RIPL-4 update on the mass, nuclear level densities and fission segments in the framework of mean field models

S. Goriely

In collaboration with

- W. Ryssens, G. Grams (ULB)
- S. Hilaire (CEA/DAM/DIF)
- A. Koning (IAEA)

Task 4: Update of the RIPL-3 mass segment

5. Update of RIPL-3 Segments

5.1. Update of the Mass segment (Coord : S. Goriely)

It is proposed to include in RIPL-4:

- AME'16 experimental and recommended masses
- FRDM'12 instead of FRDM'95 (masses and deformations)
- HFB-27 masses and densities instead of HFB-14 (plus deformations)
- D1M masses, deformation and densities
- WS4 masses & deformations (β_2, β_4, β_6)

This proposal will be revisited at each RCM for new possible updates.

→ files prepared and made available at 2d RCM

AME'20 of experimental and recommended masses

→ New updates proposed :

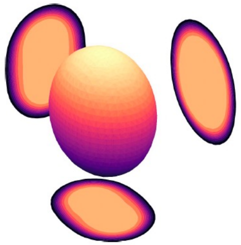
- **HFB: BSkG2 → BSkG3 mass model**
- Others ? (files available)

Brussels-**Sk**yrme-on-a-**G**rid: BSkG

BSkG1: G. Scamps et al., EPJA **57**, 333 (2021).
BSkG2: W. Ryssens et al., EPJA **58**, 246 (2022).
W. Ryssens et al., EPJA **59**, 96 (2023).
BSkG3: G. Grams et al. EPJA 59, 270 (2023)

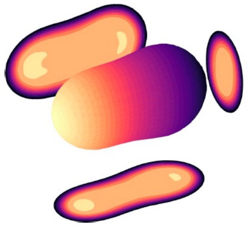
BSkG1 (2021)

- fitted to 2457 masses
- fitted to 884 charge radii
- includes triaxial deformation



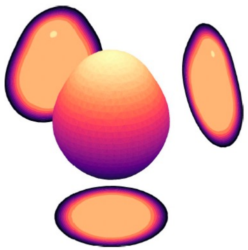
BSkG2 (2022)

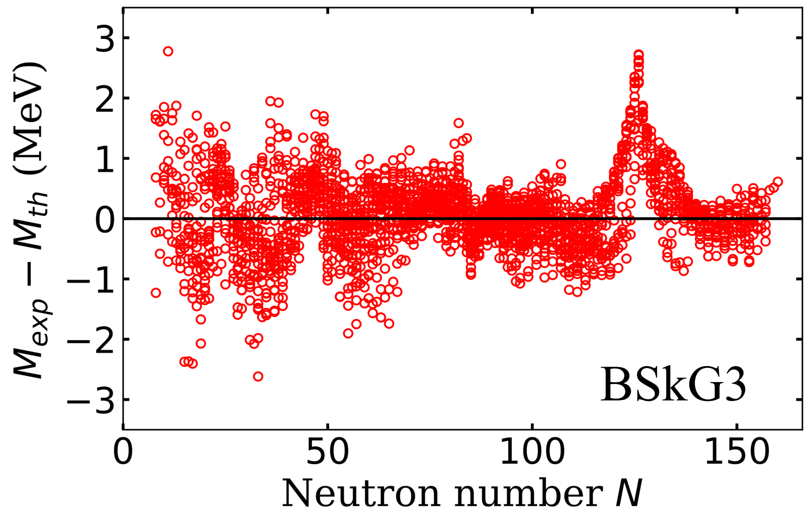
- fitted to 45 fission barriers
- includes spins, currents,...



BSkG3 (2023)

- larger max. neutron star mass
- includes octupole deformation





Rms σ	BSkG1	BSkG2	BSkG3
Masses [MeV]	0.741	0.678	0.631
Radii [fm]	0.024	0.027	0.024
Prim. barriers [MeV]	0.88	0.44	0.33
Secon. barriers [MeV]	0.87	0.47	0.51
Fission isomers [MeV]	1.0	0.49	0.34
Max. NS mass [$M_\odot$]	1.8	1.8	2.3

BSkG3 masses, deformations & densities: new Skyrme-HFB default in TALYS

Also available at: https://http://www.astro.ulb.ac.be/bruslib/nucdata/bskg03-dat

BSkG1 & 2 & 3

G. Scamps, et al. EPJA 57 (2021) 333

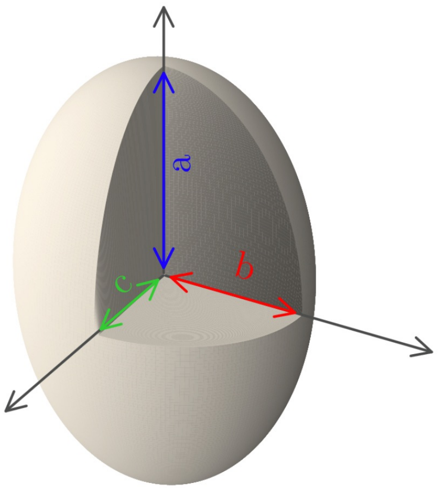
$$E_{\text{tot}} = E_{\text{HFB}} + E_{\text{collective}} \,,$$

- Skyrme + pairing energy
- kinetic energy
- Coulomb energy

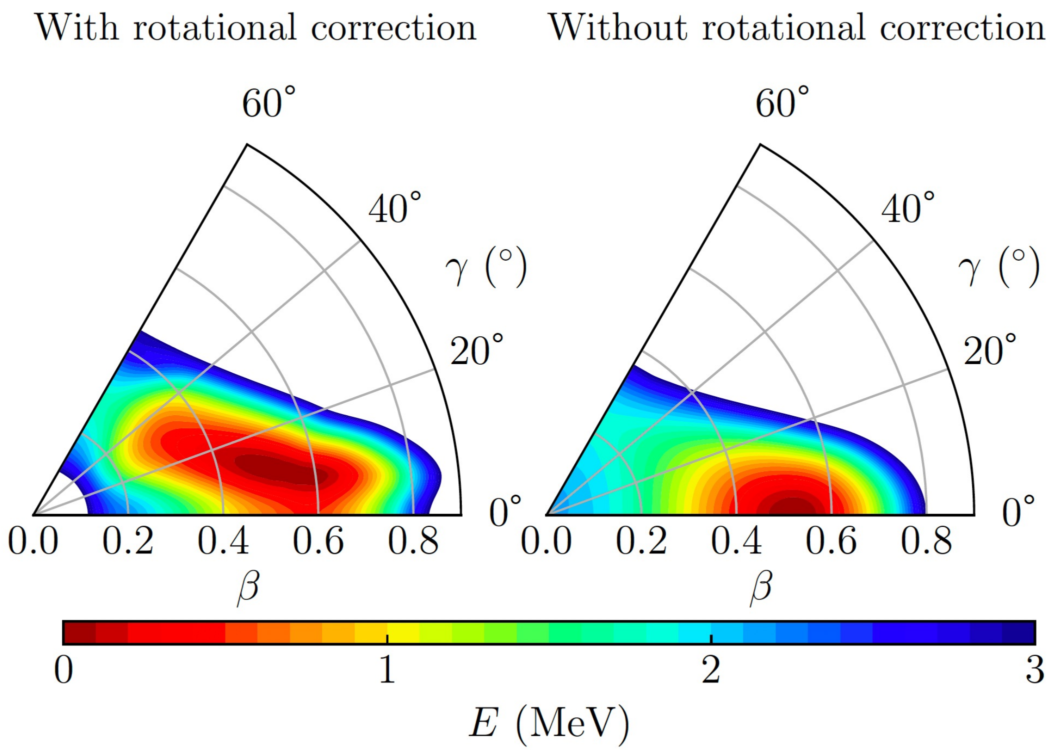
Variational!

- Centre-of-mass correction
- Rotational correction
- Vibrational correction [BSkG 2-3]

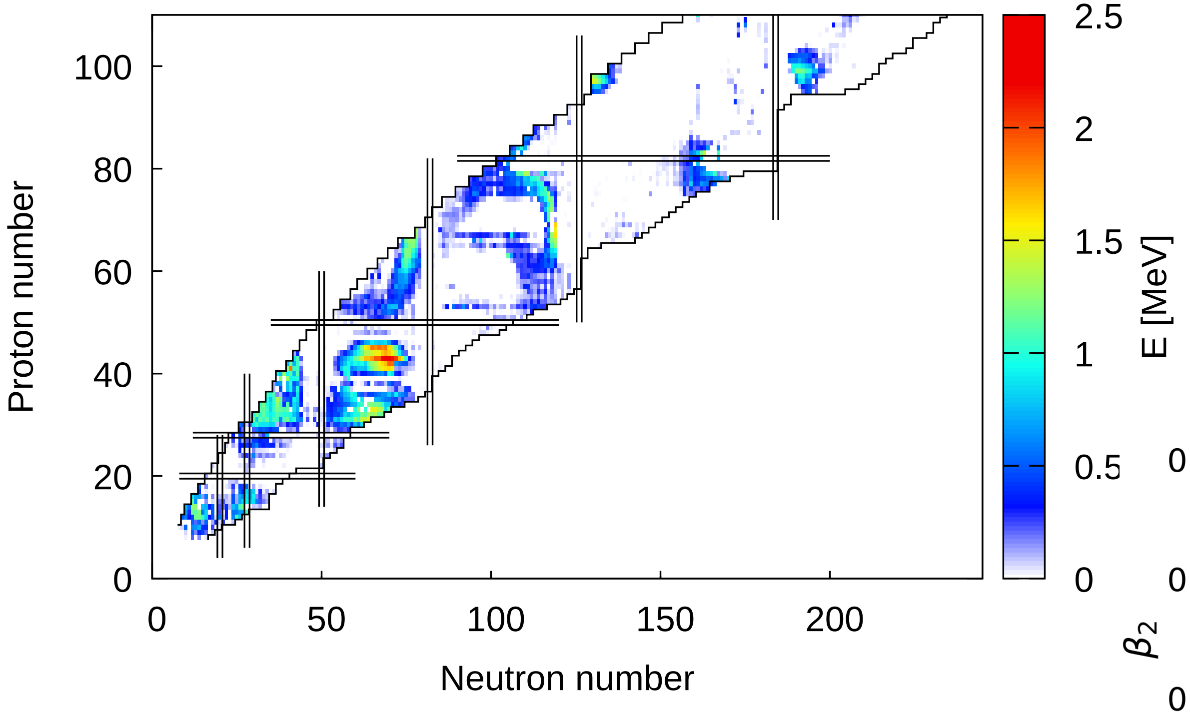
Semi-variational!

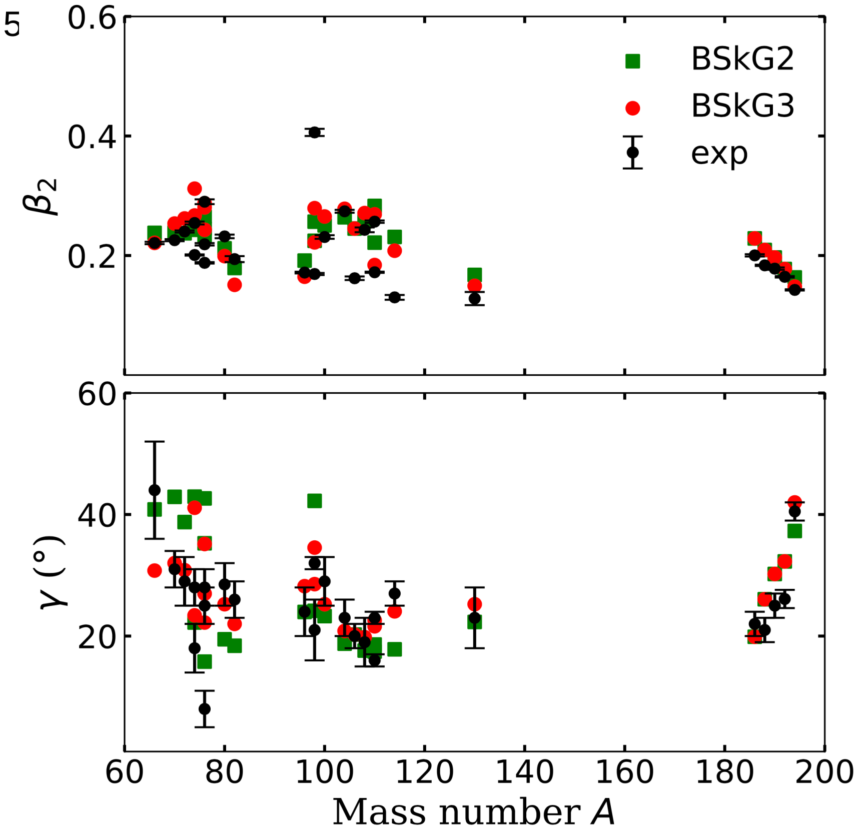


Two DOF: (β_{20}, β_{22}) or (β, γ)



Impact of Triaxiality

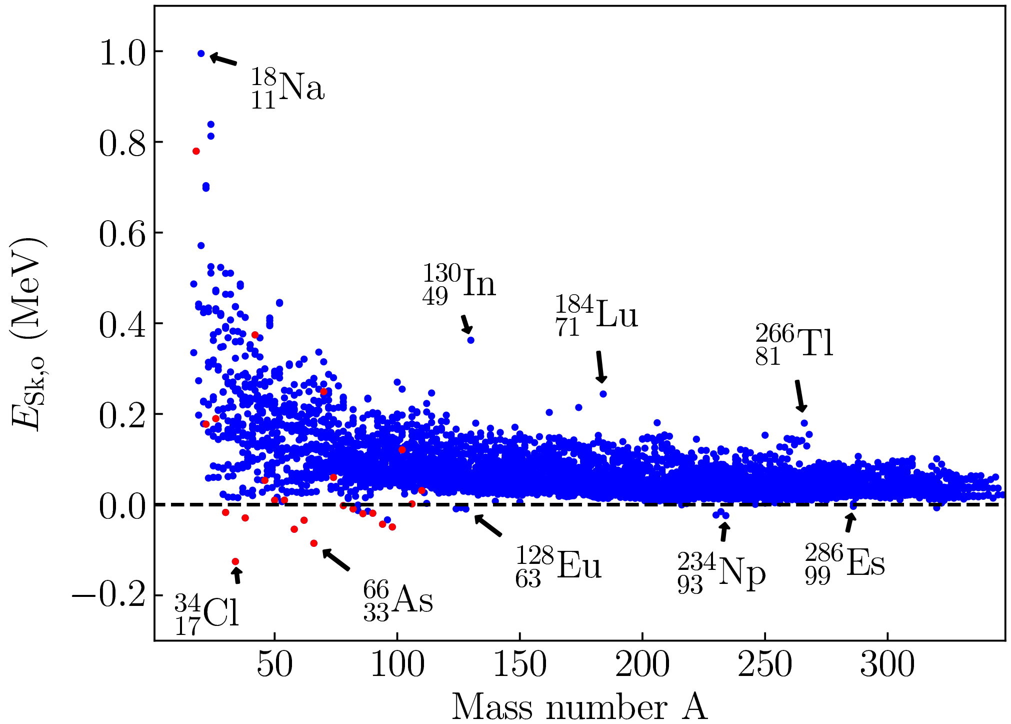




Allows for time-reversal symmetry breaking

Inclusion of ‘time-odd’ terms in the Skyrme EDF instead of Equal Filling Approximation (EFA) as almost all previous models

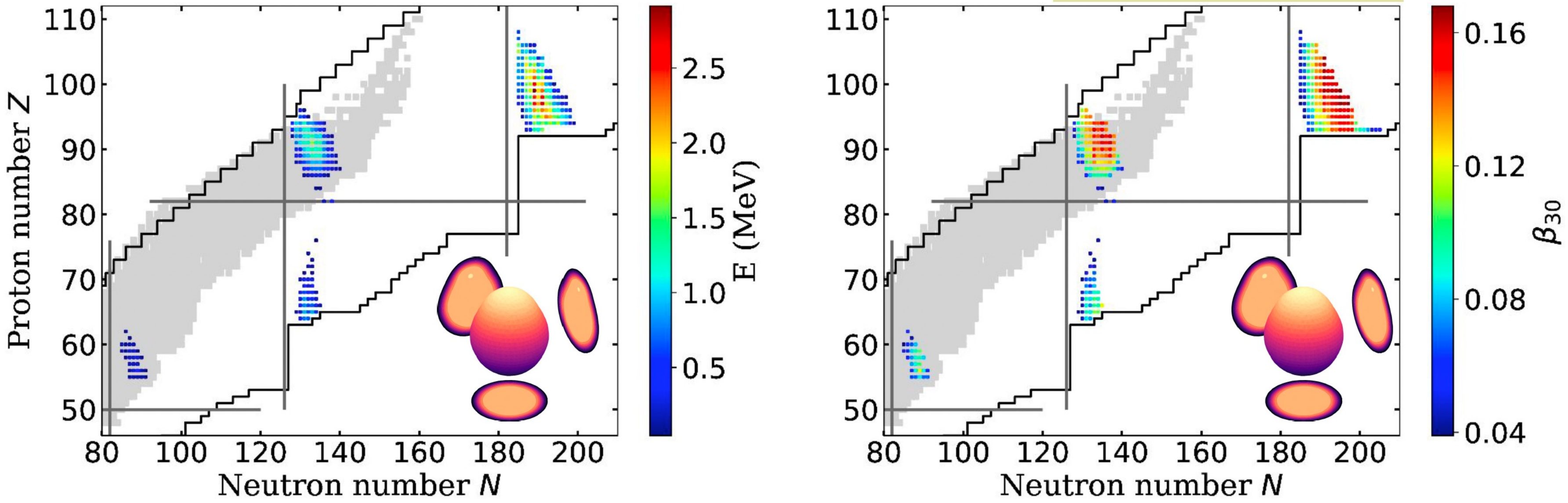
Contributions of time-odd terms to the nuclear masses



- Almost all time-odd energies are positive (repulsive)
- Effect can be negative for *Z*=*N* nuclei (red points: *Z*=*N* nuclei)
- Particularly large effect for light nuclei and just outside shell closures

BSkG3: Inclusion of octupole deformation for GS mass

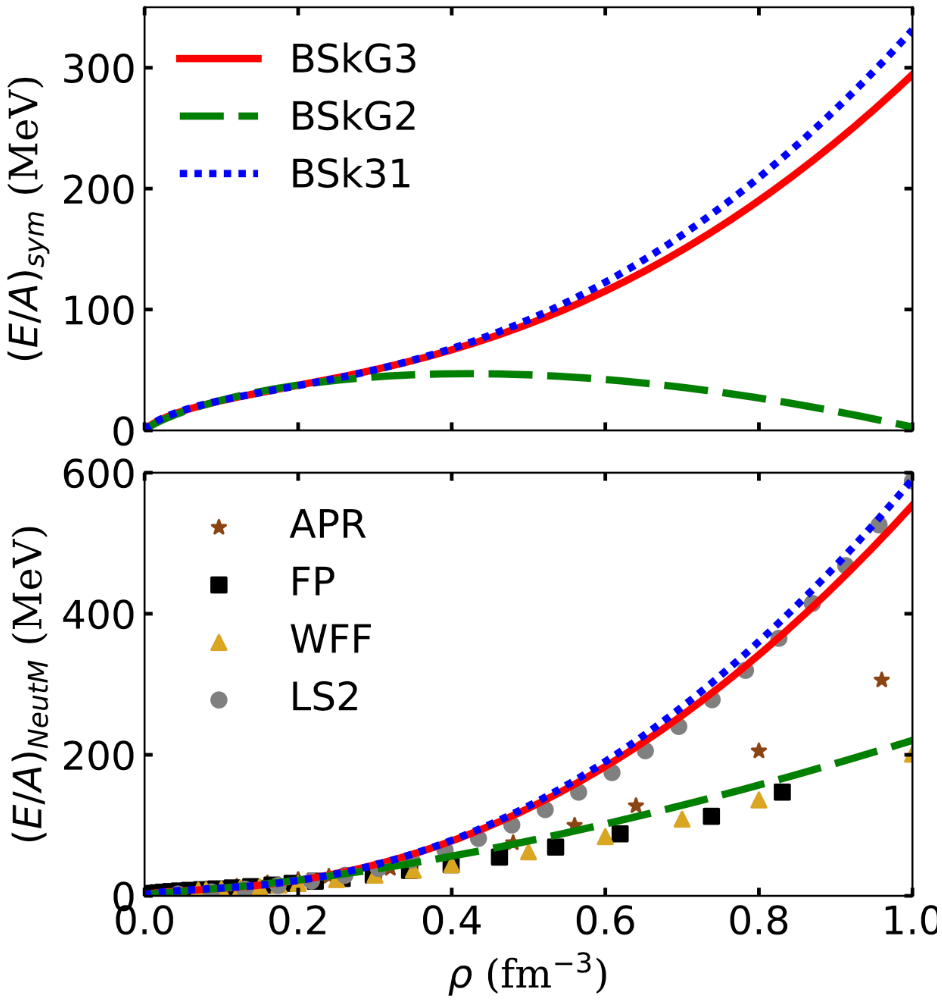
G.Grams, W.R. et al., in preparation.



Reflection asymmetry

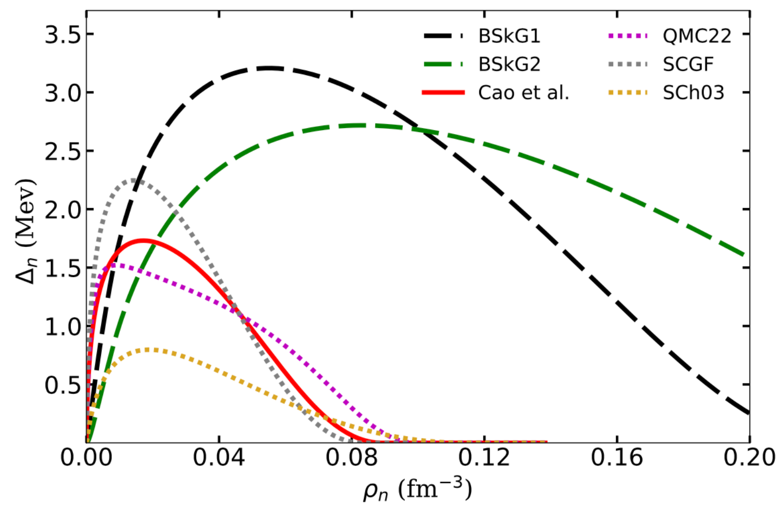
- small number of known nuclei affected
- Near N=184:
  - large effect up to 2.5 MeV
  - dripline modified
  - fission properties modified

BSkG3: Stiffer Equation of State of pure neutron matter & microscopic pairing from ab-initio calculations



Inclusion of t_4 and t_5 terms

BSkG3 reproduces exactly Cao et al. (2006)



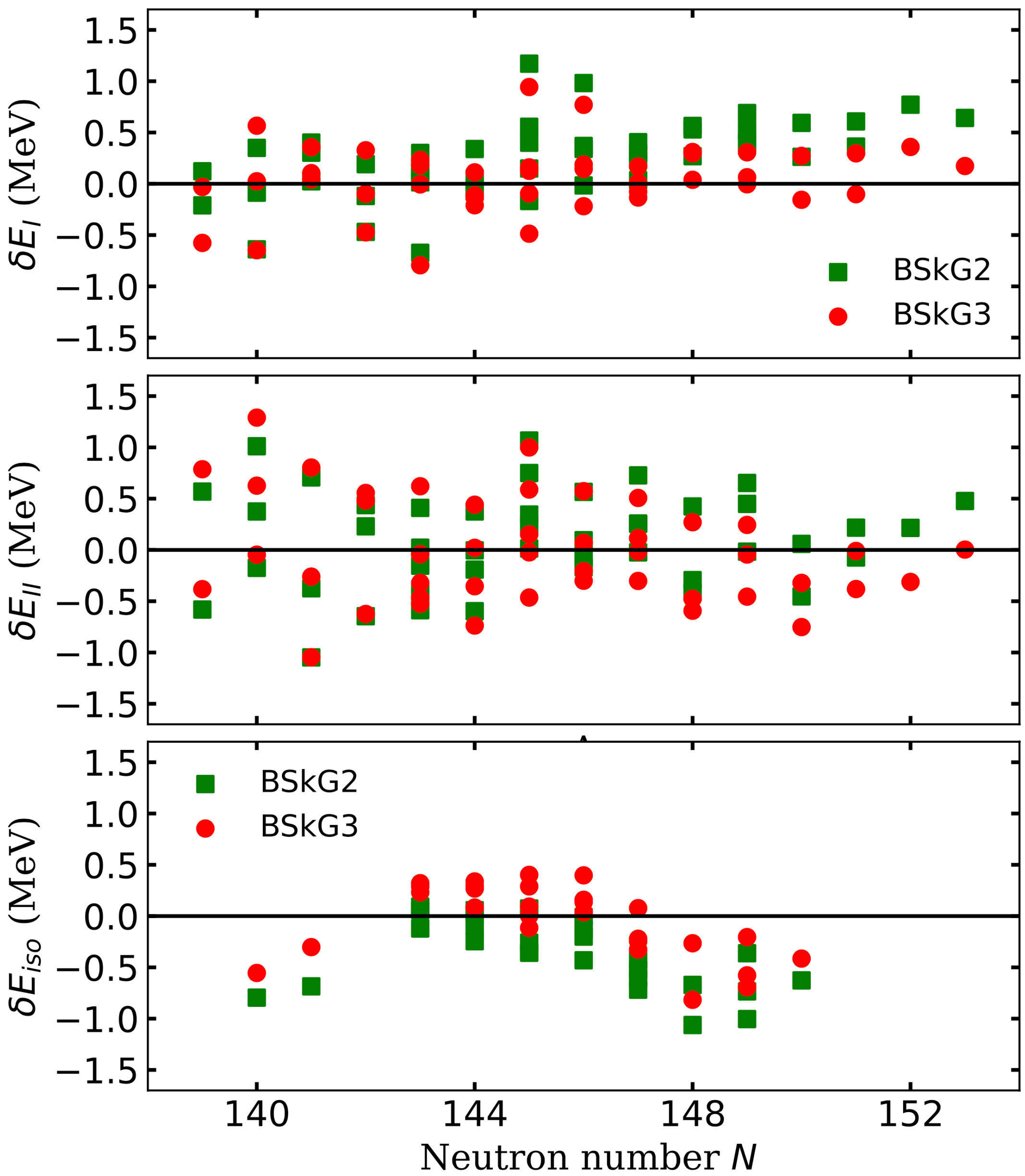
Pairing strength: $g_q(\rho_n,\rho_p) = V_q(\rho_n,\rho_p)\left[1+\kappa_q(\nabla\rho_0)^2\right]$

$$V_q(\rho_n,\rho_p) = -\frac{8\pi^2}{I_q(\rho_n,\rho_p)}\left(\frac{\hbar^2}{2M_q^*(\rho_n,\rho_p)}\right)^{3/2},$$

where

$$I_q = \int_0^{\lambda_q^{\mathrm{INM}}+E_{\mathrm{cut}}} d\xi \frac{\sqrt{\xi}}{\sqrt{(\xi-\mu_q)^2+[\Delta_q^{\mathrm{INM}}(\rho_n,\rho_p)]^2}}$$

BSkG3: Remarkable description of primary fission barriers (σ=0.33MeV)

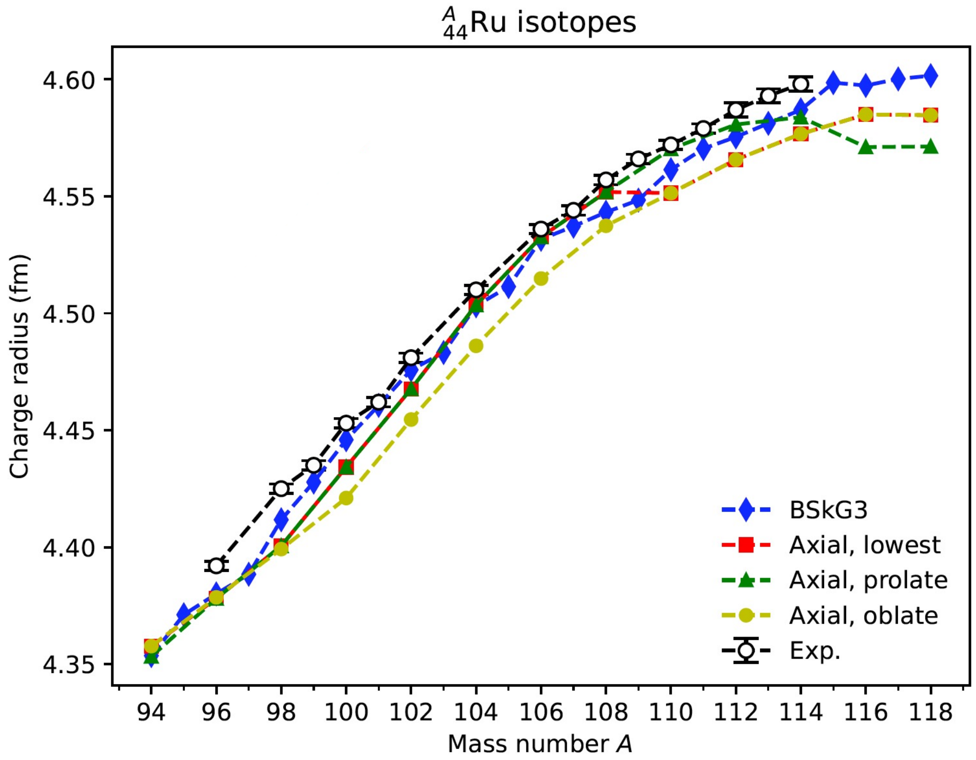


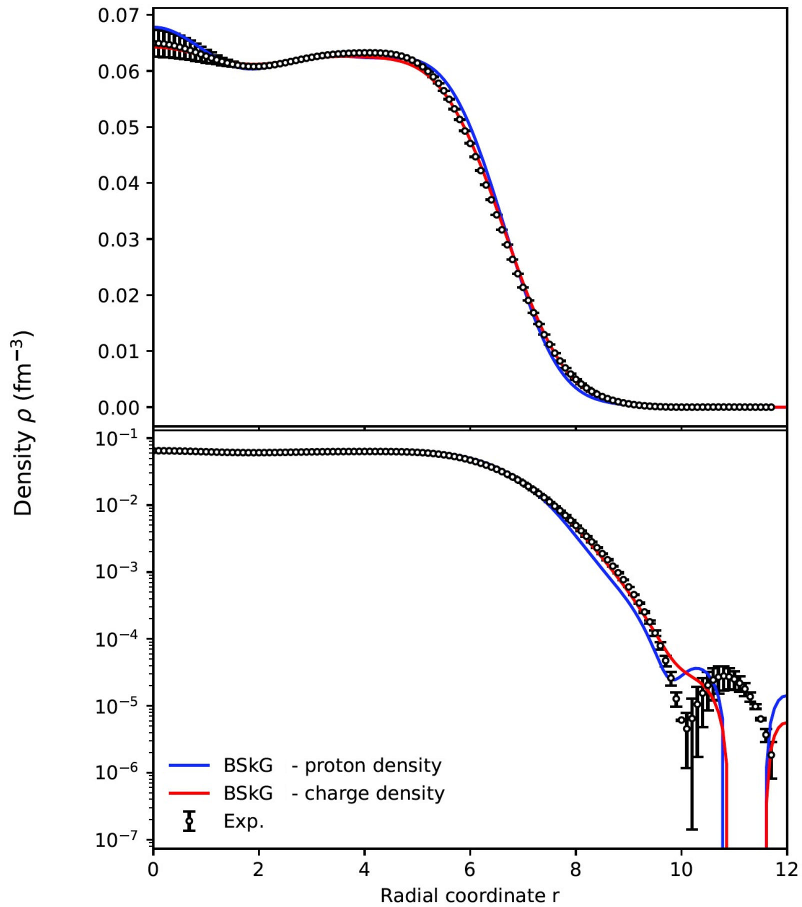
rms deviations on 45 Z>90 nuclei wrt known (RIPL3) fission barriers/wells

	BSkG2	BSkG3
σ(M) [MeV]	0.67	0.63
σ(E_I) [MeV]	0.44	0.33
σ(E_{II}) [MeV]	0.47	0.51
σ(E_{iso}) [MeV]	0.49	0.36

	HFB-14	FR(L)DM
σ(M) [MeV]	0.73	0.56
σ(E_I) [MeV]	0.59	0.76
σ(E_{II}) [MeV]	0.72	--
σ(E_{iso}) [MeV]	0.73	--

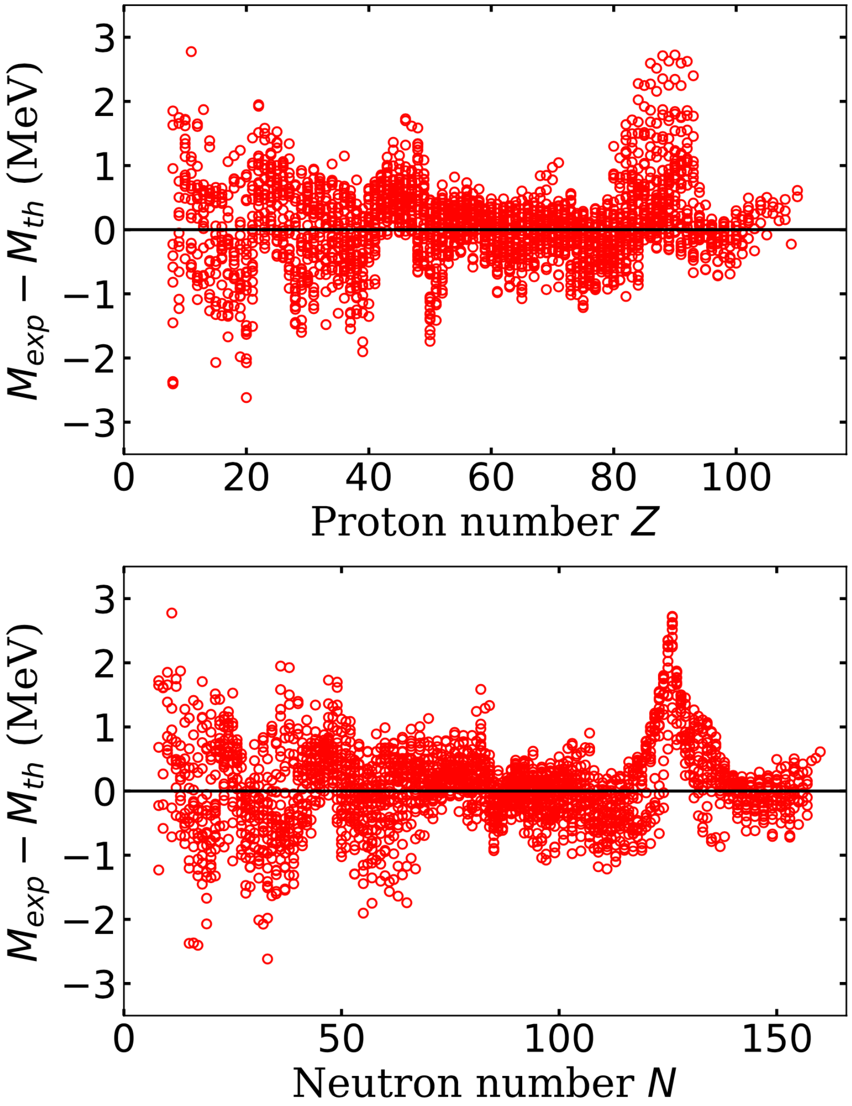
BSkG3: accurate reproduction of charged radii – σ(810 R_c) = 0.237 fm



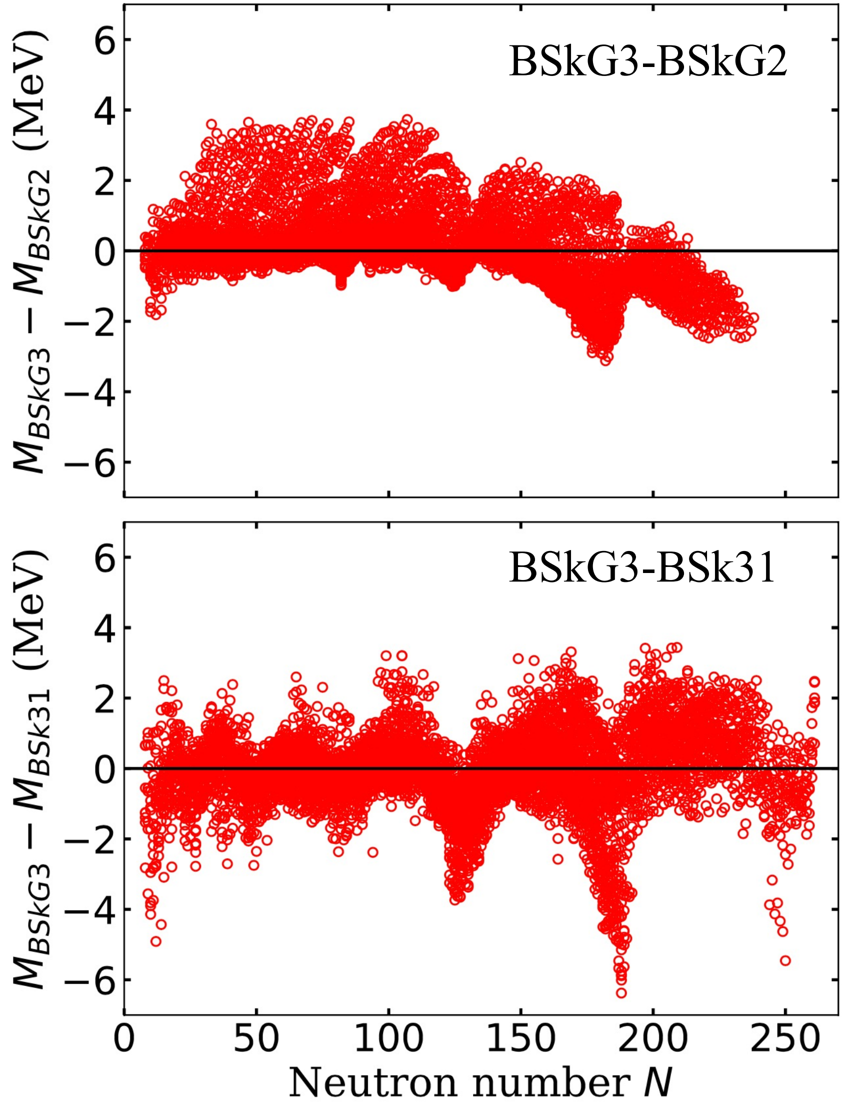


BSkG3 *deformed* densities : new Skyrme-HFB default in TALYS

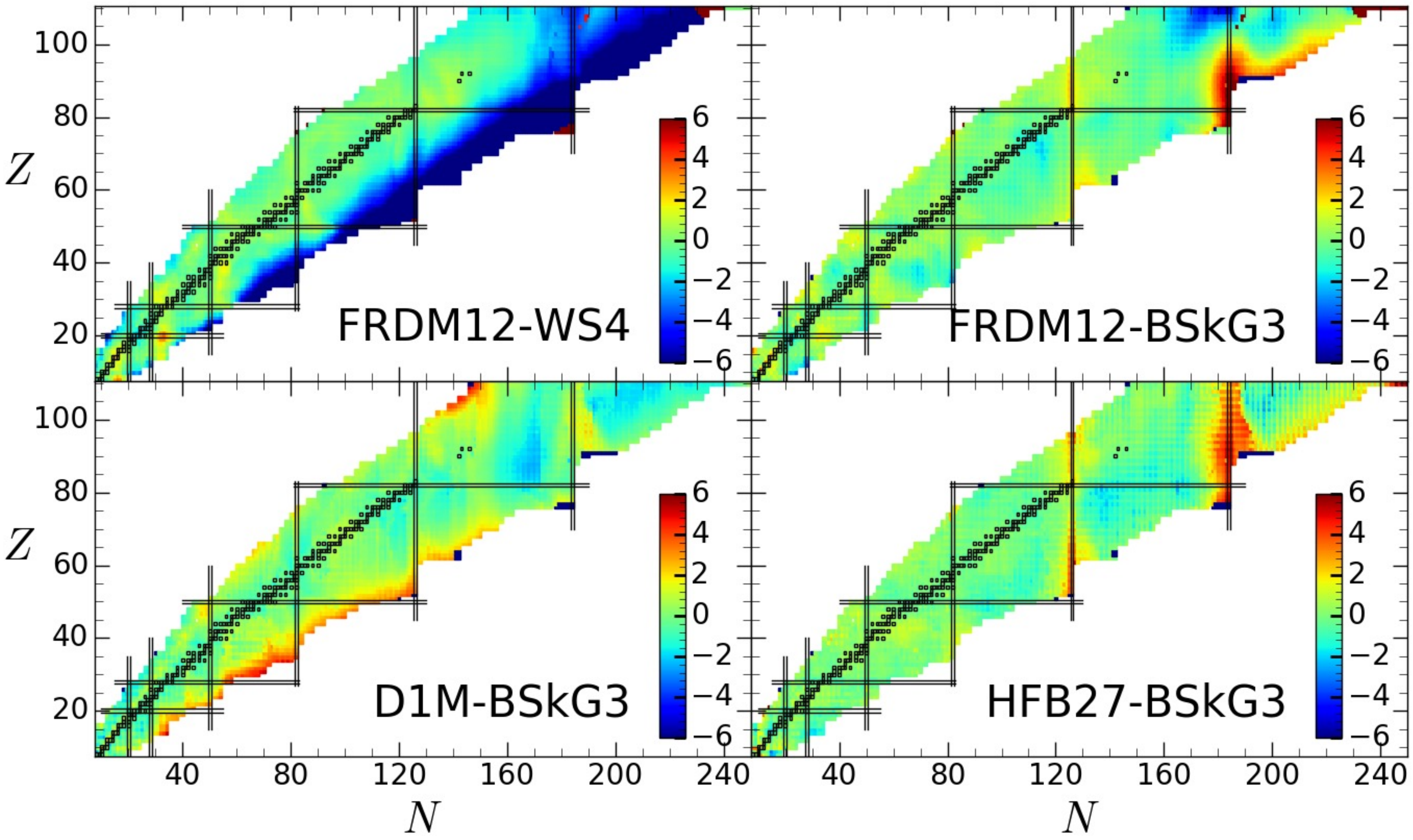
Comparison with experimental masses



Comparison with BSkG2 and BSk31 masses



Differences in mass predictions among various mass models



Nuclear Level densities

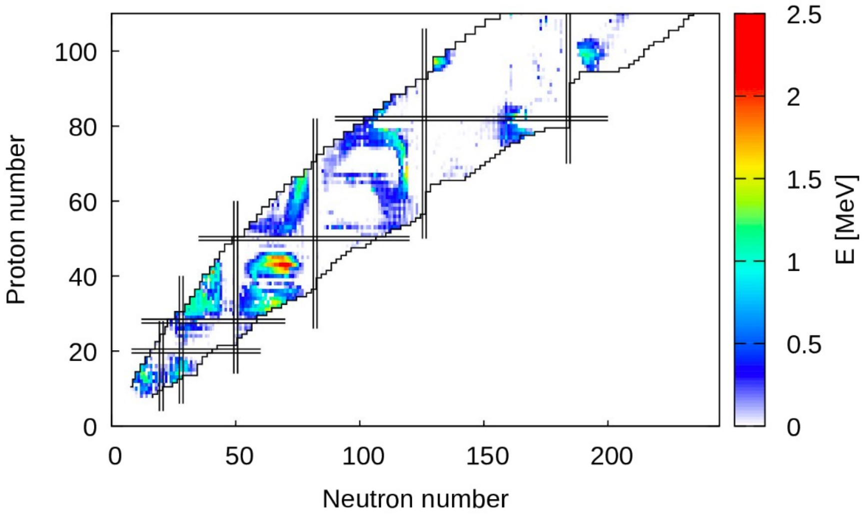
New BSkG3 predictions

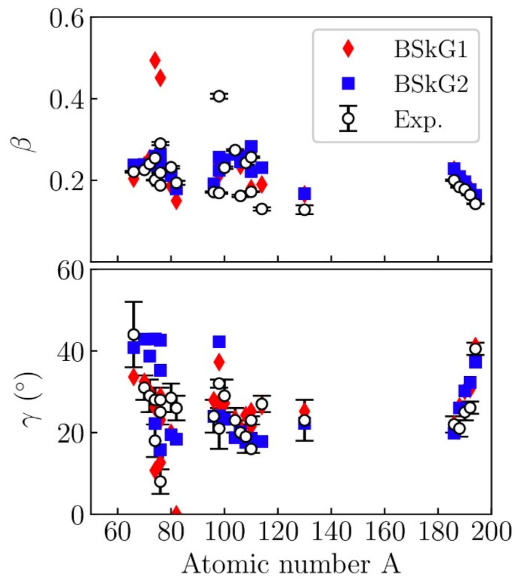
New HFB calculations allowing for triaxial deformations

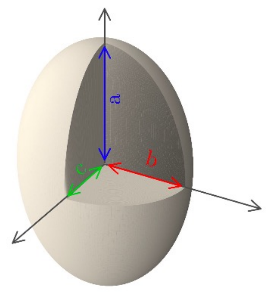
BSkG1-3 interactions (MOCCa code: Ryssens et al. 2021-2023): σ(M)~0.74-0.63 MeV

Wouter Ryssens (ULB)

Triaxial deformation







Two DOF: (β_{20}, β_{22}) or (β, γ)

Energy gain by triaxial deformation

- Many nuclei gain **0.5-2.5** MeV
- Highest gains for Z~43 (Rh)

Rotational invariants

All refs in G. Scamps et al., EPJA 57, 333 (2021).

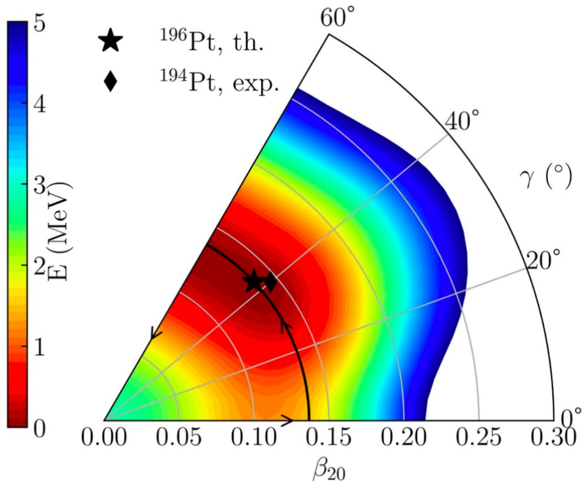
- obtained from COULEX
- data compiled by M. Zielińska

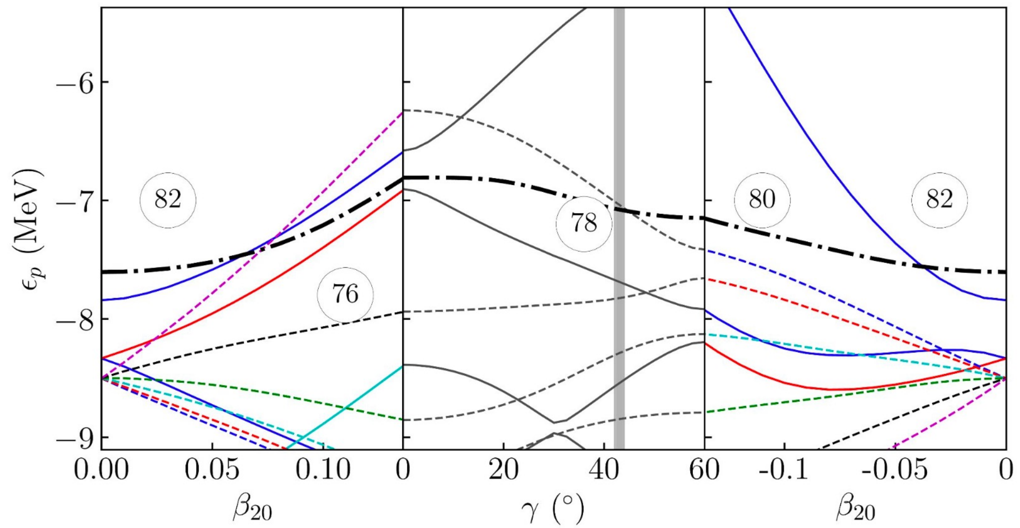
New NLD calculations allowing for triaxial deformations

BSkG1-3 interactions (MOCCa code: Ryssens et al. 2021-2023): σ(M)~0.74-0.63 MeV

NLDs for triaxial nuclei: ^{196}Pt

Wouter Ryssens (ULB)





Single-particle aspects

- Even lower single-particle density
- Lower intrinsic level density
- No more *K* quantum numbers

$$\bar{K} = \frac{1}{2}\lfloor 2\langle \hat{J}_\mu \rangle \rceil$$

where *μ*=*x*=*y*=*z* is the principal axis of the nucleus in the intrinsic frame with the lowest Belyaev moment of inertia.

→ “round to the nearest half-integer”, and reduces to the *K* quantum number in the case of axial symmetry

New NLD calculations allowing for triaxial deformations

BSkG1-3 interactions (MOCCa code: Ryssens et al. 2021-2023): σ(M)~0.74-0.63 MeV

BSkG3 + Combinatorial model

NLDs for triaxial nuclei: ^{196}Pt

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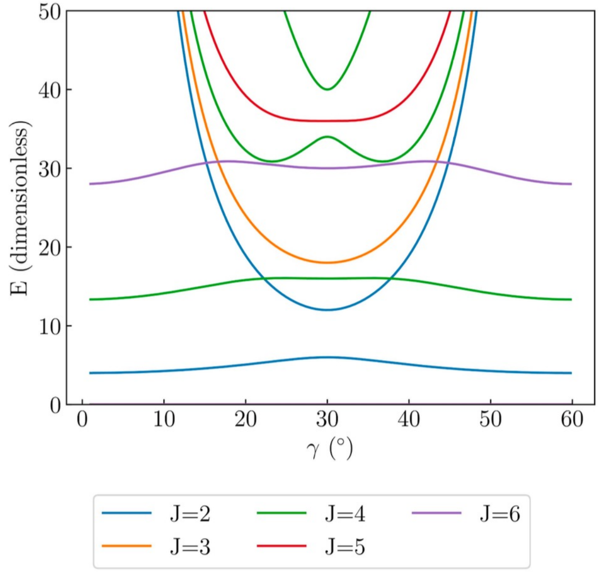
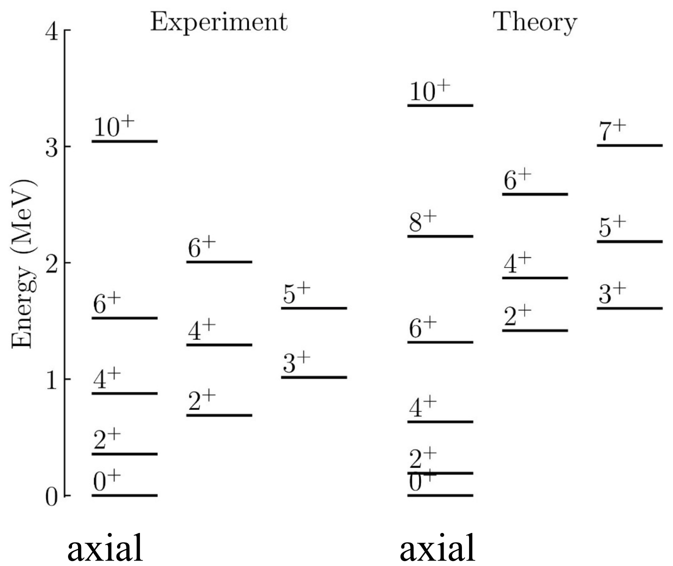




Rotational enhancement

- rigid rotor modelling
  - **three** moments of inertia
  - requires a small diagonalization
- results in (at same excitation)
  - **more states**
  - **more extended spin distribution**

$$\hat{H}_{\mathrm{rot}} = \sum_{\mu=x,y,z} \frac{\hat{J}_\mu^2}{2\mathcal{I}_\mu}$$

$$J = J_{\mathrm{rot}} + \bar{K}$$

Exp.: NNDC.

New NLD calculations allowing for triaxial deformations

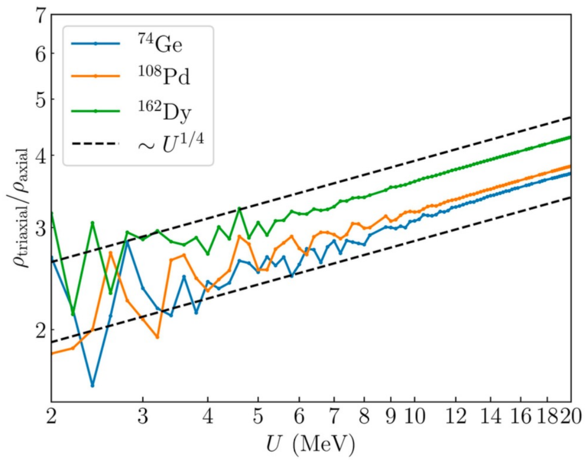
BSkG1-3 interactions (MOCCa code: Ryssens et al. 2021-2023): σ(M)~0.74-0.63 MeV

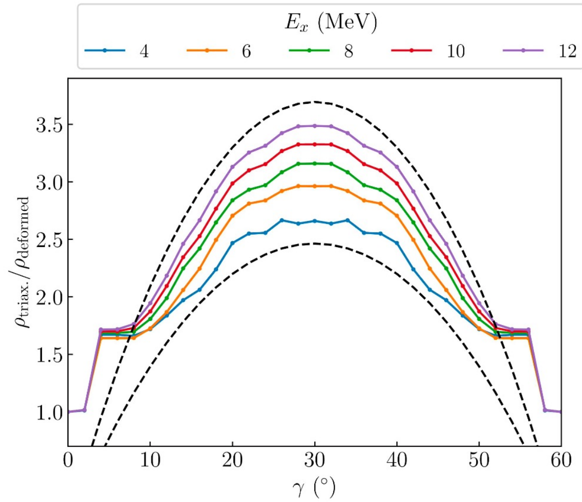
$$\rho(E_X, J, P) = \frac{1}{2} \sum_{\bar{K}=-J}^{J} \sum_{i=1}^{n^{J,\bar{K}}} \rho\left(E_X - E_i^{J,\bar{K}}, P\right)$$

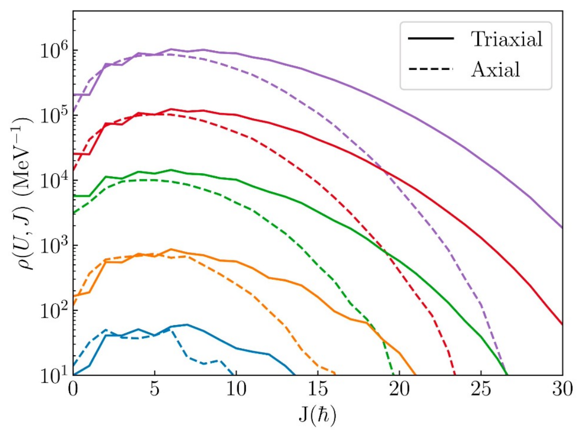
$$n^{J,\bar{K}} = \begin{cases} J_{\rm rot}+1 & \text{if } J_{\rm rot} \text{ is even, and } \bar{K} \neq 0, \\ J_{\rm rot} & \text{if } J_{\rm rot} \text{ is odd, and } \bar{K} \neq 0, \\ J_{\rm rot}/2+1 & \text{if } J_{\rm rot} \text{ is even, and } \bar{K} = 0, \\ (J_{\rm rot}-1)/2 & \text{if } J_{\rm rot} \text{ is odd, and } \bar{K} = 0. \end{cases}$$

Wouter Ryssens (ULB)

Collective enhancement for triaxial nuclei







Expectations

- from analytical models:

$$\frac{\rho_{\rm triaxial}}{\rho_{\rm axial}} \sim \frac{\sqrt{\mathcal{I}_x \mathcal{I}_y \mathcal{I}_z}}{\mathcal{I}_\perp} U^{1/4}$$

- wider spin distributions

New NLD calculations allowing for triaxial deformations

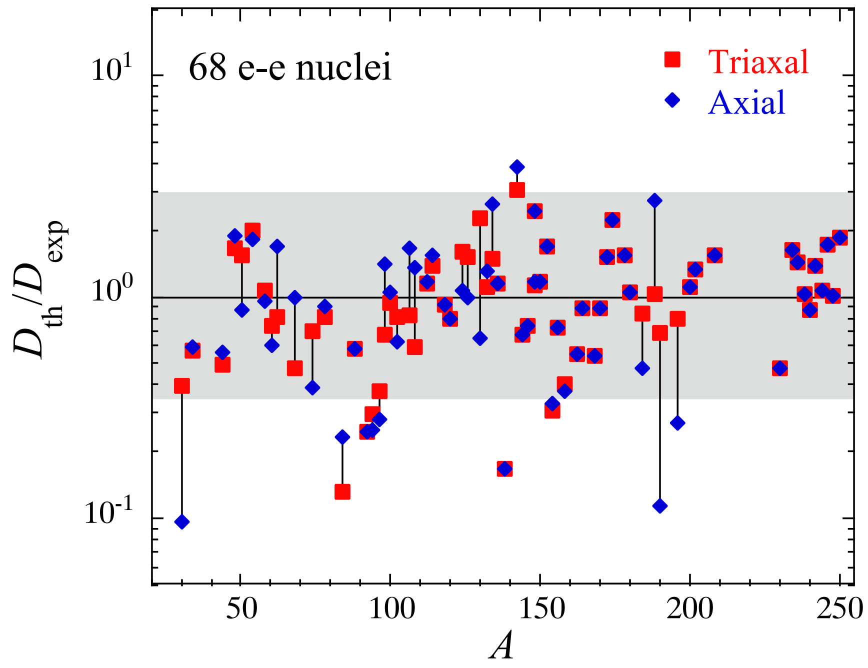
BSkG1-3 interactions (MOCCa code: Ryssens et al. 2021-2023): σ(M)~0.74-0.63 MeV

Wouter Ryssens (ULB)

Performance on mean s-wave spacings

$$f_{\rm rms} = \exp\left[\frac{1}{N_e}\sum_{i=1}^{N_e}\ln^2\frac{D^i_{\rm th}}{D^i_{\rm exp}}\right]^{1/2},$$

	f_{rms}
BSkG2 (triaxial)	**1.83**
BSkG2 (axial)	**2.13**
BSFG	1.80
HFB+comb	2.30
THFB+comb	2.70



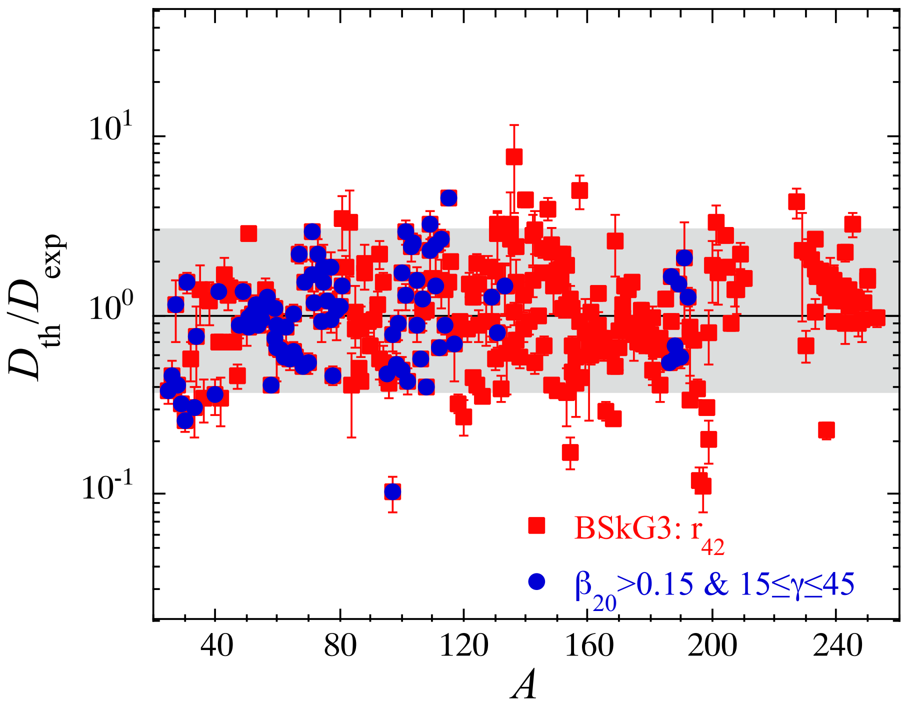
HFB+comb: S. Goriely, S. Hilaire and A. J. Koning, PRC 78, 064307 (2008).
THFB+comb: S. Hilaire, M. Girod, S. Goriely and A. J. Koning, PRC 86, 064317 (2012).
BSFG: A.J. Koning, S. Hilaire and S. Goriely, NPA810, 13-76 (2008).
Exp. data : NNDC and F. Giacoppo, PRC ***90***, 054330 (2014).

New NLD calculations allowing for triaxial deformations

BSkG1-3 interactions (MOCCa code: Ryssens et al. 2021-2023): σ(M)~0.74-0.63 MeV

299 nuclei: $f_{\rm rms}$ =1.74 including errors
=1.96 excluding errors

$$f_{\rm rms} = \exp\left[\frac{1}{N_e}\sum_{i=1}^{N_e}\ln^2\frac{D^i_{\rm th}}{D^i_{\rm exp}}\right]^{1/2}$$



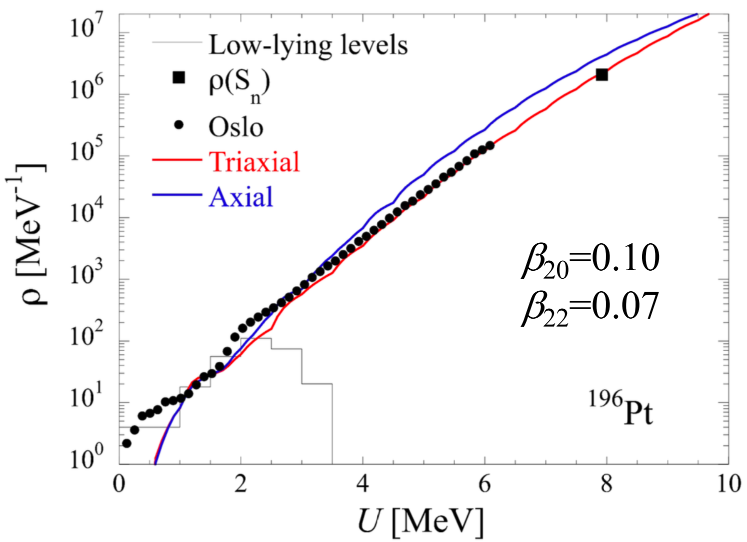
Tables ready for use: only need renormalisation coefficients (α,δ) on experimental $D_{\rm exp}$

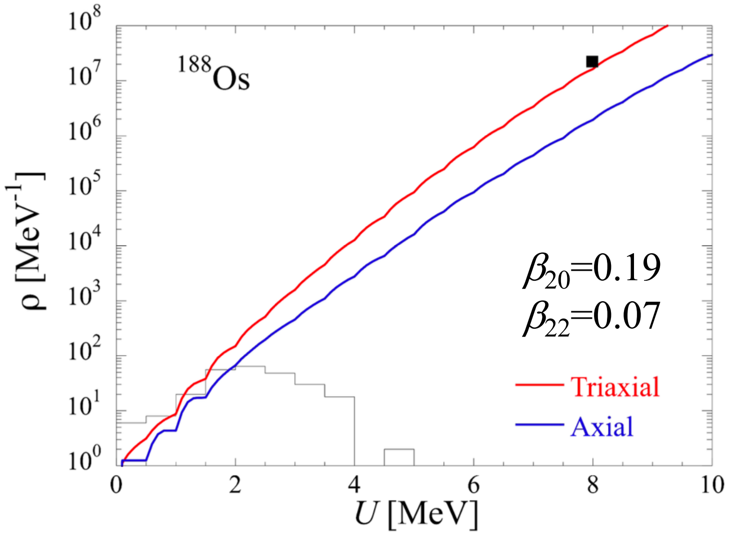
$$\rho_{\rm renorm}(U) = e^{\alpha\sqrt{(U-\delta)}}\rho_{\rm global}(U-\delta)$$

Comparison of BSkG3+Combinatorial NLD with Oslo data

The effect of triaxiality

Wouter Ryssens (ULB)





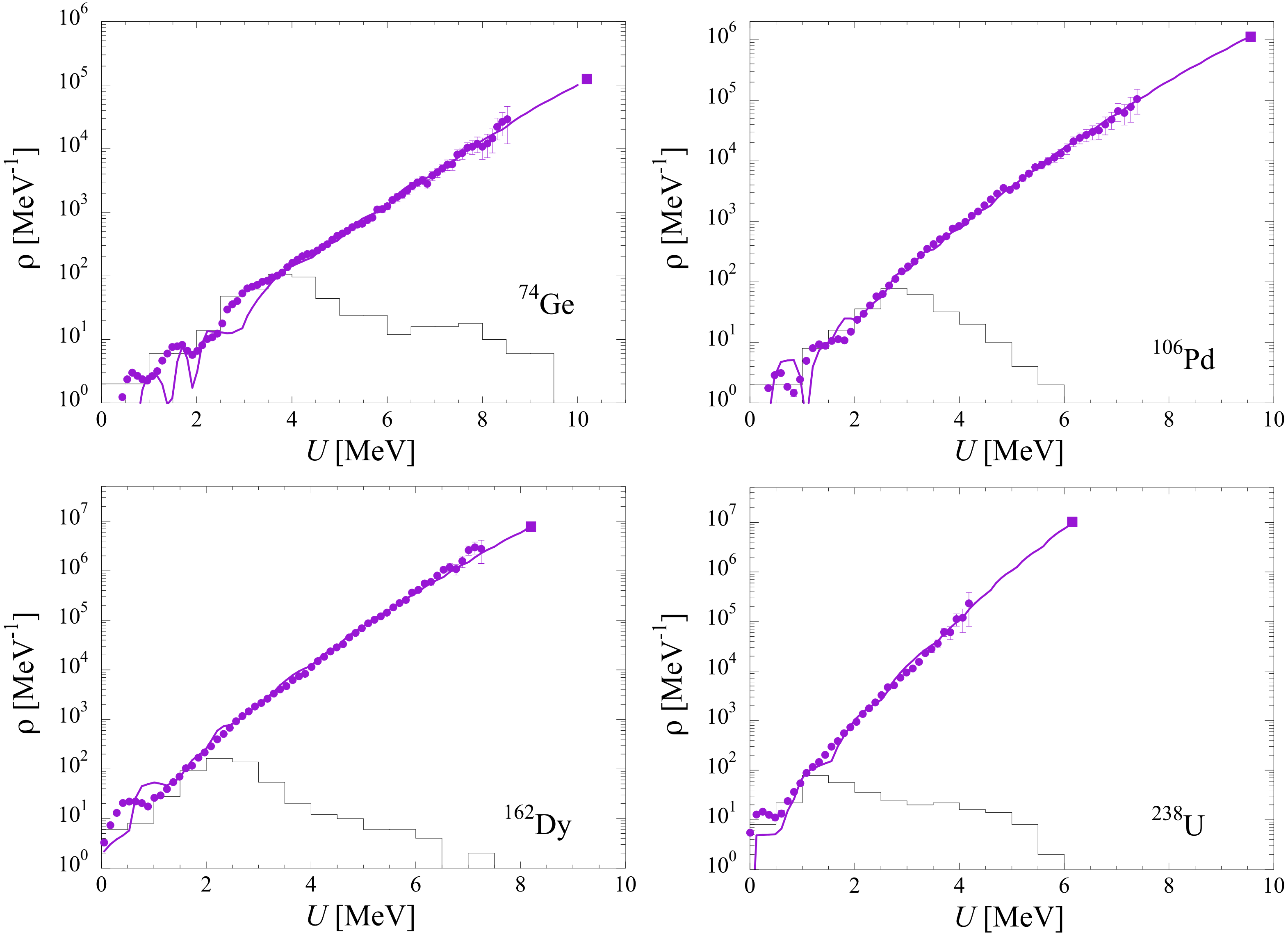
- lower intrinsic NLD
- modest deformation and MOI

Lower overall level density
with a different **U-dependence**

- lower intrinsic NLD
- large deformation and MOI

Larger overall level density
with a different **U-dependence**

Comparison of BSkG3+Combinatorial NLD with Oslo data



Fission properties

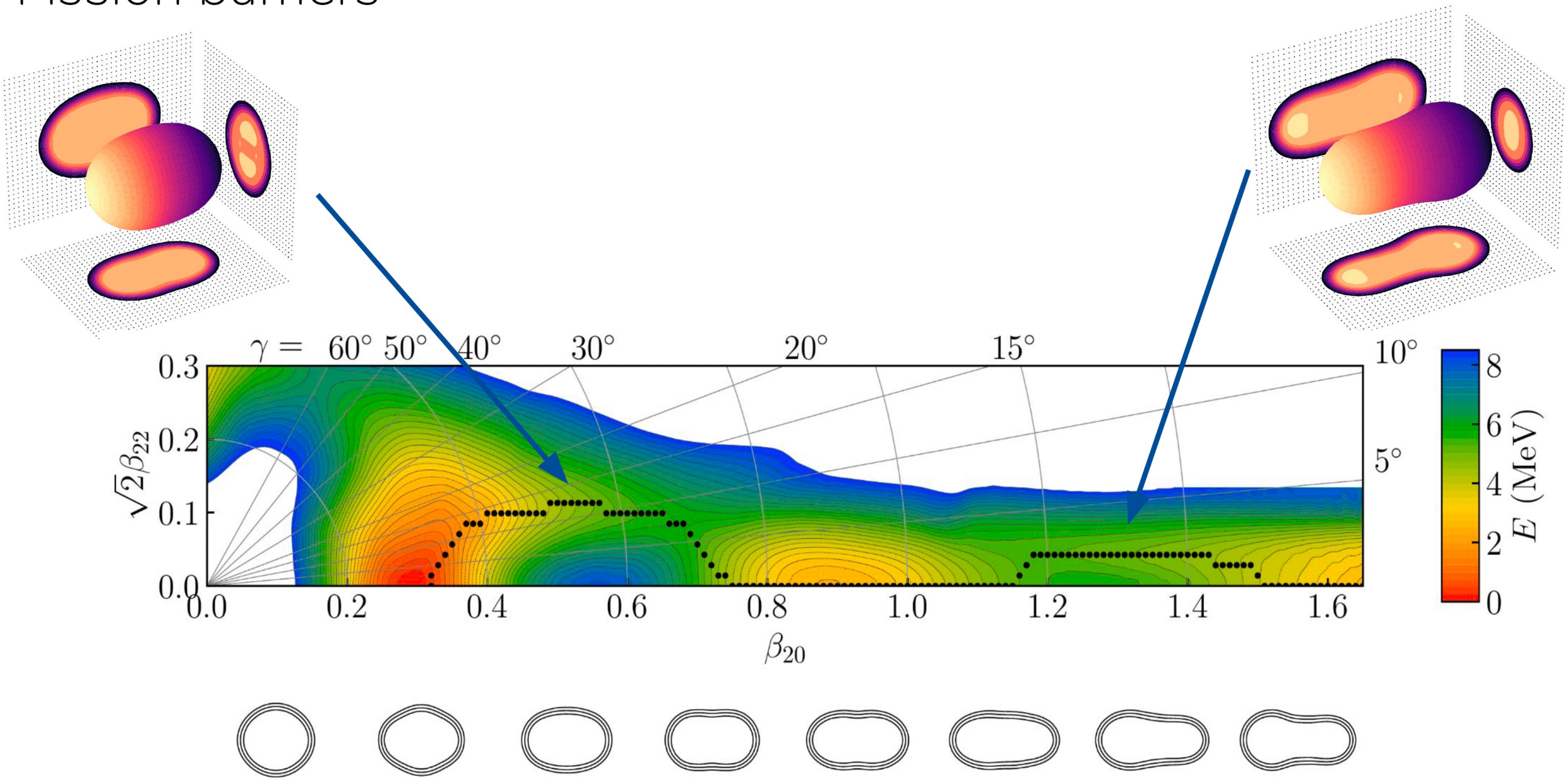
- New BSkG3 predictions

BSkG3 fission paths

Degrees of freedom: β_{20}, β_{22}, β_{30}

W. R. et al., EPJA **59**, 96 (2023).

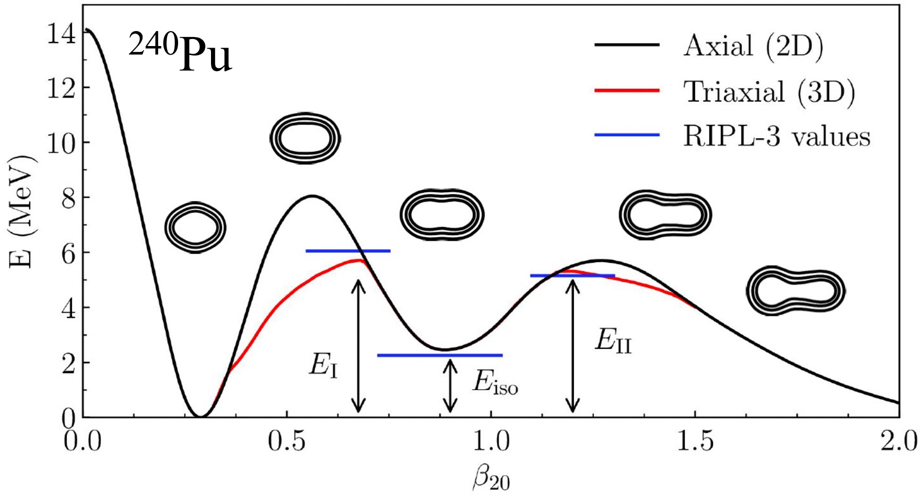
Fission barriers



BSkG3 fission paths

Fission

W. R. et al., EPJA **59**, 96 (2023).



Rms σ	BSkG1	BSkG2	BSkG3
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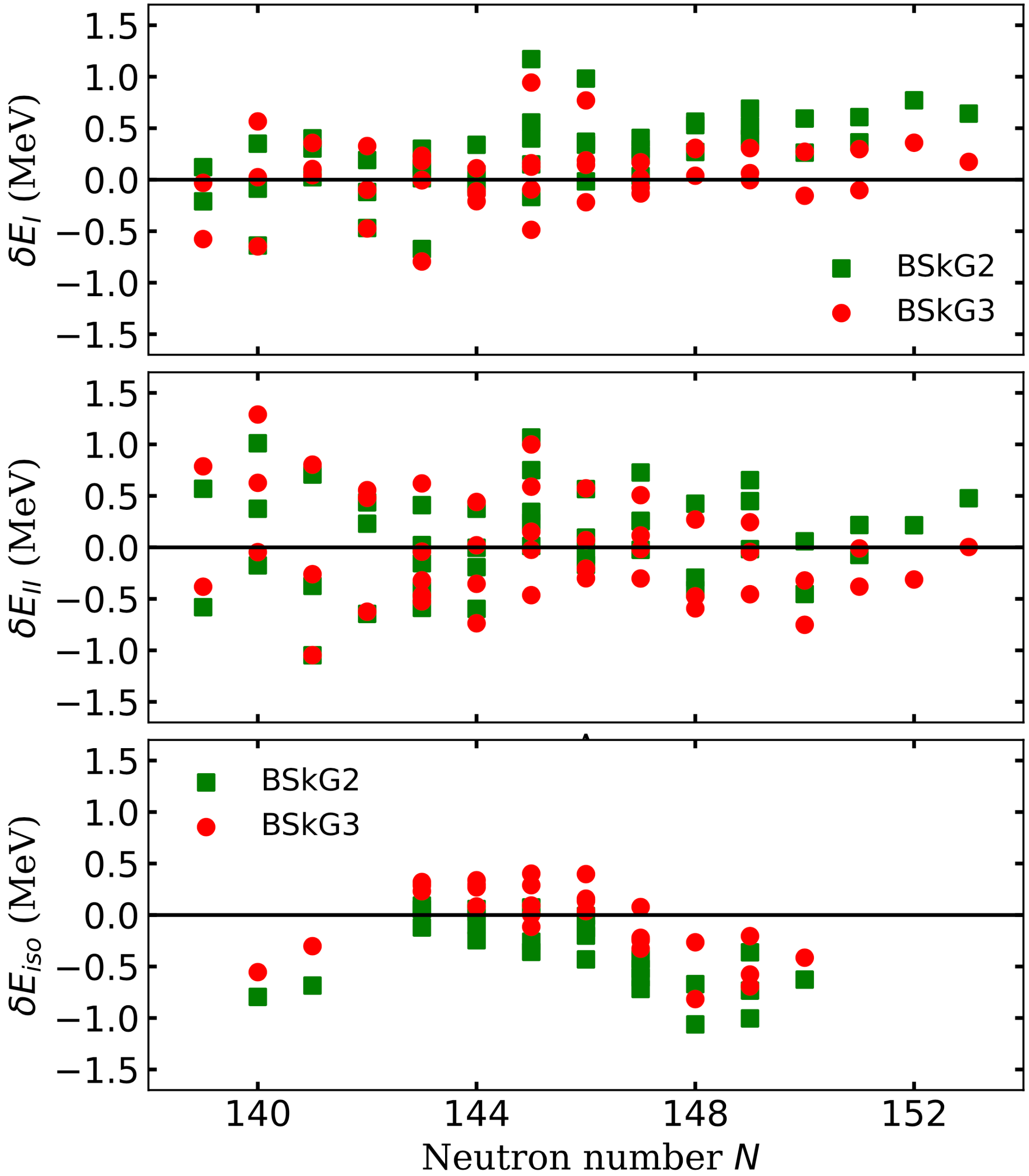
Max. NS mass [$M_\odot$]	1.8	1.8	2.3

Fission properties of 45 actinide nuclei

- includes odd-A and odd-odds
- **all** inner barriers exploit triaxiality
- **all** outer barriers exploit
  - octupole deformation
  - triaxial deformation

BSkG3: Remarkable description of primary fission barriers (σ=0.33MeV)



rms deviations on 45 Z>90 nuclei wrt known (RIPL3) fission barriers/wells

	BSkG2	BSkG3
σ(M) [MeV]	0.67	0.63
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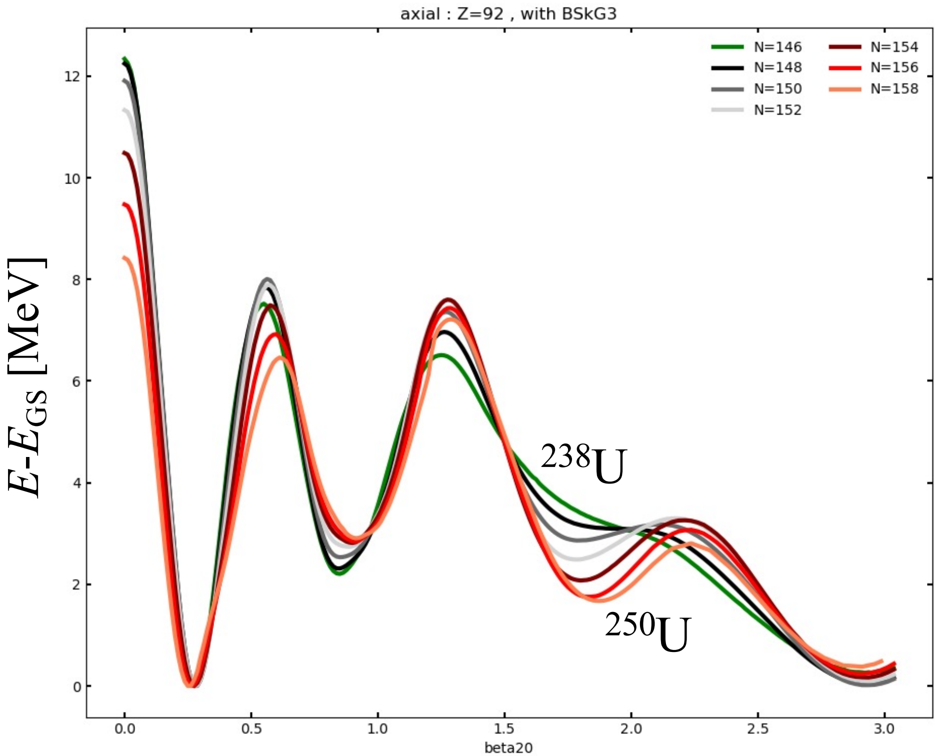
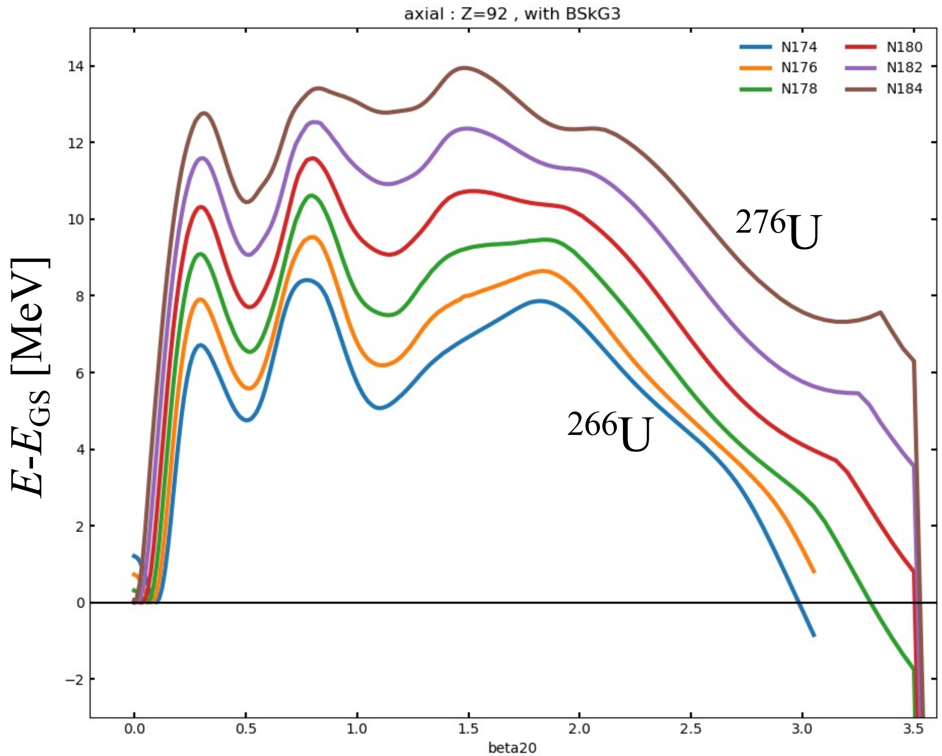
	HFB-14	FR(L)DM
σ(M) [MeV]	0.73	0.56
σ(E_{I}) [MeV]	0.59	0.76
σ(E_{II}) [MeV]	0.72	--
σ(E_{iso}) [MeV]	0.73	--

Extraction of the BSkG3 1D Lowest Energy Paths

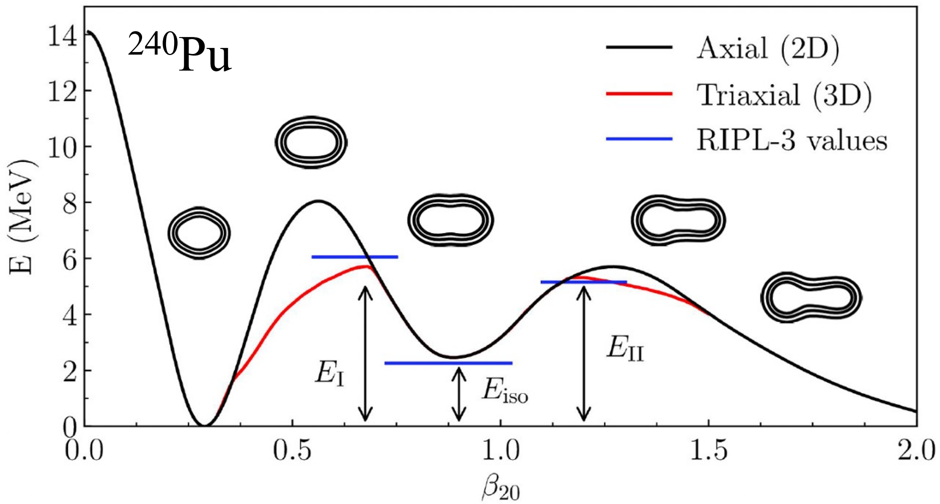
Axial (β_{20},β_{30}) paths





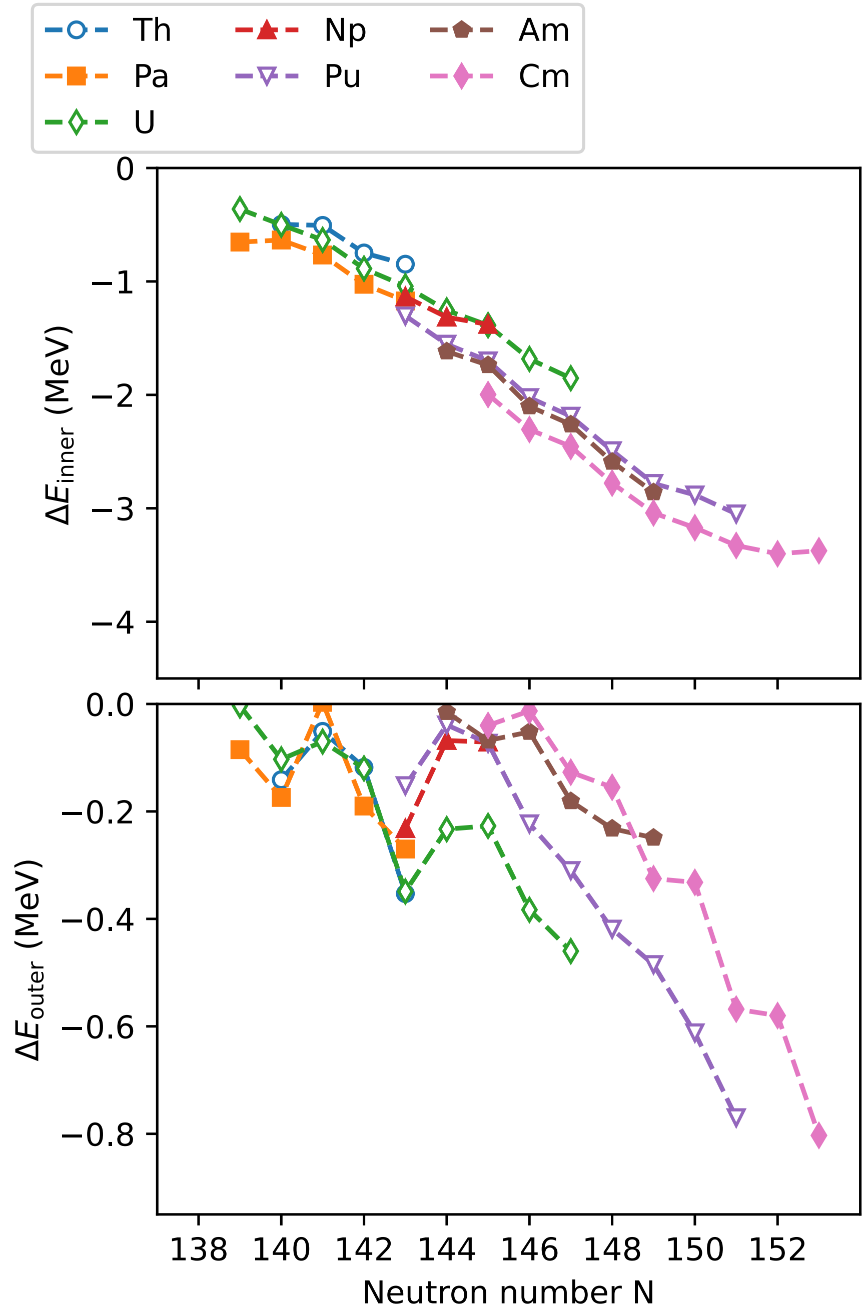
Effects of triaxiality on ***both***

- Triaxial inner barrier



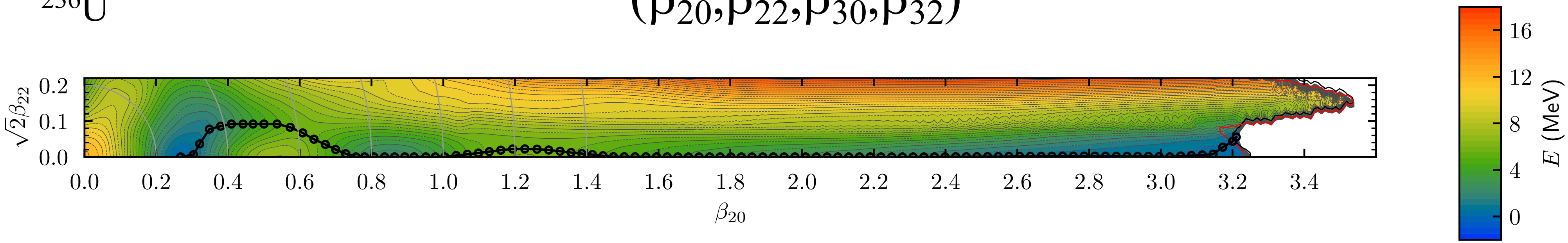
- Triaxial- and octupole-deformed outer barrier

(also for odd-*A* and dd-odd nuclei)

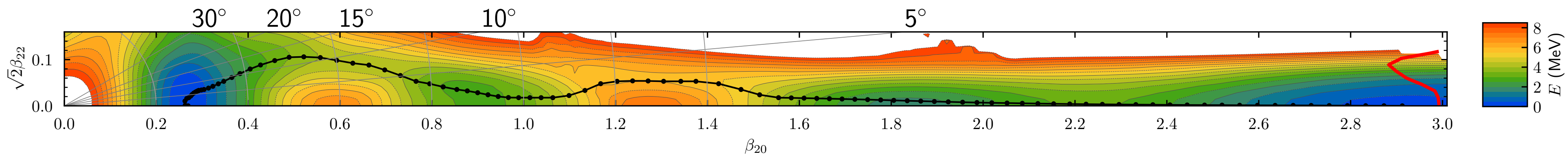


Impact of triaxial deformations on the Lowest Energy fission path (β_{20},β_{22},β_{30},β_{32})

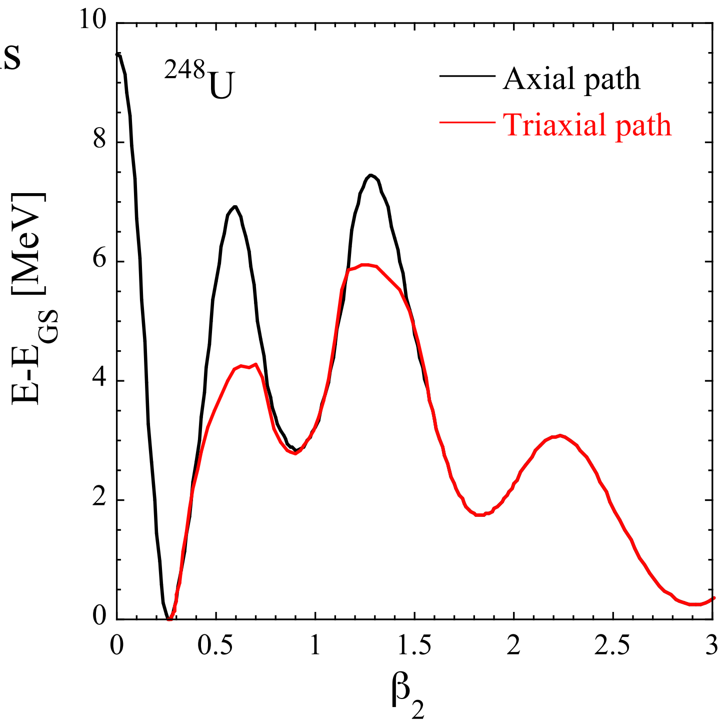
^{236}U



^{248}U

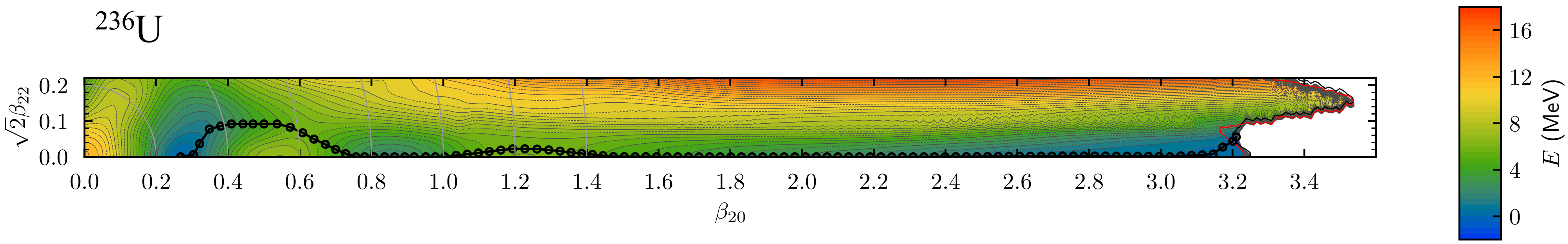


Lowest energy paths

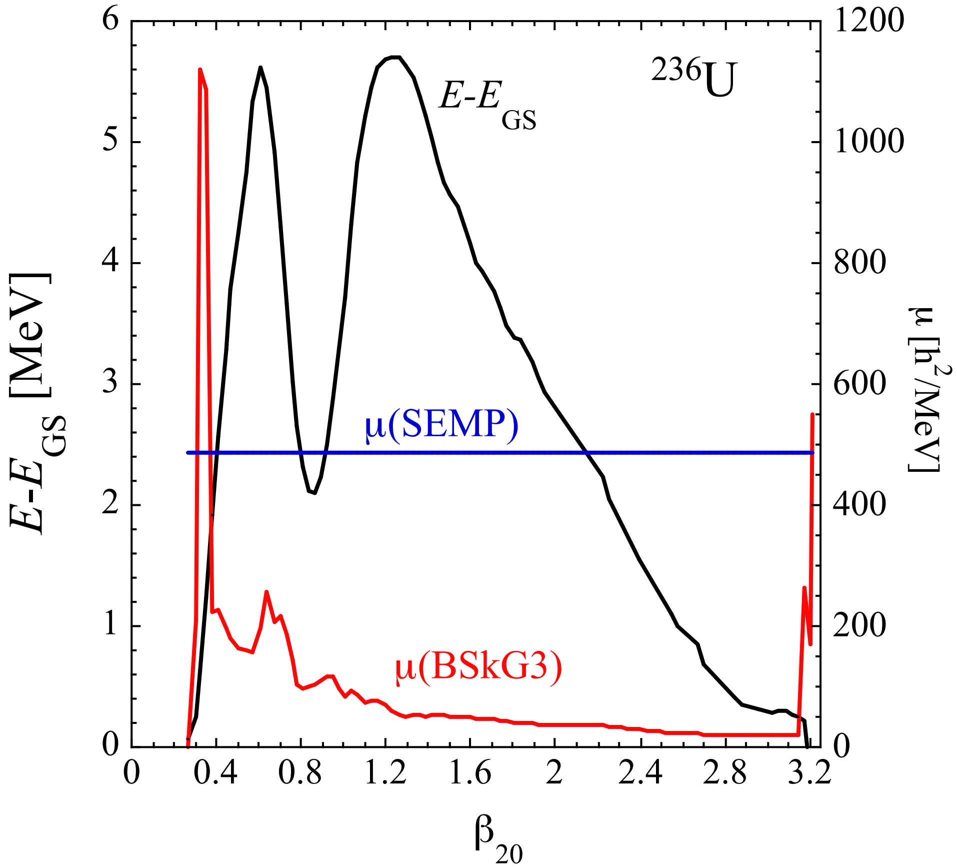


including octupole deformation for β_{20}>0.9

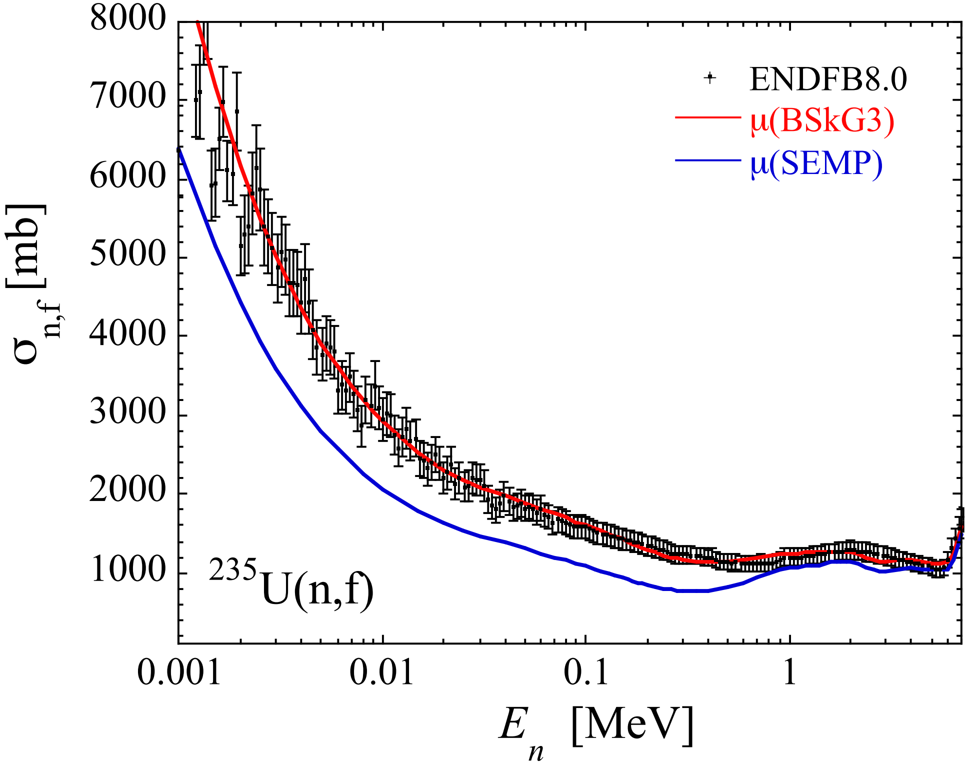
BSkG3 estimate of inertial masses and the least action path



Least action path (β_{20},β_{22},β_{30},β_{32})



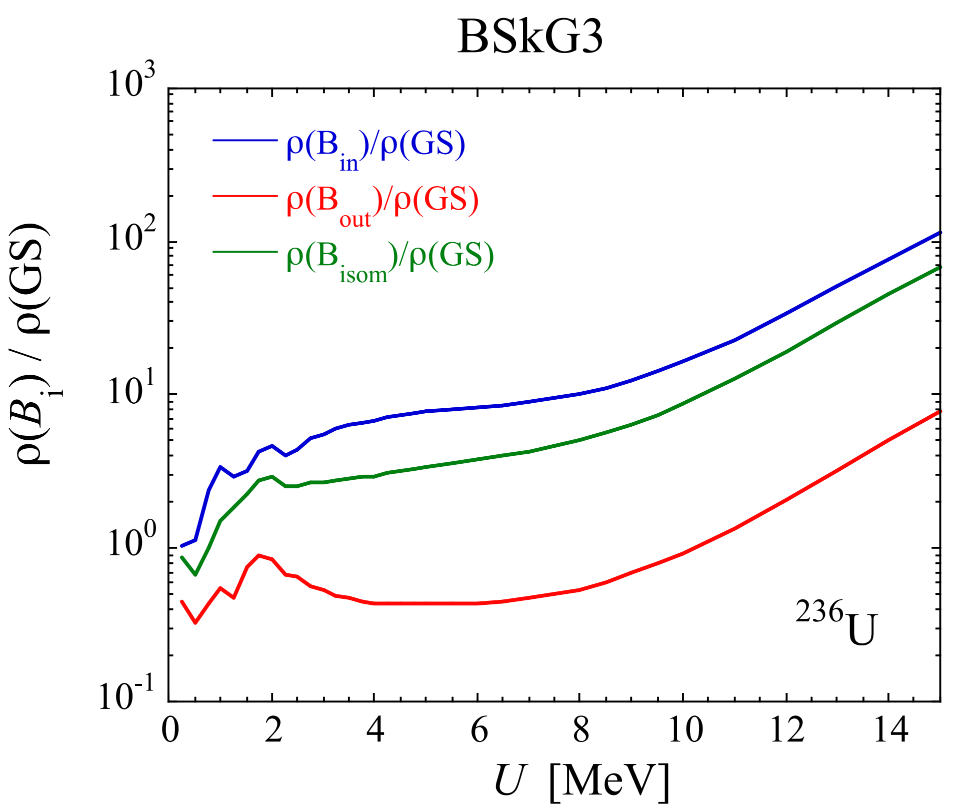
Impact of μ on (n,f) cross section

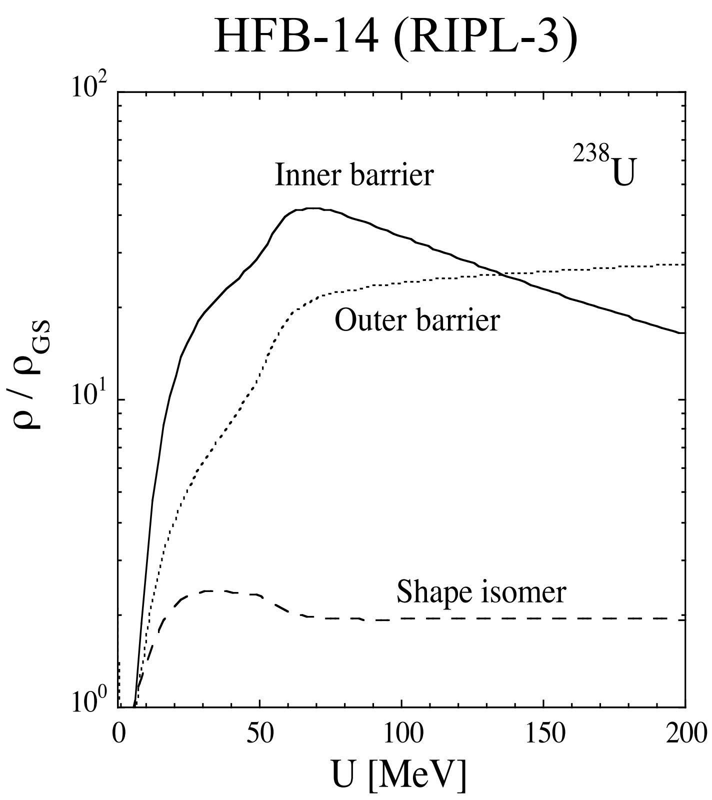


Normalisation of BSkG3 fission $B_{f\,(\sim 2\%)}$ & NLD for ^{236}U

BSkG3 estimate of NLD at fission saddle points and well

Triaxial inner barrier and octupole-triaxial outer barrier





…. MORE TO COME ….

- Determination from 2D-constrained (β_{20}, β_{22}) PES with BSkG3 :
  - fission paths (LEP & LAP) with BSkG3 inertial masses
  - 1D projection of fission path for transmission barrier calculation
  - NLD at saddle points and isomeric wells
  - Calculation of spontaneous, β-delayed and n-induced fission probabilities
- Calculations of full 3D-constrained (β_{20}, β_{22}, β_{30}) PES (~ 20 M CPU h)
- To be updated by BSkG4 (coming soon) ?

for some 2000 (e-e,e-o,o-e,o-o) nuclei ($90 \leq Z \leq 110$) from p- to n-drip lines

- New post-doc position at ULB for 3 years on "fission"
  → candidate recruited to start on 1 July, 2024

Expected outcomes for RIPL-4 : ~ end 2024...