Description of properties of heavy and very heavy nuclei: mean field and beyond

Michael Bender

Institut de Physique Nucléaire de Lyon
CNRS/IN2P3, Université de Lyon, Université Lyon 1
69622 Villeurbanne, France

Workshop on

Physics at the Super Separator Spectrometer S^3

Espace de Structure et de réactions Nucléaires Théorique
Saclay, 27-30 March 2017

Modeling of heavy and very heavy nuclei

Main ingredients:

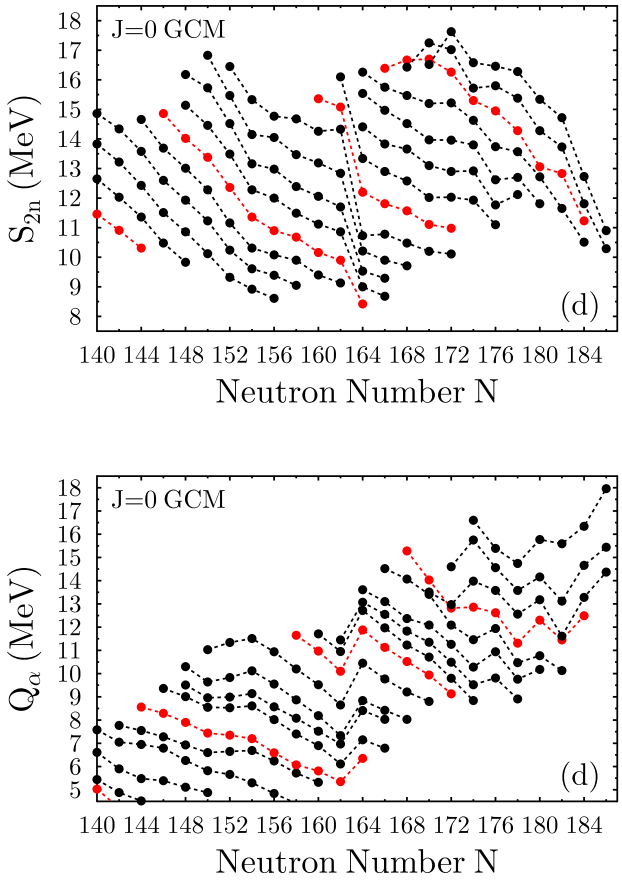
- Self-consistent mean-field
- Effective interaction / effective energy density functional
- Correlations "beyond the mean field"

Description of excited states

- single-particle excitations $\Rightarrow$ blocked HFB
- rotational bands $\Rightarrow$ cranked HFB
- small-amplitude shape vibrations $\Rightarrow$ Random Phase Approximation (RPA)
- large-amplitude shape vibrations $\Rightarrow$ Generator Coordinate Method (GCM)
- shape coexistence $\Rightarrow$ Generator Coordinate Method
- Restoration of symmetries with projection methods is always a good idea (selection rules, . . .)

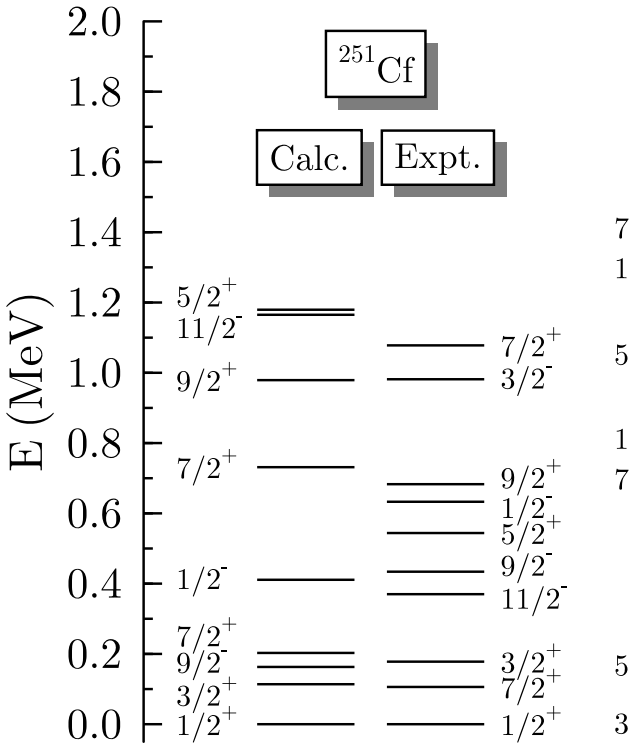
Indicators of (deformed) shell structure

Mass differences



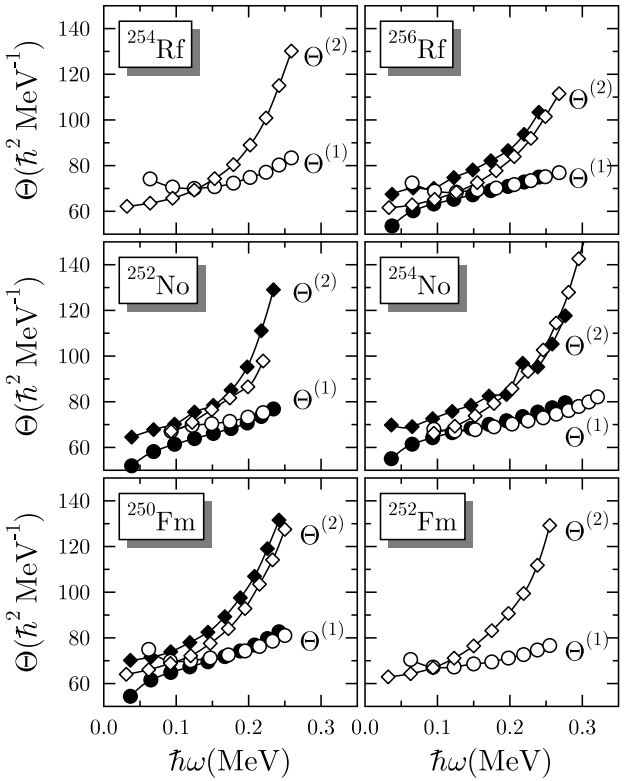
Bender and Heenen, to be published

Spectra of bandheads in odd-mass nuclei



Bender, Bonche, Duguet, Heenen, NPA723 (2003) 354

Moment of inertia

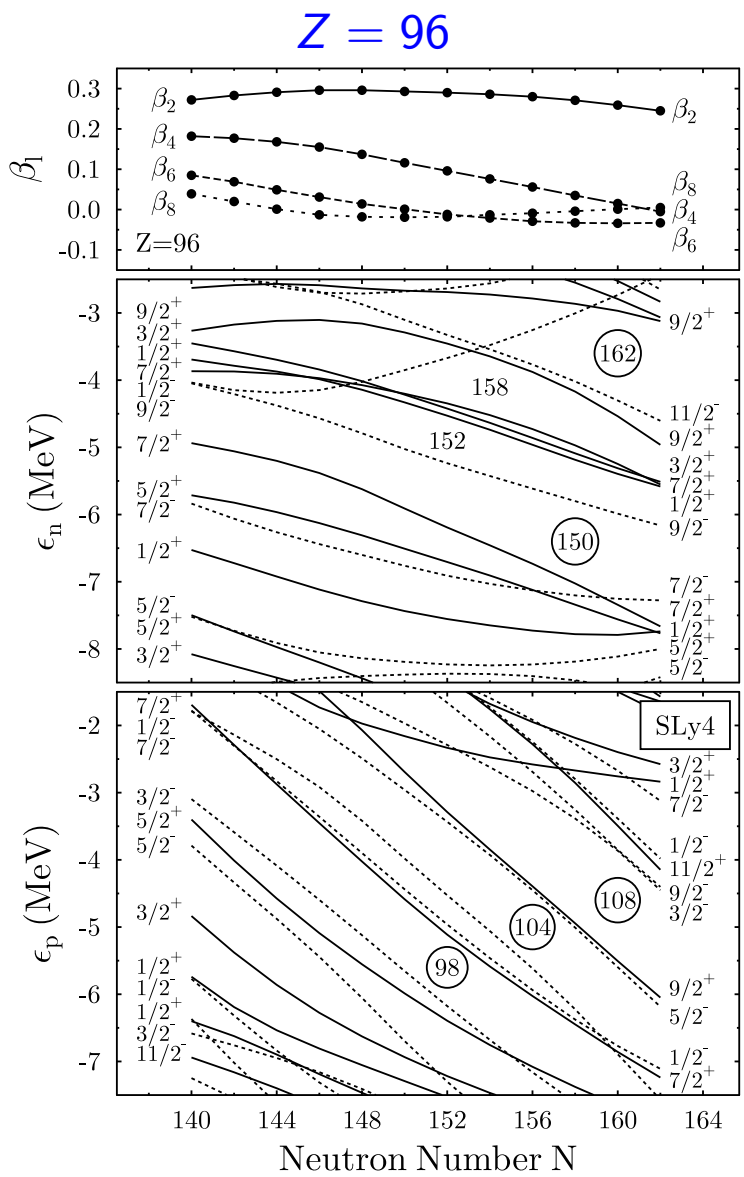


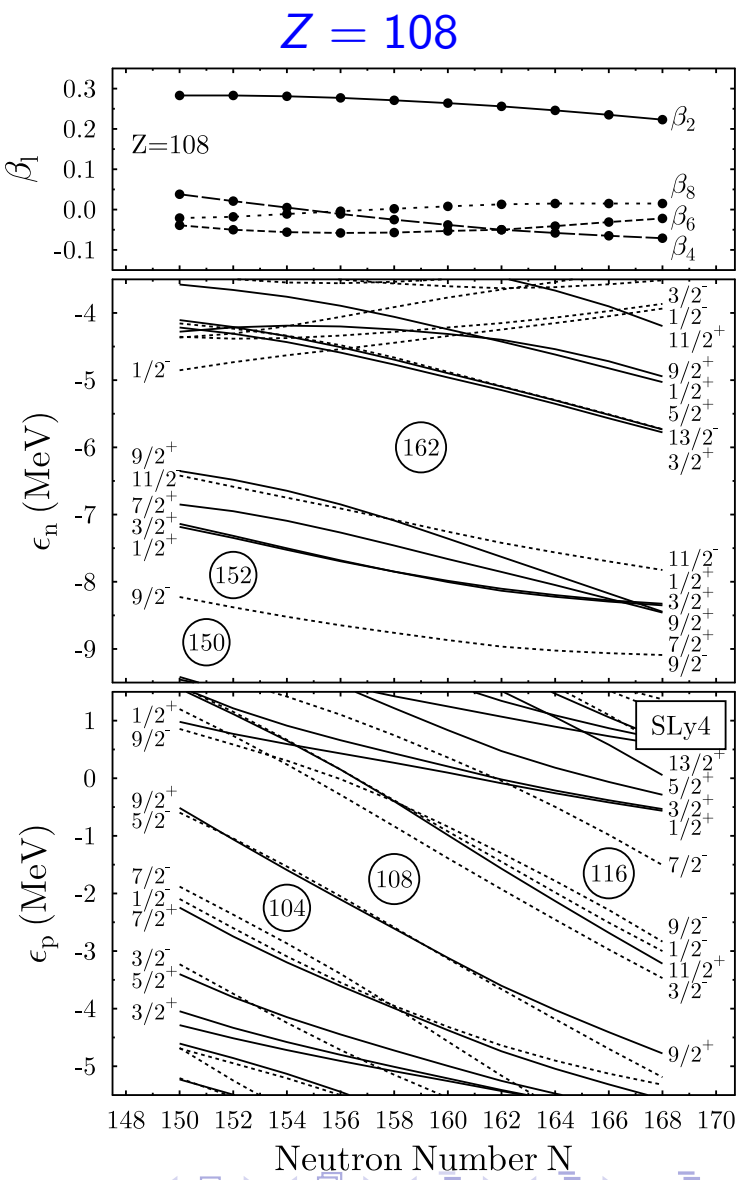
Bender and Heenen, J. Phys. Conf. Ser. 420 (2013) 012002

Some noteworthy physics to expect

Evolution of deformed shells with SLy4

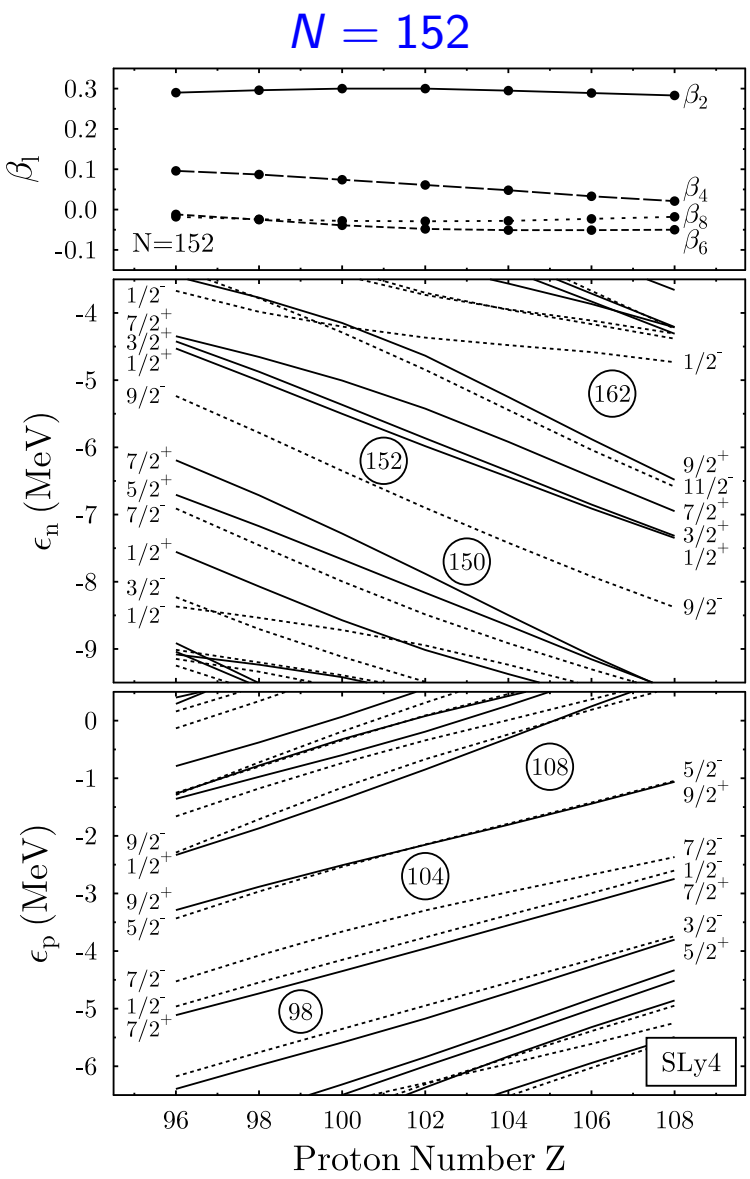
Bender and Heenen, to be published

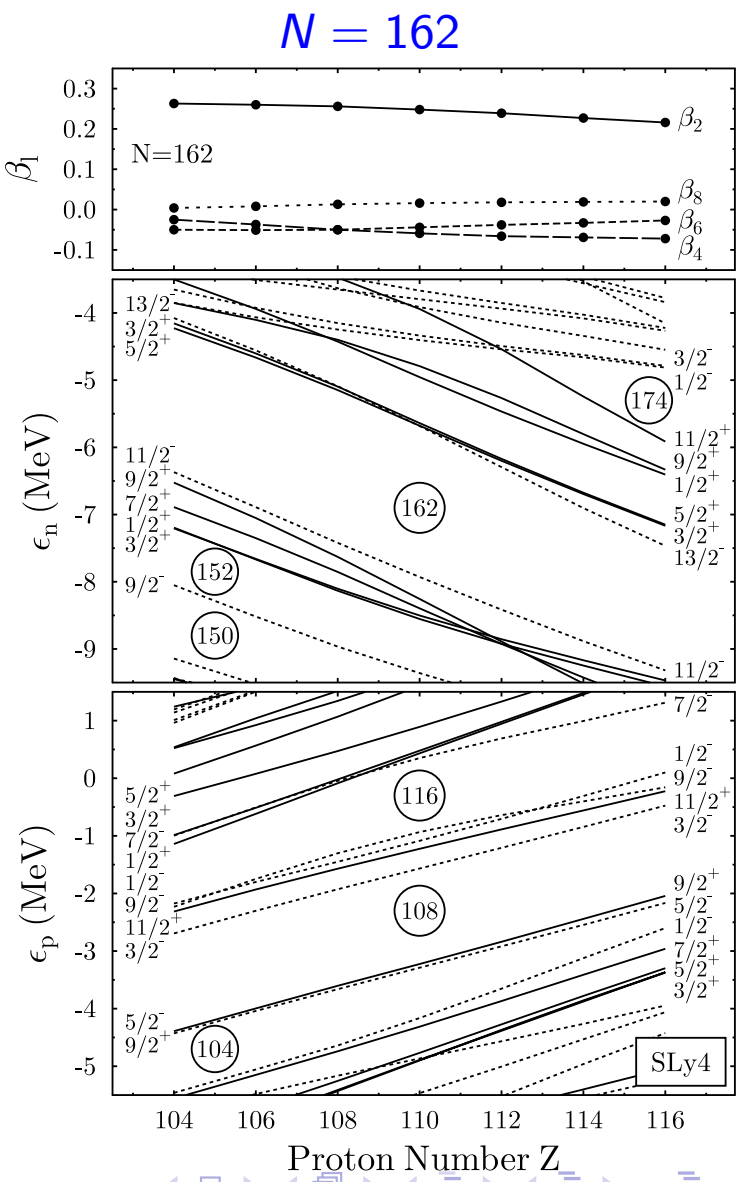




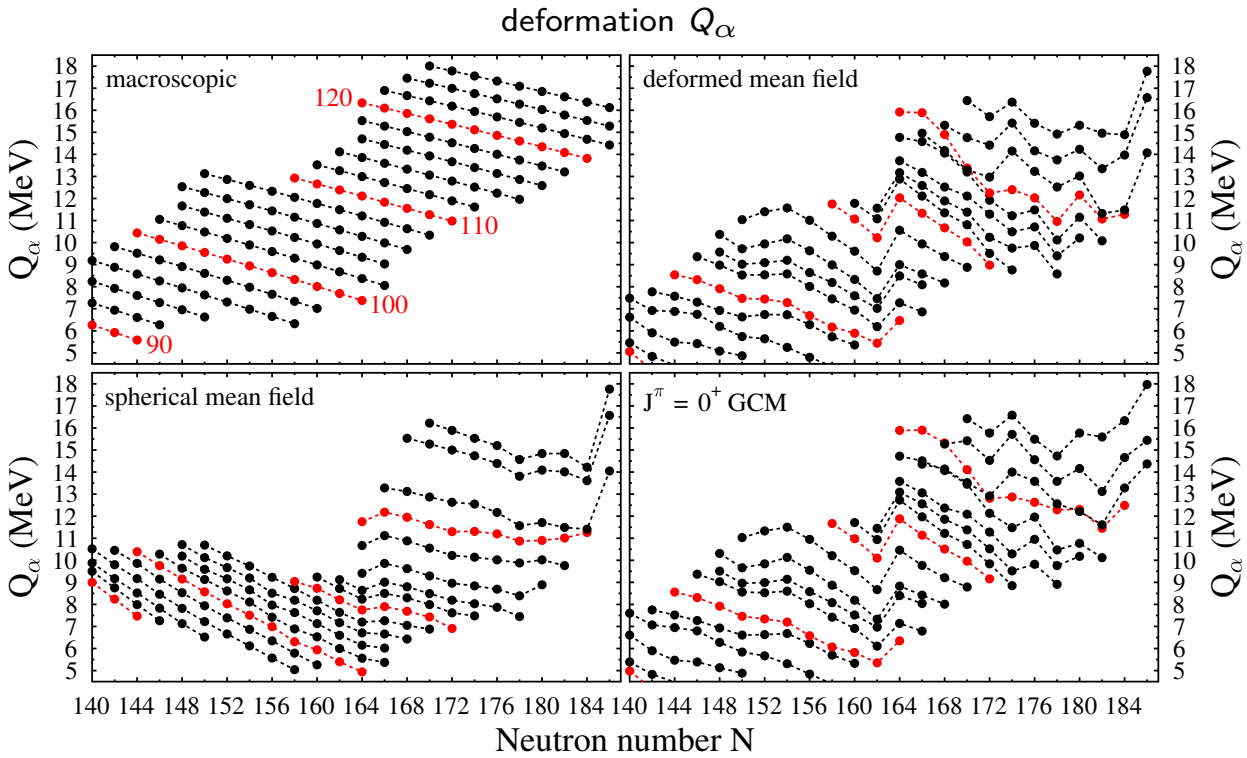
Evolution of deformed shells with SLy4

Bender and Heenen, to be published

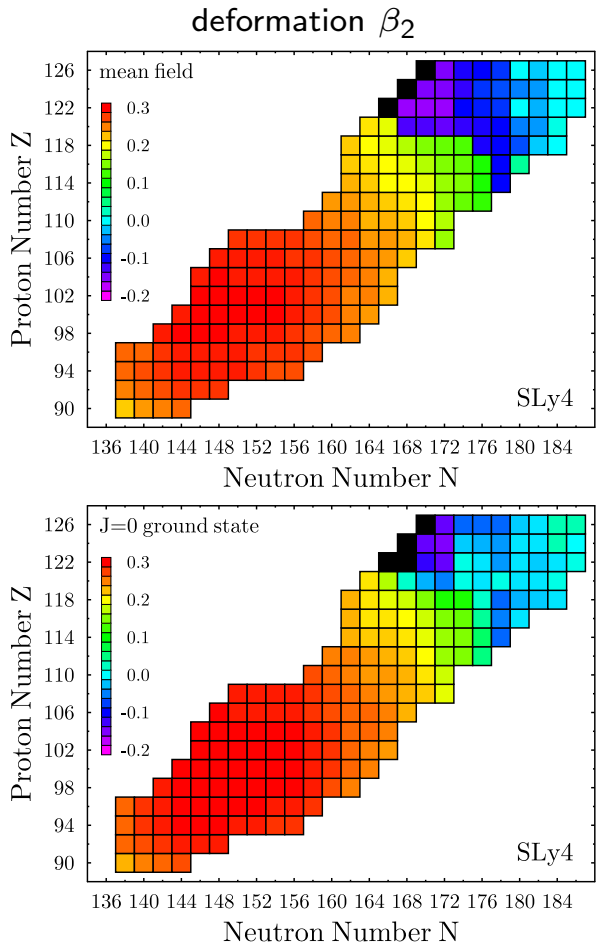




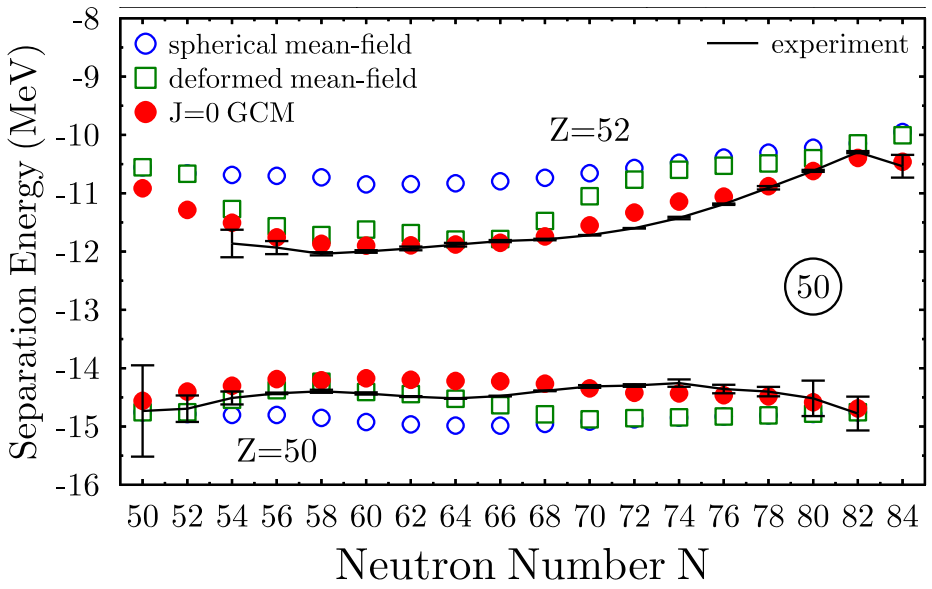
Correlations beyond the mean field



Heenen, Bender, Bally & Ryssens, EPJ WoC 131 2016 02001

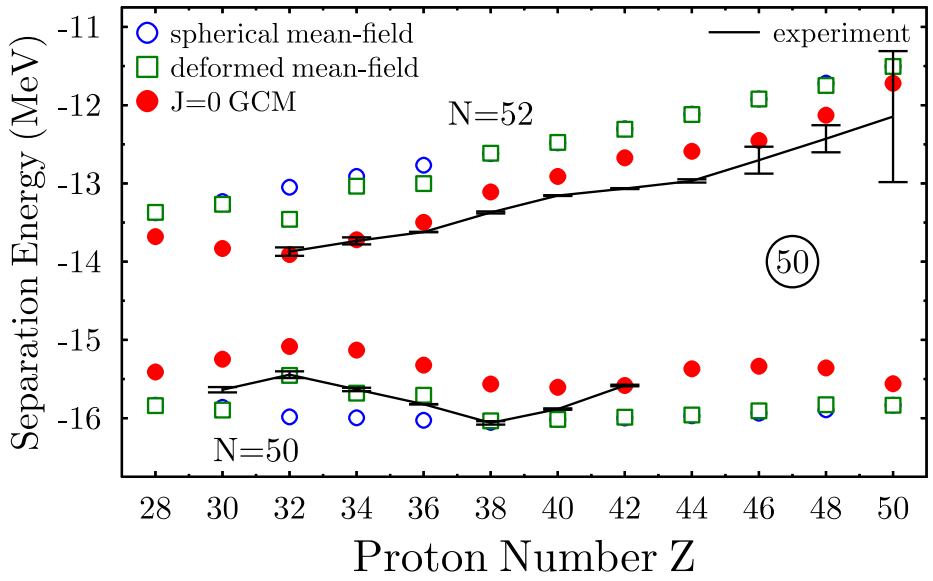


Collectivity-induced quenching of indicators of shell structure



$-S_{2p}(Z=50, N)/2$

The global linear trend is taken out subtracting $\frac{N-82}{2}\,[S_{2p}(Z{=}50, N{=}50) - S_{2p}(Z{=}50, N{=}82)]$ using the spherical mean-field values

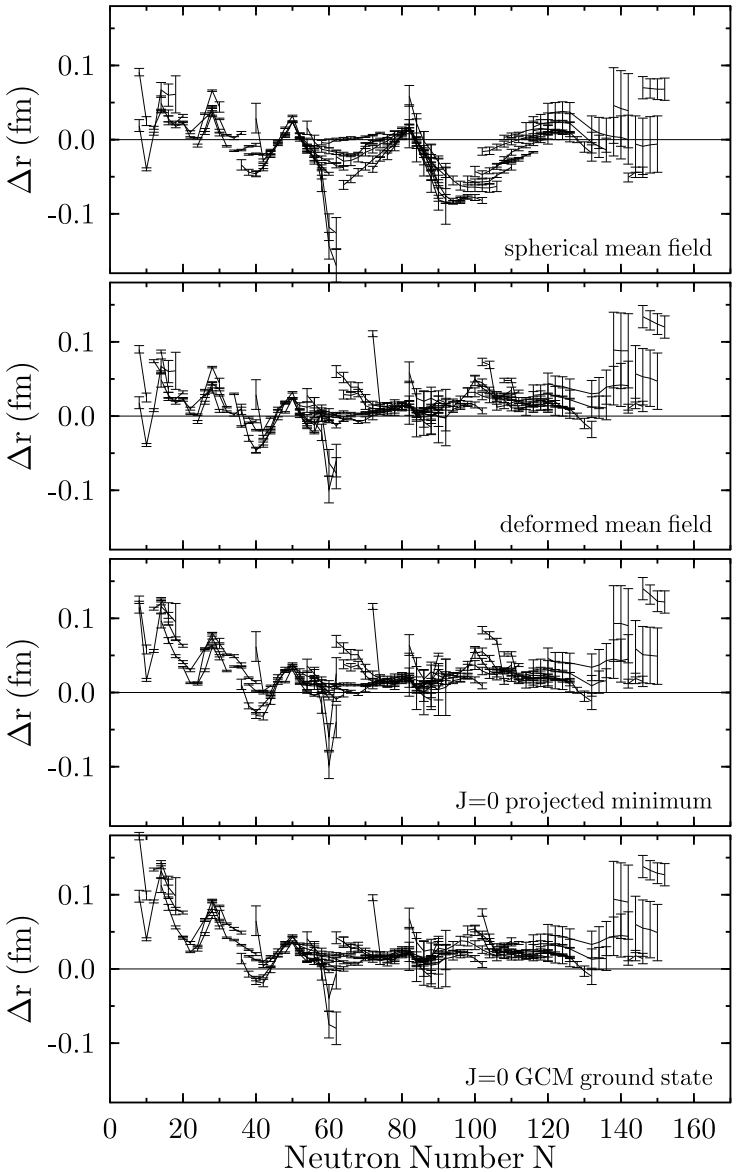


$-S_{2n}(Z, N=50)/2$

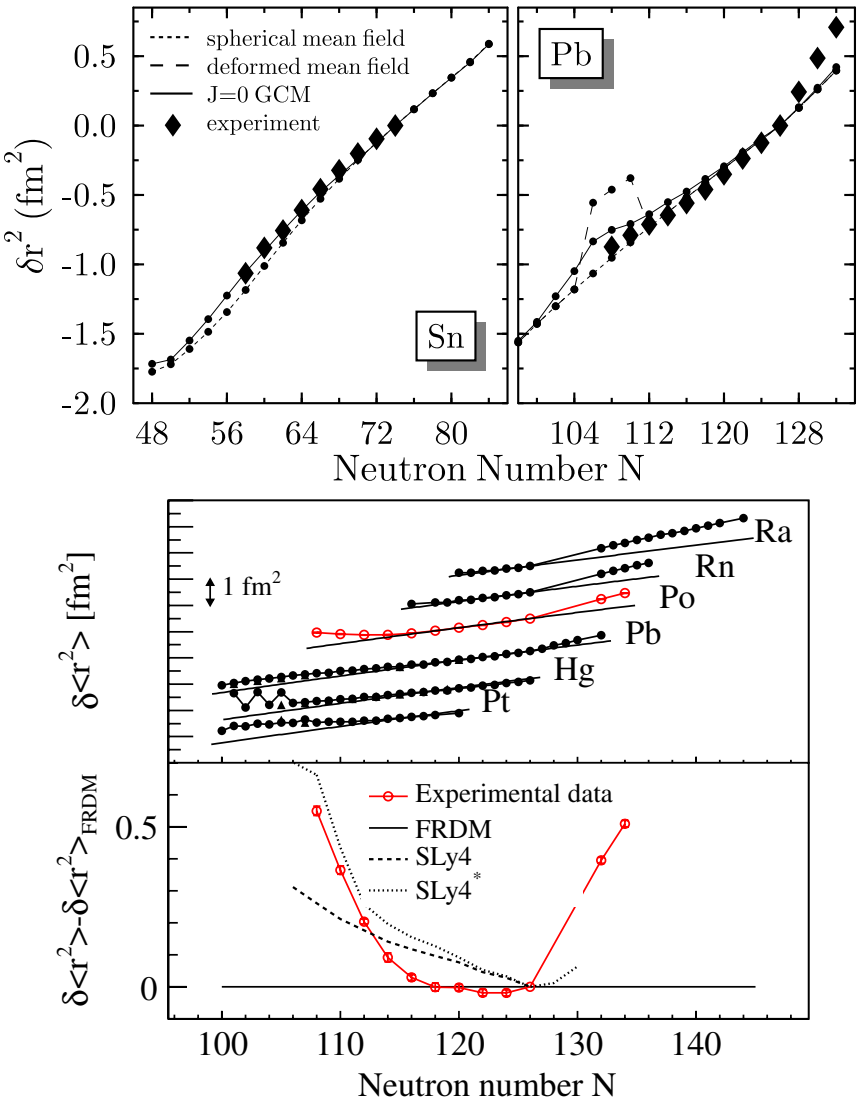
The global linear trend is taken out subtracting $\frac{N-50}{2}\,[S_{2n}(Z{=}28, N{=}50) - S_{2n}(Z{=}50, N{=}50)]$ using the spherical mean-field values

Bender, Bertsch, Heenen, PRC 78 (2008) 054312

charge radii: Experimental signatures of shape mixing



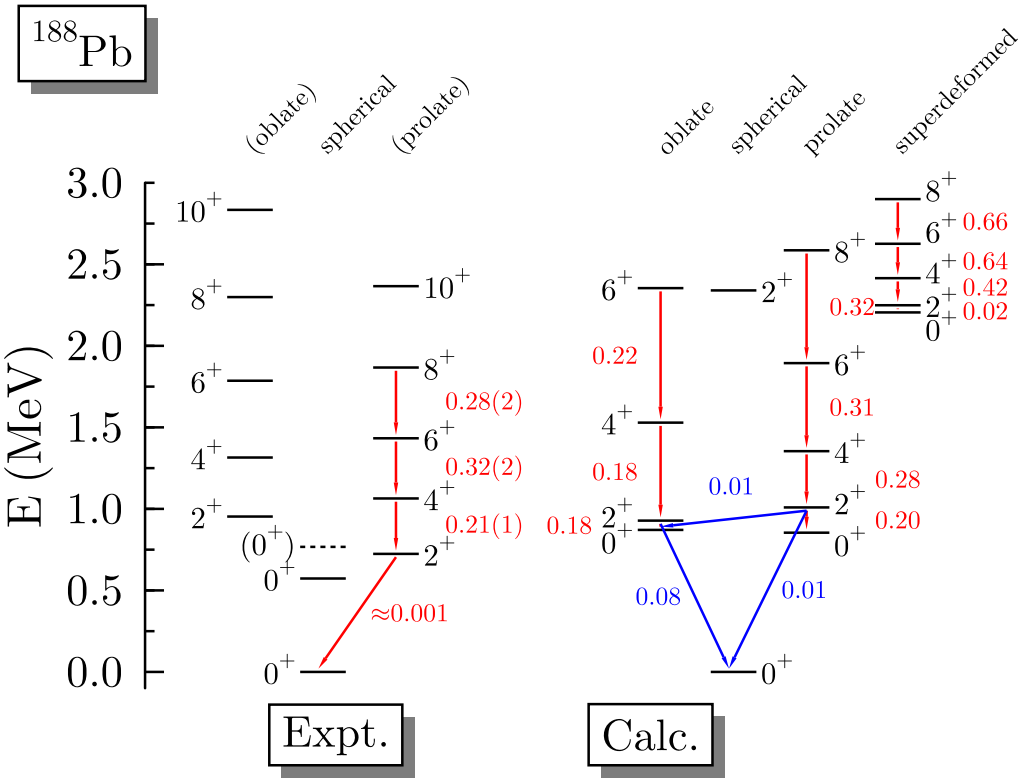
Bender, Bertsch, Heenen, PRC 78 (2008) 054312



Cocolios, *et al*, PRL 106 (2011) 052503.

Transition moments

Bender, Bonche, Duguet, Heenen, PRC 69 (2004) 064303.
Experiment: Grahn *et al*, PRL **97** (2006) 062501



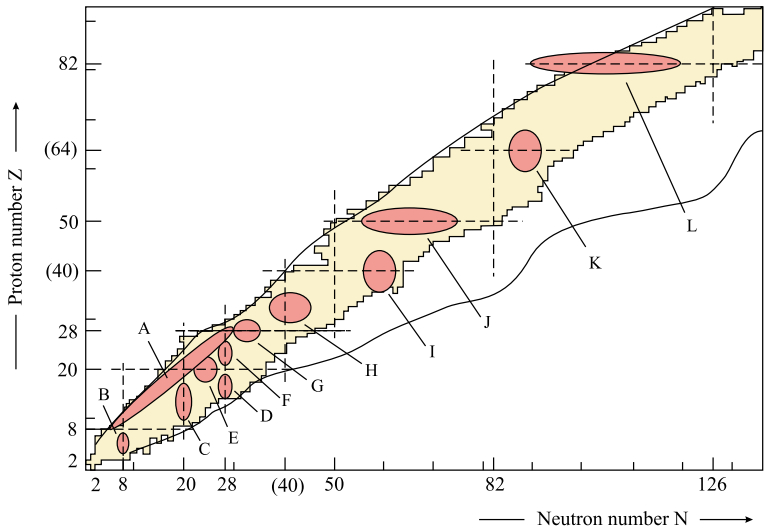
- in-band and out-of-band $E2$ transition moments calculated in the laboratory frame, respecting selection rules
- full model space of occupied particles
- only occupied single-particle states contribute to the kernels ("horizontal expansion")
- $\Rightarrow$ *no effective charges necessary*
- *no adjustable parameters*

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

$$\beta_2^{(t)} = \frac{4\pi}{3R^2A}\sqrt{\frac{B(E2; J \to J-2)}{(J\,0\,2\,0\,|(J-2)\,0)^2 e^2}} \quad \text{with} \quad R = 1.2\,A^{1/3}$$

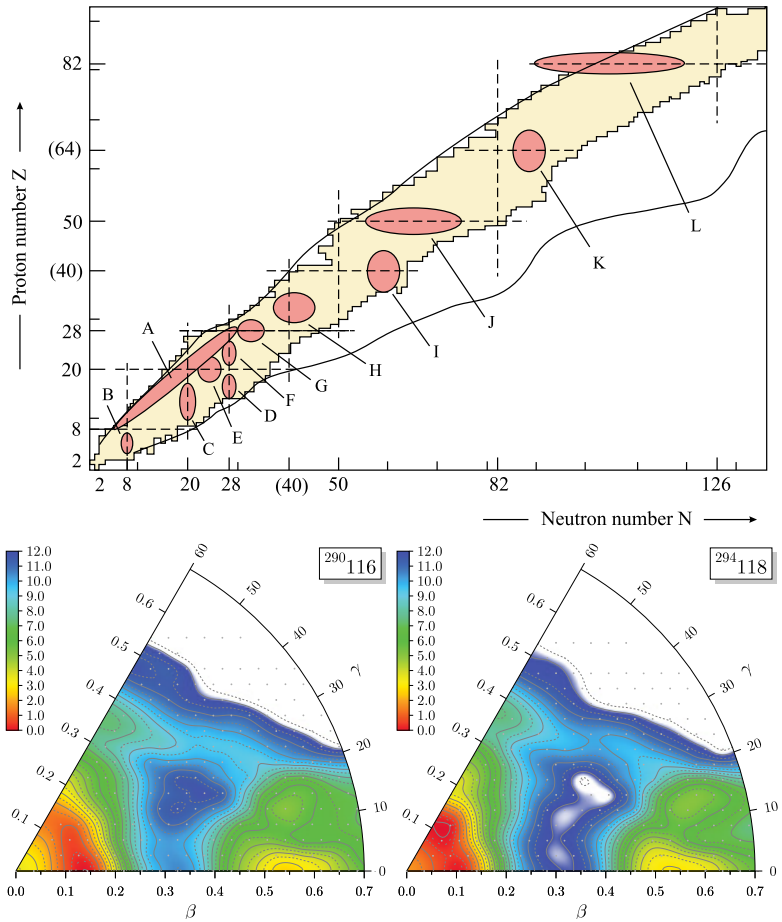
Coexistence in normal nuclei, exotic nuclei, and elsewhere

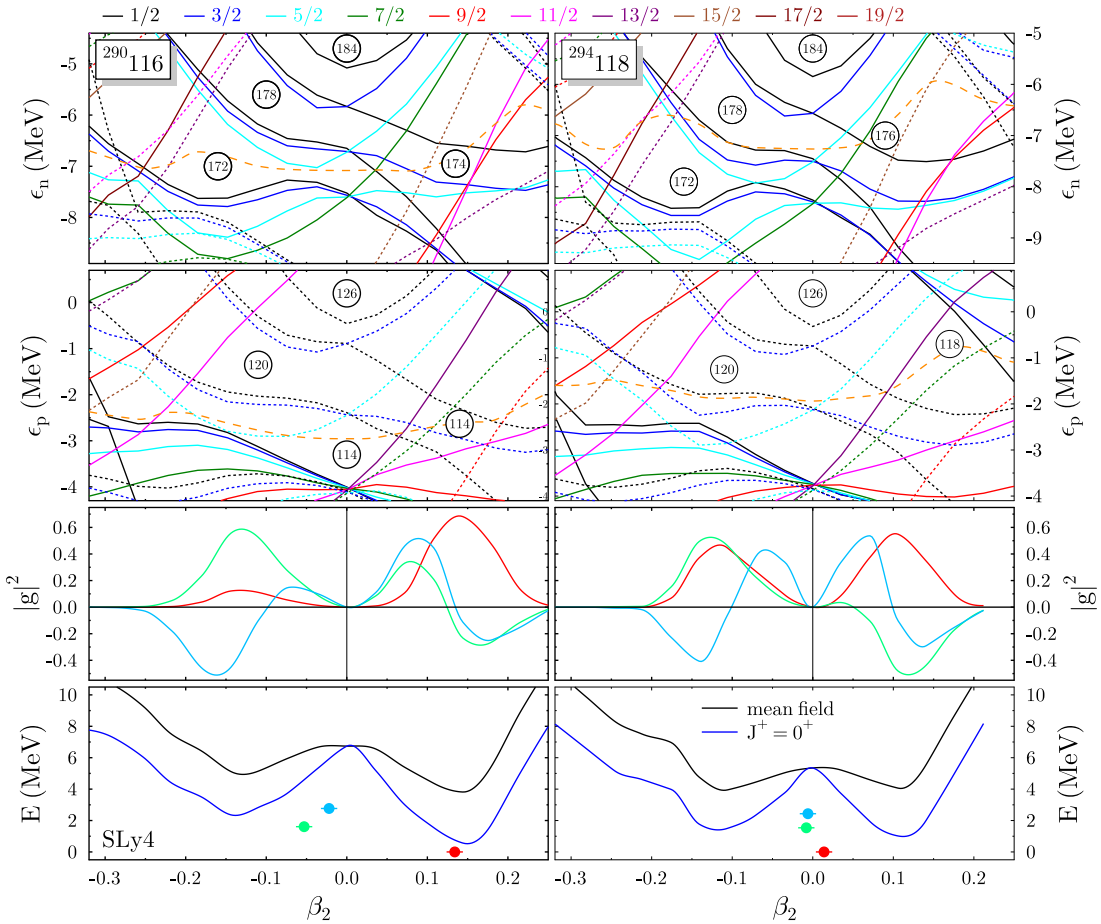
Heyde & Woods, RMP 83 (2011) 1467



Coexistence in normal nuclei, exotic nuclei, and elsewhere

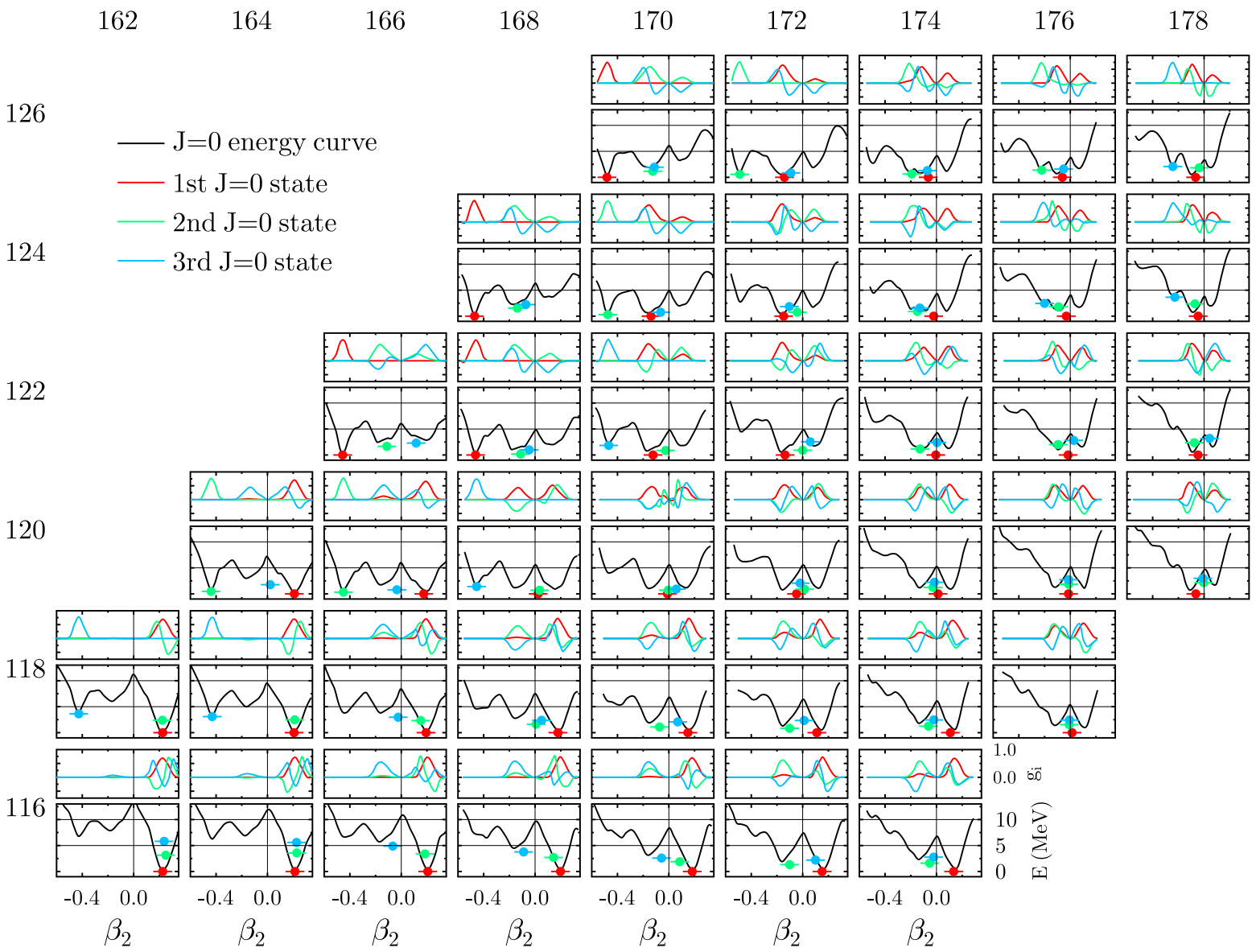
Heyde & Woods, RMP 83 (2011) 1467





Heenen, Bender, Bally & Ryssens, EPJ WoC 131 2016 02001

Configuration mixing for superheavy nuclei



Bender and Heenen, to be published
extension of Bender, Bertsch, Heenen, PRC 73 (2006) 034322 to heavier nuclei

Modeling in progress

Mean-field-based models – Ongoing research

Construction of better effective interactions

- construction of better parameterizations of existing forms (which cannot be pushed much further)
- construction of new forms of the nuclear EDF
- recognition of formal constraints on the form of the nuclear EDF

Refined modeling of the nuclear states:

- towards symmetry-unrestricted mean-field calculations
- explicit treatment of correlation effects

Symmetry considerations

- quasiparticle excitations (and odd- and odd-odd nuclei in general) $\Leftrightarrow$ broken time-reversal symmetry
- rotating nuclei ("cranking") $\Leftrightarrow$ broken time-reversal symmetry
- collectively rotating nuclei ("cranking") $\Leftrightarrow$ broken axial symmetry
- octupole correlations $\Leftrightarrow$ broken parity
- rotating quasiparticle excitations $\Leftrightarrow$ broken signature symmetry

Up to now, very few calculations combine broken time-reversal symmetry and broken parity, or broken signature in addition to broken time-reversal symmetry.

Known deficiencies: incorrect deformed shell closures

Bender and Heenen, J. Phys. Conf. Ser. 420 (2013) 012002

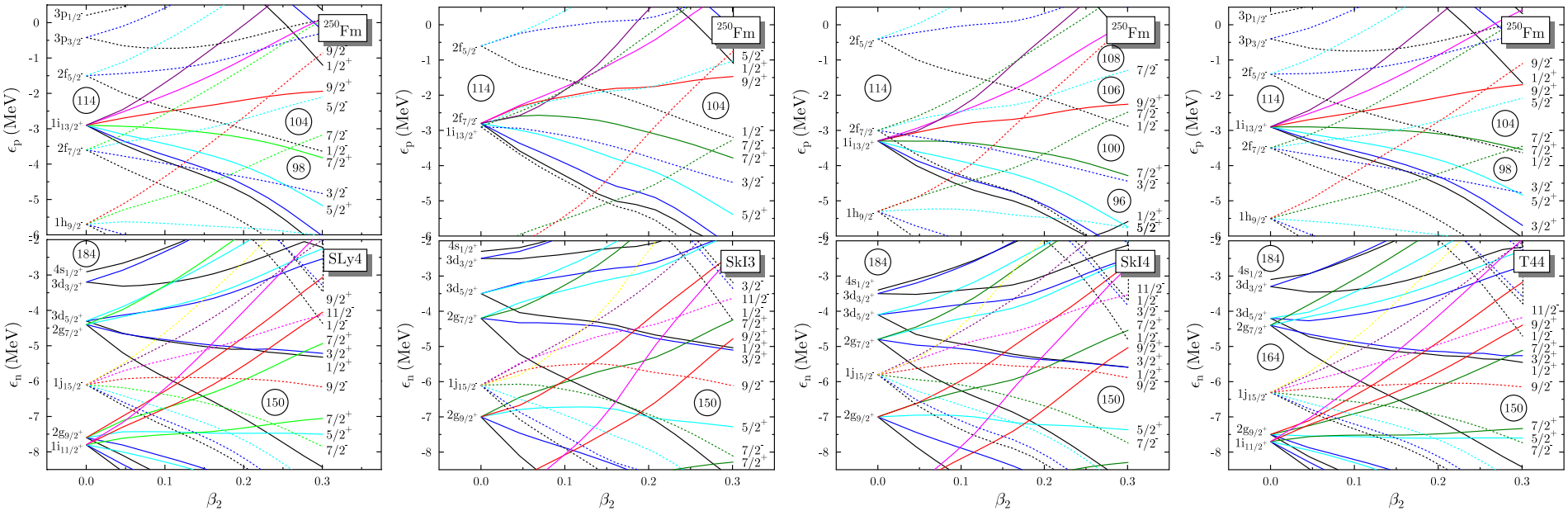
Nilsson diagrams of ^{250}Fm

SLy4
standard spin-orbit

SkI3
modified spin-orbit

SkI4
modified spin-orbit

T44
tensor force added



- Nilsson diagram of protons (top) and neutrons (bottom) going from spherical shape (left) to the prolate deformed ground state (right)
- different colours indicate different mean values of j_z
- compare bunching of levels, not the details.

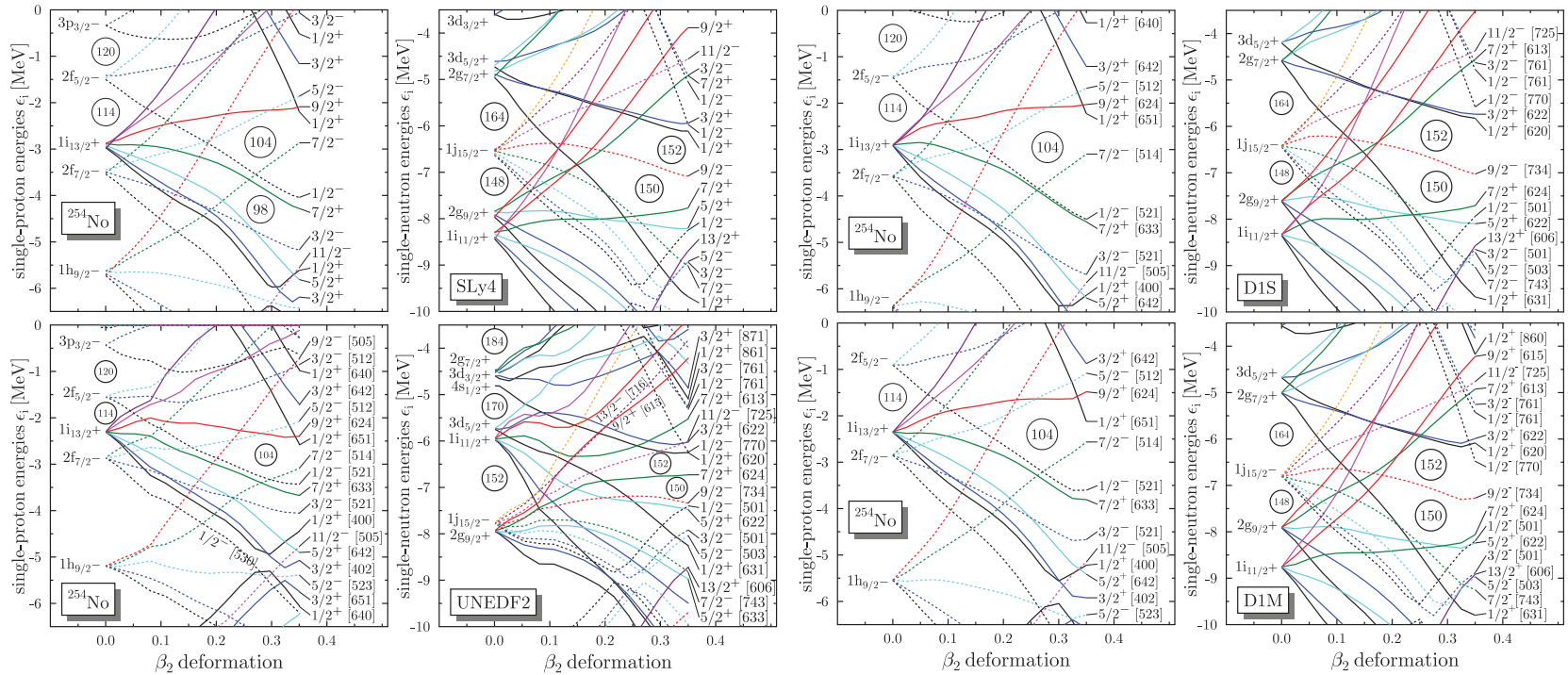
Known deficiencies: incorrect deformed shell closures

Nilsson diagrams of ^{254}No

protons neutrons protons neutrons

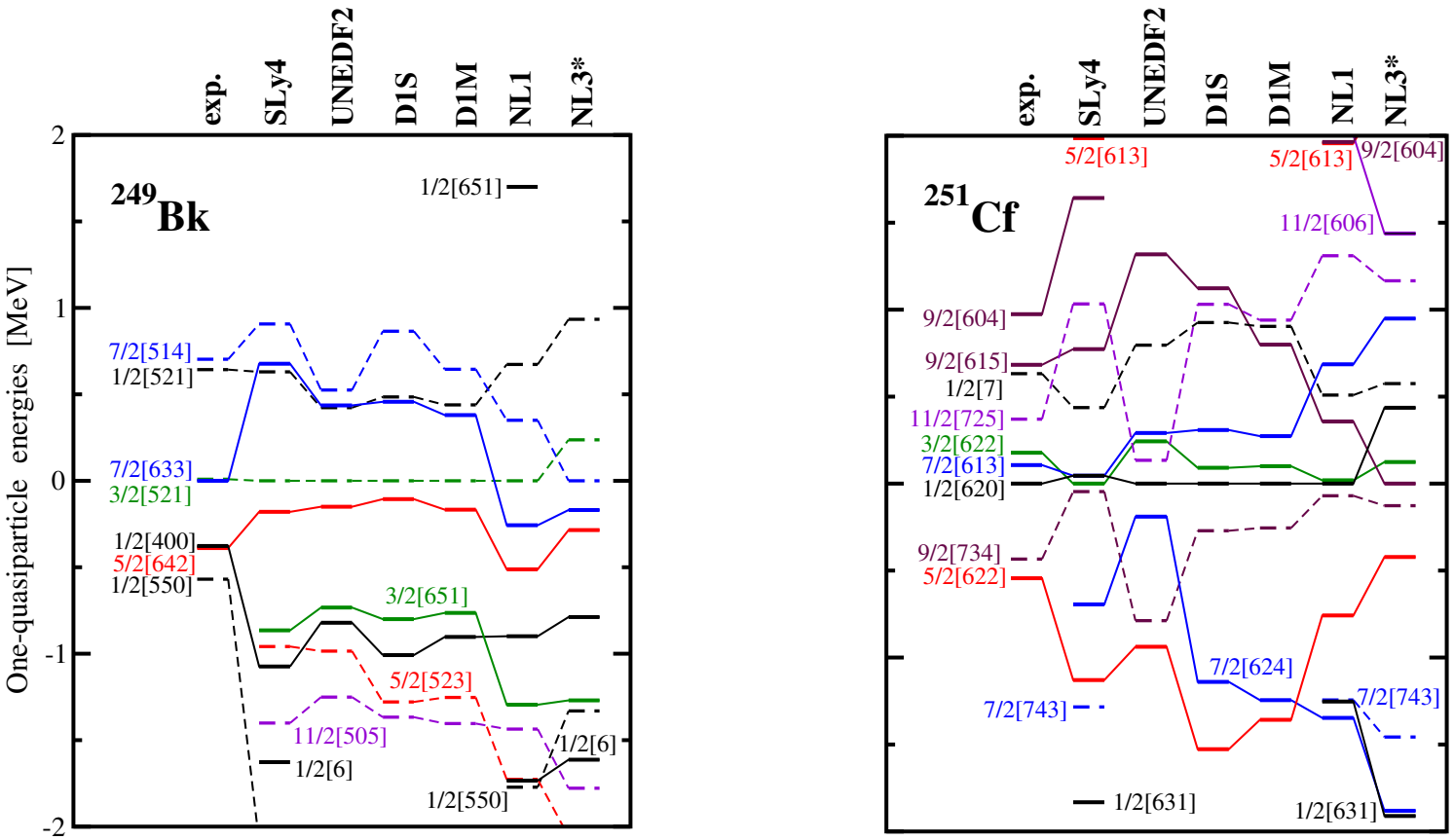
SLy4 D1S

UNEDF2 D1M



Dobaczewski, Afanasjev, Bender, Robledo, Shi, NPA944 (2015) 388

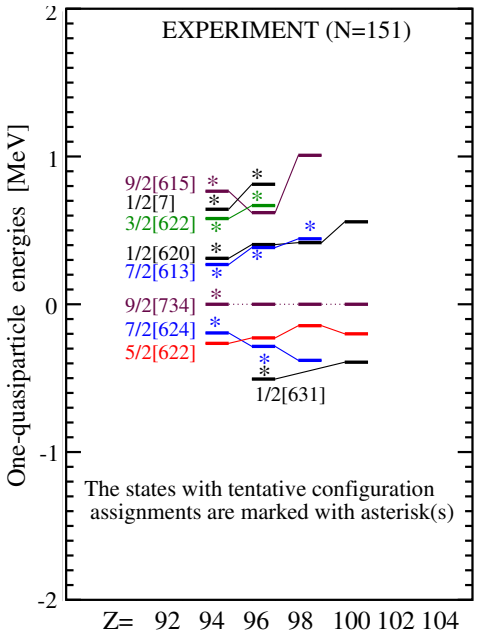
Known deficiencies: One-quasiparticle states in ^{249}Bk and ^{251}Cf

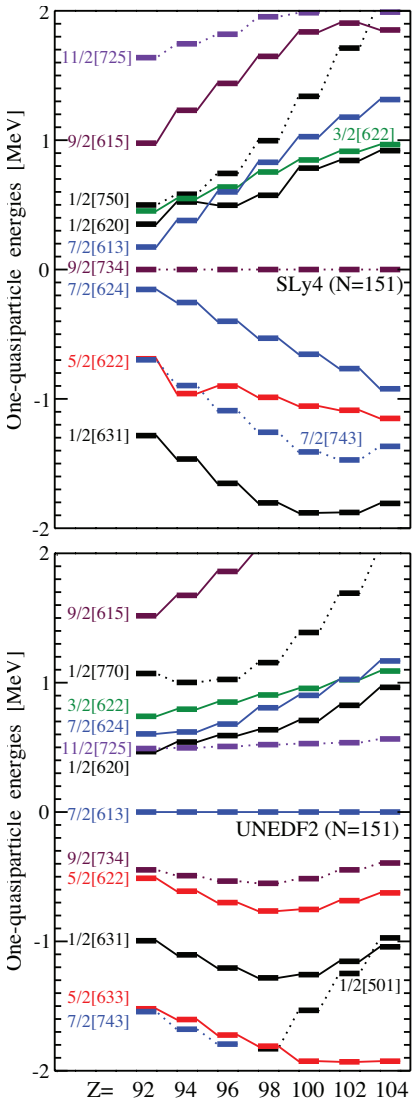


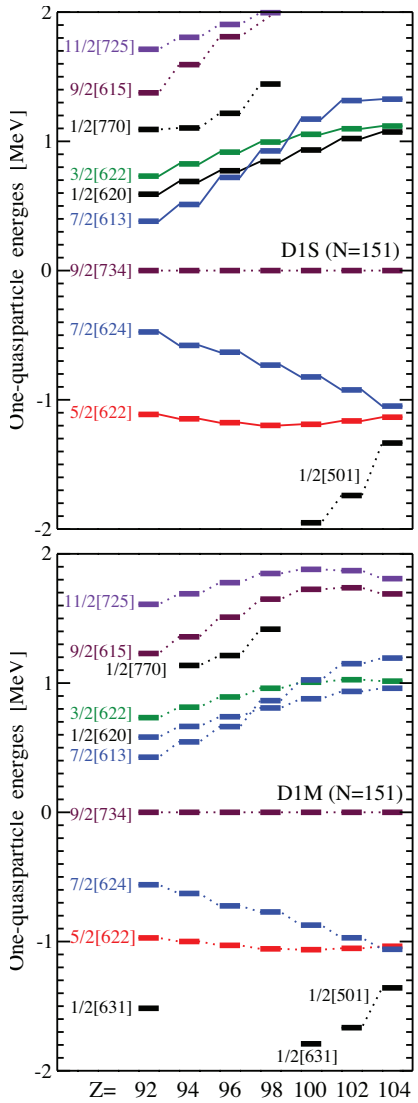
- intruder levels (π 7/2[633] and ν 11/2[725]) misplaced in the spectrum (which can be partially cured with local readjustment of the spin-orbit interaction, [Shi, Dobaczewski, Greenlees, PRC 89 (2014) 034309]), but that's not the only problem.

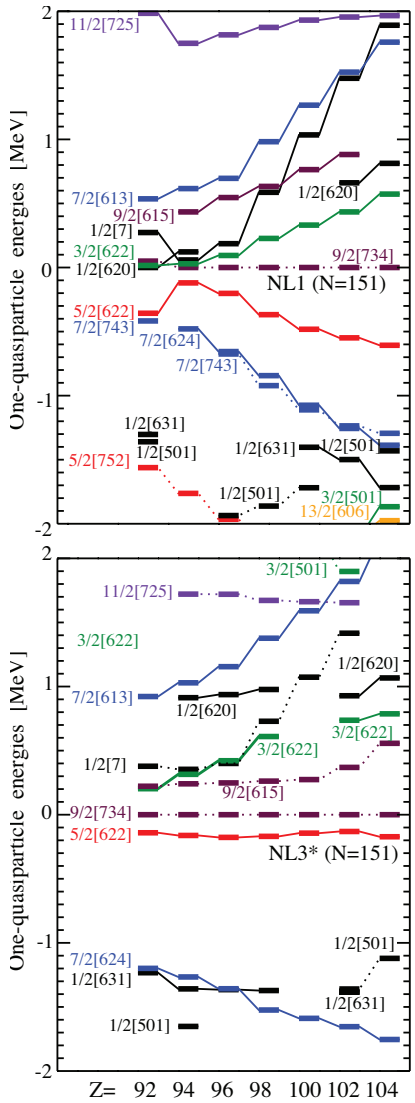
Dobaczewski, Afanasjev, Bender, Robledo, Shi, NPA944 (2015) 388

One-quasiparticle states (bandheads) in the $N = 151$ chain



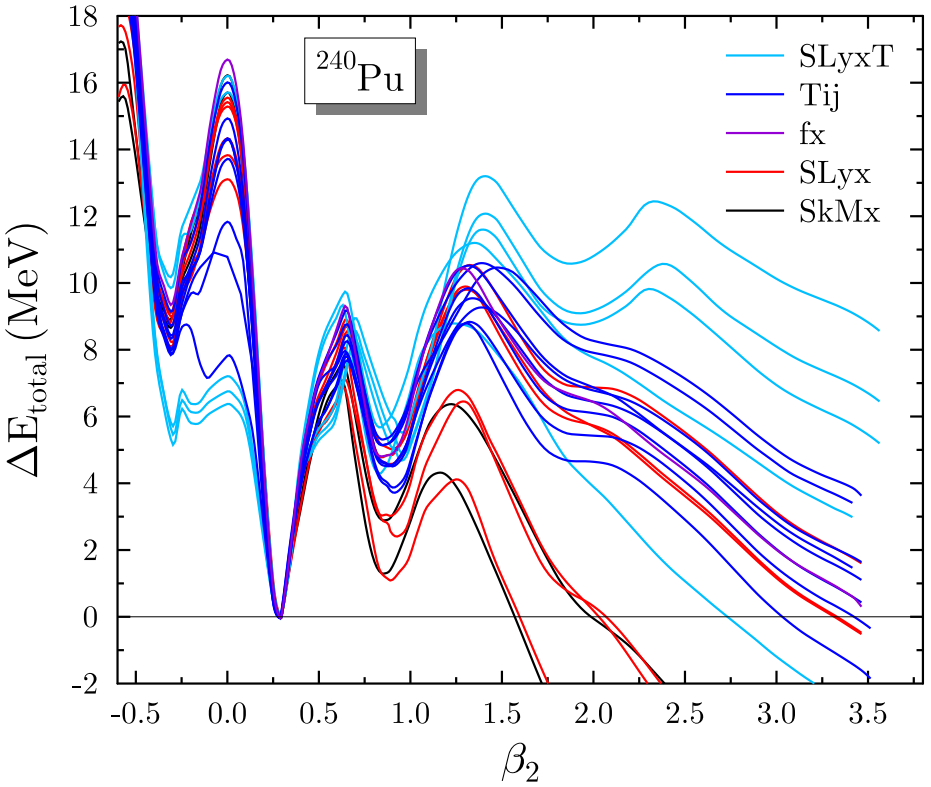




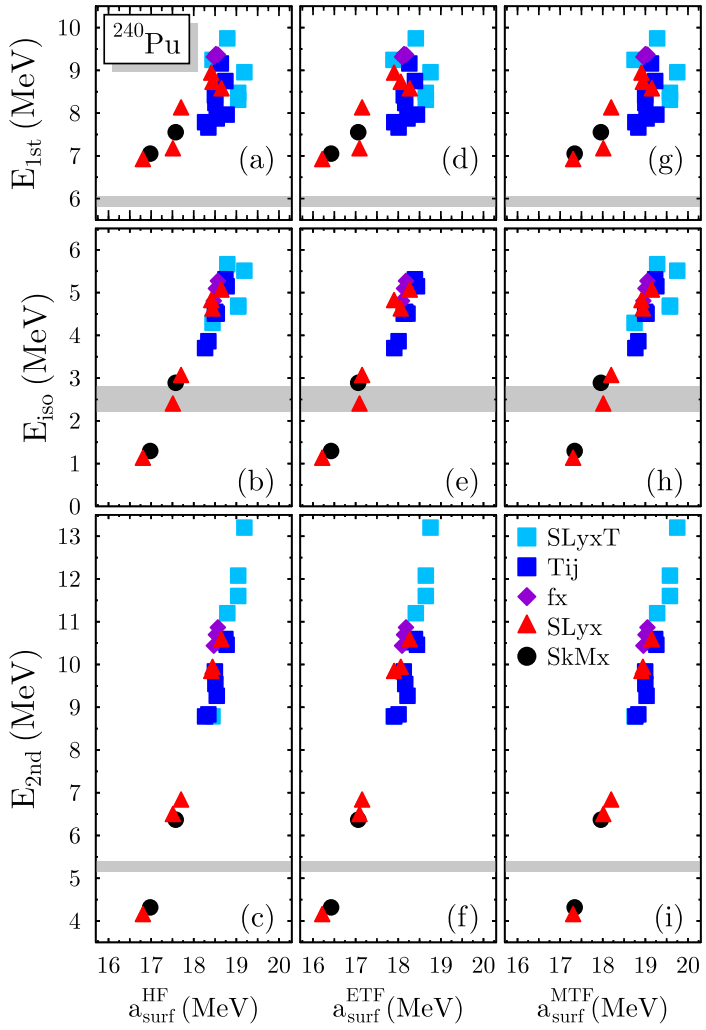


Dobaczewski, Afanasjev, Bender, Robledo, Shi, NPA944 (2015) 388

Known deficiencies: fission barrier heights

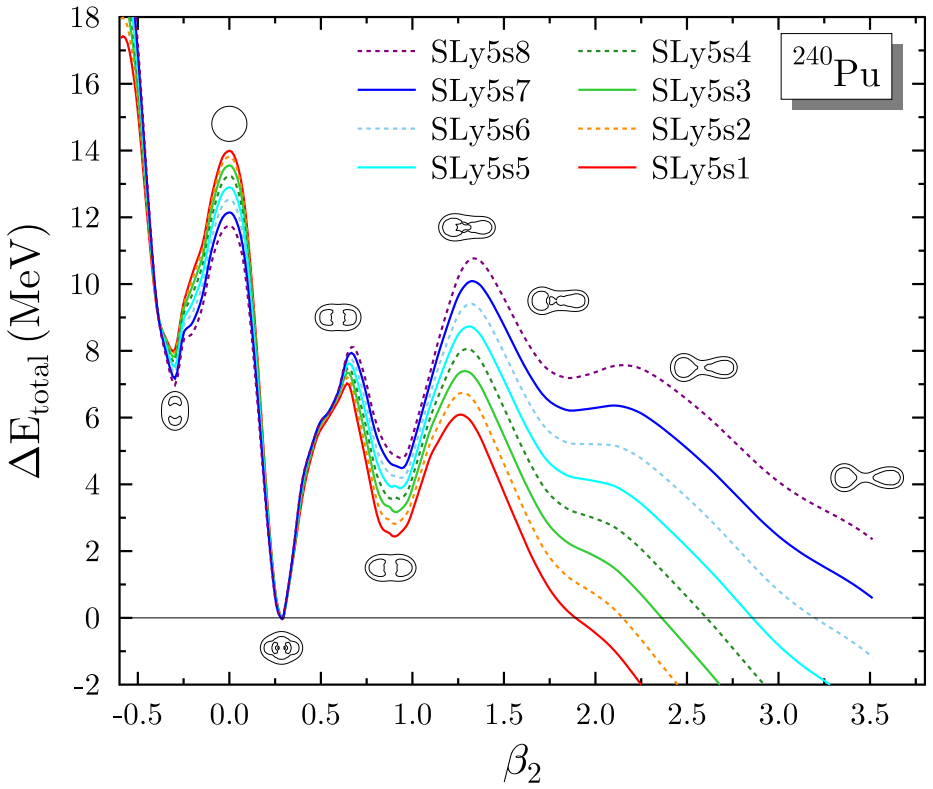


- most Skyrme parameterizations overestimate fission barriers . . .
- . . . although a few do well . . .
- and a very few even systematically underestimate them.

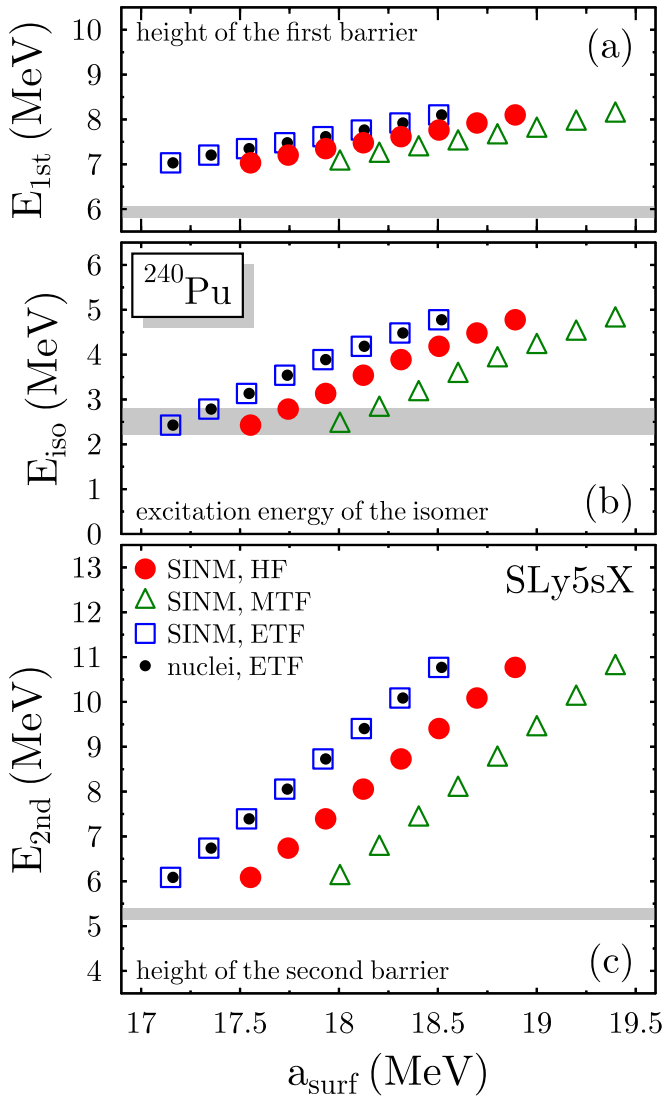


Jodon, Bennaceur, Meyer, Bender, PRC94 (2016) 024355

Construction of better parameterizations: control of surface properties

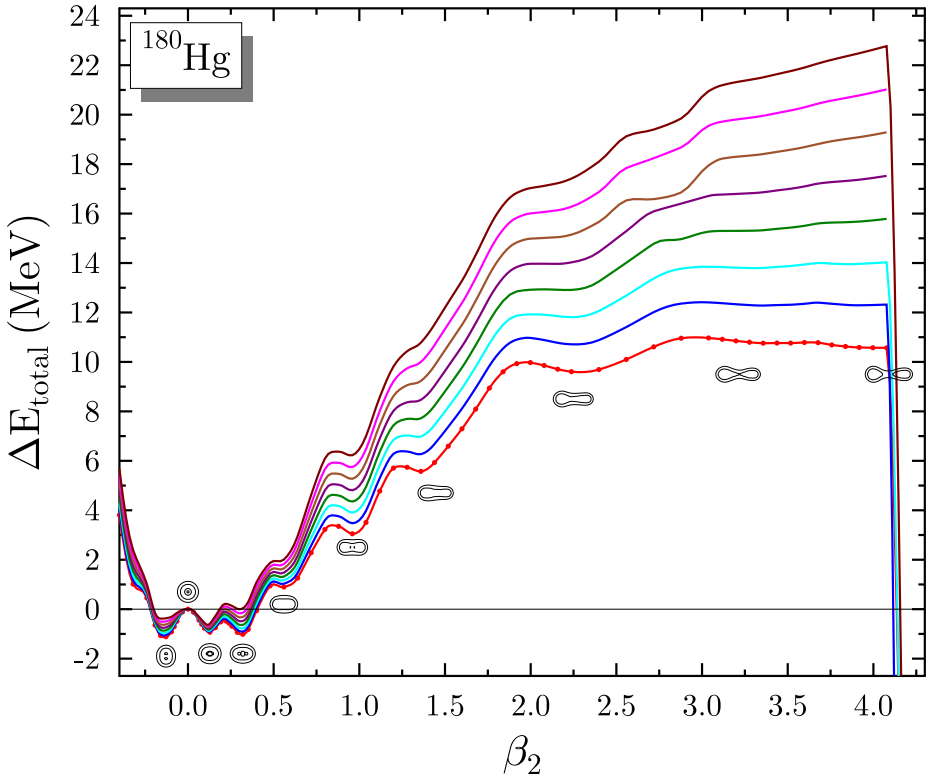


- add constraint on surface tension to the fit protocol
- (which requires understanding of the ambiguities of its determination)
- fit of SLy5s1, SLy5s2, ... SLy5s8 as proof of principle.



Jodon, Bennaceur, Meyer, Bender, PRC94 (2016) 024355

Construction of better parameterizations: control of surface properties



Ryssens, Bender, Heenen, unpublished

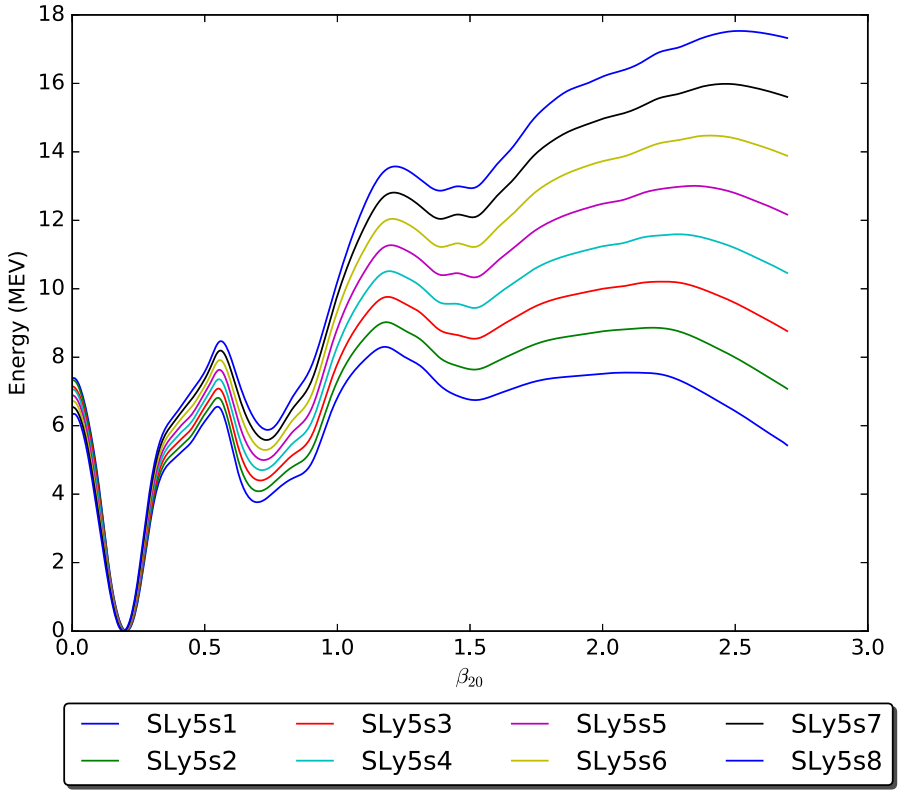


Figure 3: Fission barrier of ^{226}Ra as a function of β_{20} for the SLy5sX functionals with $X = 1,\ldots,8$ with HFB+LN pairing. Energy is relative to minimum of the deformation surface.

Ryssens, Heenen, Bender, PoS (BORMIO2016) 033

Construction of better parameterizations: how to improve shell structure

- better **local** control of single-particle structure possible,

  Shi, Dobaczewski, Greenlees, PRC 89 (2014) 034309

- . . . but better **global** control of single-particle structure is difficult

  Lesinski, M. B., Bennaceur, Duguet, Meyer, PRC 76 (2007) 014312

  M. B., Bennaceur, Duguet, Heenen, Lesinski, Meyer, PRC 80 (2009) 064302

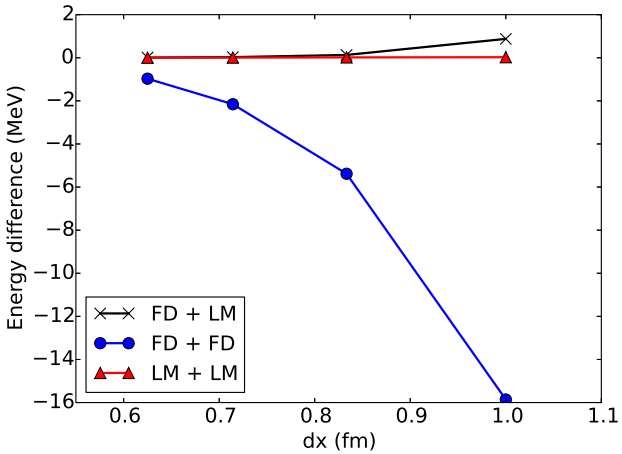
  Kortelainen, Dobaczewski, Mizuyama, Toivanen, PRC 77 (2008) 064307

  Kortelainen, McDonnell, Nazarewicz, Olsen, Reinhard, Sarich, Schunck, Wild, Davesne, Erler, Pastore, PRC 89 (2014) 054314

- . . . withing the existing forms of the nuclear EDF
- $\Rightarrow$ new forms of the EDF are needed.

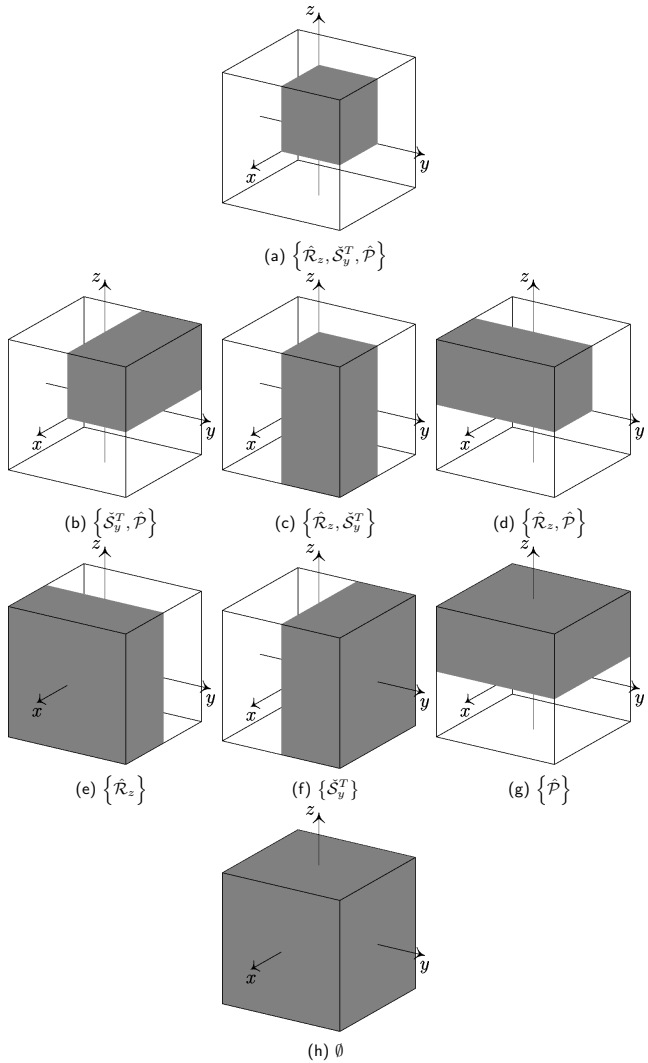
MOCCa: a new flexible HFB solver using coordinate-space representation

- coordinate space representation
- flexible description of shapes of the density and the current distribution. At present, any subgroup out of $\hat{P}$, $\hat{R}_x$, $\hat{S}_y^T$, and $\hat{T}$ is possible.
- high numerical precision obtained with Lagrange-mesh techniques



Ryssens, Heenen, and M. B., PRC 92 (2015) 064318

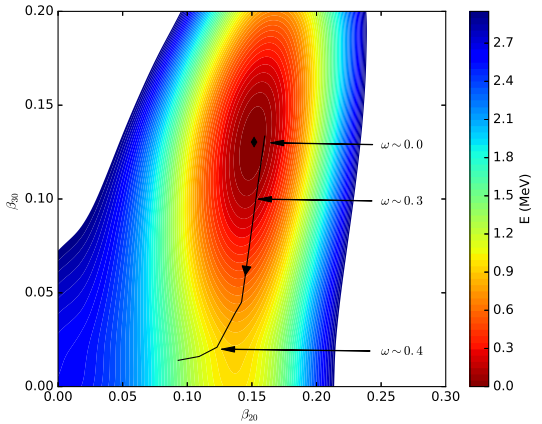
- multiple constraints on the shape of densities and currents.
- HFB.

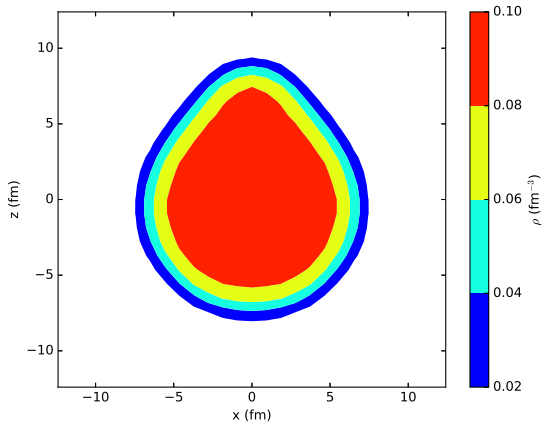


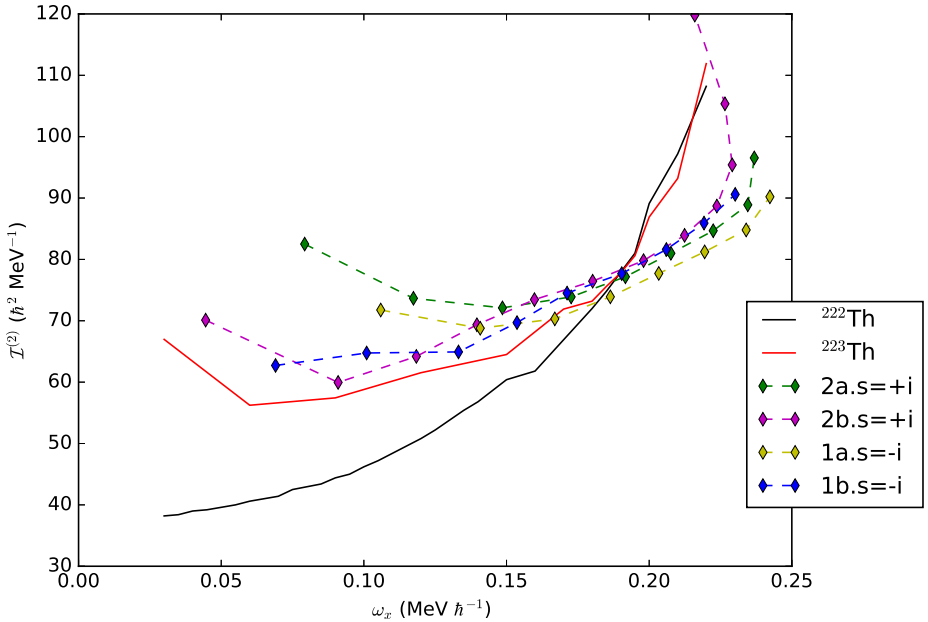
W. Ryssens, Ph.D. thesis (Université Libre de Bruxelles, 2016).

Fun with MOCCa: Broken-parity and broken time-reversal non-axial shapes

Example: rotational bands of ^{222}Th and ^{223}Th obtained in cranked HFB







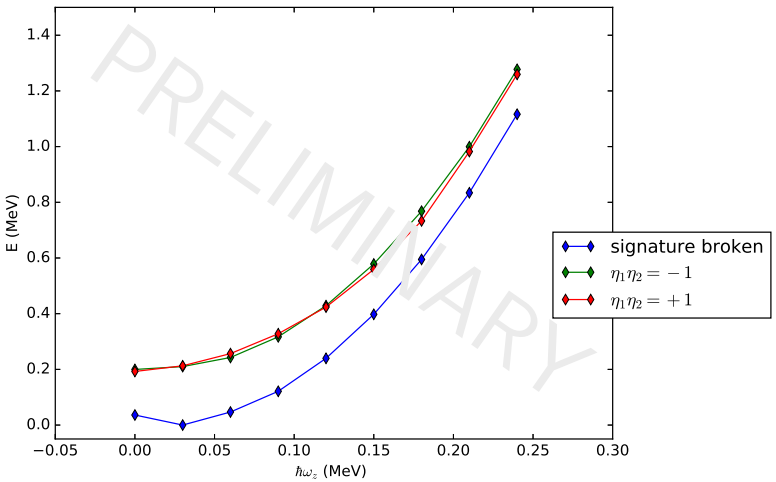
data: Marquart *et al*, PRC 95 (2017) 034304

Ryssens, Heenen, Bender, unpublished

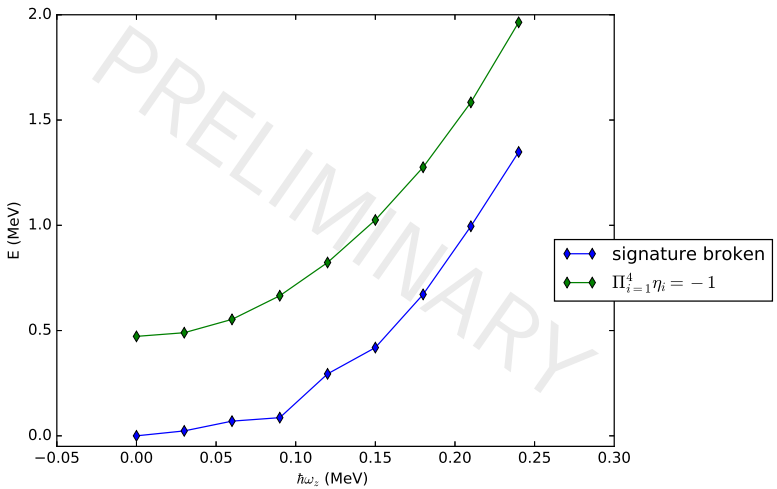
MOCCa: Broken signature and broken time-reversal non-axial shapes

Example: rotational bands build on two-quasiparticle states of ^{178}Hf obtained in cranked HFB

2qp $K = 8$ state, blocked protons



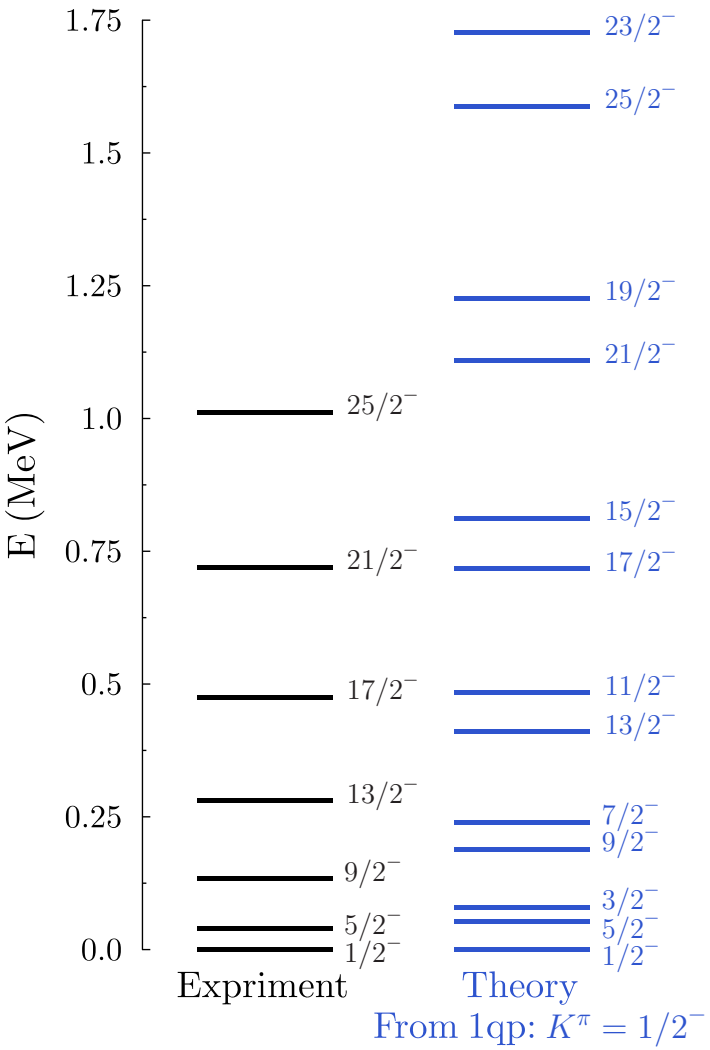
4qp $K = 16$ state

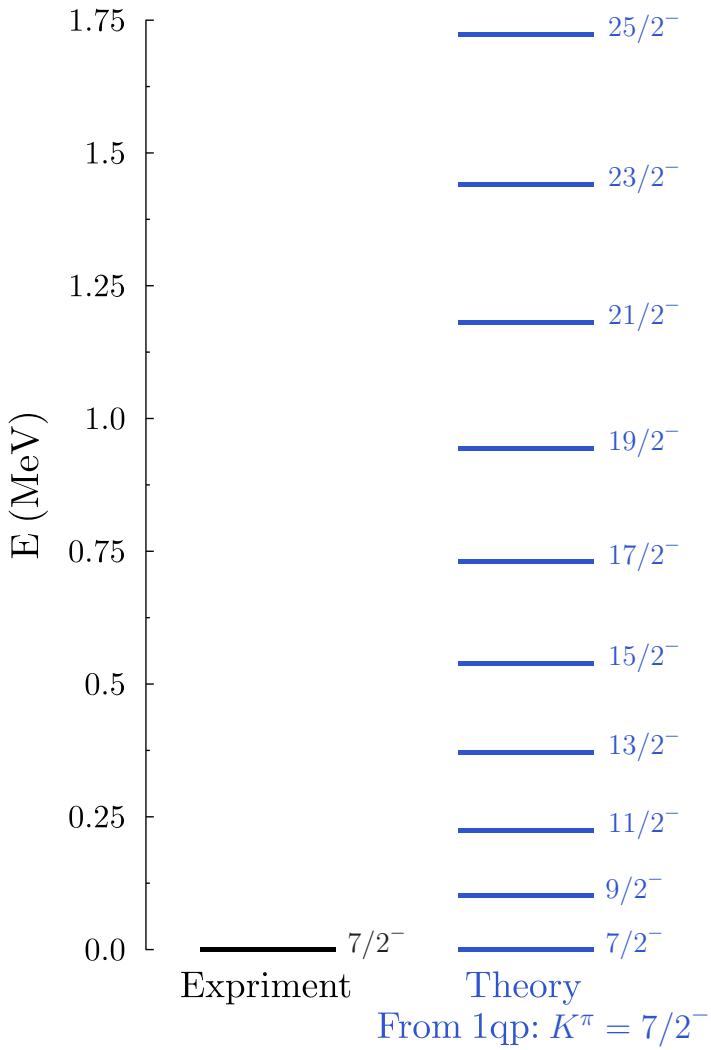


Ryssens, Heenen, Bender, unpublished

- Low-lying states also change.
- as spins have more freedom to orient themselves, magnetic moments might be sensitive (but should be calculated from projected states)

Proof-of-principle: Symmetry-restoration for ^{251}Md





Bally, M. B., Heenen, unpublished

Proof-of-principle: Symmetry-restoration for ^{251}Md

Other observables:

- radii
- magnetic moments μ
- spectroscopic quadrupole moments Q_s
- $B(E2)$ values
- $B(M1)$ values

J	rrmsp (fm)	rrmsn (fm)	mu (mu_N)	Q_s e fm^2	<Lz>	<Sz>	<Jz>	J
7/2	5.8769	6.0193	1.4540	596.84	3.835	-0.335	3.500	3.501
9/2	5.8769	6.0194	1.8407	232.67	4.753	-0.253	4.500	4.500
11/2	5.8769	6.0194	2.2308	14.27	5.692	-0.192	5.500	5.500
13/2	5.8769	6.0194	2.6230	-127.63	6.644	-0.144	6.500	6.500
15/2	5.8770	6.0194	3.0164	-225.40	7.604	-0.104	7.500	7.500
17/2	5.8770	6.0195	3.4108	-295.86	8.570	-0.069	8.500	8.500
19/2	5.8771	6.0195	3.8057	-348.48	9.539	-0.039	9.500	9.500
21/2	5.8771	6.0196	4.2011	-388.91	10.512	-0.012	10.500	10.500
23/2	5.8772	6.0196	4.5968	-420.74	11.487	0.013	11.501	11.500
25/2	5.8773	6.0197	4.9928	-446.29	12.464	0.037	12.501	12.500

transition	B(E2) (e^2 fm^4)	M(M1) (mu_N^2)
9/2 -> 7/2	55214	2.6167 E-04
11/2 -> 7/2	11834	---
11/2 -> 9/2	55760	3.9979 E-04
13/2 -> 9/2	21953	---
13/2 -> 11/2	47809	4.8087 E-04

Take-away messages

- Many efforts underway to improve the description of the properties of low-lying states in mean-field-based models
  - construction of more general (less symmetry restricted) configurations
  - improved parameterizations (better fit protocols)
  - improved effective interactions (additional terms)
- projection on good quantum numbers restores selection rules for transitions
- configuration mixing (Generator coordinate method) might significantly alter results for soft nuclei and/or nuclei exhibiting shape coexistence.

Acknowledgements

The work presented here would have been impossible without my collaborators

founding fathers

Paul Bonche	SPhT, CEA Saclay
Hubert Flocard	CSNSM Orsay
Paul-Henri Heenen	Université Libre de Bruxelles

analysis of formal aspects

Thomas Duguet	Irfu/CEA Saclay & KU Leuven & NSCL/MSU
Denis Lacroix	IPN Orsay

code development and benchmarking

Benoît Avez	CEN Bordeaux Gradignan
Benjamin Bally	CEN Bordeaux Gradignan, now SPhN, CEA Saclay
Veerle Hellemans	Université Libre de Bruxelles

development and benchmarking of new functionals

Karim Bennaceur	IPN Lyon & Jyväskylä
Dany Davesne	IPN Lyon
Robin Jodon	IPN Lyon
Jacques Meyer	IPN Lyon
Alessandro Pastore	formerly IPN Lyon, now University of York
Jeremy Sadoudi	Irfu/CEA Saclay first, then CEN Bordeaux Gradignan
Kouhei Washiyama	Université Libre de Bruxelles

color code: active (past) member of the collaboration