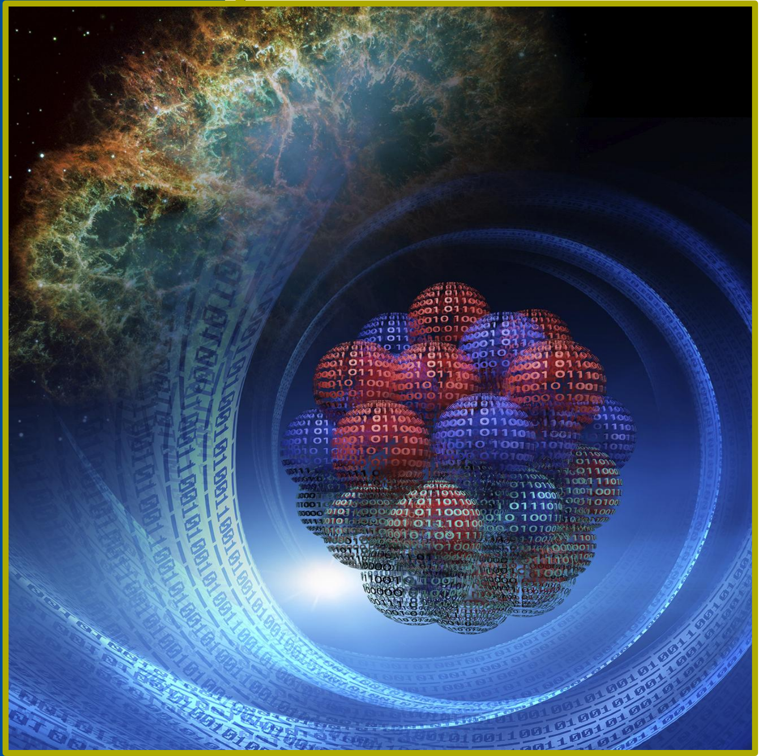
WOUTER RYSSENS



Andy Sproles, ORNL

The **Skyrme** EDF: the view from Brussels

May 31th 2022

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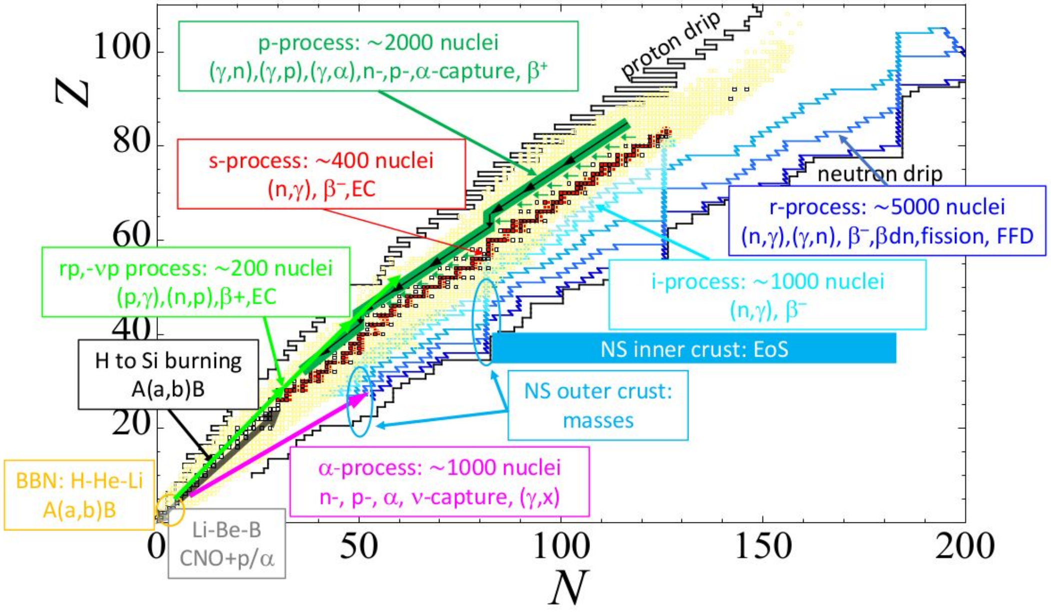
I. The call of astrophysics



M. Arnould & S. Goriely, Prog. Part. Nuc. Phys. **112,** 103766 (2020).

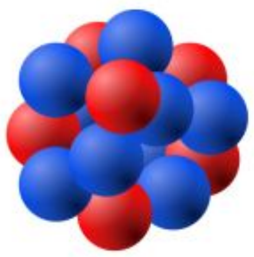
I. The call of astrophysics: **a video!**

Animation by J.-F. Lemaître (CEA)

Modelling challenge

- predictions for thousands of nuclei
- … for many **different observables**
- … in a **unified** fashion
- … founded in **microscopic** physics
- … despite **enormous extrapolations**

II. The Skyrme EDF: **so you want to describe nuclei?**



$$\hat{H}|\Psi\rangle = E|\Psi\rangle \, .$$

Interaction?

- Look at QCD, n-n scattering?
- Phenomenological?
- Global or local?

Model space?

- Include all nucleons?
- Numerical representation?
- Local or global?

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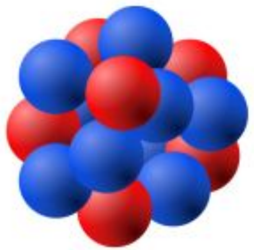

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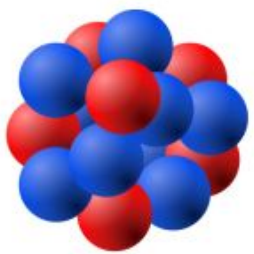

$$\hat{H}|\Psi\rangle = E|\Psi\rangle \, .$$

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- Look at QCD, n-n scattering?
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- Local or global?

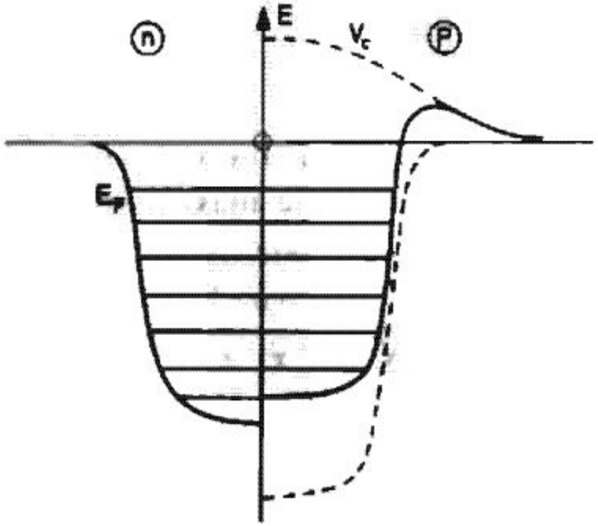
II. The Skyrme EDF: **the Skyrme interaction**

$$T = \sum_{i<j} t_{ij} + \sum_{i<j<k} t_{ijk}$$

$$t_{12} = \delta(\mathbf{r}_1 - \mathbf{r}_2)\, t(\mathbf{k}', \mathbf{k})$$

$$\begin{aligned} t(\mathbf{k}', \mathbf{k}) &= t_0(1+x_0 P^\sigma) + \tfrac{1}{2} t_1 (1+x_1 P^\sigma)(\mathbf{k}'^2 + \mathbf{k}^2) \\ &+ t_2[1+x_2(P^\sigma - \tfrac{4}{5})]\mathbf{k}' \cdot \mathbf{k} \\ &+ \tfrac{1}{2} T[\boldsymbol{\sigma}_1 \cdot \mathbf{k} \boldsymbol{\sigma}_2 \cdot \mathbf{k} - \tfrac{1}{3} \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 \mathbf{k}^2 + \text{conj.}] \\ &+ \tfrac{1}{2} U[\boldsymbol{\sigma}_1 \cdot \mathbf{k}' \boldsymbol{\sigma}_2 \cdot \mathbf{k} - \tfrac{1}{3} \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 \mathbf{k}' \cdot \mathbf{k} + \text{conj.}] \\ &+ V[i(\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2) \cdot \mathbf{k}' \times \mathbf{k}], \end{aligned}$$

= Central + Tensor + Spin-orbit interaction



"It is now clear that such interaction is **very different** from the interaction between two (free) nucleons."

T. H. R. Skyrme, Nuclear Physics 9, 615–634 (1958).
P. Ring and P. Schuck, the nuclear many-body problem (1984).

II. The Skyrme EDF

D. Vautherin and D. M. Brink, PRC 5, 626-647 (1972).

$$E = \langle HF|\hat{H}_{\mathrm{Sk.}}|HF\rangle = \int H(\mathbf{r})\, d^3\mathbf{r}\,.$$

$$H(\vec{r}) = \frac{\hbar^2}{2m}\tau + \frac{3}{8}t_0\rho^2 + \frac{1}{16}t_3\rho^3 + \frac{1}{16}(3t_1+5t_2)\rho\tau + \frac{1}{64}(9t_1-5t_2)(\vec{\nabla}\rho)^2 - \frac{3}{4}W_0\rho\vec{\nabla}\cdot\vec{J}\,.$$

= Central + Tensor + Spin-orbit **interaction**

$$E_{\mathrm{Sk}} = \int d^3\mathbf{r} \sum_{t=0,1} \mathcal{E}_t(\mathbf{r})\,,$$

$$\mathcal{E}_t(\mathbf{r}) = C_t^{\rho\rho}\,\rho_t^2(\mathbf{r}) + C_t^{\rho\rho\rho^\gamma}\,\rho_0^\gamma(\mathbf{r})\,\rho_t^2(\mathbf{r}) + C_t^{\rho\tau}\,\rho_t(\mathbf{r})\,\tau_t(\mathbf{r}) + C_t^{\rho\Delta\rho}\,\rho_t(\mathbf{r})\,\Delta\rho_t(\mathbf{r}) + C_t^{\rho\nabla\cdot J}\,\rho_t(\mathbf{r})\,\nabla\cdot\mathbf{J}_t(\mathbf{r})\,,$$

= Central + Tensor + Spin-orbit **functional**

Some remarks:

Energy Density Functional= analytical form of the energy density, **can be** linked to an interaction
Parameterization = values of the coupling constants
Nuclear DFT is significantly more **ad-hoc** than electronic DFT.

II. The Skyrme EDF: a comparison

		Pros
Skyrme	standard	Simple zero-range interaction
		=> parameter adjustment pushed farthest
		=> most applications (linear response, time-dependent MF, ...)
	Fayans	Gradients in the pairing channel
	N2/3LO	Higher-number-of-gradients expansion
	SEAL	Minimal number of parameters
	Ab initio	Forms inspired by different kinds of ab initio calculations
Gogny		Finite-range interaction (with identical interaction in pairing channel)
RMF		Lorentz-invariant (with implications for coupling constants)

III. Modelspace: mean-field theory

1. Guess some initial product wavefunction with **single-particle wavefunctions**
2. Variationally minimize the energy through variation of the spwfs
3. Restore symmetries if needed
4. Mix different solutions: **GCM**

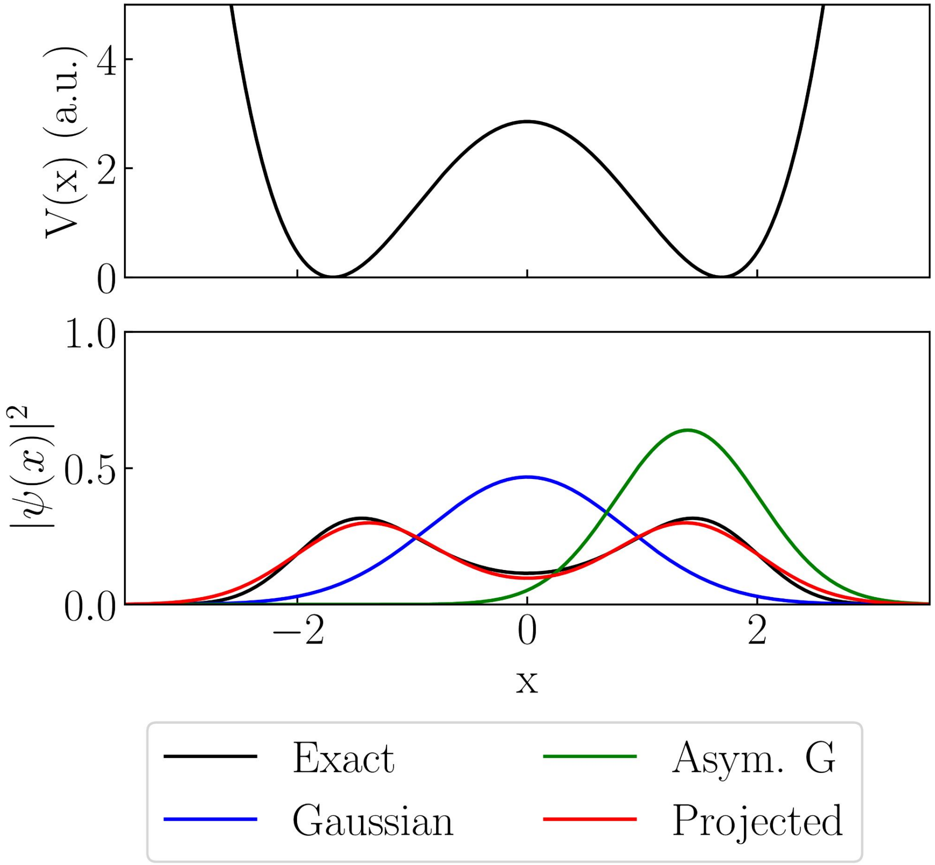
$$|\Psi\rangle = c_1^\dagger \dots c_A^\dagger |0\rangle \,.$$

$$|\Psi_{\text{opt.}}\rangle = \arg\min \left\{ \langle \Psi | \hat{H} | \Psi \rangle | \Psi = \text{simple} \right\} \,.$$

$$|\Psi_{\text{sym}}\rangle = \frac{1}{\sqrt{2}} \left[|\Psi_{\text{opt.}}\rangle + \hat{U} |\Psi_{\text{opt.}}\rangle \right] \,.$$

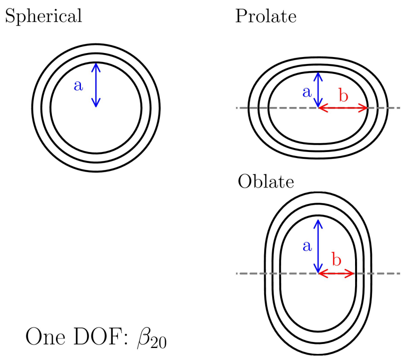
$$|\Psi_{\text{final}}\rangle = \sum_i c_i |\Psi_{\text{sym}}\rangle \,.$$

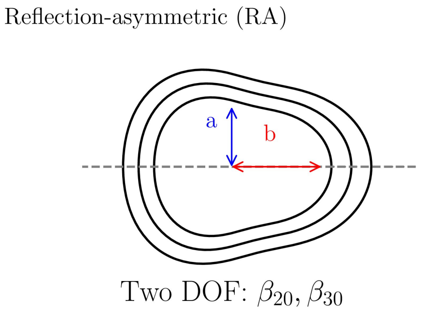
III. Modelspace: symmetry breaking and restoration

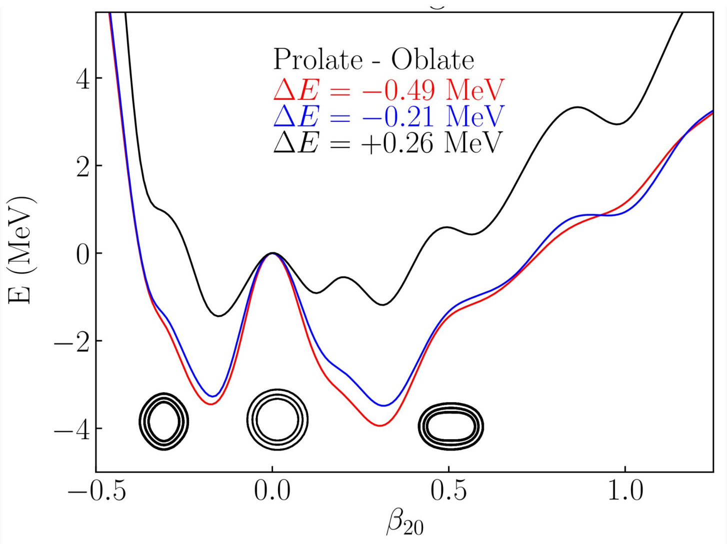


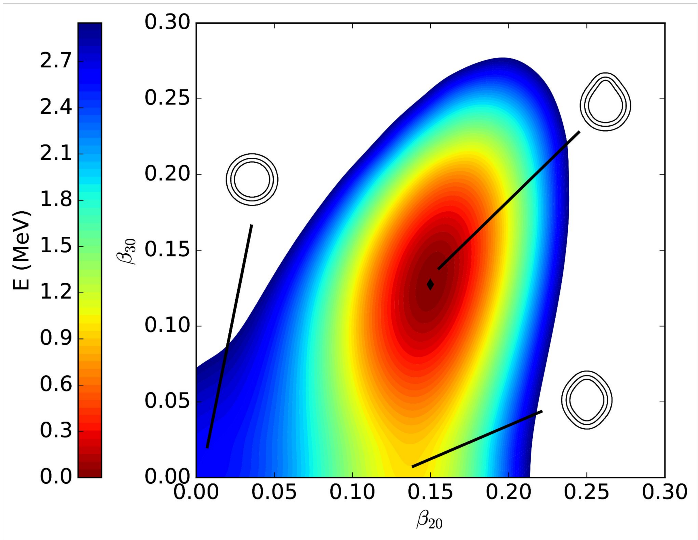
	Energy	<X^2>
Exact	1.625	1.98
Gaussian	2.152	0.727
Asym. G.	1.844	2.331
Projected	1.735	2.190

III. Modelspace: nuclear deformation





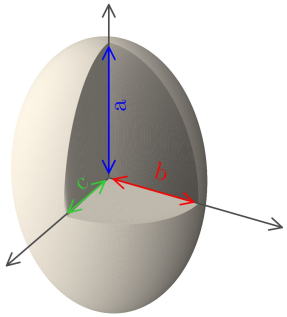




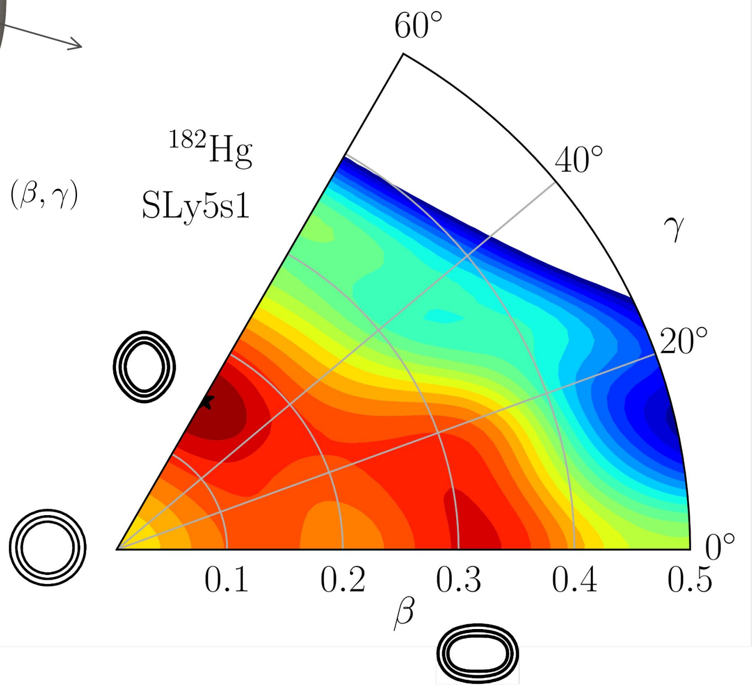
III. Modelspace: nuclear deformation

In general:

$$\beta_{\ell m} = \frac{4\pi}{3(r_0 A^{1/3})^\ell A} \int d^3\mathbf{r}\, \rho(\mathbf{r}) r^\ell \mathrm{Re}\, Y_{\ell m}(\theta, \phi)\,,$$



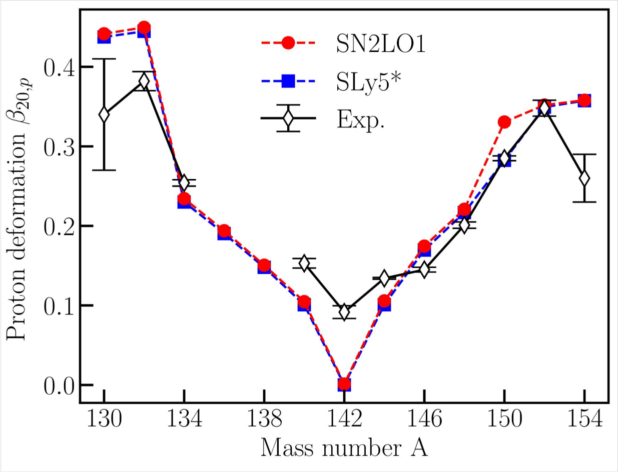
Two DOF: (β_{20}, β_{22}) or (β, γ)

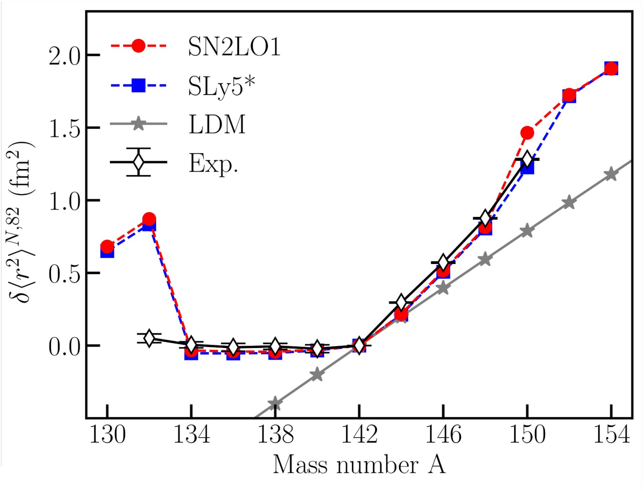


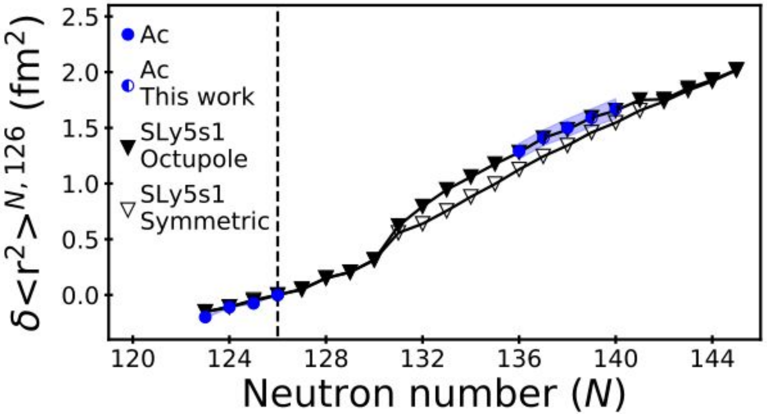
Some remarks:

- multipole expansion of the nuclear **volume**
- a priori **all** are non-zero
- these are **outputs** of the models
- but they are **inputs** for mic-mac!

III. Modelspace: deformation and radii







W. R. and M. Bender, PRC 104, 044308 (2021).
E. Verstraelen et al. PRC **100**, 044321 (2019).

III. Modelspace: MOCCa

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W. R. PhD Thesis, ULB (2016).
W. R. et. al., PRC 92, 064318 (2015).
W. R. et. al., EPJA 55, 93 (2019).
W.R. and M. Herbst, in preparation.
W.R., in preparation.

Physics

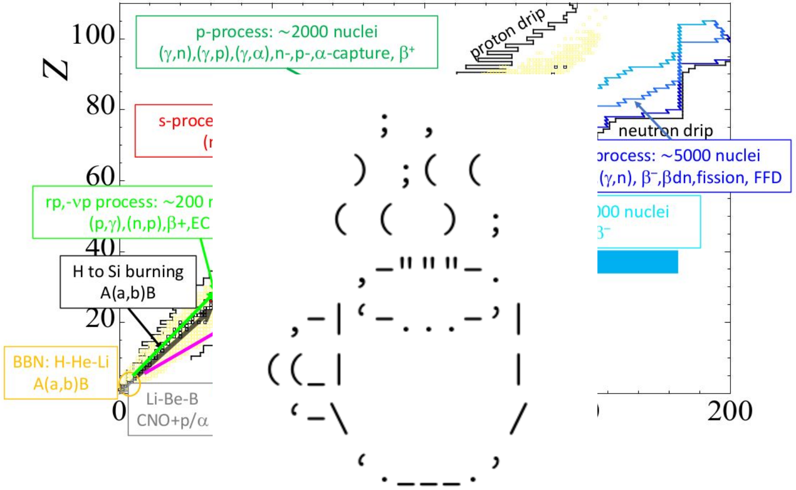
- flexibility w.r.t. **imposed symmetries**
- **unique tool** for the study of:
  - **exotic** shapes
  - **fission** properties
  - **rotational** bands
  - **electromagnetic** form factors
  - **odd-mass and odd-odd** nuclei

Technical aspects

- **3D coordinate space** representation
- developed algorithms
  - speed
  - stability (constraints, blocked states, ...)
  - numerical precision
- **automated implementation** of Skyrme EDFs

IV. The view from Brussels

- Skyrme EDF with:
  - no symmetry-restoration
  - **rotational** correction
  - **finite-size** of nucleons
- 20-25 parameters
- Fitting protocol
  - 2457 known masses
  - 884 charge radii
  - infinite nuclear matter properties
- **global** description (< 0.8 MeV rms)
- Systematic tables of 1000's of nuclei:
  - **masses**, **radii, deformations,** .....
  - **fission** properties
  - nuclear **level densities**
  - **strength** functions
- Input for:
  - r-process calculations (S. Goriely)
  - neutron star structure (N. Chamel)

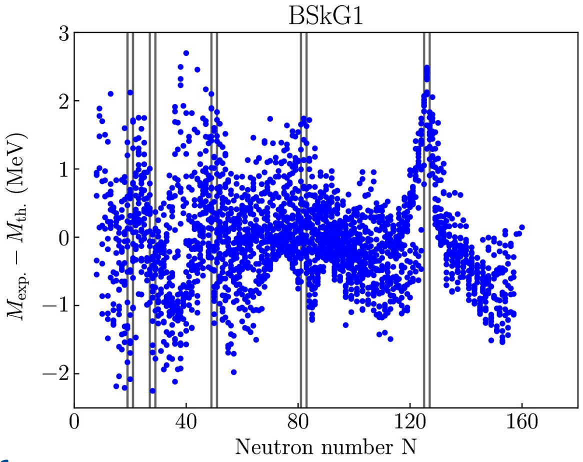


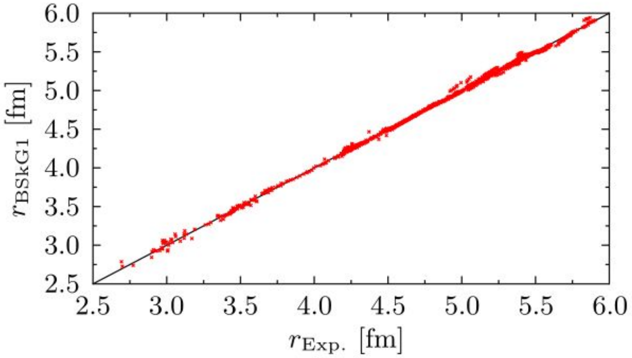
$$E_{\text{tot}} = E_{\text{HFB}} + E_{\text{corr}} \,,$$

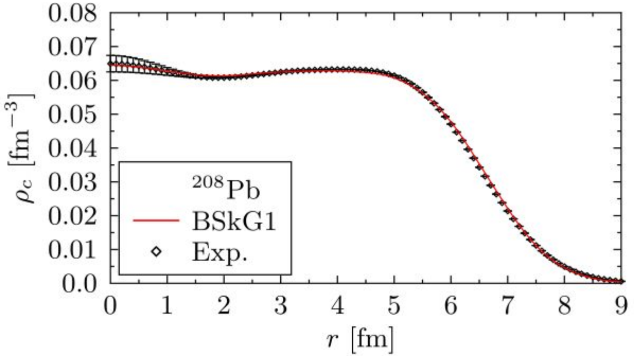
$$E_{\text{HFB}} = E_{\text{kin}} + E_{\text{Sk}} + E_{\text{pair}} + E_{\text{Coul}} + E^{(1)}_{\text{cm}} \,,$$

$$E_{\text{corr}} = E_{\text{rot}} + E^{(2)}_{\text{cm}} + E_{\text{W}} \,.$$

IV. The view from Brussels: **BSkG1/2**







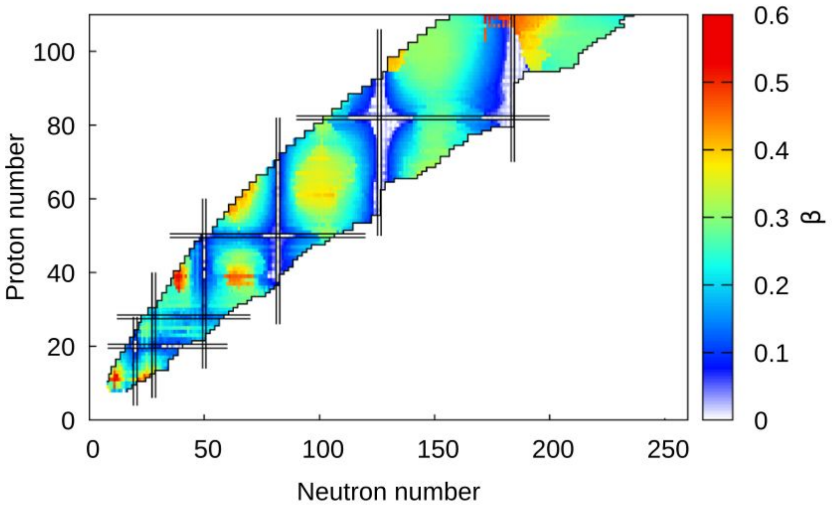
Global performance

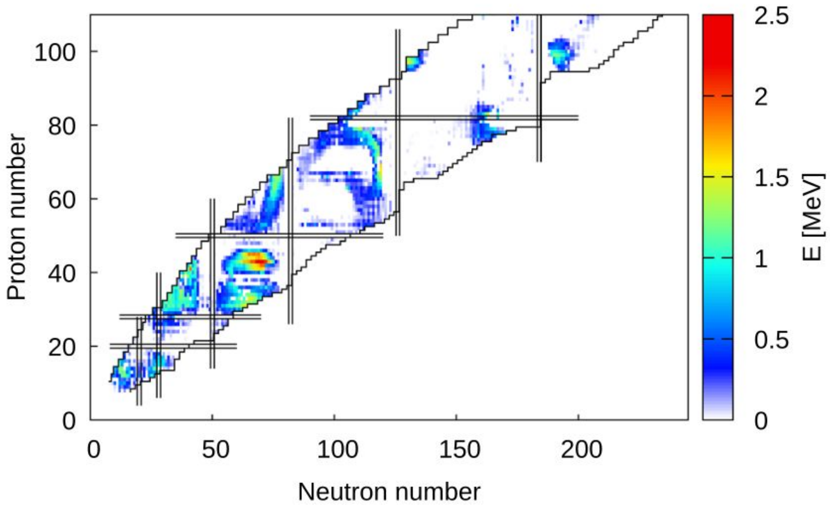
σ^2(MeV)	**BSkG1**	**BSkG2**	HFB-14	FR(L)DM
Masses	0.741	**0.678**	0.729	0.560
Charge radii (fm)	0.027	**0.027**	0.039	0.038
Primary barriers	0.87	**0.45**	0.61	0.79
Secondary barriers	0.86	**0.45**	0.70	1.35
Isomers	0.45	**0.48**	0.93	1.04

BSkG1: G. Scamps et al., EPJA 57, 333 (2021);
HFB-14: S. Goriely et al., PRC ***75***, 064312 (2007).
FRDM: P. Möller et al., At. Data Nucl. Data Tables, **109-110** (2016).

IV. The view from Brussels: **BSkG1/2**

G. Scamps et al., EPJA 57, 333 (2021).





Quadrupole deformation

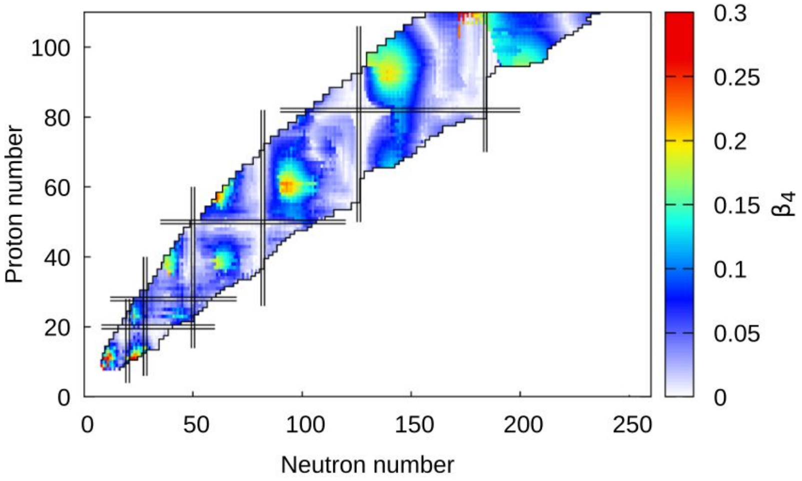
- quadrupole is everywhere
- and can get rather large!

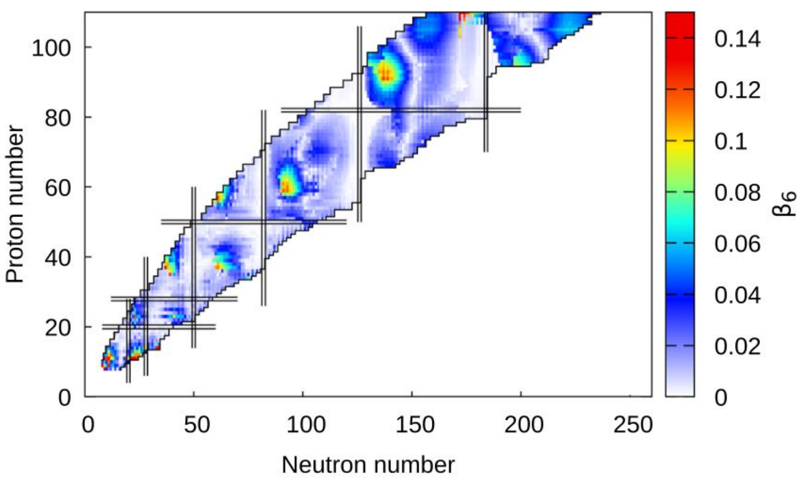
Triaxial deformation

- lots of nuclei
- significantly **more** than in mic-mac

IV. The view from Brussels: **BSkG1/2**

G. Scamps et al., EPJA **57**, 333 (2021).





Higher order multipoles

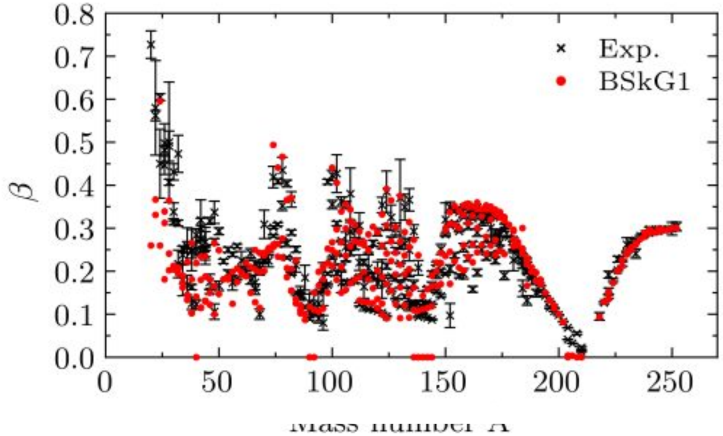
- **always** present
- though less important
- .... but not necessarily for **fission!**

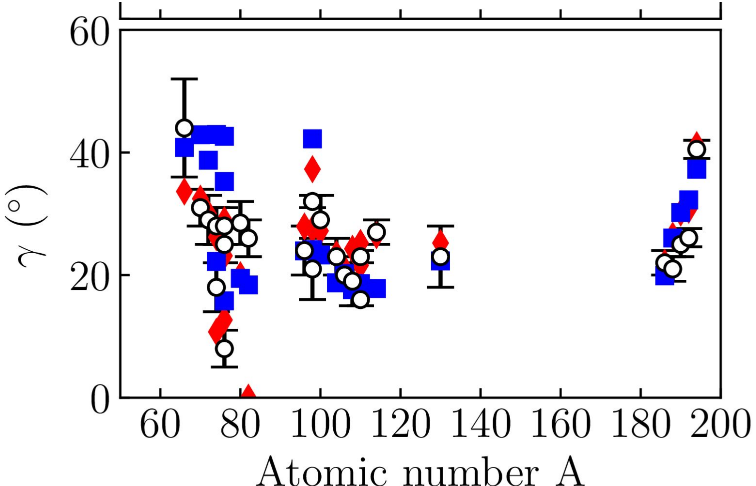
IV. The view from Brussels: **BSkG1/2**

S. Raman, At. Data Nucl. Data Tables, **78**(1), 1-128 (2001).
Many references for γ, thanks to M. Zielinska!

- average **β** from B(E2) systematics
- average **γ** from COULEX

	Exp.		BSkG1	
	β	γ	β	γ
^{96}Mo	**0.17**	**24(4)**	**0.19**	**24**
^{98}Mo	**0.17**	**32(1)**	**0.22**	**24**
^{100}Mo	**0.23**	**29(4)**	**0.25**	**23**





IV. The view from Brussels: **the rotational correction**

Wouter Ryssens (ULB)

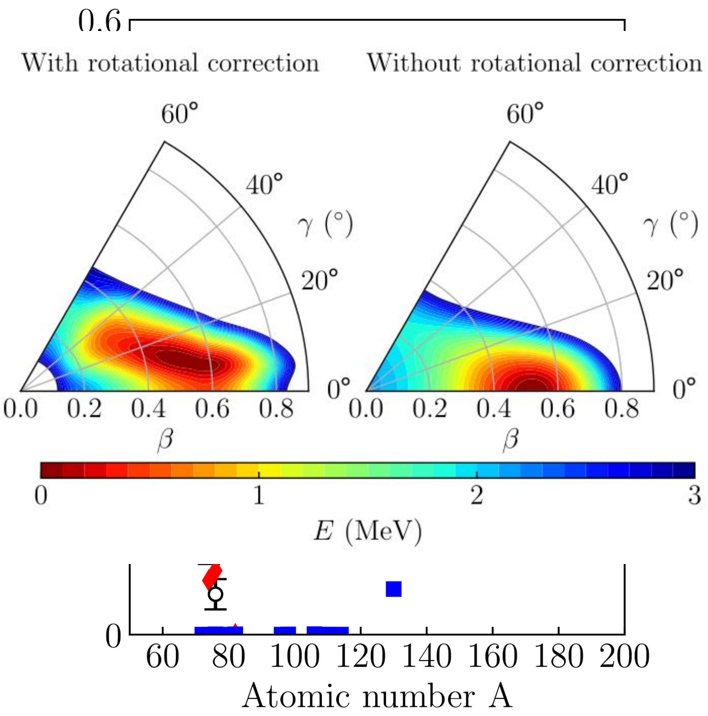
Rotational correction

- aims to mimic beyond-MF effects
- assumes rotational motion
- with consistent moments of inertia
- some parameters

Semi-variational approach:

1. construct surface in (β,γ)
2. add rotational energy
3. select minimum

$$E_{\text{tot}} = E_{\text{HFB}} + E_{\text{corr}} \, , \qquad E_{\text{rot}} \sim - \sum_{\mu=x,y,z} \frac{\langle J_\mu^2 \rangle}{2\mathcal{I}_\mu} \, .$$

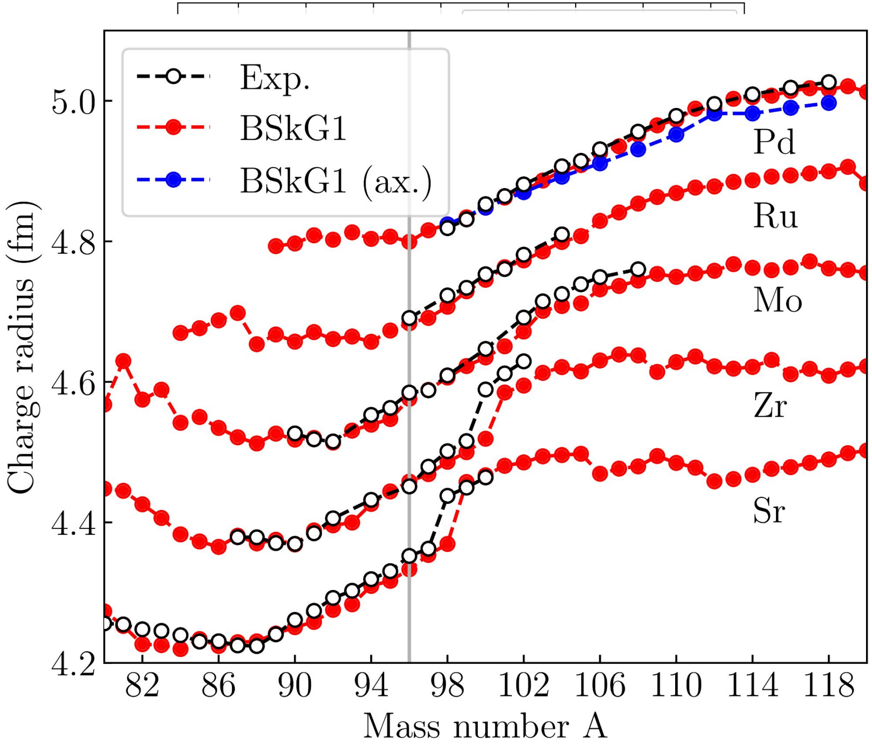


V. Some Ru's, Rh's, Pd's: **masses and radii**

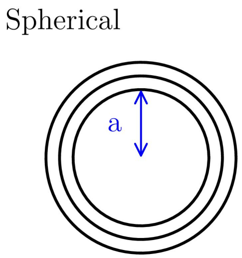
M. Hukkanen et al., in preparation.
I. Angeli and K. P. Marinova, *At. Data Nuc. Data Tables*, ***99*** (2015).
S. Geldhof et al., PRL **128,** 152501 (2022).

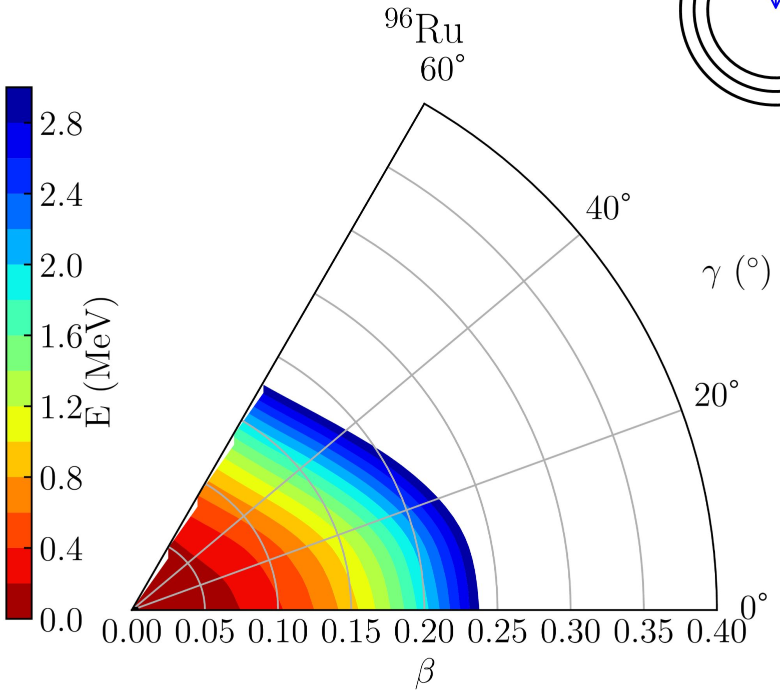
Performance in the region

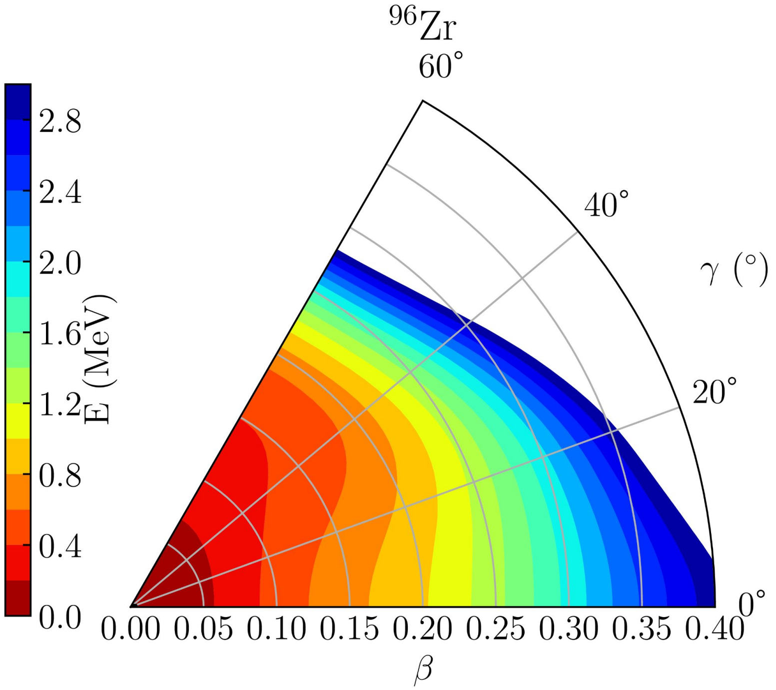
- **absolute** E about 700 keV
- triaxial model agrees **well** for S2ns
- all older **axial** models are less good
- **absolute** charge radii well-reproduced



V. .... and A=96

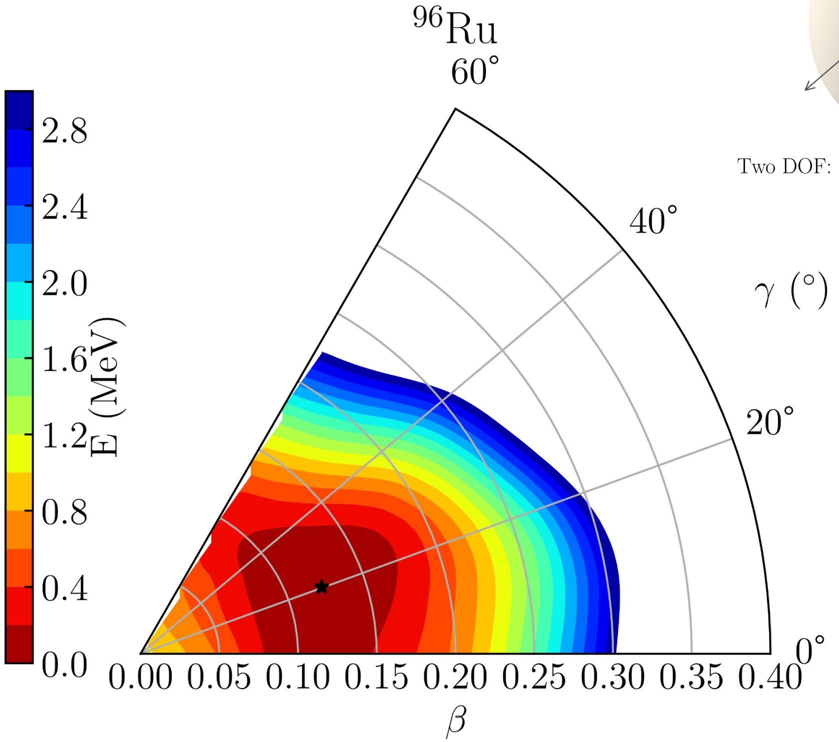


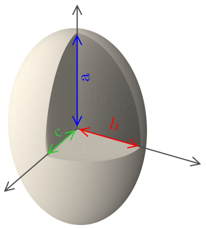




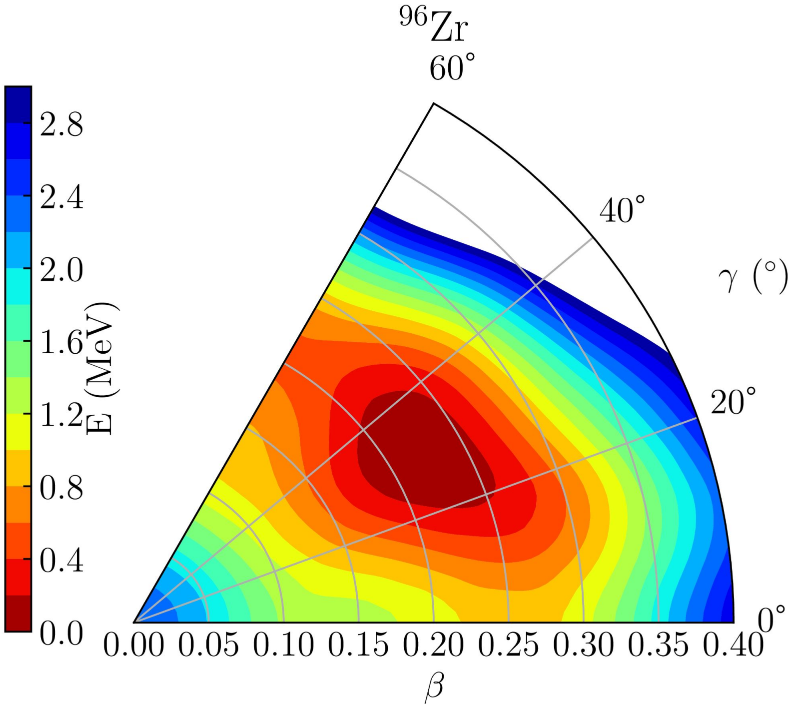
without rotational correction.

V. .... and A=96



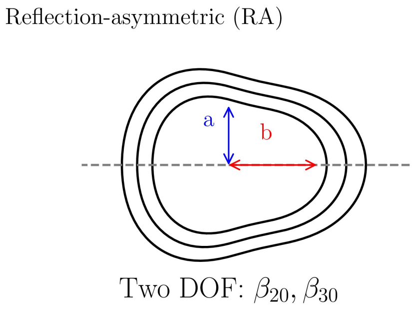


Two DOF: (β_{20}, β_{22}) or (β, γ)

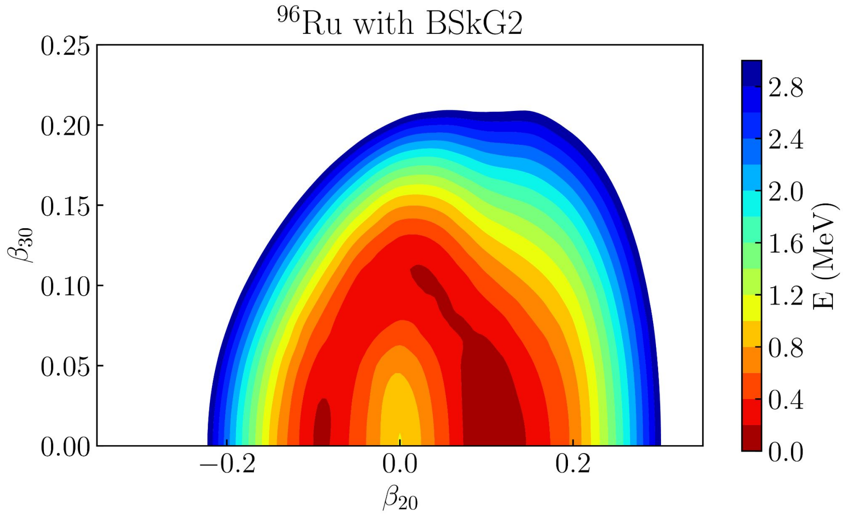


with rotational correction.

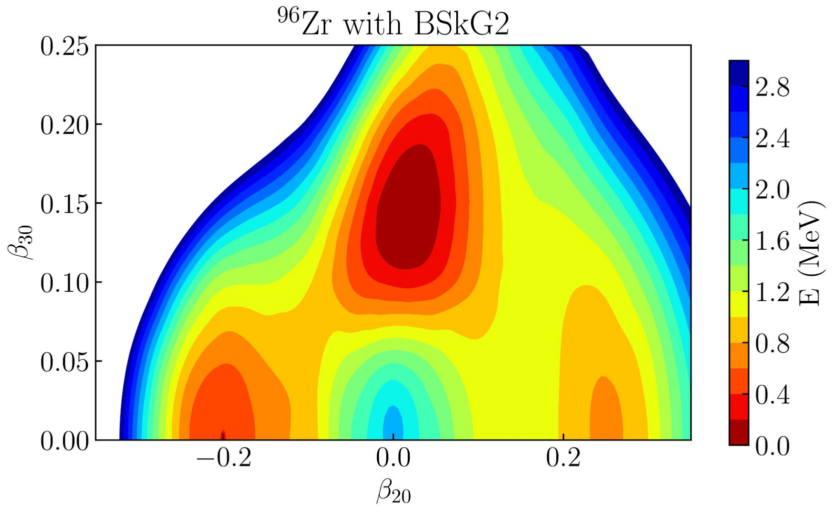
V. .... and A=96



Reflection-asymmetric (RA)
a
b
Two DOF: β_{20}, β_{30}

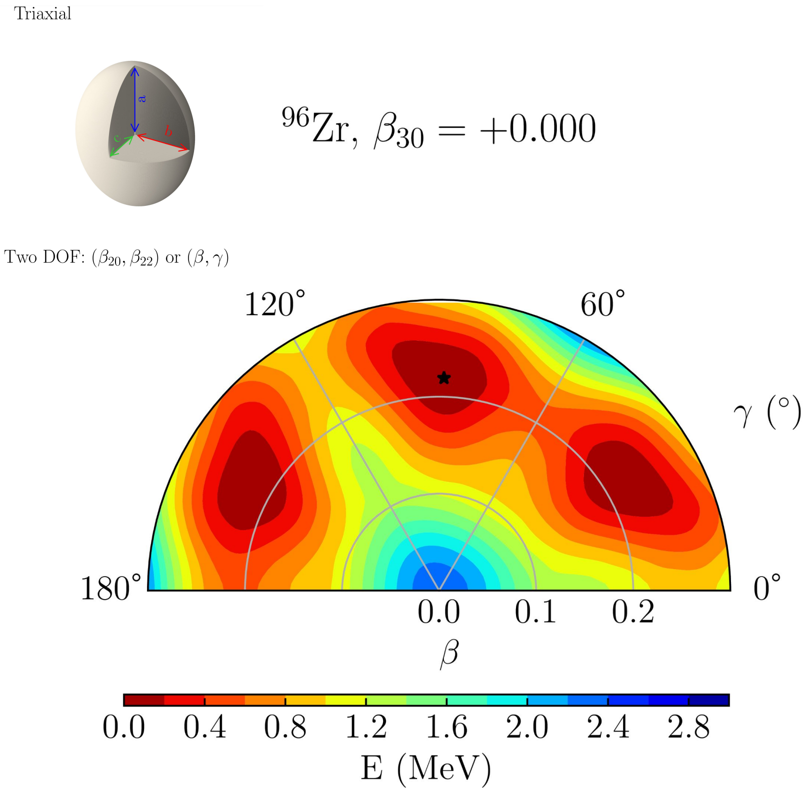


^{96}Ru with BSkG2
β_{30}
0.25
0.20
0.15
0.10
0.05
0.00
−0.2
0.0
0.2
β_{20}
E (MeV)
2.8
2.4
2.0
1.6
1.2
0.8
0.4
0.0

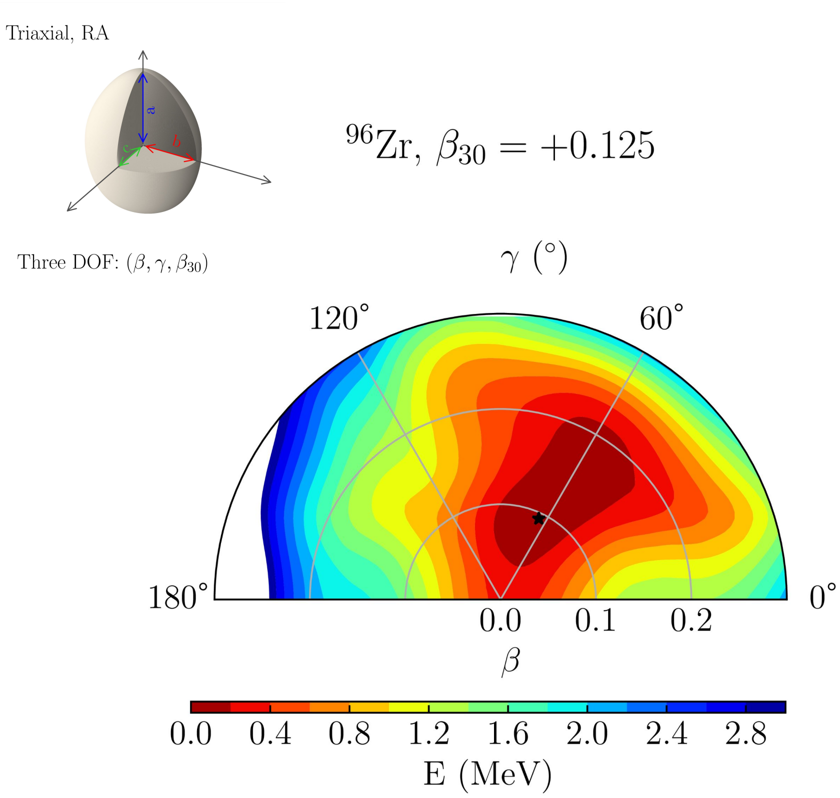


^{96}Zr with BSkG2
β_{30}
0.25
0.20
0.15
0.10
0.05
0.00
−0.2
0.0
0.2
β_{20}
E (MeV)
2.8
2.4
2.0
1.6
1.2
0.8
0.4
0.0

V. .... and A=96



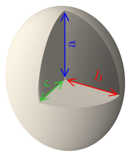
Triaxial
^{96}Zr, $\beta_{30} = +0.000$
Two DOF: (β_{20}, β_{22}) or (β, γ)
120°
60°
γ (°)
180°
0°
0.0
0.1
0.2
β
0.0 0.4 0.8 1.2 1.6 2.0 2.4 2.8
E (MeV)



Triaxial, RA
^{96}Zr, $\beta_{30} = +0.125$
Three DOF: $(\beta, \gamma, \beta_{30})$
γ (°)
120°
60°
180°
0°
0.0
0.1
0.2
β
0.0 0.4 0.8 1.2 1.6 2.0 2.4 2.8
E (MeV)

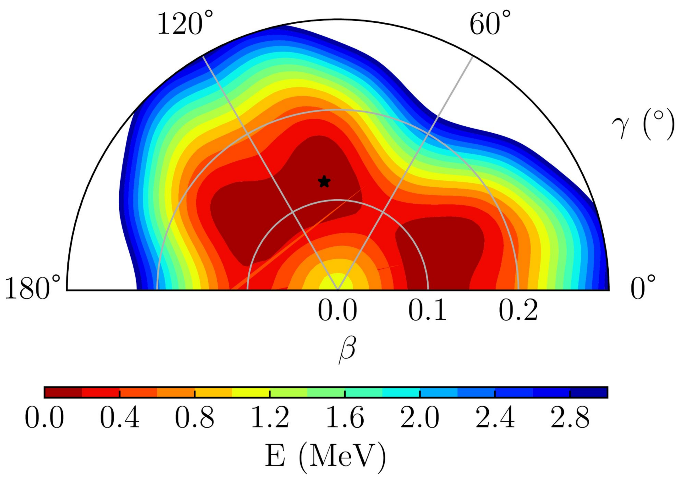
V. .... and A=96

Triaxial

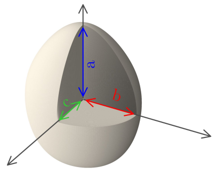


Two DOF: (β_{20}, β_{22}) or (β, γ)

$^{96}\mathrm{Ru},\ \beta_{30} = +0.000$

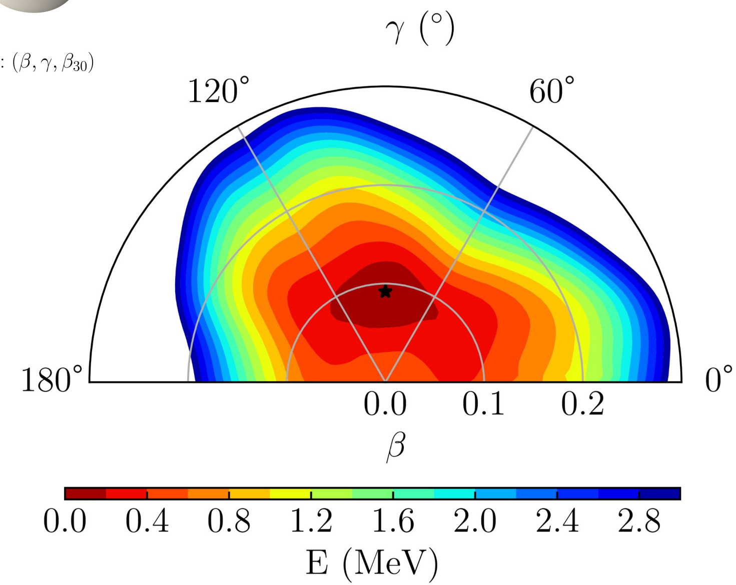


Triaxial, RA

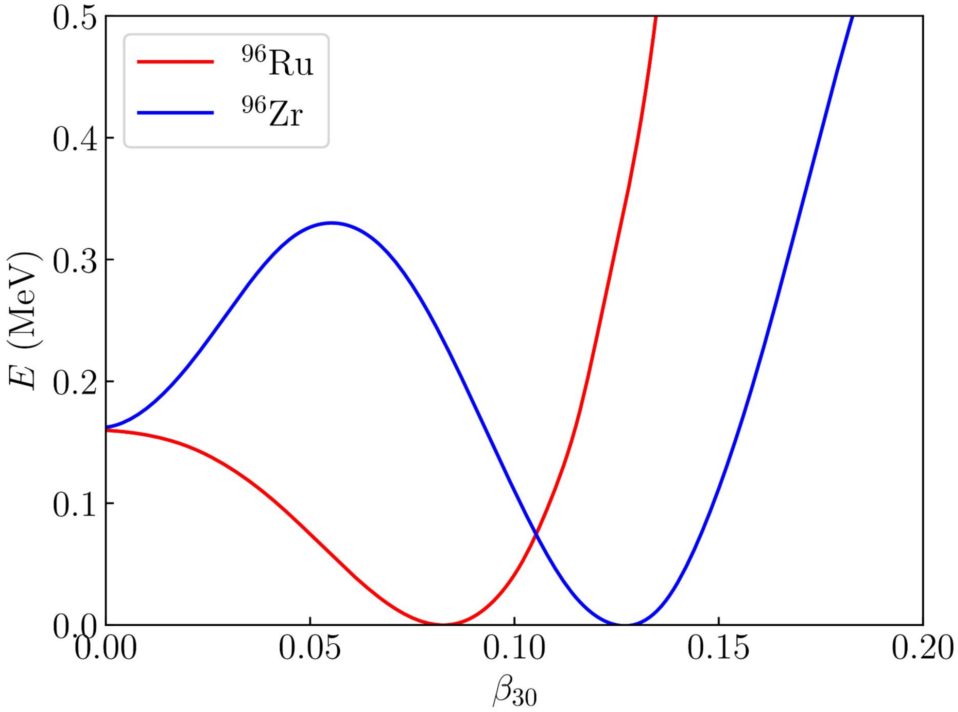


Three DOF: $(\beta, \gamma, \beta_{30})$

$^{96}\mathrm{Ru},\ \beta_{30} = +0.075$



V. …. and A=96



Conclusions

Skyrme Energy Density Functional

- simplicity as **prime quality**
- has been pushed very far
- many variants, many extensions sought for

Symmetries & deformations

- symmetry breaking captures correlations
- with simple wave-functions
- symmetry restoration highly desirable
- but many things can be studied without it

The Brussels Models

- excellent description: masses, radii, INM, ...
- geared for large-scale applications
- recent push towards exotic deformations
- pheno. corrections beyond mean-field

Ru, Rh, Pds and A=96

- overall good description of region
- unexpected ground-state deformations for 96Ru **and** 96Zr