# GLOBAL PREDICTIONS OF NUCLEAR FISSION PROPERTIES FOR ASTROPHYSICS

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Many of the topics I discuss are treated in more detail in the more recent papers on my web page: http://t16web.lanl.gov/Moller/abstracts.html

## Potential Energy of Deformation

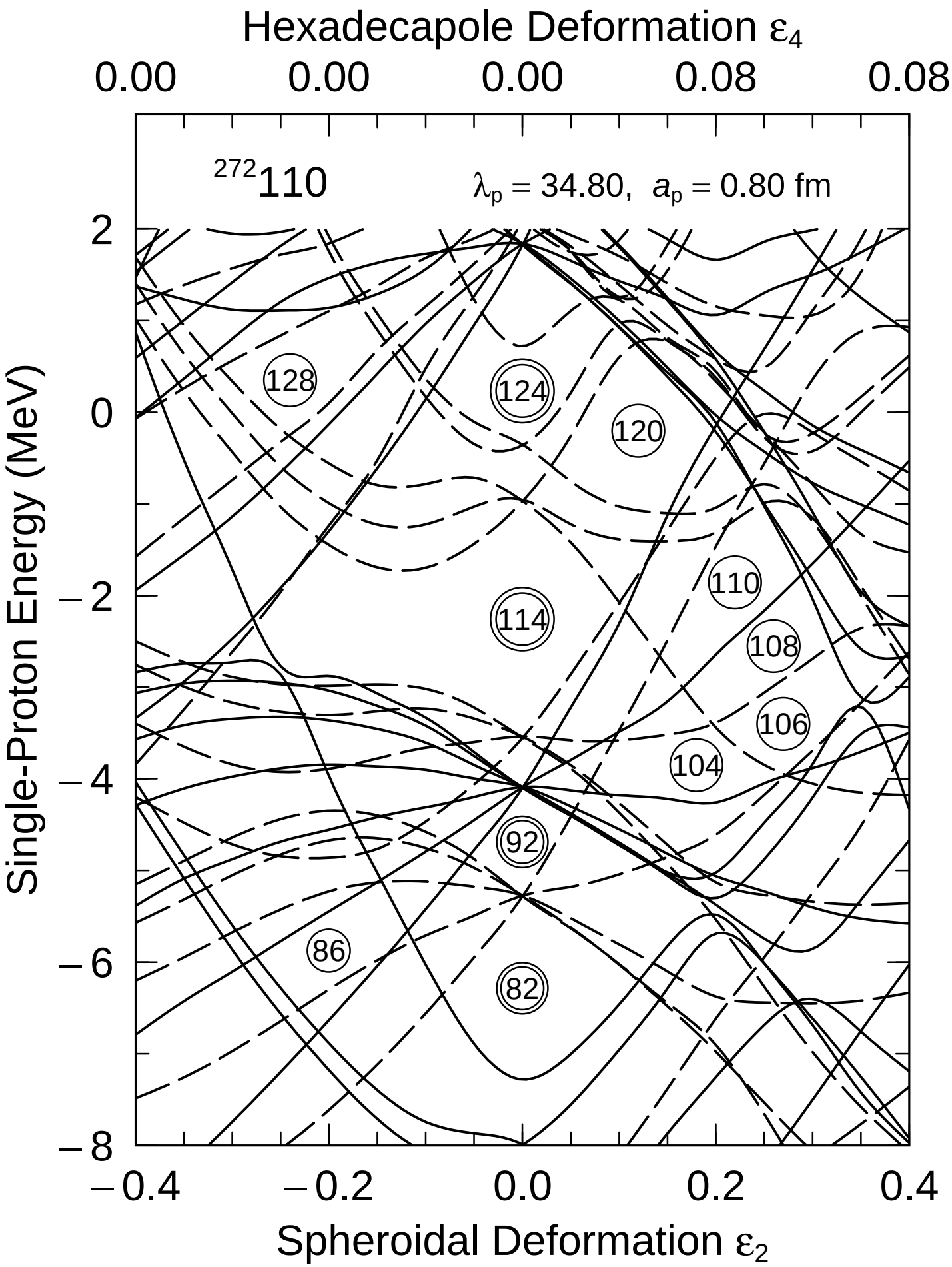
We use the macroscopic-microscopic method introduced by Swiatecki and Strutinsy:

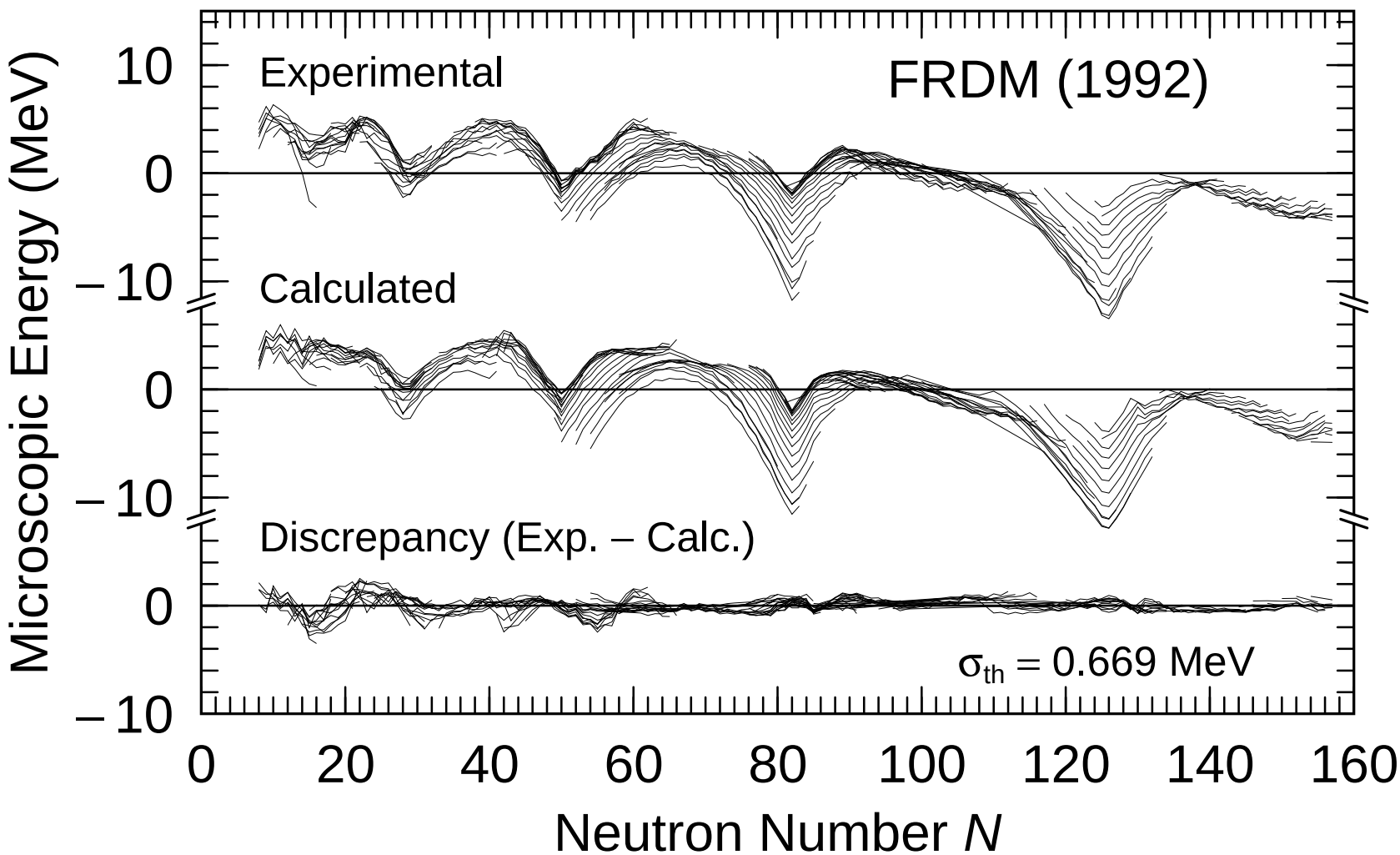
$$E_{\mathrm{pot}}(\mathrm{shape}) = E_{\mathrm{macr}}(\mathrm{shape}) + E_{\mathrm{micr}}(\mathrm{shape}) \quad (1)$$

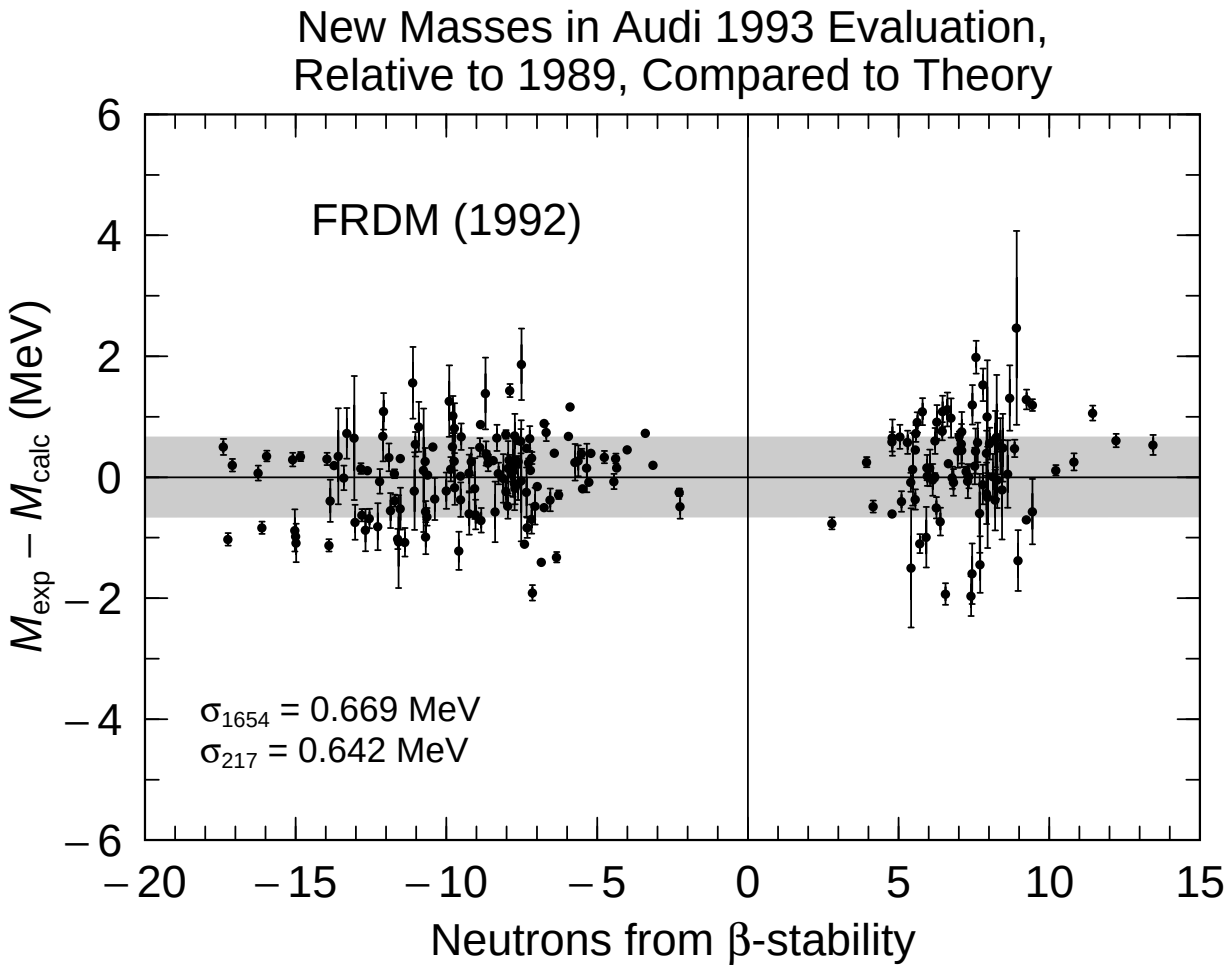
The macroscopic term is calculated in a liquid-drop type model (for a specific deformed shape).

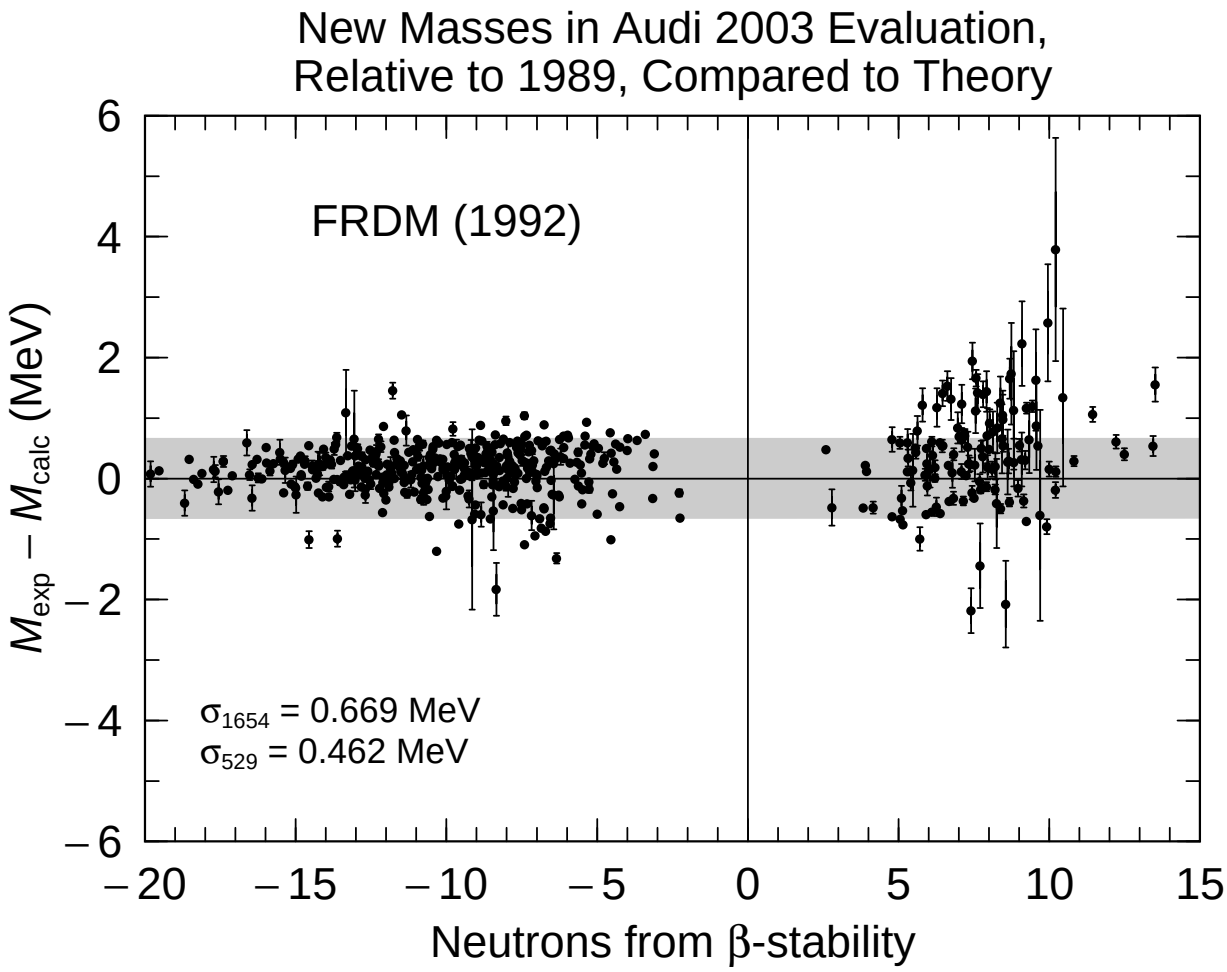
The microscopic correction is determined in the following steps

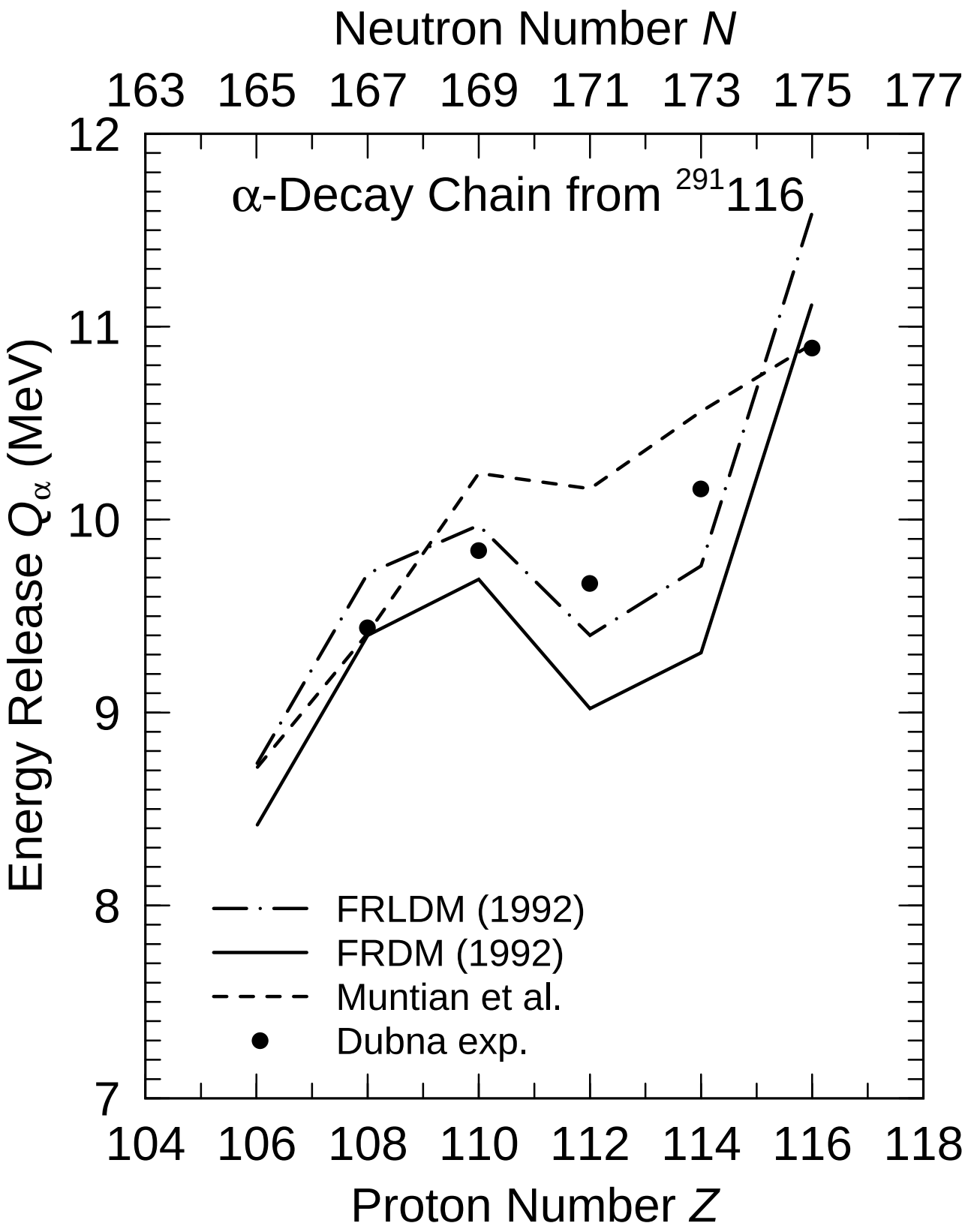
1. A shape is prescribed
2. A single-particle potential with this shape is generated. A spin-orbit term is included.
3. The Schrödinger equation is solved for this deformed potential and single-particle levels and wave-functions are obtained
4. The shell correction is calculated by use of Strutinsky's method.
5. The pairing correction is calculated in the BCS or Lipkin-Nogami method.


Hexadecapole Deformation ε4
0.00
0.00
0.00
0.08
0.08
272110
λp = 34.80, ap = 0.80 fm
128
124
120
110
114
108
106
104
92
86
82
2
0
−2
−4
−6
−8
Single-Proton Energy (MeV)
−0.4
−0.2
0.0
0.2
0.4
Spheroidal Deformation ε2


Experimental
FRDM (1992)
Calculated
Discrepancy (Exp. – Calc.)
σth = 0.669 MeV
Microscopic Energy (MeV)
10
0
– 10
0
– 10
0
– 10
0
20
40
60
80
100
120
140
160
Neutron Number N

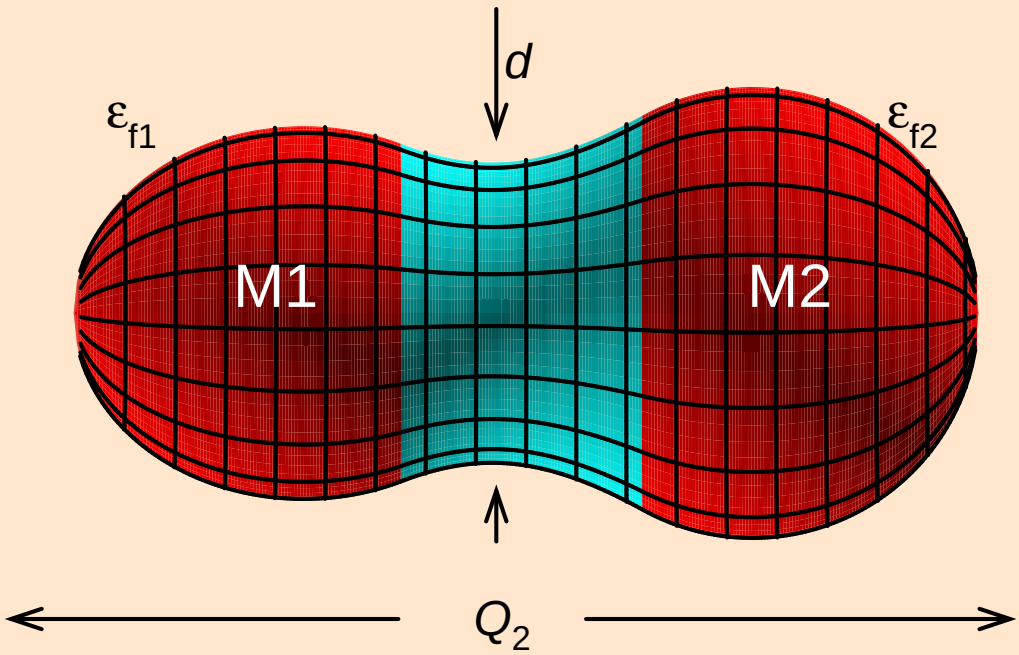

New Masses in Audi 1993 Evaluation,
Relative to 1989, Compared to Theory
FRDM (1992)
σ1654 = 0.669 MeV
σ217 = 0.642 MeV
Mexp – Mcalc (MeV)
Neutrons from β-stability
6
4
2
0
– 2
– 4
– 6
– 20
– 15
– 10
– 5
0
5
10
15


New Masses in Audi 2003 Evaluation,
Relative to 1989, Compared to Theory
FRDM (1992)
σ1654 = 0.669 MeV
σ529 = 0.462 MeV
Mexp – Mcalc (MeV)
Neutrons from β-stability
6
4
2
0
– 2
– 4
– 6
– 20
– 15
– 10
– 5
0
5
10
15


Neutron Number N
163 165 167 169 171 173 175 177
α-Decay Chain from 291116
Energy Release Qα (MeV)
12
11
10
9
8
7
FRLDM (1992)
FRDM (1992)
Muntian et al.
Dubna exp.
104 106 108 110 112 114 116 118
Proton Number Z

| Model | A/C | $a_1$ (MeV) | $a_2$ (MeV) | $J$ (MeV) | $Q$ (MeV) | $L$ (MeV) | $\mu_{\rm th}$ (MeV) | $\sigma_{{\rm th};\mu=0}$ (MeV) |
|---|---|---|---|---|---|---|---|---|
| (92) | 1/1 | 16.247 | 22.92 | 32.73 | 29.21 | 0.00 | 0.0156 | 0.6688 |
| (92) | 1/3 | | | | | | 0.1755 | 0.4617 |
| (92) | 1/2 | | | | | | 0.0607 | 0.6314 |
| (92)-a | 1/1 | 16.245 | 23.02 | 32.22 | 30.73 | 0.00 | 0.0000 | 0.6614 |
| (92)-a | 1/3 | | | | | | 0.0174 | 0.4208 |
| (92)-a | 1/2 | | | | | | 0.0114 | 0.6180 |
| (92)-b | 1/1 | 16.286 | 23.37 | 32.34 | 30.51 | 0.00 | 0.0000 | 0.6591 |
| (92)-b | 1/3 | | | | | | 0.0031 | 0.4174 |
| (92)-b | 1/2 | | | | | | 0.0076 | 0.6157 |
| (06)-a | 2/2 | 16.274 | 23.27 | 32.19 | 30.64 | 0.00 | 0.0000 | 0.6140 |
| (07)-b | 2/2 | 16.231 | 22.96 | 32.11 | 30.83 | 0.00 | 0.0000 | 0.5964 |
| (09)-a | 1/1 | 16.143 | 22.41 | 33.00 | 27.50 | 86.22 | 0.0000 | 0.6166 |
| (09)-a | 1/3 | | | | | | 0.0533 | 0.4091 |
| (09)-a | 1/2 | | | | | | 0.0230 | 0.5808 |
| (09)-b | 2/2 | 16.145 | 22.43 | 32.53 | 28.53 | 72.59 | 0.0000 | 0.5788 |

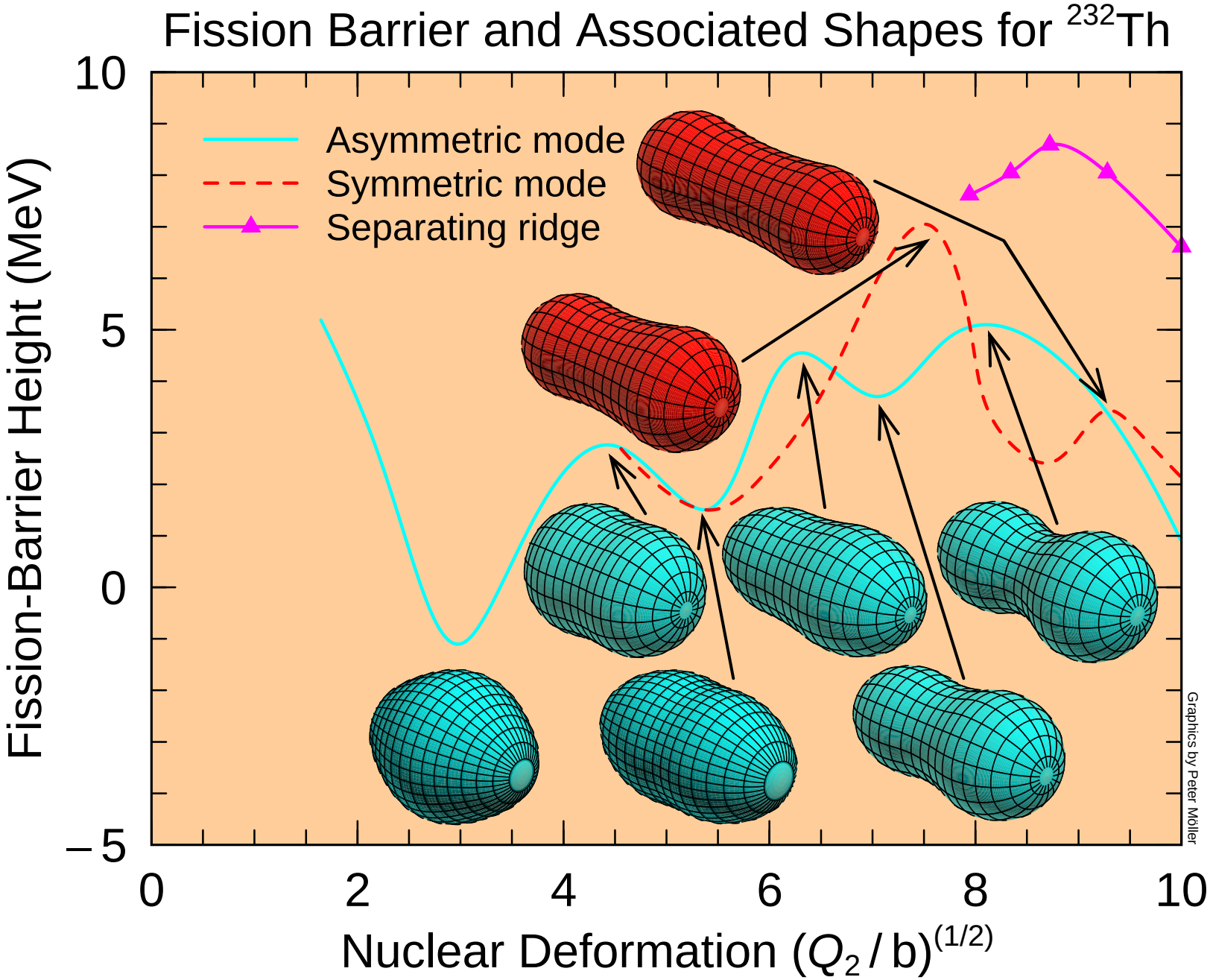
# Five Essential Fission Shape Coordinates

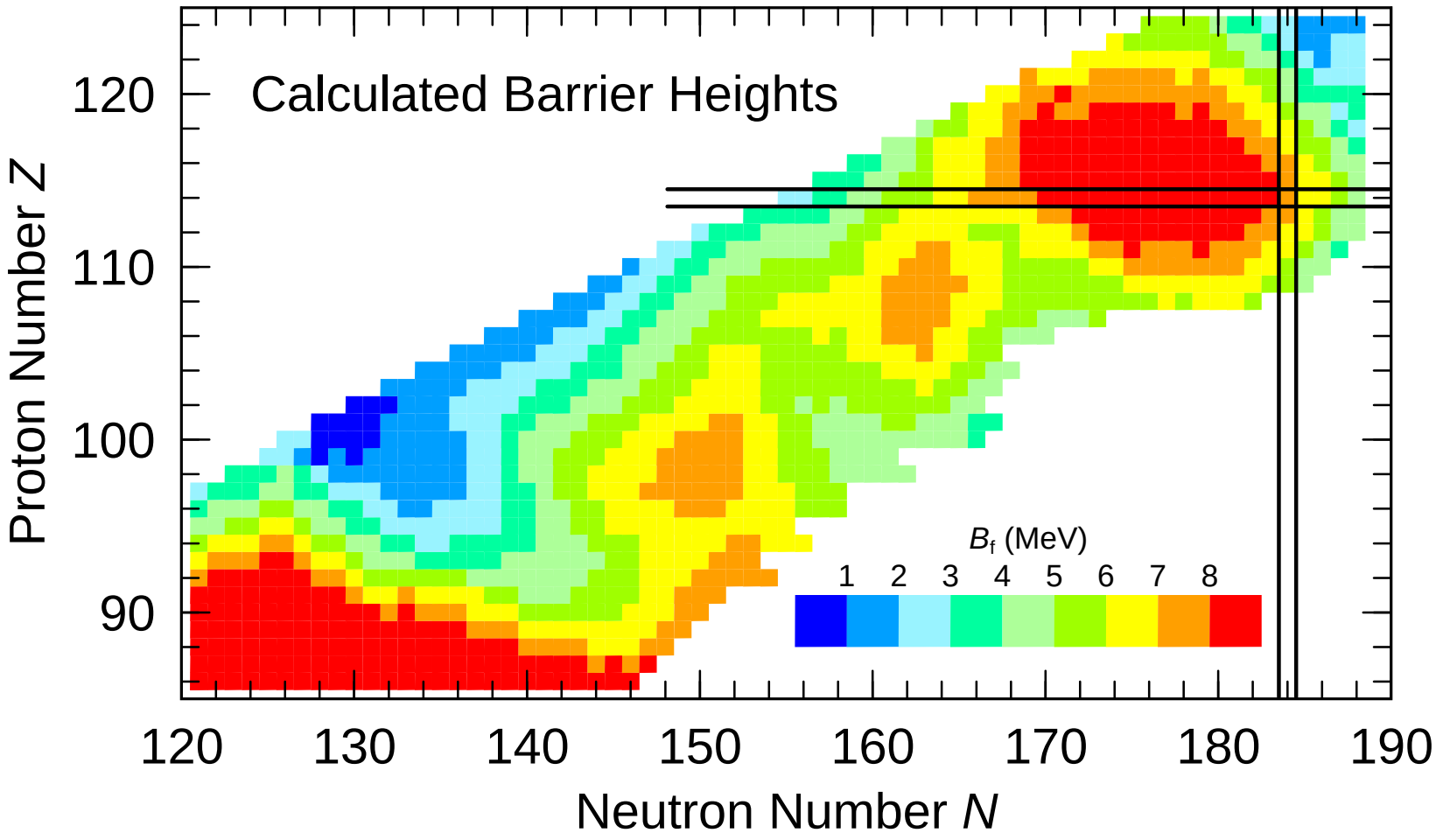



| | | |
|---|---|---|
| 45 | $Q_2$ ~ | Elongation (fission direction) |
| ⊗ | | |
| 35 | $\alpha_g$ ~ | (M1-M2)/(M1+M2) Mass asymmetry |
| ⊗ | | |
| 15 | $\varepsilon_{f1}$ ~ | Left fragment deformation |
| ⊗ | | |
| 15 | $\varepsilon_{f2}$ ~ | Right fragment deformation |
| ⊗ | | |
| 15 | $d$ ~ | Neck |

⇒ 5 315 625 grid points – 306 300 unphysical points

⇒ 5 009 325 physical grid points


Fission Barrier and Associated Shapes for $^{232}$Th
Asymmetric mode
Symmetric mode
Separating ridge
Fission-Barrier Height (MeV)
10
5
0
– 5
0
2
4
6
8
10
Nuclear Deformation $(Q_2 / \mathrm{b})^{(1/2)}$
Graphics by Peter Möller


Calculated Barrier Heights
Proton Number Z
Neutron Number N
120
110
100
90
120
130
140
150
160
170
180
190
B_f (MeV)
1 2 3 4 5 6 7 8

# SCISSION-SURFACE MODEL OF YIELD

The yield at each point on the scission surface

$$Y \approx \rho(E^*) = \exp(2\sqrt{a(E^* - E_{\mathsf{pot}}(I,J,K,L,N))})$$

The mass yield at $A_{\mathsf{H}}$, $Y(A_{\mathsf{H}})$, is then the sum of the yield at all points with asymmetry $A_{\mathsf{H}}$.

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+++++++++++++++----------------
+++++++++++++++++++------------
++++++++++++------------------
+++++++++++++++----------------
+++++++++++++++++++------------
++++++++++++++++++++----------
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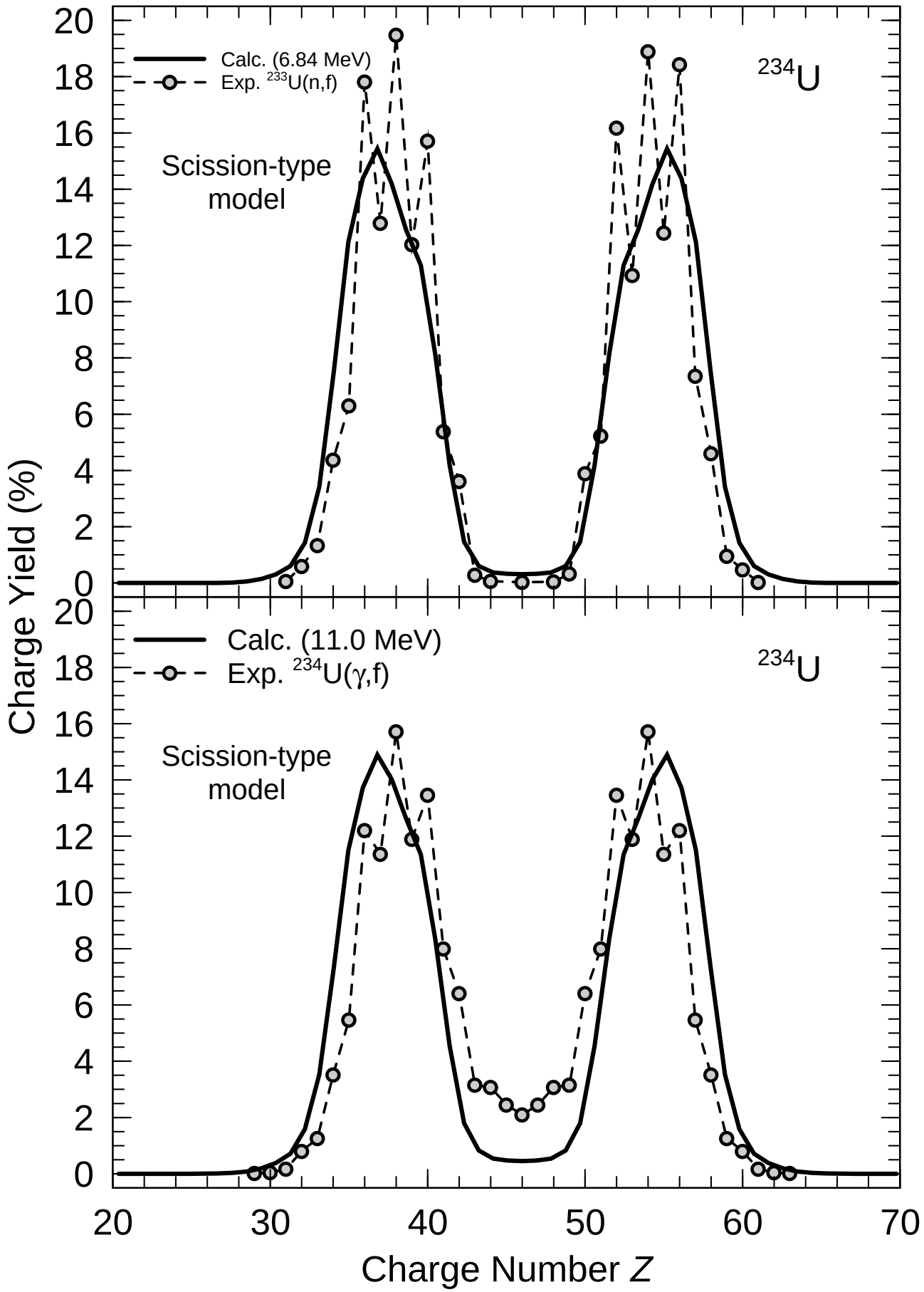

Calc. (6.84 MeV)
Exp. 233U(n,f)
234U
Scission-type model
Calc. (11.0 MeV)
Exp. 234U(γ,f)
234U
Scission-type model
Charge Yield (%)
Charge Number Z
0
2
4
6
8
10
12
14
16
18
20
20
30
40
50
60
70

We see in this approach (1) the peaks are offset from the data and (2) the energy dependence is deficient.

It is a plausible assumption that the final yields depend on the dynamical evolution of the system from the initial (ground-state-like) compound system towards separation.

Recently J. Randrup suggested a novel treatment of the dynamical evolution in the 5D energy-deformation space that is sufficiently tractable that modern computer resources permit us to explore this approach for all nuclei at all excitation energies above the barrier.

First results of our implementation of these ideas are highly encouraging.

# S U M M A R Y

On the near (1–5 years) frontier we anticipate

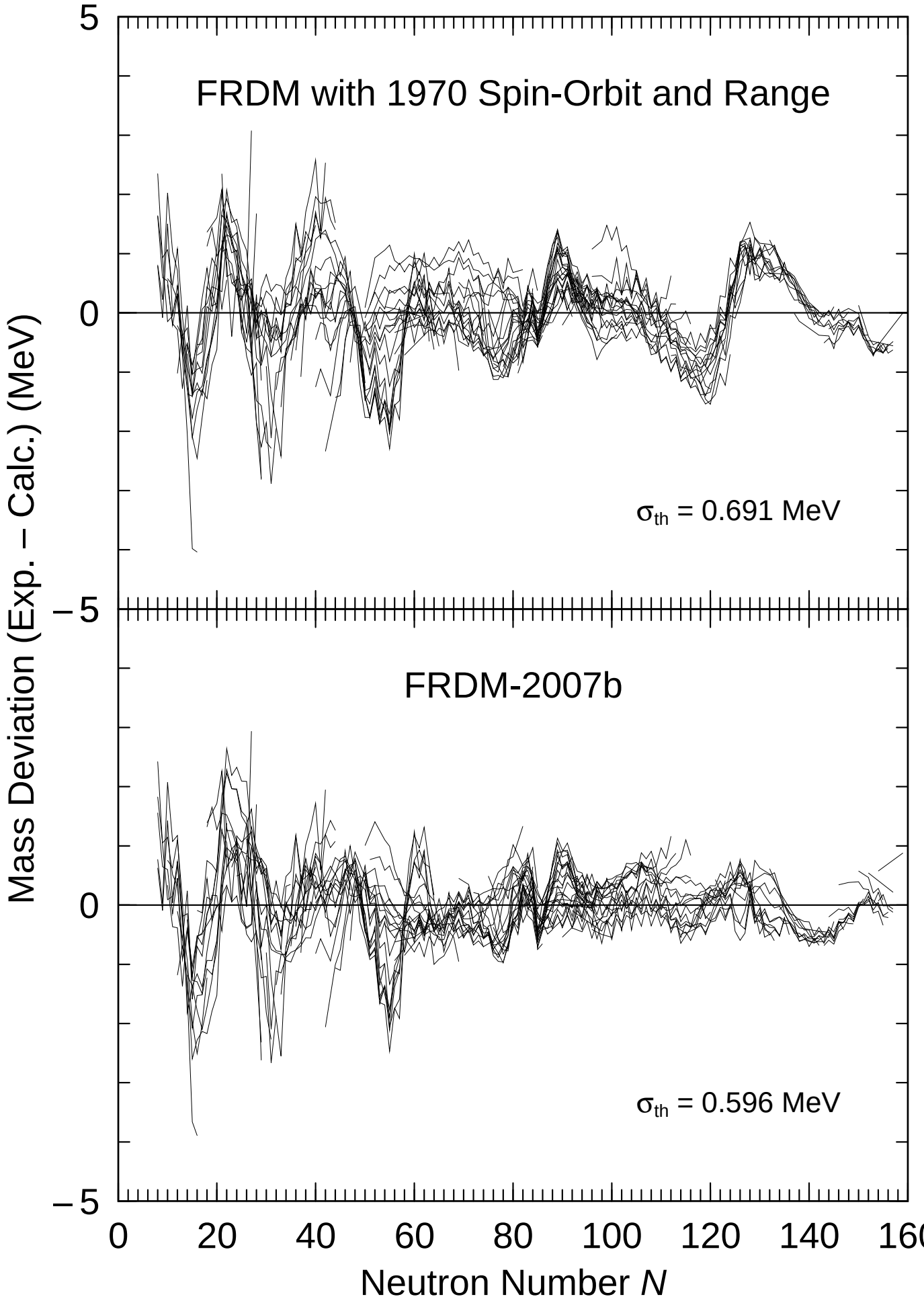
- New mass table with more accurate gs deformations and accuracy better than 0.58 MeV.

- Associated improved $\beta$-decay half-lives and EQS parameters.

- A microscopic (non-phenomenological) fission-Yield model that can be applied to all nuclei at all energies above the barrier.

- Since we have barriers and $\beta$-decay properties calculated for all heavy nuclei we will have essential new data required for network end-of-r-process calculations.

Further details can be found on:
http://t16web.lanl.gov/Moller/abstracts.html


FRDM with 1970 Spin-Orbit and Range
σth = 0.691 MeV
FRDM-2007b
σth = 0.596 MeV
Mass Deviation (Exp. – Calc.) (MeV)
5
0
–5
0
20
40
60
80
100
120
140
160
Neutron Number N