Theoretical Nuclear Level Density models for practical applications

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The Back-Shifted Fermi Gas Model

$$\boxed{\rho_F(E_x, J, \Pi) = \frac{1}{2}\,\frac{2J+1}{2\sqrt{2\pi}\sigma^3}\exp\left[-\frac{(J+\frac{1}{2})^2}{2\sigma^2}\right]\frac{\sqrt{\pi}}{12}\,\frac{\exp\left[2\sqrt{aU}\right]}{a^{1/4}U^{5/4}}}$$

where $U \approx E_x - \chi\Delta$ (χ=0, 1, 2 for o-o, odd-A, e-e) Pairing effect

$$a = a(E_x) \approx \tilde{a}\left[1 + \delta W \frac{1-\exp(-\gamma U)}{U}\right]$$ Shell effect

$$\sigma^2(T) = \frac{\mathcal{I}_{\rm rig}}{\hbar^2}\frac{a(T)}{\tilde{a}}T \approx \frac{\mathcal{I}_{\rm rig}}{\hbar^2}\frac{1}{\tilde{a}}\sqrt{aU}$$ Spin cut-off factor

Many approximations to derive an analytical expression

- Independent particle approximations
- Saddle point approximation
- Statistical distribution at all energies is assumed
- Continuous SPL density approximation
- Empirical shell effect included
- Pairing effects reduced to an energy shift Δ (no supraconducting phase)
- Similar T-dependence (hence shell effect) for the 3 a-parameters

  $a_S(T)=S(T)/2T$; $a_U(T)=U(T)/T^2$; $a_\sigma(T)=\sigma^2(T)/T$
- Equiparity
- No explicit account of collective enhancement $K_{rot}(E_x)\ K_{vib}(E_x)$
- Approximate constant-T behaviour at low energies

The Constant-Temperature approximation at low energies

- Divergence of the Fermi Gas formula at U=0

$$\rho(U) = \frac{\sqrt{\pi}}{12\ a^{1/4}\ U^{5/4}} e^{2\sqrt{a\ U}} \xrightarrow[U \to 0]{} \infty$$

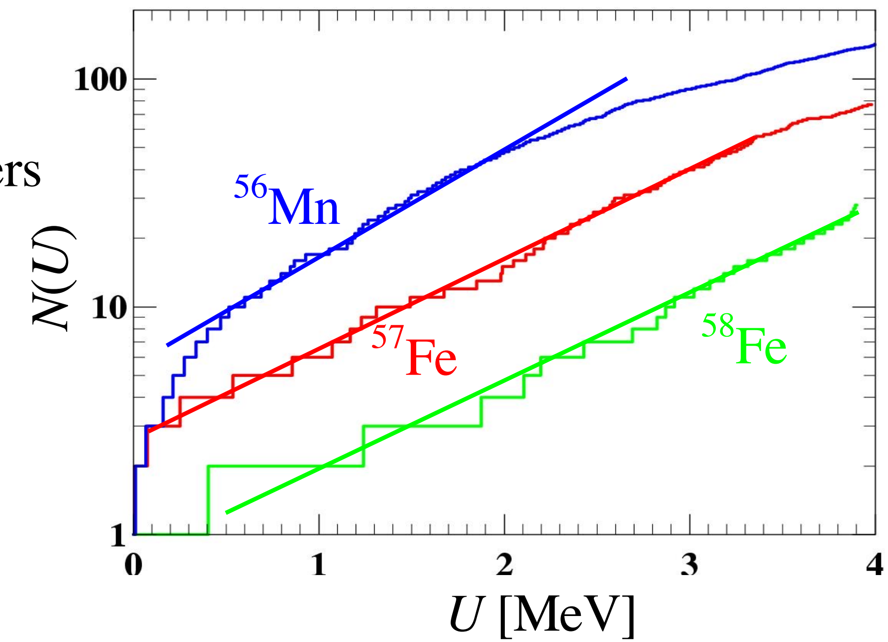
- Data on the cumulative numbers of low-lying nuclear levels are also very important for level density analyses. The observed energy dependence of the cumulative number of levels can be described rather well by the function

$$N(U) = \exp\left[(U - U_0)/T\right]$$

where U_0 and T are free parameters

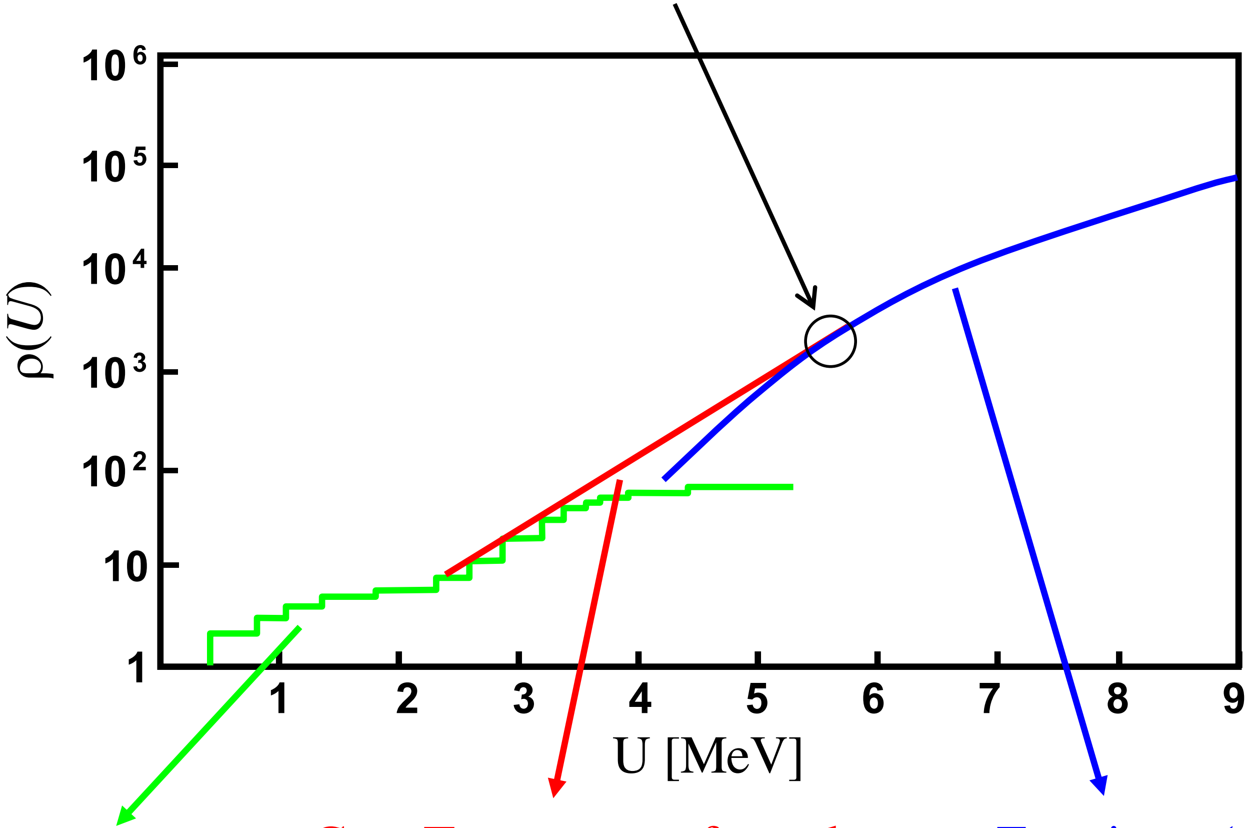
at low energies:

$$\rho(U) = \frac{dN(U)}{dU} = \frac{1}{T}\exp\left[(U - U_0)/T\right]$$



The Constant-Temperature approximation at low energies

Matching conditions : continuity of ρ and of its derivative (sometimes difficult)



Discrete levels (spectroscopy)

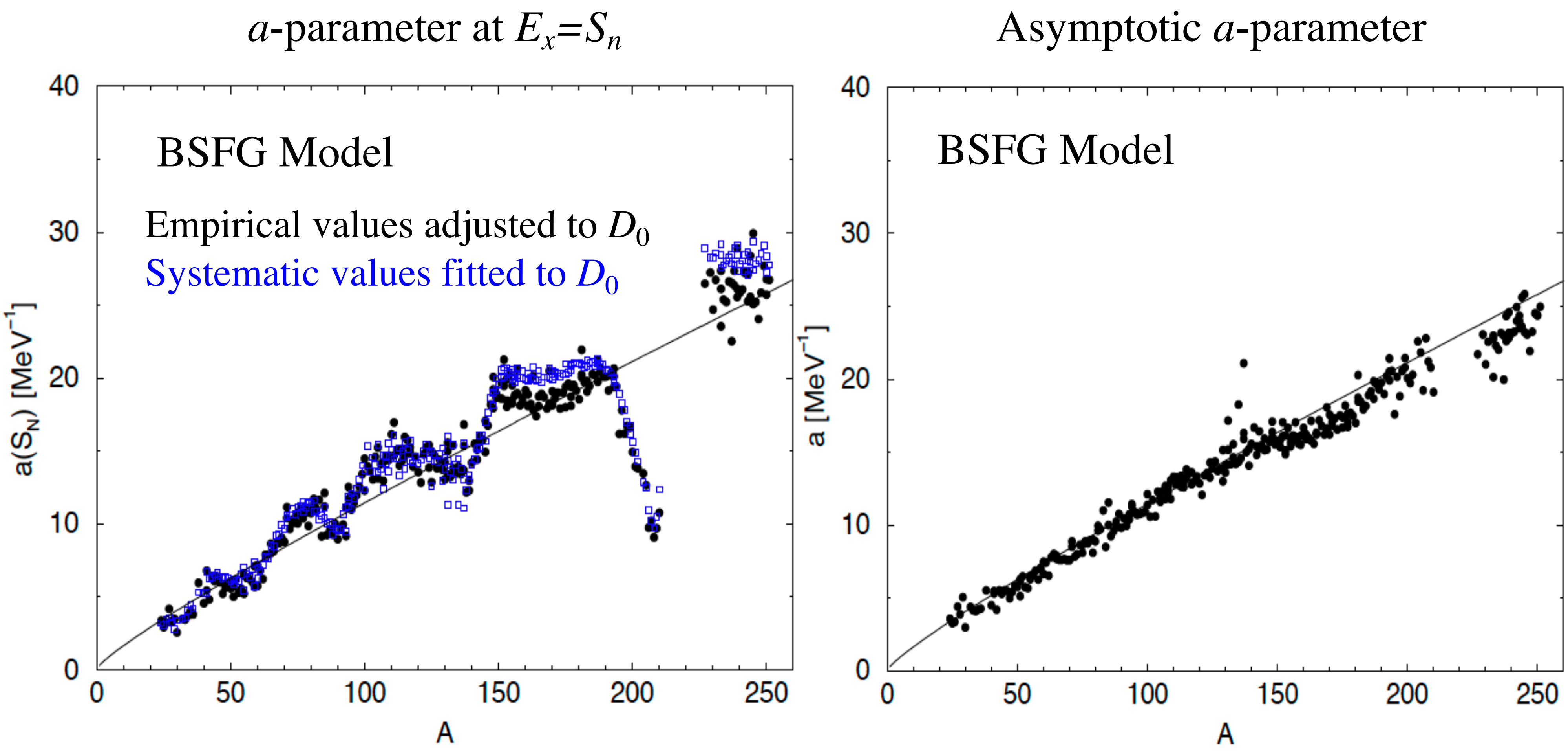
Cst - Temperature formula

$$\rho(U) = \frac{1}{T}\exp\left[(U - U_0)/T\right]$$

Fermi gas (adjusted at S_n)

$$\rho(U) = \frac{\sqrt{\pi}}{12\ a^{1/4}\ U^{5/4}} e^{2\sqrt{a\ U}}$$

Shortcoming in the BSFG approximation compensated by parameter adjustment



Quite successful description of cumulative number of low-lying levels and s-wave spacings … BUT ... What is the predictive power outside the fitted range and for nuclei where no experimental data exists (especially isospin dependence !) ??

Mean Field + Statistical NLD formula

Partition function method applied to the discrete SPL scheme predicted by a MF model

$$\omega(U) = \frac{\mathrm{e}^{S(U)}}{(2\pi)^{3/2}\sqrt{D(U)}} \qquad\qquad U(T) = E(T) - E(T=0)$$

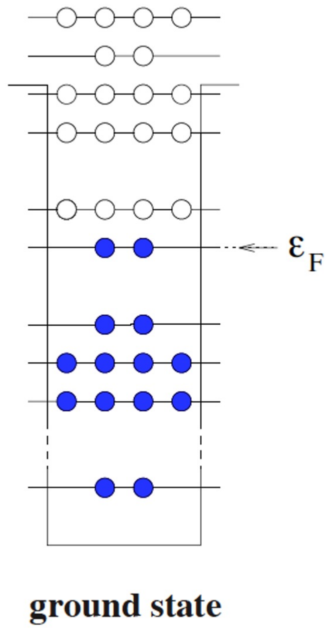
$$S(T) = 2\sum_{q=n,p}\sum_k \ln\Big[1+\exp(-E_q^k/T)\Big] + \frac{E_q^k/T}{1+\exp(-E_q^k/T)}$$

$$E(T) = \sum_{q=n,p}\sum_k \varepsilon_q^k \left[1 - \frac{\varepsilon_q^k - \lambda_q}{E_q^k}\tanh(\frac{E_q^k}{2T})\right] - \frac{\Delta_q^2}{G}$$

$$N_q = \sum_k\left[1 - \frac{\varepsilon_q^k - \lambda_q}{E_q^k}\tanh(\frac{E_q^k}{2T})\right]$$

$$\frac{2}{G_q} = \sum_k \frac{1}{E_q^k}\tanh(\frac{E_q^k}{2T})$$

$$\sigma^2(T) = \frac{1}{2}\sum_{q=n,p}\sum_k \omega_q^{k^2}\,\mathrm{sech}^2(\frac{E_q^k}{2T})$$



→ Exact solution the analytical formulas try to reproduce

→ Tables of NLD (no analytical approximation) !

Mean Field + Statistical NLD formula

Reliability: Exact solution the analytical formulas try to mimic
Accuracy: Competitive with parametrized formulas in reproducing experimental data

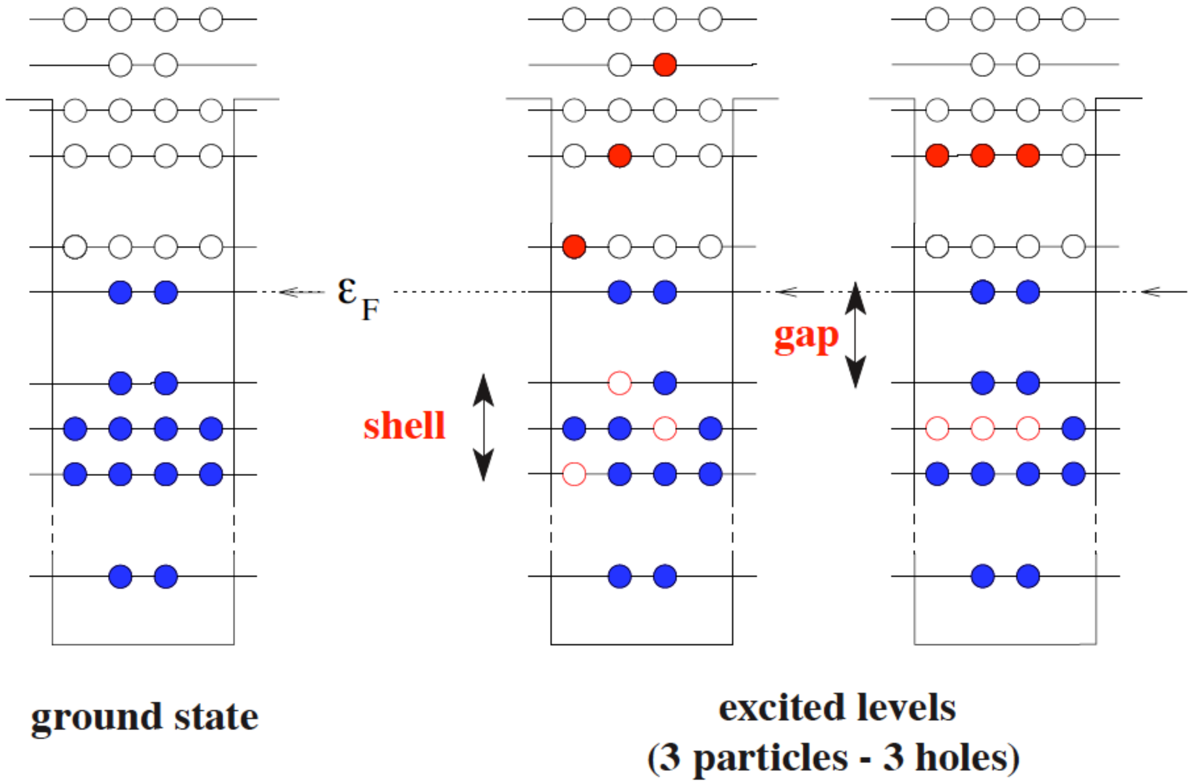
But the MF + Statistical approach still makes fundamental approximations :

- Saddle point approximation & Statistical distribution
- Simple vibrational enhancement
- Equiparity
- Sensitive to the adopted potential, i.e SPL and pairing scheme
- Phenomenological deformed-to-spherical transition at increasing energies
- Etc…

Global combinatorial NLD formula

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



→ Tables of NLD (no analytical approximation) !

- **Skyrme / Gogny HFB**
  $\Rightarrow$ **SPL scheme; Pairing strength & GS deformation**

- **HFB + Combinatorial calculation**
  $\Rightarrow$ **Incoherent particle-hole $\omega_{ph}(U,M,\pi)$**
  $\Rightarrow$ **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 λ=2, 3 and 4 phonons**
  - **Folding of the total incoherent $\omega_{tot}(U,M,\pi)$ with $\omega_{vib}(U,M,\pi)$**
  $\Rightarrow$ **band-head state densities $\omega_{bh}(U,M,\pi)$**

- **Construction of spherical level densities :**
  $\Rightarrow$ $\rho_{sph}(U,J,\pi) = \omega_{bh}(U,M=J,\pi) - \omega_{bh}(U,M=J+1,\pi)$

- **Construction of deformed level densities, i.e. rotational bands on top of every band-head state**

  $\Rightarrow$ $\rho_{def}(U,J,\pi) = ½ \, \Sigma_K \, \omega_{tot}(U-E_{rot}(J,K),K,\pi)$

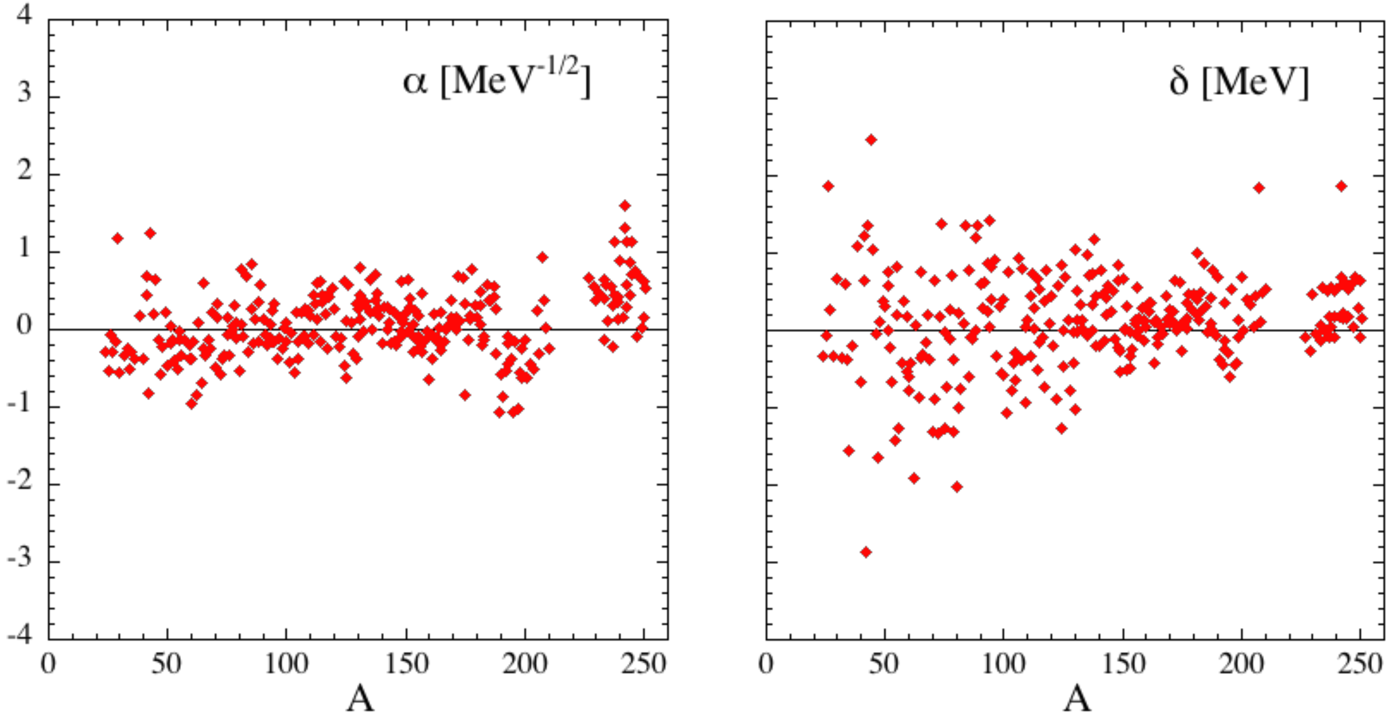
- **Mixing of deformed and spherical level densities using a phenomenological expression and/or phenomenological transition from deformed to spherical shape at increasing energy.**

→ Tables of NLD (no analytical approximation) !

Global adjustment for practical applications

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

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



Extension to T-dependent HFB calculations based on the D1M Gogny force

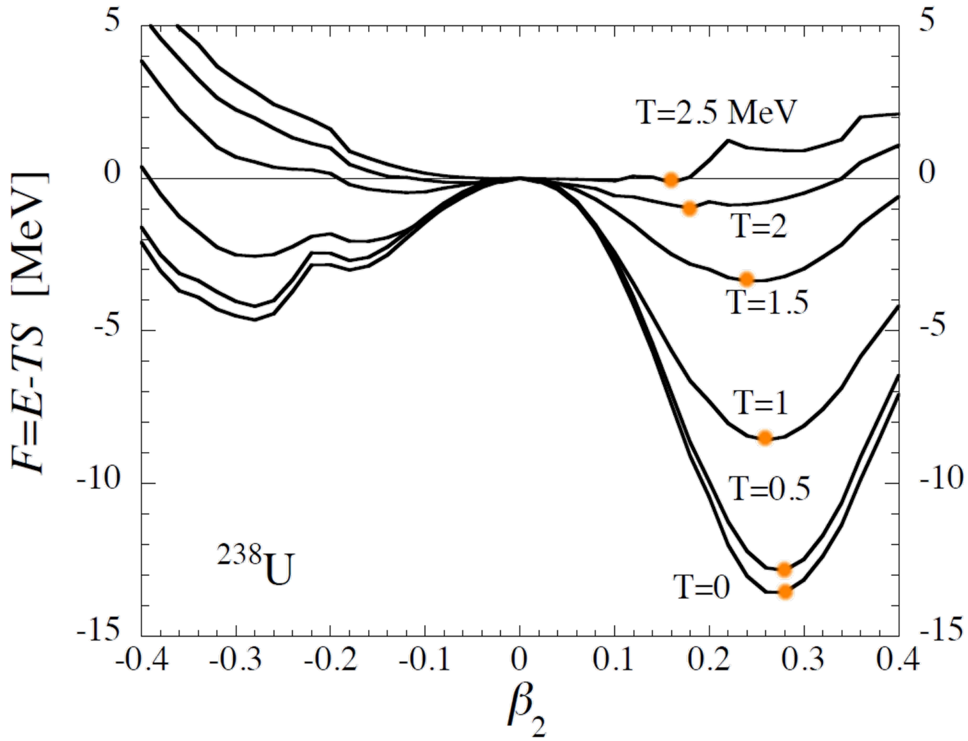
Temperature-dependent HFB calculations as input to NLD model: (Martin et al. 2003)

→ the free energy $F=E\text{-}TS$ is minimized as a function of the deformation for each temperature T

→ average value of any observable given by $\langle \mathcal{O} \rangle = \frac{\int \mathcal{O} \exp[-F(q)/T] dq}{\int \exp[-F(q)/T] dq}$ (q = quad def)

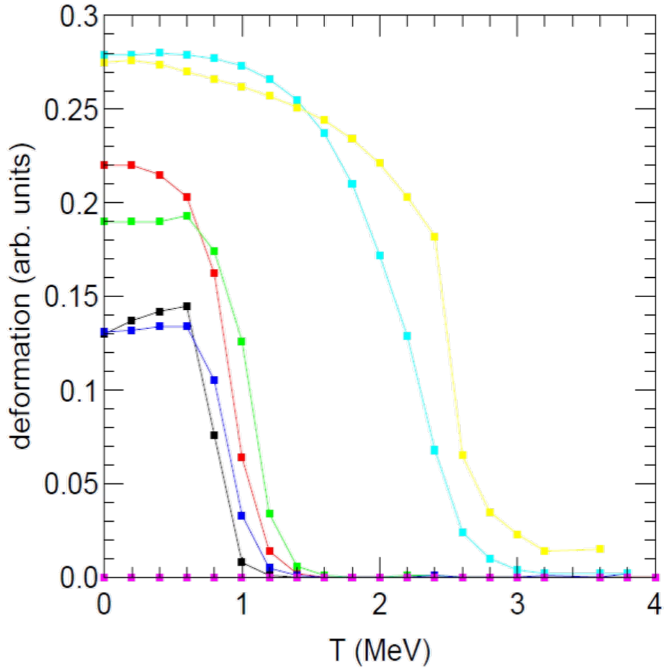
→ nuclear deformation approximated at the lowest free energy F

→ equilibrium shape of the nucleus at each temperature.

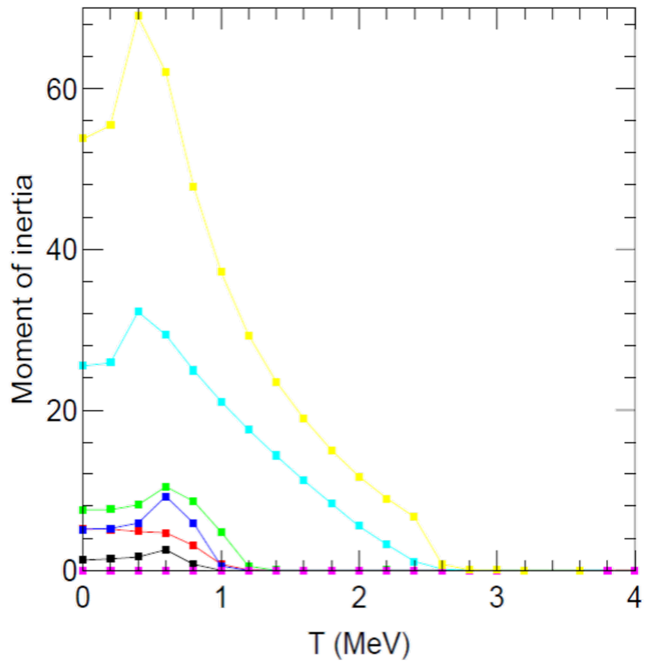


Temperature evolution of nuclear structure properties relevant for level density calculations within the combinatorial model

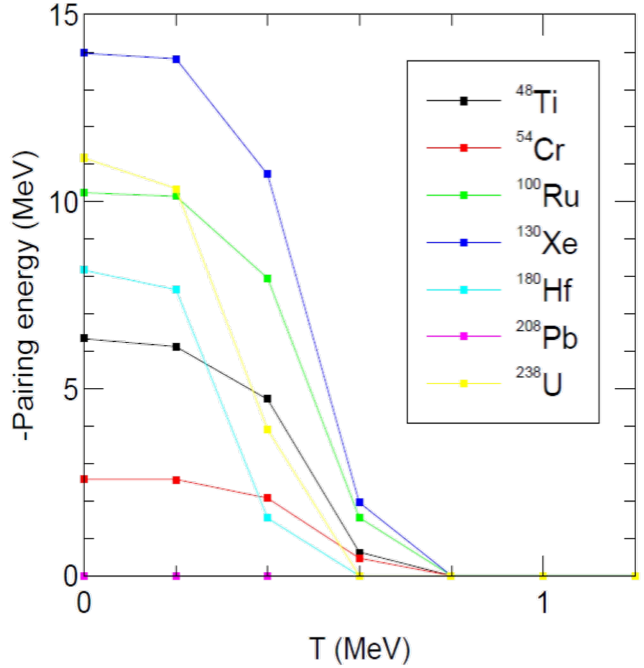
Quadrupole deformation



Cranking moment of Inertia

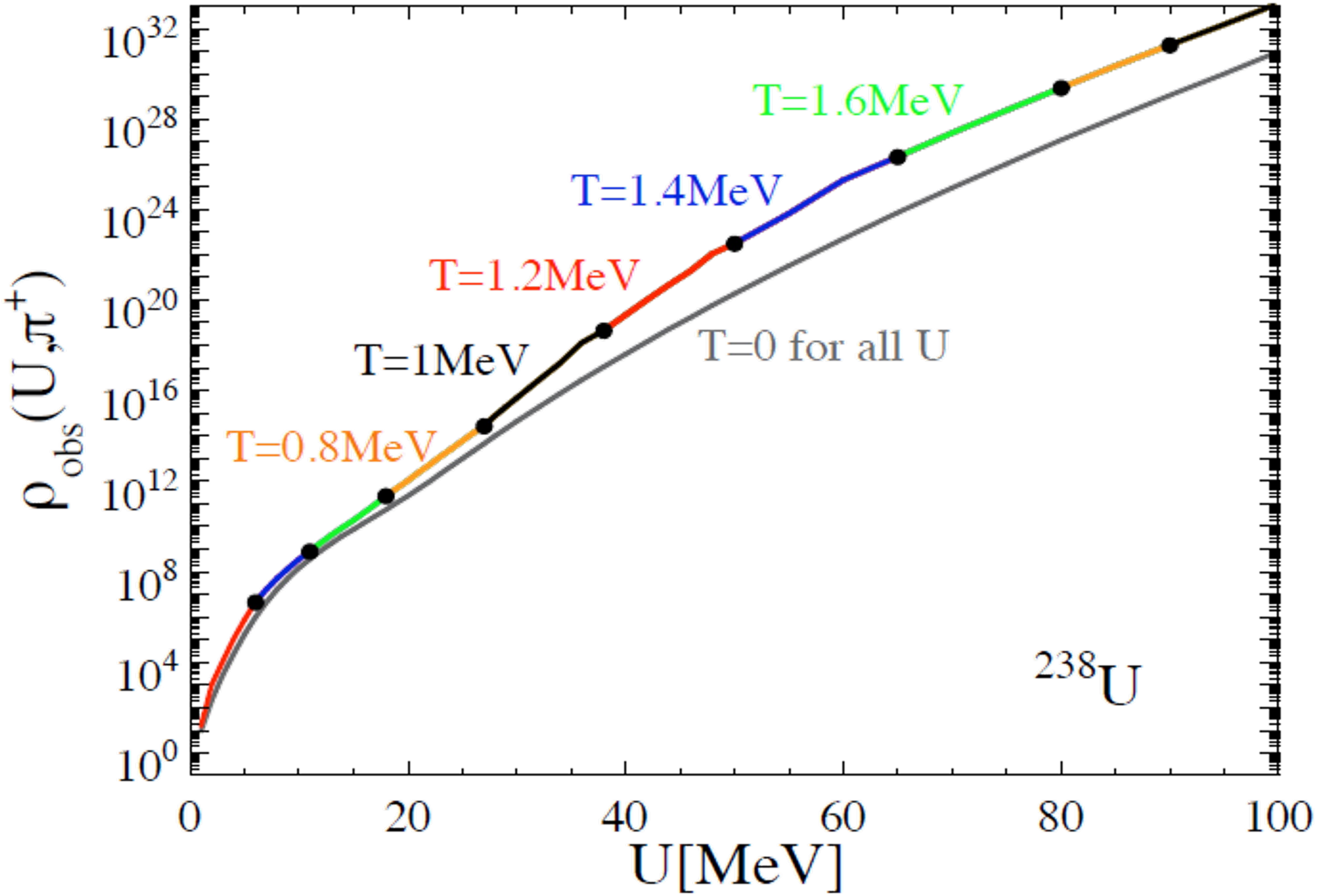


Total pairing energy



T-dependent HFB calculation and the Combinatorial Approach

^{238}U level densities calculated over a restricted energy range according to the correspondance between the excitation energy *U* and the temperature *T*

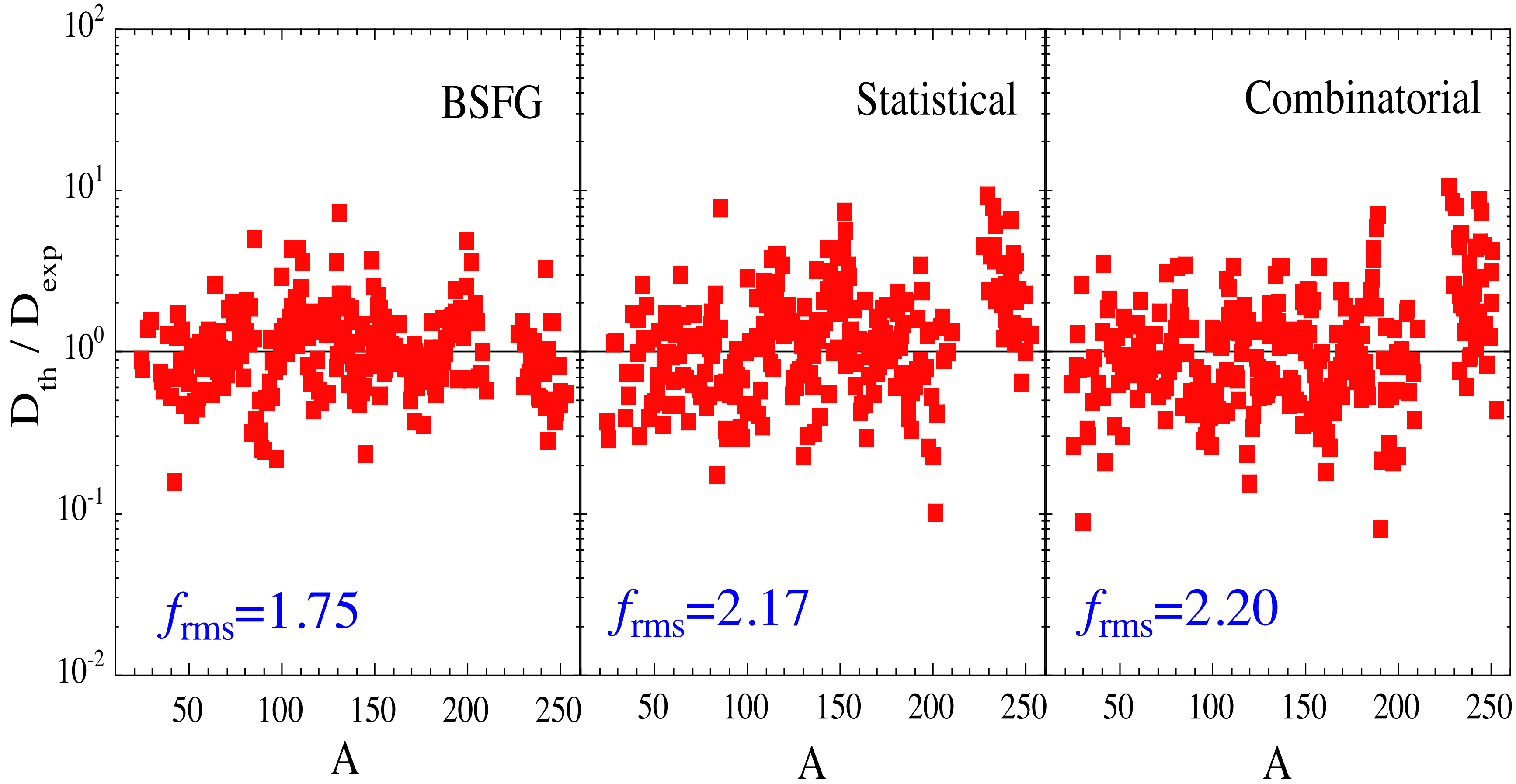


Comparison with experimental neutron resonance spacings

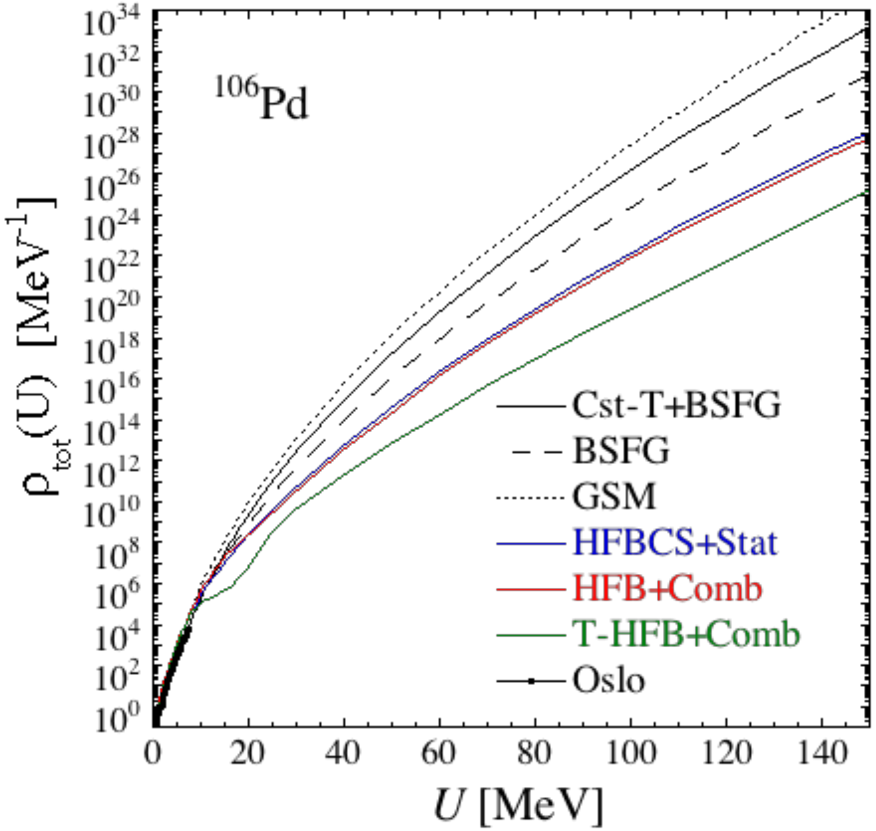
~300 exp. D_0 from RIPL-3 at $U=S_n$ from thermal n-capture data on a target of spin J_0 and parity π_0

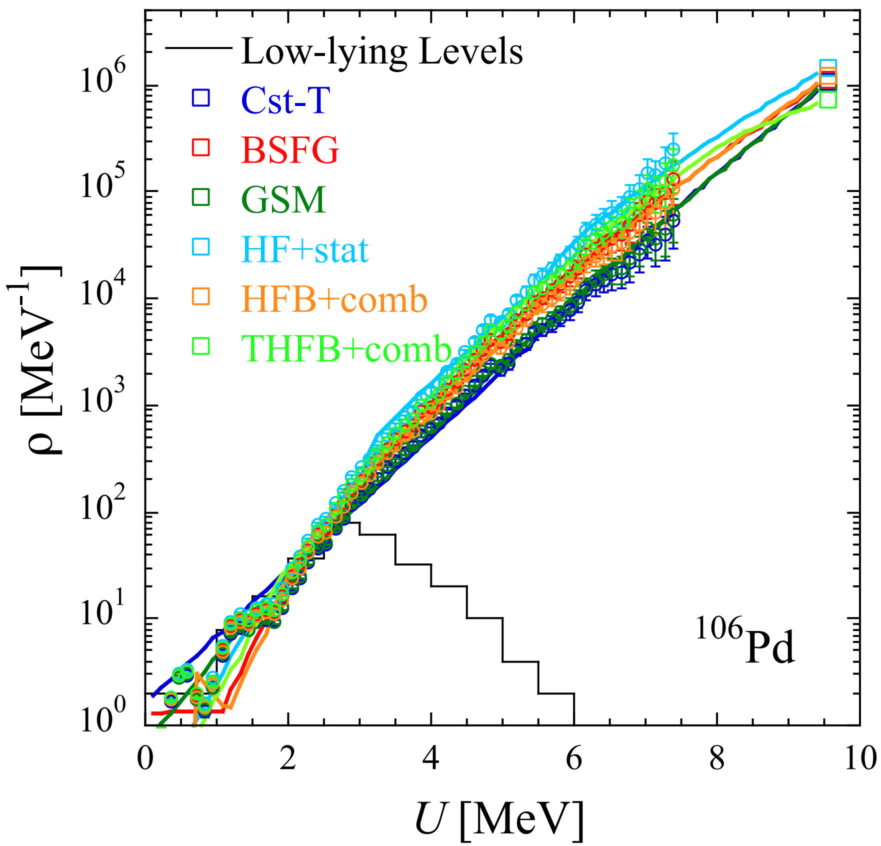
$$D_0 = \frac{1}{\rho(S_n, J_0+1/2, \pi_0) + \rho(S_n, J_0-1/2, \pi_0)} \quad J_0>0$$

$$= \frac{1}{\rho(S_n, J_0+1/2, \pi_0)} \quad J_0=0$$

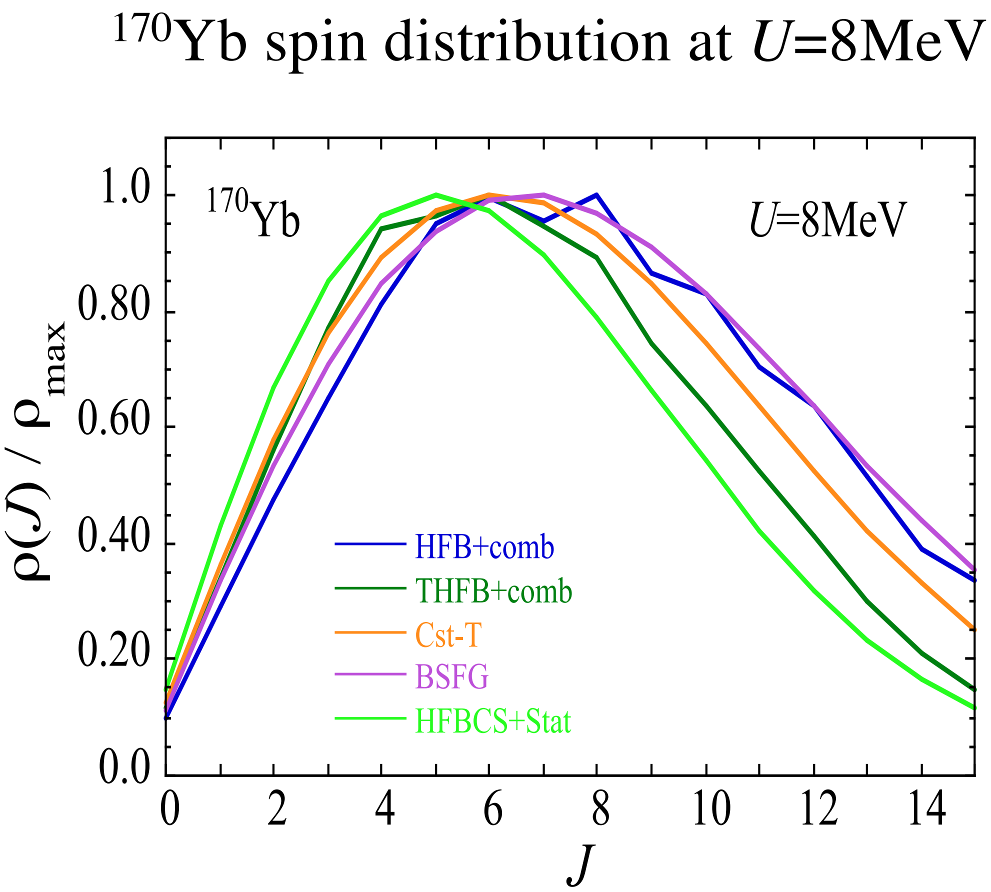


^{106}Pd total nuclear level density

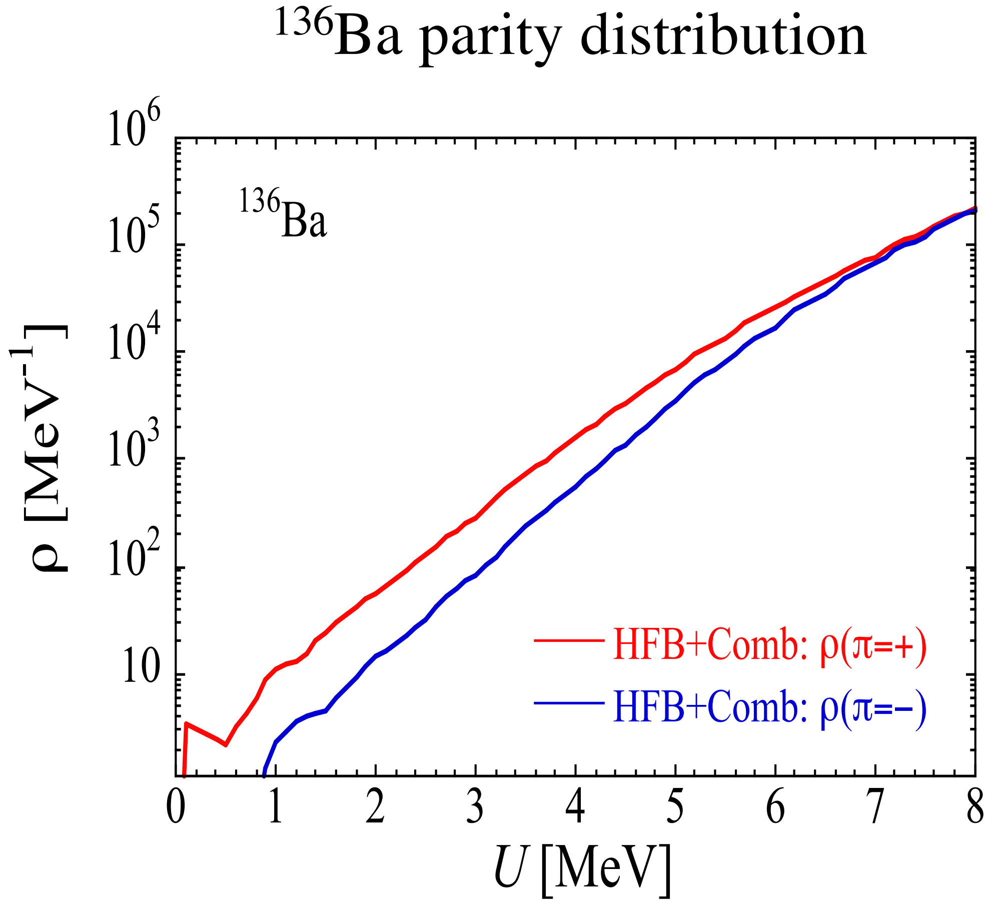




S_n=9.56MeV



^{170}Yb spin distribution at U=8MeV
^{170}Yb
U=8MeV
$\rho(J) / \rho_{max}$
J
1.0
0.80
0.60
0.40
0.20
0.0
0
2
4
6
8
10
12
14
HFB+comb
THFB+comb
Cst-T
BSFG
HFBCS+Stat



^{136}Ba parity distribution
^{136}Ba
ρ [MeV^{-1}]
U [MeV]
10^6
10^5
10^4
10^3
10^2
10
0
1
2
3
4
5
6
7
8
HFB+Comb: $\rho(\pi=+)$
HFB+Comb: $\rho(\pi=-)$

Nuclear Level Densities

Experimental data

- Low-lying levels
- *s*/*p*-wave resonance spacings
- Oslo data (+ Shape Method)

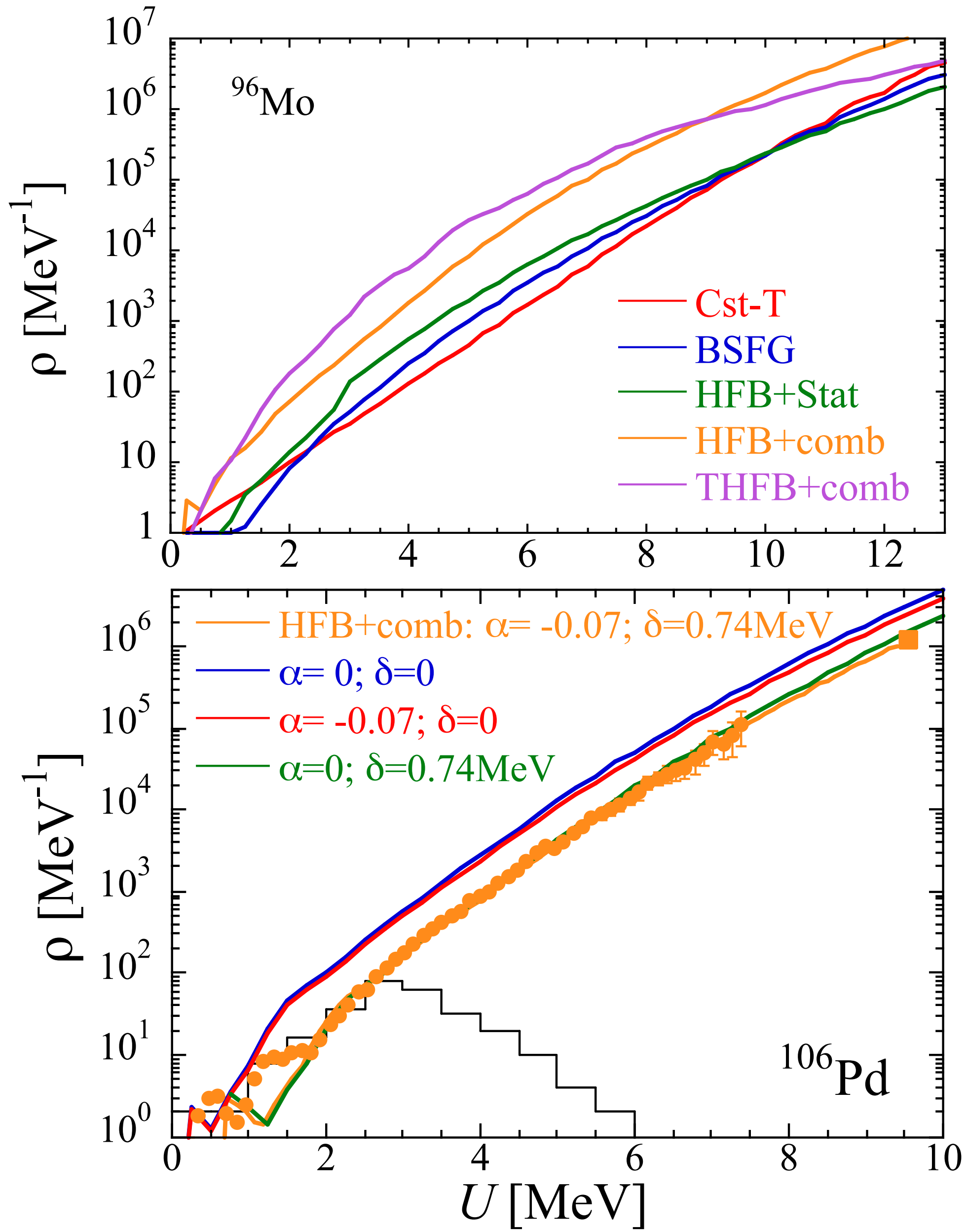
Models

- Constant-T + BSFG
- BSFG
- Mean-Field+statistical
- Mean-Field+combinatorial
- (Moments methods)
- (Shell model)

Parameter adjustment

- GS properties: β_2, δW, *SPL*, ...
- Analytical: a, Δ, T, ...
- Tables: α and δ

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



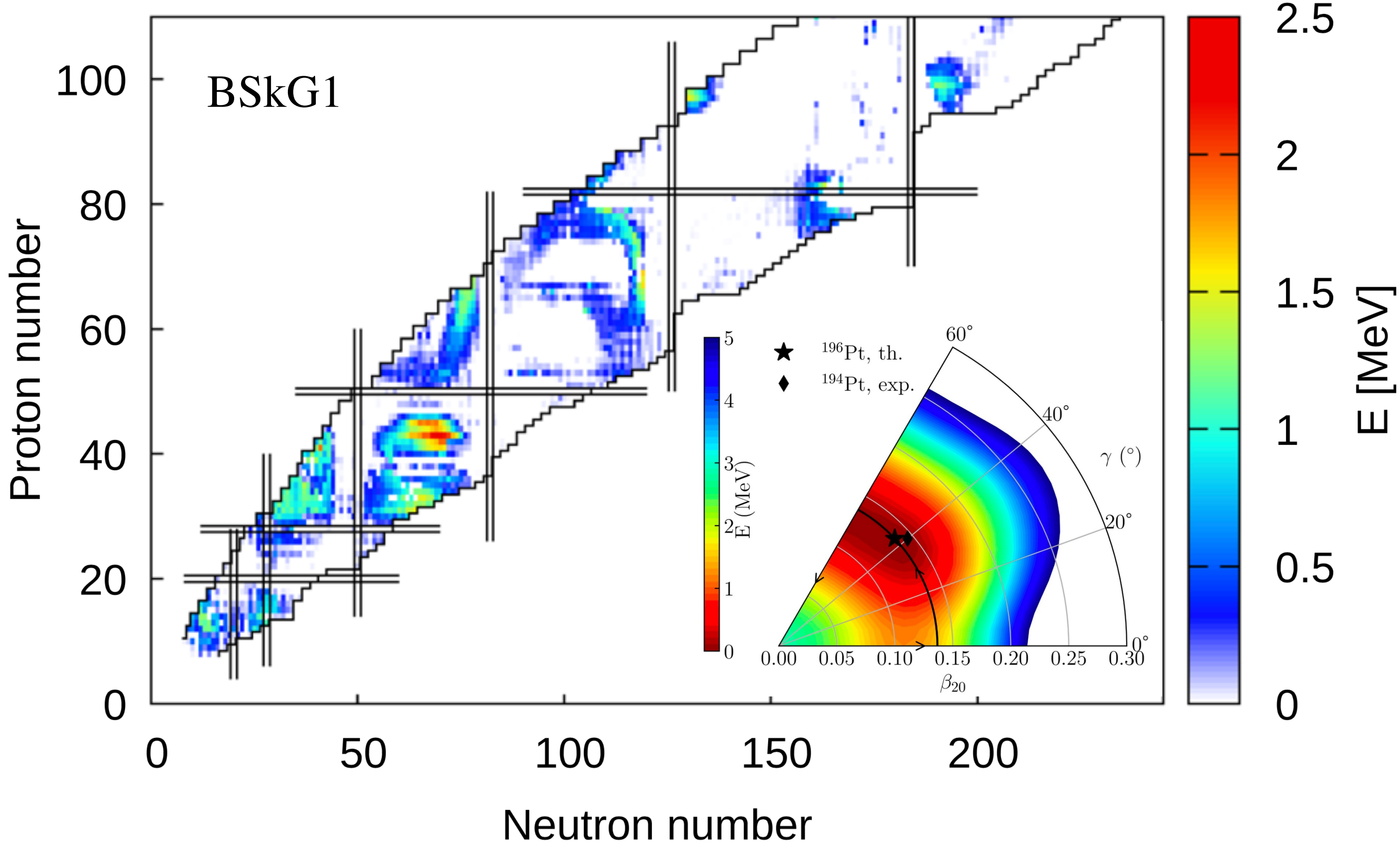
New developments in Nuclear Level Density models

- BSkG2 + Combinatorial model including triaxility
  (W. Ryssens, S. Hilaire, S. Goriely)
- QRPA + Boson Exchange model
  (S. Hilaire, S. Péru, S. Goriely)

New HFB calculations allowing for triaxial deformations

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

Binding energy differences between calculations restricted to axial quadrupole deformations and unrestricted calculations (triaxial)



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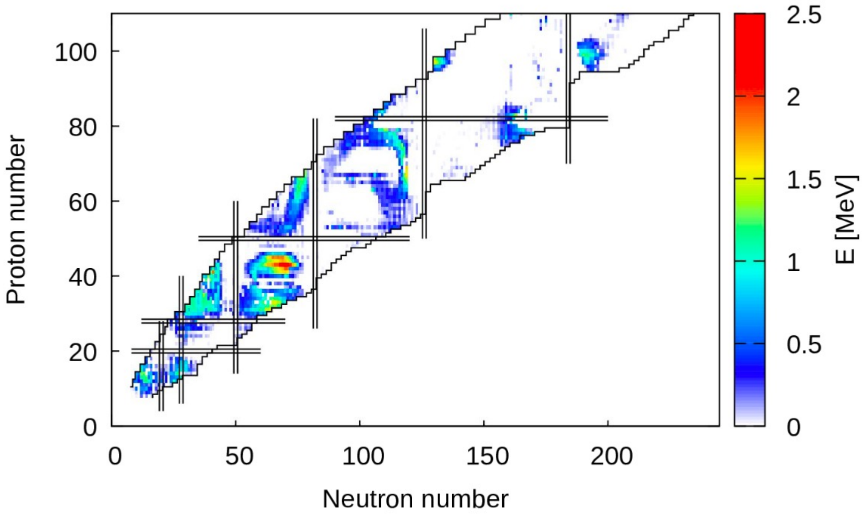
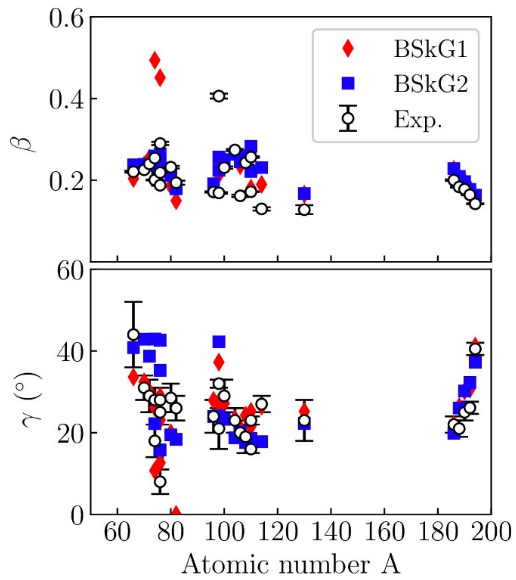
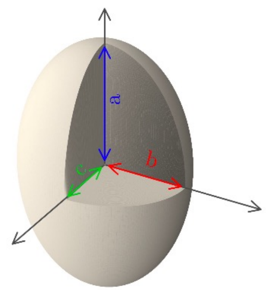
Wouter Ryssens (ULB)

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

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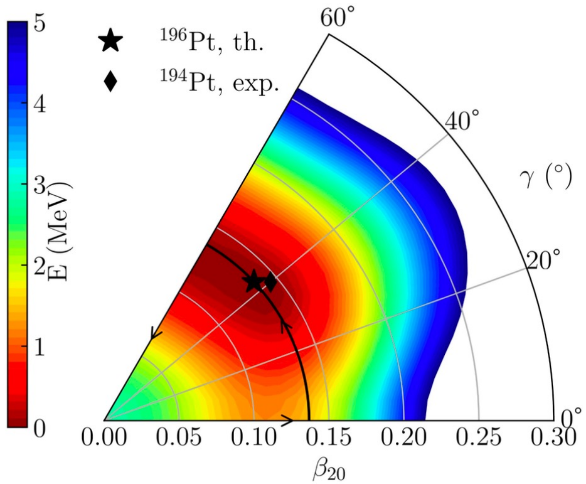
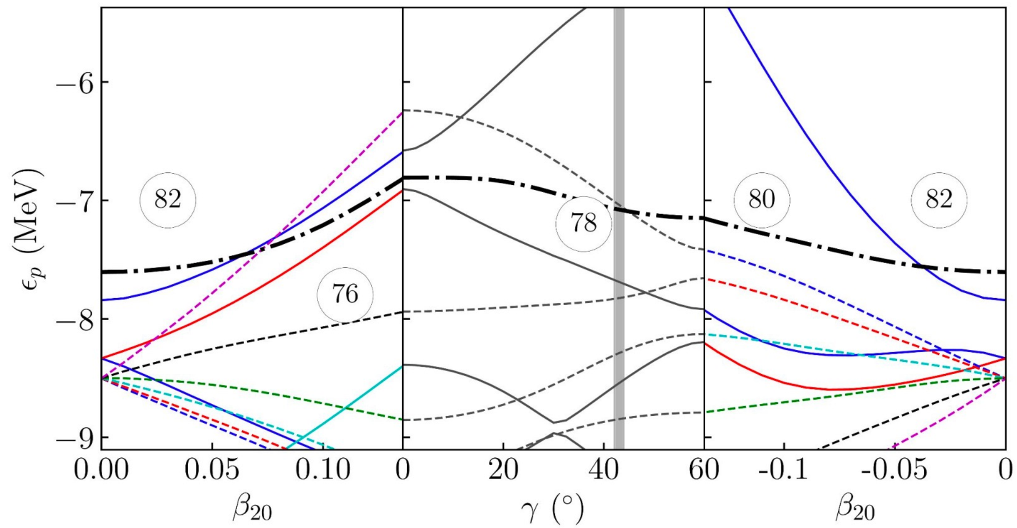
BSkG1-3 interactions (MOCCa code: Ryssens et al. 2021-2023): σ(M)~0.74-0.63 MeV

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

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BSkG2 + Combinatorial model

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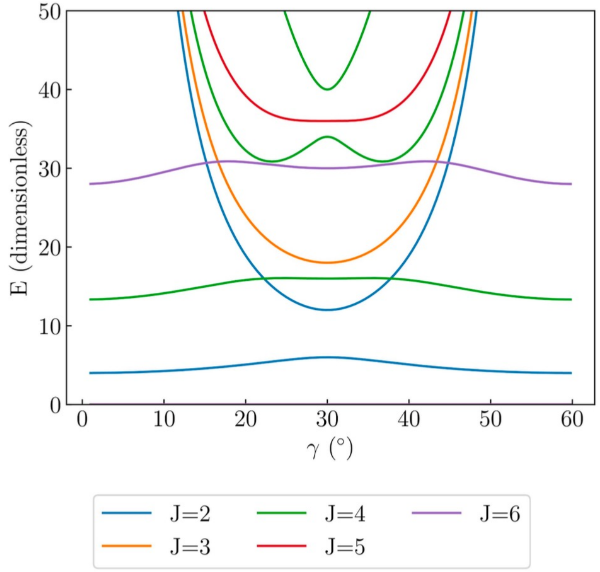

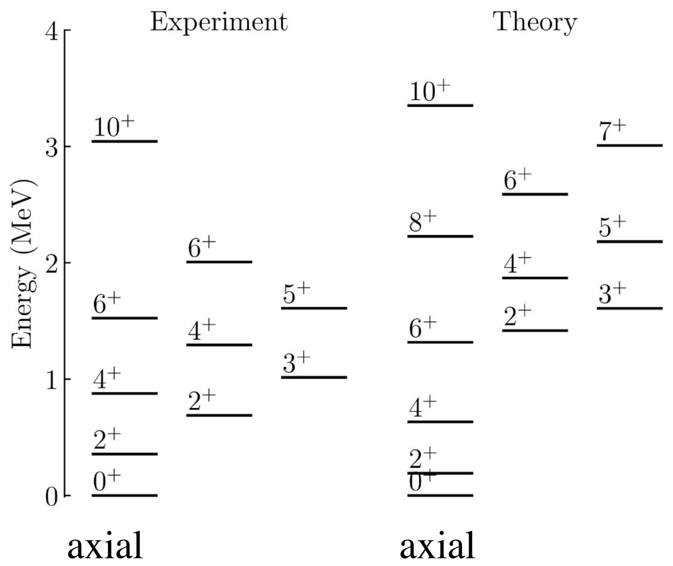

Rotational enhancement

- 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

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

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

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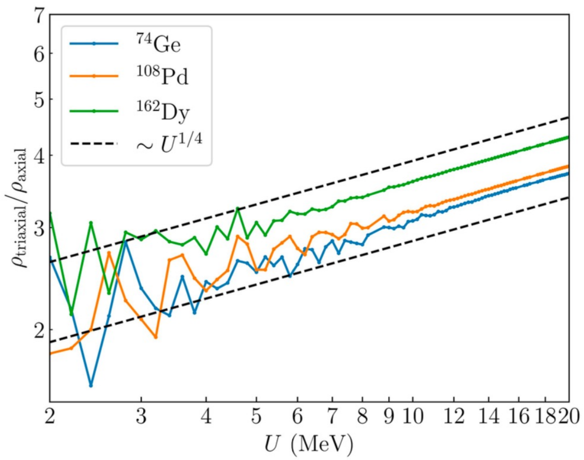
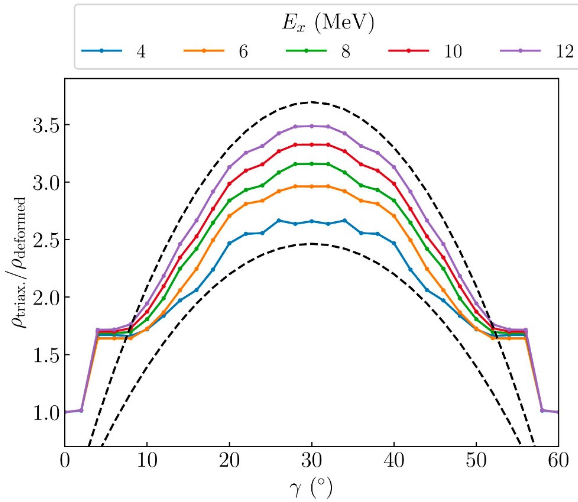
Collective enhancement for triaxial nuclei



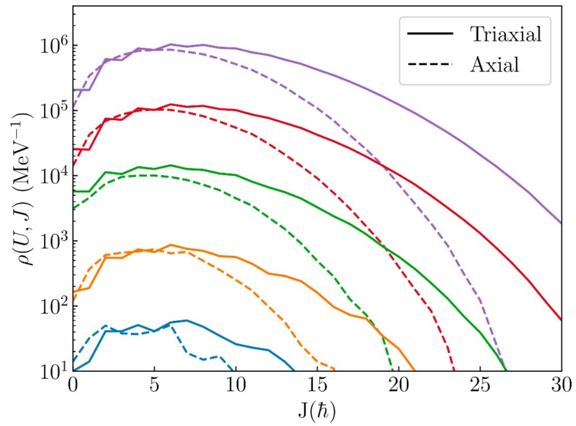


Expectations

- 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

Performance on mean s-wave spacings

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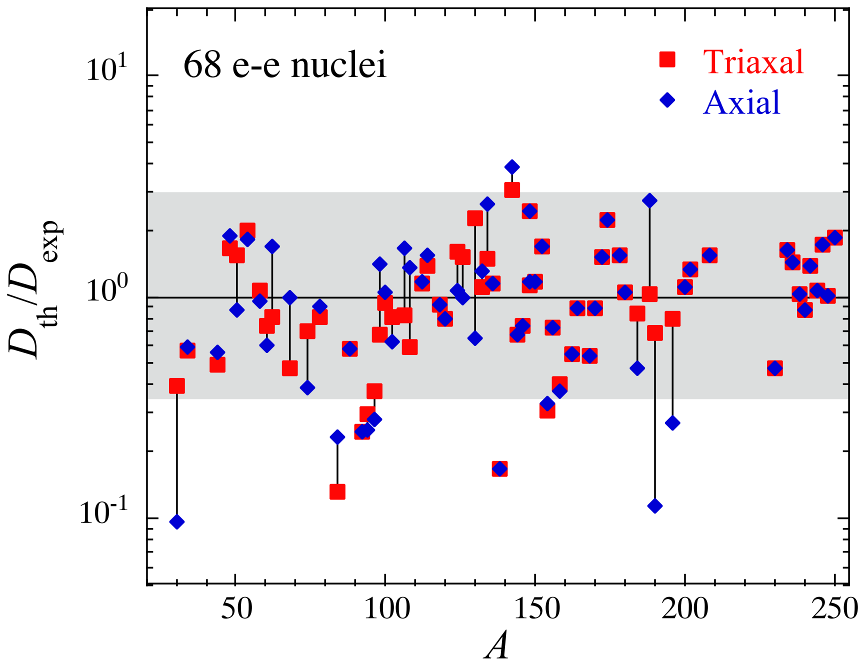
$$f_{\mathrm{rms}} = \exp\left[\frac{1}{N_e}\sum_{i=1}^{N_e}\ln^2\frac{D^i_{\mathrm{th}}}{D^i_{\mathrm{exp}}}\right]^{1/2},$$

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



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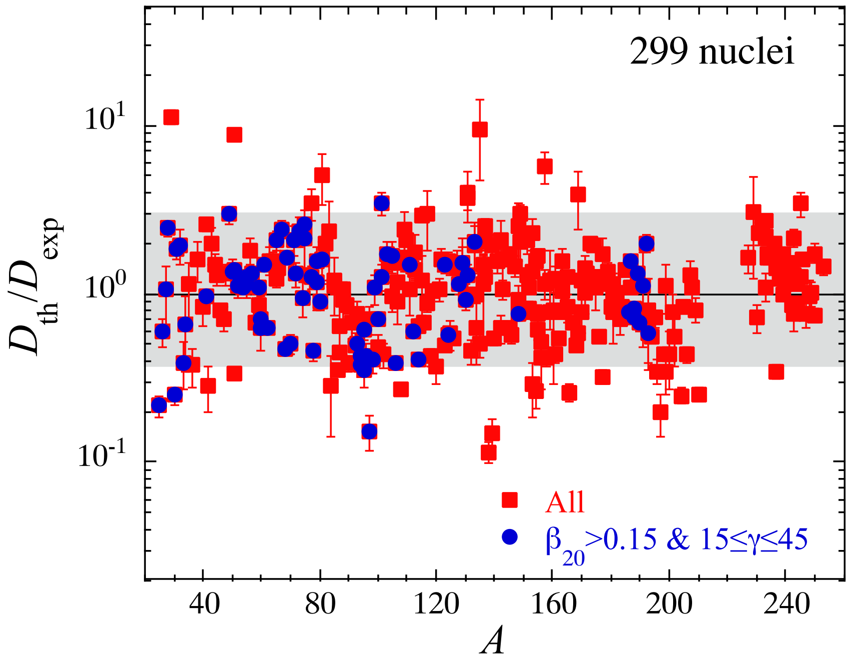

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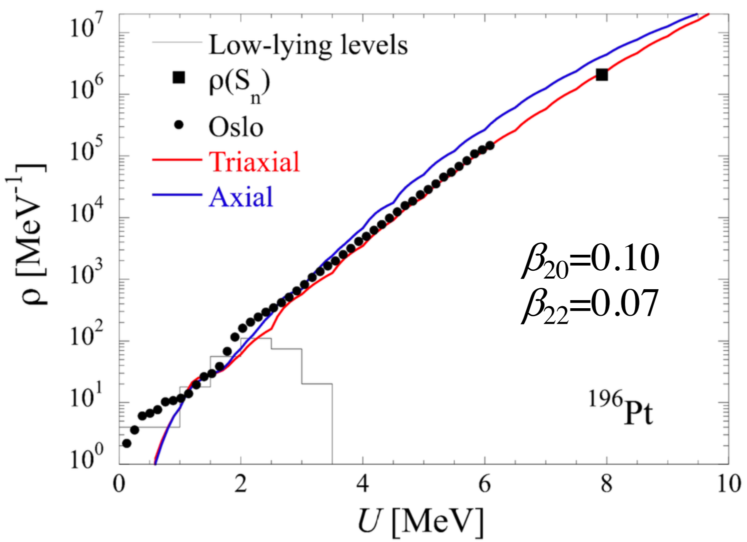
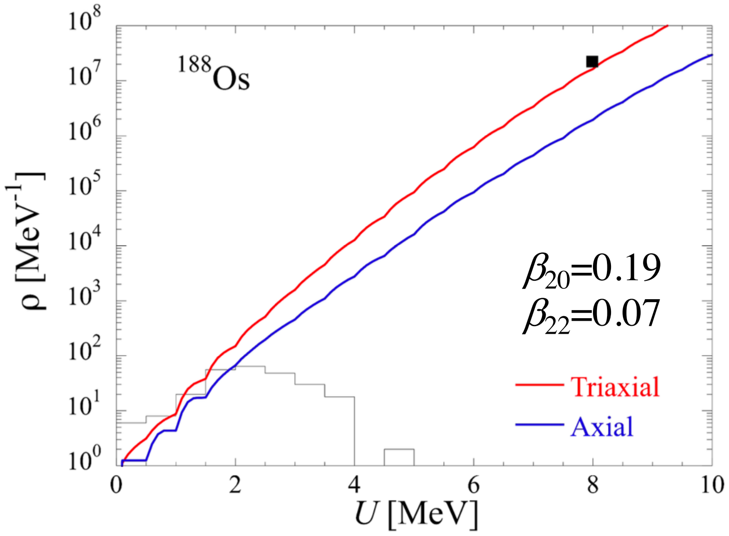
Comparison of BSkG2+Combinatorial NLD with Oslo data

The effect of triaxiality





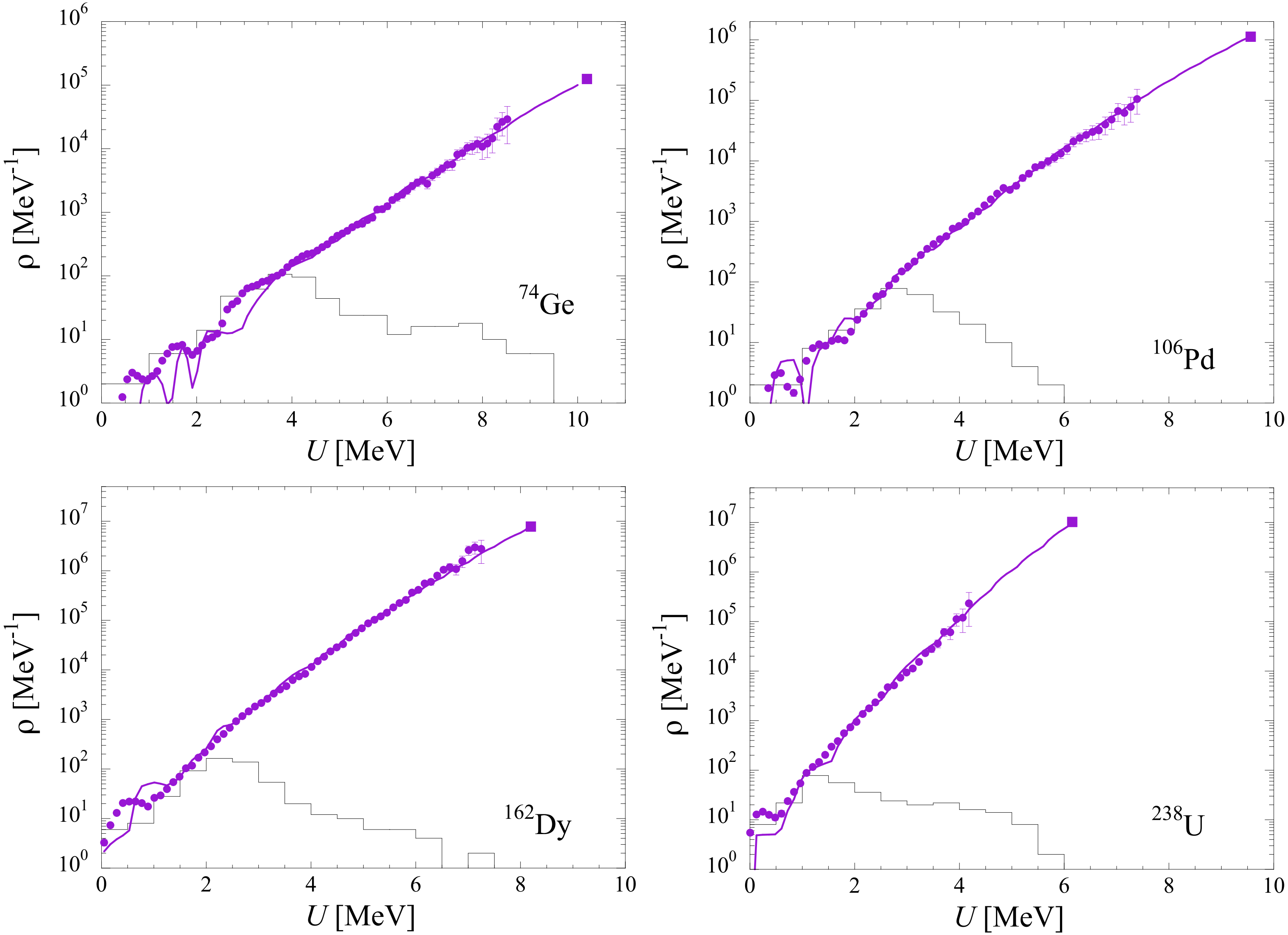
- lower intrinsic NLD
- modest deformation and MOI

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 BSkG2+Combinatorial NLD with Oslo data



Conceptually new approach: QRPA + Boson Expansion Method

- **QRPA calculations** => collective levels (***Bosons***) for various given multipolarities and parities: K=$0^{+/-}$ up to $9^{+/-}$ for even-even nuclei (Gogny D1M+QRPA)

- **Boson Expansion** : Coupling Bosons through a generalized boson partition function

$$\mathcal{Z}_{\text{boson}} = \prod_{\lambda} \prod_{\mu=-\lambda}^{\lambda} \sum_{N_{\text{boson}}} \left[y^{\varepsilon_{\lambda\mu}} t^{\mu} p_{\lambda}\right]^{N_{\text{boson}}}$$

- **Construction of rotational bands** for well deformed nuclei

$$\rho_{\text{d}}(U,J,\pi) = \frac{1}{2}\left[\sum_{K=-J,K\neq 0}^{J} \omega_{\text{tot}}(U - E_{rot}^{J,K}, K, \pi)\right] + \omega_{\text{tot}}(U - E_{rot}^{J,0}, 0, \pi)\left[\delta_{(J\,even)}\,\delta_{(\pi=+)} + \delta_{(J\,odd)}\,\delta_{(\pi=-)}\right]$$

- **Phenomenological mixing** between spherical and well deformed nuclei

$$\rho(U,J,\pi) = \left[1-\mathcal{F}\right]\rho_s(U,J,\pi) + \mathcal{F}\rho_d(U,J,\pi) \qquad \text{where} \qquad \mathcal{F} = 1 - \left[1 + \mathrm{e}^{(\beta_2 - 0.18)/0.04}\right]^{-1}$$

Gogny-HFB (D1M) + QRPA *E*1 and *M*1 strength functions

ARC data

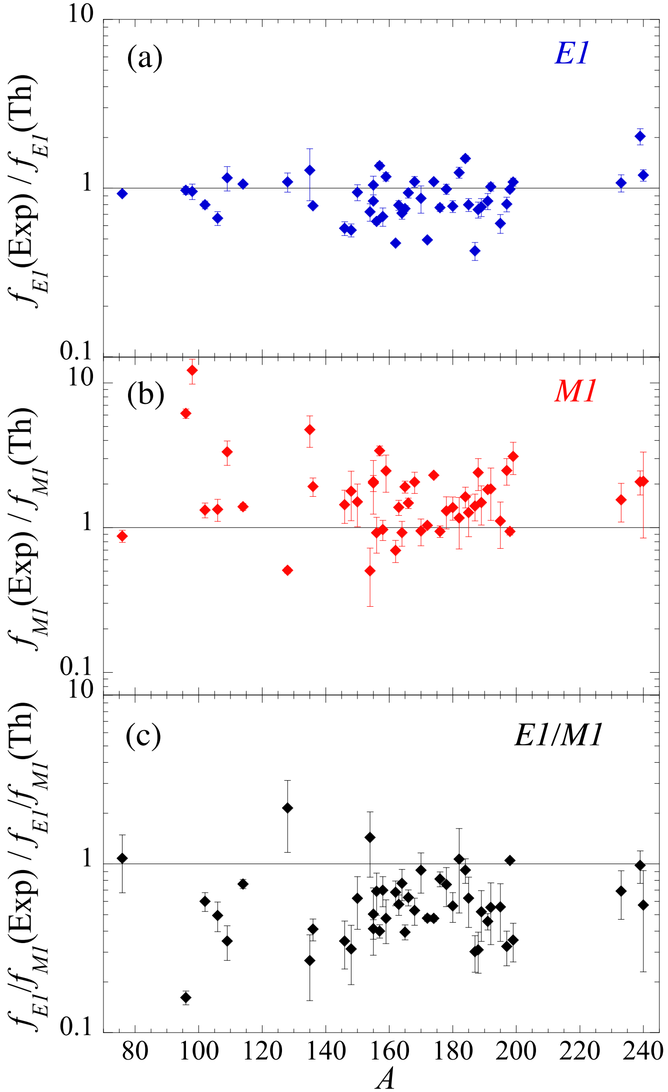
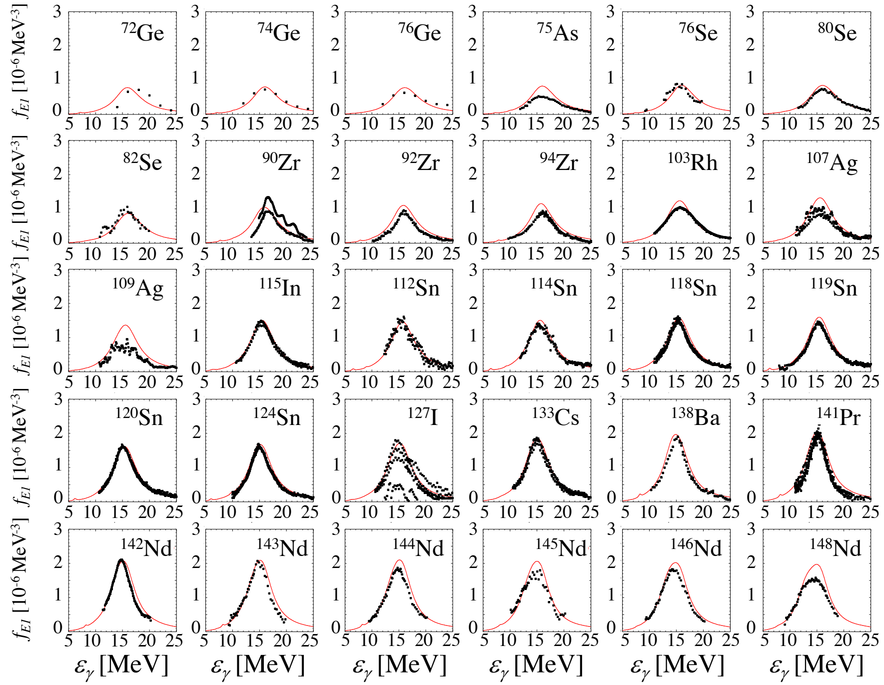
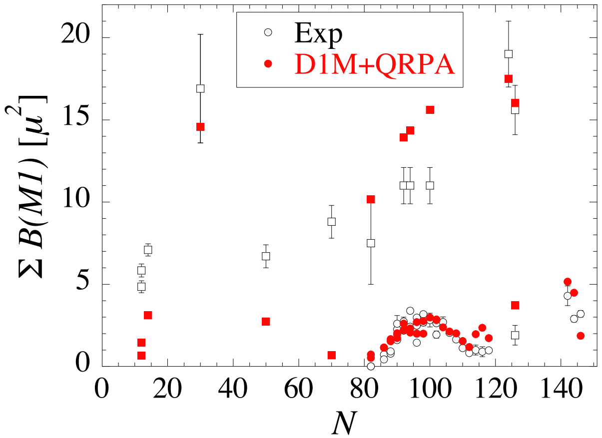


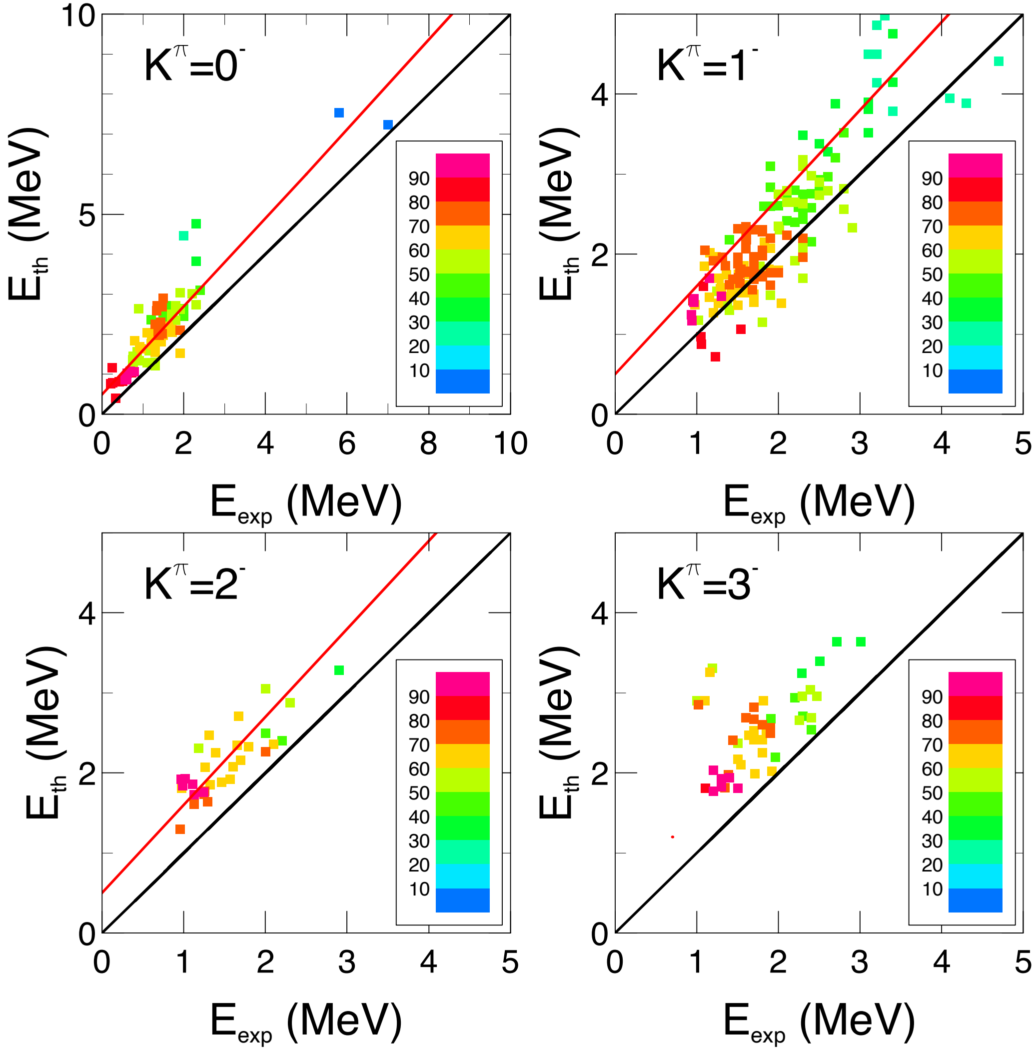
Photo data



NRF data



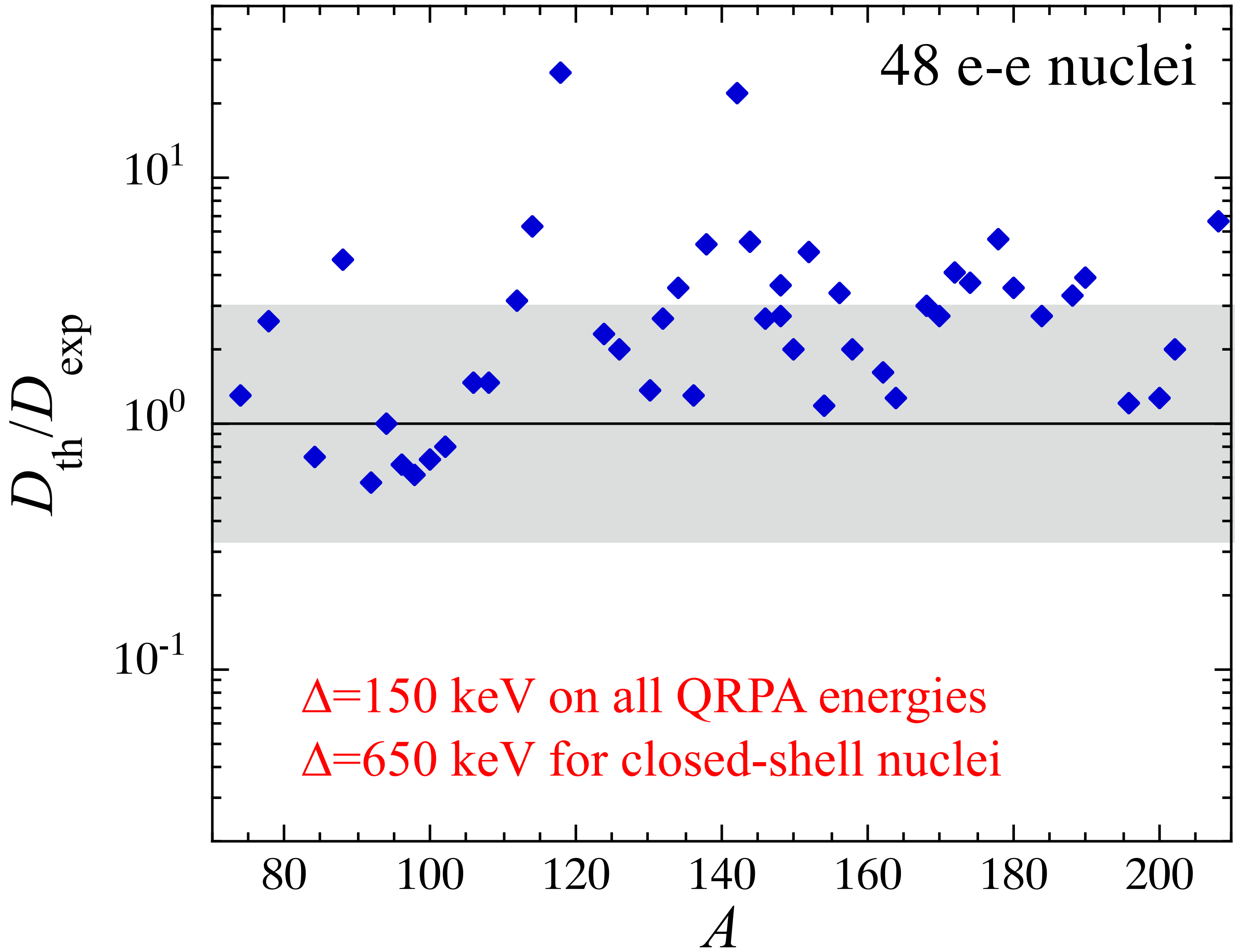
Rather satisfactory QRPA predictions of low-energy spectroscopy

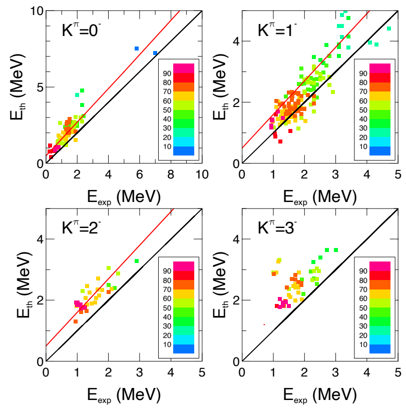


Though some systematic overestimate of spectroscopic data with D1S/D1M (Δ~few 100keV)

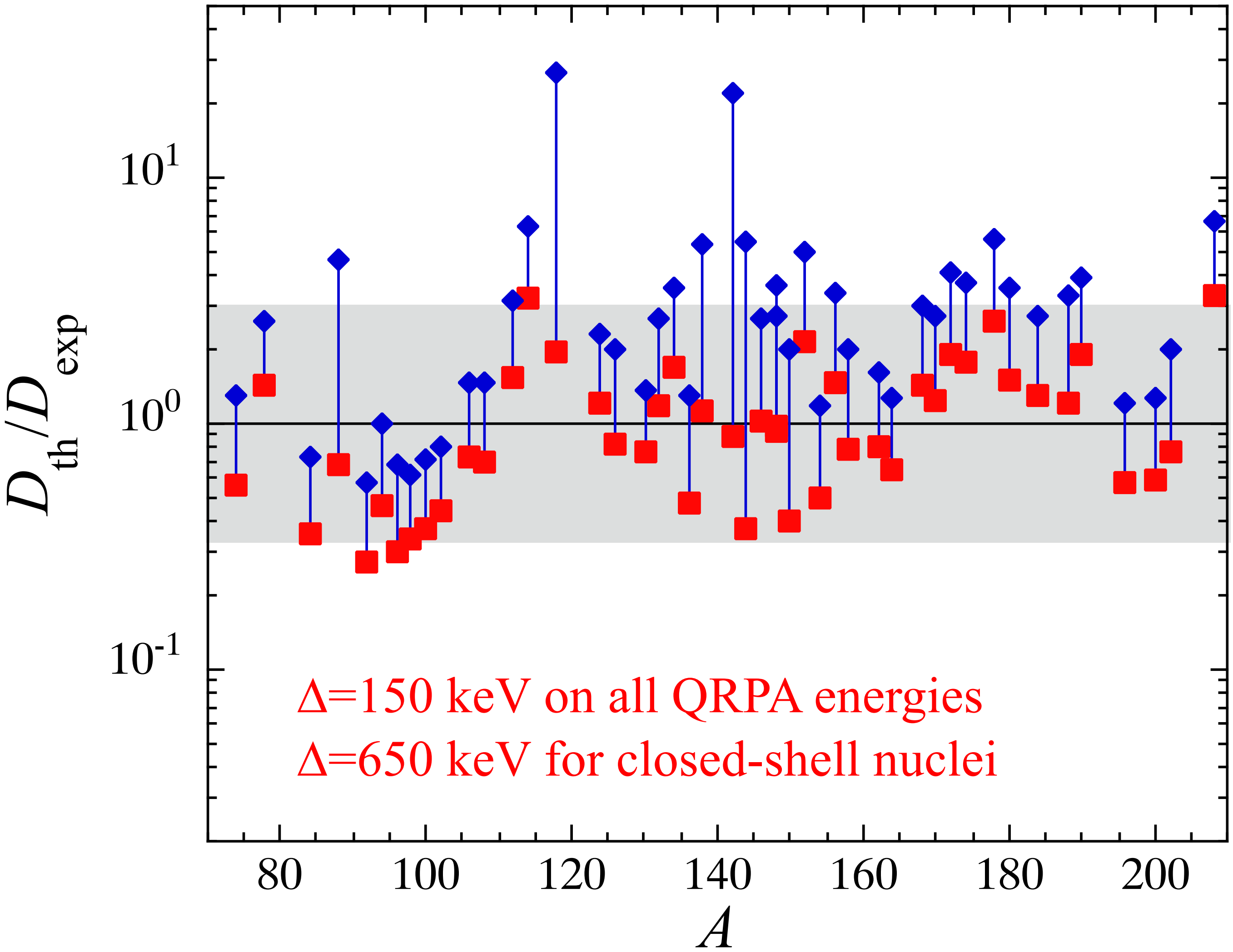
The QRPA + Boson Expansion Method

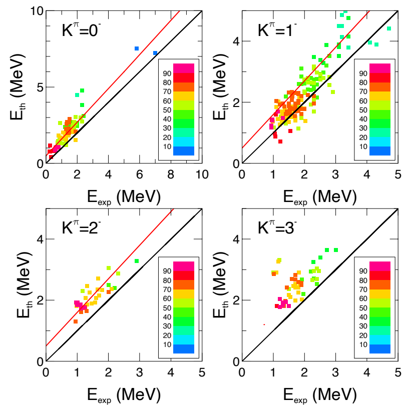
Relatively satisfactory description of D_0, but overall overestimation (*i.e.* underestimation of ρ)





The QRPA + Boson Expansion Method

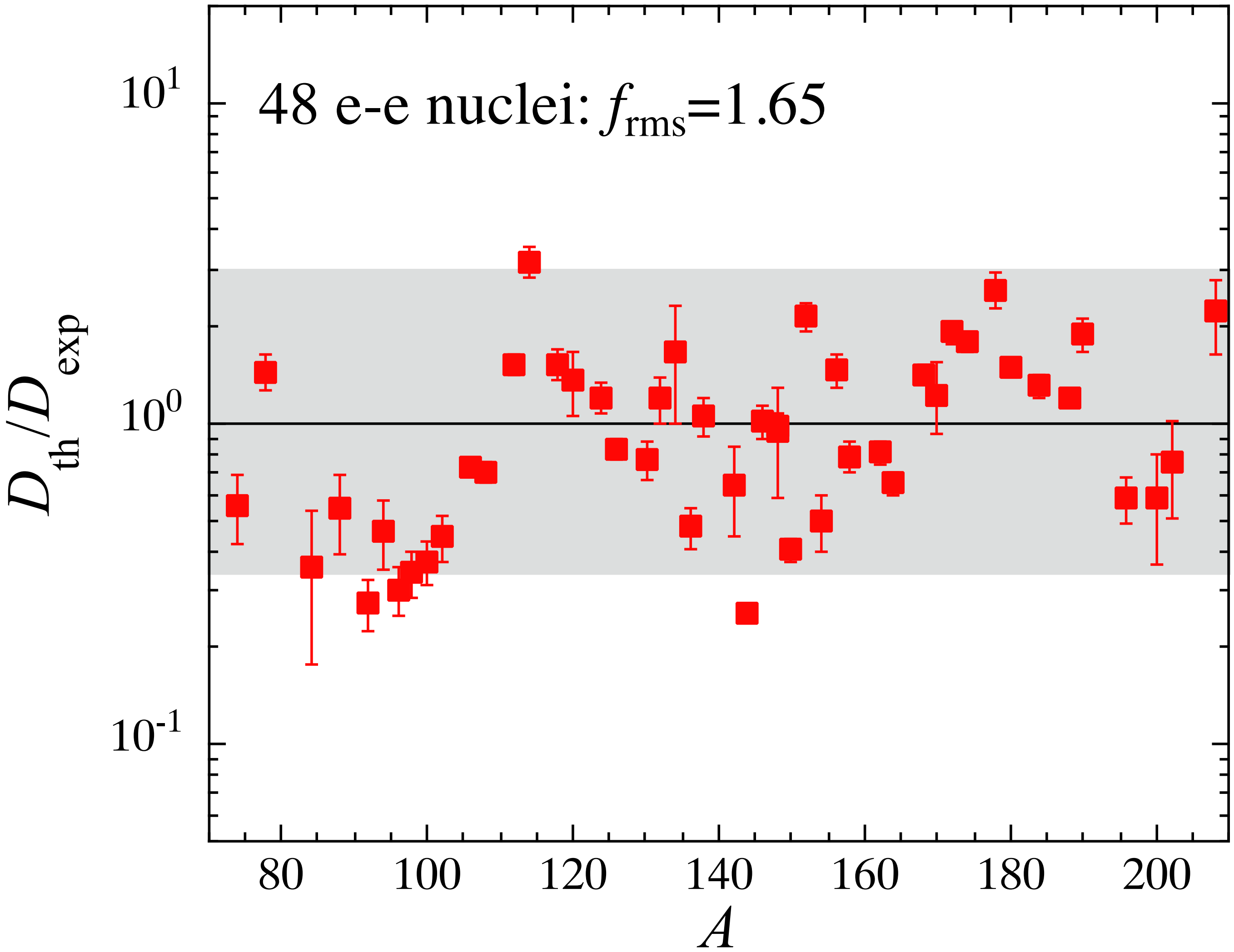




→ Need for an accurate estimate of the lowest QRPA exitations energies

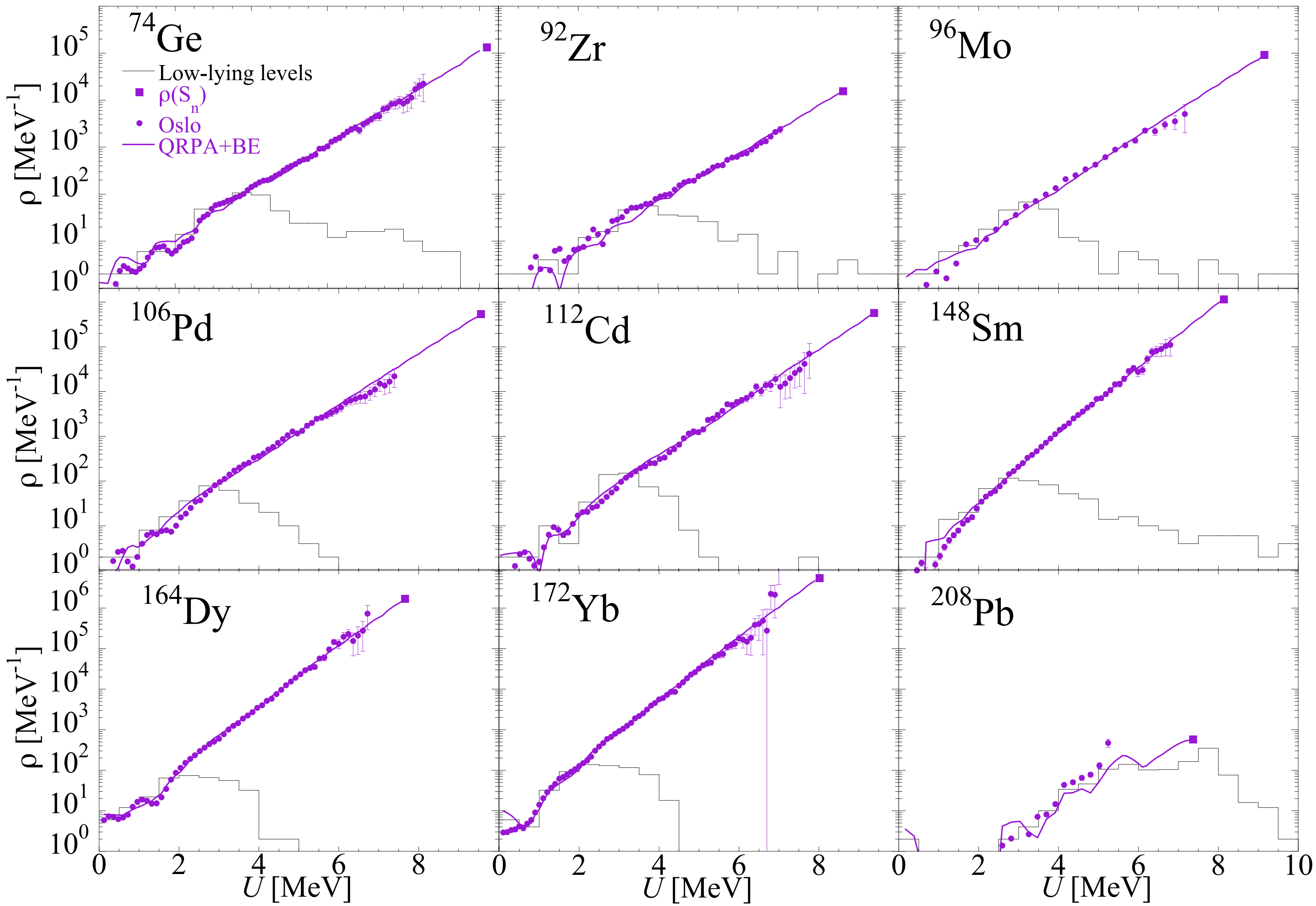
The QRPA + Boson Expansion Method

Finally, including experimental uncertainties



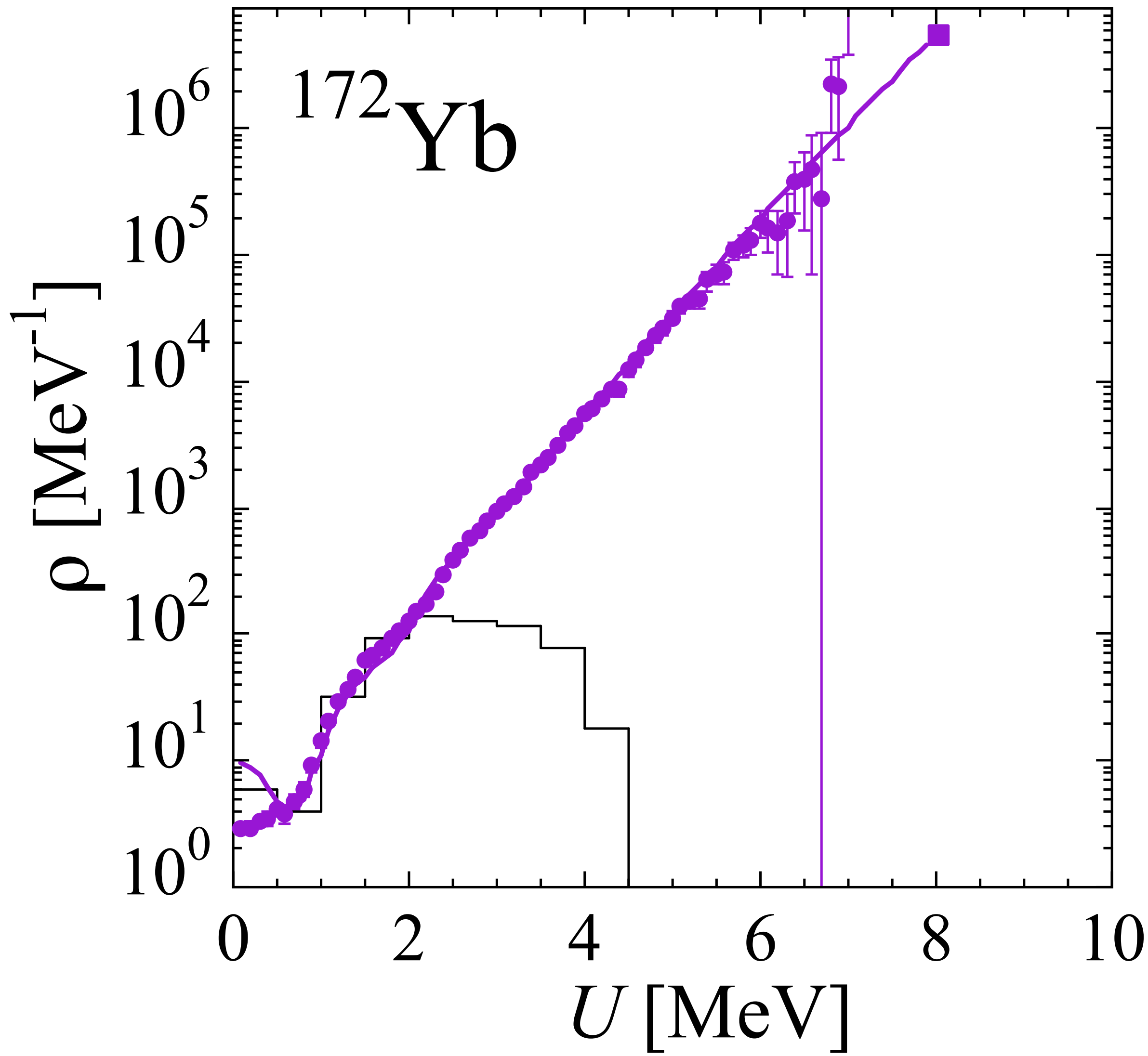
On the same data set: Cst-T: f_{rms}=1.5 - HFB+Comb: f_{rms}=2.4

The QRPA + Boson Expansion Method



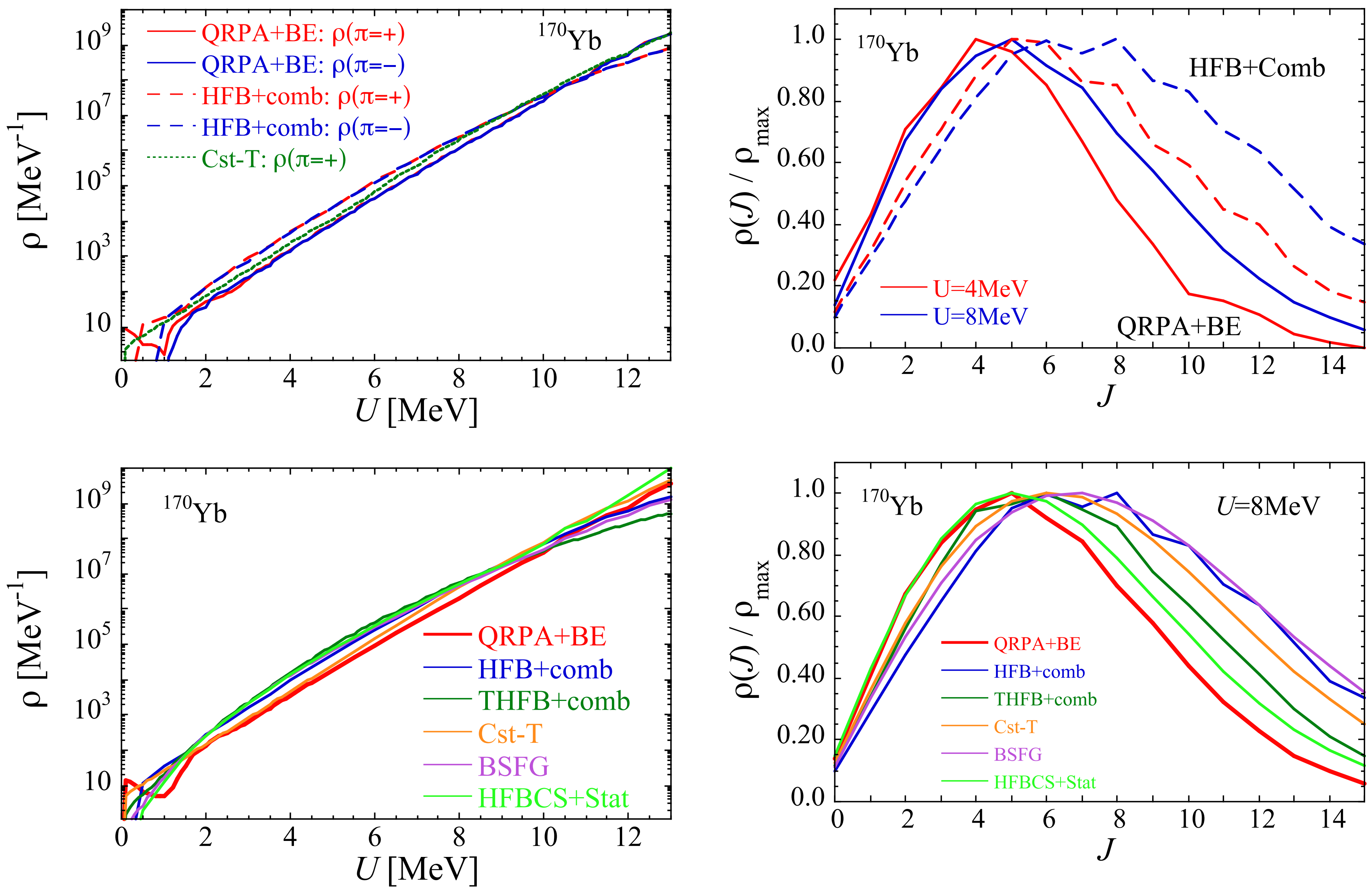
The QRPA + Boson Expansion Method

Normalisation of the QRPA+BE energies on D0 & Oslo data on theoretical NLDs



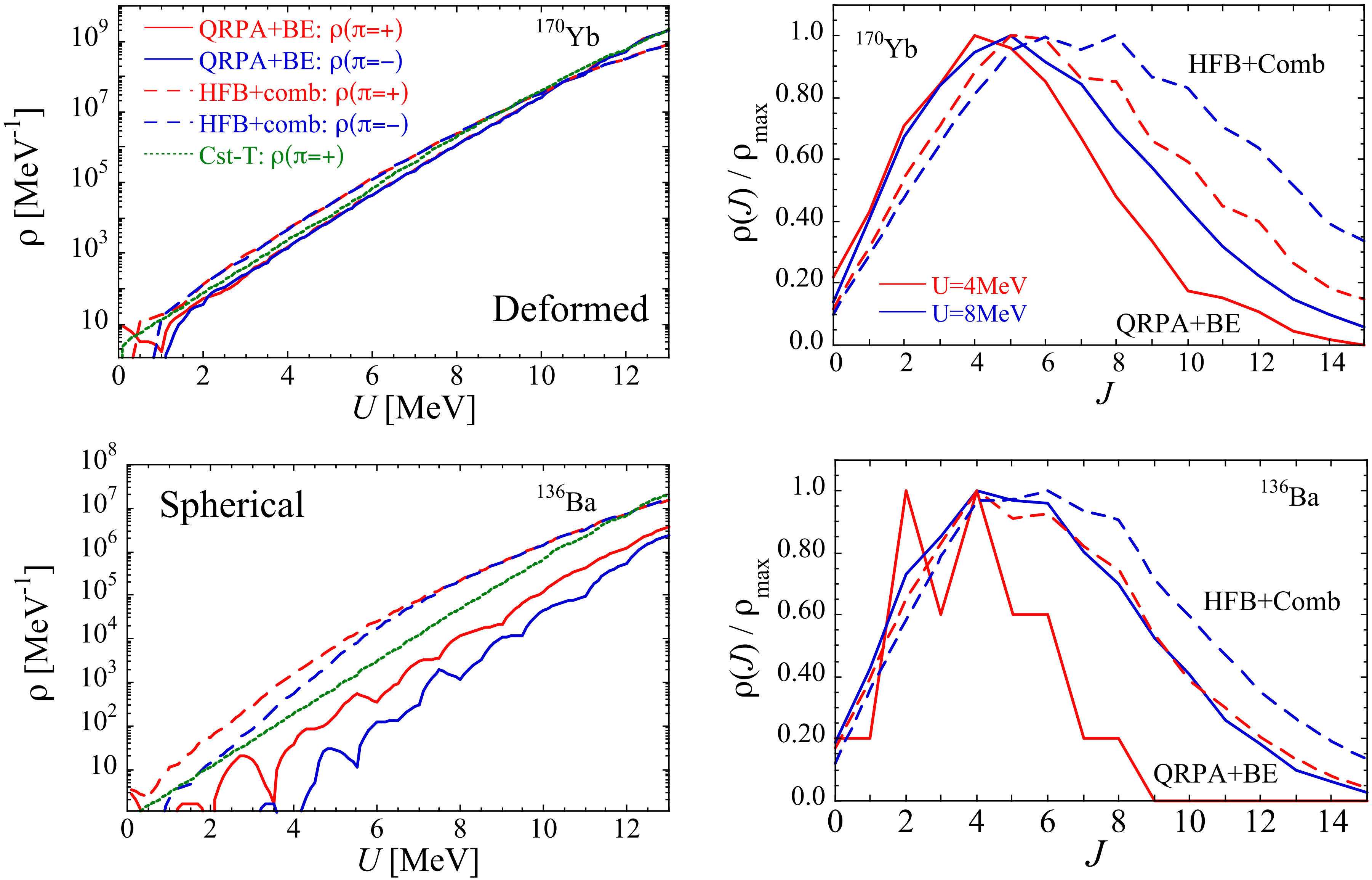
The QRPA + Boson Expansion Method

(assuming a global shift of QRPA energies)



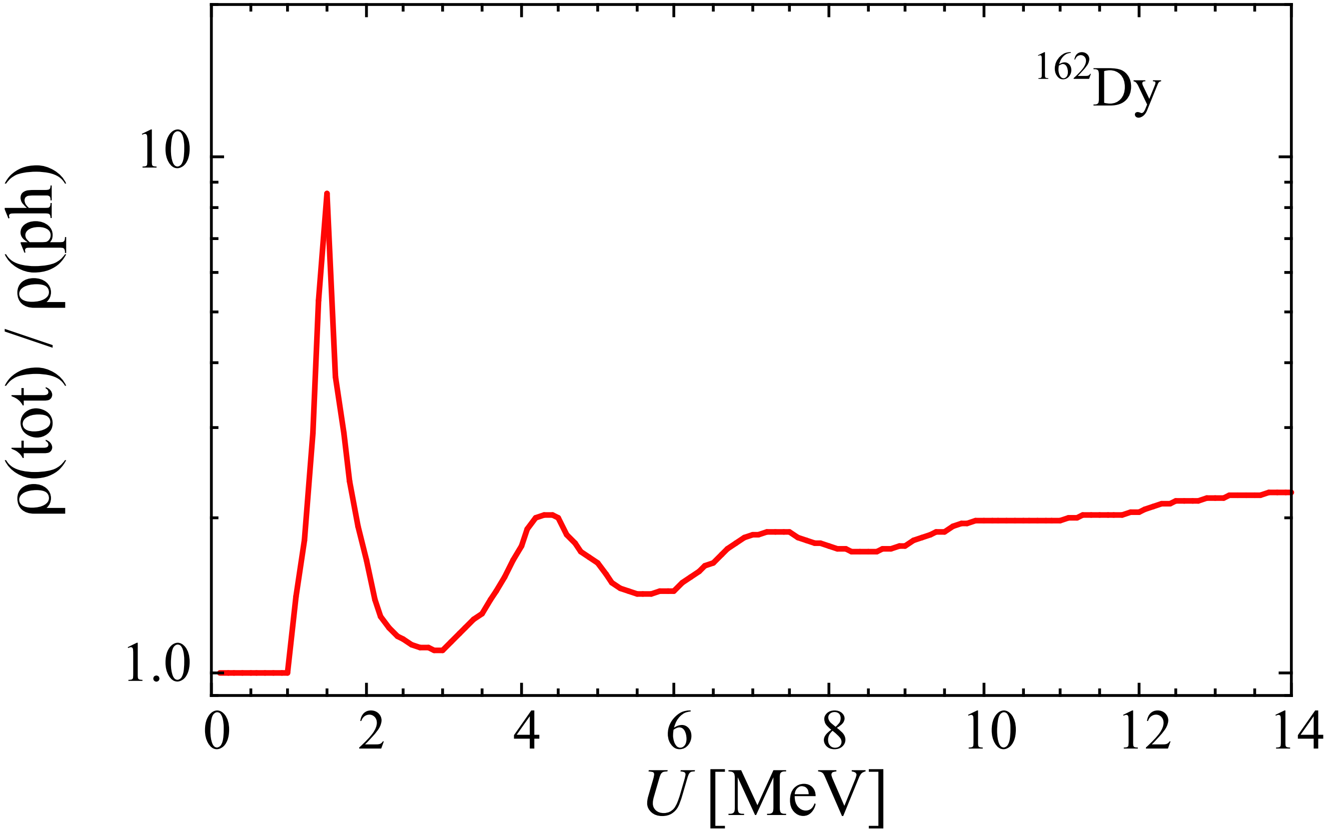
The QRPA + Boson Expansion Method

(assuming a global shift of QRPA energies)

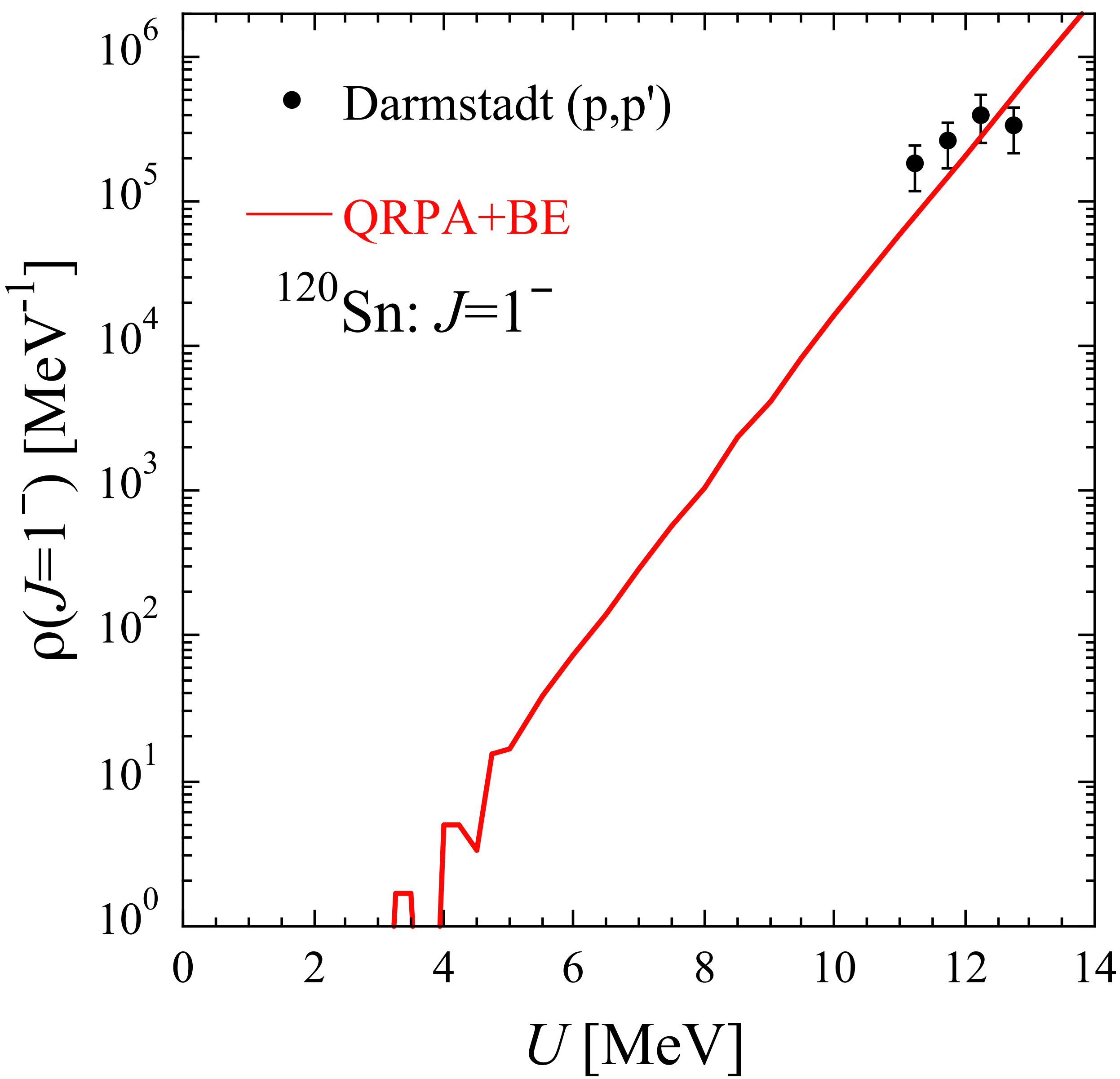


The QRPA + Boson Expansion Method

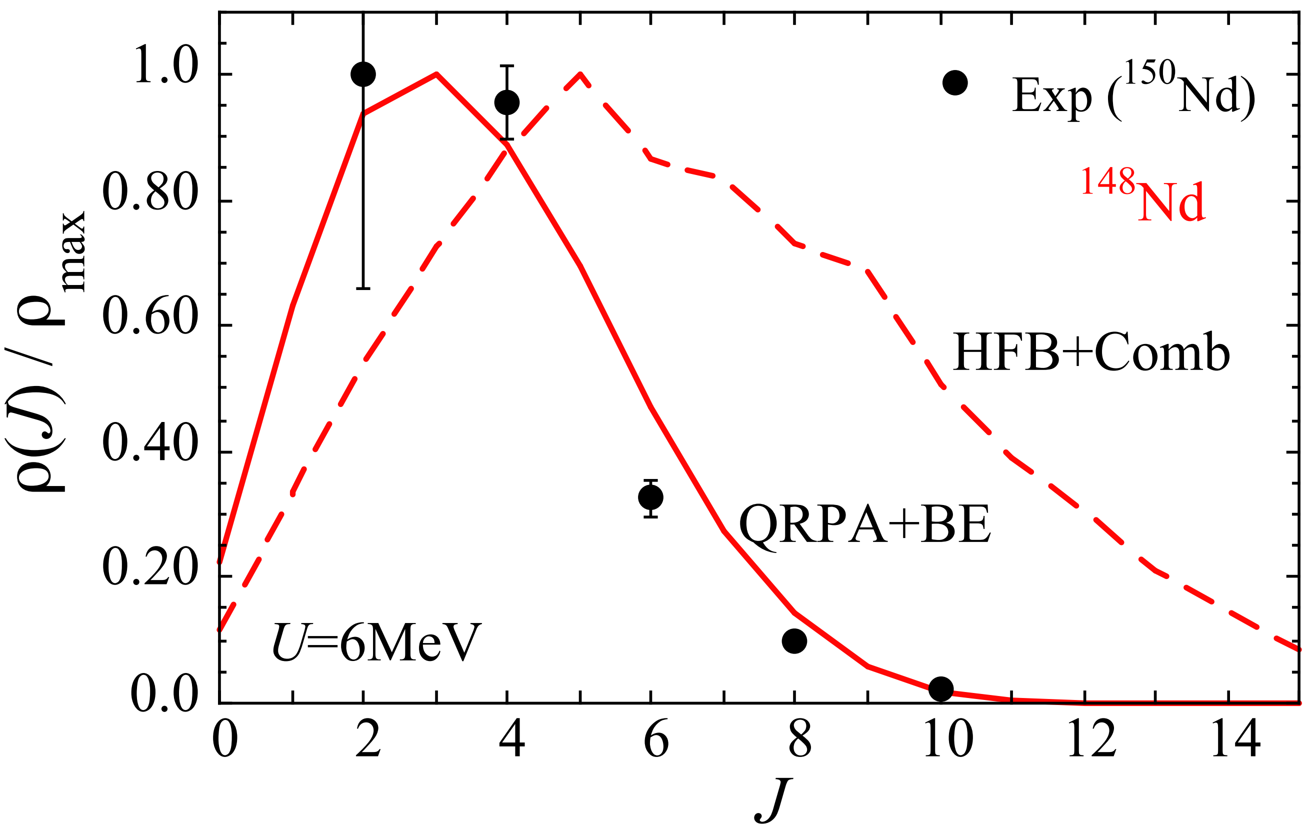
Total to intrinsic NLD ratio



Comparison with NLD extracted from Darmstadt (p,p') reactions

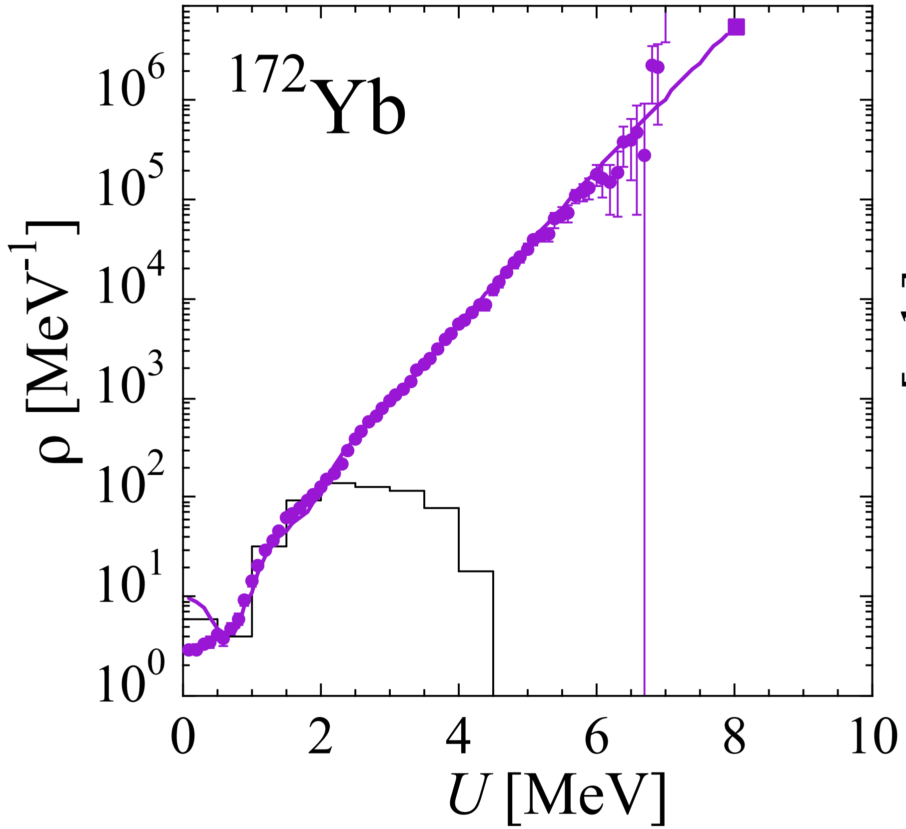


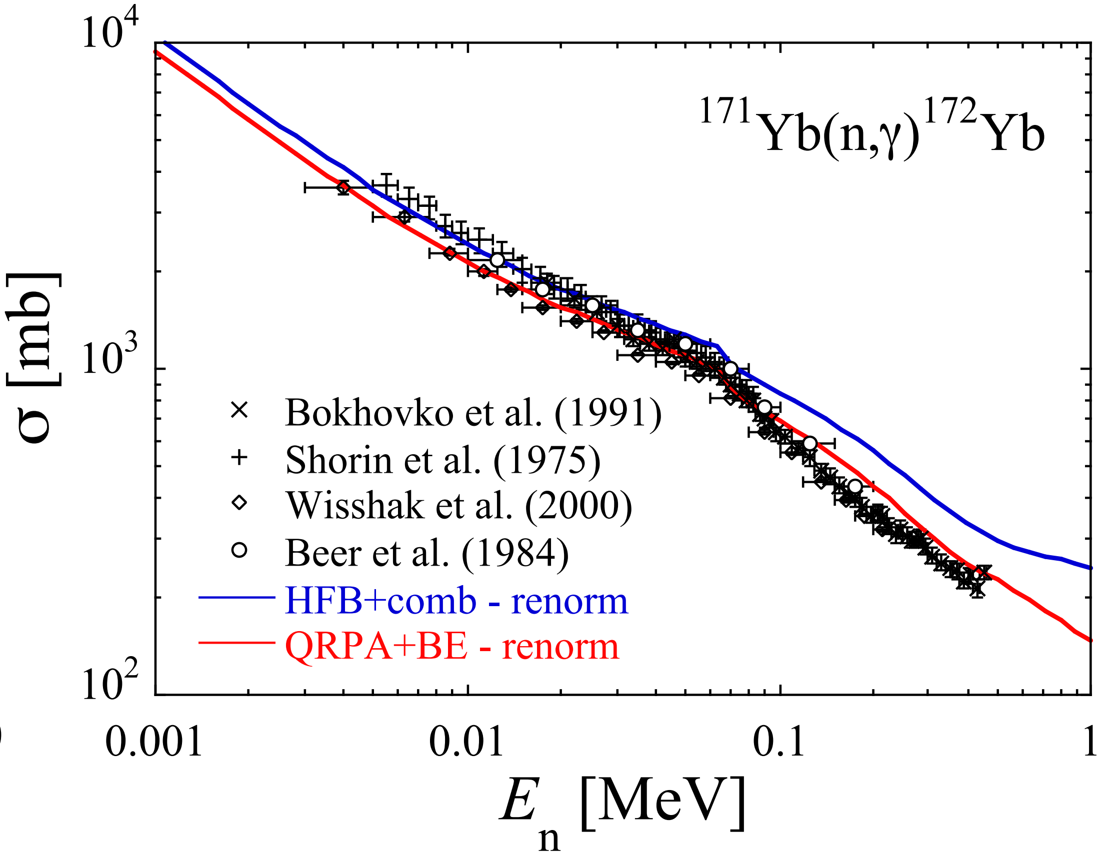
The QRPA + Boson Expansion Method



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

The QRPA + Boson Expansion Method

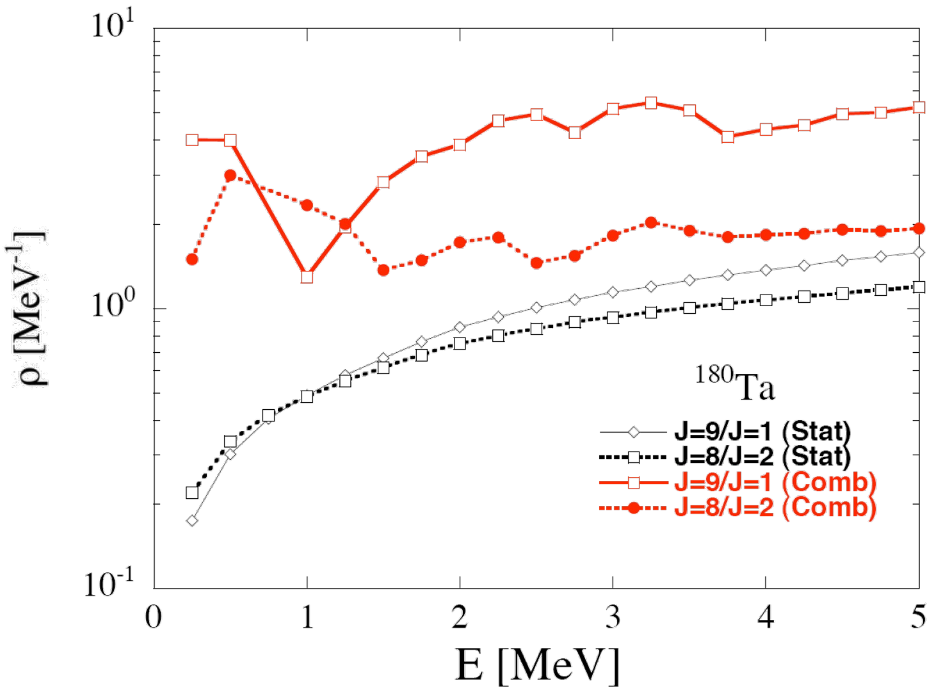




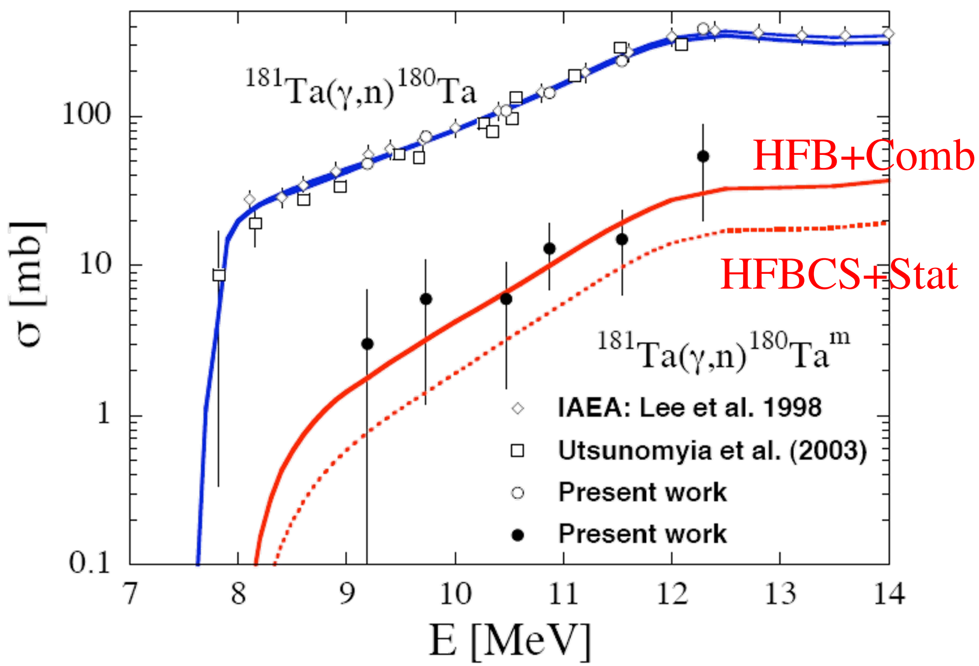
NLD renormalized on known D_0

Possibility to test NLD spin dependence on isomeric ratios

Non statististical spin dependence in the combinatorial level densities



Impact on the photoneutron cross sections for the isomeric state $^{180}Ta^m$



➡ Deviations from the usual gaussian spin dependence can have large impact on isomeric level production cross sections

Conclusions

- **Conceptually new approach to NLD : QRPA + Boson Expansion**

- **Advantages:**
  - Go beyond the Independent Particle Approximation
  - Significantly more physical at the lowest energies of interest in applications

- **Not free from uncertainties:**
  - Quality of the interaction to predict correct QRPA energies
  - Overestimate of QRPA energies (~150keV; closed shell: ~600keV)
  - QRPA treatment of triaxial and γ-soft nuclei, ...
  - Truncations of HFB+QRPA calculation needed for heavy (actinide) nuclei
  - NLD description of slightly deformed nuclei

- **Extension to *A*-odd systems, odd-odd systems to follow...**

- **Still need more experimental data to guide and constrain models** (e.g. Shape Method, spin cut-off determination, etc...)

Major questions related to the NLD estimates

Structure properties of nuclei

→ GS deformation, shell effect, pairing, SPL, ...

→ T-evolution of the GS

Energy dependence

→ Energy dependence: $exp(U/T)$ vs $\exp(2\sqrt{aU})$ (+ K_{rot}) ?

→ Impact of going beyond "Independent Particle Approximation"

Spin dependence

→ Non-Gaussian spin distribution ?

→ Energy, shell and pairing dependence of the spin cutoff factor ?

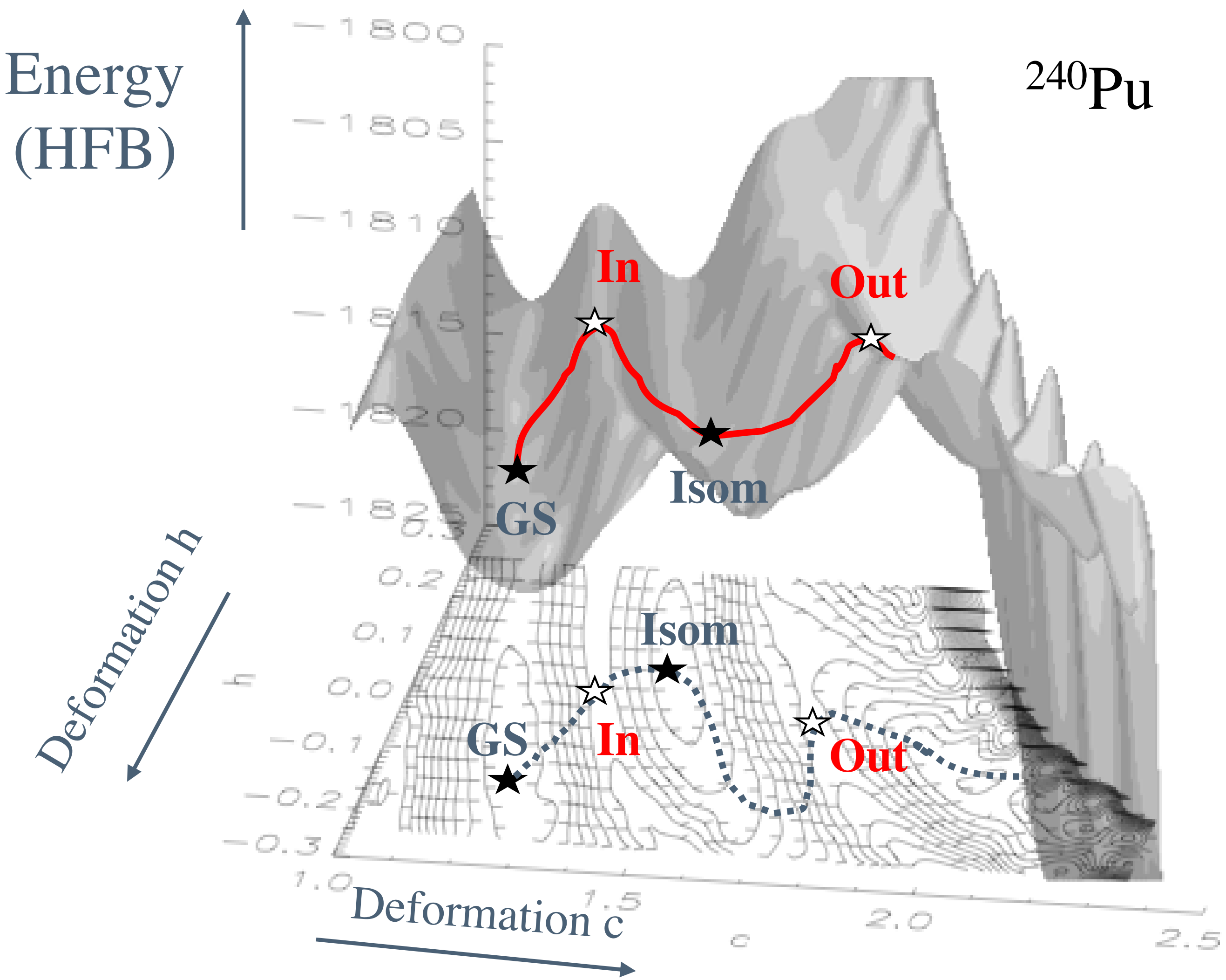
Parity dependence

→ Non-equiparity distribution ?

HFB calculation of the Fission Barriers

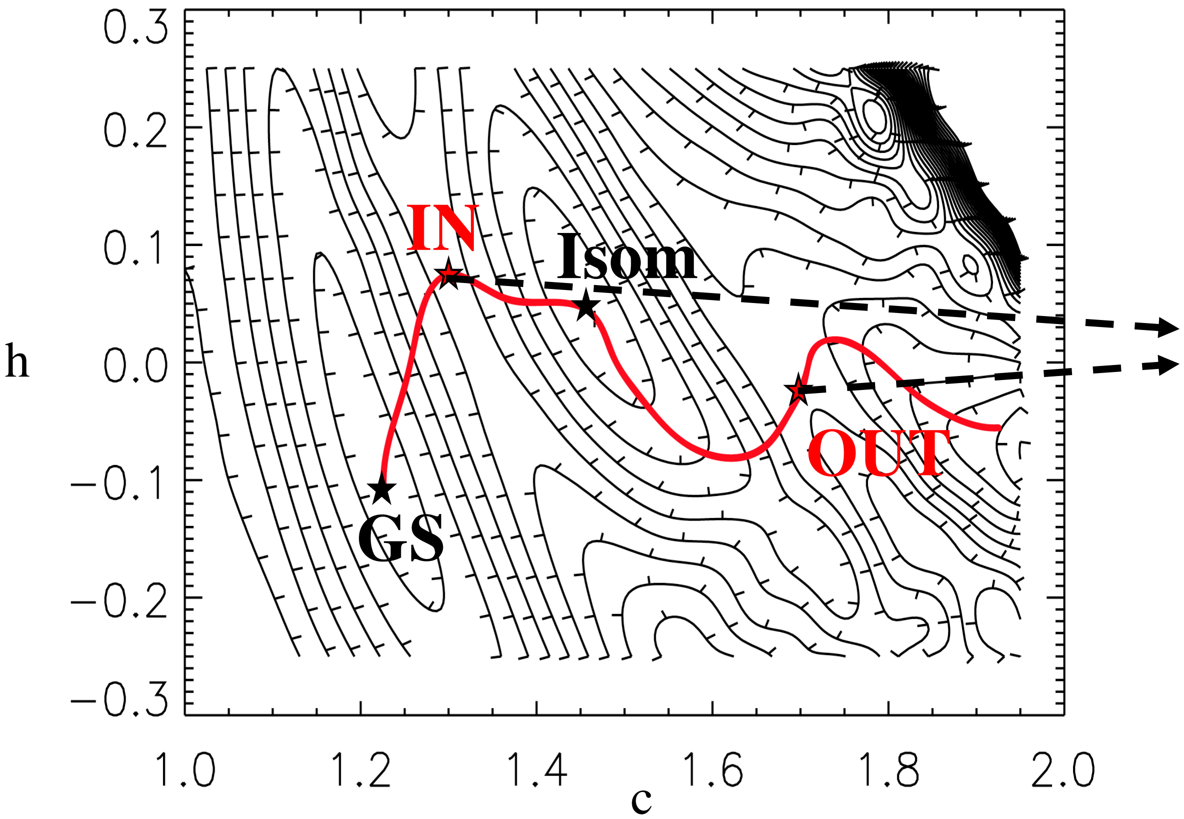
Determination of the full energy surface within the (Q,O,H) deformed HFB model

based on the same effective interaction as the one determined by the mass fit (HFB14) !

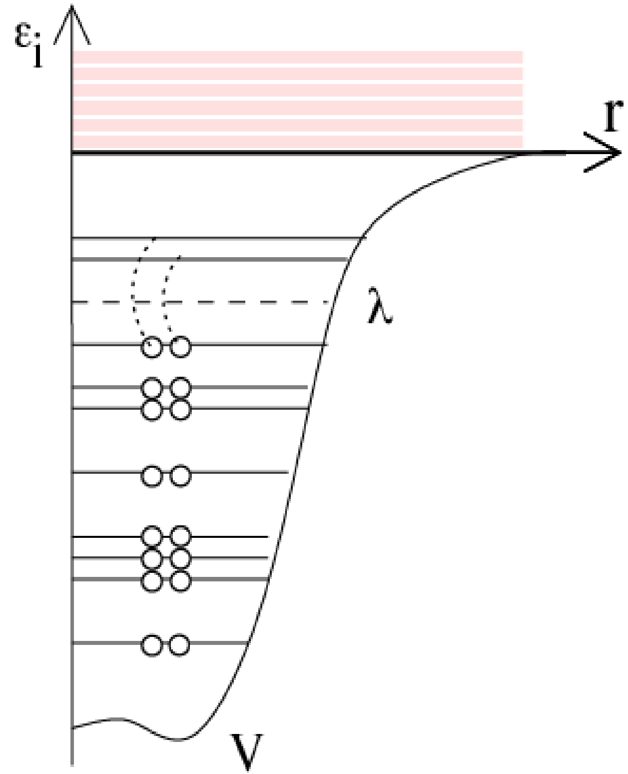


Nuclear level densities at the saddle points

HFB model provides at each deformation (including saddle points)
all nuclear properties needed to estimate the NLD



single-particle scheme
at saddle point deformation



Possibility to estimate NLD at the saddle point within the HFB+Combinatorial model

Nuclear Level Density at Saddle Points

- Fission Barriers and saddle point deformations (Q,O,H) determined within HFB method
- Nuclear properties (spl, pairing) at the inner and outer saddle points with constrained HFB model
- NLD in the framework of the microscopic combinatorial model based on HFB single-particle level and pairing predictions at the HFB saddle points (plus collective rotational and vibrational enhancement)

All ingredients described on the basis of the

same Skyrme effective interaction (e.g BSkG3) at GS and Saddle Points

→ **NLD in a table format at inner and outer saddle points**

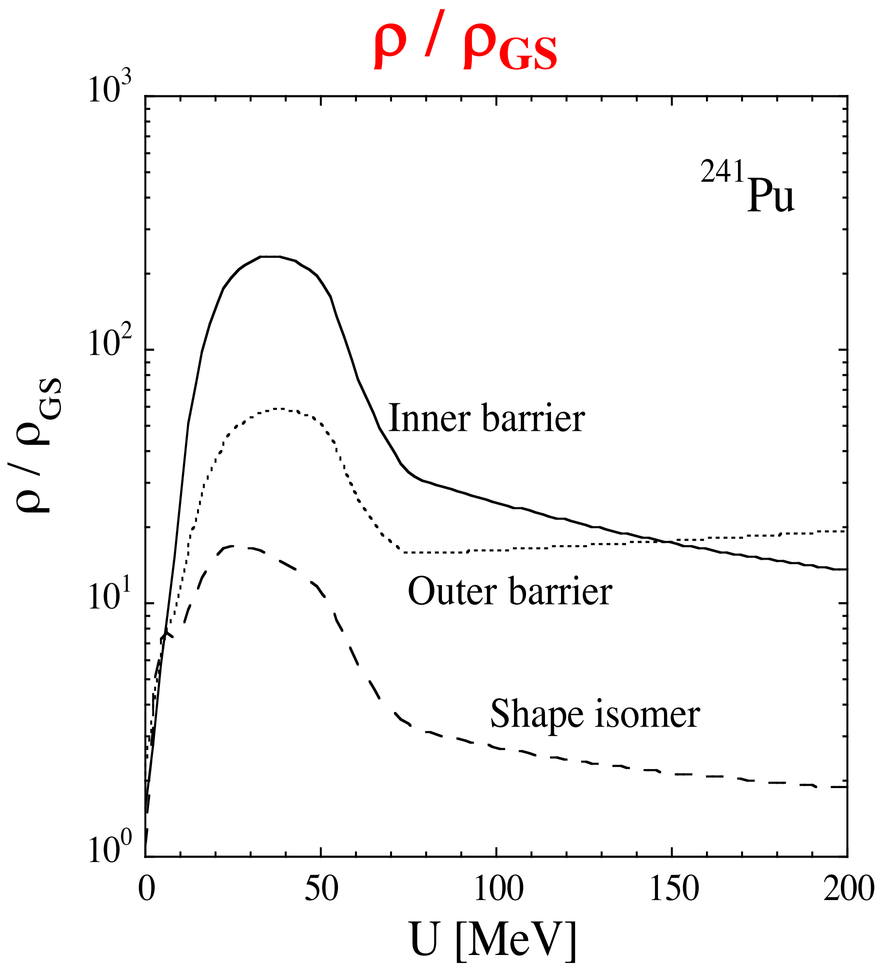
(~ 2000 nuclei : 2–3 saddle points & 1–2 shape isomers)

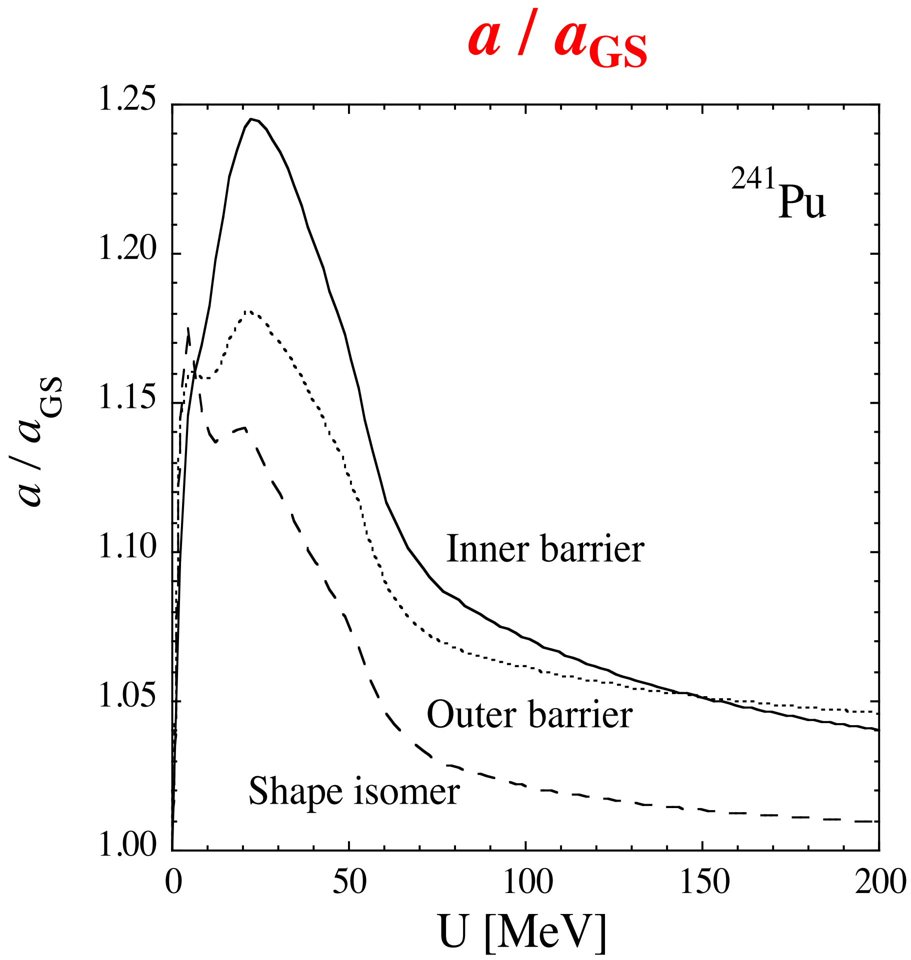
For inner barrier, usually predicted to be triaxial: $\rho_{triax} = \sqrt{\frac{\pi}{2}}\sigma_{\perp} \times \rho_{Comb}$ → New HFB+Comb

For outer barrier, usually predicted to be left-right asymmetric: $\rho_{asym} = 2 \times \rho_{Comb}$

Björnholm & Lynn (1980)

Prediction of the NLD at the fission saddle point and shape isomer





***a*-parameter deduced from the TOTAL level density:** $\rho(U) = \frac{\sqrt{\pi}}{12\, a^{1/4}\, U^{5/4}} e^{2\sqrt{a\, U}}$

THANK YOU
FOR
YOUR ATTENTION