Beyond mean-field methods: success and problems

- Basis: Skyrme density functional

(but not many differences for RMF methods or Gogny force)

- M. Bender and P-H Heenen
- P. Bonche and H. Flocard

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- What is our goal ?
- How do we proceed ?
- What's next?

What do we want to do?

Some successful applications: spectra
transition probabilities
systematic calculations

Requirements: no ad hoc parameters
numerical accuracy
link to "simpler" models

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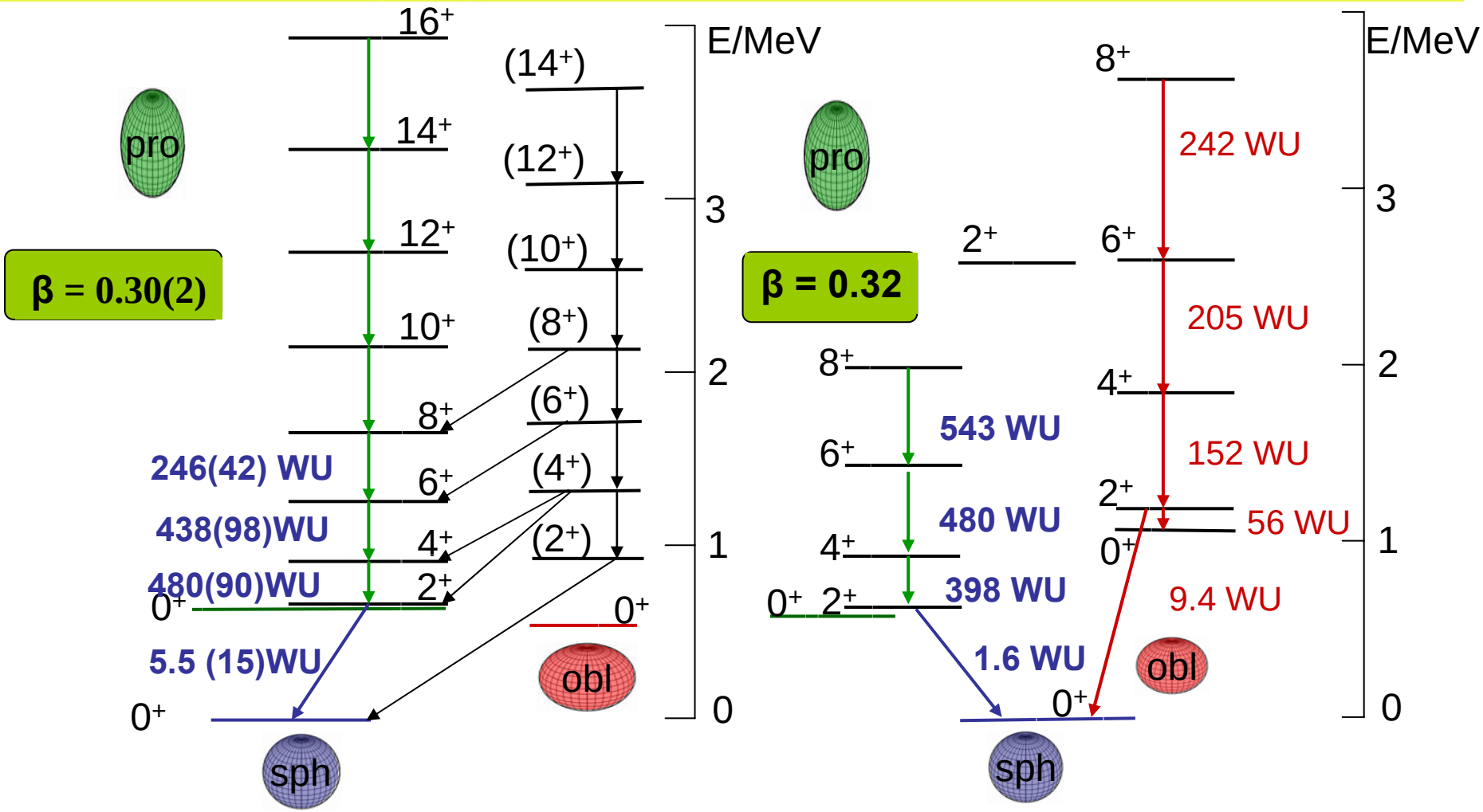
^{186}Pb

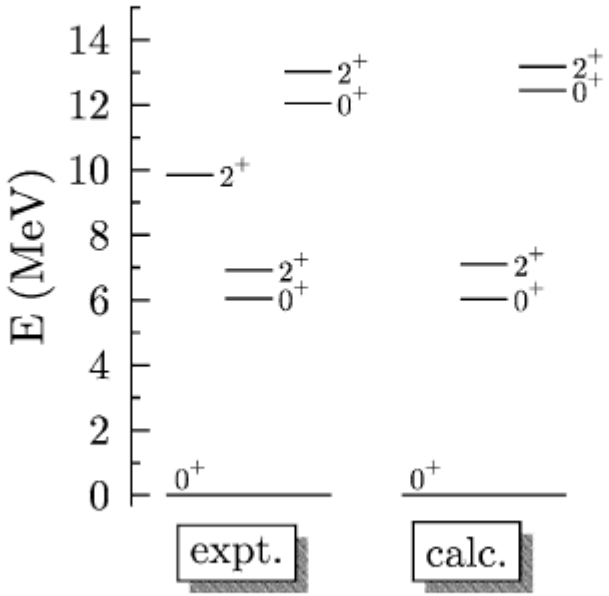
exp.

cal.

conf. mix of mean field states (Skyrme intera.SLy6)

M. Bender et al. PRC 69 (2004), 064303 & privat com.



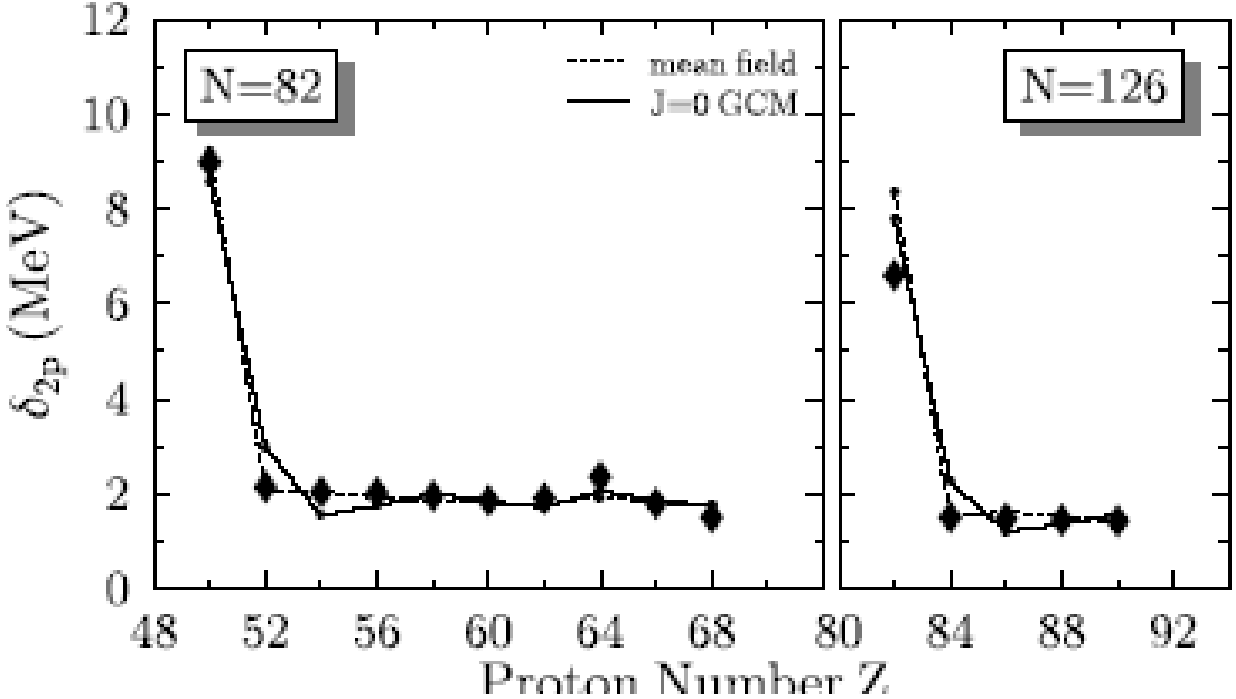


Comparison between the experimental and theoretical low-lying 0^+ and 2^+ states in ^{16}O.

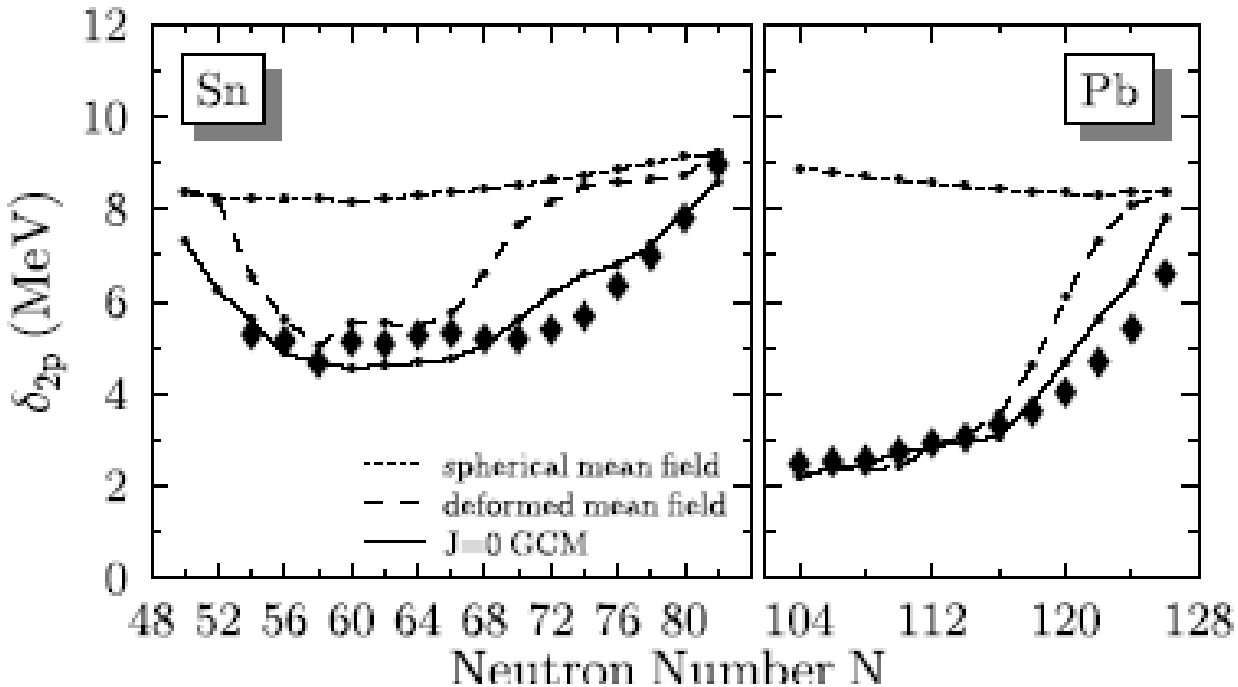
Transition	$B(\mathrm{E2})\uparrow/(e^2\,\mathrm{fm}^4)$		$Q_0(t)$ $(e\,\mathrm{fm}^2)$	$\beta_2(t)$	Transition	$M(\mathrm{E0})/\mathrm{fm}^2$	
	Expt.	Calc.				Expt.	Calc.
$2_1^+ \to 0_1^+$	42 ± 1.4	65.8	25.7	0.47	$0_2^+ \to 0_1^+$	3.55 ± 0.21	5.735
$2_2^+ \to 0_1^+$	21 ± 7	0.27	1.6	0.03	$0_3^+ \to 0_1^+$	4.03 ± 0.09	0.690
$2_1^+ \to 0_2^+$	370 ± 4	426	65.5	1.82			
$2_2^+ \to 0_2^+$	42 ± 7	6.7	8.2	0.15			
$2_2^+ \to 0_3^+$	–	1110	106	1.91			

Two-proton gap for chains

Isotonic



Isotopic



M. Bender, G. Bertsch and PHH

Phys. Rev. C 73 024322 (2006)

How to proceed?

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Starting point:

- Skyrme “HFB”
- Pairing with a density-dependent zero range interaction
- Solution of the HF equations on a 3D cartesian mesh (unrestricted nuclear shape)
- Lipkin Nogami method to simulate a Variation after N,Z projection
- Breaking of time-reversal invariance (cranking or qp excitations)

The energy functional:

$$\mathcal{E} = \mathcal{E}_{\rm kin} + \mathcal{E}_{\rm Sk} + \mathcal{E}_{\rm pairing} + \mathcal{E}_{\rm Coulomb} + \mathcal{E}_{\rm corr}\,.$$

The Skyrme functional:

$$\mathcal{E}_{\rm Sk} = \int d^3r \sum_{t=0,1} \left[\mathcal{H}_t^c(\mathbf{r}) + \mathcal{H}_t^{ls}(\mathbf{r}) + \mathcal{H}_t^t(\mathbf{r})\right].$$

$$\begin{aligned}\mathcal{H}_t^{\rm Sk} \;=\; & C_t^\rho[\rho_0]\,\rho_t^2 + C_t^{\Delta\rho}\rho_t\Delta\rho_t + C_t^\tau\,\rho_t\tau_t + C_t^{\nabla\cdot J}\rho_t\nabla\cdot\mathbf{J}_t \\ & -C_t^T\sum_{\mu,\nu=x}^{z} J_{t,\mu\nu}J_{t,\mu\nu} - C_t^F\left[\tfrac{1}{2}\Big(\sum_{\mu=x}^{z} J_{t,\mu\mu}\Big)^2 + \tfrac{1}{2}\sum_{\mu,\nu=x}^{z} J_{t,\mu\nu}J_{t,\nu\mu}\right].\end{aligned}$$

8 parameters for the central part
2 parameters for the spin orbit
2 parameters for the tensor (if considered as an interaction)

Fitting protocol

- Masses and radii of ^{40}Ca, ^{48}Ca, ^{56}Ni, ^{90}Zr, ^{132}Sn, ^{208}Pb
- Mass of ^{100}Sn
- Spin orbit splitting neutron 3p state in ^{208}Pb
- Empirical values of E/A and ρ_0 of symmetric nuclear matter
- Equation of state of pure neutron matter of Wiringa
- Incompressibility, symmetry energy and isovector effective of nuclear matter are fixed to specific values.

- Tensor ????

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:

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

(cut-off in κ in J and q)

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:

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

Core of the problem: determination of the kernels:

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

Projection on angular momentum

=

From intrinsic to laboratory frame of reference

No approximation based on the collective model for transition probabilities.

The HWG solutions permit to calculated EM transition probabilities:

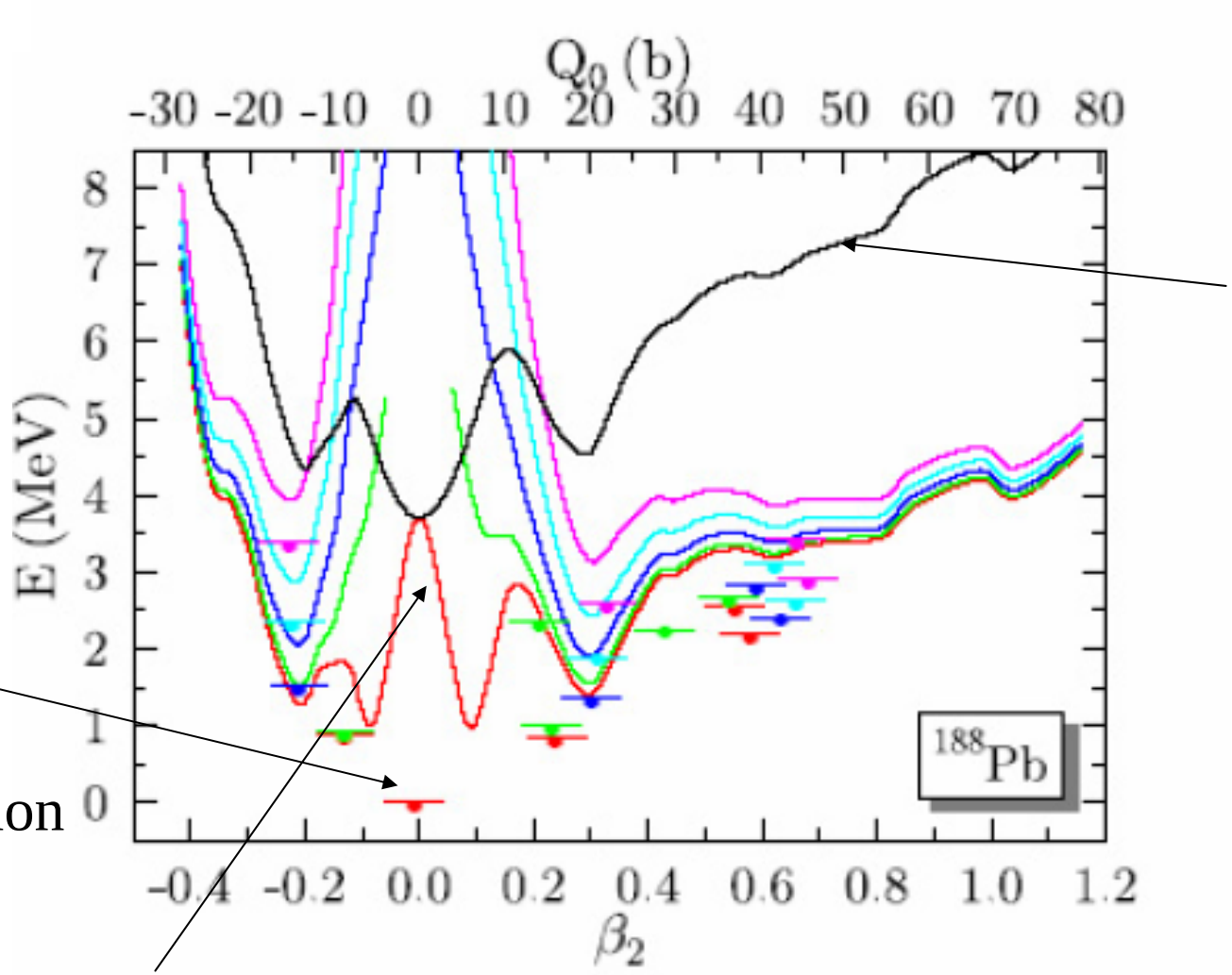
$$B(E2; J'_{\nu'} \rightarrow J_{\nu}) = \frac{e^2}{2J'+1} \sum_{M=-J}^{+J} \sum_{M'=-J'}^{+J'} \sum_{\mu=-2}^{+2} \left| \langle JM\nu \middle| \hat{Q}_{2\mu} | J'M'\nu' \rangle \right|^2$$

Spectroscopic Q moments:

$$Q_s(J_{\nu}) = \sqrt{\frac{16\pi}{5}} \, \langle JM = J \, \nu | \hat{Q}_{20} | JM = J \, \nu \rangle \, .$$

$$B(M1; J'_{\nu'} \rightarrow J_{\nu}) = \frac{3}{4\pi} \frac{1}{2J'+1} \sum_{M=-J}^{+J} \sum_{M'=-J'}^{+J'} \sum_{\mu=-1}^{+1} \left| \langle JM\nu | \hat{\mu}_{\mu} | J'M'\nu' \rangle \right|^2$$

Up to now: restrictions to axial deformations

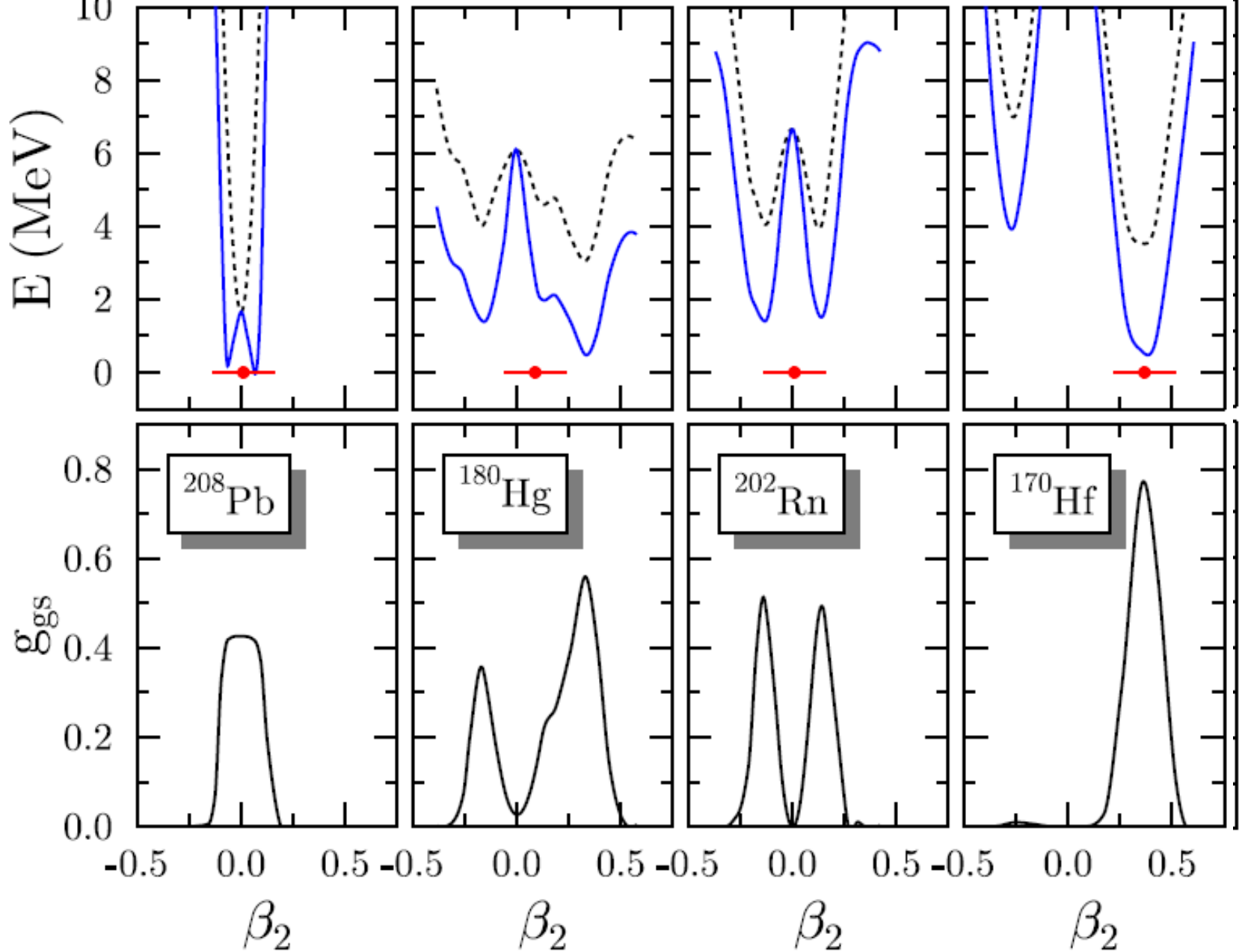


Mean field

Bars at a "mean" deformation

Mean field projected on J=0

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


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

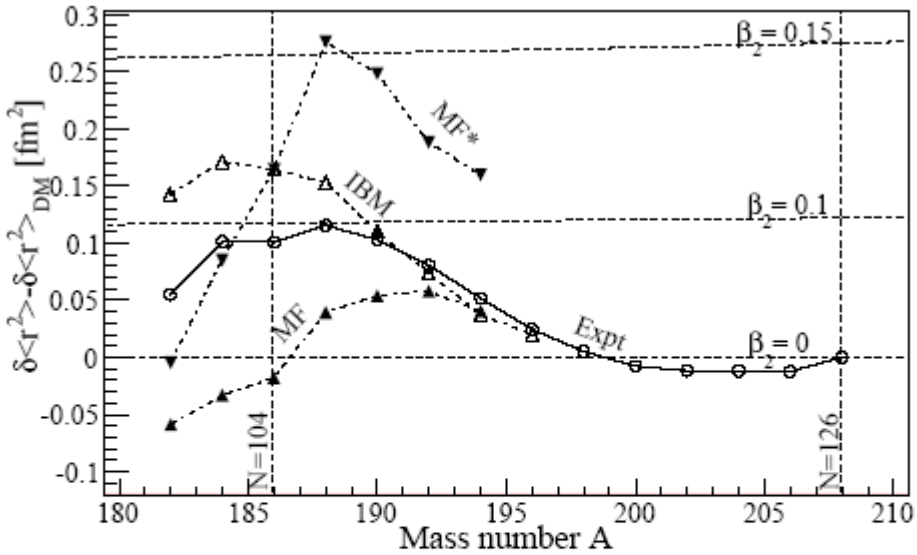


FIG. 3: Difference from the experimental mean square charge radii (*Expt*), the beyond mean field calculations with normal [4] (*MF*) and decreased pairing [18] (*MF**) and the IBM calculations (*IBM*) to the droplet model calculations for a spherical nucleus. Isodeformation lines from the droplet model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

H. De Witte et al. Phys. Rev. Lett. **98**, 112502 (2007)

What's next?

Main drawback is related to the modeling of the strong interaction.

Link with non empirical interactions?
How to define properly an EDF? Divergence and steps?
Density dependence in multi reference calculations?
On which data to adjust an EDF?

T. Lesinski: Non-empirical pairing functional and first-order contribution to pairing in finite nuclei
T. Duguet: Nuclear EDF

New terms in the EDF/interaction: "l^2 terms"

Developments seem to be compatible with our method.

Breaking of symmetries:

Triaxiality
Time reversal invariance (spectra)
New modes (pairing vibrations)

Already included, although at a prohibitive computational cost
Require to solve the divergence/step problems to be applied systematically.

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