Woods-Saxon Potential, Shell Correction Theory Atomic Masses and Deformation of Nuclei

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PLAN

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2. Woods-Saxon Potential.
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1. Introduction

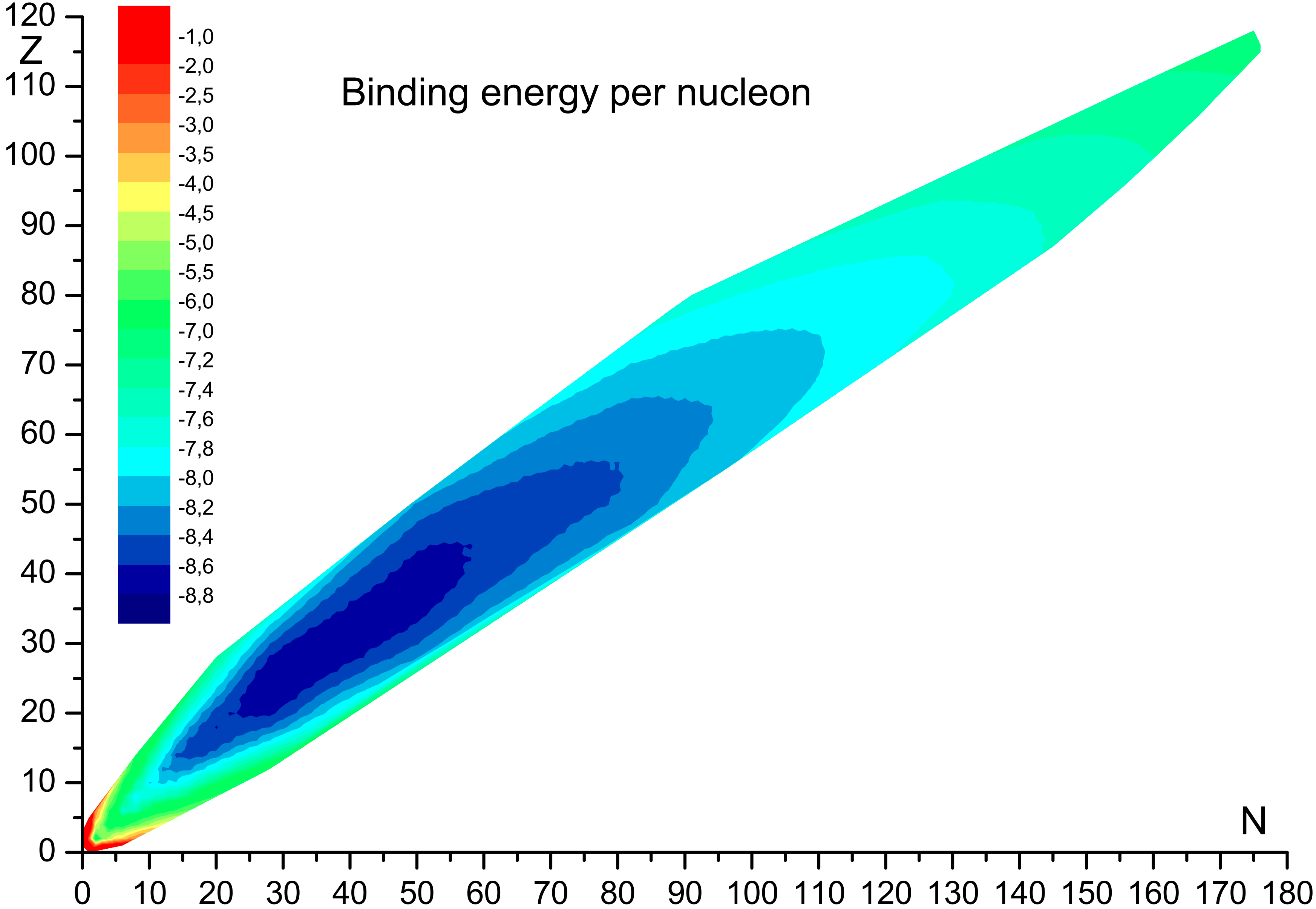
Mass of Nucleus $M_{Nucl}c^2$ is less than the mass of all protons and all neutrons, which compose the nucleus, i.e.

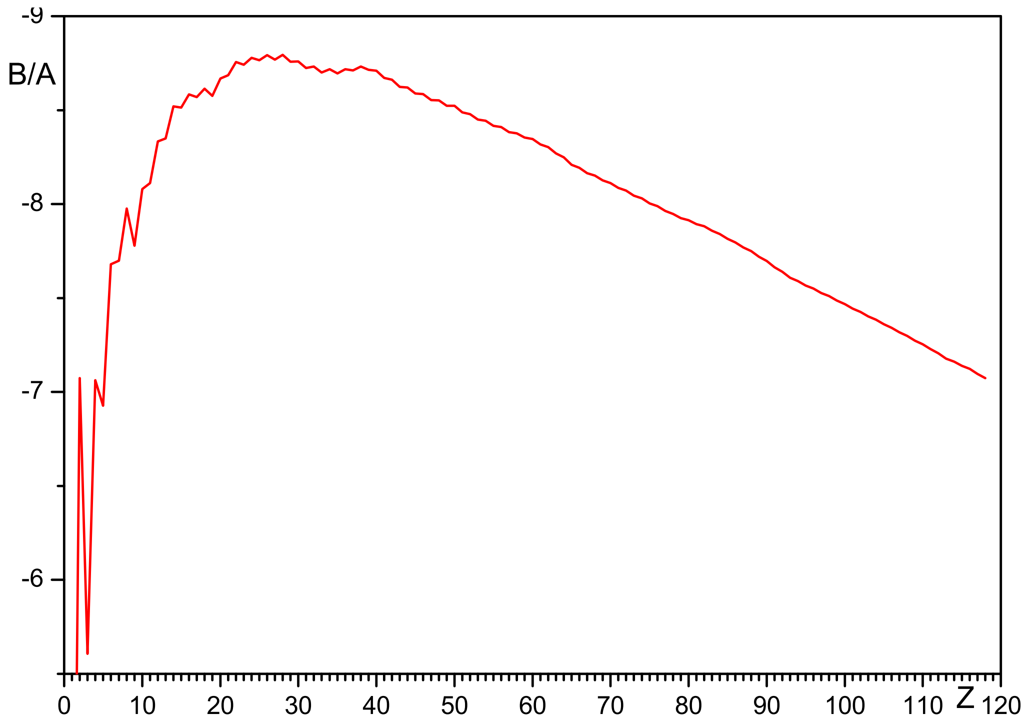
$$M_{\mathrm{Nucl}}c^2 < Z \cdot m_P c^2 + N \cdot m_N c^2.$$

The difference of these masses is binding energy of nucleus

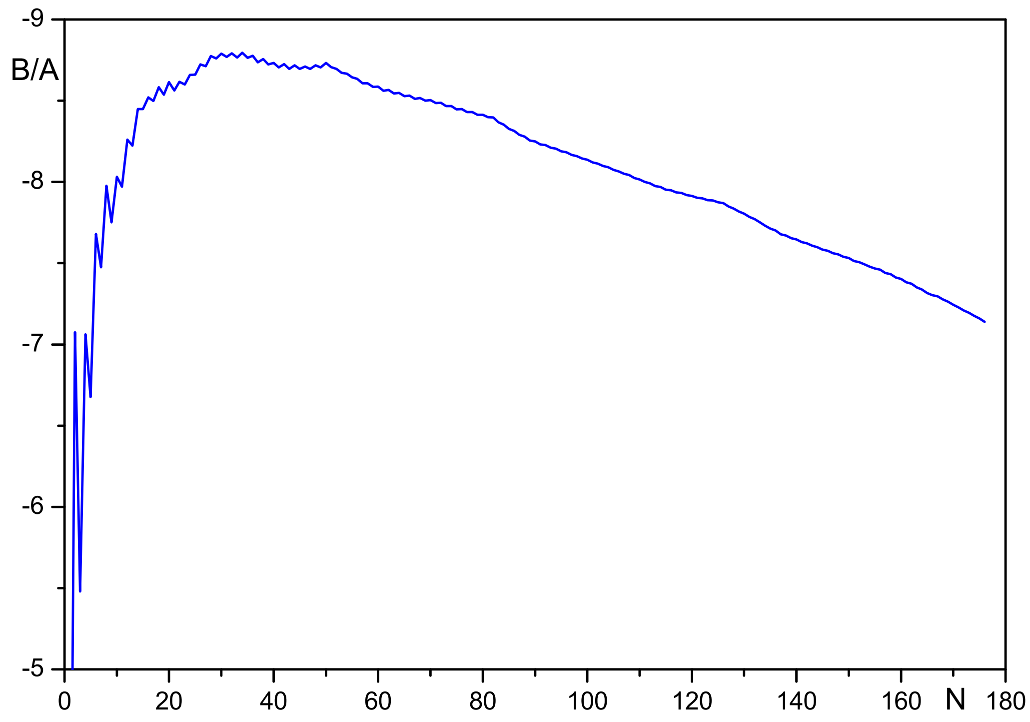
$$E(Z,N) = M_{\mathrm{Nucl}}c^2 - (Z \cdot m_P c^2 + N \cdot m_N c^2).$$

Binding energy per nucleon

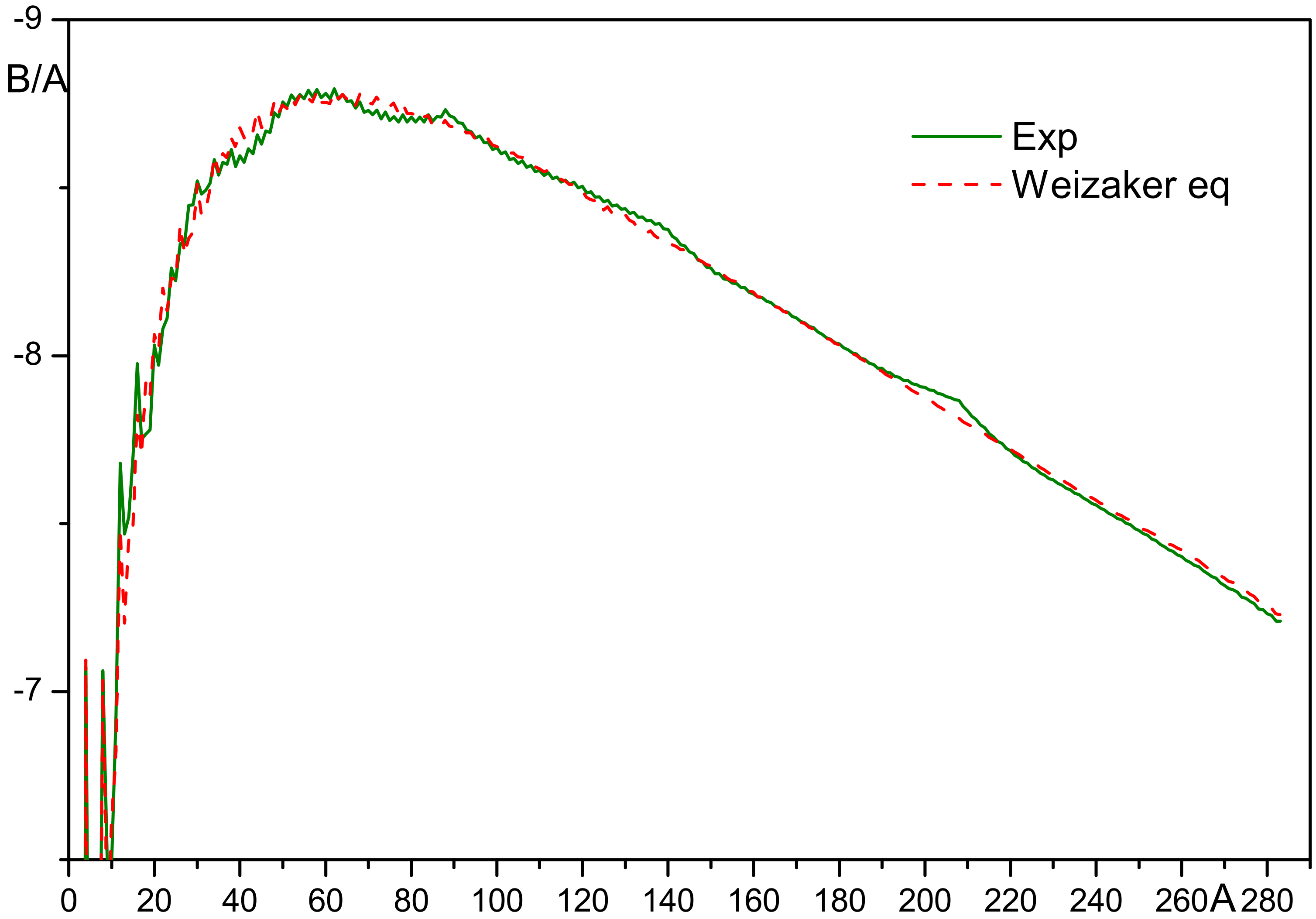




B/A
-9
-8
-7
-6
0
10
20
30
40
50
60
70
80
90
100
110
Z
120



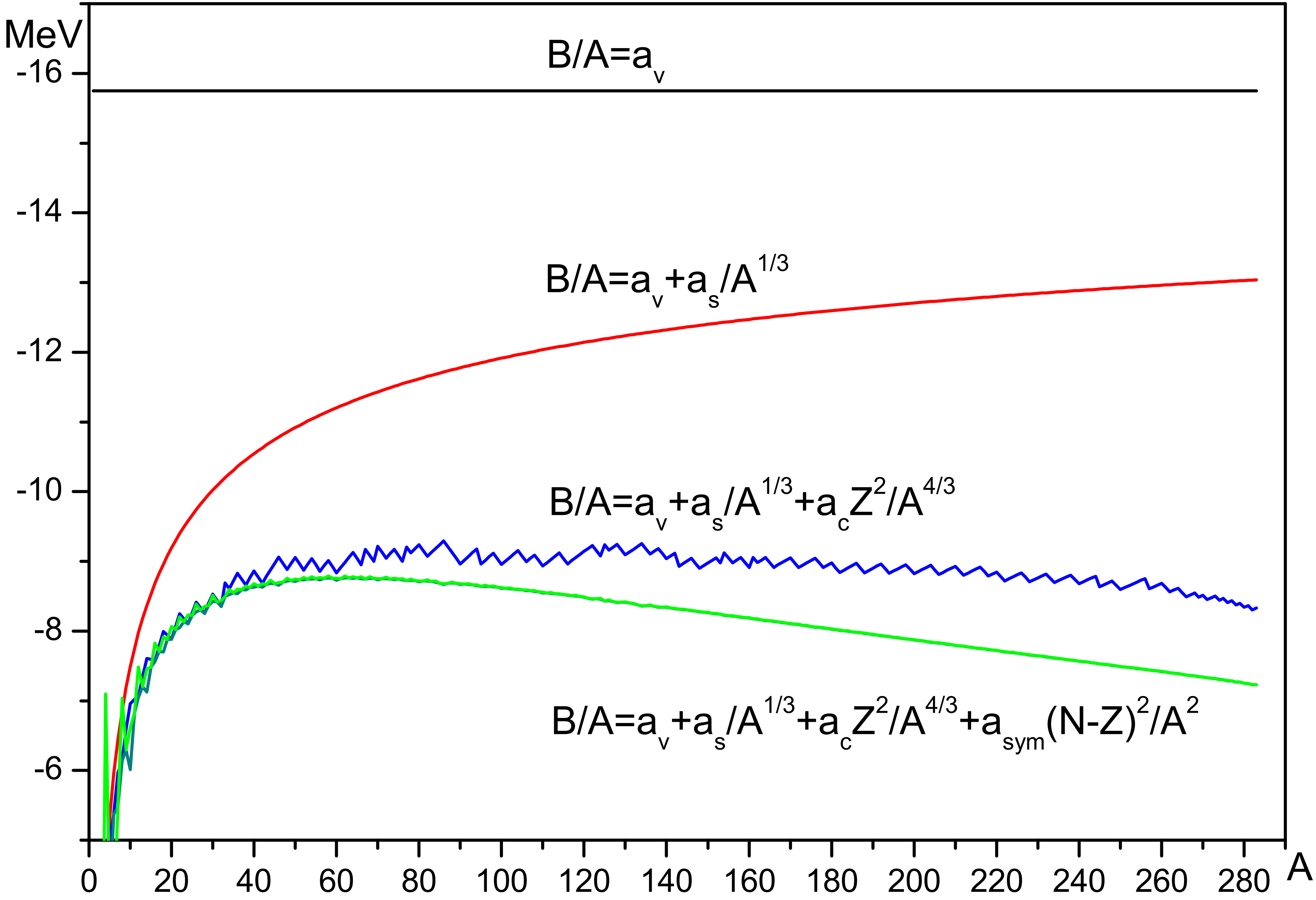
B/A
-9
-8
-7
-6
-5
0
20
40
60
80
100
120
140
160
N
180



Weizäcker expression for binding energy of nuclei is

$$B = a_v A + a_s A^{2/3} + a_c \frac{Z^2}{A^{1/3}} + a_{sym} \frac{(N-Z)^2}{A} - \begin{cases} 34A^{-3/4} & \text{foreven} - \text{even} \\ 0 & \text{forodd} \\ -34A^{-3/4} & \text{forodd} - \text{odd} \end{cases} .$$

where $a_v = -15.75$ MeV, $a_s = 17.8$ MeV, $a_c = 0.71$ MeV and $a_{sym} = 23.7$ MeV.


MeV
B/A=a_v
B/A=a_v+a_s/A^{1/3}
B/A=a_v+a_s/A^{1/3}+a_cZ^2/A^{4/3}
B/A=a_v+a_s/A^{1/3}+a_cZ^2/A^{4/3}+a_sym(N-Z)^2/A^2
-16
-14
-12
-10
-8
-6
0
20
40
60
80
100
120
140
160
180
200
220
240
260
280
A

2. Woods-Saxon Potential.

Let's consider for simplicity Schrödinger equation for proton in nucleus with Z protons

$$[-\frac{\hbar^2}{2m}\nabla^2 + V]\Psi = E\Psi$$

where

$$V = V_{\rm Coul}(r) + V_{\rm CR}(r) + V_{\rm SR}(r)\hbar^2(\vec{S}\vec{L}),$$

$$V_{\rm Coul}(r) = \begin{cases} \frac{(Z-1)e^2}{r}, & r \geq R_{\rm Coul}, \\ \frac{(Z-1)e^2}{R_{\rm Coul}}\left[\frac{3}{2} - \frac{r^2}{2R_{\rm Coul}^2}\right], & r \geq R_{\rm Coul}, \end{cases}$$

is the Coulomb energy,

$$V_{\rm CR}(r) = \frac{V_0}{1+\exp\left((r-R_C)/d_C\right)}, \quad V_{\rm LS}(r) = \frac{d}{dr}\frac{V_{\rm SR}}{1+\exp\left((r-R_{\rm SR})/d_{\rm SR}\right)}.$$

are the central and spin-orbital potentials.

If we evaluate the single-particle energy E_i and summate all energies than the energy

$$E_{\rm tot} = \sum_i^{i_F} E_i.$$

is not equated to the binding energy of nuclei, because the potential is not self-consistent.

Note that the binding energy can be evaluated in the framework of the Hartree-Fock approximation with high accuracy. However the Hartree-Fock approximation approximation is rather complex.

However many various quantities:

- single-particle levels,
- fission barriers, fission half-life,
- binding energies (using the shell correction approach)
- various dynamics parameters,
- energy of single-particle and excited states
- can be evaluated within the simple Woods-Saxon approximation with high precision.

So, the Woods-Saxon approximation is rather both simple and useful!

3. Strutinsky Shell Correction Theory.

Vilen Mitrofanovich Stutinsky introduced the shell-correction approach in 1965-1968 (16 October 1929, Danilova Balka, Kirovograd district, Ukraine - 28 June 1993, Roma, Italy) Member-correspondent NASU, Head of Theoretical Nuclear Physics Department of KINR

Main idea: As we pointed that

$$E_{\rm tot} = \sum_i^{i_F} E_i.$$

is not equated to the binding energy of nuclei, because the potential is not self-consistent, but we consider

$$\begin{aligned} E_{\rm tot} &= \sum_i^{i_F} \tilde{E}_i + \left[\sum_i^{i_F} E_i - \sum_i^{i_F} \tilde{E}_i\right] \\ &\Downarrow \text{substitution} \Downarrow \\ &= \text{Macro Mass Formula} + \left[\sum_i^{i_F} E_i - \sum_i^{\tilde{i}_F} \tilde{E}_i\right] \\ &= \text{Macro Mass Formula} + \delta E_{\rm shell}. \end{aligned}$$

Note Macro Mass Formula is rather accurate in general.

$\sum \tilde{E}_i$ is energy evaluated using smooth single-particle energies, averaged on energy.

The shell-model single-particle level density

$$g(E) = \sum_i \delta(E - E_i)$$

gives the single-particle energy, E_i. In this case

$$\sum_i E_i = \int dE\ g(E)E.$$

The smooth single-particle energy, $\tilde{E}$ is given by the mean single-particle level density, $\tilde{g}(\epsilon)$, obtained from $g(E)$ by folding with a smoothing function $f(x)$:

$$\tilde{g}(E) = \frac{1}{\gamma}\int_{-\infty}^{+\infty} dE'\ g(E')f\left(\frac{E - E'}{\gamma}\right) = \frac{1}{\gamma}\sum_i f\left(\frac{E - E_i}{\gamma}\right),$$

where $\gamma \sim (1 \div 2)\hbar\Omega = (1 \div 2)E_F A^{1/3}$ is the averaging parameter, which are close to the distance between shells $8 \div 10$ MeV. So, the averaging is going over the bound single-particle states as well as over the positive-energy single-particle continuum. Therefore

$$\delta E_{\text{shell}} = \sum_i^{i_F} E_i - \int_{-\infty}^{\tilde{\lambda}} dE\ \tilde{g}(E)\ E,$$

where $\tilde{\lambda}$ is the smoothed Fermi level defined through the particle number equation:

$$N = \int_{-\infty}^{\tilde{\lambda}} dE\ \tilde{g}(E).$$

The folding function $f(x)$ can be written as a product

$$f(x) = \omega(x)P_p(x),$$

where

$$\omega(x) = \pi^{-1/2}\exp(-x^2)$$

is a weighting function and

$$P_m(x) = \sum_{k=0,2,\ldots}^{m} \frac{(-1)^{k/2}}{2^k(k/2)!} H_k(x)$$

is the so-called curvature-correction polynomial of the mth order (typical values of the polynomial order are $m = 6, 8$).

The smoothed single-particle energy can be expressed in the form:

$$\tilde{E} = \int_{-\infty}^{\tilde{\lambda}} E\,\tilde{g}(E)dE = \sum_i E_i\tilde{n}_i + \gamma\frac{d\tilde{E}}{d\gamma},$$

where the smoothed distribution numbers are

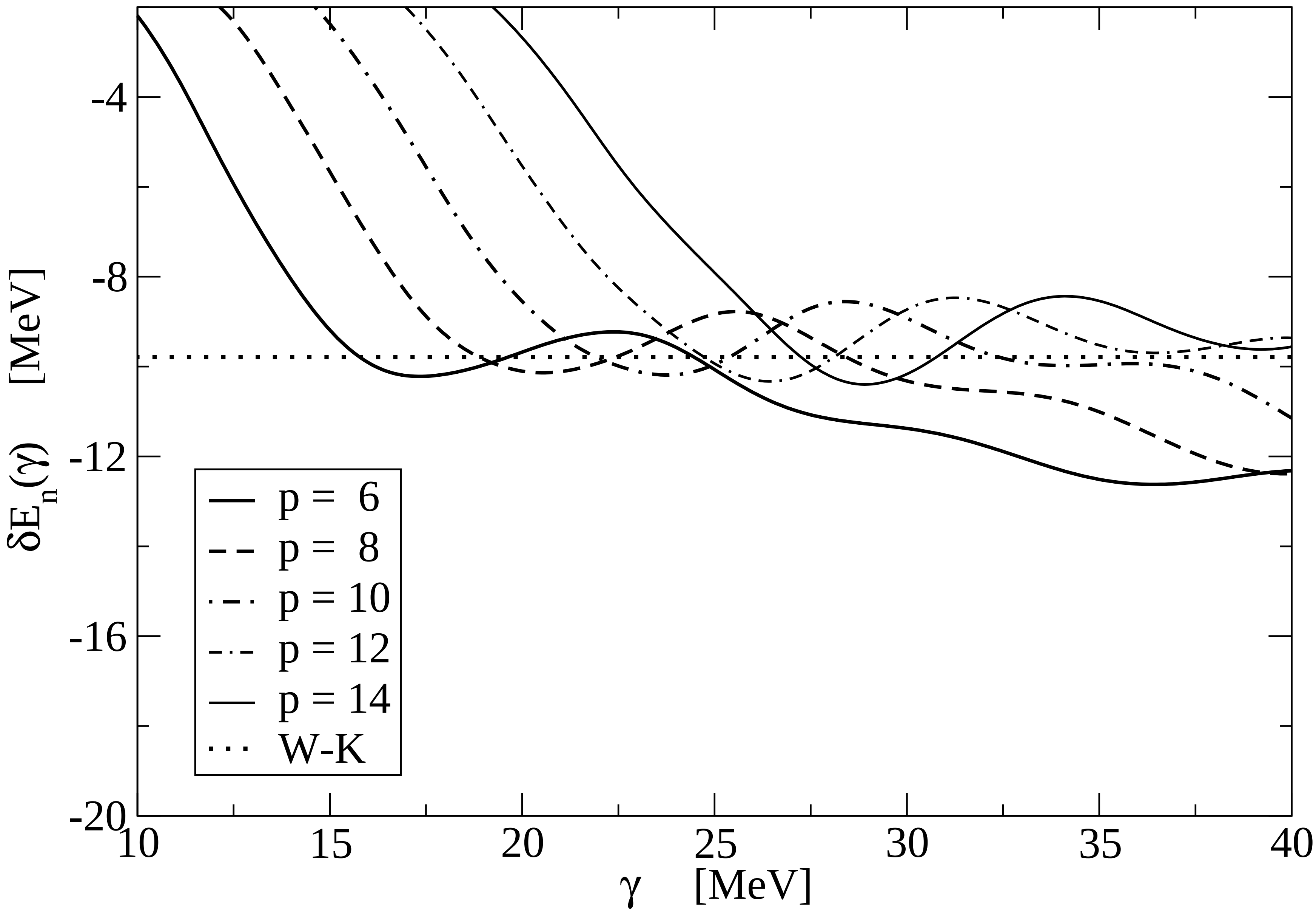
$$\tilde{n}_i = \frac{1}{\gamma}\int_{-\infty}^{\tilde{\lambda}} dE\,f\left(\frac{E-E_i}{\gamma}\right).$$

Since the value of $\tilde{E}$ should not depend on the smoothing range γ (nor on the order of curvature correction m), the second term in must vanish, i.e.

$$\frac{d\tilde{E}}{d\gamma} = 0 \text{ and } \frac{d\tilde{E}}{dm} = 0.$$

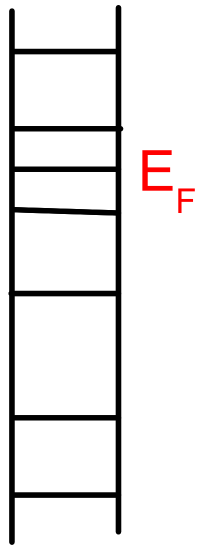
If **plateau condition** does not hold, the Strutinsky averaging method does not yield an unambiguous result.

As a rule, the accuracy os Strutinsky shell correction method (or accuracy of plateau) is $\sim$0.5 MeV in very heavy nuclei and $\sim$1.5 MeV in light and medium nuclei. However often such accuracy is enough. The choice of γ and m on practice defines as corresponding values where the functions $\tilde{E}(\gamma) \simeq constant$ and $\tilde{E}(m) \simeq constant$.



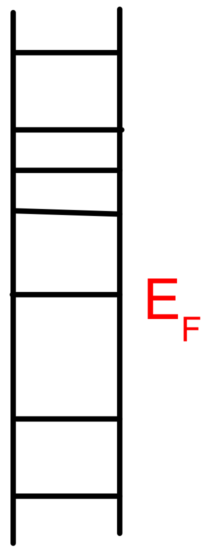
Dependence of Shell-Correction on the averaging parameter γ and order of the curvature-correction polynomial p.

Shell features $\delta E_{\text{shell}} = \sum_i^{i_F} E_i - \int_{-\infty}^{\tilde{\lambda}} dE\, \tilde{g}(E)\, E.$



energy level delsity is higher than average

System stability is less than average shell correction $\delta E_{\text{shell}} > 0$



energy level delsity is lower than average

System stability is higher than average shell correction $\delta E_{\text{shell}} < 0$

The highest value of shell correction is $\delta E_{\rm shell} = -13 \div -14$ Mev evaluated for the ground-state of ^{208}Pb.

For comparison, the binding energy of ^{208}Pb is -1636 MeV.

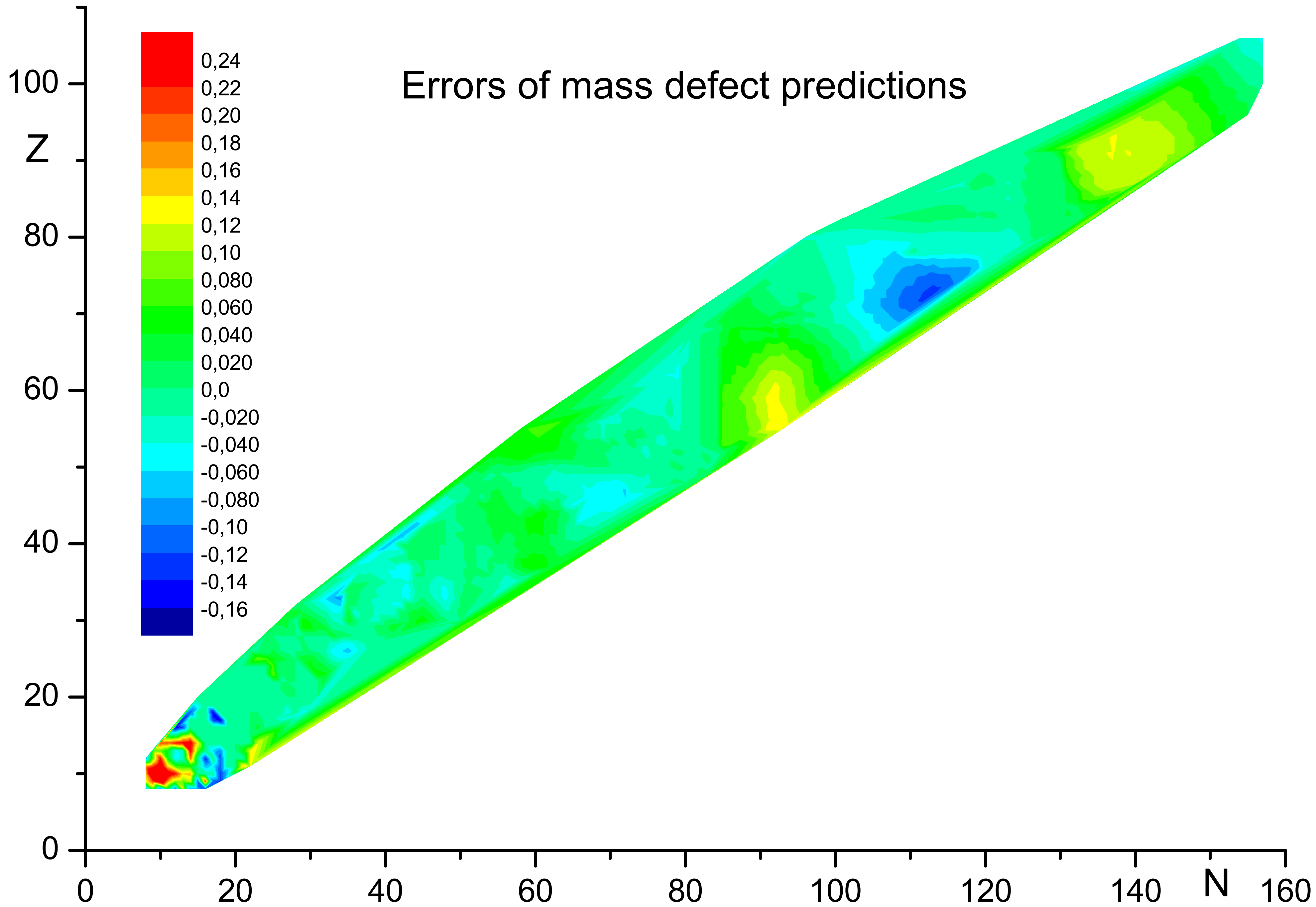
The shell correction method was extremely useful.

By using this method was

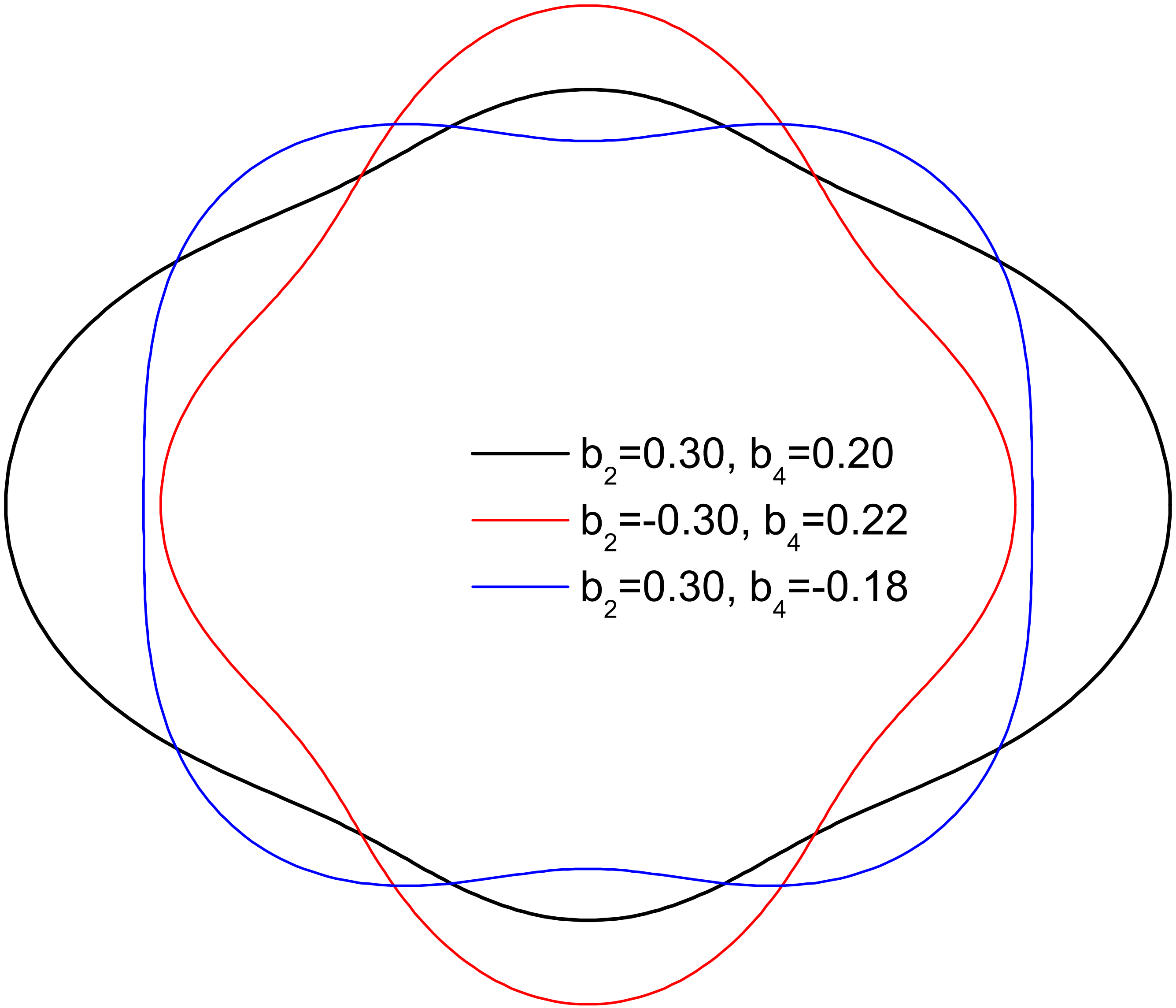
- built the mass formulas with extremely high precision ~0.5 MeV;
- evaluated the equilibrium deformation parameters;
- obtained the fission barriers;
- and etc.

Axial Deformations:

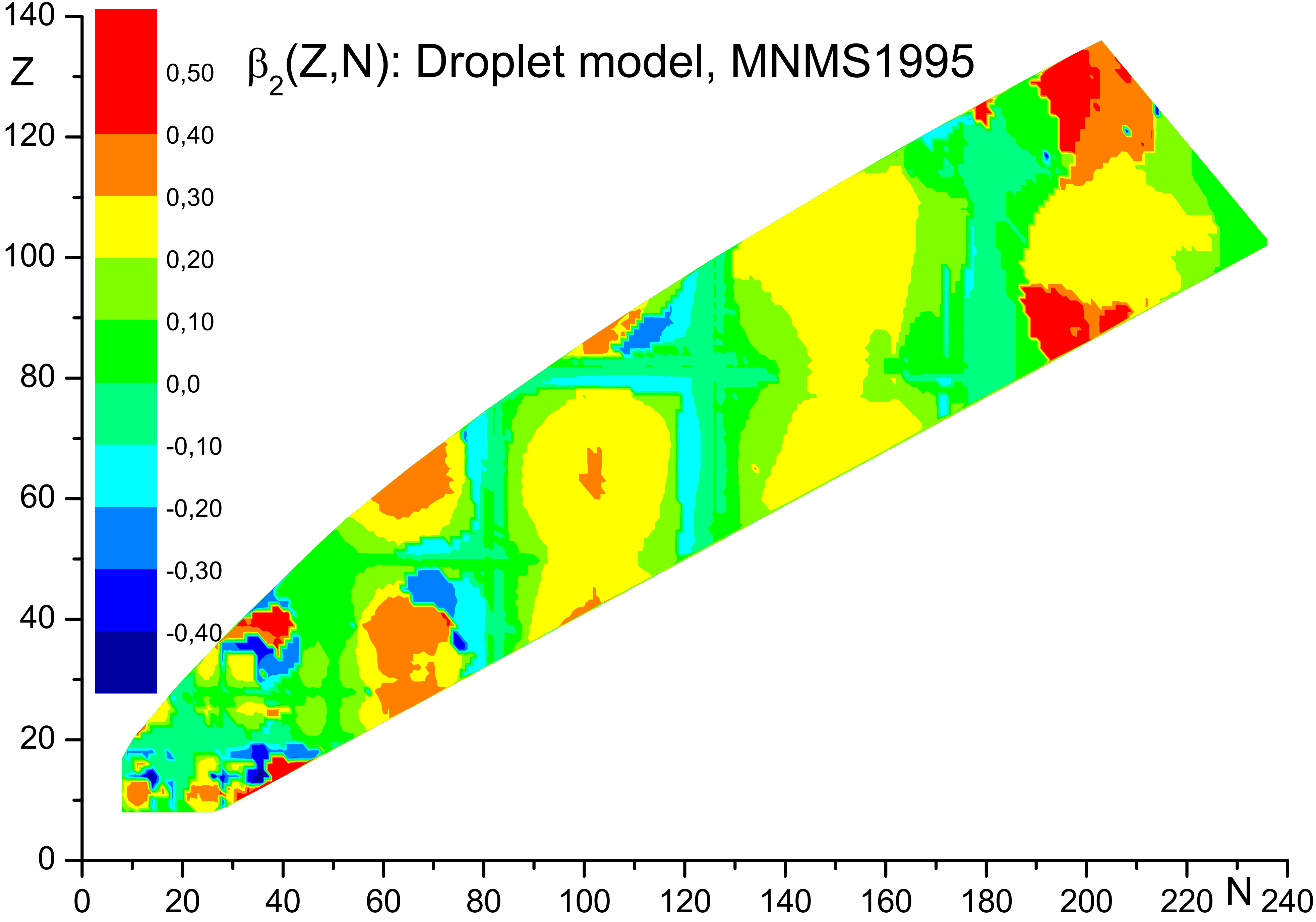
$$
\begin{aligned}
R(\theta) &= R_0[1 + \beta_2 Y_{20}(\theta) + \beta_4 Y_{40}(\theta)], \\
Y_{20}(\theta) &= \sqrt{\frac{5}{16\pi}}(3\cos^2\theta - 1), \\
Y_{40}(\theta) &= \frac{9}{256\sqrt{\pi}}(35\cos^4\theta - 30\cos^2\theta + 3).
\end{aligned}
$$



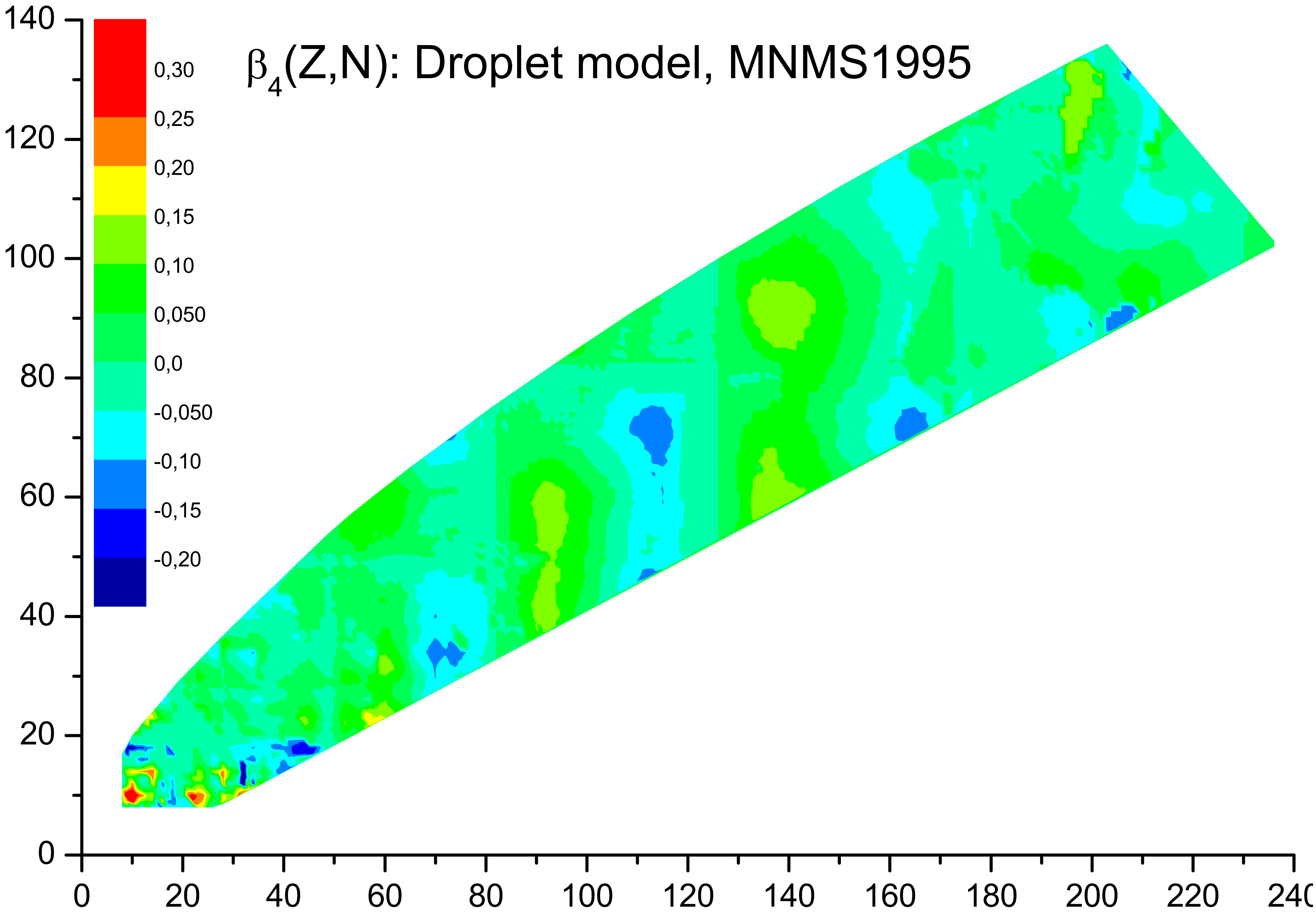
Errors of mass defect predictions
Z
N
100
80
60
40
20
0
0
20
40
60
80
100
120
140
160
0,24
0,22
0,20
0,18
0,16
0,14
0,12
0,10
0,080
0,060
0,040
0,020
0,0
-0,020
-0,040
-0,060
-0,080
-0,10
-0,12
-0,14
-0,16



b2=0.30, b4=0.20
b2=-0.30, b4=0.22
b2=0.30, b4=-0.18



β2(Z,N): Droplet model, MNMS1995
Z
N
0,50
0,40
0,30
0,20
0,10
0,0
-0,10
-0,20
-0,30
-0,40
0
20
40
60
80
100
120
140
160
180
200
220
240



β4(Z,N): Droplet model, MNMS1995
0,30
0,25
0,20
0,15
0,10
0,050
0,0
-0,050
-0,10
-0,15
-0,20
140
120
100
80
60
40
20
0
0
20
40
60
80
100
120
140
160
180
200
220
240

Non-Axial Deformations:

$$
\begin{aligned}
R(\theta, \varphi) &= R_0[1 + \beta_2 Y_{20}(\theta) + \beta_{22}(Y_{22}(\theta, \varphi) + Y_{2-2}(\theta, \varphi))], \\
Y_{22}(\theta, \varphi) &= \sqrt{\frac{3 \cdot 5}{32\pi}} \sin^2\theta e^{2i\phi}, \\
Y_{2-2}(\theta, \varphi) &= \sqrt{\frac{3 \cdot 5}{32\pi}} \sin^2\theta e^{-2i\phi}.
\end{aligned}
$$

Beta vibrations $\beta_2 = \beta_{20} + \beta_{20}^t \cos(\omega_\beta t)$, ω_β is the frequency of beta-vibrations.

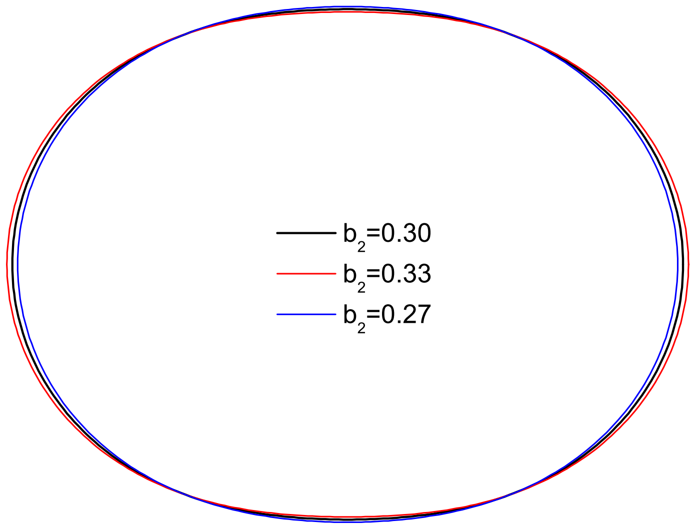
Classical Hamiltonian is

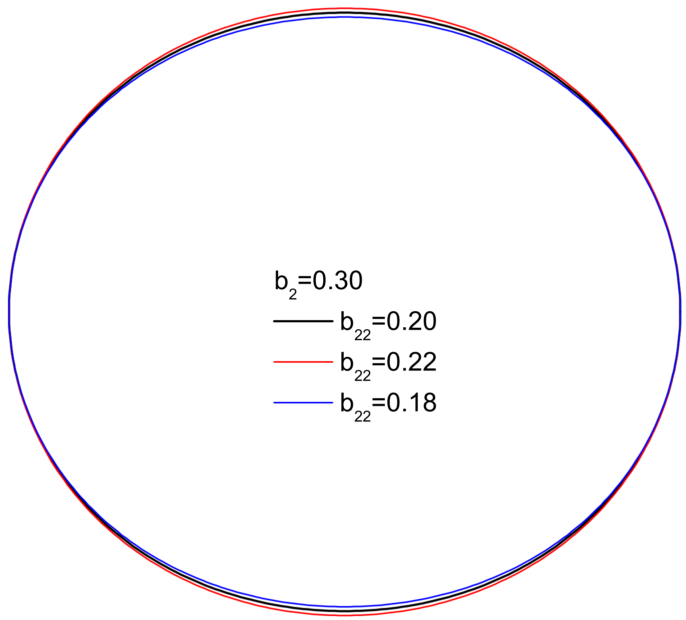
$$
H = \frac{\mathcal{M}_\beta}{2} \left(\frac{d\beta_{20}^t \cos \omega_\beta t}{dt} \right)^2 + \frac{\mathcal{C}_\beta}{2} \left(\beta_{20}^t \cos \omega_\beta t \right)^2.
$$

If $\beta_{22} = \beta_{22}^0 + \beta_{22}^t \cos \omega_\gamma t$ - gamma vibrations, ω_γ is the frequency of gamma-vibrations.

Classical Hamiltonian is

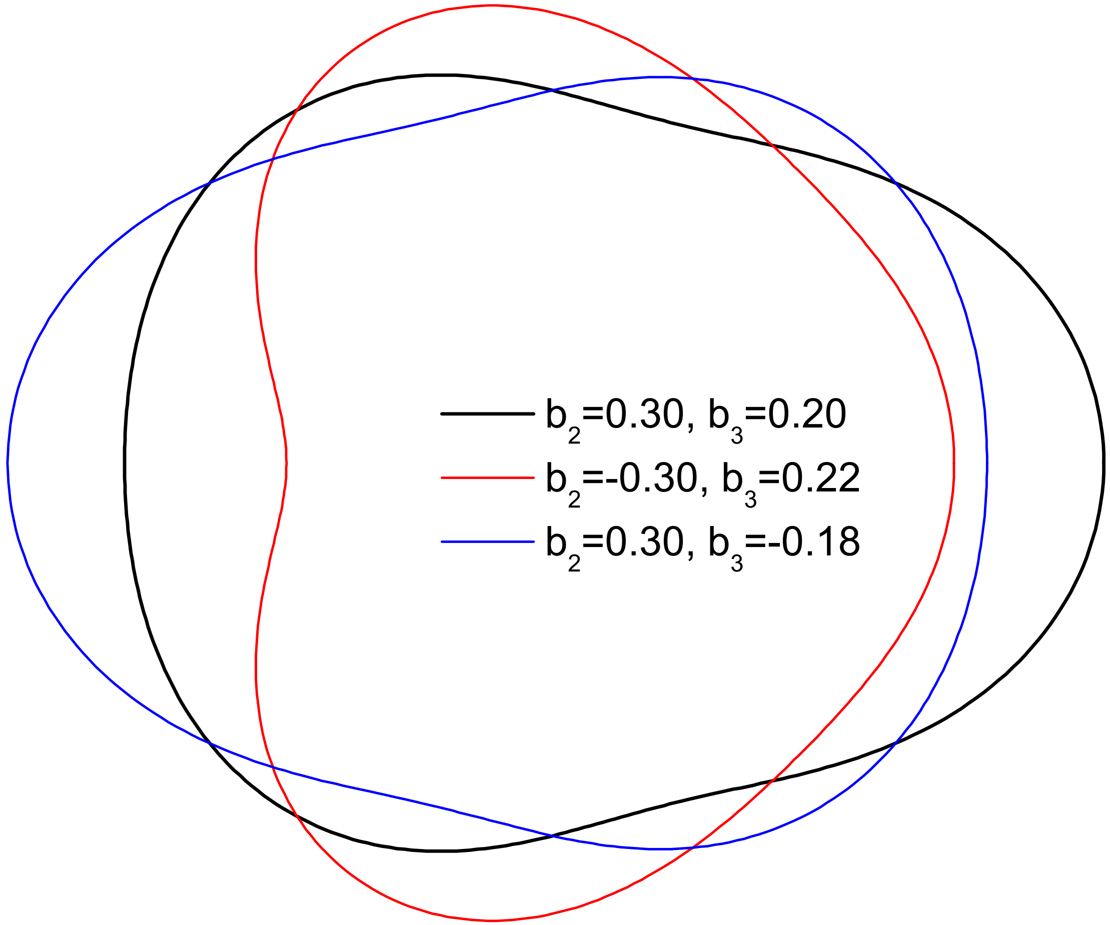
$$
H = \frac{\mathcal{M}_\gamma}{2} \left(\frac{d\beta_{22}^t \cos \omega_\gamma t}{dt} \right)^2 + \frac{\mathcal{C}_\gamma}{2} \left(\beta_{22}^t \cos \omega_\gamma t \right)^2.
$$


b2=0.30
b2=0.33
b2=0.27


b2=0.30
b22=0.20
b22=0.22
b22=0.18

Axial Reflection Asymmetric Deformation (Pear-shaped)

$$R(\theta) = R_0[1 + \beta_2 Y_{20}(\theta) + \beta_3 Y_{30}(\theta)],$$
$$Y_{30}(\theta) = \sqrt{\frac{7}{64\pi}}(5\cos^2\theta - 3)\cos\theta.$$



Non-Axial Reflection Asymmetric Deformation (Banana-shaped)

$$
\begin{aligned}
R(\theta) &= R_0[1 + \beta_2 Y_{20}(\theta) + \beta_3 Y_{30}(\theta) + \beta_{31}(Y_{31}(\theta,\varphi) - Y_{3-1}(\theta,\varphi))], \\
Y_{31}(\theta) &= -\sqrt{\frac{3\cdot 7}{16\pi}}(5\cos^2\theta - 1)\sin\theta e^{i\phi}, \\
Y_{3-1}(\theta) &= \sqrt{\frac{3\cdot 7}{16\pi}}(5\cos^2\theta - 1)\sin\theta e^{-i\phi}.
\end{aligned}
$$

R. R. Chasman, Physics Letters B, Volume 266, Issues 3-4, 29 August 1991, Pages 243-248.

The effects of $Y_{3\pm1}(\theta,\varphi)$ deformations on the energy surface of nuclides in the A = 190 region has been studied. Many nuclides with superdeformed and hyperdeformed minima have been found. The states associated with these minima are found to be near yrast at $I = 40$.

There are various more accurate approaches to description of atomic masses

- Thomas-Fermi + Strutinsky Shell Corrections
- Extended Thomas-Fermi + Strutinsky Shell Corrections
- Hartree-Fock and Hartree-Fock-Bogoliubov
- Relativistic Mean Field Theory

7. Fission of Nuclei.

Fission on two fragments, energy condition:

$$\text{Released Energy at Fission} = E(Z,N) - E(Z_1,N_1) - E(Z_2,N_2).$$

Action:

$$\mathcal{A}(E) = (2/\hbar)\int_a^b \sqrt{2\mu(s)(\mathcal{V}(s)-E)}ds,$$

where s is the fission trajectory in the deformation space $\beta_2, \beta_3, ..., \beta_\ell$, $\mu = \sum_{\ell,\ell'} B_{\ell,\ell'}\frac{d\beta_\ell}{ds}\frac{d\beta_{\ell'}}{ds}$.

Transmission coefficient:

$$T(E) = 1/\{1+\exp[\mathcal{A}(E)]\}$$

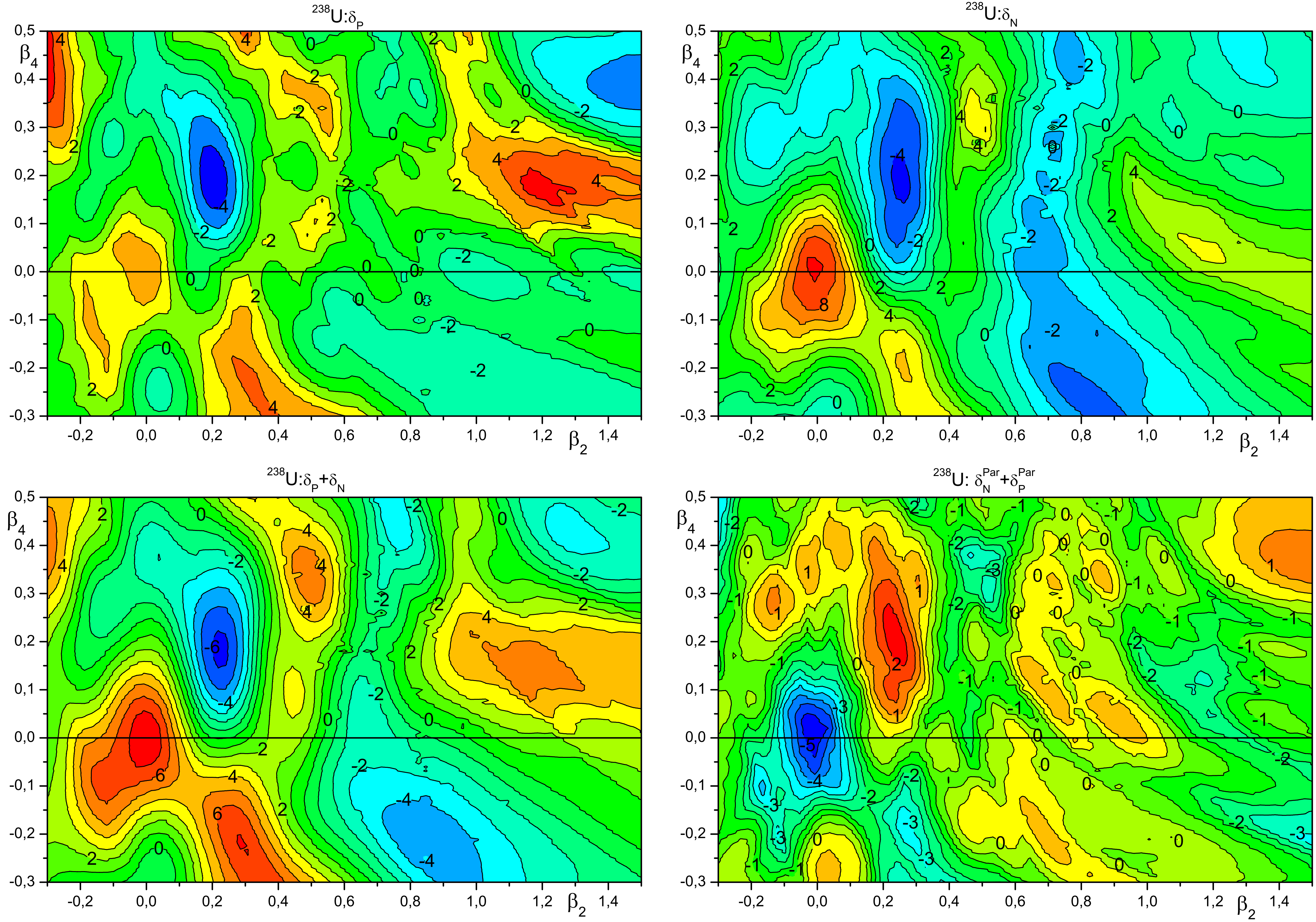
Number of assaults of a nucleus on fission barrier in the unit time $\omega_0/(2\pi)$:

$$\nu_{\rm sf} = \frac{2\pi\ln 2}{\omega_0},$$

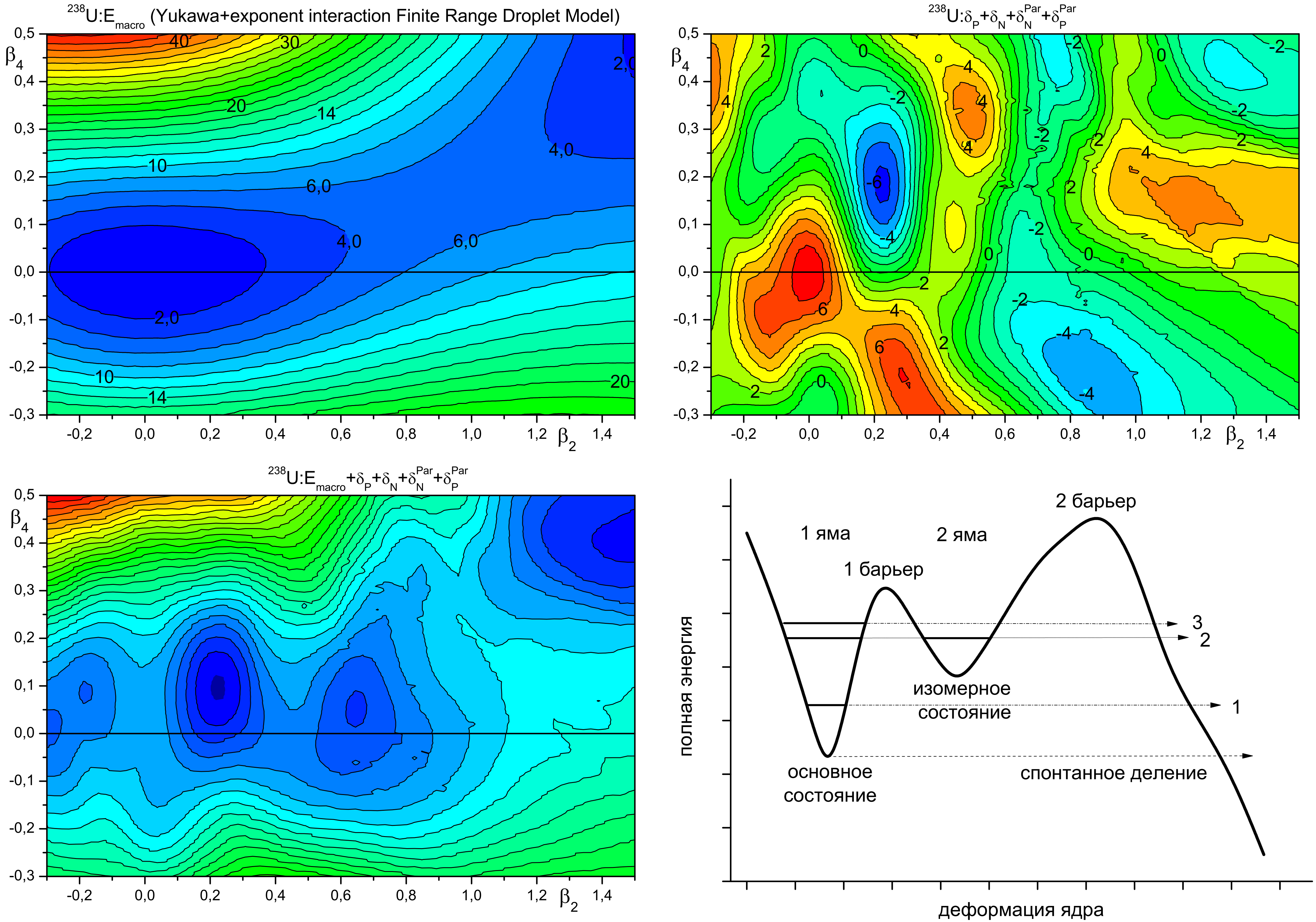
where $E_{zp} = 0.5\hbar\omega_0 \approx 0.7$ MeV.

Fission half-life:

$$t_{sf}(E) = \nu_{\rm sf}/T(E)$$

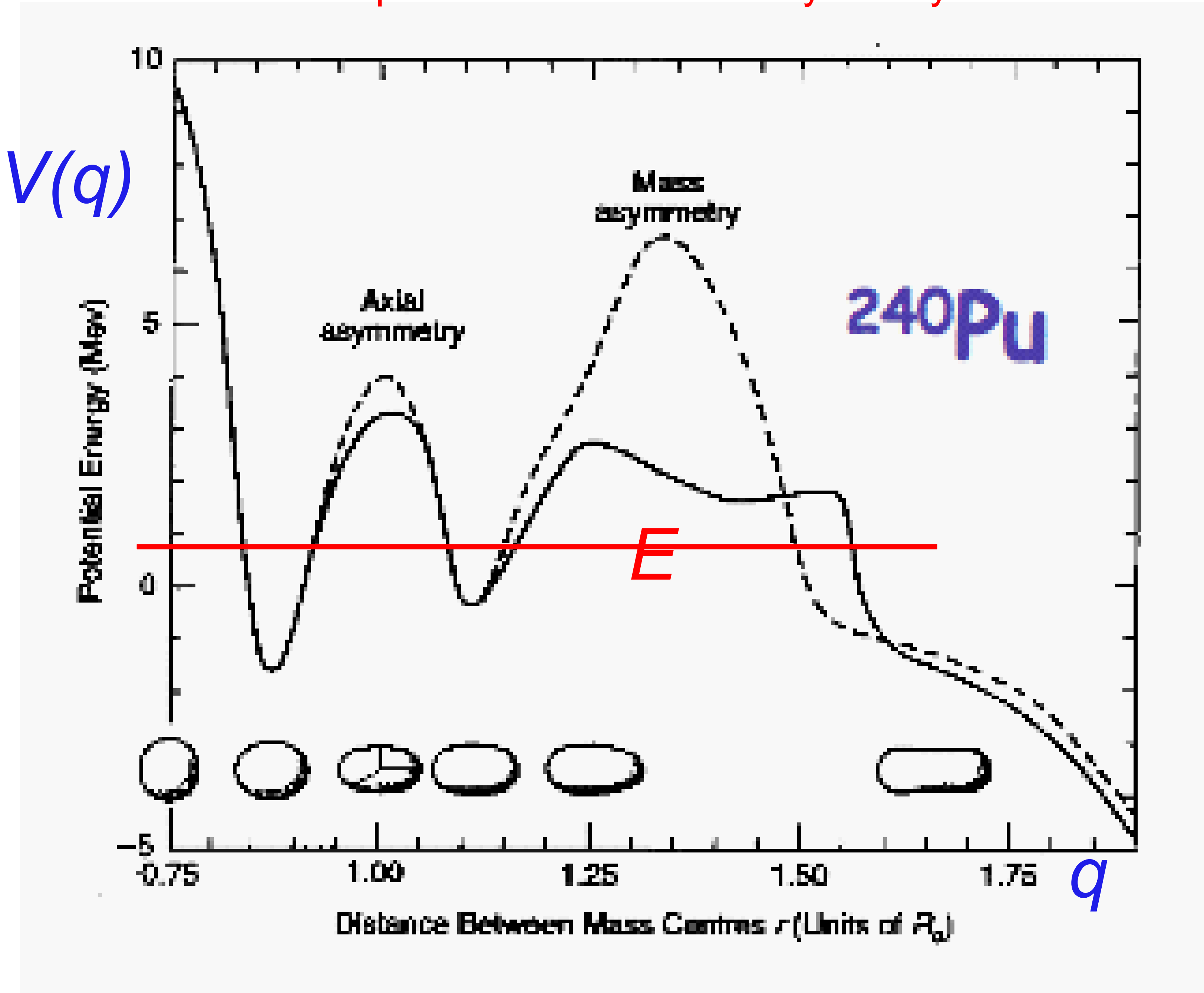


$^{238}U:\delta_P$
$^{238}U:\delta_N$
$^{238}U:\delta_P+\delta_N$
$^{238}U: \delta_N^{Par}+\delta_P^{Par}$
β_4
β_2
0,5
0,4
0,3
0,2
0,1
0,0
-0,1
-0,2
-0,3
-0,2
0,0
0,2
0,4
0,6
0,8
1,0
1,2
1,4

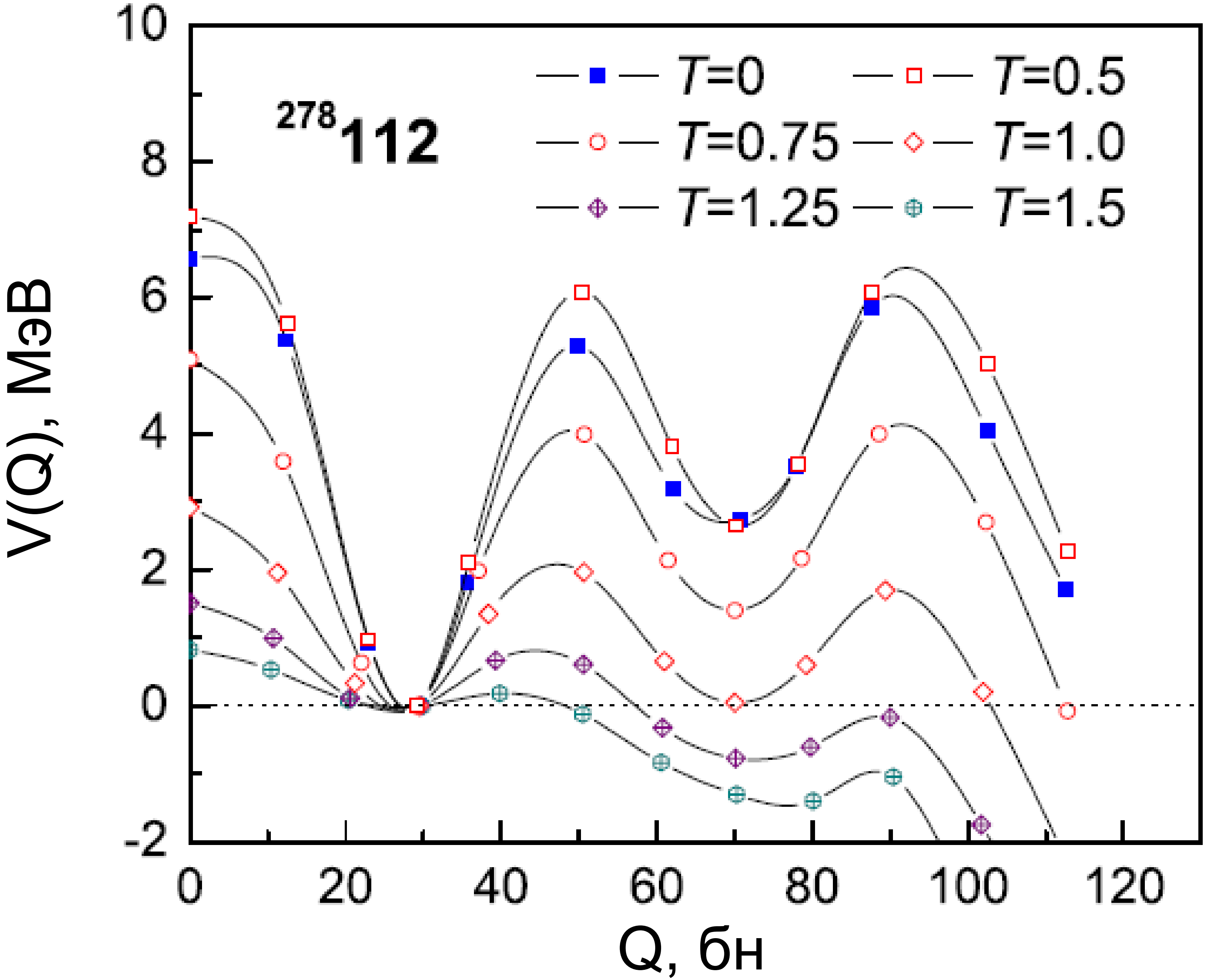


238U:E macro (Yukawa+exponent interaction Finite Range Droplet Model)
238U:δP+δN+δN Par+δP Par
238U:E macro+δP+δN+δN Par+δP Par
β4
β2
1 яма
2 яма
1 барьер
2 барьер
изомерное состояние
основное состояние
спонтанное деление
полная энергия
деформация ядра

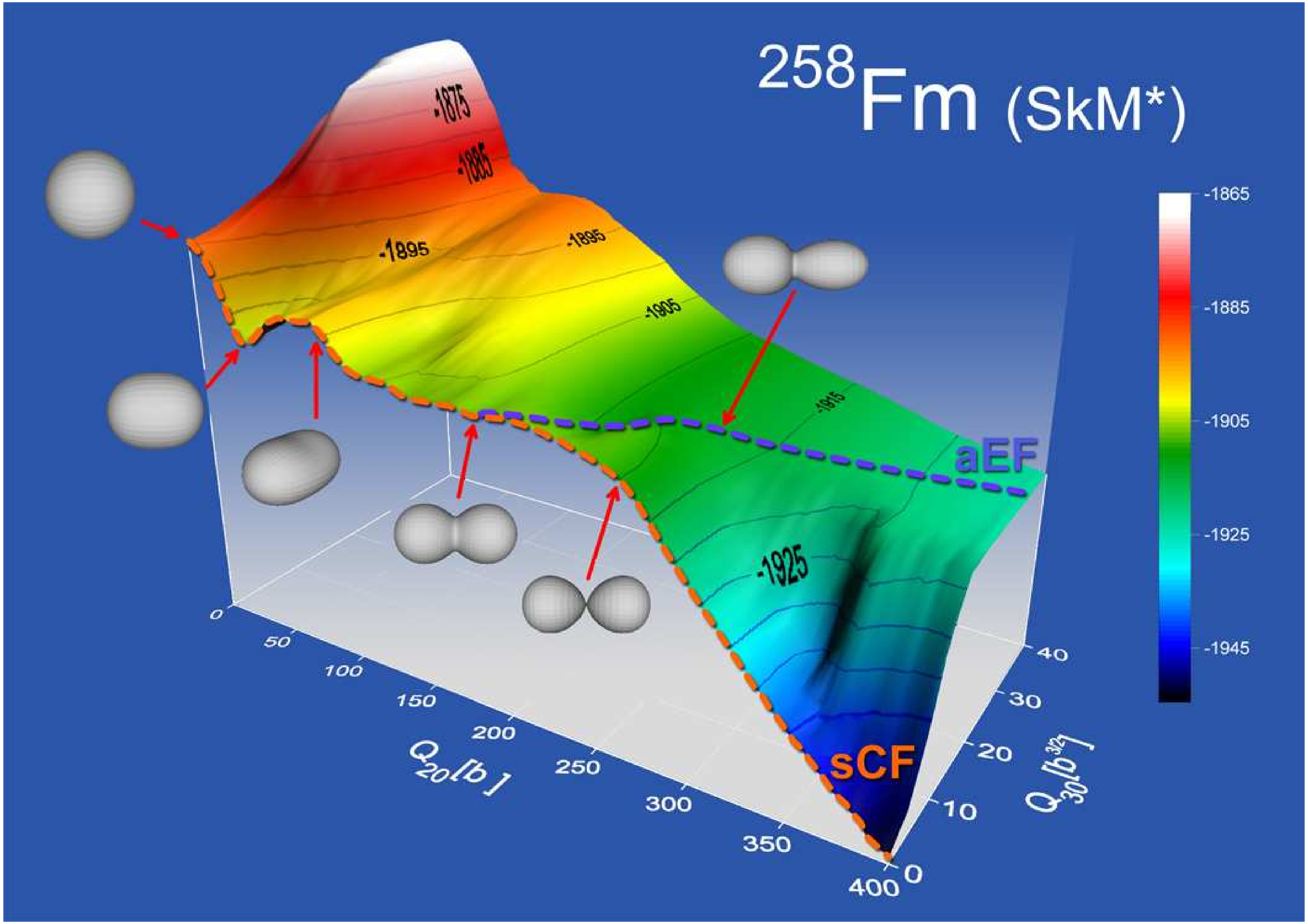
Fission Barrier: impotance of dimensionality and symmetries

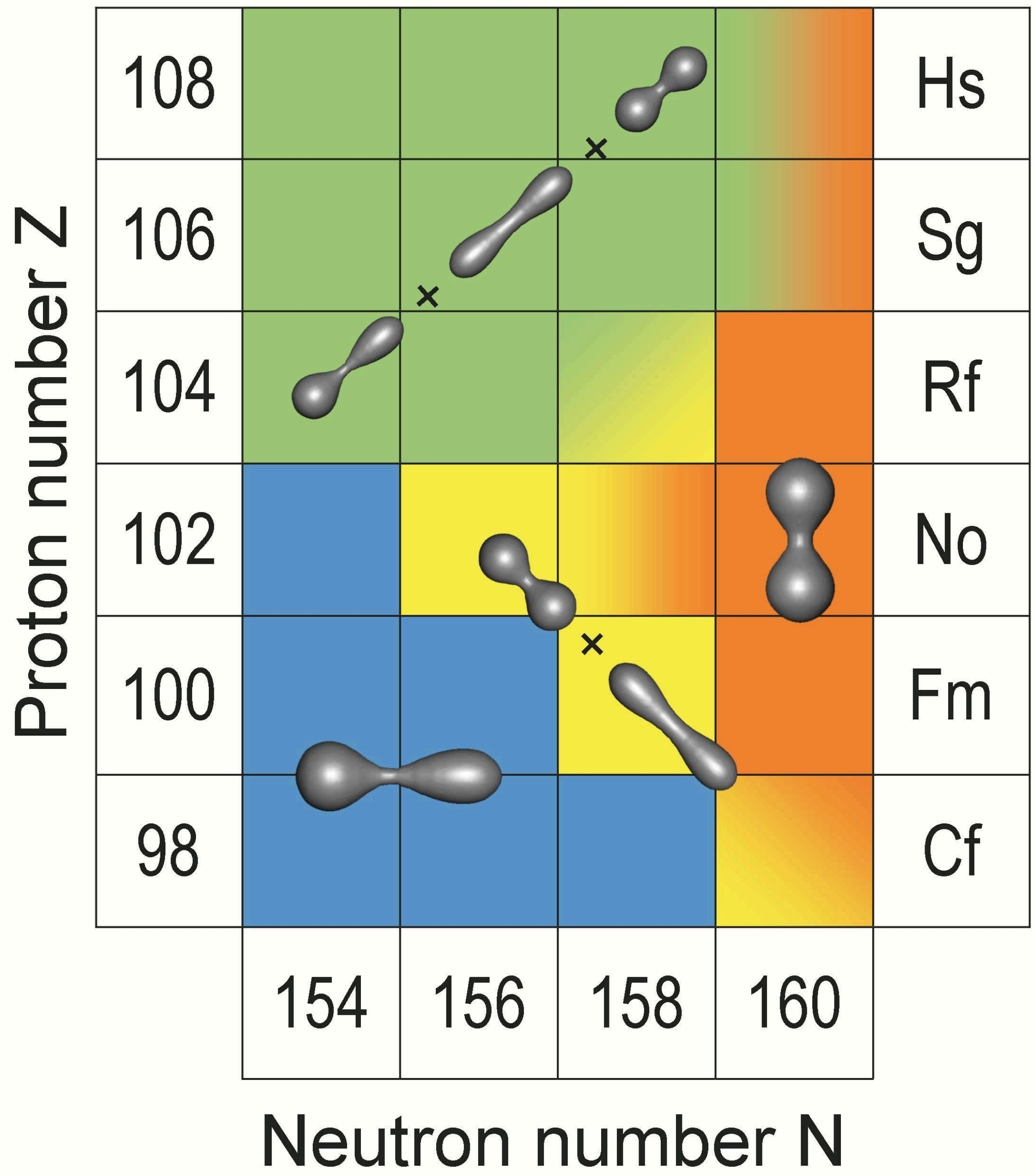


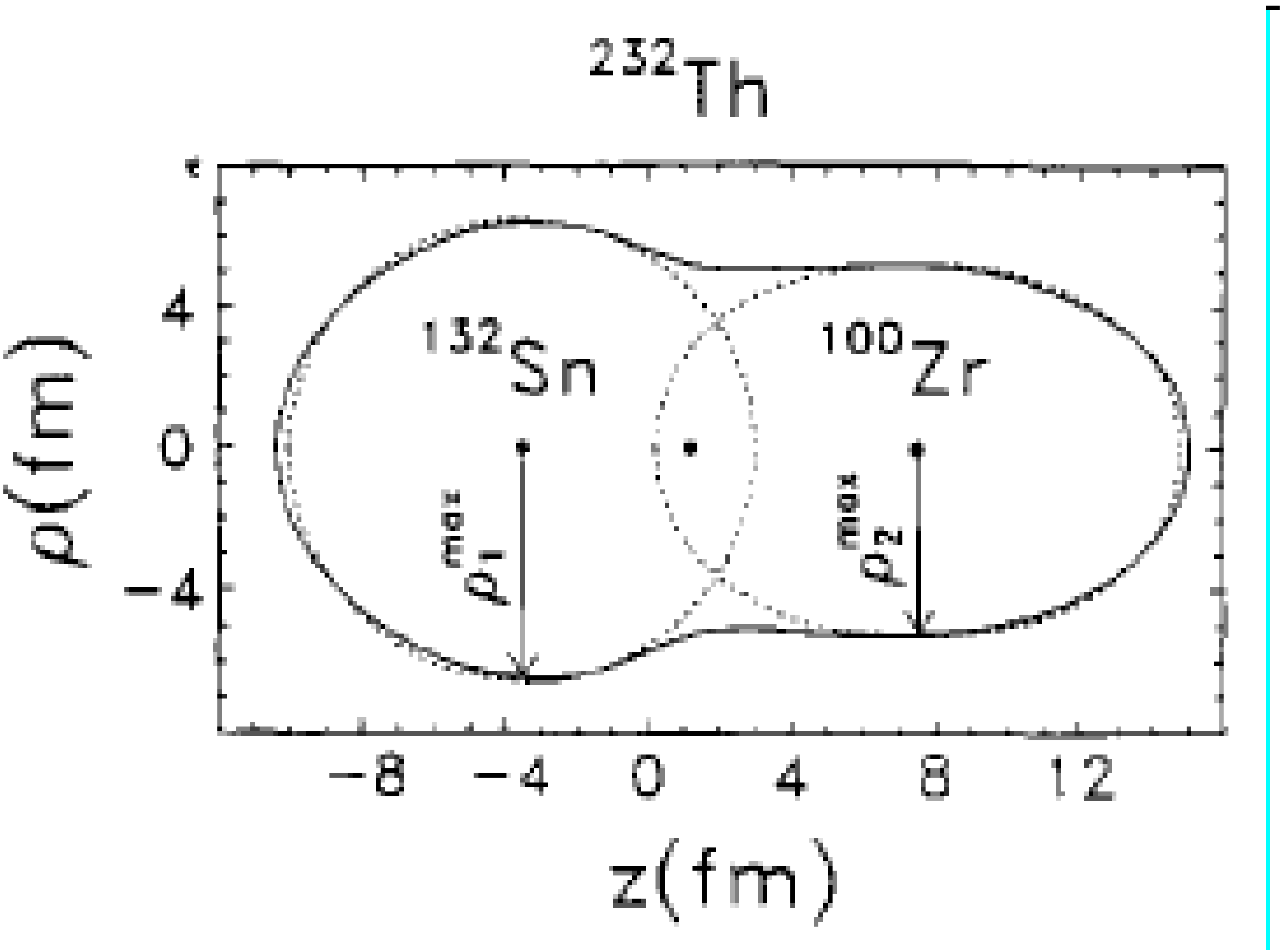
Dependence on the excitation energy $E^* = aT^2$, T – temperature



Bimodal fission



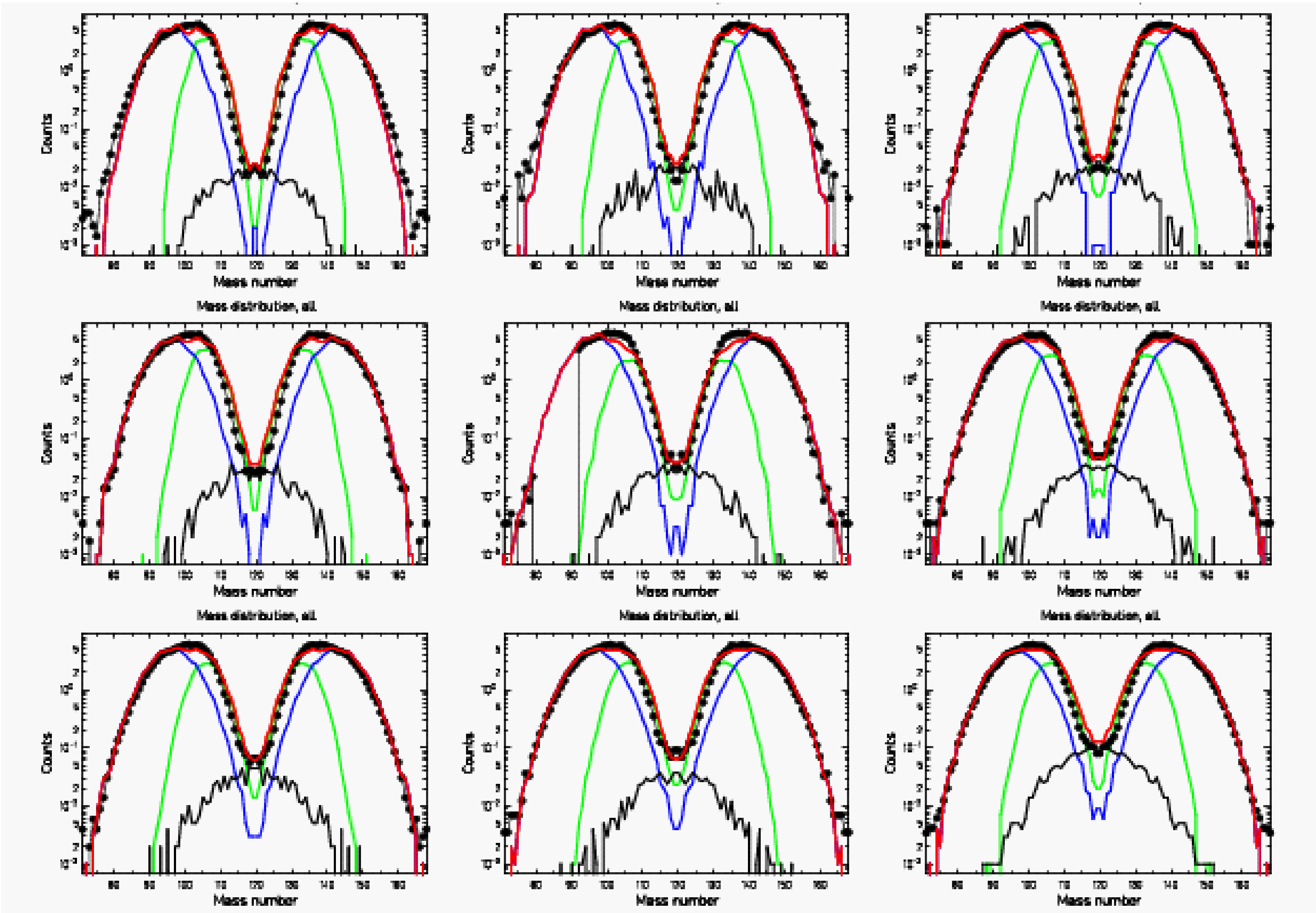

Proton number Z
108
106
104
102
100
98
Hs
Sg
Rf
No
Fm
Cf
154
156
158
160
Neutron number N



^{232}Th
^{132}Sn
^{100}Zr
ρ_1^{max}
ρ_2^{max}
4
0
−4
−8
−4
0
4
8
12
ρ(fm)
z(fm)

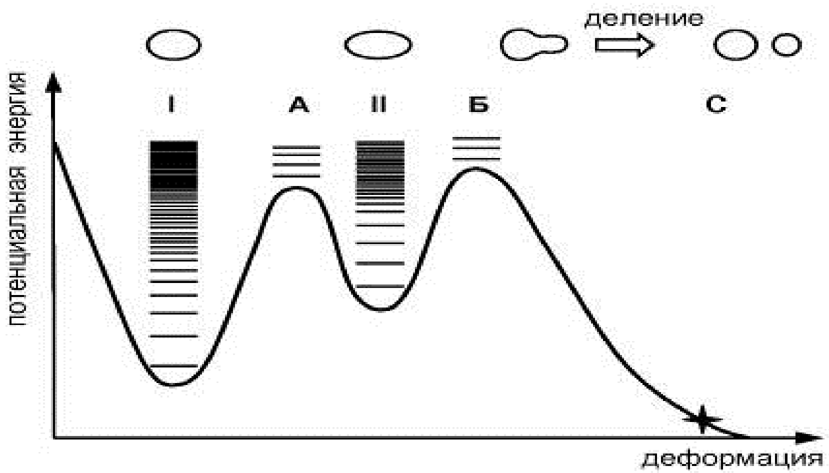
Fission fragment modes

Data - F. Vives et al, Nucl. Phys. A662 (2000) 63;   Lines - Model calculations

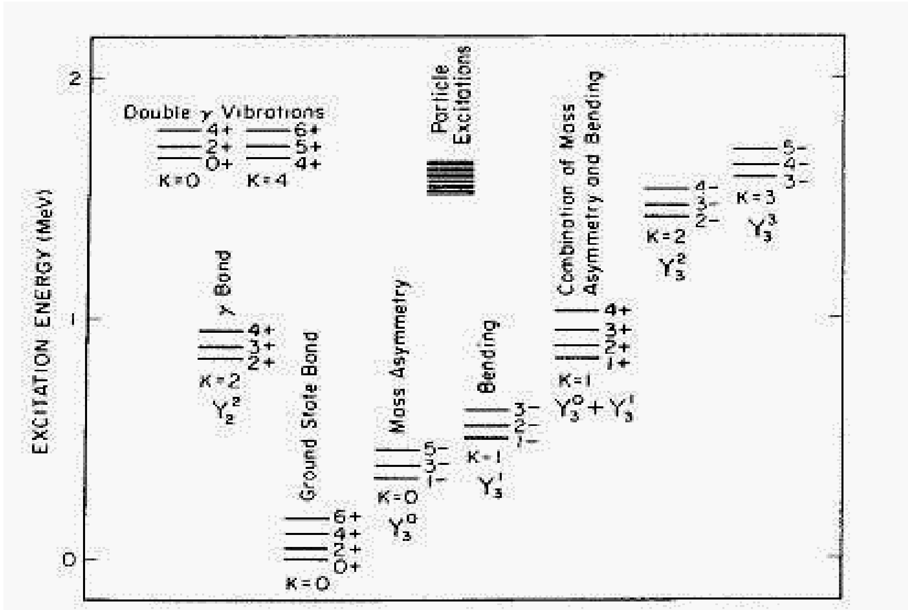


$$Y_{sym}(A) = \frac{1}{\sqrt{\pi}\sigma} \exp^{\left[-\left(\frac{A-A_0/2}{\sigma}\right)^2\right]}; \quad Y_{asym}(A) = \frac{1}{\sqrt{\pi}\sigma} \exp^{\left[-\left(\frac{A-A_a}{\sigma}\right)^2\right]} + \frac{1}{\sqrt{\pi}\sigma} \exp^{\left[-\left(\frac{A-(A_0-A_a)}{\sigma}\right)^2\right]}$$

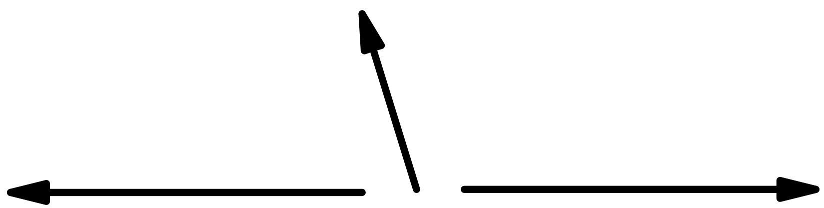
Fission isomers

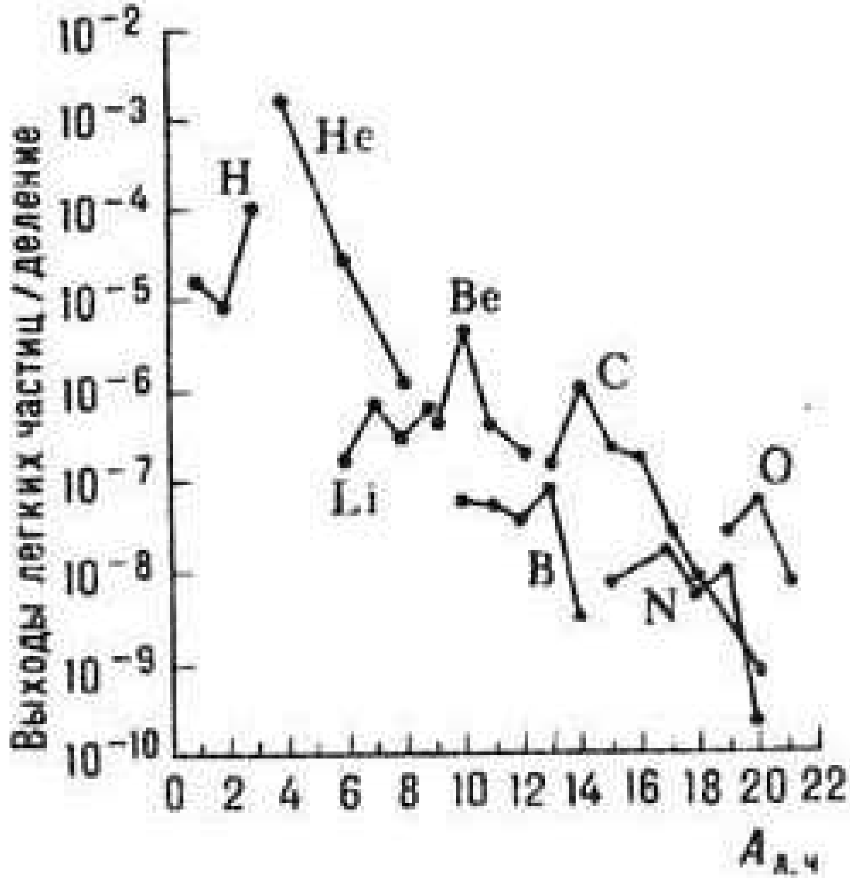


Rotational structure of fissionisomers



Ternary fission: 1event for few hundrents of binary fission events





Typically the probabilities for ternary (α and etc) and quaternary (α+α or $\alpha + t$ or $t + t$) fission are $\sim 10^{-3}$ per fission and 10^{-7} per fission, respectively.

Thanks for your attention!