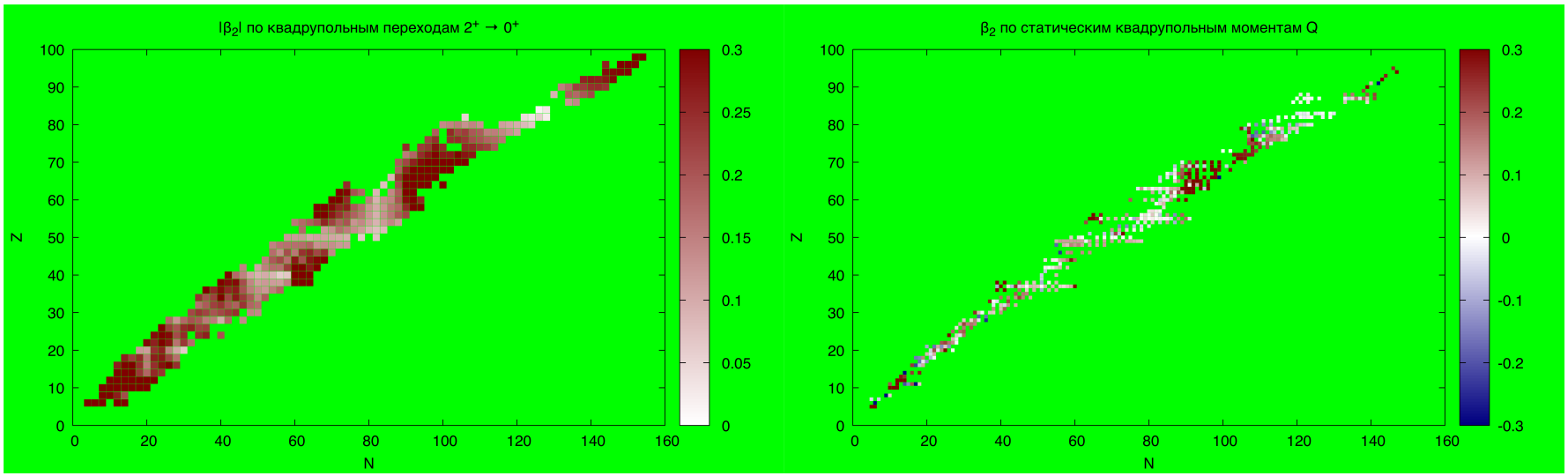
Introduction

- Models used for large-scale prediction of nuclear deformations: macro-microscopic (e.g., Finite Range Droplet Model FRDM), Hartree–Fock–Bogolyubov calculations with different effective interaction potentials.
- Purpose of this work: construct simple phenomenological model capable of prediction of deformation of majority of medium and heavy nuclei through extension of a simple Nilsson model.



Nilsson deformed shell model

- Single-particle Hamiltonian of the spherical SM with the harmonic oscillator potential (Göppert–Mayer & Jensen, 1949):

$$\hat{H} = -\frac{\hbar^2}{2m}\Delta + V_{ls}\frac{\partial V(r)}{\partial r}(\hat{\mathbf{l}}\cdot\hat{\mathbf{s}}) + D\hat{\mathbf{l}}^2 + \frac{m}{2}\omega^2 r^2.$$

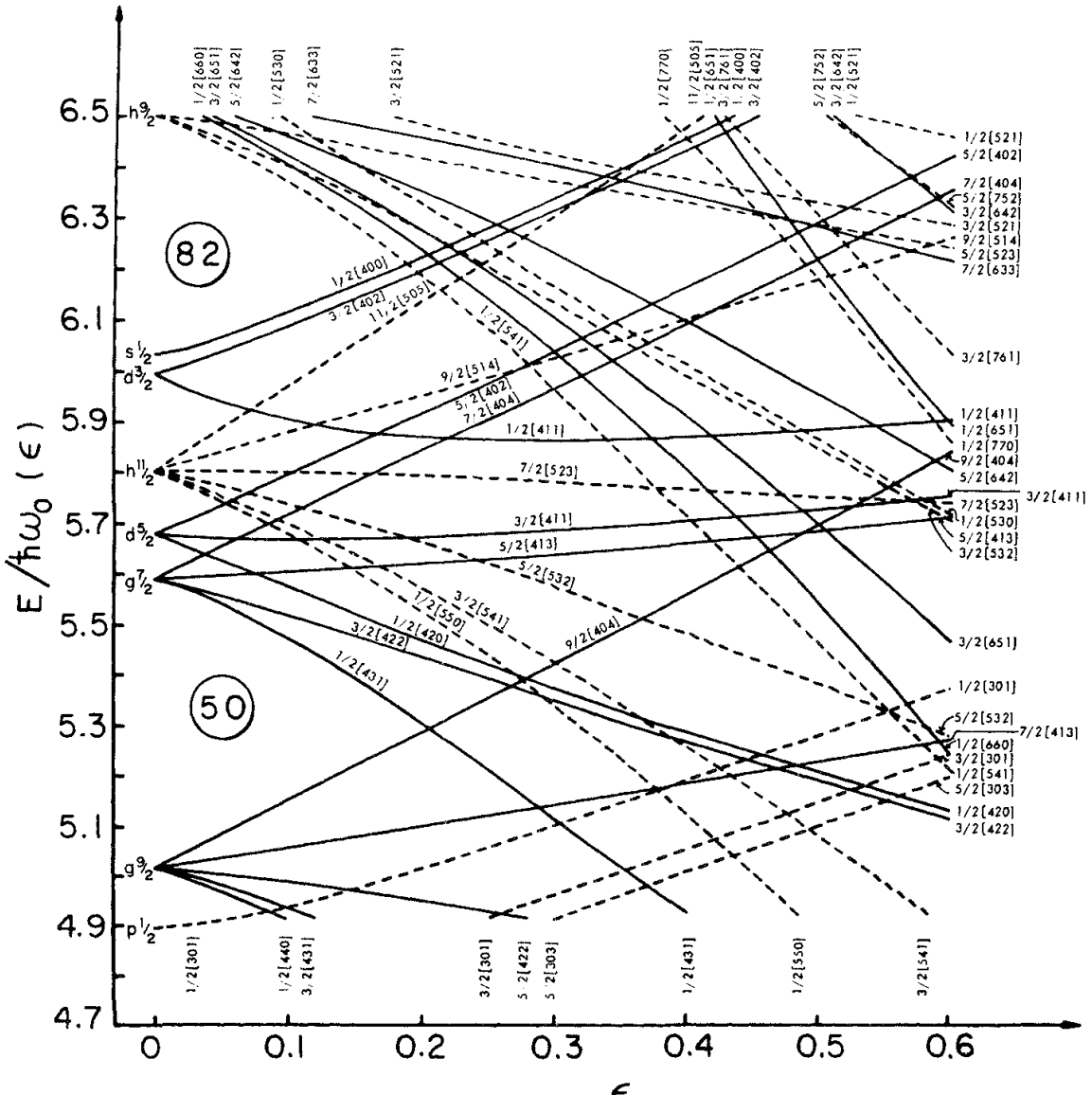
- Axially-deformed potential of the Nilsson model (1955):

$$\hat{H} = -\frac{\hbar^2}{2m}\Delta + C(\hat{\mathbf{l}}\cdot\hat{\mathbf{s}}) + D\hat{\mathbf{l}}^2 + \frac{m}{2}(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2),$$

  where $\omega_x = \omega_y = \omega_\perp = \omega_0\left(1 + \frac{\beta_2}{3}\right)$, and $\omega_z = \omega_\parallel = \omega_0\left(1 - \frac{2\beta_2}{3}\right)$.
- conservation of volume after deformation: $\omega_x\omega_y\omega_z = \text{const}$. Then $\omega_0 = \mathring{\omega}_0\left(1 - \frac{\beta_2^2}{3} - \frac{2\beta_2^3}{27}\right)^{-\frac{1}{6}}$, where $\mathring{\omega}_0 \approx 41A^{-\frac{1}{3}}$ to reproduce rms radius of magic nuclei.

Nilsson deformed shell model

Solution of the Schrödinger equation via diagonalization of the Hamiltonian in the axially-deformed oscillator basis $\langle \mathbf{r} | N l \Lambda \Sigma \rangle$ with different β_2 leads to the Nilsson diagrams $\epsilon_i(\beta_2)$:



[C. Gustafson *et al.*, Ark. Fys. **36**, 613 (1967)]

Nilsson deformed shell model

Location of the equilibrium deformation point

Total nuclear energy in the ground state is defined as $E(\beta_2) = \sum \epsilon_i(\beta_2)$. Minimum of the function corresponds to the equilibrium deformation point.

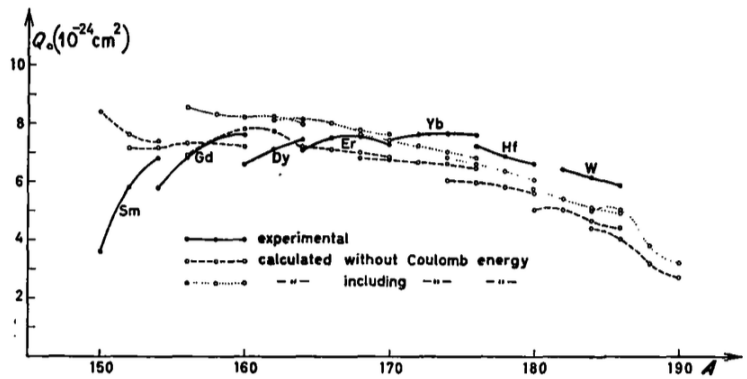


Fig. 3. The electric quadrupole moments for the shifts I+IV. The experimental values are taken from ref. [25]). The Coulomb effects are included in the dotted curve, but not in the dashed curve.

[D. R. Bès, Z. Szymański, Nucl. Phys. **28**, 42 (1961)]

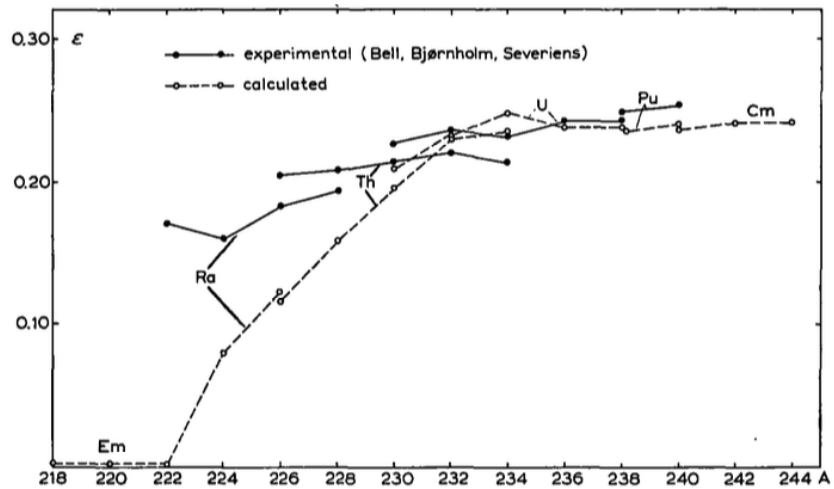


Fig. 4. Equilibrium deformations versus A. The solid line refers to the values of the density deformation parameter $\bar{\varepsilon}$ computed from the experimental quadrupole moments [1]) by means of eq. (11). They are to be compared with the calculated potential deformation ε (dashed line). The level scheme corresponds to the variant 2 of table 1.

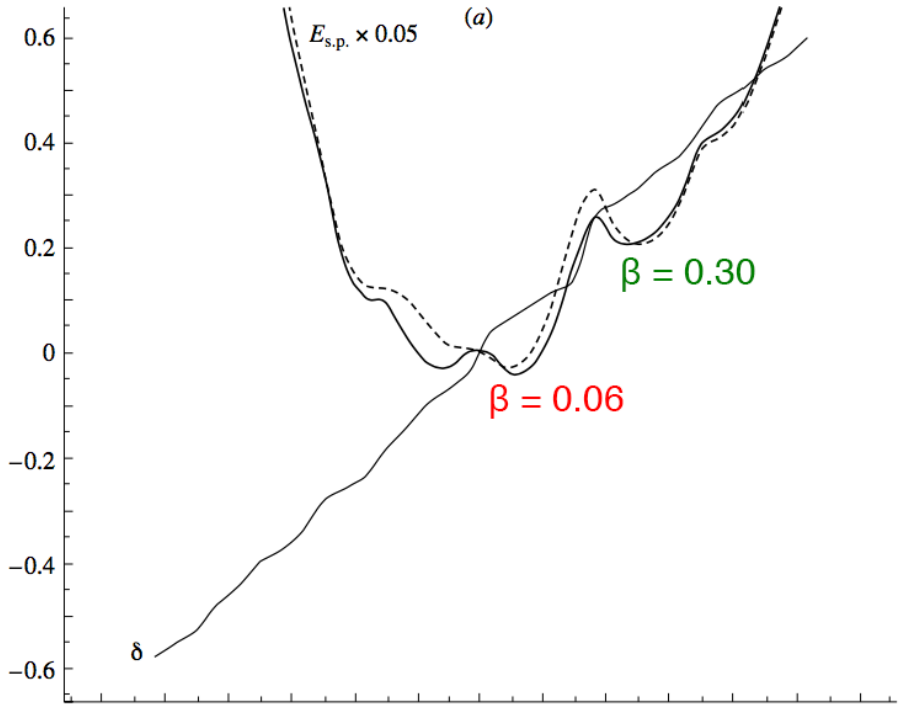
[Z. Szymański, Nucl. Phys. **28**, 63 (1961)]

Good agreement with data in the region of strongly deformed rare-earth and actinide nuclei. (BCS treatment of pairing correction is included.)

Nilsson deformed shell model

Location of the equilibrium deformation point

Less satisfactory agreement in other regions of the *NZ* chart. The minimum of the potential energy curve can be too shallow. Example: ^{77}Kr.



[РҪ. Рғ. РЧСЇСЖҚРѳР„,Р«Рў, РЎ. Р№. Р¤СҐРњРчР„, PsPh **68**, 1407 (2005)]

(Here axially deformed Woods–Saxon potential is used instead of the Nilsson potential.)

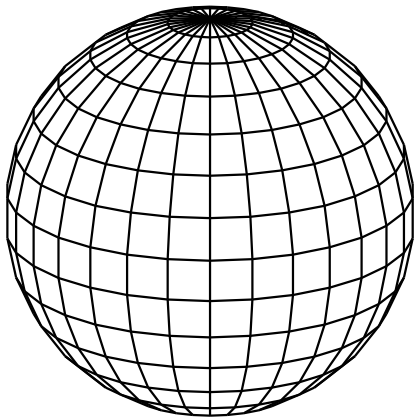
Nilsson deformed shell model

Reasons of the failure

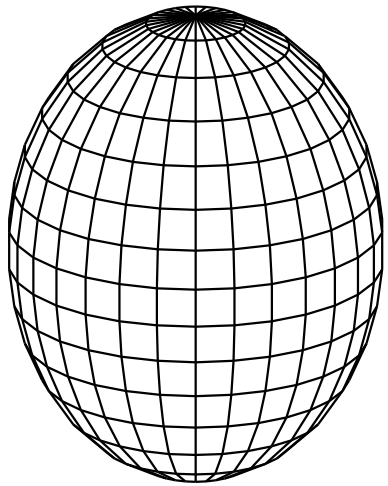
- Inaccurate approximation of the average nuclear field, lacking description of two-body interactions, etc.
- One of the main reasons: total single-particle energy does not form a correct expression of the nuclear energy due to double summation of the interaction energy. In reality $E = \sum_i \epsilon_i - \frac{1}{2} \sum_{i \neq j} \langle i, j | \hat{V} | i, j \rangle$.
- The approach practically not used after introduction of the Strutinsky shell correction method.

Parameterization of the nuclear shape

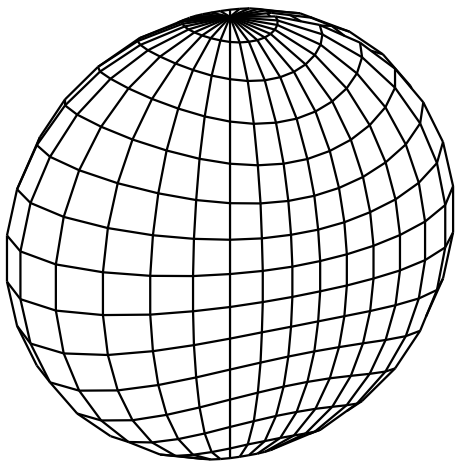
Non-axial ellipsoid



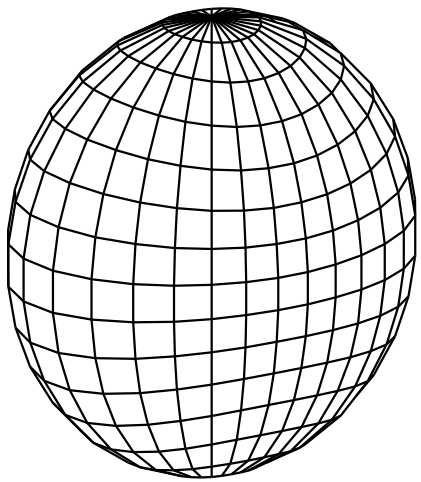
β = 0; γ = 0



β = 0,4; γ = 0



β = 0,4; γ = 60



β = 0,4; γ = 30

Axial deformation
$\beta \geq 0$
Non-axiality $0 \leq \gamma \leq \frac{\pi}{3}$

Ellipsoid semi-axes

$$a_0 = \beta \cos\gamma$$

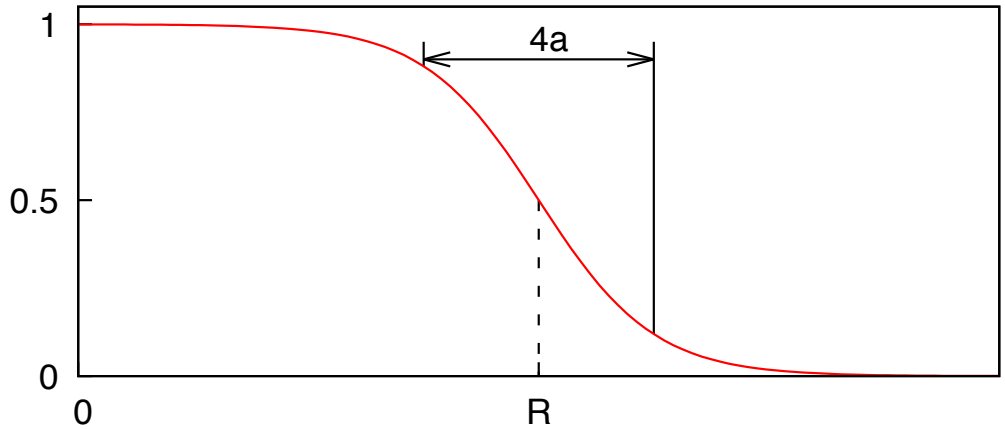
$$a_2 = \frac{1}{\sqrt{2}} \beta \sin\gamma$$

$$a^2 = 1 - \sqrt{\frac{5}{4\pi}} a_0 + \sqrt{\frac{15}{2\pi}} a_2$$

$$b^2 = 1 - \sqrt{\frac{5}{4\pi}} a_0 - \sqrt{\frac{15}{2\pi}} a_2$$

$$c^2 = 1 + \sqrt{\frac{5}{\pi}} a_0$$

Deformed Woods–Saxon form-factor



Single-particle potentials defined in terms of the form-factor

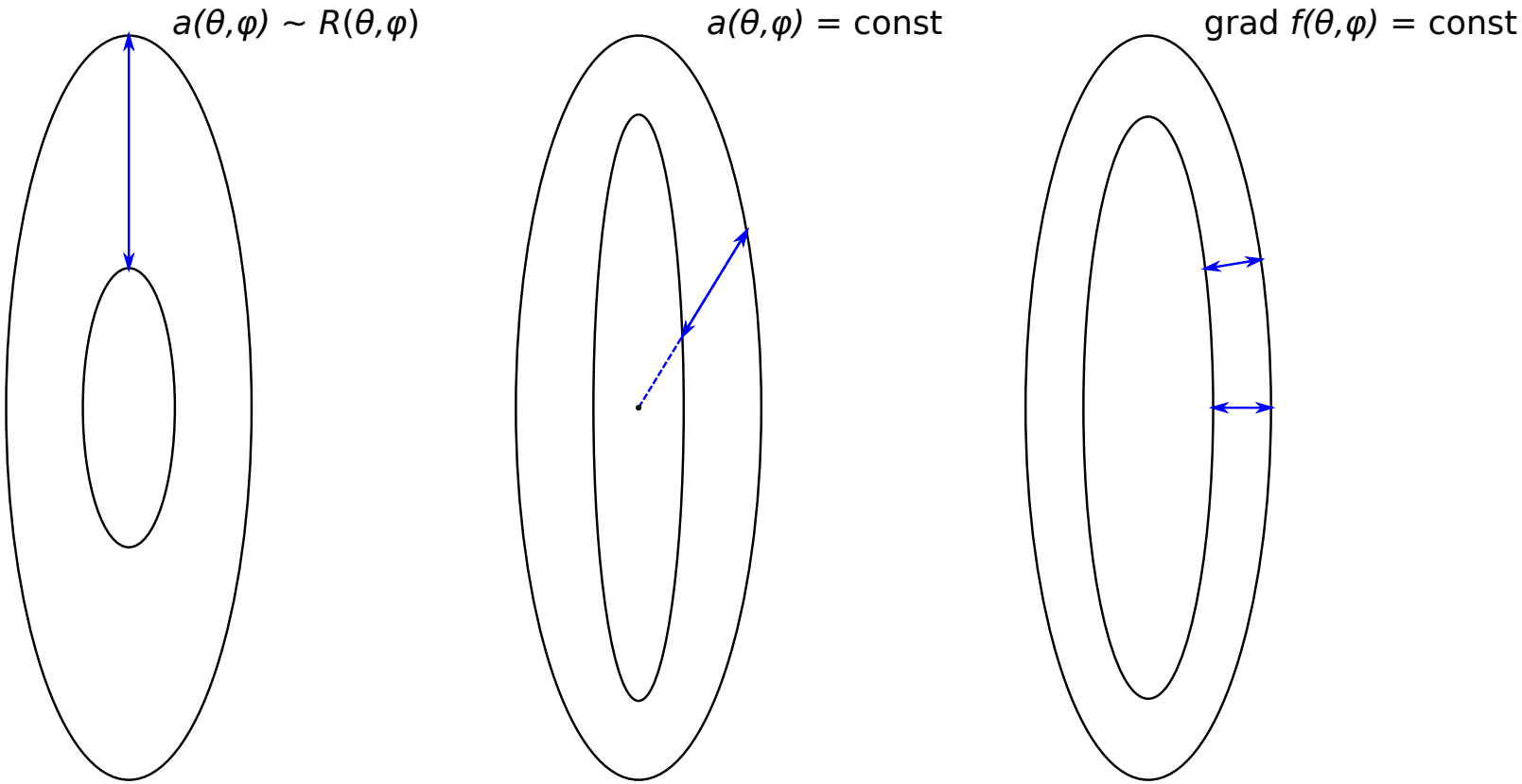
$$f(\theta,\phi) = \frac{1}{1+e^{\frac{r-R(\theta,\phi)}{a(\theta,\phi)}}},$$

where $R(\theta,\phi)$ is the radius (with restriction of volume conservation $abc = \text{const}$)

$$R = R_0\left(\frac{\sin^2\theta\cos^2\phi}{a^2} + \frac{\sin^2\theta\sin^2\phi}{b^2} + \frac{\cos^2\theta}{c^2}\right)^{-\frac{1}{2}};$$

$a(\theta,\phi)$ is the diffuseness parameter ("thickness of the surface layer").

Choice of the angular dependence of the diffuseness



$r_{\text{CSPYPXCГP}_{\prime\prime}} \approx 1$ fm $\Longrightarrow$ thickness of the surface layer is constant at different points of the surface:

$$\left(\text{grad } f(r,\theta,\phi)|_{r=R(\theta,\phi)}\right)^2 = \frac{1}{16a^2(\theta=0,\phi=0)} = \text{const.}$$

Single-particle shell-model potential

Parameters of the potential

- Use the real part of the spherical global optical potential from [A. Koning, J. Delaroche, Nucl. Phys. **A 713**, 231 (2003)]

$$U(r,E) = -V_V(r,E) - iW_V(r,E) - iW_D(r,E) + \\ + V_{SO}(r,E)(\mathbf{l}\cdot\mathbf{s}) + iW_{SO}(r,E)(\mathbf{l}\cdot\mathbf{s}) + V_C(r),$$

  where each term $V(r,E) \equiv V(E)f(a,R,r)$.

- Parameterized $V(E) = V(E,A,Z)$, $R = R(A,Z)$, $a = a(A,Z)$ for p and n from experimental cross sections of nucleon scattering on spherical nuclei $24 \leq A \leq 209$.
- Parameter values at $E = \epsilon_F$ approximately correspond to the average nuclear potential in the near-surface area which affects deformation the most.

Single-particle shell-model potential

Terms of the potential

$$V(r,\theta,\phi) = V_{\text{nucl}}(r,\theta,\phi) + V_{\text{ls}}(r,\theta,\phi) + V_{\text{Coul}}(r,\theta,\phi)$$

- Nuclear interaction

$$V_{\text{nucl}}(r,\theta,\phi) = -U_{\text{nucl}} f_{\text{nucl}}(r,\theta,\phi).$$

- Spin-orbit interaction

$$V_{\text{ls}}(r,\theta,\phi) = \lambda\!\!\!^{-2}_{\pi} U_{\text{ls}}(\hat{F} + \hat{F}^{+}),$$

  PγPψPχ $\hat{F} = ([\nabla f_{\text{ls}}(r,\theta,\phi) \times \hat{\mathbf{p}}] \cdot \hat{\mathbf{s}})$.

- Coulomb potential

$$V_{\text{Coul}}(r,\theta,\phi) = \frac{3}{4\pi}\frac{qZe^2}{R^3_{\text{Coul}}} \times \int_0^{2\pi} d\phi' \int_0^{\pi} \sin\theta' d\theta' \int_0^{R(\theta'\phi')} \frac{(r')^2 dr'}{\sqrt{r^2 + (r')^2 - 2rr'\cos\beta}}.$$

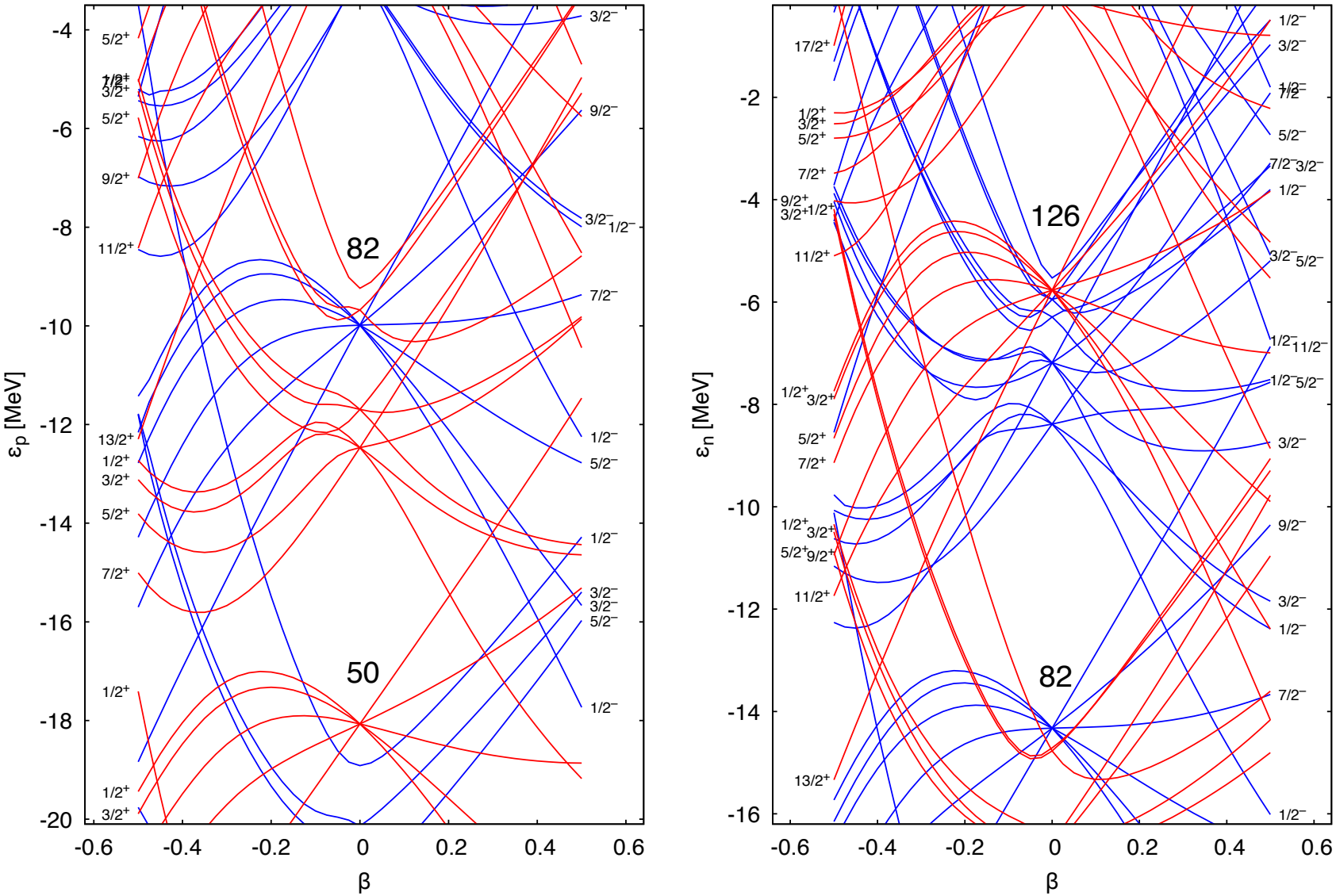
Calculation of single-particle states

- Schrödinger equation solved by diagonalization of the Hamiltonian $\hat{H} = \hat{T} + \hat{V}$.
- Matrix elements $\langle N'l'm's'|\hat{H}|Nlms\rangle$ calculated in the isotropic harmonic oscillator basis.

$$\langle \mathbf{r}\sigma|Nlms\rangle = U_{Nl}(r)Y_{lm}(\theta,\phi)\langle\sigma|s\rangle.$$

- Cut-off $N_{\max} = 11$.
- Volume integration reduced to calculation of spherical harmonic expansion coefficients $\alpha(r)$ of functions of f, $\frac{\partial f}{\partial\theta}$, $\frac{\partial f}{\partial\phi}$, K_λ and subsequent 1D integration wrt. r.
- Full time of eigenvalue computation for p and n at a fixed deformation 5–10 s.

Single-particle levels of ^{150}Sm



(Negative β values taken along the $\gamma = 60^\circ$ line.)

Pairing correction

Levels of the single-particle spectrum are double degenerate (Cramers). Nucleon pairing taken into account using the BCS method:

$$\Delta E = \sum_{k=N_1}^{N_2} (2v_k^2 - n_k)e_k - \frac{\Delta^2}{G} - G\sum_{k=N_1}^{N_2} v_k^4 + \frac{1}{2}G\sum_{k=N_1}^{N_2} n_k,$$

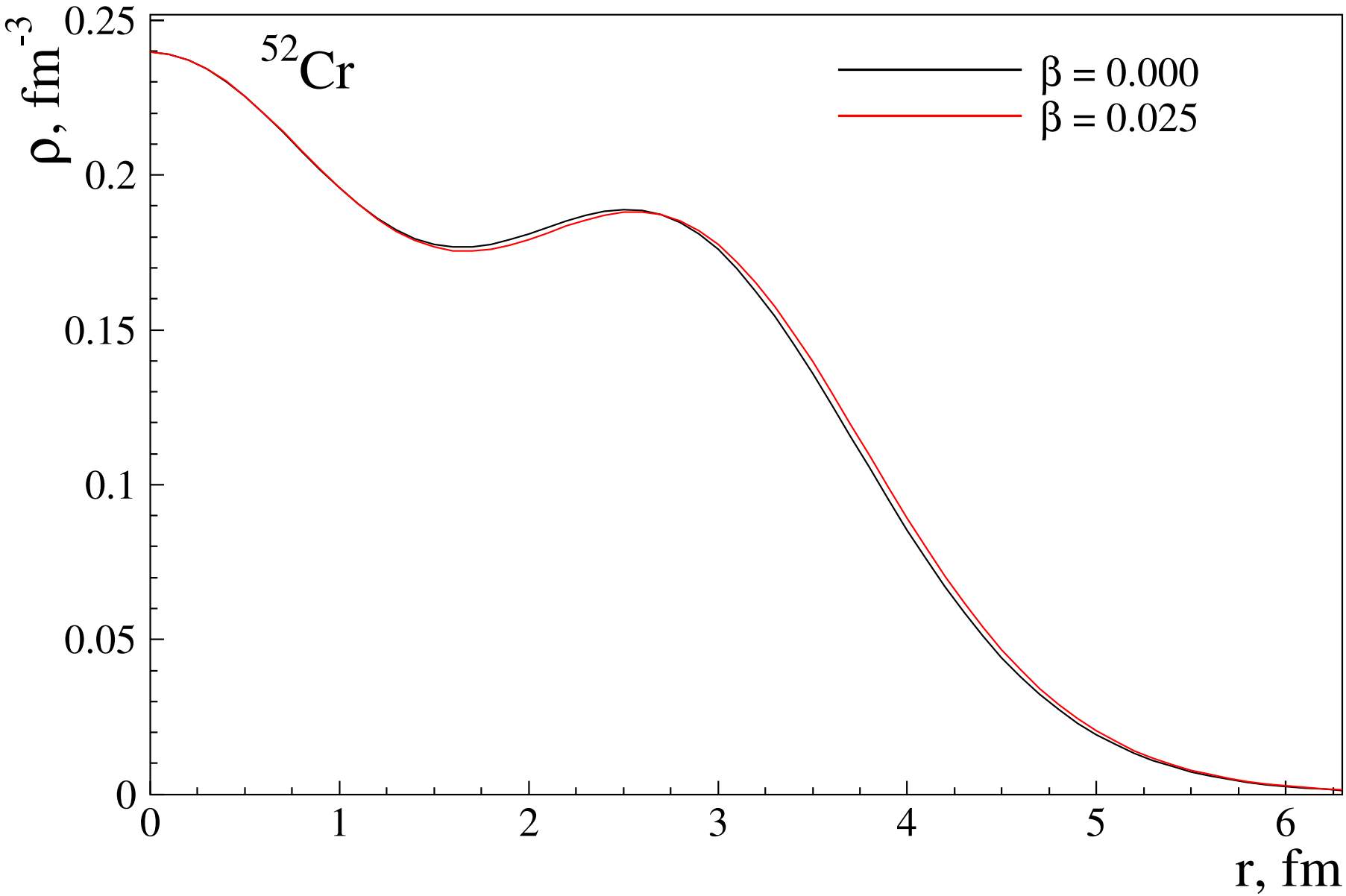
where the pairing gap width Δ is estimated from difference of masses of 4 neighbour nuclei, and the interaction constant G, particle numbers v_k, and energies of quasiparticle levels e_k are determined by solution of the BCS equations.
N_1 Рч N_2 determine the range of interacting states.

$$N_1 = 1,$$

$$N_2 = 2N_F.$$

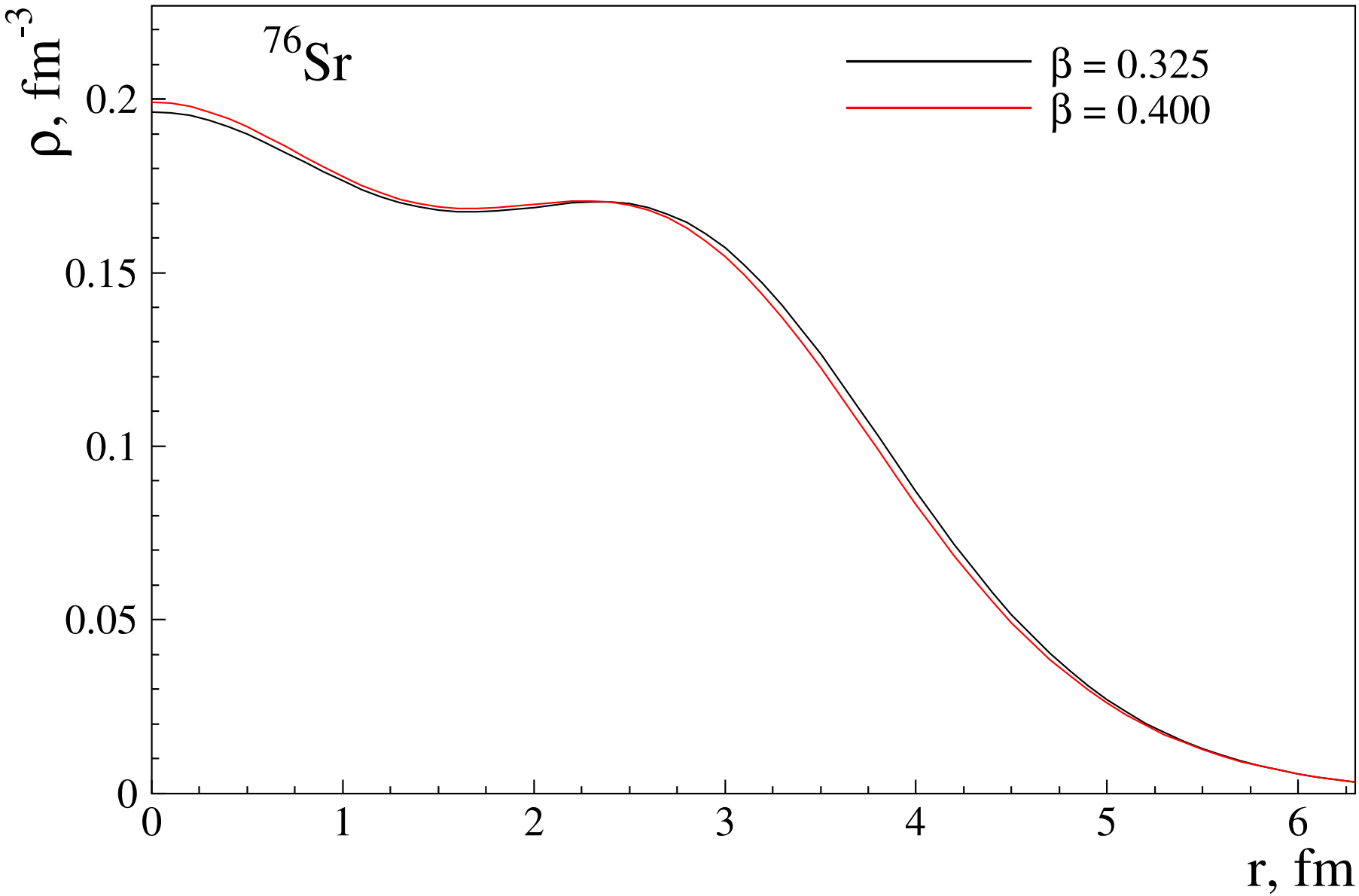
Surface diffuseness as a function of deformation

Spherical $^{52}_{24}Cr_{28}$



Surface diffuseness as a function of deformation

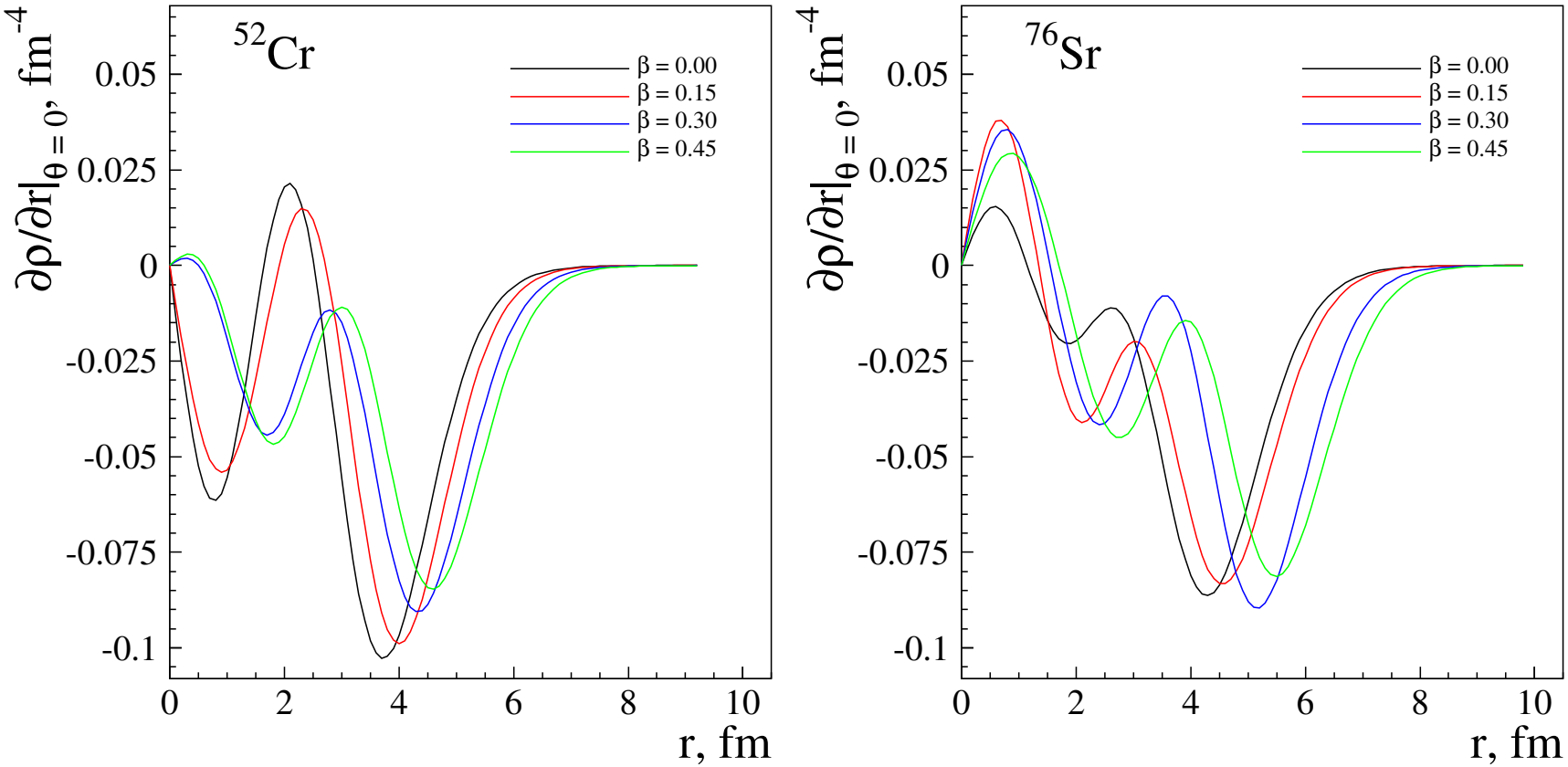
Deformed $^{76}_{38}Sr_{38}$



Surface diffuseness as a function of deformation

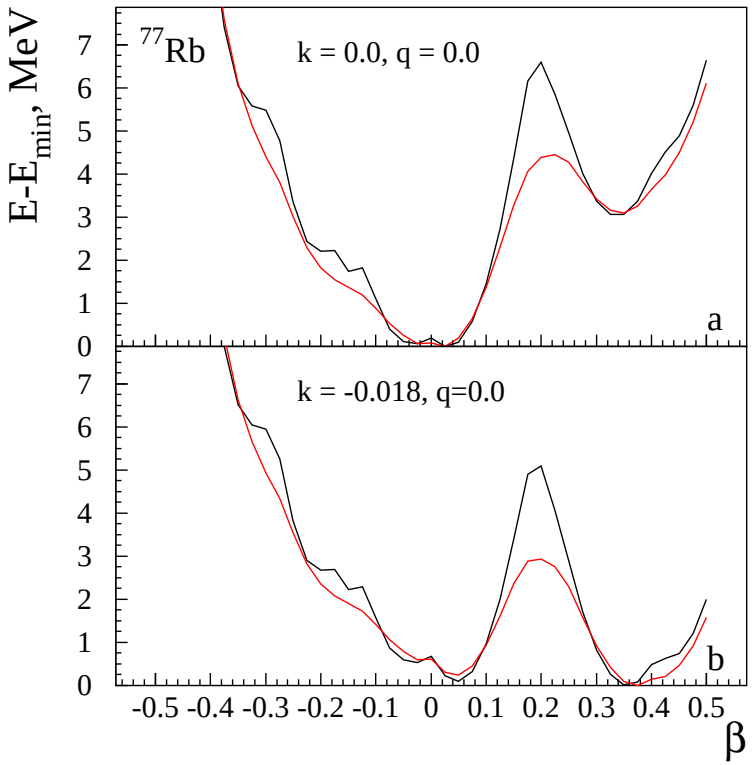
- Which parameter of the WS potential to adjust — R, V, or a?
- Deformation $\Longleftrightarrow$ increased density of single-particle states near the Fermi surface.
- Diffuseness $\Longleftrightarrow$ surface energy (i. e., total energy of nucleons in the surface layer).
- Connection between the deformation and the diffuseness parameter a which was measured only for spherical nuclei. Its value should have a minimum near the equilibrium deformation point.

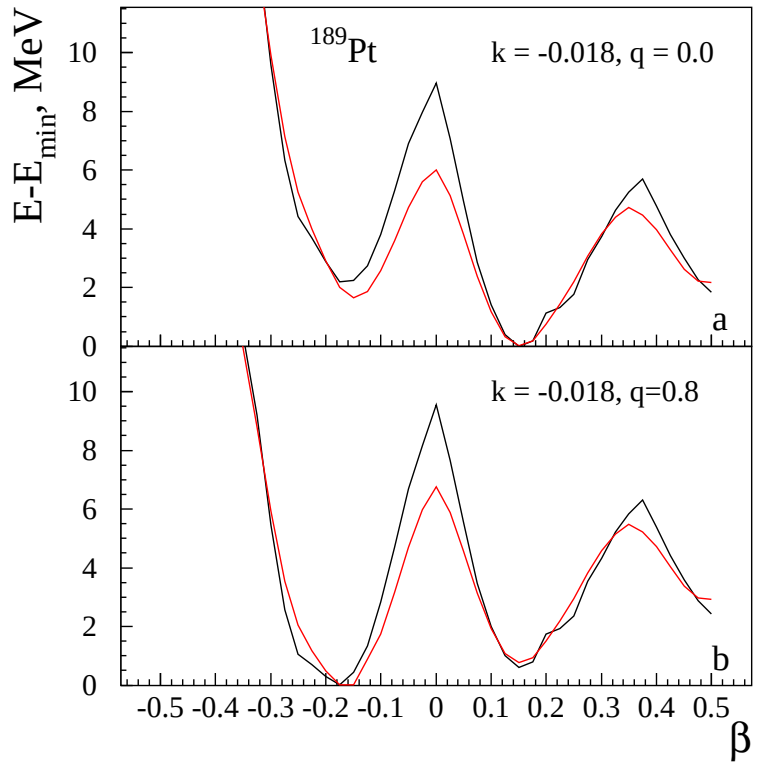
Surface diffuseness as a function of deformation



We choose $a(\beta,\gamma) = a_0\left(1 + k\beta\psi\left(\frac{3\gamma}{\pi}\right)\right)$, where $\psi(x) = 1 + p_1 x + p_2 x^2 + p_3 x^3$. Derivative ψ' should be negative at $\gamma = 0^\circ$ and positive at $\gamma = 60^\circ$ with the same absolute value. Finally, $p_2 = -3(1-q) - p_1$, $p_3 = 2(1-q)$.

Surface diffuseness as a function of deformation



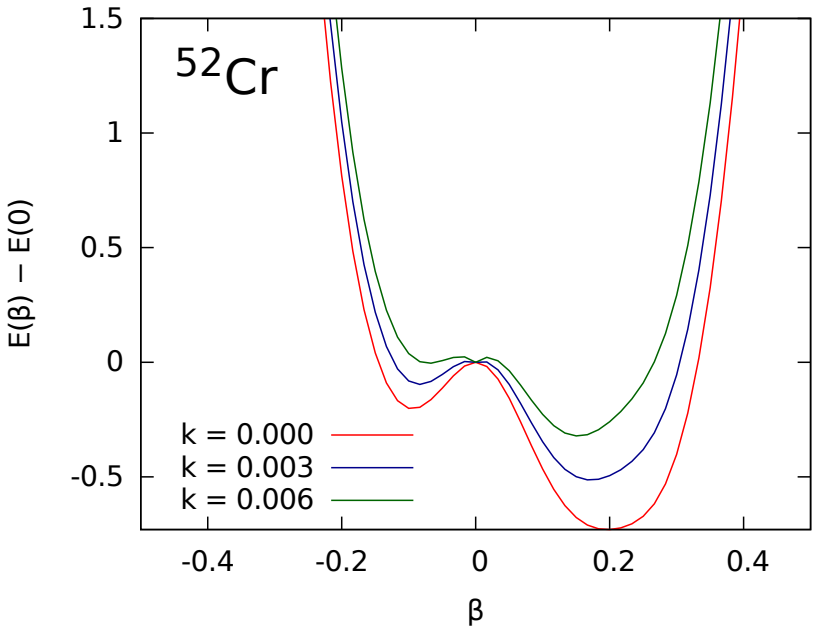


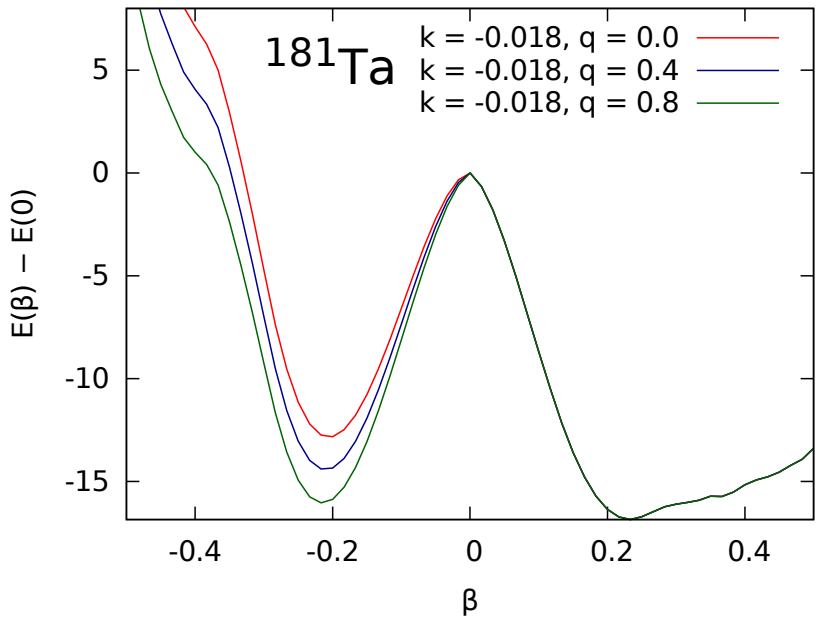
Based on key nuclei ^{52}Cr (spherical), ^{77}Rb (prolate), ^{189}Pt (oblate) Рч ^{181}Ta (prolate) two strategies of variation of diffuseness are proposed.

(a) Magic nuclei: $k = +0.006$.

(b) All others: $k = -0.018$, $q = 0.8$, $p_1 = -0.4$.

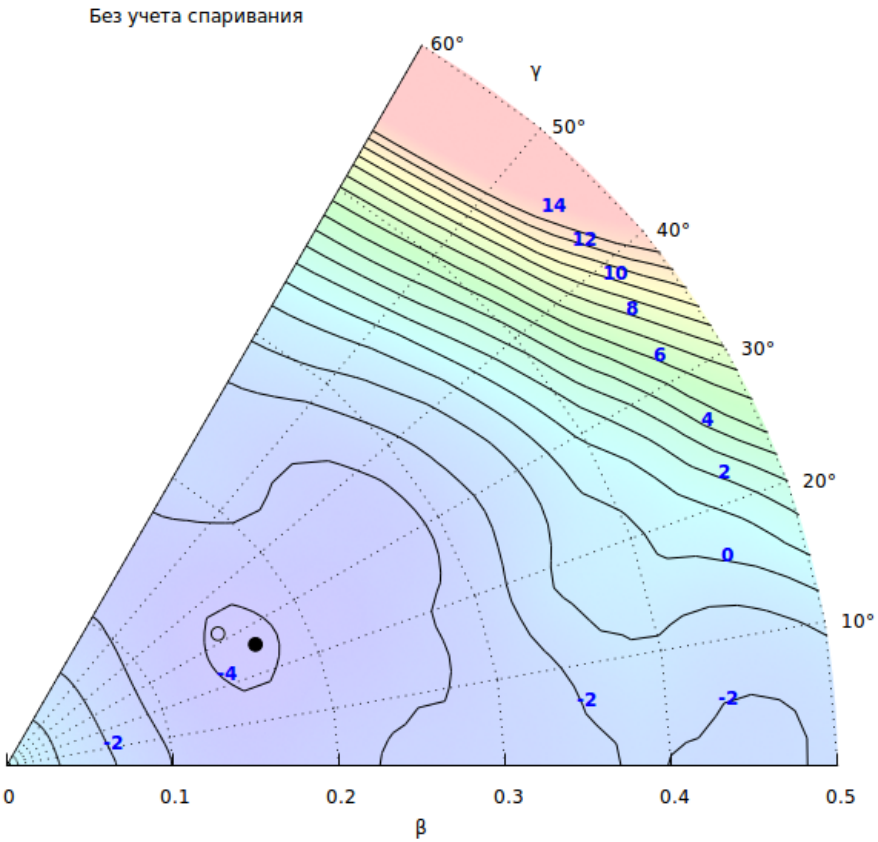
Surface diffuseness as a function of deformation

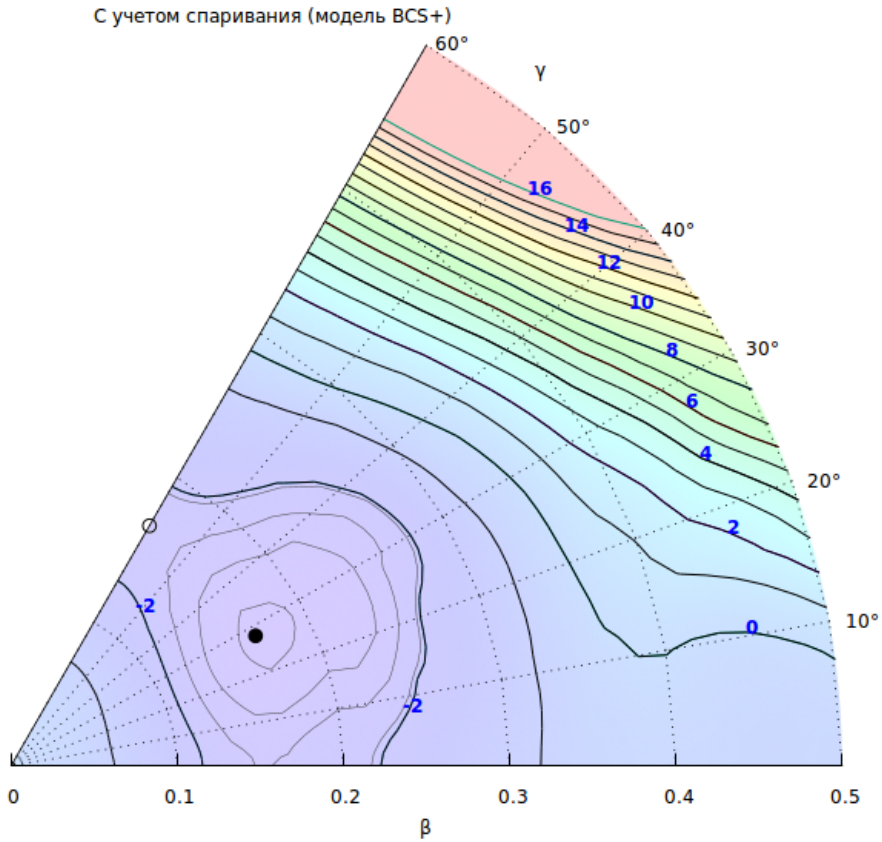




Results

^{68}Ga

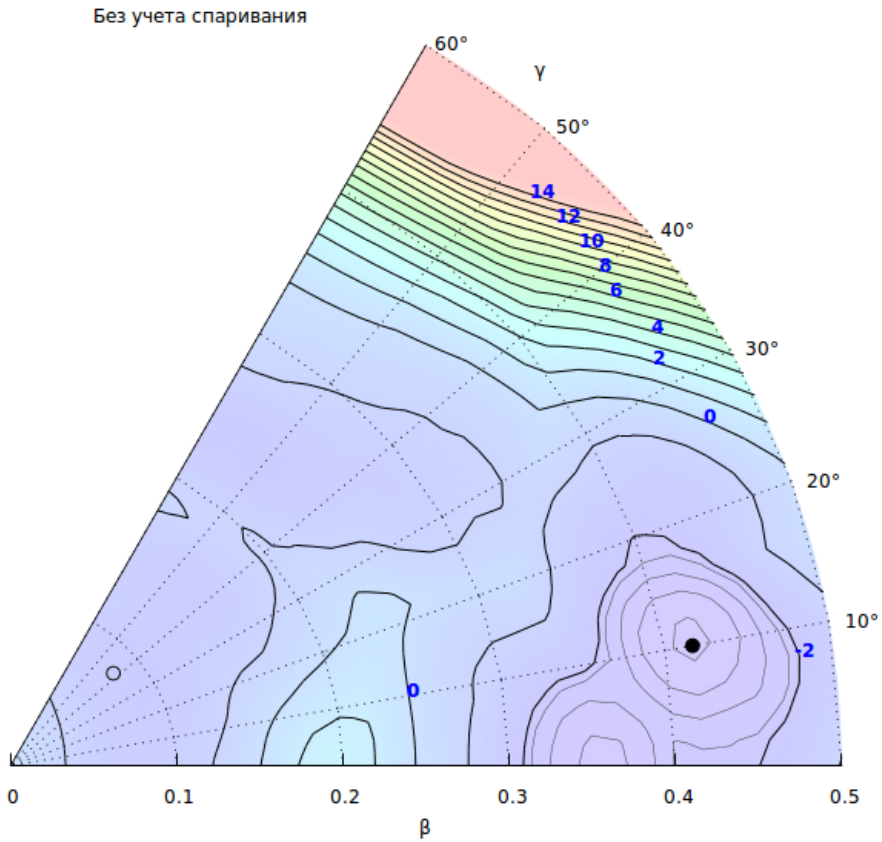


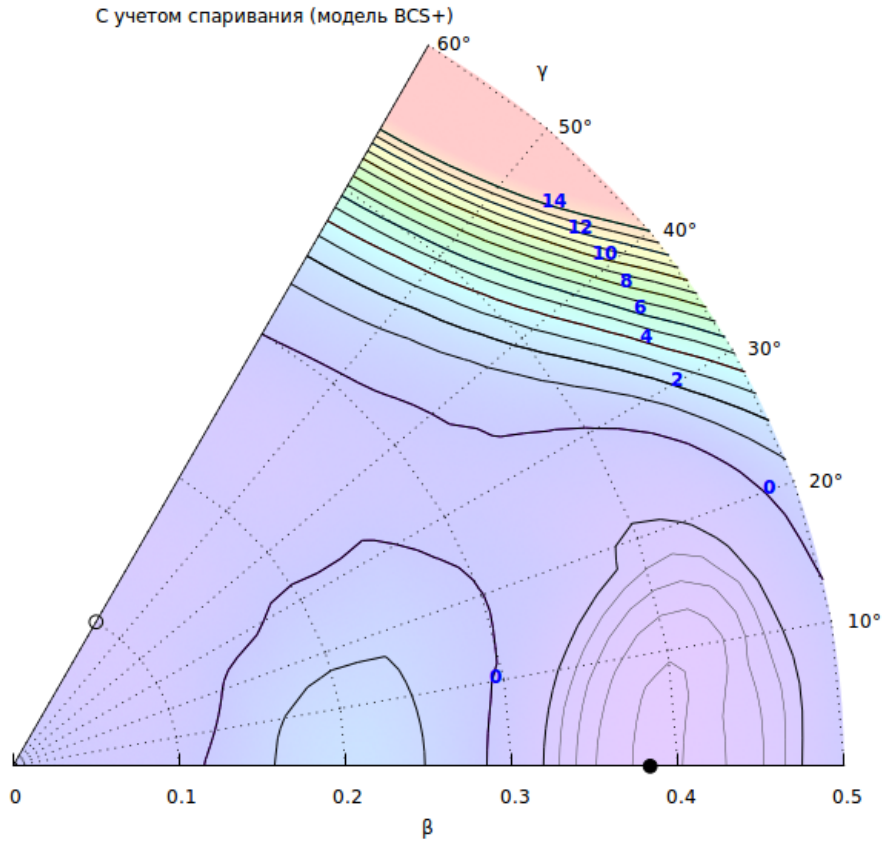


This work				FRDM			BRUSLIB		AMEDEE		CDFE
β	γ	β_2	β_4	β_2	γ	β_4	β_2	β_4	β_2	γ	β_2
0.17	34	0.165	0.027	-0.207	45	-0.006	-0.23	0.04	-0.20		0.022 ± 0.002

Results

^{75}Kr

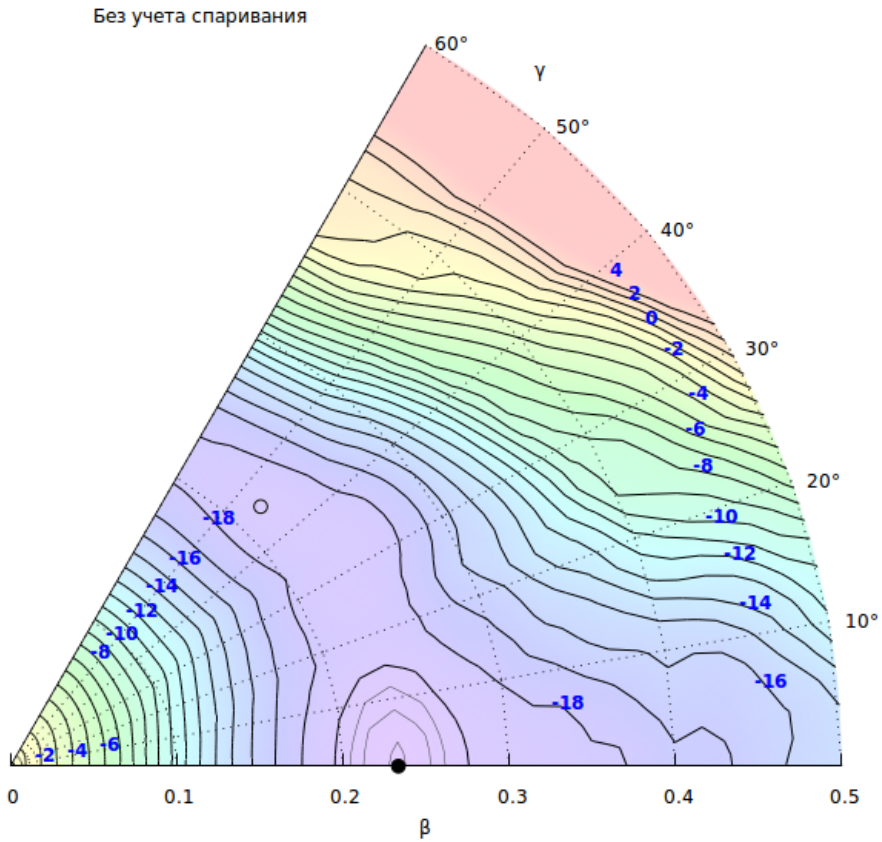


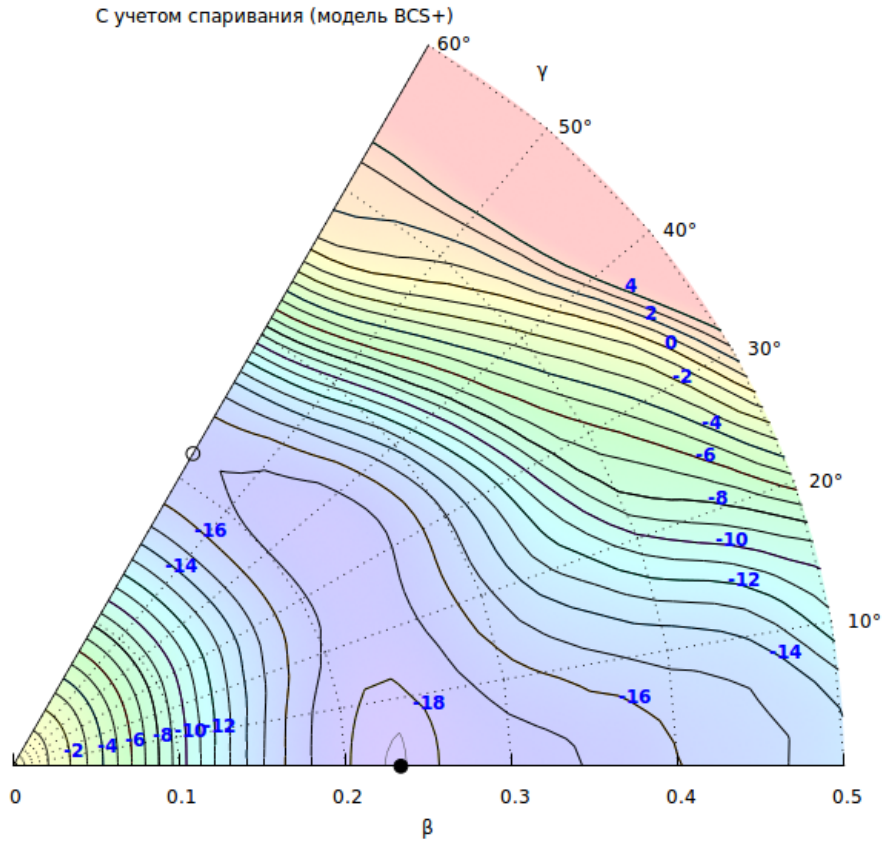


This work				FRDM			BRUSLIB		AMEDEE		CDFE
β	γ	β_2	β_4	β_2	γ	β_4	β_2	β_4	β_2	γ	β_2
0.38	0	0.406	0.168	0.402	0	-0.010	-0.20	0.01	-0.15		0.412 ± 0.065

Results

^{181}Ta

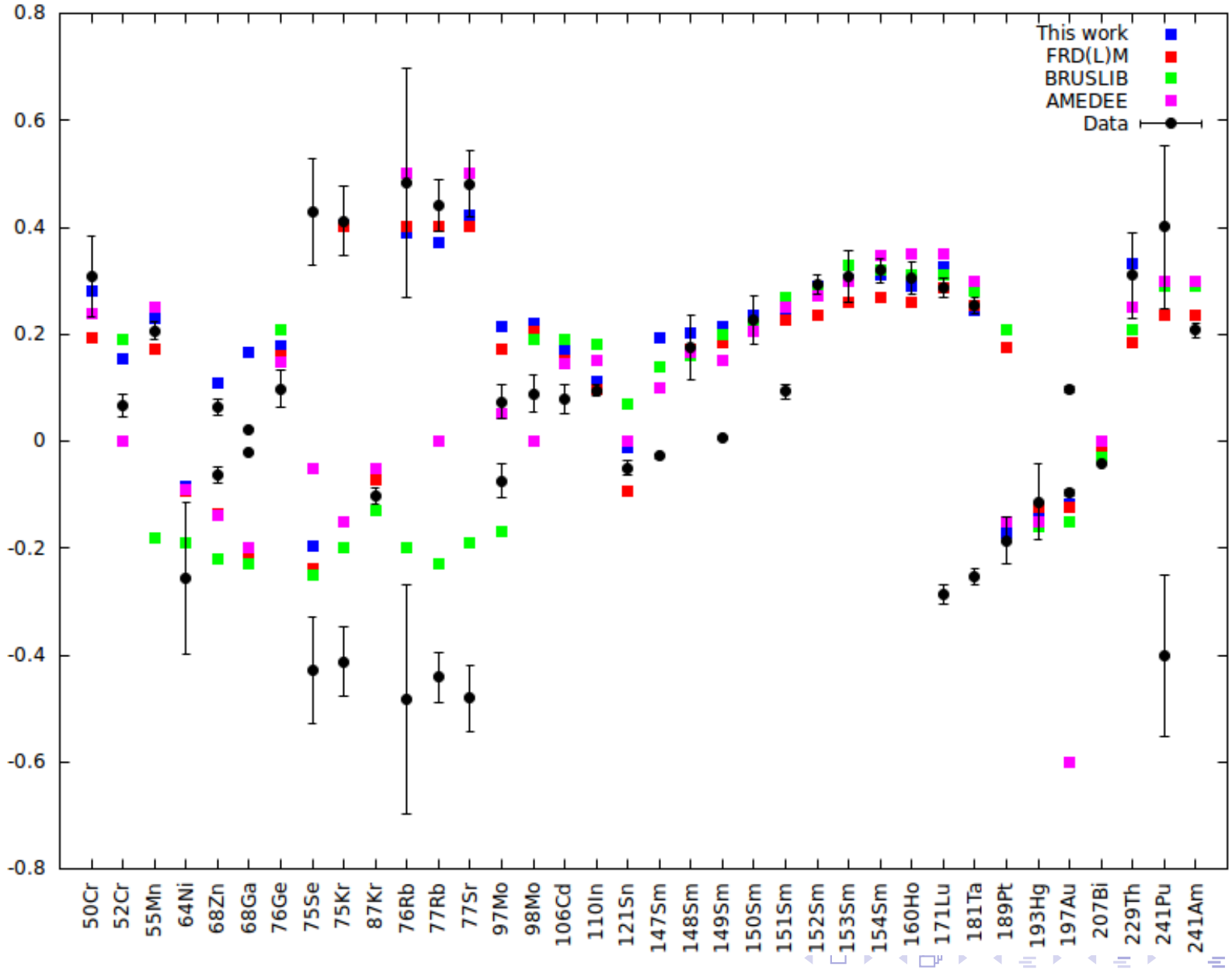




This work				FRDM			BRUSLIB		AMEDEE		CDFE
β	γ	β_2	β_4	β_2	γ	β_4	β_2	β_4	β_2	γ	β_2
0.23	0	0.245	0.043	0.255	0	-0.076	0.28	-0.04	0.30		0.253 ± 0.015

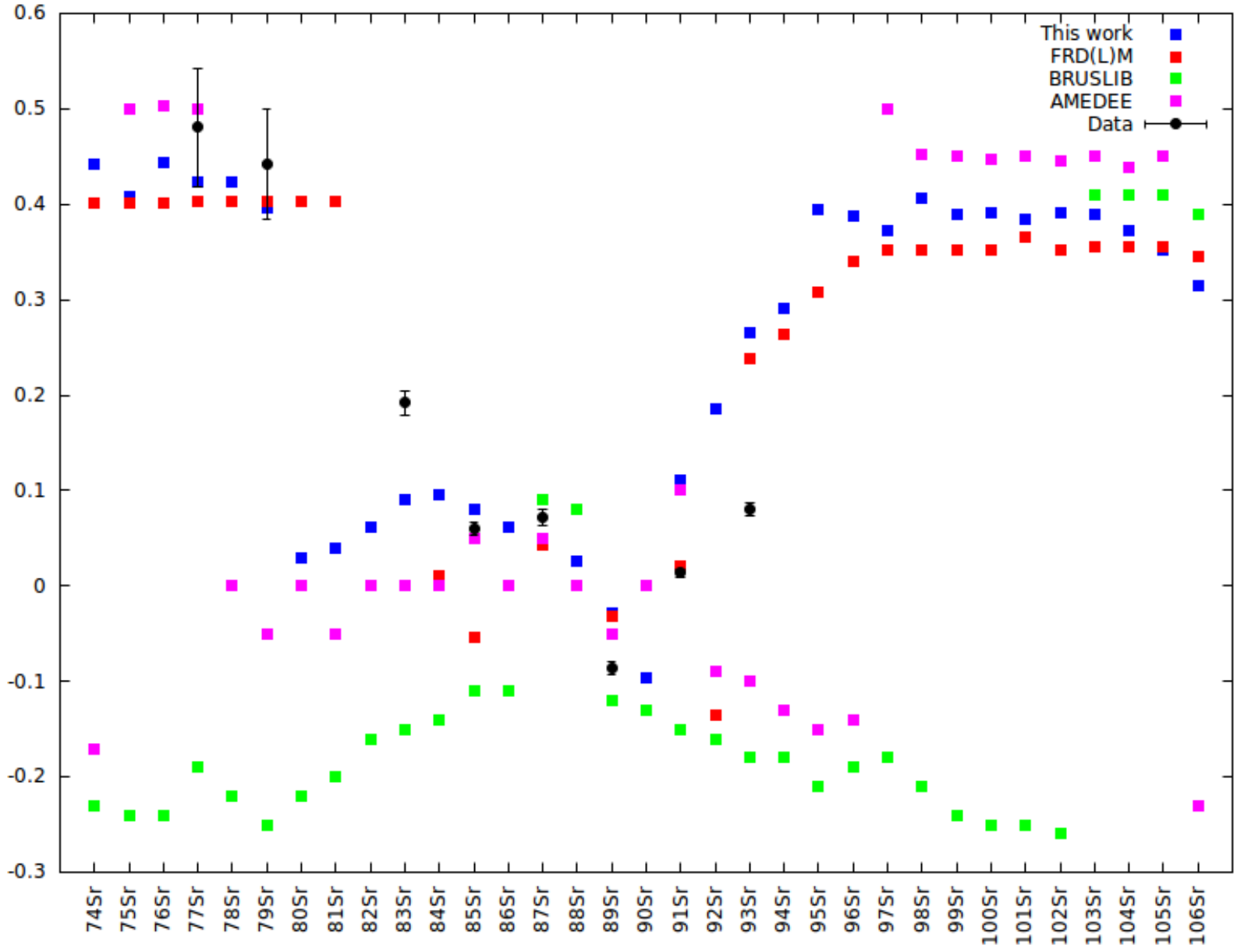
Overall evaluation

^{50}Cr — ^{241}Am



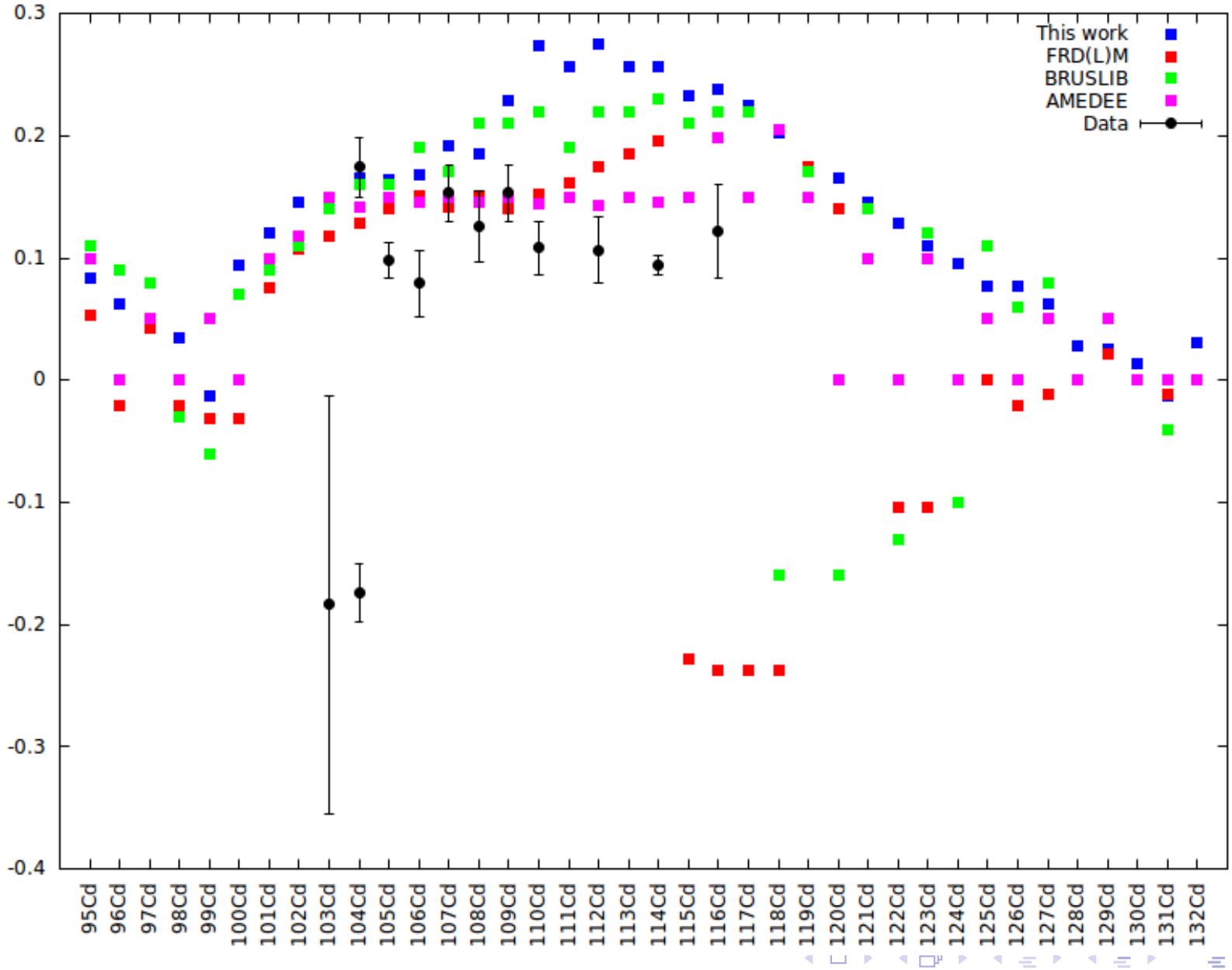
Overall evaluation

^{74}Sr — ^{106}Sr



Overall evaluation

^{95}Cd — ^{132}Cd



Conclusions

- A simple model of deformation of medium and heavy nuclei based on the Nilsson model is formulated.
- Connection between deformation energy and surface diffuseness is shown.
- Only 3 additional parameters are introduced.
- Calculations of potential energy surfaces are performed on 107 nuclei from ^{50}Cr to ^{241}Am.
- Very small variation ($< 1\%$) of the diffuseness parameter was enough for satisfactory description of wide range of data, comparable with much more complex models.

Thank you!