# Symmetry unrestricted Skyrme mean-field study of heavy nuclei

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## Summary

- 1 Density Functional Theory
- 2 SLy5sX Functionals
- 3 Symmetries Rotational Symmetry Parity
- 4 Fission of <sup>226</sup>Ra with the Sly5sX
- 5 Conclusion



## The nuclear landscape



Figure from G.F. Bertsch et al., SciDAC Review 6, 48 (2007).



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 $\Psi_{many-body} = \mathsf{Slater} \; \mathsf{Determinant}$ 



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$$\psi_i(\vec{r}), i = 1, \dots, A$$



 $\Psi_{many-body} = \text{Slater Determinant}$   $\rho(\vec{r}), \tau(\vec{r}), \dots$   $\psi_i(\vec{r}), i = 1, \dots, A$ 









![](_page_8_Figure_1.jpeg)

$$E(\rho) = E_{kinetic} + E_{Coulomb} + E_{Skyrme} + E_{pairing}$$

![](_page_9_Picture_2.jpeg)

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• 
$$E_{kinetic} = \frac{\hbar^2}{2m_n} \int d\vec{r} \,\tau(\vec{r})$$

![](_page_10_Picture_3.jpeg)

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![](_page_11_Picture_4.jpeg)

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![](_page_12_Picture_5.jpeg)

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![](_page_13_Picture_6.jpeg)

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- ( $\approx$ ) 10 parameters

![](_page_14_Picture_7.jpeg)

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- ( $\approx$ ) 10 parameters
- fitted on doubly-magic binding energies and charge radii

![](_page_15_Picture_8.jpeg)

## The Sly5sX family

![](_page_16_Picture_1.jpeg)

- General EDF
- Widely used and succesful
- Rather bad at fission
- Unsafe to use! (2011)
- E. Chabanat et al., Nucl. Phys. A. 635 (1998)

![](_page_16_Picture_7.jpeg)

## The Sly5sX family

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- General EDF
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- E. Chabanat et al., Nucl. Phys. A. 635 (1998)

![](_page_17_Picture_7.jpeg)

- Refit of SLy5
- Similar properties
- Safe!
- Even worse at fission ... A. Pastore *et al.*, Phys. Scr. T154, 014014 (2013)

![](_page_17_Picture_12.jpeg)

#### The Sly5sX family

![](_page_18_Figure_1.jpeg)

## Symmetries

## #{Symmetric Slater Determinants} $\leq$ #{Asymmetric Slater Determinants}

![](_page_19_Picture_2.jpeg)

## Symmetries

![](_page_20_Picture_1.jpeg)

![](_page_20_Picture_2.jpeg)

![](_page_20_Picture_3.jpeg)

## Rotational Symmetry

![](_page_21_Figure_1.jpeg)

![](_page_21_Picture_2.jpeg)

## Rotational Symmetry

![](_page_22_Figure_1.jpeg)

### Rotational Symmetry

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![](_page_23_Figure_1.jpeg)

Figure from M. Bender et al., PRC 69, 064303 (2004)

![](_page_23_Picture_3.jpeg)

## Parity

![](_page_24_Picture_1.jpeg)

![](_page_24_Picture_2.jpeg)

## Parity

![](_page_25_Picture_1.jpeg)

![](_page_25_Picture_2.jpeg)

## Deformation of <sup>226</sup>Ra

![](_page_26_Figure_1.jpeg)

### **Fission Barriers**

![](_page_27_Figure_1.jpeg)

### **Fission Barriers**

![](_page_28_Figure_1.jpeg)

### **Fission Barriers**

![](_page_29_Figure_1.jpeg)

![](_page_29_Figure_2.jpeg)

## Conclusion

Density Functional Theory

- Tool to study the entirety of the nuclear chart.
- Symmetry breaking is essential to capture the physics.

![](_page_30_Picture_4.jpeg)

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Density Functional Theory

- Tool to study the entirety of the nuclear chart.
- Symmetry breaking is essential to capture the physics.

What is new?

- Possibility of breaking all discrete symmetries
- Generalized pairing (HFB) calculations.
- Controllable  $a_s$  for improved description of fission (with stable functionals).

![](_page_31_Picture_8.jpeg)

#### Prospects

In progress/Immediate future:

- Rotational bands in parity broken nuclei,
- Parity broken odd nuclei.

![](_page_32_Picture_4.jpeg)

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In progress/Immediate future:

- Rotational bands in parity broken nuclei,
- Parity broken odd nuclei.

Long-term future:

- Restoration of broken symmetries
- Investigation of nuclear Schiff moment.

![](_page_33_Picture_7.jpeg)

## Thanks!

Thanks to my collaborators:

- P.-H. Heenen (ULB)
- M. Bender (IPNL)
- K. Bennaceur (IPNL & Jyväskylä)

![](_page_34_Picture_5.jpeg)

![](_page_34_Picture_6.jpeg)

![](_page_34_Picture_7.jpeg)

![](_page_34_Picture_8.jpeg)

![](_page_35_Figure_0.jpeg)

Figure from M. Kortelainen et al., Phys. Rev. C 85, 024304

![](_page_35_Picture_2.jpeg)

![](_page_36_Figure_0.jpeg)

## Form of SLy5sX

$$E(\rho,\tau,\vec{j},J_{\mu\nu},\vec{s},\vec{T})_{T=0} = b_1\rho^2 + b_3(\rho\tau - \vec{j}^2) + b_5\rho\Delta\rho + b_7\rho^{2+\alpha} + b_9(\rho\nabla\vec{J} + \vec{j}\cdot\nabla\times\vec{s}) + b_{10}\vec{s}^2 + b_{12}\rho^{\alpha}\vec{s^2} + b_{14}\left(\sum_{\mu\nu}J_{\mu\nu}J_{\mu\nu} - \vec{s}\cdot\vec{T}\right) + b_{18}\vec{s}\cdot\Delta\vec{s} + b_{20}(\nabla\cdot\vec{s})^2$$

![](_page_37_Picture_2.jpeg)

### Mesh calculations

![](_page_38_Figure_1.jpeg)

![](_page_38_Picture_2.jpeg)