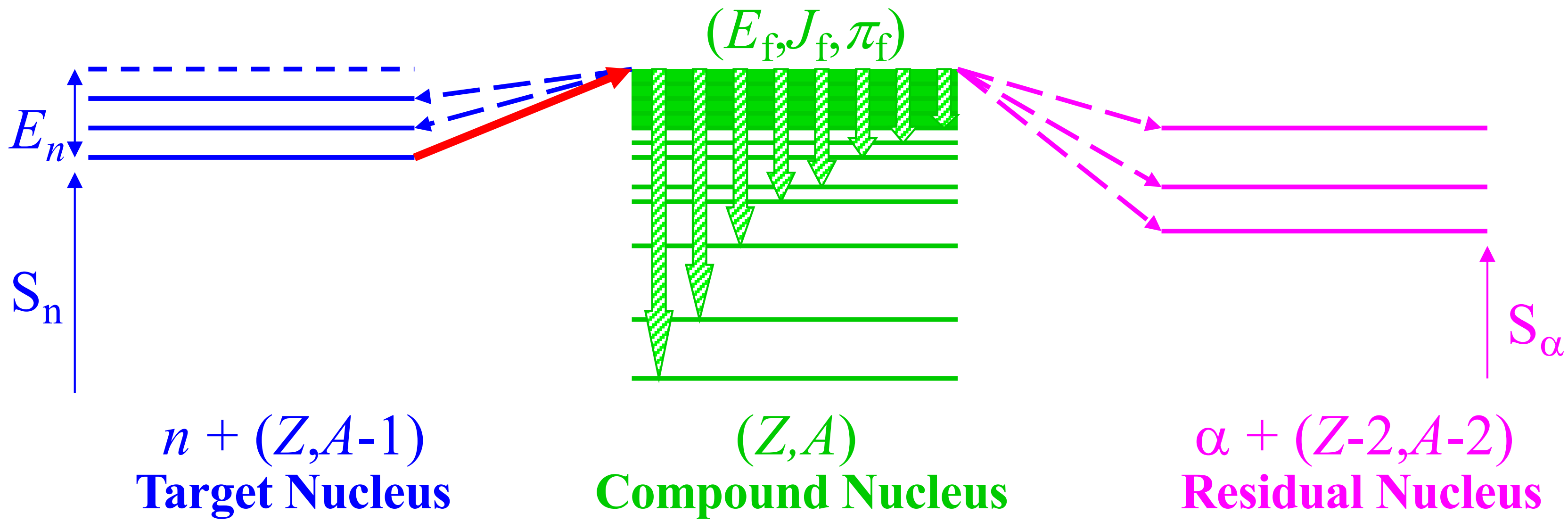
Prediction of Nuclear Level Densities within the QRPA + Boson Expansion method

S. Goriely, S. Hilaire, S. Péru
ULB, Belgium
CEA,DAM, DIF, France

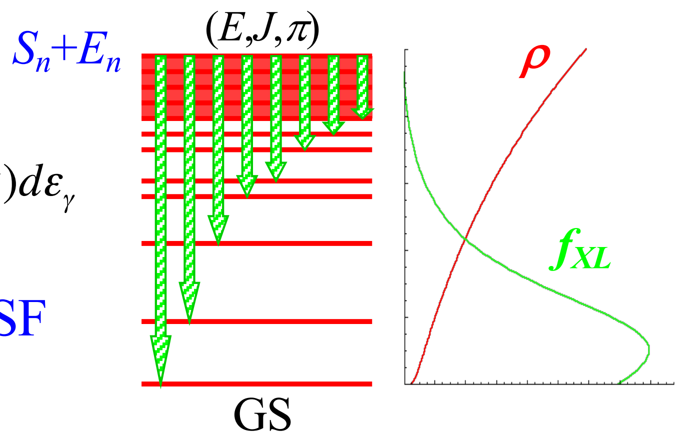
Hauser-Feshbach model for radiative neutron capture reactions



$$\sigma_{(n,\gamma)} \propto \sum_{J,\pi} \frac{T_n(J^\pi)T_\gamma(J^\pi)}{T_n(J^\pi)+T_\gamma(J^\pi)} \approx \sum_{J,\pi} T_\gamma(J^\pi)$$ since $T_n(J^\pi) >> T_\gamma(J^\pi)$: $E_n \sim$ keV

$$T_\gamma = \sum_{J^\pi XL} \int_0^{S_n+E_n} 2\pi\varepsilon_\gamma^{2L+1} f_{XL}(\varepsilon_\gamma)\rho(S_n+E_n-\varepsilon_\gamma, J, \pi)d\varepsilon_\gamma$$

Nuclear astrophysics apps require NLDs & GSF for ~ 8000 nuclei



The Back-Shifted Fermi Gas Model

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

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
- Assumption of a statistical distribution at all energies
- Continuous SPL density approximation
- Approximate empirical shell effect included
- Approximate pairing effects reduced to an energy shift Δ (no supra phase)
- Approximate similar T-dependence for the 3 a-parameters
  $a_S(T)=S(T)/2T$; $a_U(T)=U(T)/T^2$; $a_\sigma(T)=\sigma^2(T)/T$
- Assumption of equiparity
- Assumption collective enhancements [$K_{rot}(E_x)$ $K_{vib}(E_x)$] implicitly included
- Approximate constant-T behaviour at low energies

Mean Field + Statistical NLD formula

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

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

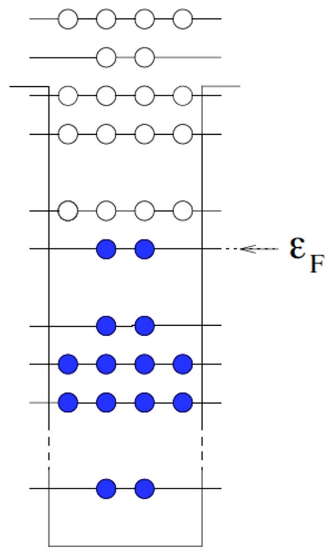
$$S(T) = 2\sum_{q=n,p}\sum_{k} \ln\left[1+\exp(-E_q^k/T)\right] + \frac{E_q^k/T}{1+\exp(-E_q^k/T)}$$

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

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

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

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



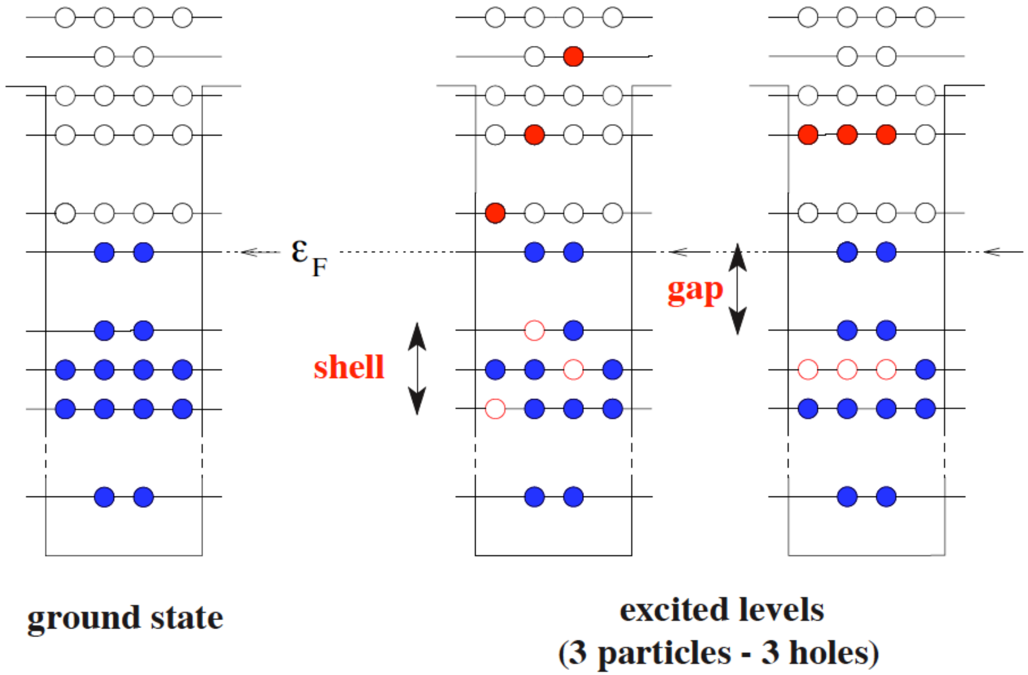
ground state

→ Still statistical approach (Solution the analytical formulas try to reproduce)
→ Still Independent Particle Approximation
→ Tables of NLD (no analytical approximation) !

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



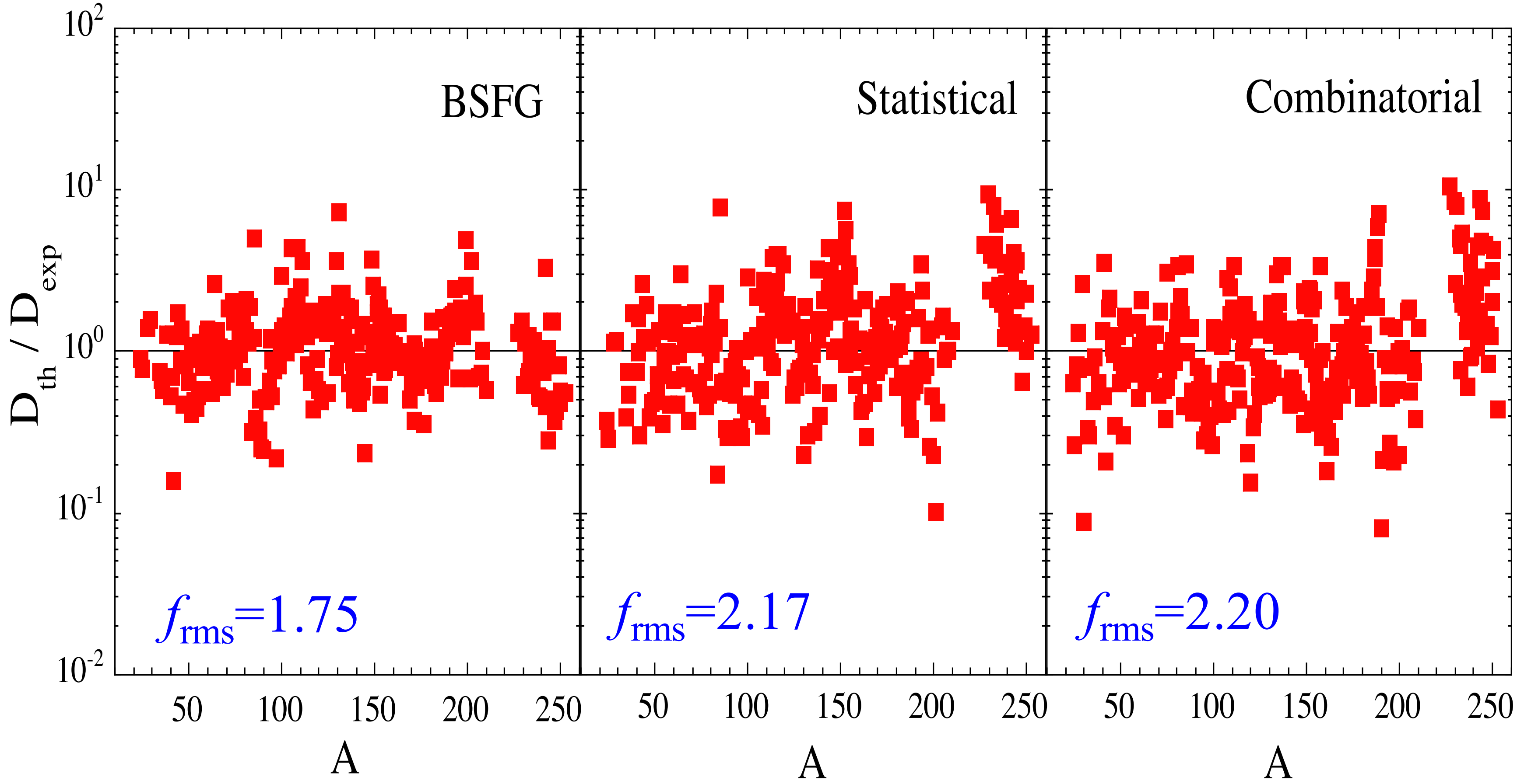
→ No more a statistical approach
→ Still Independent Particle Approximation
→ Tables of NLD (no analytical approximation)

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

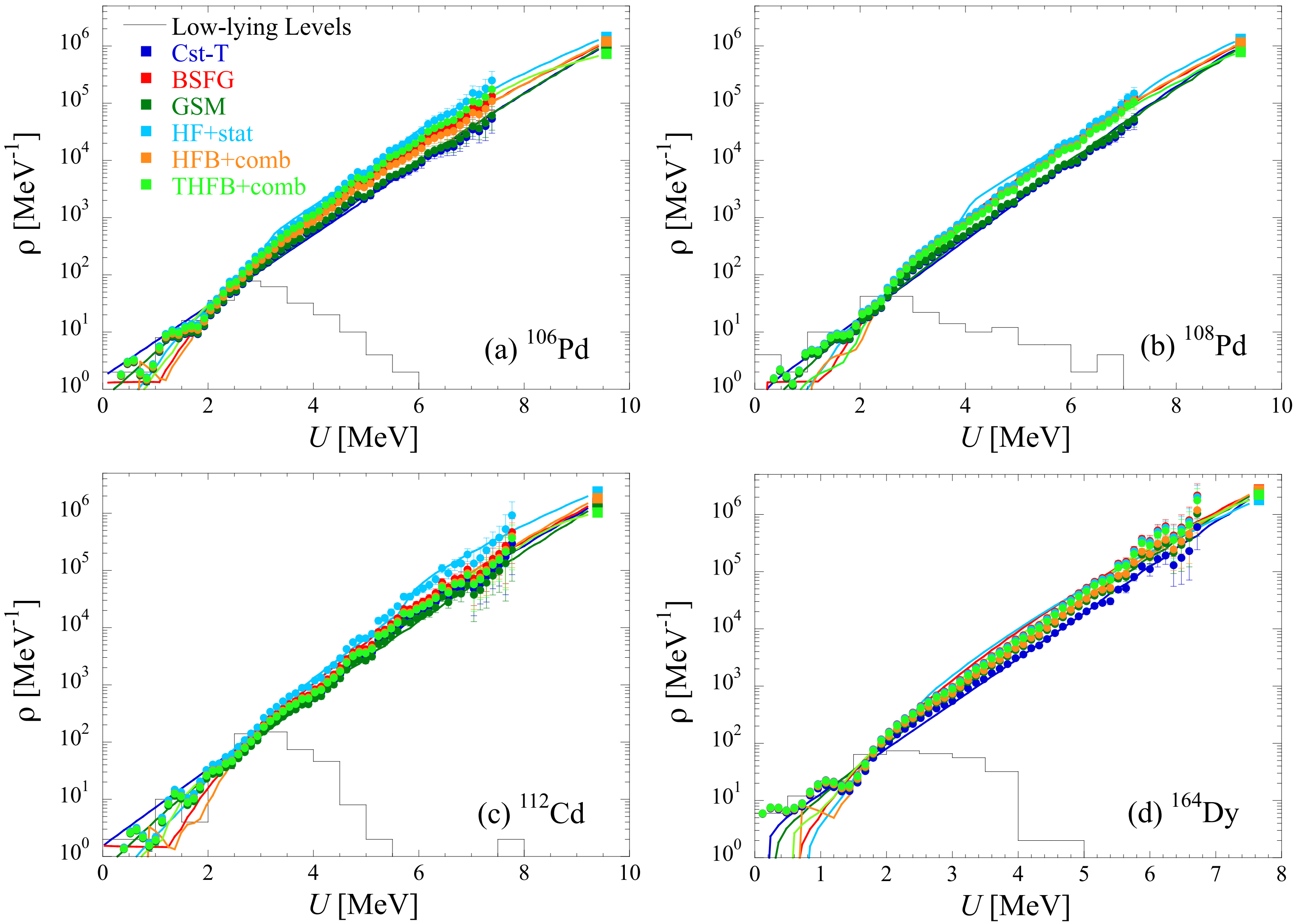
$$D_0 = \frac{1}{\rho(S_n, J_0+1/2, \pi_0) + \rho(S_n, J_0-1/2, \pi_0)} \qquad J_0>0$$

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



Testing NLD models on Oslo data

cf PRC106, 0443115 (2022)



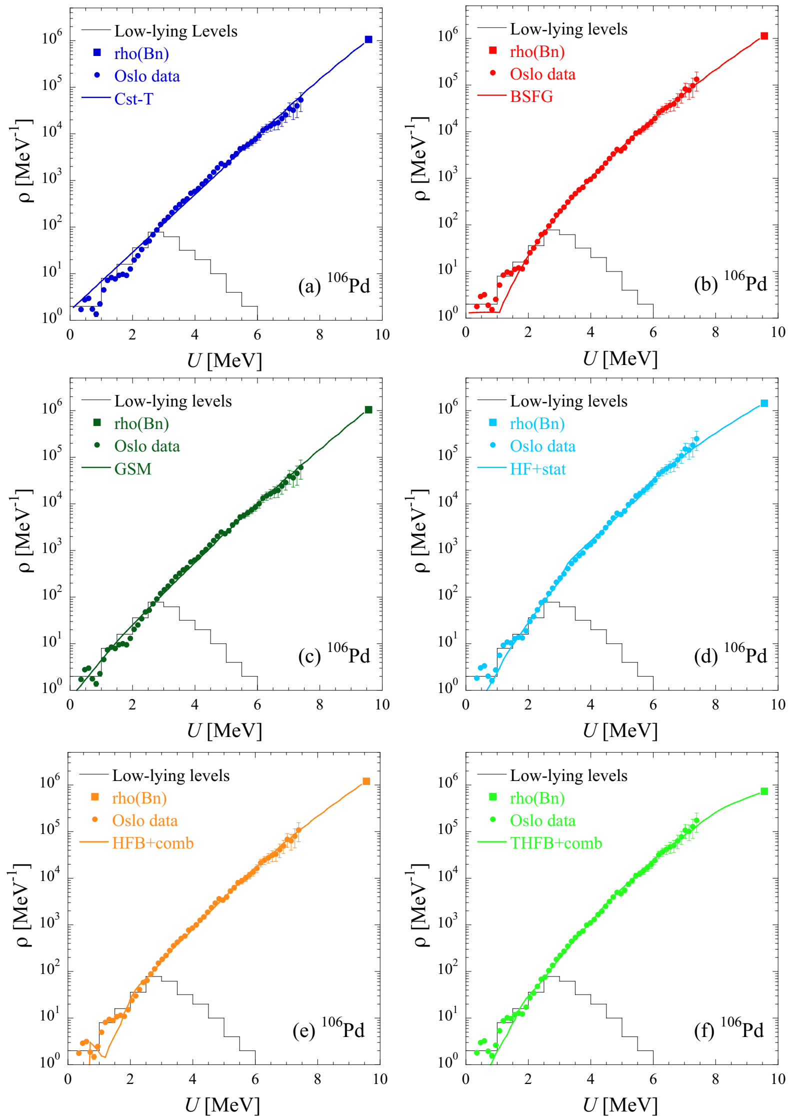
Most of Oslo data (except SM) still affected by renormalisation uncertainties

$$\tilde{\rho}(E_i - E_\gamma) = A \exp[\alpha\,(E_i - E_\gamma)]\,\rho(E_i - E_\gamma)$$

A statistical f_{rms} test of the “quality” of the NLD model vs Oslo data

Mean ε and rms σ deviations between the NLD predictions and the renormalized Oslo data for all the $N_e = 42$ nuclei for which Oslo & D_0 values are available.

NLD model	ε(all)	σ(all)
Cst-T	1.02	1.45
BSFG	0.92	1.68
GSM	0.97	1.69
HF+stat	0.94	1.53
HFB+comb	0.94	1.47
THFB+comb	0.95	1.64

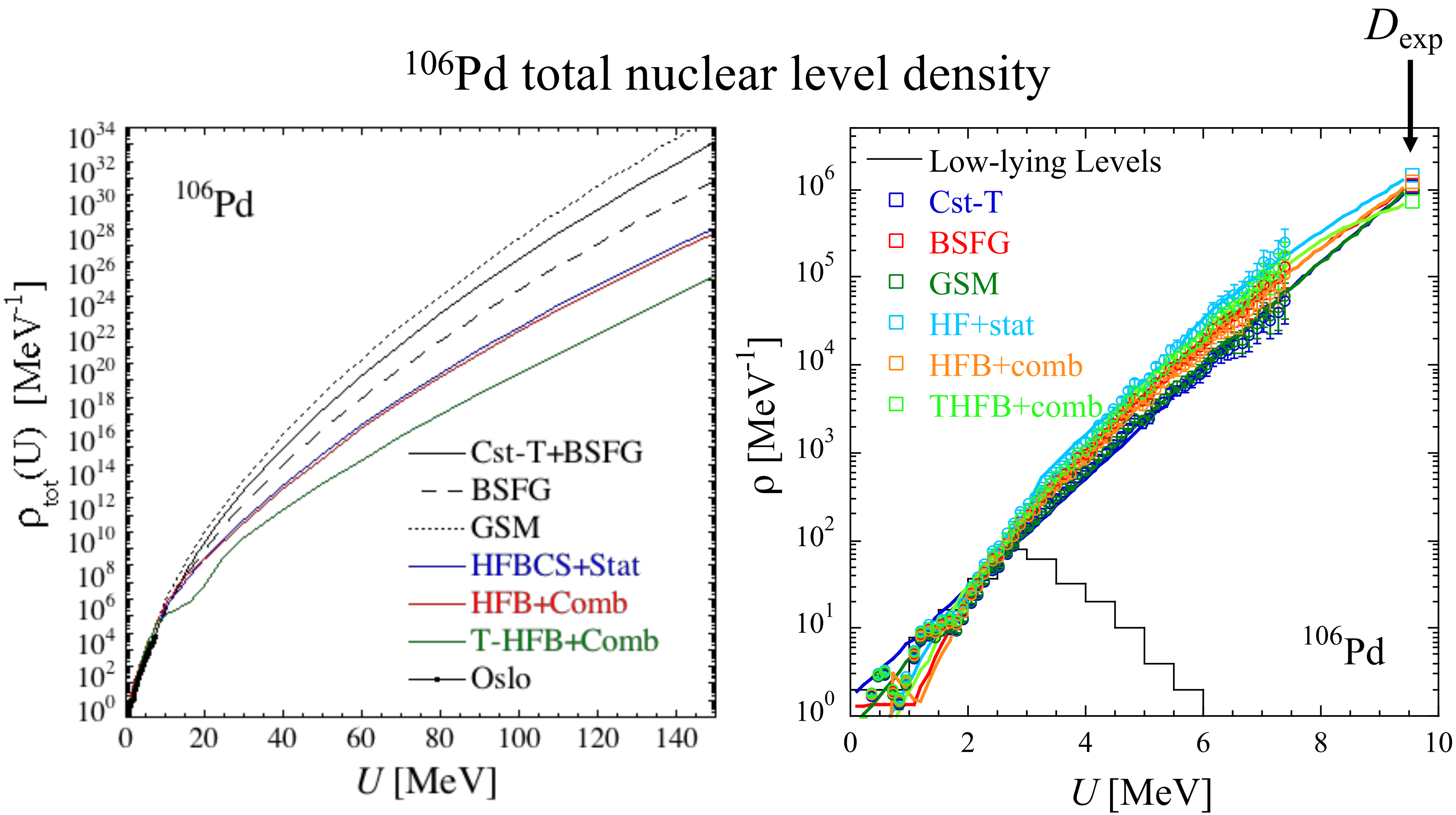


But the Shape Method should be able to reduce the uncertainties related to the renormalisation

cf PRC106, 0443115 (2022)

Different models, different predictions

^{106}Pd total nuclear level density



^{105}Pd(n,γ): Model uncertainty: $<\sigma>_{30keV} = 0.6 - 1.5$ b

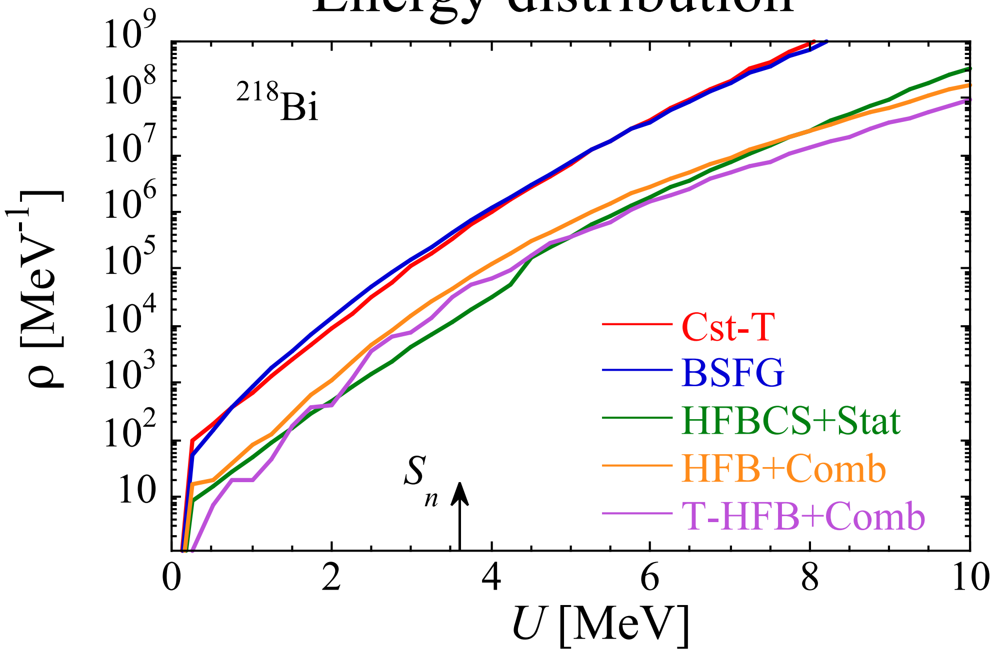
(available low-lying states and s-wave spacings)

Different models, different predictions

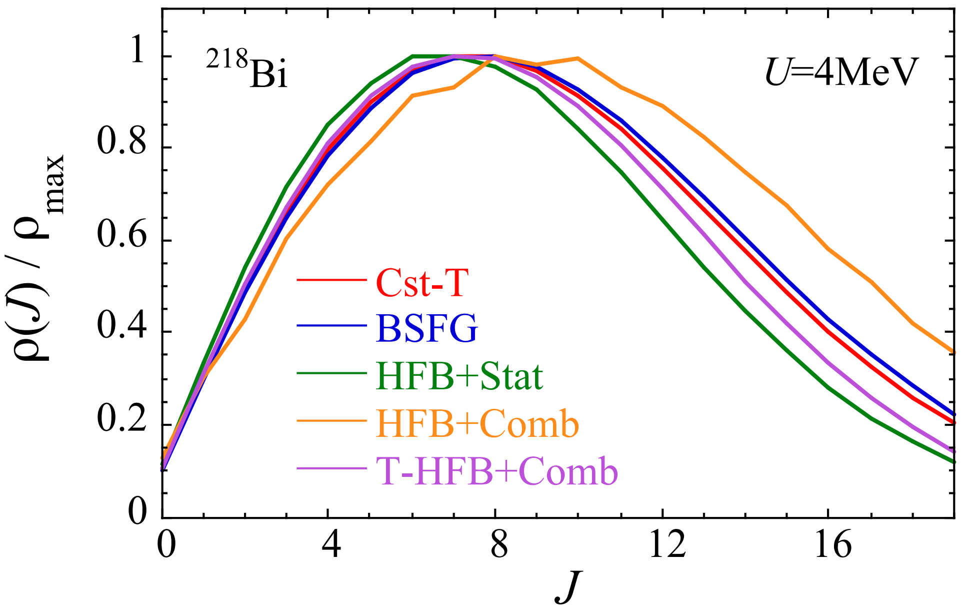
Obviously worse for unknown nuclei

^{218}Bi nuclear level density

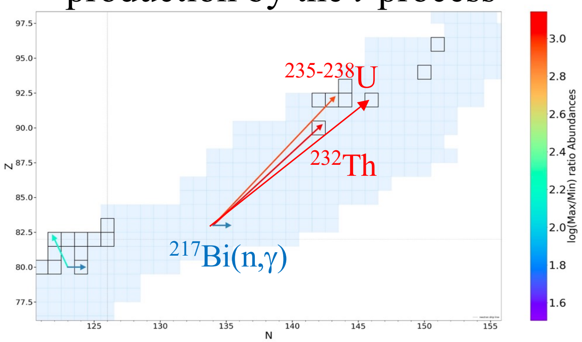
Energy distribution



Spin distribution



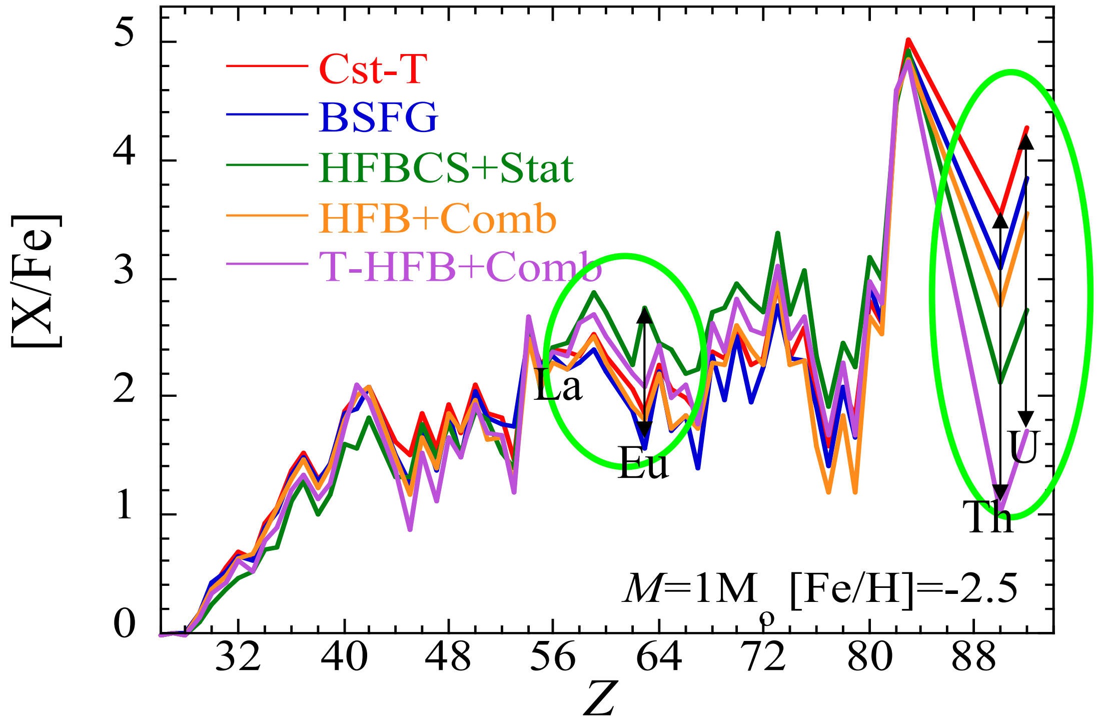
^{218}Bi of particular relevance for the Th/U production by the *i*-process



^{217}Bi(n,γ) model uncertainty:

$<\sigma>_{30keV}$ = 2.5 – 58 mb (factor 23 !)

Impact of NLD on the ***i*-process** in low-*Z* AGB stars



Significant impact on the production of "*r*"-elements by the *i*-process:

- Sm-Eu-Dy region of spectroscopic interest: e.g [La/Eu]=0.7 vs -0.3
- Actinide production of chronometric interest (though Th/U ~ cst)

- **All NLD models still unsatisfactory → Priority: improve NLD models !**
- **All NLD models based on the Independent Particle Approximation**
- **All NLD models fail at the lowest energies**

Conceptually new approach: QRPA + Boson Expansion Method

- **deformed QRPA calculations** => collective levels (***Bosons***) for various given multipolarities and parities: K=0$^{+/-}$ up to 9$^{+/-}$ for even-even nuclei (Gogny D1M+QRPA) with a energy cut-off ε_c=200MeV

- **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 spin-dependent NLD**

spherical nuclei: $$\rho_{\text{s}}(U,J,\pi) = \omega_{\text{tot}}(U,M=J,\pi) - \omega_{\text{tot}}(U,M=J+1,\pi)$$

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

- **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

Axially deformed QRPA calculations (Peru et al.)

ARC data

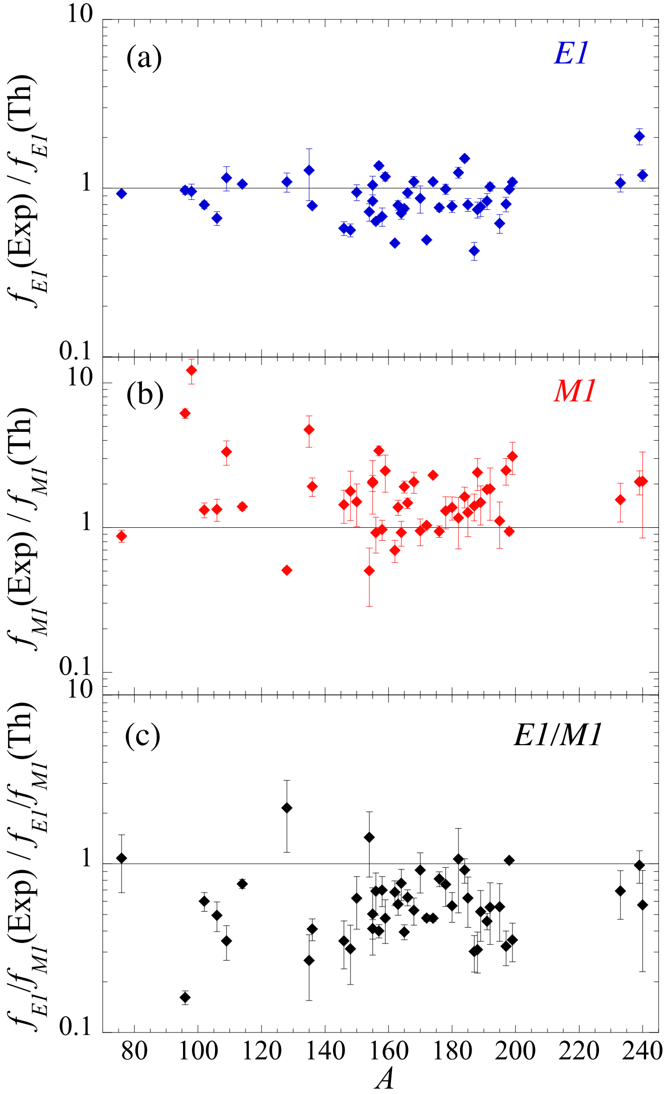
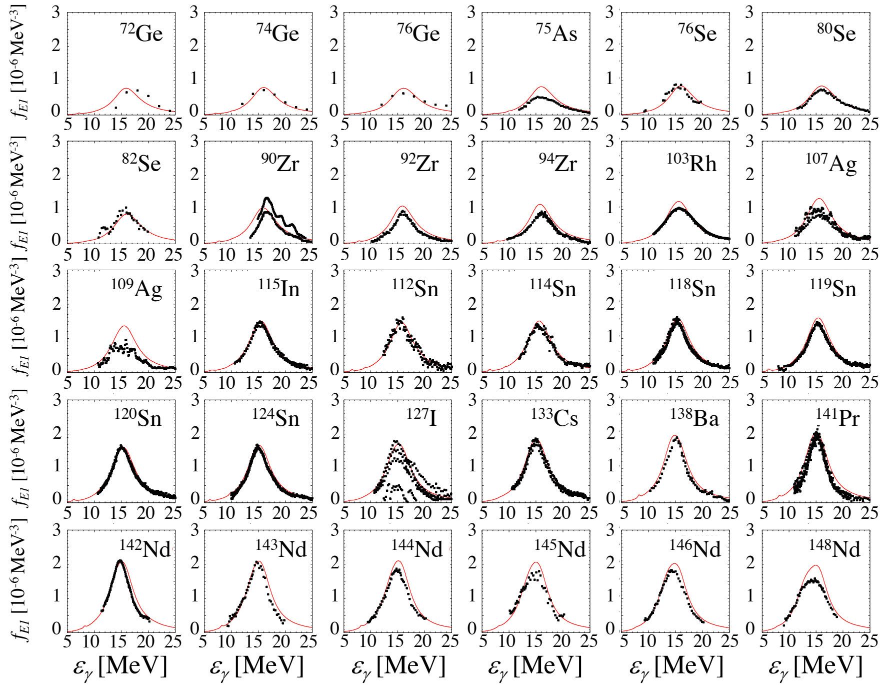
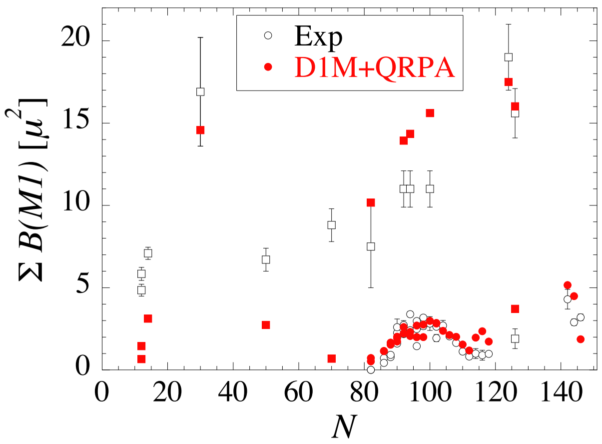


Photo data

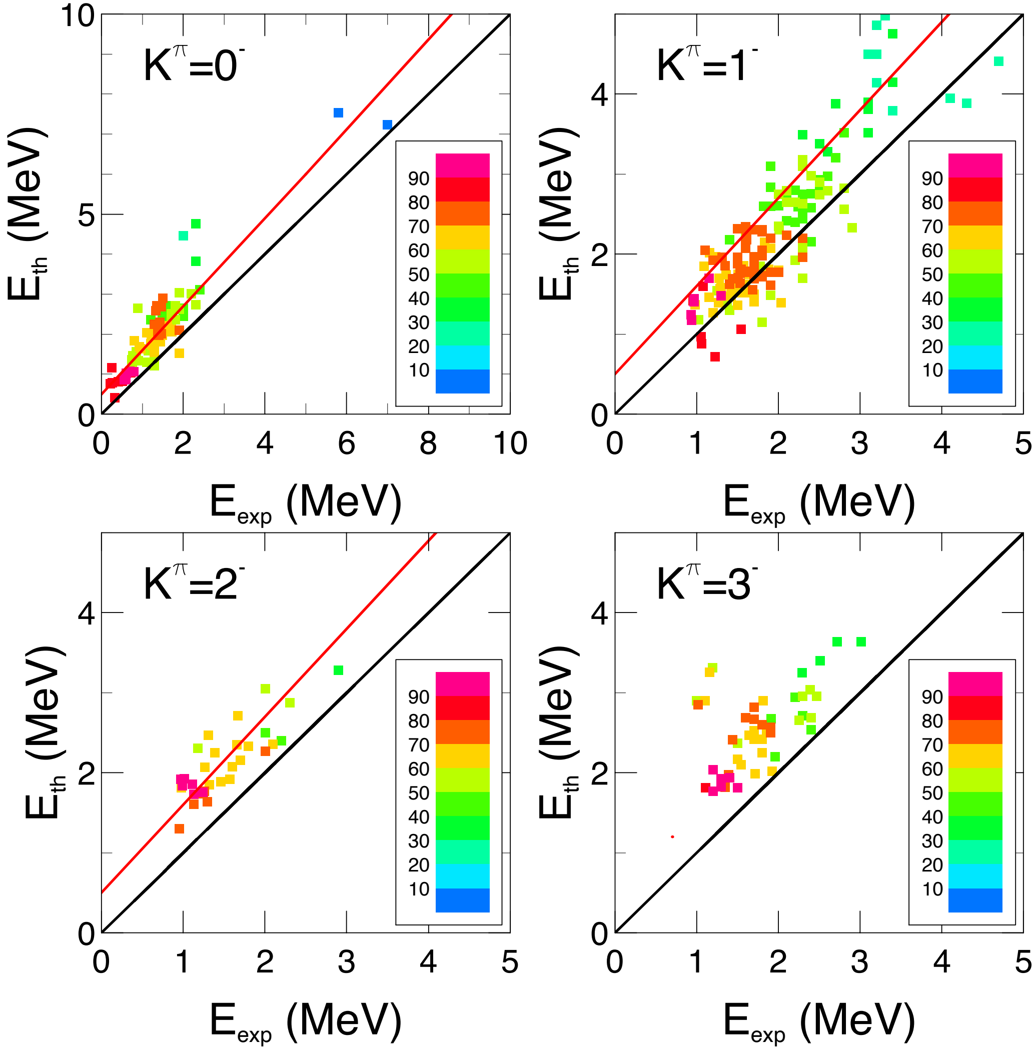


NRF data



Rather satisfactory QRPA predictions of low-energy spectroscopy

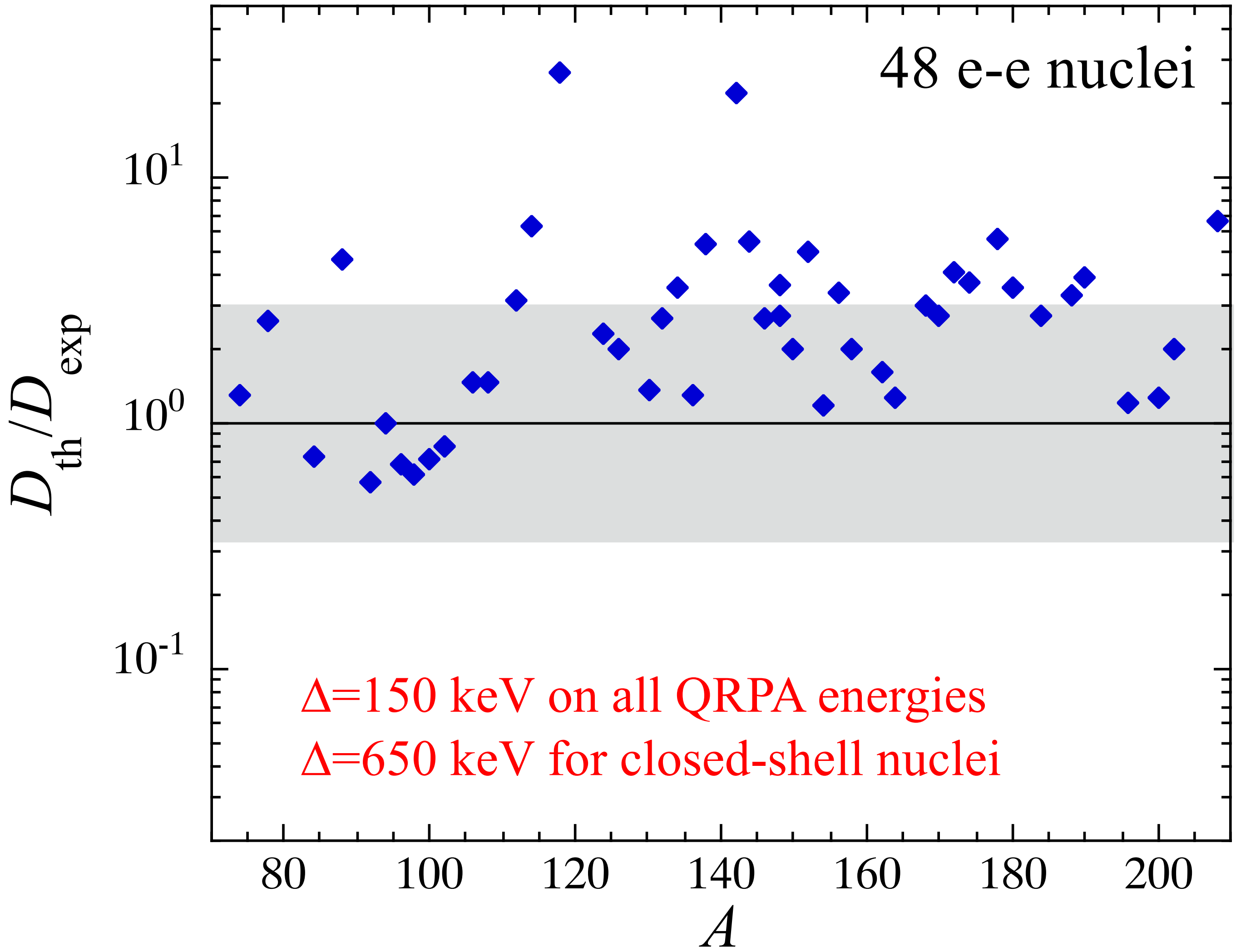
D1M+QRPA

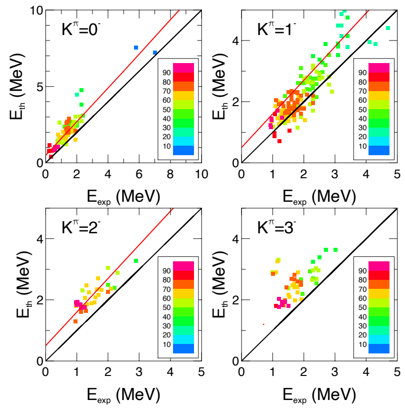


Though D1S/D1M+QRPA tends to systematically overestimate spectroscopic data (Δ ~ few 100keV)

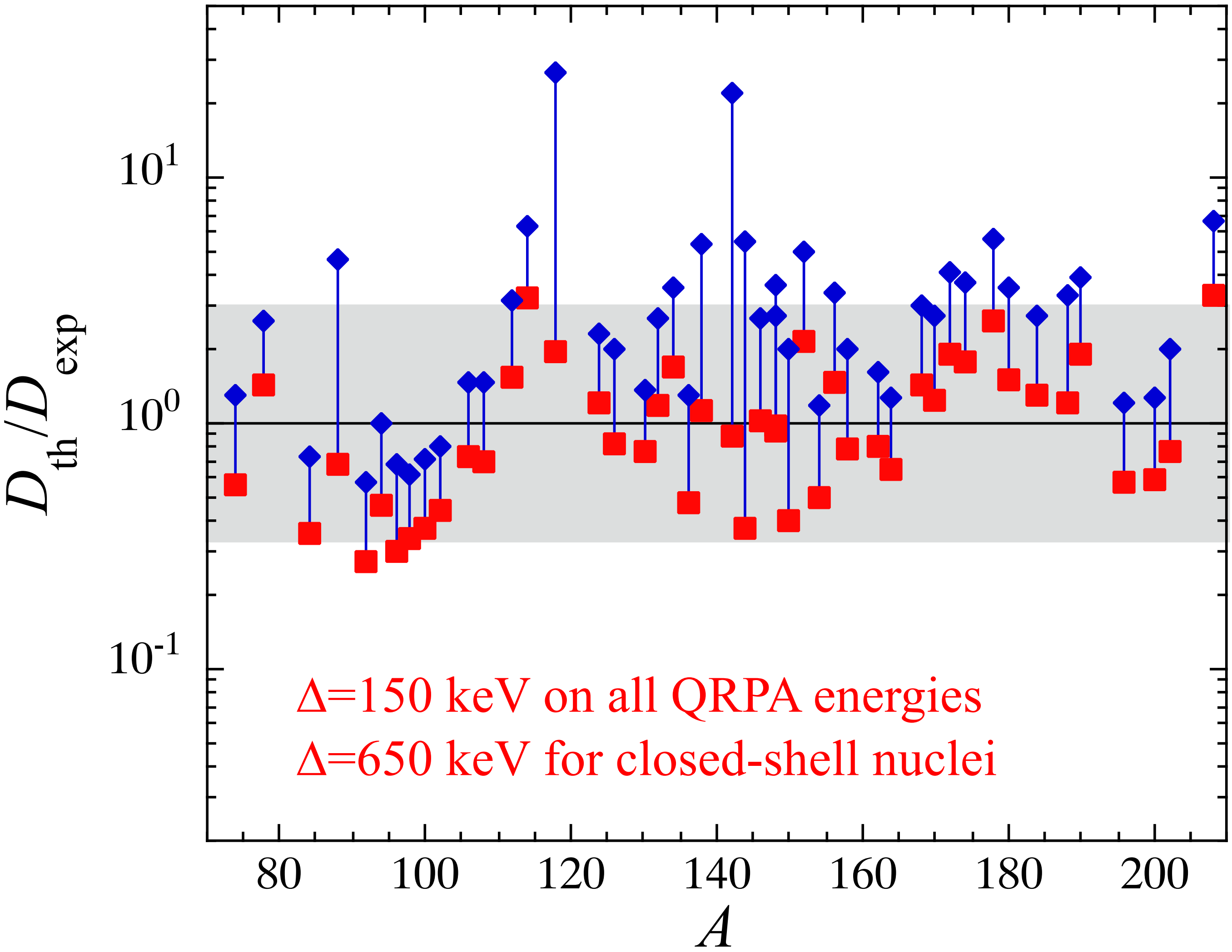
The QRPA + Boson Expansion Method

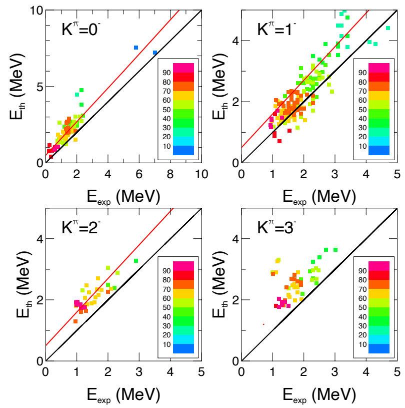
Relatively satisfactory description of D_0, but overall overestimation (*i.e.* underestimation of ρ)





The QRPA + Boson Expansion Method

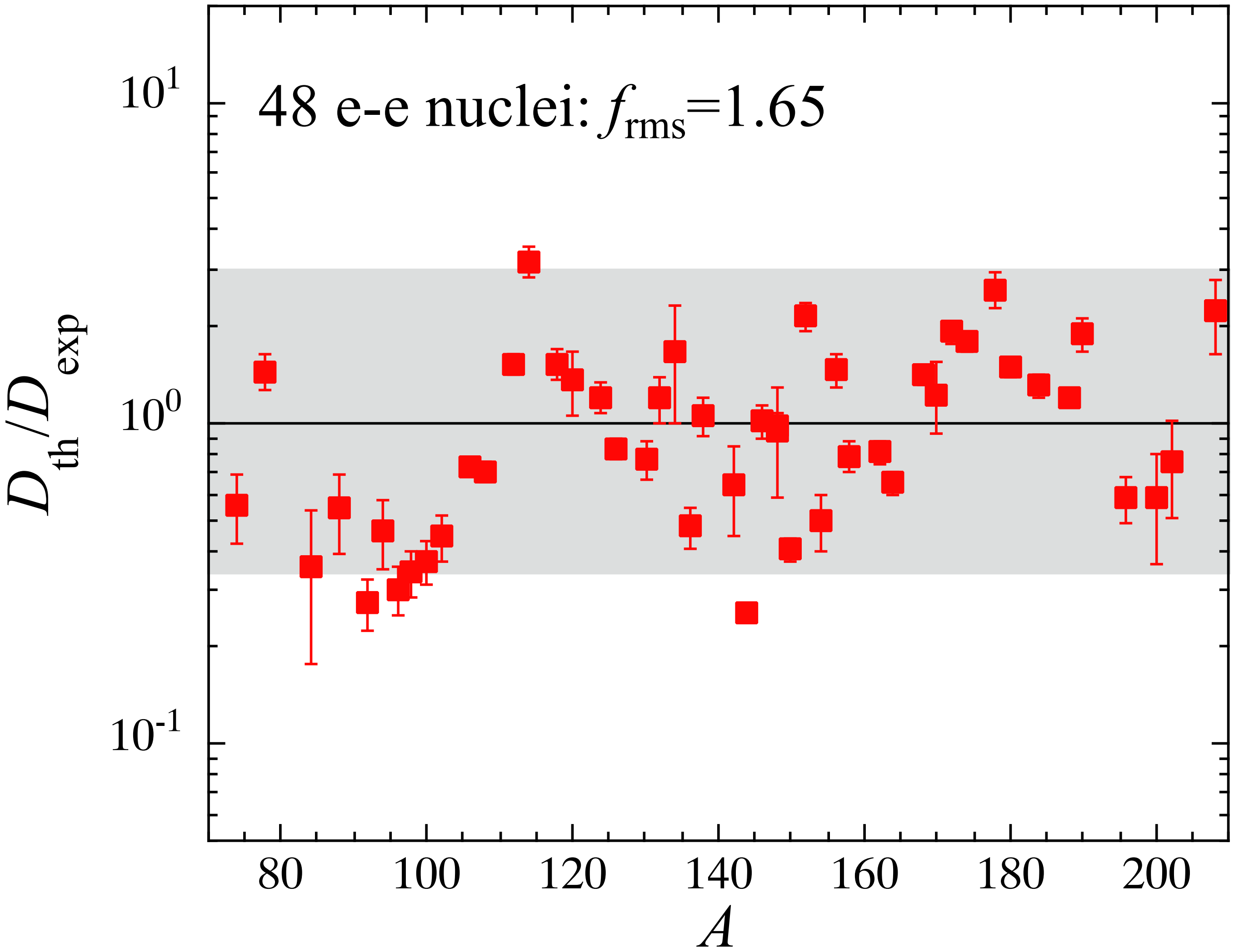




→ Need for an accurate estimate of the lowest QRPA exitations energies

The QRPA + Boson Expansion Method

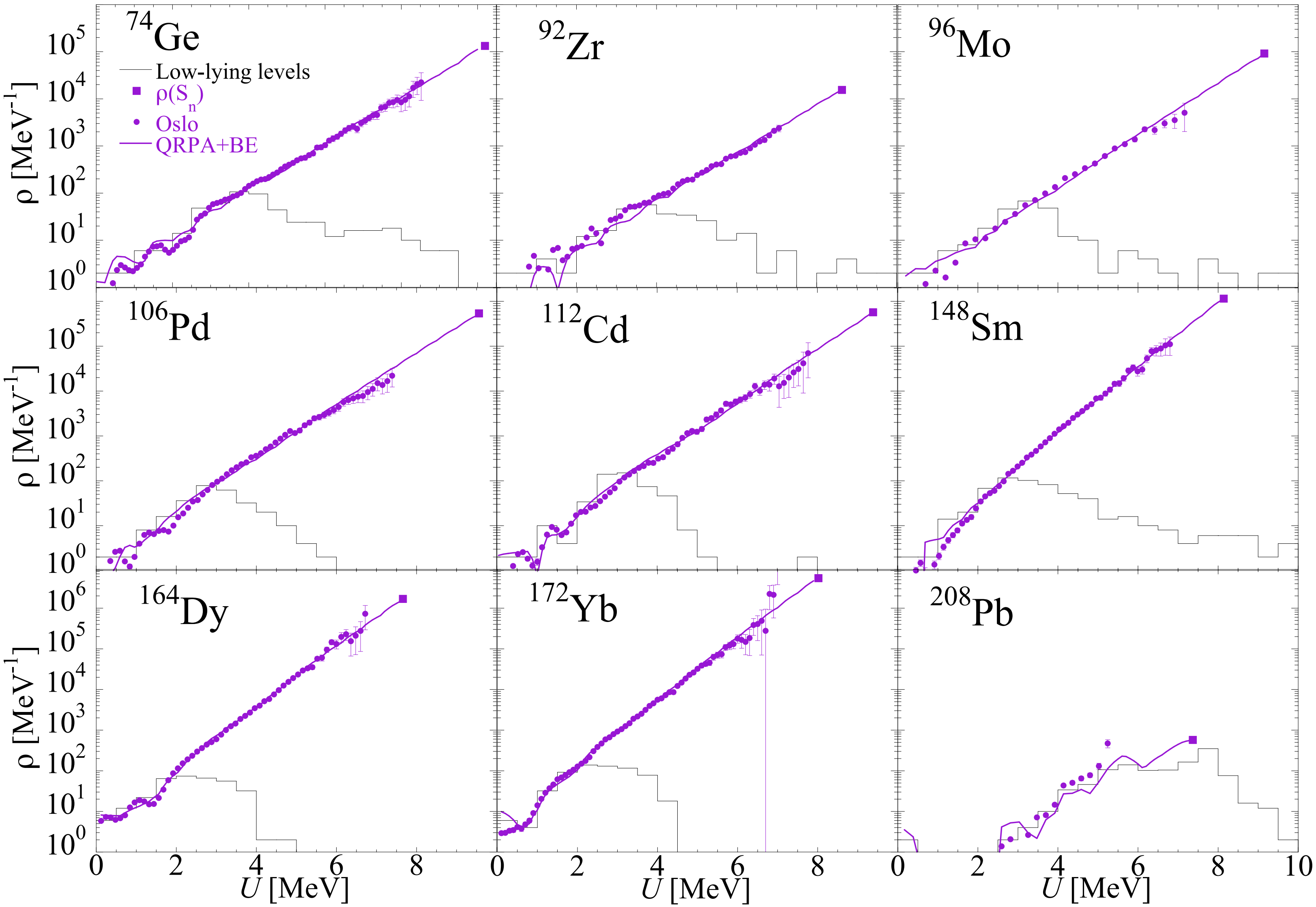
Finally, including experimental uncertainties



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

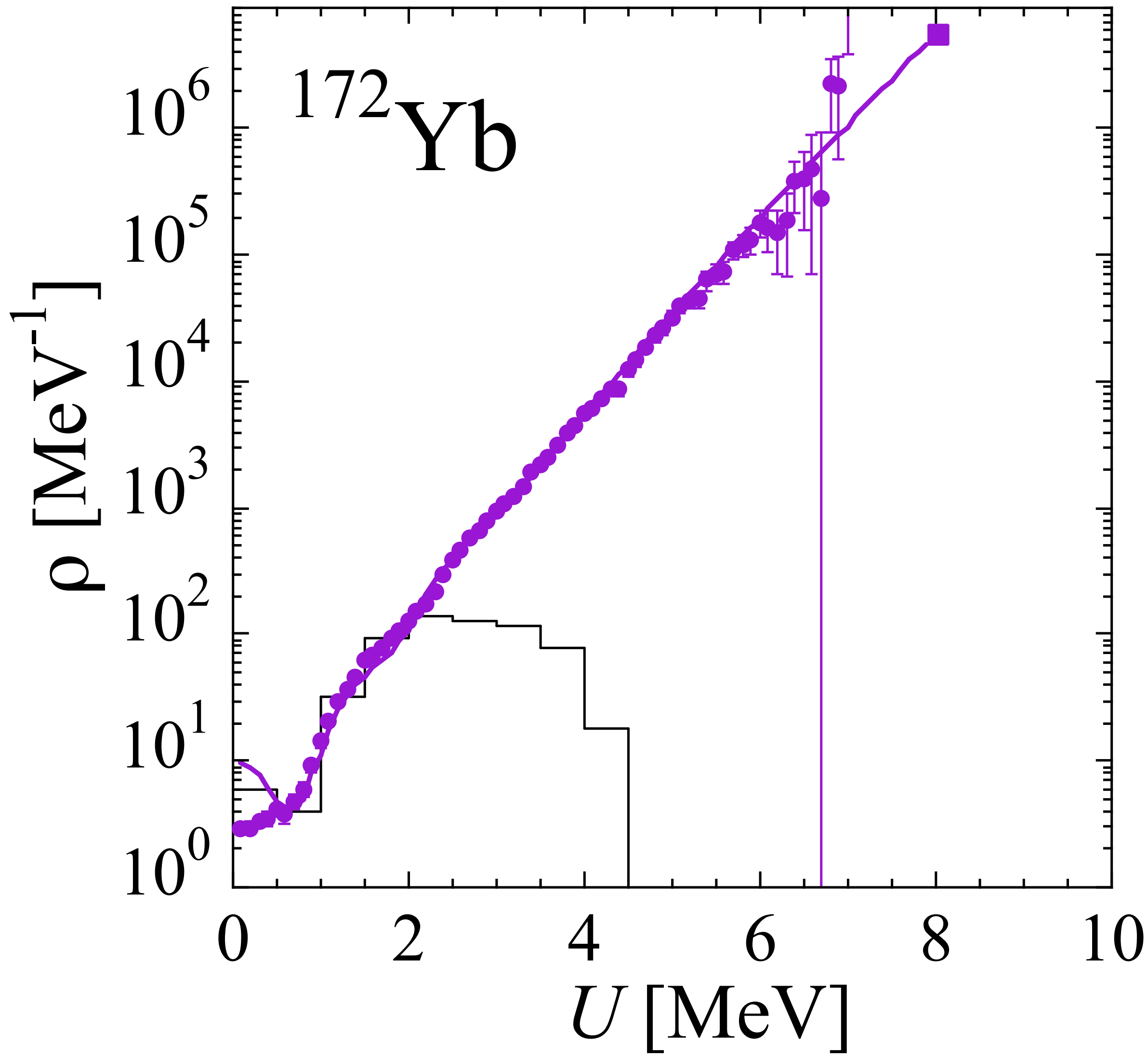
The QRPA + Boson Expansion Method

Normalisation of the QRPA+BE energies on D_0 & Oslo data on theoretical NLDs



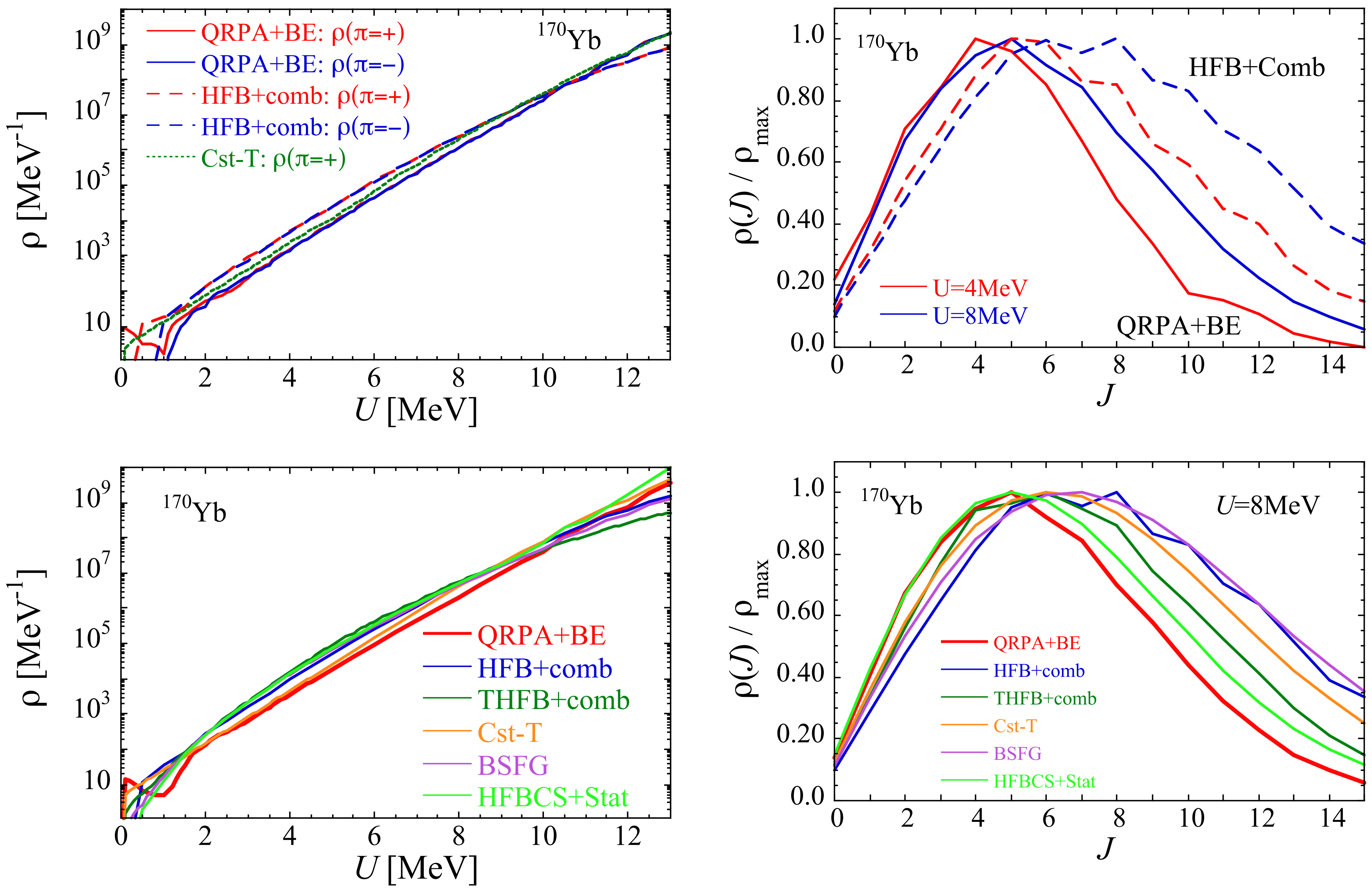
The QRPA + Boson Expansion Method

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



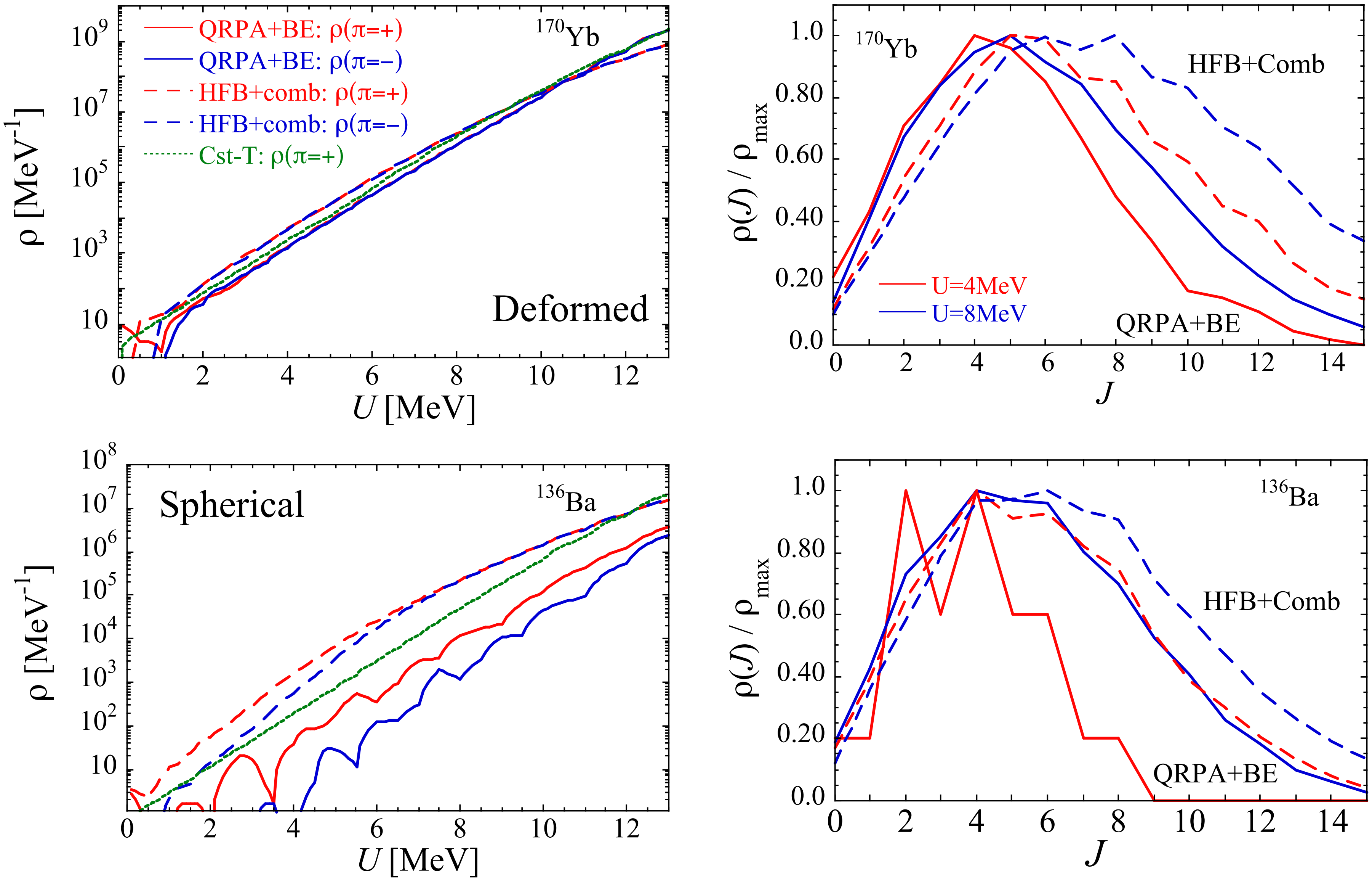
The QRPA + Boson Expansion Method

(assuming a global shift of QRPA energies)

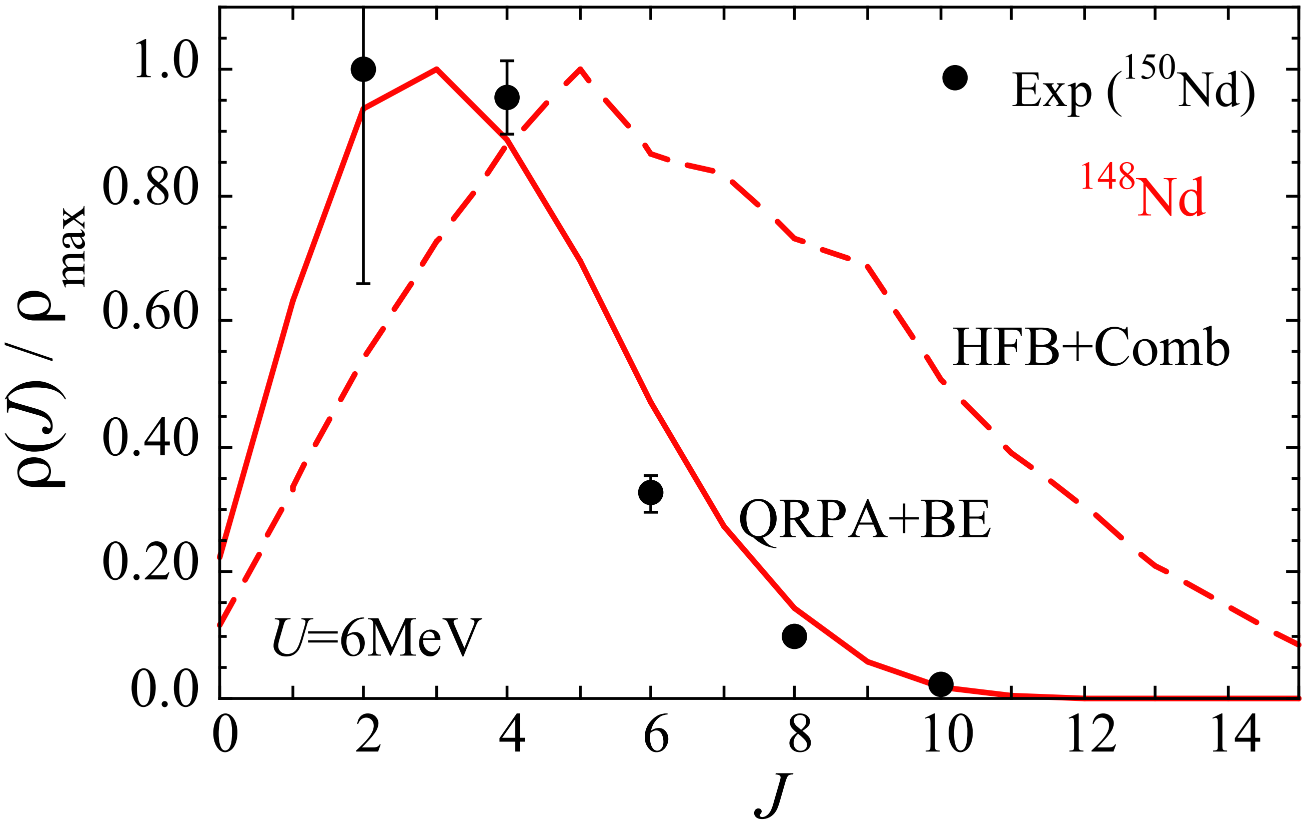


The QRPA + Boson Expansion Method

(assuming a global shift of QRPA energies)

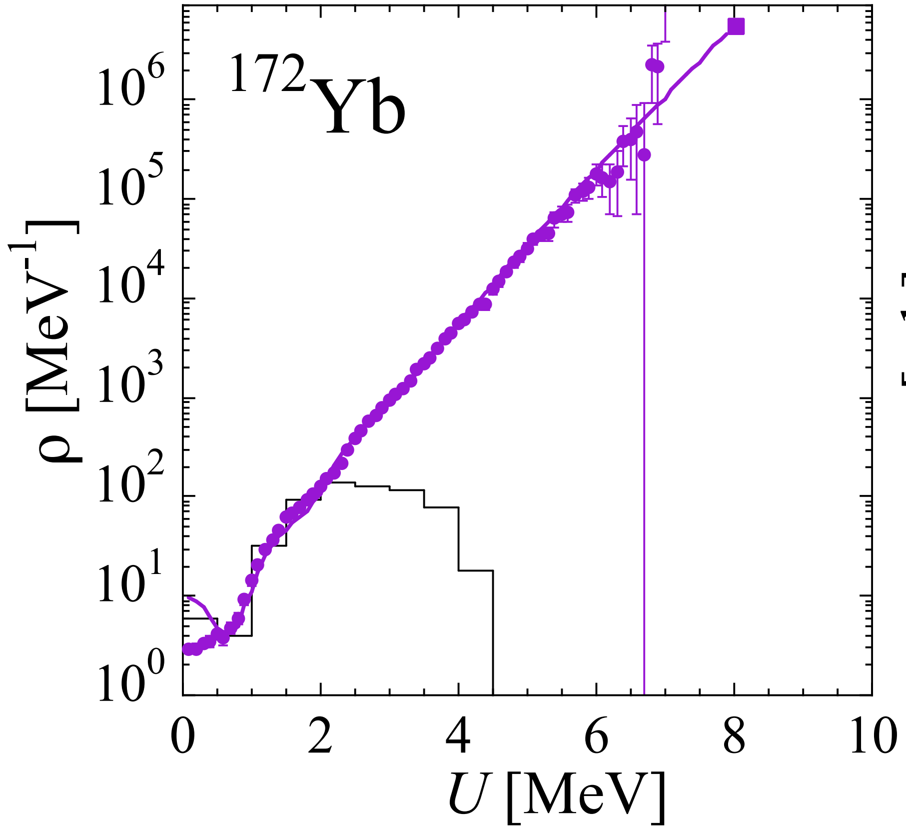


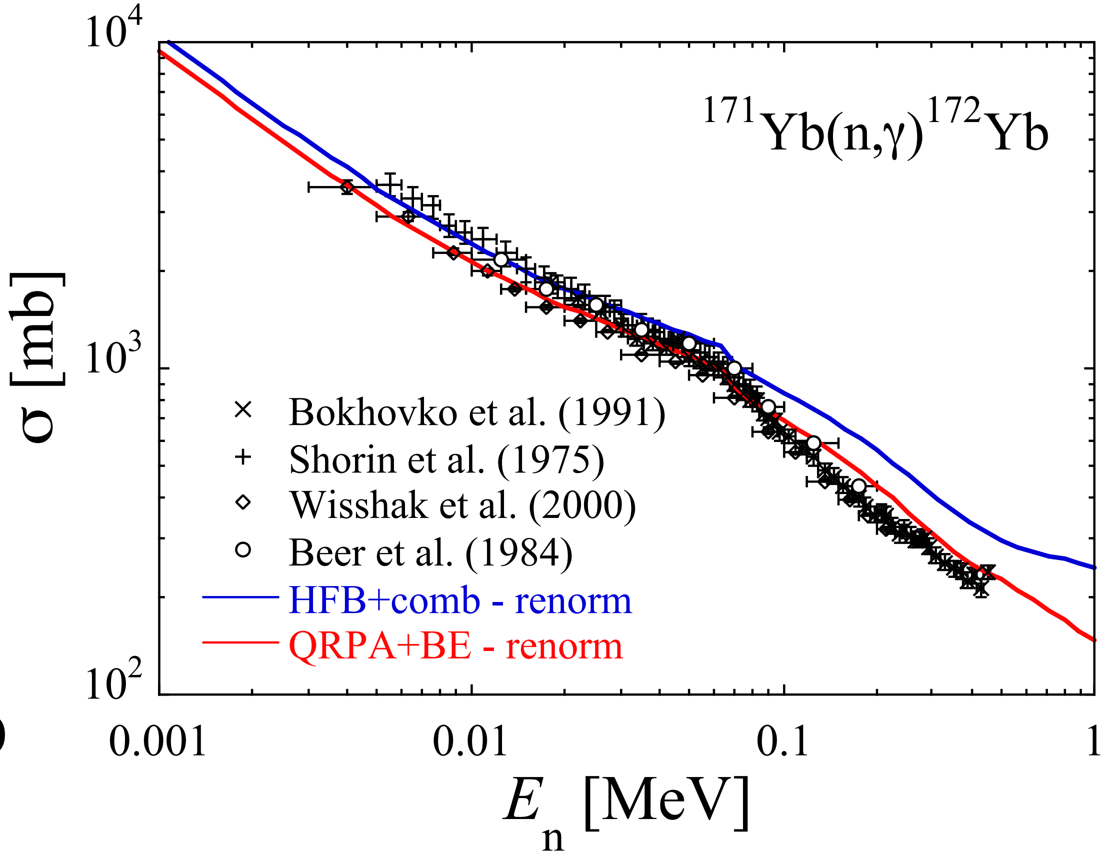
The QRPA + Boson Expansion Method



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

Application of the QRPA + Boson Expansion Method to cross section calculations





NLD renormalized on known D_0

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...)