# Microscopic mass model for astrophysics

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# Nuclear mass models

**Nuclear mass models provide all basic nuclear ingredients:**

**Mass excess (Q-values), deformation, GS spin and parity**

**but also**

**single-particle levels, pairing strength, density distributions, … in the GS as well as non-equilibrium (e.g fission path) configuration**

***Building blocks for the prediction of ingredients of relevance in the determination of nuclear reaction cross sections and β-decay rates, such as***

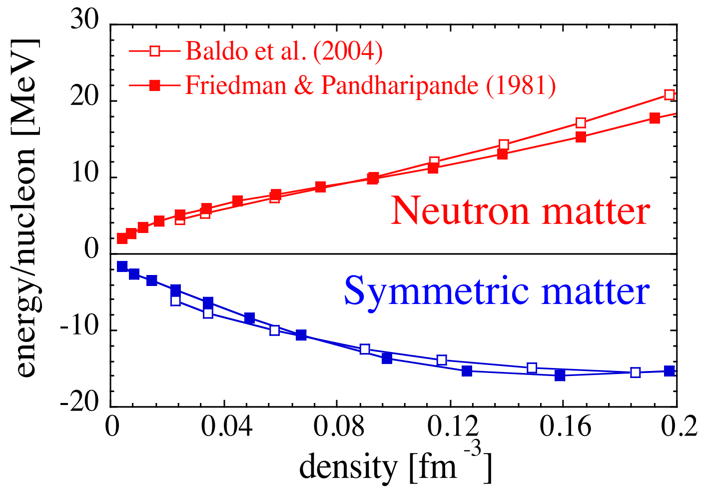
- nuclear level densities
- γ-ray strengths
- optical potentials
- fission probabilities
- etc …

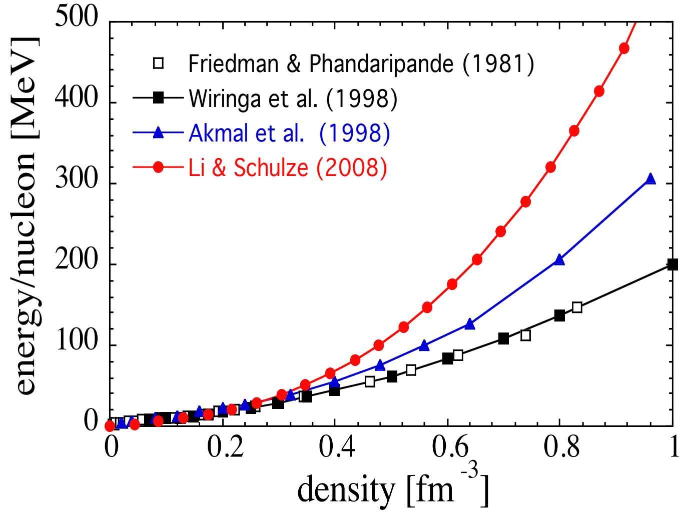
***as well as for the nuclear/neutron matter Equation of State* (NEUTRON STARS)**

**The criteria to qualify a mass model should NOT be restricted to the rms deviation wrt to exp. masses, but also include**
**- the quality of the underlying physics (sound, coherent, "microscopic", …)**
**- all the observables of relevance in the specific applications of interest (e.g astro)**

# Challenge for modern mass models: to reproduce as many observables as possible

- 2353 experimental masses from AME'2012
- 782 exp. charge radii, as well as ~26 neutron skins
- Isomers & Fission barriers (scan large deformations)
- Symmetric nuclear matter properties
    - $m^* \sim 0.6 - 0.8$ (BHF, GQR) & $m^*_n(\beta) > m^*_p(\beta)$
    - $K \sim 230 - 250$ MeV (breathing mode)
    - $E_{pot}$ from BHF calc. & in 4 $(S,T)$ channels
    - Landau parameters $F_l(S,T)$
        - stability condition: $F_l^{ST} > -(2l+1)$
        - empirical $g_0 \sim 0$; $g_0' \sim 0.9$-$1.2$
        - sum rules $S_1 \sim 0$; $S_2 \sim 0$
    - Pairing gap (with/out medium effects)
    - Pressure around 2-3$\rho_0$ from heavy-ion collisions
- Neutron matter properties
    - $J \sim 29 - 32$MeV
    - $E_n/A$ from realistic BHF-like calculations
    - Pairing gap
    - Stability of neutron matter at all polarizations
- Giant resonances
    - ISGMR, IVGDR, ISGQR
- Additional model-dependent properties
    - Nuclear Level Density (pairing-sensitive)
    - Properties of the lowest $2^+$ levels (519 e-e nuclei)
    - Moment of inertia in superfluid nuclei (back-bending)



# HFB mass models

**Adjustement of an effective interaction to all (2353) experimental masses within the Hartree-Fock-Bogolyubov approach**

**rms(M) = 0.5-0.8 MeV on 2353 ($Z \geq 8$) experimental masses**

(definition of a “mass model” in contrast to a calculation with a given force)

To be compared with

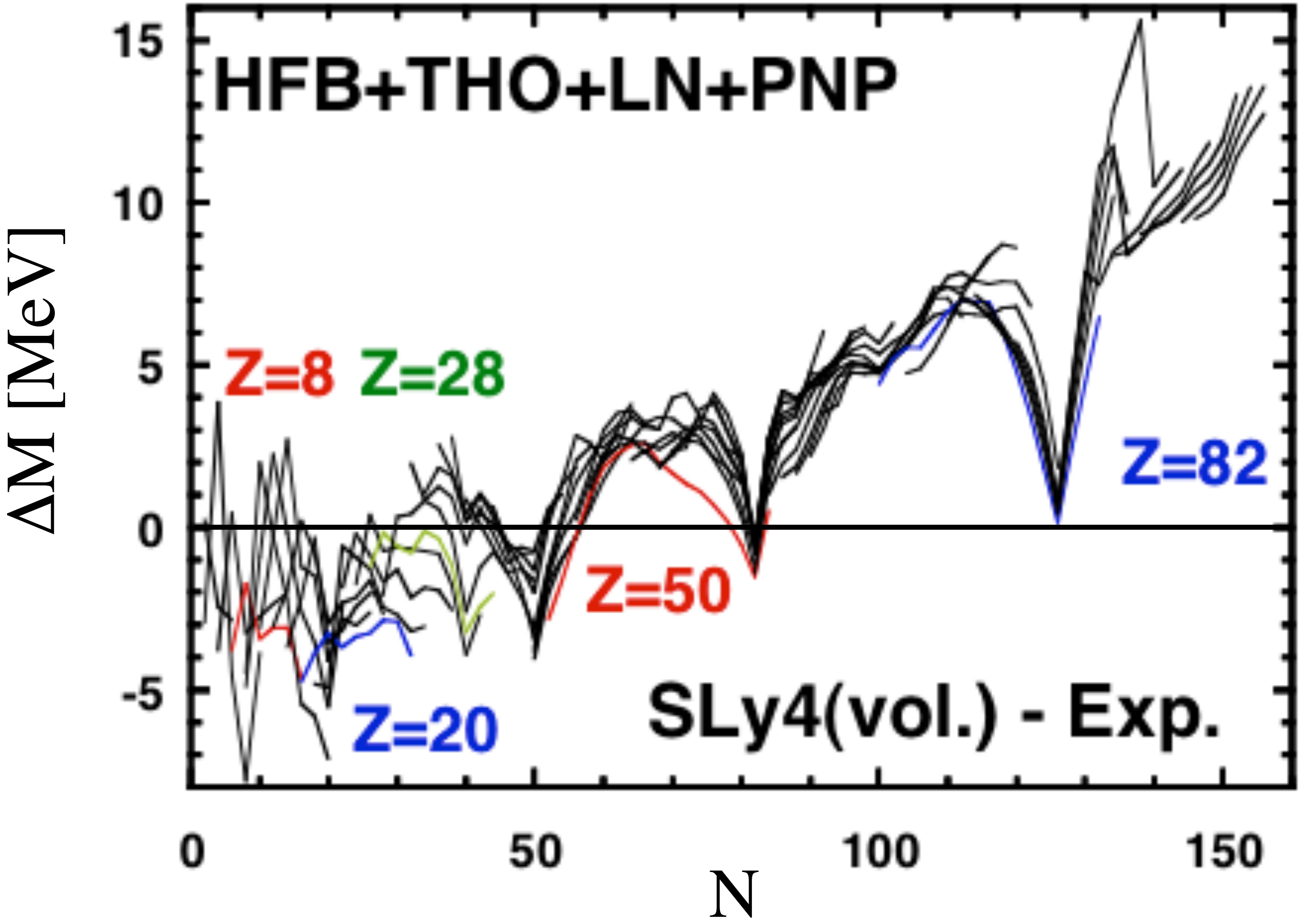
- FRDM predictions: rms(M)=0.65 MeV
- Other mean-field predictions:

Traditional Skyrme or Gogny forces: rms > 2 MeV

e.g. Oak Ridge "Mass Table" based on HFB with SLy4

rms(M)=5.1MeV on 570 e-e sph+def nuclei

# M(SLy4) – M(exp)




Dobaczewski et al., 2004

# Skyrme-HFB mass model

**Adjustement of an effective force to all (2353) experimental masses within the Hartree-Fock-Bogolyubov approach**

Standard Skyrme force (10 parameters)

$$
\begin{aligned}
v_{ij} &= t_0(1+x_0P_\sigma)\delta(\boldsymbol{r}_{ij}) + \frac{1}{2}t_1(1+x_1P_\sigma)\frac{1}{\hbar^2}\left[p_{ij}^2\,\delta(\boldsymbol{r}_{ij}) + \delta(\boldsymbol{r}_{ij})\,p_{ij}^2\right] \\
&+ t_2(1+x_2P_\sigma)\frac{1}{\hbar^2}\boldsymbol{p}_{ij}.\delta(\boldsymbol{r}_{ij})\,\boldsymbol{p}_{ij} + \frac{1}{6}t_3(1+x_3P_\sigma)\,n(\boldsymbol{r})^\alpha\,\delta(\boldsymbol{r}_{ij}) \\
&+ \frac{\mathrm{i}}{\hbar^2}W_0(\boldsymbol{\sigma_i}+\boldsymbol{\sigma_j})\cdot\boldsymbol{p}_{ij}\times\delta(\boldsymbol{r}_{ij})\,\boldsymbol{p}_{ij} \quad ,
\end{aligned}
$$

# HFB mass model: potentially a very powerful mass model

**Adjustement of an effective force to all (2353) experimental masses within the Hartree-Fock-Bogolyubov approach**

Standard Skyrme force or Extended Skyrme force including $t_4$- & $t_5$-terms

$$
\begin{aligned}
v_{ij} \quad = \quad & t_0(1+x_0P_\sigma)\delta(\boldsymbol{r}_{ij}) + \frac{1}{2}t_1(1+x_1P_\sigma)\frac{1}{\hbar^2}\left[p_{ij}^2\,\delta(\boldsymbol{r}_{ij}) + \delta(\boldsymbol{r}_{ij})\,p_{ij}^2\right] \\
+ \quad & t_2(1+x_2P_\sigma)\frac{1}{\hbar^2}\boldsymbol{p}_{ij}.\delta(\boldsymbol{r}_{ij})\,\boldsymbol{p}_{ij} + \frac{1}{6}t_3(1+x_3P_\sigma)\,n(\boldsymbol{r})^\alpha\,\delta(\boldsymbol{r}_{ij}) \\
+ \quad & \frac{1}{2}\,t_4(1+x_4P_\sigma)\frac{1}{\hbar^2}\left[p_{ij}^2\,n(\boldsymbol{r})^\beta\,\delta(\boldsymbol{r}_{ij}) + \delta(\boldsymbol{r}_{ij})\,n(\boldsymbol{r})^\beta\,p_{ij}^2\right] \\
+ \quad & t_5(1+x_5P_\sigma)\frac{1}{\hbar^2}\boldsymbol{p}_{ij}.n(\boldsymbol{r})^\gamma\,\delta(\boldsymbol{r}_{ij})\,\boldsymbol{p}_{ij} \\
+ \quad & \frac{\mathrm{i}}{\hbar^2}W_0(\boldsymbol{\sigma_i}+\boldsymbol{\sigma_j})\cdot\boldsymbol{p}_{ij}\times\delta(\boldsymbol{r}_{ij})\,\boldsymbol{p}_{ij} \quad ,
\end{aligned}
$$

$t_4$- & $t_5$-terms needed to describe the neutron matter EoS, not for masses

## Pairing strength deduced from "realistic" calculation of screened symmetric matter and screened neutron matter

$$\Delta_q(\rho_n,\rho_p) = \Delta_{SM}(\rho)\left[1-|\eta|\right] \pm \Delta_{NM}(\rho_q)\eta\frac{\rho_q}{\rho} \qquad \eta = \frac{\rho_n-\rho_p}{\rho}$$

$\Delta_q(\rho_n,\rho_p)$ such that

$$\begin{cases} \Delta_n(\rho_n,\rho_p) = \Delta_p(\rho_p,\rho_n) & \text{charge symmetry} \\ \Delta_q(\rho/2,\rho/2) = \Delta_{SM}(\rho) & \text{for Symmetric matter} \\ \Delta_n(\rho,0) = \Delta_{NM}(\rho) & \text{for Pure neutron matter} \\ \Delta_p(\rho,0) = 0 & \text{for Pure neutron matter} \end{cases}$$

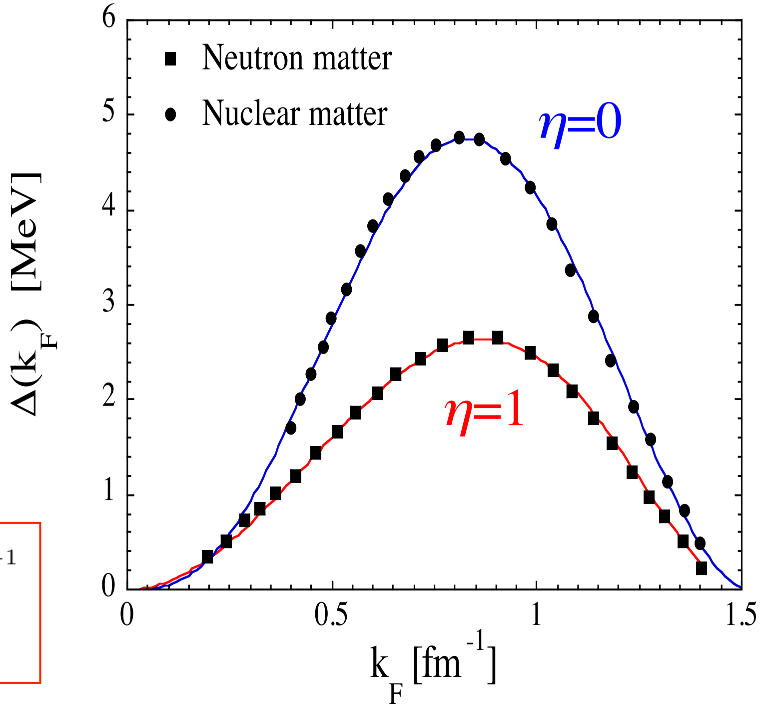
Pairing strength for screened

- symmetric matter
- neutron matter

obtained with *free spectrum* from BHF calculations with realistic 2- and 3-nucleon forces (Cao et al. 2006)

↓ Pairing strength for nuclei

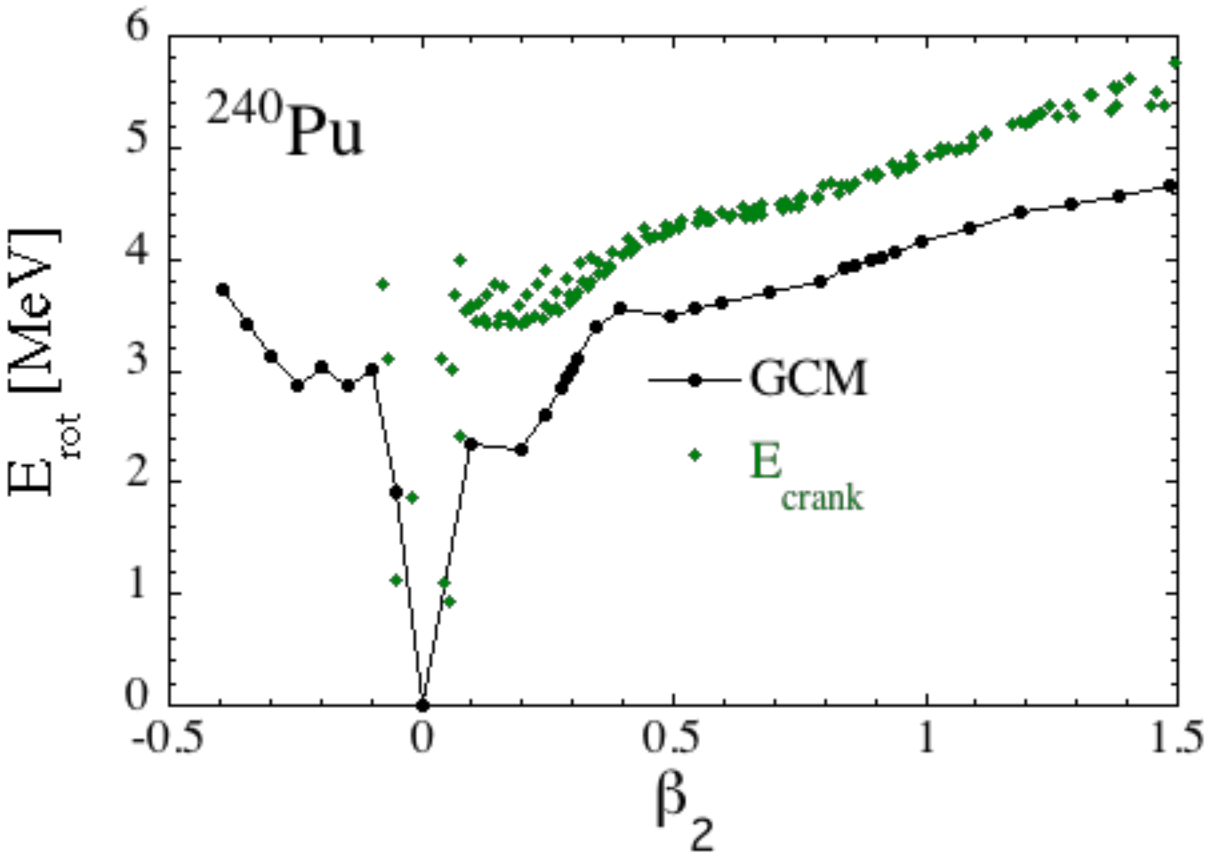
$$v^{\pi\, q}[\rho_n,\rho_p] = -8\pi^2\left(\frac{\hbar^2}{2M_q^*(\rho_n,\rho_p)}\right)^{3/2} \times \left(\int_0^{\mu_q+\varepsilon_\Lambda} \mathrm{d}\xi \frac{\sqrt{\xi}}{\sqrt{(\xi-\mu_q)^2+\Delta_q(\rho_n,\rho_p)^2}}\right)^{-1}$$



# Correction for quadrupole correlations

a perturbative *cranking* correction for rotational correlations

$$E_{rot}^{crank} = \frac{\langle \hat{J}^2 \rangle}{2I}$$



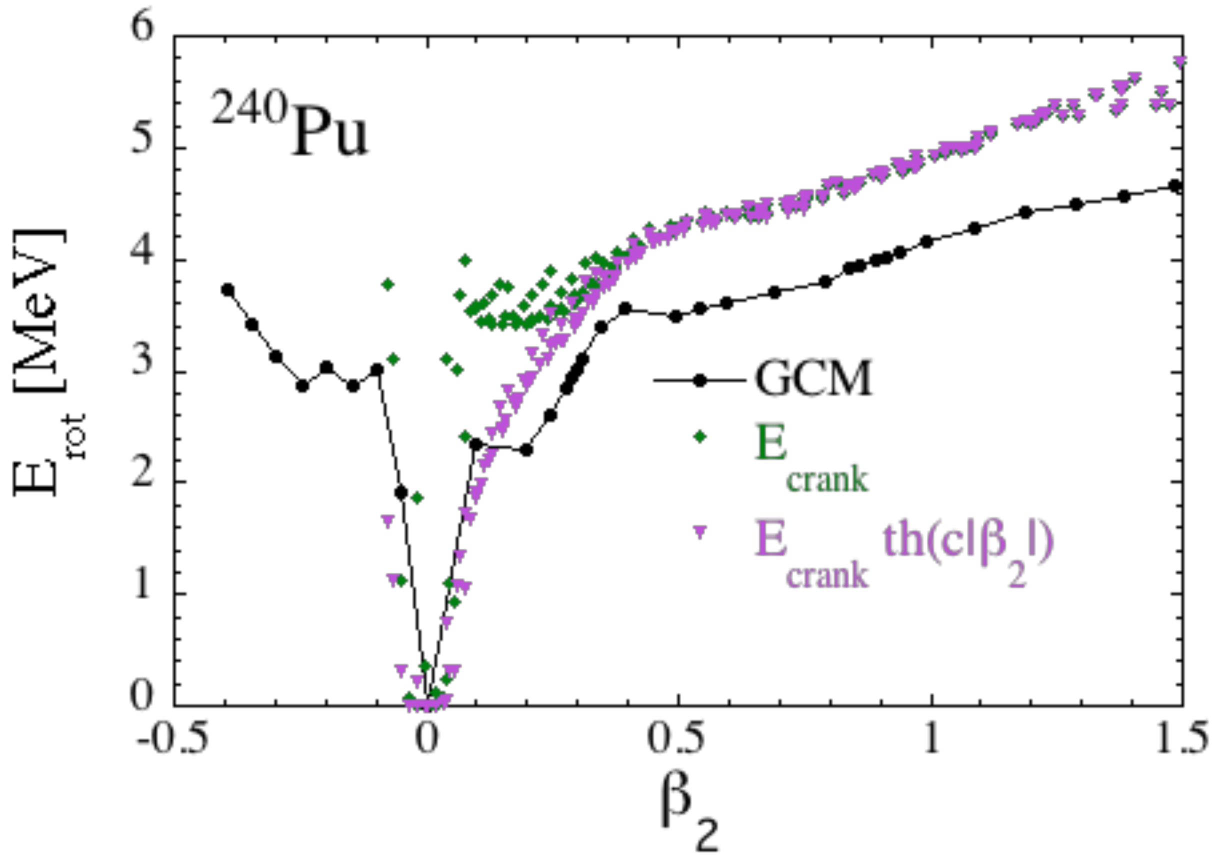

**rotational**

$$E_{coll} = E_{rot}^{crank}$$

# Correction for quadrupole correlations

a perturbative *cranking* correction for rotational correlations

$$E_{rot}^{crank} = \frac{\langle \hat{J}^2 \rangle}{2I}$$



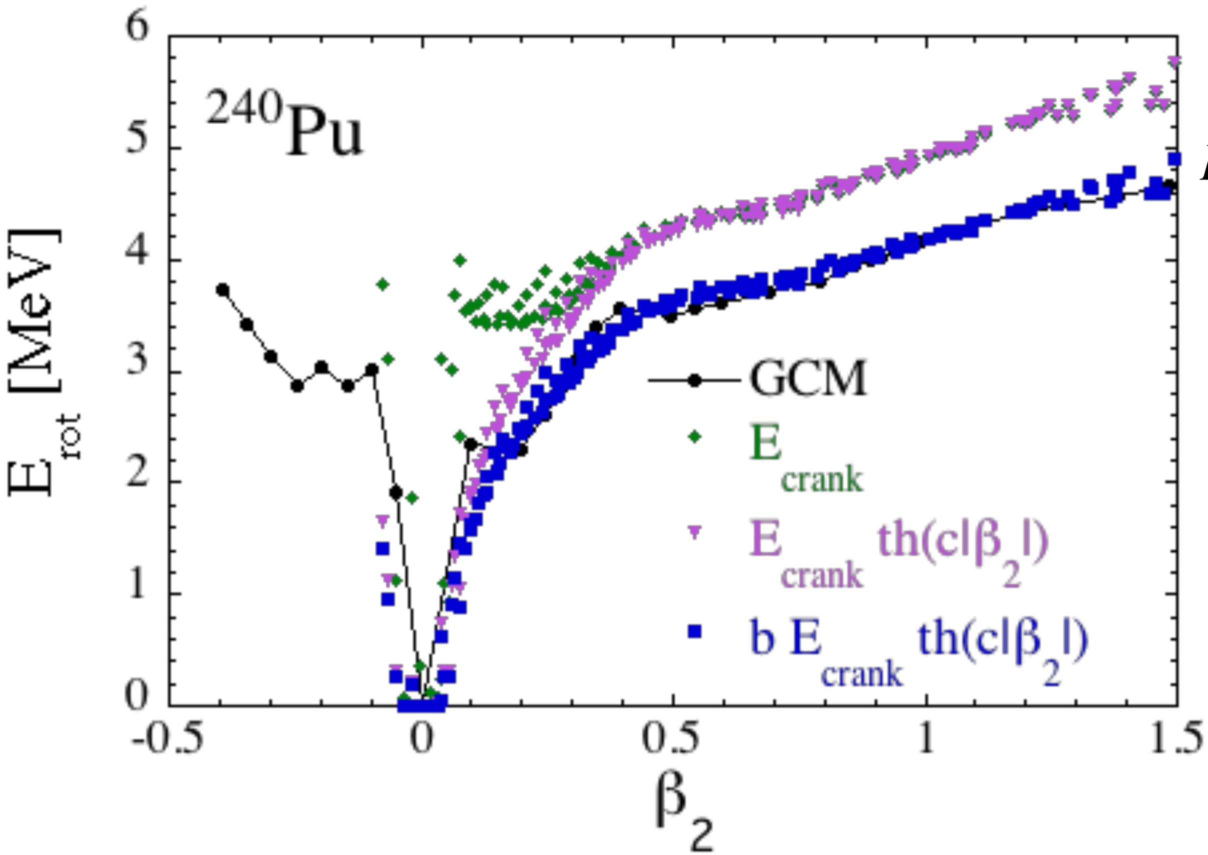

**rotational**

$$E_{coll} = E_{rot}^{crank} \tanh(c\beta_2)$$

## Correction for quadrupole correlations

a perturbative *cranking* correction for rotational correlations

$$E_{rot}^{crank} = \frac{\langle \hat{J}^2 \rangle}{2I}$$



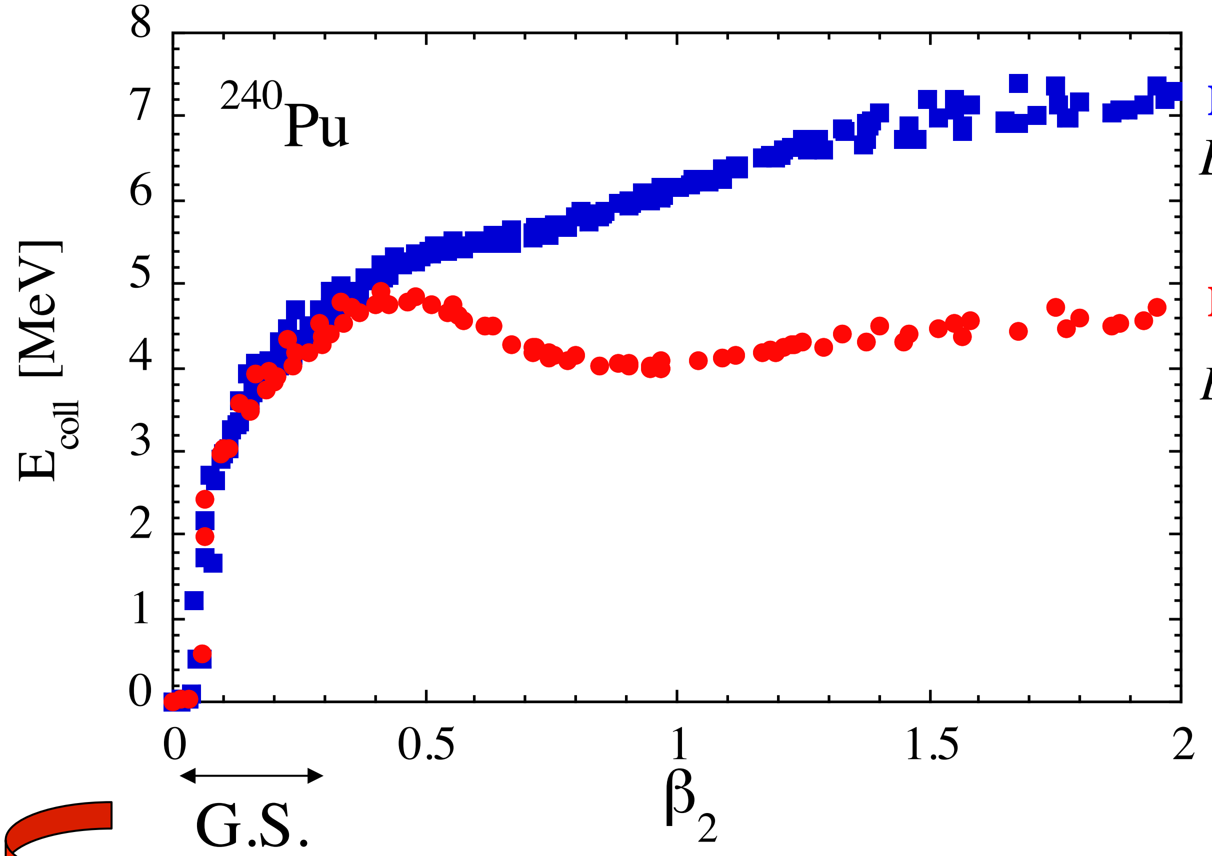

**rotational**

$$E_{coll} = b\, E_{rot}^{crank} \tanh(c\beta_2)$$

# Correction for quadrupole correlations

**!! of particular relevance at large deformation --> Fission calculations !!**

- a perturbative *cranking* correction for rotational correlations
- a *phenomenological* correction for "vibrational" correlations




**rotational**

$$E_{coll} = b\, E_{rot}^{crank} \tanh(c\beta_2)$$

**rotational + vibrational**

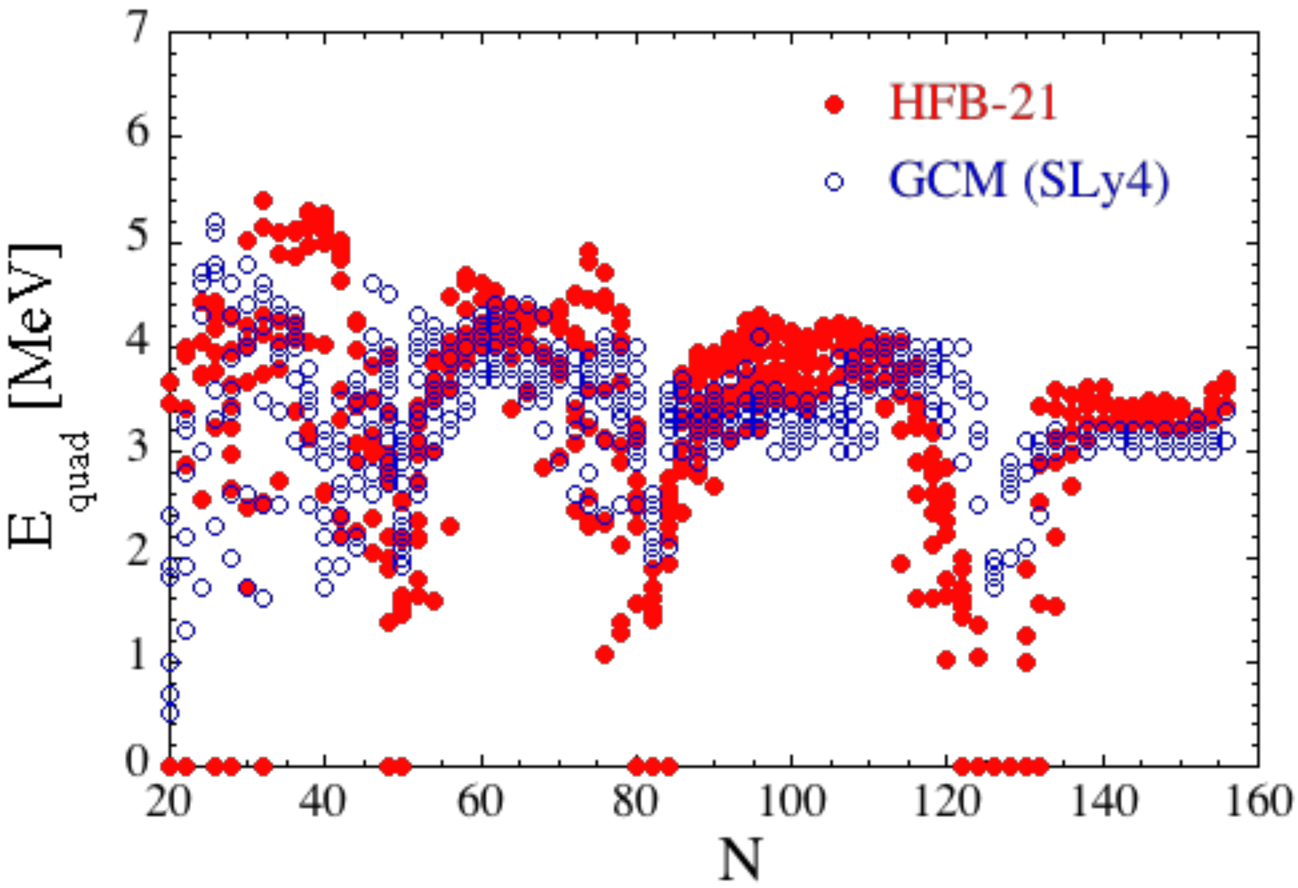
$$E_{coll} = b\, E_{rot}^{crank} \tanh(c\beta_2) + d\, E_{rot}^{crank} \exp\left[-l(\beta_2 - \beta_2^0)^2\right]$$

(still unsatisfactory description)

**Small impact on GS energy, but significant on Isomers and fission barriers**

# Quadrupole corrections to the binding energy

Comparison with the GCM (SLy4) calculation of Bender (2004)




606 e-e nuclei with $8 \leq Z \leq 108$

# Final estimate of the binding energy

$$E = E_{HFB} - E_{coll} - E_W$$

where the Wigner correction $E_W$ contributes significantly only for nuclei along the Z~N line or for light nuclei with $A < A_0 \sim 26$

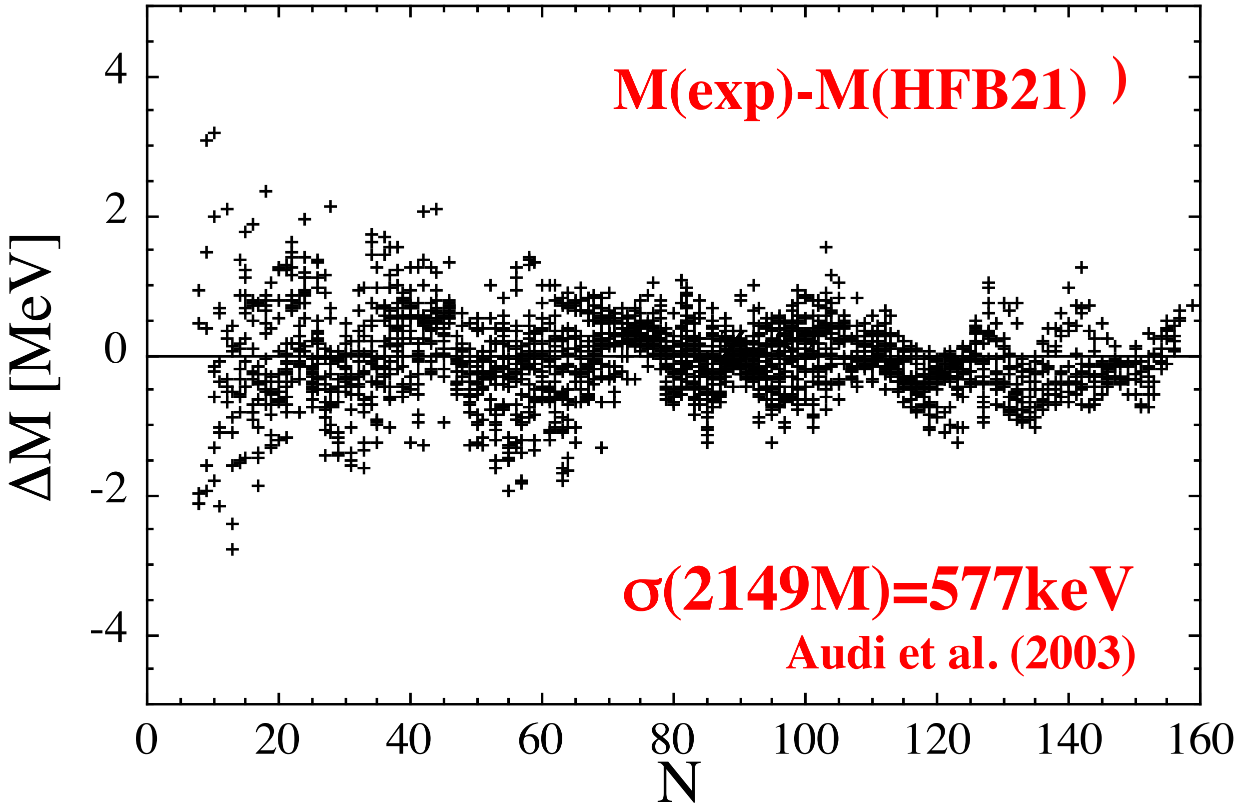
$$E_W = V_W \exp\left\{ -\lambda \left( \frac{N-Z}{A} \right)^2 \right\} + V'_W |N-Z| \exp\left\{ -\left( \frac{A}{A_0} \right)^2 \right\}$$

# HFB model: a weapon of mass production

| The long road in the HFB mass model development | | $\sigma_{rms}$ (2149 AME'03) | |
|---|---|---|---|
| HFB-1-2 : | Possible to fit all 2149 exp masses Z≥8 | 659 keV | ↑ |
| HFB-3: | Volume versus surface pairing | 635 keV | |
| HFB-4-5: | Nuclear matter EoS: $M^*$=0.92 | 660 keV | |
| HFB-6-7: | Nuclear matter EoS: $M^*$=0.80 | 657 keV | |
| HFB-8: | Introduction of number projection | 635 keV | ↓ |
| HFB-9: | Neutron matter EoS - $J$=30 MeV | 733 keV | ↗ |
| HFB-10-13: | Low pairing & NLD | 717 keV | ~ |
| HFB-14: | Collective correction and Fission $B_f$ | 729 keV | ~ |
| HFB-15: | Including Coulomb Correlations | 678 keV | |
| HFB-16: | with Neutron Matter pairing | 632 keV | |
| HFB-17: | with Neutron & Nuclear Matter pairing | 581 keV | |
| HFB-18-21: | Non-Std Skyrme ($t_4$-$t_5$ terms) - Fully stable | 577 keV | ↓ |

↳ Maximum Constraints on both Nuclei and Infinite Nuclear Matter
But also fission barriers, shape isomers, NLD, GR

# Comparison with experimental masses

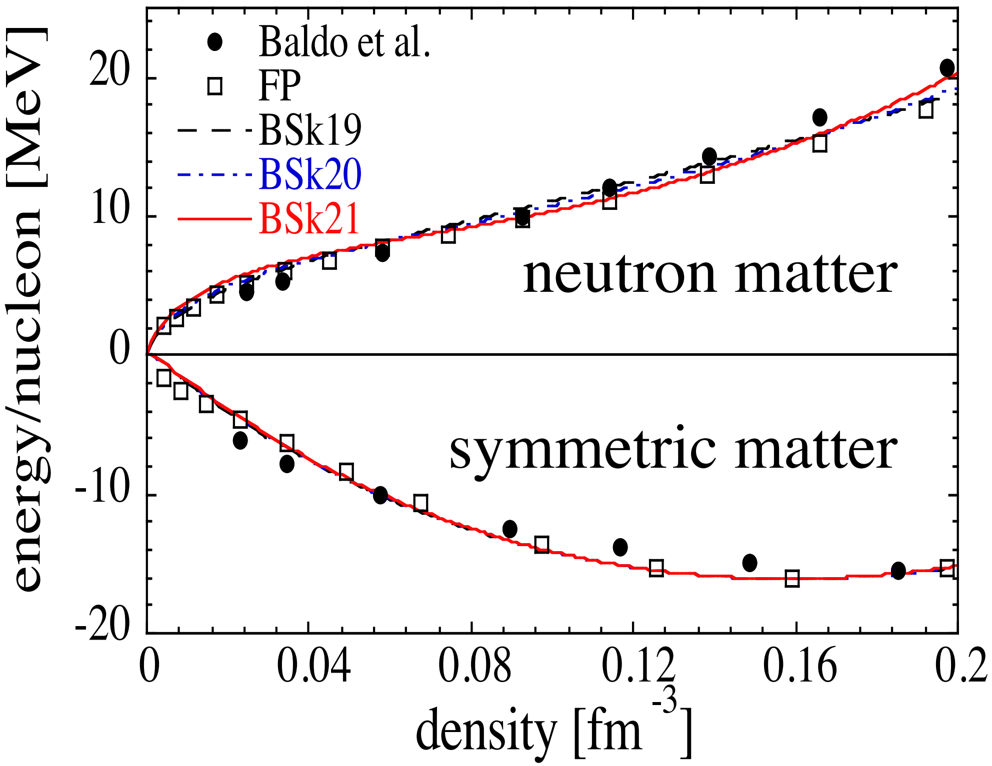



| | σ(HFB21) | σ(FRDM) |
|---|---|---|
| **2149 M (AME 2003):** | **577 keV** | **656 keV** |
| **2353 M (AME 2012):** | **572 keV** | **654 keV** |
| **128 M (28≤Z≤46, n-rich) at JYFLTRAP (2012):** | **620 keV** | **698 keV** |

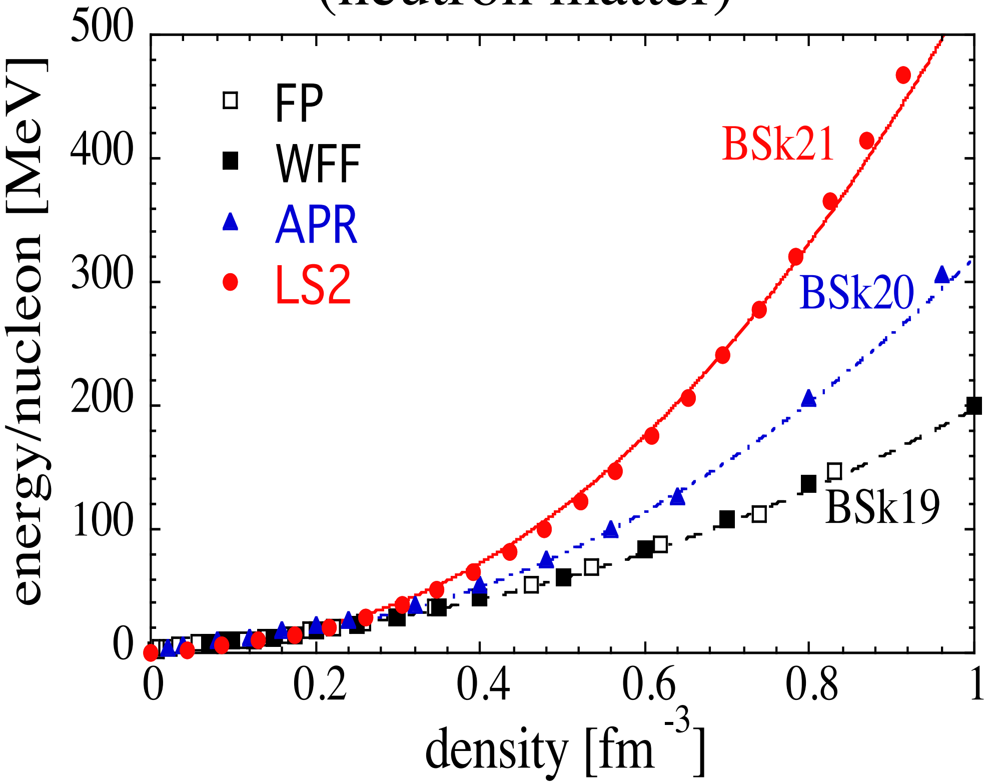
# HFB19-21: Stiffness of the neutron matter energy density

## (all characterized by *J*=30MeV)

Low-density regime

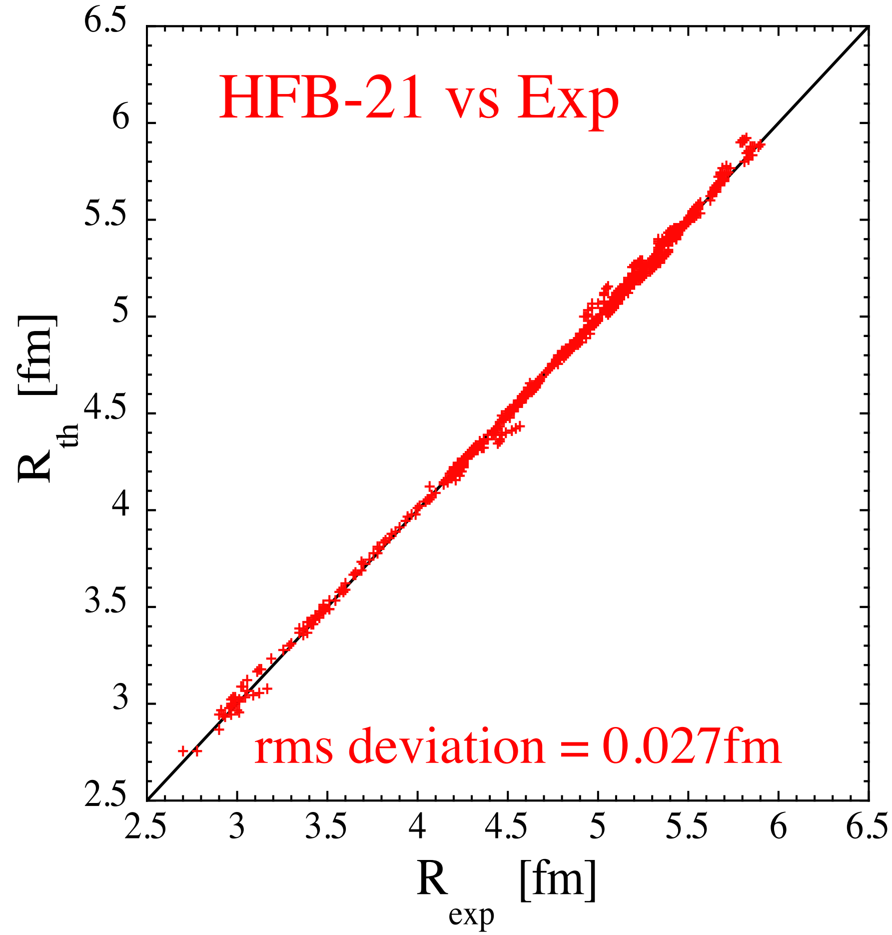



High-density regime (neutron matter)

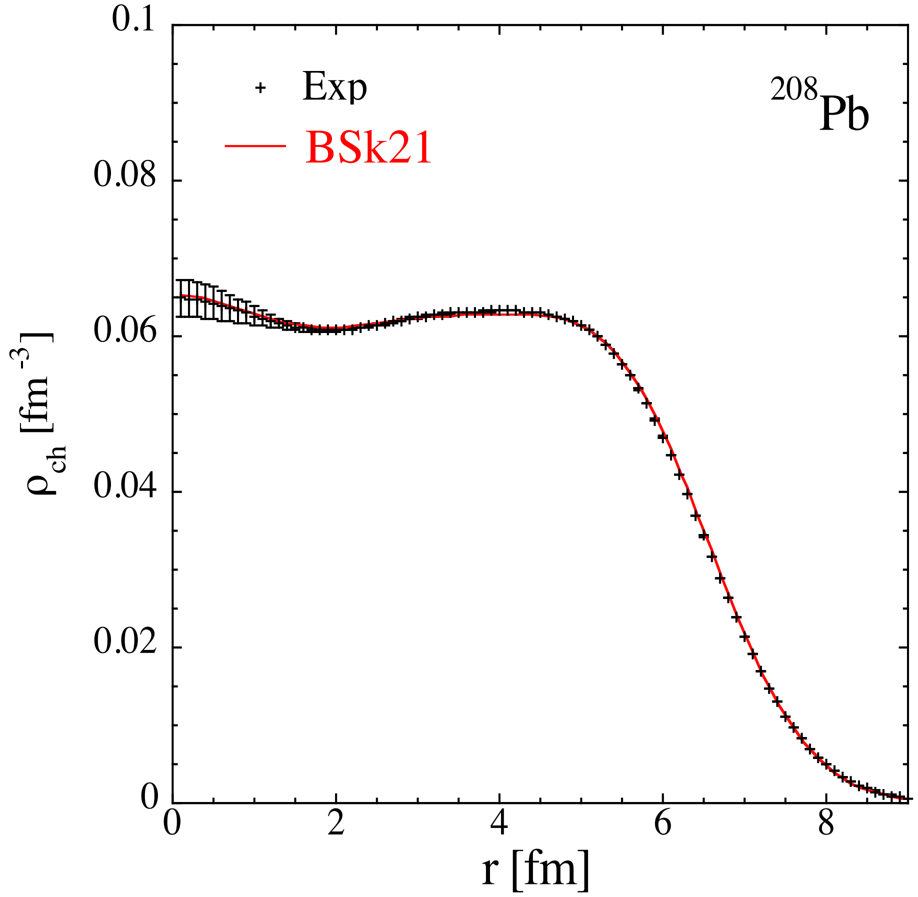


# Some examples for nuclear structure properties of interest for applications

Charge radii for 782 nuclei




Charge distribution of $^{208}$Pb



## Some significant developments since our last mass fits

i) New AME 2012 with 2353 masses ($Z$, $N \geq 8$), compared to 2149 masses in AME2003

ii) Discovery of PSR J1614-2230 with $M = 1.97 \pm 0.04\ M_o$
(a new NS with $M = 2.01 \pm 0.04\ M_o$ has been announced)

Maximum NS mass : $M_{max} = 1.86\ M_o$ for HFB-19
$M_{max} = 2.15\ M_o$ for HFB-20
$M_{max} = 2.28\ M_o$ for HFB-21

This could exclude HFB-19, at least *if the NS core is made of nucleons only:, i.e there is no transition to an exotic phase with a stiff EoS (e.g hyperons, deconfined quarks)*

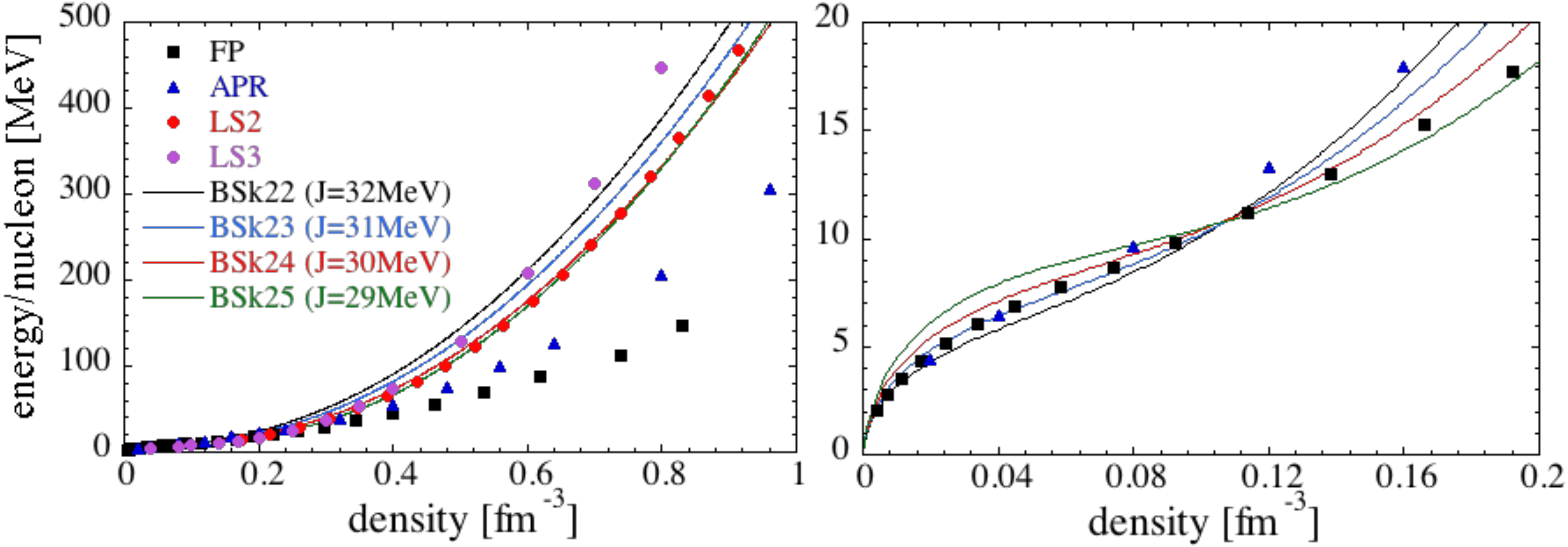
*– STILL AN OPEN QUESTION –*

**New mass fits including constraints on the rigid NeuM EoS**

# The new HFB-22 – 25 mass models

Extended Skyrme interaction with « realistic » pairing force

EoS of infinite neutron matter




Fit to 2353 exp masses (AME'12)

**σ(HFB-22) = 629 keV (J=32MeV)**

**σ(HFB-23) = 569 keV (J=31MeV)**

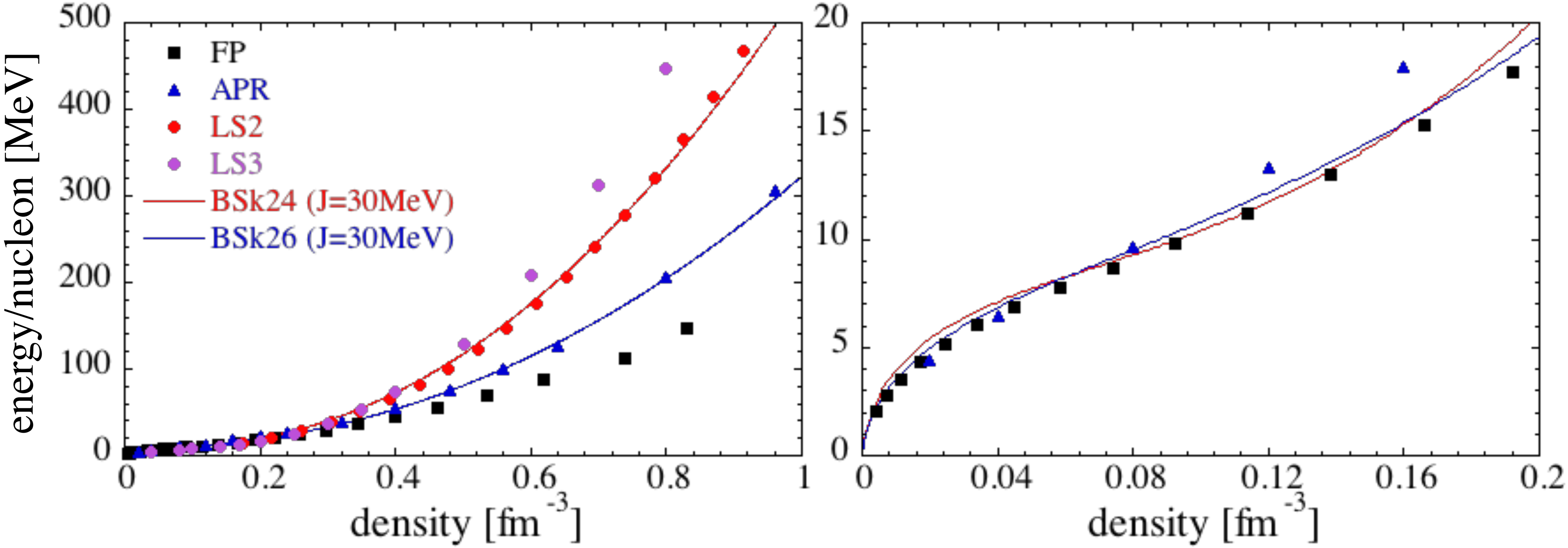
**σ(HFB-24) = 549 keV (J=30MeV)**

**σ(HFB-25) = 544 keV (J=29MeV)**

# The new HFB-24 & HFB-26 mass models

Extended Skyrme interaction with « realistic » pairing force

EoS of infinite neutron matter




Fit to 2353 exp masses (AME'12)

**σ(HFB-24) = 549 keV (J=30MeV)**

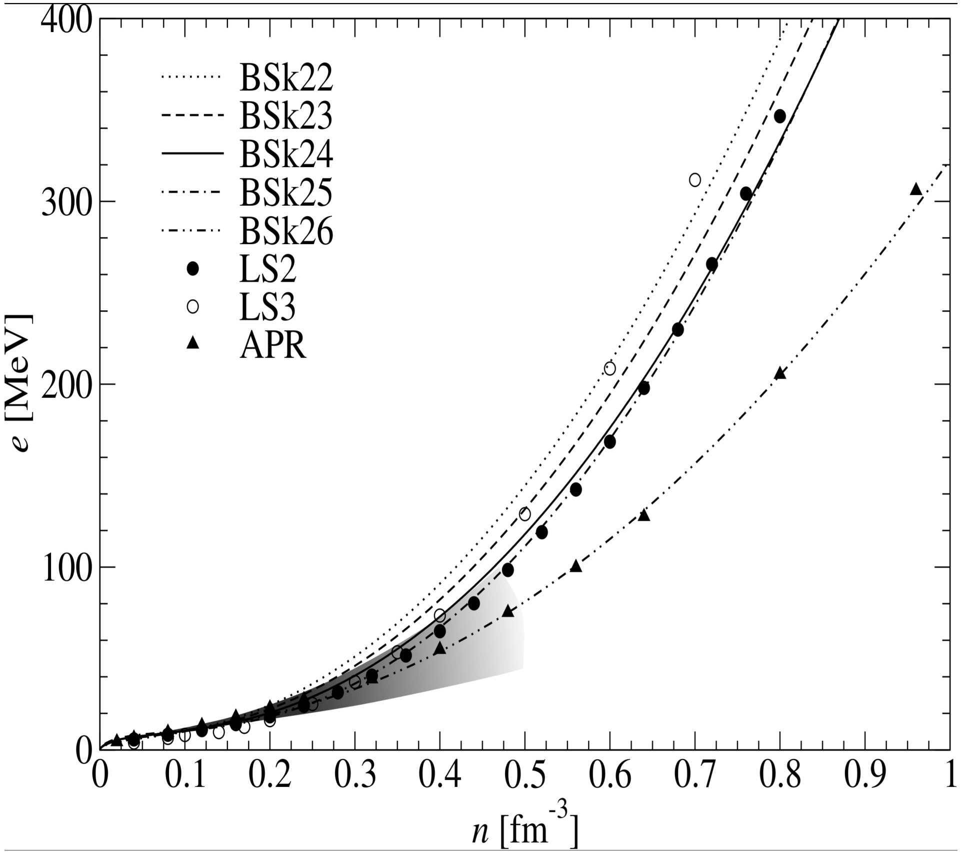
**σ(HFB-26) = 564 keV (J=30MeV)**

Maximum NS mass : $M_{max}$= 2.22-2.28 $M_o$ for HFB-22–25

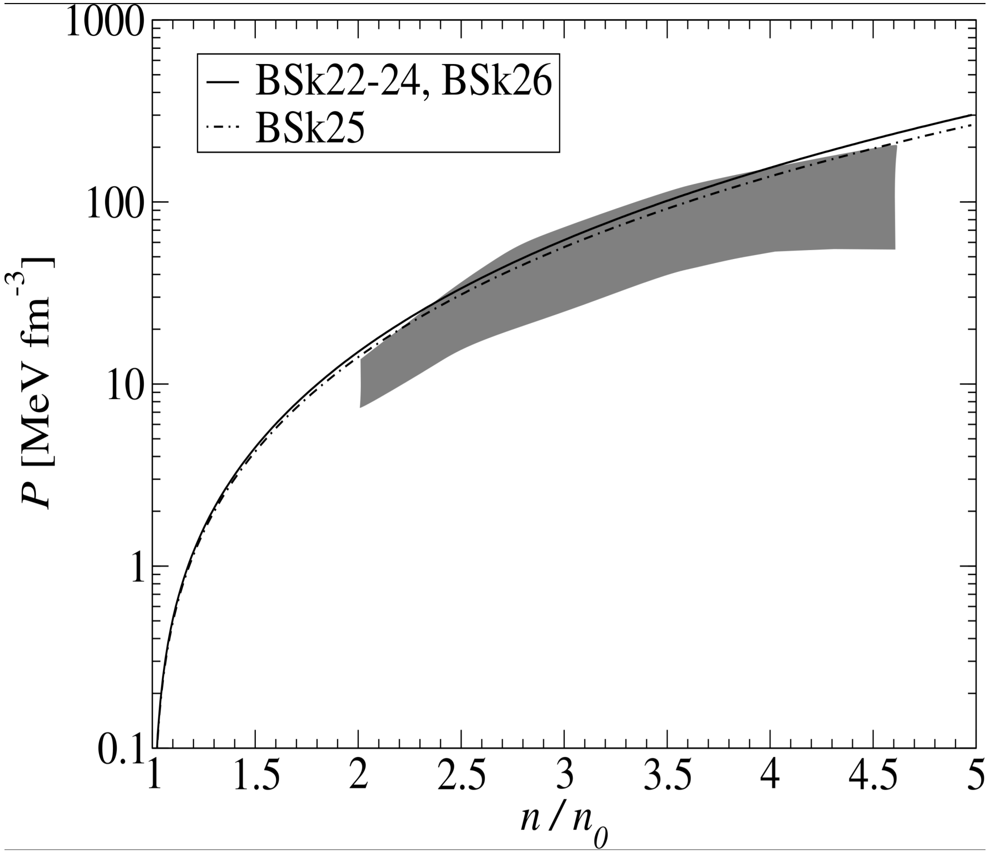
$M_{max}$= 2.15 $M_o$ for HFB-26

# Nuclear matter properties

Energy per nucleon in neutron matter




Pressure in symmetric nuclear matter




- Stable neutron matter at all polarisations (no ferromagnetic instability)
- Effective masses in agreement with realistic predictions

$$M_s^* / M = 0.80 \quad \& \quad M_v^* / M \sim 0.70$$

# Neutron skins obtained with the new HFB mass model

$$\theta \equiv R_n^{rms} - R_p^{rms} \Rightarrow \theta = \frac{3}{2} r_0 \frac{J}{Q} \left| \frac{N-Z}{A} \right|$$

with $r_0 = (3/4\pi\, n_0)^{1/3}$

$Q$ = surface stiffness coeff.

| | | $\sigma_{rms}$ (26) | $\bar{\epsilon}$ (26) | $\sigma_{mod}$ (26) | $\sigma_{rms}$ (10) | $\bar{\epsilon}$ (10) | $\sigma_{mod}$(10) |
|---|---|---|---|---|---|---|---|
| J=32MeV | BSk22 | 0.0495 | -0.0266 | 0.0205 | 0.0429 | -0.030 | 0.0244 |
| J=31MeV | BSk23 | 0.0447 | -0.0142 | 0.0090 | 0.0342 | -0.017 | 0.0128 |
| J=30MeV | BSk24 | 0.0437 | -0.0031 | 0.0047 | 0.0270 | -0.0030 | 0.0087 |
| J=29MeV | BSk25 | 0.0469 | 0.0088 | 0.0170 | 0.0277 | 0.011 | 0.0194 |
| J=30MeV | BSk26 | 0.0415 | -0.0038 | 0.0044 | 0.0265 | -0.0040 | 0.0084 |

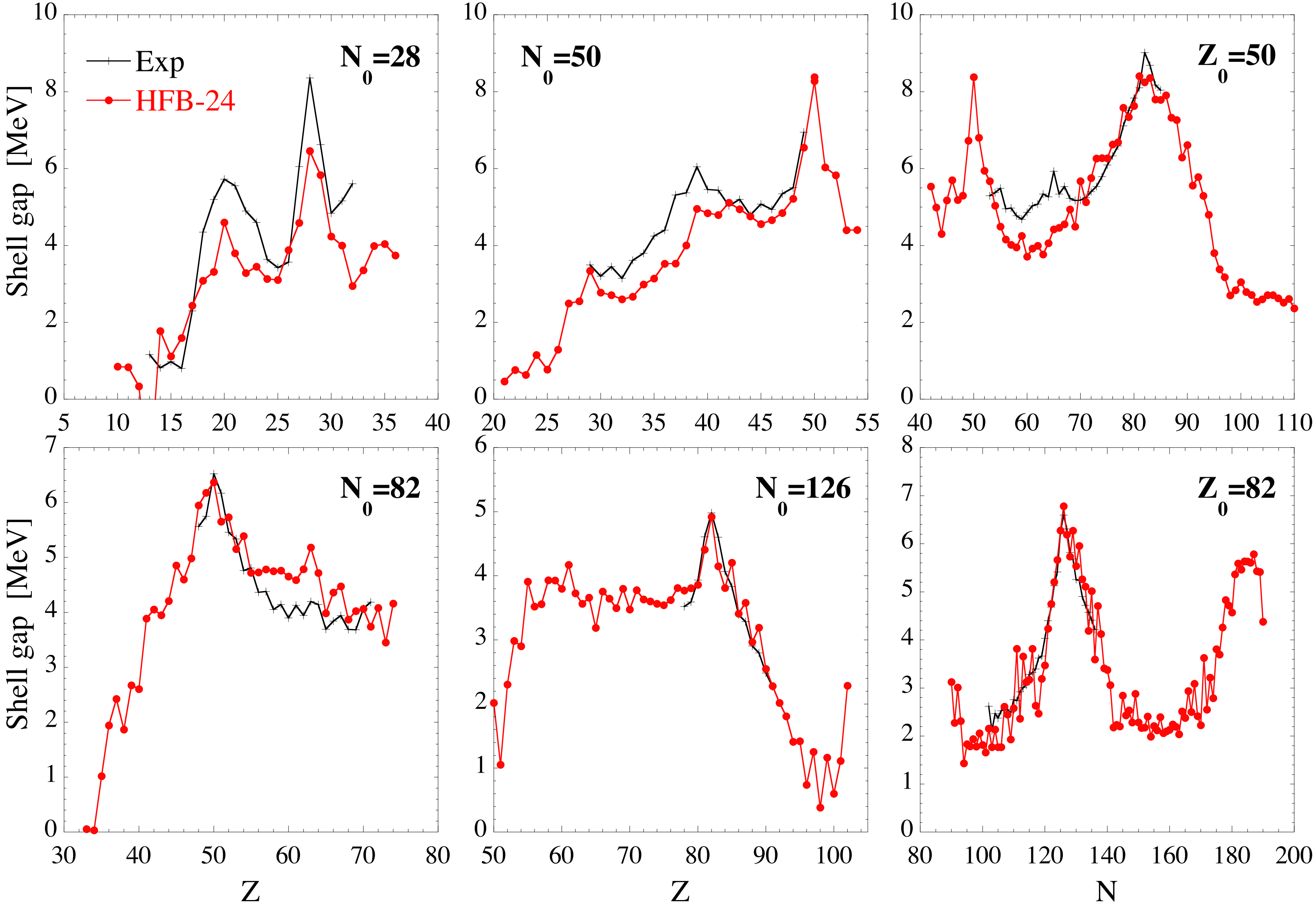
Exp. Errors up to 0.16 fm　　　Exp. Errors ≤ 0.04 fm

Exp neutron skin data from Jastrzebski et al. (2004)

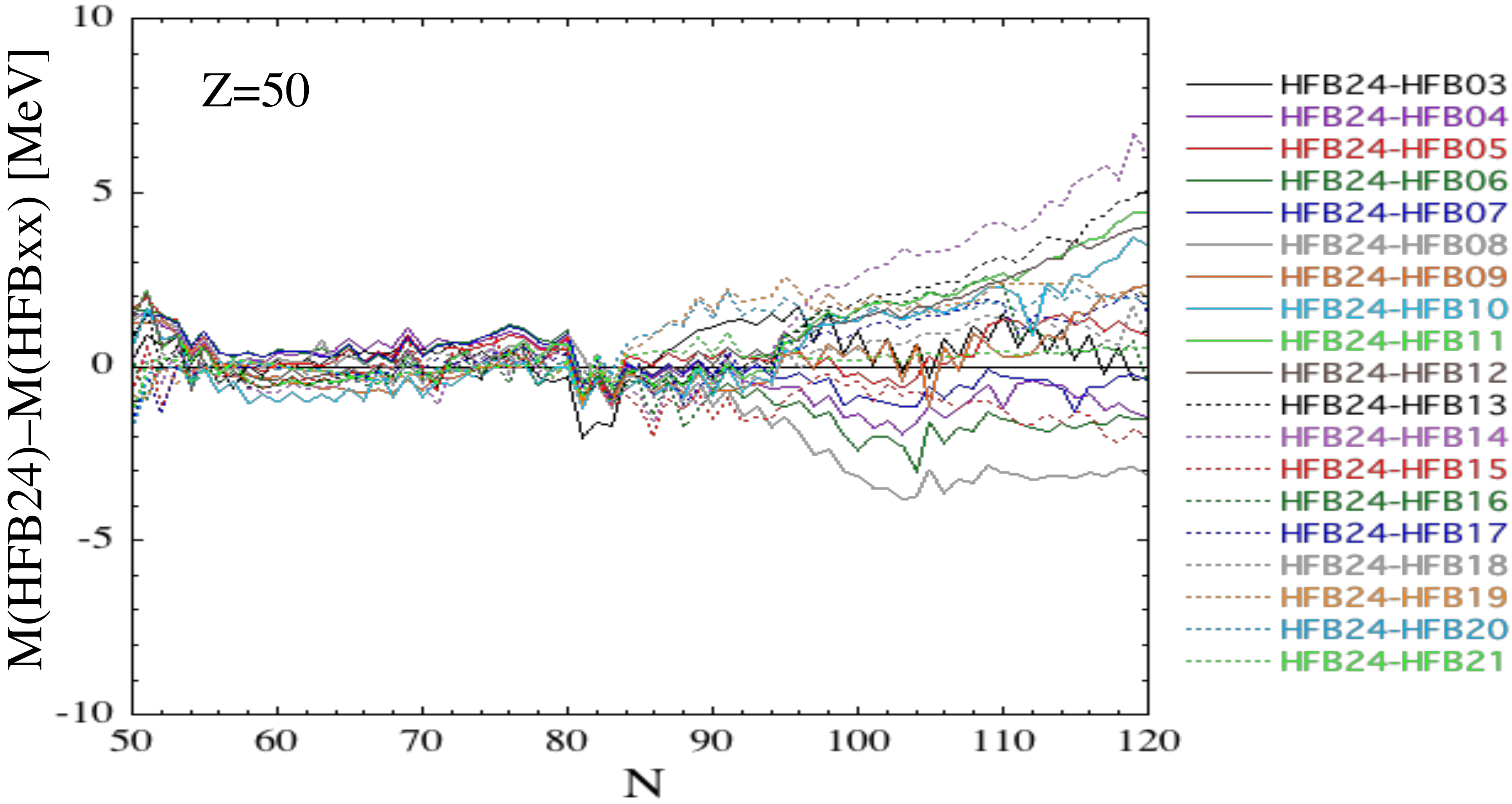
**Masses and neutron skin favour J=30MeV in this framework !!**

# Shell gaps obtained with HFB-24 mass model

$$\Delta_n(N_0, Z) = S_{2n}(N_0, Z) - S_{2n}(N_0 + 2, Z)$$



# Sensitivity of the HFB mass models to the parameter uncertainties



Skyrme-HFB mass models: a first step towards "microscopic" models for practical applications

… but there is obviously still room for many improvements:

- Pairing interaction (contact force, cut-off dependence)
- Improved treatment of odd nuclei
- Phenomenological Wigner correction
- Finite-range forces of Gogny-type
- Correlation effects beyond mean field
- Etc…

# A new generation of mass models

# Gogny-HFB mass table beyond mean field !

(M. Girod, S. Hilaire, S. Péru: Bruyères-le-Châtel, France)

Beyond the mean field, the total binding energy is estimated from

$$E_{tot} = E_{HFB} - E_{Quad}$$

where • $E_{HFB}$: deformed HFB binding energy obtained with a *finite-range* standard Gogny-type force

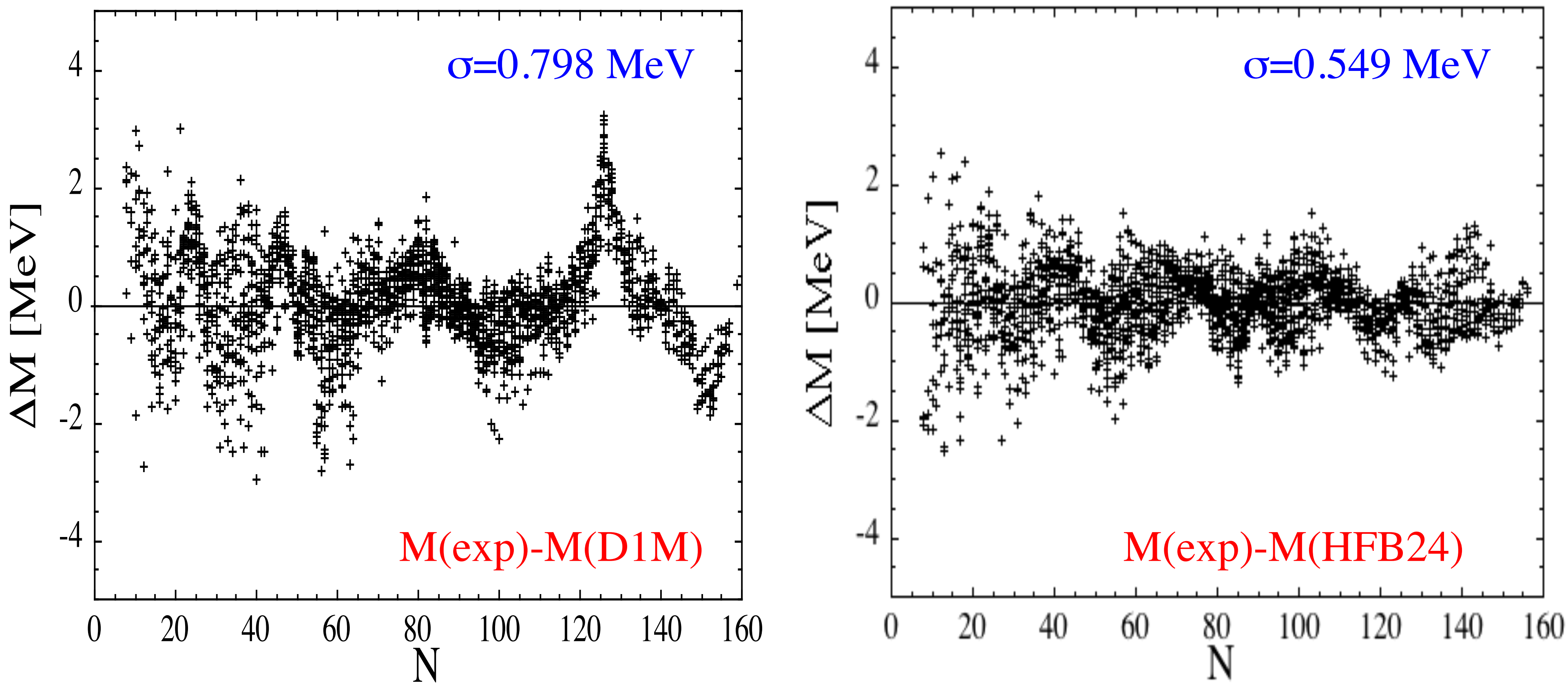
$$V(1,2)=\sum_{j=1,2} e^{-\frac{(\vec{r}_1-\vec{r}_2)^2}{\mu_j^2}}(W_j+B_jP_\sigma-H_jP_\tau-M_jP_\sigma P_\tau)$$
$$+t_0\,(1+x_0P_\sigma)\,\delta\,(\vec{r}_1-\vec{r}_2)\left[\rho\left(\frac{\vec{r}_1+\vec{r}_2}{2}\right)\right]^\alpha$$
$$+i\,W_{LS}\overleftarrow{\nabla}_{12}\,\delta\,(\vec{r}_1-\vec{r}_2)\times\overrightarrow{\nabla}_{12}.\,(\overrightarrow{\sigma}_1+\overrightarrow{\sigma}_2)\,.$$

• $E_{Quad}$ : quadrupolar correction energy determined with the *same* Gogny force (no "double counting") in the framework of the GCM +GOA model for the five collective quadrupole coordinates, i.e. rotation, quadrupole vibration and coupling between these collective modes (axial and triaxial quadrupole deformations included)

Girod, Berger, Libert, Delaroche

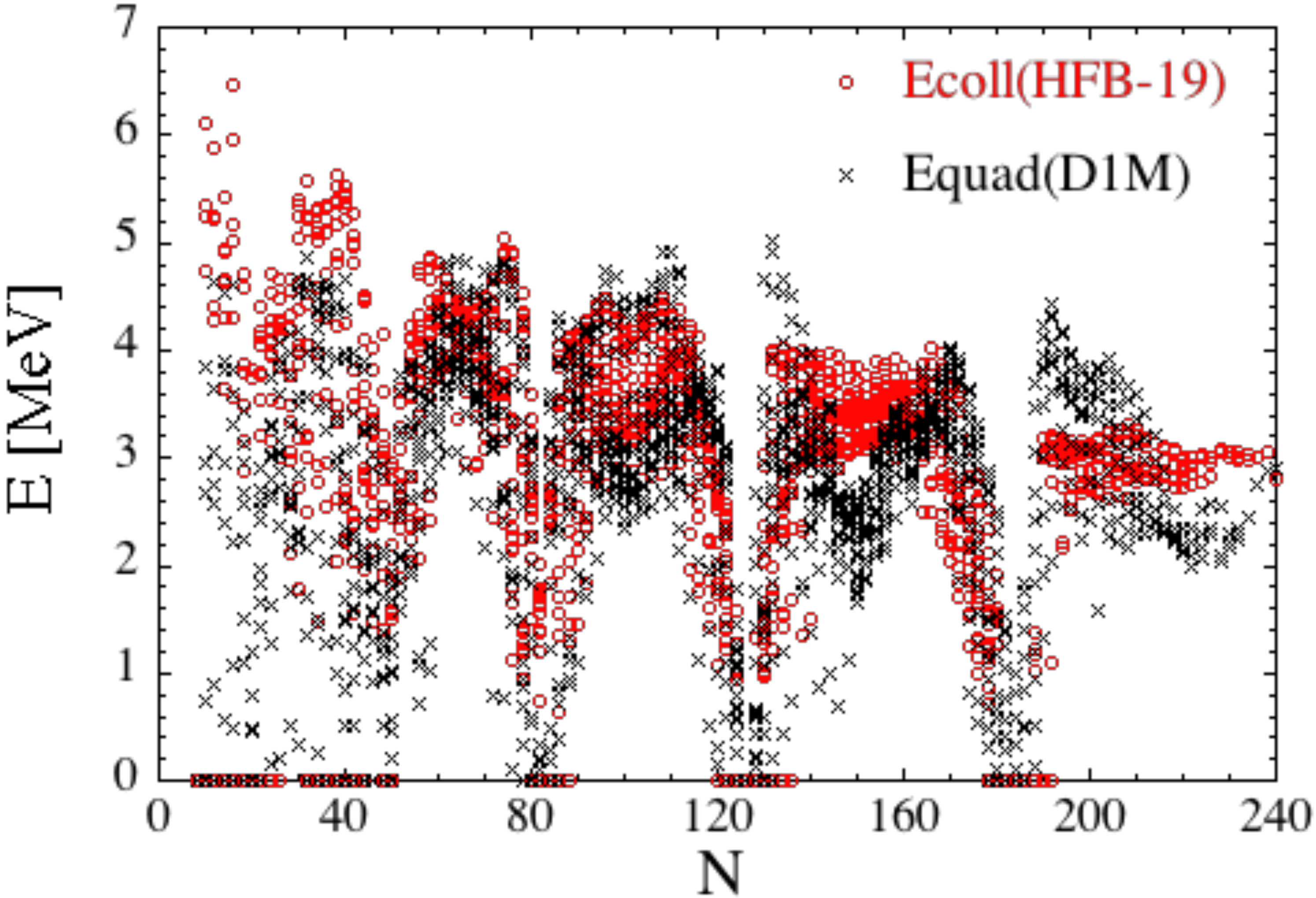
# First Gogny-HFB mass formula (D1M force)

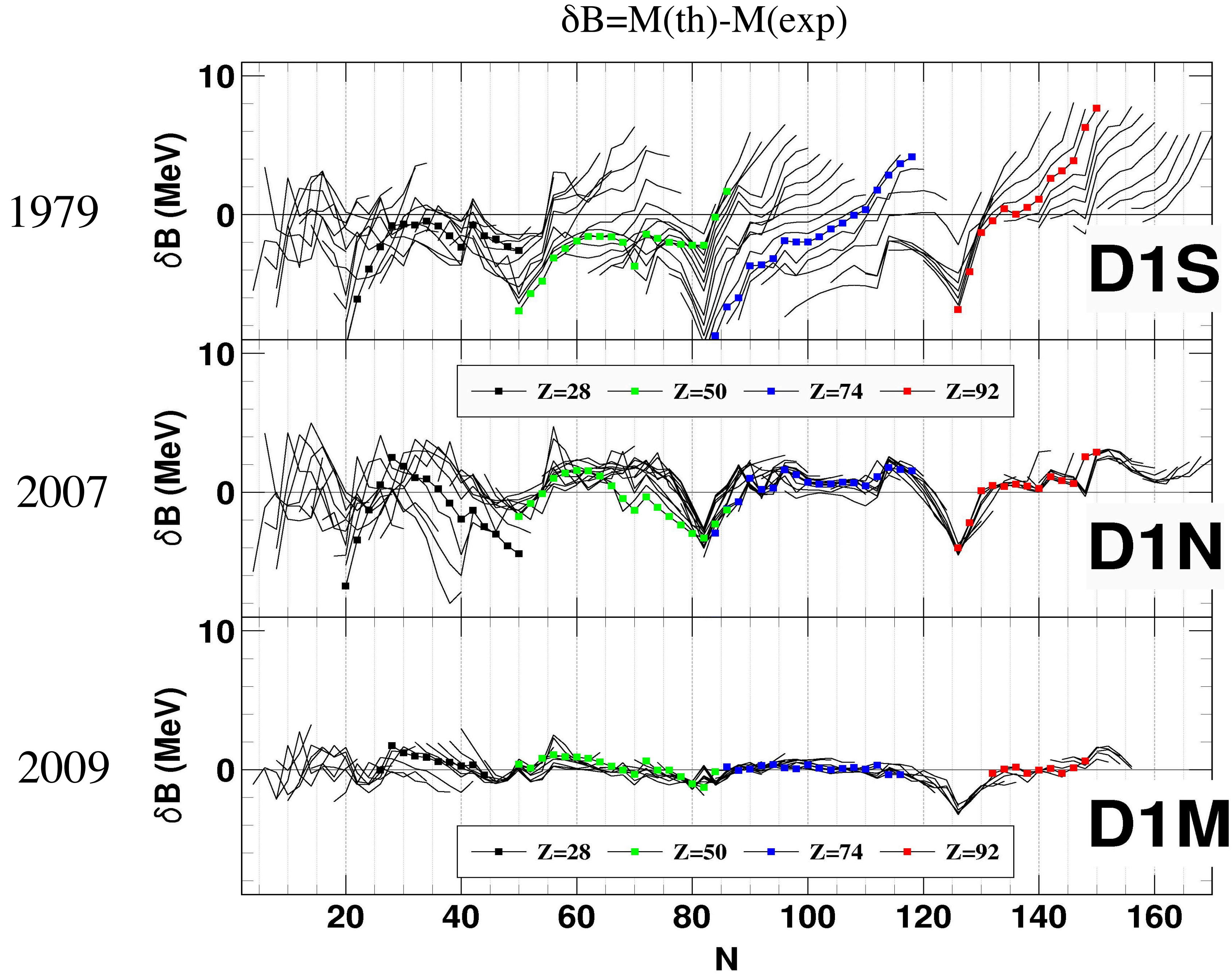
2149 Masses: ε=0.126 MeV  σ=0.798 MeV
with coherent $E_{Quad}$ & $E_{HFB}$ !
707 Radii: ε=-0.008 fm  σ=0.031 fm (with Q corrections)




--> It is possible to adjust a Gogny force to reproduce all experimental masses accurately

# Quadrupole corrections to the binding energy

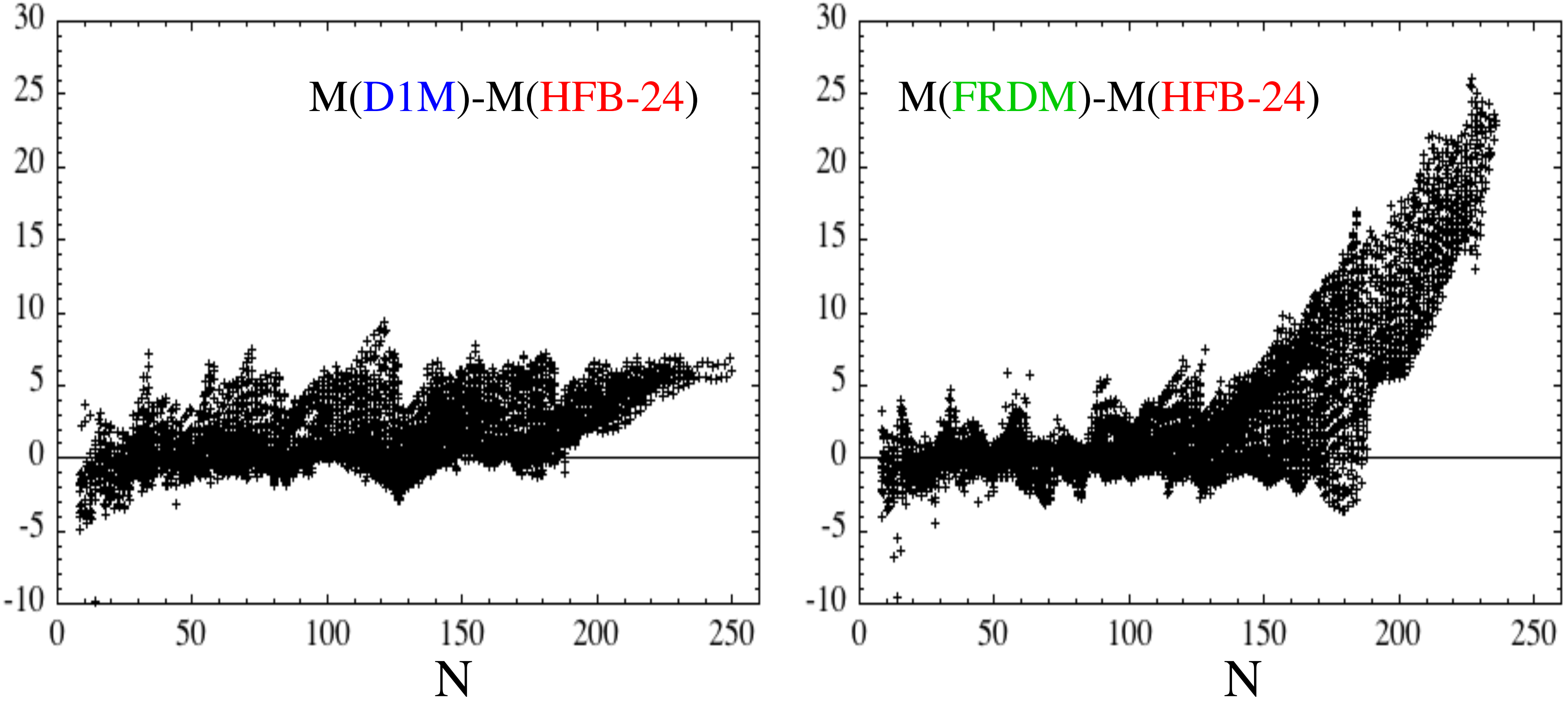



δB=M(th)-M(exp)
1979
2007
2009
δB (MeV)
D1S
D1N
D1M
Z=28
Z=50
Z=74
Z=92
N
0
10
20
40
60
80
100
120
140
160

# Comparison between Skyrme-HFB, Gogny-HFB and FRDM

| | |
|---|---|
| HFB-24: Skyrme HFB mass model | σ(2353 exp masses)=549keV |
| HFB-D1M: Gogny HFB mass model | σ(2353 exp masses)=789keV |
| FRDM: Finite Range Droplet mass model | σ(2353 exp masses)=654keV |

$8 \leq Z \leq 110$



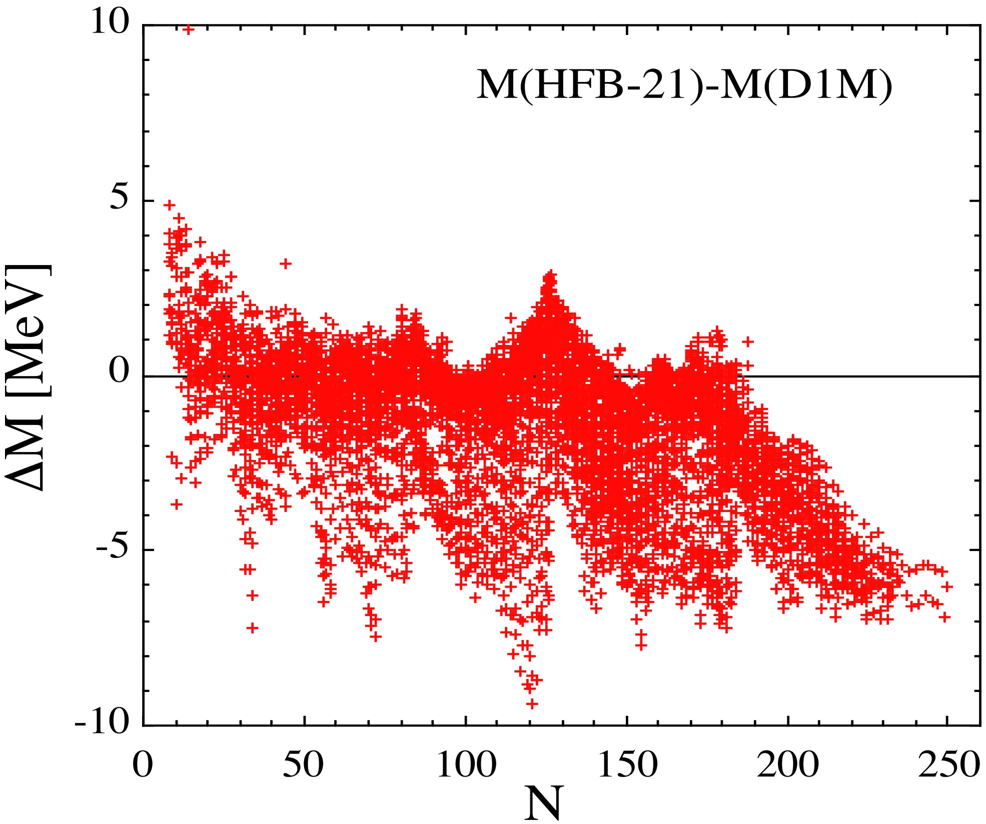

Different trends due to different INM, shell & correlation energies

# Sensitivity to the masses and corresponding reaction rates

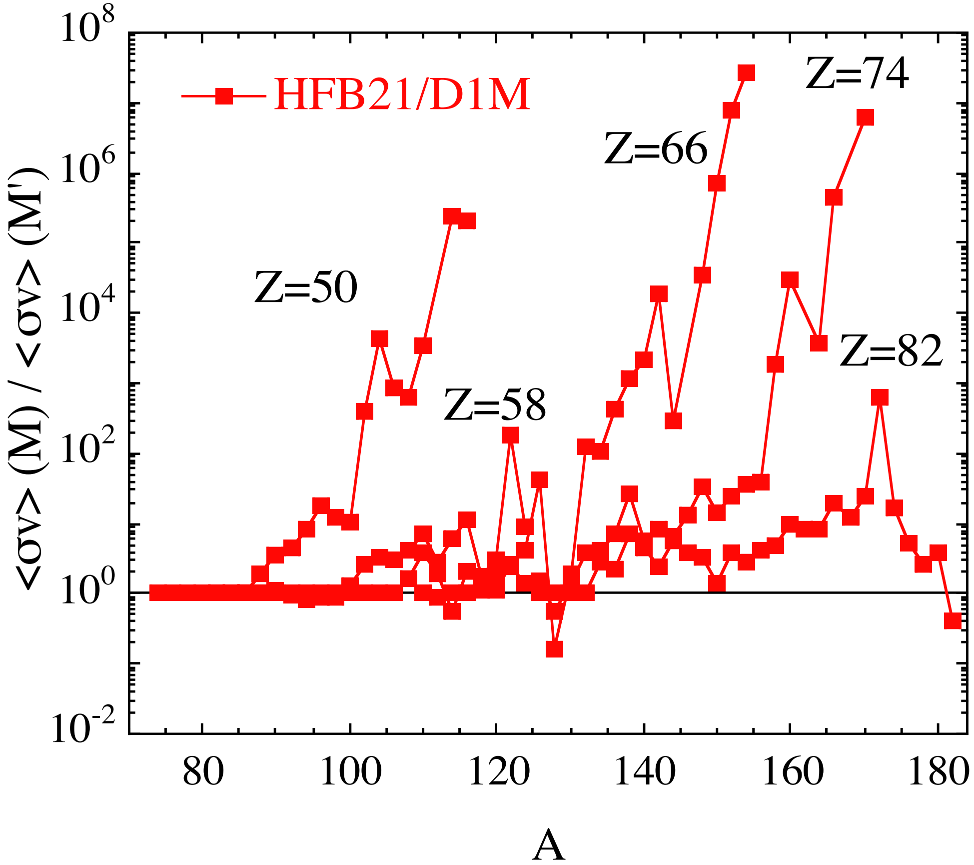
HFB-21: Skyrme HFB mass model — σ(2149 exp masses)=577keV

HFB-D1M: Gogny HFB mass model — σ(2149 exp masses)=798keV

Mass differences between HFB21 & D1M




TALYS(n,γ) rates at $T_9$=1 on Sn-Pb isotopes




Different trends due to different shell & correlation energies

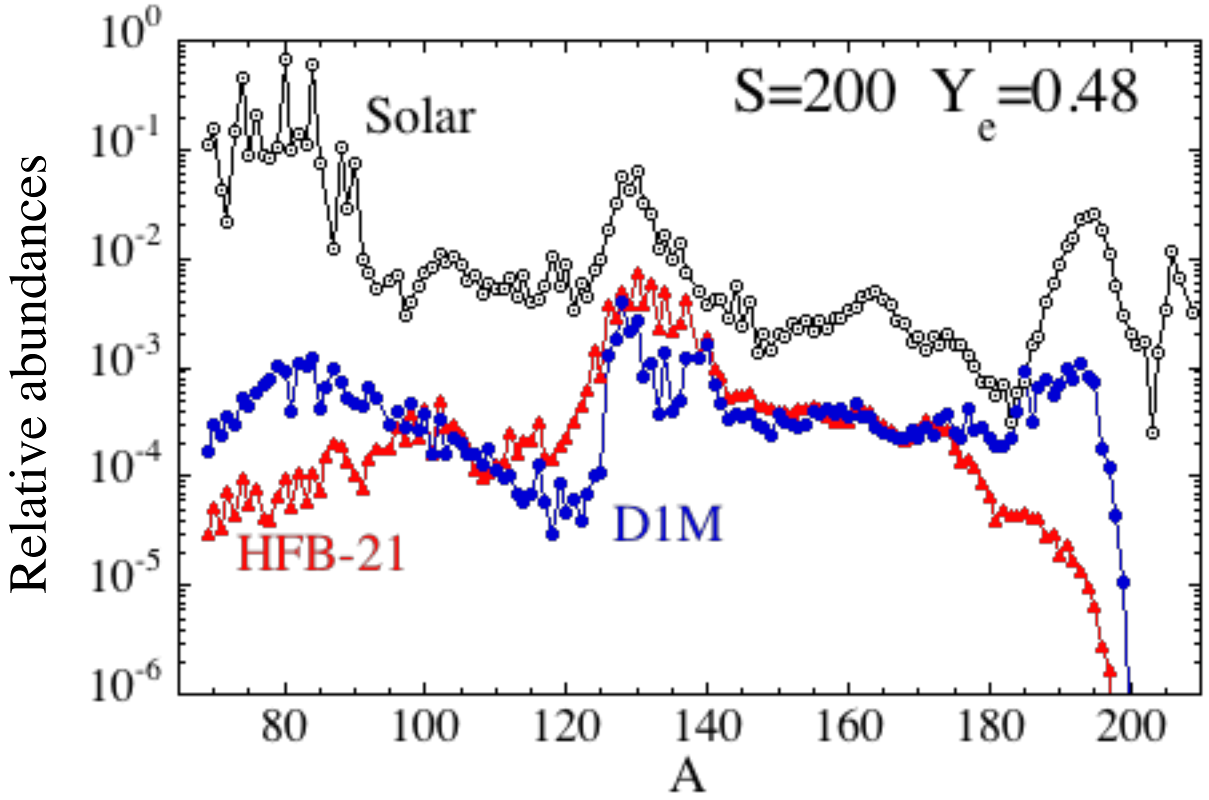
## Sensitivity to nuclear masses and corresponding rates

Comparison for 2 different mass models:

HFB-21: Skyrme HFB mass model — σ(2149 nuclei)=577keV

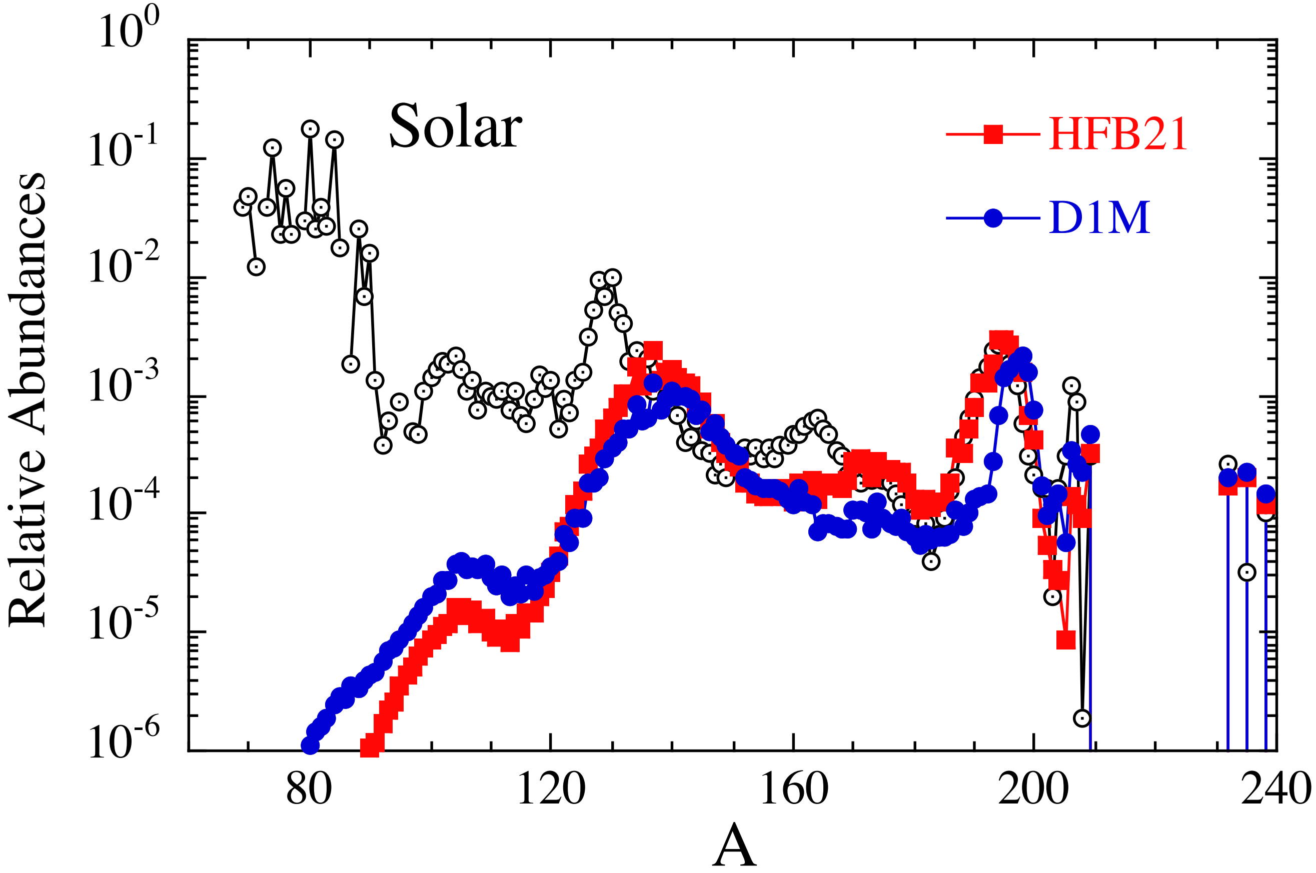
HFB-D1M: Gogny HFB mass model — σ(2149 nuclei)=798keV

r-abundance distribution from 1 specific ν-driven wind



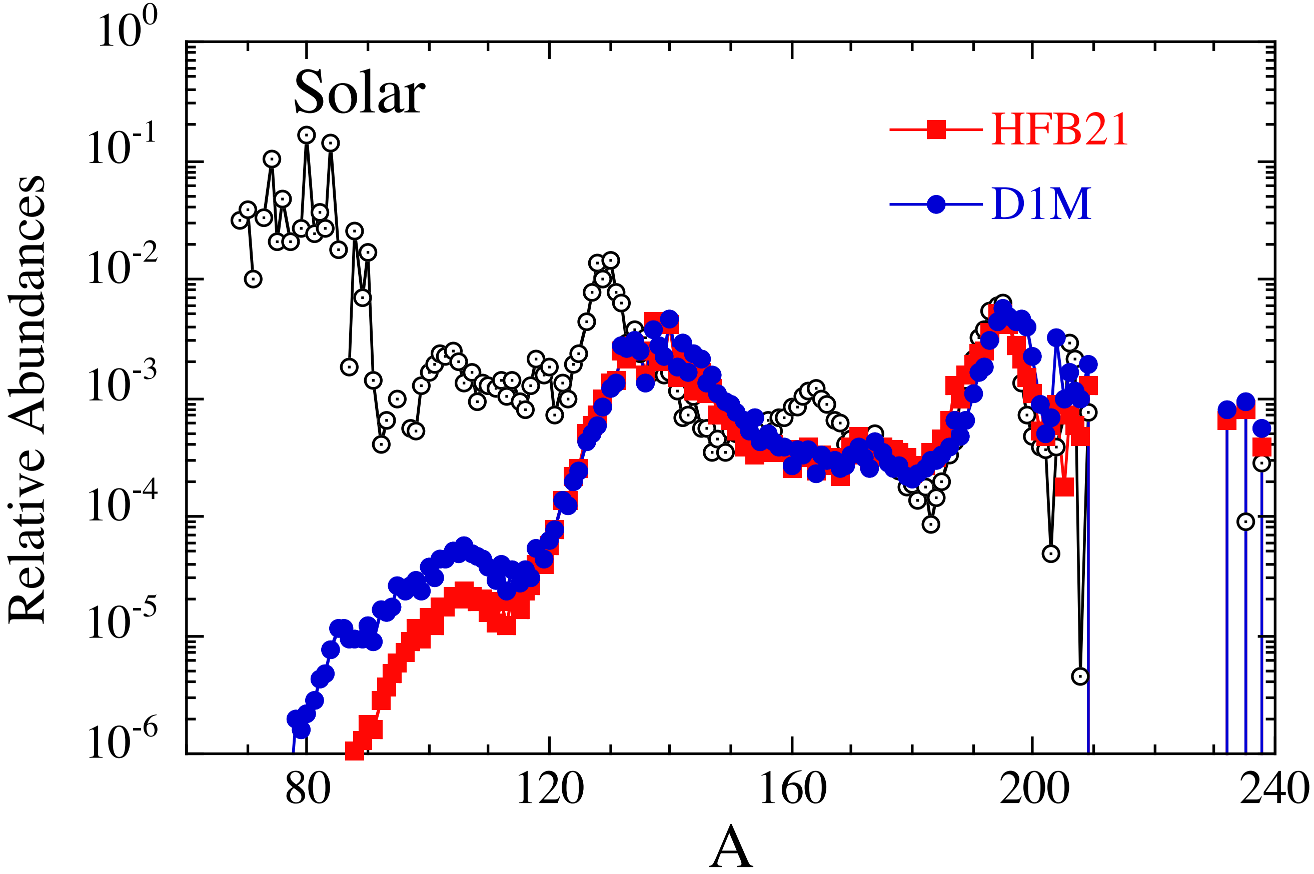
# Impact of masses/rates on the r-process nucleosynthesis in NS mergers

r-abundance distributions from **1** typical ejected "mass element"



# Impact of masses/rates on the r-process nucleosynthesis in NS mergers

r-abundance distributions from hundreds of “mass elements”)

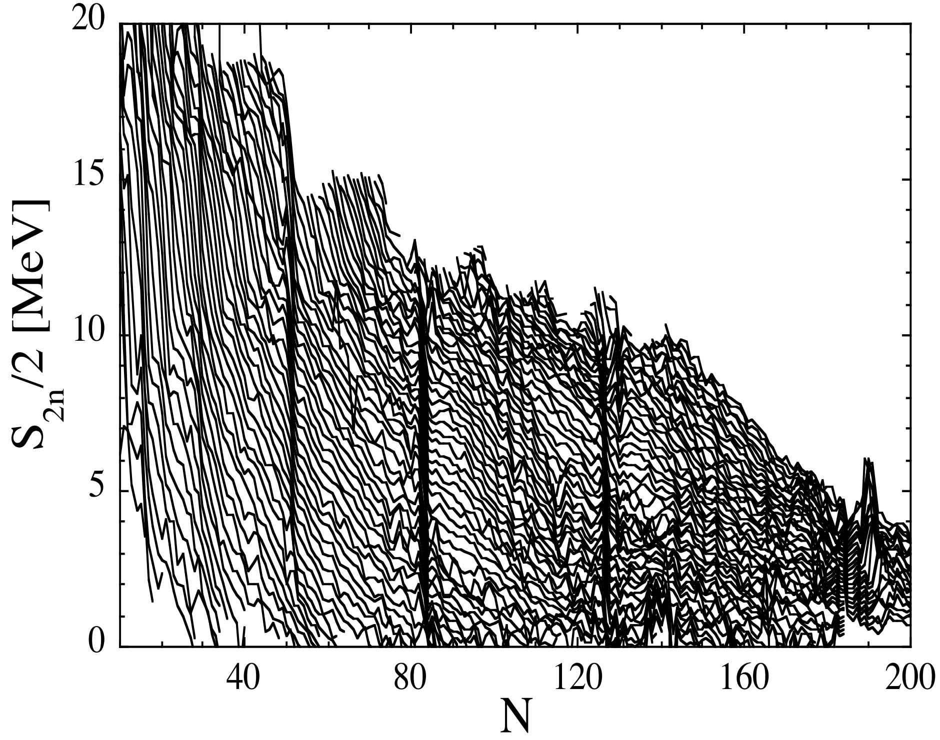



Local differences, but smoothed out by fission recycling and mass-averaging

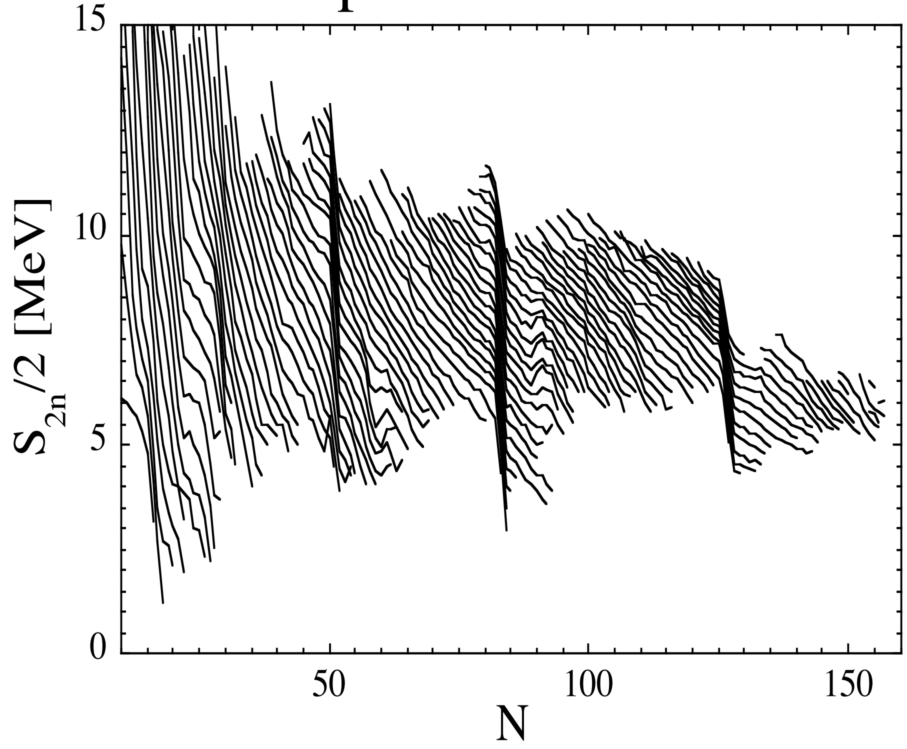
$S_{2n}$ surfaces from microscopic calculations affected by numerical noise

(resolution of Schrodinger equations, determination of equilibrium deformation, optimized wave function, perturbative rotational correction, …)

HFB-21 masses




Experimental masses




--> for practical applications, the mass surface may need to be smoothed

# Garvey-Kelson relations between nuclear masses

Z

| | | | | |
|---|---|---|---|---|
| +1 | -2 | +2 | -2 | +1 |
| -2 | | +4 | | -2 |
| +2 | +4 | **-12** | +4 | +2 |
| -2 | | +4 | | -2 |
| +1 | -2 | +2 | -2 | +1 |

N

The GK relations take advantage of the cancellation to first order of the most important interactions

21-mass relation verified for exp. masses with an rms accuracy ~ 90keV

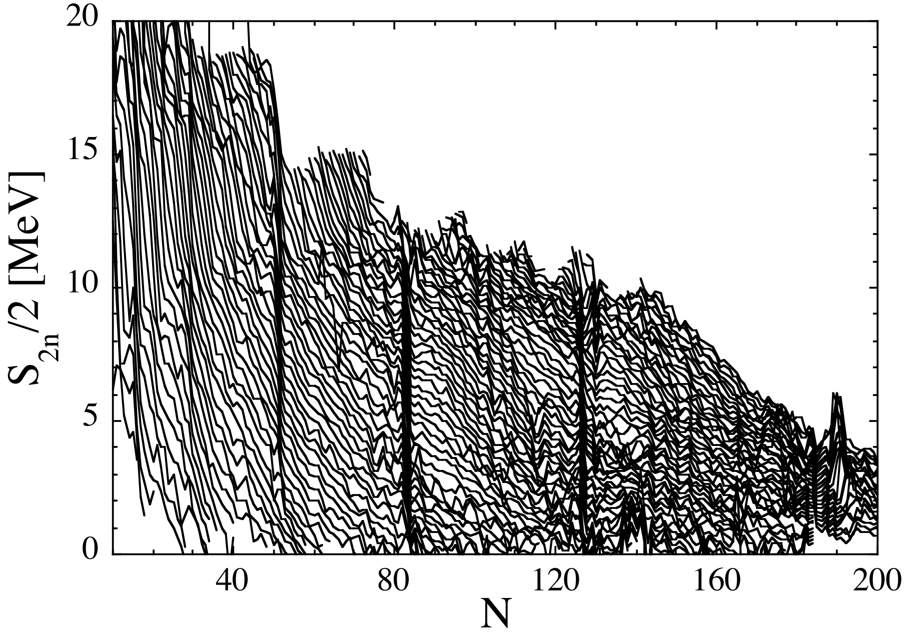
--> possibility to use an iterative procedure based on GK relations to correct the masses at iteration *i* from the masses at iteration *i*-1,
i.e to smooth the mass surface
i.e to filter model noise

$$
\begin{aligned}
M_i(Z,N) = \\
\frac{1}{12}\,[M_{i-1}(Z+2,N-2) + M_{i-1}(Z+2,N+2) \\
+M_i(Z-2,N-2) + M_i(Z-2,N+2) \\
-2\ M_{i-1}(Z+2,N-1) - 2\ M_{i-1}(Z+2,N+1) \\
-2\ M_{i-1}(Z+1,N-2) - 2\ M_{i-1}(Z+1,N+2) \\
-2\ M_i(Z-1,N-2) - 2\ M_i(Z-1,N+2) \\
-2\ M_i(Z-2,N-1) - 2\ M_i(Z-2,N+1) \\
+2\ M_{i-1}(Z,N+2) + 2\ M_{i-1}(Z+2,N) \\
+2\ M_i(Z,N-2) + 2\ M_i(Z-2,N) \\
+4\ M_{i-1}(Z,N+1) + 4\ M_{i-1}(Z+1,N) \\
+4\ M_i(Z,N-1) + 4\ M_i(Z-1,N)]
\end{aligned}
$$

# Smoothing of the HFB masses on the basis of the GK relations

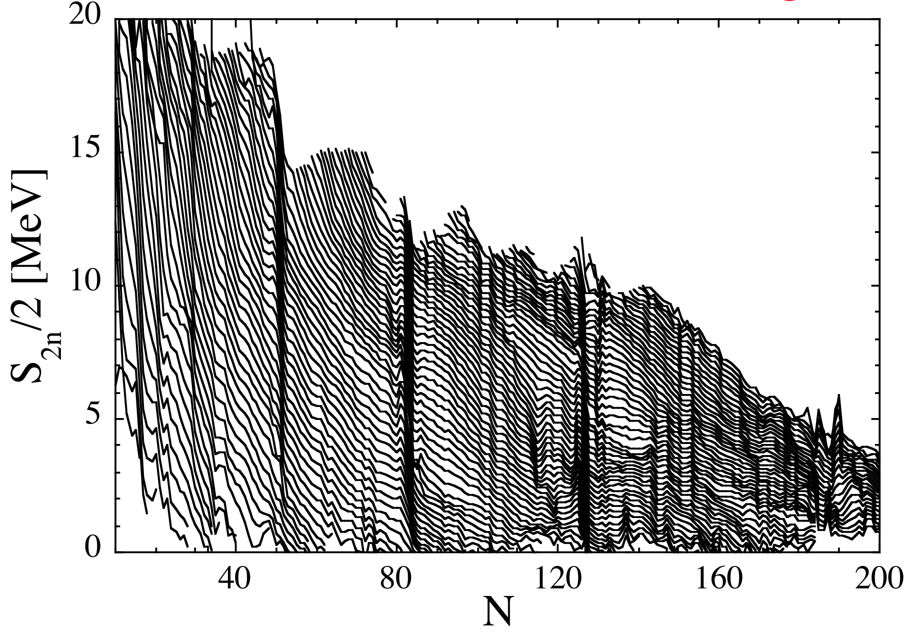
(independent of experimental masses)

HFB-21



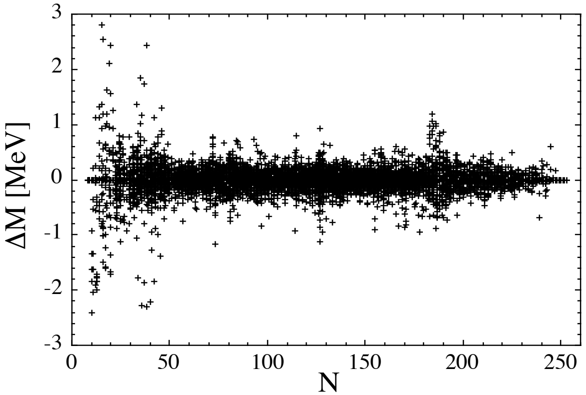

$\sigma_{exp}$ (2149 nuc)=0.577MeV

HFB-21 after noise-filtering

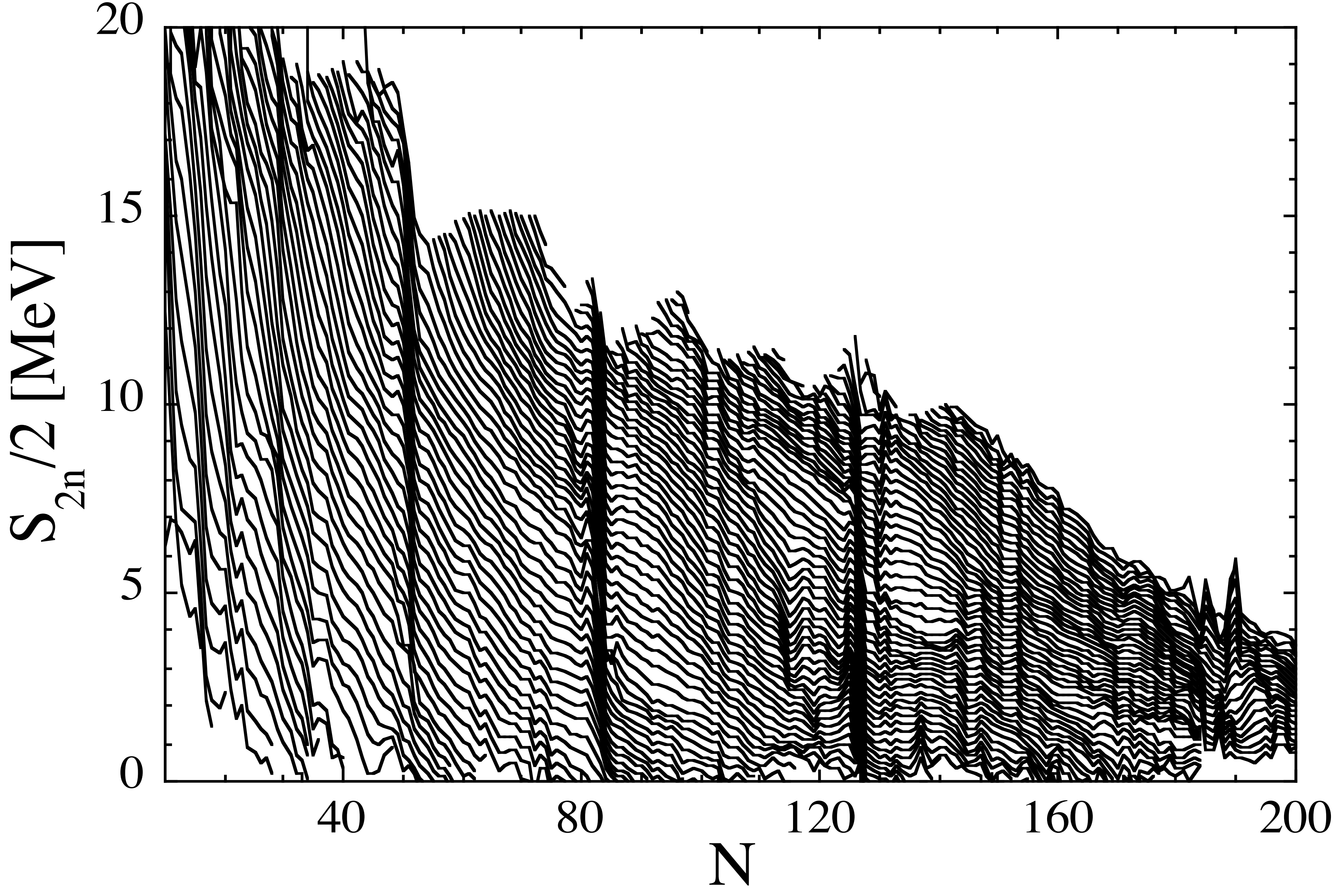



$\sigma_{exp}$ (2149 nuc)=0.581MeV

**No modification of the mass extrapolation !!**




$\sigma_{HFB\text{-}GK}$ (8509M)=0.270MeV


20
15
10
5
0
40
80
120
160
200
N
$S_{2n}/2$ [MeV]

# Conclusions

**Experimental masses on more than 2300 nuclei provide a wealth of information that can help us to further constrain theoretical models and shed light on microscopic physics**

**The future challenge lies in a unified description of masses and all other nuclear properties, such as deformations, densities, quadrupole moments, spins, nuclear and neutron matter properties, but also Level Densities, Fission, GR…**

**A new generation of mass models beyond mean field is emerging**
**A mass model within the relativistic mean field still need to be built**

**More experimental data & theoretical works are needed**