M/SR-EDF calculations for (super)heavy nuclei

Things we control and things we do not (yet): an overview.

W. Ryssens[1], M. Bender[1] and P.-H. Heenen [2].

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23th of April 2018

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MR-EDF with Skyrme EDFs.

1. Select
   a) a functional $E(\rho, \tau, \ldots)$
   b) (multiple) symmetries $\hat{U}_j$ to break
   c) Numerical representation
2. Obtain HF(B) 'product' states

$$\Omega = \{|\Phi_i\rangle \,|i = 1, \ldots, \text{ a lot}\}$$

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3. Restore symmetries by projection

$$|\Phi_i\rangle \rightarrow \Omega_i^P = \left\{ |\Phi_i^{J_a}\rangle \, | J_a = 0, 2, \ldots \right\} .$$

4. Mix the obtained states of same quantum numbers with a GCM

$$|\Phi_{\text{final}}^{J_a}\rangle = \sum_i a_i |\Phi_i^J\rangle \, .$$

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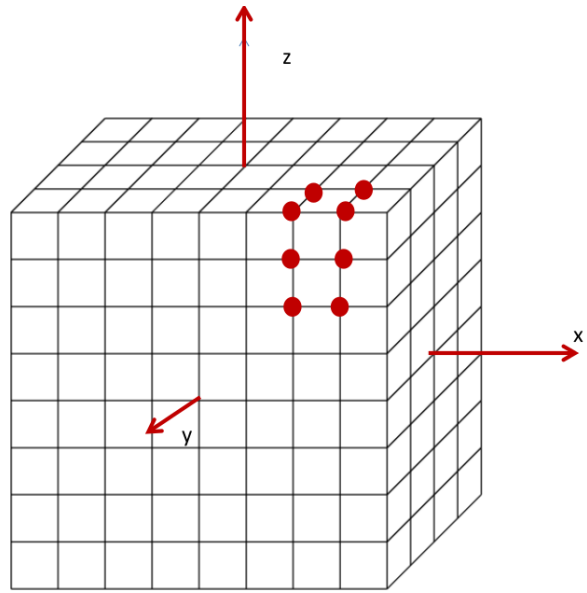
We select
a) Skyrme functionals
b) J, M, Z, N and ...
c) Coordinate space



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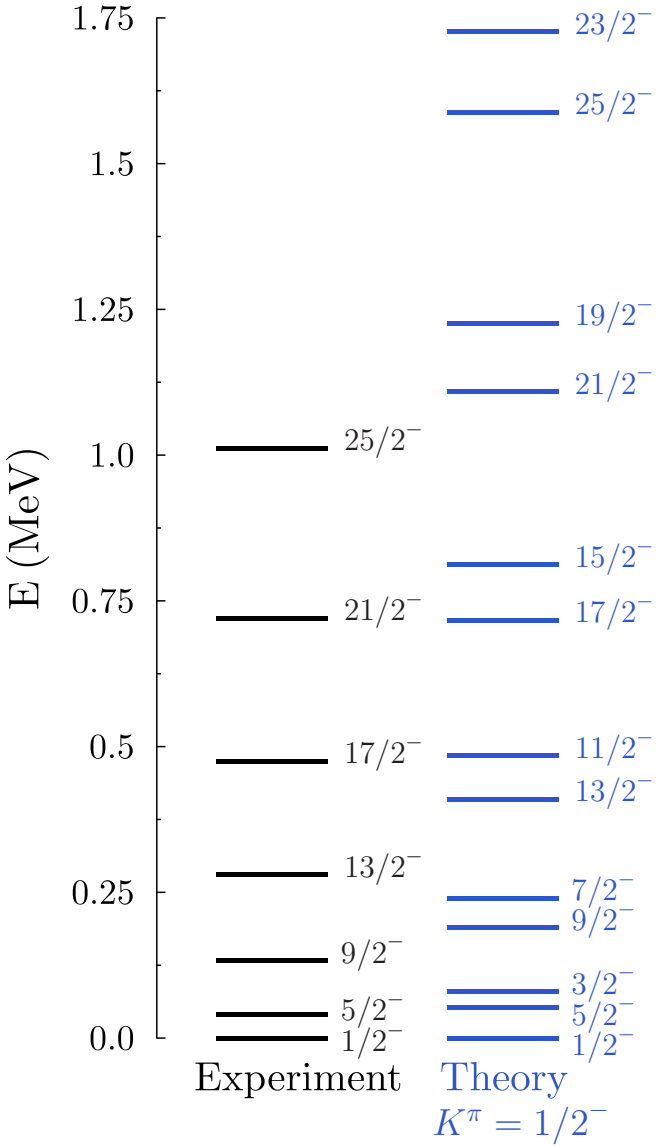
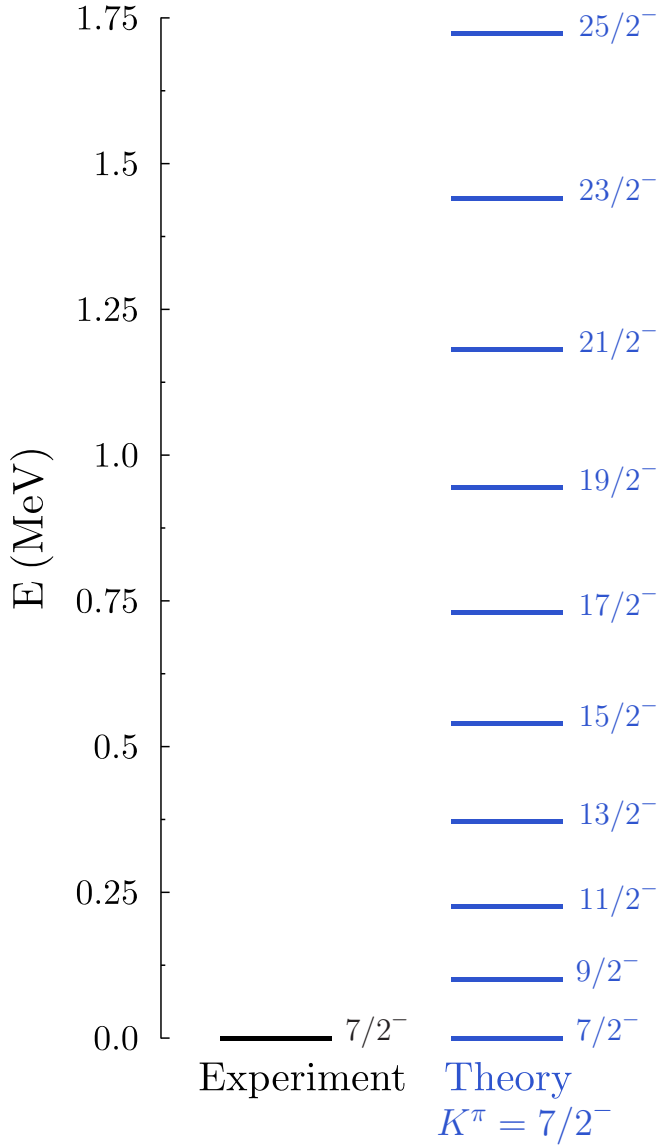
^{251}Md with SLyMR1.





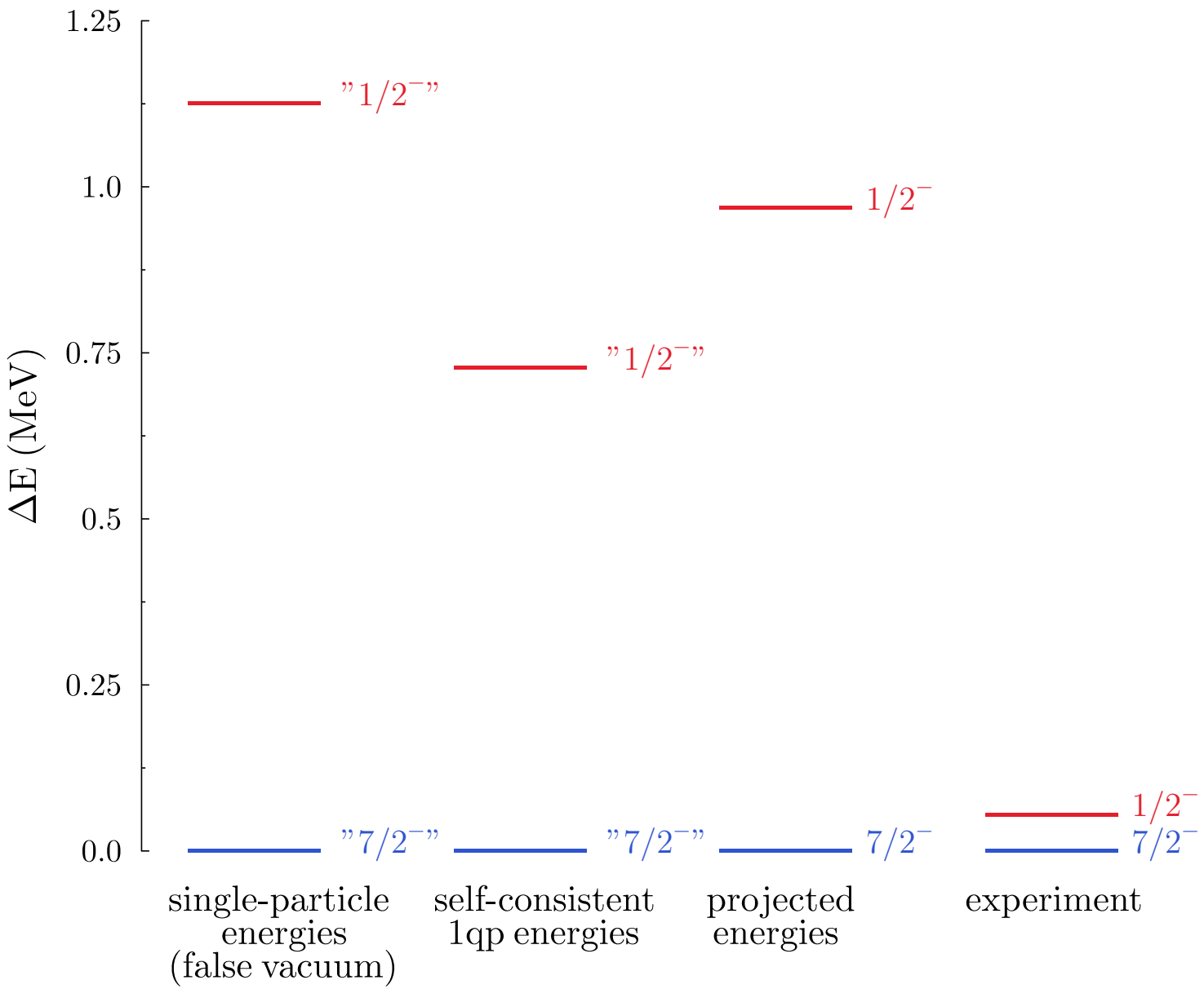
Th. B. Bally (unpublished), Exp. data: A. Chatillon et al. Phys. Rev. Lett. 98, 132503 (2007).

^{251}Md with SLyMR1.

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

^{251}Md with SLyMR1.



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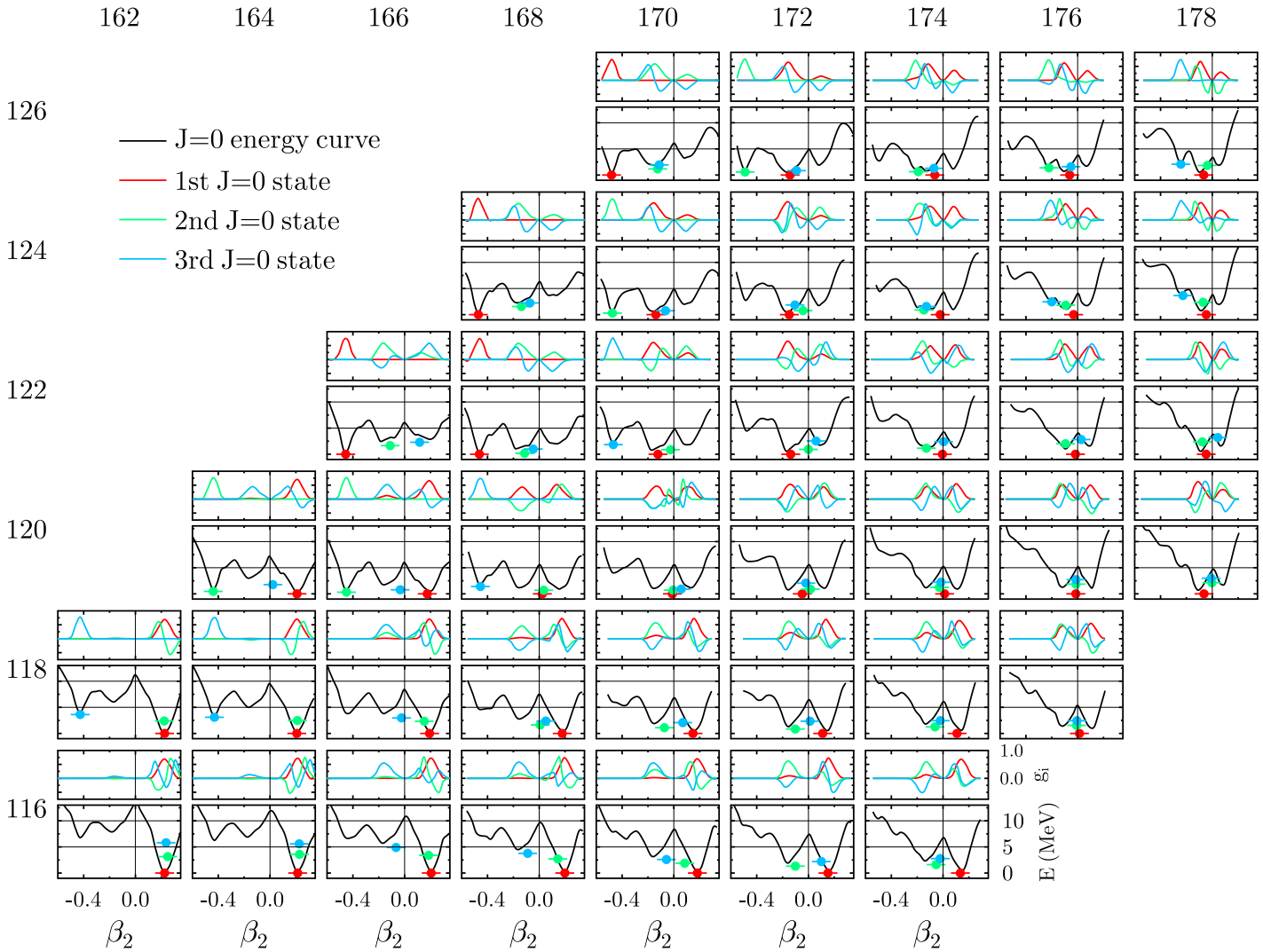
EDFs can explode: part I.



M. Bender and P.-H. Heenen (unpublished).

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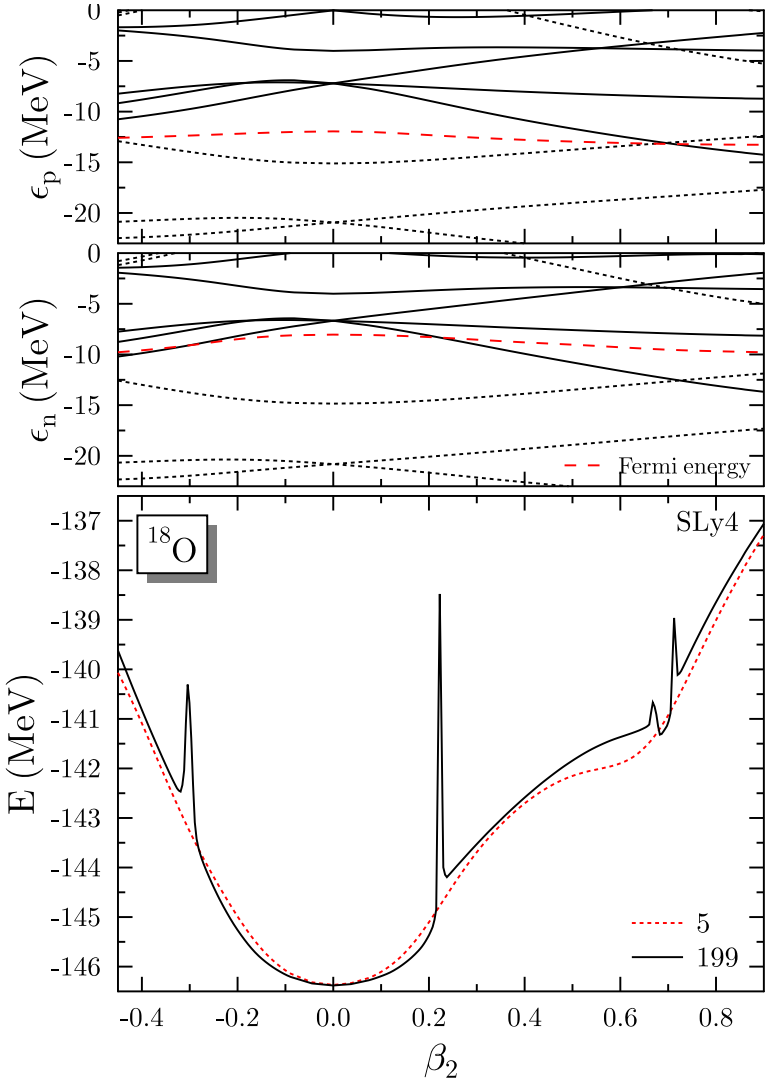

From M. Bender *et al.* PRC 79, 044319 (2009).

EDFs can explode: part I.

One way to guarantee a problem-free calculation

$$E^{ab}[\rho,\kappa,\kappa^*] = \frac{\langle\Phi_a|\hat{H}|\Phi_b\rangle}{\langle\Phi_a|\Phi_b\rangle}\,.$$

$$\rho^{ab}=\frac{\langle\Phi_a|c^\dagger c|\Phi_b\rangle}{\langle\Phi_a|\Phi_b\rangle} \qquad \kappa^{ab}=\frac{\langle\Phi_a|cc|\Phi_b\rangle}{\langle\Phi_a|\Phi_b\rangle}, \qquad \kappa^{ab}=\frac{\langle\Phi_a|cc|\Phi_b\rangle}{\langle\Phi_a|\Phi_b\rangle}\,.$$

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1. Relations between coupling constants
2. No density dependent coupling constants
3. Pairing $\leftrightharpoons$ Particle-Hole linked
4. Exact Coulomb Exchange (CPU!)

Functionals available

- SLyMR0
- SLyMR1
- SV

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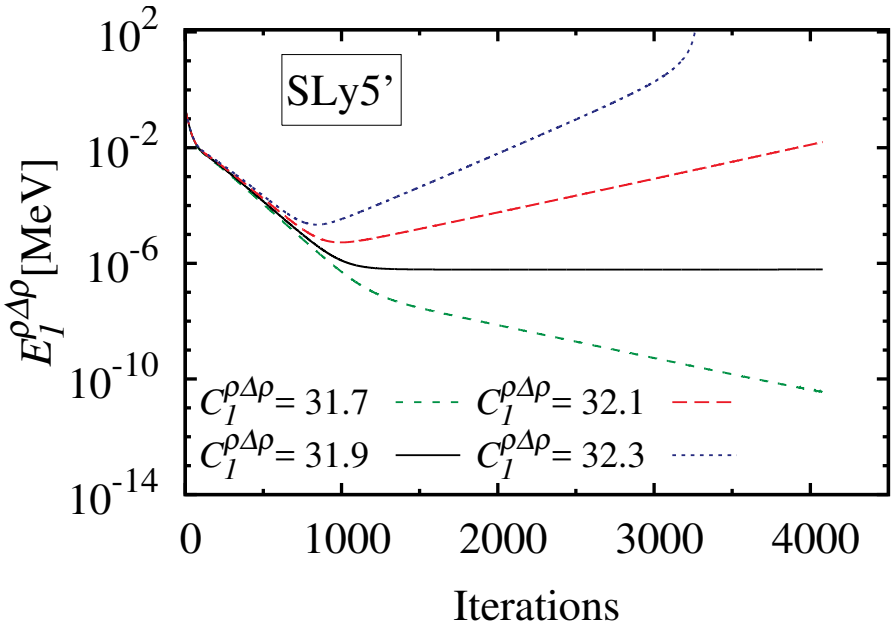
Stopgap procedure might work when time-reversal is conserved!
J.L. Egido, Phys. Scripta T 91, 7 (2016).

EDFs can explode, part II.



Instabilities on the SR-EDF level

a No stable solutions

b Calculations are impossible

c Can be hidden by (too small) variational space

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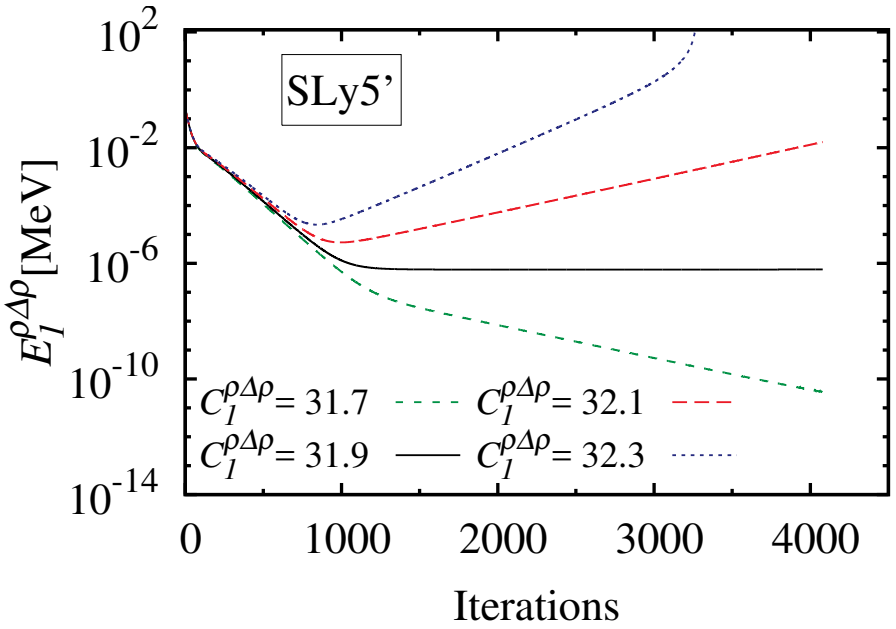

Instabilities on the SR-EDF level

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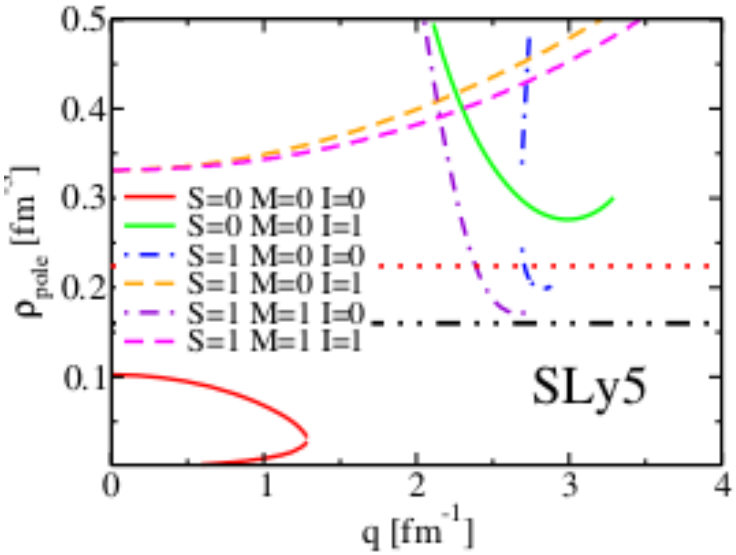
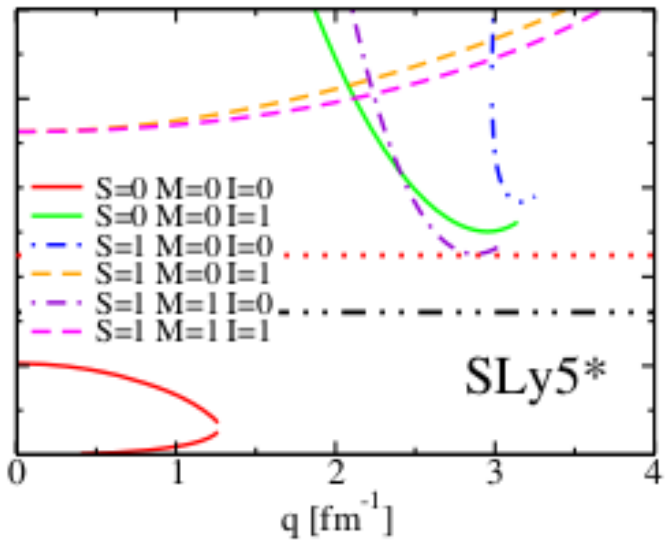
→ Linear response of SNM in the fitting protocol





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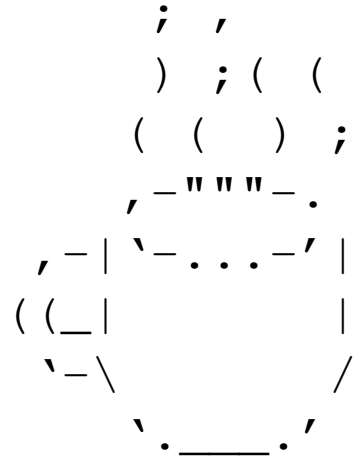
Development of MOCCa



MOCCa

a SR-EDF on the 3D mesh

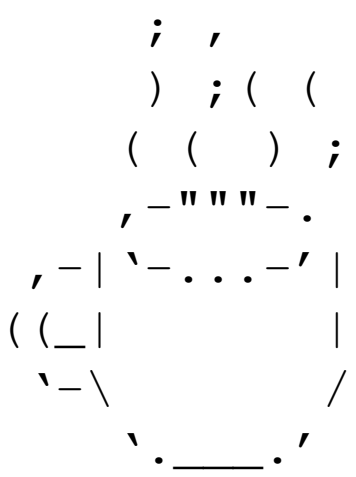
b 16 symmetry options

c HFB pairing in all cases

d Fast in CPU time...

e ...and human time(!)

Development of MOCCa



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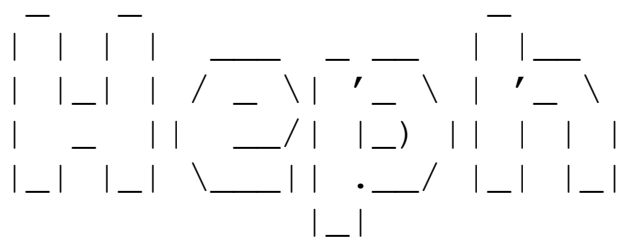

Hephaestos

a Code generator for MOCCa

b Automatic implementation of new functionals

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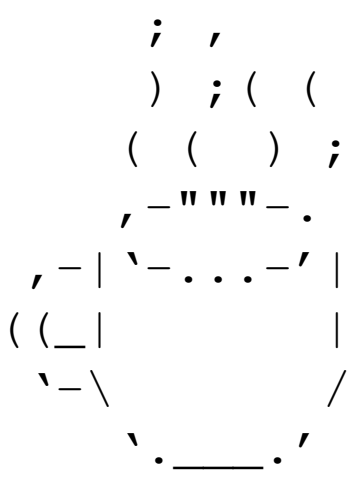

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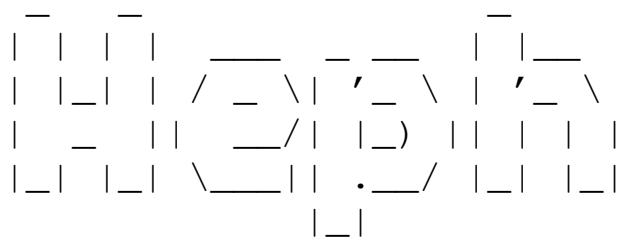


Hephaestos

a Code generator for MOCCa

b Automatic implementation of new functionals

MOCCa + Hephaestos = Unprecedented freedom

a in choosing symmetries

b in implementing EDFs

SR-Possibilities

Even-even ground states

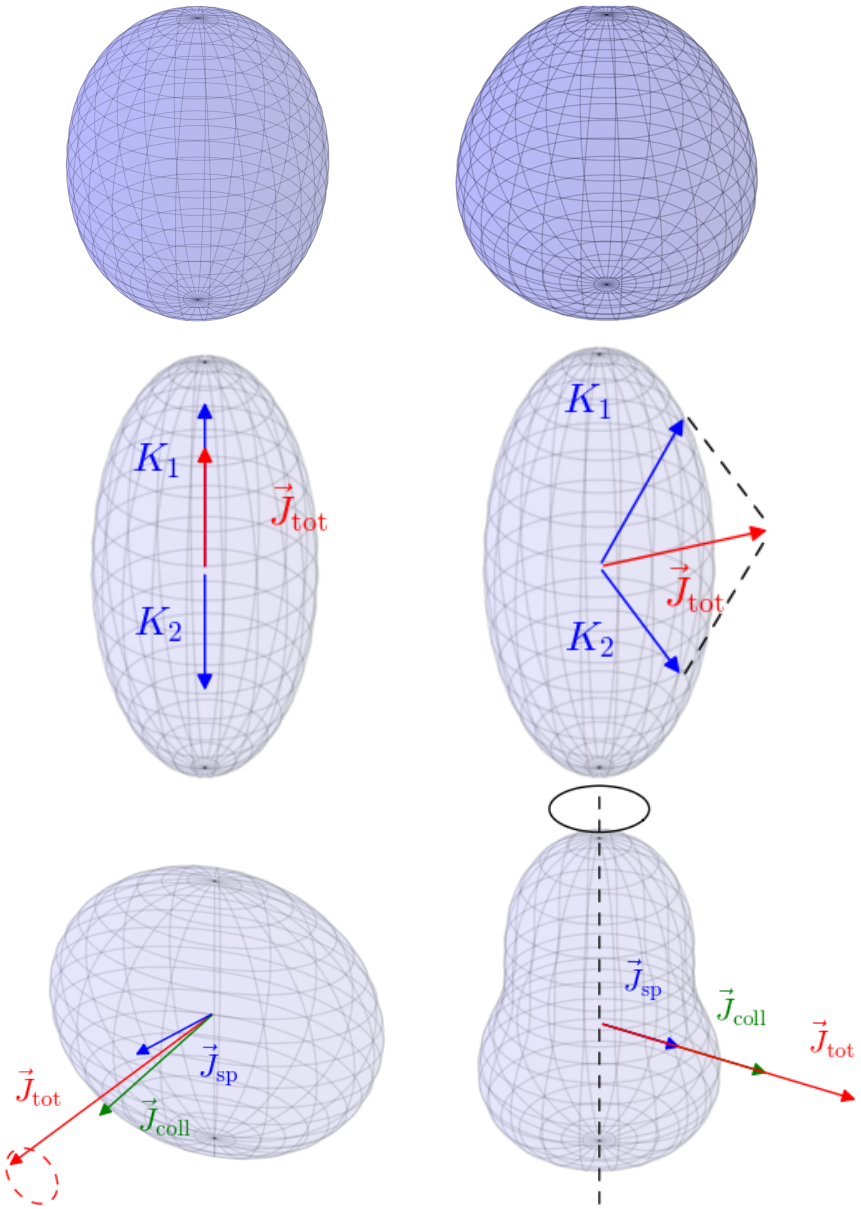
a Triaxiality
b Octupole
c Non-axial octupole

Quasi-particle excitations

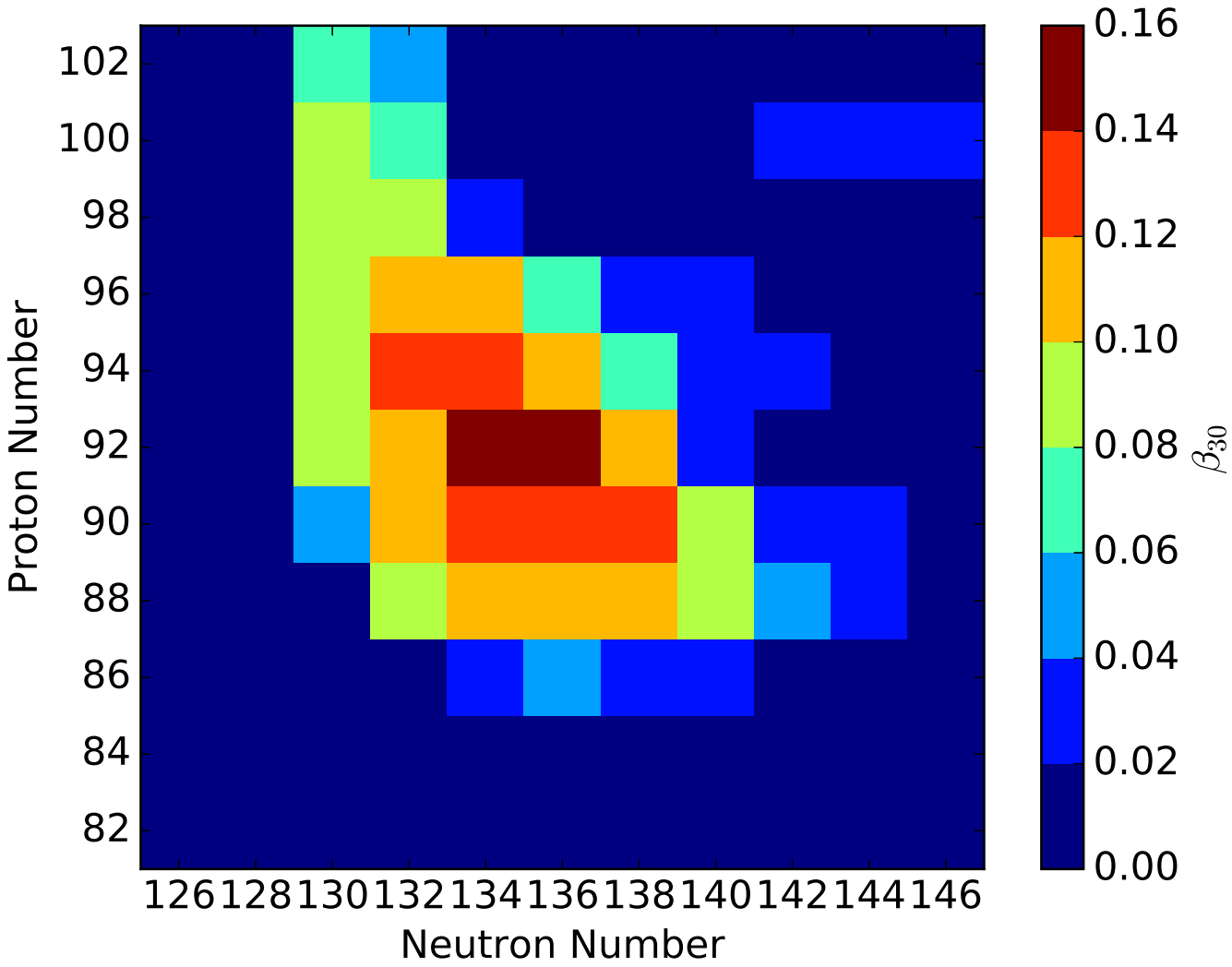
a Odd & Odd-odd nuclei
b Multi-quasiparticle excitations ...
c ...without signature symmetry!

Rotational bands

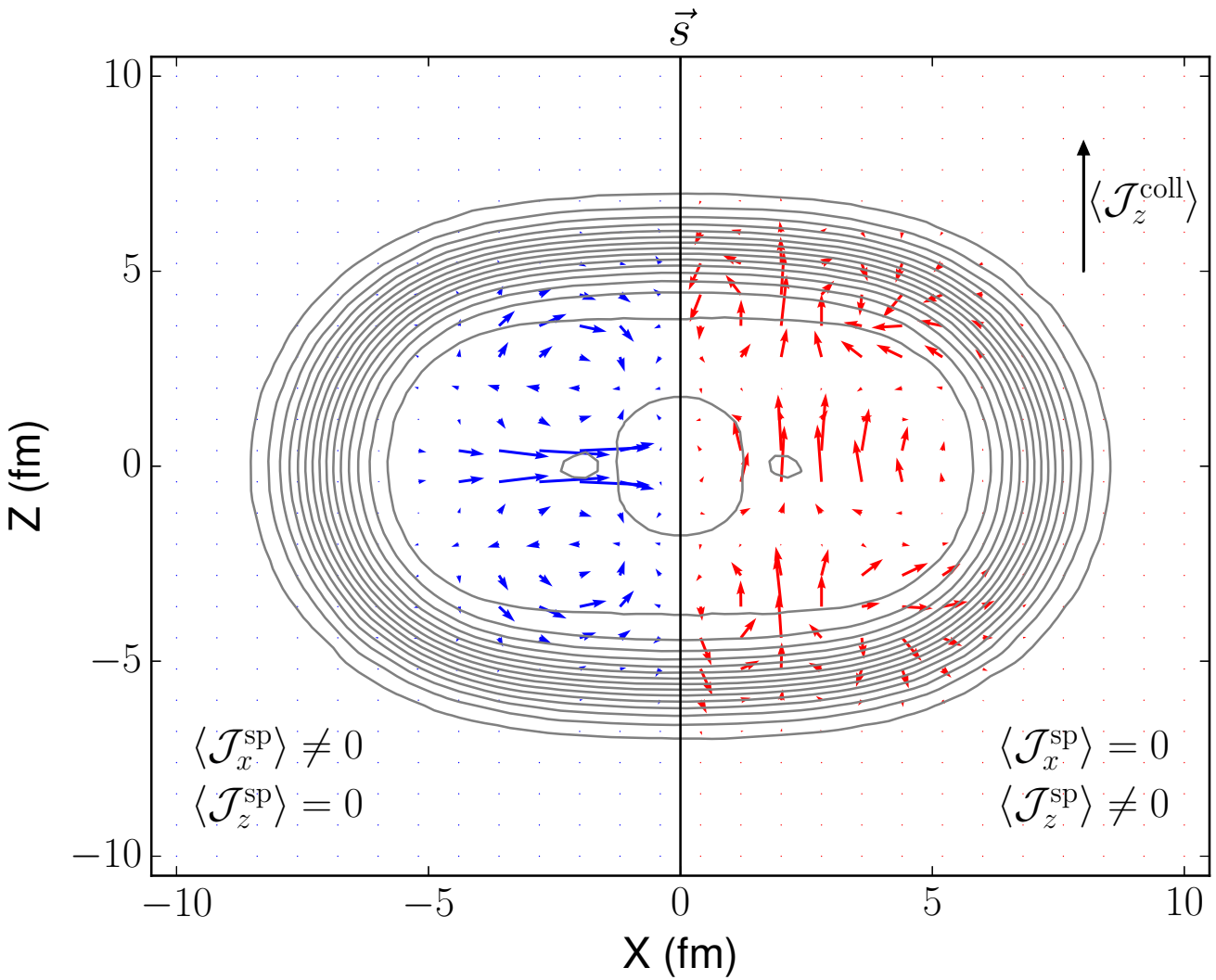
a Axial
b 'Wobbling' triaxial
c Octupole bands



Octupole deformation in the region



Multi-qp-excitations: ^{178}Hf

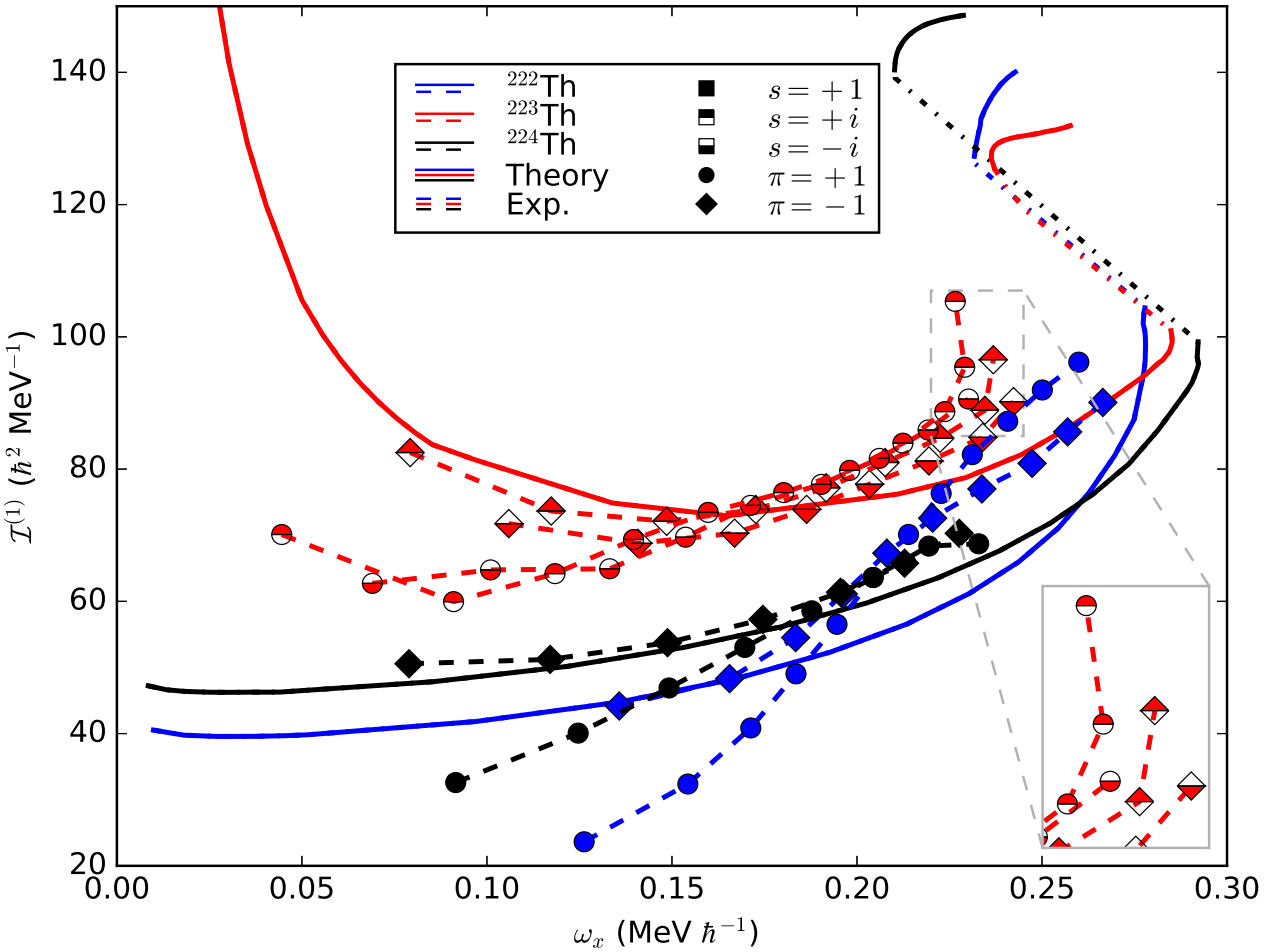


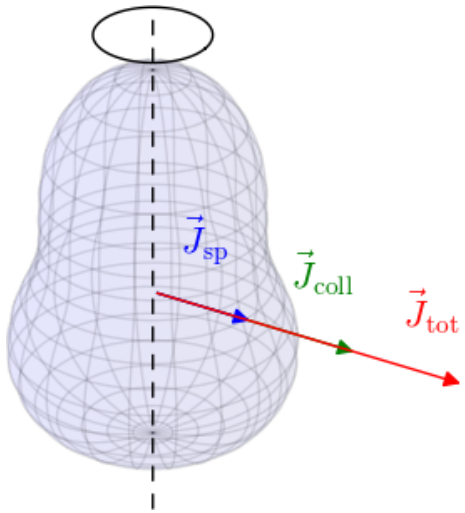
^{178}Hf

a $\frac{7}{2}^+$ and $\frac{9}{2}^-$ quasiprotons

b Spin distribution is totally different!

Rotational bands





Data from
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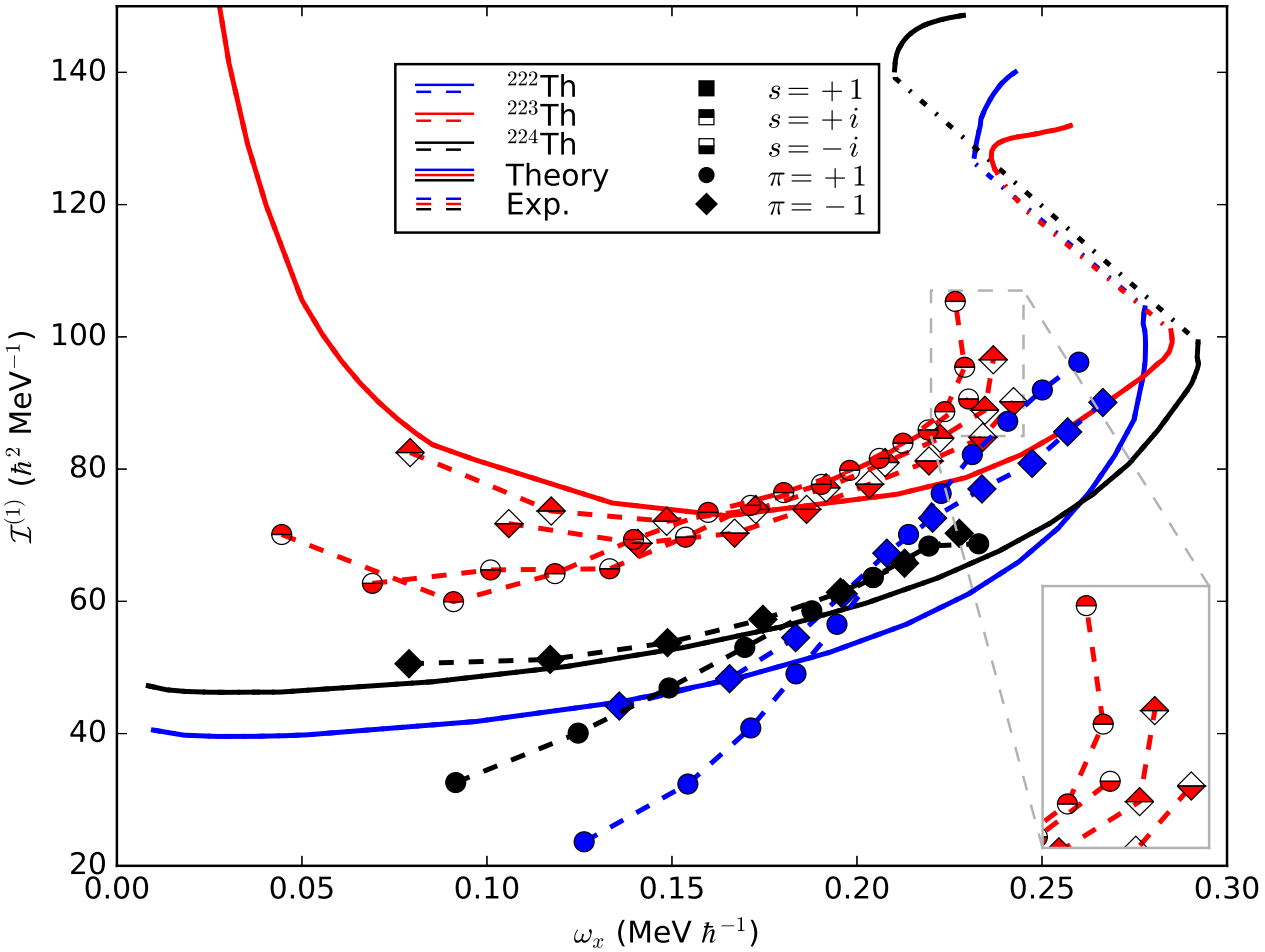
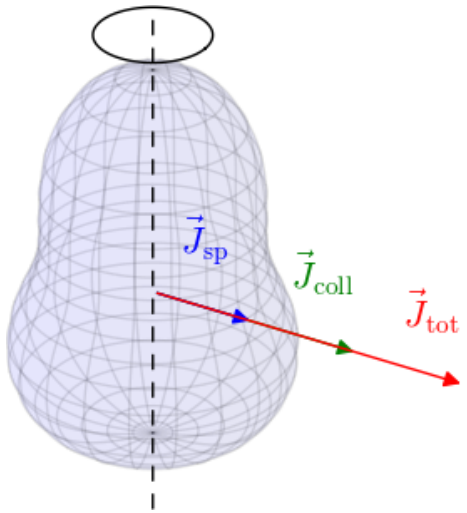
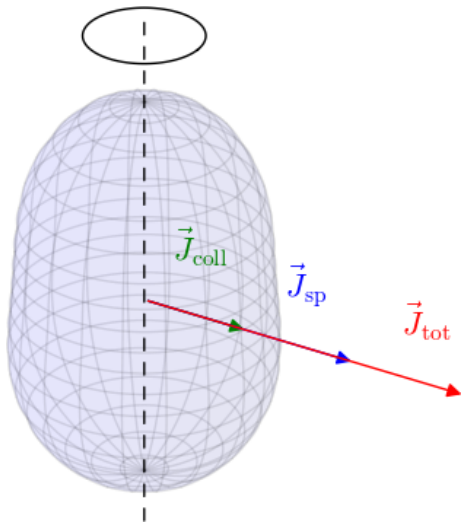
J.F. Smith *et al.*, Phys. Rev. Lett. 75, 1050-1053 (1995).

Rotational bands







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Controlling the surface tension: SLy5s1-8

'How' a system deforms (semi-classical) is a competition

$$\text{Coulomb repulsion} \Longleftrightarrow \text{Surface tension}$$

Controlling the surface tension: SLy5s1-8

'How' a system deforms (semi-classical) is a competition

Coulomb repulsion $\Longleftrightarrow$ Surface tension

(MeV)	$a_{\rm surf}^{\rm (MTF)}$		$a_{\rm surf}^{\rm (MTF)}$
SLy5s1	18.0	SLy5s5	18.8
SLy5s2	18.2	SLy5s6	19.0
SLy5s3	18.4	SLy5s7	19.2
SLy5s4	18.6	SLy5s8	19.4

Parameterizations from R. Jodon *et al.*, PRC **94** 024335 (2016).

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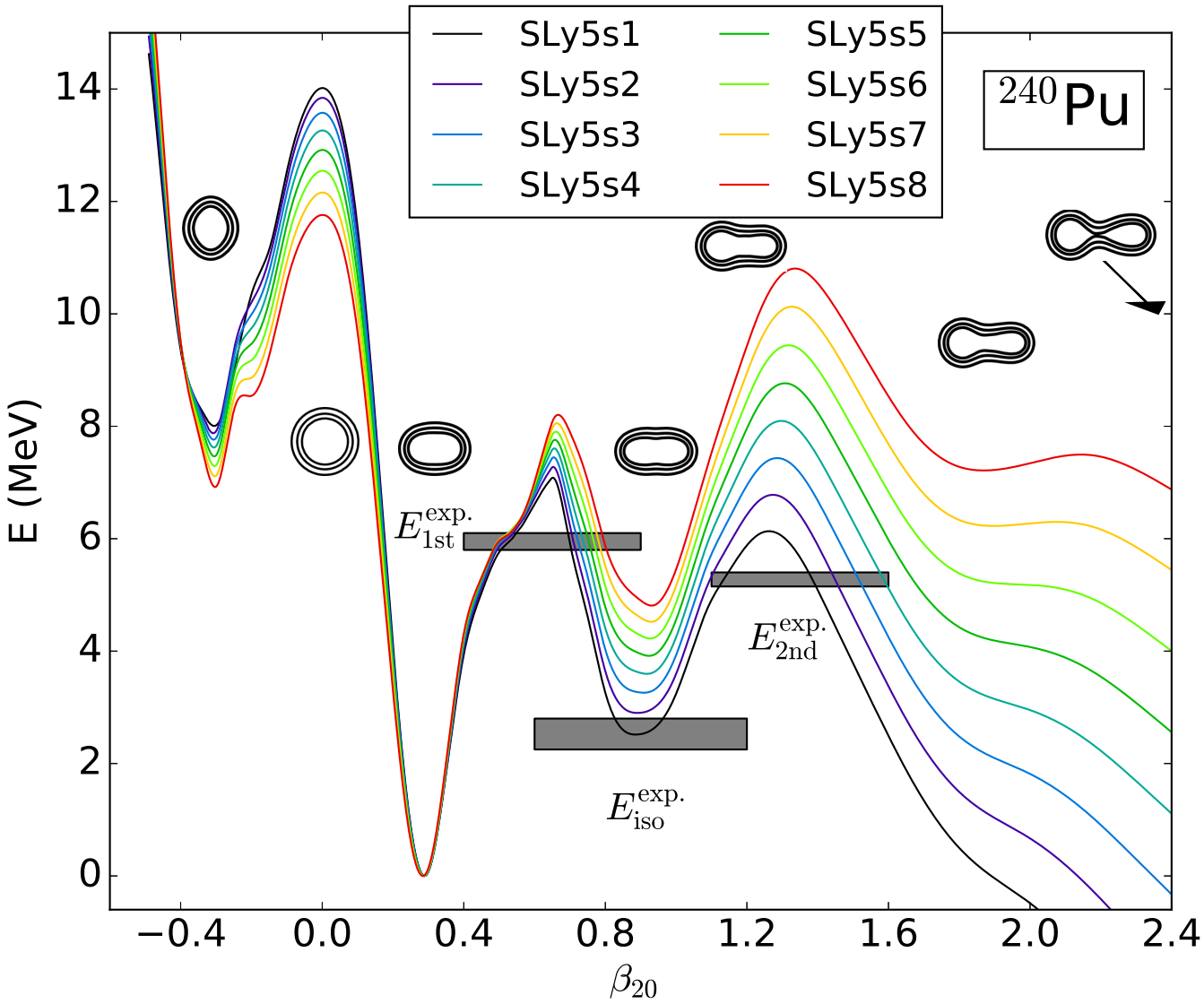
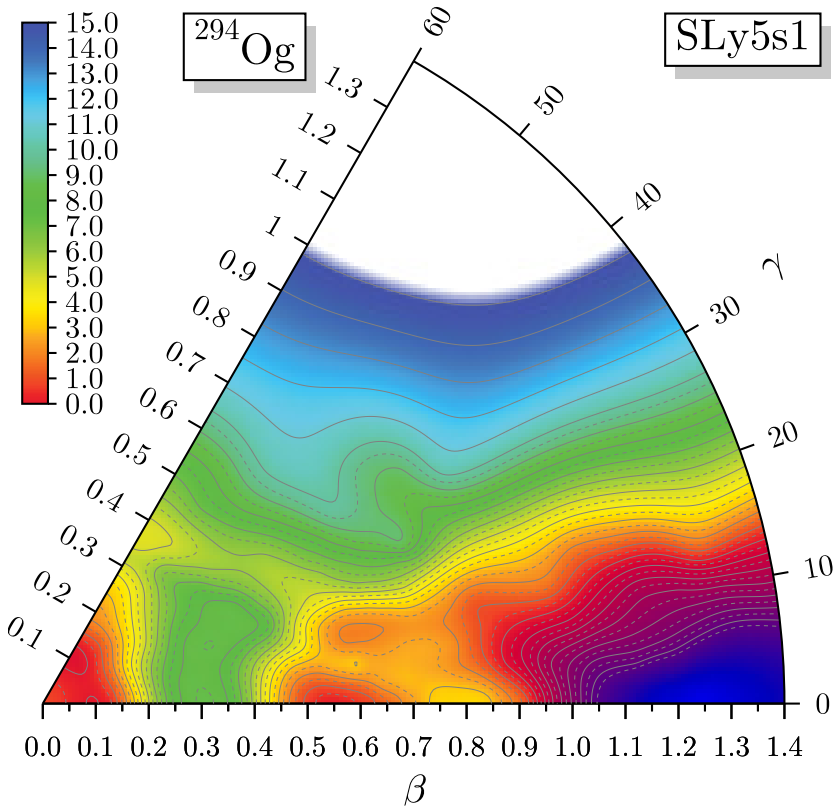
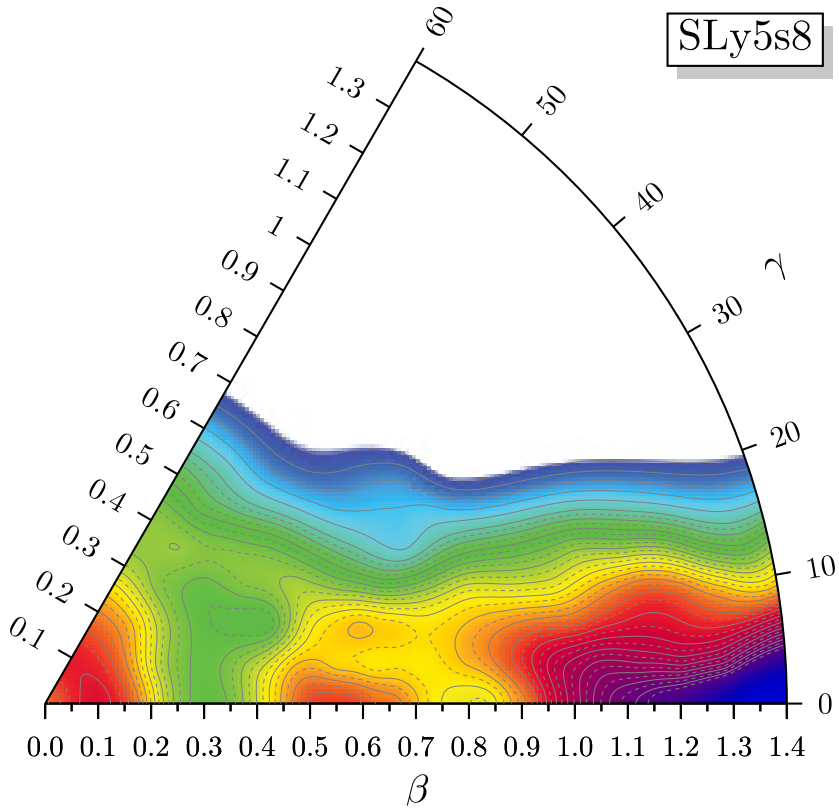


Controlling the surface tension: SLy5s1-8





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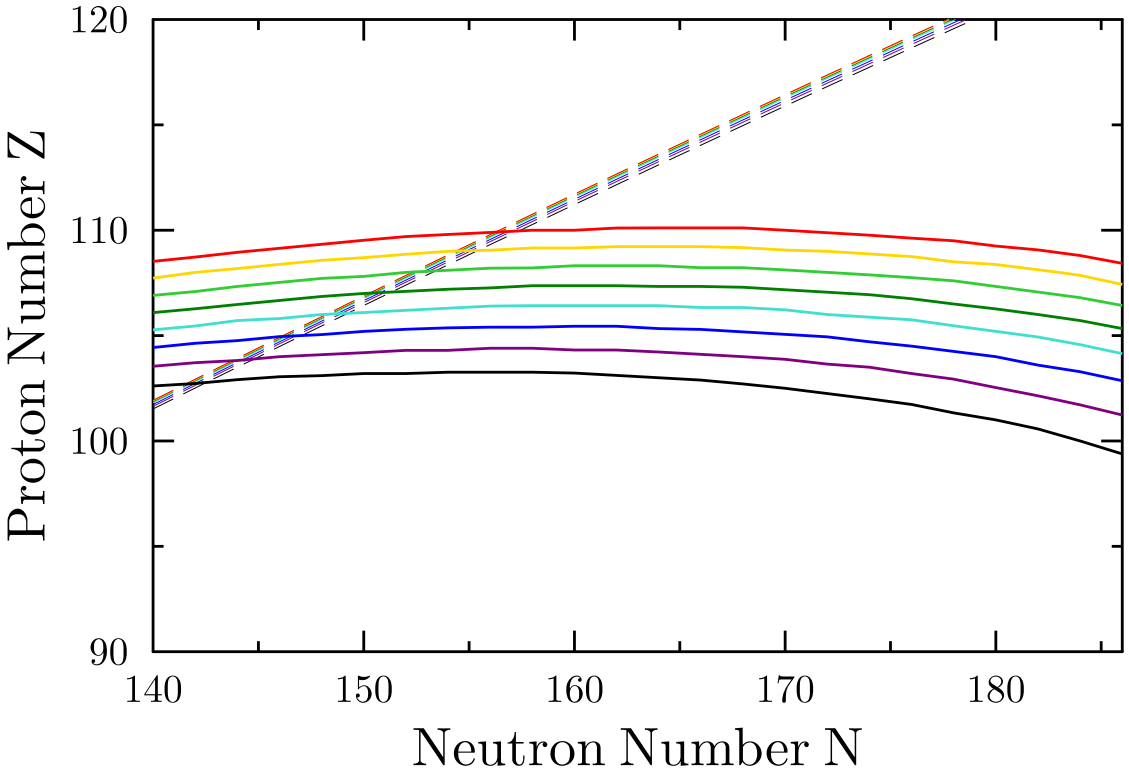


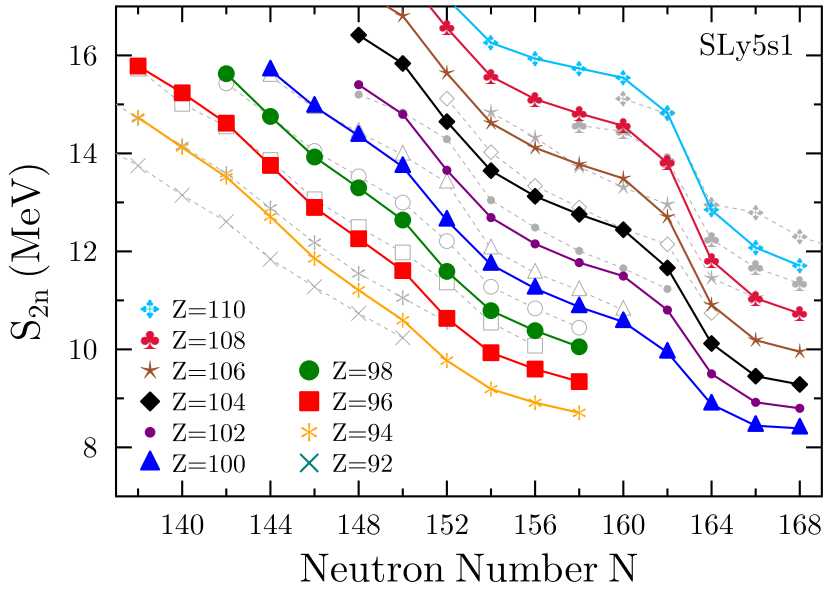
Surface tension

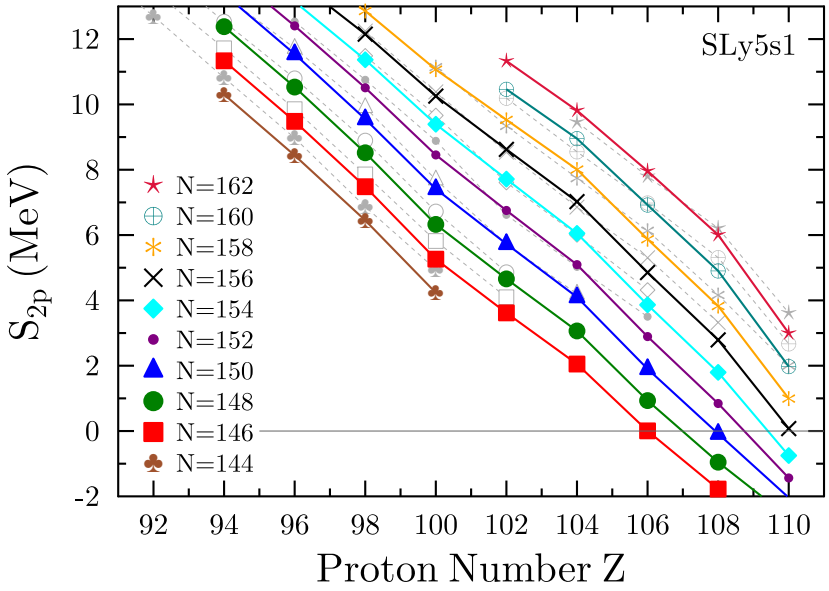
a Easy to control in a parameter fit

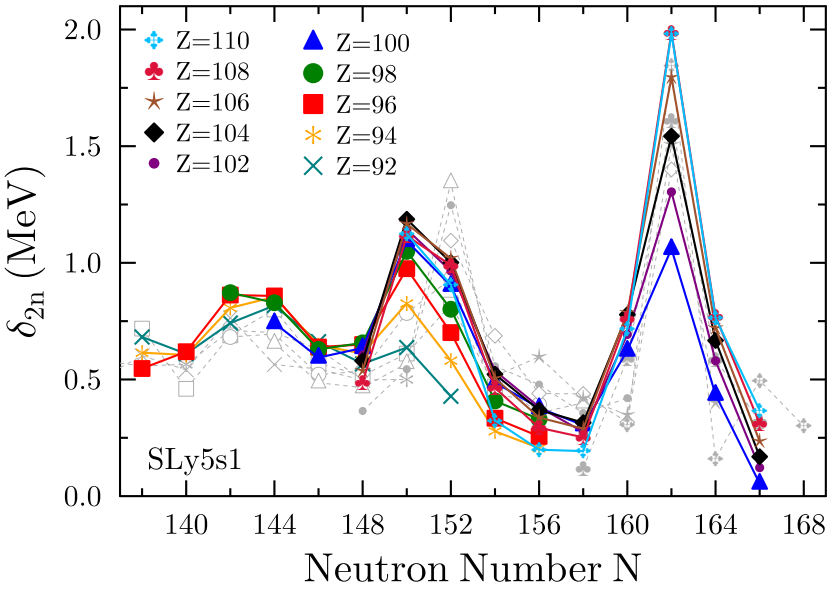
b Only slightly influences ordinary deformations

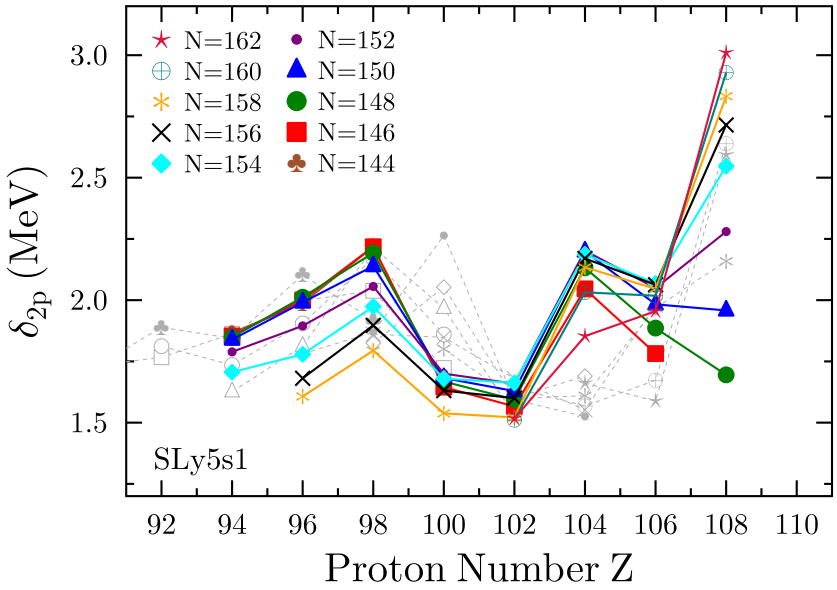
c Lower values of surface tension clearly preferred for fission

Gaps around N=152 & Z=100









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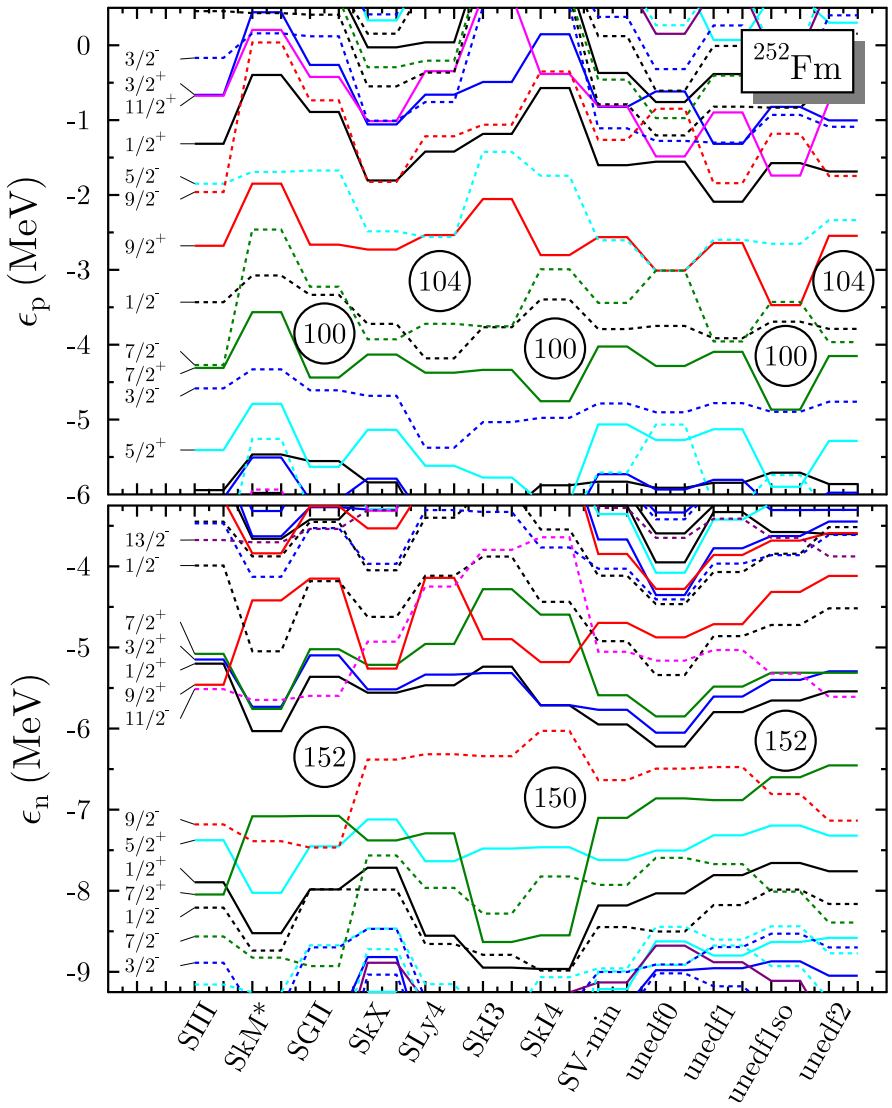

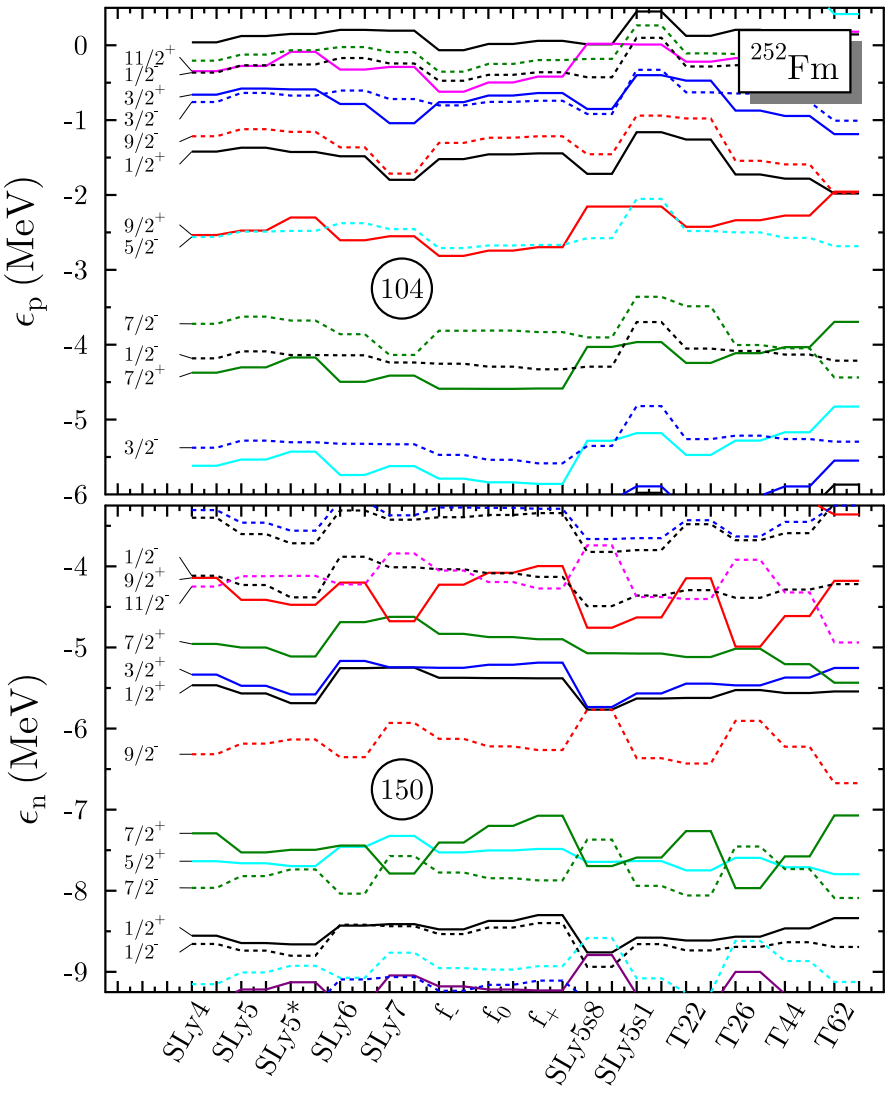

Systematically adding terms to the Skyrme functional with more derivatives

$$E^{\text{N2LO}}_{\text{local, central}} = \int dr \left[C_t^{(4)\Delta\rho} (\Delta\rho_t)^2 + C_t^{(4)M\rho} M_t(\rho) \right]$$

$$M_t[\rho] = \rho_t Q_t + \tau^2 + 2\sum_{\mu\nu} \Re\tau_{\mu\nu}\Re\tau_{\mu\nu} - 2\sum_{\mu\nu} \Im\tau_{\mu\nu}\Im\tau_{\mu\nu} - 2\sum_{\mu\nu} \Re\tau_{\mu\nu}\nabla_\mu\nabla_\nu\rho$$

NXLO functionals

a. Terms up to 2X derivatives
b. One N2LO EDF available
   PhD of P. Becker
c. Extra degrees of freedom
   specifically suited to s.p. spectra

SHEET and N2LO

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SHEET project
Coming soon^{TM} ...

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Conclusion

Contributions

I MOCCa with Hephaestos
- a Versatile in functionals
- b Fast in CPU time...
- c ...and human time(!)

II Exotic symmetry breaking
- a Deformations (triax, octupole)
- b Rotational bands
- c (Multi-)qp-excitations

III Beyond-mean-field codes
- a Projection and GCM
- b Triaxiality and odd nuclei
- c Limited by functionals
- d Limited by CPU time

IV Parameter-adjustment
- a Stable MF calculations through linear response
- b Control of the surface tension (fission!)

Challenges

I Deficient sp. spectra

→ SHEET project

II Paradigm shift needed for Hamiltonian-based EDFs

III Mitigating the CPU cost of Coulomb exchange

Thank you!

The presentation covered work of many people. Those still active are:
(red =explicit contribution for today)

Paul-Henri Heenen	ULB
Michael Bender	IPN Lyon
Benjamin Bally	UA Madrid
Thomas Duguet	Irfu/CEA Saclay & KULeuven & NSCL/MSU
Denis Lacroix	IPN Orsay
Karim Bennaceur	IPN Lyon
Dany Davesne	IPN Lyon
Jacques Meyer	IPN Lyon
Alessandro Pastore	University of York
P. Becker	University of York

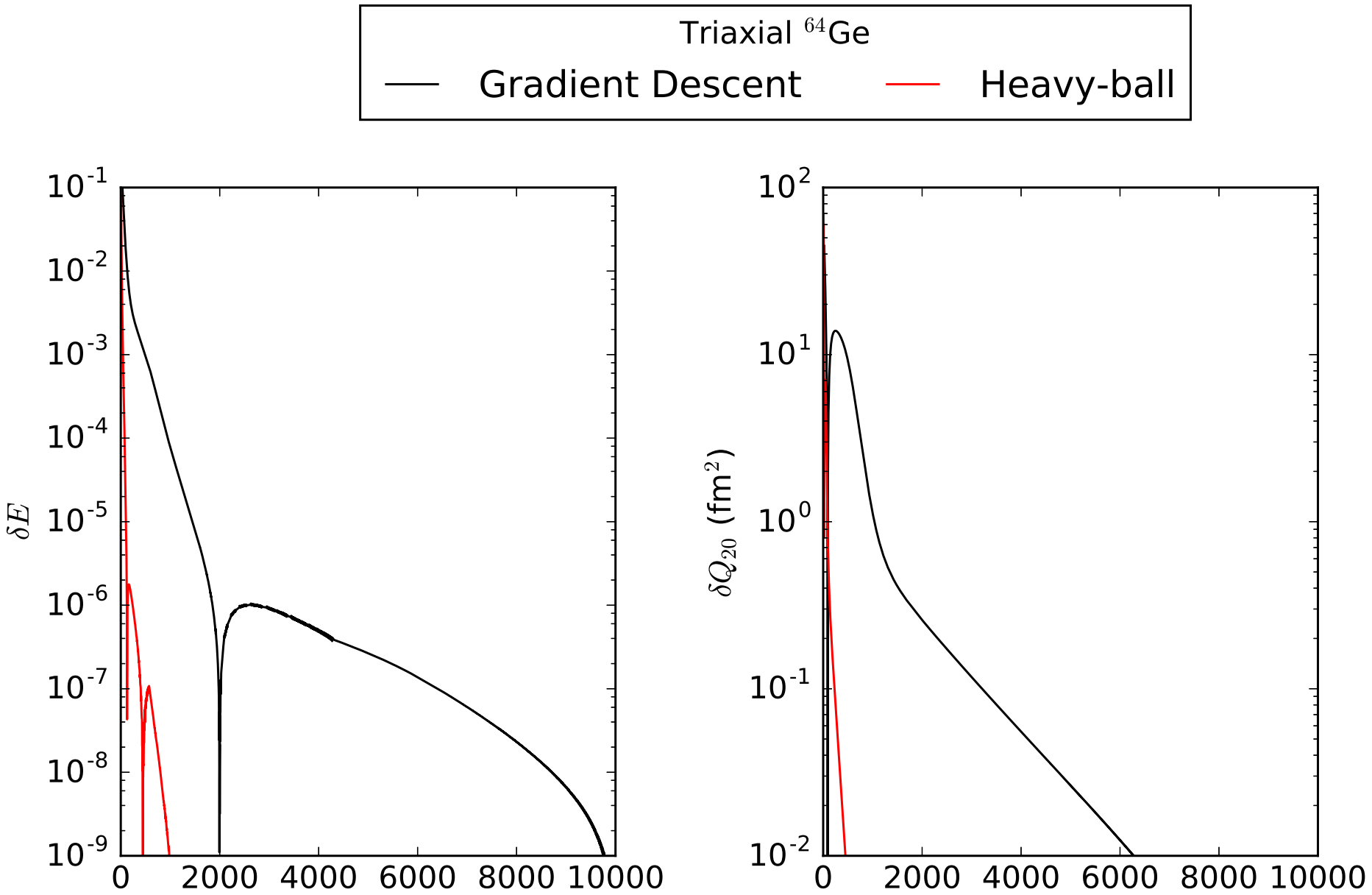
No longer active :(

Benoît Avez	Robin Jodon
Veerle Hellemans	Jeremy Sadoudi

Thanks for the support in form of CPU time (for W.R.)

CC of the IN2P3	CNRS, France
CECI network	FNRS, Belgium

Speed


Triaxial ^{64}Ge
Gradient Descent
Heavy-ball
δE
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
10^{-8}
10^{-9}
0
2000
4000
6000
8000
10000
δQ_{20} (fm^2)
10^{2}
10^{1}
10^{0}
10^{-1}
10^{-2}

Constraints