Mean-field and Beyond for heavy nuclei Present and Future

- Mean-field methods: codes
- Good reasons to go beyond mean-field
- How to do it Applications

Our group:

The precursors: P. Bonche, H. Flocard,
M. Weiss, J. Dobaczewski

The successors: M. Bender , T. Duguet

Many collaborators: G. Bertsch, S. Cwiok, W. Nazarewicz,
J. Skalski, P. Magierski…

Recent Ph D and Post Doc collabotators
V. Hellemans, W. Ryssen, B. Avez, B. Bally, K. Washiama,
J. Yao, S. Baroni, …

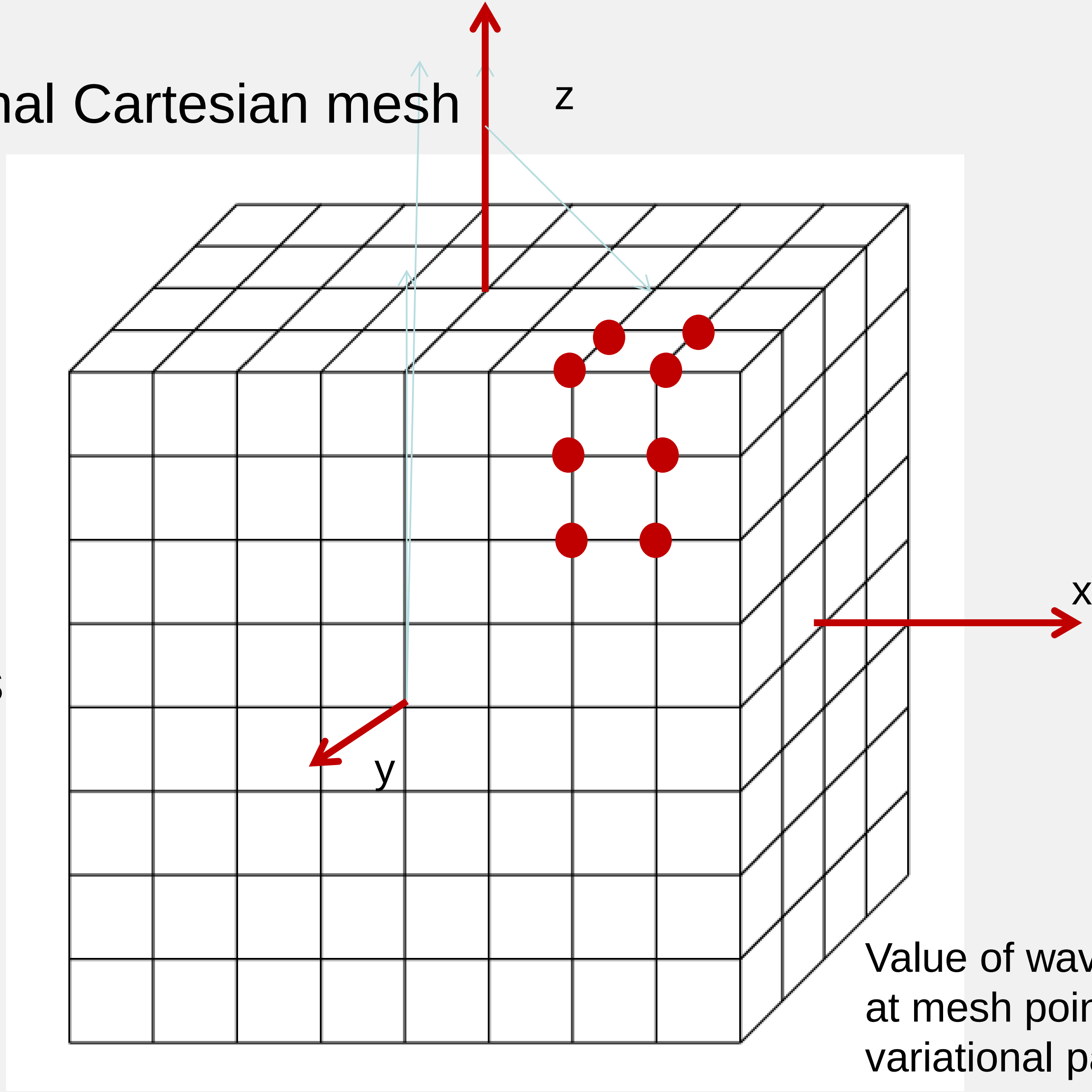
Mean-field Methods

• Based on an “effective interaction” or a “density functional”
The (small number of) parameters of the effective interaction are fixed by general considerations (no local adjustments)
• Pairing correlations are included at the BCS or better HFB level
• Full self-consistency

Our method: discretization on a 3-dimensional mesh (no expansion on a basis)
• No restrictions to a few shells, mean-field equations are solved as precisely as one wishes.
• Spherical and deformed nuclei are treated on the same footing, no “parametric deformation”

3-dimensional Cartesian mesh

Codes:
ev8, ev4
cr8, cr4
GCM codes



Value of wave functions at mesh points= variational parameters

Numerical accuracy of the codes

HOSPHE spherical oscillator
Lenteur 1d (spherical) mesh
EV8 3d (cartesian) mesh

HOSPHE shells		Lenteur dr		EV8 dx	
10	-343,6343232	0,5	-344,6723824	1	-343,4911
15	-343,9616588	0,25	-344,0789679	0,9	-343,6463
20	-344,0759899	0,1	-344,0779376	0,8	-343,7597
40	-344,0836702	0,01	-344,0844223	0,7	-343,8380
60	-344,0837838	0,005	-344,084479	0,6	-343,8996
70	-344,0837891	0,002	-344,0844949	0,5	-343,9500
				0,4	-343,9887

40Ca, SLy4

Test MOCCa new Coulomb, Skm* dx=0.8 fm -341.064
To be compared to Lenteur converged: -341.080

In preparation: rewriting of all the codes in a modern way

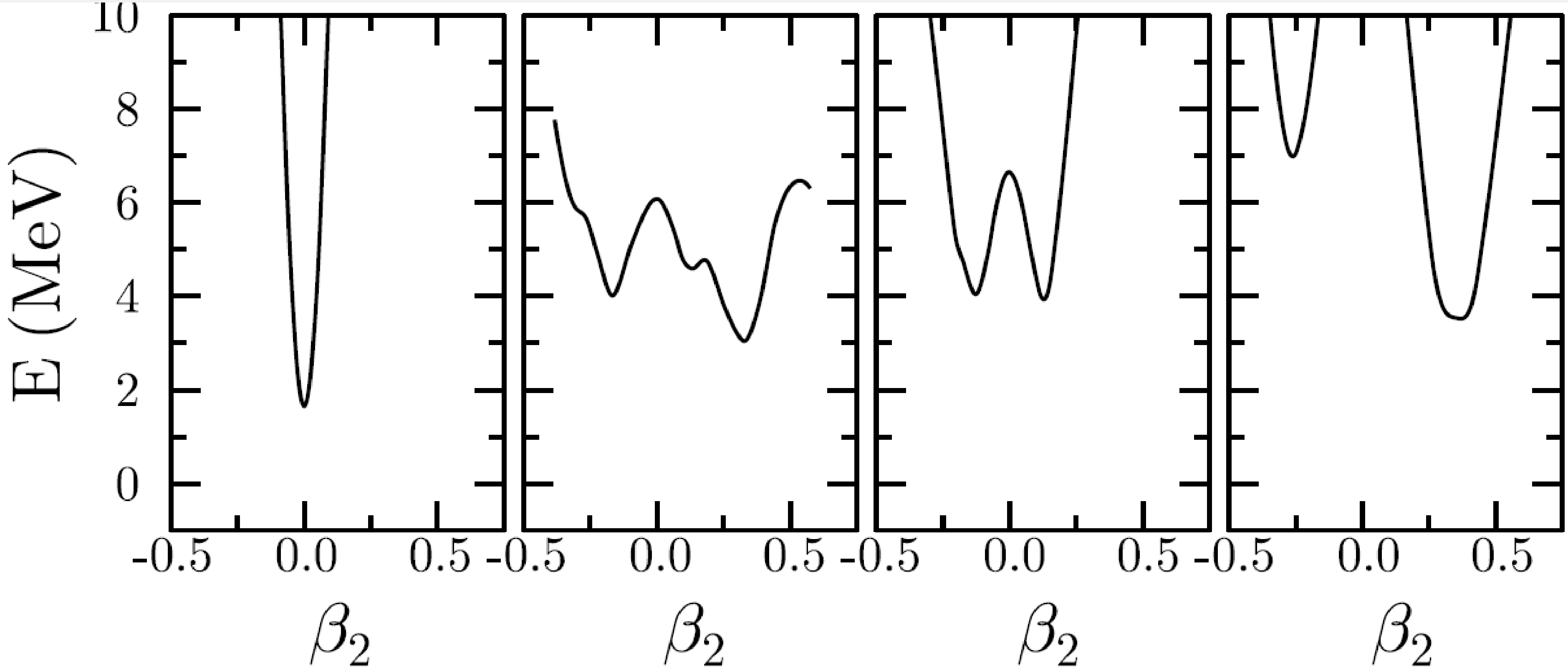
Single code with all possibility of symmetry breaking in a box

Modular code that will replace all the exiting ones and extends them

Already operational without pairing.

(Thesis of Wouter Ryssen)

^{208}Pb ^{180}Hg ^{202}Rn ^{170}Hf



Mean-field energy curves (β_2 proportional to Q)

Plus and minus of the mean-field approach:

Plus:

Starts from an effective interaction: generality
Can describe any kind of shapes (from ground state to fission)
Cranking (or qp excitations) well justified for deformed nuclei

Minus:

Valid only for energy (variational) and one-body operators
Breaking of symmetries (no direct determination of transitions)
Soft nuclei? Shape coexistence?
Effects of correlations beyond mean-field on masses?

Correlations

Explicitly included at the mean-field level:

- Statistics (fermions)
- Pairing (BCS or HFB)
- Deformation (can bring up to 20 MeV!)

Absent:

- Symmetry restoration (rotational correlations)
- Configuration mixing (shape, multi qp excitations, …)

  (vibrational correlations)

Can all missing correlations be included in the interaction?

(“DFT spirit”)

Mean-field wave-functions generated by a double constraint:

$$q_1 = Q_0 \cos(\gamma) - \frac{1}{\sqrt{3}} Q_0 \sin(\gamma)$$
$$q_2 = \frac{2}{\sqrt{3}} Q_0 \sin(\gamma) .$$

$$\beta_2 = \sqrt{\frac{5}{16\pi}} \frac{4\pi Q_0}{3R^2 A}$$

and projected on good angular momentum with the projector:

$$\hat{P}^J_{MK} = \frac{2J+1}{16\pi^2} \int_0^{4\pi} d\alpha \int_0^{\pi} d\beta \, \sin(\beta) \int_0^{2\pi} d\gamma \, \mathcal{D}^{J\,*}_{MK} \, \hat{R}$$

projected also on N and Z

Three steps:

1. Projection on N, Z, J, K and M of the mean-field wave functions

$$|JMKq\rangle = \hat{P}^J_{MK}\,\hat{P}^Z\,\hat{P}^N|q\rangle$$

after projection, *q* is a label (reminder) of the mean-field state
Non orthogonal basis as a function of *q* before and after projection!

2. K-mixing:

$$|JM\kappa q\rangle = \sum_{K=-J}^{+J} f^J_\kappa(K)\,|JMKq\rangle$$

3. Selection of the relevant states (truncation on κ) and mixing on the deformation:

$$|JM\nu\rangle = \sum_q \sum_{\kappa=1}^{\kappa^{J,q}_m} F^J_\nu(\kappa,q)\,|JM\kappa q\rangle$$

The coefficients *F* are determined by minimizing the energy:

$$\frac{\delta}{\delta F_\nu^{J*}(K,q)} \frac{\langle JM\nu|\hat{H}|JM\nu\rangle}{\langle JM\nu|JM\nu\rangle} = 0$$

and are obtained by solving the HWG equation:

$$\sum_{q'} \sum_{\kappa'=1}^{\kappa_m^{J,q}} \left[\mathcal{H}_J(\kappa,q;\kappa',q') \quad - E_\nu^J \mathcal{I}_J(\kappa,q;\kappa',q')\right] F_\nu^J(\kappa',q') = 0$$

Core of the problem: determination of the kernels:

$$\begin{aligned} \mathcal{H}^J(\kappa,q;\kappa',q') &= \langle JM\kappa q|\hat{H}|JM\kappa' q'\rangle \\ \mathcal{I}^J(q,\kappa;q',\kappa') &= \langle JM\kappa q|JM\kappa' q'\rangle\,. \end{aligned}$$

PLUS:

-Very rich basis with many ph components
 (more precisely qp excitations with respect
 to a spherical basis)
-GCM is not limited to small amplitude motion
 as the QRPA
- multi np-mh excitations are automatically included

MINUS:

-Kind of ph excitations determined by the constraint
 used in the mean-field
-Only time reversed pairs are excited
-Up to now, (nearly) only axially deformed states

Projection on angular momentum

=

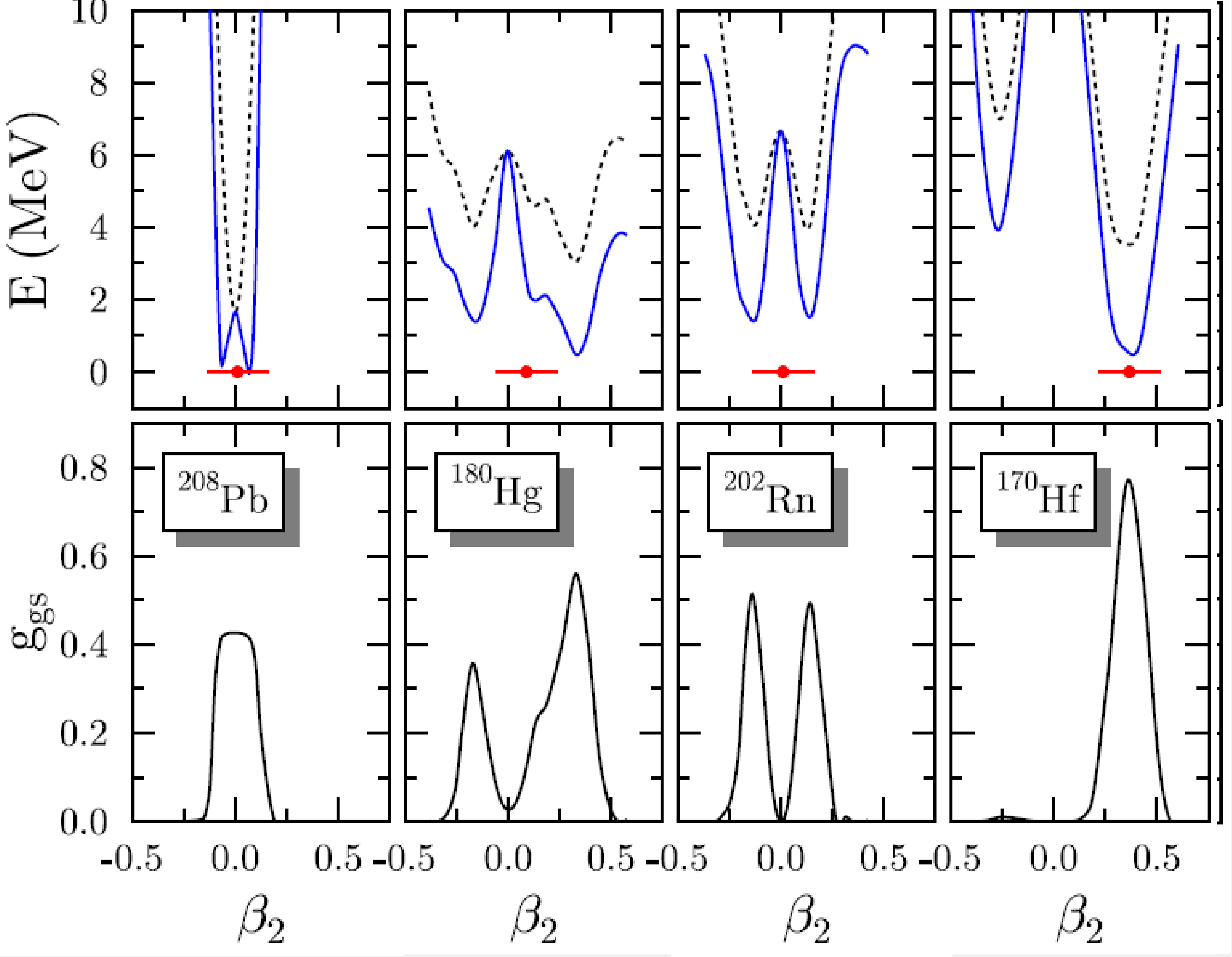
From intrinsic to laboratory frame of reference

No approximation based on the collective model

for transition probabilities.

Selected applications

- Shape coexistence in neutron deficient Pb region
- Breaking of translational invariance
- 240 Pu fission barrier
- Superheavy elements
- 180Hg



E (MeV)
10
8
6
4
2
0
g_{gs}
0.8
0.6
0.4
0.2
0.0
208Pb
180Hg
202Rn
170Hf
-0.5
0.0
0.5
β_2

Neutron-deficient Pb region

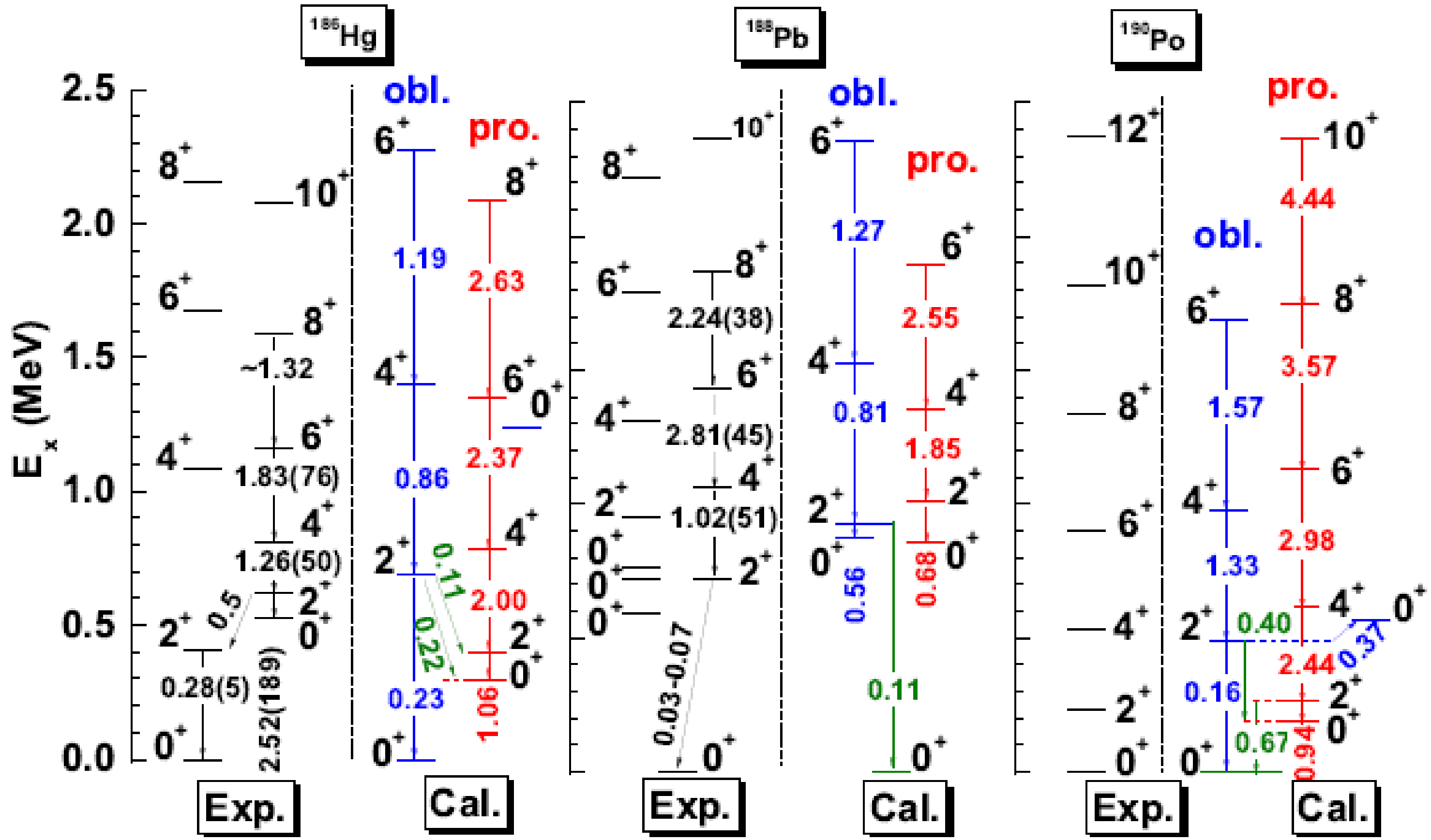


FIG. 16: (Color online) Comparison between the calculated and the measured low-lying spectra for ^{186}Hg, ^{188}Pb, and ^{190}Po. The $B(E2)$ values are given in e^2b^2 units. The experimental data are taken from Refs. [8, 17, 52–54].

Yao, Bender, Heenen, PRC 2013

Restoration of translational invariance

Generator coordinate:

r translation of the mean-field wave function

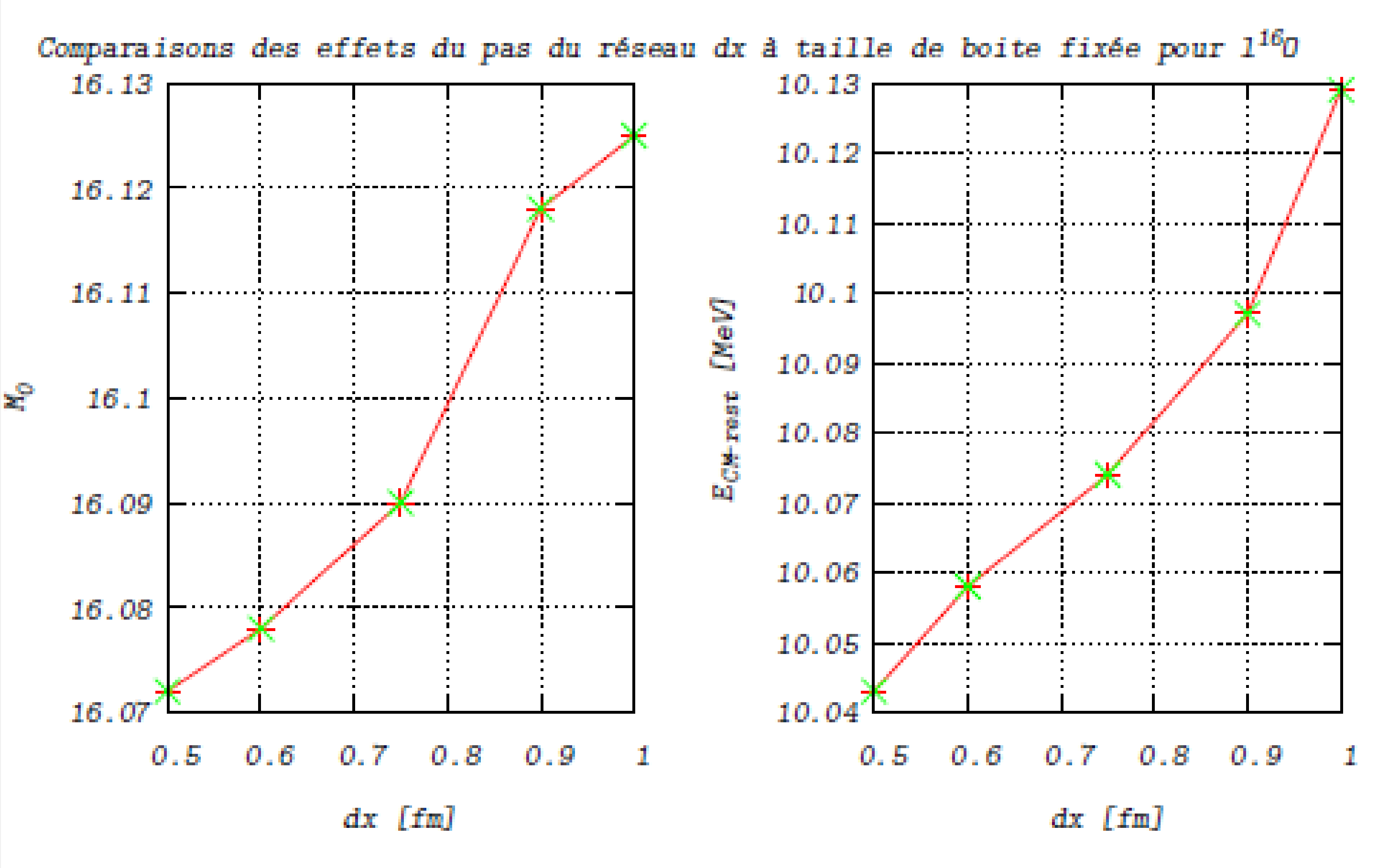
$$|\Psi_k\rangle = cst. \int d^3\mathbf{r} e^{i\mathbf{k}.\mathbf{r}} |\Phi(\mathbf{r})\rangle$$

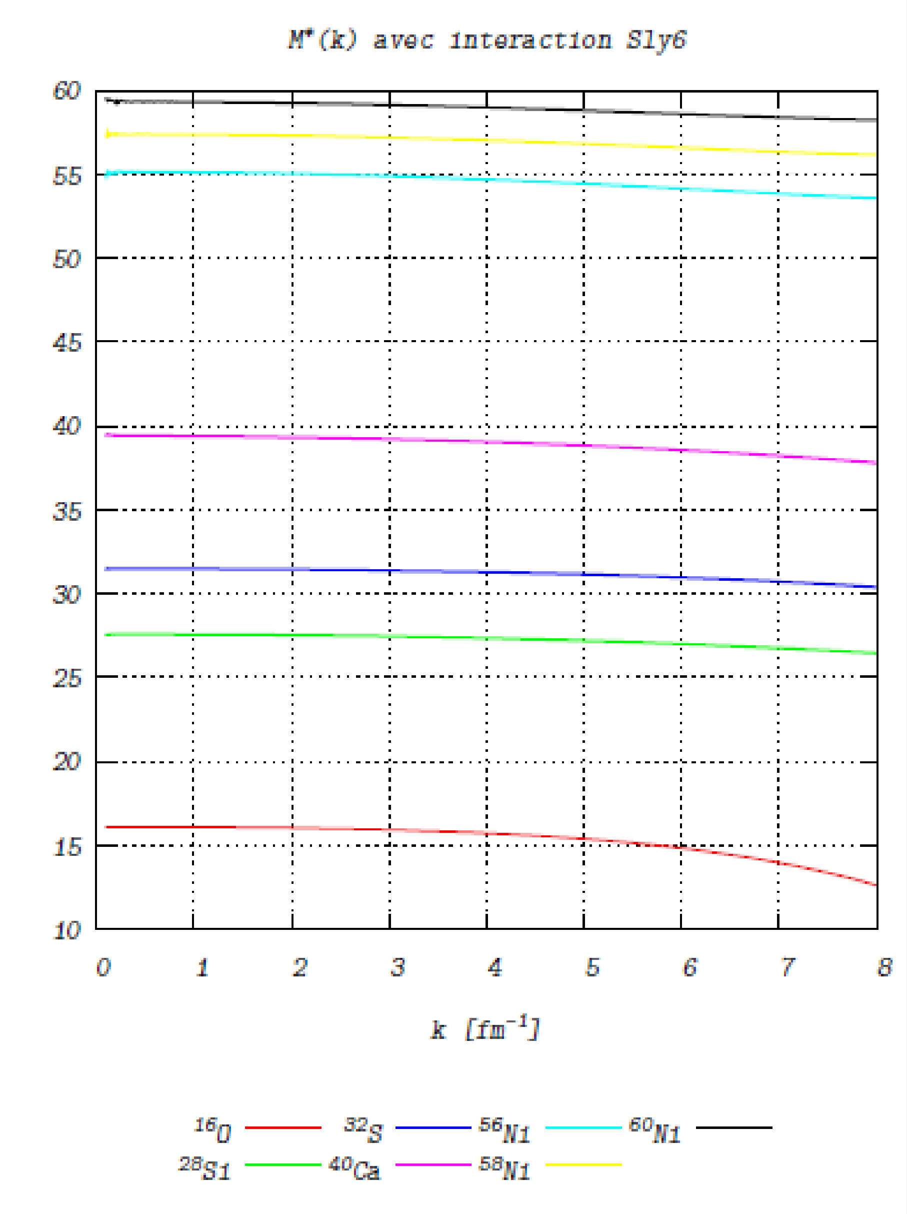
$$E_k = \frac{\int d^3r \langle\Phi(0)|H|\Phi(\mathbf{r})\rangle . e^{i\mathbf{k}.\mathbf{r}}}{\int d^3r \langle\Phi(0)|\Phi(\mathbf{r})\rangle . e^{i\mathbf{k}.\mathbf{r}}}$$

$$E_k = E_0 + \frac{1}{2}\frac{\mathbf{k}^2}{M^*(k)}$$

$$M^*(0) = 3\frac{\left(\int_0^\infty R^2 dR \mathcal{I}(R)\right)^2}{\left[\left(\int_0^\infty R^4 dR \mathcal{I}(R)\right)\left(\int_0^\infty R^2 dR \mathcal{H}(R)\right) - \left(\int_0^\infty R^2 dR \mathcal{I}(R)\right)\left(\int_0^\infty R^4 dR \mathcal{H}(R)\right)\right]}$$

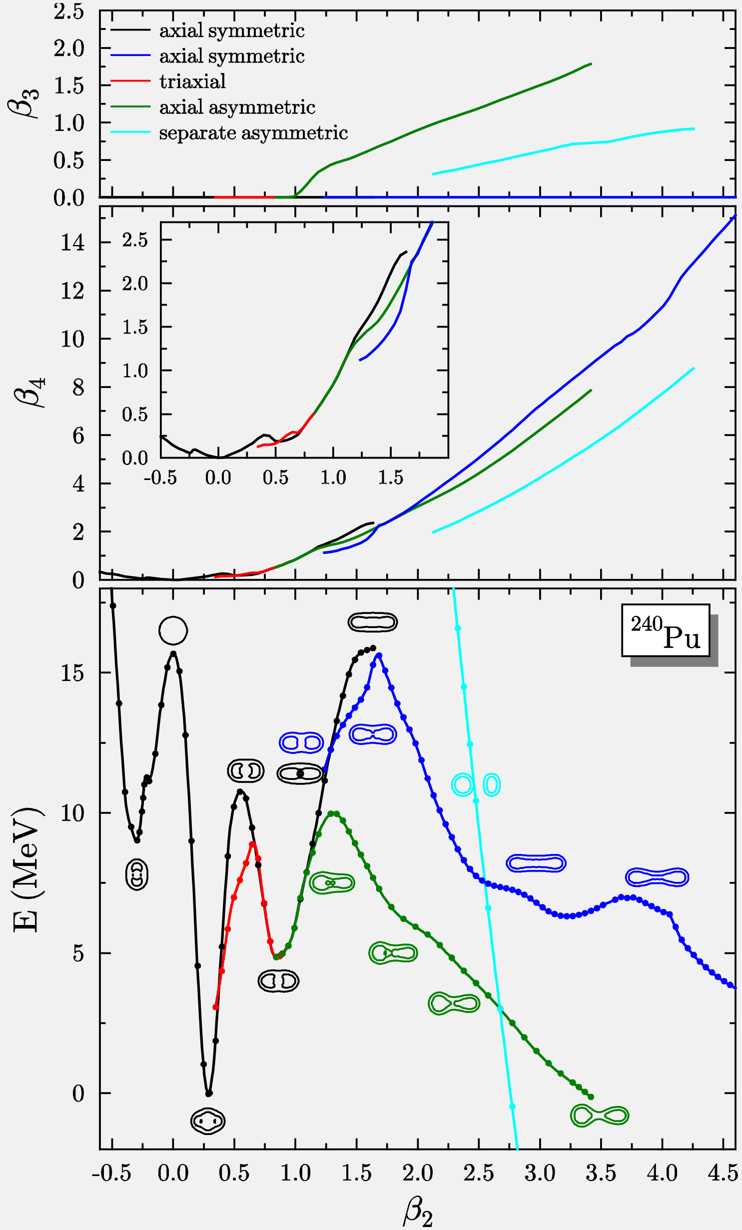
$$E_0 = \frac{\int d^R R^2 \mathcal{H}(R)}{\int d^R R^2 \mathcal{I}(R)}$$


Comparaisons des effets du pas du réseau dx à taille de boite fixée pour 1^16O
16.13
16.12
16.11
16.1
16.09
16.08
16.07
M_0
0.5
0.6
0.7
0.8
0.9
1
dx [fm]
10.13
10.12
10.11
10.1
10.09
10.08
10.07
10.06
10.05
10.04
E_CM-rest [MeV]
0.5
0.6
0.7
0.8
0.9
1
dx [fm]

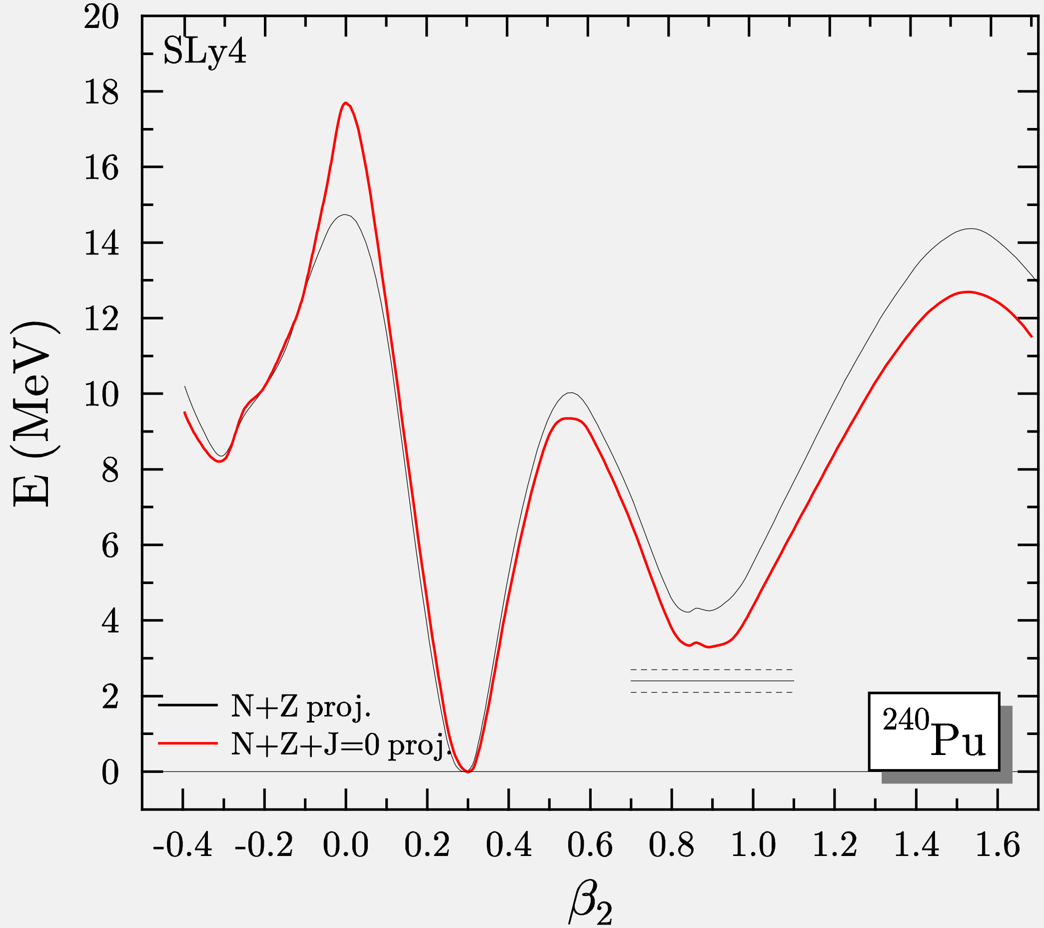


M*(k) avec interaction Sly6
60
55
50
45
40
35
30
25
20
15
10
0
1
2
3
4
5
6
7
8
k [fm^-1]
16O
32S
56Ni
60Ni
28Si
40Ca
58Ni

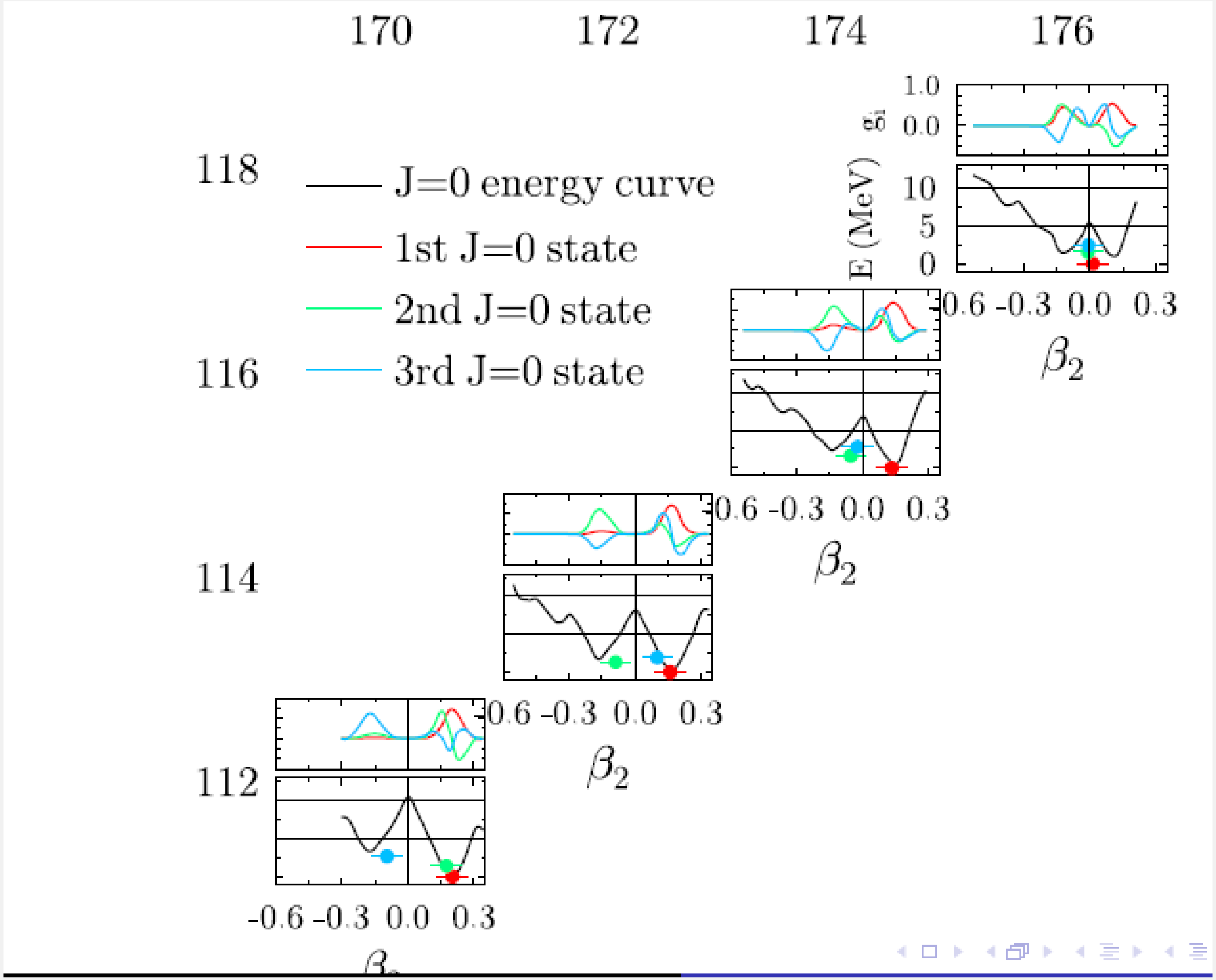
^{240}Pu



axial symmetric
axial symmetric
triaxial
axial asymmetric
separate asymmetric
β_3
β_4
E (MeV)
^{240}Pu
β_2

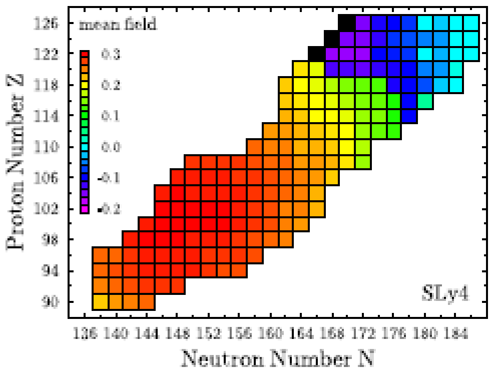


SLy4
E (MeV)
N+Z proj.
N+Z+J=0 proj.
^{240}Pu
β_2

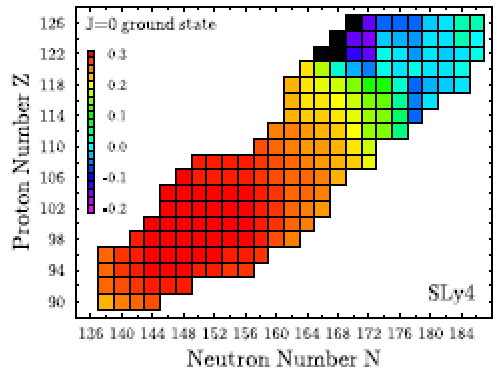


170
172
174
176
118
116
114
112
J=0 energy curve
1st J=0 state
2nd J=0 state
3rd J=0 state
E (MeV)
10
5
0
1.0
0.0
-0.6 -0.3 0.0 0.3
β_2

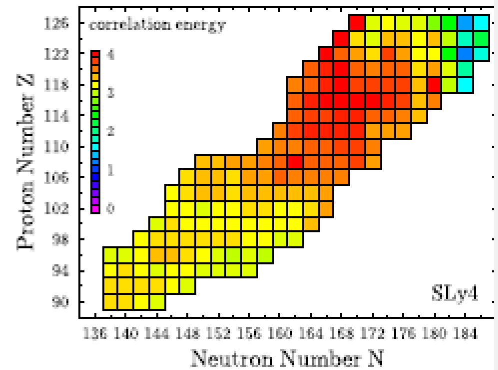
β_2 mean-field ground state



average (axial) deformation of the mean-field states the correlated $J = 0$ GCM ground state is constructed from



correlation energy (MeV)

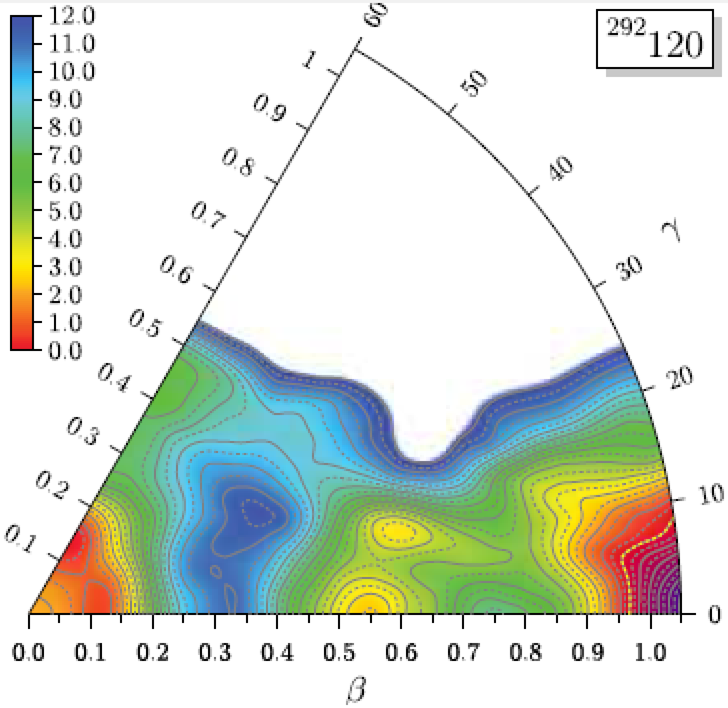


$$\beta_{\ell m} \equiv \frac{4\pi}{3R^{\ell}A} \Re\{\langle Q_{\ell m}\rangle\}$$

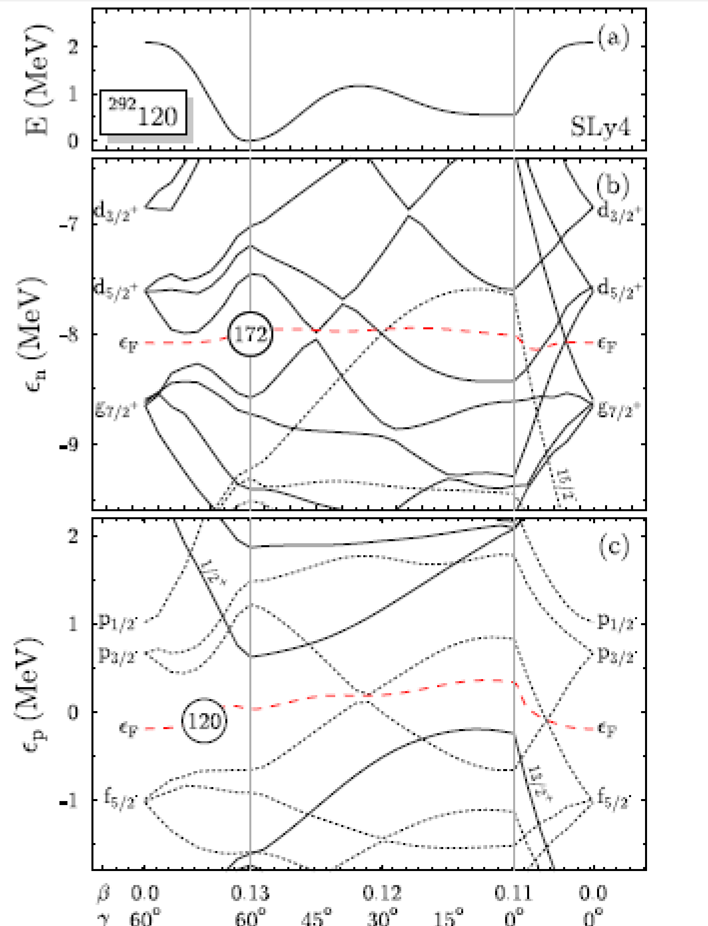
with $R = 1.2\,A^{1/3}$ fm.

two conventions used throughout this talk

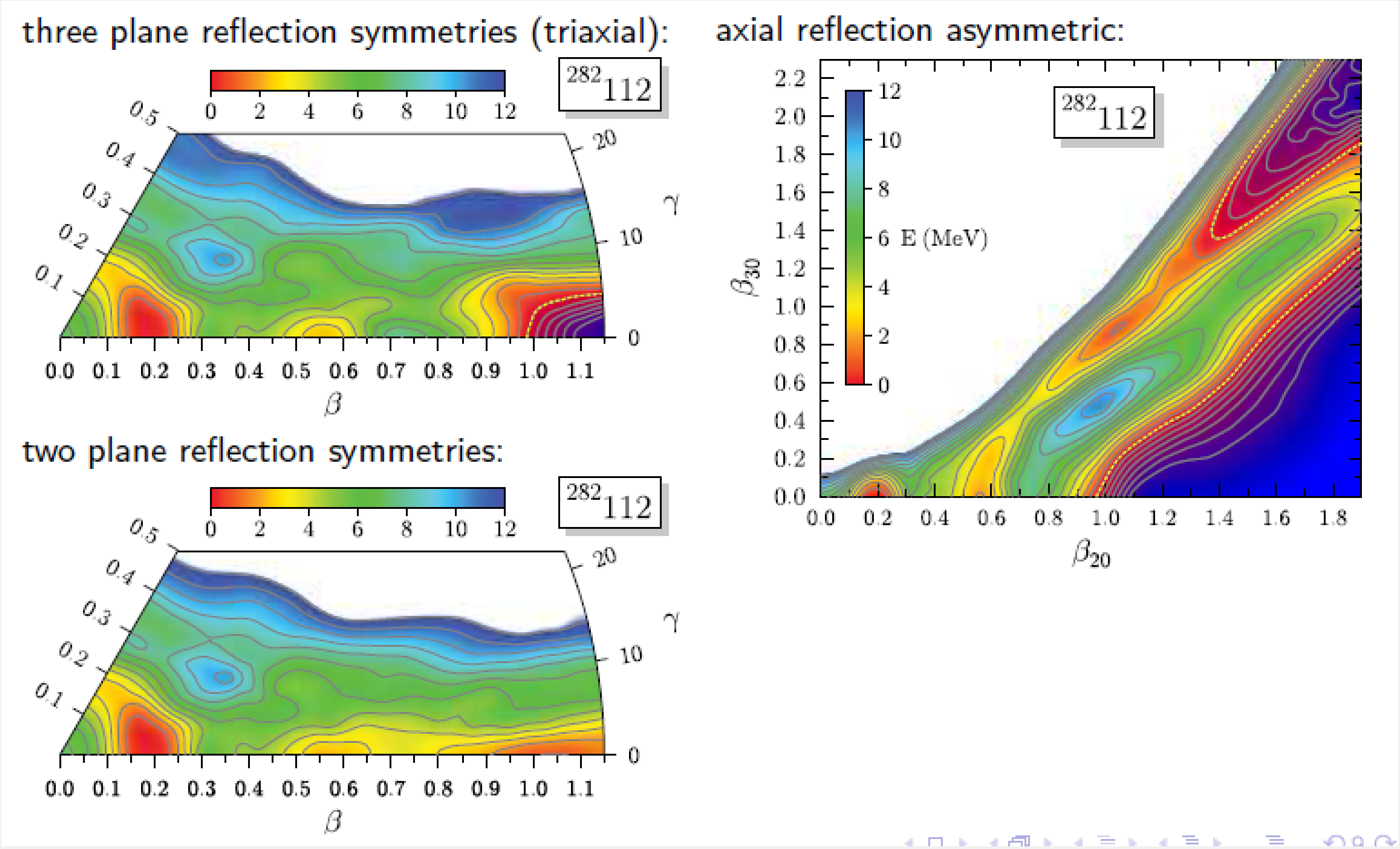
1. axial: $\beta_2 < 0$: oblate, $\beta_2 > 0$: prolate
2. triaxial: $\beta_2 > 0$, $\gamma = 60^o$: oblate, $\beta_2 > 0$, $\gamma = 0^o$: prolate

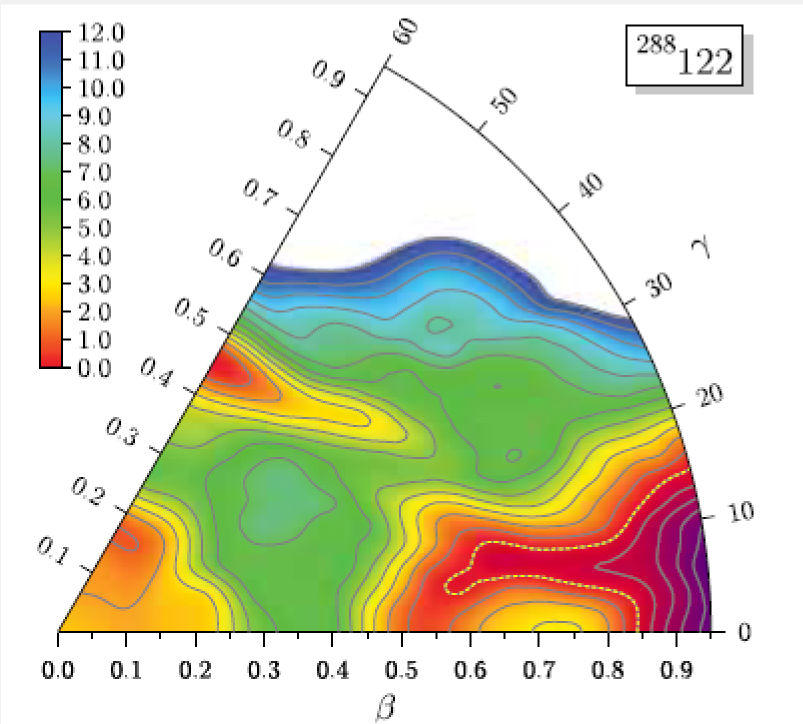


- calculation assuming triaxial shapes
- Second barrier disappears almost completely when considering also octupole deformation

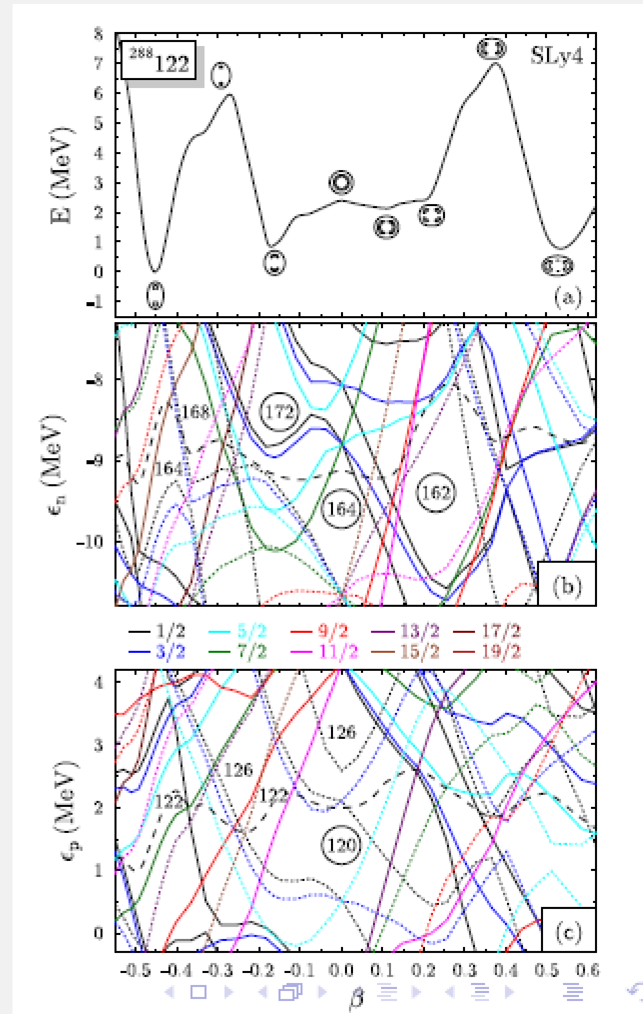


Relevant degrees of freedom for $^{282}_{112}Cn$

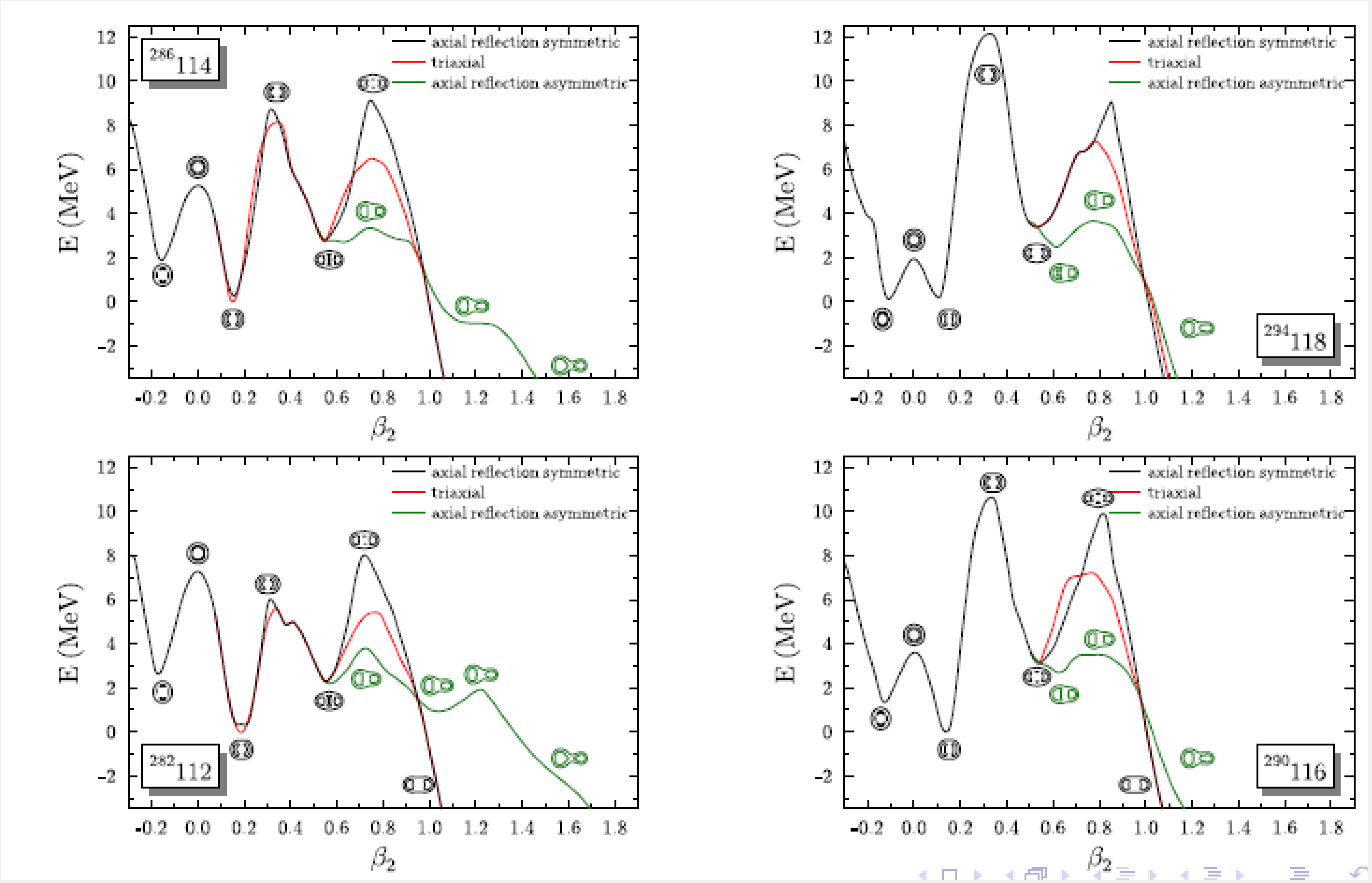




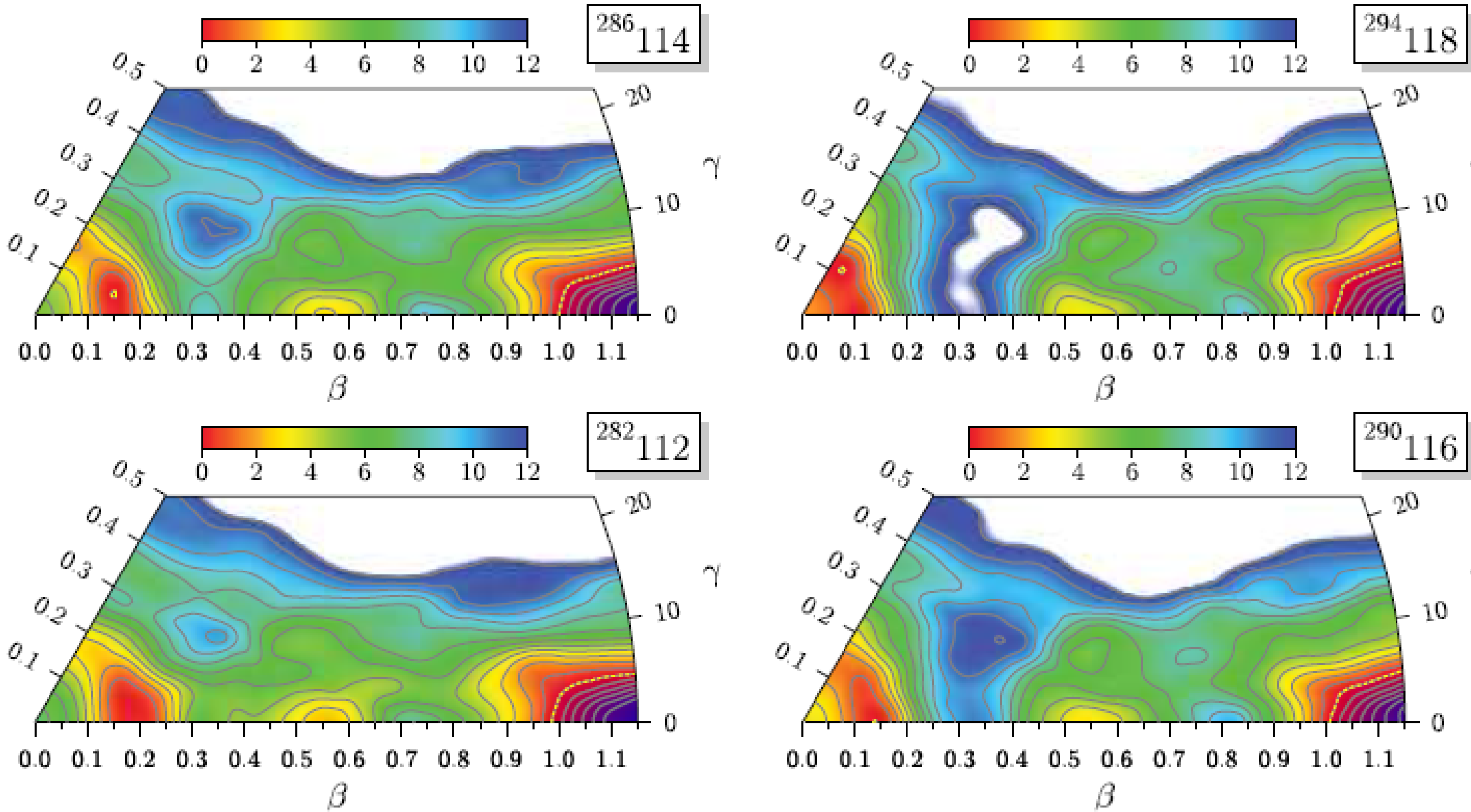
288 122
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
β
γ
0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9
0 10 20 30 40 50 60



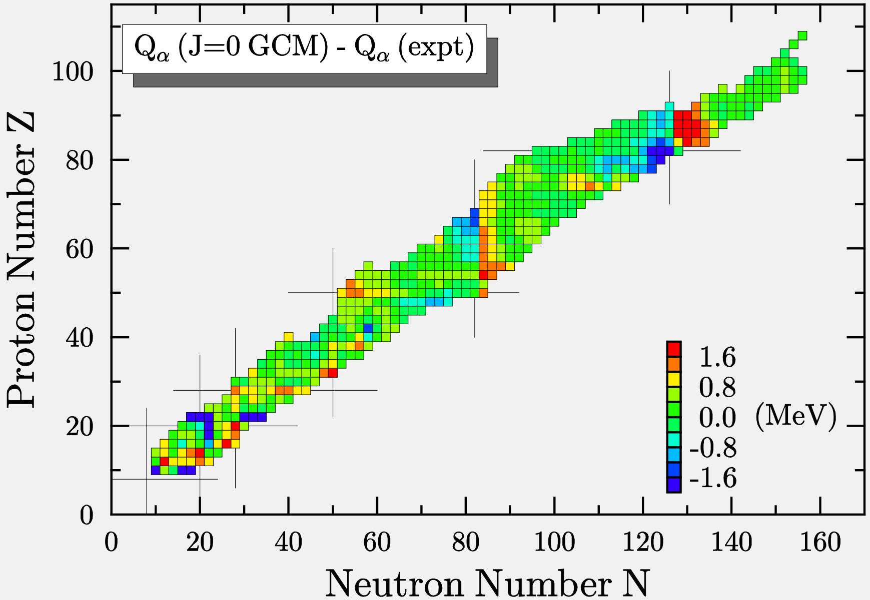
288 122
SLy4
E (MeV)
(a)
ϵ_n (MeV)
168
172
164
164
162
(b)
1/2 5/2 9/2 13/2 17/2
3/2 7/2 11/2 15/2 19/2
ϵ_p (MeV)
126
126
122
122
120
(c)
β
-0.5 -0.4 -0.3 -0.2 -0.1 0.0 0.1 0.2 0.3 0.4 0.5 0.6

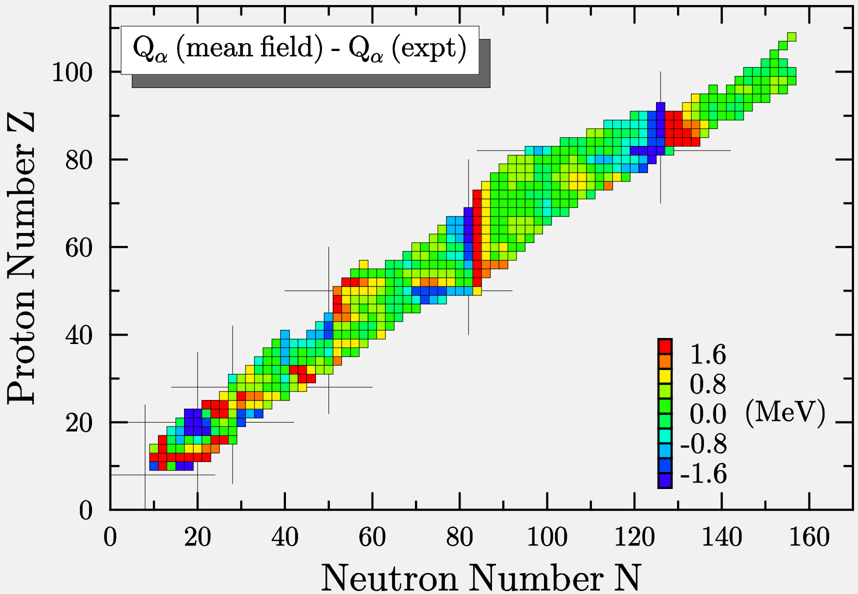


286 114
294 118
282 112
290 116
axial reflection symmetric
triaxial
axial reflection asymmetric
E (MeV)
β_2

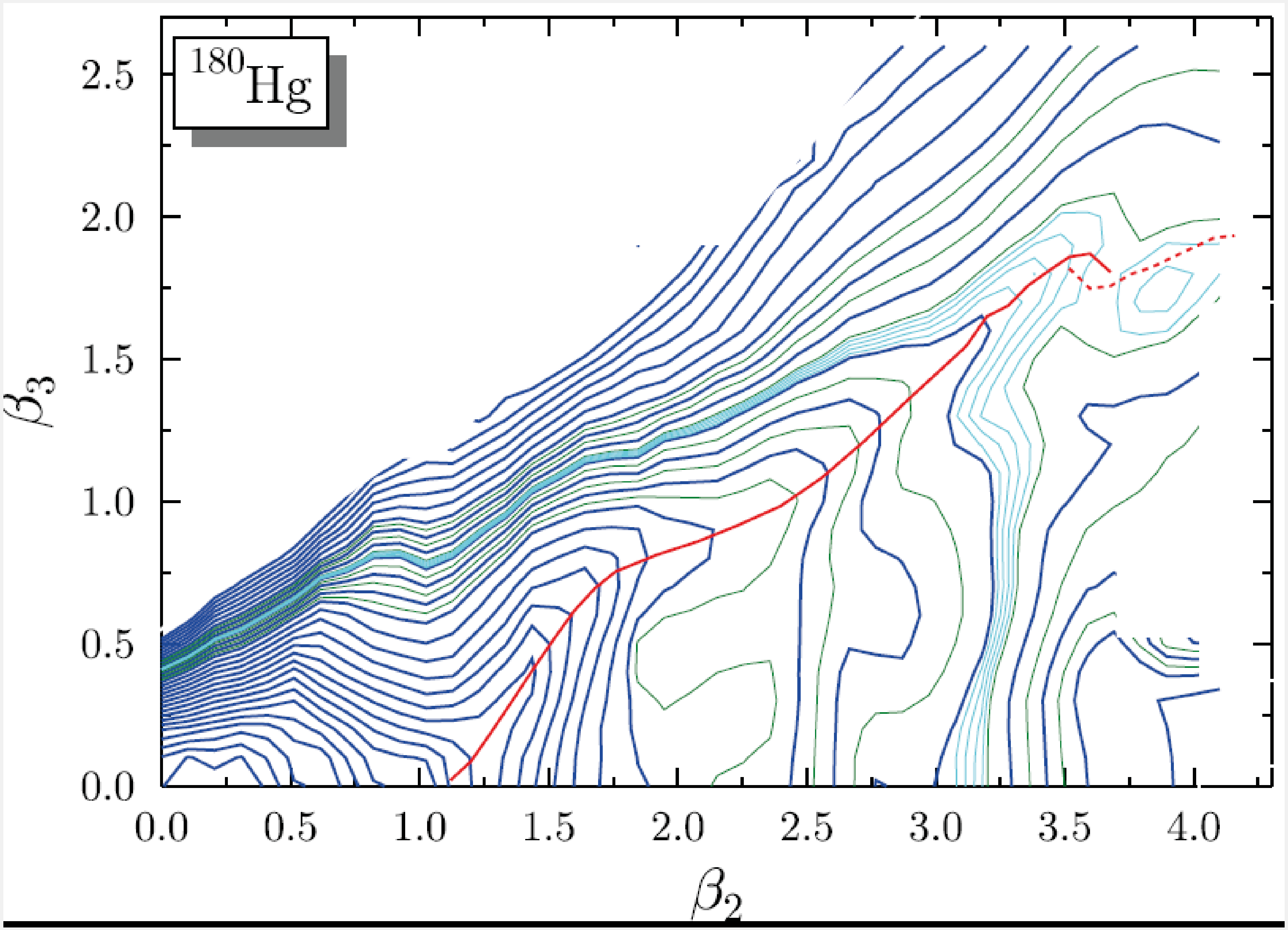


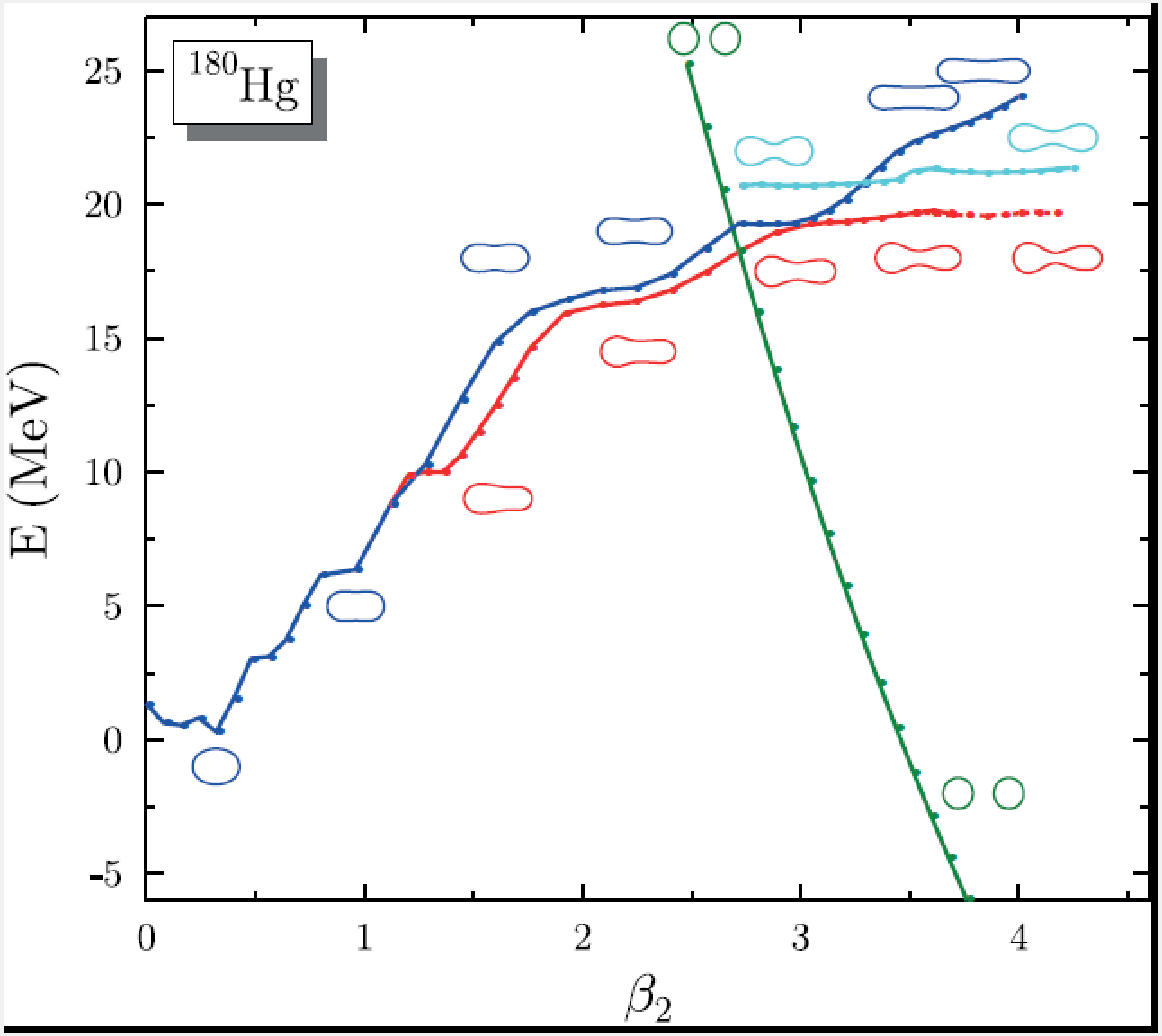
286114
294118
282112
290116
0 2 4 6 8 10 12
0.1 0.2 0.3 0.4 0.5
0 10 20
γ
0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.1
β


Q_α (J=0 GCM) - Q_α (expt)
Proton Number Z
Neutron Number N
1.6
0.8
0.0
-0.8
-1.6
(MeV)

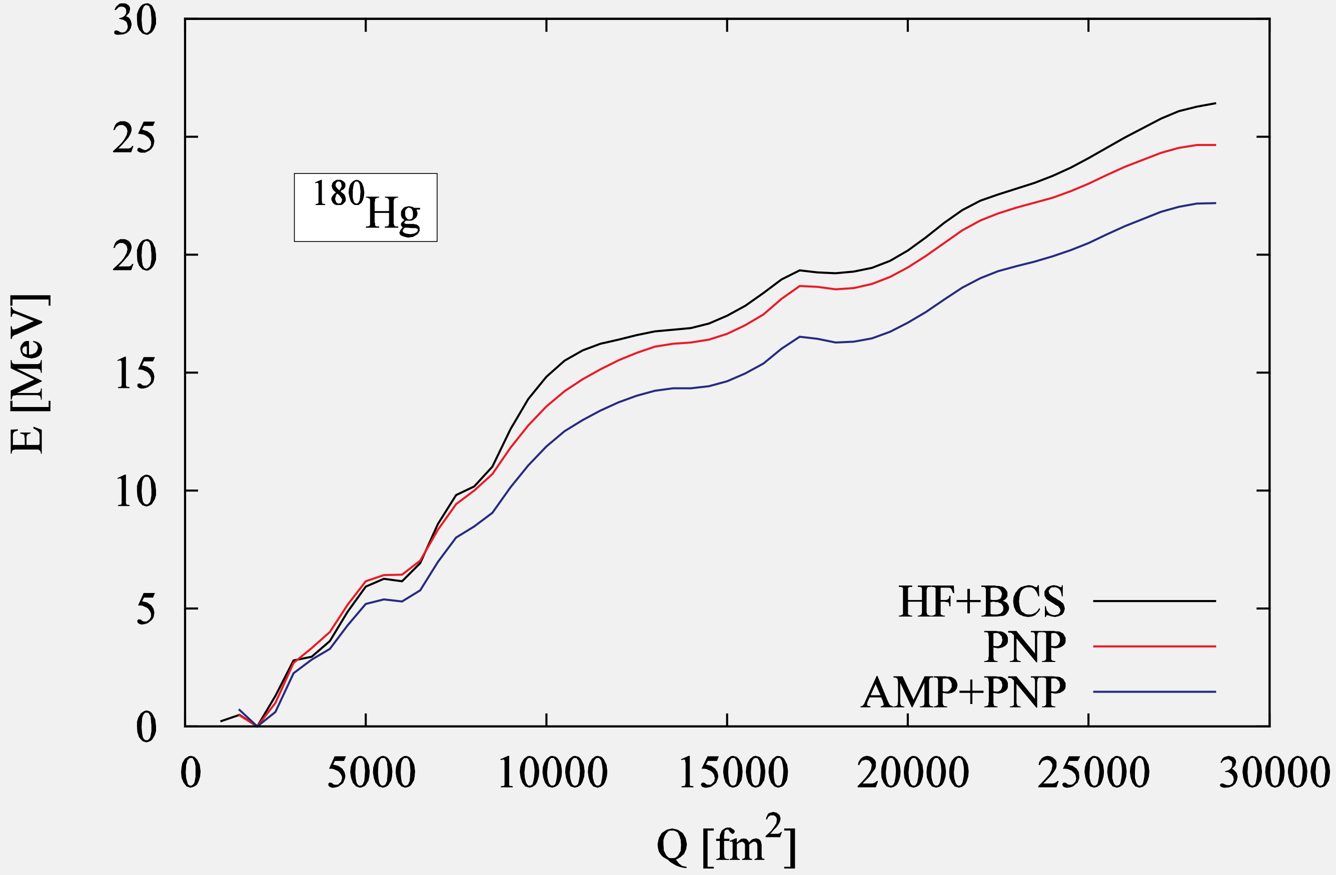

Q_α (mean field) - Q_α (expt)
Proton Number Z
Neutron Number N
1.6
0.8
0.0
-0.8
-1.6
(MeV)

Fission and octupole





^{180}Hg
E (MeV)
25
20
15
10
5
0
-5
0
1
2
3
4
β_2


30
25
20
15
10
5
0
E [MeV]
180Hg
HF+BCS
PNP
AMP+PNP
0
5000
10000
15000
20000
25000
30000
Q [fm2]

The future

Triaxiality also plays a role and has to be included for many nuclei

    done, but very time-consuming

Description of odd nuclei (1qp excitations) requires:

-to break time-reversal invariance (cranked HFB as a mean-field tool)

    done, but very time-consuming

    will improve also the description of spectra of even nuclei

- to break more symmetries of the mean-field

Readjustment of the effective interaction (correlations increase the binding energy

Effective interactions based on realistic nucleon-nucleon interactions