Nuclear structure with MOCCa at ULB

W. Ryssens

Université Libre de Bruxelles

January 2021

Nuclear theory & astrophysics

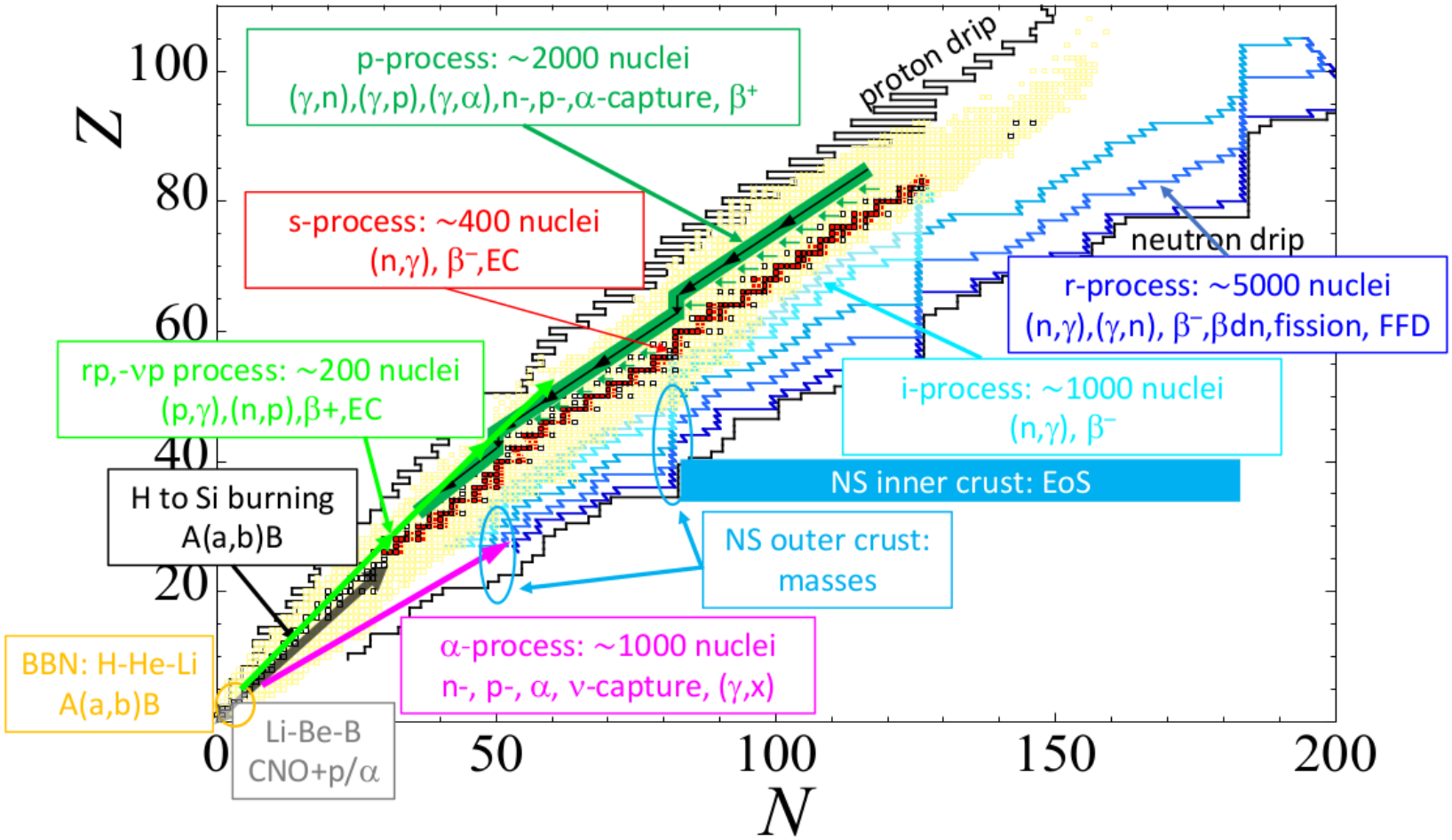
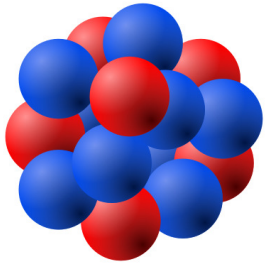


Figure from M. Arnould & S. Goriely, Prog. Part. Nuc. Phys. **112**, 103766 (2020)

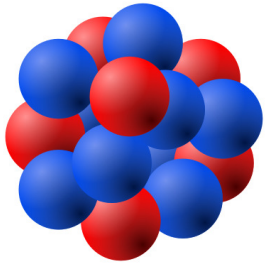
Table of contents

Planning

So you want to describe nuclei?

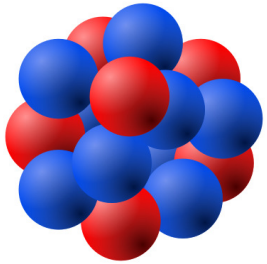


So you want to describe nuclei?



$$\hat{H}|\Psi_{N,Z}\rangle = E|\Psi_{N,Z}\rangle \begin{cases} \text{for } Z = 1, \ldots, 120, \ldots \\ \text{for } N = 0, \ldots, 200, \ldots \end{cases}$$

So you want to describe nuclei?

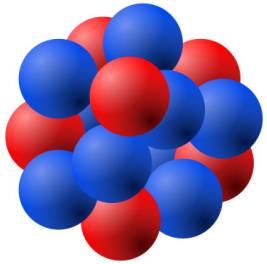


$$\hat{H}|\Psi_{N,Z}\rangle = E|\Psi_{N,Z}\rangle \begin{cases} \text{for Z} = 1, \ldots, 120, \ldots \\ \text{for N} = 0, \ldots, 200, \ldots \end{cases}$$

$\hat{H}$

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

So you want to describe nuclei?



$$\hat{H}|\Psi_{N,Z}\rangle = E|\Psi_{N,Z}\rangle \begin{cases} \text{for Z} = 1, \ldots, 120, \ldots \\ \text{for N} = 0, \ldots, 200, \ldots \end{cases}$$

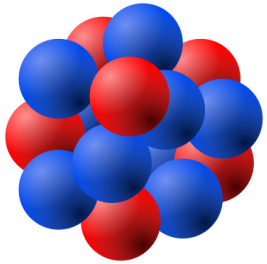
$\hat{H}$

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

$|\Psi_{N,Z}\rangle$

- What modelspace?
- Include all nucleons?
- Global or local?

So you want to describe nuclei?



$$\hat{H}|\Psi_{N,Z}\rangle = E|\Psi_{N,Z}\rangle \begin{cases} \text{for Z} = 1, \ldots, 120, \ldots \\ \text{for N} = 0, \ldots, 200, \ldots \end{cases}$$

$\hat{H}$

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

$|\Psi_{N,Z}\rangle$

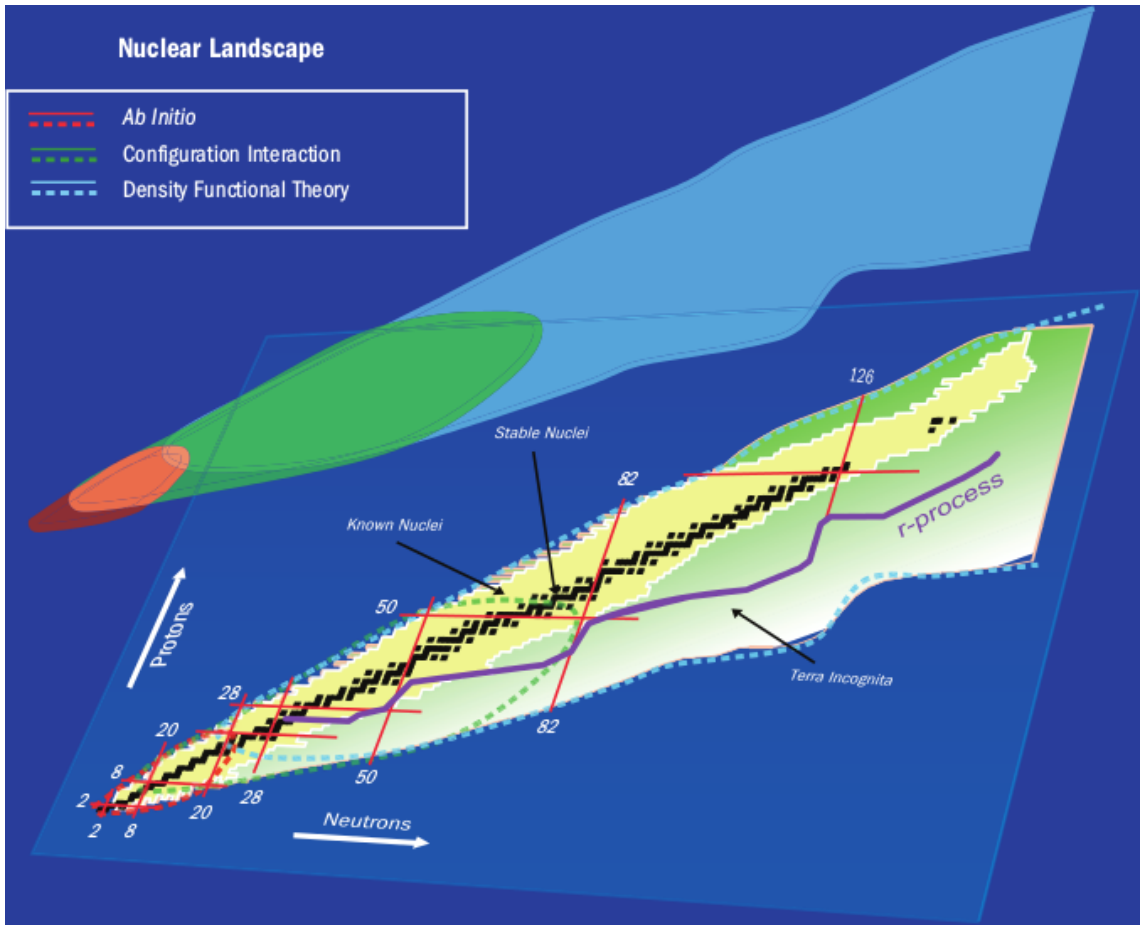
- What modelspace?
- Include all nucleons?
- Global or local?

Obtaining a solution?

- Exactly?
- Semi-classically?
- Different variational ansatzes?

Reach of approaches

	Interaction	Global?	Many-body	nucleons?
Ab initio	scattering	Depends	Exact (often)	All
Shell model	Phenom.	Local	Exact	Valence
DFT	Phenom.	Global	Mean-field	All



Ab initio: reach in 2020

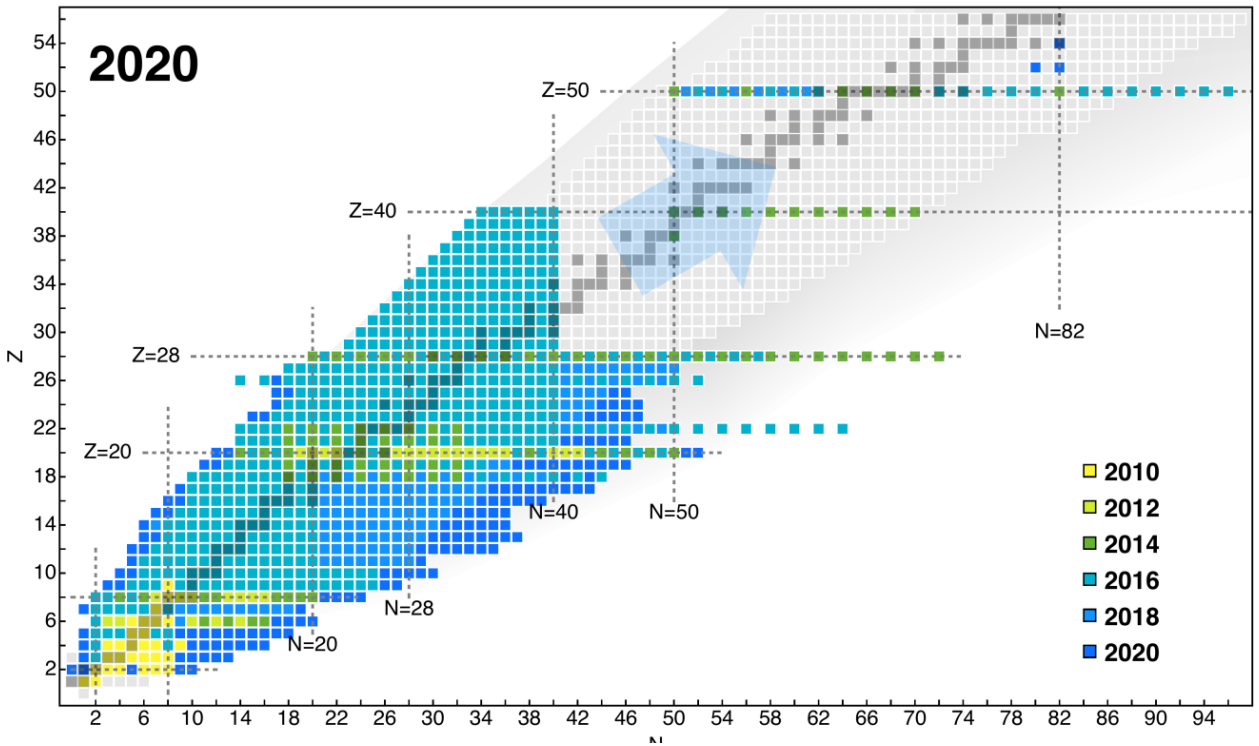


Figure from H. Hergert, Frontiers in Physics **8**:379 (2020).

Planning

Skyrme functionals

We model the energy as

$$E = E_{\text{kinetic}} + E_{\text{Coulomb}} + E_{\text{Skyrme}} + E_{\text{pairing}} + E_{\text{corrections}}$$

Skyrme functionals

We model the energy as

$$E = E_{\text{kinetic}} + E_{\text{Coulomb}} + E_{\text{Skyrme}} + E_{\text{pairing}} + E_{\text{corrections}}$$

To model the strong interaction, we have E_{Skyrme}

$$\hat{v}^{\text{Sk}} \sim t_0(1 + x_0\hat{P}_\sigma)\delta_{\boldsymbol{r}}$$
$$+ \text{terms dependent on momentum, spin-orbit, } \ldots$$

Skyrme functionals

We model the energy as

$$E = E_{\text{kinetic}} + E_{\text{Coulomb}} + E_{\text{Skyrme}} + E_{\text{pairing}} + E_{\text{corrections}}$$

To model the strong interaction, we have E_{Skyrme}

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

Skyrme functionals

We model the energy as

$$E = E_{\text{kinetic}} + E_{\text{Coulomb}} + E_{\text{Skyrme}} + E_{\text{pairing}} + E_{\text{corrections}}$$

To model the strong interaction, we have E_{Skyrme}

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

Skyrme part

- Bilinear in densities $\rho, \tau, J_{\mu\nu}$
- $\sim$ 10 parameters
- . . . fitted to experiment

Mean-field theory

Simple product state as variational ansatz

$$|\Psi_{N,Z}\rangle = \prod_{i=1}^{A} \hat{c}_i^\dagger |0\rangle$$

Mean-field theory

Simple product state as variational ansatz

$$|\Psi_{N,Z}\rangle = \prod_{i=1}^{A} \hat{c}_i^\dagger |0\rangle = \text{VERY simple state}$$

Mean-field theory

Simple product state as variational ansatz

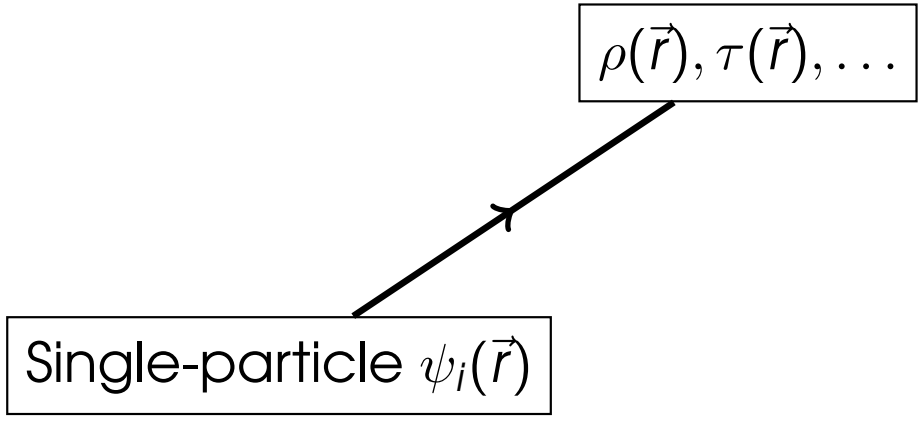
$$|\Psi_{N,Z}\rangle = \prod_{i=1}^{A} \hat{c}_i^\dagger |0\rangle = \text{VERY simple state}$$

Single-particle $\psi_i(\vec{r})$

Mean-field theory

Simple product state as variational ansatz

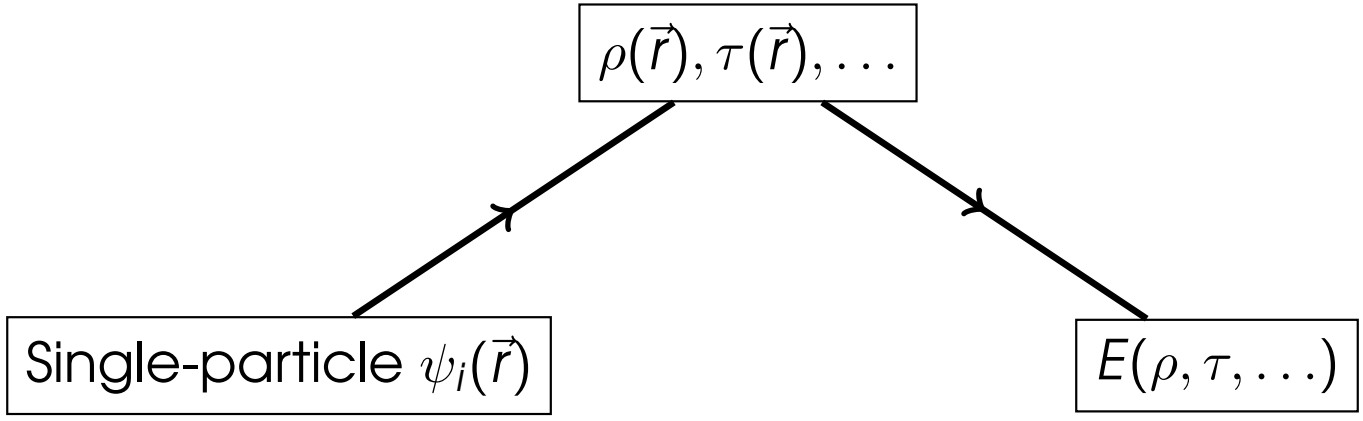
$$|\Psi_{N,Z}\rangle = \prod_{i=1}^{A} \hat{c}_i^\dagger |0\rangle = \text{VERY simple state}$$



Mean-field theory

Simple product state as variational ansatz

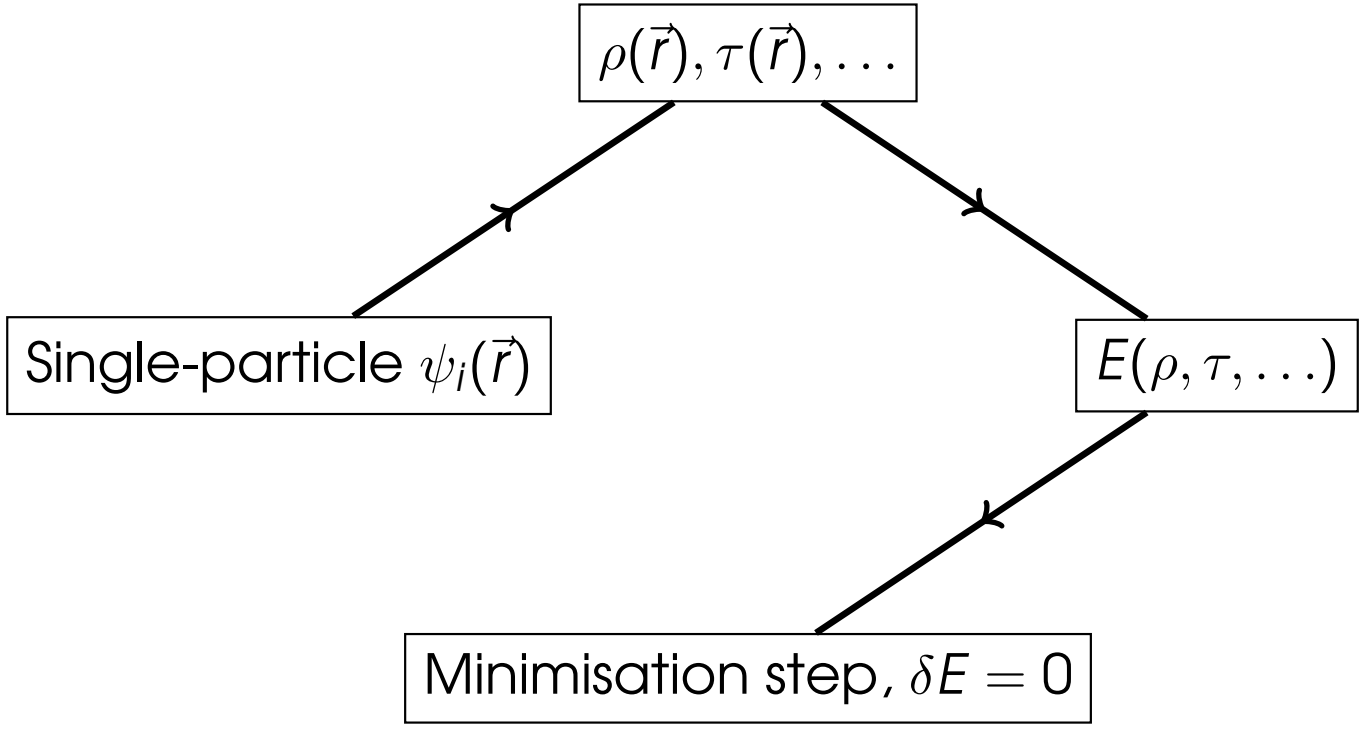
$$|\Psi_{N,Z}\rangle = \prod_{i=1}^{A} \hat{c}_i^\dagger |0\rangle = \text{VERY simple state}$$



Mean-field theory

Simple product state as variational ansatz

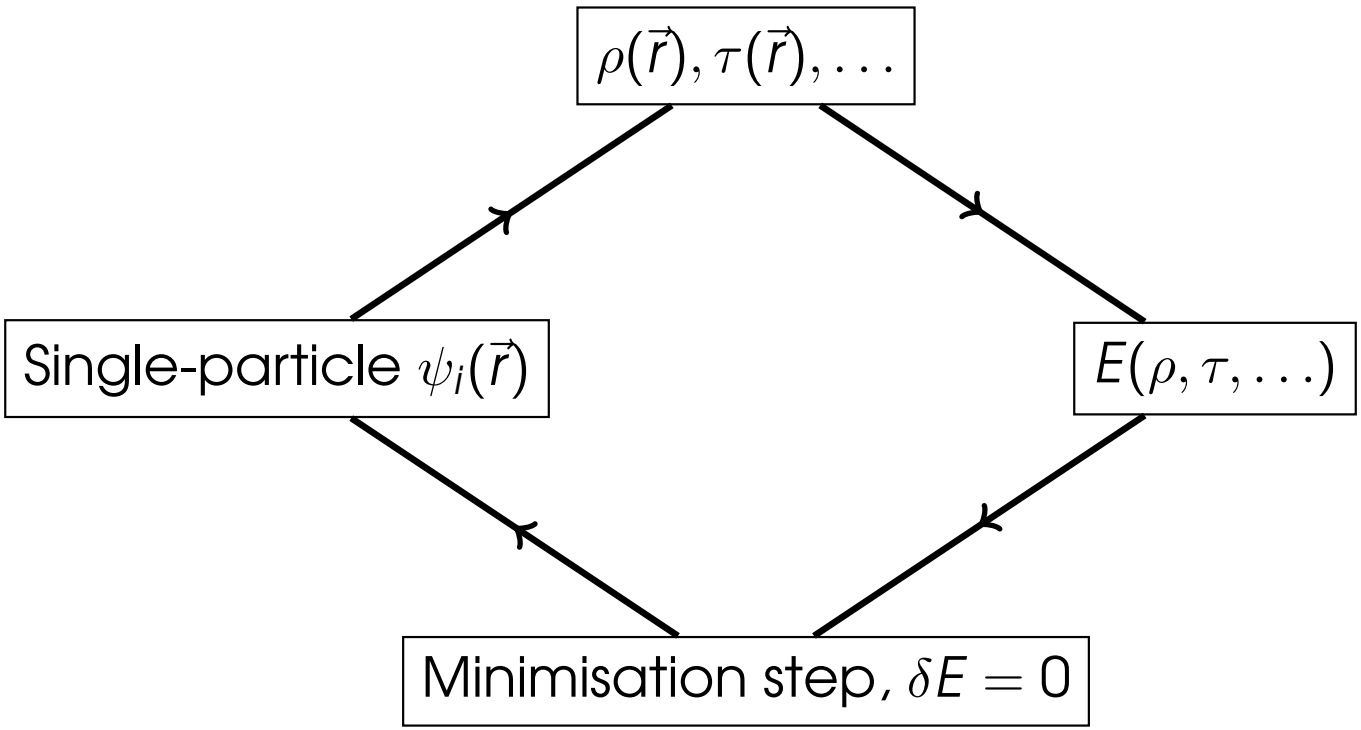
$$|\Psi_{N,Z}\rangle = \prod_{i=1}^{A} \hat{c}_i^\dagger |0\rangle = \text{VERY simple state}$$



Mean-field theory

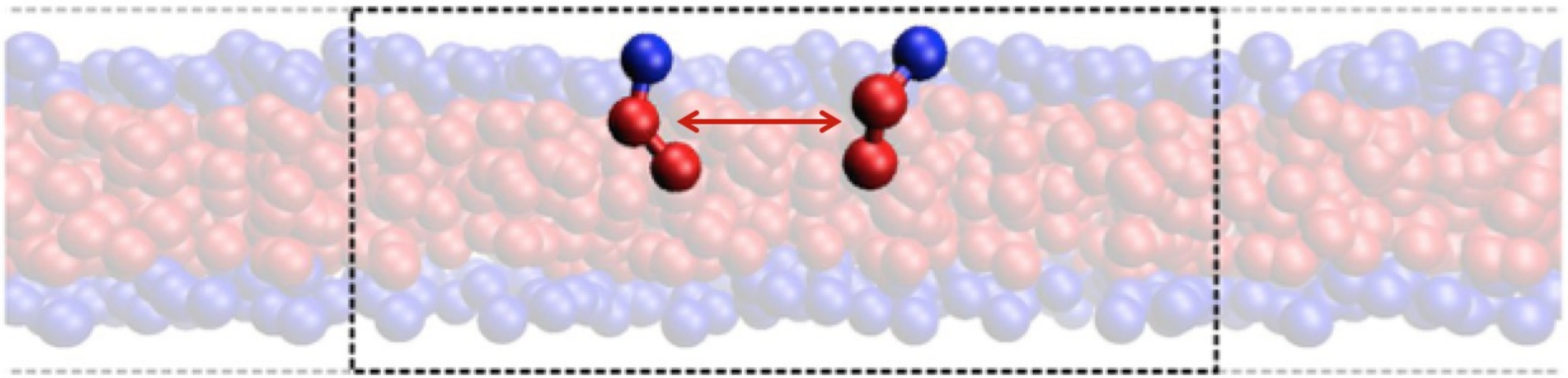
Simple product state as variational ansatz

$$|\Psi_{N,Z}\rangle = \prod_{i=1}^{A} \hat{c}_i^\dagger |0\rangle = \text{VERY simple state}$$



Mean-field

Every pair of molecules interact at a close distance.
To take into account all these interactions is computationally expensive



Mean-field approach: every molecule interacts only with the average distribution of other molecules

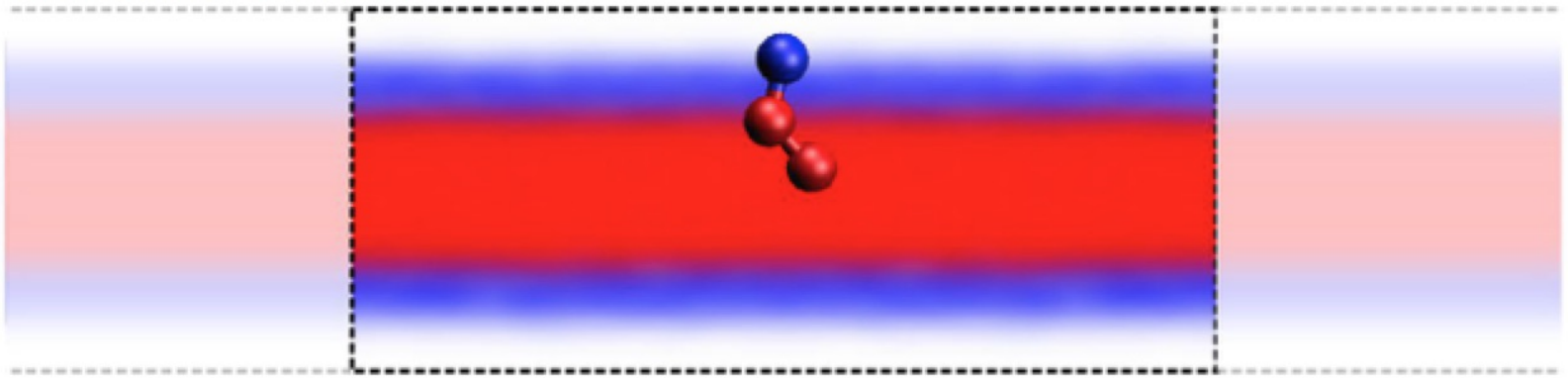
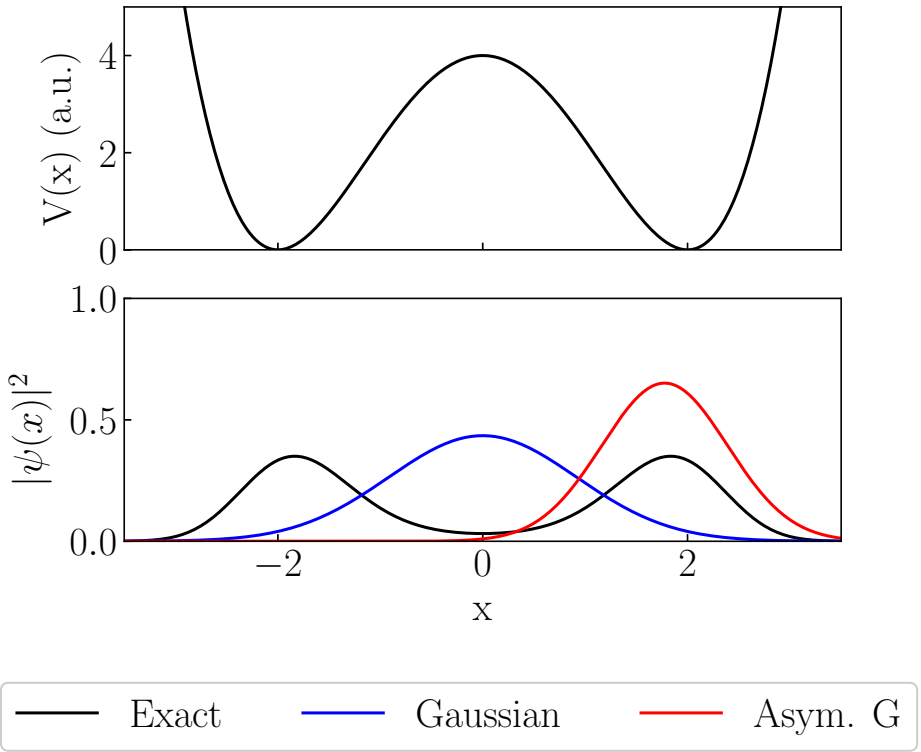


Figure from the ITN-SNAL, https://itn-snal.net/

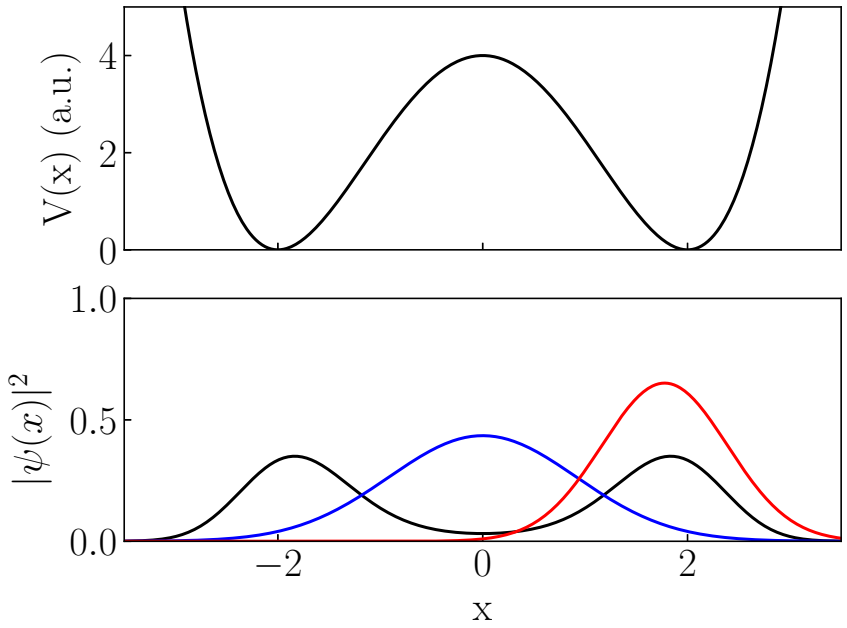
Planning

Symmetry breaking



$$\psi \sim \begin{cases} e^{-\frac{x^2}{\sigma^2}} & \text{(1 parameter)} \\ e^{-\frac{(x-x_0)^2}{\sigma^2}} & \text{(2 parameters)} \end{cases}$$

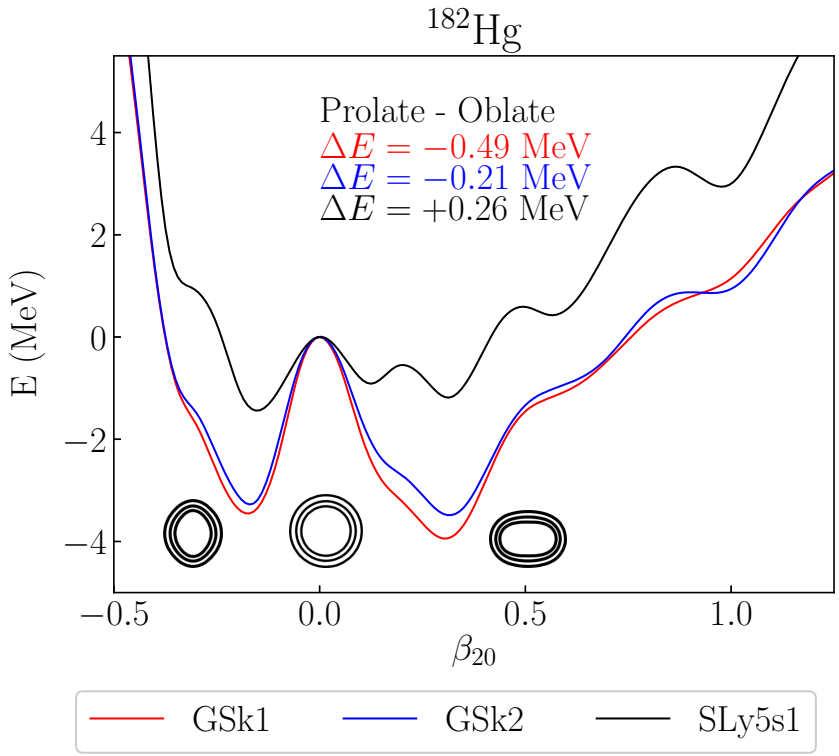
Symmetry breaking



$$\psi \sim \begin{cases} e^{-\frac{x^2}{\sigma^2}} & \text{(1 parameter)} \\ e^{-\frac{(x-x_0)^2}{\sigma^2}} & \text{(2 parameters)} \end{cases}$$

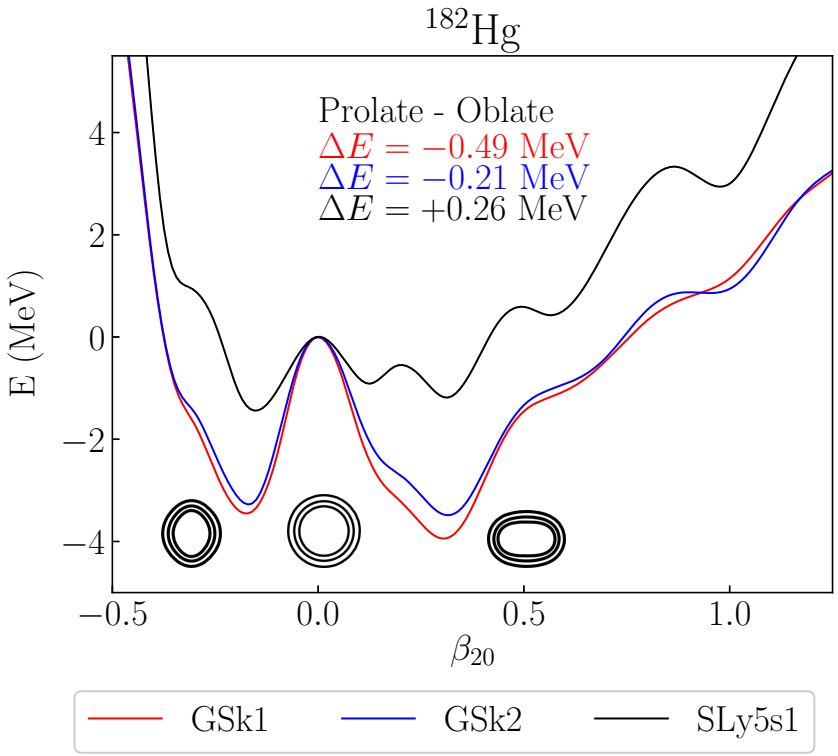
	$\langle \hat{H} \rangle$	$\langle \hat{x}^2 \rangle$
Exact	1.80	3.25
Gaussian	2.84	0.84
Asymmetric G.	1.85	3.53

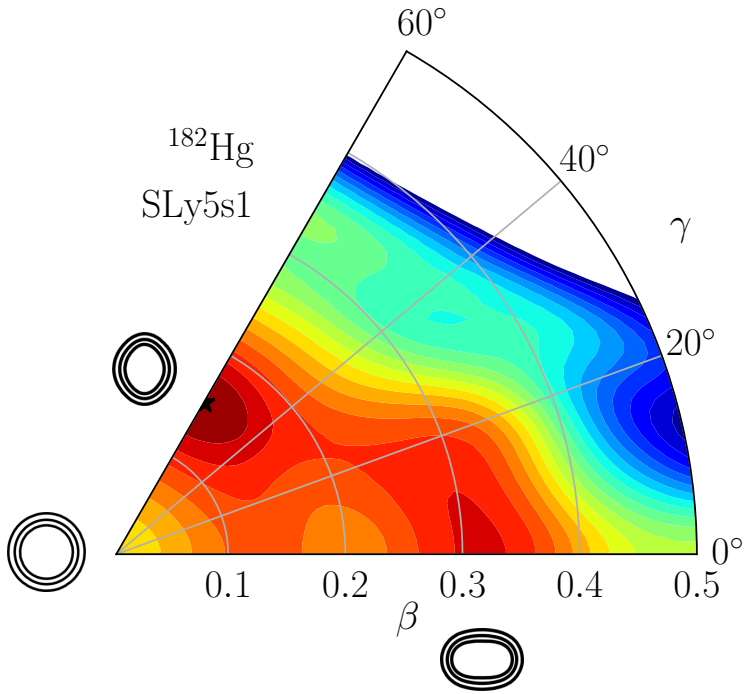
Nuclear shapes



$$\beta_{\ell m} = N(A) \int d\vec{r}\, \rho(\vec{r}) r^{\ell} Y_{\ell m}(\vec{r})$$

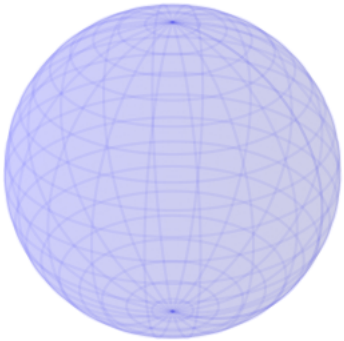
Nuclear shapes

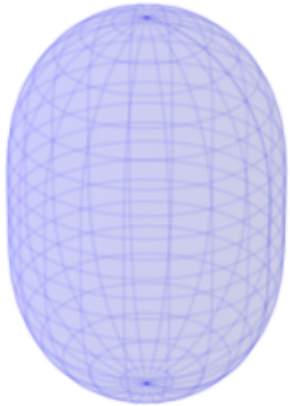


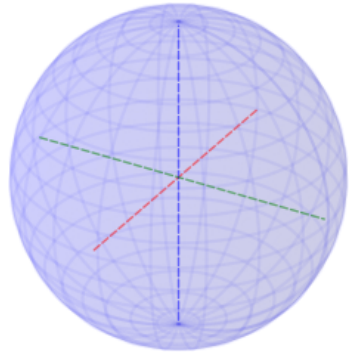


$$\beta_{\ell m} = N(A) \int d\vec{r}\, \rho(\vec{r}) r^{\ell} Y_{\ell m}(\vec{r})$$

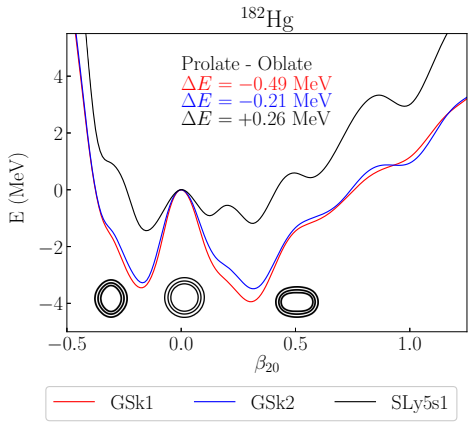
Rotational symmetry

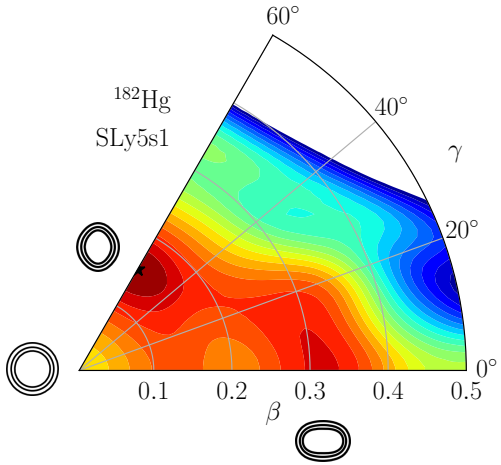






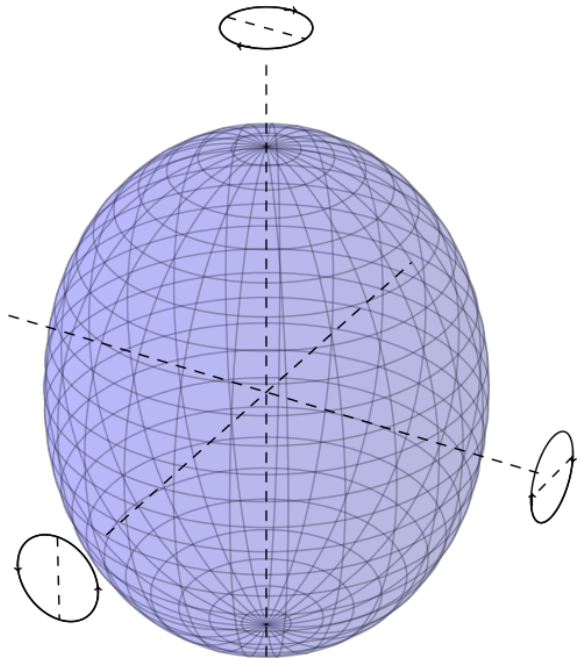
Dimensions	1	2	3
CPU time	$\leq$1 s	$\leq$1 min	tens of minutes
EDFs fitted	Most EDFs	ULB EDFs	None published





Single-particle symmetry operators

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



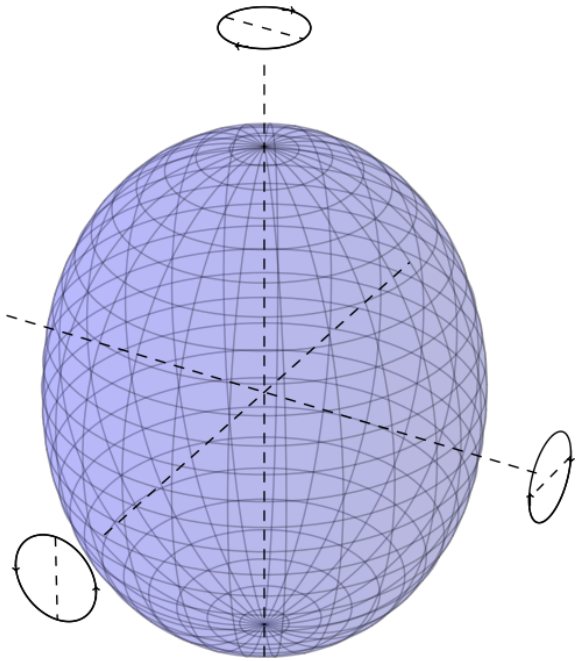
Single-particle symmetry operators

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

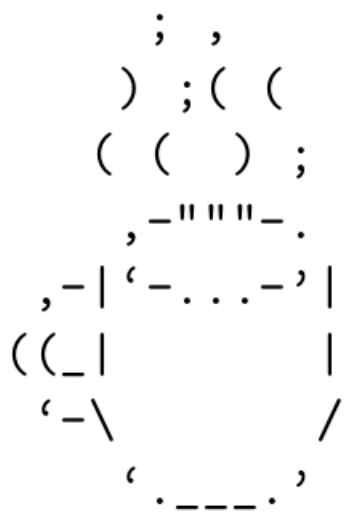
give rise to many-body groups

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

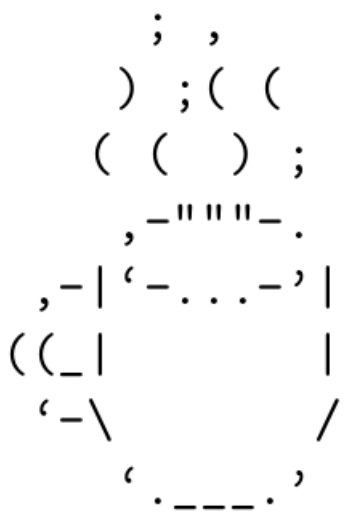
$$\mathcal{D}_{2h}^{TD} = \left\{ \hat{1}, -\hat{1}, \hat{\mathcal{P}}, -\hat{\mathcal{P}}, \check{\mathcal{T}}, -\check{\mathcal{T}}, \hat{\mathcal{R}}_{\mu}, -\hat{\mathcal{R}}_{\mu}, \check{\mathcal{R}}_{\mu}^{T}, -\check{\mathcal{R}}_{\mu}^{T}, \right.$$
$$\left. \hat{\mathcal{S}}_{\mu}, -\hat{\mathcal{S}}_{\mu},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



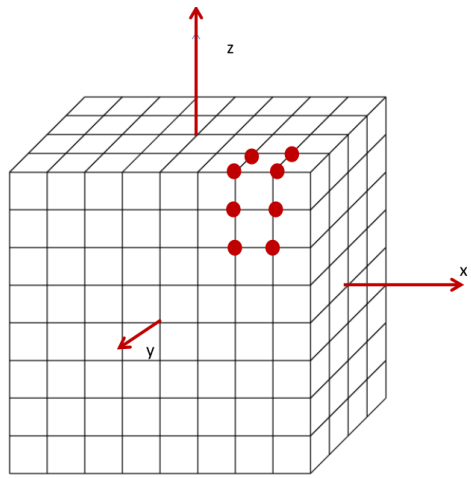
All subgroups in principle contain different correlations/physics.



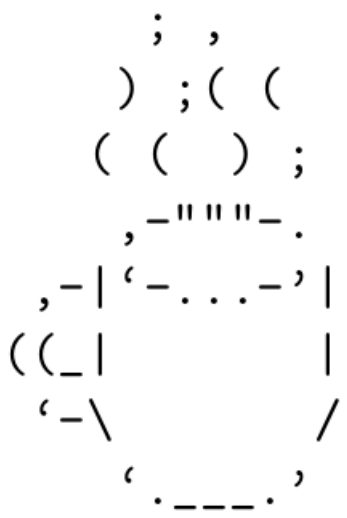
- Mean-field with Skyrme EDFs
- 3D coordinate mesh
  $\sim 16 \times 16 \times 16$ points and $dx = 0.8$ fm
  triaxial shapes naturally included



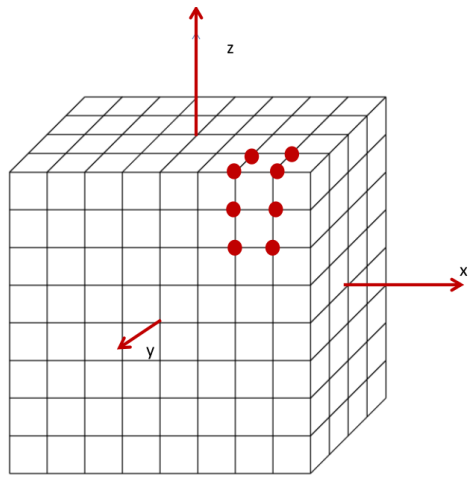
- Mean-field with Skyrme EDFs
- 3D coordinate mesh
  $\sim 16 \times 16 \times 16$ points and $dx = 0.8$ fm
  triaxial shapes naturally included



D. Baye et al. J. Phys. A 19 (1986).



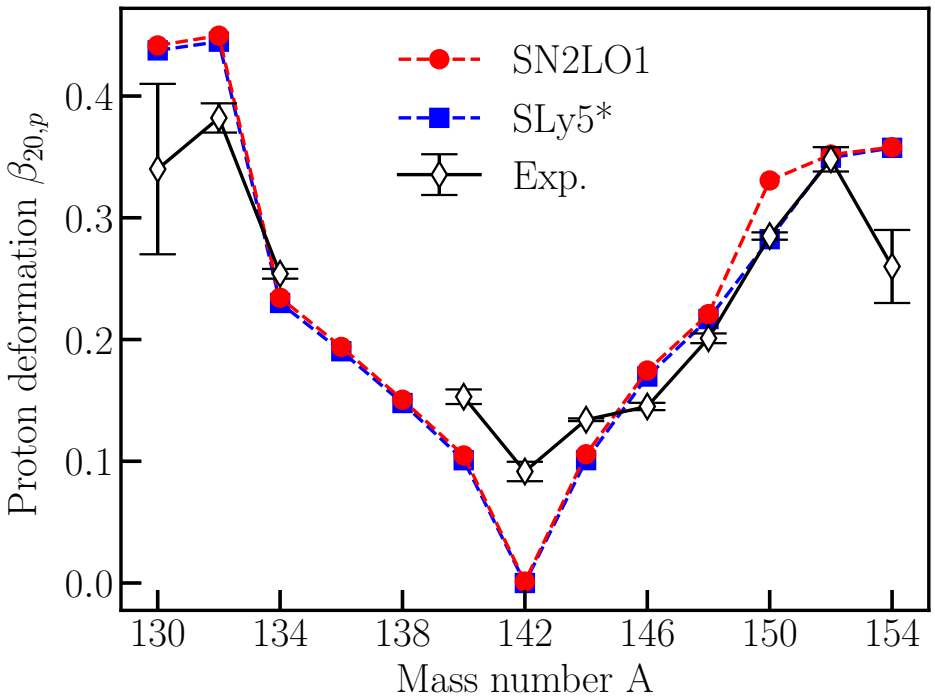
- Mean-field with Skyrme EDFs
- 3D coordinate mesh
  $\sim 16 \times 16 \times 16$ points and $dx = 0.8$ fm
  triaxial shapes naturally included
- 16 possible symmetry combinations
- Fast and easy to use
- Extremely accurate
- Developed on the 6th floor!

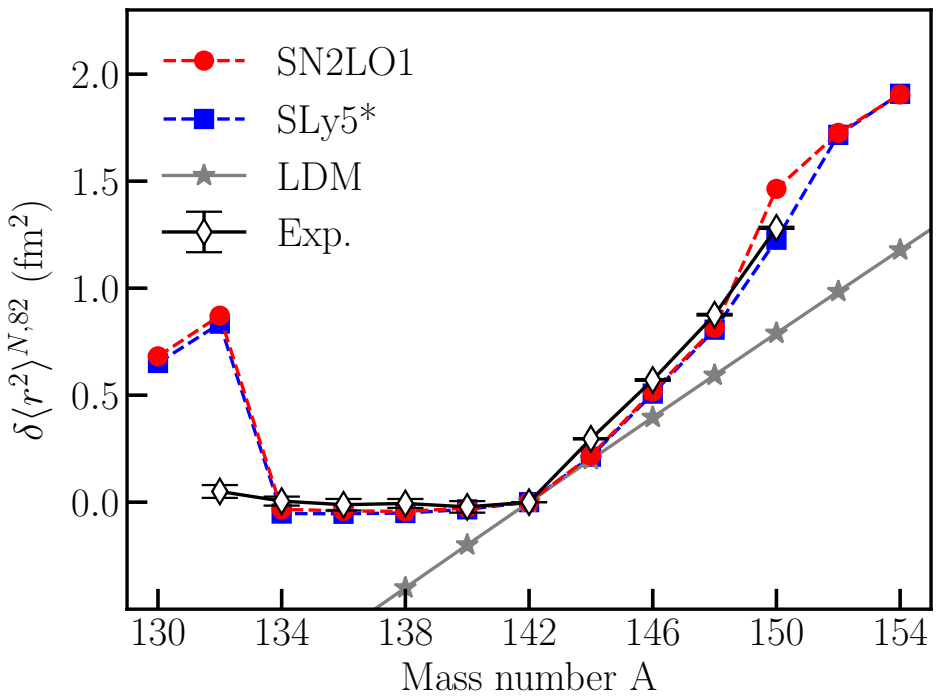


D. Baye et al. J. Phys. A 19 (1986).

Planning

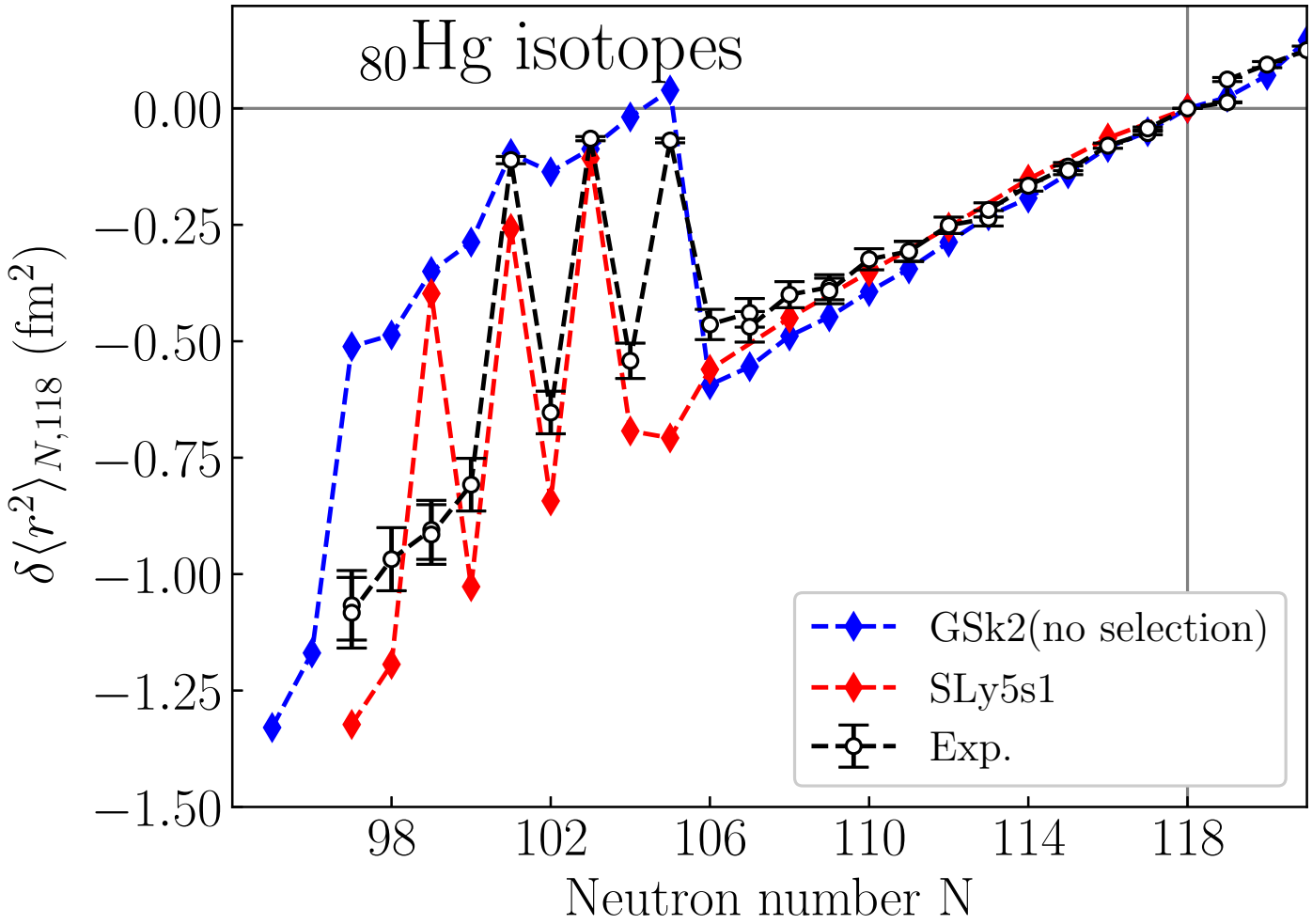
Nuclear radii: $^{A}_{60}$Nd





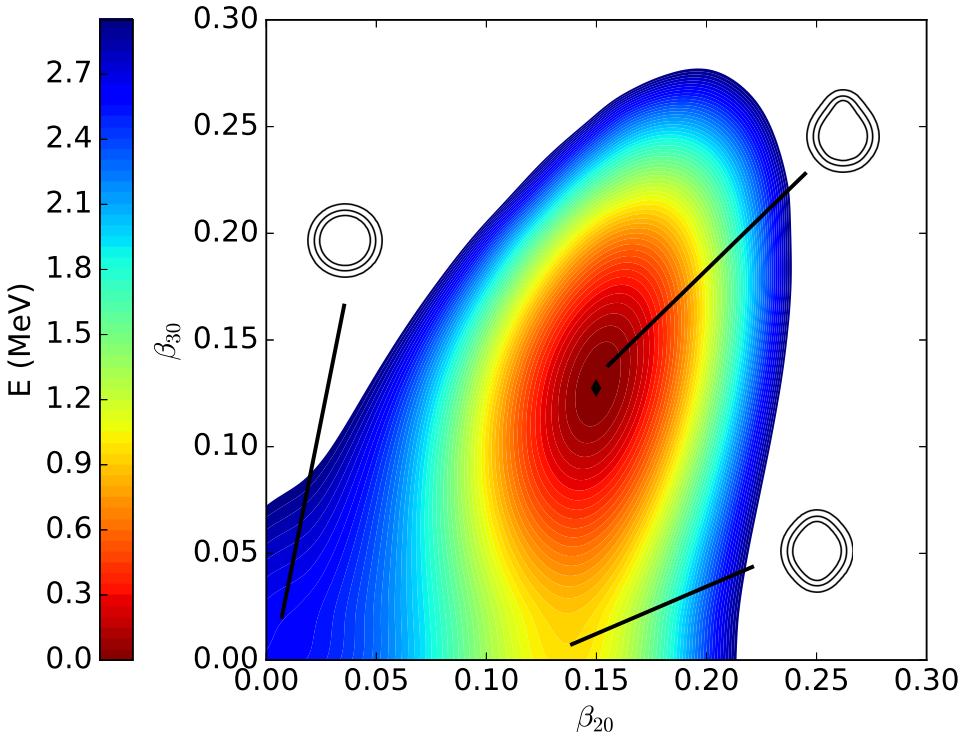
Calculations from W. Ryssens & M. Bender, in preparation.
Exp. data from I. Angeli, At. Data Nucl. Data Tables **87**, 185-193 (2004).

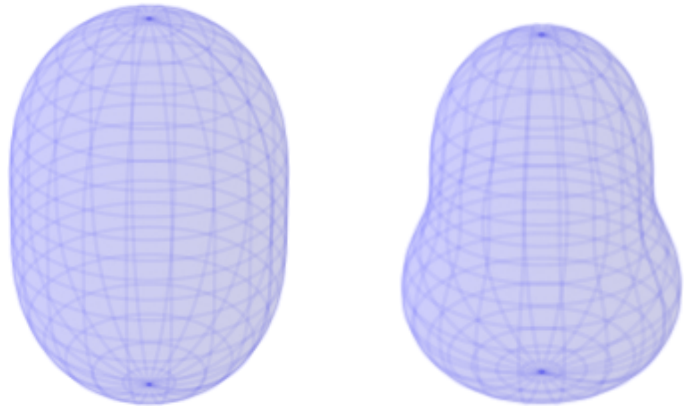
Nuclear radii: ${}^{A}_{60}$Hg



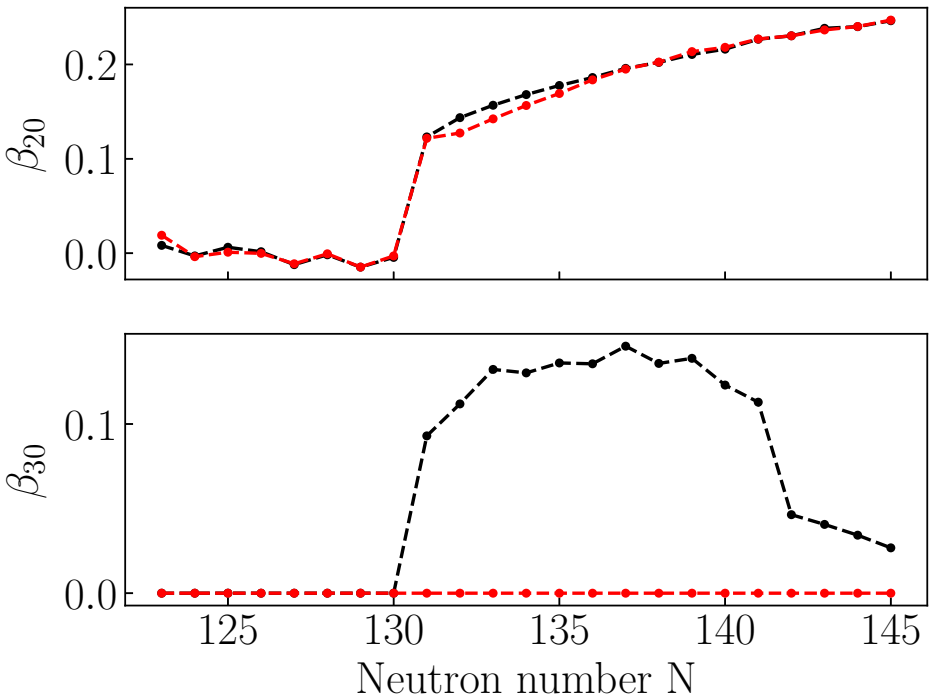
Exp. data and SLy5s1 calculations from S. Sels et al. PRC **99**, 044306 (2019).

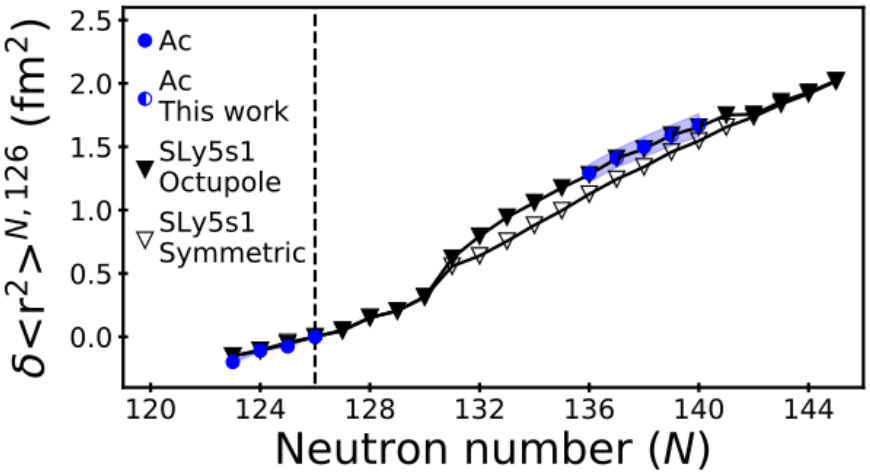
Octupole deformation





$^{A}_{89}$Ac isotopes





Exp. data and calculations from E. Verstraelen et al. PRC 100, 044321 (2019).

Planning

What am I doing here on the 4th floor?

Long tradition of nuclear models based on configurations that are

- axially symmetric
- time-reversal invariant

What am I doing here on the 4th floor?

Long tradition of nuclear models based on configurations that are

- axially symmetric
- time-reversal invariant

Can we improve EDFs for astrophysical needs by breaking symmetries?

What am I doing here on the 4th floor?

Long tradition of nuclear models based on configurations that are

- axially symmetric
- time-reversal invariant

Can we improve EDFs for astrophysical needs by breaking symmetries?
Can we use MOCCa to fit better EDF models?

What am I doing here on the 4th floor?

Long tradition of nuclear models based on configurations that are

- axially symmetric
- time-reversal invariant

Can we improve EDFs for astrophysical needs by breaking symmetries?
Can we use MOCCa to fit better EDF models?

Observables of focus

- Binding energies?
- Fission barriers?
- Radii?
- Spins and parities for odd systems?

The GSk1&2 models

	GSk1	GSk2	HFB-27
$\sigma(M)$ (MeV)	0.662		0.512
$\bar{\epsilon}(M)$ (MeV)	−0.027		−0.005
$\sigma(R_c)$ (fm)	0.0248		0.028
$\bar{\epsilon}(R_c)$ (fm)	−0.0030		0.010

AI work & fit mostly by G. Scamps

- First models fit to 3D-calculations
- GSk1 = best fit to **all known** masses
- GSk2 = compromise masses vs. MOI

G. Scamps, E. Olsen, W.R., M. Bender and S. Goriely *et al.*, submitted to PRL.
HFB-27 from S. Goriely, N. Chamel and J. M. Pearson, PRC **88**, 061302(R) (2015).

The GSk1&2 models

	GSk1	GSk2	HFB-27
$\sigma(M)$ (MeV)	0.662		0.512
$\bar{\epsilon}(M)$ (MeV)	−0.027		−0.005
$\sigma(R_c)$ (fm)	0.0248		0.028
$\bar{\epsilon}(R_c)$ (fm)	−0.0030		0.010

AI work & fit mostly by G. Scamps

- First models fit to 3D-calculations
- GSk1 = best fit to **all known** masses
- GSk2 = compromise masses vs. MOI

G. Scamps, E. Olsen, W.R., M. Bender and S. Goriely *et al.*, submitted to PRL.
HFB-27 from S. Goriely, N. Chamel and J. M. Pearson, PRC **88**, 061302(R) (2015).

The GSk1&2 models

	GSk1	GSk2	HFB-27
$\sigma(M)$ (MeV)	0.662	0.731	0.512
$\bar{\epsilon}(M)$ (MeV)	−0.027	0.031	−0.005
$\sigma(R_c)$ (fm)	0.0248	0.0242	0.028
$\bar{\epsilon}(R_c)$ (fm)	−0.0030	−0.0009	0.010

All work & fit mostly by G. Scamps

- First models fit to 3D-calculations
- GSk1 = best fit to **all known** masses
- GSk2 = compromise masses vs. MOI

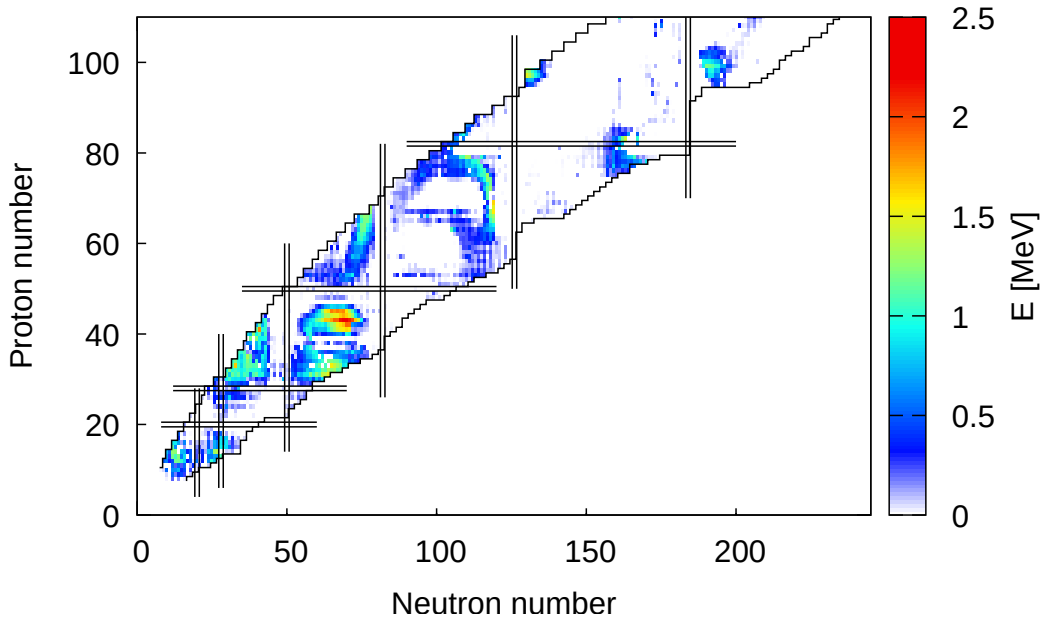
G. Scamps, E. Olsen, W.R., M. Bender and S. Goriely *et al.*, submitted to PRL.
HFB-27 from S. Goriely, N. Chamel and J. M. Pearson, PRC **88**, 061302(R) (2015).

The GSk1&2 models

	GSk1	GSk2	HFB-27
$\sigma(M)$ (MeV)	0.662	0.731	0.512
$\bar{\epsilon}(M)$ (MeV)	−0.027	0.031	−0.005
$\sigma(R_c)$ (fm)	0.0248	0.0242	0.028
$\bar{\epsilon}(R_c)$ (fm)	−0.0030	−0.0009	0.010

Al work & fit mostly by G. Scamps

- First models fit to 3D-calculations
- GSk1 = best fit to **all known** masses
- GSk2 = compromise masses vs. MOI
- Triaxiality important in several regions



G. Scamps, E. Olsen, W.R., M. Bender and S. Goriely *et al.*, submitted to PRL.
HFB-27 from S. Goriely, N. Chamel and J. M. Pearson, PRC **88**, 061302(R) (2015).

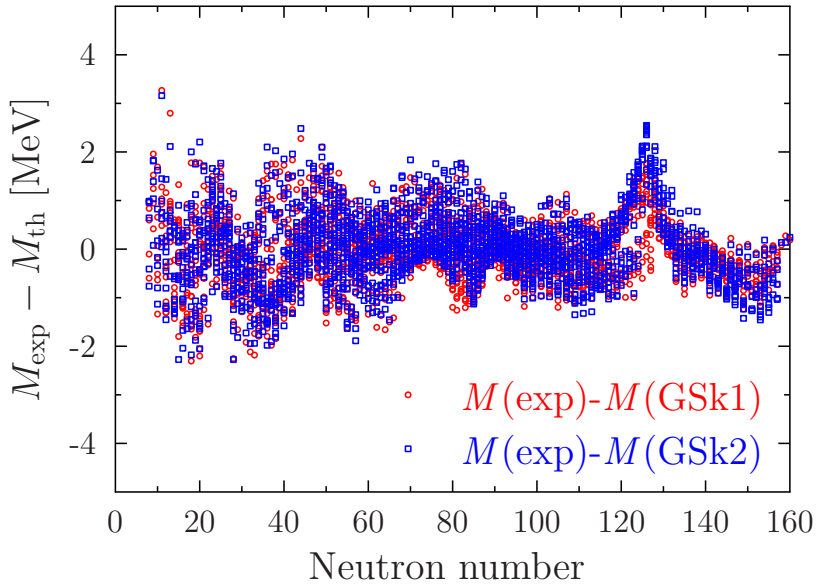
Relative success of this approach

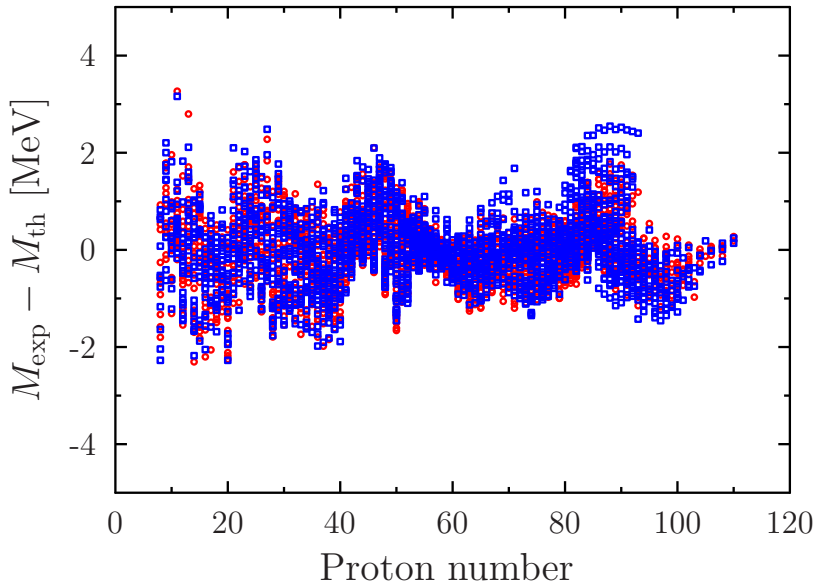
2408 masses

- RMS deviation $\sim$ 0.731 MeV
- Vast majority within 2 MeV of experiment
- cf. total binding energy of ^{208}Pb = 1.6 GeV
- Relative error: $<$ 1%

884 charge radii

- RMS deviation $\sim$ 0.0242 fm
- cf. charge radius of ^{208}Pb = 5.5 fm
- Relative error: $<$ 1%





Conclusion

Mean-field approaches with Skyrme functionals

- are truly simple wavefunctions

Conclusion

Mean-field approaches with Skyrme functionals

- are truly simple wavefunctions
- but (global) excellent description

Conclusion

Mean-field approaches with Skyrme functionals

- are truly simple wavefunctions
- but (global) excellent description
- because of the power of symmetry breaking

Conclusion

Mean-field approaches with Skyrme functionals

- are truly simple wavefunctions
- but (global) excellent description
- because of the power of symmetry breaking
- which we'll take further in the coming years

Thanks!

Thanks for. . .

. . . the **help**:

GSk1 & 2

- S. Goriely ULB
- G. Scamps ULB
- E. Olsen ULB

MOCCa

- P.-H. Heenen ULB
- M. Bender IP2I

Thanks!

Thanks for. . .

. . . the **help**:

GSk1 & 2

- S. Goriely ULB
- G. Scamps ULB
- E. Olsen ULB

MOCCa

- P.-H. Heenen ULB
- M. Bender IP2I

. . . the **CPU time**!

- CÉCI network, Belgium.
- and in particular its Zenobe Tier1 cluster.

Thanks!

Thanks for. . .

. . . the **help**:

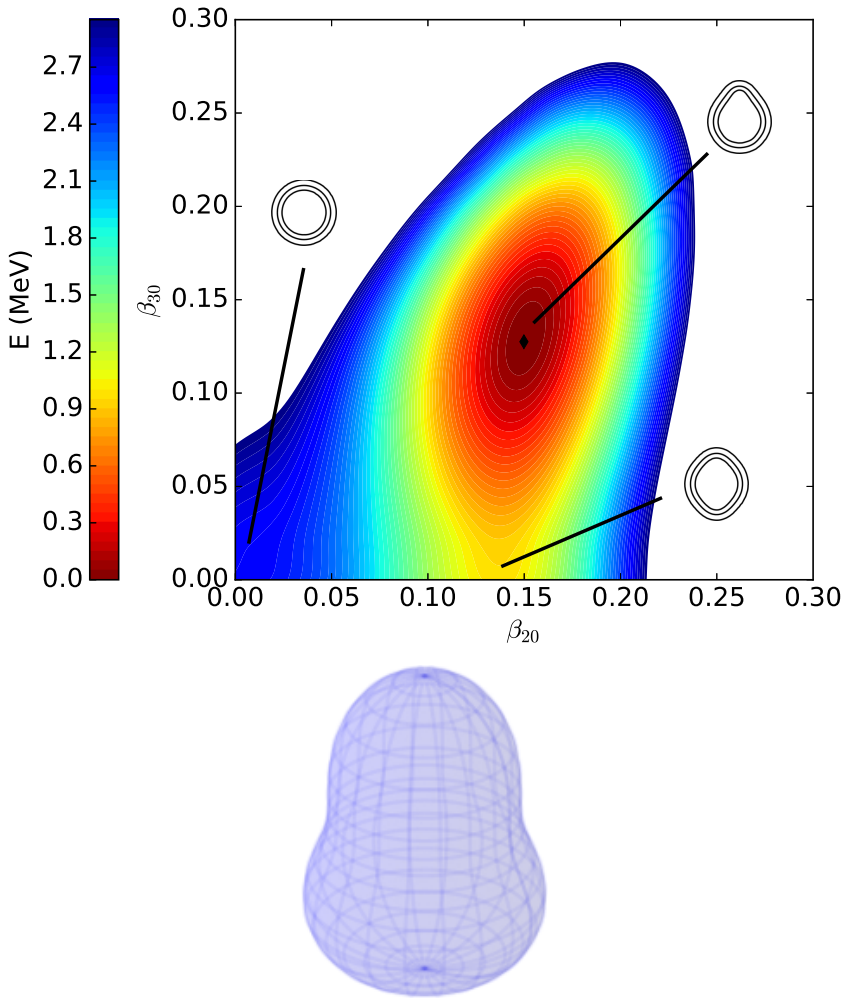
GSk1 & 2		**MOCCa**	
• S. Goriely	ULB	• P.-H. Heenen	ULB
• G. Scamps	ULB	• M. Bender	IP2I
• E. Olsen	ULB		

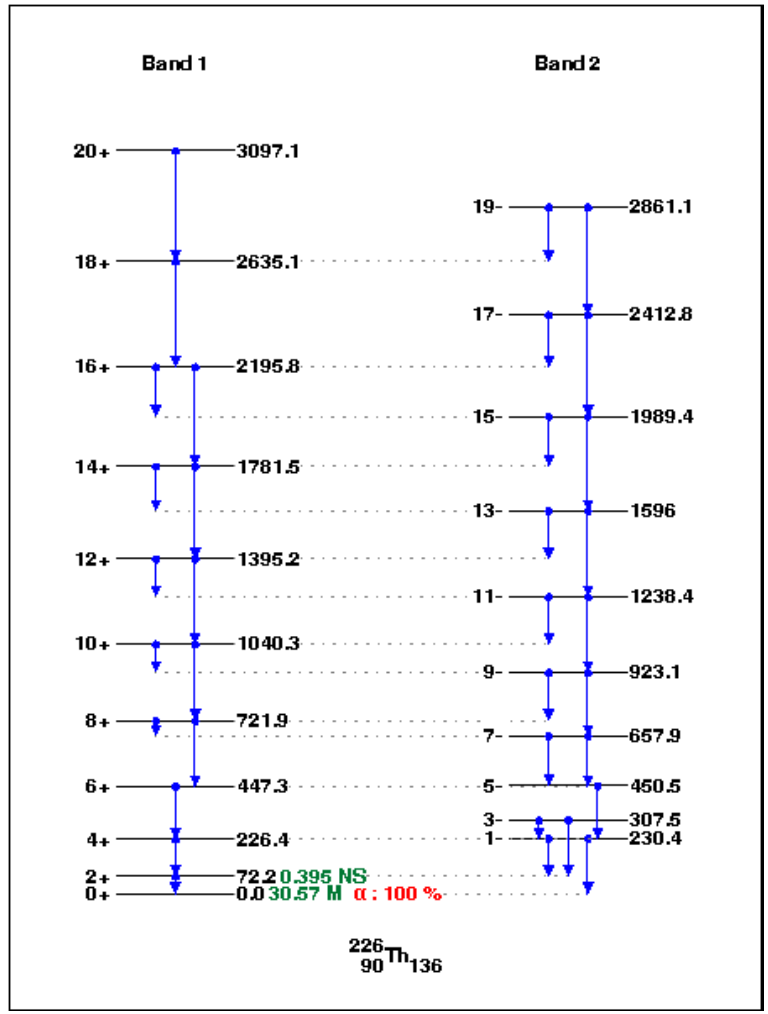
. . . the **CPU time**!

- CÉCI network, Belgium.
- and in particular its Zenobe Tier1 cluster.

. . . your **attention**!

Octupole deformation





f