Unified, global calculations of nuclear-structure data

P. Möller (LANL)

Collaborators on this and other projects: W. D. Myers, H. Sagawa (Aizu), S. Yoshida (Hosei), T. Ichikawa(YITP), A. J. Sierk(LANL), A. Iwamoto (JAEA), S. Aberg (Lund), R. Bengtsson (Lund), J. Randrup(LBL), S. Gupta (IIT, Ropar), and many experimental groups (e. g. K.-L. Kratz (Mainz), H. Schatz (MSU) . . .).

Please look on my web page for more details about the mass model and other projects (beta-decay, fission)

http://t16web.lanl.gov/Moller/abstracts.html

Potential Energy of Deformation

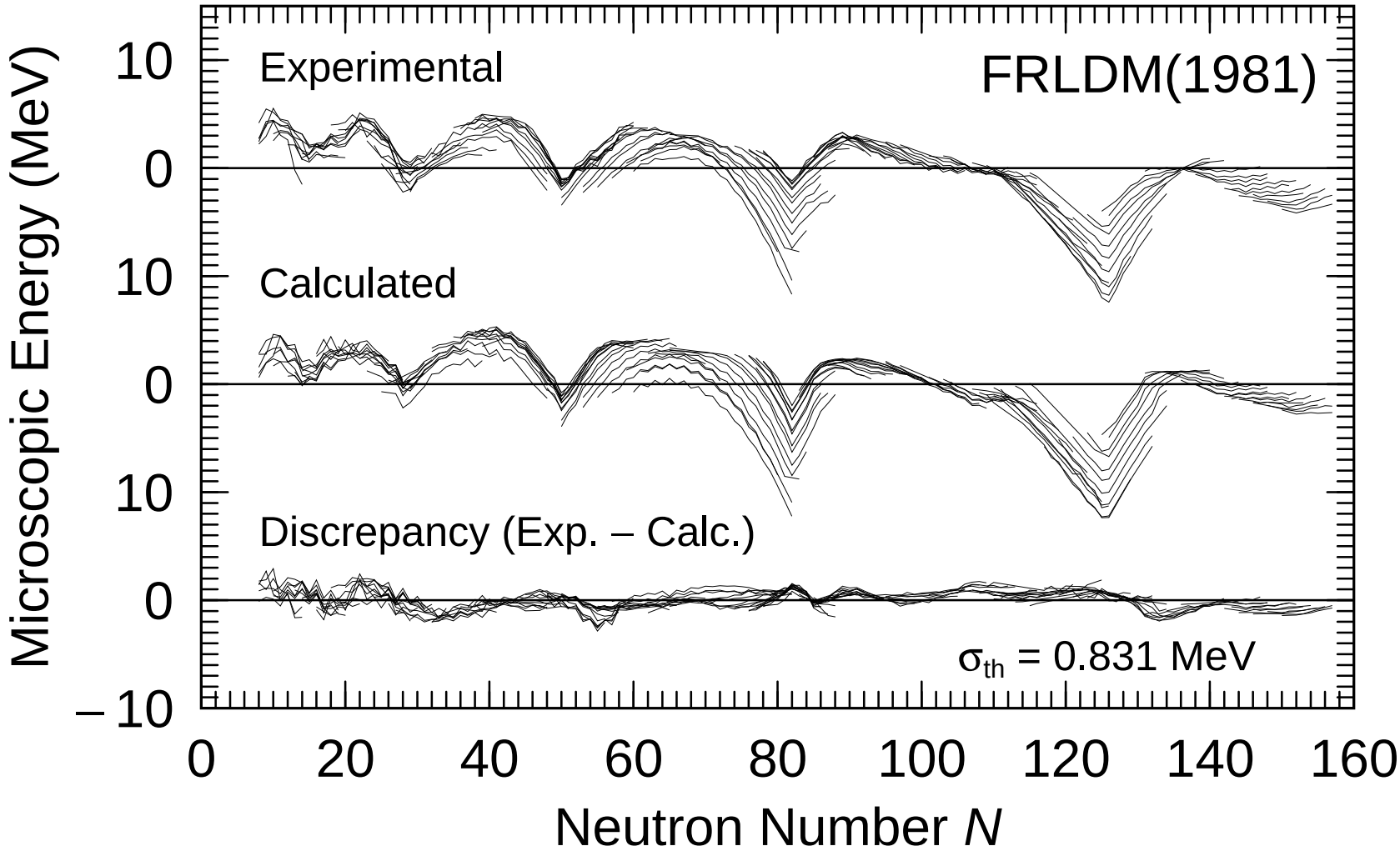
We use the macroscopic-microscopic method introduced by Swiatecki and Strutinsky:

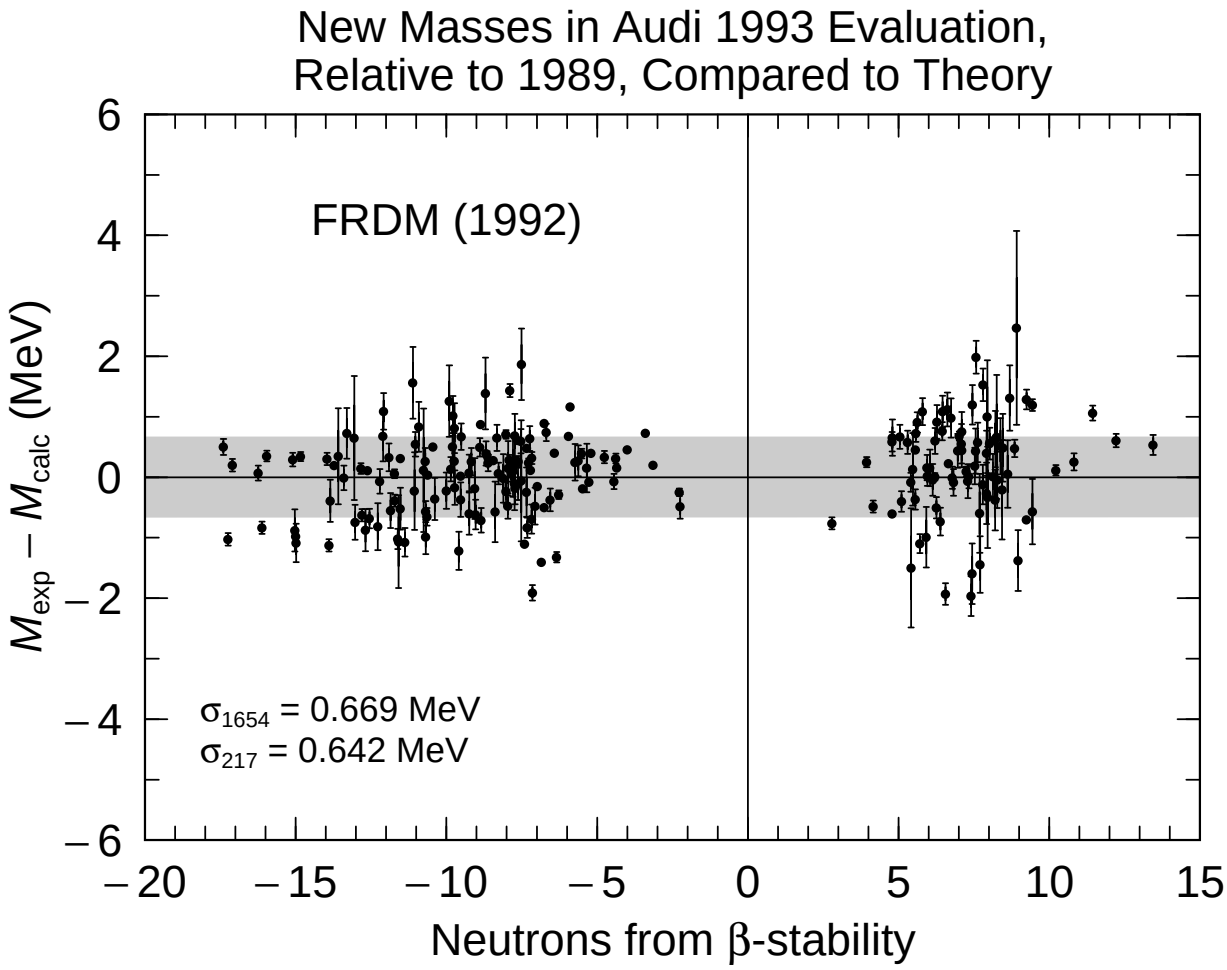
$$E_{\mathrm{pot}}(\mathrm{shape}) = E_{\mathrm{macr}}(\mathrm{shape}) + E_{\mathrm{micr}}(\mathrm{shape}) \quad (1)$$

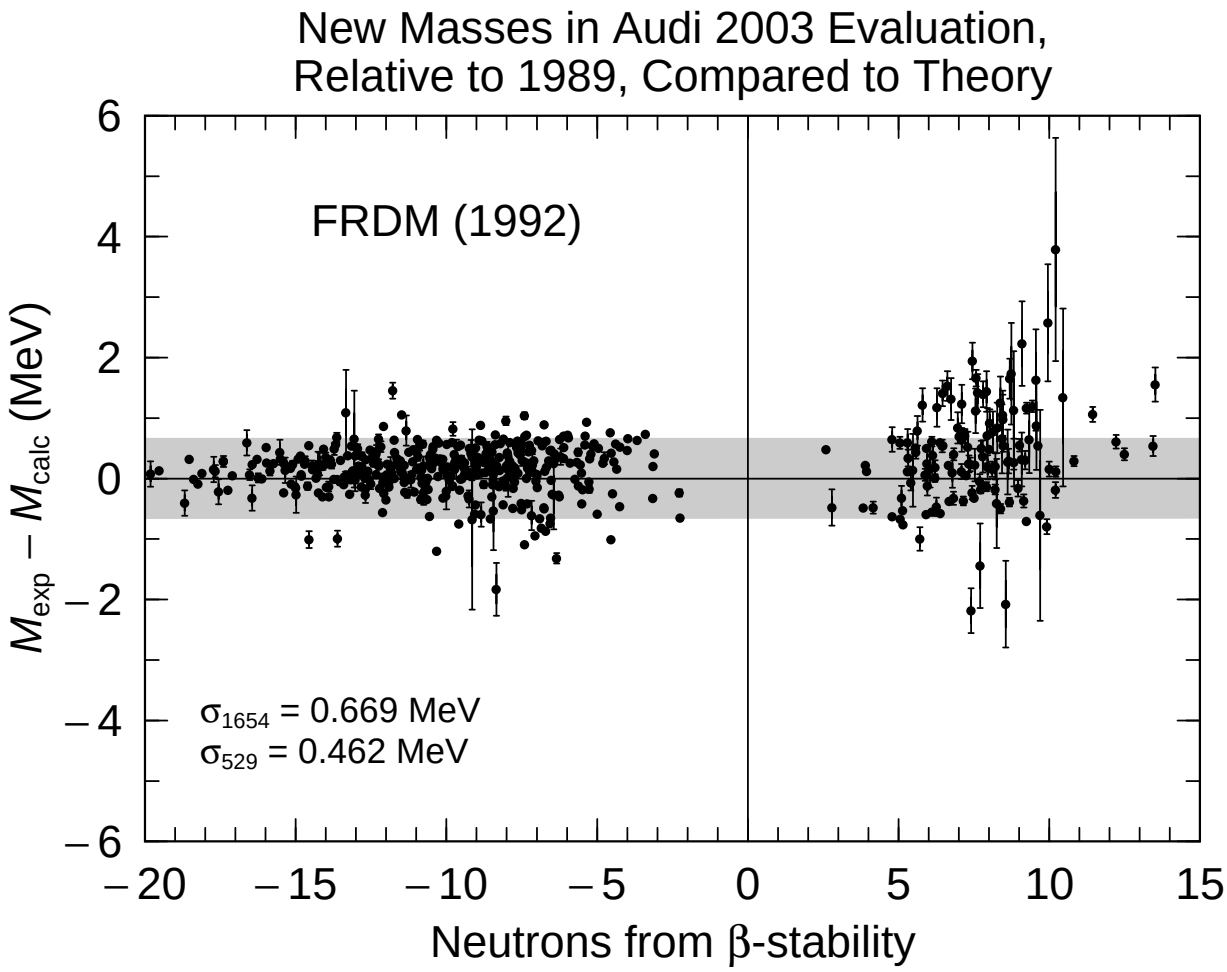
The macroscopic term is calculated in a liquid-drop type model (for a specific deformed shape).

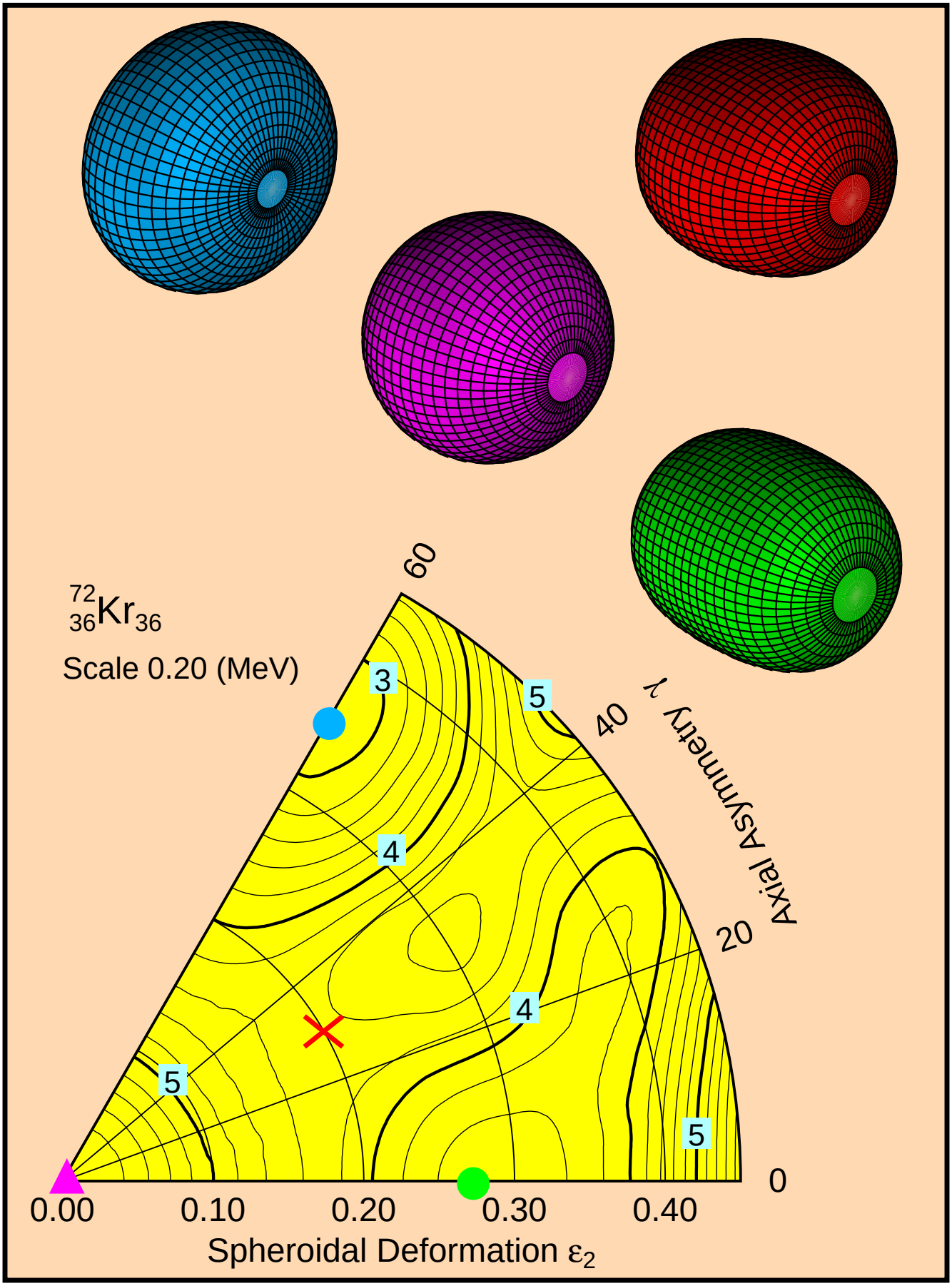
The microscopic correction is determined in the following steps

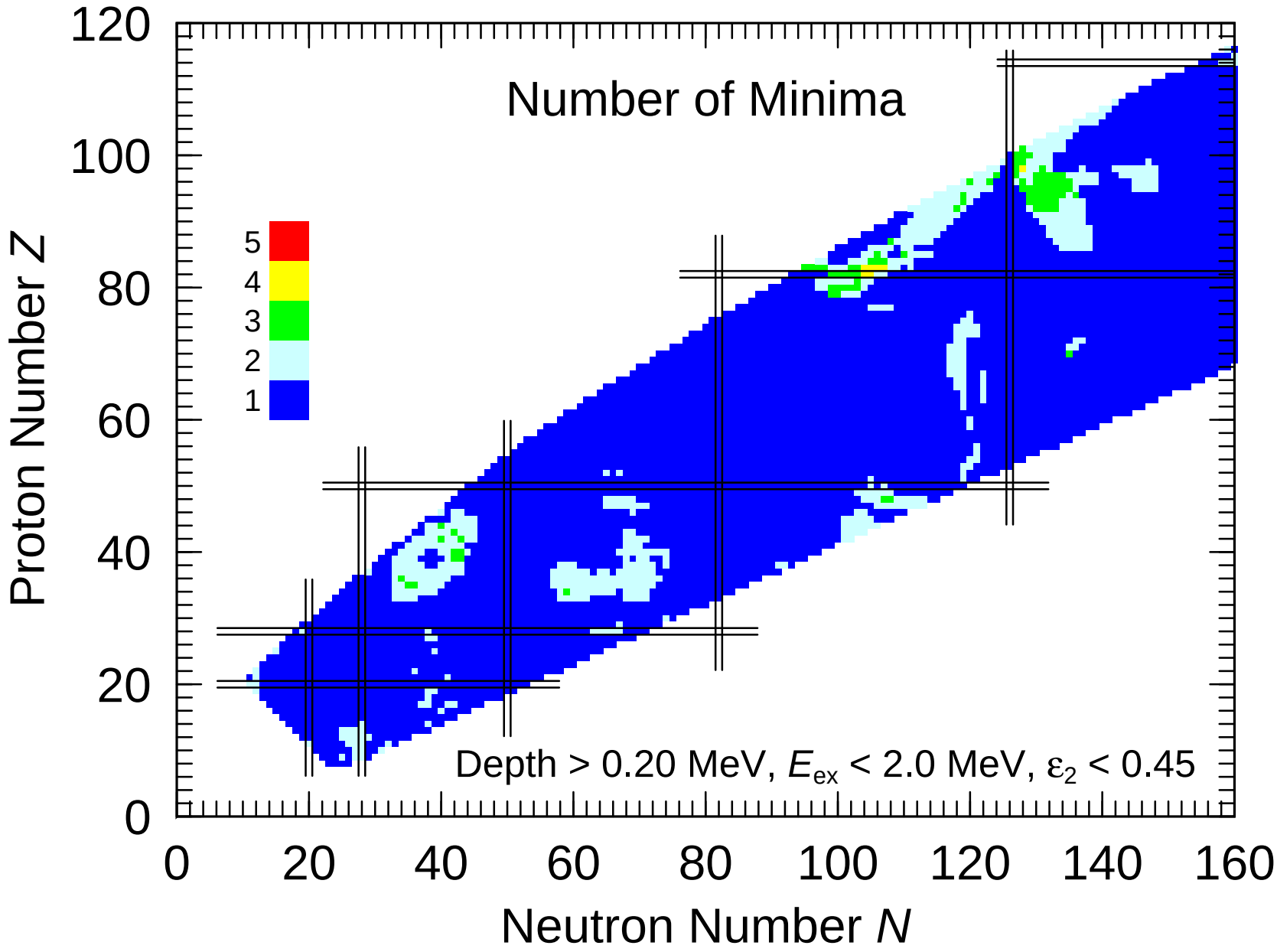
1. A shape is prescribed
2. A single-particle potential with this shape is generated. A spin-orbit term is included.
3. The Schrödinger equation is solved for this deformed potential and single-particle levels and wave-functions are obtained
4. The shell correction is calculated by use of Strutinsky's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


Experimental
FRLDM(1981)
Calculated
Discrepancy (Exp. – Calc.)
σth = 0.831 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


$^{72}_{36}Kr_{36}$
Scale 0.20 (MeV)
3
4
5
4
5
5
0.00
0.10
0.20
0.30
0.40
Spheroidal Deformation ε_2
0
20
40
60
Axial Asymmetry γ


Number of Minima
5
4
3
2
1
Depth > 0.20 MeV, E_{ex} < 2.0 MeV, ε_2 < 0.45
Proton Number Z
Neutron Number N
0
20
40
60
80
100
120
140
160

Typical Level Spectra for 3 Major Types of Deviation from Spherical Symmetry

Spherical

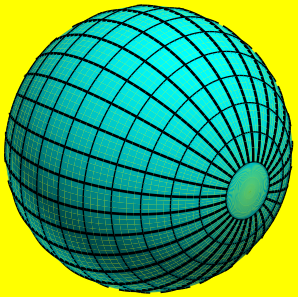
^{128}Te

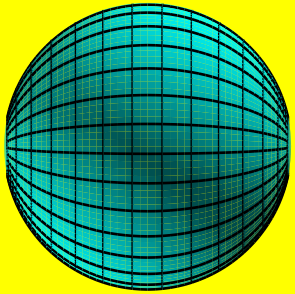
4+ 1497.04

2+ 743.22

0+

Vibrational band





Spheroidal

^{238}U

8+ 518.3

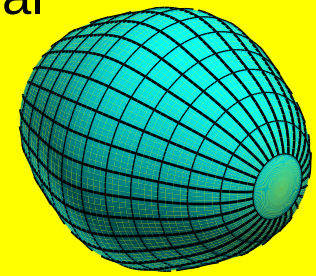
6+ 307.21

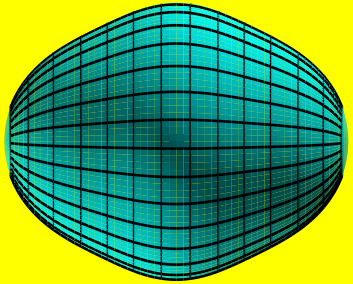
4+ 148.41

2+ 44.91

0+

Rotational band





Reflection Asymmetric

^{222}Ra

4+ 301.42

317.27 3-

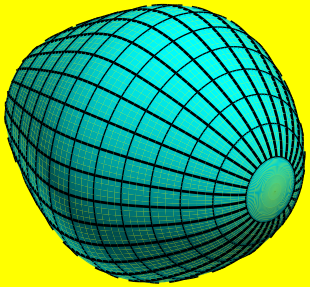
242.13 1-

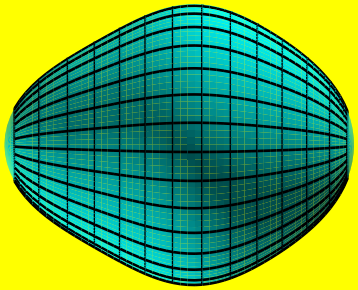
Negative-parity band

2+ 111.12

0+

Positive-parity band





Axially Asymmetric

^{140}Gd

10+ 2796.8

8+ 2139.7

6+ 1464.0

4+ 836.2

2+ 328.6

0+

GS band

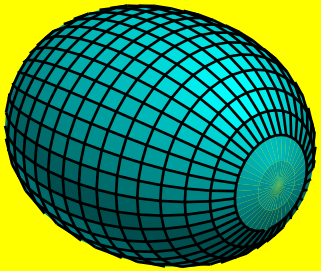
7+ 2412

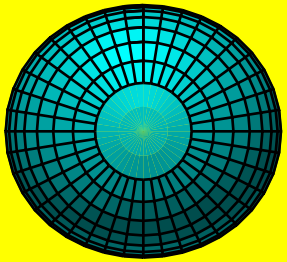
5+ 1882 6+

3+ 1281.5 4+

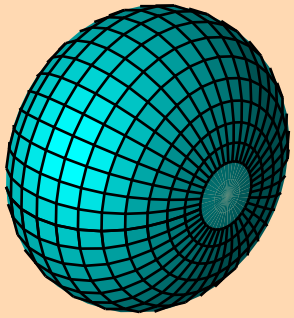
713.4 2+

γ band

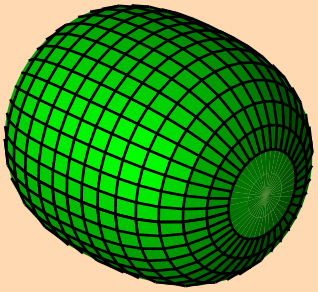




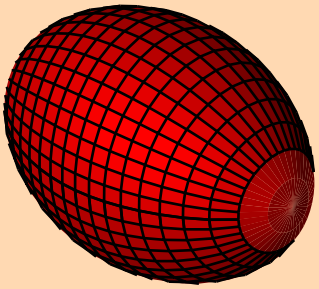
Krypton Equilibirium-Point Shapes



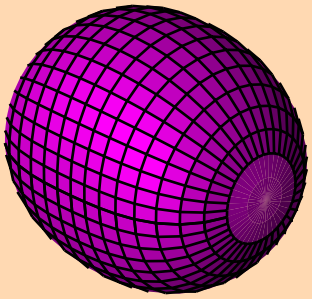
Oblate ground state



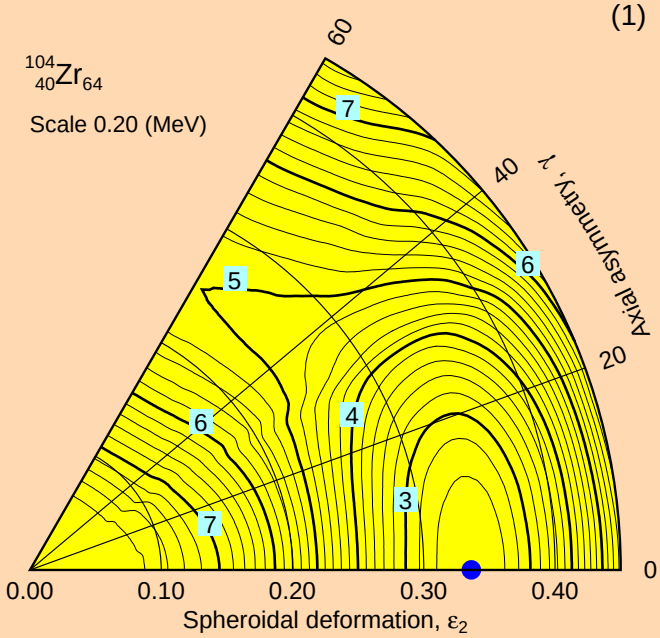
Prolate minimum

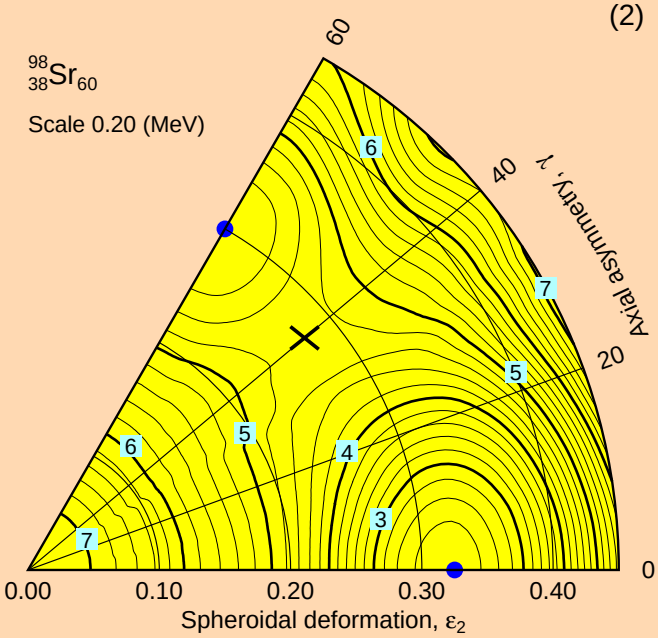


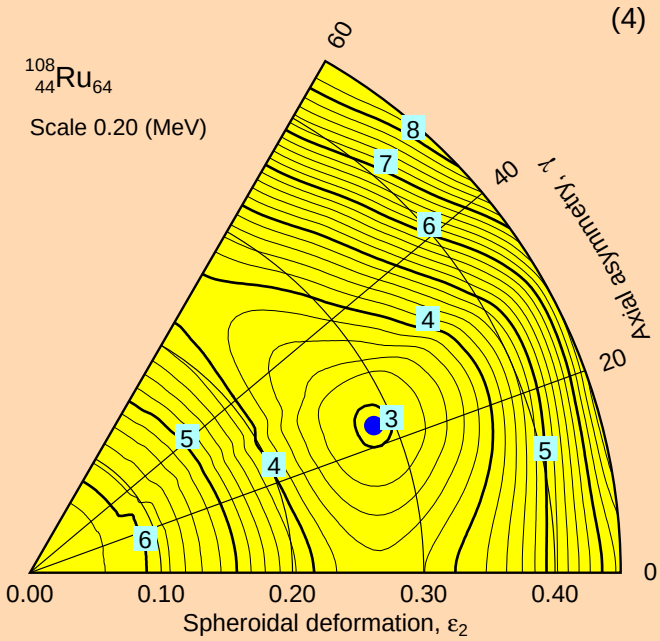
Axially asymmetric minimum

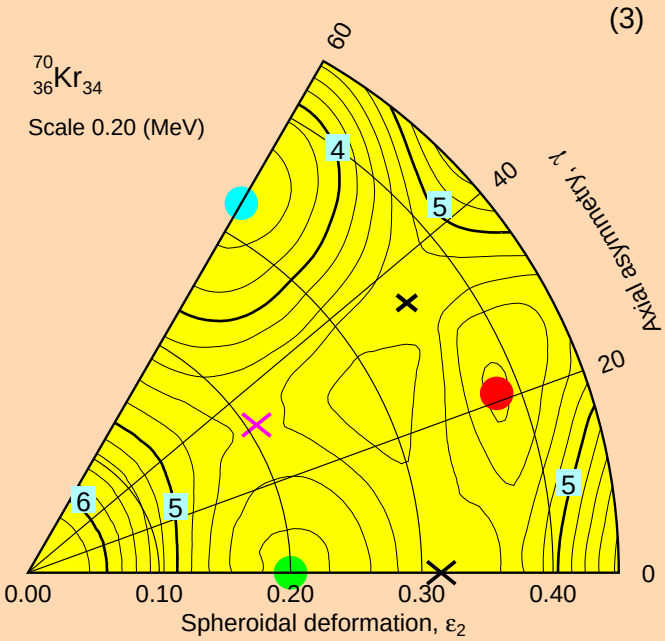


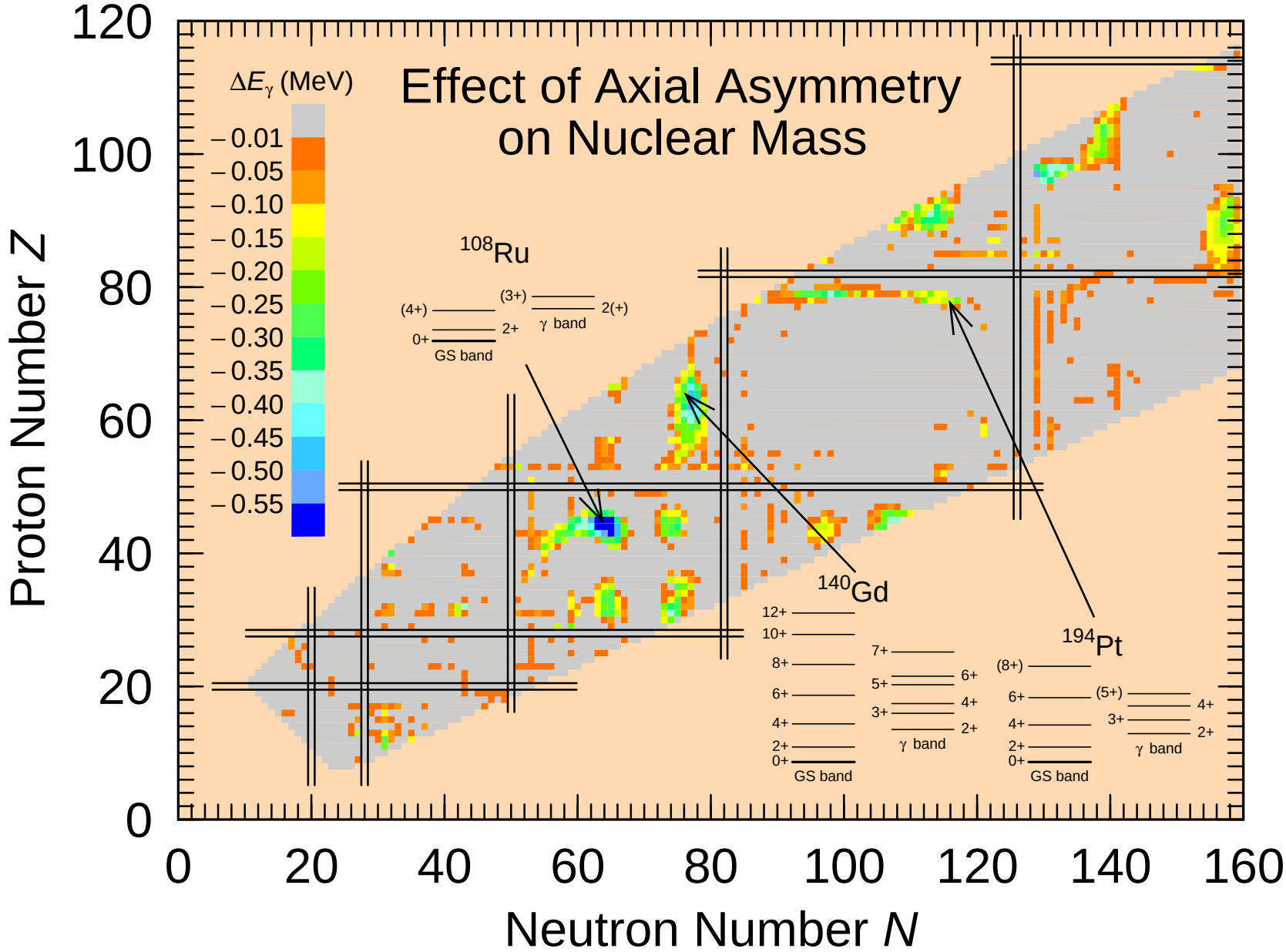
Axially asymmetric saddle

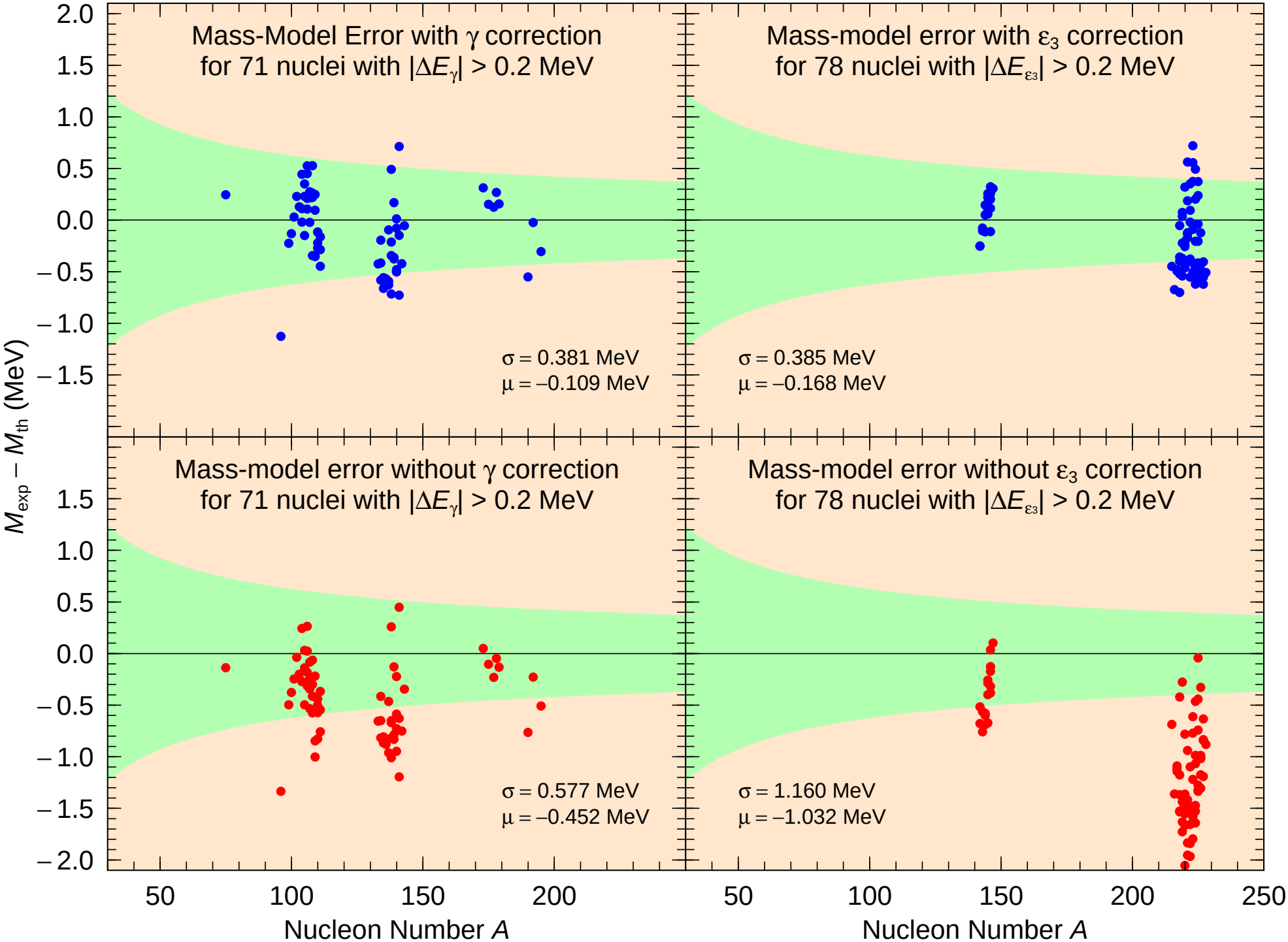


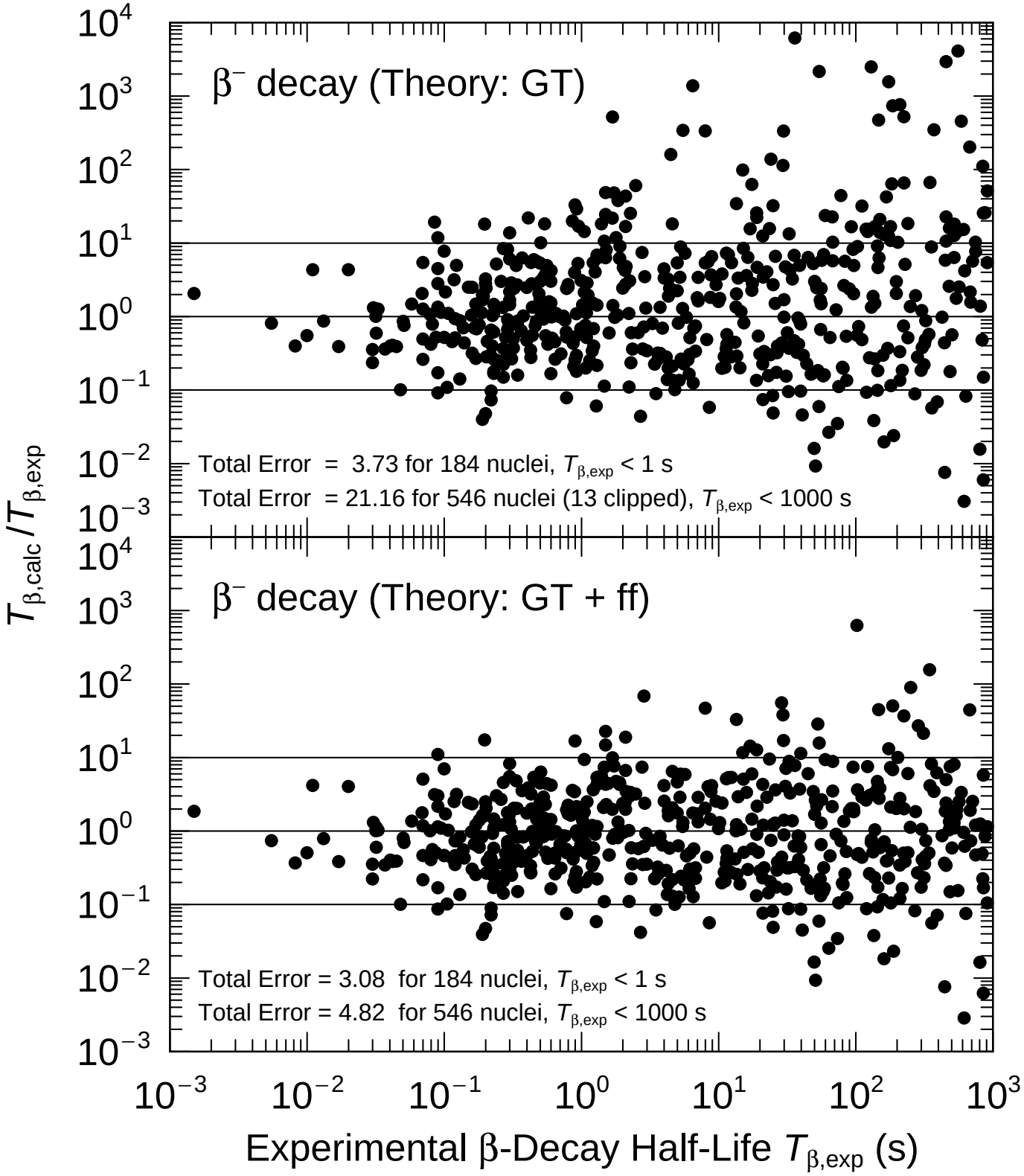


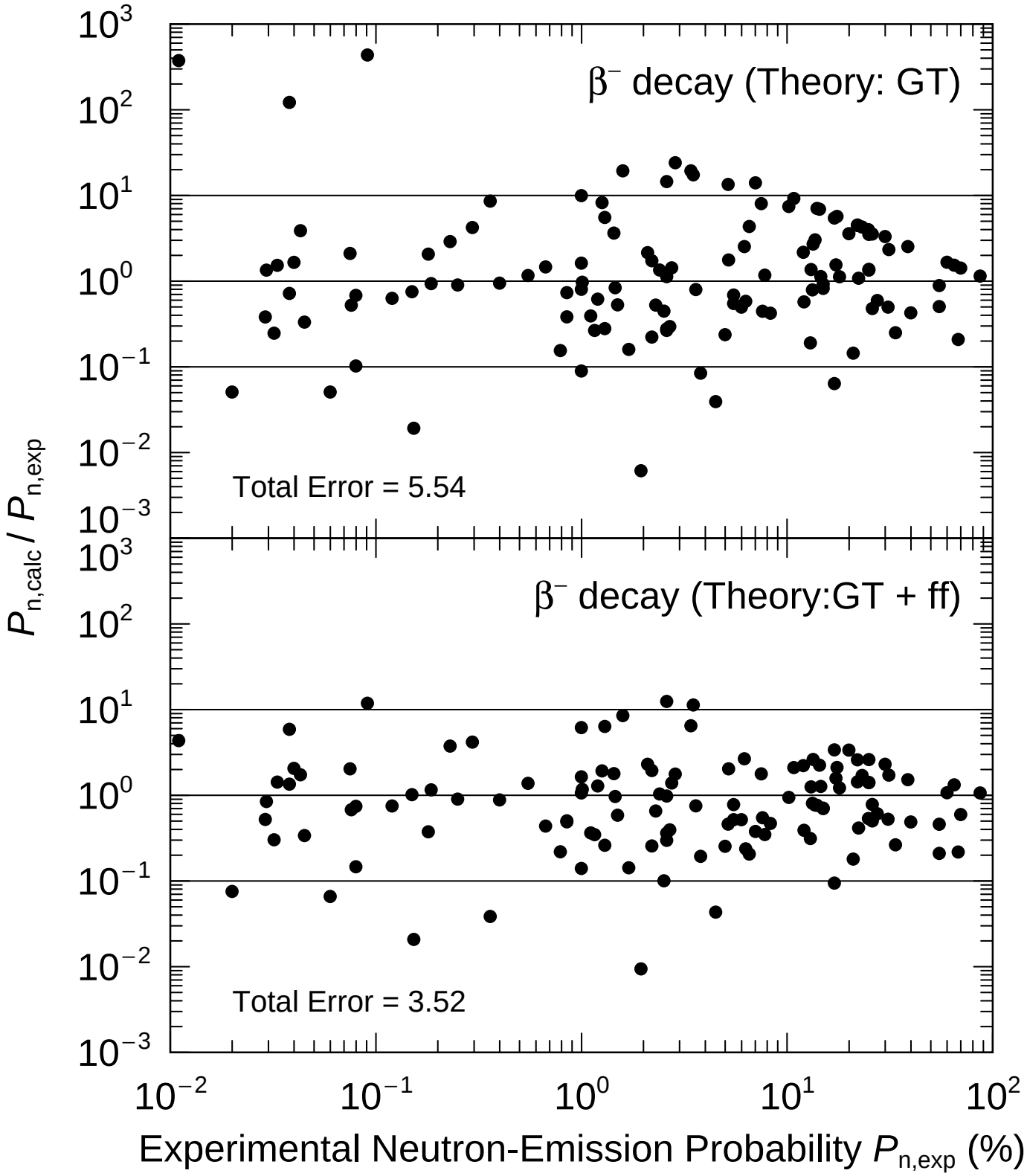





Effect of Axial Asymmetry
on Nuclear Mass
ΔEγ (MeV)
– 0.01
– 0.05
– 0.10
– 0.15
– 0.20
– 0.25
– 0.30
– 0.35
– 0.40
– 0.45
– 0.50
– 0.55
108Ru
(4+)
(3+)
2(+)
2+
0+
γ band
GS band
140Gd
12+
10+
8+
6+
4+
2+
0+
GS band
7+
5+
3+
6+
4+
2+
γ band
194Pt
(8+)
6+
4+
2+
0+
GS band
(5+)
3+
4+
2+
γ band
Proton Number Z
Neutron Number N
0
20
40
60
80
100
120
140
160


Mass-Model Error with γ correction
for 71 nuclei with |ΔE_γ| > 0.2 MeV
σ = 0.381 MeV
μ = –0.109 MeV
Mass-model error with ε3 correction
for 78 nuclei with |ΔE_ε3| > 0.2 MeV
σ = 0.385 MeV
μ = –0.168 MeV
Mass-model error without γ correction
for 71 nuclei with |ΔE_γ| > 0.2 MeV
σ = 0.577 MeV
μ = –0.452 MeV
Mass-model error without ε3 correction
for 78 nuclei with |ΔE_ε3| > 0.2 MeV
σ = 1.160 MeV
μ = –1.032 MeV
M_exp – M_th (MeV)
Nucleon Number A
Nucleon Number A

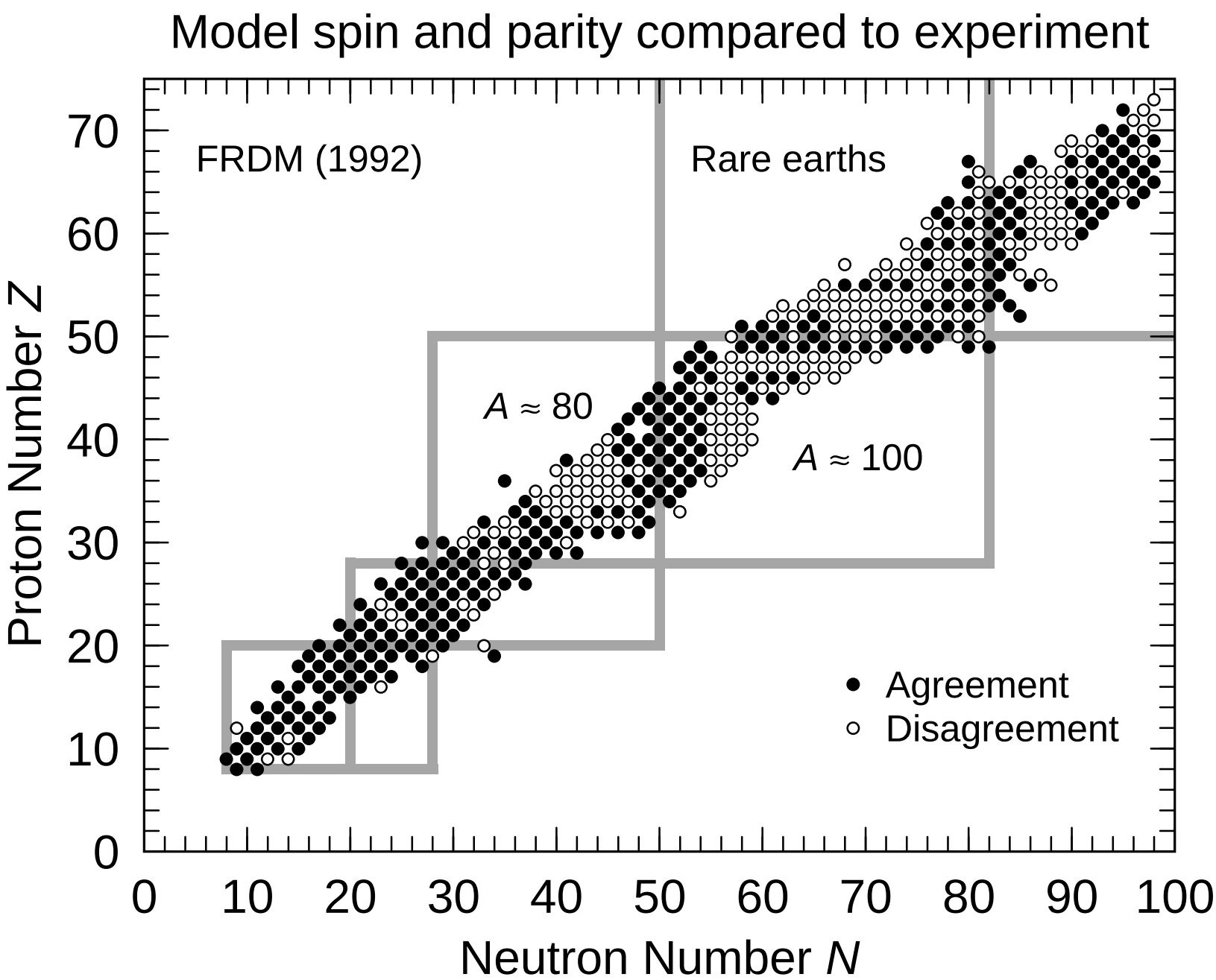

β⁻ decay (Theory: GT)
Total Error = 3.73 for 184 nuclei, $T_{\beta,exp}$ < 1 s
Total Error = 21.16 for 546 nuclei (13 clipped), $T_{\beta,exp}$ < 1000 s
β⁻ decay (Theory: GT + ff)
Total Error = 3.08 for 184 nuclei, $T_{\beta,exp}$ < 1 s
Total Error = 4.82 for 546 nuclei, $T_{\beta,exp}$ < 1000 s
$T_{\beta,calc}/T_{\beta,exp}$
Experimental β-Decay Half-Life $T_{\beta,exp}$ (s)

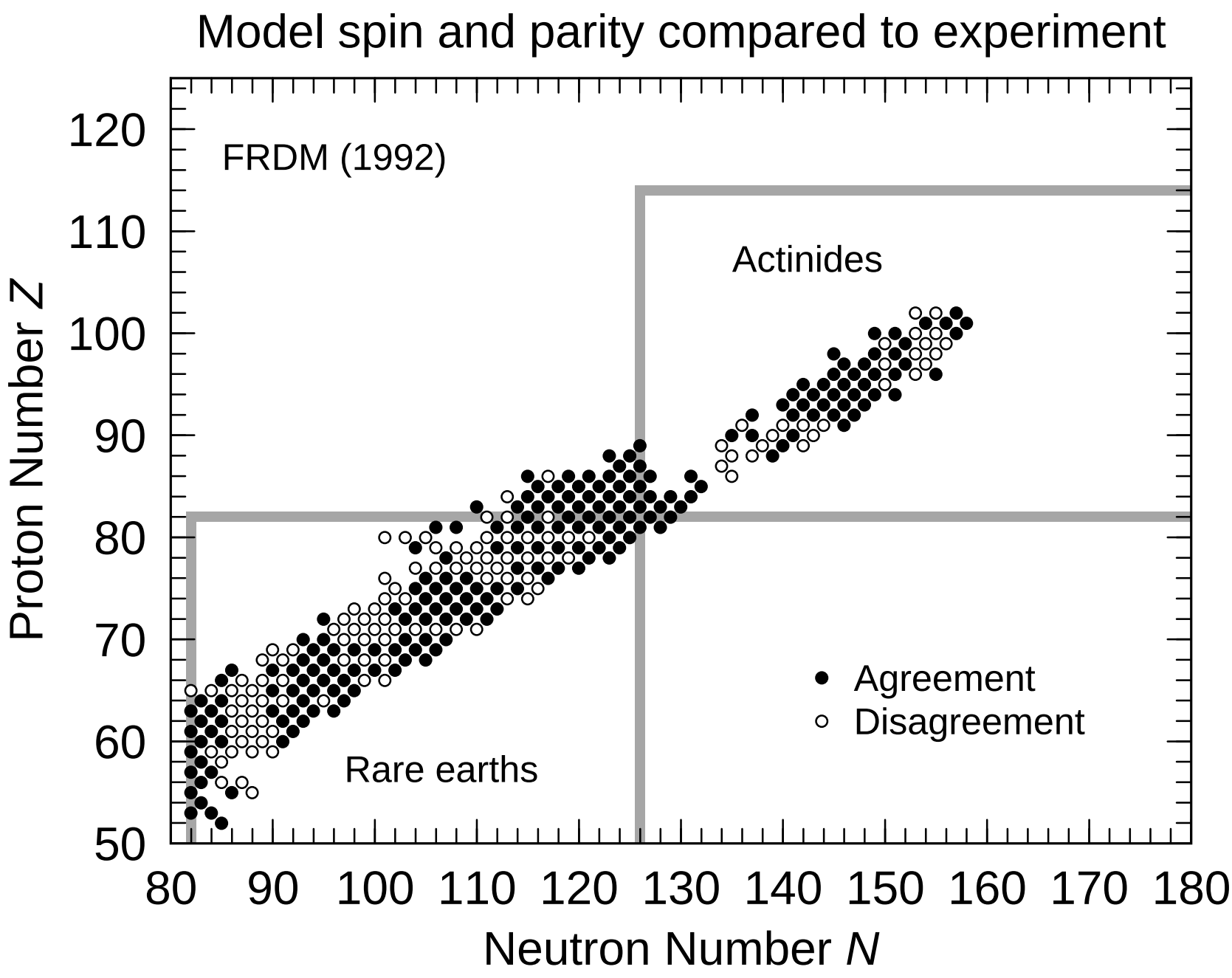

β⁻ decay (Theory: GT)
Total Error = 5.54
β⁻ decay (Theory:GT + ff)
Total Error = 3.52
$P_{n,calc} / P_{n,exp}$
Experimental Neutron-Emission Probability $P_{n,exp}$ (%)

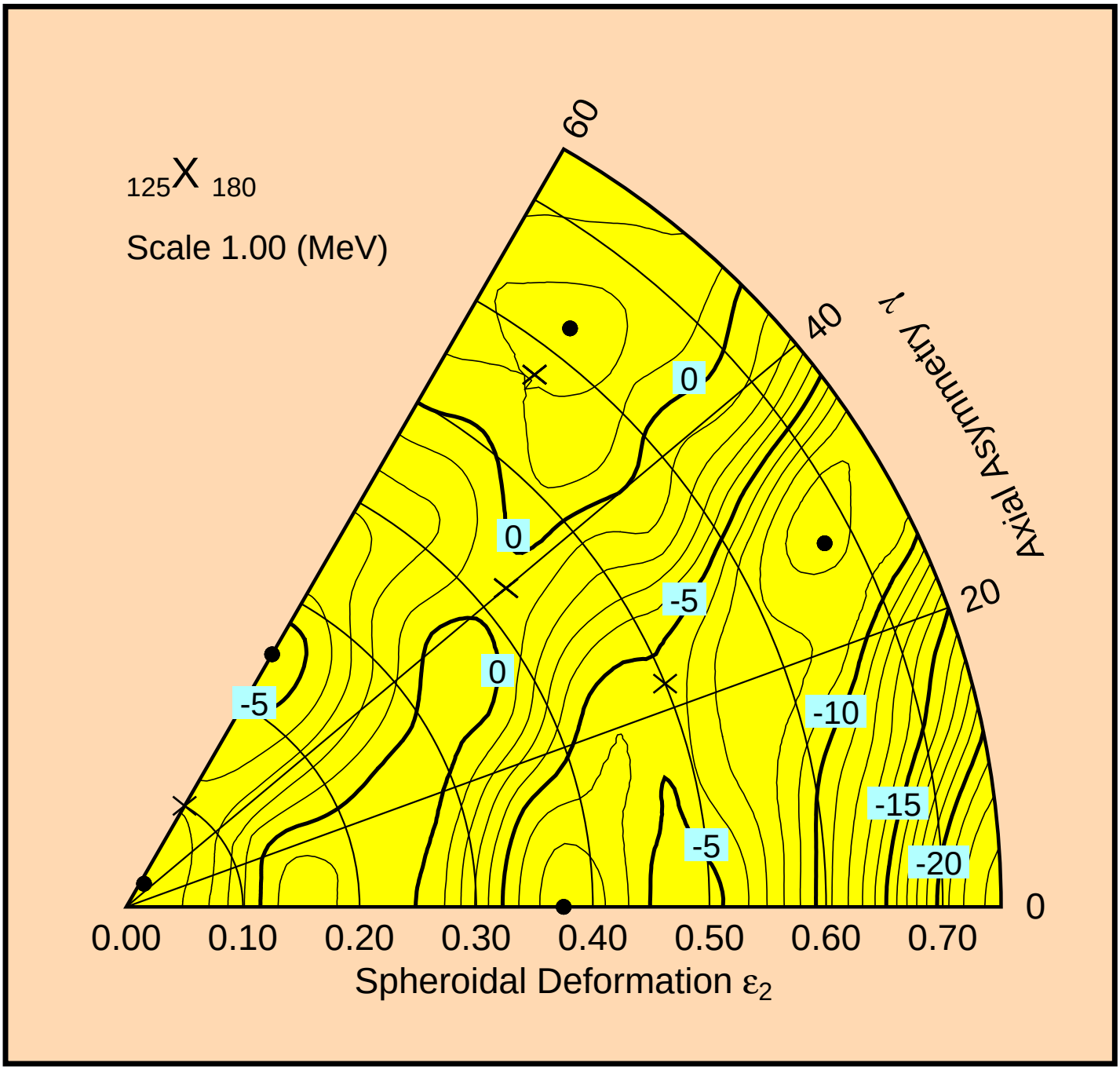
GS SPIN OF O-E NUCLEI

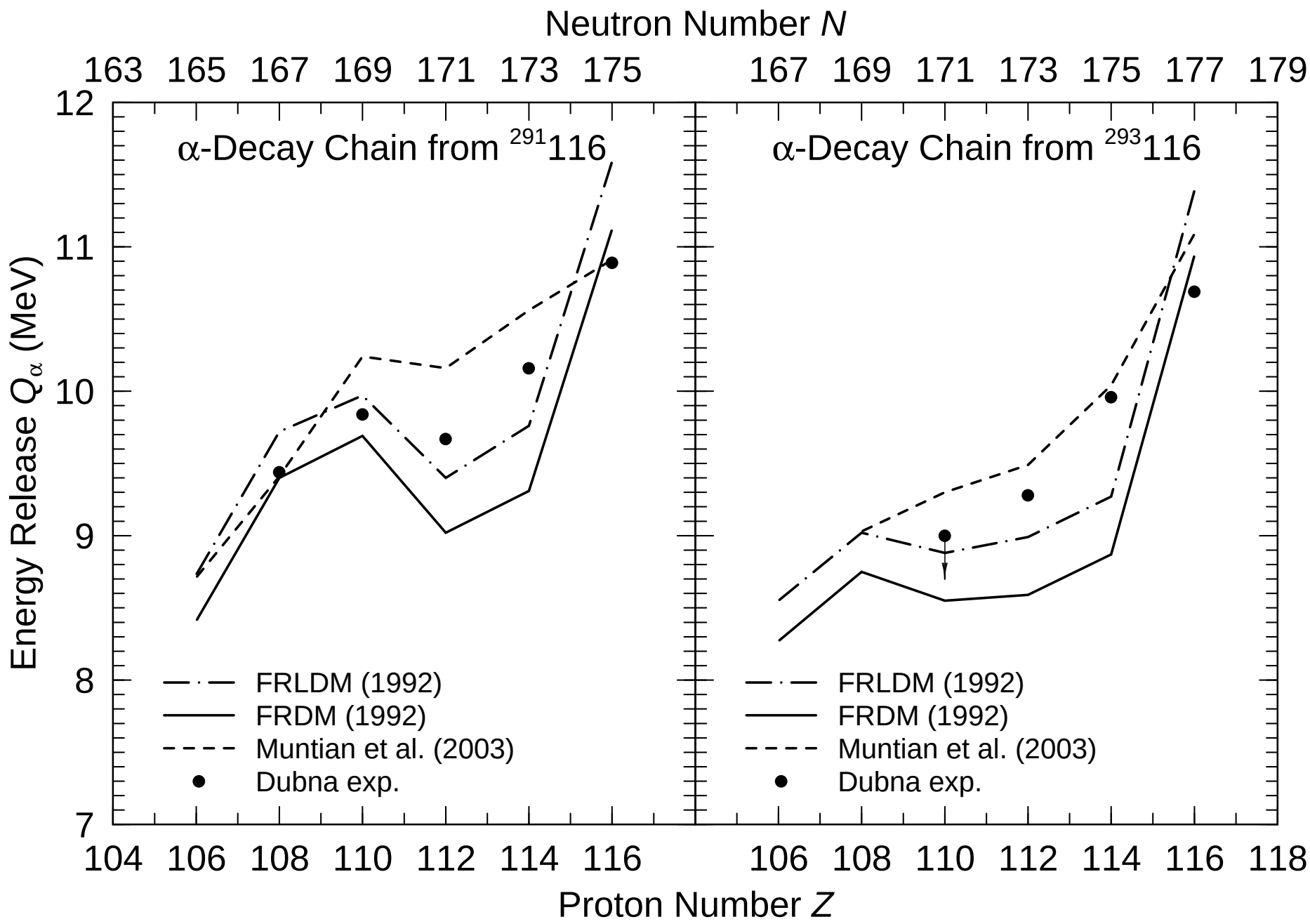
Calculated spins of odd-even nuclei agree with experiment to about 60% for about 700 nuclei.

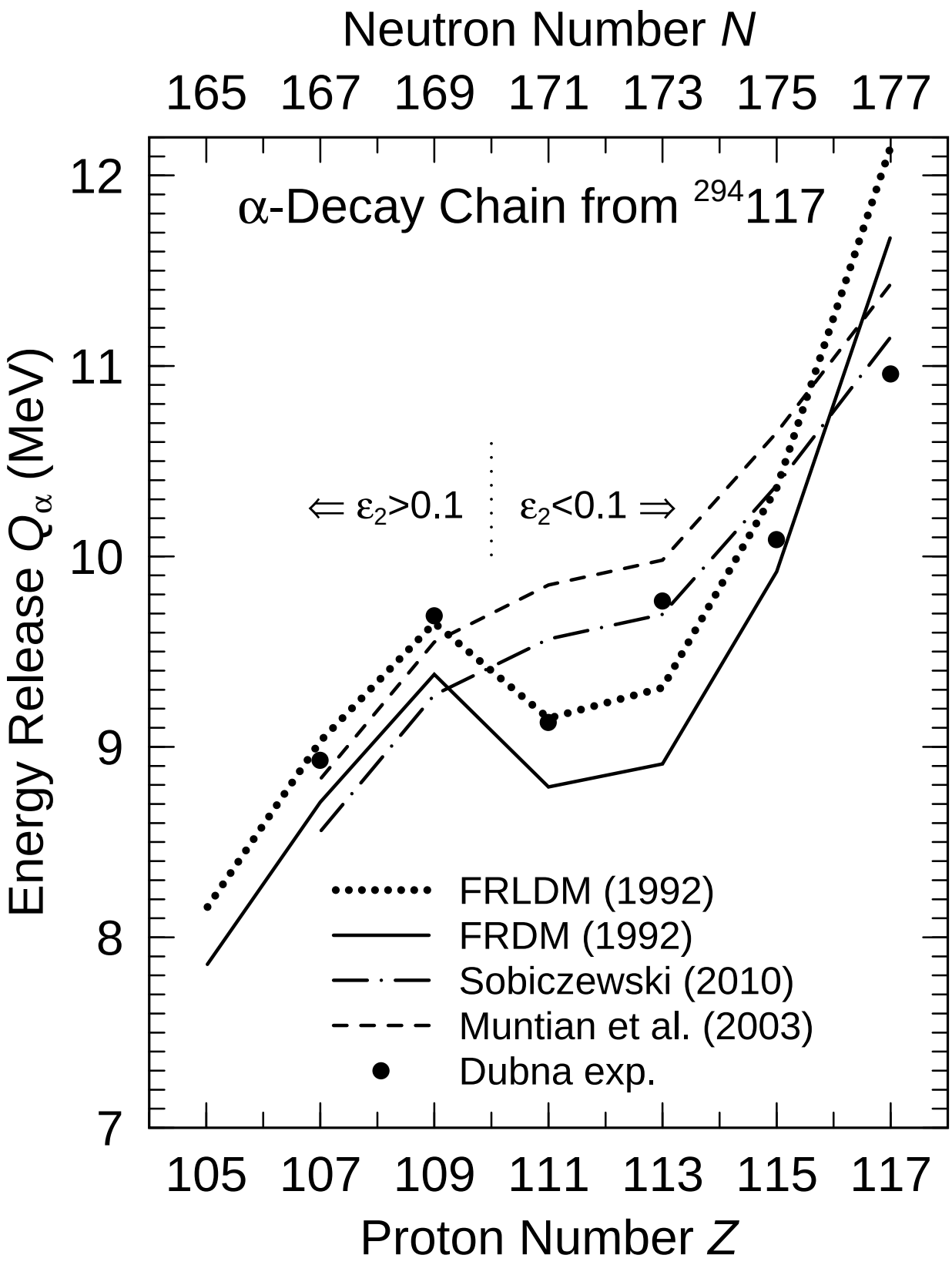
Correct results for these spins are of paramount importance in many cases, for example β-decay. Selection rules for the odd nucleon determine the decays to low-lying states in the daughter, incorrect gs spin can have substantial consequences for predictions of half-life and delayed-neutron emission probabilities.

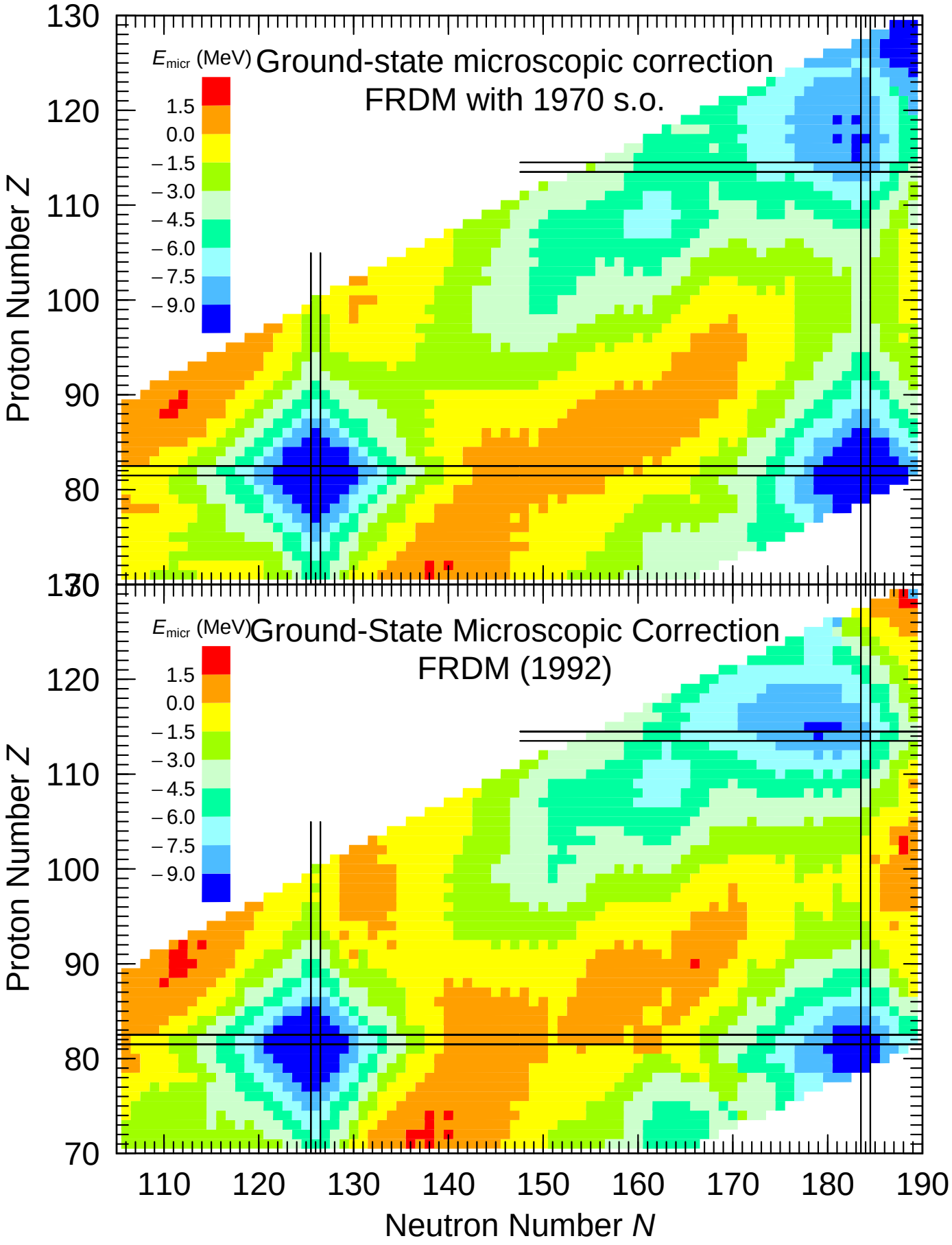

Model spin and parity compared to experiment
FRDM (1992)
Rare earths
A ≈ 80
A ≈ 100
Agreement
Disagreement
Proton Number Z
Neutron Number N
0
10
20
30
40
50
60
70
80
90
100


Model spin and parity compared to experiment
FRDM (1992)
Actinides
Rare earths
Agreement
Disagreement
Proton Number Z
Neutron Number N
120
110
100
90
80
70
60
50
80
90
100
110
120
130
140
150
160
170
180


125X 180
Scale 1.00 (MeV)
60
40
20
0
Axial Asymmetry γ
0
0
-5
0
-5
-10
-15
-20
-5
0.00
0.10
0.20
0.30
0.40
0.50
0.60
0.70
Spheroidal Deformation ε2


Neutron Number N
163 165 167 169 171 173 175
167 169 171 173 175 177 179
α-Decay Chain from 291116
α-Decay Chain from 293116
Energy Release Qα (MeV)
12
11
10
9
8
7
FRLDM (1992)
FRDM (1992)
Muntian et al. (2003)
Dubna exp.
FRLDM (1992)
FRDM (1992)
Muntian et al. (2003)
Dubna exp.
104 106 108 110 112 114 116
106 108 110 112 114 116 118
Proton Number Z


Neutron Number N
165 167 169 171 173 175 177
α-Decay Chain from 294117
⇐ ε2>0.1
ε2<0.1 ⇒
Energy Release Qα (MeV)
12
11
10
9
8
7
FRLDM (1992)
FRDM (1992)
Sobiczewski (2010)
Muntian et al. (2003)
Dubna exp.
105 107 109 111 113 115 117
Proton Number Z


Ground-state microscopic correction
FRDM with 1970 s.o.
E_{micr} (MeV)
1.5
0.0
−1.5
−3.0
−4.5
−6.0
−7.5
−9.0
Ground-State Microscopic Correction
FRDM (1992)
Proton Number Z
Neutron Number N
130
120
110
100
90
80
70
110
120
130
140
150
160
170
180
190

Now let us address the determination of the symmetry term parameters. To do this we have in successive steps improved the FRDM(1992), the current interim “table” is FRDM(2011a). Once we have more consistently recalculated the “beyond-mean-field” zero-point vibrational-energy corrections we are planning to submit FRDM(2012) for publication.

FRDM enhancements

Optimization

The search for optimum FRDM macroscopic parameters has been improved.

Accuracy improvement: 0.01 MeV

New exp. mass data base

We agree better with the new mass data base

Accuracy improvement: 0.04 MeV

Full 4D energy minimization

Search for minimum energy versus $\epsilon_2, \epsilon_3, \epsilon_4, \epsilon_6$, full 4D in steps of 0.01.

Accuracy improvement: 0.02 MeV

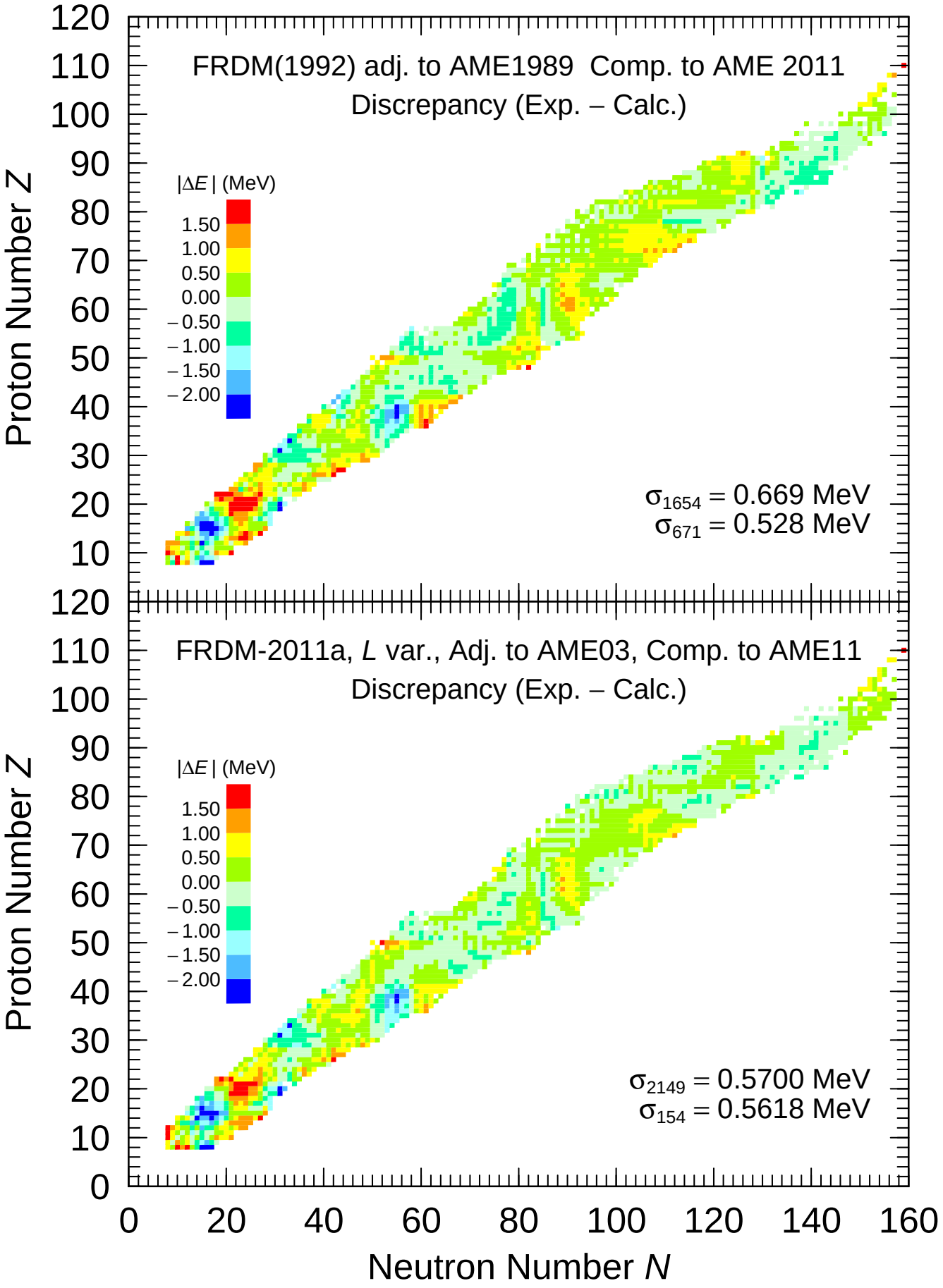
Axial asymmetry

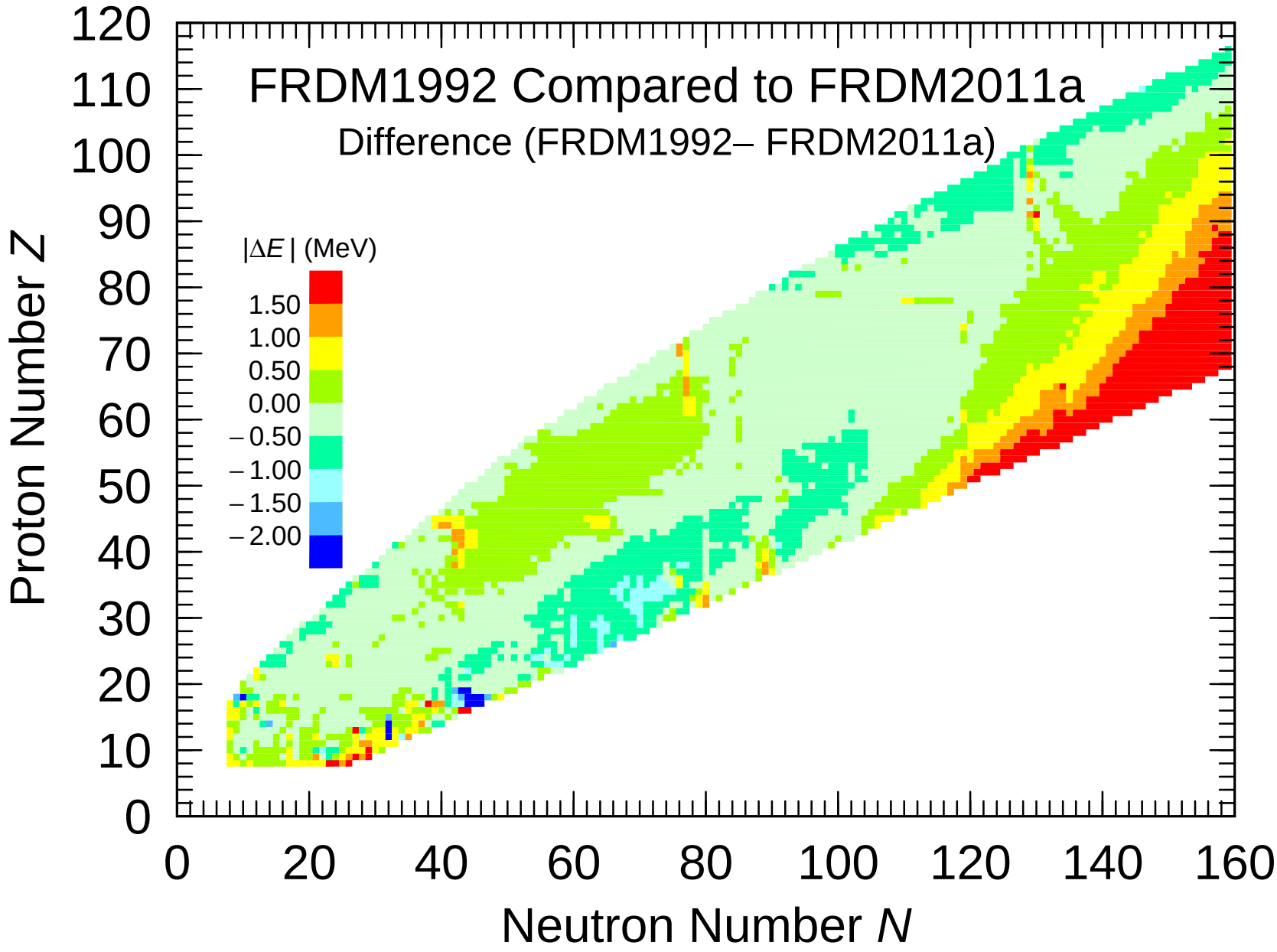
Results in correct gs assignments in SHE regions, and mass improvements.

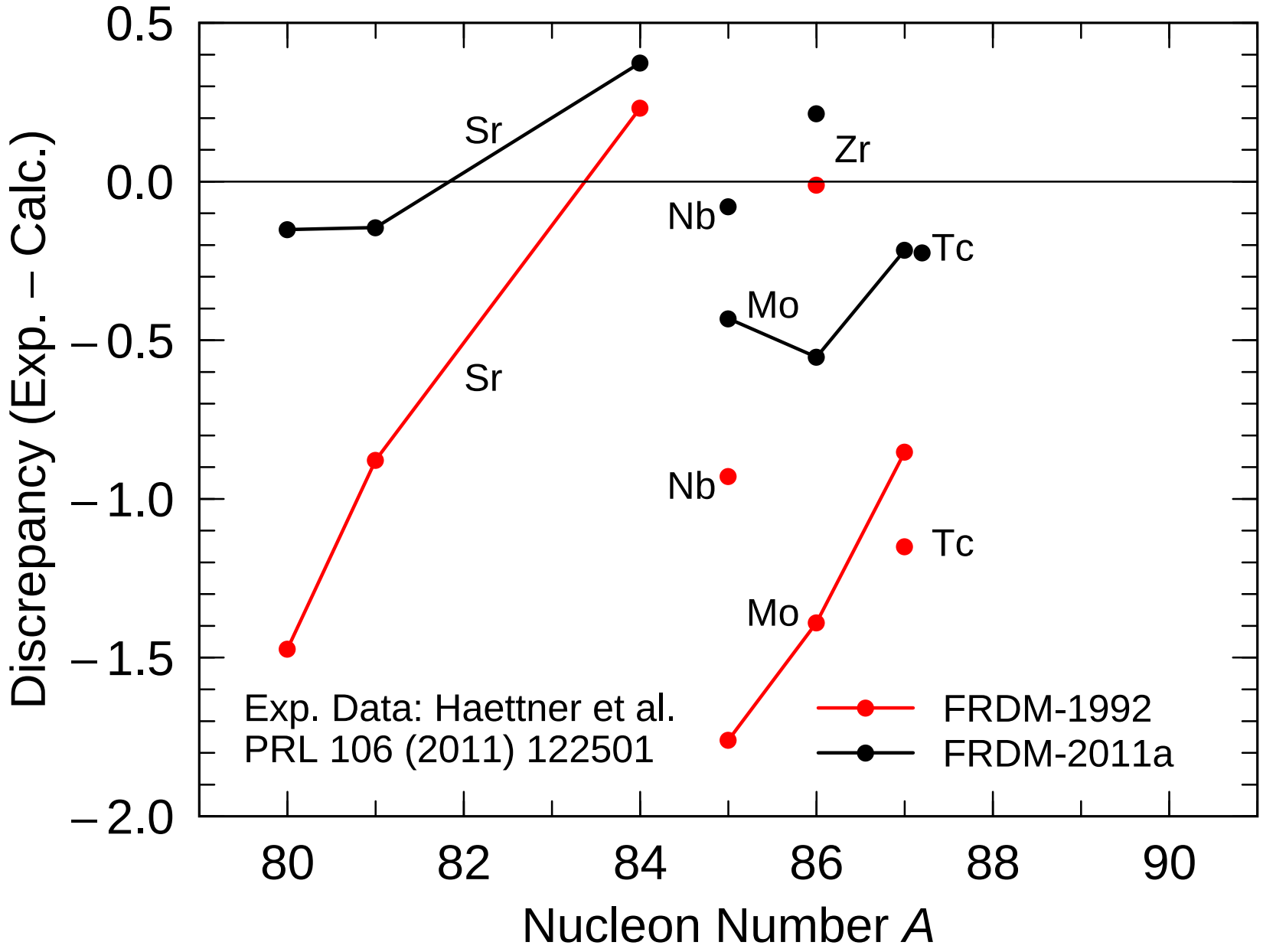
Accuracy improvement: 0.01 MeV

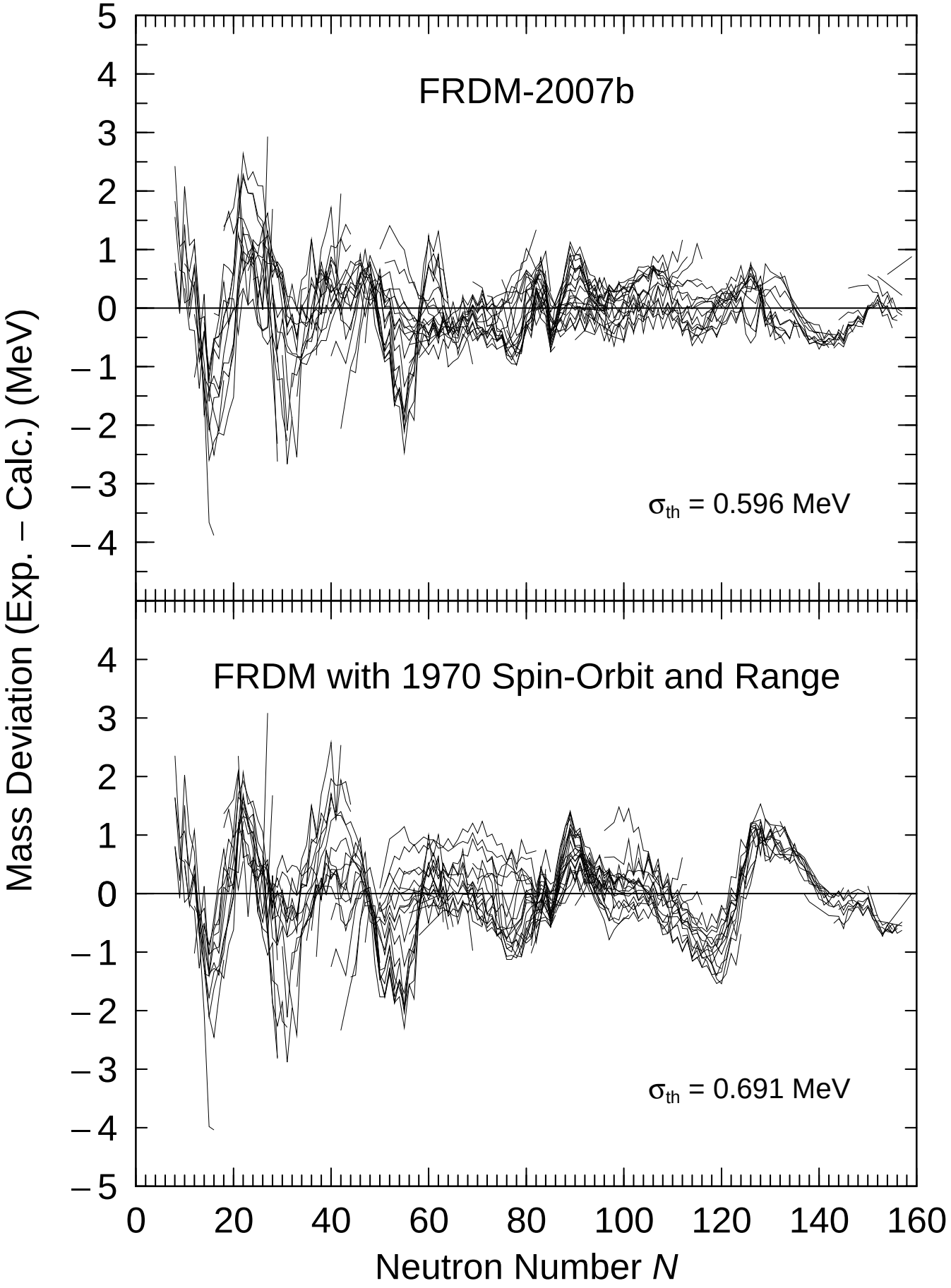
L variation

Accuracy improvement 0.02 MeV


FRDM(1992) adj. to AME1989 Comp. to AME 2011
Discrepancy (Exp. – Calc.)
|ΔE| (MeV)
1.50
1.00
0.50
0.00
– 0.50
– 1.00
– 1.50
– 2.00
σ1654 = 0.669 MeV
σ671 = 0.528 MeV
FRDM-2011a, L var., Adj. to AME03, Comp. to AME11
Discrepancy (Exp. – Calc.)
|ΔE| (MeV)
1.50
1.00
0.50
0.00
– 0.50
– 1.00
– 1.50
– 2.00
σ2149 = 0.5700 MeV
σ154 = 0.5618 MeV
Proton Number Z
Neutron Number N
0
10
20
30
40
50
60
70
80
90
100
110
120
0
20
40
60
80
100
120
140
160


FRDM1992 Compared to FRDM2011a
Difference (FRDM1992– FRDM2011a)
|ΔE| (MeV)
1.50
1.00
0.50
0.00
– 0.50
– 1.00
– 1.50
– 2.00
Proton Number Z
Neutron Number N
0
10
20
30
40
50
60
70
80
90
100
110
120
0
20
40
60
80
100
120
140
160


0.5
0.0
– 0.5
– 1.0
– 1.5
– 2.0
Discrepancy (Exp. – Calc.)
80
82
84
86
88
90
Nucleon Number A
Sr
Sr
Zr
Nb
Nb
Tc
Tc
Mo
Mo
Exp. Data: Haettner et al.
PRL 106 (2011) 122501
FRDM-1992
FRDM-2011a


FRDM-2007b
σth = 0.596 MeV
FRDM with 1970 Spin-Orbit and Range
σth = 0.691 MeV
Mass Deviation (Exp. – Calc.) (MeV)
Neutron Number N
5
4
3
2
1
0
–1
–2
–3
–4
–5
0
20
40
60
80
100
120
140
160

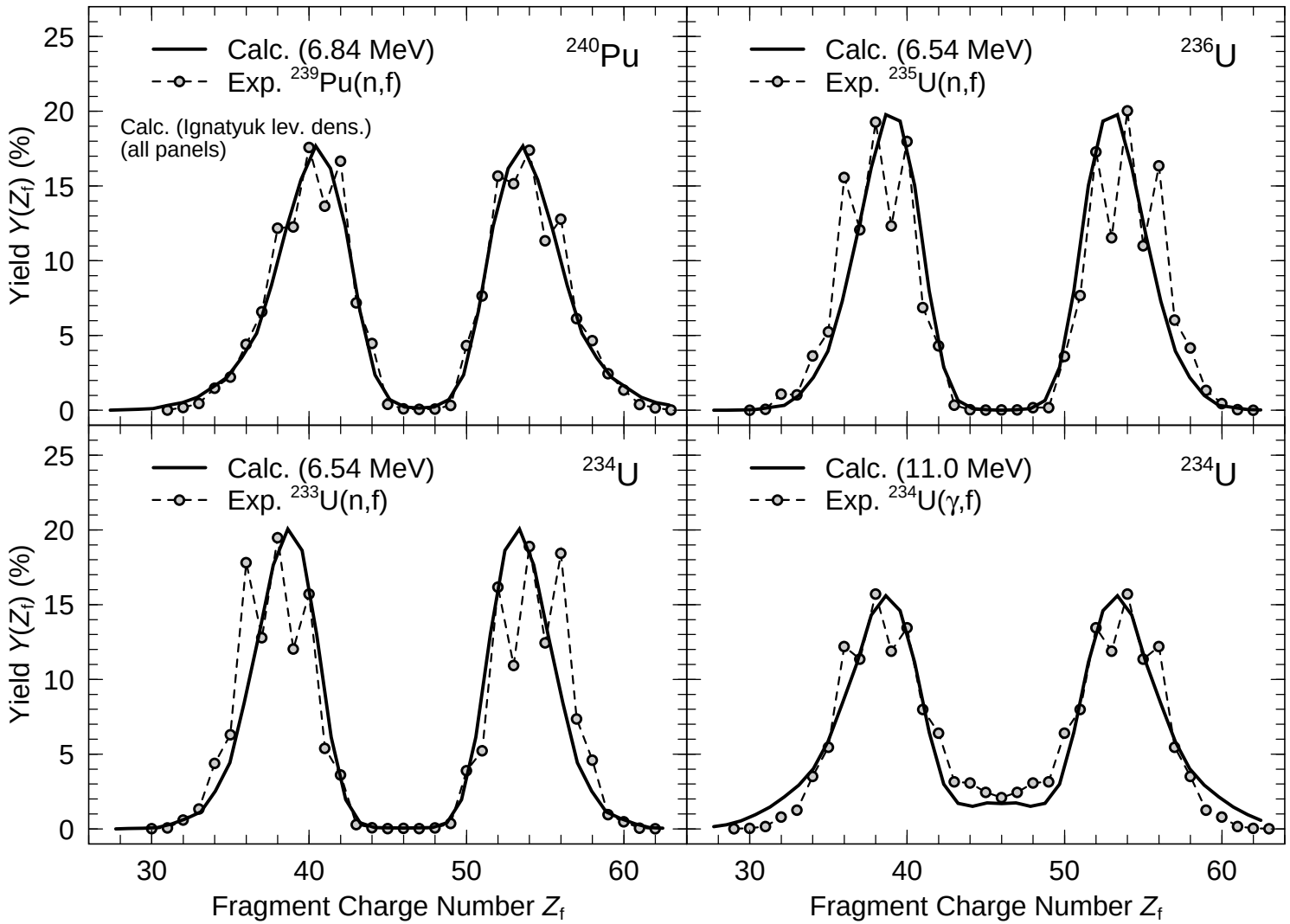
Potential Surface away from GS??

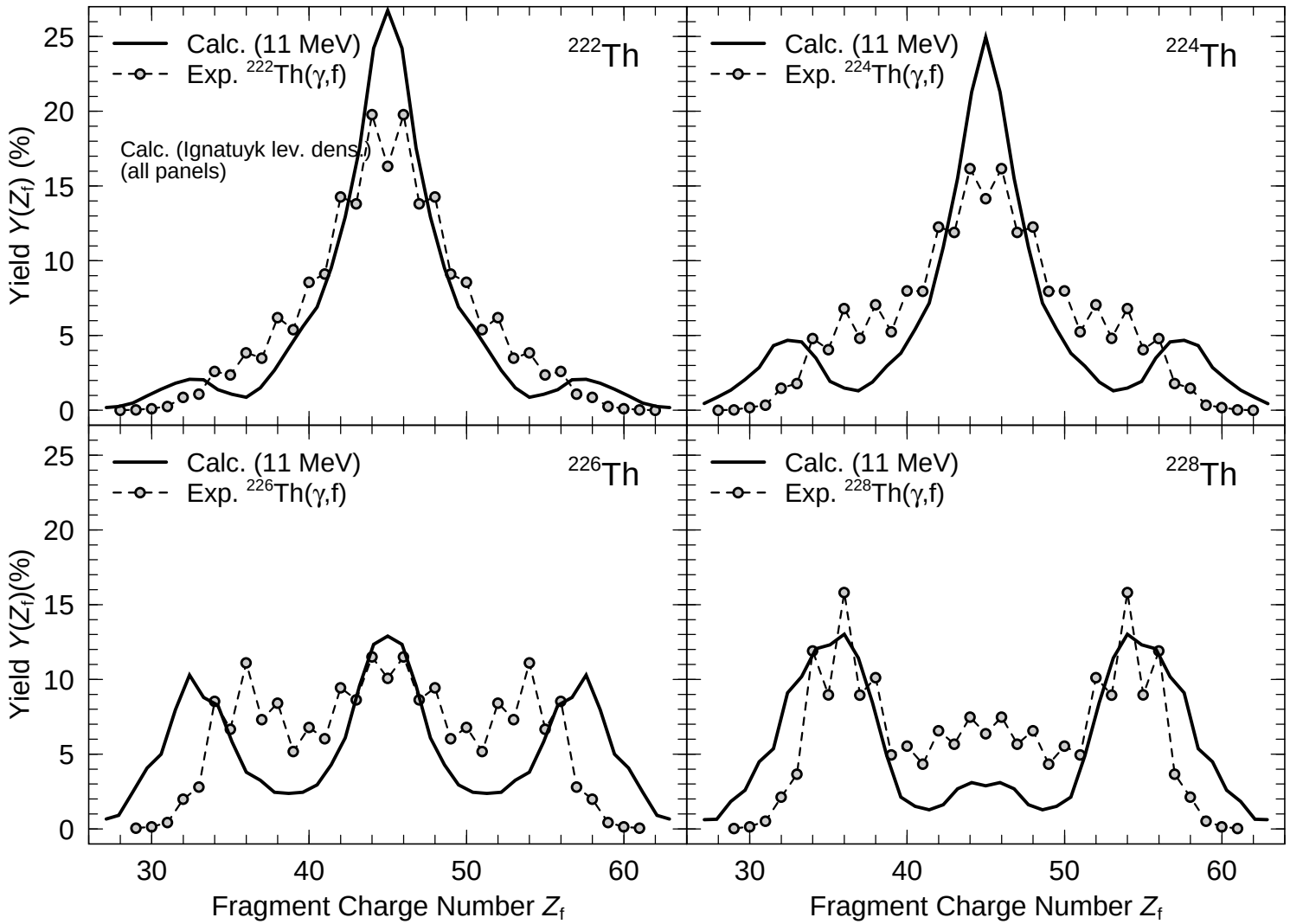
Our calculations of gs properties have over the years yielded data bases that are sufficiently realistic to be useful in many types of simulations (reactor, astrophysics).

Are the calculated potential surfaces realistic far away from the ground-state?

Recent studies of fission yields show they are. In calculations of fission yields based on Brownian-shape-motion and 5D potential-energy surfaces the structure in the calculated yields depends crucially on the calculated structure in the potential-energy surface (Randrup & Möller PRL 106-2011-132503).

The calculations very accurately reproduce the onset of asymmetry versus neutron number for Th isotopes, and, for example, the different widths of the symmetric valley for ^{234}U and ^{240}Pu. (Relative to the PRL we have implemented an improved level density model, PRC-84-2011-034613)


Calc. (6.84 MeV)
Exp. 239Pu(n,f)
240Pu
Calc. (Ignatyuk lev. dens.)
(all panels)
Calc. (6.54 MeV)
Exp. 235U(n,f)
236U
Calc. (6.54 MeV)
Exp. 233U(n,f)
234U
Calc. (11.0 MeV)
Exp. 234U(γ,f)
234U
Yield Y(Zf) (%)
Fragment Charge Number Zf
0
5
10
15
20
25
30
40
50
60


Calc. (11 MeV)
Exp. 222Th(γ,f)
222Th
Calc. (Ignatuyk lev. dens.)
(all panels)
Calc. (11 MeV)
Exp. 224Th(γ,f)
224Th
Calc. (11 MeV)
Exp. 226Th(γ,f)
226Th
Calc. (11 MeV)
Exp. 228Th(γ,f)
228Th
Yield Y(Zf) (%)
Yield Y(Zf)(%)
Fragment Charge Number Zf
Fragment Charge Number Zf
0
5
10
15
20
25
30
40
50
60

S U M M A R Y

- A macroscopic model reproduces binding energies to about 3 MeV. The Strutinsky shell correction method based on a simple single-particle potential (deformed well + spin-orbit force) increases the accuracy to 0.6 MeV, that is 80% of the microscopic effects are obtained in this simple model.

- One remaining issue is what is the origin of remaining correlated fluctuating deviations whose magnitude increases for lighter systems.

- Another observation is that some remaining deviations such as the strengthening of the $N = 56$ subshell near $Z = 40$ cannot be described within the present framework, possible a new term in the s.p. potential will be needed.

- Phenomenological terms, such as the Wigner term need to be described microscopically.

- We expect to release a new mass table FRDM-2012 next year. We are just doing some minor touch-ups to FRDM-2011a.