Mean-field and Beyond
Past, Present and Future

- Mean-field methods: what can and what cannot be calculated
- Applications and good reasons to go beyond mean-field
- How to do it (today)
- Applications

- The density functional theory: theorems

- Missing ingredients, new developments
- What remains to be done

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…

Today:
the working tools

- Mean-field with effective interactions
- Typical applications
- First step beyond mean-field
  - symmetry restorations
  - configuration mixing
- Selected applications

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
• 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”

An example of an effective interaction: the Gogny force

It contains:

- A finite range central term:

10

$$V_C = \sum_{i=1,2} (V_W^i + V_M^i P^r + V_B^i P^\sigma + V_H^i P^\sigma P^r) exp(-r^2/b_i^2)$$

- A zero range density dependent term

1-3

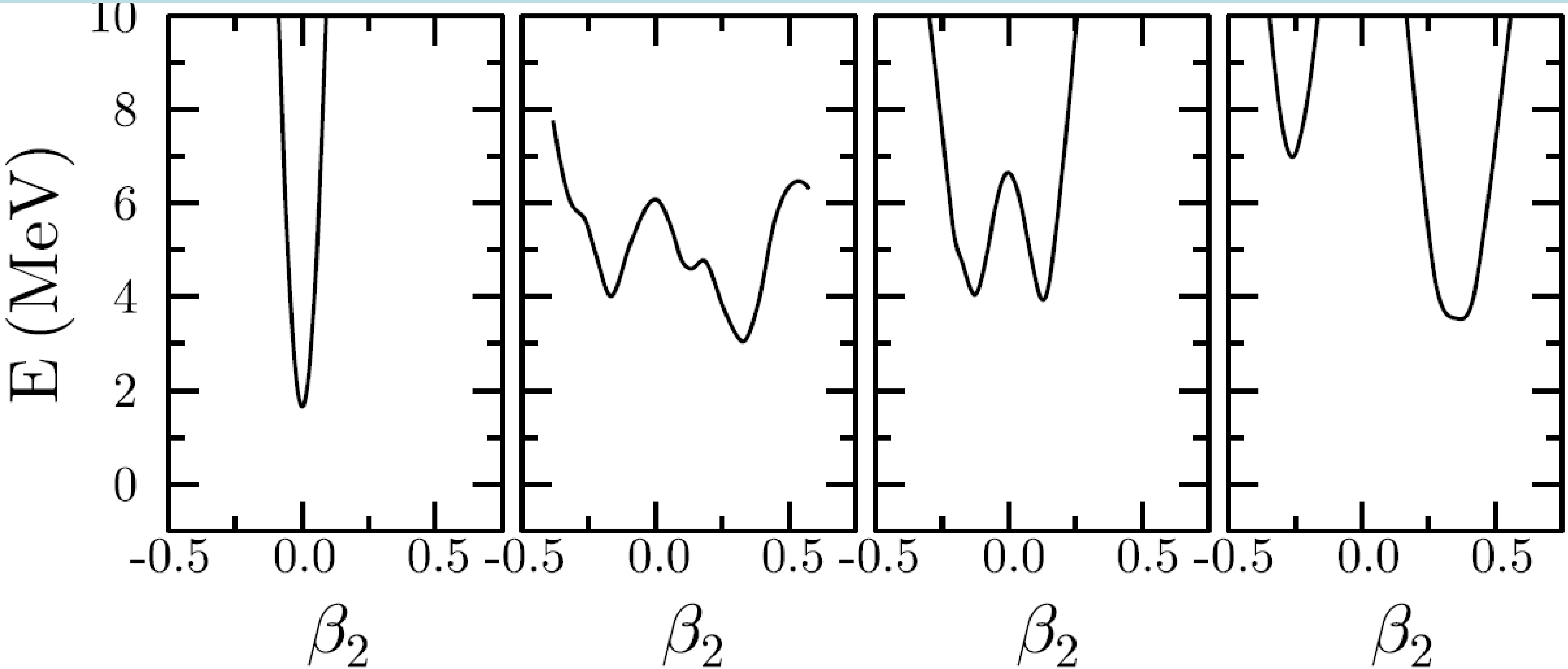
$$t_3(1 + x_3 P^\tau)\rho(\overrightarrow{r})^\alpha$$

1

- Spin orbit and Coulomb

Parameters are adjusted on nuclear matter properties (saturation, …)
properties of a few magic nuclei

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



Mean-field energy curves (β_2 proportional to Q)

The competitors

Three families:

- Gogny: finite range including a density dependence, same interaction for HF and pairing

(Bruyères le Chatel, Madrid, some Japanese groups)

- Skyrme: zero range, specific interaction for pairing, easy

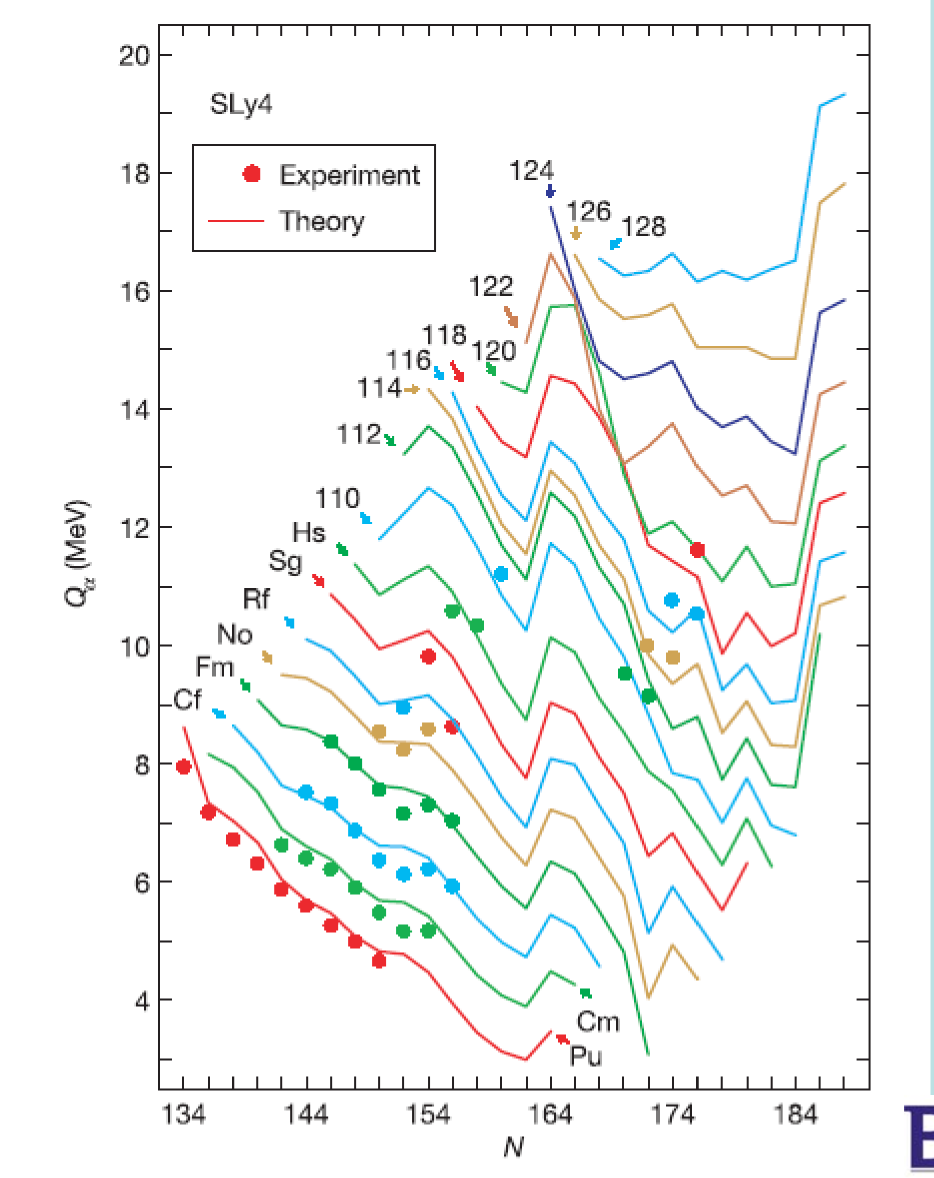
("French group", "Polish group", P. Rheinardt et al., Japanese groups,…)

- RMF: relativistic but no exchange, pairing non relativistic

(Munich-Zagreb, ….)

Skyrme HFB

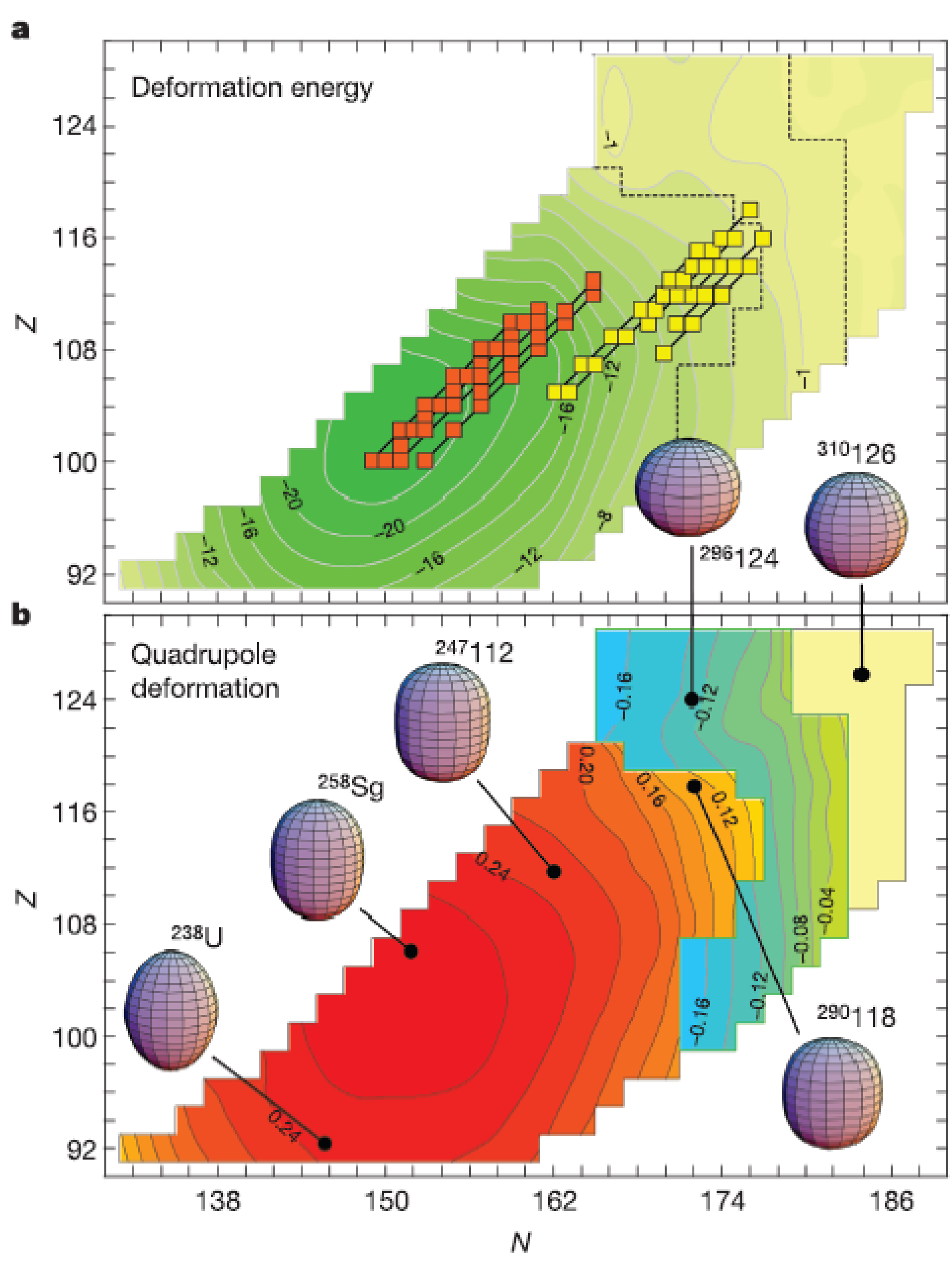
Q_α for isotopic chains for super heavy elements (only even-even)



Cwiok, Heenen, Nazarewicz
Nature 2005

Skyrme HFB

Deformation properties of super-heavies



Beyond ground state properties of even-even nuclei

Breaking of time reversal invariance

by a cranking constraint:

$H' = H - \omega J_x$ rotational bands for deformed nuclei

by quasi particle excitations:

Odd nuclei : 1 qp states: $\beta_i^\dagger |0\rangle$

Even nuclei: 2qp states

Still a mean-field method

Full self-consistency for mean-field and pairing

Moments of inertia

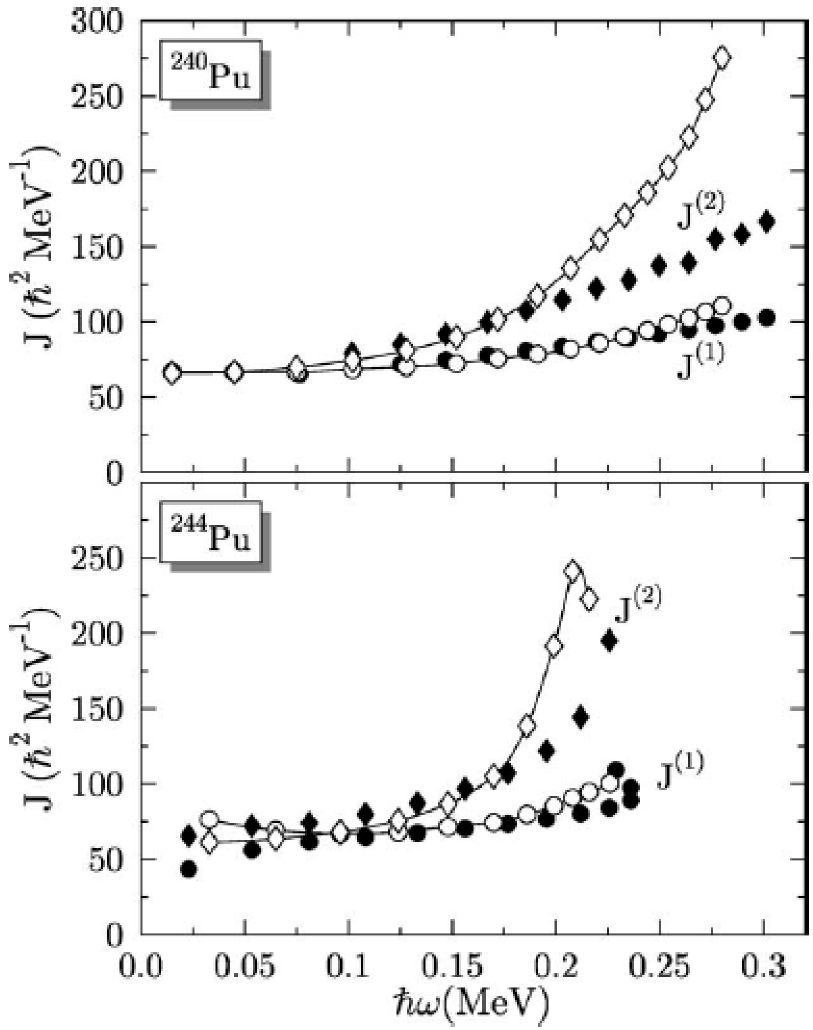
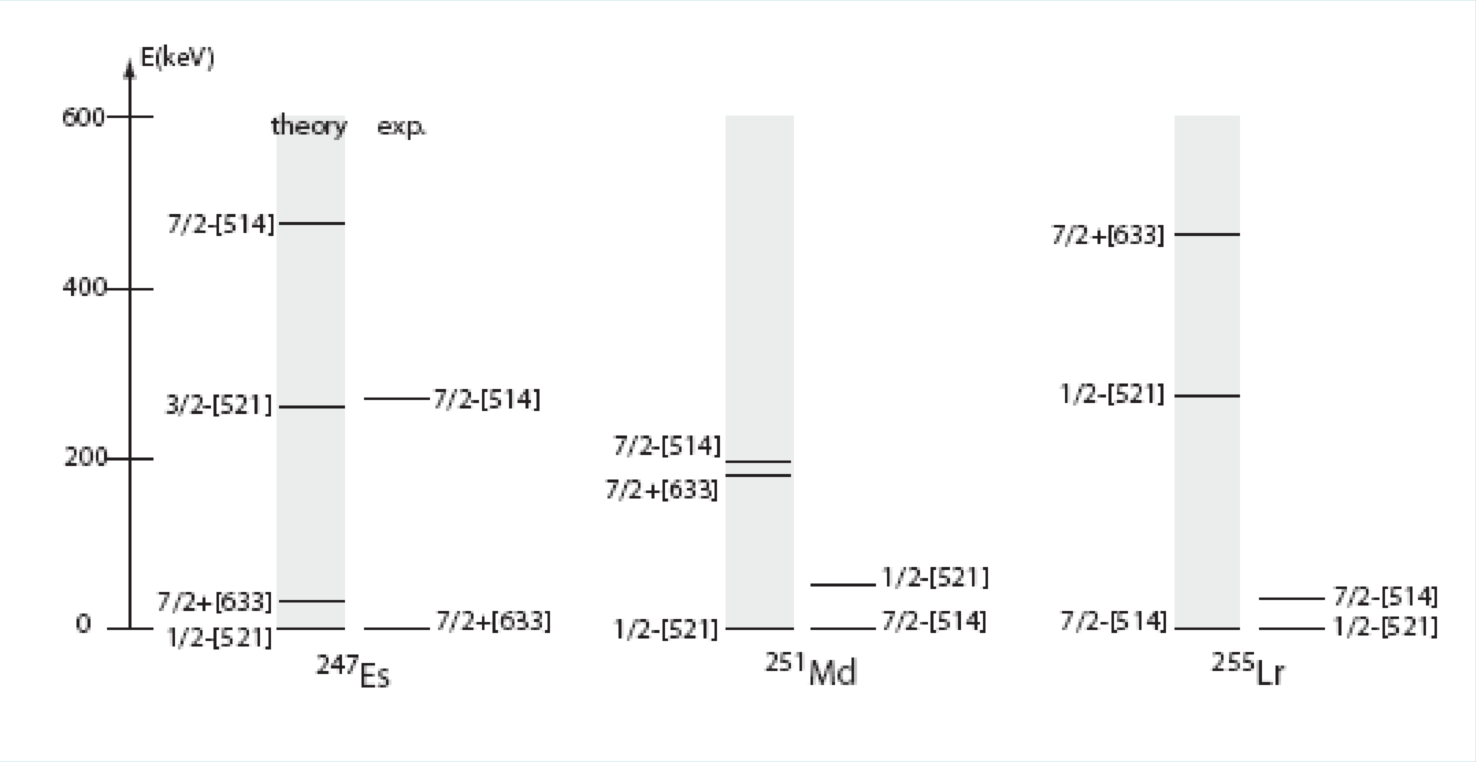


Fig. 3. Kinematical (circles) and dynamical (diamonds) moment of inertia for ^{240}Pu (top) and ^{244}Pu (bottom). Open (filled) markers denote calculated (experimental) values.

Spectra of odd Z nuclei



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:

Validity 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
- Configuration mixing (shape, multi qp excitations, …)

Can all missing correlations be included in the interaction?

(“DFT spirit”)

Beyond mean-field

Set of mean-field wave functions depending on axial *q*

- Projection on N, Z, J:

$$|J0q\rangle = \frac{1}{N_{J0q}} \hat{P}^{J}_{00} \hat{P}_{Z} \hat{P}_{N} |q\rangle ,$$

- New wave functions by mixing on q:

$$|J0k\rangle = \sum_q f_{J,k}(q) |J0q\rangle$$

with $f_{J,k}(q)$ determined by minimizing the energy:

$$E_{J,k} = \frac{\langle J0k|\hat{H}|J0k\rangle}{\langle J0k|J0k\rangle}$$

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

MINUS:

-Kind of ph excitations determined by the constraint
used in the mean-field

-Only time reversed pairs are excited

-Up to now, only axial states

Projection on angular momentum

=

From intrinsic to laboratory frame of reference

No approximation based on the collective model for transition probabilities.

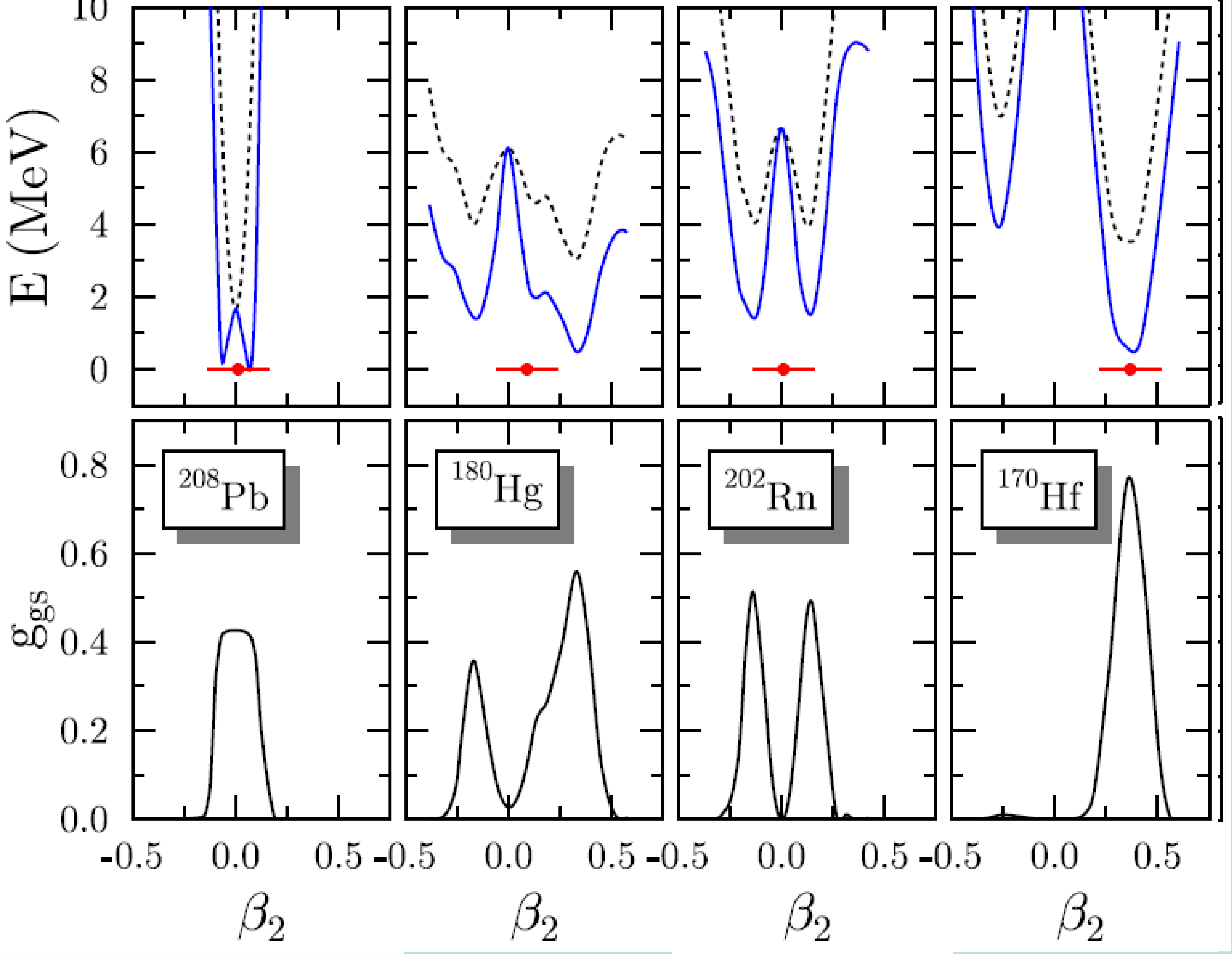
The spectroscopic quadrupole moment is given by:

$$
\begin{aligned}
Q_c(J_k) &= \sqrt{\frac{16\pi}{5}}\,\langle J, M=J, k|\hat{Q}_{20}|J, M=J, k\rangle \\
&= \sqrt{\frac{16\pi}{5}}\,\frac{\langle JJ20|JJ\rangle}{\sqrt{2J+1}} \\
&\quad \times \sum_{q,q'} f^*_{J,k}(q)\, f_{J,k}(q')\, \langle Jq||\hat{Q}_{20}||Jq'\rangle,
\end{aligned}
$$

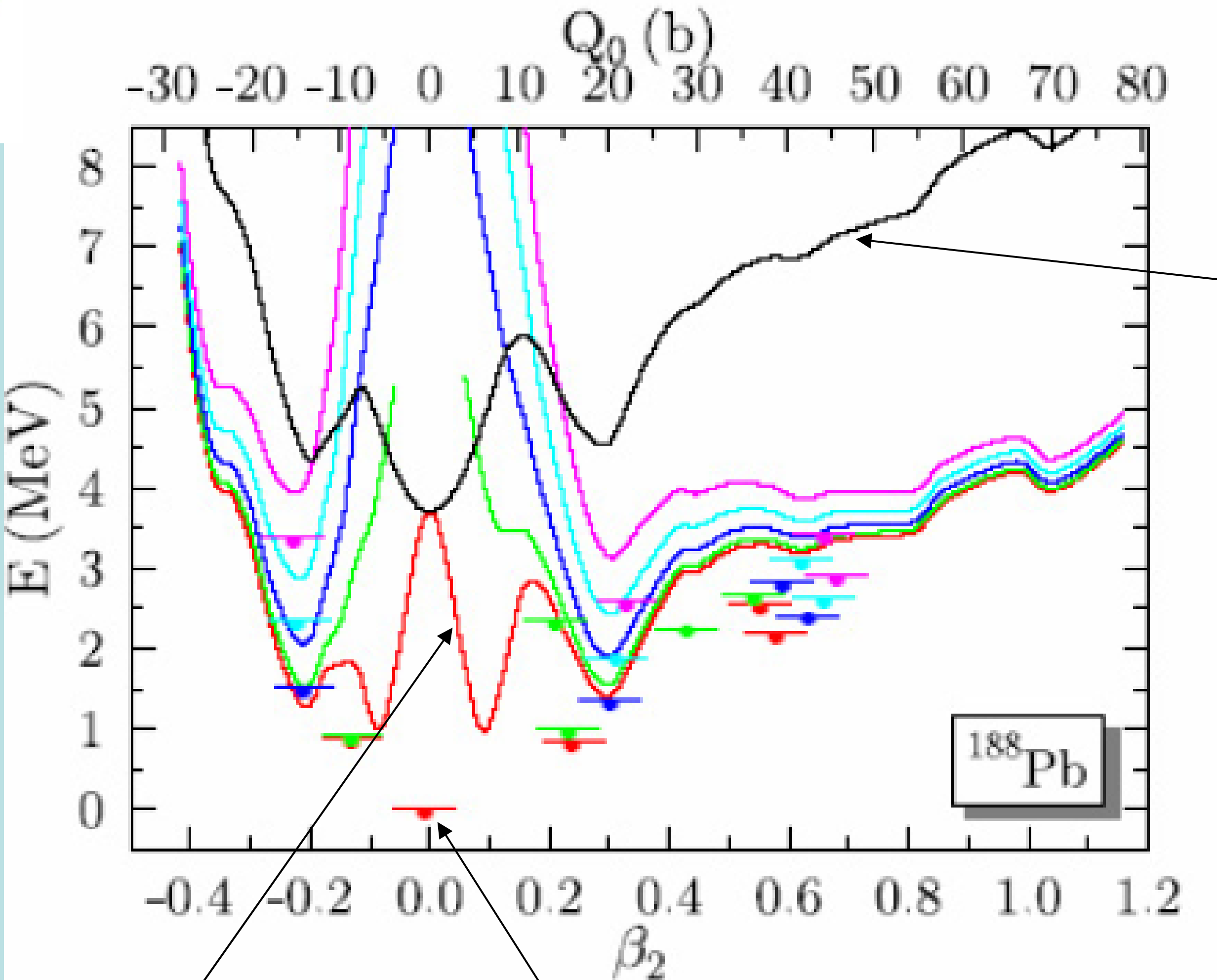
Deformation parameters similar to collective ones have to be defined:

$$
\begin{aligned}
\beta_2^{(s)}(J_k) &= \sqrt{\frac{5}{16\pi}}\,\frac{4\pi Q_2^{(s)}(J_k)}{3R^2 Z} \\
Q_2^{(s)}(J_k) &= -\frac{2J+3}{J}\,Q_c(J_k)
\end{aligned}
$$

with $R = 1.2\,A^{1/3}$ and $K = 0$.



E (MeV)
g_{gs}
^{208}Pb
^{180}Hg
^{202}Rn
^{170}Hf
β_2



Mean field

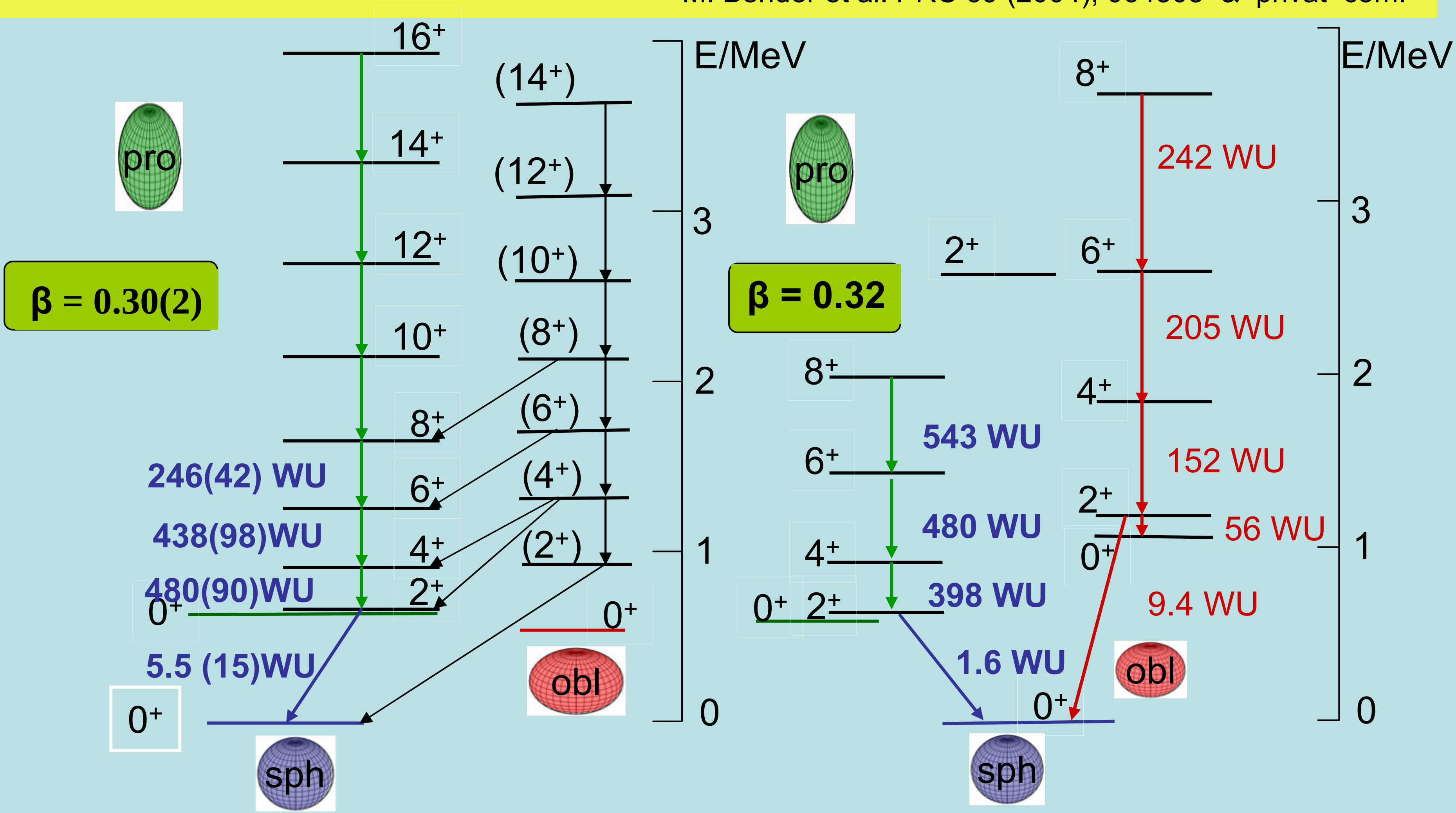
Mean field projected on J=0

Bars in red: 0^+ states obtained after configuration mixing

^{186}Pb

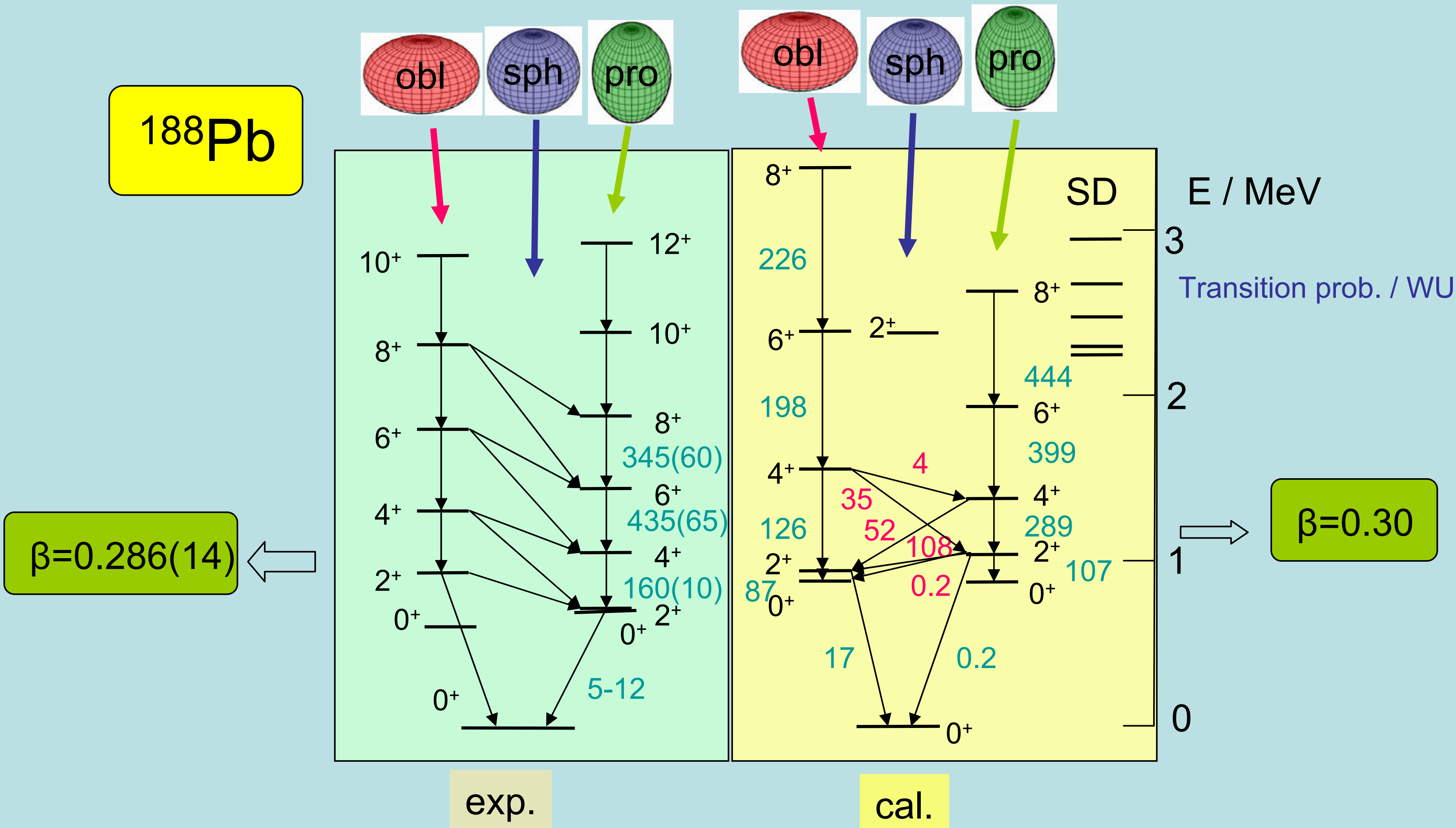
exp. | cal.

conf. mix of mean field states (Skyrme intera.SLy6)
M. Bender et al. PRC 69 (2004), 064303 & privat com.



Hartree-Fock + BCS (Skyrme SLy6 interaction + density dependent zero-range pairing force)
⇒configuration mixing of angular-momentum and particle-number projected self-consistent mean field states

(M. Bender, P. Bonche, T. Duguet, and P.H. Heenen, PRC 69, 2004, 064303)



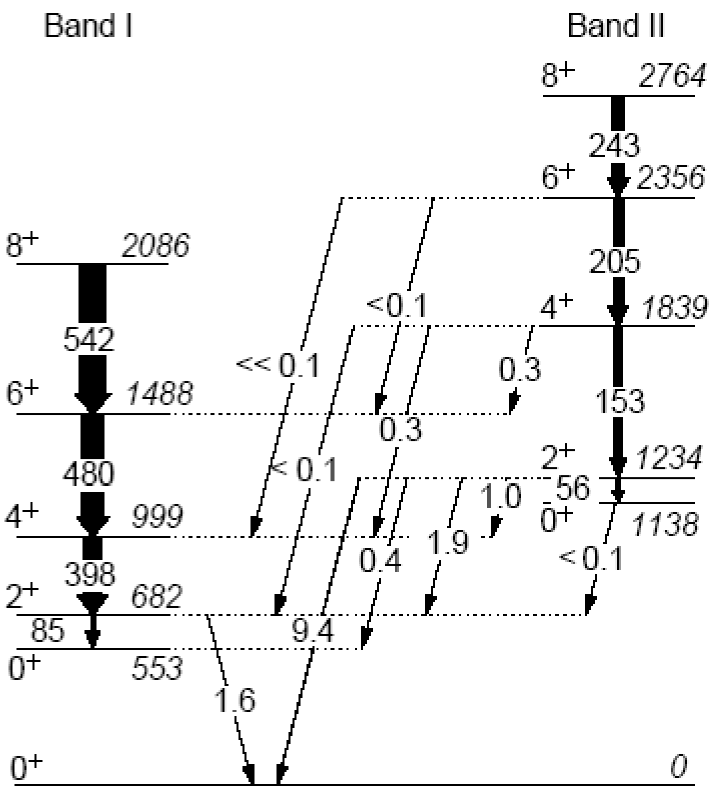
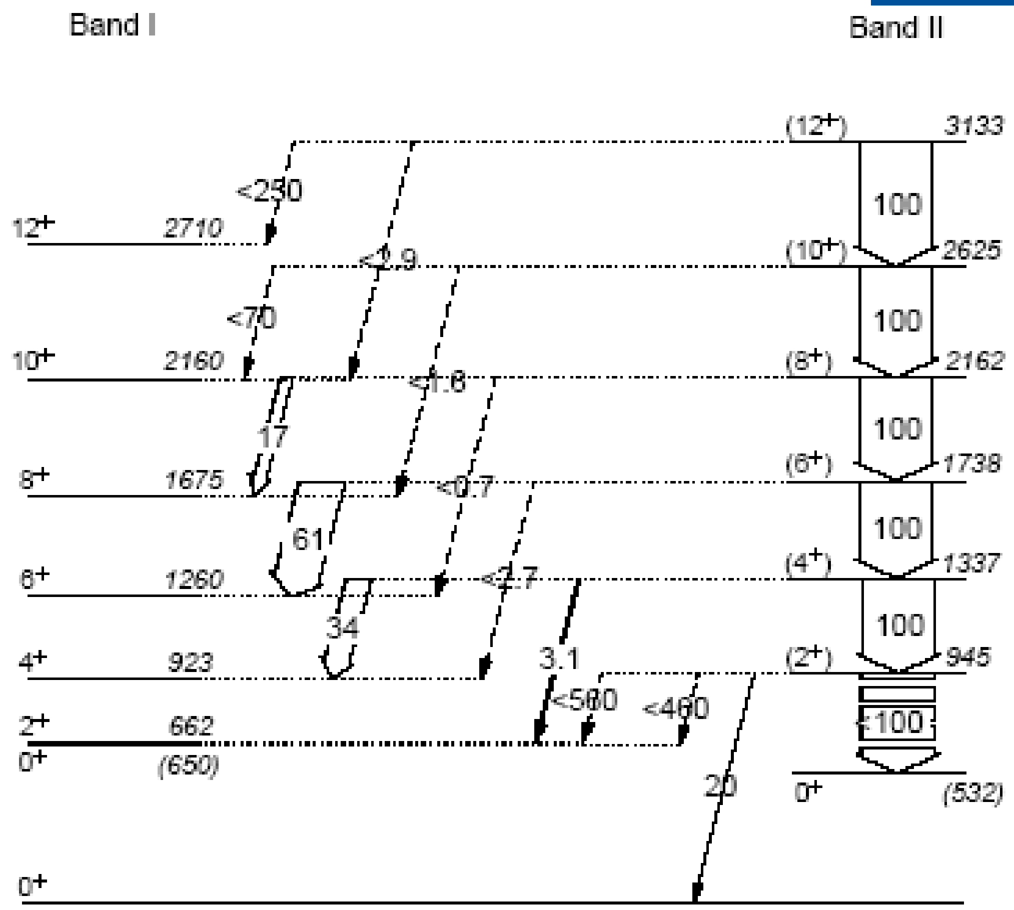


FIG. 14: Partial level scheme of ^{186}Pb obtained by configuration mixing. The values of the B(E2) between all the states are given in Weisskopf units.



Pb isotopic shifts

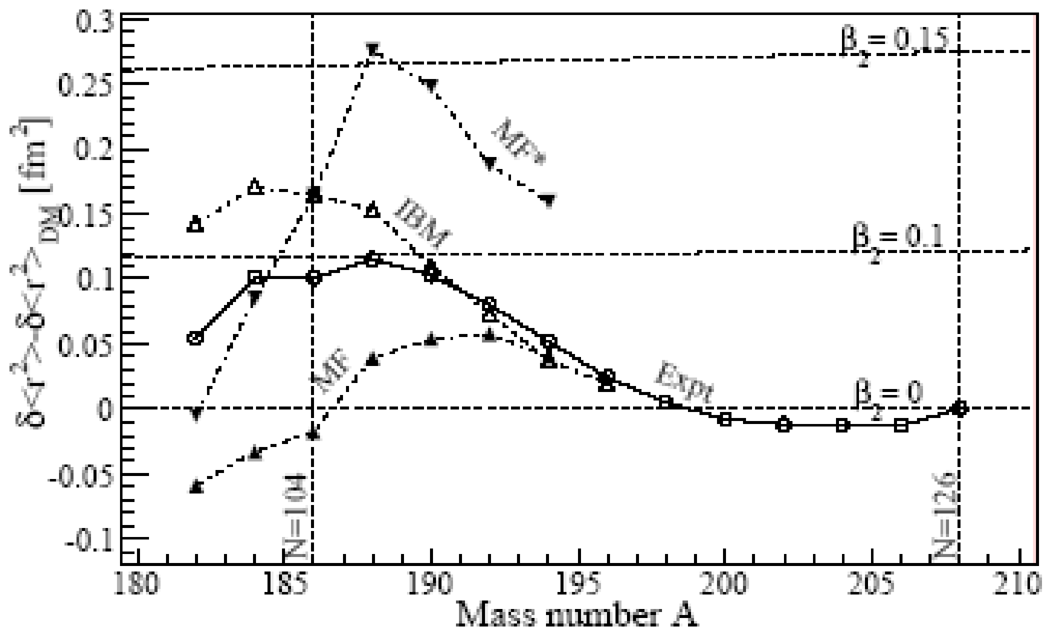
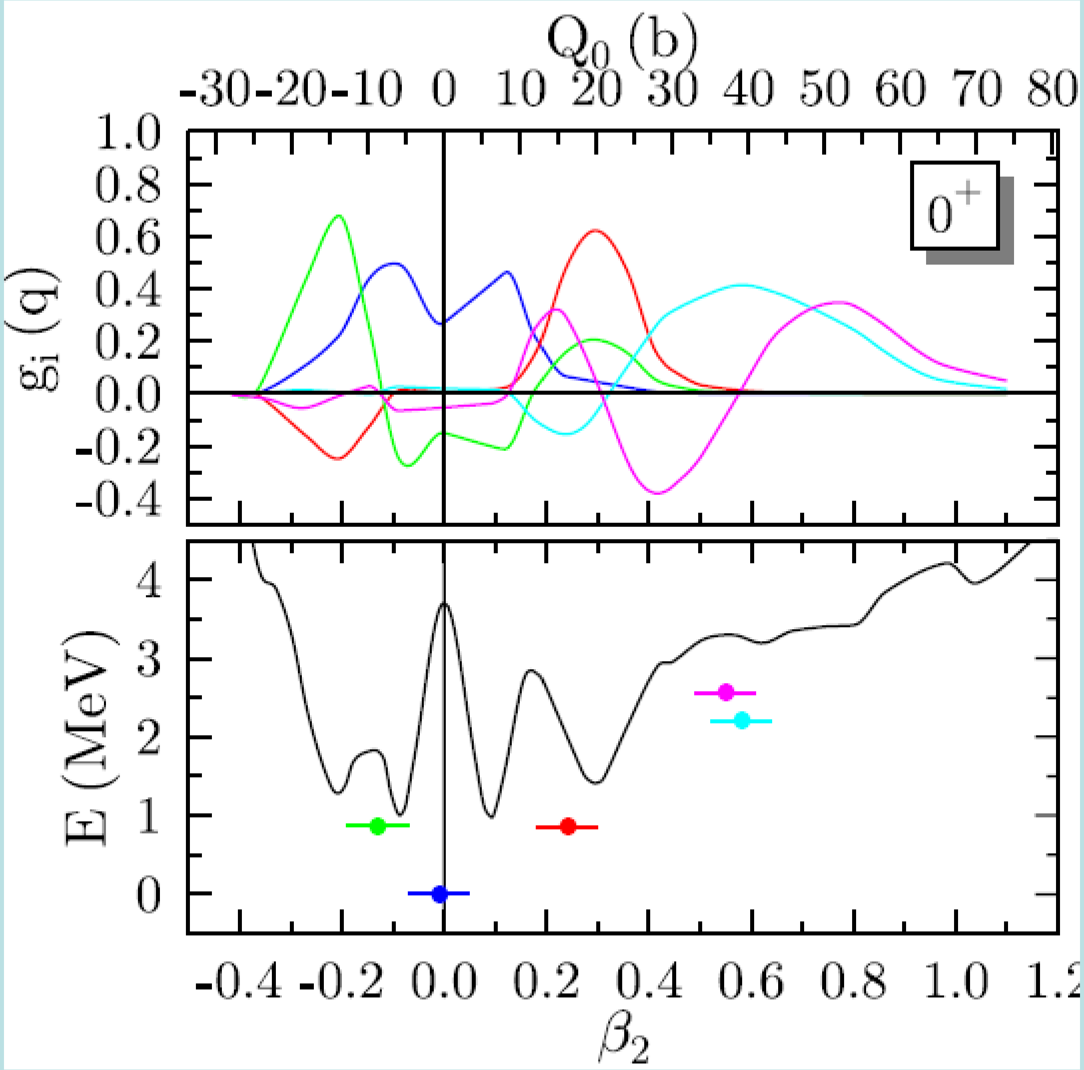
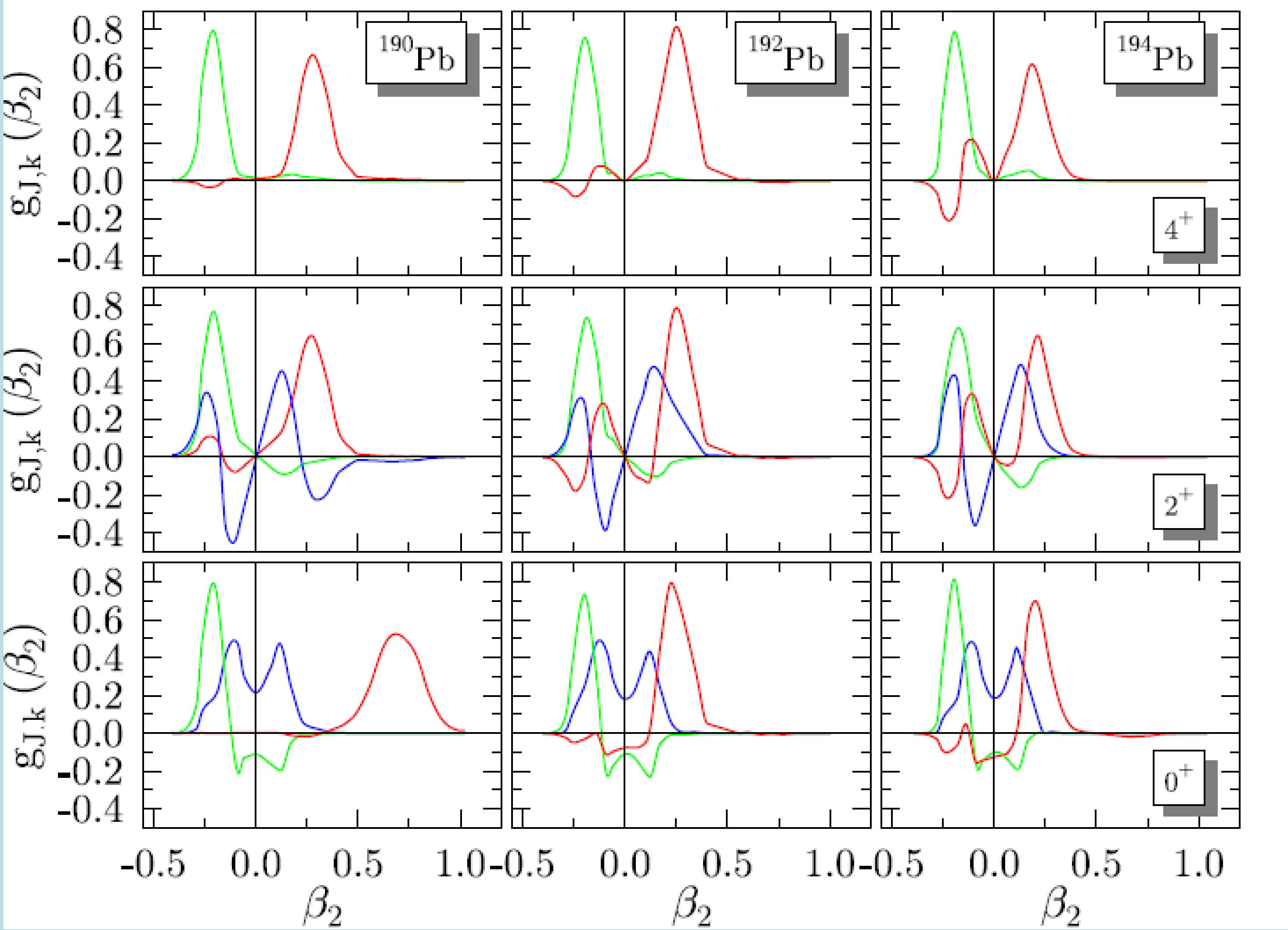


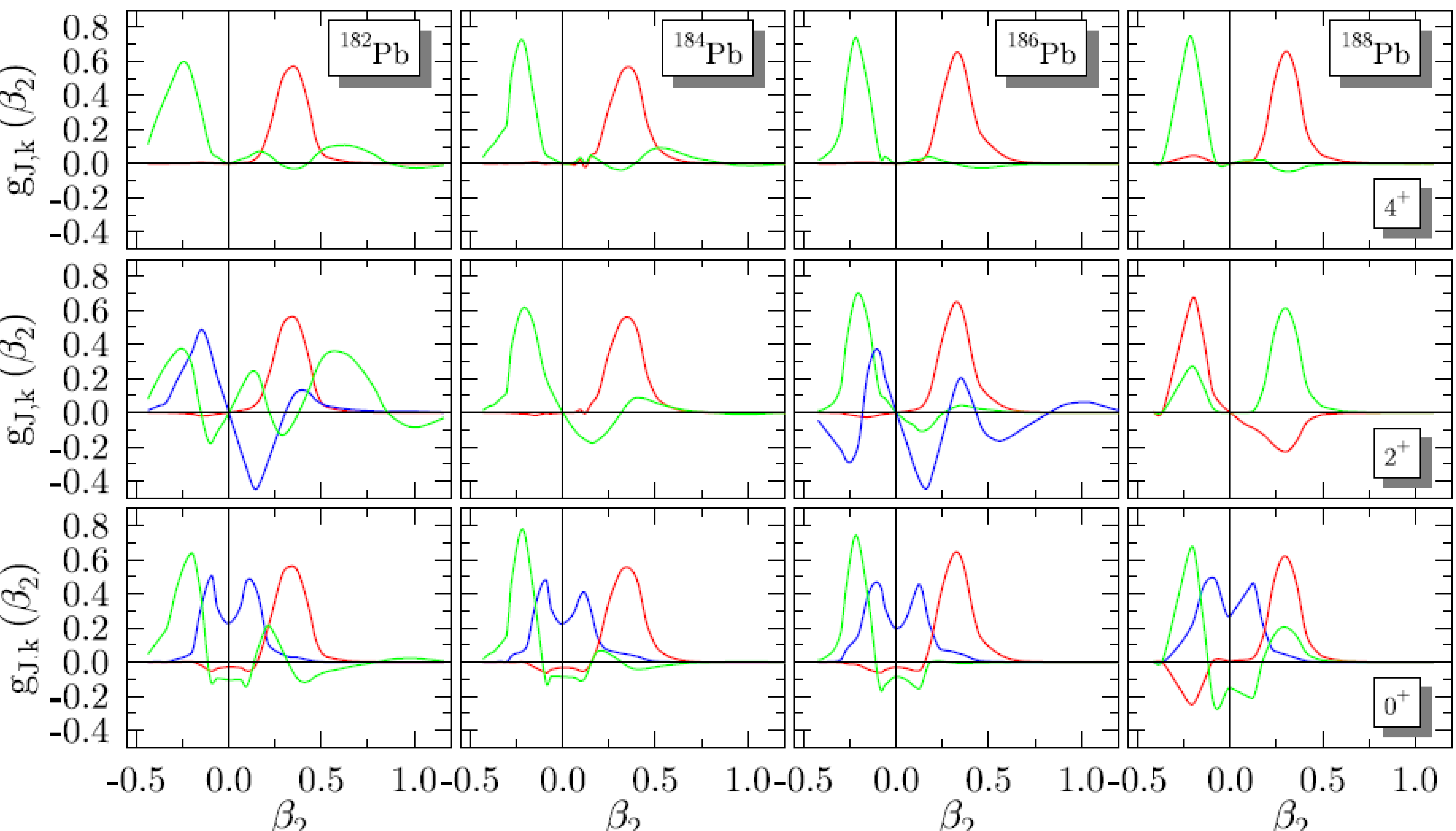
FIG. 3: Difference from the experimental mean square charge radii (*Expt*), the beyond mean field calculations with normal [4] (*MF*) and decreased pairing [18] (*MF**) and the IBM calculations (*IBM*) to the droplet model calculations for a spherical nucleus. Isodeformation lines from the droplet model at β_2=0.1 and 0.15 are shown.

Collective wave functions



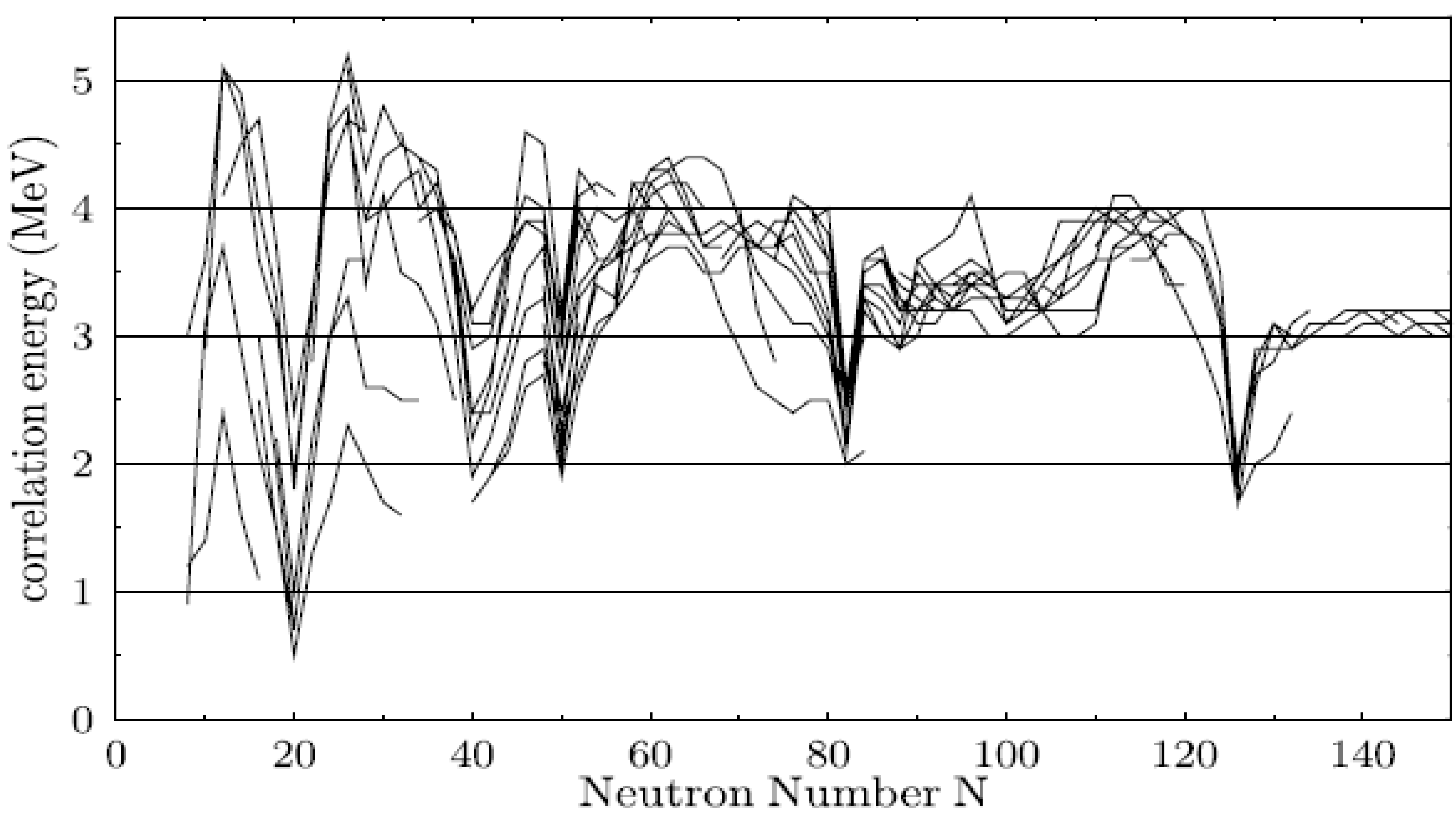


^{190}Pb
^{192}Pb
^{194}Pb
4^+
2^+
0^+
$g_{J,k}(\beta_2)$
β_2
0.8
0.6
0.4
0.2
0.0
-0.2
-0.4
-0.5
0.0
0.5
1.0



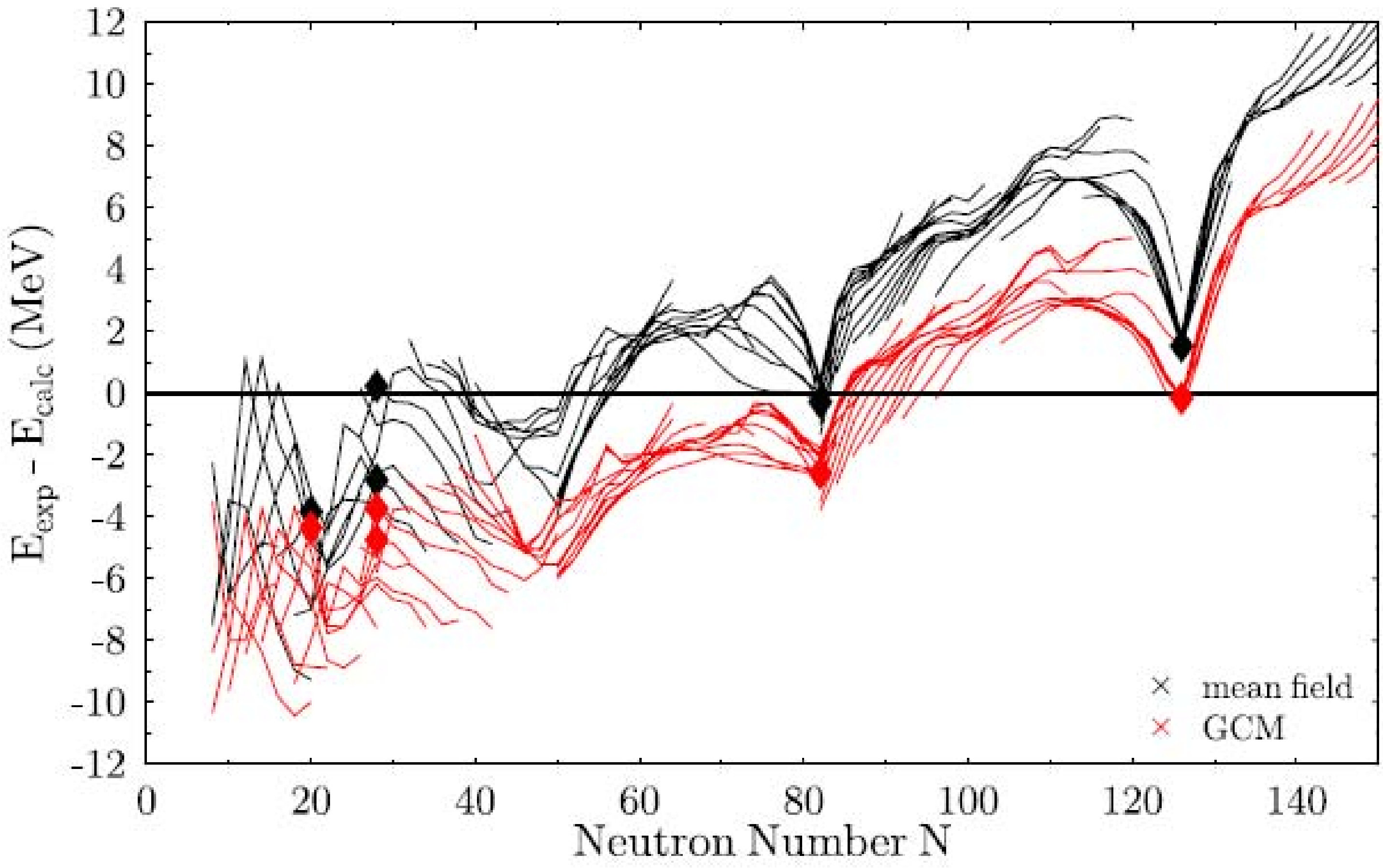
^{182}Pb
^{184}Pb
^{186}Pb
^{188}Pb
4^+
2^+
0^+
$g_{J,k}(\beta_2)$
β_2
0.8
0.6
0.4
0.2
0.0
-0.2
-0.4
-0.5
0.0
0.5
1.0

Global calculations



Correlations due to - symmetry restorations

- configuration mixing

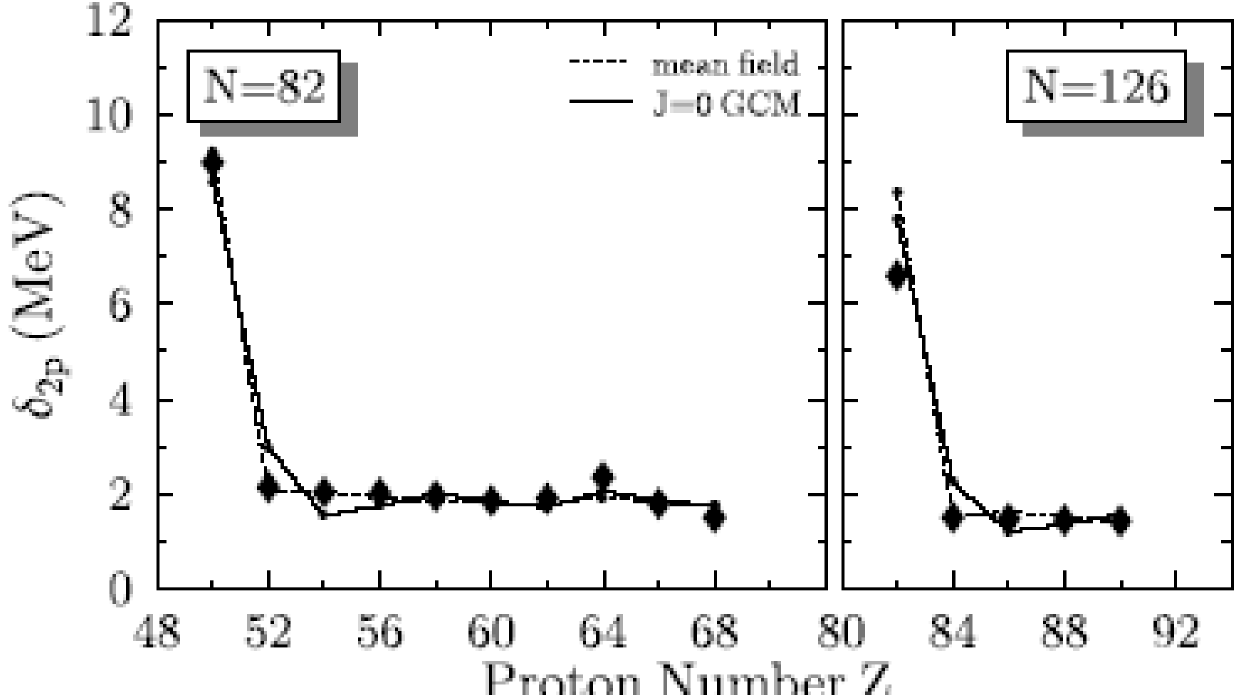


Difference between exp and theory for masses

Red: with correlations

Two-proton gap for chains

Isotonic



Isotopic