Broken symmetries in nuclear mean field approaches with Skyrme functionals.

Successes, failures and what we learn from them.

W. Ryssens[1]

[1]IPNL, Université de Lyon, Université Lyon 1, CNRS/IN2P3, F-69622 Villeurbanne, France

29th of August 2018

Mean-field with MOCCa.

Things that work and things that don't.

W. Ryssens[1]

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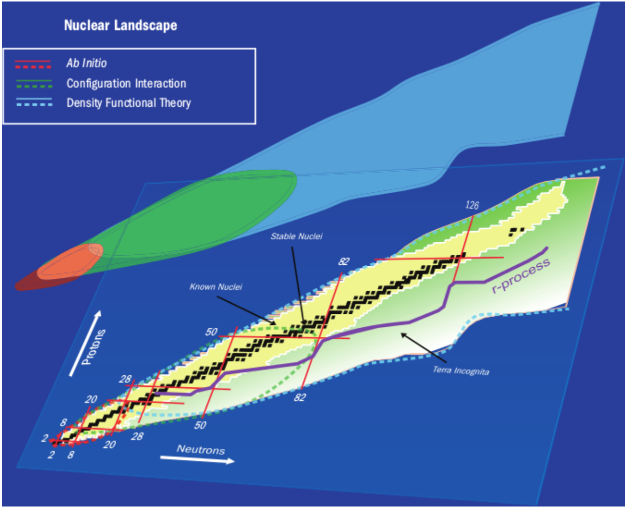
Table of contents

Planning

The nuclear chart



(Outdated) Figure of the UNEDF project from G .F. Bertsch et al., SciDAC Review 6, 48 (2007).

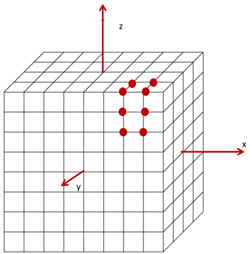
Find the **minimum** of $E(\rho, \tau, J_{\mu\nu})$ in a given **variational** space

EDF optimization

Find the **minimum** of $E(\rho, \tau, J_{\mu\nu})$ in a given **variational** space

Variational space $\rightarrow$ Single-particle states

- represented on a 3D mesh.
- form many-body states ...
- ... as (generalized) product states
- Also determined by **symmetries** !



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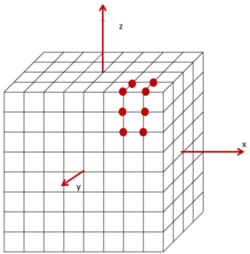
Products states maintain simplicity, . . .
Symmetry breaking to enrich!



Self-consistent EDF calculations

$\boxed{\Psi_{\text{many-body}} = \text{Product wavefunction}}$

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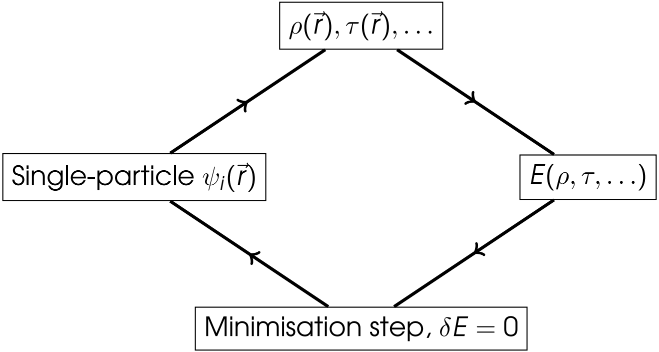

Self-consistent EDF calculations

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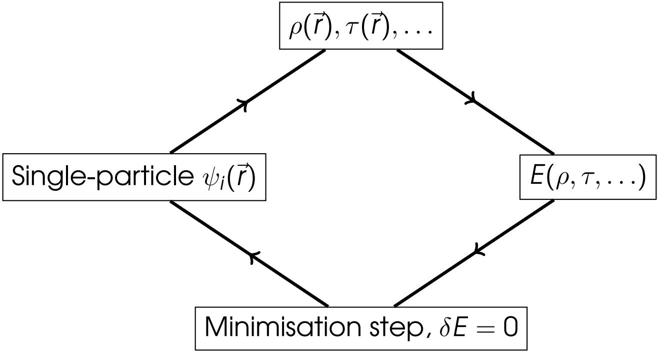

Complexity determined by the single-particle space!

Skyrme (NLO) functional

Multiple terms

$$E_{\text{tot}} = E_{\text{kin}} + E_{\text{Skyrme}} + E_{\text{Coul}} + E_{\text{cm}} + E_{\text{pair}} \,,$$

The more or less standard Skyrme part is the following

$$E_{\text{Skyrme}} = \sum_{t=0,1} \int d^3 r \left[C_t^{\rho} \, \rho_t^2(\vec{r}) + C_t^{\rho^{\alpha}} \, \rho_0^{\alpha}(\vec{r}) \, \rho_t^2(\vec{r}) + C_t^{\tau} \, \rho_t(\vec{r}) \, \tau_t(\vec{r}) \right.$$
$$\left. + \, C_t^{\Delta\rho} \, \rho_t(\vec{r}) \, \Delta \rho_t(\vec{r}) + C_t^{\nabla \cdot J} \rho_t(\vec{r}) \, \nabla \cdot \vec{J}_t(\vec{r}) - C_t^{T} \sum_{\mu,\nu} J_{t,\mu\nu}(\vec{r}) \, J_{t,\mu\nu}(\vec{r}) \right] .$$

which has

- Densities: $\rho, \tau, J_{\mu\nu}$
- $\sim$ **10** parameters ...
- ... fitted to a few masses and radii.

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$$+ C_t^{\Delta\rho}\, \rho_t(\vec{r})\, \Delta\rho_t(\vec{r}) + C_t^{\nabla\cdot J} \rho_t(\vec{r})\, \nabla \cdot \vec{J}_t(\vec{r}) - C_t^{J} \sum_{\mu,\nu} J_{t,\mu\nu}(\vec{r})\, J_{t,\mu\nu}(\vec{r}) \Big] \,.$$

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Only half of the story; also time-odd terms!

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

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

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(MeV)	$a_{\mathrm{surf}}^{(\mathrm{MTF})}$		$a_{\mathrm{surf}}^{(\mathrm{MTF})}$
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).

Controlling the surface tension: SLy5s1-8

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- Comparable shell structure
- **Easily** deformable (s1) vs. ...
- **Stiff** deformation (s8).

Parameterizations from
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What we try to reach

Global microscopic framework to describe

Bulk properties

- Masses
- Radii

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Low-energy spectroscopy

- Ground states

  0^+ for even-even nuclei
  J^π for even-odd
- Low-lying excitations
  - Isomers of various kinds
  - Rotational bands

What we try to reach

Global microscopic framework to describe

Bulk properties

- Masses
- Radii

Rather good: **HFB17** describes

S.Goriely et al., PRL **102**, 152503 (2009).

- **2149** masses
  RMS deviation = **0.581** MeV
  Cf. BE(^{208}Pb) $\sim$ **1.6 G**eV.
- **792** charge radii
  RMS deviation = **0.0313** fm
  Cf. $R_{\rm rms}$ (^{208}Pb) = $\sim$ **5.5** fm.

Low-energy spectroscopy

- Ground states
  0^+ for even-even nuclei
  J^π for even-odd
- Low-lying excitations
  - Isomers of various kinds
  - Rotational bands

This is not easy at all . . .

L. Bonneau et al., PRC **76**, 024320.

- Correct J^π $\sim$ 80% (spherical)
- Correct J^π $\sim$ 40% (deformed)
- Similar performance as MIC-MAC.

The N2LO extension

$$\begin{aligned}
E_{\text{Skyrme}} &= E^{\text{NLO}}_{\text{Skyrme}} + E^{\text{N2LO}}_{\text{Skyrme}} \\
E^{\text{N2LO}}_{\text{Skyrme}} &= \sum_{t=0,1} \Big[C_t^{\Delta\rho\Delta\rho} (\Delta \rho_t(\vec{r}))^2 + C_t^{\tau\tau} \tau_t^2(\vec{r}) + C_t^{\rho Q} \rho_t(\vec{r})\, Q_t(\vec{r}) \\
&\quad + 2C^{\tau_{\mu\nu}\tau_{\mu\nu}} \sum_{\mu,\nu} \tau^2_{t,\mu\nu}(\vec{r}) - 2C^{\tau\nabla\nabla\rho} \sum_{\mu,\nu} \tau_{t,\mu\nu}(\vec{r}) \nabla_\mu \nabla_\nu \rho_t(\vec{r}) \\
&\quad + 2C_t^{KK} \sum_{\mu,\nu,\kappa} \big(K_{t,\mu\nu\kappa}(\vec{r})\big)^2 - 2C_t^{JV} \sum_{\mu,\nu} J_{t,\mu\nu}(\vec{r}) V_{t,\mu\nu}(\vec{r}) \Big] ,
\end{aligned}$$

which has

- Densities: Q, $V_{\mu\nu}$, $K_{\mu\nu\kappa}$
- **14** (cf. 10) parameters . . .
- . . . fitted to a few masses and radii.
- But what new information to include?

Skyrme (N2LO) functional

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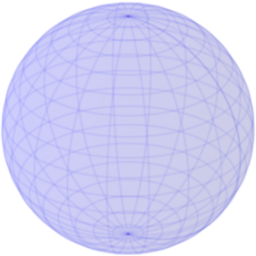
Planning

Spherical symmetry

a. Ultra-Fast calculations ($\sim$seconds)
b. Symmetries respected
c. Most EDFs fitted at this level
d. Single-particle quantum numbers J, J_z, π

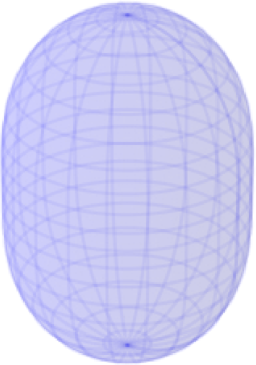


Axial symmetry: Ellipsoids

a Fast calculations ($\sim$minutes)

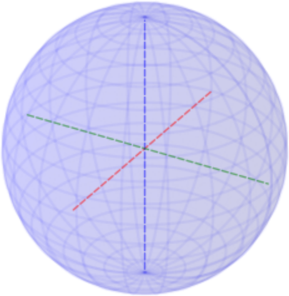
b One symmetry axis

c Single-particle quantum numbers
$K = J_z, \pi$



Triaxial shapes

a Slow calculations ($\sim$ hours/days)
b No more continuous symmetries



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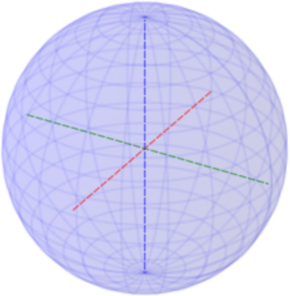
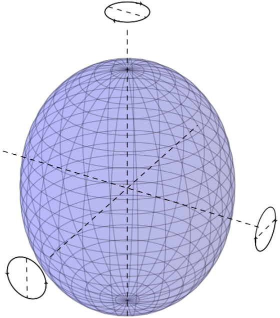


$\mathcal{D}_{2h}^{T(D)}$ for nuclei

Single-particle symmetry operators

$$\hat{P}, \hat{R}_{x/y/z}, \check{T}$$



$\mathcal{D}_{2h}^{T(D)}$ for nuclei

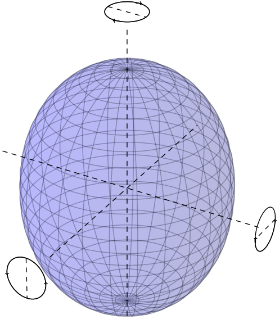
Single-particle symmetry operators

$$\hat{P}, \hat{R}_{x/y/z}, \check{T}$$

give rise to many-body groups

$$\mathcal{D}_{2h}^{T} = \left\{ \hat{1}, \hat{\mathcal{P}}, \check{\mathcal{T}}, \check{\mathcal{P}}^{T}, \hat{\mathcal{R}}_{\mu}, \check{\mathcal{R}}_{\mu}^{T}, \hat{\mathcal{S}}_{\mu}, \check{\mathcal{S}}_{\mu}^{T} \right\} \text{ (even)}$$

$$\mathcal{D}_{2h}^{TD} = \left\{ \hat{1}, -\hat{1}, \hat{\mathcal{P}}, -\hat{\mathcal{P}}, \check{\mathcal{T}}, -\check{\mathcal{T}}, \hat{\mathcal{R}}_{\mu}, -\hat{\mathcal{R}}_{\mu}, \check{\mathcal{R}}_{\mu}^{T}, -\check{\mathcal{R}}_{\mu}^{T}, \hat{\mathcal{S}}_{\mu}, -\hat{\mathcal{S}}_{\mu}, \check{\mathcal{S}}_{\mu}^{T}, -\check{\mathcal{S}}_{\mu}^{T}, \check{\mathcal{P}}^{T}, -\check{\mathcal{P}}^{T} \right\} \text{ (odd)}$$



All subgroups in principle contain different correlations/physics.

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MOCCa

* 3D coordinate representation
* Discrete symmetry breaking
    16(!) different combinations
* Easy to use and fast
    W. Ryssens et al., (almost) Submitted to EPJA.

The hero of the story

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  NLO functionals
  SLy5s1-8 today
  R. Jodon et al. , PRC **94**, 024335 (2016)
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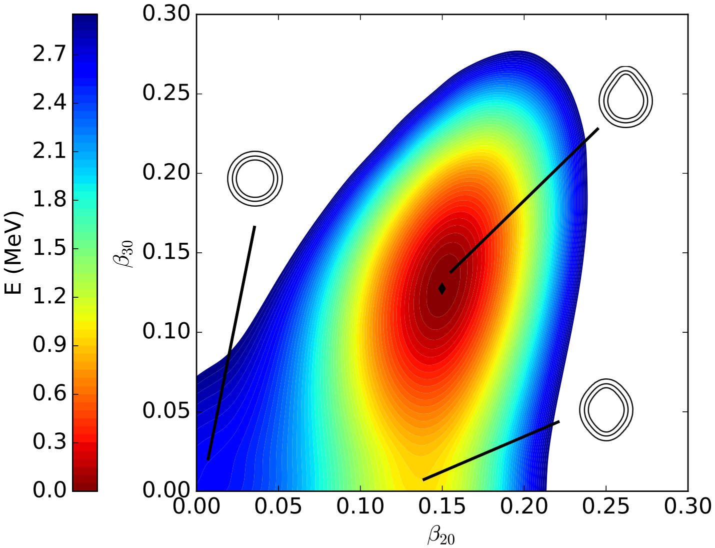
* MOCCa v2, *Tantalus*
  N2LO functionals.
  N3LO, N4LO, . . .
  Automation from formula to code

Planning

Even-even Thoriums



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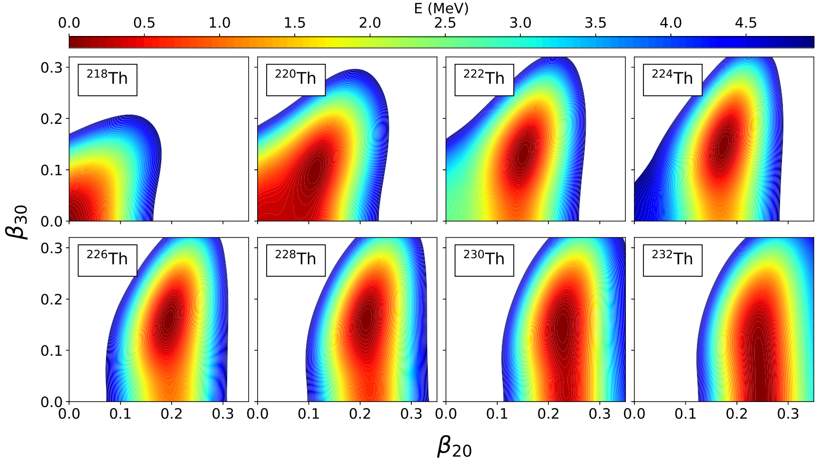

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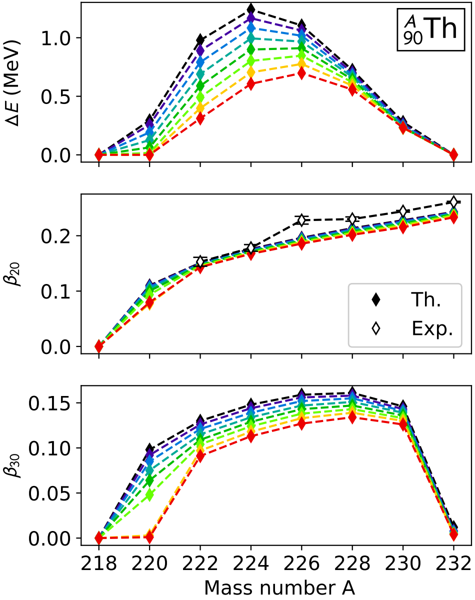
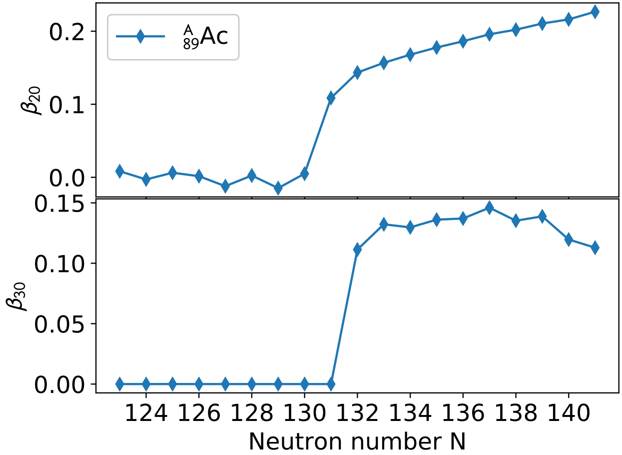
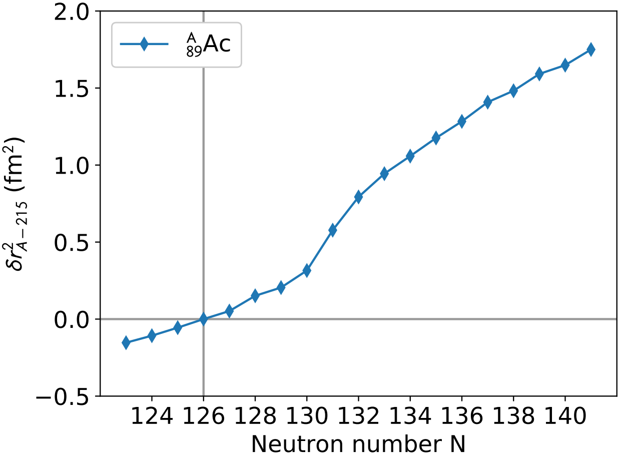


Deformations of the Ac isotopes



Isotopic shifts



(Preliminary) Data from E. Verstraelen, A. Teigelhoefer et al. (unpublished).

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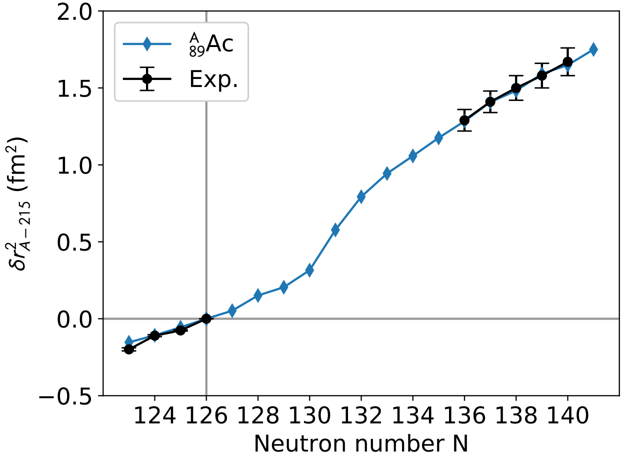


(Preliminary) Data from E. Verstraelen, A. Teigelhoefer et al. (unpublished).

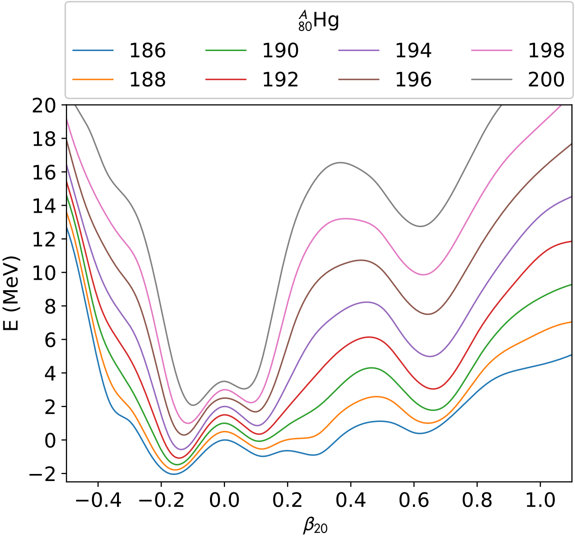
Ground states of odd Thorium isotopes

Odd Th isotopes		
A	Exp.	Th.
221	$7/2^+$	1/2
223	$5/2^+$	5/2
225	$3/2^+$	3/2
227	$1/2^+$	1/2
229	$5/2^+$	1/2
231	$5/2^+$	1/2

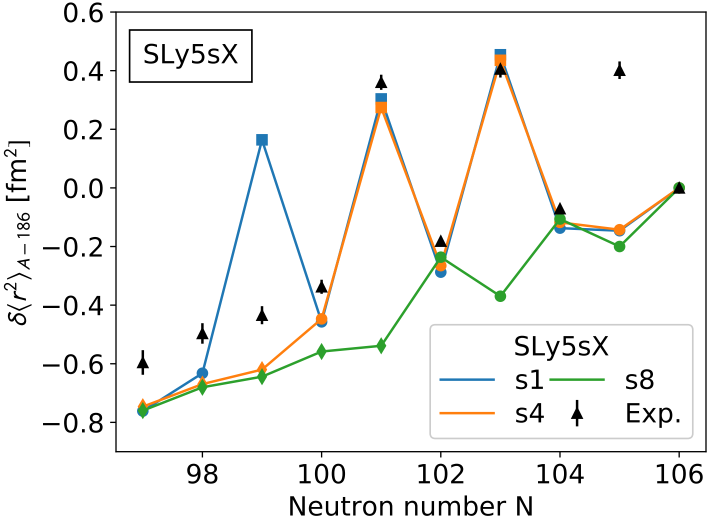
Ac isotopes		
A	Exp.	Th.
212	(7)	(4)
213	(9/2)	1/2
214	5	(4)
215	9/2	5/2
225	3/2	3/2
226	(1)	(2)
227	3/2	3/2
228	3	(2)
229	3/2	3/2

Planning

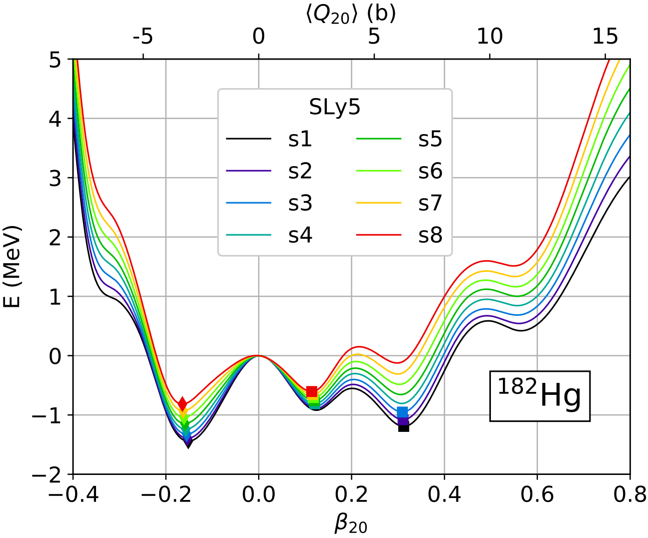
Shape coexistence in the Hg isotopes



Radii/shifts in the Hg isotopes

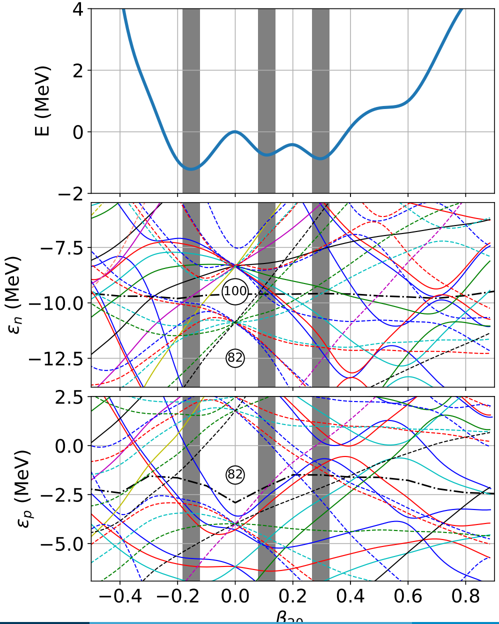


S. Sels et al., (almost) submitted to PRC.



⟨Q_{20}⟩ (b)
-5
0
5
10
15
E (MeV)
SLy5
s1
s2
s3
s4
s5
s6
s7
s8
^{182}Hg
β_{20}

Single-particle structure



Ground states of Hg isotopes

A	Exp.	SLy5s1	SLy5s8.
177	(7)/2$^-$	1/2$^-$	1/2$^-$
179	(7)/2$^-$	1/2$^-$	1/2$^-$
181	1/2$^-$	5/2$^-$	1/2$^-$
183	1/2$^-$	5/2$^-$	3/2$^-$
185	1/2$^-$	3/2$^-$	3/2$^-$

Planning

Modelling rotation with
Skyrme-HFB cranking Routhian.

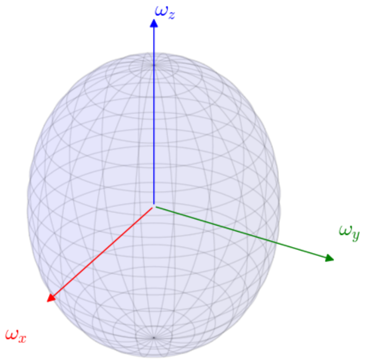
$$R = E - \omega_x \langle \hat{J}_x \rangle - \omega_y \langle \hat{J}_y \rangle - \omega_z \langle \hat{J}_z \rangle$$

Preferred directions $\Rightarrow$ ~~signatures~~

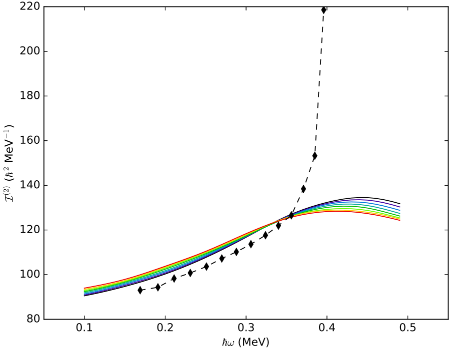
Compared to experiment

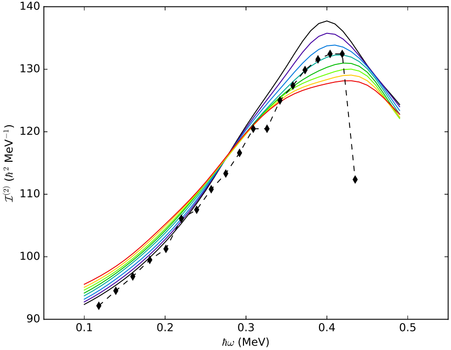
$$\omega(J) = \frac{E(J+1) - E(J-1)}{I(J+1) - I(J-1)} .$$

$$I(J) = \sqrt{J^2 - J_{\mathrm{sp}}^2}$$



Superdeformed bands: Hg isotopes





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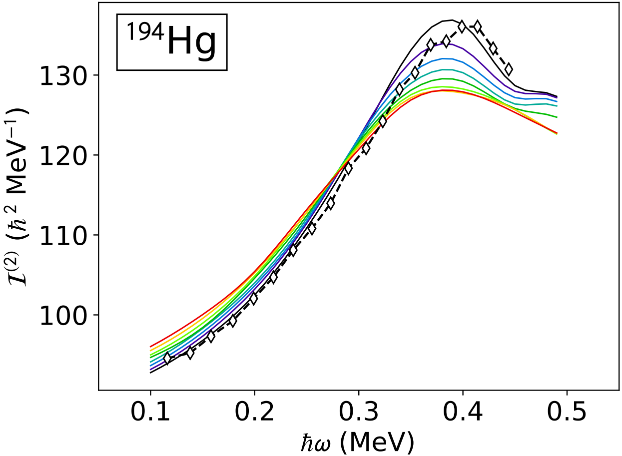
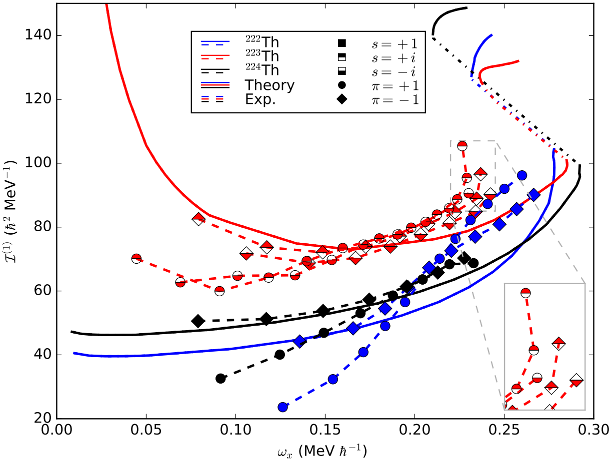
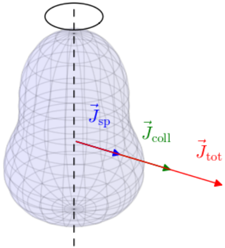


Moments of inertia





Data from
G. Maquart *et al.*, Phys. Rev. C **95**, 034304 (2017),
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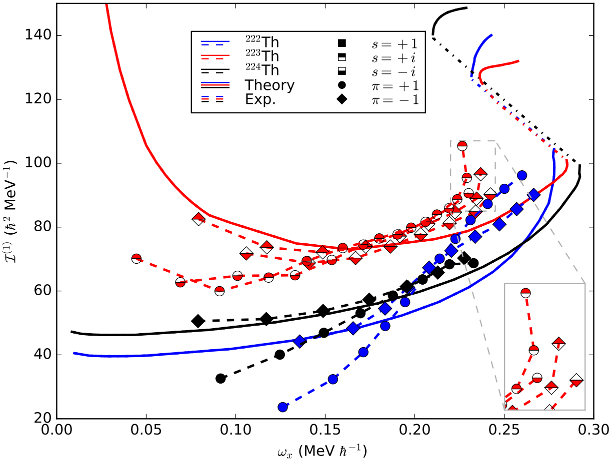

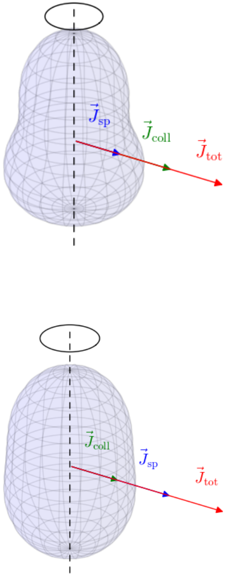

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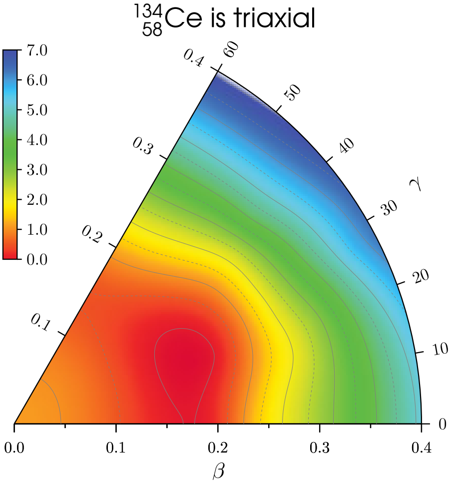
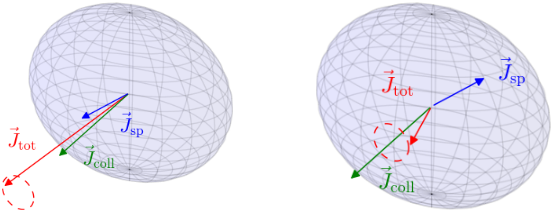

$^{134}_{58}$Ce is triaxial
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
0.0
0.1
0.2
0.3
0.4
β
0
10
20
30
40
50
60
γ

Tilted-axis cranking: $^{135}_{59}\mathrm{Pr}$

Two ways of combining rotation with an odd particle



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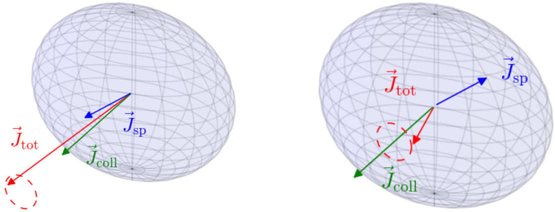
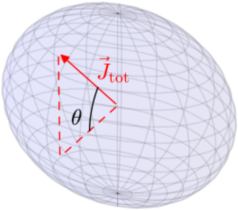
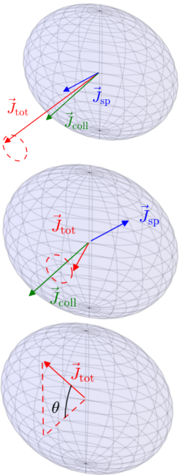
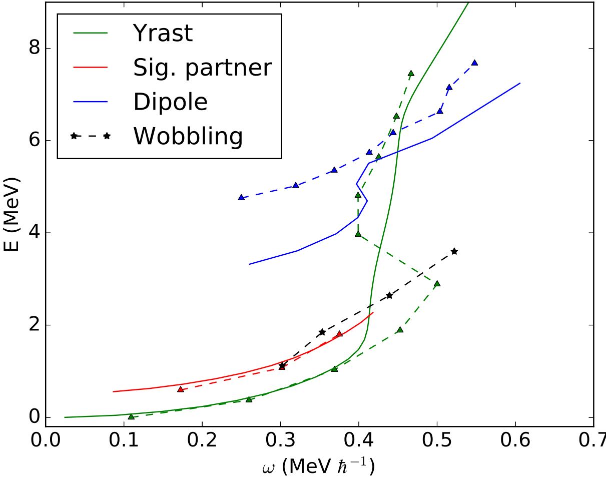


But on top of that options to spin about non-principal axes







Exp. data from
PRL **114**, 082501 (2015).

Planning

Conclusion

Nuclear structure calculations with EDFs:

- Applicable to ALL nuclei
- Symmetry breaking is key
- Bulk properties ✓
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Thank you!

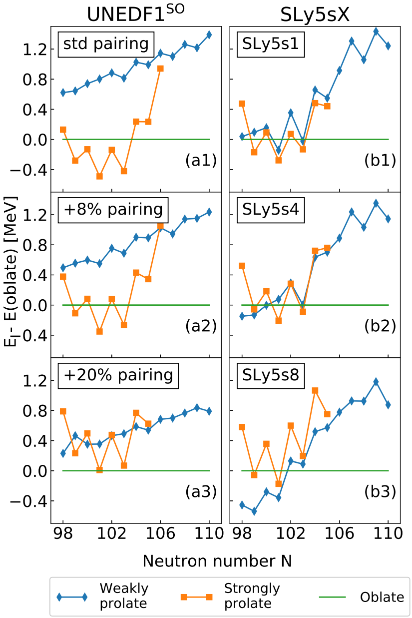
Direct contributions from

Paul-Henri Heenen	ULB
Michael Bender	IPN Lyon
Karim Bennaceur	IPN Lyon
Jacques Meyer	IPN Lyon

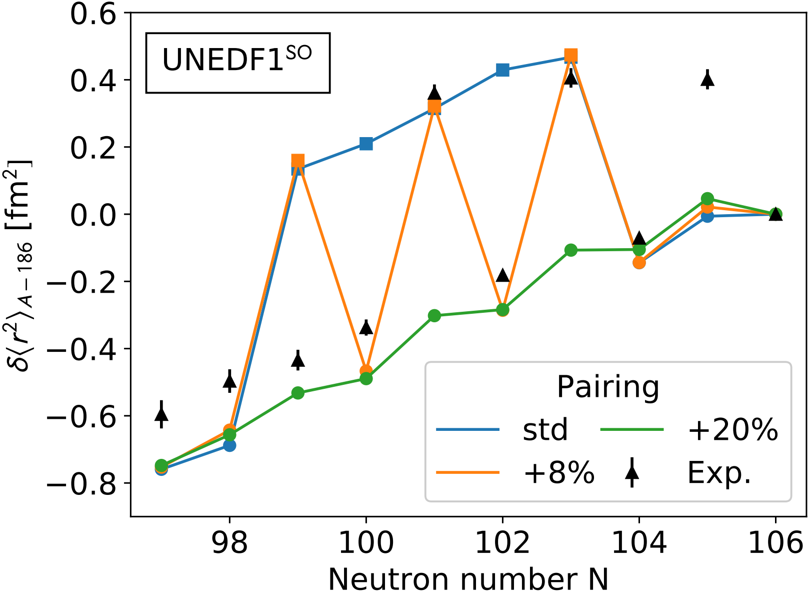
Thanks for the CPU time! (for W.R.)

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

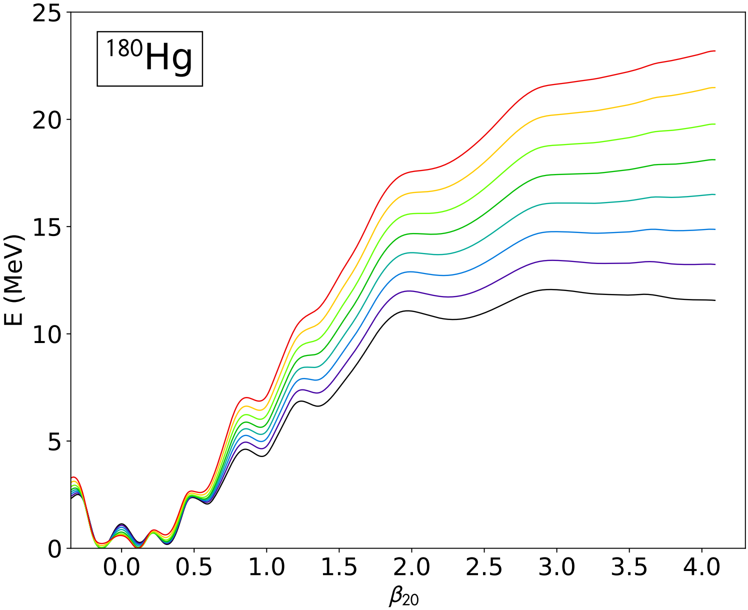
Hg radii: energy differences



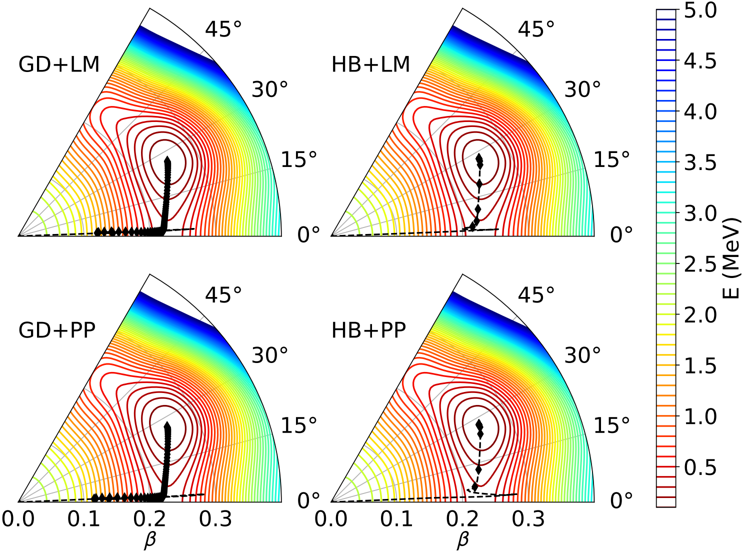
Hg staggering with UNEDF1^{SO}



Hg fission



Heavy-Ball



GD+LM
HB+LM
GD+PP
HB+PP
45°
30°
15°
0°
0.0
0.1
0.2
0.3
β
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
E (MeV)