Theoretical Nuclear Level Density models for practical applications

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New developments in Nuclear Level Density models

1. QRPA + Boson Expansion model

   (S. Hilaire, S. Péru, S. Goriely)

2. BSkG3 + Combinatorial model including triaxiality

   (S. Goriely, W. Ryssens, S. Hilaire, A. Sánchez Fernández)

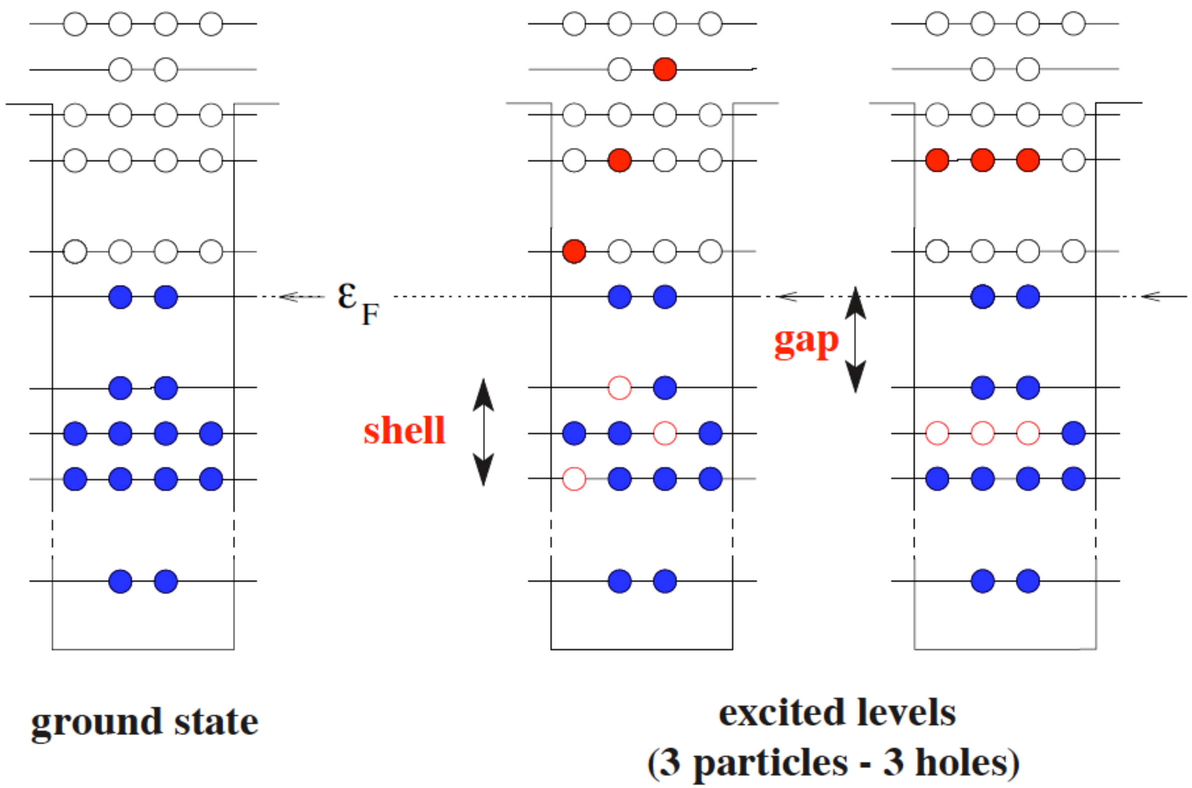
3. Testing the quality of Nuclear Level Density models on Oslo data

   (S. Goriely, A.-C. Larsen, D. Mücher)

Global HFB + Combinatorial NLD model

Level density estimate is a counting problem: $\rho(U)=\mathrm{d}N(U)/\mathrm{d}U$

$N(U)$ is the number of ways to distribute the nucleons among the available levels for a fixed excitation energy U



- **Skyrme / Gogny HFB**
  - ⇒ **GS properties: SPL scheme, Pairing strength, MoI, deformation, ...**
- **HFB + Combinatorial calculation**
  - ⇒ **Incoherent particle-hole $\omega_{ph}(U,M,\pi)$**
  - ⇒ **Incoherent total state densities $\omega_{tot}(U,M,\pi)$**
- **Vibrational enhancement**
  - **Construction of multiphonon state densities $\omega_{vib}(U,M,\pi)$ using a boson partition function with $\lambda=2$, 3 and 4 phonons**
  - **Folding of the total incoherent $\omega_{tot}(U,M,\pi)$ with $\omega_{vib}(U,M,\pi)$**
  - ⇒ **band-head state densities $\omega_{bh}(U,M,\pi)$**
- **Construction of spherical level densities :**
  - ⇒ $\rho_{sph}(U,J,\pi) = \omega_{bh}(U,M=J,\pi) - \omega_{bh}(U,M=J+1,\pi)$
- **Construction of deformed level densities, i.e. rotational bands on top of every band-head state**
  - ⇒ $\rho_{def}(U,J,\pi) = ½ \sum_K \omega_{bh}(U-E_{rot}(J,K),K,\pi)$
- **Mixing of deformed and spherical level densities using a phenomenological transition from deformed to spherical shape**

$$\rho(U,J,\pi) = \left[1-\mathcal{F}\right]\rho_{\rm sph}(U,J,\pi) + \mathcal{F}\rho_{\rm def}(U,J,\pi) \text{ with } \mathcal{F} = 1 - \frac{1}{1+\mathrm{e}^{(E_{def}-E^*_{def})/e}}$$

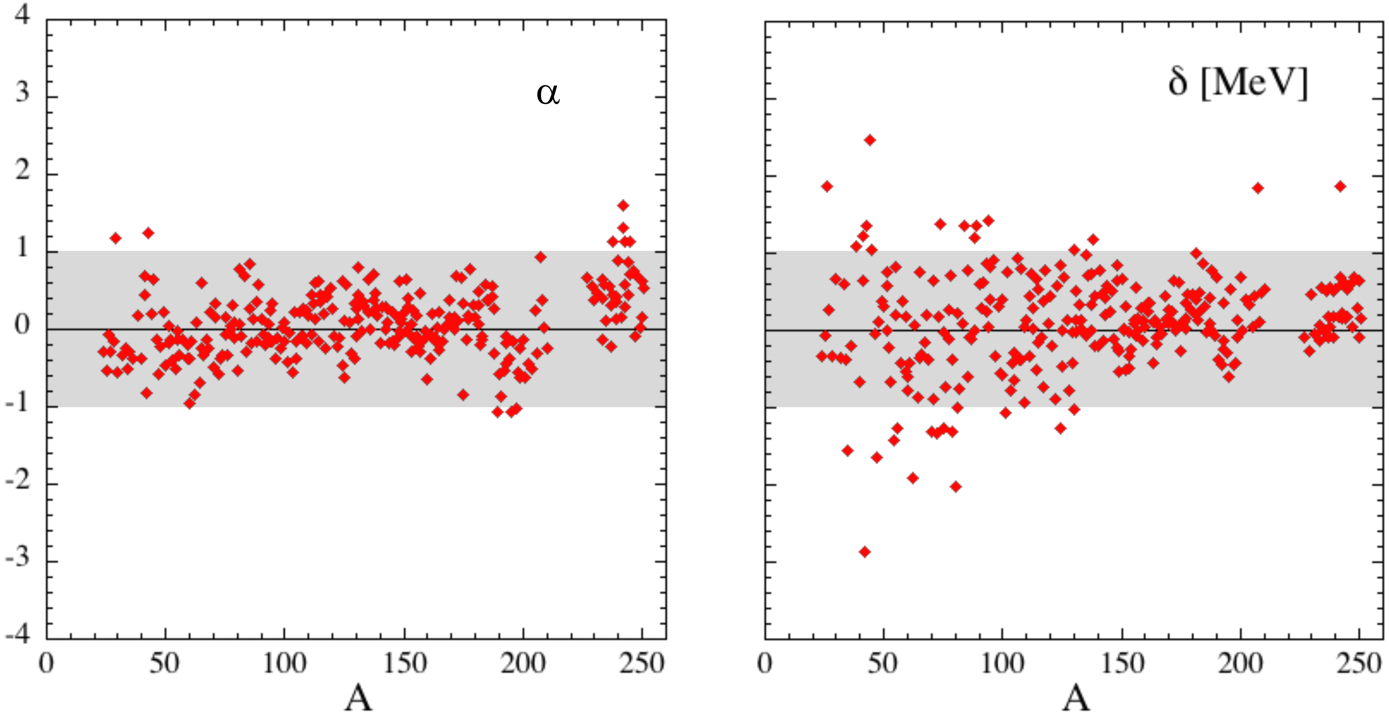
$$\text{or} \quad \mathcal{F} = 1 - \frac{1}{1+\mathrm{e}^{(\beta_2-\beta_2^*)/b}}$$

→ Tables of NLD obtained with BSk14+HFB & D1M+T-HFB

Global adjustment for practical applications

$$\rho^*(U) = e^{\alpha\sqrt{U-\delta}} \times \rho(U - \delta)$$

α and δ adjusted to fit - discrete levels (≈ 1200 nuclei) and
- D_0's (≈ 300 nuclei)



(not a trivial problem: cf Arjan's talk)

Nuclear Level densities

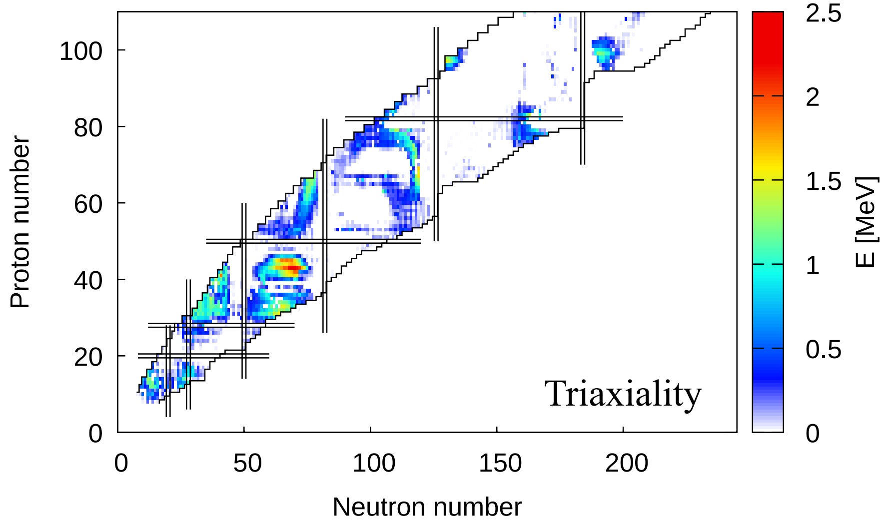
New combinatorial predictions based on the BSkG3 nuclear structure properties

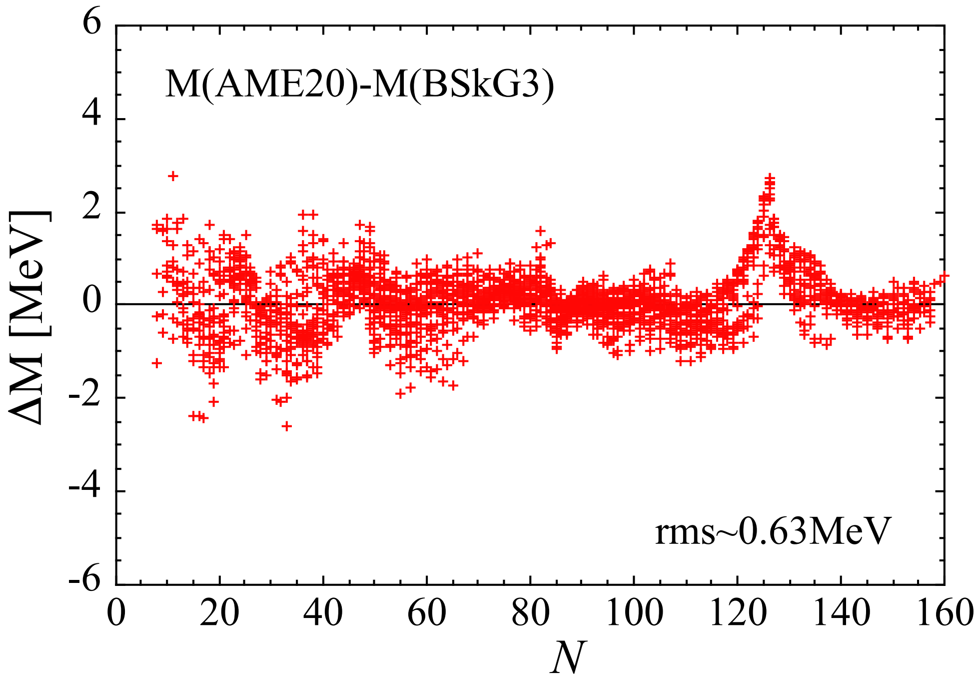
New HFB nuclear mass models

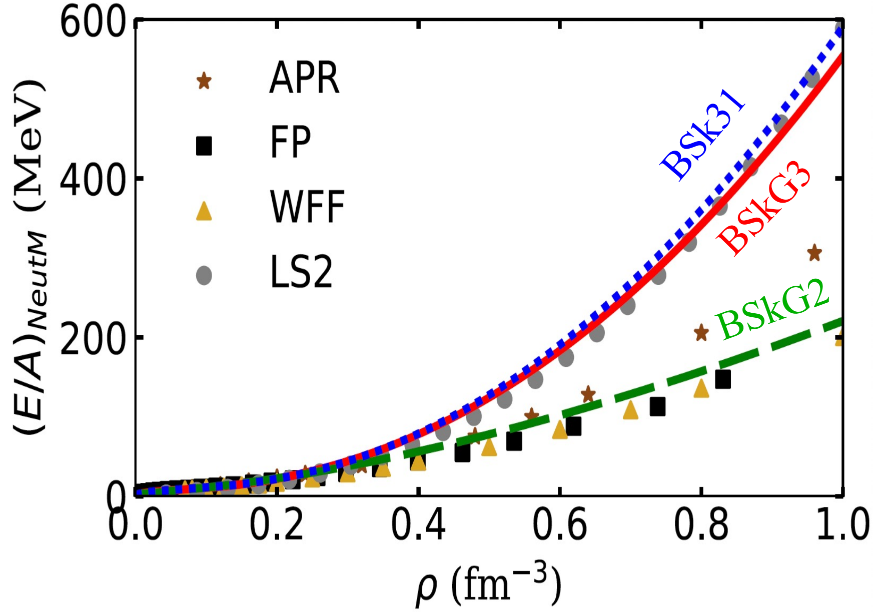
MOCCa code on a Grid representation: Ryssens et al. 2021-2025

New Syrme-HFB mass model: BSkG3

- Triaxiality, time-reversal symmetry breaking & octupole GS deformation
- Microscopic pairing from “realistic” calculations
- Stiff EoS
- Accurate masses: σ(2457*M*)=0.63MeV







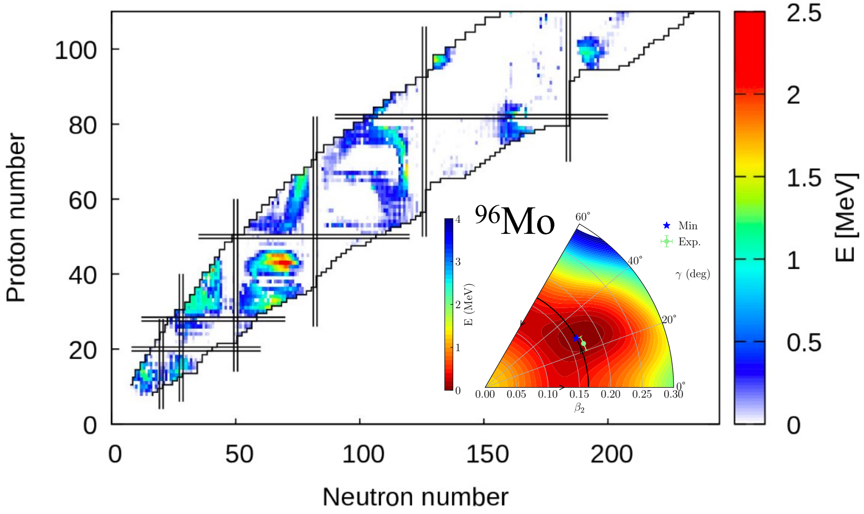
Grams, Ryssens et al. (EPJA 59, 270, 2023)

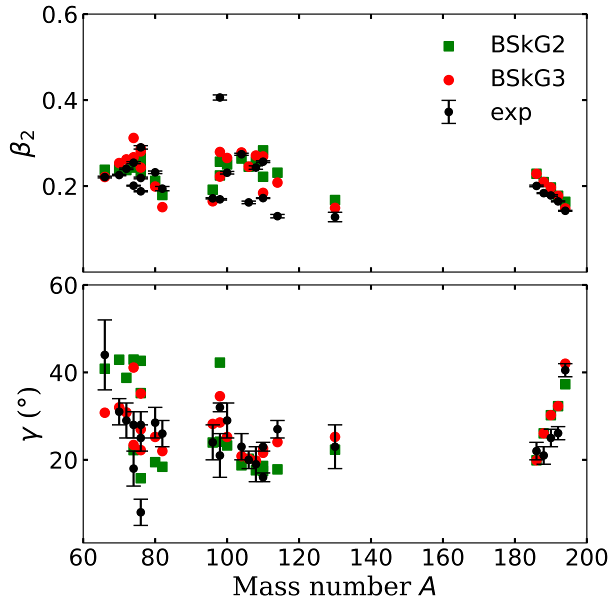
New HFB calculations allowing for triaxial deformations

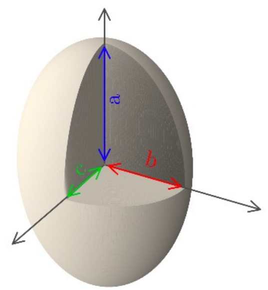
BSkG3 interactions (MOCCa code: Ryssens et al. 2021-2025): σ(M)=0.63 MeV

Triaxial deformation

Wouter Ryssens (ULB)







Two DOF: (β_{20}, β_{22}) or (β, γ)

Energy gain by triaxial deformation

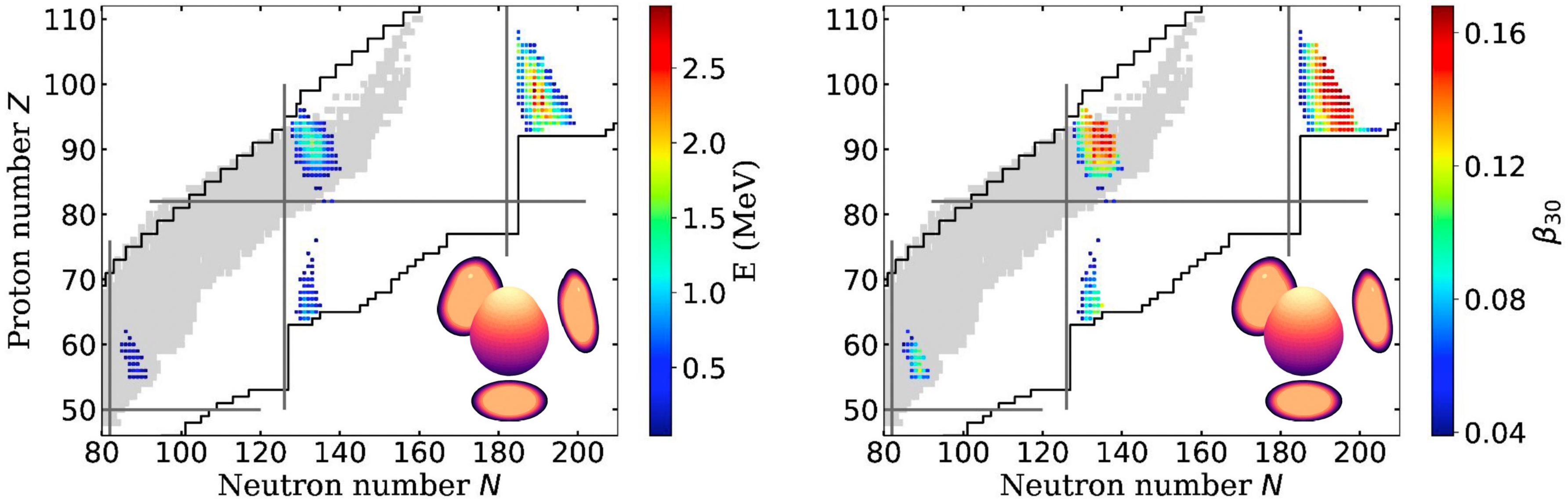
- Many nuclei gain **0.5-2.5** MeV
- Highest gains for Z~43 (Rh)

Rotational invariants

- obtained from COULEX
- data compiled by M. Zielińska

BSkG3: Inclusion of octupole deformation for GS configuration

Masses

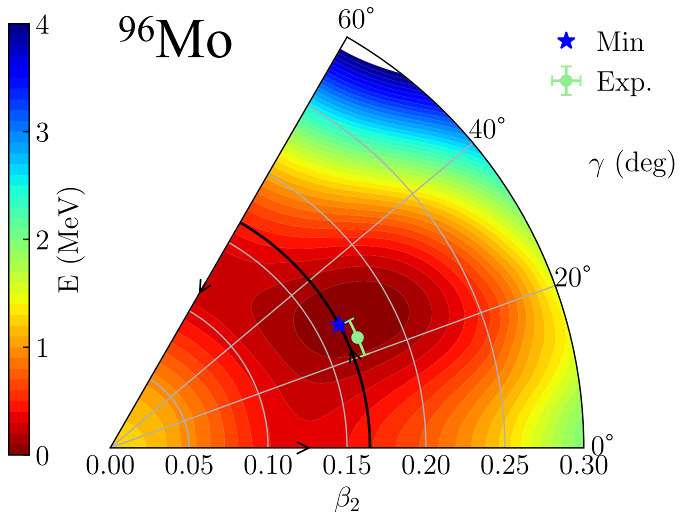


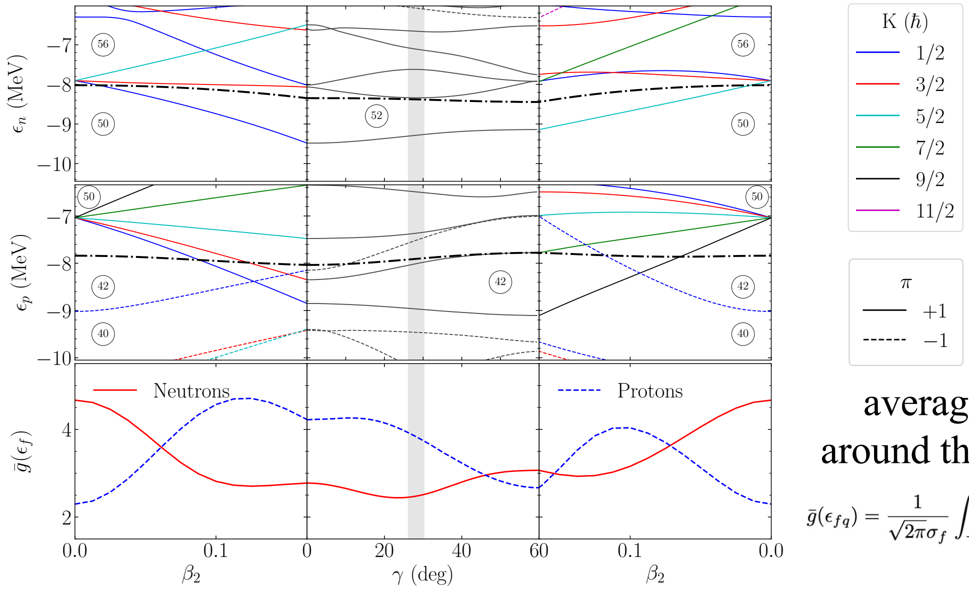
Reflection asymmetry

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

New NLD calculations allowing for triaxial deformations

BSkG3 interactions (MOCCa code: Ryssens et al. 2021-2025): σ(M)=0.63 MeV





average spl density around the Fermi energy

$$\bar{g}(\epsilon_{fq}) = \frac{1}{\sqrt{2\pi}\sigma_f}\int_{-\infty}^{\infty} f_{\mathrm{spl,q}}(\epsilon)\ \exp\left[-\frac{(\epsilon-\epsilon_f)^2}{2\sigma_f^2}\right] d\epsilon$$

- Lower single-particle density
- No more *K* quantum numbers

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

where $\mu = x=y=z$ 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

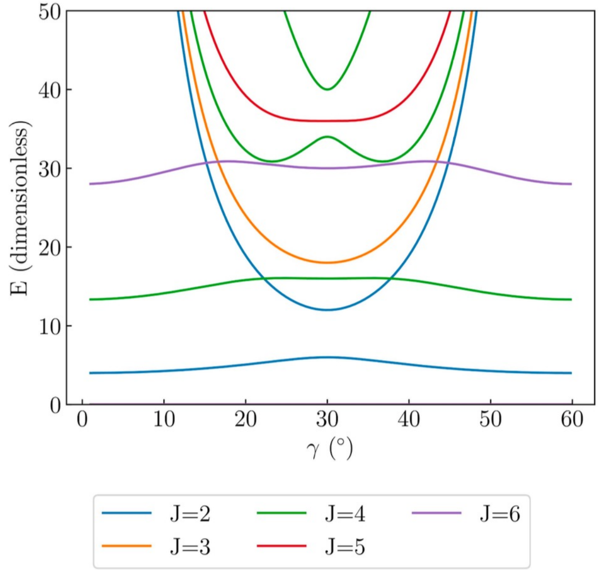
New NLD calculations allowing for triaxial deformations

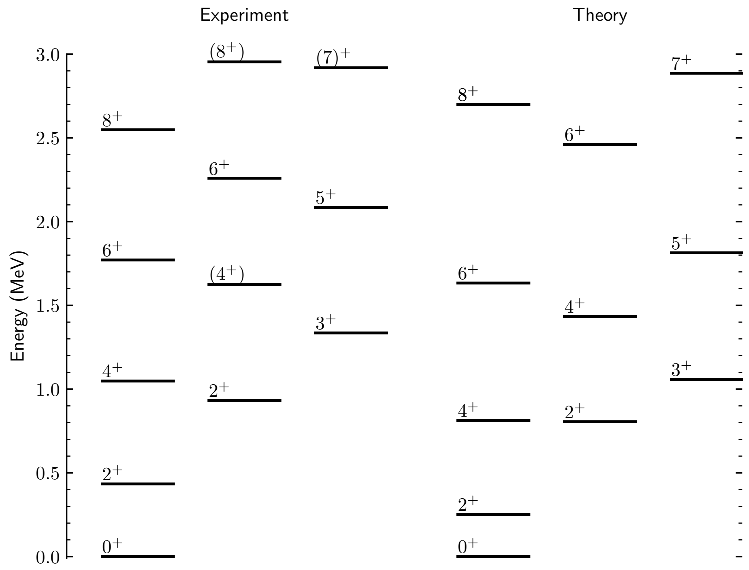
BSkG3 interactions (MOCCa code: Ryssens et al. 2021-2025): σ(M)=0.63 MeV

BSkG3 + Combinatorial model

Wouter Ryssens (ULB)

NLDs for triaxial nuclei: ^{108}Pd





Rotational enhancement

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

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

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

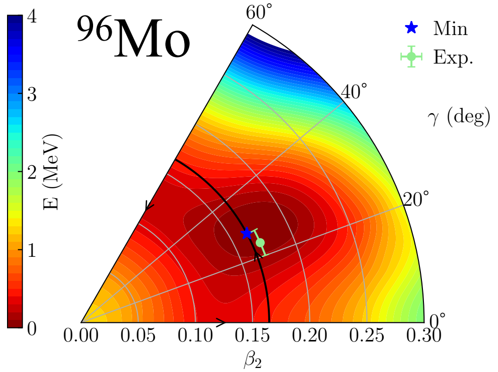
Exp.: NNDC.

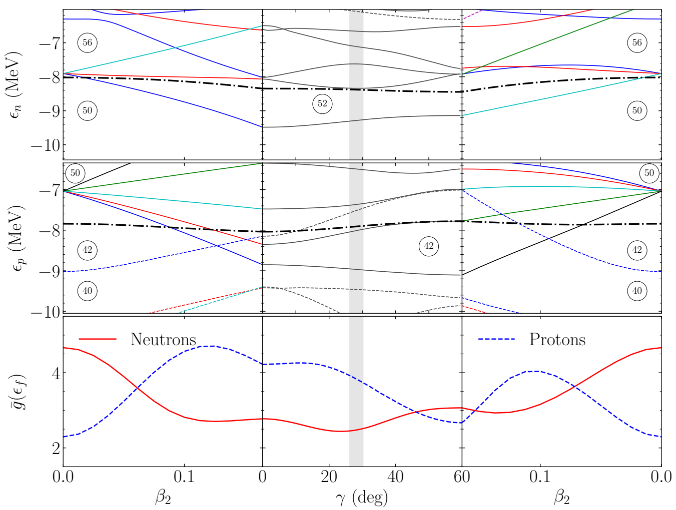
New NLD calculations allowing for triaxial deformations

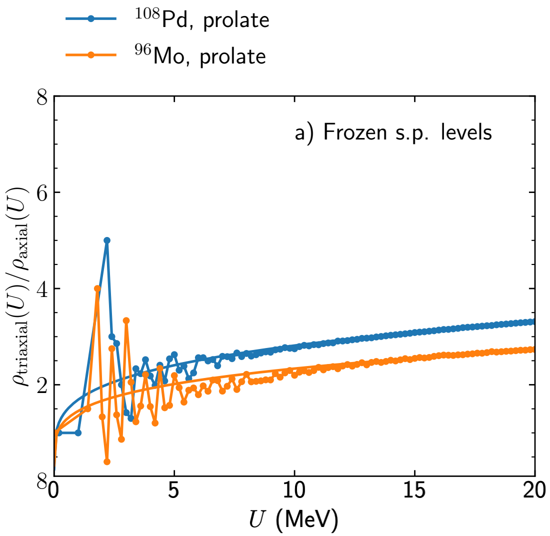
BSkG3 interactions (MOCCa code: Ryssens et al. 2021-2025): σ(M)=0.63 MeV

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

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







Phenomenological collective enhancement

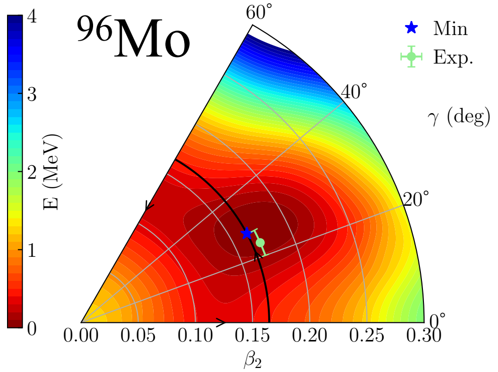
$$\frac{\rho_{\rm triaxial}}{\rho_{\rm axial}} \sim \frac{\sqrt{\mathcal{I}_x \mathcal{I}_y \mathcal{I}_z}}{\mathcal{I}_\perp} U^{1/4}$$

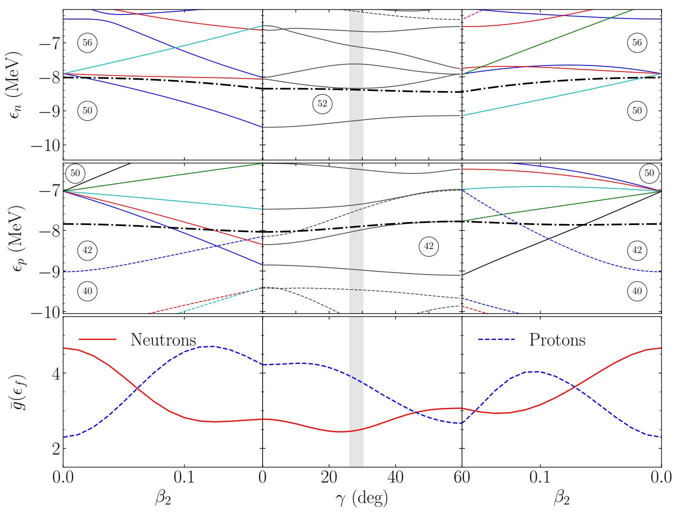
"Frozen" SPL taken from prolate configurations with triaxial GS moments of inertia $\mathcal{I}$

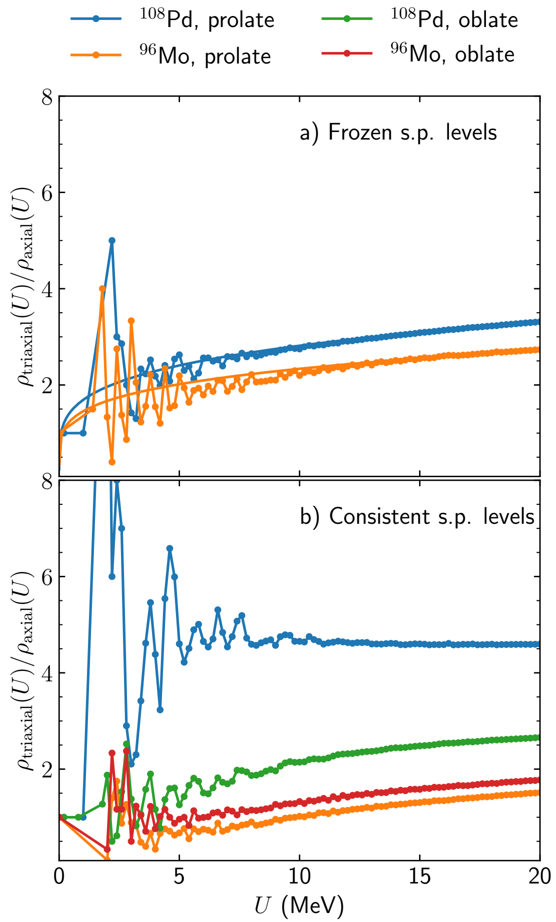
New NLD calculations allowing for triaxial deformations

BSkG3 interactions (MOCCa code: Ryssens et al. 2021-2025): σ(M)=0.63 MeV

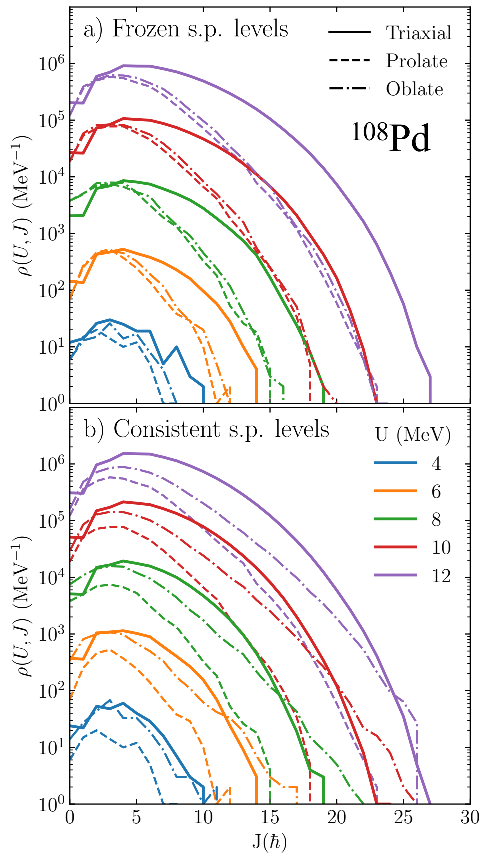
$$\rho(E_X, J, P) = \frac{1}{2}\sum_{\bar{K}=-J}^{J}\sum_{i=1}^{n^{J,\bar{K}}}\rho\left(E_X - E_i^{J,\bar{K}}, P\right) \qquad n^{J,\bar{K}} = \begin{cases} J_{\rm rot}+1 & \text{if } J_{\rm rot} \text{ is even, and } \bar{K}\neq 0,\\ J_{\rm rot} & \text{if } J_{\rm rot} \text{ is odd, and } \bar{K}\neq 0,\\ J_{\rm rot}/2+1 & \text{if } J_{\rm rot} \text{ is even, and } \bar{K}=0,\\ (J_{\rm rot}-1)/2 & \text{if } J_{\rm rot} \text{ is odd, and } \bar{K}=0. \end{cases}$$



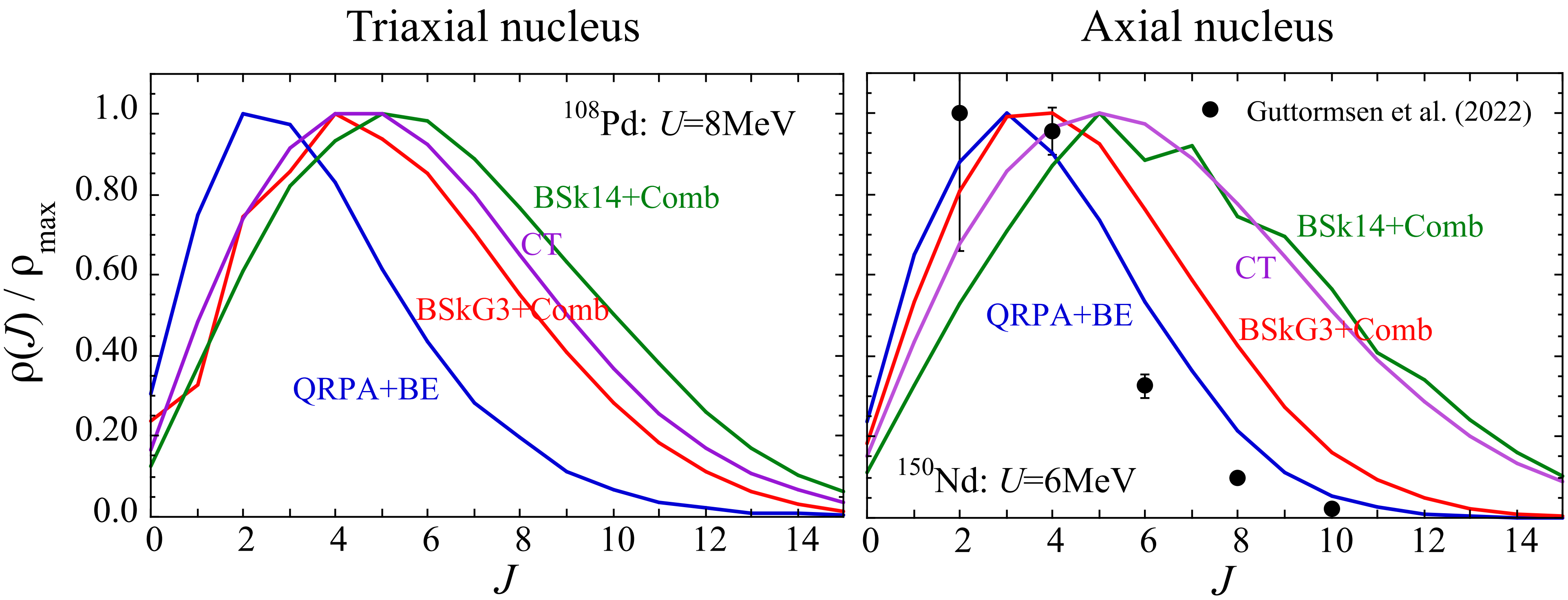




Wider Spin Distribution



Spin distribution



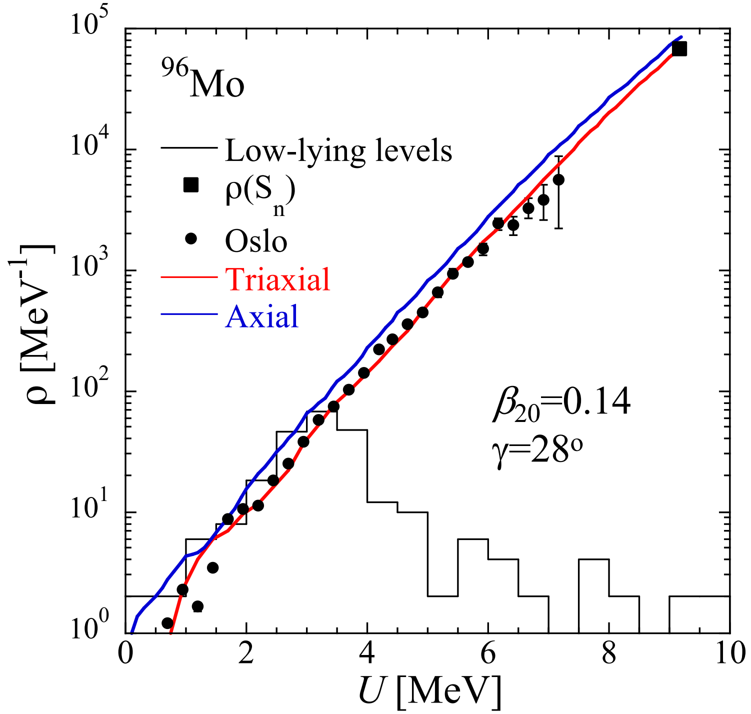
Deeper analysis of the spin cut-off
and its energy dependence ?

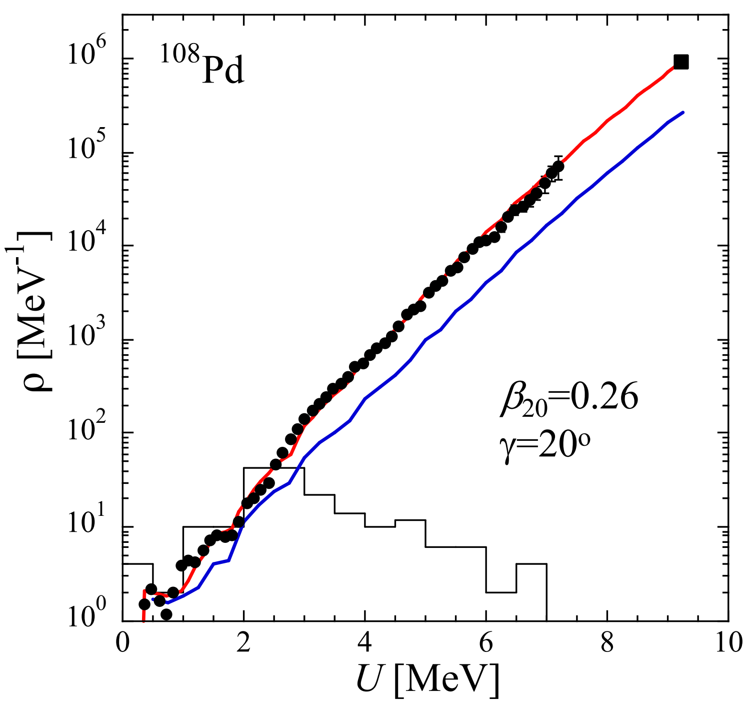
Experimental spin distribution from
(p,p') reaction: σ=2.9 ± 0.2
(Guttormsen et al., 2022)

Effects of traxiality on BSkG3+Combinatorial NLD

Main impact of the triaxiality on the NLD:

- Reduction of the spl density → Lower intrinsic NLD
- Additional collective enhancement → Increase total NLD



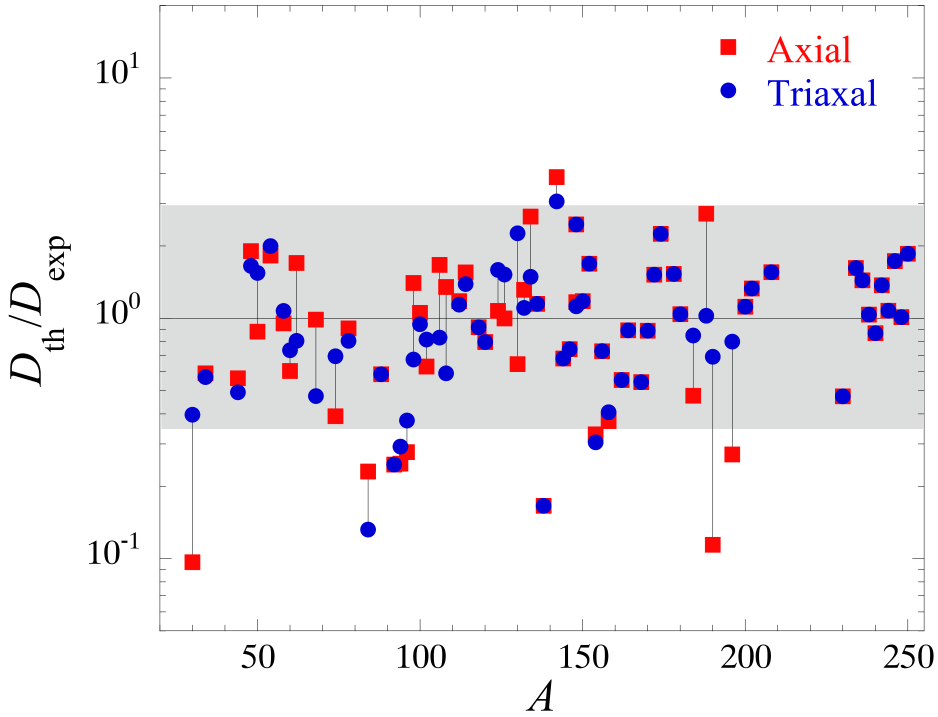


For modestly deformed nuclei:
Decrease of NLD

For well deformed nuclei:
Increase of NLD

Effects of triaxiality on s-wave resonance spacings

D_0 = *s*-wave neutron resonance spacings



$$\rho(U,J,\pi) = \Big[1-\mathcal{F}\Big]\rho_{\text{sph}}(U,J,\pi) + \mathcal{F}\rho_{\text{def}}(U,J,\pi)$$

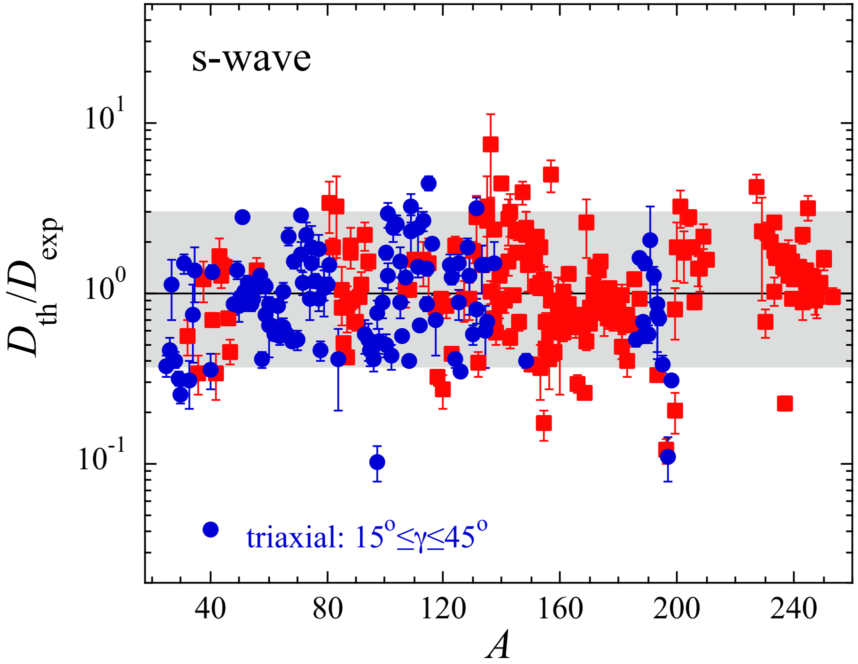
with $\mathcal{F} = 1 - \dfrac{1}{1+\mathrm{e}^{\frac{r_{42}-r^*_{42}}{d^*}}}$

$r_{42} = E_1(4^+)/E_1(2^+)$ from D1M 5DCH

r^*_{42}=3.0 & d^*=0.4

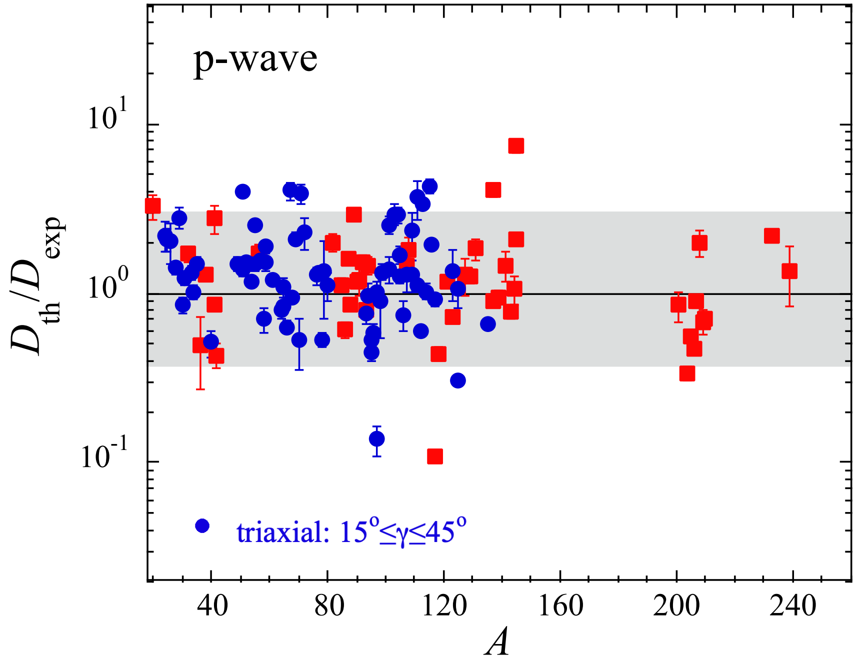
Comparison with RIPL-3 resonance spacings

D_0 = *s*-wave neutron resonance spacings



299 nuclei: f_{mean}=1.03 - f_{rms}=1.96

D_1 = *p*-wave neutron resonance spacings



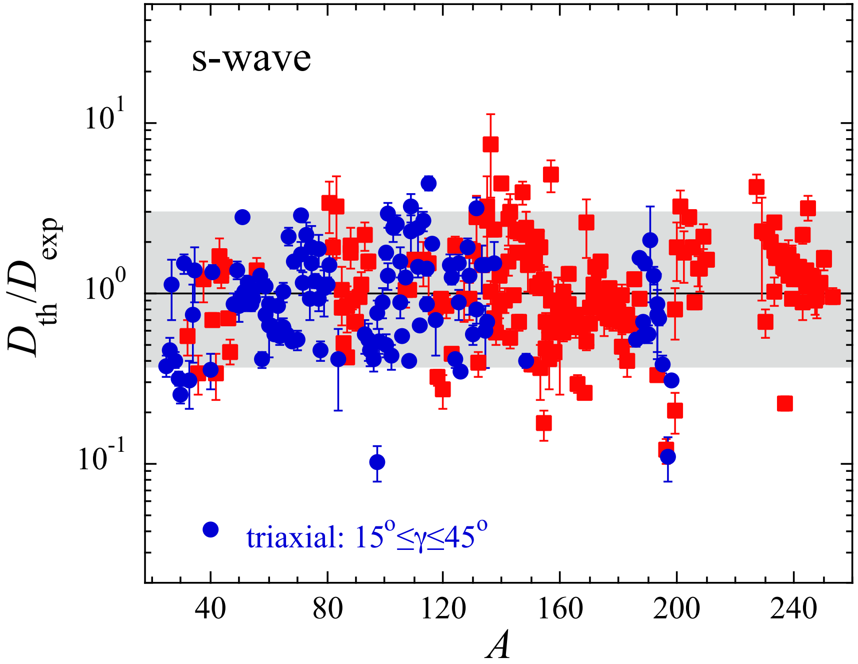
116 nuclei: f_{mean}=1.21 - f_{rms}=1.99

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

PS: Experimental uncertainties not included in the calculation of f_{mean} and f_{rms}

Comparison with RIPL-3 resonance spacings

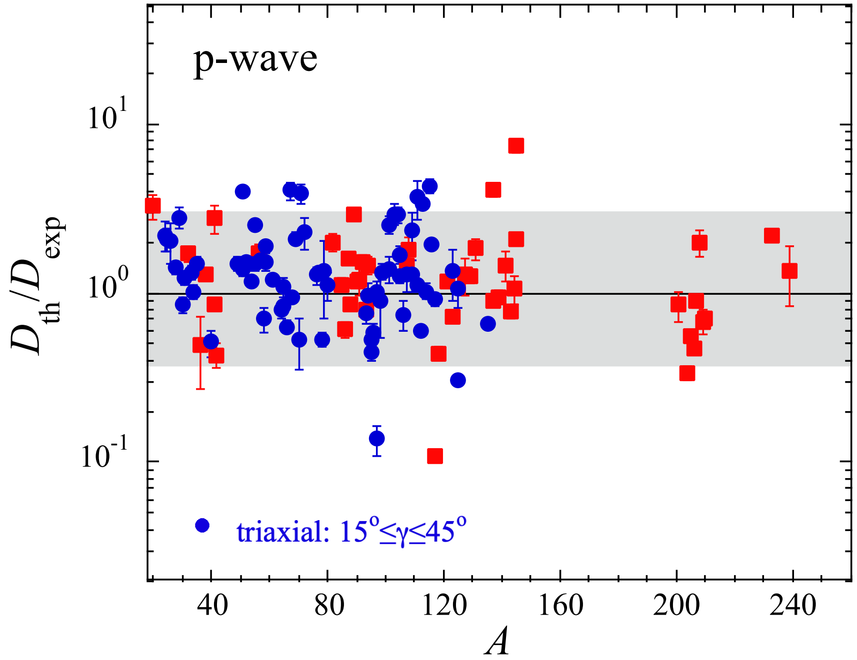
D_0 = *s*-wave neutron resonance spacings



299 nuclei

D_0	f_{mean}	f_{rms}
BSkG3	1.03	1.96
HFB+Comb	0.95	2.34
T-HFB+Comb	1.11	2.58
QRPA+BE	1.12	2.50

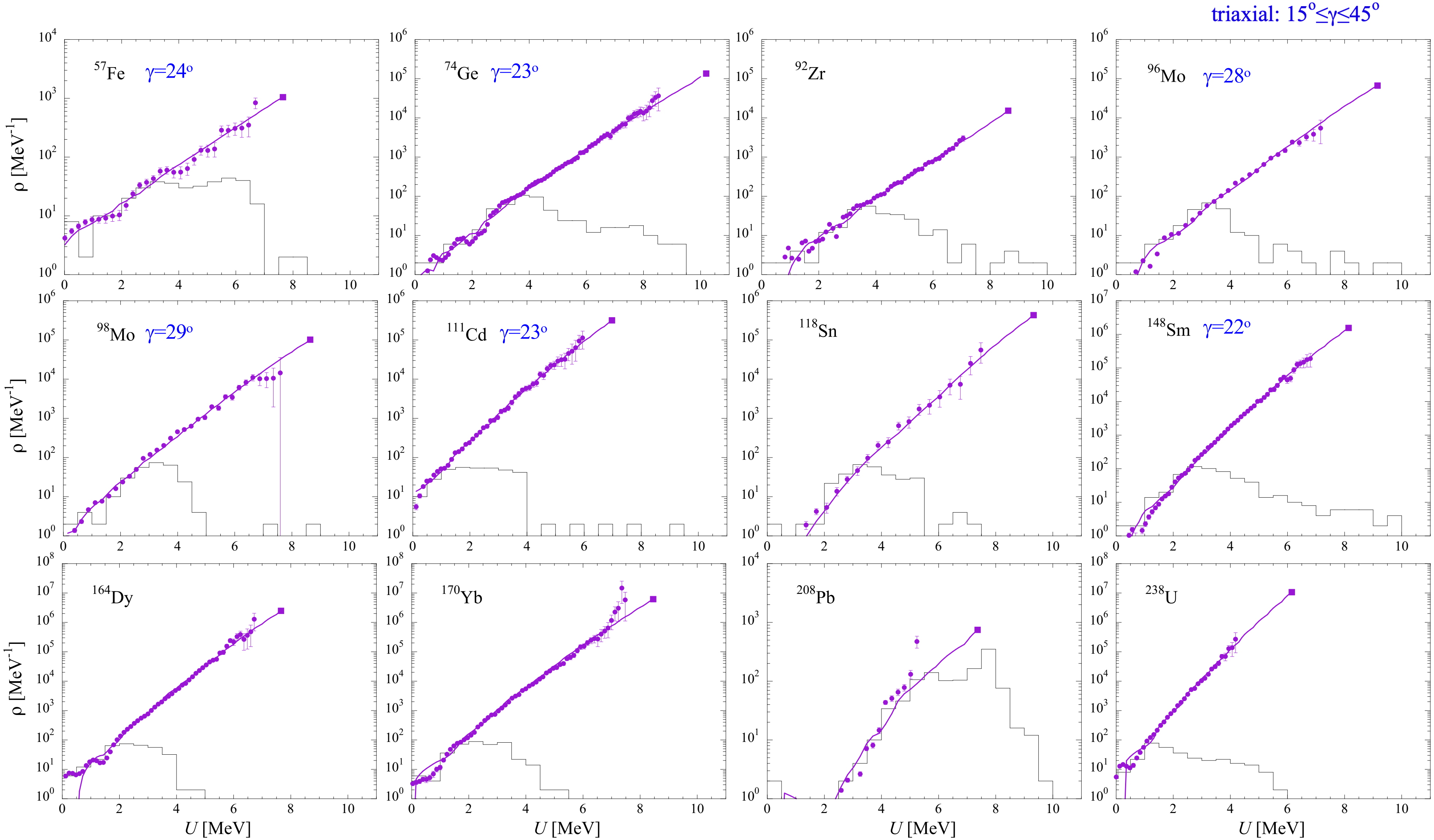
D_1 = *p*-wave neutron resonance spacings



116 nuclei

D_0	f_{mean}	f_{rms}
BSkG3	1.21	1.99
HFB+Comb	1.01	2.24
T-HFB+Comb	1.62	4.38
QRPA+BE	1.72	3.75

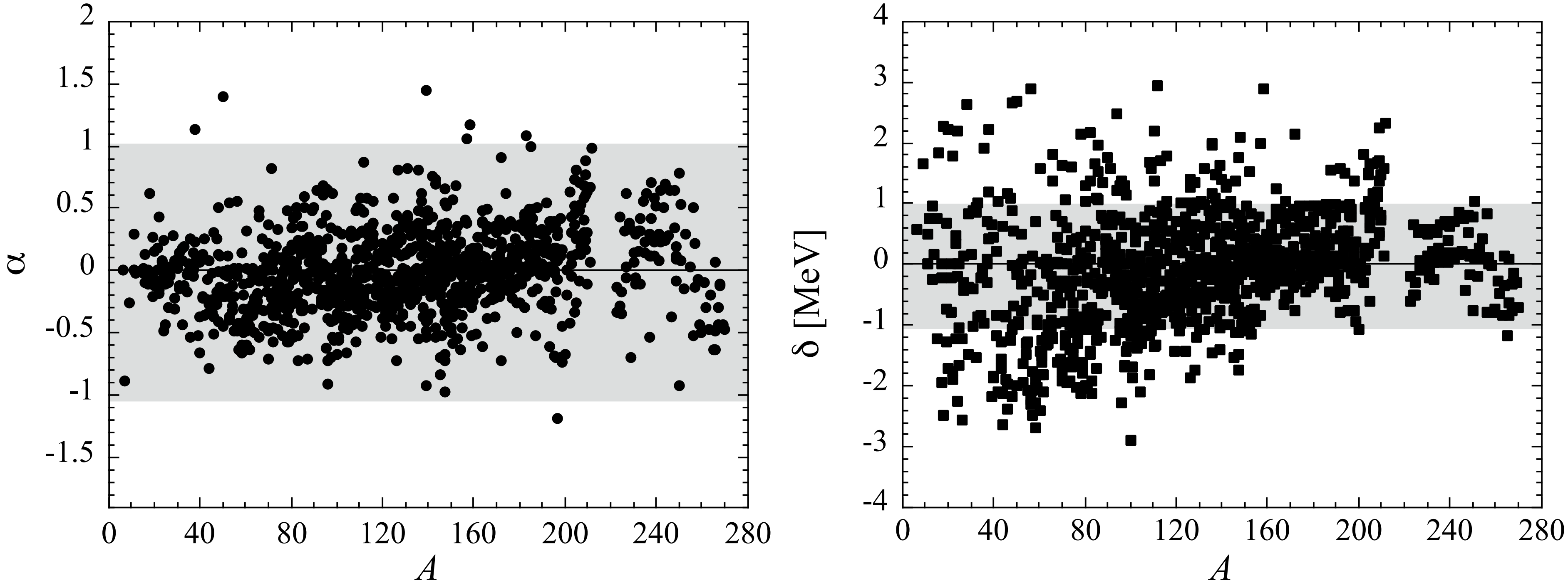
Comparison of BSkG3+Combinatorial NLD with Oslo data



Following the normalisation procedure of Oslo data (SG, Larsen, Mücher, PRC106, 044315, 2022)

Renormalisation of BSkG3 NLD on D_0's and low-lying levels

$$\rho^*(U) = e^{\alpha\sqrt{U-\delta}} \times \rho(U-\delta)$$



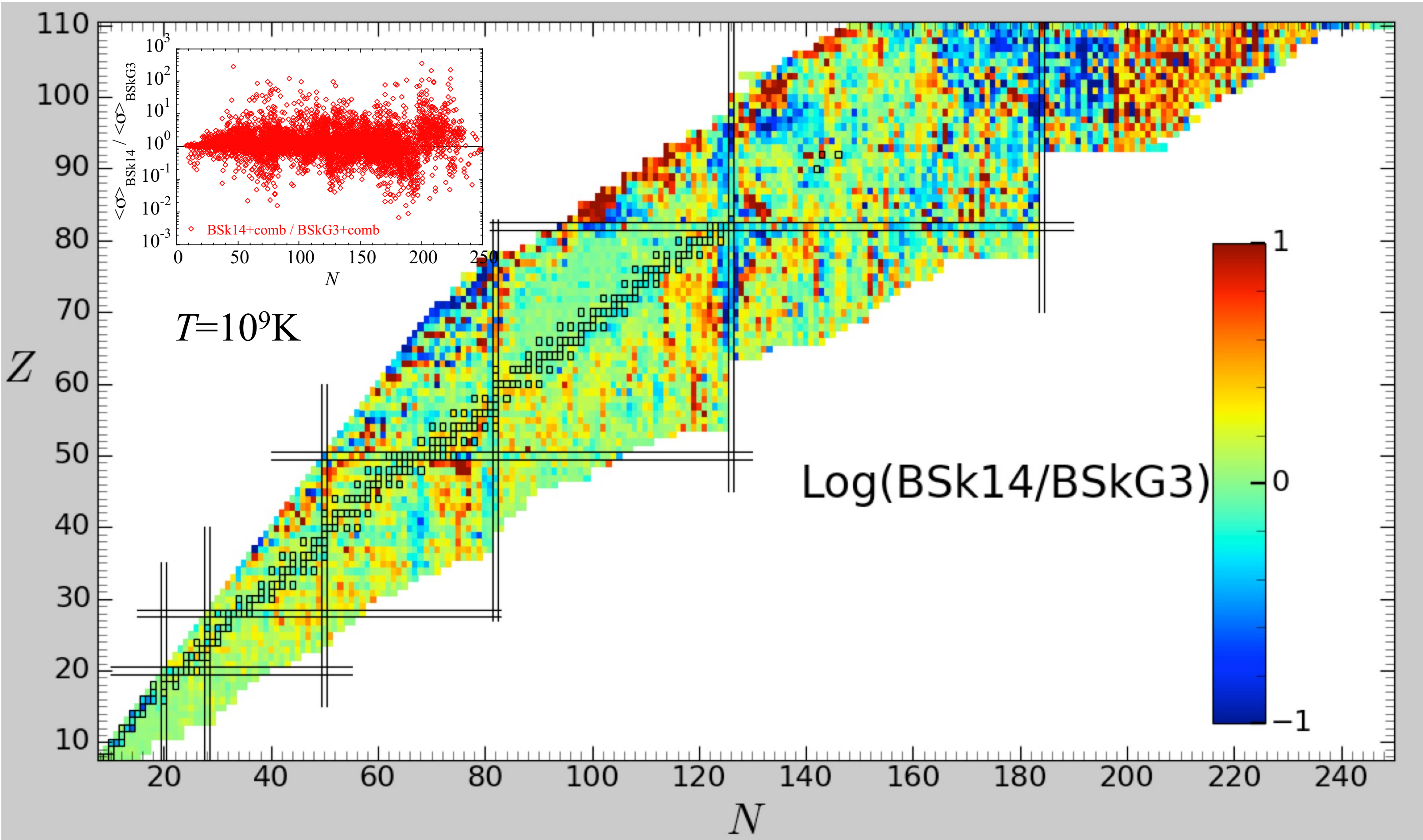
(not a trivial problem: cf Arjan's talk)

Impact of the BSkG3+combinatorial on HF (n,γ) reaction rates (T_9=1)

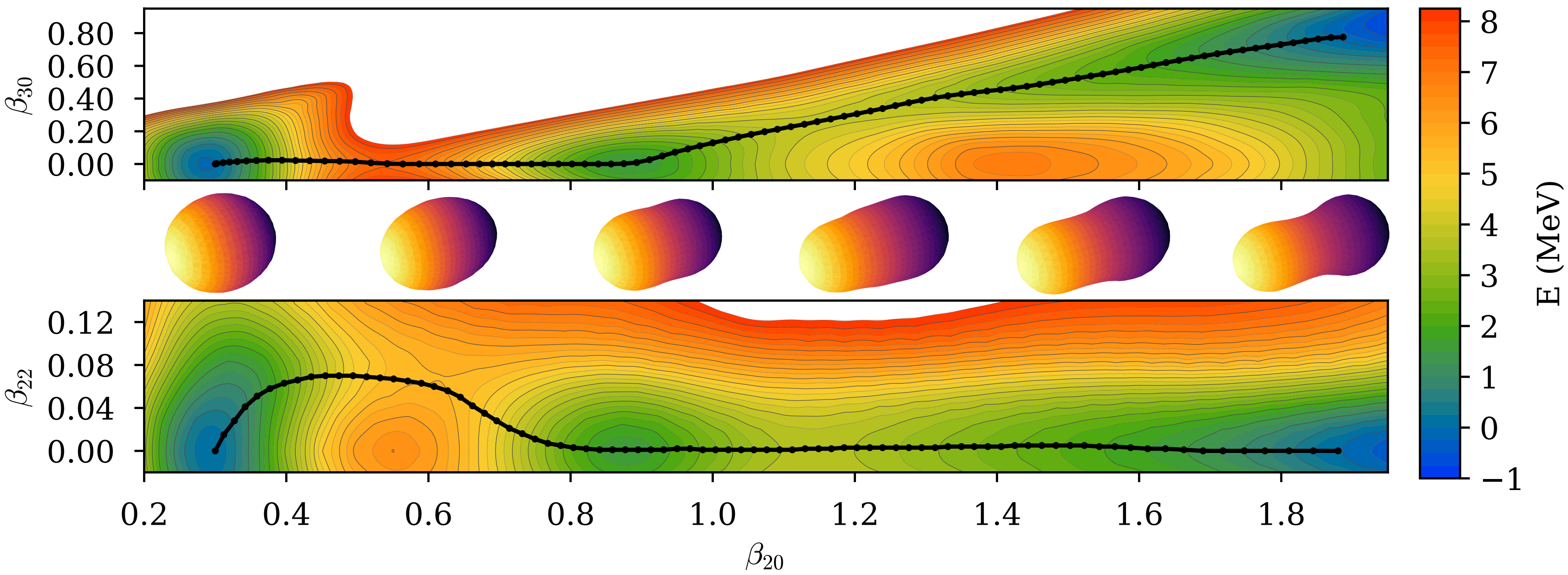
Energy-, spin- and parity-depencent NLD tables ready for use for 7677 nuclei ($8 \le Z \le 110$) including renormalisation coefficients (α,δ) on experimental D_{exp} & LLL (when available)

$0.25 \le U \le 200$MeV; $0 \le J \le 50$; $\pi = \pm$

Impact of BSk14+comb (2008) vs BSkG3+comb (2025) on N_a<σv>

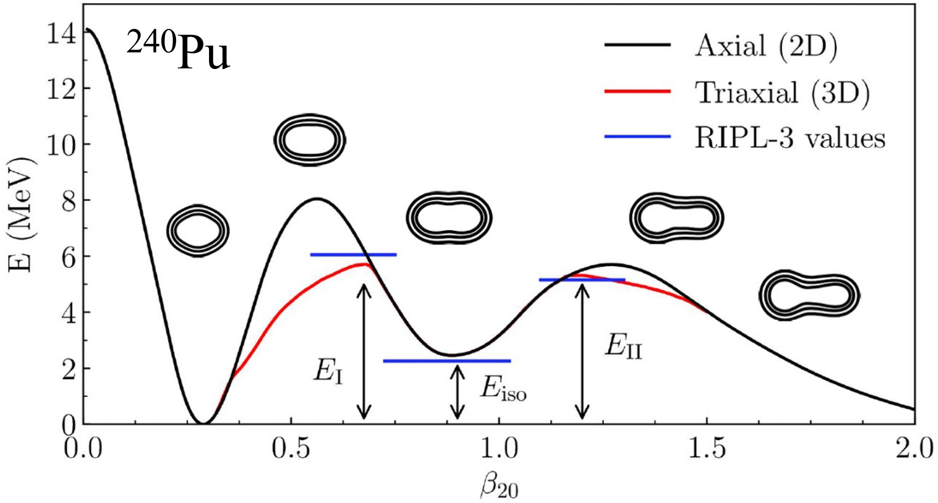


Extension of BSkG3 predictions to fission properties



BSkG3 prediction of fission paths

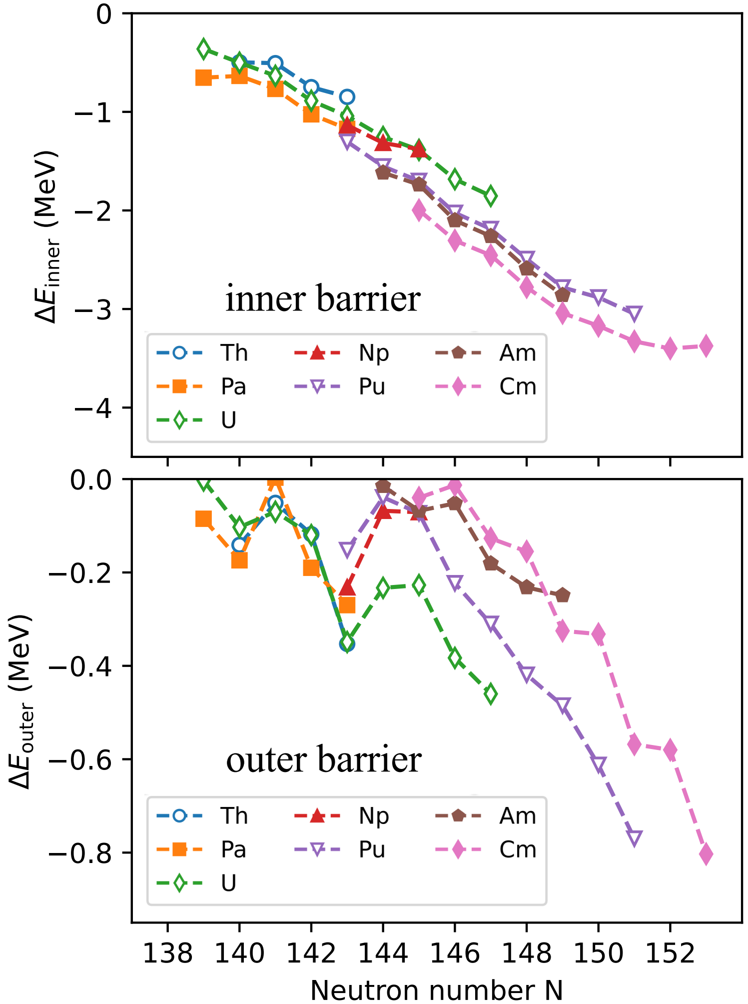
- Triaxial inner barrier



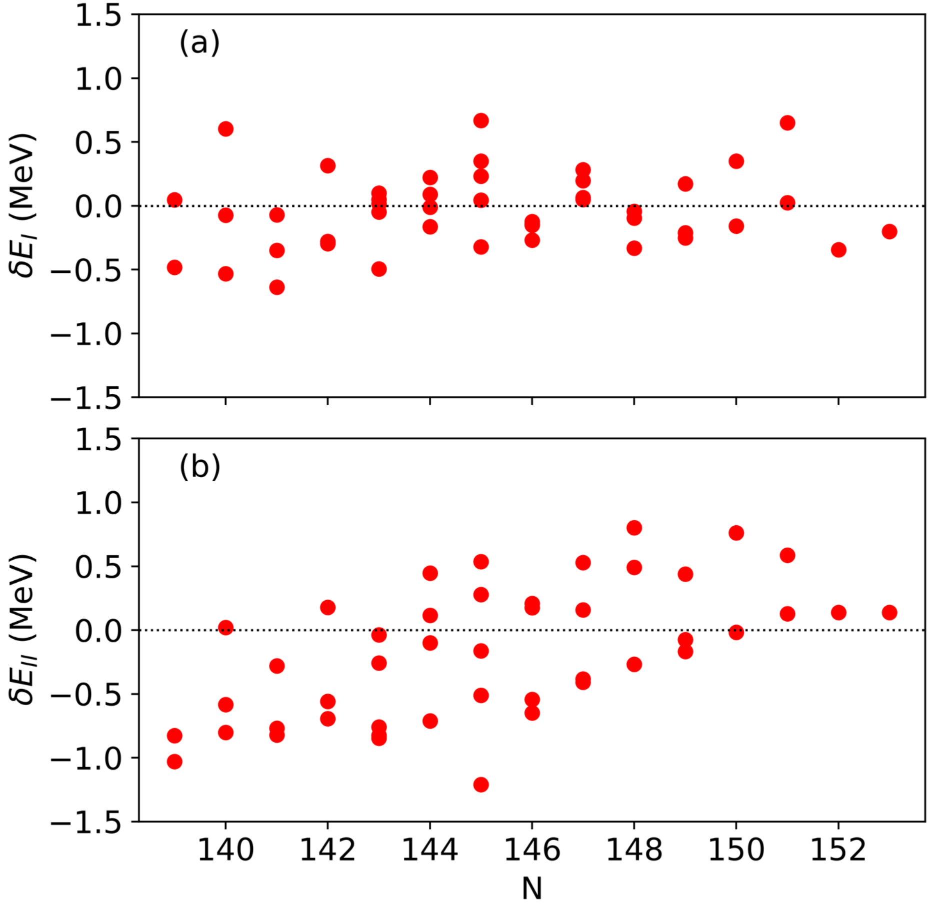
- Triaxial- **and** octupole-deformed outer barrier

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

Impact of triaxiality on the barrier height



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

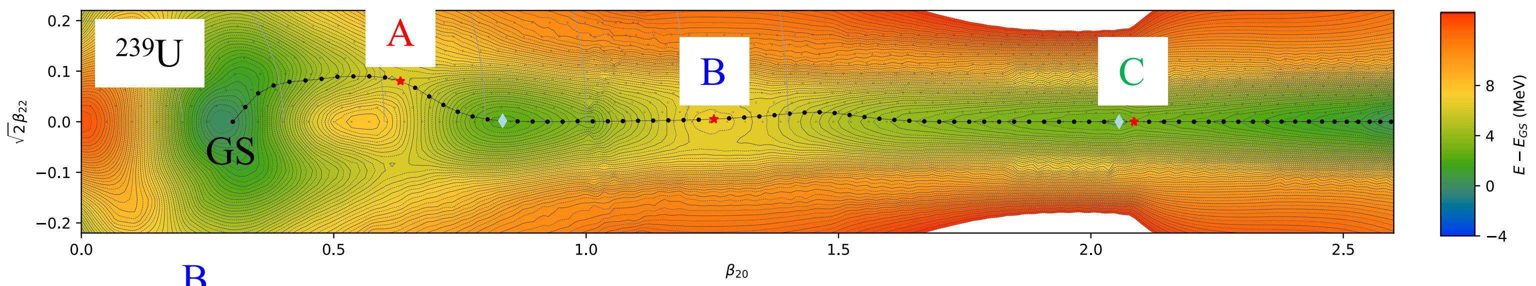


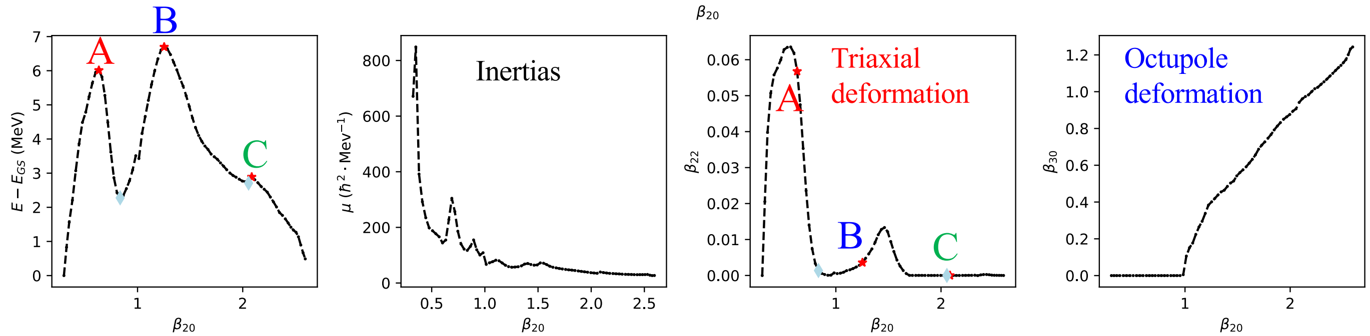
rms deviations on 45 Z>90 nuclei wrt known (RIPL3) fission barriers/wells

	BSkG3
σ(M) [MeV]	0.63
σ(E_I) [MeV]	**0.33**
σ(E_{II}) [MeV]	0.51
σ(E_{iso}) [MeV]	0.36

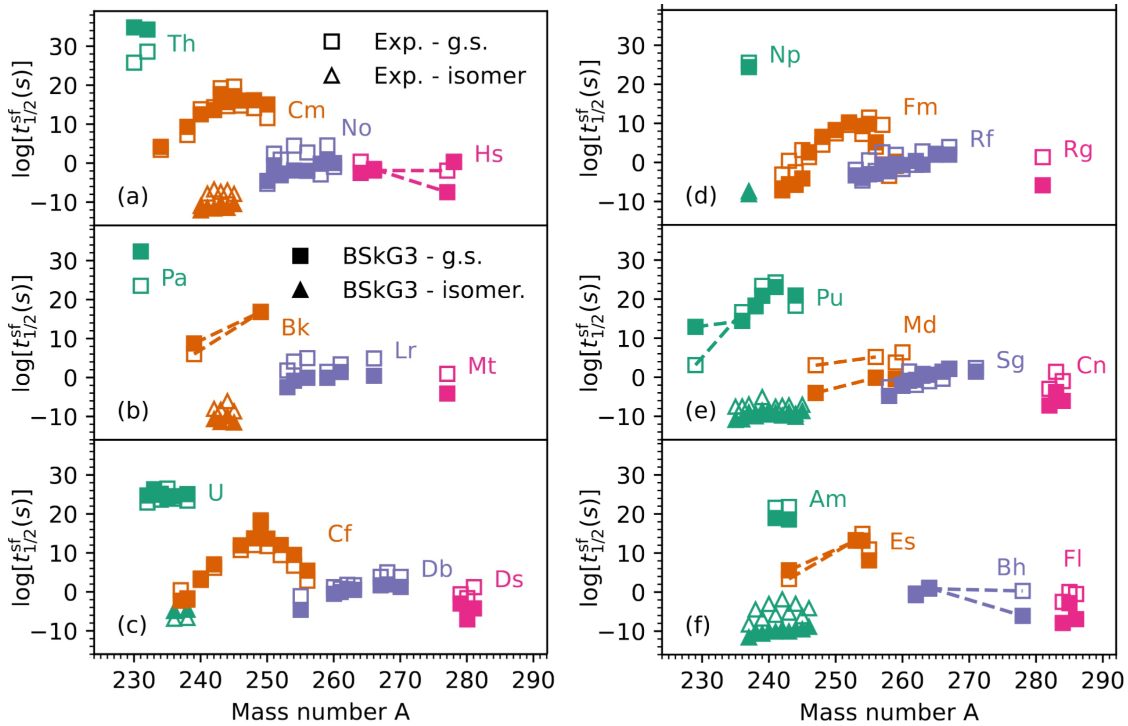
	HFB-14	FRLDM
σ(M) [MeV]	0.76	0.81
σ(E_I) [MeV]	0.59	0.76
σ(E_{II}) [MeV]	0.72	--
σ(E_{iso}) [MeV]	0.73	--

BSkG3: Remarkable description of spontaneous fission half-lives





$t_{1/2}$(SF) not sensitive to NLD



For GS:

124 $t_{1/2}$ (all nuclei):

f_{mean}=0.07 - f_{rms}=3.1 10^3

59 $t_{1/2}$ (e-e nuclei):

f_{mean}=1.5 - f_{rms}=7.6 10^2

For fission isomers:

34 $t_{1/2}$ (all nuclei):

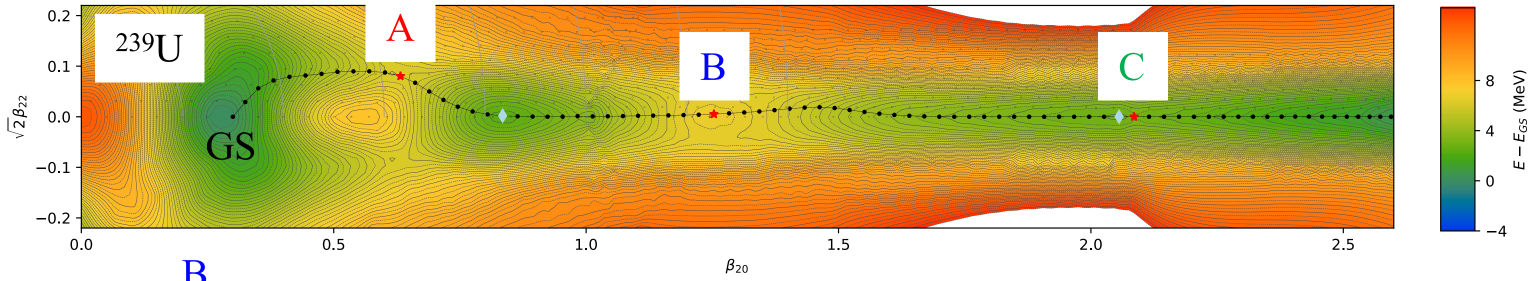
f_{mean}=0.02 - f_{rms}=5.1 10^2

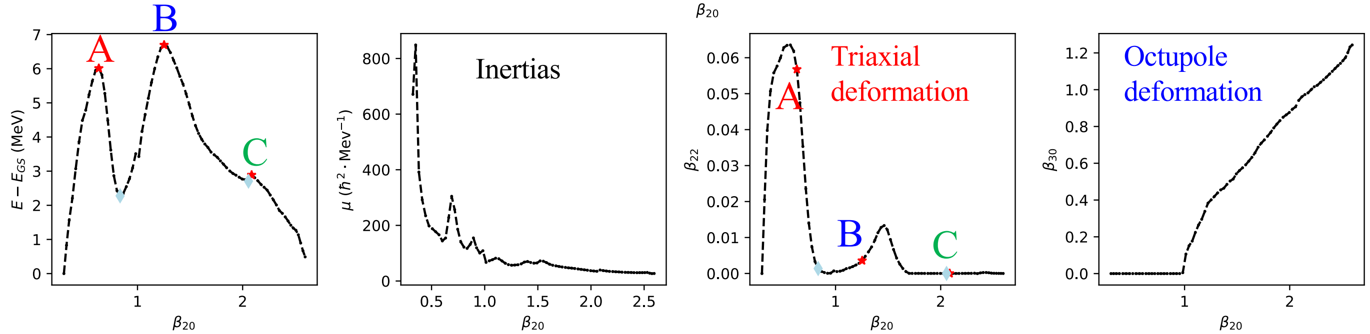
10 $t_{1/2}$ (e-e nuclei):

f_{mean}=0.6 - f_{rms}=1.8 10^2

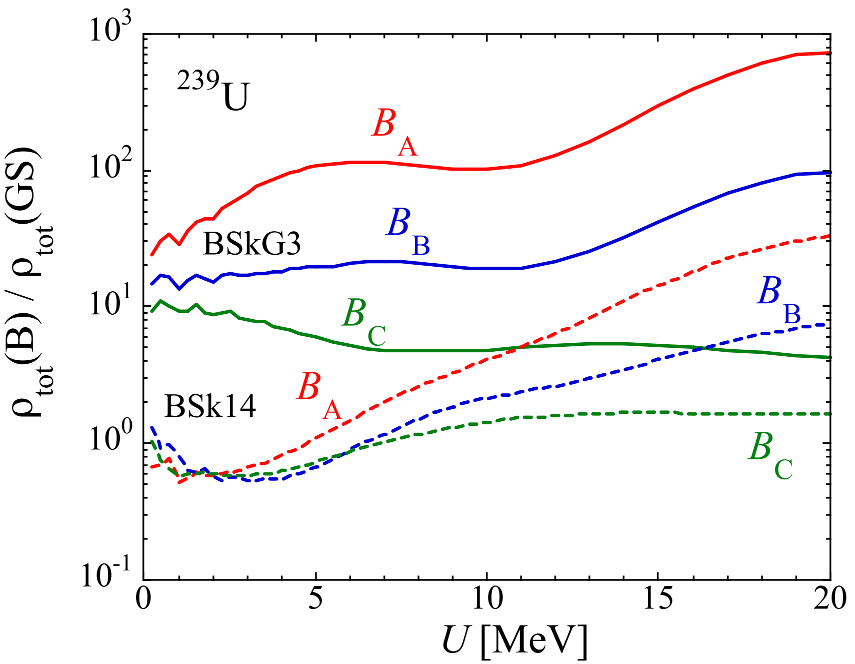
$$f_{\rm rms} = \exp\left[\frac{1}{N}\sum_i^N (\ln r_i)^2\right]^{1/2}$$

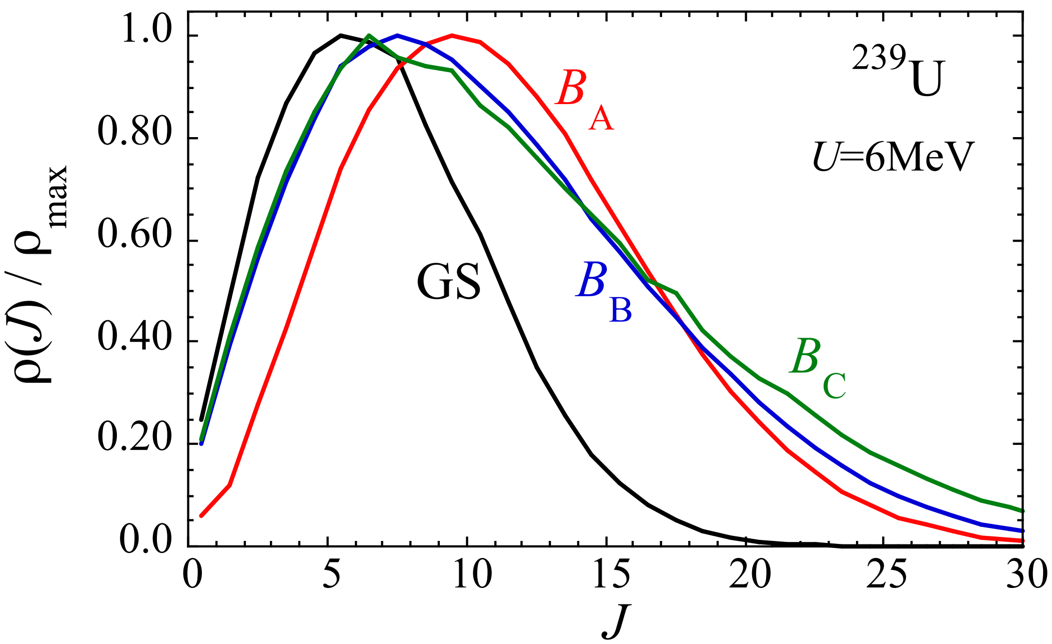
NLD at the fission saddle points: coherent treatment of triaxiality



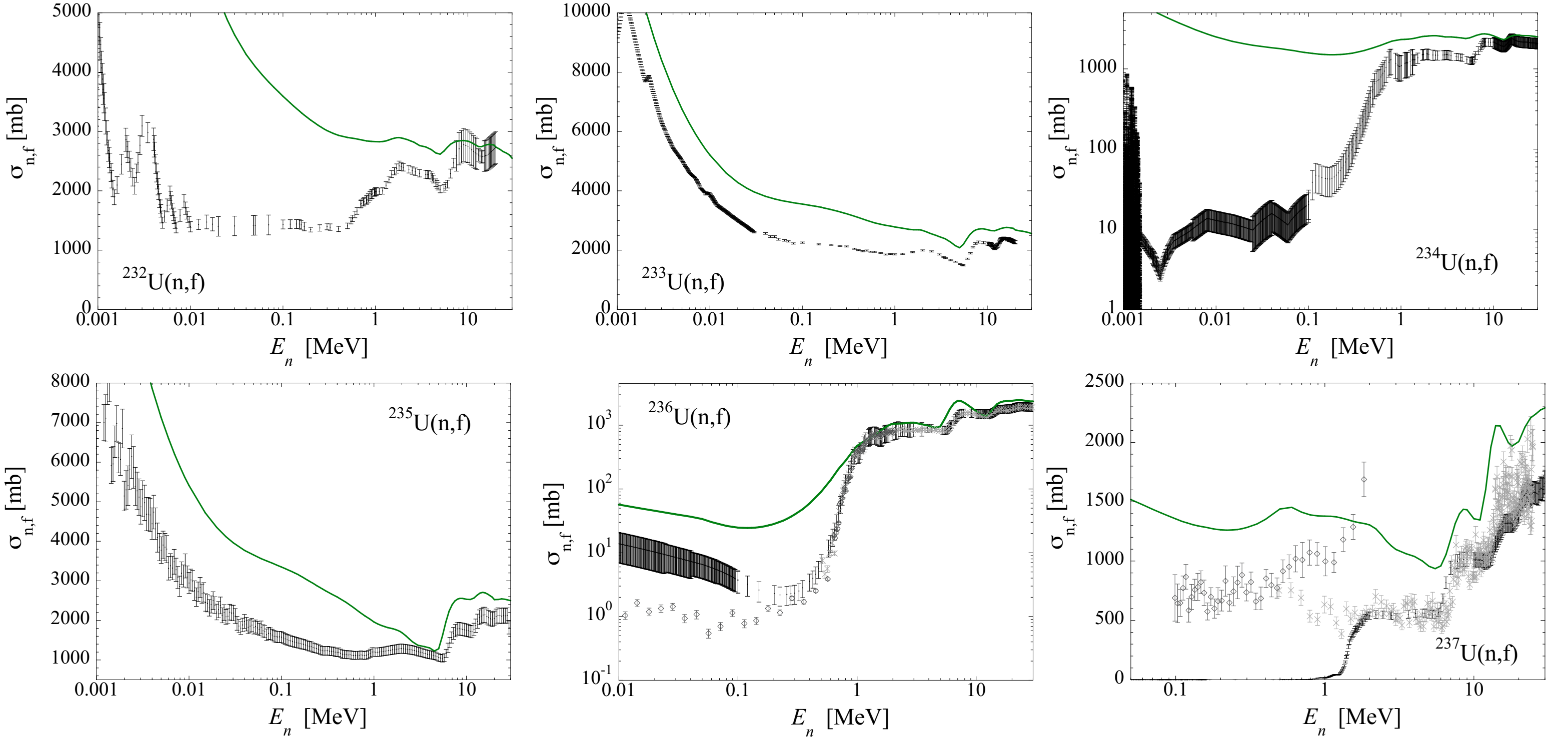


NLD for octupole deformations:
ρ x 2



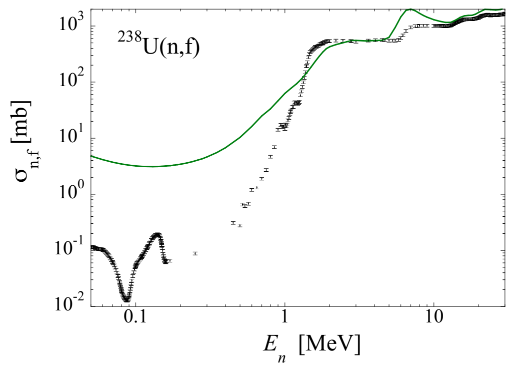


Default calculation of ^{xxx}U(n,f) cross sections with BSkG3 fission path [$E(\beta_{20}),\mu(\beta_{20})$] and NLD at saddle points



No adjustment on any of U parameters:

- f_B=1
- f_μ=1
- α=0, δ=0 inner *B*
- α=0, δ=0 outer *B*



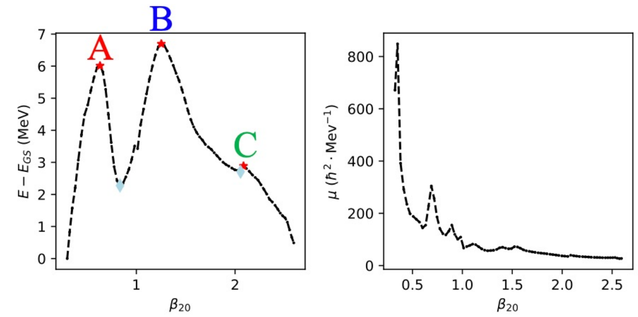
$$T(E,J,\pi) = \frac{T_A T_B}{T_A + T_B}$$

$$T(E,J,\pi) = \sum_d P(E-\varepsilon_d^{J,\pi}) + \int_{E_d}^{E} P(E-\varepsilon)\rho(\varepsilon,J,\pi)d\varepsilon$$

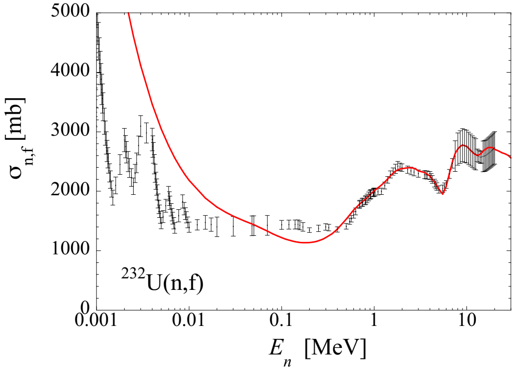
$$P_j(E) = \frac{1}{1+\exp(2K_j)}$$

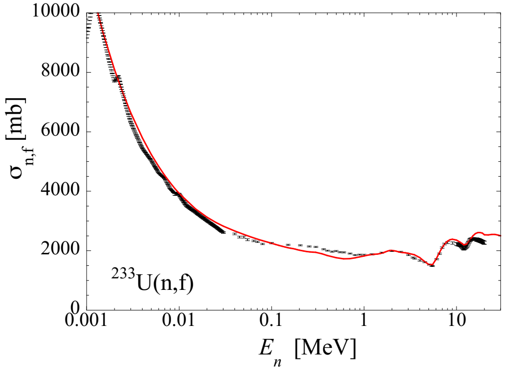
$$K_j = \pm\int_{a_j}^{b_j}\sqrt{2f_\mu\mu[f_B V(\beta_{20})-E_{GS}]/\hbar^2}d\beta_{20}$$

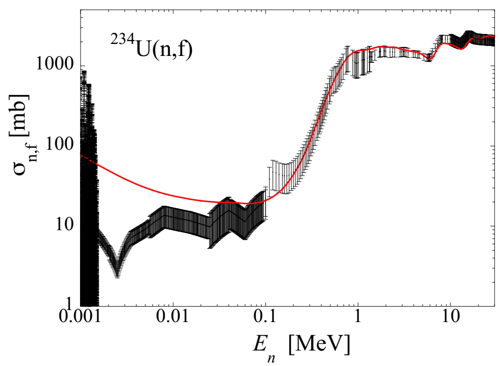
$$\rho^*(U) = e^{\alpha\sqrt{U-\delta}} \times \rho(U-\delta)$$



Coherent fit to $^{xxx}U(n,f)$ cross sections with BSkG3 fission path $[E(\beta_{20}),\mu(\beta_{20})]$ and NLD at saddle points

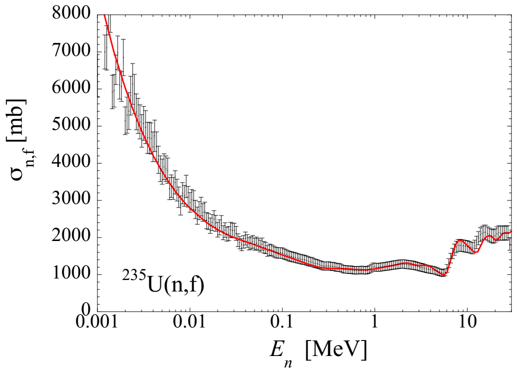


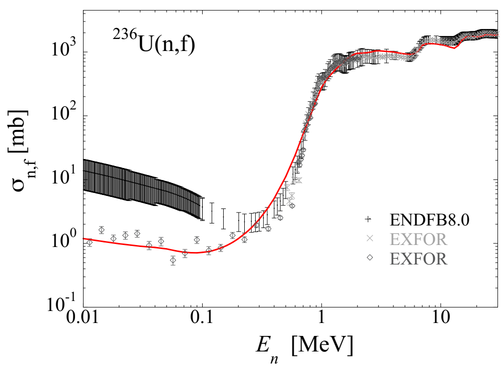


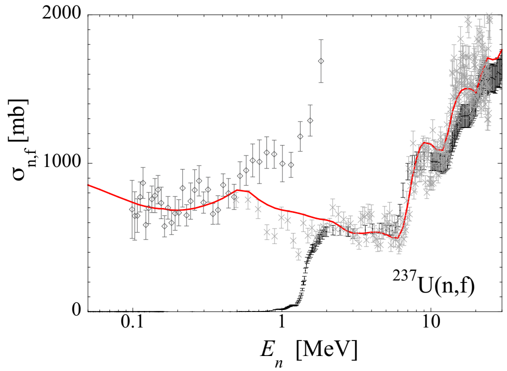


Adjustment for each U:

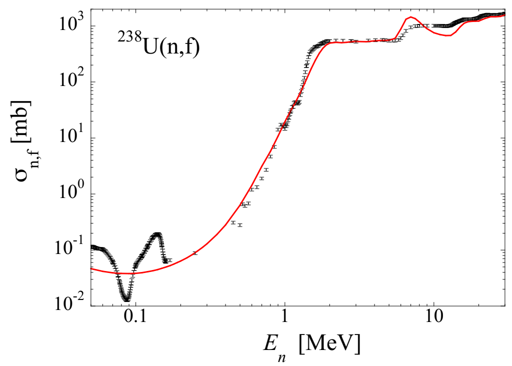
- f_B
- f_μ
- α,δ inner B
- α,δ outer B

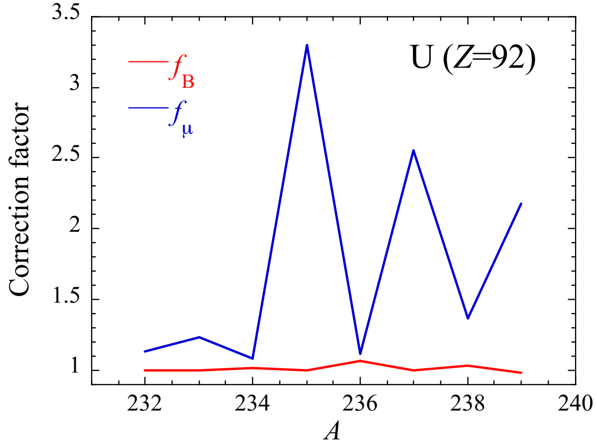


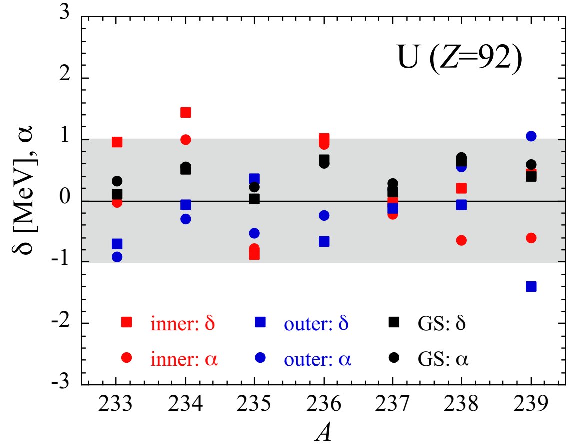




One unique set
$f_B, f_\mu, \alpha_i, \delta_i, \alpha_o, \delta_o$
for each U isotope, irrespective of the channel





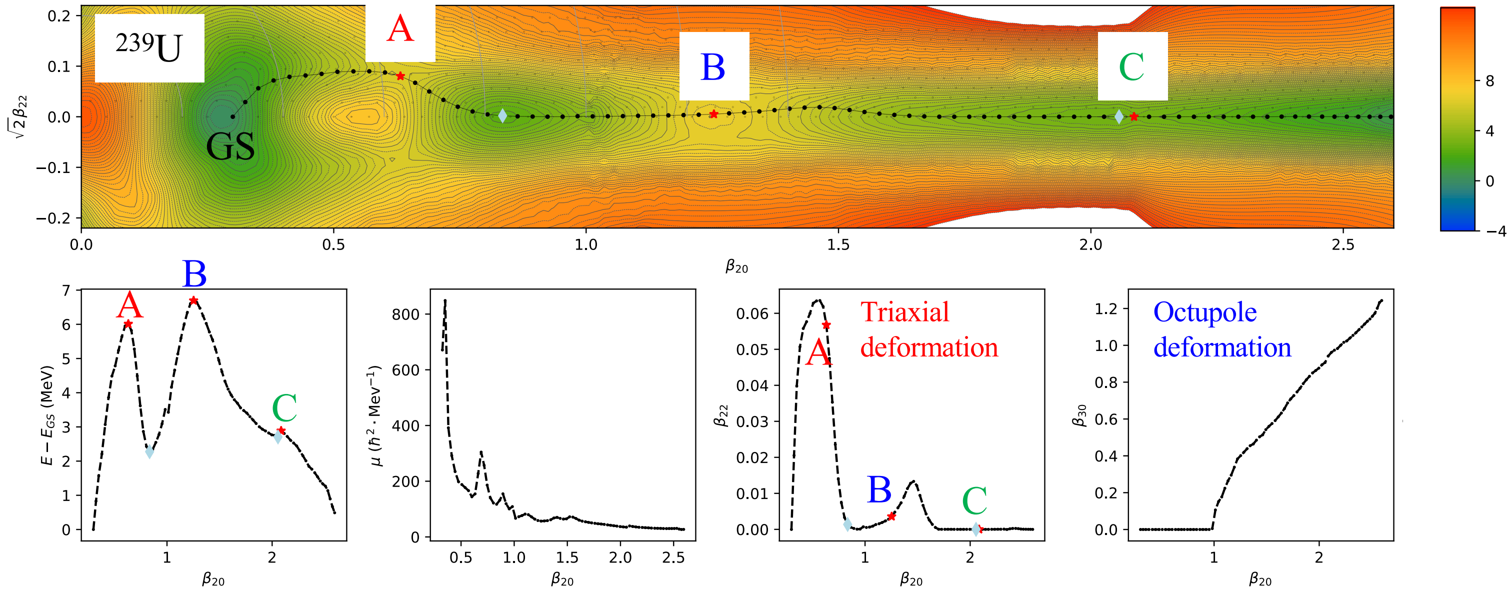


$$K_j = \pm \int_{a_j}^{b_j} \sqrt{2 f_\mu \mu [f_B V(\beta_{20}) - E_{GS}]/\hbar^2} d\beta_{20}$$

$$P_j(E) = \frac{1}{1+\exp(2K_j)}$$

$$\rho^*(U) = e^{\alpha\sqrt{U-\delta}} \times \rho(U-\delta)$$

NLD tables at the fission saddle points and isomers



Energy-, spin- and parity-depencent NLD tables calculated for ~ 1600 PES ($90 \le Z \le 110$)

→ to be extended to ~2000 nuclei ($90 \le Z \le 118$) ?

$0.25 \le U \le 200$MeV; $0 \le J \le 50$; $\pi = \pm$

```
*****************************************************************************************************
*  Z= 92 A=236: Positive-Parity Spin-dependent Level Density [MeV-1] for U 236 b2 = 0.61 b2 = 0.61 b30= 0.00 b40= 0.26 Icr=  41.61  *
*****************************************************************************************************
```

U[MeV]	T[MeV]	NCUMUL	RHOOBS	RHOTOT	J=00	J=01	J=02	J=03	J=04	J=05	J=06	J=07	J=08	J=09	J=10	J=11	J=12	J=13	J=14
0.25	0.108	1.10E+01	8.69E+01	1.03E+03	3.08E+00	7.69E-01	8.46E+00	6.92E+00	1.46E+01	1.23E+01	1.46E+01	8.46E+00	7.69E+00	3.08E+00	3.08E+00	7.69E-01	1.54E+00	7.69E-01	7.69E-01
0.50	0.153	3.80E+01	1.29E+02	1.74E+03	4.67E+00	1.33E+00	1.13E+01	8.67E+00	1.53E+01	1.27E+01	1.67E+01	1.27E+01	1.47E+01	1.00E+01	8.00E+00	5.33E+00	3.33E+00	1.33E+00	1.33E+00
0.75	0.187	8.80E+01	2.66E+02	3.56E+03	7.22E+00	3.89E+00	2.22E+01	2.22E+01	3.61E+01	2.94E+01	3.50E+01	2.50E+01	2.44E+01	1.44E+01	1.39E+01	1.06E+01	9.44E+00	5.56E+00	3.89E+00
1.00	0.216	1.74E+02	4.28E+02	6.05E+03	9.00E+00	6.00E+00	2.90E+01	3.10E+01	5.15E+01	4.80E+01	5.40E+01	4.35E+01	4.40E+01	3.15E+01	2.70E+01	1.70E+01	1.45E+01	8.00E+00	6.50E+00
1.25	0.241	3.83E+02	1.24E+03	1.76E+04	2.55E+01	1.85E+01	7.95E+01	8.85E+01	1.44E+02	1.40E+02	1.56E+02	1.34E+02	1.27E+02	9.45E+01	8.25E+01	5.15E+01	3.90E+01	2.10E+01	1.55E+01
1.50	0.264	8.33E+02	2.36E+03	3.45E+04	4.60E+01	3.60E+01	1.46E+02	1.68E+02	2.64E+02	2.52E+02	2.84E+02	2.44E+02	2.32E+02	1.82E+02	1.59E+02	1.16E+02	8.85E+01	5.70E+01	3.75E+01
1.75	0.286	1.88E+03	6.05E+03	9.07E+04	9.95E+01	8.35E+01	3.36E+02	4.06E+02	6.34E+02	6.38E+02	7.38E+02	6.42E+02	6.21E+02	4.88E+02	4.10E+02	2.98E+02	2.26E+02	1.55E+02	1.12E+02
2.00	0.305	4.07E+03	1.14E+04	1.73E+05	1.88E+02	1.64E+02	6.36E+02	7.64E+02	1.16E+03	1.17E+03	1.34E+03	1.19E+03	1.16E+03	9.32E+02	7.94E+02	5.87E+02	4.48E+02	3.02E+02	2.18E+02
2.25	0.324	9.10E+03	2.89E+04	4.54E+05	4.14E+02	3.69E+02	1.42E+03	1.75E+03	2.71E+03	2.82E+03	3.30E+03	3.05E+03	3.01E+03	2.47E+03	2.15E+03	1.64E+03	1.28E+03	8.92E+02	6.29E+02
2.50	0.341	1.93E+04	5.29E+04	8.39E+05	7.42E+02	6.78E+02	2.60E+03	3.23E+03	4.98E+03	5.13E+03	5.90E+03	5.41E+03	5.33E+03	4.47E+03	3.92E+03	3.03E+03	2.39E+03	1.71E+03	1.25E+03
2.75	0.358	4.16E+04	1.25E+05	2.05E+06	1.53E+03	1.44E+03	5.45E+03	7.01E+03	1.10E+04	1.16E+04	1.36E+04	1.27E+04	1.28E+04	1.08E+04	9.62E+03	7.57E+03	6.10E+03	4.46E+03	3.31E+03
3.00	0.374	8.52E+04	2.24E+05	3.70E+06	2.75E+03	2.62E+03	9.86E+03	1.26E+04	1.95E+04	2.05E+04	2.38E+04	2.24E+04	2.23E+04	1.92E+04	1.73E+04	1.37E+04	1.11E+04	8.18E+03	6.12E+03
3.25	0.389	1.76E+05	5.07E+05	8.67E+06	5.45E+03	5.25E+03	1.98E+04	2.58E+04	4.04E+04	4.37E+04	5.19E+04	5.00E+04	5.10E+04	4.46E+04	4.06E+04	3.30E+04	2.72E+04	2.05E+04	1.56E+04
3.50	0.404	3.48E+05	8.62E+05	1.49E+07	9.20E+03	8.89E+03	3.35E+04	4.35E+04	6.81E+04	7.36E+04	8.68E+04	8.35E+04	8.50E+04	7.50E+04	6.88E+04	5.65E+04	4.69E+04	3.58E+04	2.77E+04
3.75	0.418	6.87E+05	1.86E+06	3.30E+07	1.81E+04	1.75E+04	6.61E+04	8.71E+04	1.38E+05	1.51E+05	1.81E+05	1.77E+05	1.82E+05	1.63E+05	1.50E+05	1.25E+05	1.06E+05	8.22E+04	6.46E+04
4.00	0.432	1.30E+06	3.08E+06	5.53E+07	2.99E+04	2.90E+04	1.09E+05	1.43E+05	2.25E+05	2.46E+05	2.94E+05	2.88E+05	2.97E+05	2.67E+05	2.49E+05	2.09E+05	1.78E+05	1.40E+05	1.11E+05

To be ready in a few weeks/months... (today ~ 1300 nuclei)

THANK YOU
FOR
YOUR ATTENTION