DE LA RECHERCHE À L'INDUSTRIE

Optimization at the multireference level

S. Hilaire

CEA,DAM,DIF

Workshop ESNT

27 NOVEMBRE 2014

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How we fitted D1M ?

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27 NOVEMBRE 2014

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J.P. Ebran

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GENERAL MOTIVATION

Providing nuclear reaction models with **« credible and coherent »** microscopic inputs

- makes (really) senses when dealing with unmeasured target
- the sounder the underlying physics the better the predictive power
- no direct link between xs and n-n interaction for **all nuclei**
- **many inputs** needed
  - . Discrete levels properties (masses, J, p, deformation etc …)
  - . Nuclear level densities up to 200MeV
  - . Gamma strength functions
  - . Fission properties (barriers, broken symetries, = path)
  - . Optical potential (spherical and deformed)
- all this can be derived from nuclear structure more or less directly
- all this can be used mostly through tables
- robust codes needed
- robust methodolodgy (recipes)
  - . to reduce human intervention while producing tables
  - . to fill gaps (even-even limitation for instance)

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All this has been done with Skm for all nuclei (S. Goriely) !

Let's do it with Gogny !

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All this has been done with Skm for all nuclei (S. Goriely) !

Let's do it with Gogny !

$\Rightarrow$ We have codes
$\Rightarrow$ We have computers
$\Rightarrow$ We have experts (not me !)
$\Rightarrow$ We have motivation (me !)

PLAN

PLAN

- Motivation

PLAN

- Motivation

- The starting point : D1S, D1N

PLAN

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- Methodolodgy, codes

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- Results
- Perspectives

THE STARTING POINT : D1S, D1N

A little bit of history

D1 type Gogny interaction

D1 type Gogny interaction

- **First interaction D1 in 1980 (***Dechargé et al., PRC21 (1980) 1568***)**
  - Phenomenologic effective interaction
  - 14 parameters adjusted on nuclear matter properties and few data for ^{16}O, ^{48}Ca, ^{90}Zr, ^{208}Pb
  - Specificity : finite range in central term :
    ⇒interaction usable for mean field and pairing (HFB) and beyond
  - provide globally good results
  - requires significant computation time (up to 10' for 14 H.O shells)

D1 type Gogny interaction

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- **D1S in 1991 (***Berger et al., CPC 63 (1991) 365***)**
  > fission barriers problem of D1 reduced

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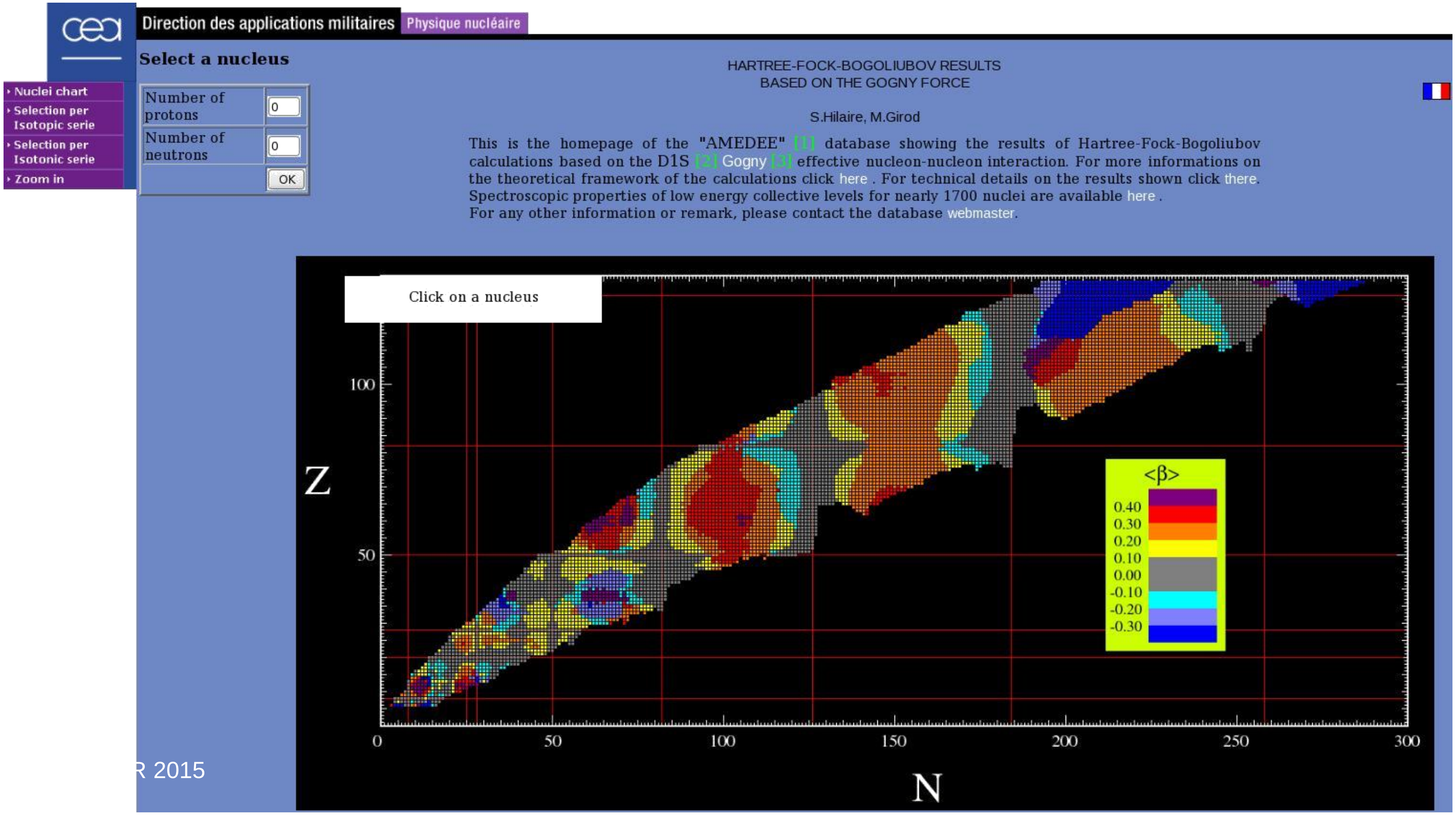

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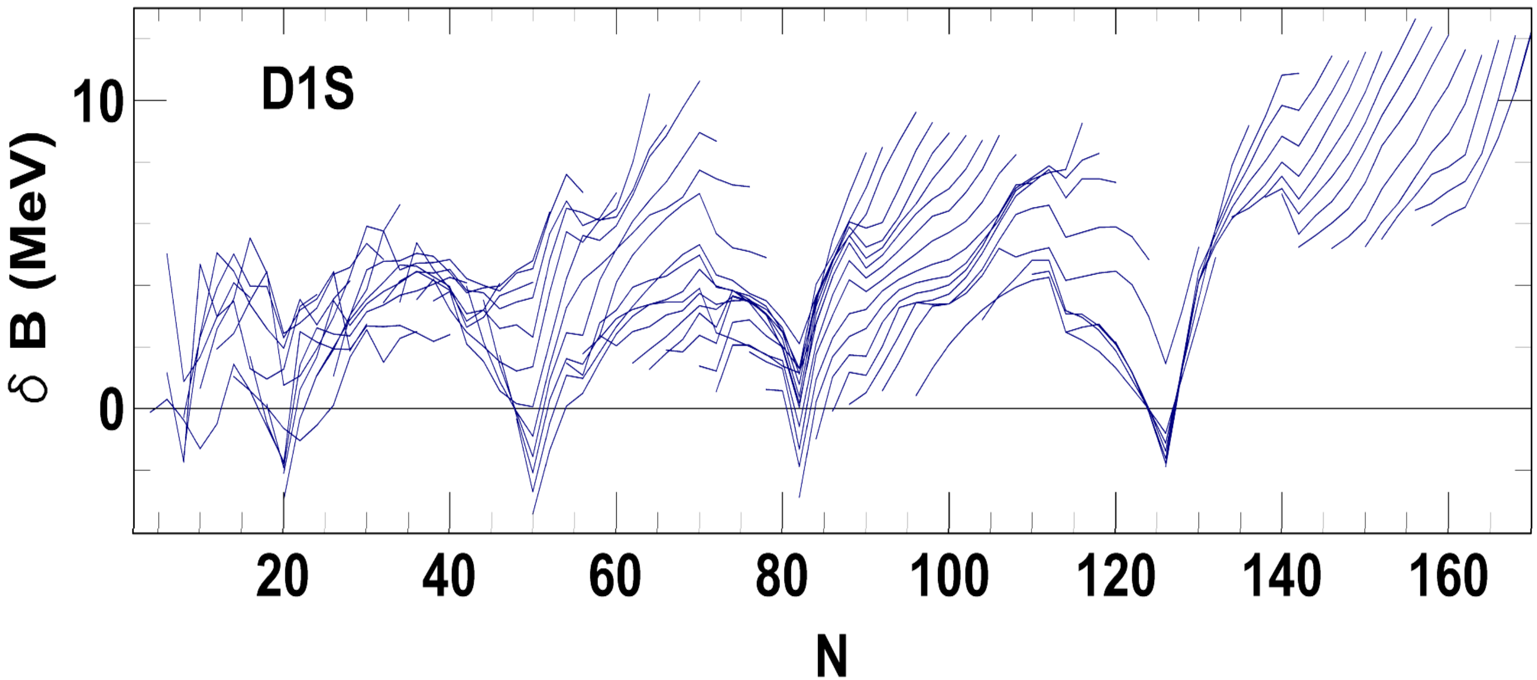

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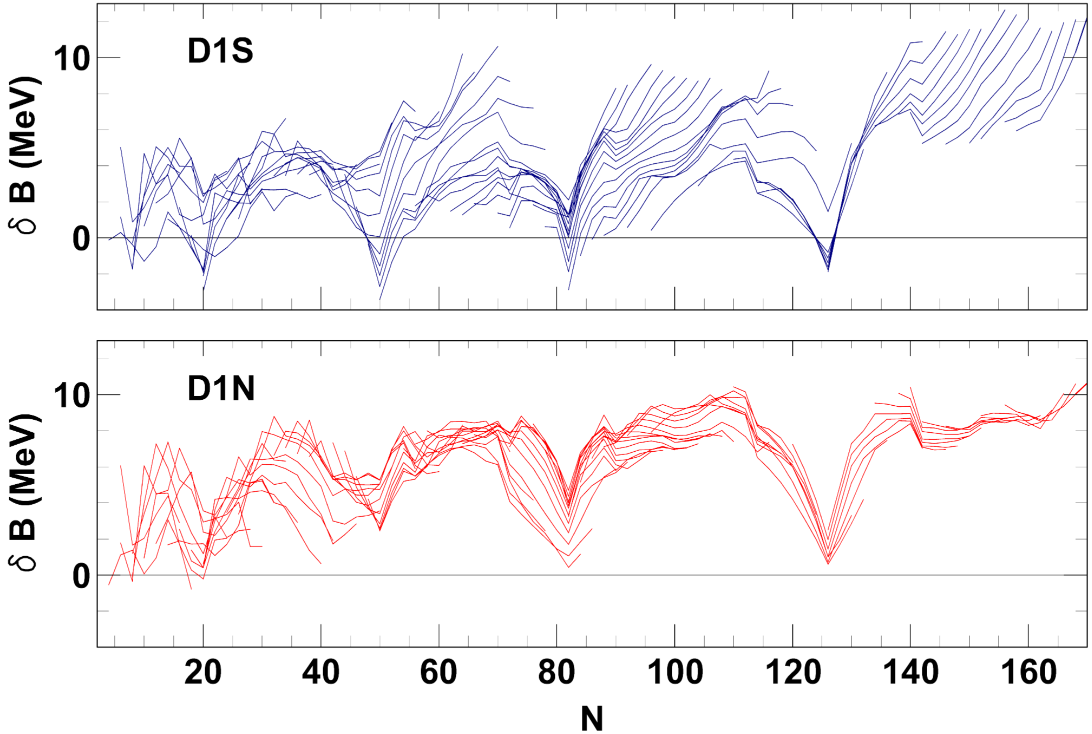

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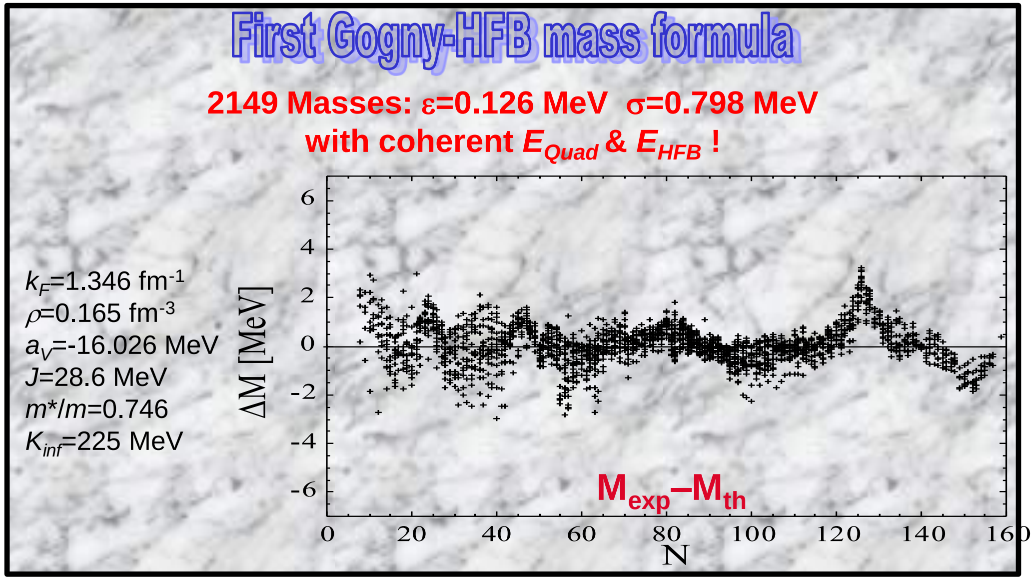
  > r.m.s masses reduction to 800 keV (D1S ≈ 4 MeV)



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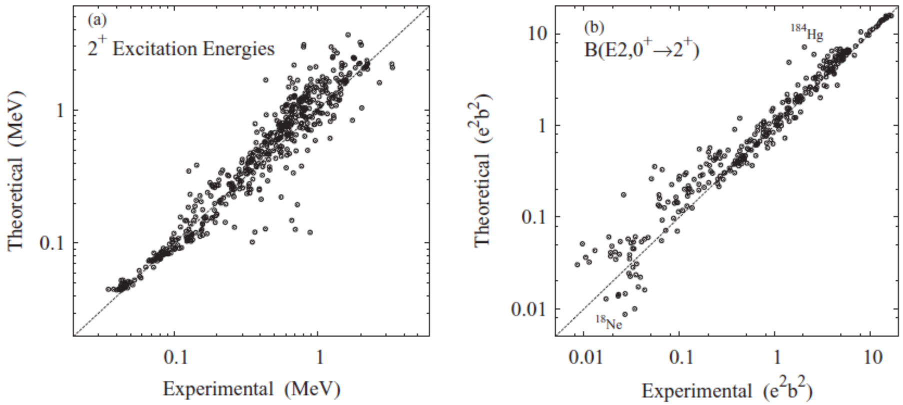

FIG. 11. (a) Theoretical 2_1^+ excitation energies of 537 even-even nuclei as a function of their experimental values. (b) Theoretical $B(E2;0_1^+ \to 2_1^+)$ transition strengths of 320 even-even nuclei as a function of their experimental values. Several cases showing deviations are labeled by the nucleus. Experimental data are from Refs. [56,57].

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➡ **New interactions more frequently**

➡ **Clear will to reduce pathologies**

➡ **Link with computer power**

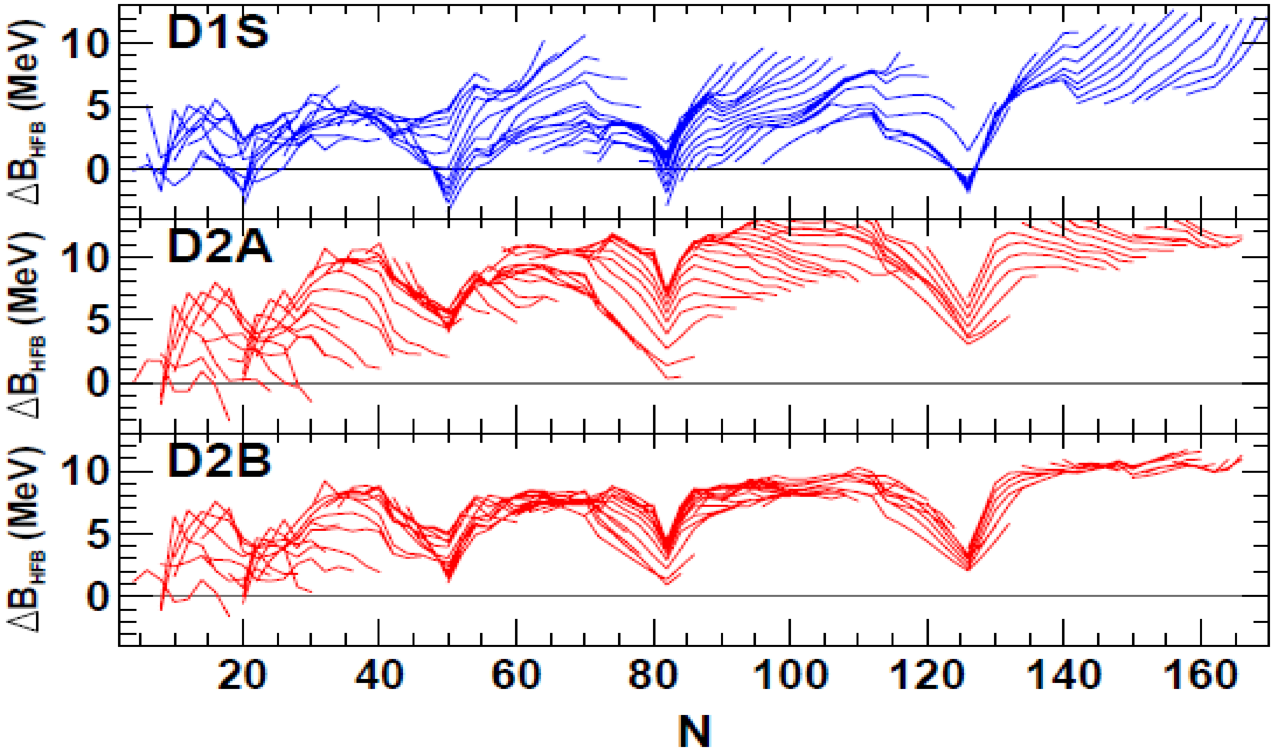
➡ **Things have not been made in order**

D2 type interaction(s)

D1 (1980)

D1S (1991) : surface properties improved (fission)

D2 (2007) : finite range in density dependent term (PRC 2015)



D2 type interaction(s)

D1 (1980)

D1S (1991) : surface properties improved (fission)

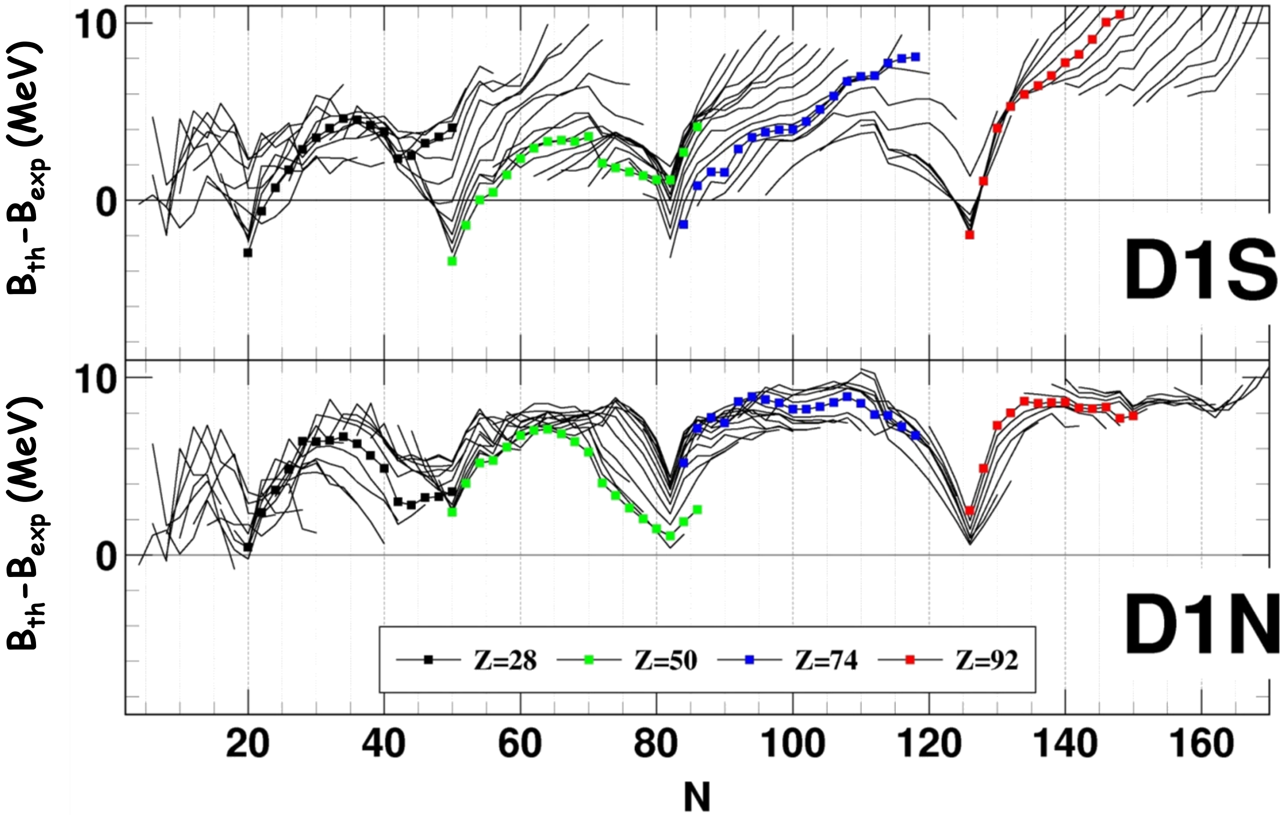
D2 (2007) : finite range in density dependent term (PRC 2015)

D1N (2008) : better neutron matter EOS description

D1M (2009) : better description of binding energies and $Q_{reaction}$

- **New interactions more frequently**
- **Clear will to reduce pathologies**
- **Link with computer power**
- **Things have not been made in order**

Summary : D1S, D1N



⇒ Challenge in 2008 : Reduce the r.m.s of binding energies differences

Other properties similar or better

Cope with local criticisms

Obey Bruyères Golden Rule

Summary : D1S, D1N

ONE SHALL ONLY DESIGN EFFECTIVE INTERACTIONS

- *for both mean field and beyond mean field predictions*
- *for all nuclei*
- *for all nuclear properties*

⇒ Challenge in 2008 : Reduce the r.m.s of binding energies differences
Other properties similar or better
Cope with local criticisms
Obey Bruyères Golden Rule

METHODOLOGY, CODES

Methodology used to fit D1S or D1N

$$v_{12} = \sum_{j=1}^{2} exp\left[-\left(\frac{|\vec{r_1}-\vec{r_2}|}{\mu_j}\right)^2\right](W_j + B_j P_\sigma - H_j P_\tau - M_j P_\sigma P_\tau)$$

$$+t_3 \left(1 + x_3 P_\sigma\right) \delta\left(\vec{r_1} - \vec{r_2}\right) \rho^\alpha \left(\frac{\vec{r_1}+\vec{r_2}}{2}\right)$$

$$+iW_{ls} \overleftarrow{\nabla}_{12} \cdot \delta\left(\vec{r_1} - \vec{r_2}\right) \bigwedge \vec{\nabla}_{12} \cdot \left(\vec{\sigma_1} + \vec{\sigma_2}\right)$$

$$+\frac{\left(1 - 2\tau_1^z\right)\left(1 - 2\tau_2^z\right)}{4} \frac{e^2}{|\vec{r_1} - \vec{r_2}|}$$

➲ **Finite range :** avoid pathologies “beyond HF” due to unrealistic behavior of 0-range forces at high relative momenta

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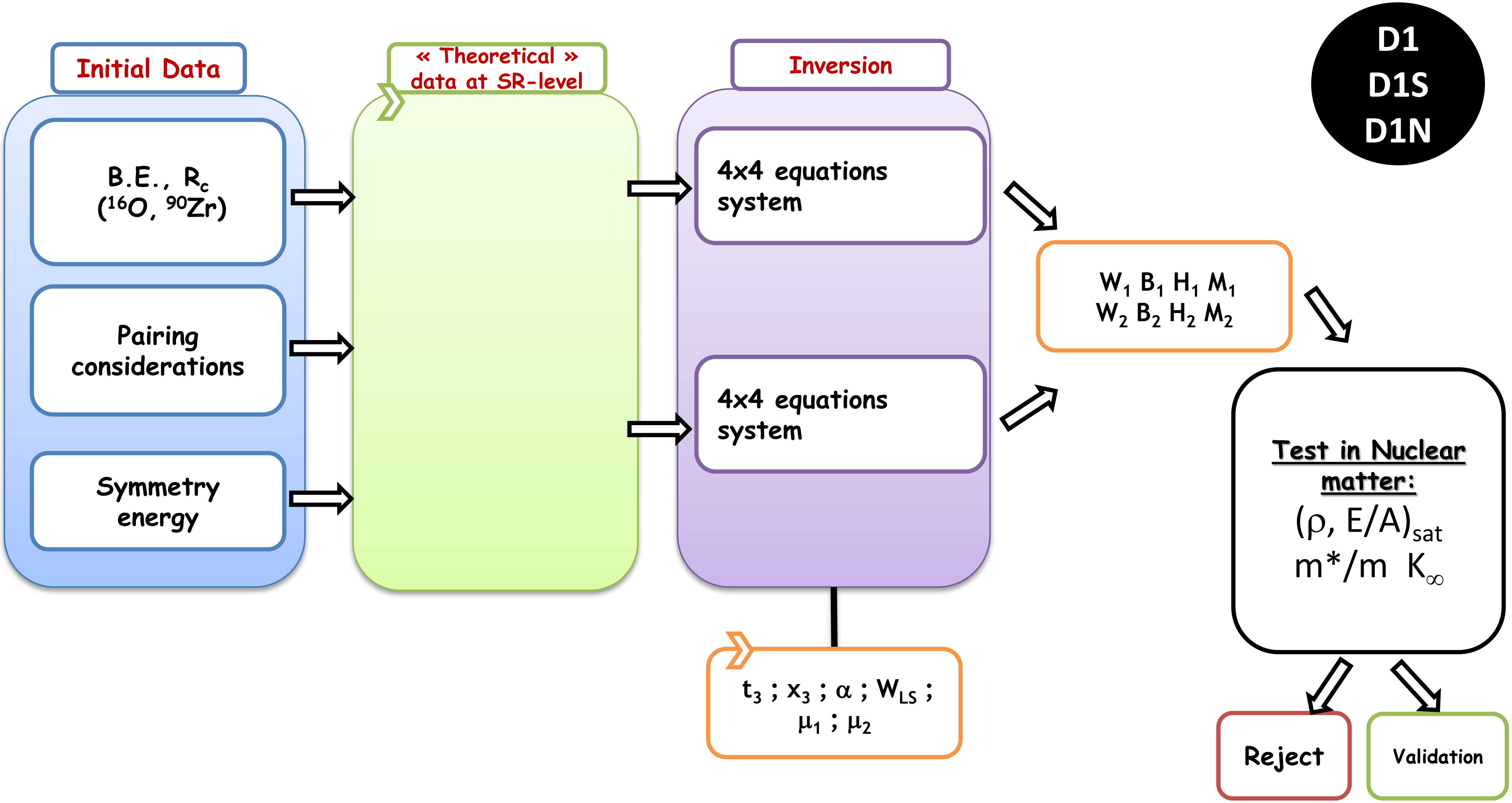
$$+ \frac{\left(1 - 2\tau_1^z\right)\left(1 - 2\tau_2^z\right)}{4} \frac{e^2}{|\vec{r_1} - \vec{r_2}|}$$

14 parameters to fit

➲ **Finite range :** avoid pathologies "beyond HF" due to unrealistic behavior of 0-range forces at high relative momenta

Methodology used to fit D1S or D1N

➲ "Traditional" method involving small set of magic nuclei (!!!) at SR-level



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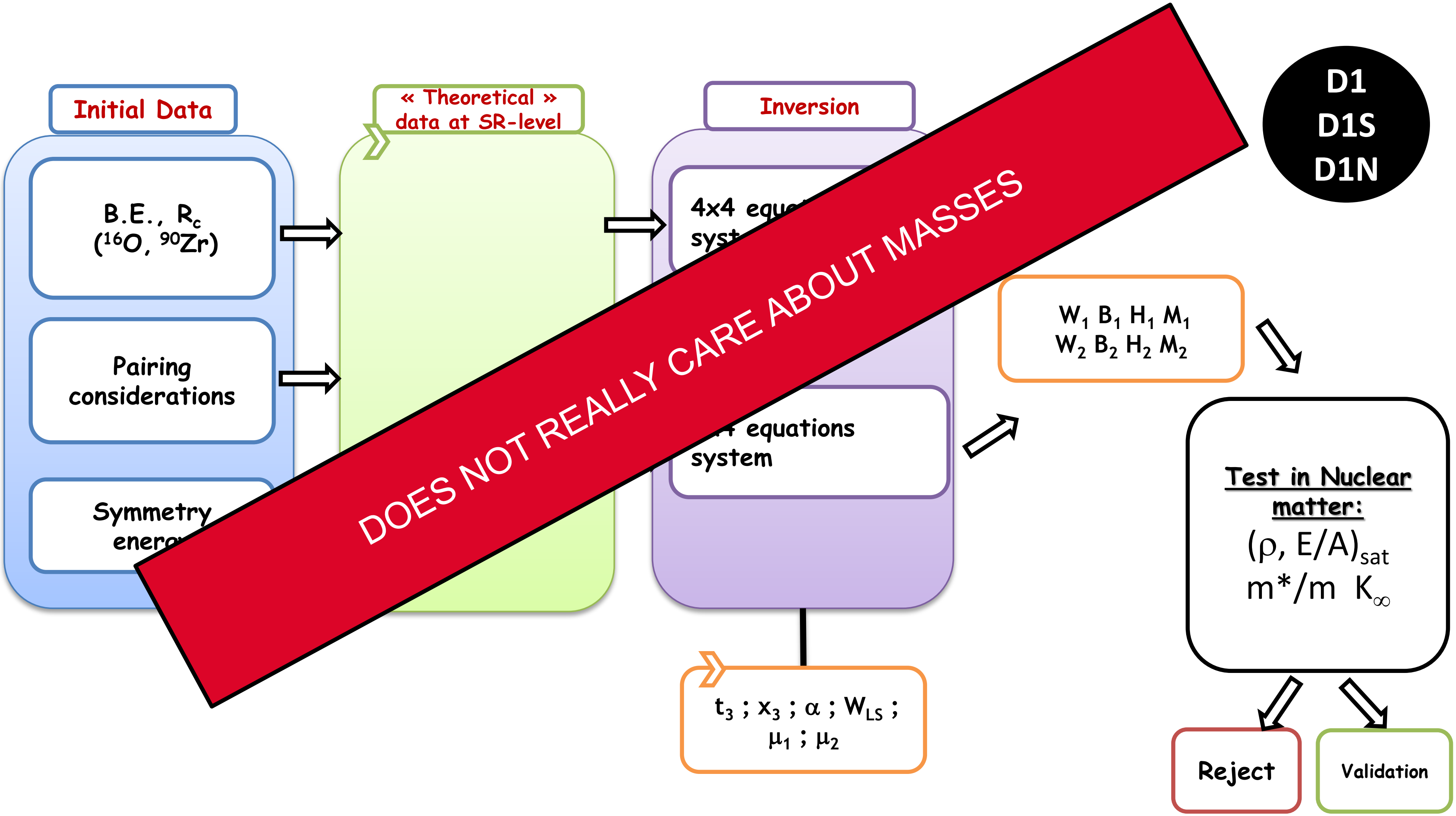

How can we compute binding energies ?

$$B = B(N_0) + \Delta_\infty + \Delta_{\mathrm{quad}}$$

➲ Infinite basis correction : code AMEDEE

$$\Delta_\infty = E(N_0) - E(N = +\infty)$$

➲ Assumption

$$\Delta_\infty = 2[E(N_0) - E(N_0 + 2)]$$

How can we compute binding energies ?

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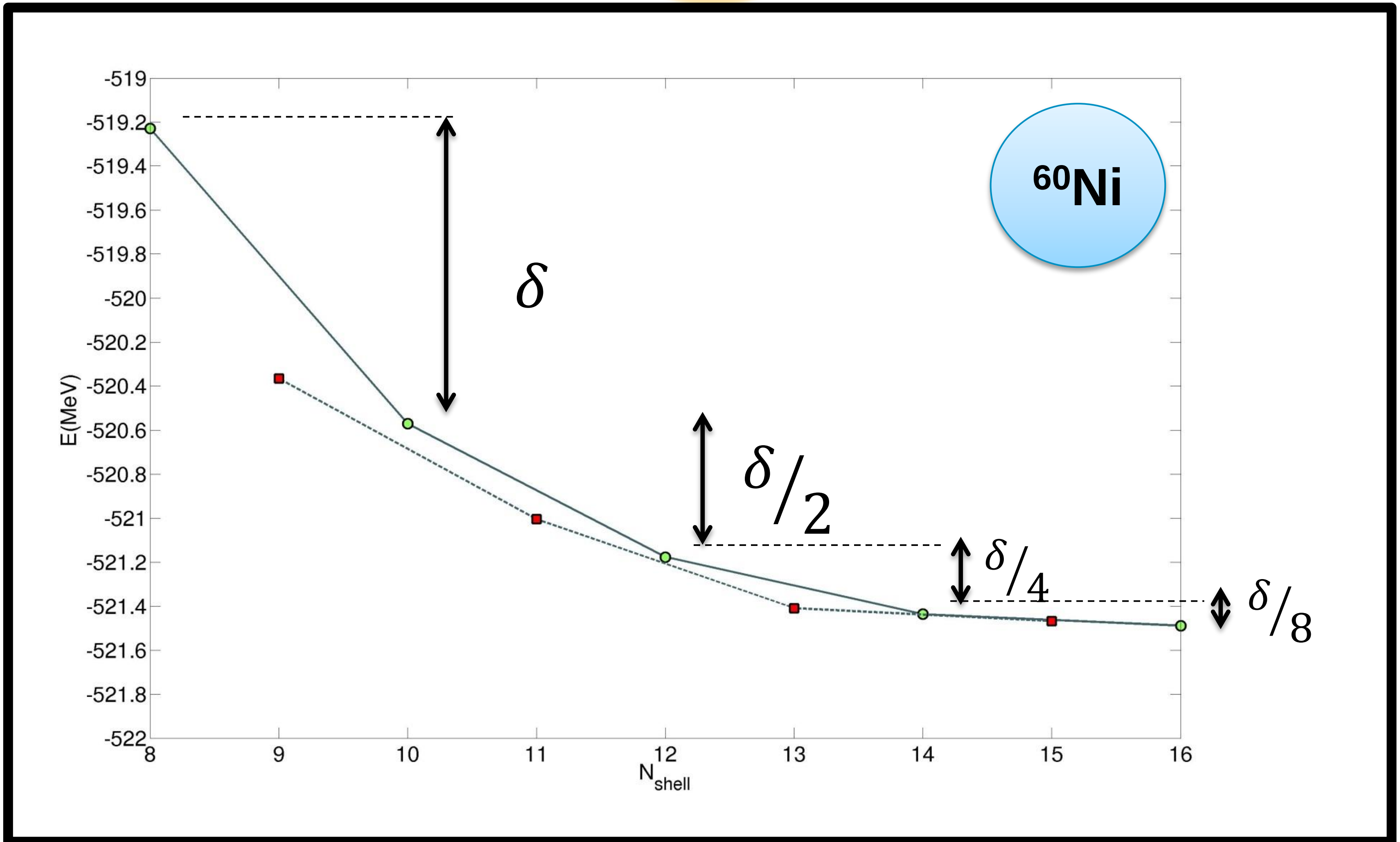

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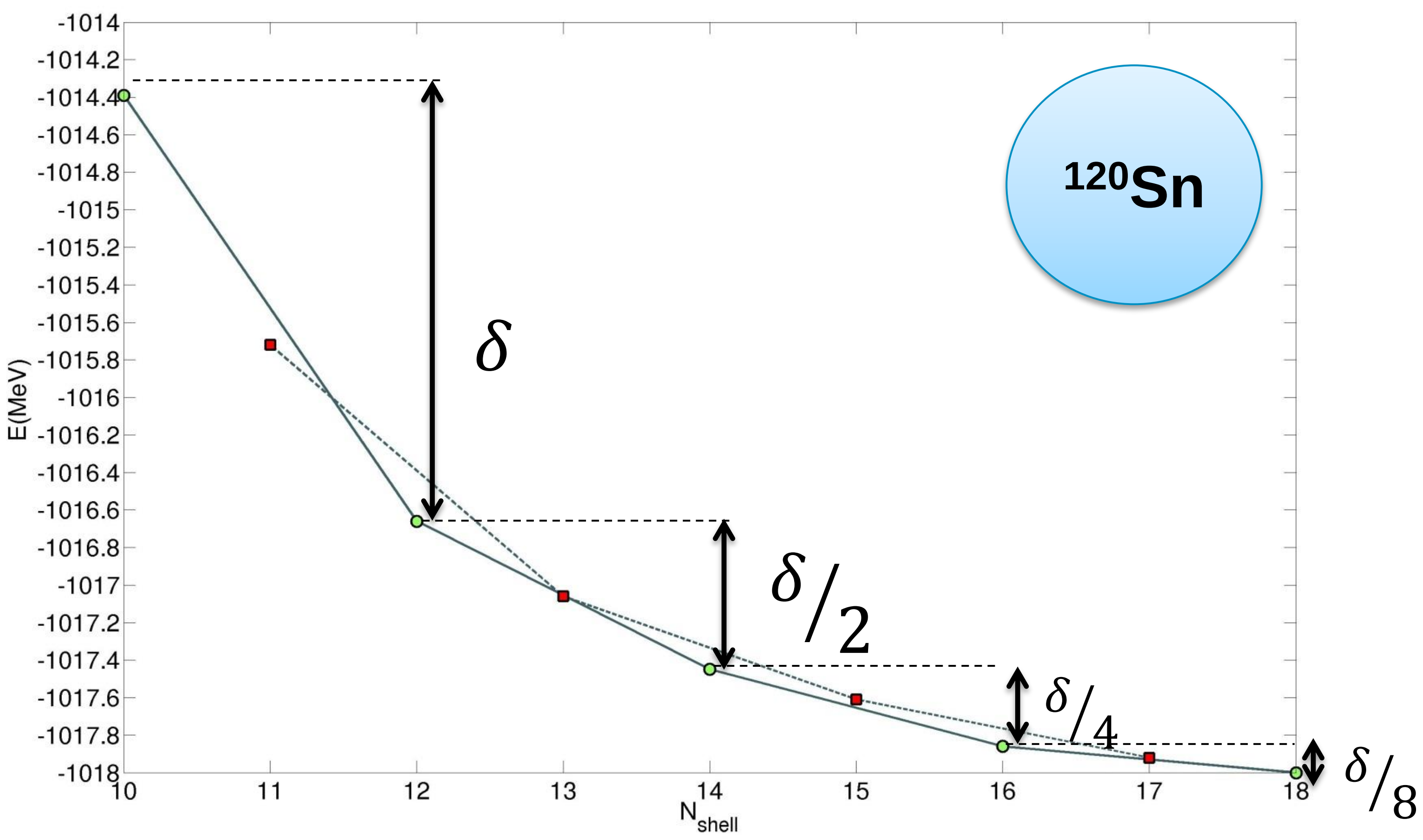

How can we compute binding energies ?

$$B = B(N_0) + \Delta_\infty + \Delta_{\text{quad}}$$

$$\Delta_{quad} = ESR - EMR$$

➲ GCM + GOA : code THEOPHIL + KUMAR

$$\hat{\mathcal{H}}_{\text{coll}} = -\frac{\hbar^2}{2}\sum_{i,j}\frac{\partial}{\partial q_i}[M^{-1}(q)]_{ij}\frac{\partial}{\partial q_j} + \mathcal{V}(q)$$

➲ M. Girod and B. Grammaticos, Nucl. Phys. A**330** 40 (1979)

➲ J. Libert, M. Girod and J.-P. Delaroche, Phys. Rev. C**60** 054301 (1999)

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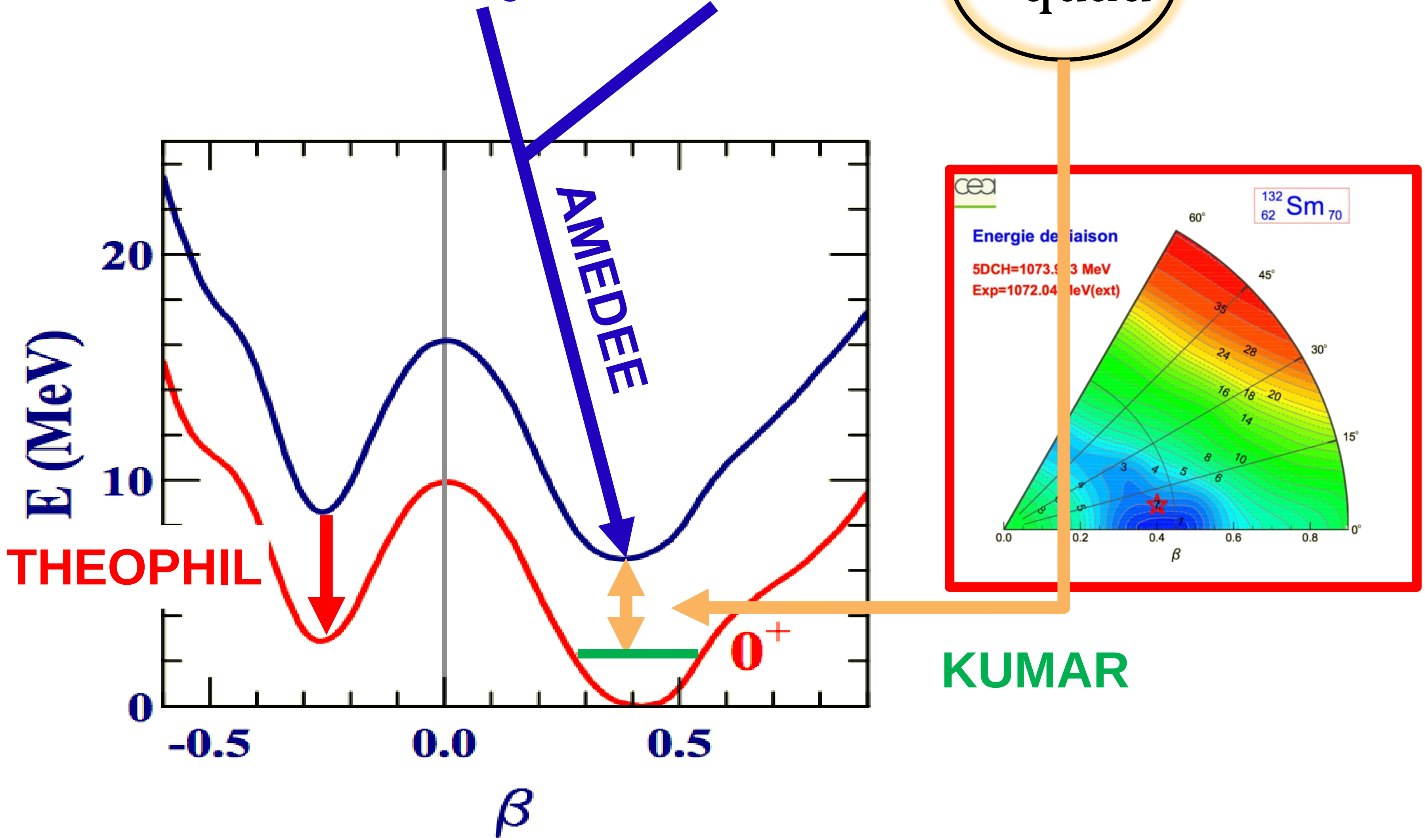
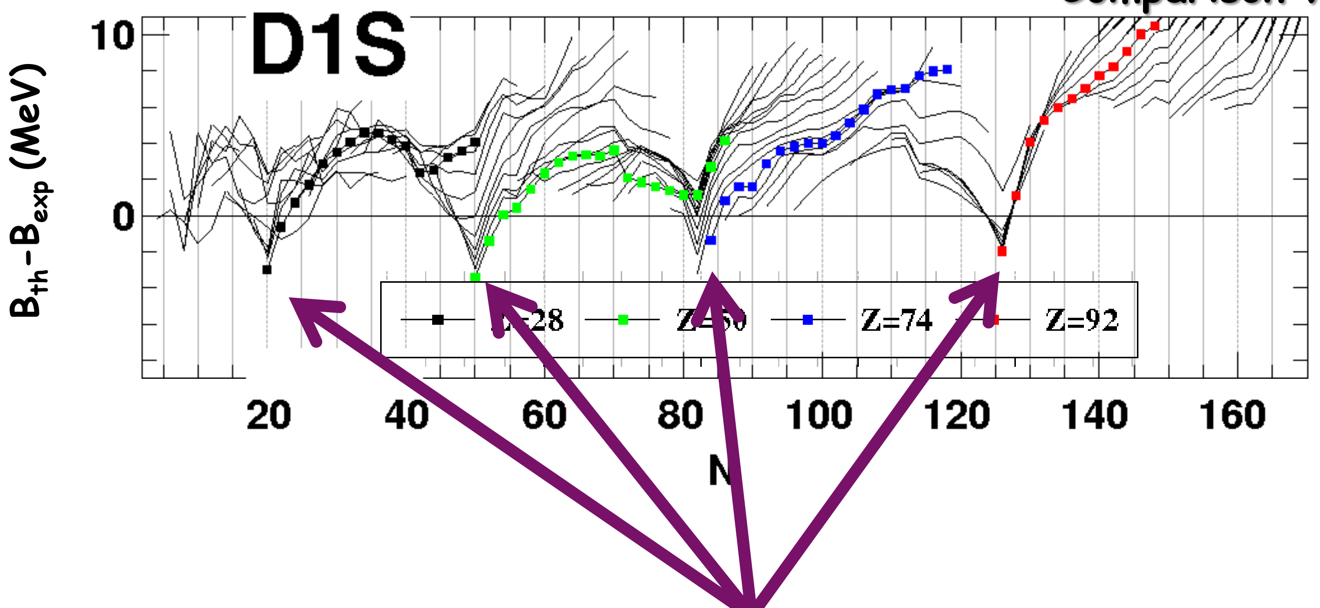


Consequences illustrated with D1S

D1S

Comparison with 2149 Exp. Masses



- $E_{th} = E_{HFB}$

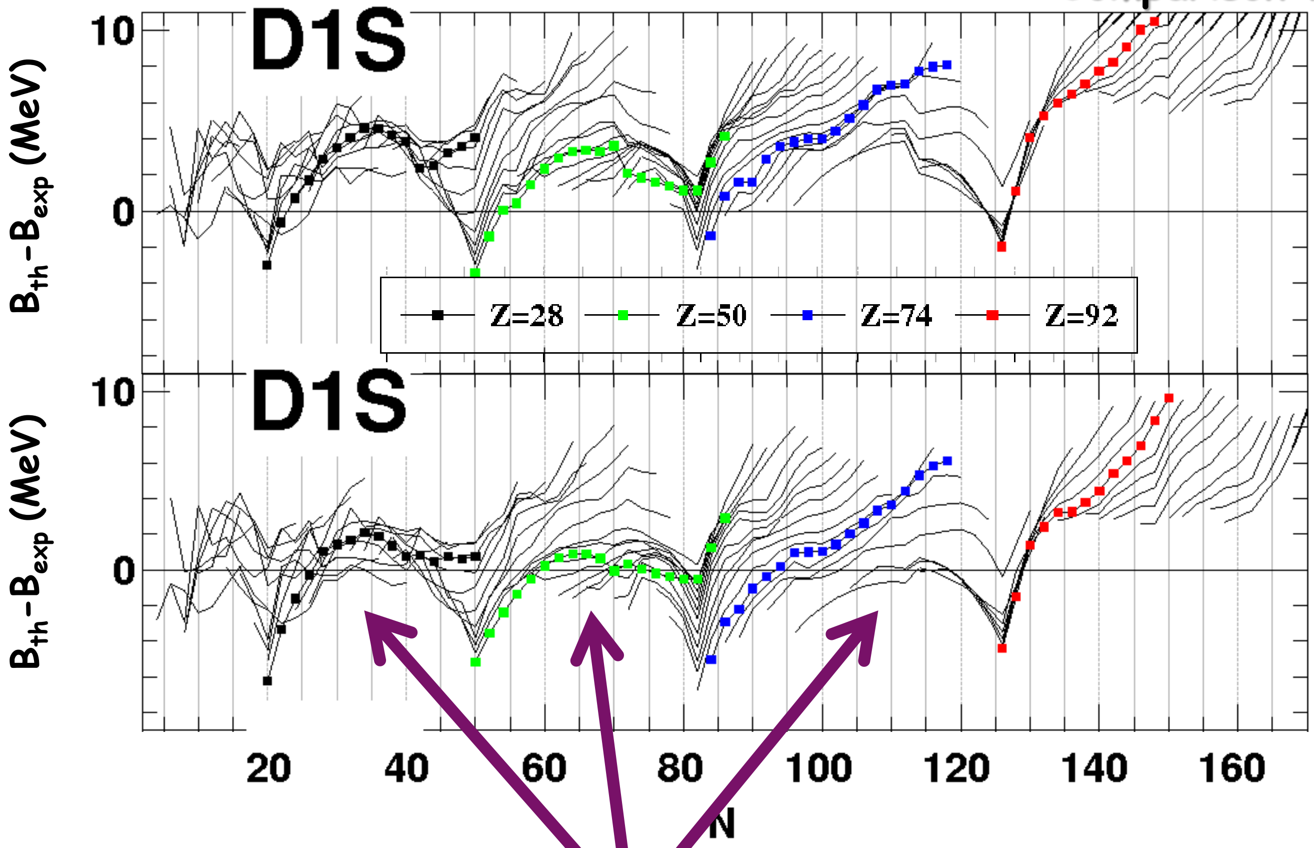
r.m.s ~ 4.4 MeV

Adjustment performed without infinite basis effect estimation
⇒ Overbinding of 1-3 MeV

Consequences illustrated with D1S

D1S

Comparison with 2149 Exp. Masses



- $E_{th} = E_{HFB}$

  r.m.s ~ 4.4 MeV

- $E_{th} = E_{HFB} - \Delta_\infty$

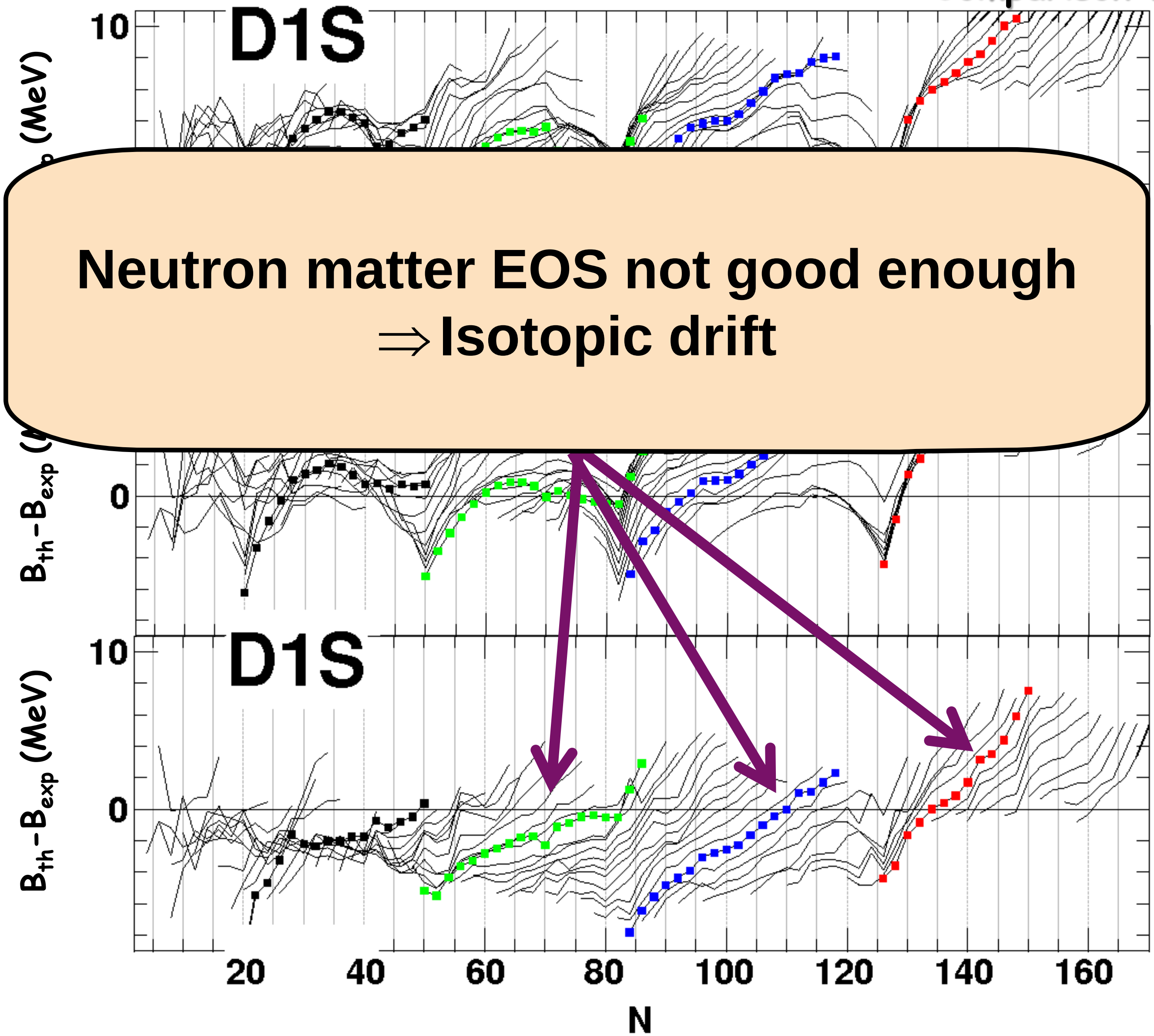
  r.m.s ~ 2.6 MeV

Quadrupole correlations missing
$\Rightarrow$ Arches between magic nuclei

Consequences illustrated with D1S

D1S

Comparison with 2149 Exp. Masses



Neutron matter EOS not good enough
$\Rightarrow$ Isotopic drift

- $E_{th} = E_{HFB}$

  r.m.s ~ 4.4 MeV

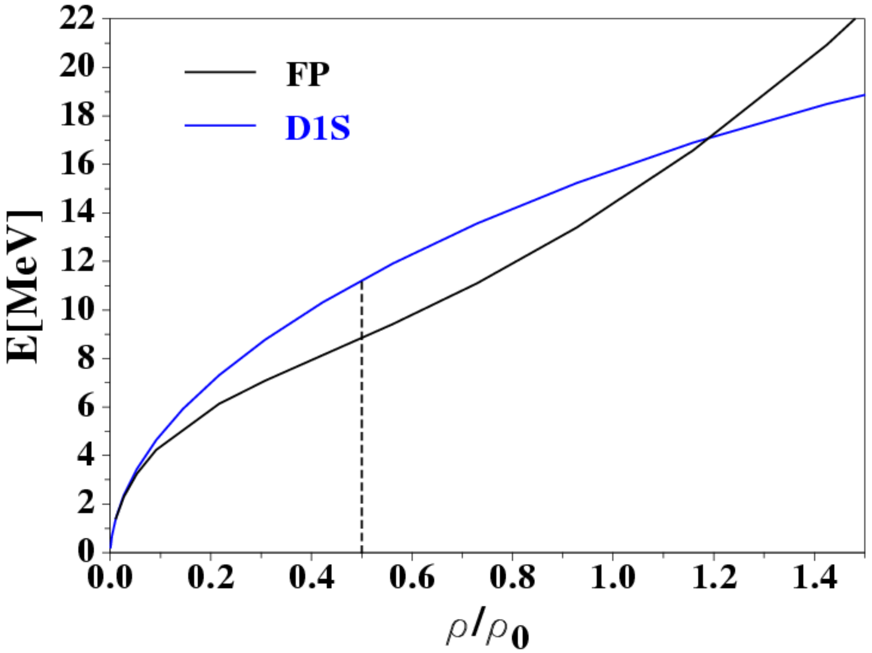
- $E_{th} = E_{HFB} - \Delta_\infty$

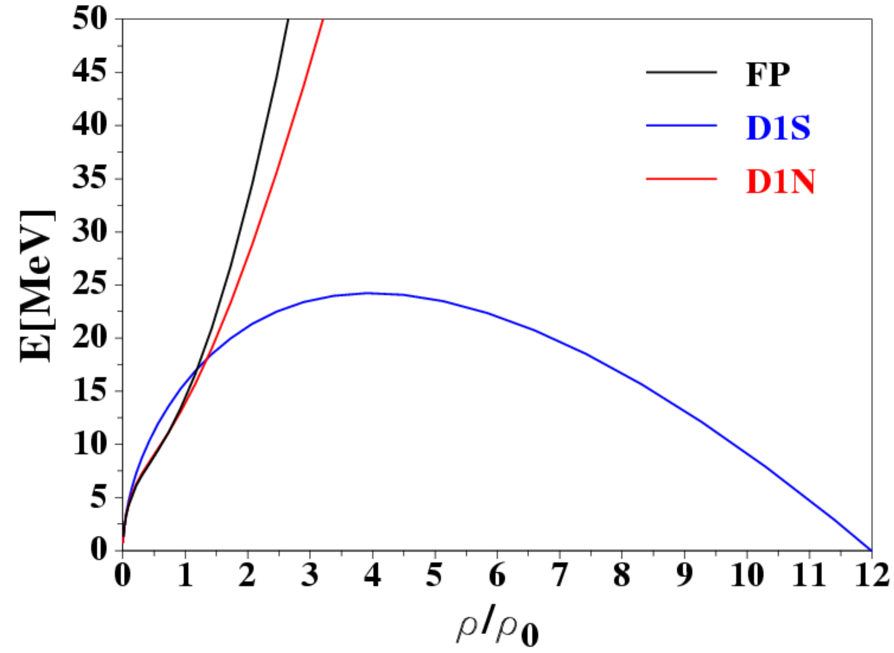
  r.m.s ~ 2.6 MeV

- $E_{th} = E_{HFB} - \Delta_\infty - \Delta_{quad}$

  r.m.s ~ 2.9 MeV

D1N : better neutron matter EOS !

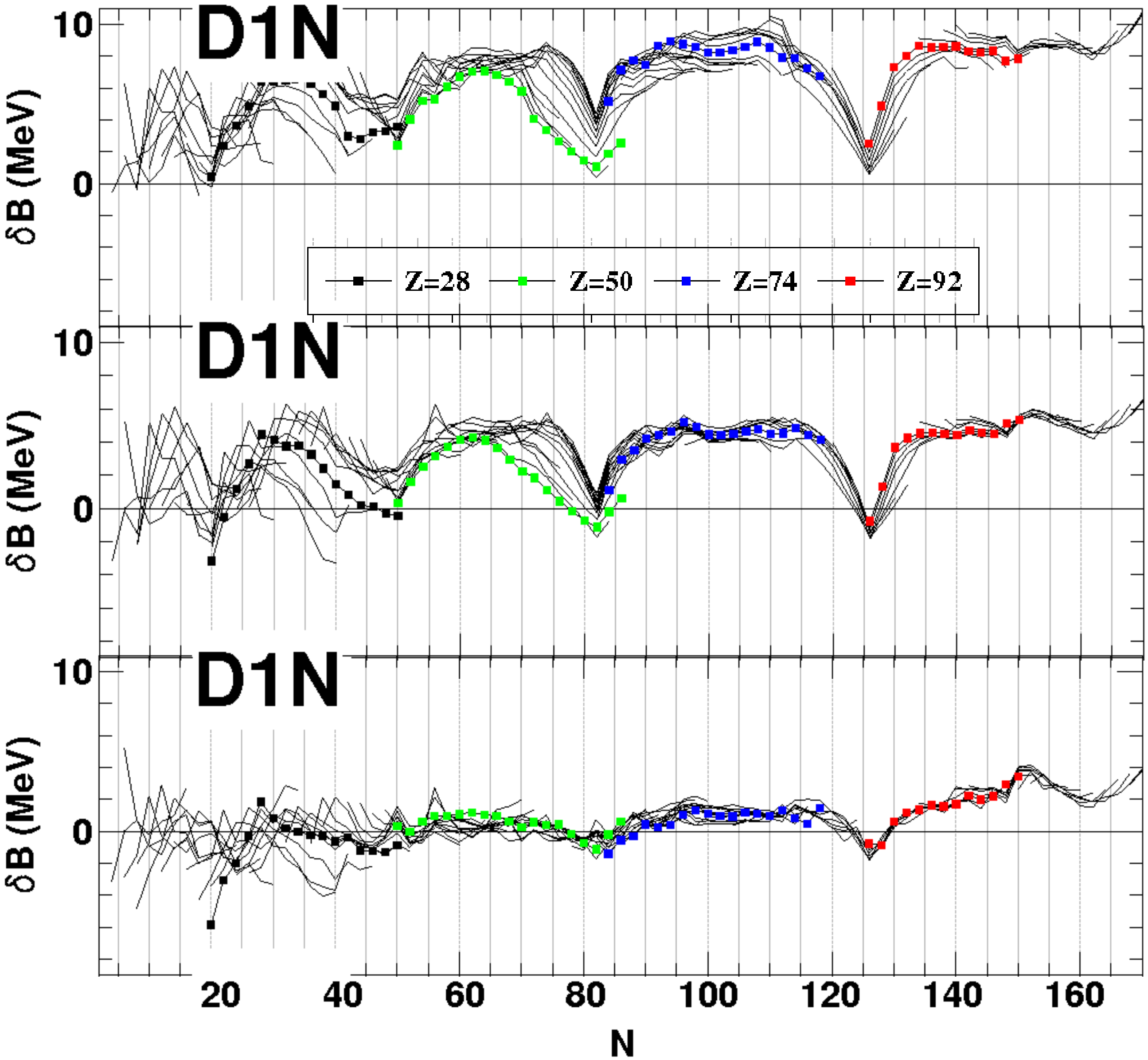




➲ F. Chappert, M. Girod & S. Hilaire, Phys. Lett. B**668** (2008) 420.

Consequences illustrated with D1N

D1N



- $E_{th} = E_{HFB}$

r.m.s ~ 2.5 MeV

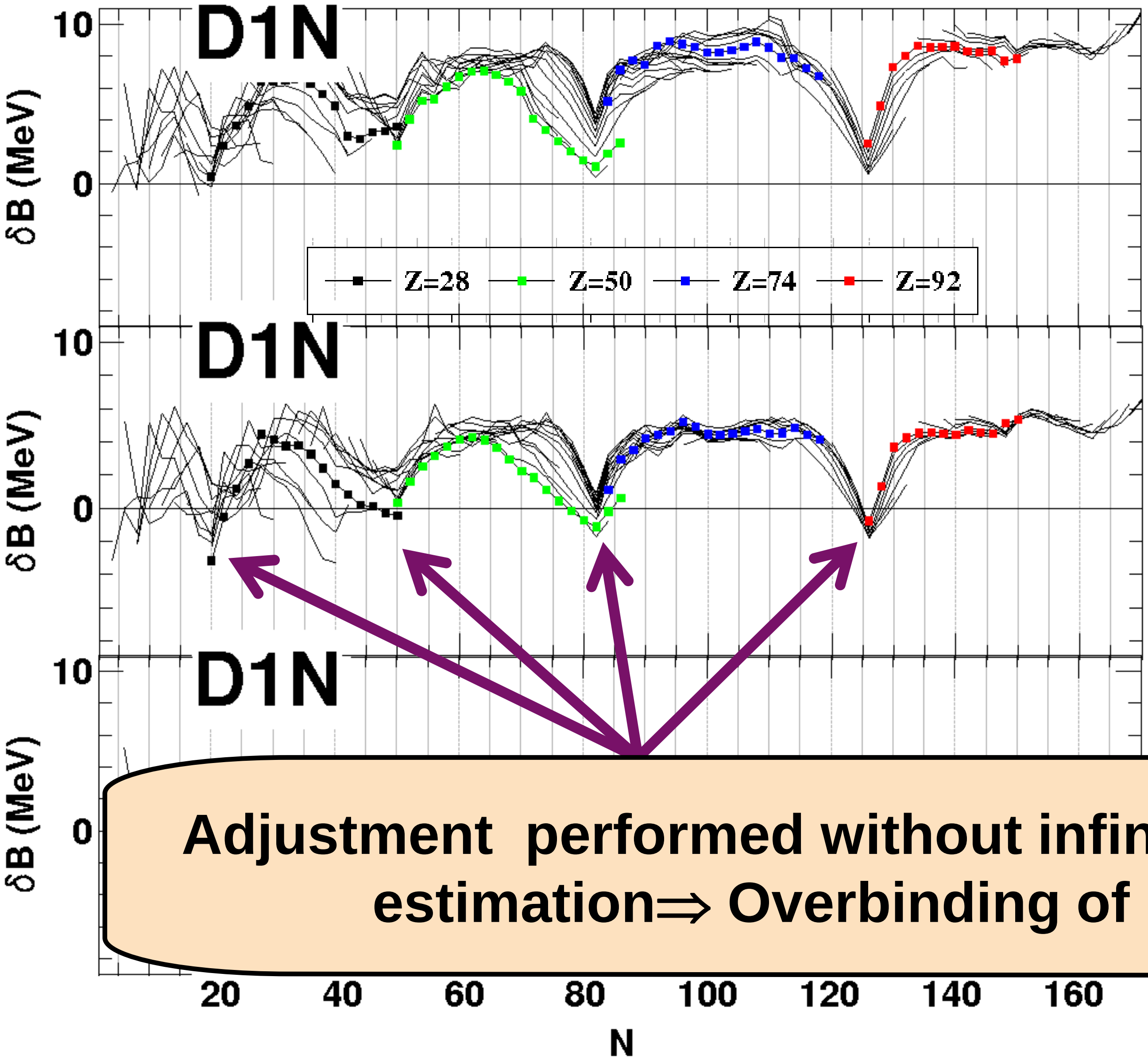
- $E_{th} = E_{HFB} - \Delta_{\infty}$

- $E_{th} = E_{HFB} - \Delta_{\infty} - \Delta_{quad}$

r.m.s ~ 1 MeV

Consequences illustrated with D1N

D1N



- $E_{th} = E_{HFB}$

  r.m.s ~ 2.5 MeV

- $E_{th} = E_{HFB} - \Delta_{\infty}$

- $E_{th} = E_{HFB} - \Delta_{\infty} - \Delta_{quad}$

Adjustment performed without infinite basis effect estimation⇒ Overbinding of 1-3 MeV

The new fitting procedure

➲ Make use of the huge data on masses and incorporate a minimum of effectivity in the functional ⇒ MR-level = the best formalism we can use

Parameters kept constant: 4 (can be included in the fit)

4 μ_1=0.7-0.8 ; μ_2=1.2 ; x_3=1 ; α=1/3 (0.2-0.5 investigated)

D1M

Parameters constrained: 3

- J ~ 29 - 32 MeV to reproduce at best neutron matter EoS
- K ~ 230 - 240 MeV as expected from exp. breathing mode data
- k_F kept constant to reproduce charge radii at best (manually adjusted)

Parameters directly fitted to nuclear masses at MR-level: 7

5 $(a_v, m^*, W_1, M_1, B_2, H_2, W_{so})$

Matrix inversion gives the rest

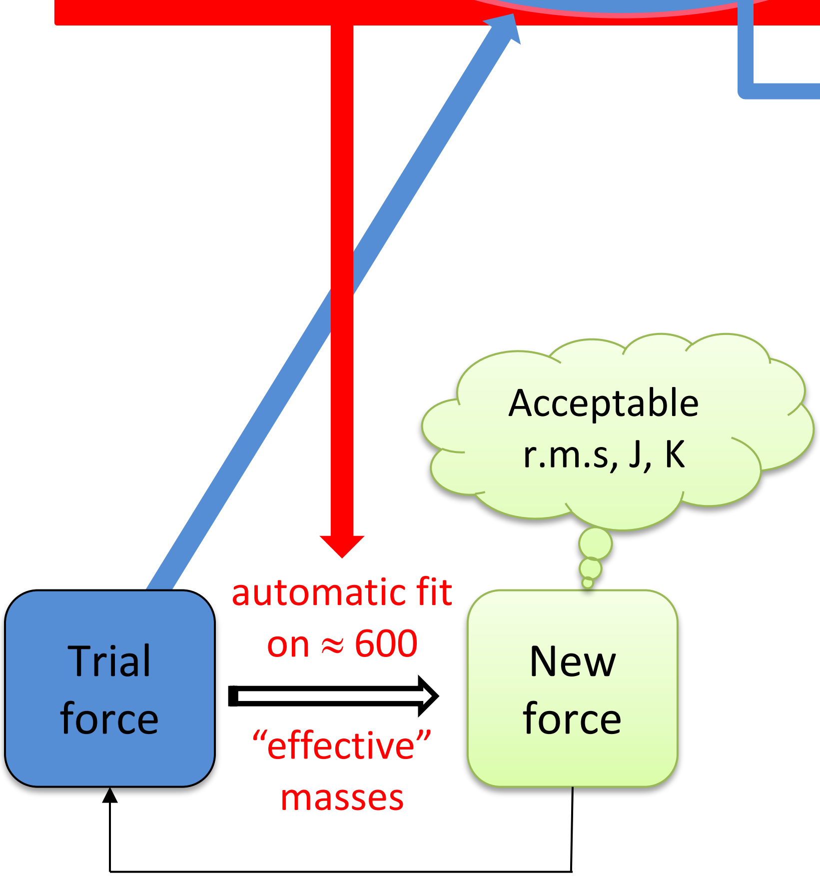
5 $(a_v, J, m^*, K, k_F) \longleftrightarrow (B_1, H_1, W_2, M_2, t_3)$

The new fitting procedure

$$\{B_{exp} + \Delta_\infty + \Delta_{quad}\}$$

For 1/3 of 2149 exp masses (Audi *et al* 2003) excluding N=Z,N=Z±1, N=Z±2 nuclei

Interpolated for odd-odd and odd-even using neighboring even-even nuclei



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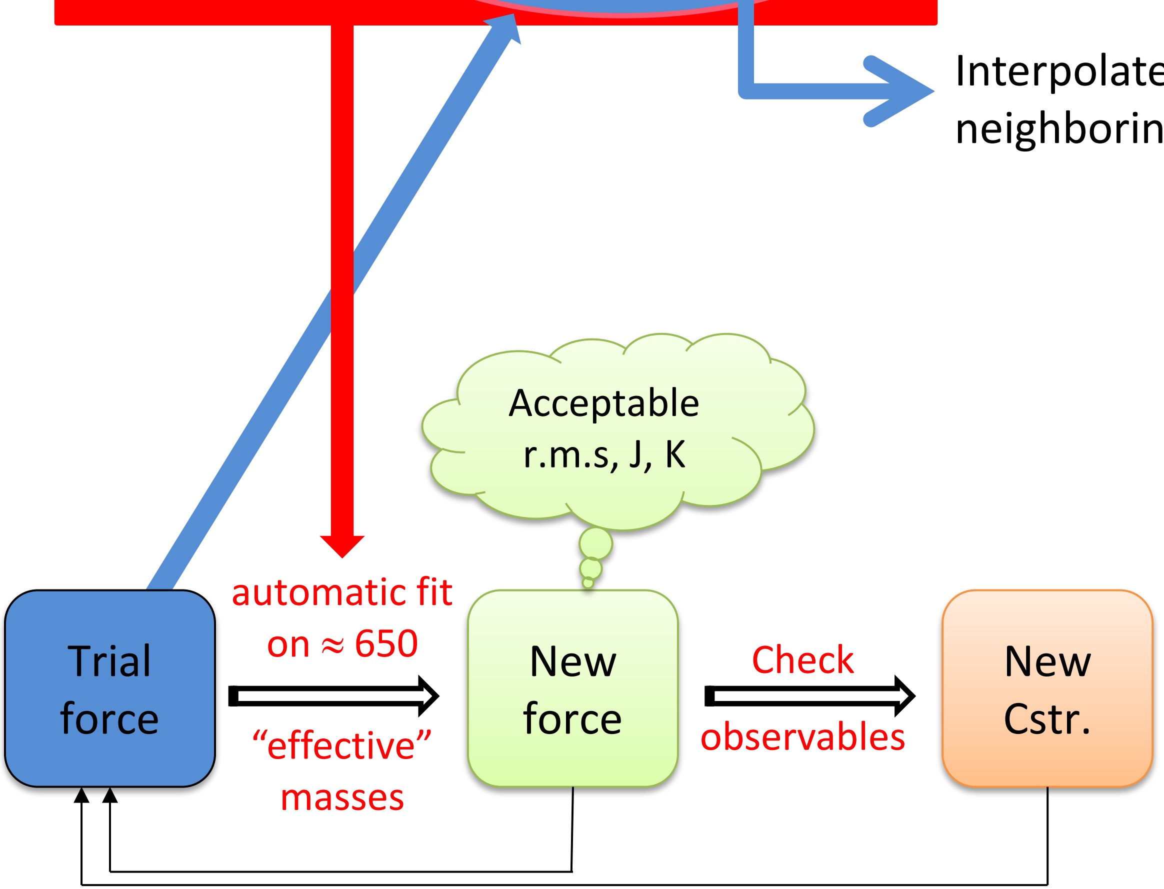

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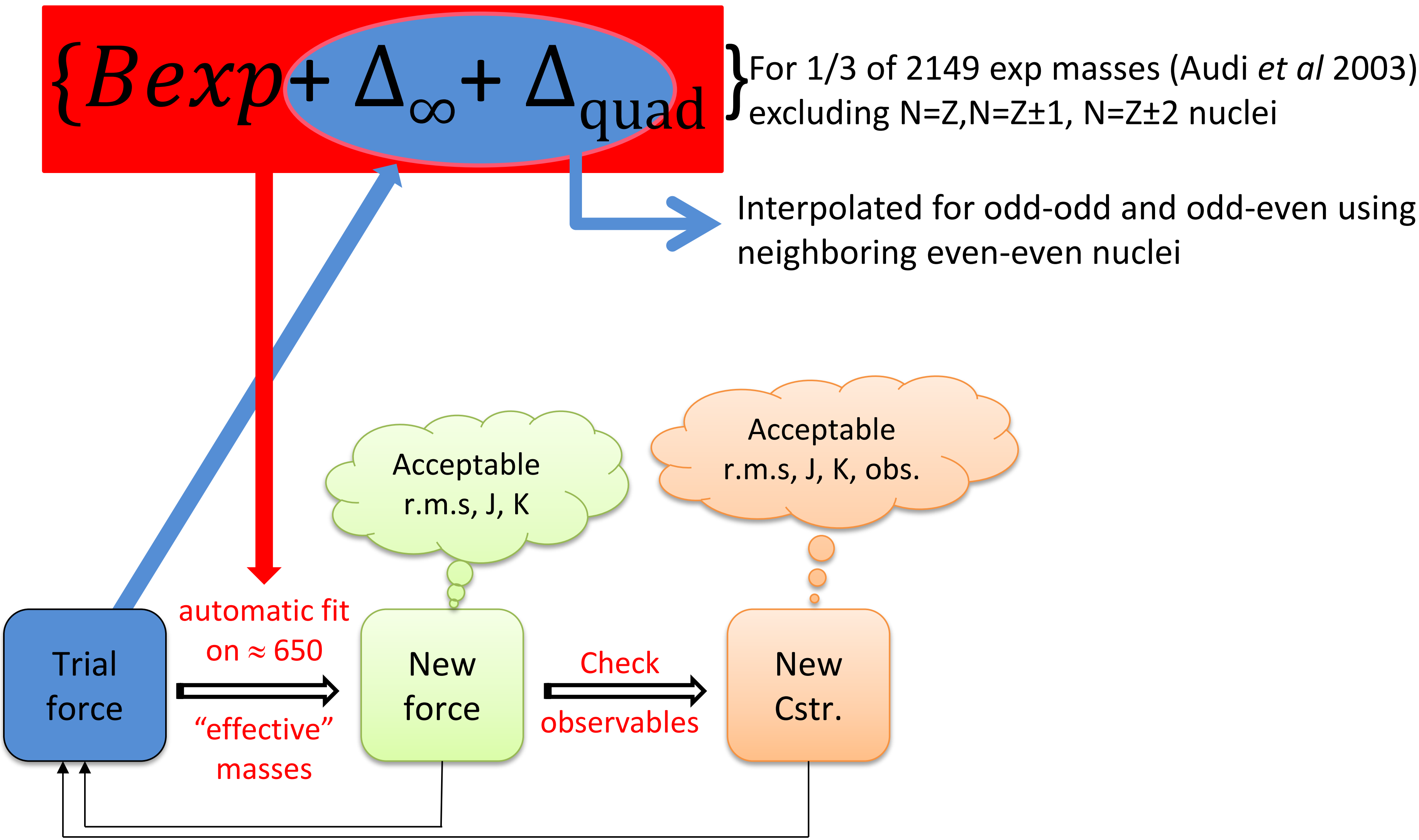


The new fitting procedure

$\{Bexp + \Delta_\infty + \Delta_{quad}\}$ For... exp...

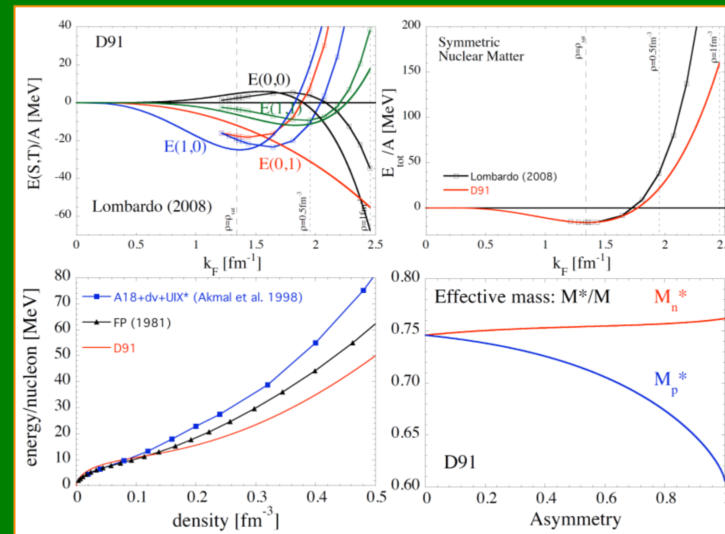
Inte... neig...

≈ 200/782 exp. charge radii
with dynamical correction
Play on k_F to adjust globally

Acc... r.m.s...

r.m.s, J, K

Nuclear Matter Properties



+

Landau Parameters (stability, sum rules, $G_0 \sim 0$; $G_0' \sim 0.9$-1 (Borzov et al. 1981))

Trial force

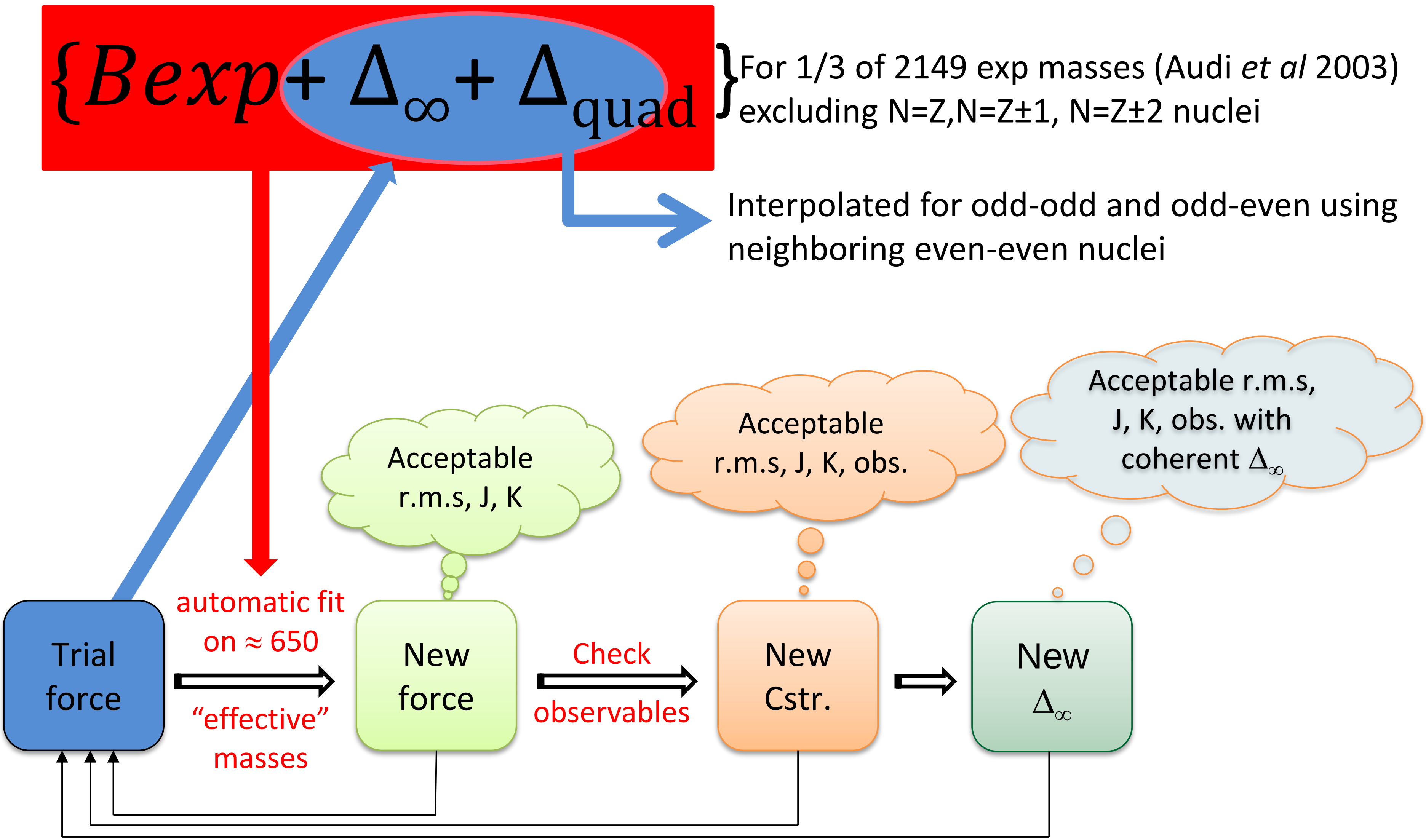
automatic fit on ≈ 650 "effective" masses

New force

Check observables

New Cstr.

The new fitting procedure



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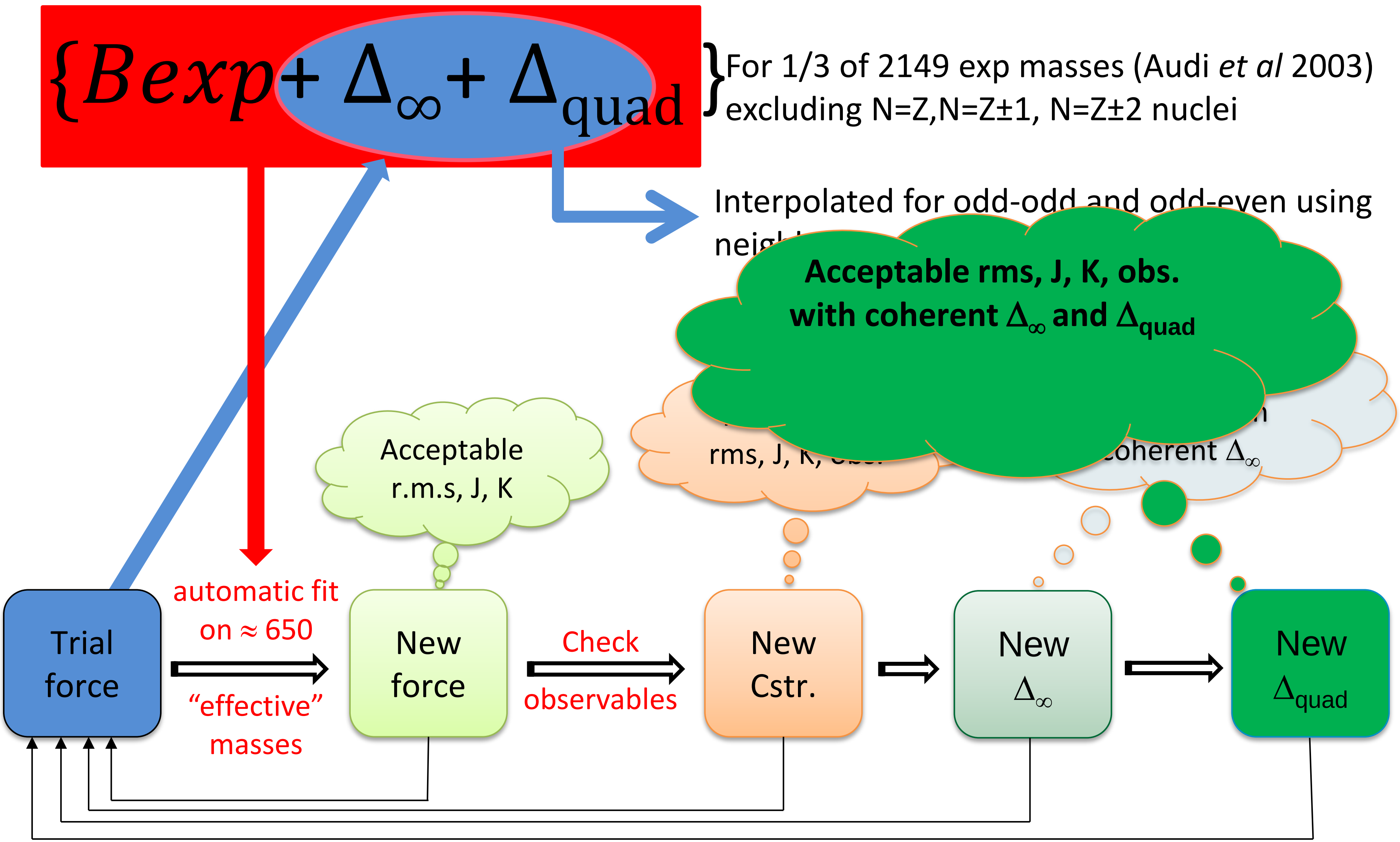
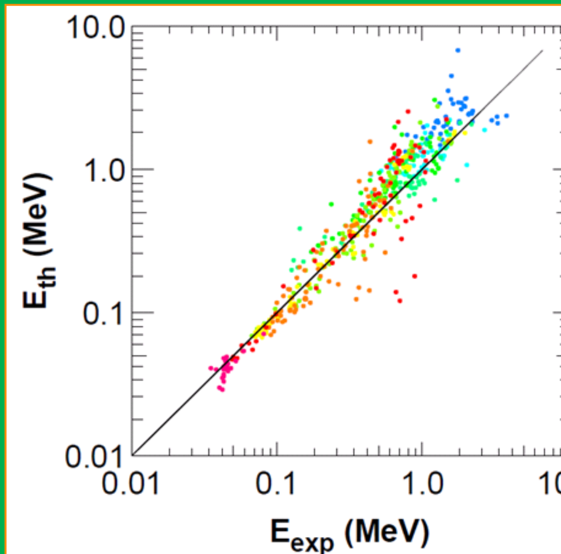


...ocedure

Energy of 2^+ levels



For 1/3 of 2149 exp masses (Audi *et al* 2003) excluding N=Z,N=Z±1, N=Z±2 nuclei

Interpolated for odd-odd and odd-even using neig...

Acceptable rms, J, K, obs. with coherent Δ_∞ and Δ_{quad}

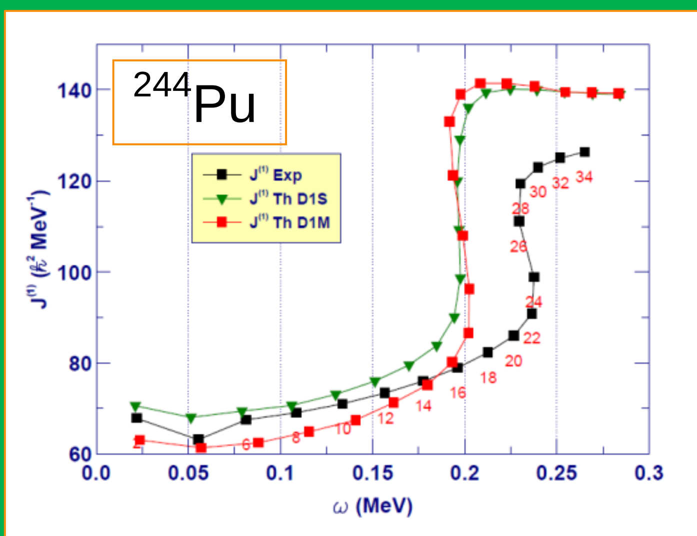
+

New observables

rms, ...

...coherent Δ_∞

Moment of inertia



New Cstr.

New Δ_∞

New Δ_{quad}

The new fitting procedure : time scales

$$\{B_{exp} + \Delta_\infty + \Delta_{quad}\}$$

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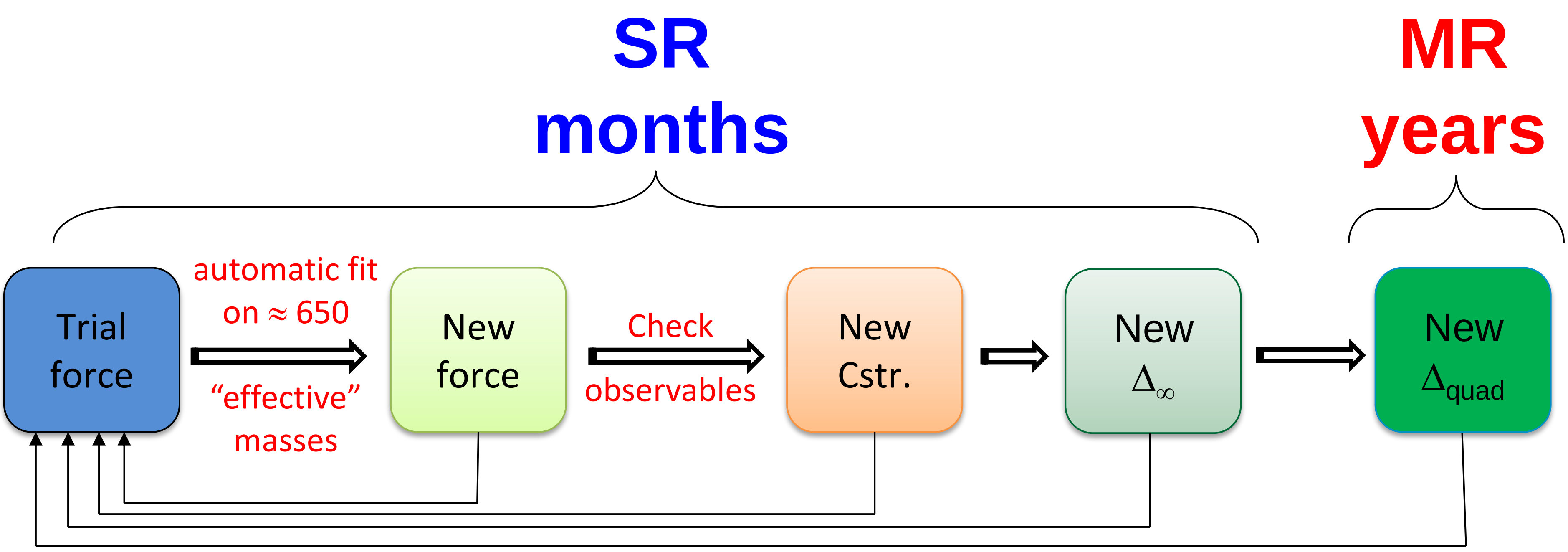
Interpolated for odd-odd and odd-even using neighboring even-even nuclei



Convergence issues : first steps on CCRT

r.m.s(F45)~1.36 MeV with E_{Quad}(D1N) but ~2.68 MeV with E_{Quad}(F45)

r.ms.(F60)~0.97 MeV with E_{Quad}(F45) but ~1.32 MeV with E_{Quad}(F60)

r.m.s(F78)~0.90 MeV with E_{Quad}(F60) but ~1.08 MeV with E_{Quad}(F78)

Convergence issues : first steps on CCRT

r.m.s(F45)~1.36 MeV with E_{Quad}(D1N) but ~2.68 MeV with E_{Quad}(F45)

r.ms.(F60)~0.97 MeV with E_{Quad}(F45) but ~1.32 MeV with E_{Quad}(F60)

r.m.s(F78)~0.90 MeV with E_{Quad}(F60) but ~1.08 MeV with E_{Quad}(F78)

SLOW CONVERGENCE (1 year)

COHERENCE DEGRADING r.m.s

Convergence issues : next steps on TERA

CCRT : 4 Interactions in 1 year

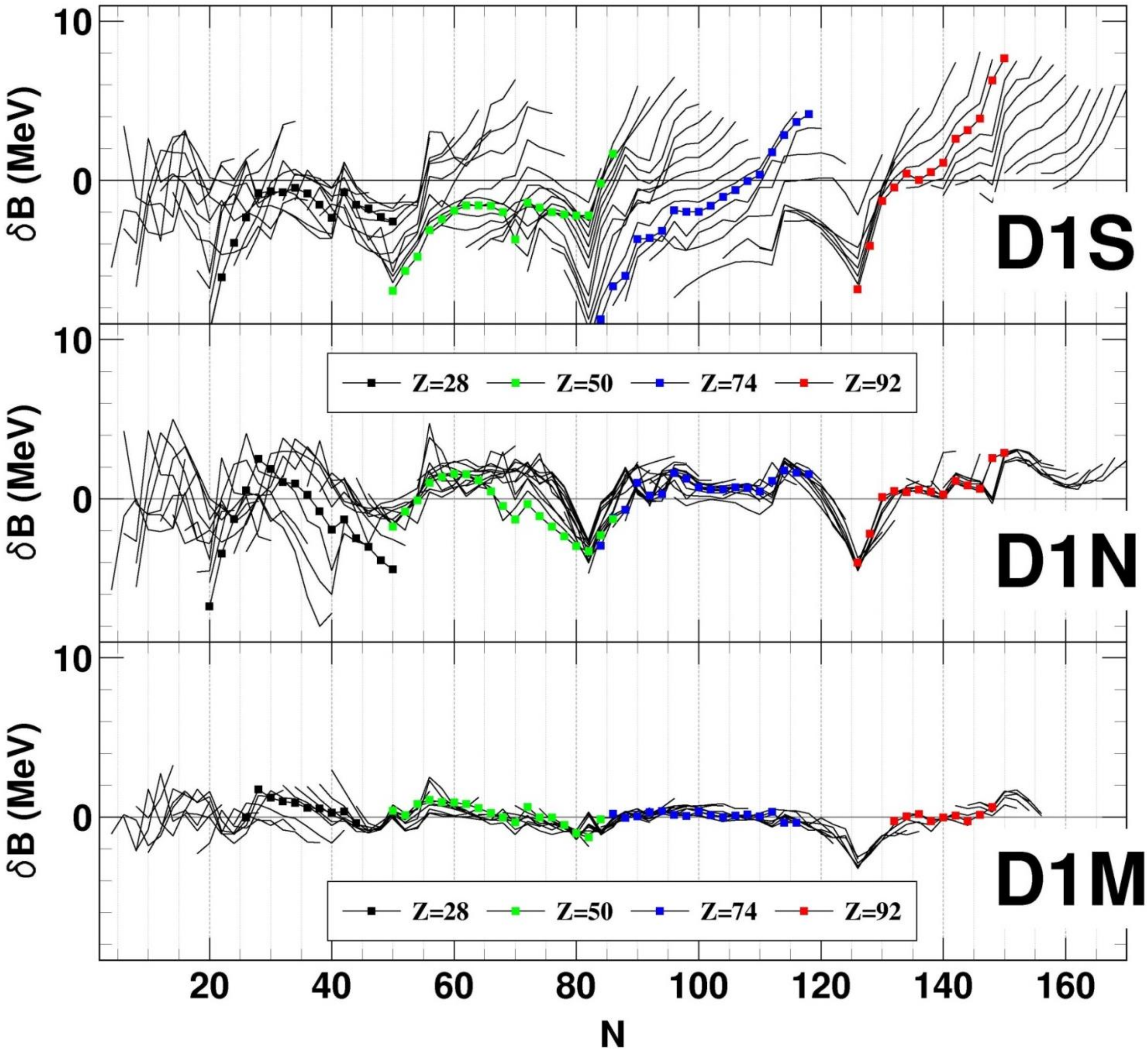
TERA : 15 Interactions in 3 months

	r.m.s masses	r.m.s radii
D08	1.027 MeV	0.0302 fm
D19	1.026 MeV	0.0328 fm
D23	0.857 MeV	0.0302 fm
D28	0.990 MeV	0.0377 fm
D32	0.846 MeV	0.0378 fm
D36	0.954 MeV	0.0385 fm
D38	0.939 MeV	0.0358 fm
D39	0.909 MeV	0.0377 fm
D44	0.853 MeV	0.0312 fm
D45	1.364 MeV	0.0295 fm
D52	0.813 MeV	0.0308 fm
D59	0.893 MeV	0.0304 fm

	r.m.s masses	r.m.s radii
F45	1.365 MeV	0.0295 fm
F60	1.376 MeV	0.0299 fm
F78	1.049 MeV	0.0321 fm
F87	1.360 MeV	0.0299 fm
F91	1.262 MeV	0.0386 fm
F101	1.319 MeV	0.0320 fm

RESULTS

Major goal reached : first Gogny mass model !

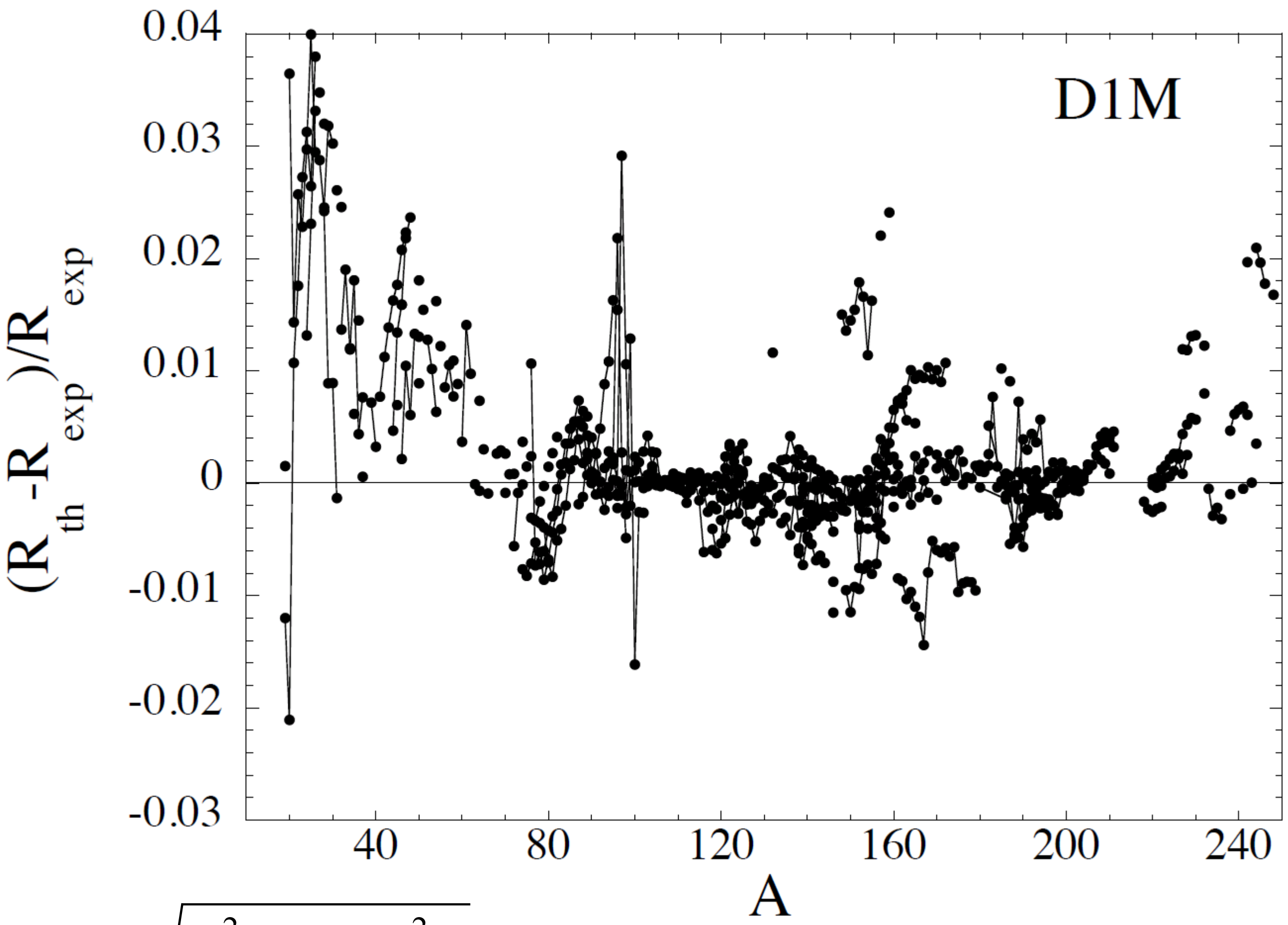


r.m.s ~ 3 MeV

r.m.s ~ 1 MeV

r.m.s = 0.798 MeV

Comparison with 707 Exp. Charge Radii



r.m.s = 0.031 fm

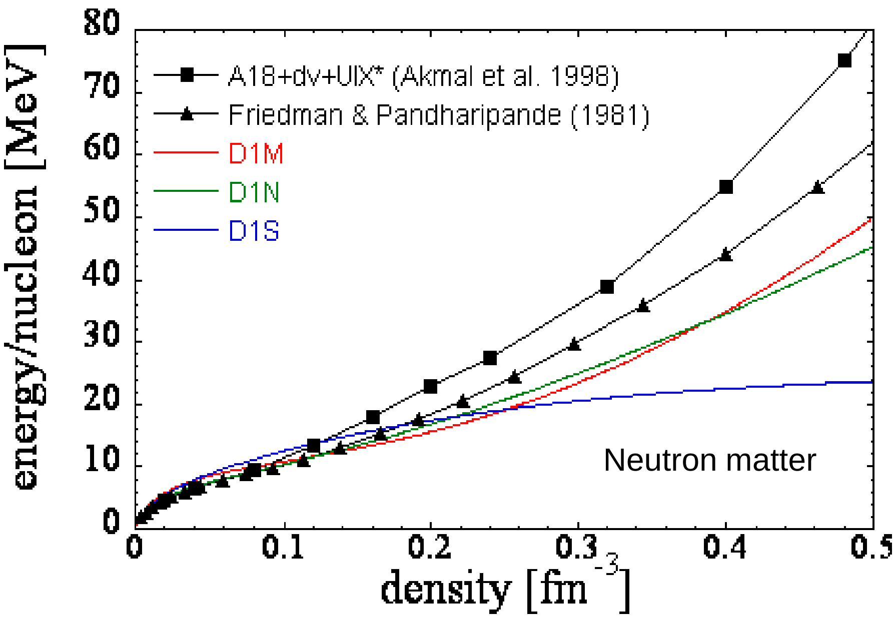
$$R_{ch} = \sqrt{R_{HFB}^2 + \Delta R_{corr}^2}$$

$$\Delta R_{corr} = \sqrt{R_{dyn}^2 - R_{HFB}^2}$$

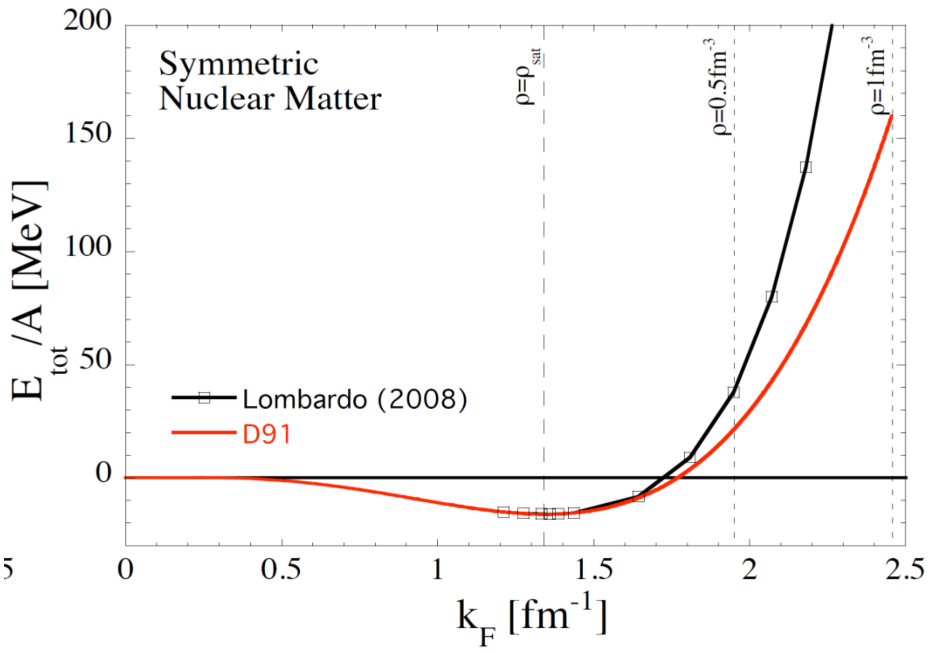
NUCLEAR MATTER EOS

k_F=1.346 fm^{-1} J=28.6 MeV m^*/m=0.746 K_{inf}=225 MeV

Neutron matter EOS

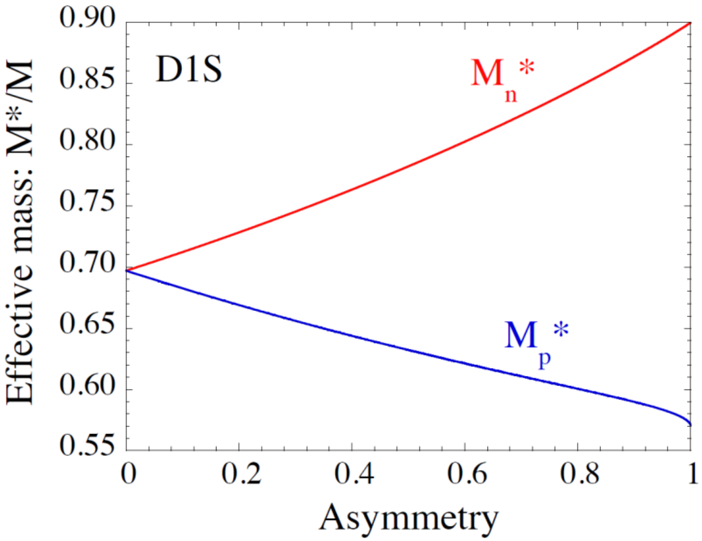


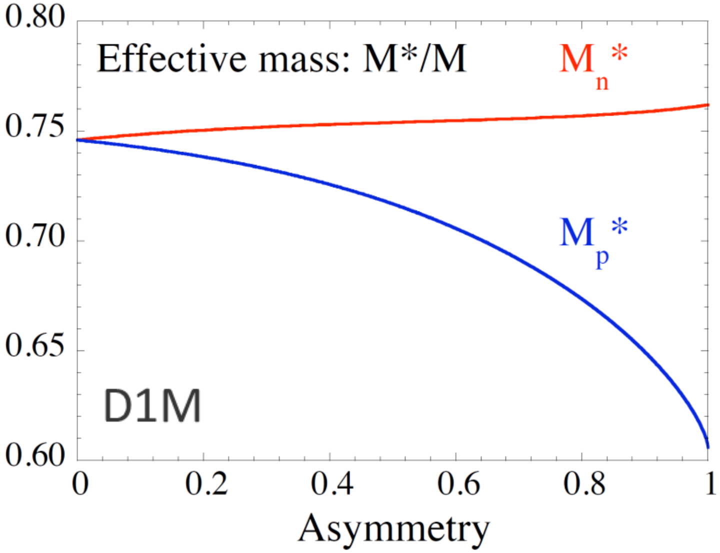
Symmetric nuclear matter EOS

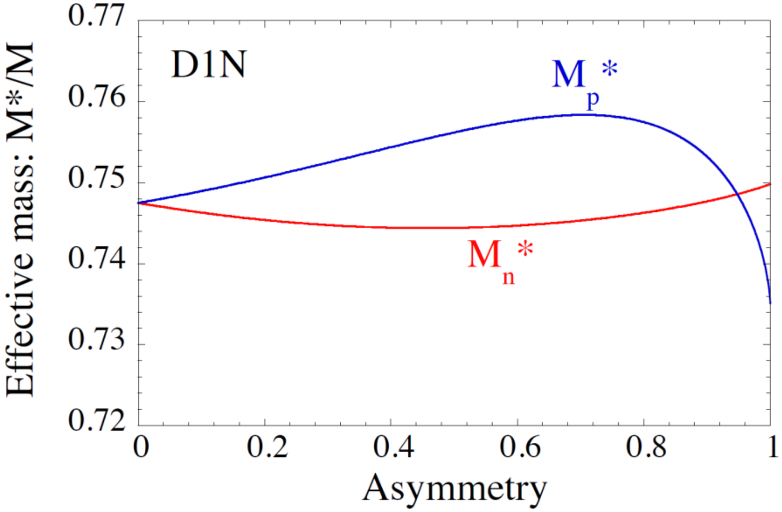


NUCLEAR MATTER : effective masses

k_F=1.346 fm^{-1} J=28.6 MeV m^*/m=0.746 K_{inf} =225 MeV

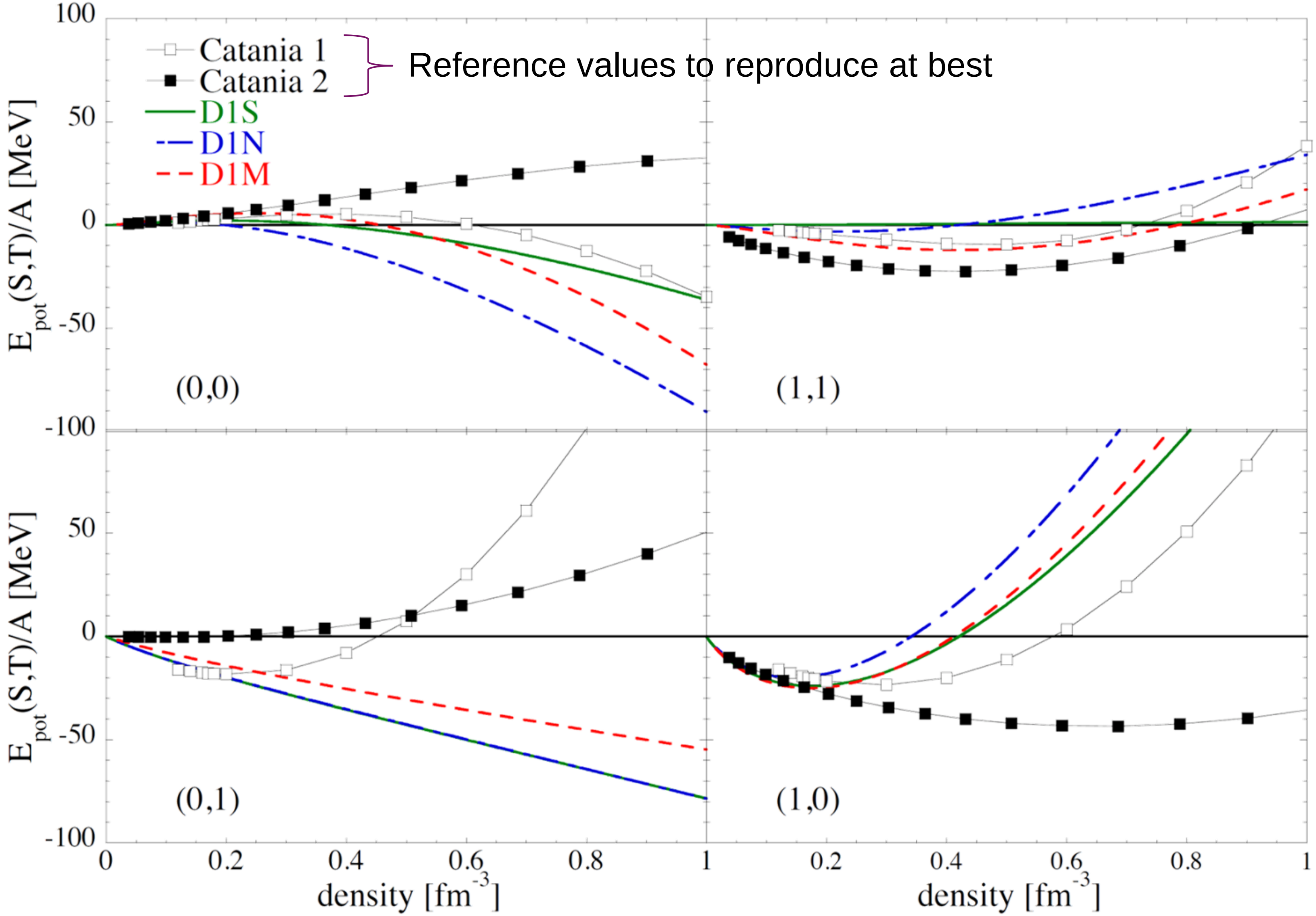




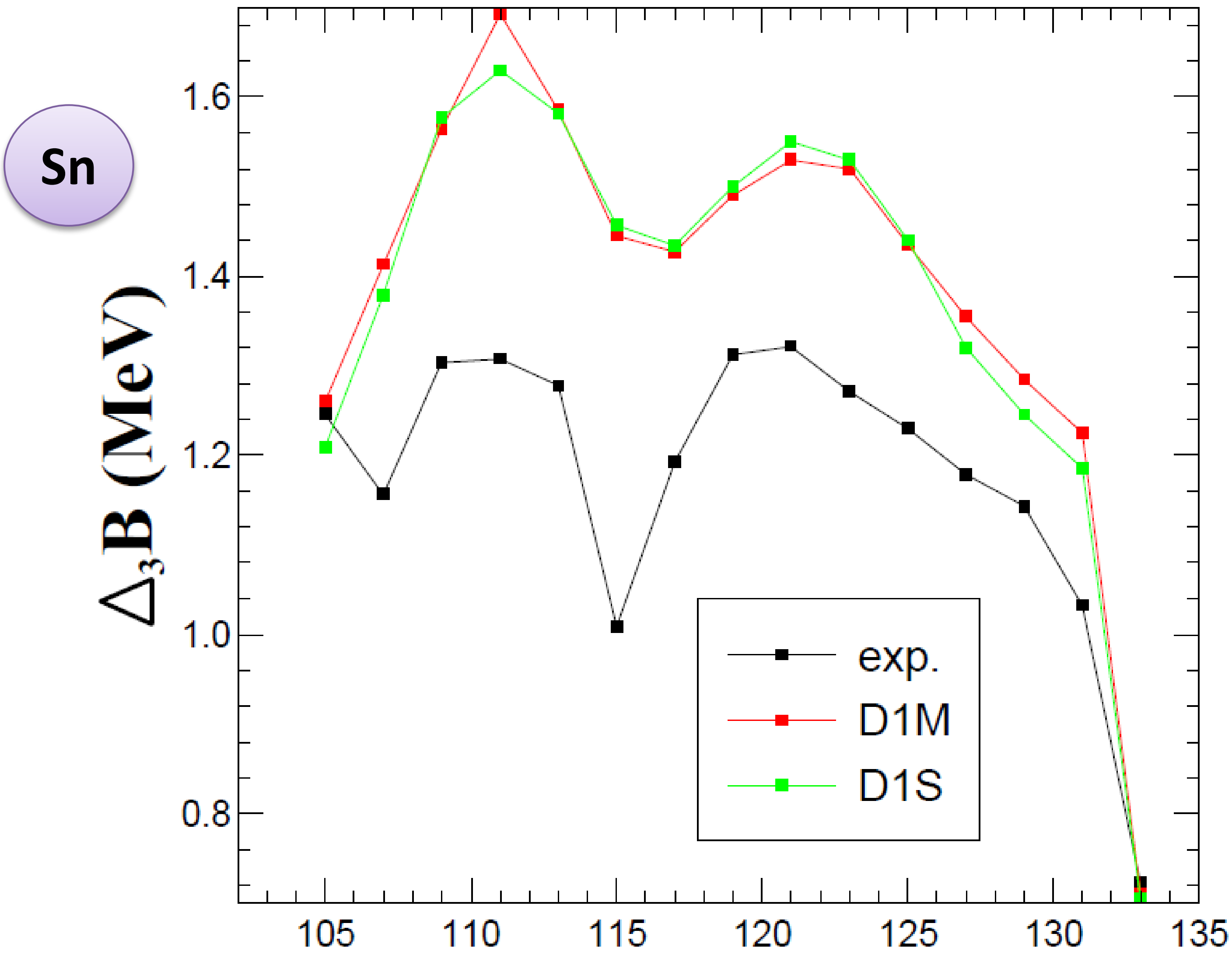


NUCLEAR MATTER EOS in the 4 (S,T) channels

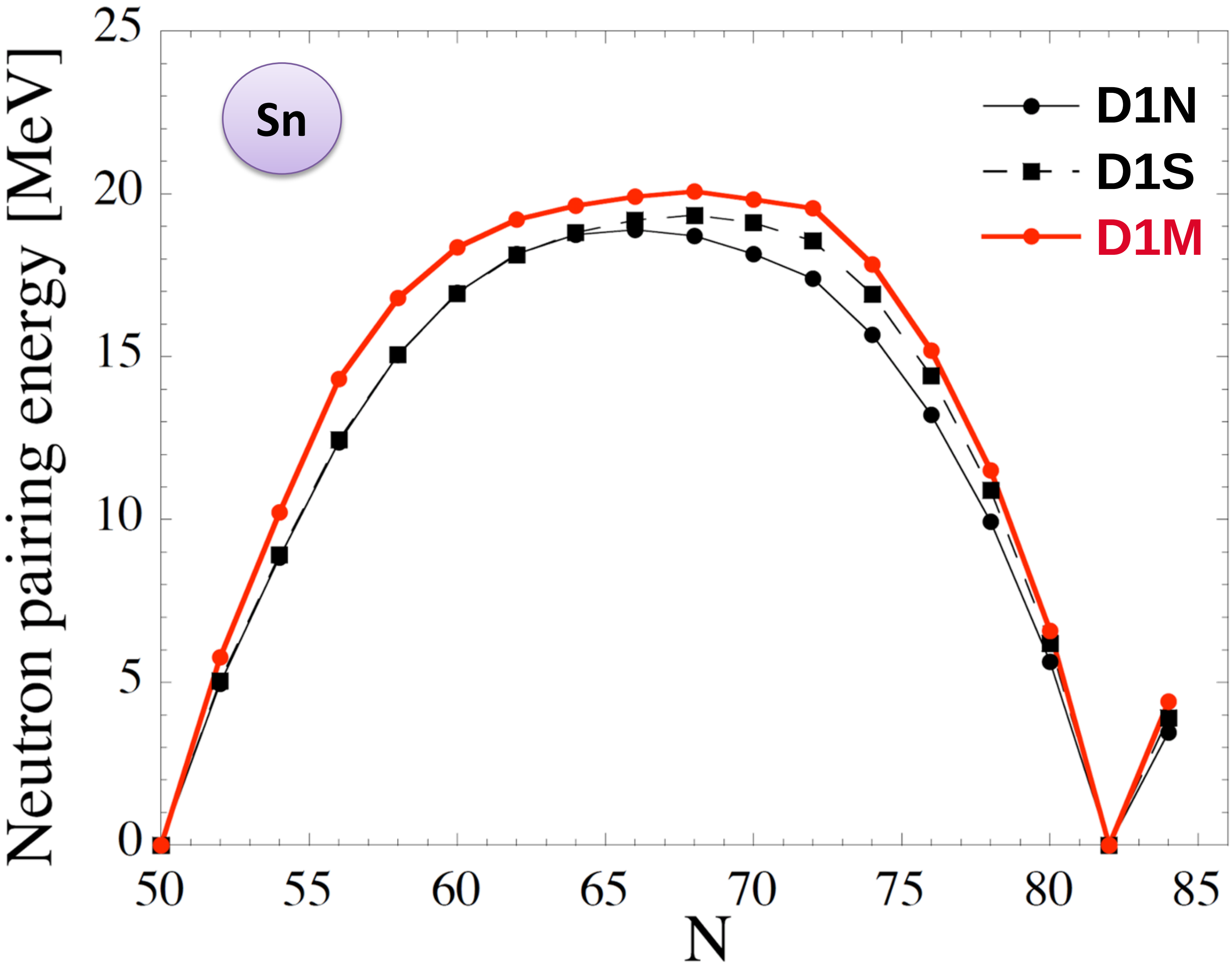
k_F=1.346 fm^{-1} J=28.6 MeV m^*/m=0.746 K_{inf}=225 MeV



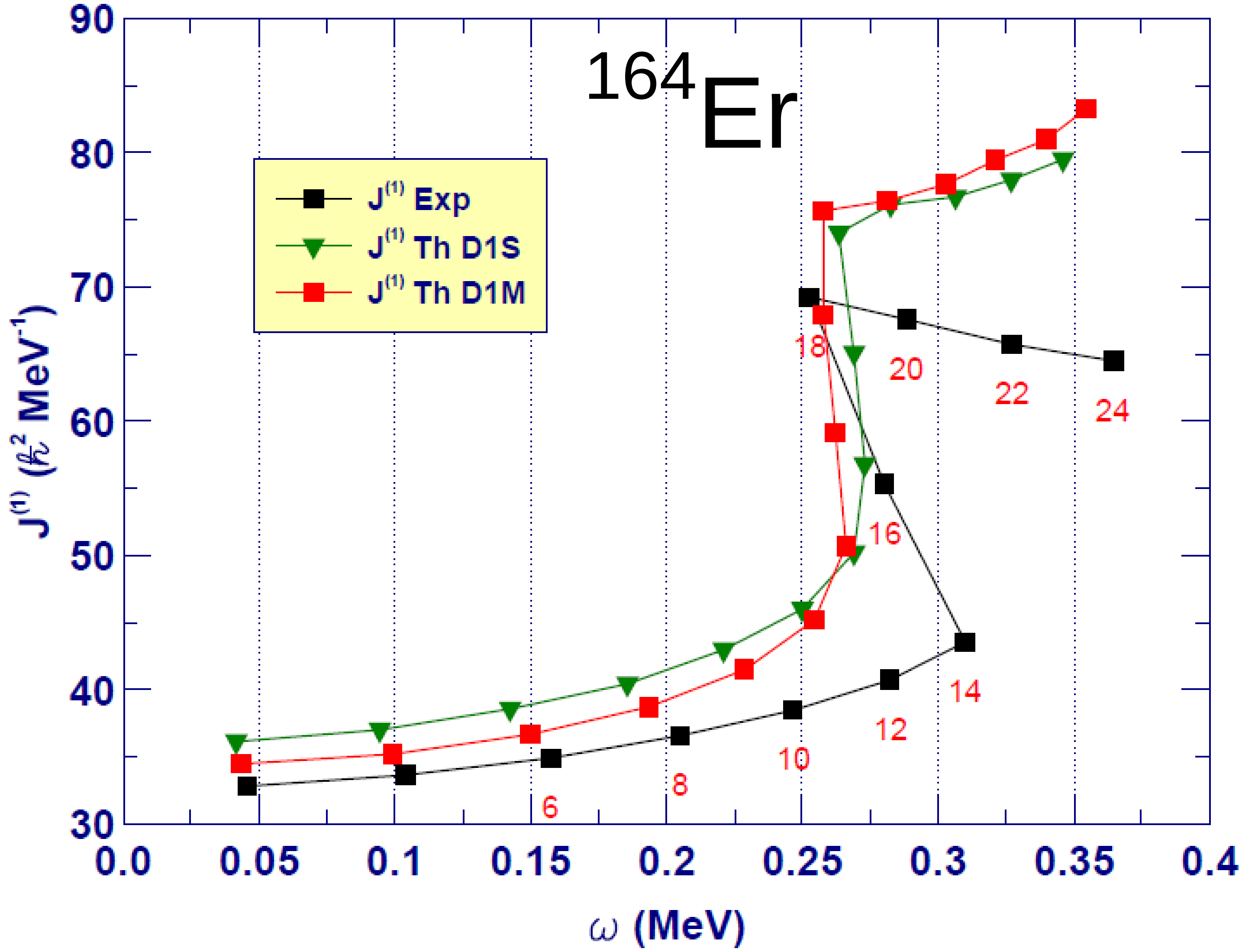
PAIRING


Sn
$\Delta_3 B$ (MeV)
1.6
1.4
1.2
1.0
0.8
105
110
115
120
125
130
135
exp.
D1M
D1S

PAIRING

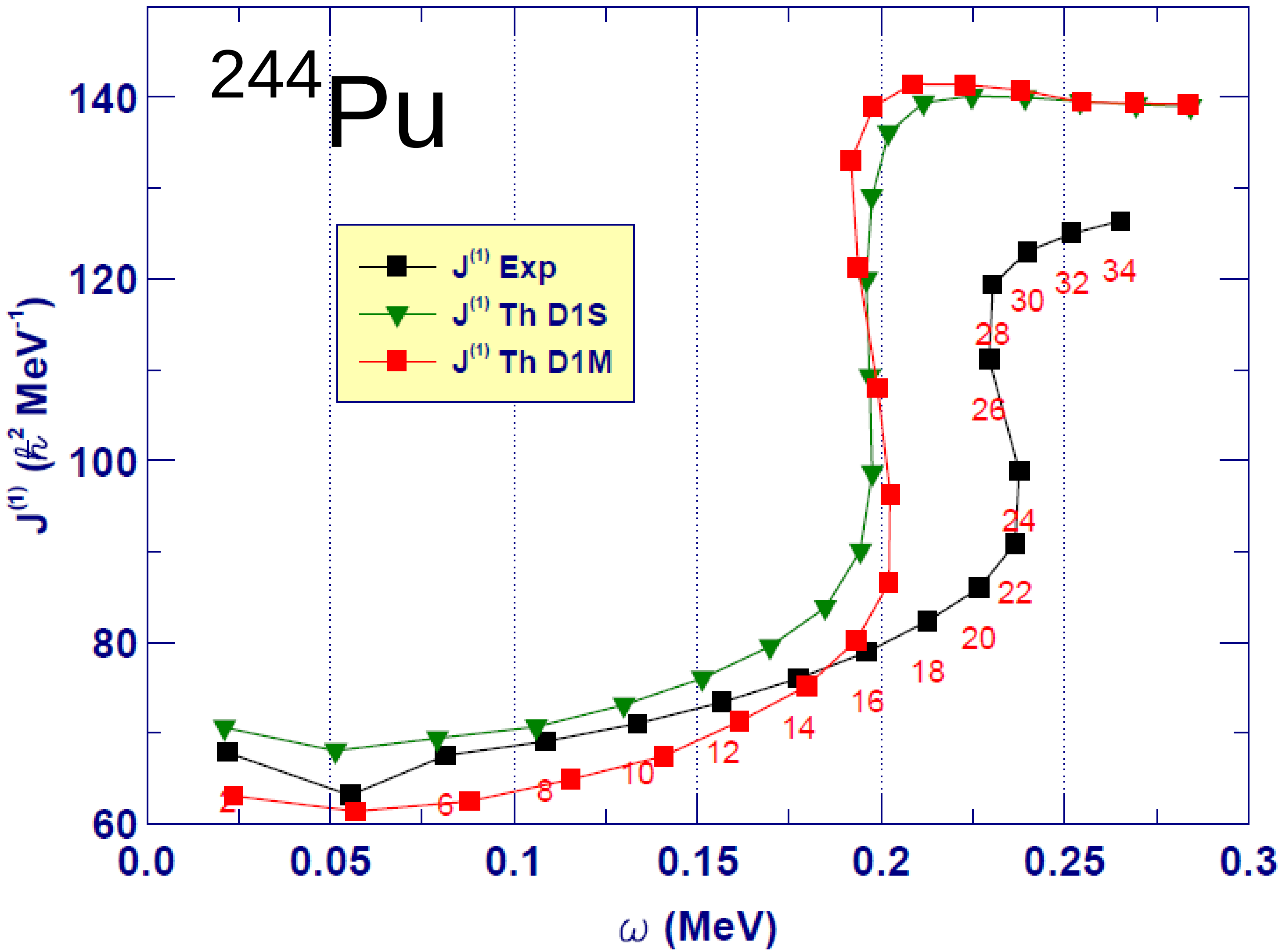

Sn
D1N
D1S
D1M
Neutron pairing energy [MeV]
N
0
5
10
15
20
25
50
55
60
65
70
75
80
85

PAIRING



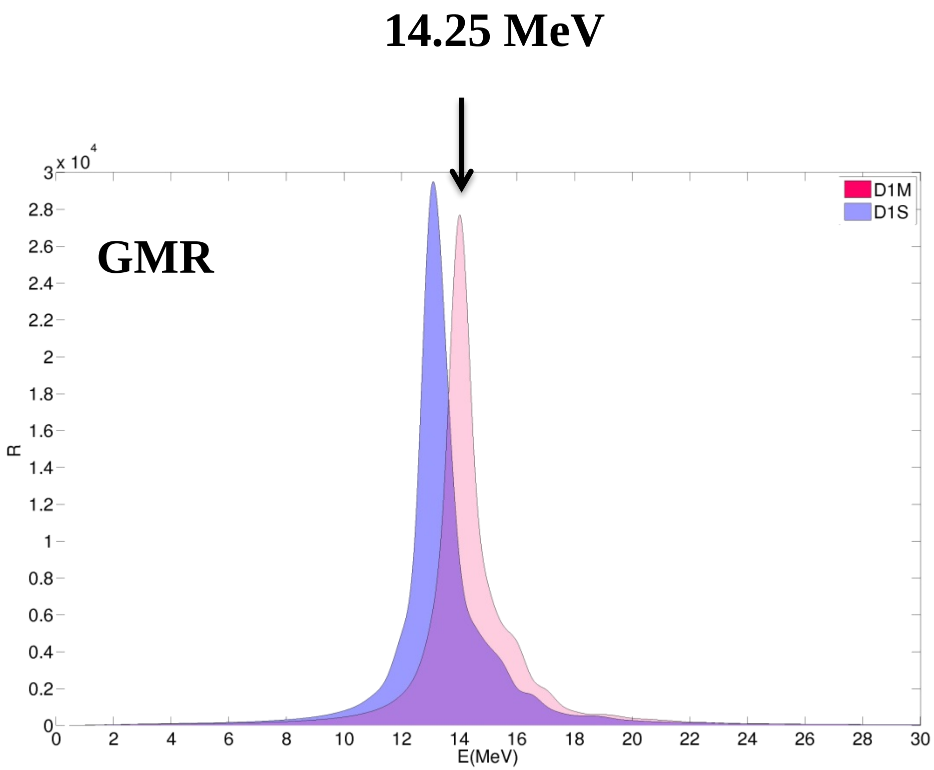
164Er
J(1) Exp
J(1) Th D1S
J(1) Th D1M
J(1) (ℏ2 MeV-1)
ω (MeV)
90
80
70
60
50
40
30
0.0
0.05
0.1
0.15
0.2
0.25
0.3
0.35
0.4
6
8
10
12
14
16
18
20
22
24

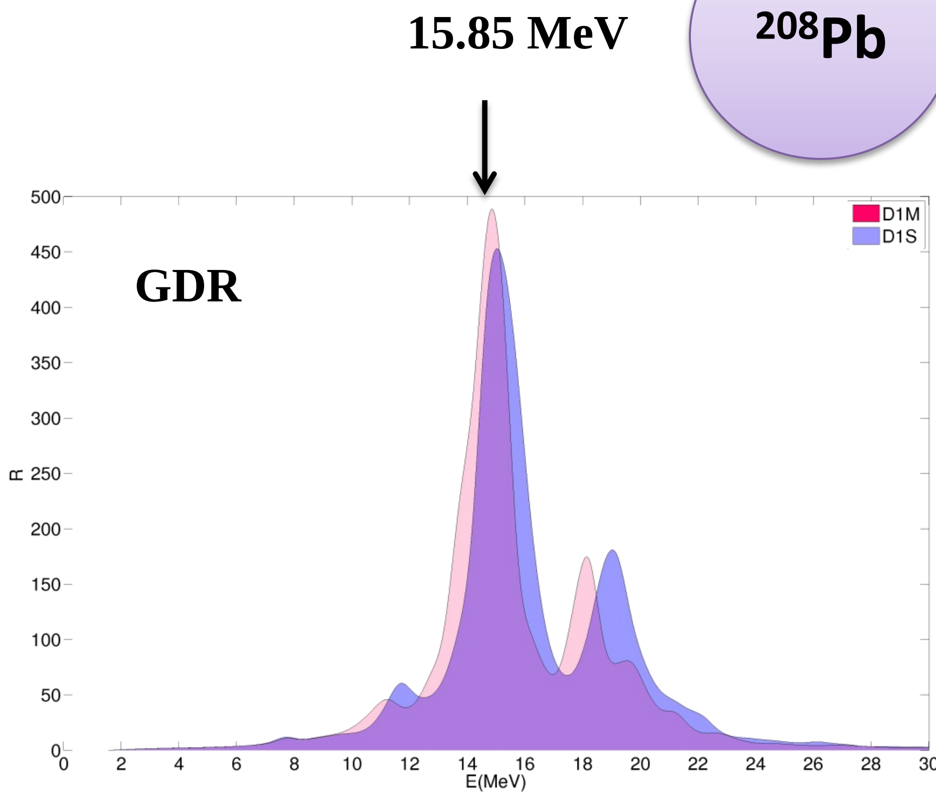
PAIRING



^{244}Pu
$J^{(1)}$ Exp
$J^{(1)}$ Th D1S
$J^{(1)}$ Th D1M
$J^{(1)}$ ($\hbar^2$ MeV^{-1})
ω (MeV)
60
80
100
120
140
0.0
0.05
0.1
0.15
0.2
0.25
0.3
2
6
8
10
12
14
16
18
20
22
24
26
28
30
32
34

GIANT RESONANCES



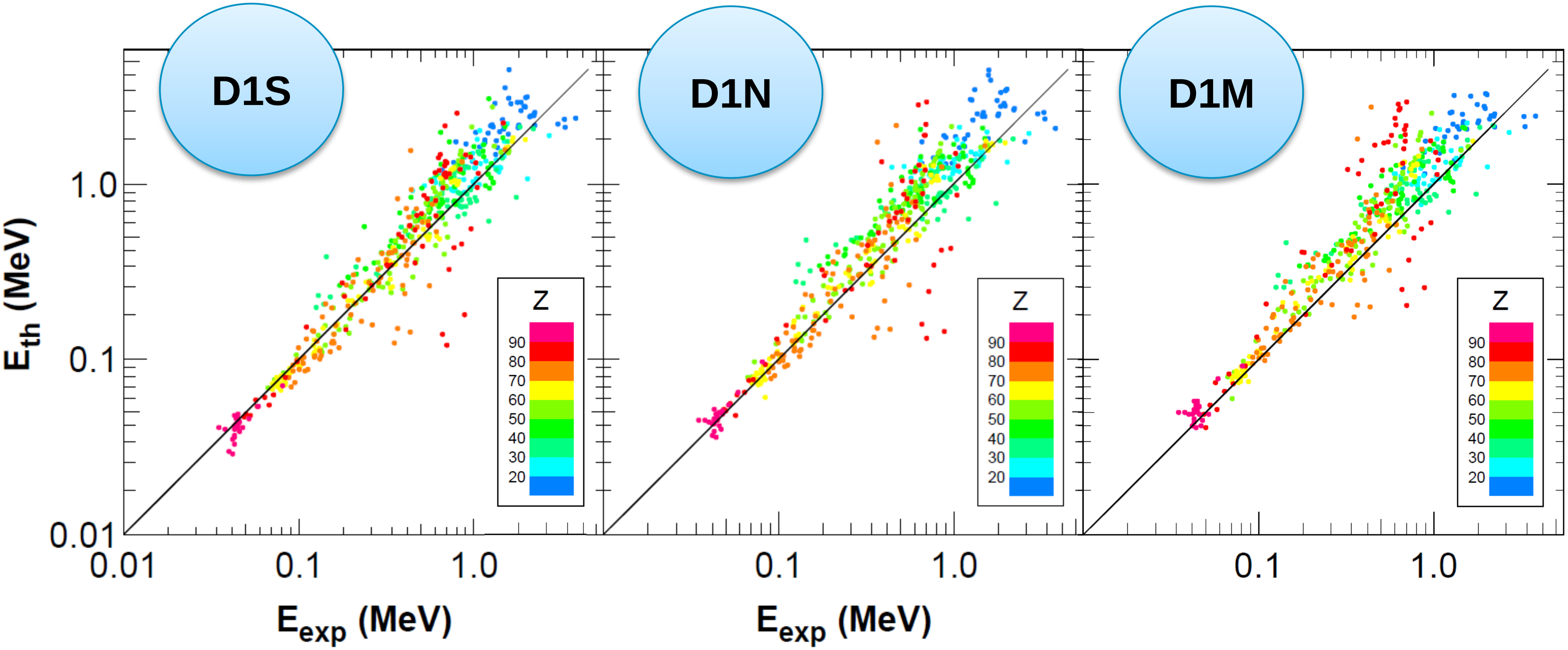


E_{exp} = 14.17 MeV D. H. Youngblood et al., Phys. Rev. Lett. 82, 691 (1999).

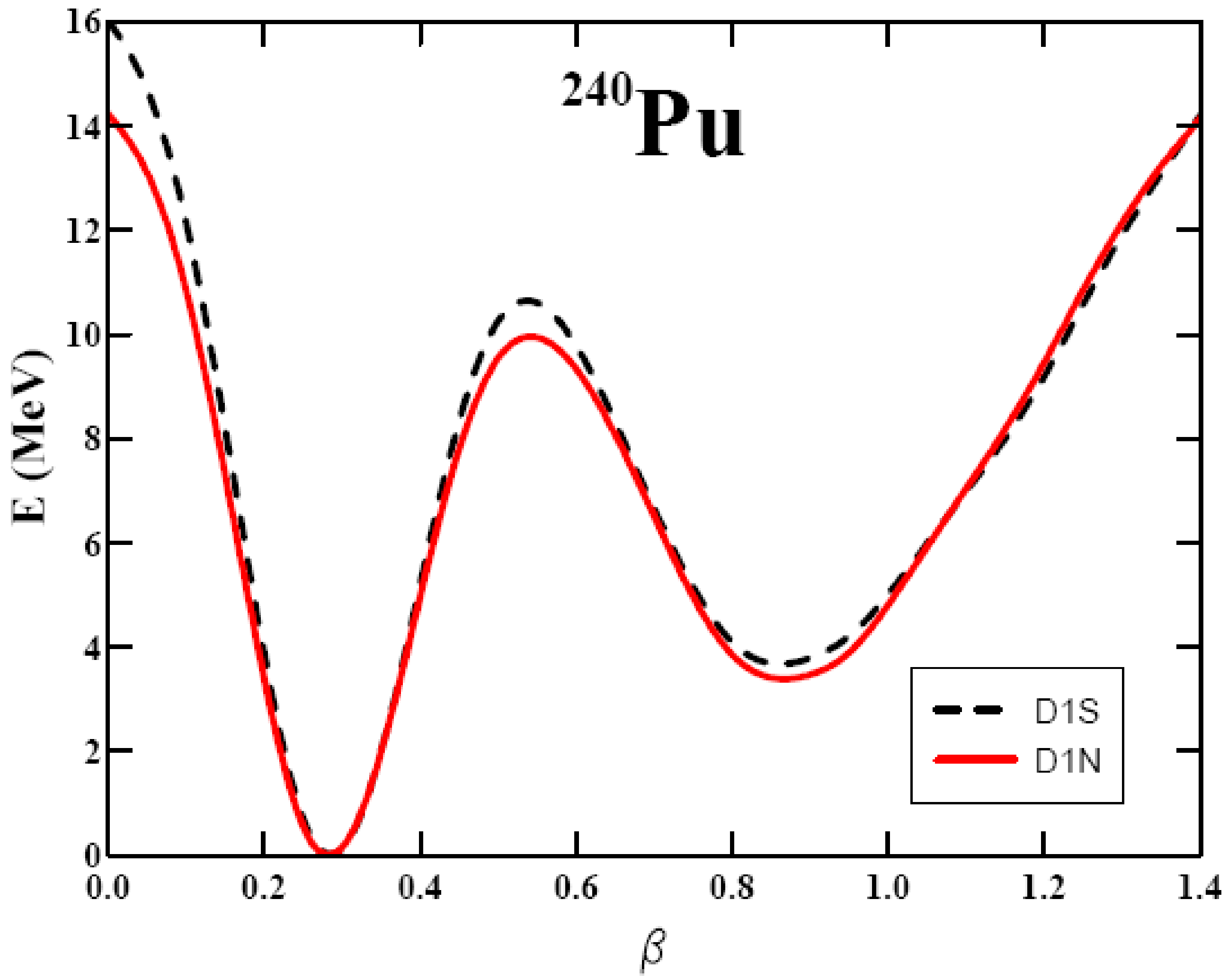
E_{exp} = 13.43 MeV B. L. Berman and S. C. Fultz, Rev. Mod. Phys. 47, 713 (1975).

SPECTROSCOPY

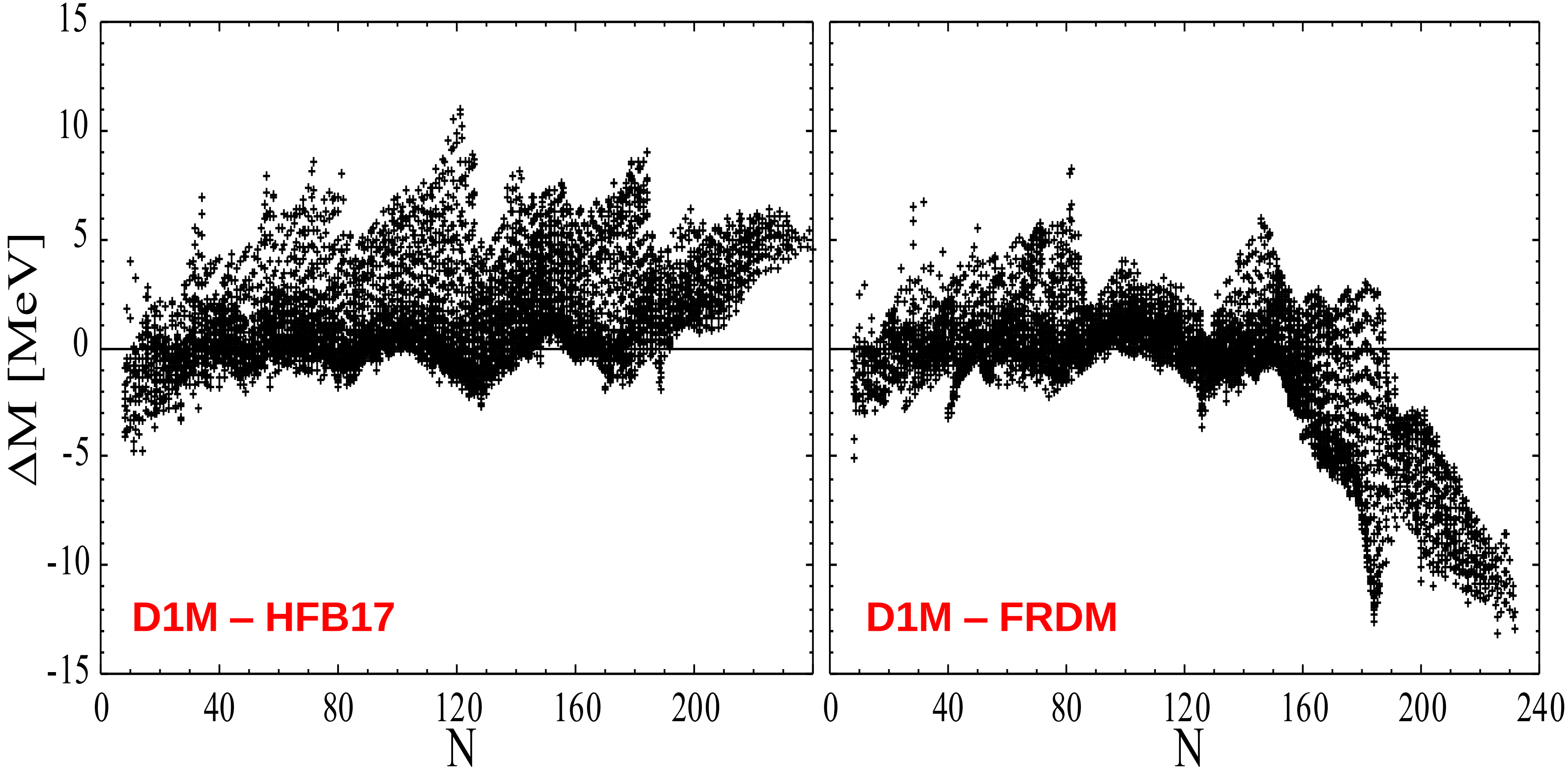
Excitation energies of the first 2^+ for 519 e-e nuclei



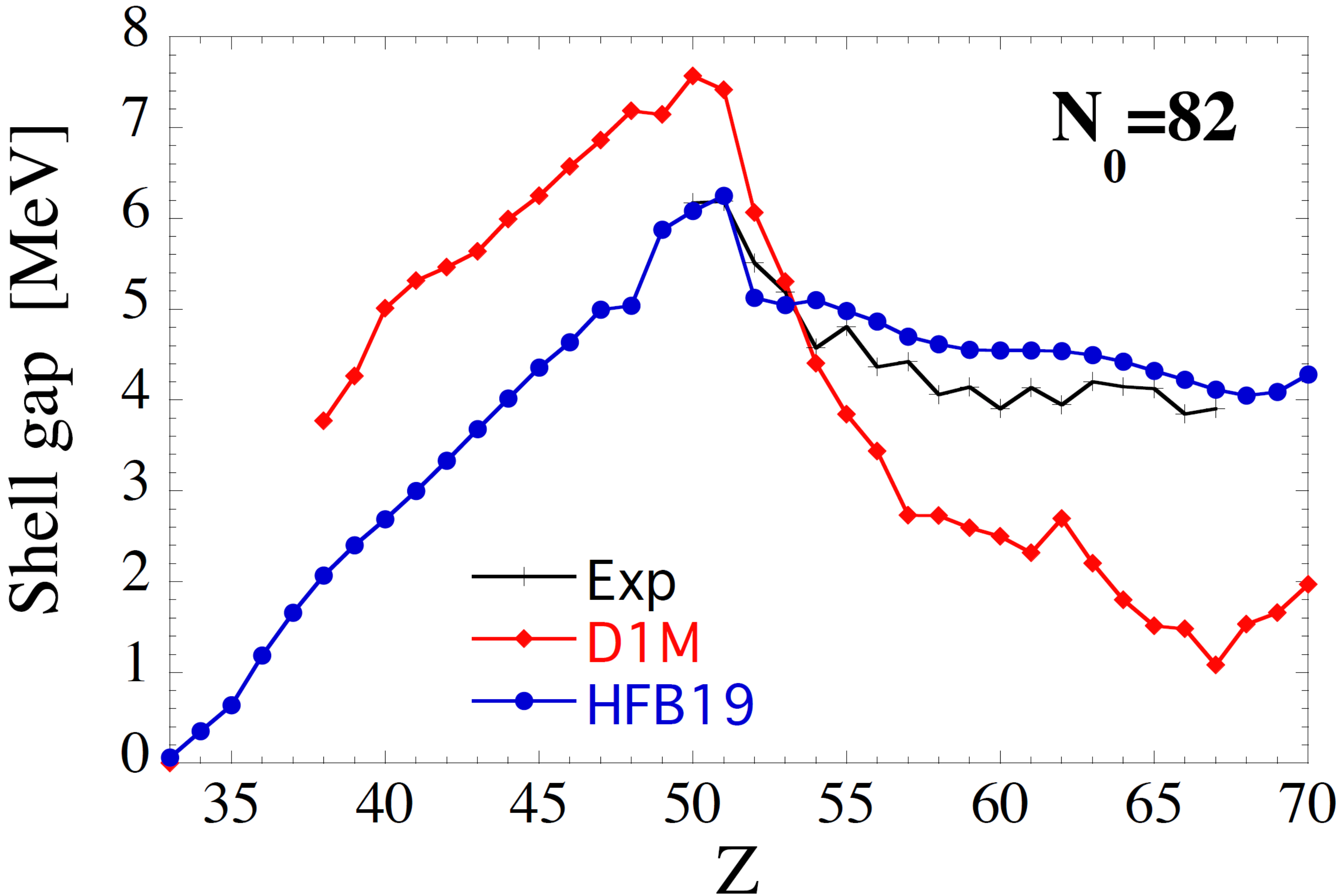
FISSION BARRIERS



COMPARISON WITH OTHER MASS FORMULAE

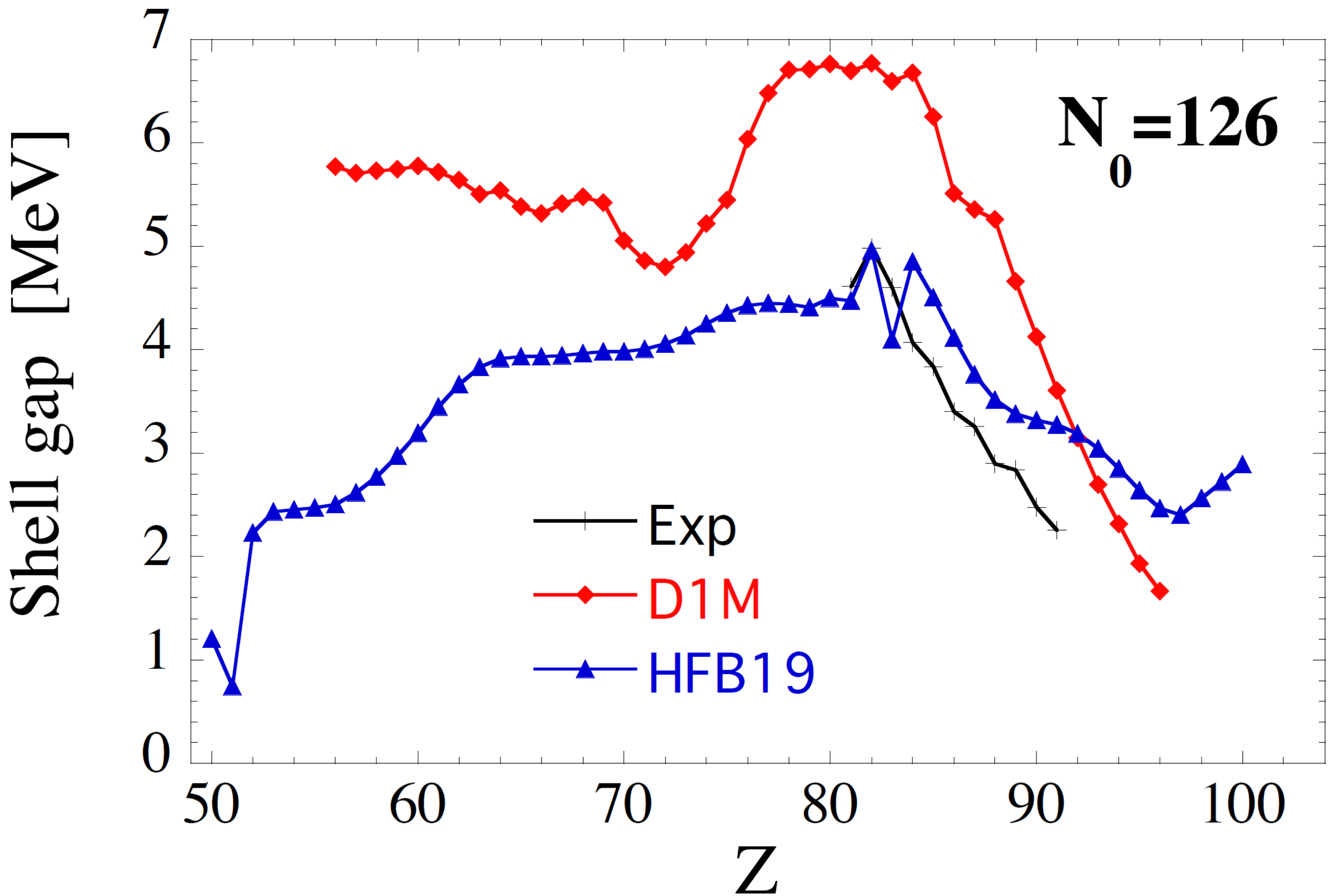


SHELL GAPS

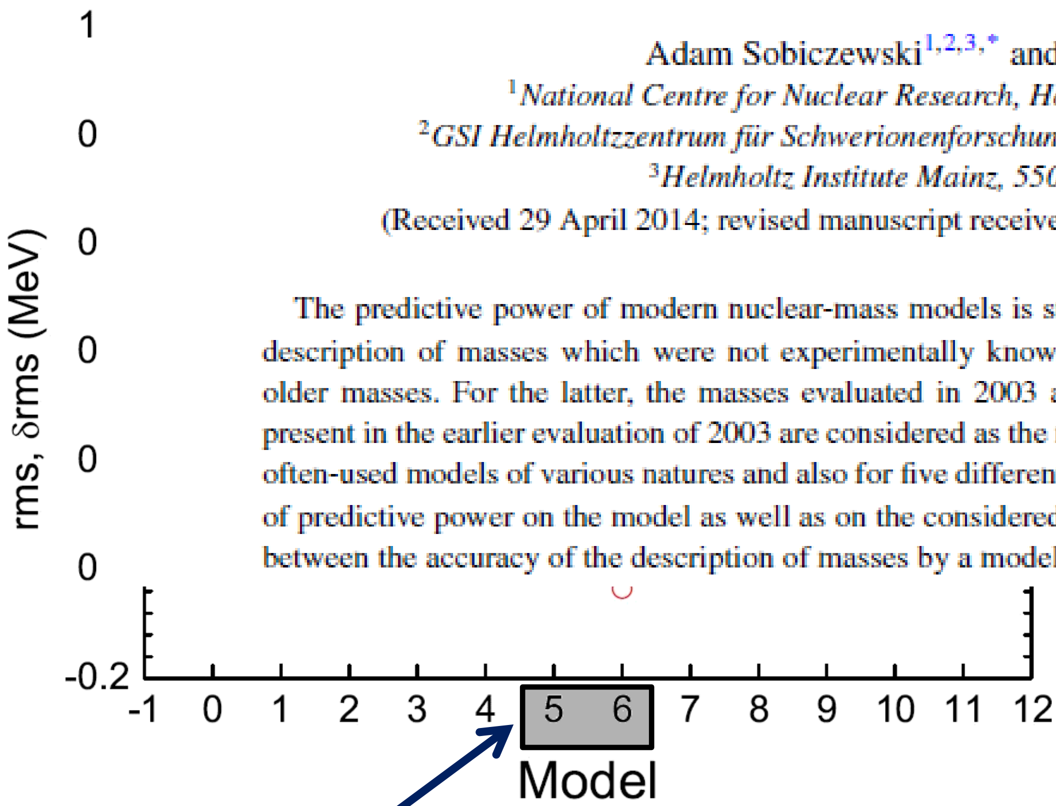


Shell gap [MeV]
Z
N_0=82
Exp
D1M
HFB19
0
1
2
3
4
5
6
7
8
35
40
45
50
55
60
65
70

SHELL GAPS



PREDICTIVE POWER ?



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Predictive power of nuclear-mass models

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[1] *National Centre for Nuclear Research, Hoża 69, 00-681 Warsaw, Poland*

[2] *GSI Helmholtzzentrum für Schwerionenforschung GmbH, 64291 Darmstadt, Germany*

[3] *Helmholtz Institute Mainz, 55099 Mainz, Germany*

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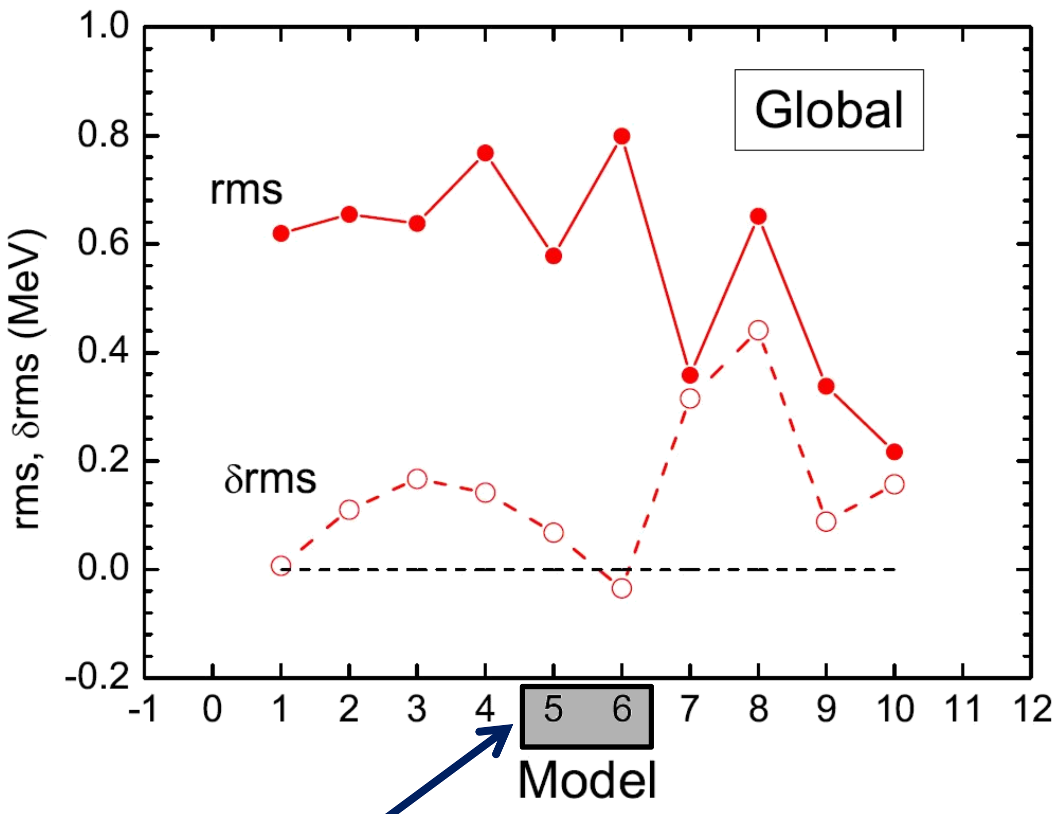
The predictive power of modern nuclear-mass models is studied. To quantify this property, we compare the description of masses which were not experimentally known at the time of the model adjustment to that of older masses. For the latter, the masses evaluated in 2003 are taken. The masses evaluated in 2012 and not present in the earlier evaluation of 2003 are considered as the new ones. The predictive power is analyzed for ten often-used models of various natures and also for five different regions in the nuclear chart. A strong dependence of predictive power on the model as well as on the considered region of nuclei is observed. No clear correlation between the accuracy of the description of masses by a model and its predictive power is found.

Microscopic models

PREDICTIVE POWER ?

Comparison between several mass models adjusted with 2003 exp and tested with 2012 exp masses



Current status

- **rms < 1 MeV (masses ≈ GeV)**
- **micro ~ macro**
- **micro more predictive**

Microscopic models

PERSPECTIVES

FURTHER IMPROVEMENTS

3 axes

D1 type with less approximations (exact Coulomb exchange and pairing)

New analytical form D2 (F. Chappert thesis + accepted in PRC)

Finite range everywhere DG (no code yet)

⇓

JPE and SP under pressure !

HFB3 under development !
D2N available ?
DG to do !

FURTHER IMPROVEMENTS

3 axes

D1 type with less approximations (exact Coulomb exchange and pairing)

New analytical form D2 (F. Chappert thesis + accepted in PRC)

Finite range everywhere DG (no code yet)

+ Sensitivity analysis v.s number of major shells

- **N basis = N(N-1) Δ_∞ values $\Rightarrow$ mean r.m.s and dispersion**
- **Δ_{quad} also sensitive to basis size**
- **Beyond 5DCH ?**
- **Same with RMF ?**

FURTHER IMPROVEMENTS

3 axes

D1 type with less approximations (exact Coulomb exchange and pairing)

New analytical form D2 (F. Chappert thesis + accepted in PRC)

Finite range everywhere DG (no code yet)

FURTHER IMPROVEMENTS

3 axes

D1 type with less approximations (exact Coulomb exchange and pairing)

New analytical form D2 (F. Chappert thesis + accepted in PRC)

Finite range everywhere DG (no code yet)

The 11th commandment :

ONE SHALL ONLY DESIGN EFFECTIVE INTERACTIONS

- *for both mean field and beyond mean field predictions*
- *for all nuclei*
- *for all nuclear properties*