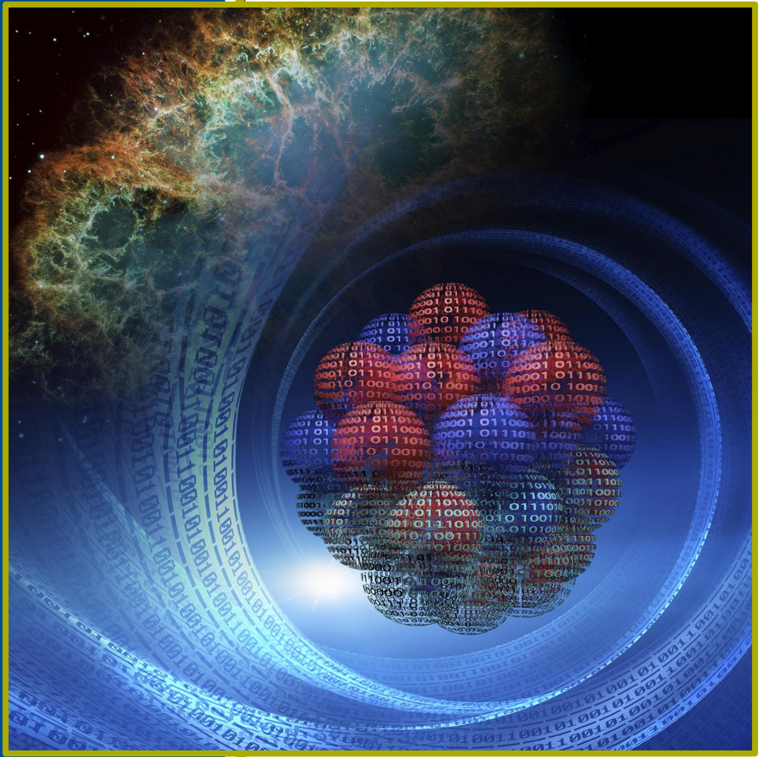
WOUTER RYSSENS



Andy Sproles, ORNL

Nuclear Density Functional Theory: **shapes and radii**

November 2022

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ULB

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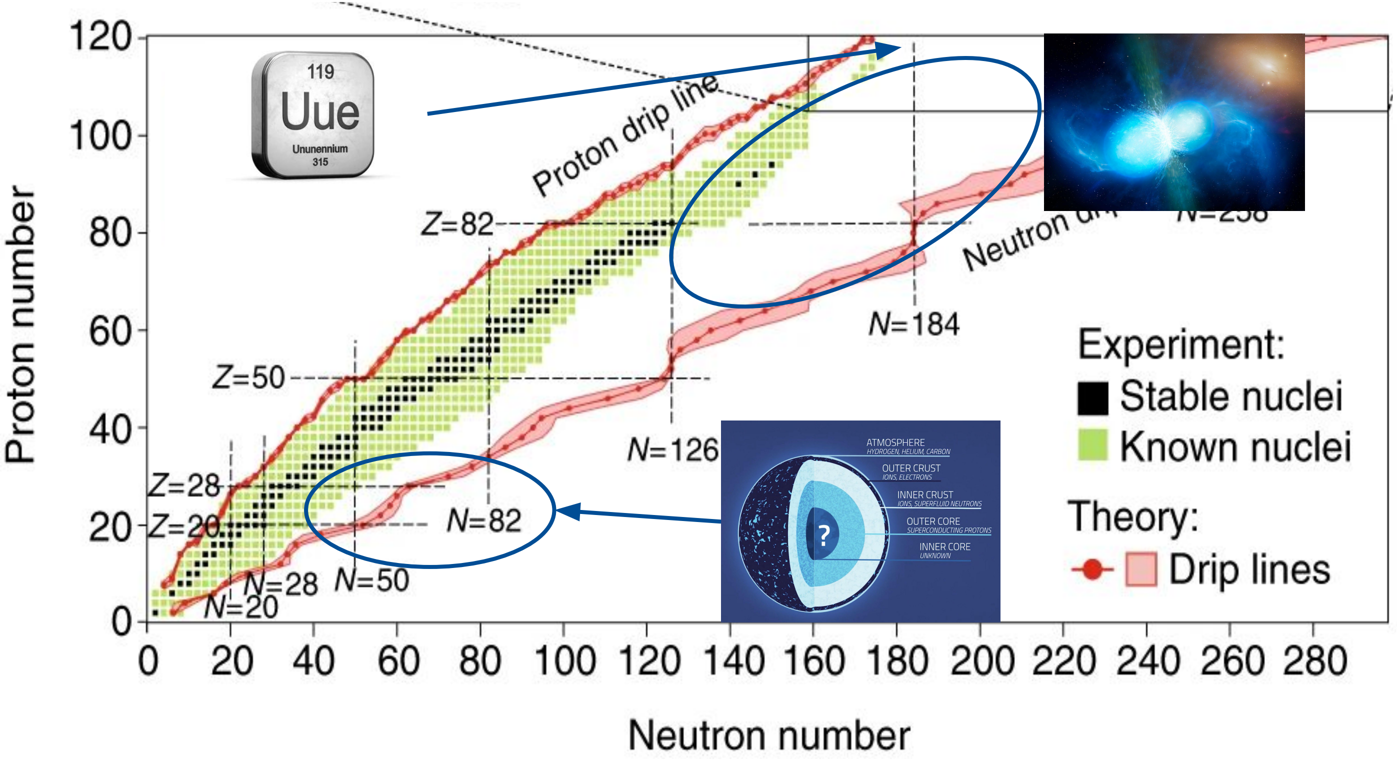
The nuclear chart

Image adapted from W. Nazarewicz, Nature 14, 537-541 (2018)



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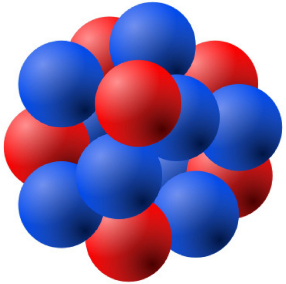


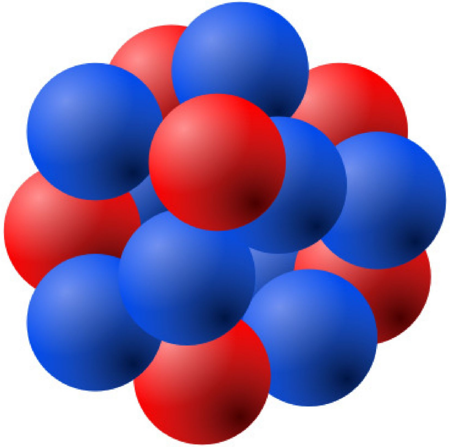
$$|\Psi_{N,Z}\rangle$$

The nuclear many-body problem

Wouter Ryssens (ULB)

How do we represent the nucleons?

- As a collections of quarks?
- In what kind of modelspace?
- Do we describe them all?



$$\hat{H}|\Psi_{N,Z}\rangle = E|\Psi_{N,Z}\rangle$$

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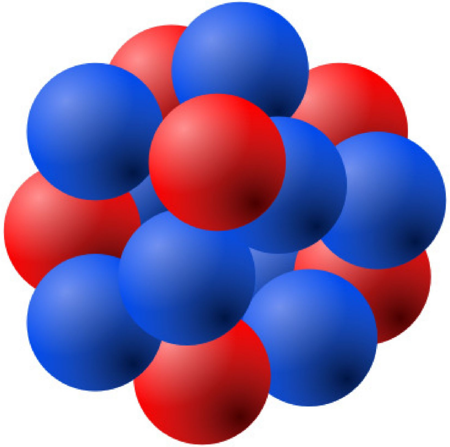

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<u>Solve Schrödingers equation?</u>

- Can we do it exactly?
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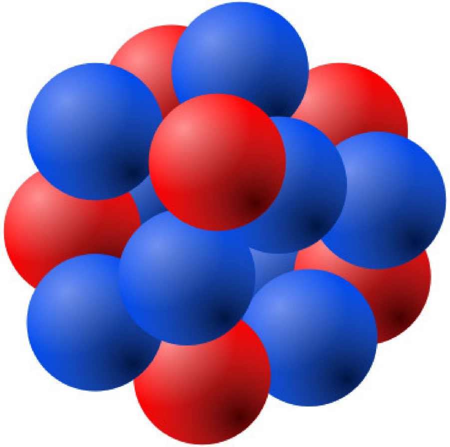

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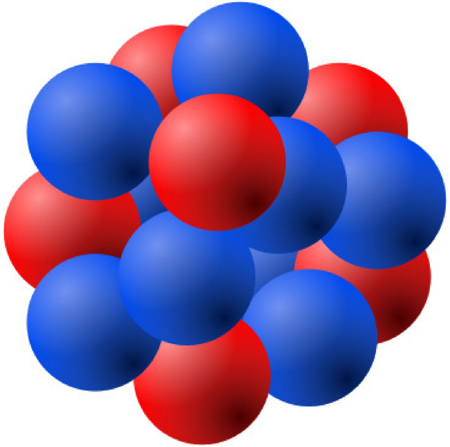


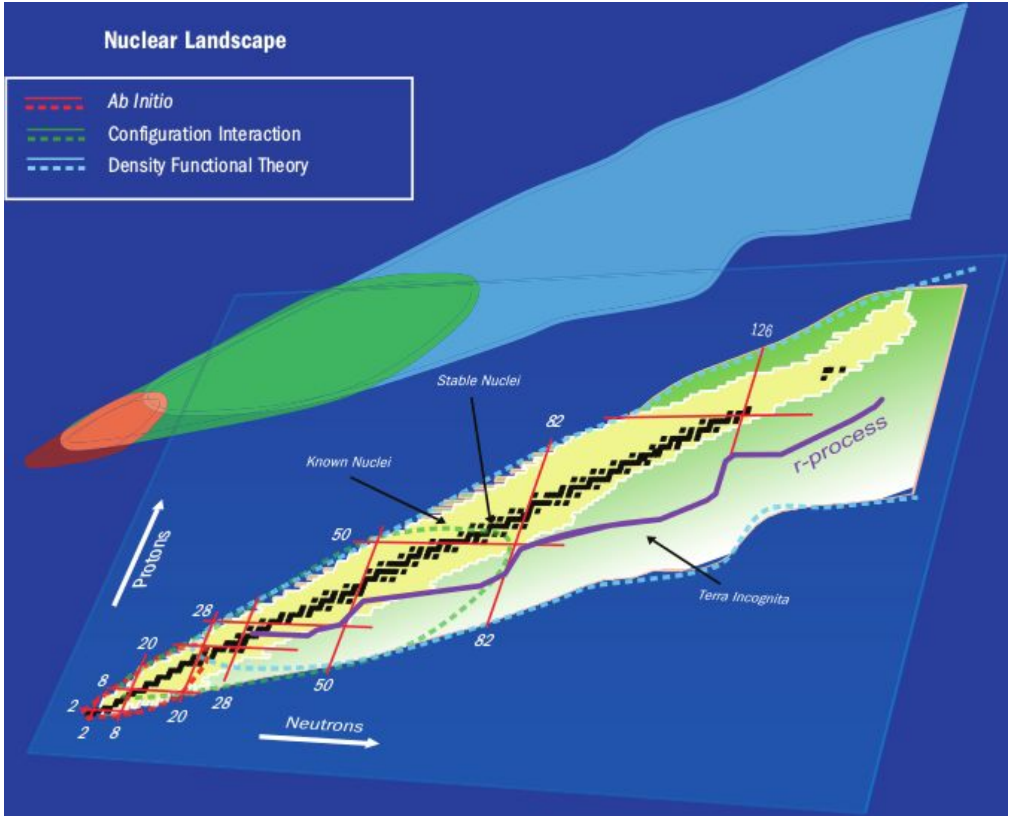
$$\hat{H}|\Psi_{N,Z}\rangle = E|\Psi_{N,Z}\rangle$$

Remark: (semi-)classical approaches exist too.

A quick look at some existing approaches

Ab initio

- Hamiltonian from n-n scattering
- Explicitly describe all nucleons
- Exact many-body solution



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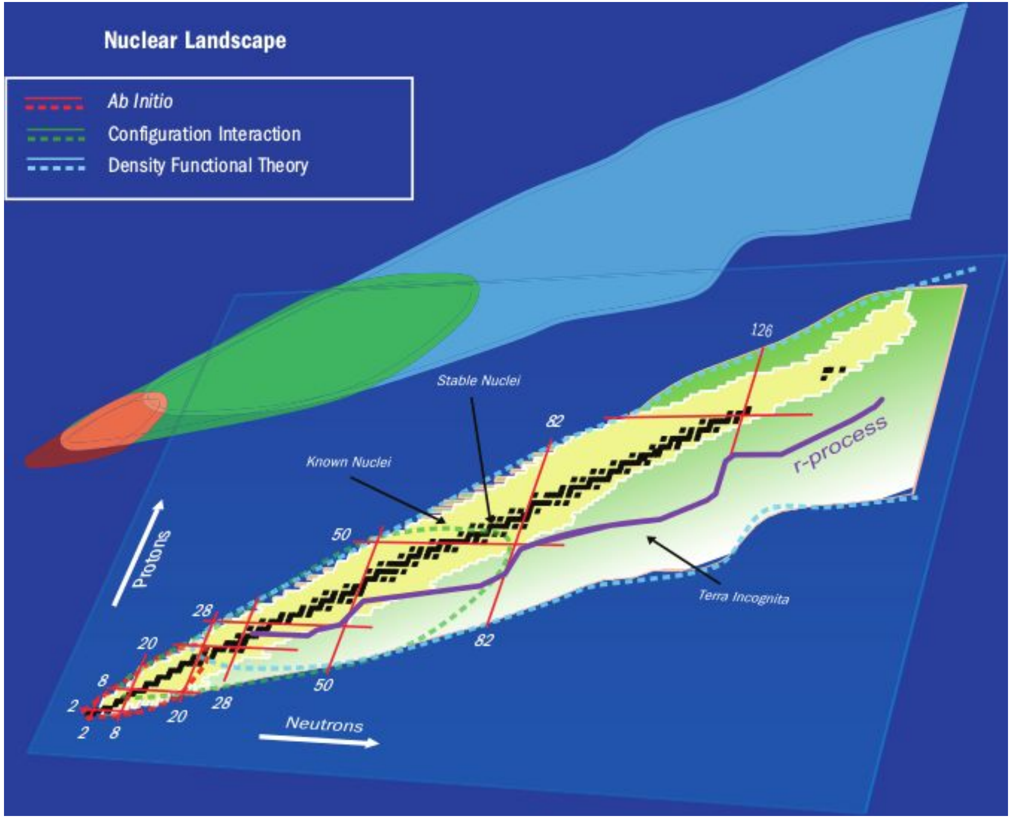

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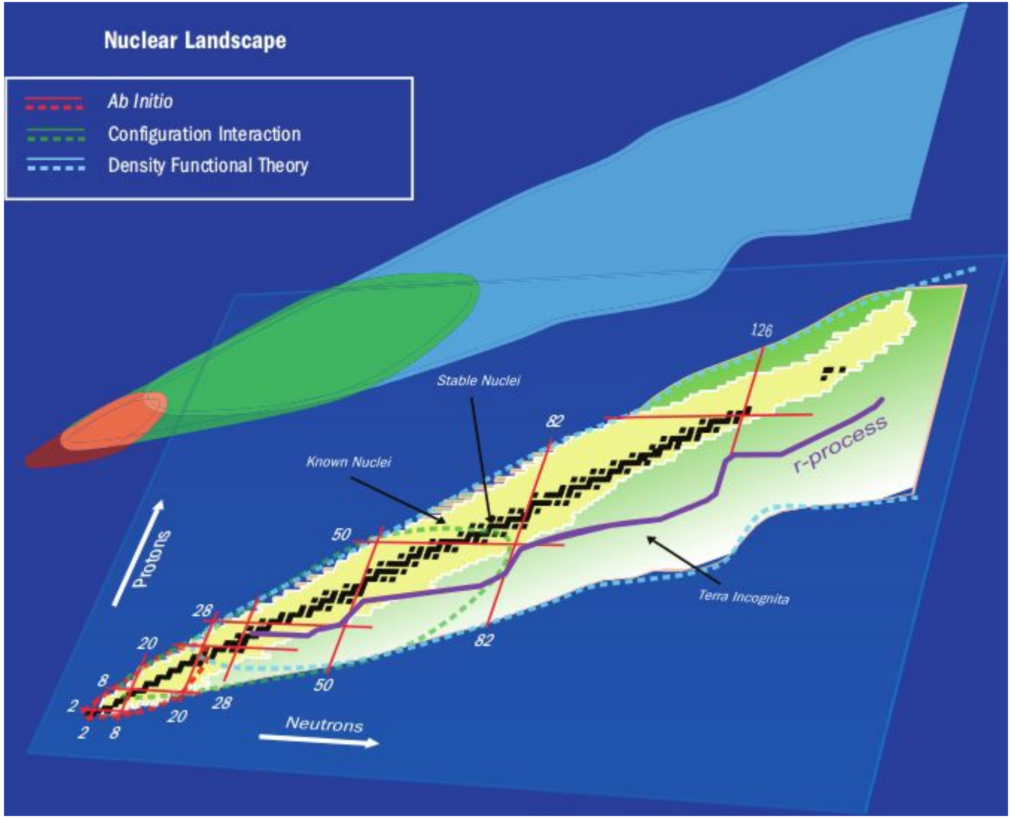
Nuclear Density Functional Theory

- Phenomenological interaction
- Explicitly describe all nucleons
- Mean-field solutions



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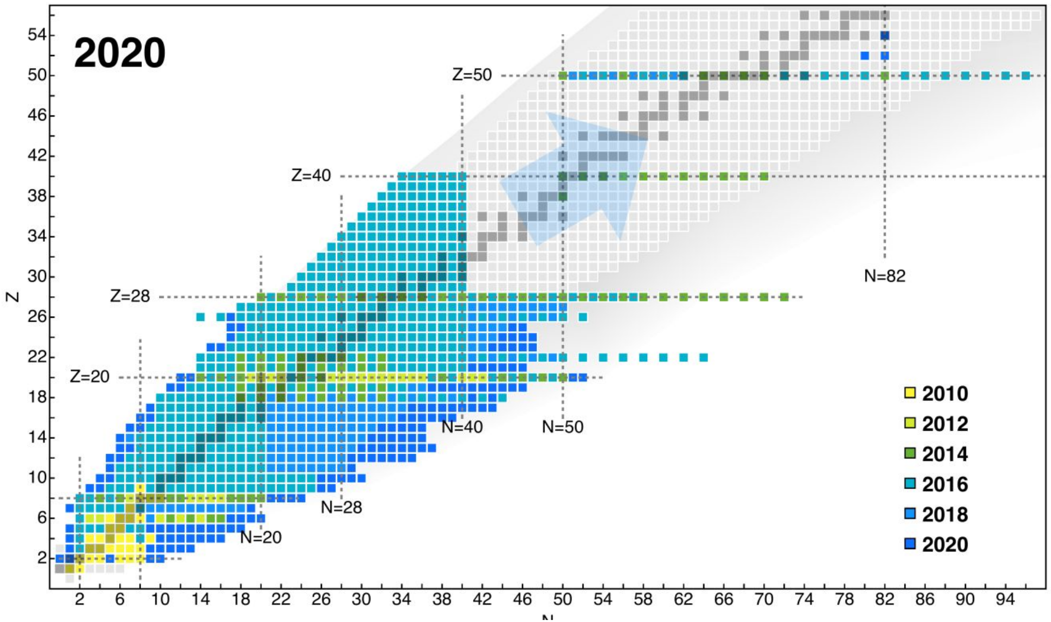

Mean-field theory

- general many-body wavefunctions are ORDERS OF MAGNITUDE too complex to handle

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_A) \longrightarrow \text{A x (3+1) dimensional}$$

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    - “independent particle”
    - no “correlations”
    - simplest possible

  A-body wavefunctions

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_A) \longrightarrow \textbf{A x (3+1)} \text{ dimensional}$$

$$\Psi_{\text{Slater}}(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_A) = \mathcal{A}\Big[\psi_1(\mathbf{r}_1)\psi_2(\mathbf{r}_2)\ldots\psi_A(\mathbf{r}_A)\Big] \, .$$

A functions of **(3+1)** dimensions

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- Including pairwise correlations:
  - HF+**BCS: B**ardeen-**C**ooper-**S**chrieffer
  - HF**B:** Hartree-Fock-**B**ogoliubov

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Effective interaction(s)

- Kinetic and Coulomb parts are known, the strong interaction part is not

$$\hat{H} = \hat{H}_{\text{kin}} + \hat{H}_{\text{strong}} + \hat{H}_{\text{Coulomb}} \, .$$

T. H. R. Skyrme, Nuclear Physics 9, 615–634 (1958).

Effective interaction(s)

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- Kinetic and Coulomb parts are known, the strong interaction part is not
- The Skyrme interaction is
  - simple **zero-range** ansatz
  - parameters: x_0, x_1, x_2, x_3, t_1, t_2, t_3, V
  - Central, Tensor and Spin-orbit part

$$\hat{H} = \hat{H}_{\text{kin}} + \hat{H}_{\text{strong}} + \hat{H}_{\text{Coulomb}}\,.$$

$$\downarrow$$

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

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

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

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- Other type of interactions exist:
  - generalized Skyrme forms
  - Gogny interaction
  - Relativistic interactions
  - ……

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Such effective interactions are **ad-hoc**, they do not constitute an approximation of the interaction between (free) nucleons.

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Energy **density** functionals

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\begin{aligned}
E &= \langle \Psi_{\text{Slater}} | \hat{H} | \Psi_{\text{Slater}} \rangle \\
&= E_{\text{kin}} + E_{\text{Coulomb}} + E_{\text{strong}} \\
&= E_{\text{kin}} + E_{\text{Coulomb}} + E_{\text{Skyrme}} + E_{\text{pairing}} + E_{\text{corrections}} \\
&= \int d^3r \, \mathcal{E}(\rho(\mathbf{r}), \tau(\mathbf{r}), J_{\mu\nu}(\mathbf{r})) \, .
\end{aligned}
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- Parameterisation
  - a set of values for the coupling constants.
  - there are several **hundreds**
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- In principle, the coupling constants are functions of the Skyrme parameters
- ..... but people take the C-s as **independent degrees of freedom**

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$$E = \langle \Psi_{\text{Slater}} | \hat{H} | \Psi_{\text{Slater}} \rangle \rightarrow C_t(t_0, x_0, \ldots)$$

$$E \neq \langle \Psi_{\text{Slater}} | \hat{H} | \Psi_{\text{Slater}} \rangle .$$

Successes of nuclear DFT

BSkG1 parameterisation: G. Scamps et al., EPJA 57, 333 (2021).

σ^2	# exp. data points	BSkG1
Masses (MeV)	2457	0.741
Charge radii (fm)	813	0.027
Fission barriers (MeV)	45	0.87

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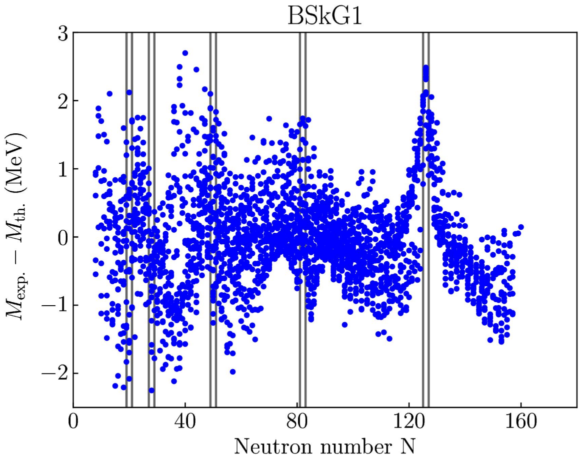

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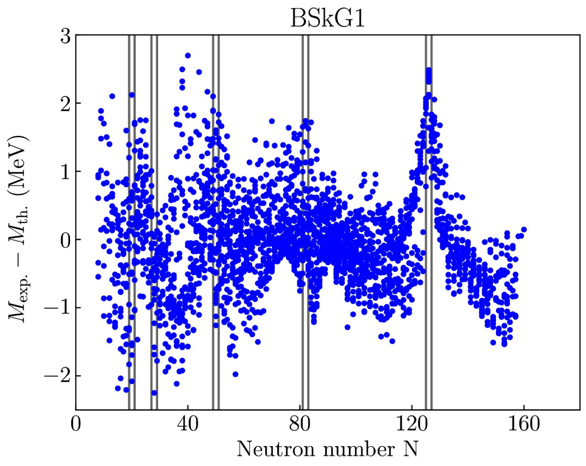
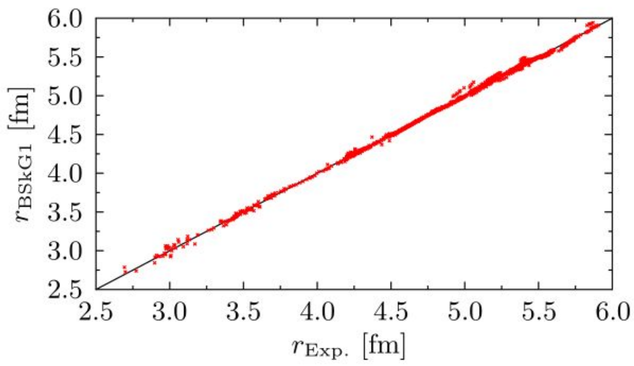




Successes of nuclear DFT

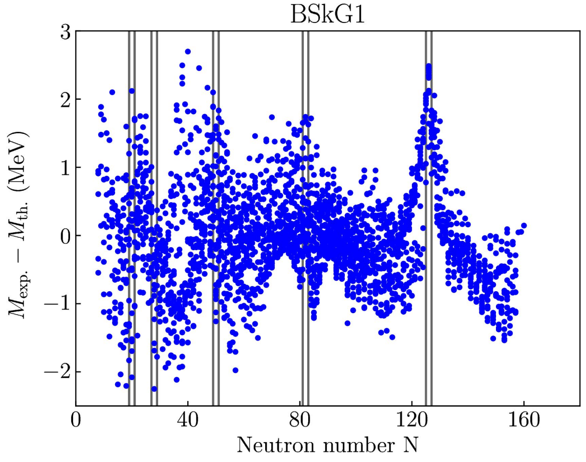
BSkG1 parameterisation: G. Scamps et al., EPJA 57, 333 (2021).

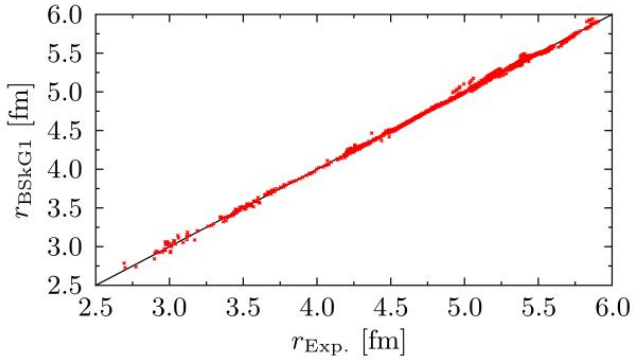
σ^2	# exp. data points	BSkG1
Masses (MeV)	2457	0.741
Charge radii (fm)	813	0.027
Fission barriers (MeV)	45	0.87

These numbers are tiny compared to typical values for heavy nuclei!

E.g. for ^{208}Pb:

- Binding energy ~ 1.6 GeV
- Charge radius ~ 5.5 fm





The mean-field equations and their solution

Varying the energy leads to

- 1-body eigenvalue problem for
- … single-particle hamiltonian h

$$\hat{h}(\rho, \tau, J_{\mu\nu})|\psi_i\rangle = \epsilon_i|\psi_i\rangle \, .$$

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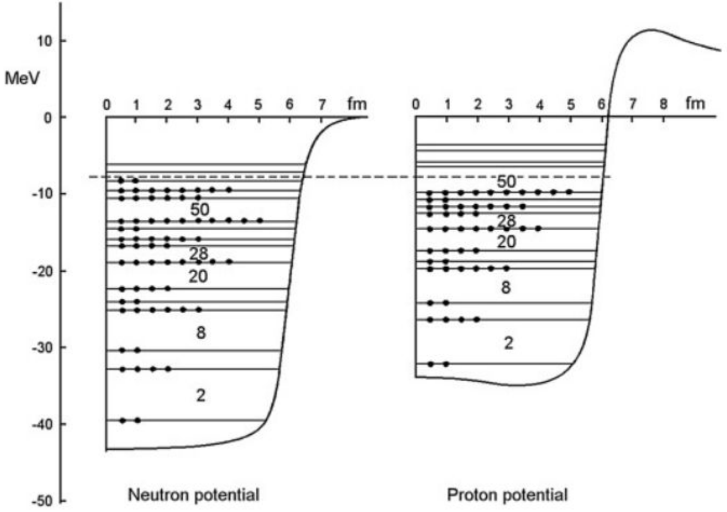
$$\hat{h}(\mathbf{r}) = -\boldsymbol{\nabla} \cdot B(\mathbf{r}) \boldsymbol{\nabla} + U(\mathbf{r}) - i \sum_{\mu\nu} W_{\mu\nu}(\mathbf{r}) \nabla_\mu \hat{\sigma}_\nu \,,$$

$$U(\mathbf{r}) = \frac{\partial E}{\partial \rho}, \qquad B(\mathbf{r}) = \frac{\partial E}{\partial \tau}, \qquad W_{\mu\nu}(\mathbf{r}) = \frac{\partial E}{\partial J_{\mu\nu}},$$



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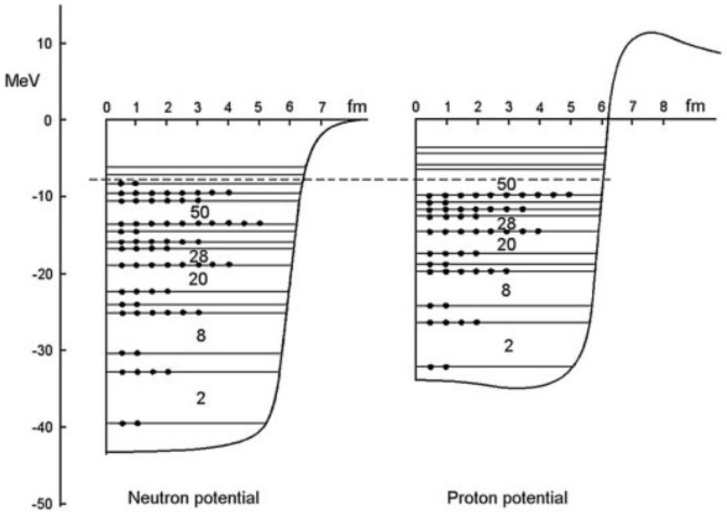

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The solution to this complicated equations: the **self-consistent** configuration

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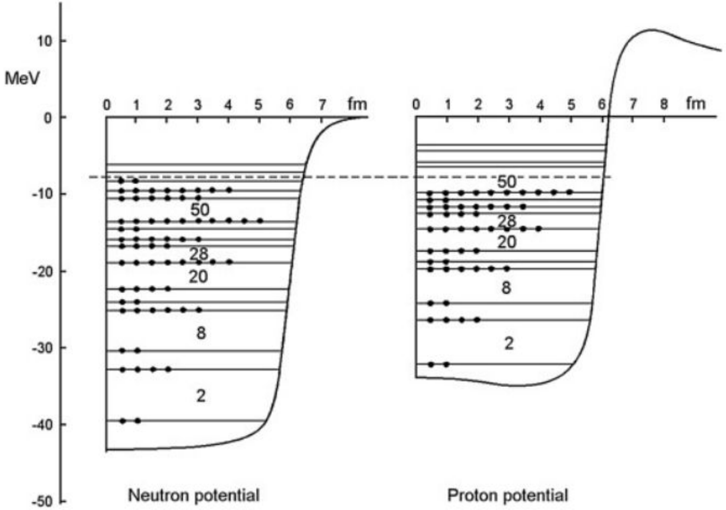

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The solution to this complicated equations: the **self-consistent** configuration

We have replaced

- **1 linear A-body** diagonalisation
- **A non-linear 1-body** diagonalisations

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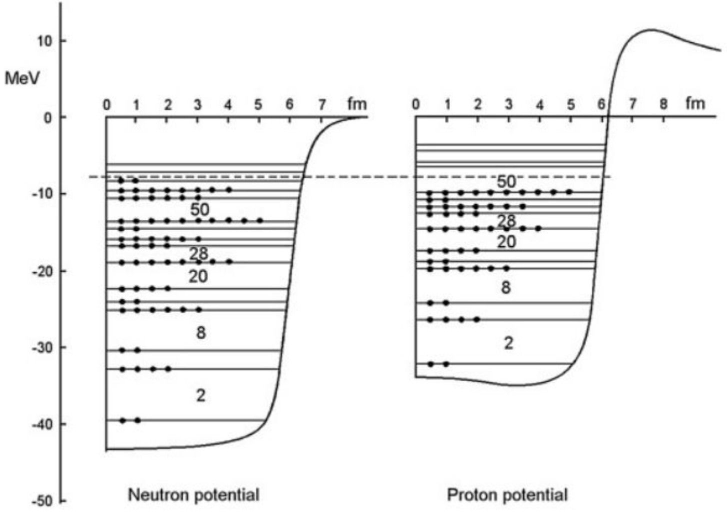
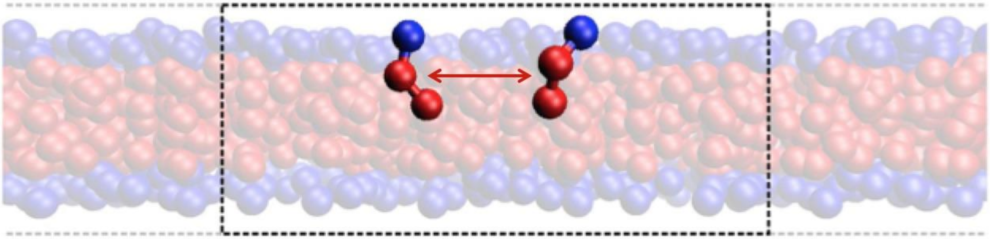


Mean-field**(?)** theory

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



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

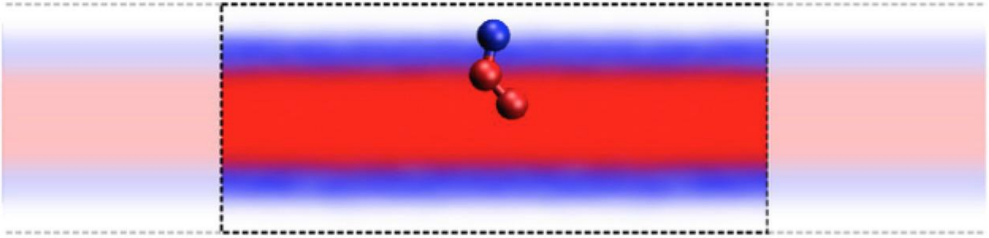
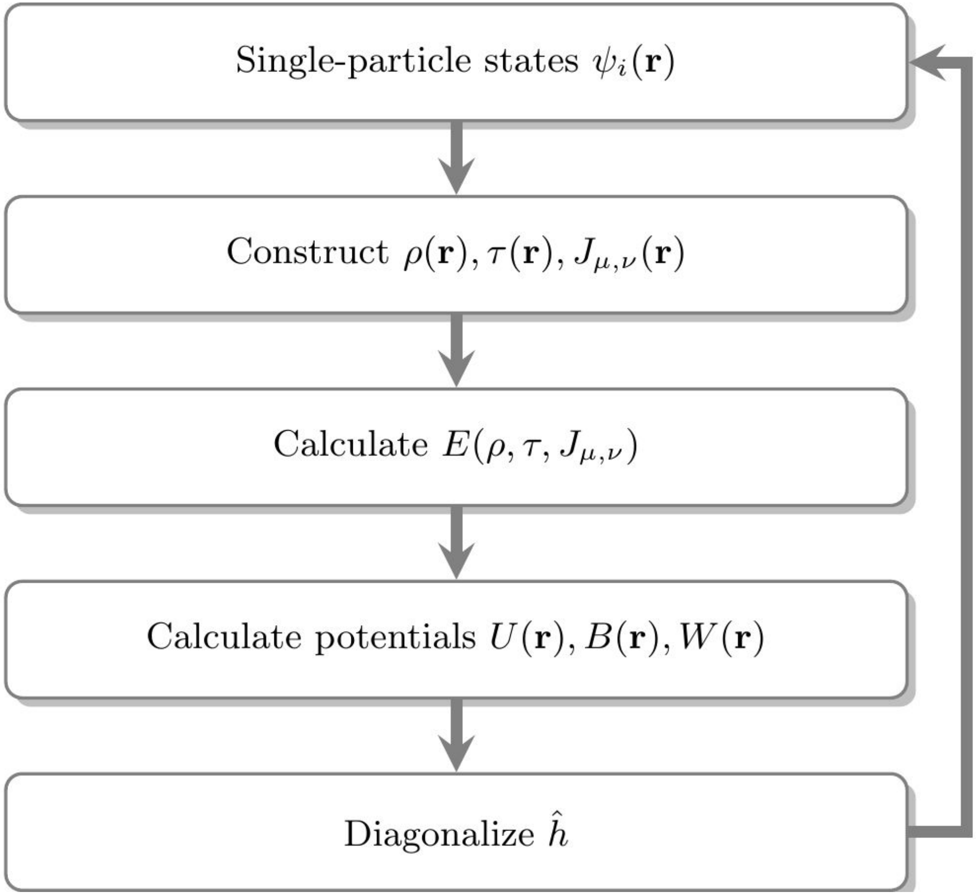


Figure from the ITN-SNAL, https://itn-snal.net/

Solving the mean-field equations

- The only hope is **iterative** techniques



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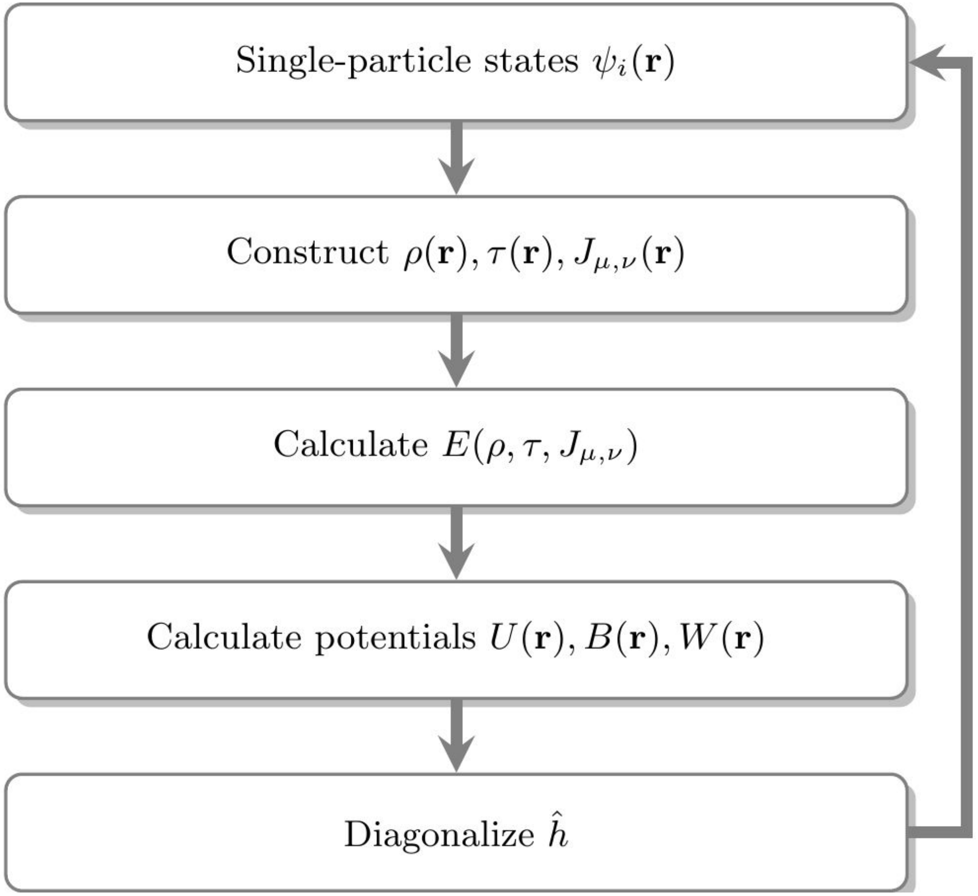

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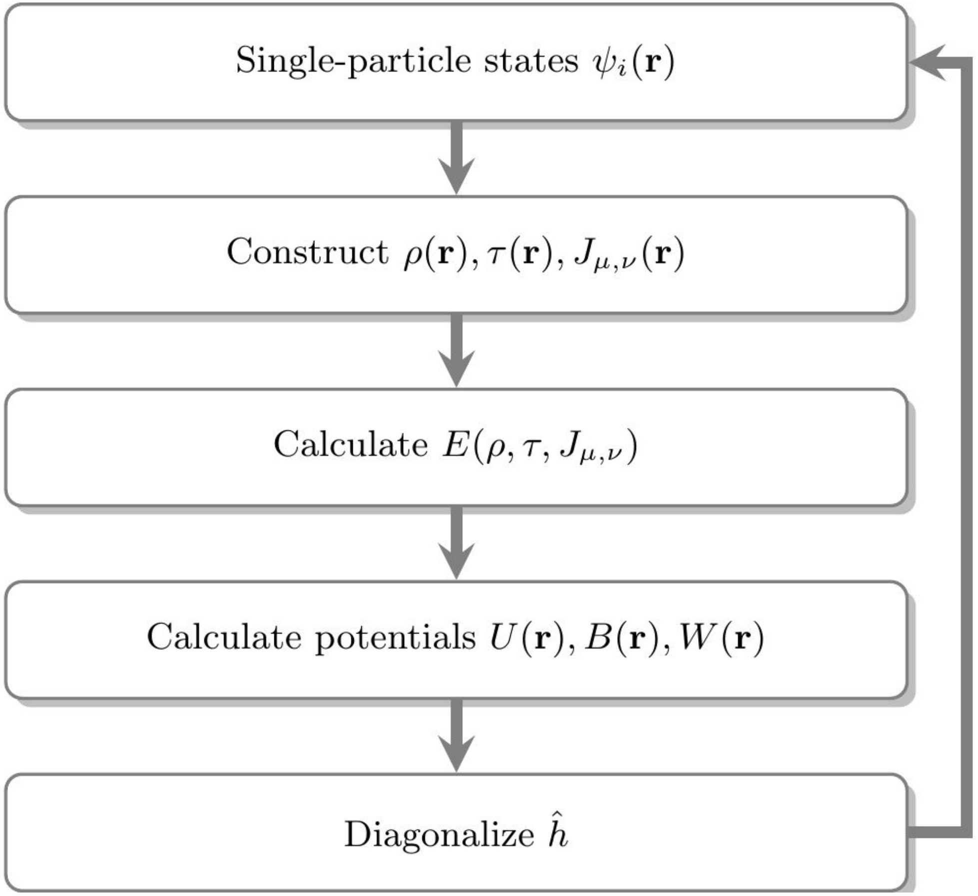
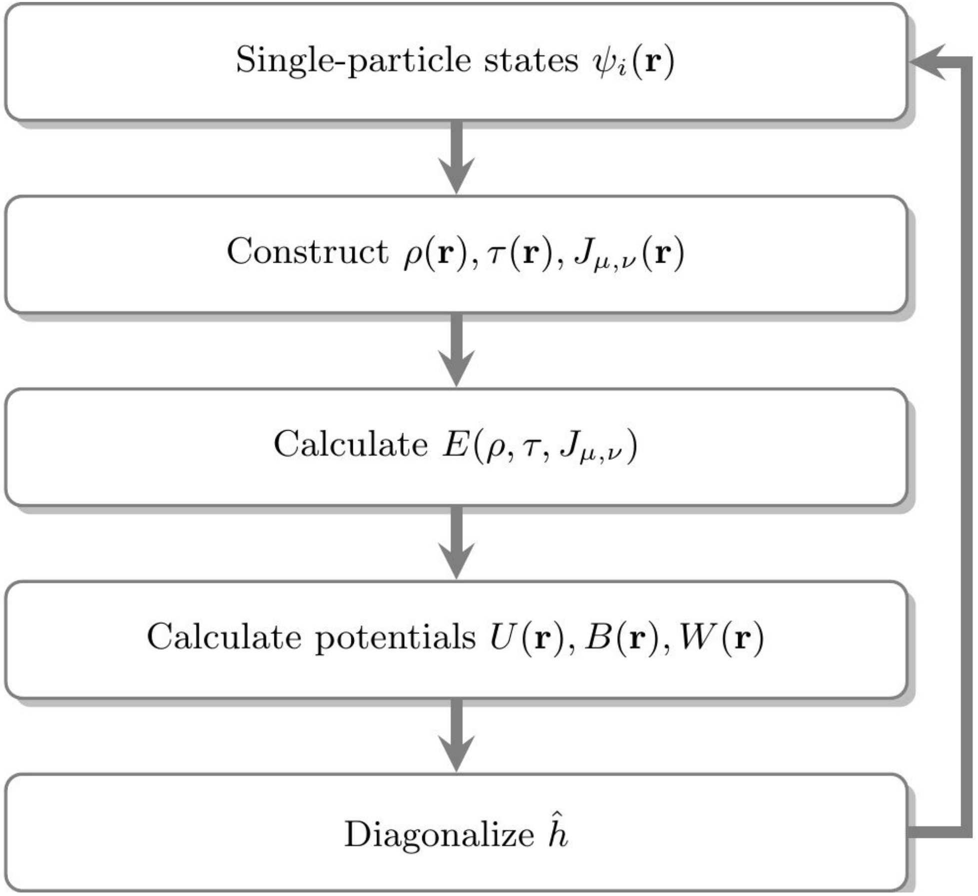
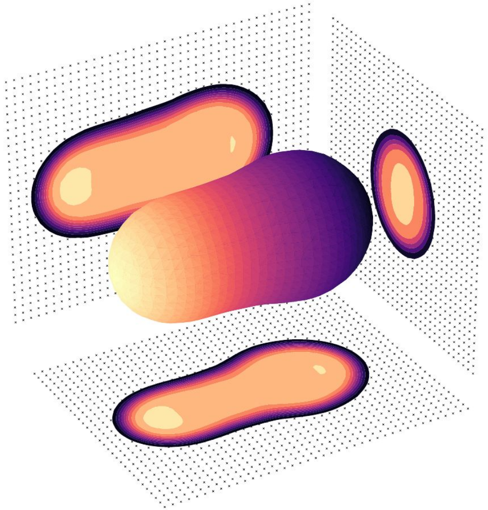


Solving the mean-field equations

- The only hope is **iterative** techniques
- Requires an initial guess
  - “good” guesses make things easier
- Finishes when [Input = Output]
- convergence is non-trivial
  - needs design of dedicated algorithms
  - usually depends on parameters
  - the **user should check!**



Nuclear shapes



Self-consistent symmetries

Nature has many symmetries

- rotational symmetry
- reflection/parity symmetry
- ....

which is reflected in quantum numbers.

If our initial guess is **symmetric**

- densities are symmetric
- potentials are symmetric
- s.p. hamiltonian h symmetric

and the solution will be **symmetric**!

The symmetry is **self-consistent.**

$$\hat{U}|\Psi\rangle = u|\Psi\rangle$$

$$\left[\hat{U}, \hat{h}(\rho, \tau, J_{\mu\nu})\right] = 0\,.$$

Symmetry breaking

If the initial guess is **NOT symmetric,** the solution will in general **NOT be symmetric.**

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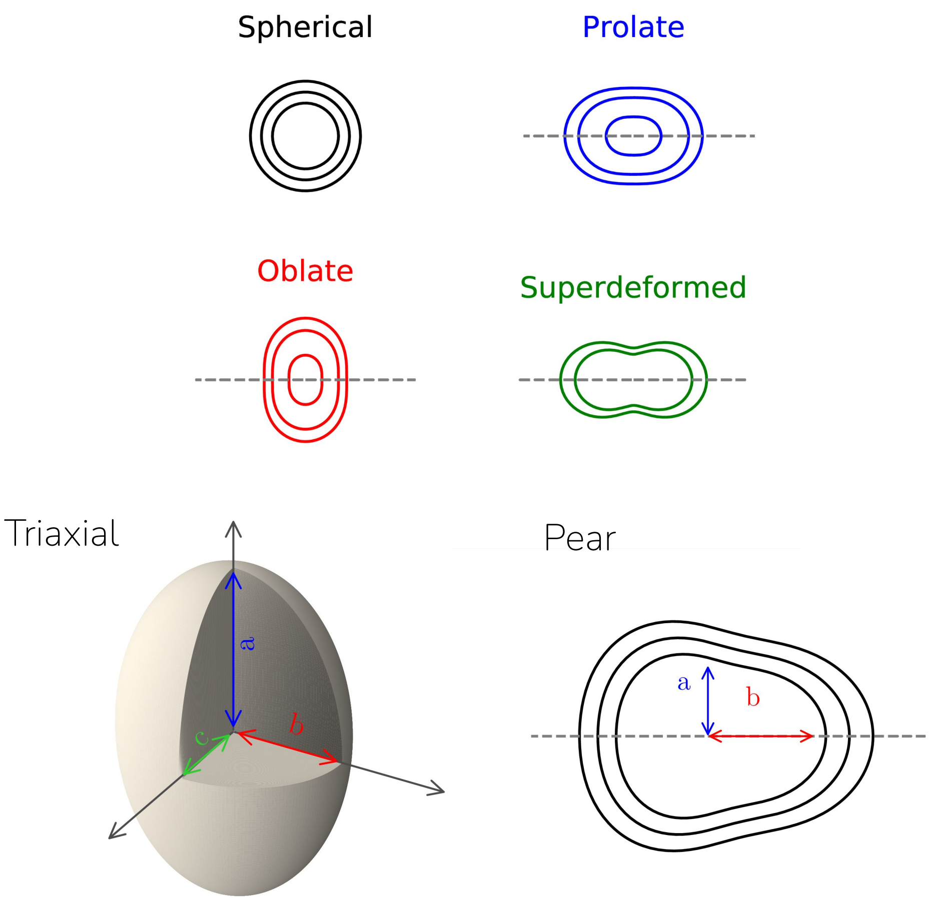
Possible configurations:

- prolate ellipsoids
- oblate ellipsoids
- superdeformed ellipsoids
- pear-like shapes
- triaxial ellipsoids
- ……



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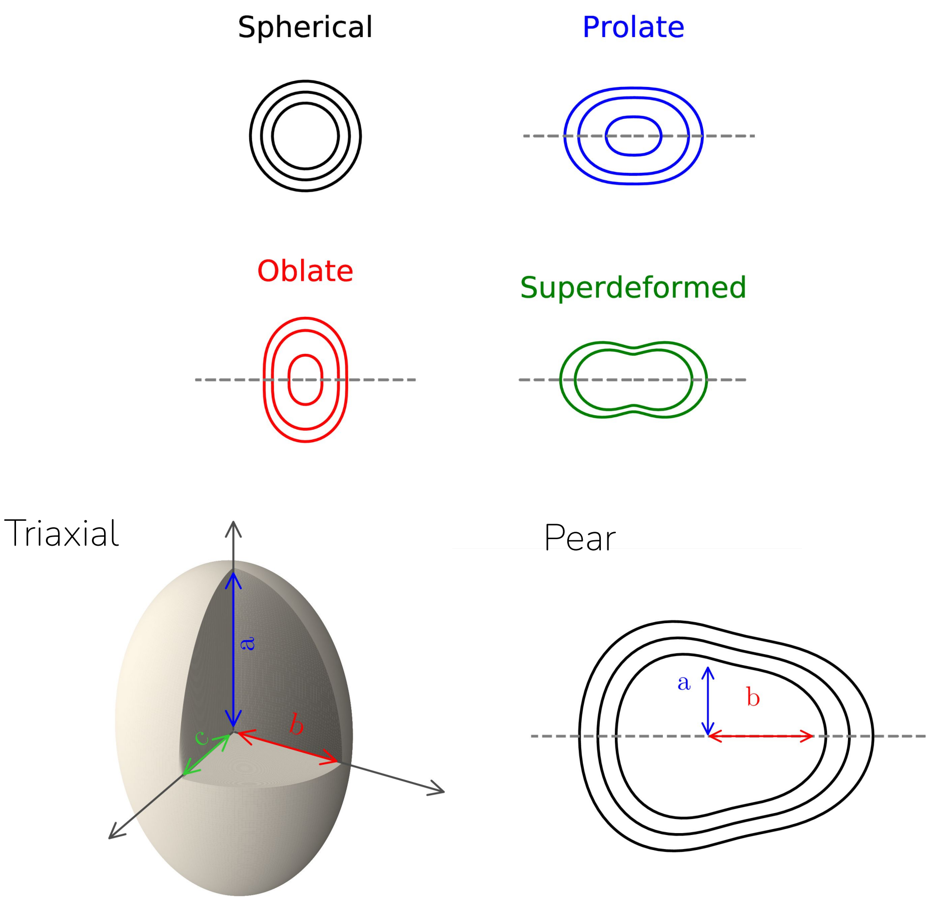
Finding the shape of lowest energy requires repeated calculations with different initial guesses!



Multipole moments

$$Q_{\ell m} = \int d^3r \, \rho(\mathbf{r}) r^l \mathrm{Re} Y_{\ell m}(\theta, \phi) \, .$$

$$\beta_{\ell m} = \frac{4\pi}{3AR^\ell} Q_{\ell m} \, .$$

$$R = 1.2 \times A[\mathrm{fm}].$$

Multipole moments characterize shapes

- quantities related to potential theory
- dimensionless quantities β_{lm}

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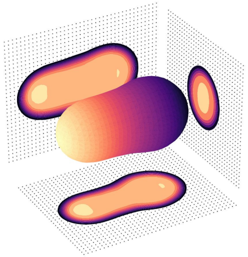

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- can all occur together....
- .... but quadrupole dominates.

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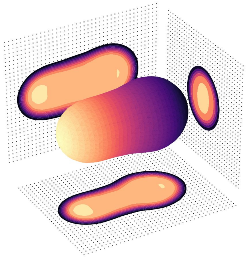

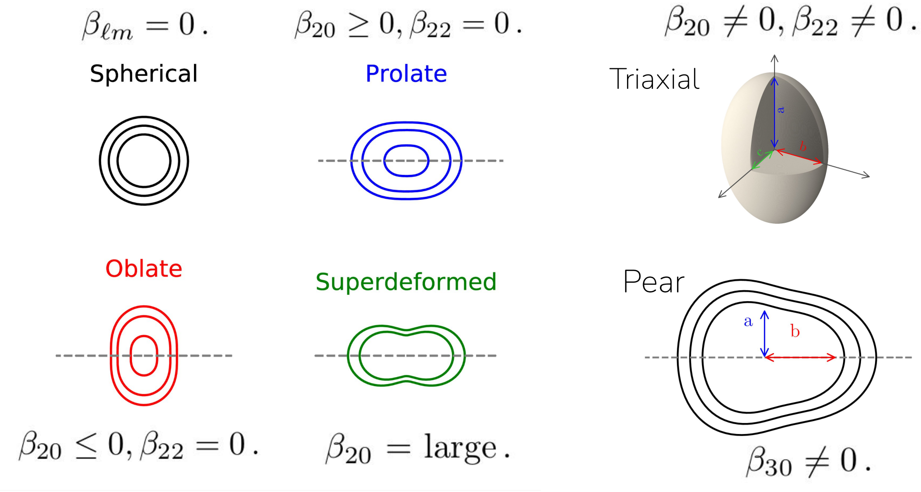

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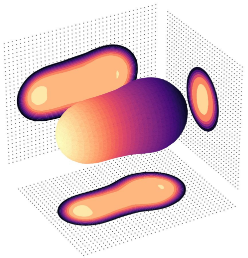

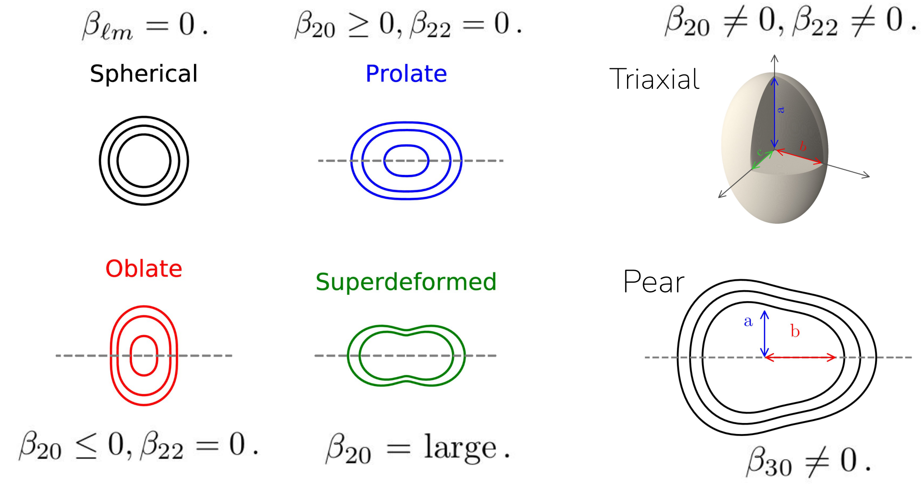

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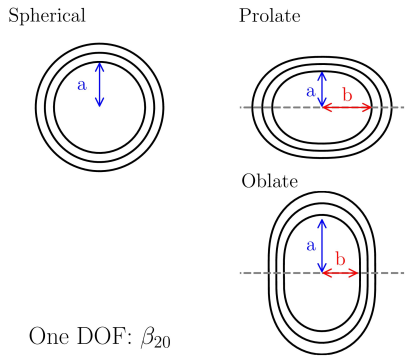
Lowest energy shape ⇔ nuclear ground state

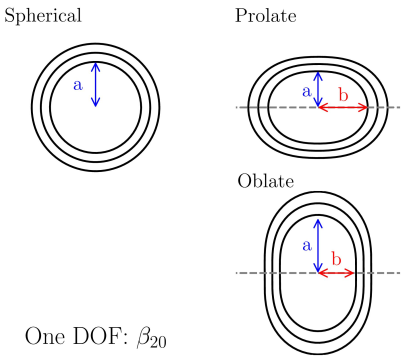
- Nuclear density is an output of DFT
- β_{lm} are **<u>predictions</u>** of DFT calculations
- and can be compared to experiment

Nuclear deformation



One DOF: β_{20}

Nuclear deformation



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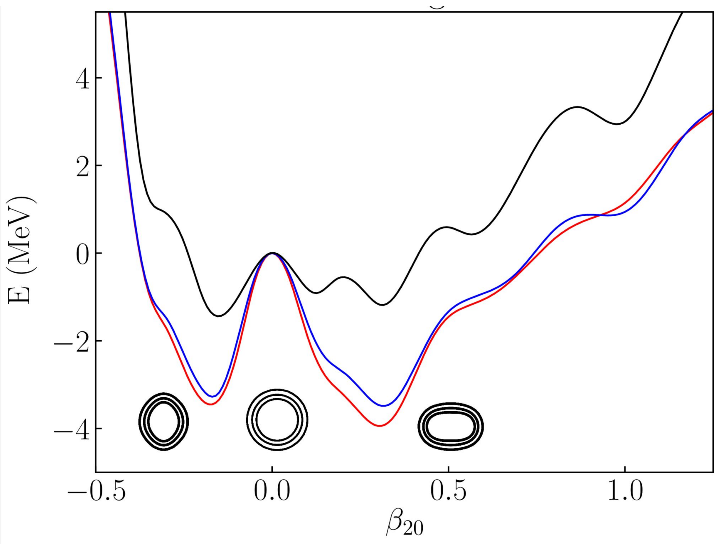

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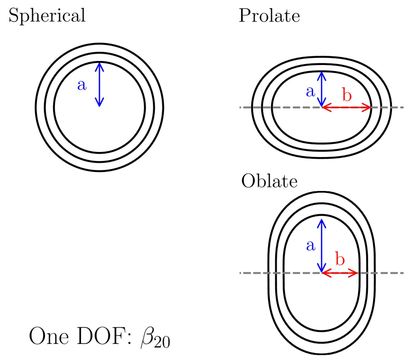

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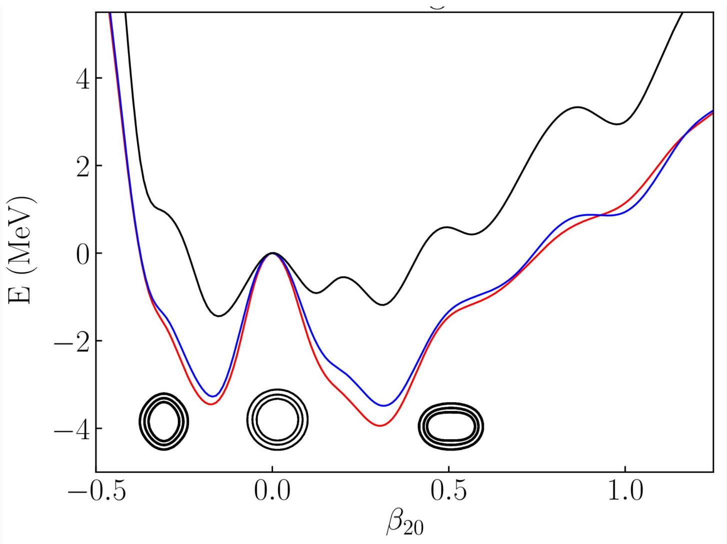
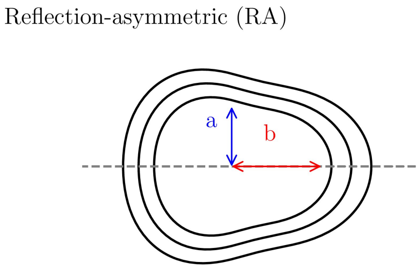
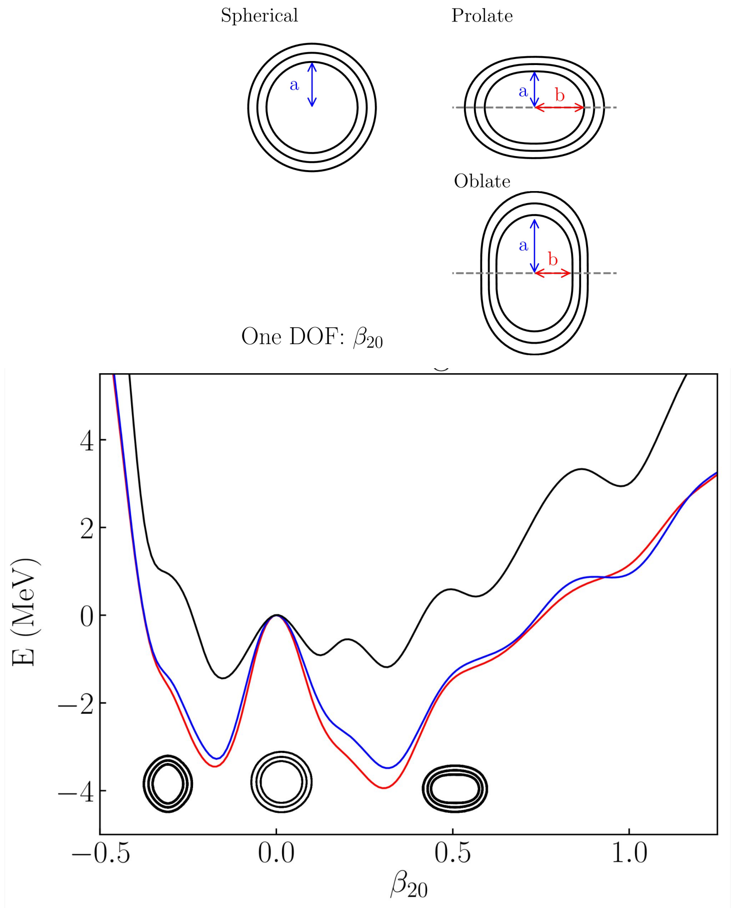
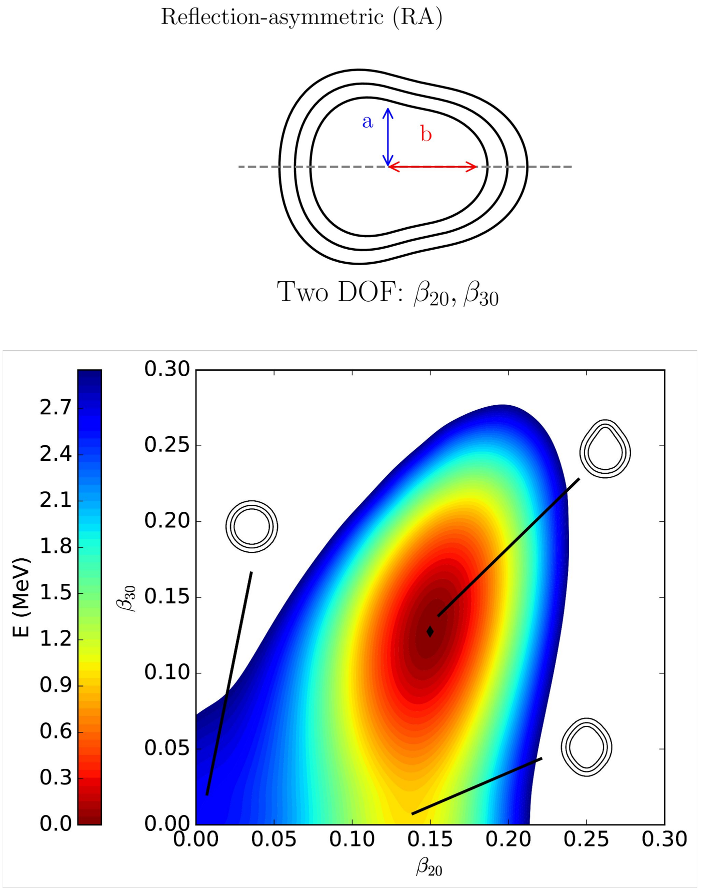




Two DOF: β_{20}, β_{30}

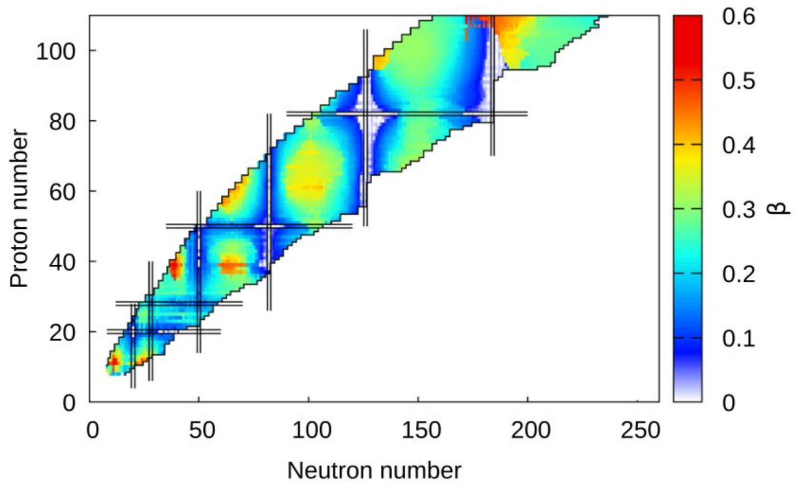
Nuclear deformation





(Quadrupole) deformation is everywhere!

BSkG1: G. Scamps et al., EPJA 57, 333 (2021).



Almost all nuclei have <u>some</u> deformation

- mostly quadrupole (l=2)
- some hexadecupole (l=4)
- a few octupole (l=3)

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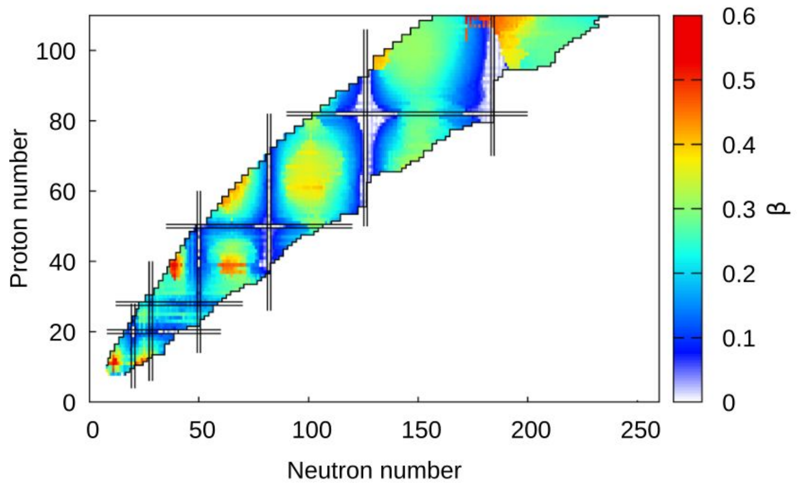

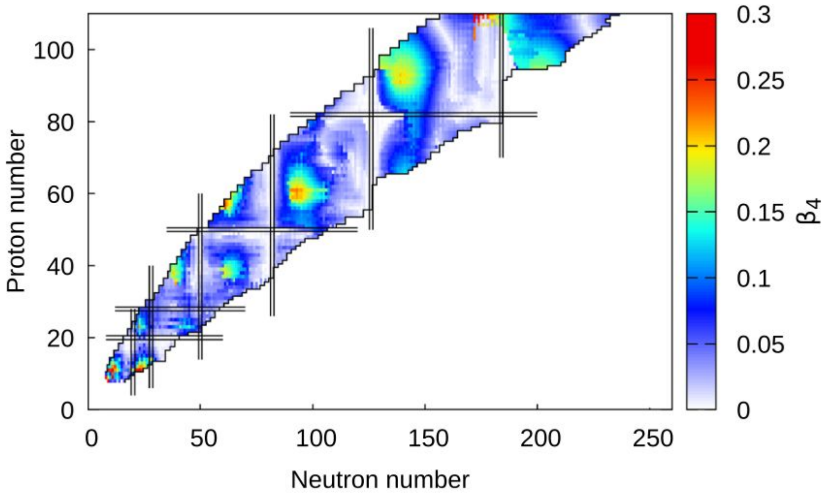

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The exception are (semi-)magic nuclei

N/Z = 8,20,28,50,82,126,....

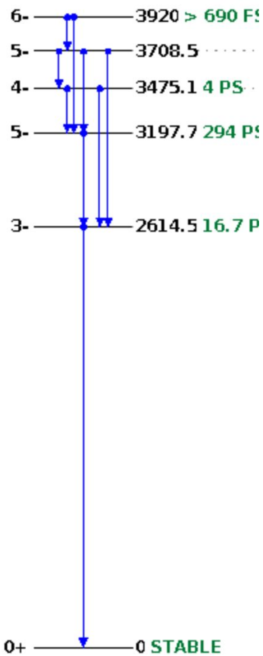
which remain perfectly spherical in DFT.

Phenomenology of nuclear deformation

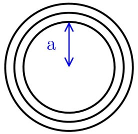
Data from NNDC, www.nndc.bnl.gov.

- Spectra can be very sparse at low energy
  - levels ~ excitations of individual nucleons
  - typical energy scale ~ 1-2 MeV

^{208}Pb



Spherical



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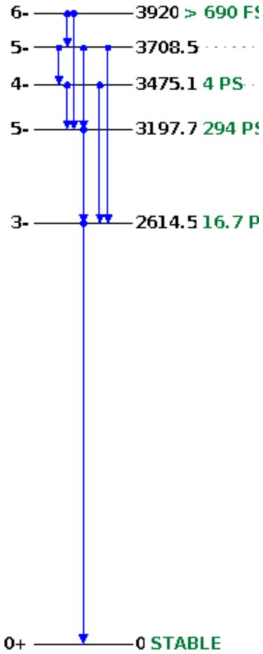
  - typical energy scale ~ 50-100 keV
  - resemble rotational spectra

^{208}Pb



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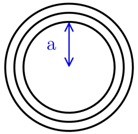
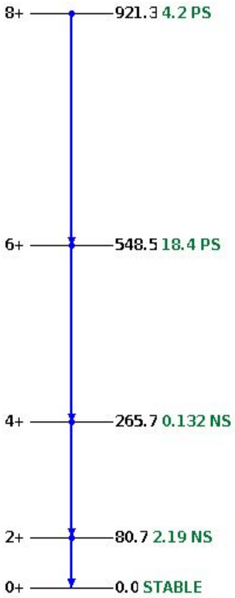
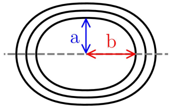


^{162}Dy



Prolate



Phenomenology of nuclear deformation

Wouter Ryssens (ULB)

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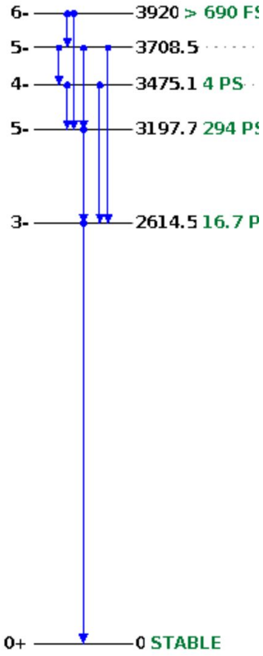
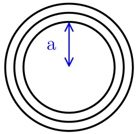


Spherical



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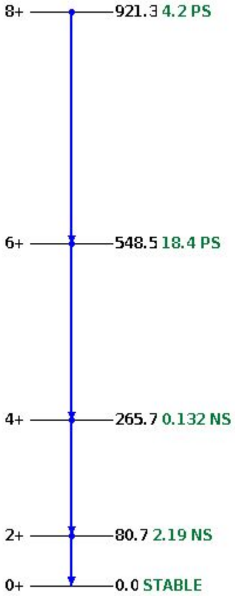

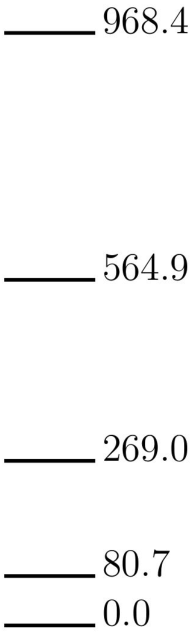

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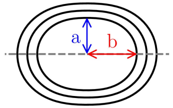

$$\hat{H}_{\rm rot} = \frac{1}{2\mathcal{I}}\left(\hat{J}_x^2 + \hat{J}_y^2\right) .$$

Phenomenology of nuclear deformation

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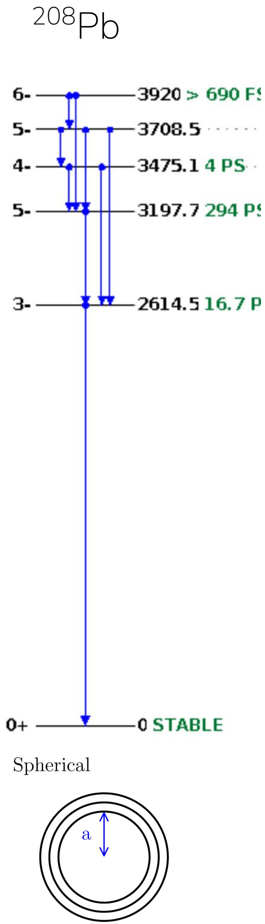
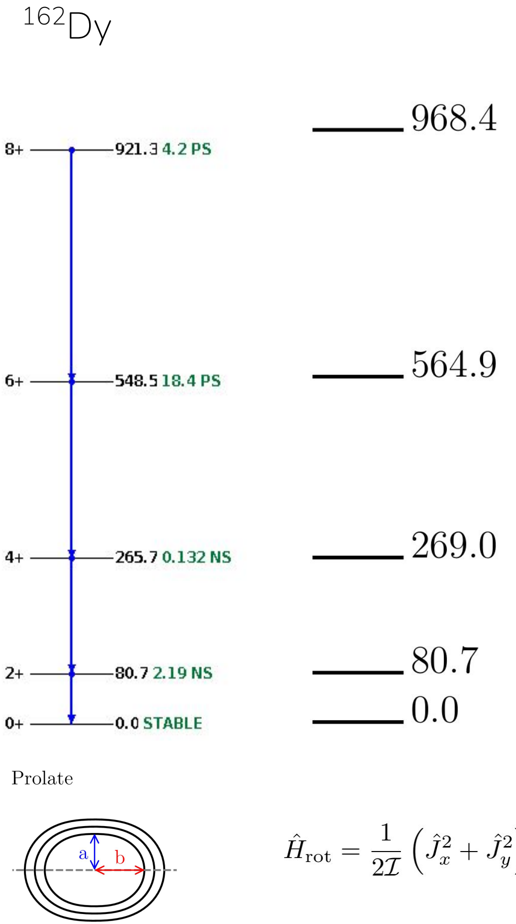
- Often, **very regular** bands appear
  - levels ~ excitations of many nucleons
  - typical energy scale ~ 50-100 keV
  - resemble rotational spectra
- Q_{lm} impact transition rates
- Also observed:
  - Asymmetric rotation
    L. P. Gaffney et al., Nature **497**, 199 (2013).
  - Triaxial rotation
    A. D. Ayangeakaa et al., PRL **123**, 102501 (2019).
  - Different kinds of vibration





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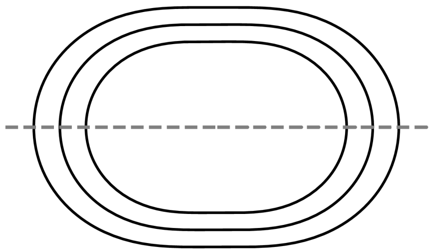
Symmetry restoration

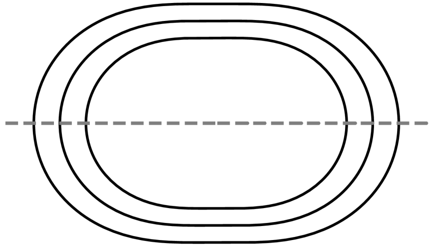
Wouter Ryssens (ULB)

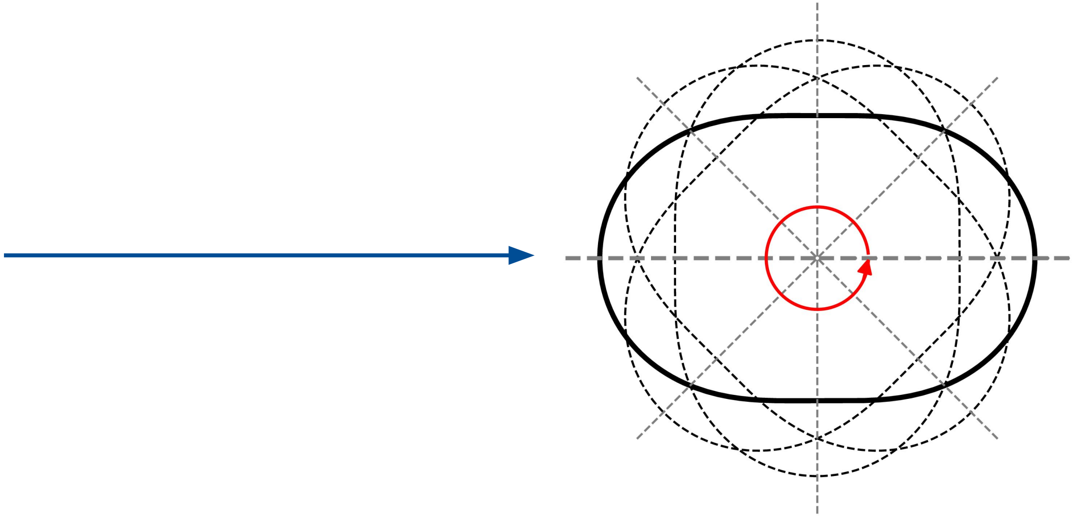


A significant problem with mean-field theory

- symmetries of nature broken
  - rotational symmetry
  - reflection symmetry
- No quantum numbers in the model!

Symmetry restoration





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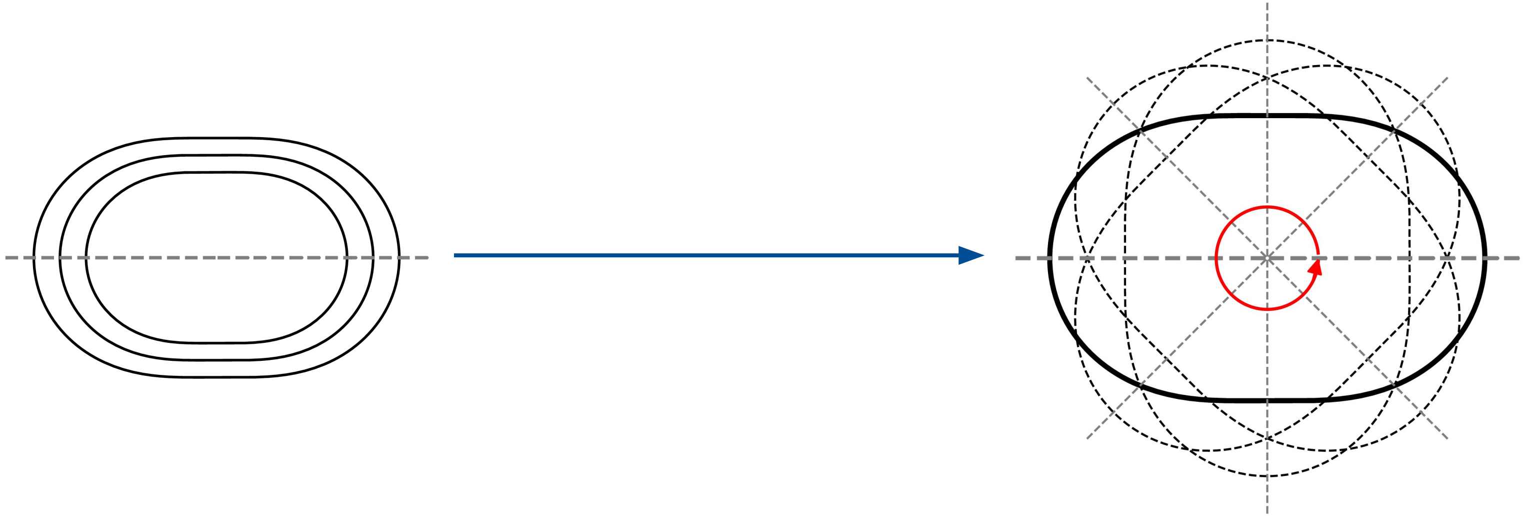
Explicit symmetry restoration

- superpositions of mean-field wavefunctions
- enlarging of the variational space

Symmetry restoration



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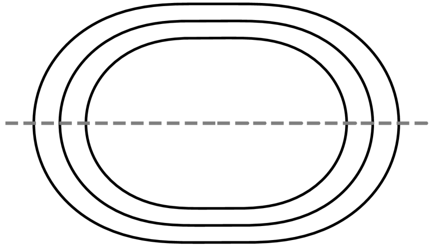

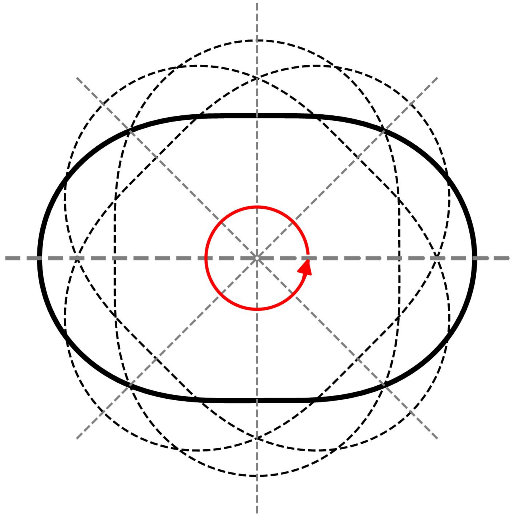

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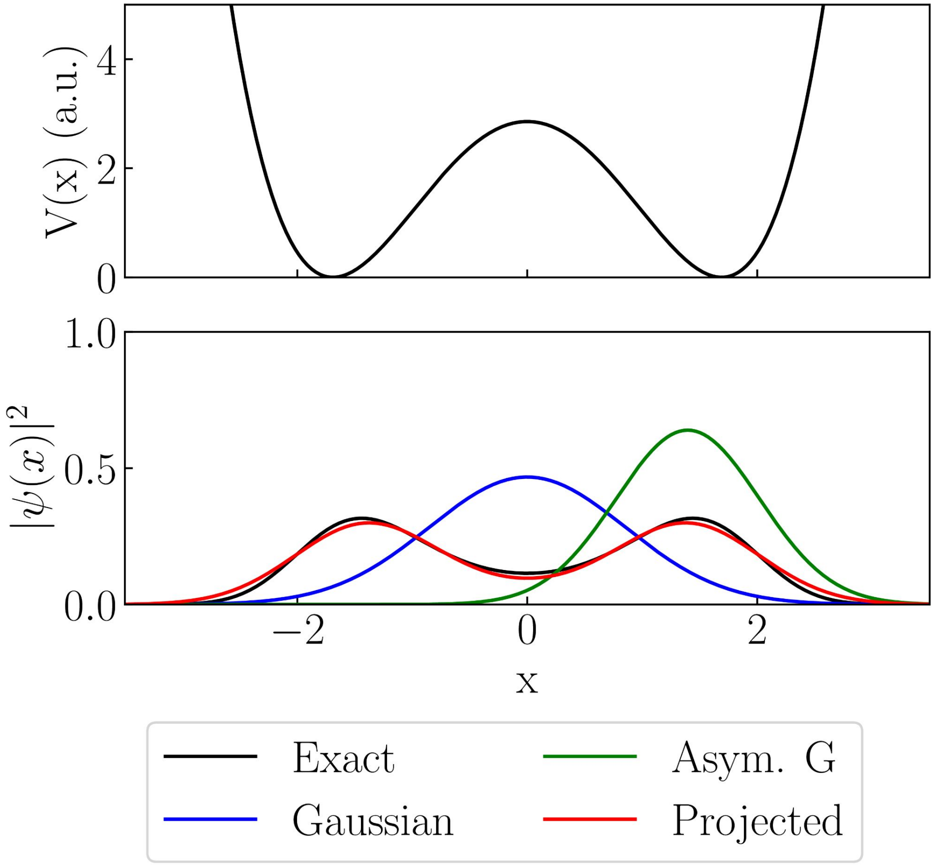
Explicit symmetry restoration

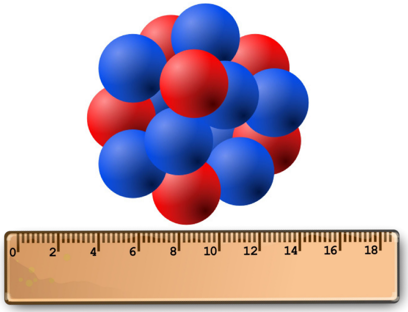
- superpositions of mean-field wavefunctions
- enlarging of the variational space
- … which are symmetric again!
- … and have quantum numbers!
- calculations become **much** harder.

A simple example



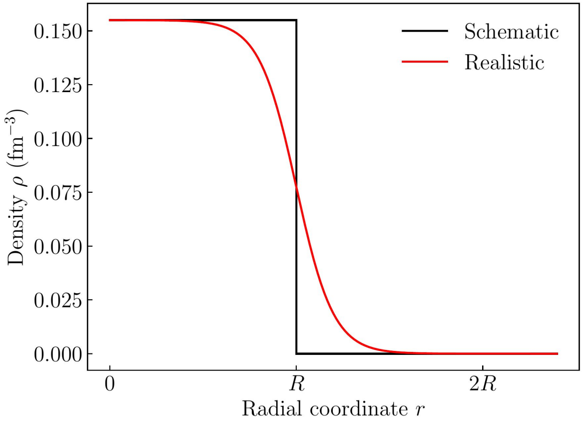
	Energy	$\langle X^2 \rangle$
Exact	1.625	1.98
Gaussian	2.152	0.727
Asym. G.	1.844	2.331
Projected	1.735	2.190

Nuclear charge radii



The size of the nucleus

- Assume the nucleus ~ liquid drop
  a. constant density for r < R
  b. vanishing density for r > R



$$A = \int d^3 r \, \rho(\mathbf{r}) = \frac{4\pi}{3} \rho_0 R^3 \, .$$

$$\downarrow$$

$$R \sim R_0 A^{1/3} \, ,$$

$$R_0 = 1.26 \text{ fm} \, .$$

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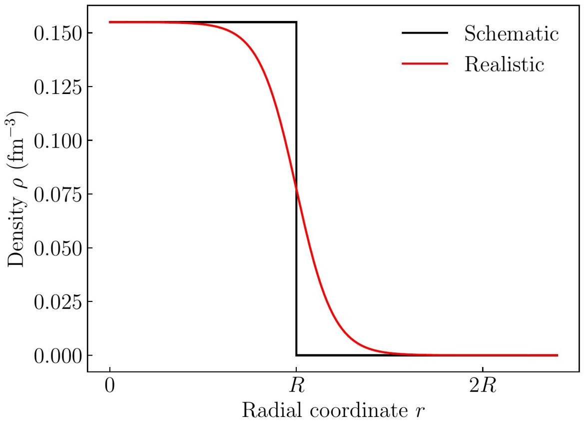
Of course, this picture is too simple.



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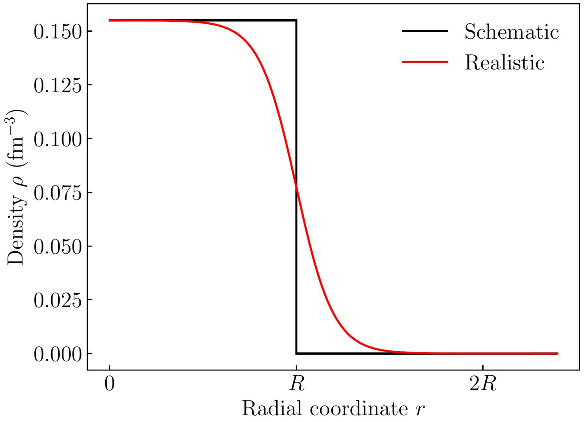
  a. laser spectroscopy
  b. x-rays from muonic atoms
  c. electron scattering
  d. hadronic scattering



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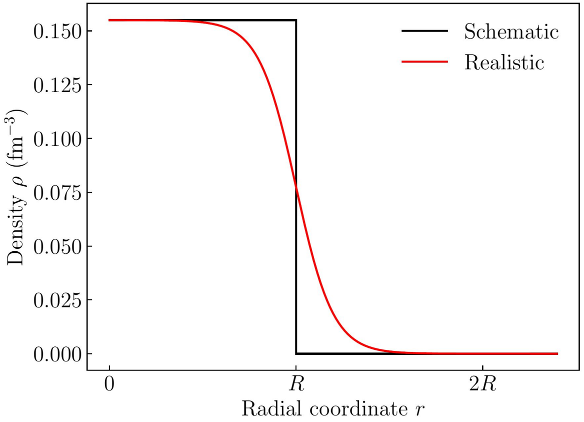
- (a-b-c) probe the **rms** radii of the **charge** densities



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$$r_{\mathrm{c,rms}} = \sqrt{\frac{\int d^3r\, r^2 \rho_c(\mathbf{r})}{\int d^3r\, \rho_c(\mathbf{r})}} \sim R_0 A^{1/3} .$$

$$\delta \langle r_{\mathrm{c}}^2 \rangle^{N,N_0}(N,Z) = r^2_{\mathrm{c,rms}}(N,Z) - r^2_{\mathrm{c,rms}}(N_0,Z) .$$

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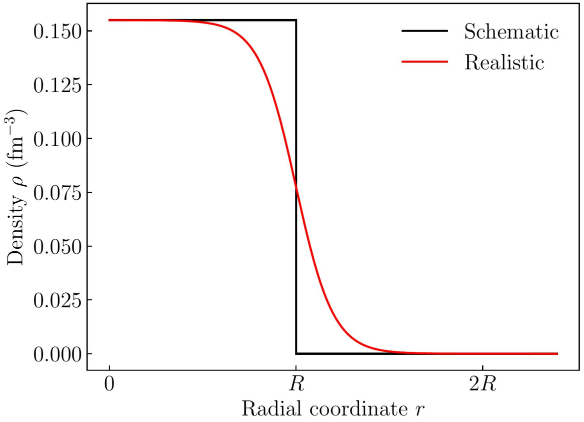
- (a-b-c) probe the **rms** radii of the **charge** densities

- (a) is only sensitive to the **isotopic shift,** differences of rms charge radii in isotopic chains



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Extracting charge radii from EDF calculations

BSkG1: G. Scamps et al., EPJA 57, 333 (2021).

$$r_{\mathrm{c,rms}}^{\mathrm{DFT}} = \sqrt{\frac{\int d^3r\, r^2 \rho_c^{\mathrm{DFT}}(\mathbf{r})}{\int d^3r\, \rho_c^{\mathrm{DFT}}(\mathbf{r})}}\,.$$

- EDF calculations provide densities
- …. so it is easy to calculate radii!

Extracting charge radii from EDF calculations

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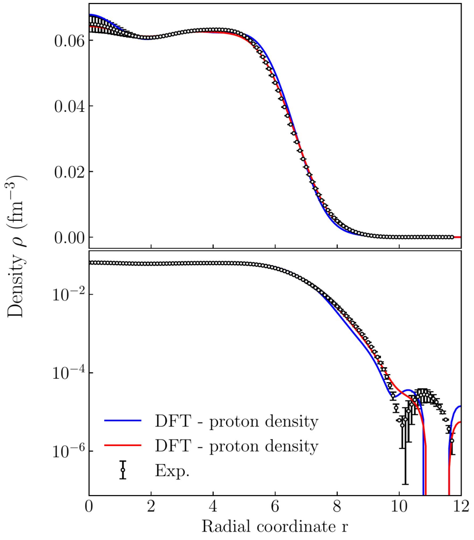
$$r_{\mathrm{c,rms}}^{\mathrm{DFT}} = \sqrt{\frac{\int d^3r\, r^2 \rho_p^{\mathrm{DFT}}(\mathbf{r})}{\int d^3r\, \rho_p^{\mathrm{DFT}}(\mathbf{r})} + r_p^2}\,,$$

$$r_p^2 = 0.74\mathrm{fm}^2\,.$$

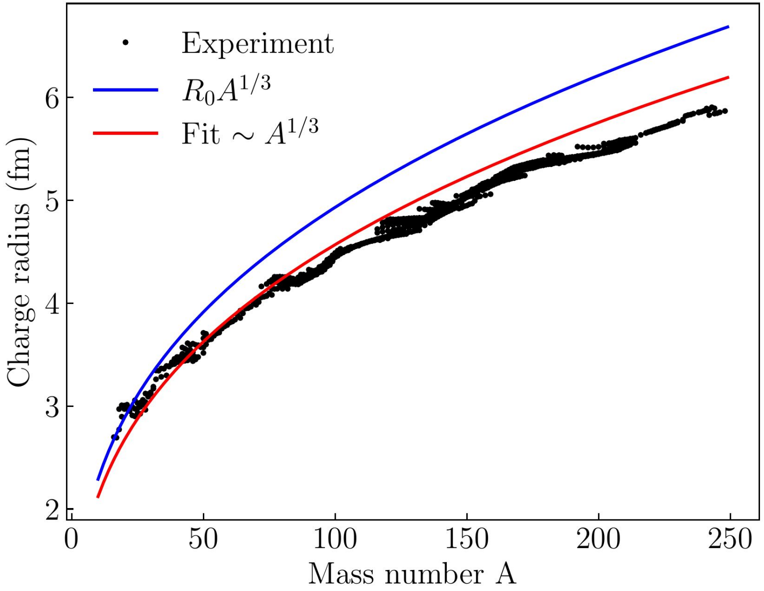


- EDF calculations provide densities
- .... so it is easy to calculate radii!

- Corrections can be made for
  - finite size of the proton
  - finite size of the neutron
  - spin-orbit currents
- Only the first is important

Global trends

I. Angeli and K. P. Marinova, *At. Data Nuc. Data Tables*, *99* (2015).
G. Scamps et al., EPJA 57, 333 (2021).



- Experiment confirms the $A^{1/3}$ picture.
- ... but fitting does a better job
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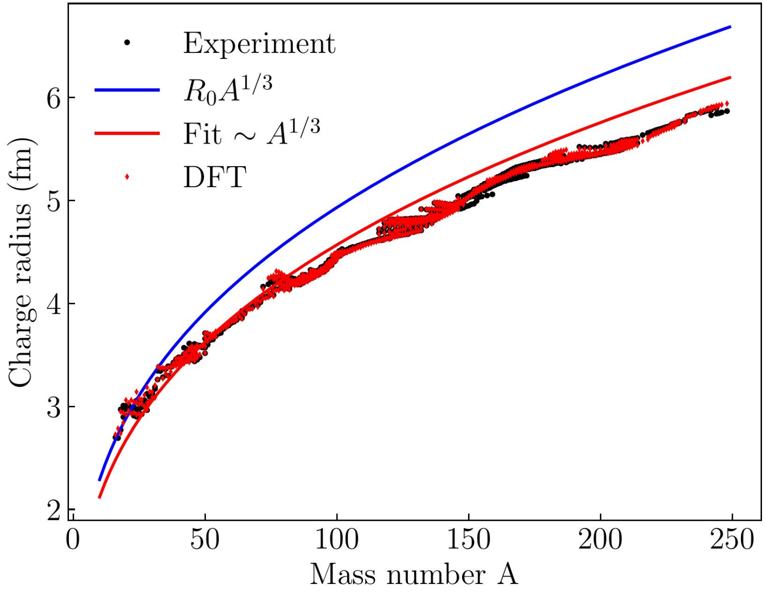

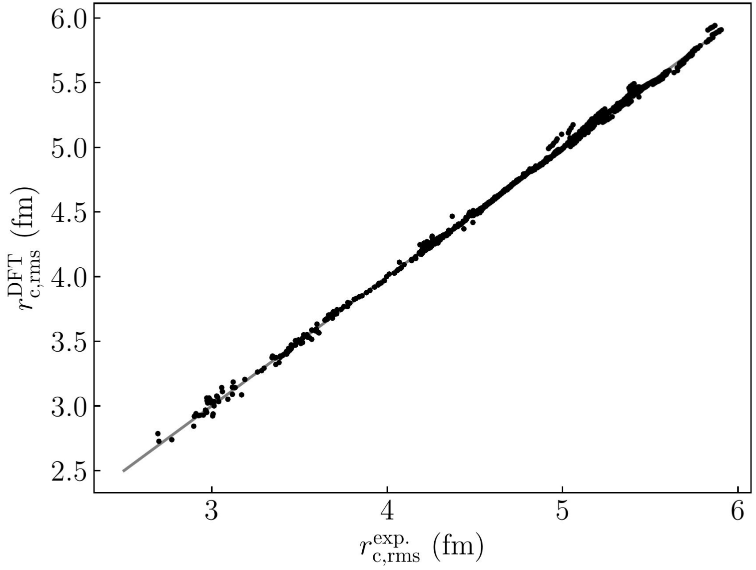

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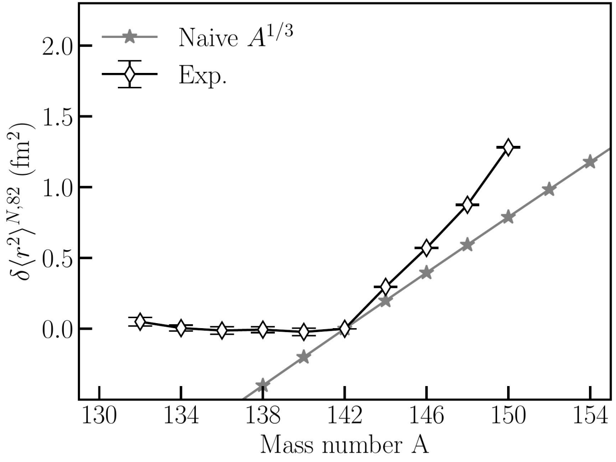
DFT calculations match global trend!

Detailed evolution

The details are much more intricate

1. strange variations with neutron number

1. Nd isotopes



Detailed evolution

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1. strange variations with neutron number
2. odd-even staggering

2. Ca isotopes

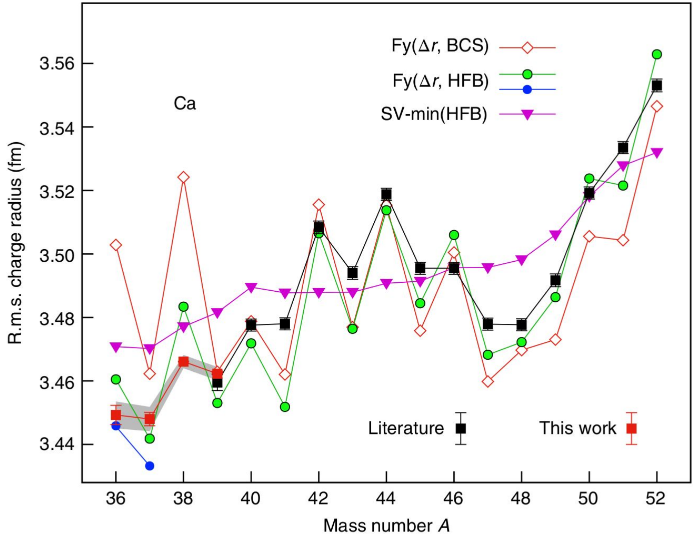

Fig. from A. J. Miller et al., Nat. Phys. 15, 432 (2019).

Detailed evolution

The details are much more intricate

1. strange variations with neutron number
2. odd-even staggering
3. extreme odd-even staggering

3. Hg isotopes

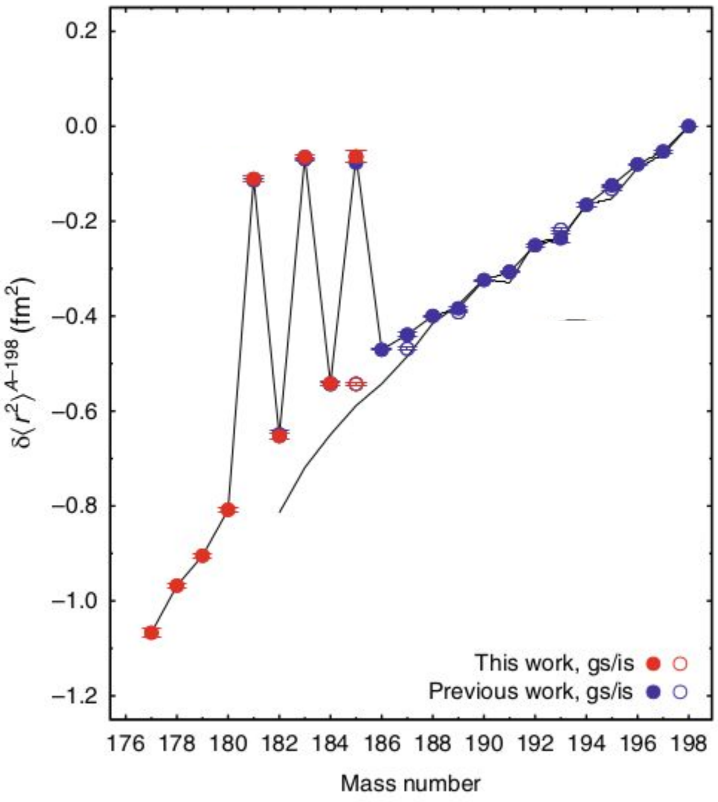

Fig. adapted from B. Marsh et al, Nat. Phys. **14**, 1163-1167 (2018)

Detailed evolution

The details are much more intricate

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3. extreme odd-even staggering
4. kinks for (semi-)magic nuclei

4. Sn and Pb isotopes

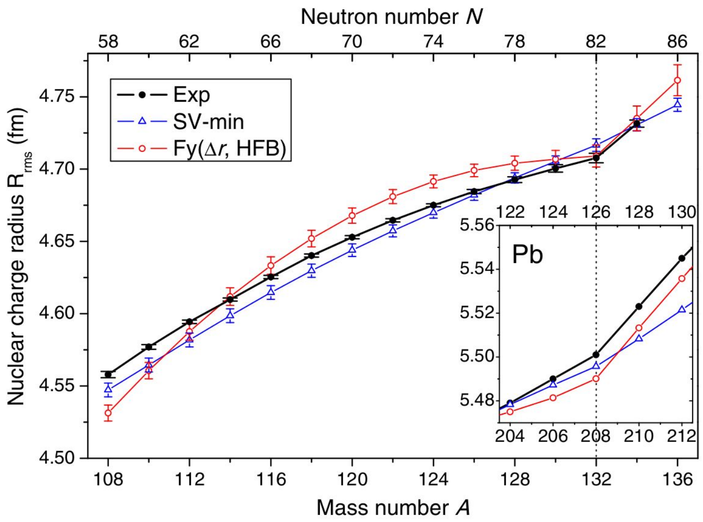


Fig. from C. Gorges et al., PRL 122, 192502 (2019).

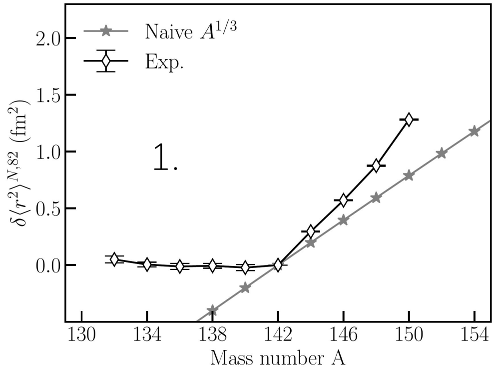
Detailed evolution

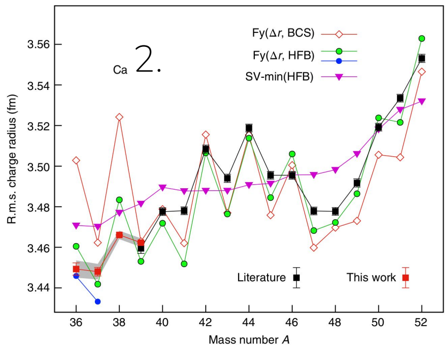
The details are much more intricate

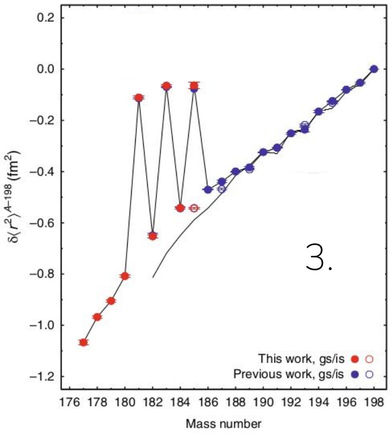
1. strange variations with neutron number
2. odd-even staggering
3. extreme odd-even staggering
4. kinks for (semi-)magic nuclei

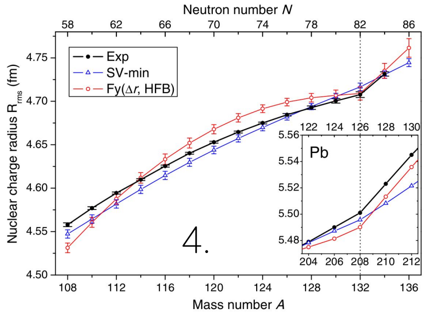
1.,2.,3. are related to deformation
4. is maybe related to deformation

1. is well described by DFT
2. can be described by **some** EDFs
3. can be qualitatively understood with DFT
4. is an open challenge for theory in general









Including deformation in our naive theory

Assume the nucleus ~ **deformed** liquid drop

- constant density for r < R(θ,ϕ)
- vanishing density for r > R(θ,ϕ)

$$R(\theta, \phi) = R_0 \left[1 + \sum_{\ell=2}^{\ell_{\max}} \beta_{\ell 0} Y_{\ell 0}(\theta, \phi) \right] .$$

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- deformation changes the rms radius
- but in a non-trivial way
- all (l,m)-moments contribute in theory

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quadrupole

mixing terms

$$r^2_{\mathrm{c,rms}} \sim R_0^2 A^{2/3}\left[1 + C_{22}\beta_{20}^2 + C_{44}\beta_{40}^2 + C_{24}\beta_{20}\beta_{40} + \ldots\right] .$$

spherical drop

hexadecapole

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- quadrupole moments dominate in practice
- C_{22} > 0, charge radius enhanced!

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Caveats:

- radius not sensitive to signs of β_{20}
- ansatz for R(θ,ϕ) not necessarily realistic

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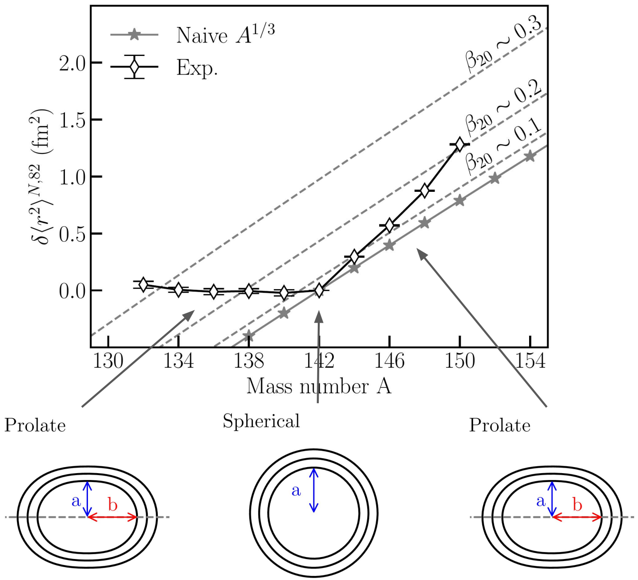
$$r^2_{\mathrm{c,rms}} \sim R_0^2 A^{2/3} \Big[\underbrace{1}_{\text{spherical drop}} + \underbrace{C_{22}\beta_{20}^2}_{\text{quadrupole}} + \underbrace{C_{44}\beta_{40}^2}_{\text{hexadecapole}} + \underbrace{C_{24}\beta_{20}\beta_{40}}_{\text{mixing terms}} + \dots \Big] .$$

Charge radii, deformation and DFT

W. R. and M. Bender, PRC 104, 044308 (2021).



- Deformation can explain the trend.

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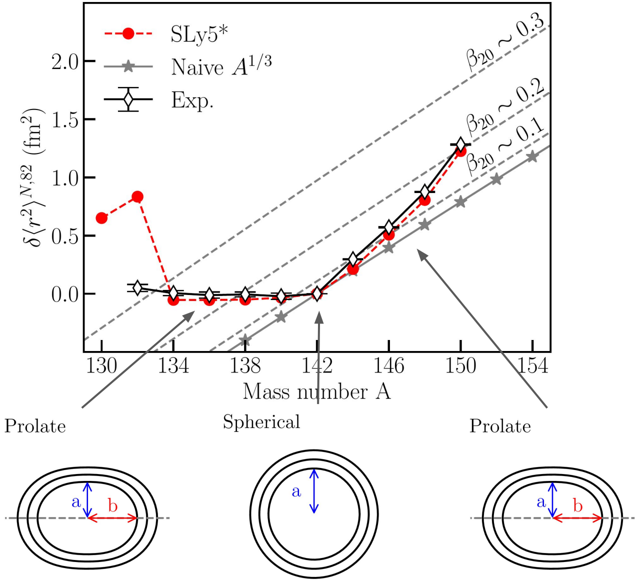

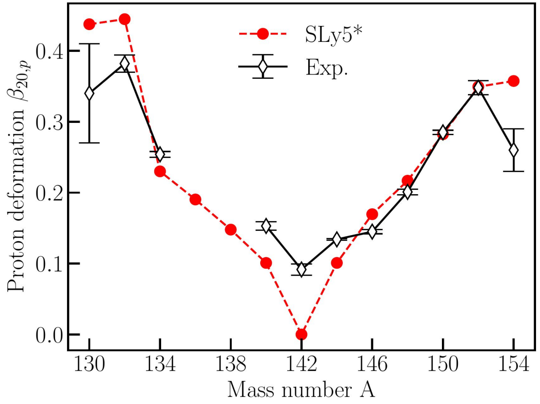

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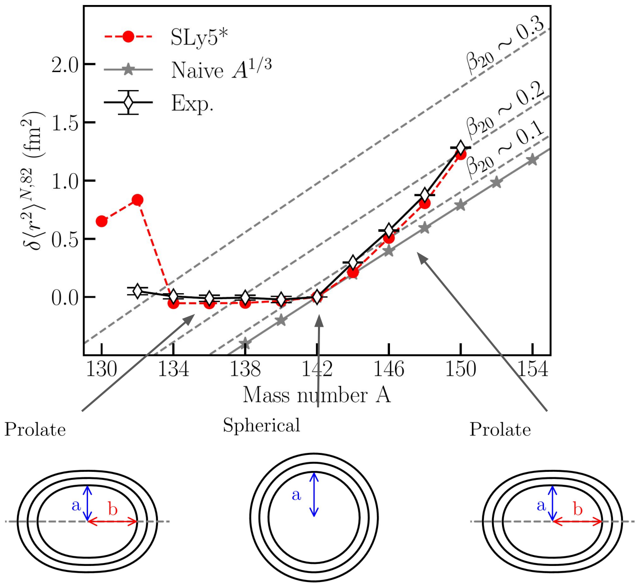

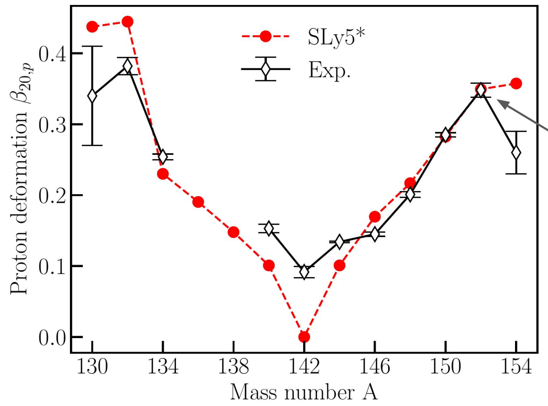

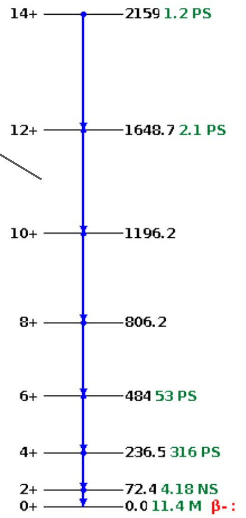

- Deformation can explain the trend.
- .... and DFT can match it

- DFTs mechanism is deformation
- which also matches spectroscopic data!

Other multipole moments

$$r^2_{\mathrm{c,rms}} \sim R_0^2 A^{2/3} \left[1 + \sum_{\ell_1 m_1} \sum_{\ell_2 m_2} C_{\ell_1 m_1 \ell_2 m_2} \beta_{\ell_1 m_1} \beta_{\ell_2 m_2} \right] .$$

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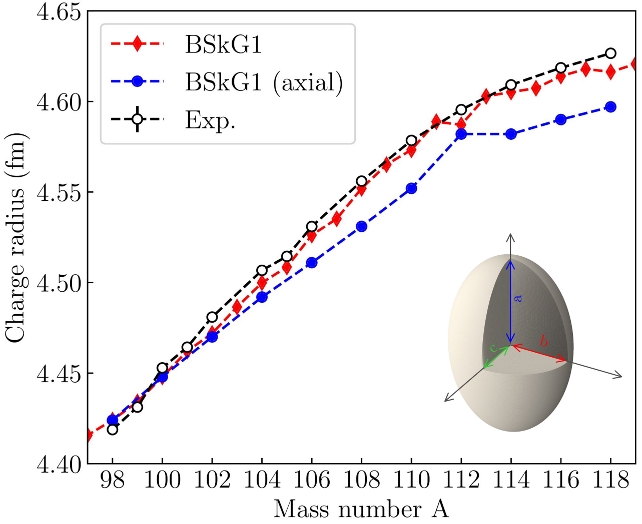

S. Geldhof et al., PRL 128, 152501 (2022).

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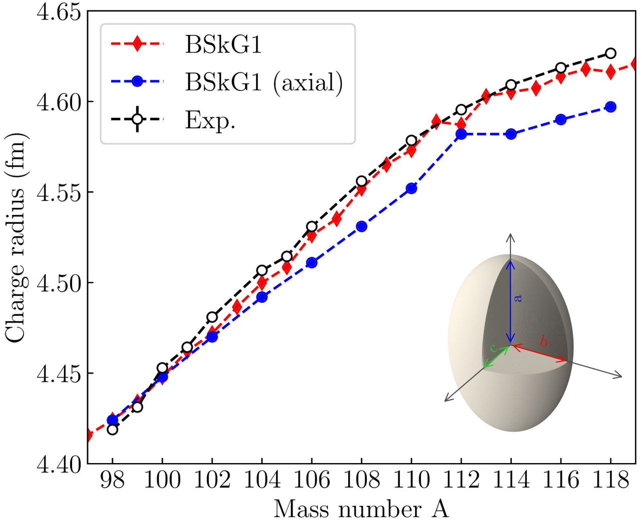

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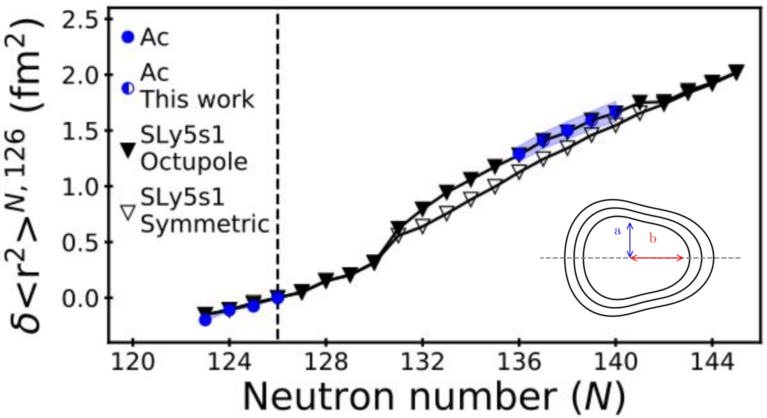
Ac isotopes



E. Verstraelen et al. PRC **100**, 044321 (2019).

EV8: a practical introduction

Computer Physics Communications
Volume 171, Issue 1, 1 September 2005, Pages 49-62

Solution of the Skyrme HF + BCS equation on a 3D mesh ☆

P. Bonche [a], H. Flocard [b], P.H. Heenen [c]

Computer Physics Communications
Volume 187, February 2015, Pages 175-194

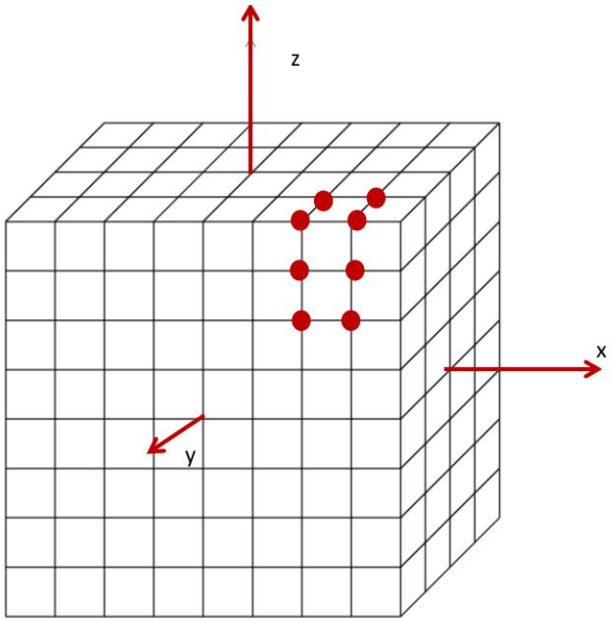
Solution of the Skyrme–HF+BCS equation on a 3D mesh, II: A new version of the Ev8 code ☆

W. Ryssens [a], V. Hellemans [a], M. Bender [b, c], P.-H. Heenen [a]

EV8: a Skyrme HF+BCS code

EV8 solves the mean-field equations

- for nuclei with **N = even and Z = even**
- for EDFs of the Skyrme type
- using HF+BCS many-body wavefunctions



V1: P. Bonche et al., CPC 171, 49 (2005).
V2: W. R. et al., CPC 187, 175 (2015).

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Wouter Ryssens (ULB)

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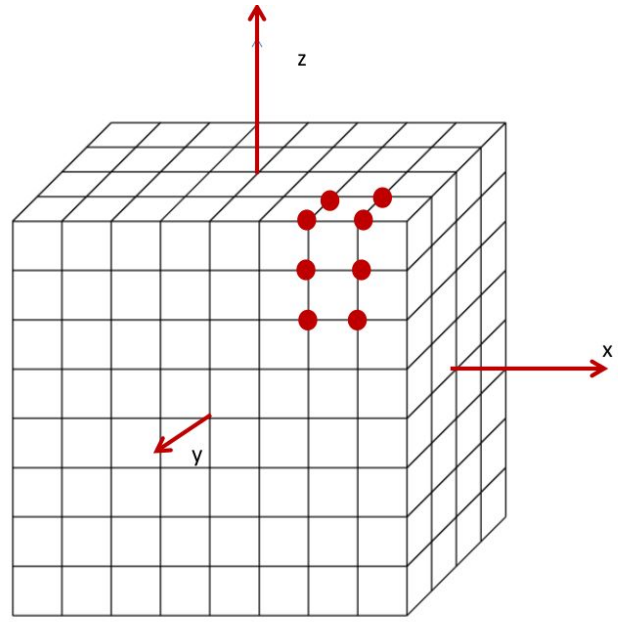
- built from single-particle wavefunctions represented in coordinate-space
  - mesh points nx, ny, nz ~ 16
  - mesh spacing dx ~ 0.8 fm



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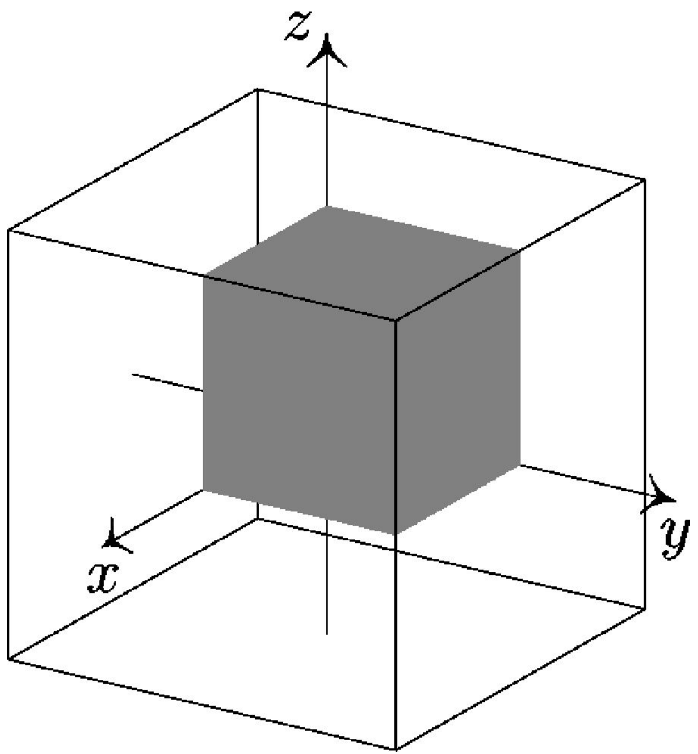
- but restricts the mesh to x > 0, y > 0, z > 0.
- for nuclear shapes with 3 plane symmetries
  - allows for β_{20}, β_{22}, β_{40}, β_{42}, ...
  - but not for β_{30}, β_{32}, β_{41}, β_{43}, ...



V1: P. Bonche et al., CPC 171, 49 (2005).
V2: W. R. et al., CPC 187, 175 (2015).

EV8: a Skyrme HF+BCS code

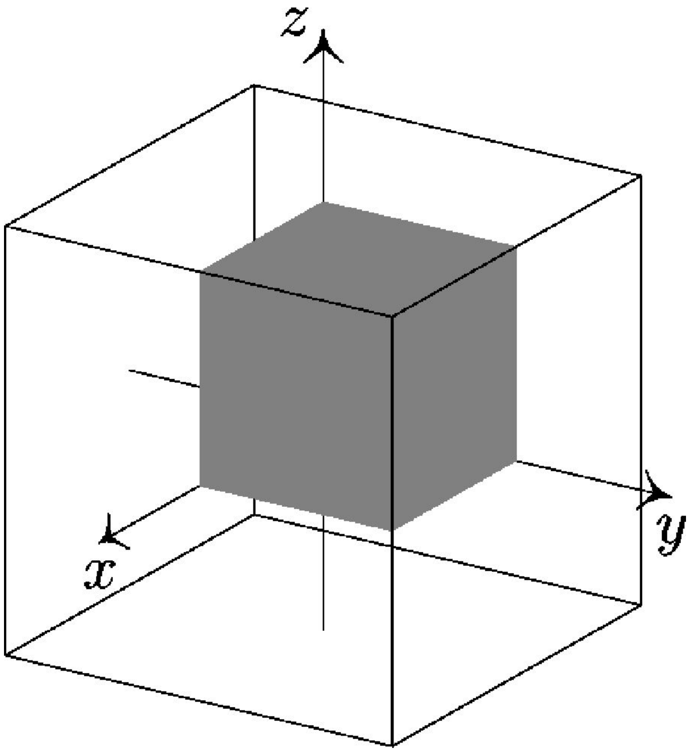
EV8 solves the mean-field equations

- for nuclei with **N = even and Z = even**
- for EDFs of the Skyrme type
- using HF+BCS many-body wavefunctions

- built from single-particle wavefunctions represented in coordinate-space
  - mesh points nx, ny, nz ~ 16
  - mesh spacing dx ~ 0.8 fm

- but restricts the mesh to $x > 0$, $y > 0$, $z > 0$.
- for nuclear shapes with 3 plane symmetries
  - allows for β_{20}, β_{22}, β_{40}, β_{42}, ...
  - but not for β_{30}, β_{32}, β_{41}, β_{43}, ...

BUT: EV8 is no longer under active development.



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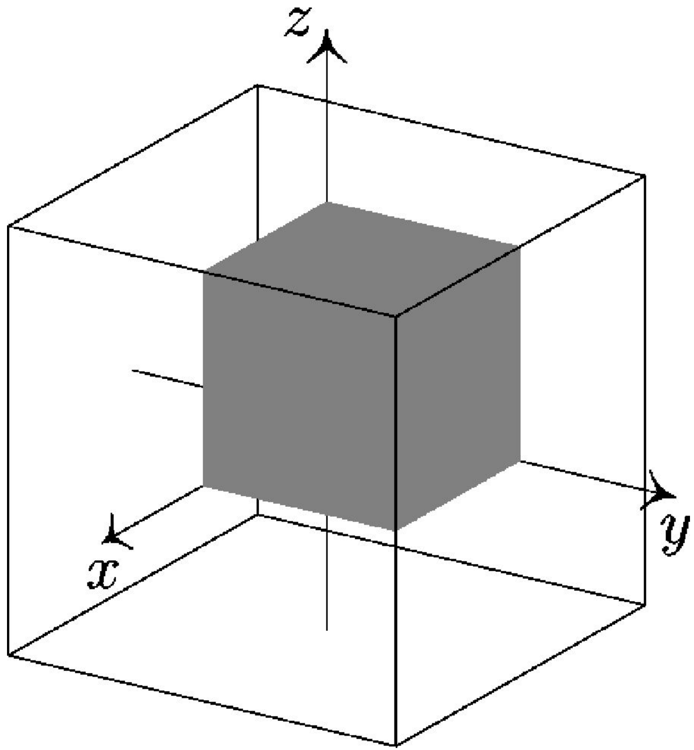
BUT: EV8 is no longer under active development.

Other codes with different EDFs/numerics/...

- HFBTHO: P. Marevic et al., CPC **276**, 108367 (2022).
- Sky3D: J. A. Maruhn et al., CPC **185**, 2195 (2014).
- HFODD: J. Dobaczewski et al., J. Phys. G **48**, 102001 (2021).
- ....

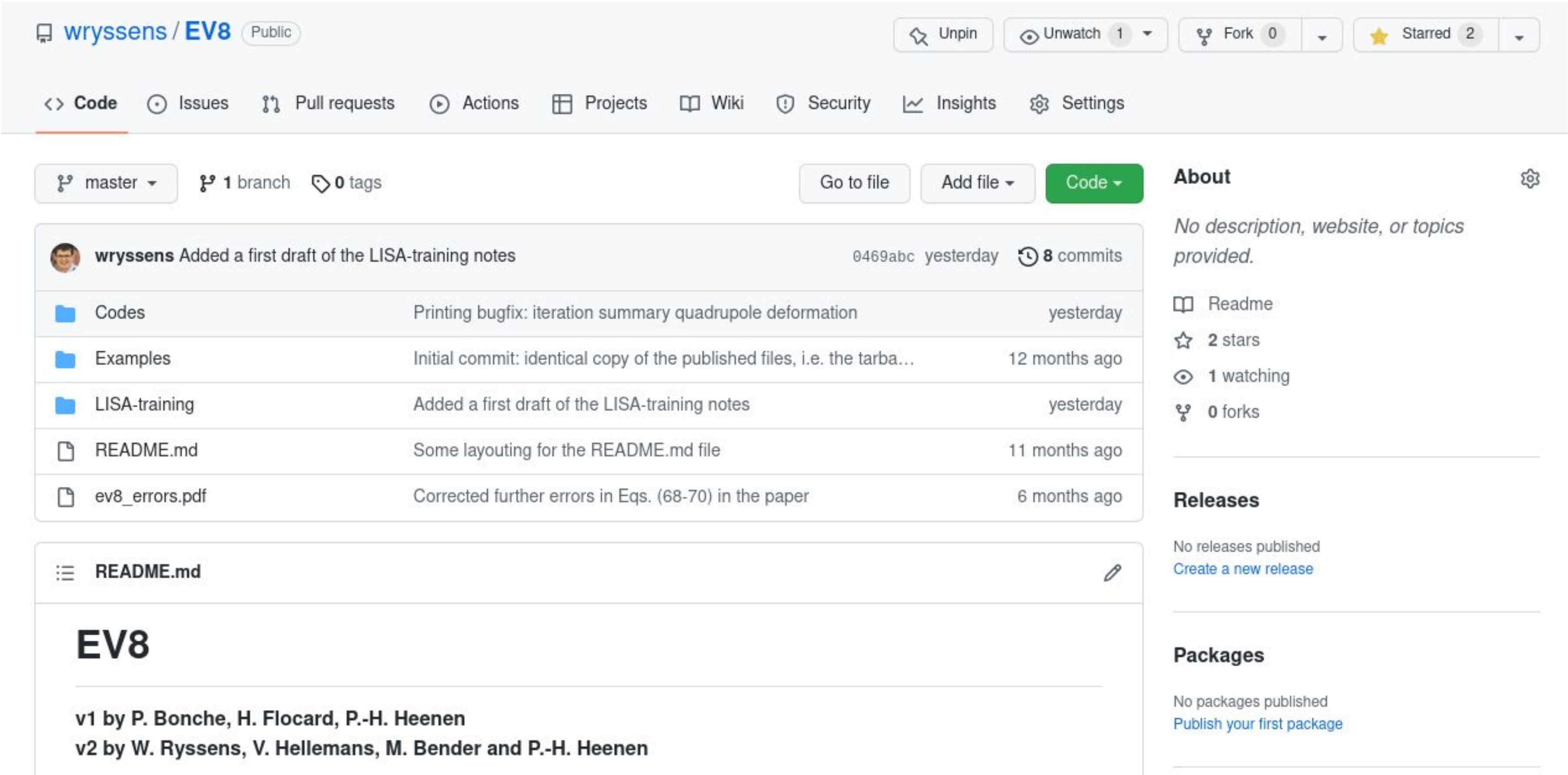


V1: P. Bonche et al., CPC 171, 49 (2005).

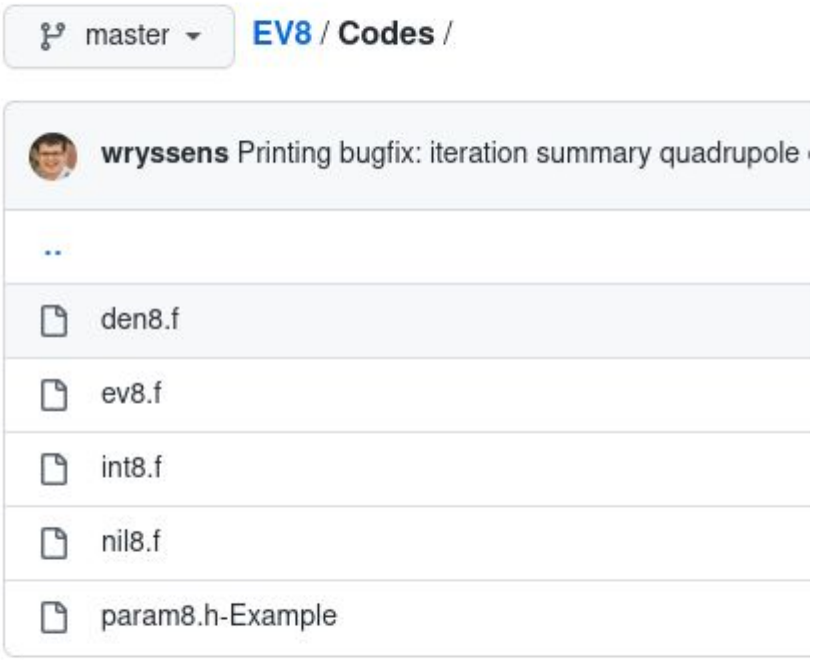
V2: W. R. et al., CPC 187, 175 (2015).

Wouter Ryssens (ULB)

www.github.com/wryssens/EV8



Contents


master
EV8 / Codes /
wryssens Printing bugfix: iteration summary quadrupole
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den8.f
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master **EV8** / **LISA-training** /

wryssens Update of LISA-training tasks

..

- EV8.example.data
- compile.sh
- nil8.oblate.data
- nil8.prolate.data
- tasks.pdf

Compilation: compile.sh

```
echo '-----------------------------------------------'
echo ' Creating the compilation parameters.'

cat <<eof  >param8.h
      parameter (mx=10,my=10,mz=14,mc=10,mv=mx*my*mz,mq=4*mv,mw=220)
      parameter (meven=5,modd=5)
eof
echo ' Done!'
echo '-----------------------------------------------'
echo 'Compiling nil8!'
echo '-----------------------------------------------'
gfortran -O3 -o nil8.exe nil8.f &> nil8.diag
echo '-----------------------------------------------'
echo 'Compiling ev8!'
echo '-----------------------------------------------'
gfortran -O3 -o ev8.exe ev8.f&> ev8.diag
echo 'Done!'
```

mesh points

FORTRAN compiler to use

nil8.exe: creates an initial guess for the calculations
ev8.exe: performs the actual DFT calculations

Typical workflow

```
# Run nil8.exe for a prepared set of input data: "nil8.data"
./nil8.exe < nil8.data > nil8.out
# This has created
#   (i)    fort.13: the initial guess for the single-particle wavefunctions
#   (ii)   nil8.out: some diagnostic information

# Move the nil8 output wavefunction to an EV8 input wavefunction
mv fort.13 fort.12

# Run nil8.exe for a prepared set of input data: "ev8.data"
./ev8.exe < ev8.data > ev8.out
# This has created
# (i)  fort.13 : the final state of the single-particle wavefunctions
# (ii) ev8.out : output of the calculations!
```

Proper preparation of initial guess is important:

- Calculations initialized with spherical symmetry will **remain spherical.**
- Calculations initialized with a prolate shape will (generally) **remain prolate.**
- Calculations initialized with a oblate shape will (generally) **remain prolate.**

EV8: input data

Maximum iteration number

Neutron and proton number

Parameterization name

Pairing information

```
 Title
 0002 0002 0002 0002
 0.03000000E+00
 0500 0025 0000
 0100 0000
 0166 0092
Sly4
 0004 0001 0000
 1.25000000E+03 0.05000000E+02 0.00000000E+00 1.00000000E+00
 1.25000000E+03 0.05000000E+02 0.00000000E+00
 5.00000000E-08 3.00000000E-03 0.01000000E+00 1.00000000E-05
 0001 0000 0000
 0.10000000E+00 0.02000000E+00 4.00000000E+00
 0.00000000E+00 0.00000000E+00
 0.00000000E+00 1.00000000E+00
 0.00000000E+03 0.00000000E+00
```

Spacing and formatting is IMPORTANT!

Reading the EV8 output: the top

```
 ______________________________________________________
|                                                      |
|  Program ev8      CPC version 2                      |
|  August 2014                                         |
|______________________________________________________|


compilation parameters:
mx=   10 my=   10 mz=   14
Maximum number of extra coulomb points:    10
Total number of wavefunctions:   220


____________________________________________________________________________________
tape information (version 5)
```

Reading the EV8 output: the run information

mesh properties

iteration count

neutron and proton number

parameterization name

```
run information

Title

nx=   10        ny=   10        nz=   14
dx=   1.000 Fm
dt=   0.030 10-22s,  number of iterations =  500
Convergence output:               Normal
number of extra points for coulomb
nx=    2        ny=    2        nz=    2
Order of the laplacian discretisation for Coulomb:     2


nxmu   =    25
ndiag  =     0
nprint =   100

number of wave-functions n=  120  p=  100
nucleus n=  144  z =   92  a =  236

Skyrme force:                  Sly4
 t0 = -2488.913000 x0 =     0.834000
 t1 =   486.818000 x1 =    -0.344000
 t2 =  -546.395000 x2 =    -1.000000
 t3a= 13777.000000 x3a=     1.354000  et3a =  0.166667
 t3b=     0.000000 x3b=     0.000000  et3b =  0.000000
 te =     0.000000 to =     0.000000
 w  =   123.000000 wq =   123.000000

EDF coefficients read:
 b14=     0.000000 b15=     0.000000
 b16=     0.000000 b18=     0.000000

nfunc  =     1 -- EDF option --

njmunu =     0 no tensor terms in the functional
ncm2   =     0 -- 1-body c.m. correction only --
nmass  =     0 m_n = m_p
ncoex  =     0 Coulomb exchange in Slater approximation

npair  =     4 -- BCS delta force --
vn   =1250.000MeV Fm3,  encut=   5.000MeV
vp   =1250.000MeV Fm3,  epcut=   5.000MeV
dcut =   0.500MeV
rhoc =   1.000

cutoff above and below the fermi level
```

Reading the EV8 output: the end of the calculation

Starts with:

```
 **final**
parameters: mx,my,mz ( 10 10 14 ) mw ( 220 ) mc ( 10 )
Neutron & proton wavefunctions 120100
```

Ends with:

```
Energies with Lagrange derivatives

                              neutron      proton       total
kinetic                      2904.507    1513.014    4417.522
1-body c.m.                   -12.412      -6.466     -18.878
2-body c.m.                     0.000       0.000       0.000
pairing                        -2.965      -0.000      -2.965

Coulomb direct                            996.042
Coulomb exchange                          -35.159

Skyrme energies
E_[rho rho]       =  -25430.125 E_[ rho tau ]    =    1528.162
E_[rho^(2+alpha)]=    16525.759 E_[rho^(2+beta)] =       0.000
E_[rho Delta rho]=      353.490 E_[rho Nabla J]  =    -101.457
E_Skyrme          =   -7124.172

total energy (Lagrange)          -1767.610056
             (Non-Lagrange)      -1786.162932


 =====  S T O P  =====

  ***** THE END *****
```

Final energy

$$E_{\mathrm{HF}} = \min\left\{\langle\Psi|\hat{H}|\Psi\rangle|\Psi = \Psi_{\mathrm{Slater}}\right\} .$$

In between these, there is tons of info that is not directly relevant to today.

Reading the EV8 output: the end of the calculation

$$r^2_{\rm rms} = \frac{\int d^3r\, r^2 \rho(\mathbf{r})}{\int d^3r\, \rho(\mathbf{r})} \, .$$

$$r_{\rm rms} = \sqrt{\frac{\int d^3r\, r^2 \rho(\mathbf{r})}{\int d^3r\, \rho(\mathbf{r})}} \, .$$

$$Q_{\ell m} = \int d^3r\, \rho(\mathbf{r}) r^l \mathrm{Re} Y_{\ell m}(\theta, \phi) \, .$$

$$\beta_{\ell m} = \frac{4\pi}{3AR^\ell} Q_{\ell m} \, .$$

```
Moments of the density

                              neutron      proton       total
particle number    :       142.000001   92.000000  234.000001

Radii
ms  radius (fm2)  :          34.7403     33.1601     34.1190
rms radius (fm)   :           5.8941      5.7585      5.8411
skin       (fm)   :                                   0.1356

Cartesian multipole moments
Qx         (fm2)  :         -791.688    -525.875   -1317.562
Qy         (fm2)  :         -791.688    -525.875   -1317.562
Qz         (fm2)  :         1583.375    1051.749    2635.124
Q0         (fm2)  :         1583.375    1051.749    2635.124
gamma      (deg)  :           -0.000      -0.000      -0.000

Quadrupole moment as used in constraints(with cutoff)
q1=iq1*delq(fm2)  :         1582.480    1051.676    2634.156
q2=iq1*delq(fm2)  :           -0.000      -0.000      -0.000
q0         (fm2)  :         1582.480    1051.676    2634.156
gamma      (deg)  :           -0.000      -0.000      -0.000

Spherical multipole moments
Q20        (fm2)  :          499.424     331.739     831.163
Q22        (fm2)  :           -0.000      -0.000      -0.000

Q40        (fm4)  :        19488.438   13143.275   32631.713
Q42        (fm4)  :           -0.000      -0.000      -0.000
Q44        (fm4)  :         -417.573    -156.811    -574.384

Q60        (fm6)  :       512758.632  386656.994  899415.626
Q62        (fm6)  :           -0.000      -0.000      -0.000
Q64        (fm6)  :         4327.881    1175.197    5503.078
Q66        (fm6)  :            0.000      -0.000       0.000

Deformation parameters
beta20            :           0.2694      0.2762      0.2721
beta22            :          -0.0000     -0.0000     -0.0000

beta40            :           0.1923      0.2001      0.1954
beta42            :          -0.0000     -0.0000     -0.0000
beta44            :          -0.0041     -0.0024     -0.0034

beta60            :           0.0925      0.1077      0.0985
beta62            :          -0.0000     -0.0000     -0.0000
beta64            :           0.0008      0.0003      0.0006
beta66            :           0.0000     -0.0000      0.0000
```

Reading the EV8 output: during the iterations

(change) in energy in MeV

quadrupole deformation $\beta_{20,}\beta_{22}$

```
-----------------------------------------------------------------------------
Sum. it   : Iter    =   85
Sum. E    : Etot    = -1799.633 dE      =-0.666E-04
Sum. Quad: Qxx      = -1142.678 Qy      = -1142.678 Qz      =  2285.357
Sum. Beta: B20      =     0.233 B22     =     0.000
Sum. Misc: Sum D2H= 0.102E+01 dFermi N= 0.555E-02 dFermi P= 0.728E-02
-----------------------------------------------------------------------------
Sum. it   : Iter    =   86
Sum. E    : Etot    = -1799.518 dE      =-0.640E-04
Sum. Quad: Qxx      = -1144.767 Qy      = -1144.767 Qz      =  2289.533
Sum. Beta: B20      =     0.233 B22     =     0.000
Sum. Misc: Sum D2H= 0.101E+01 dFermi N= 0.532E-02 dFermi P= 0.705E-02
-----------------------------------------------------------------------------
Sum. it   : Iter    =   87
Sum. E    : Etot    = -1799.408 dE      =-0.615E-04
Sum. Quad: Qxx      = -1146.837 Qy      = -1146.837 Qz      =  2293.674
Sum. Beta: B20      =     0.233 B22     =     0.000
Sum. Misc: Sum D2H= 0.101E+01 dFermi N= 0.511E-02 dFermi P= 0.683E-02
-----------------------------------------------------------------------------
Sum. it   : Iter    =   88
Sum. E    : Etot    = -1799.301 dE      =-0.591E-04
Sum. Quad: Qxx      = -1148.890 Qy      = -1148.890 Qz      =  2297.780
Sum. Beta: B20      =     0.234 B22     =     0.000
Sum. Misc: Sum D2H= 0.100E+01 dFermi N= 0.490E-02 dFermi P= 0.663E-02
-----------------------------------------------------------------------------
```

"Good" convergence:

- $\beta_{20,}\beta_{22}$ stable over many iterations
- energy change on the order of a **keV**

"typically" takes **several hundred** iterations.

Conclusion

- Nuclear DFT: an approach to the many-body problem
  - mean-field theory
  - (Skyrme) effective interactions
  - Functionals and parameterizations

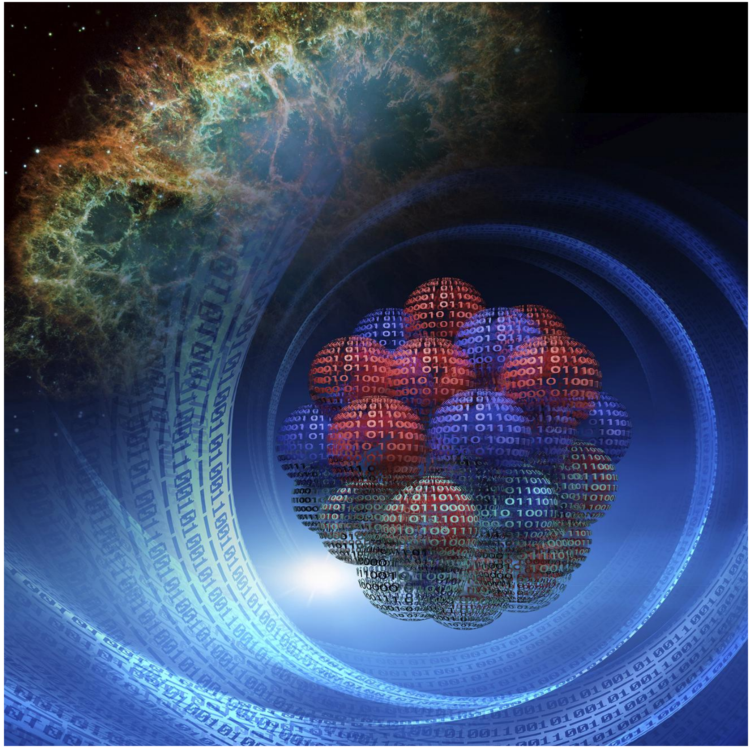

Image credit: Andy Sproles, ORNL

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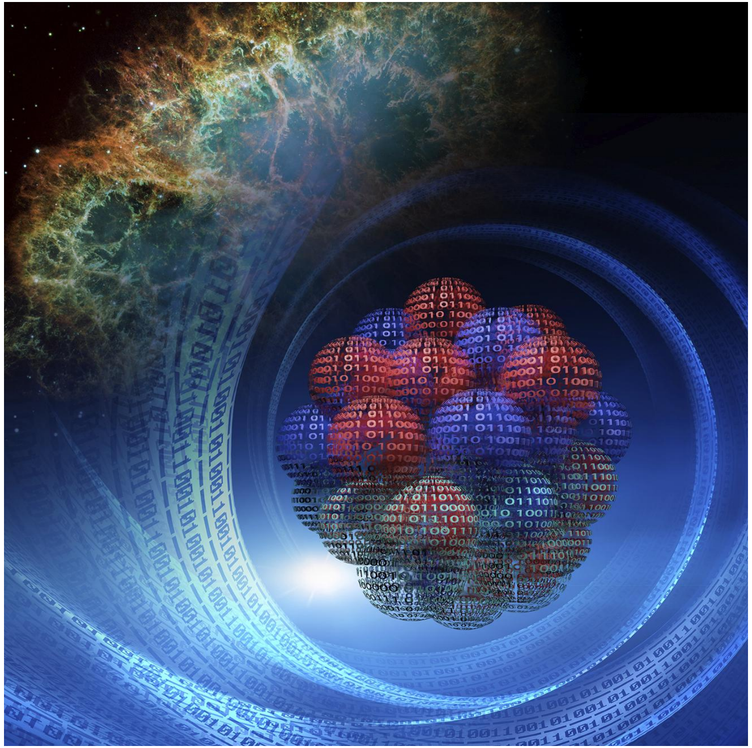

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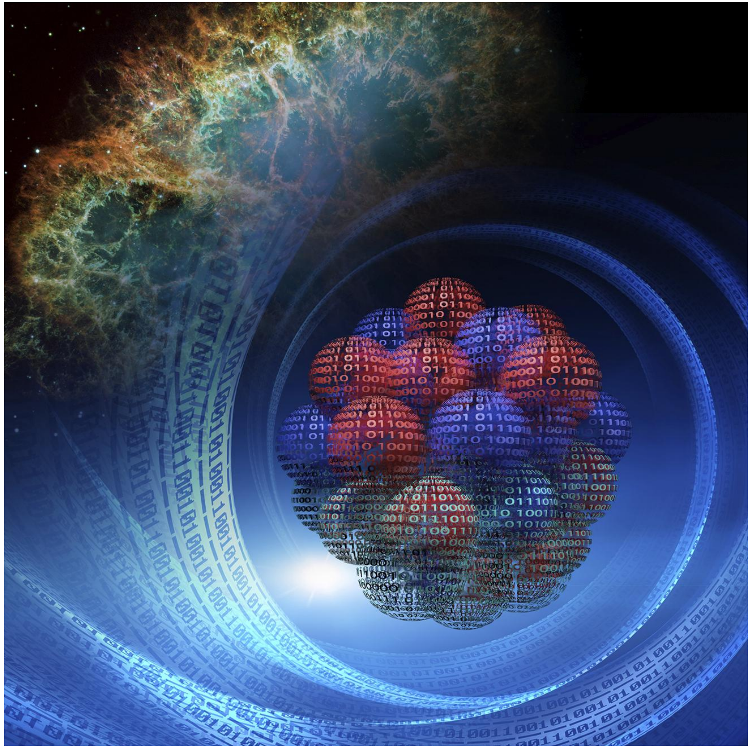

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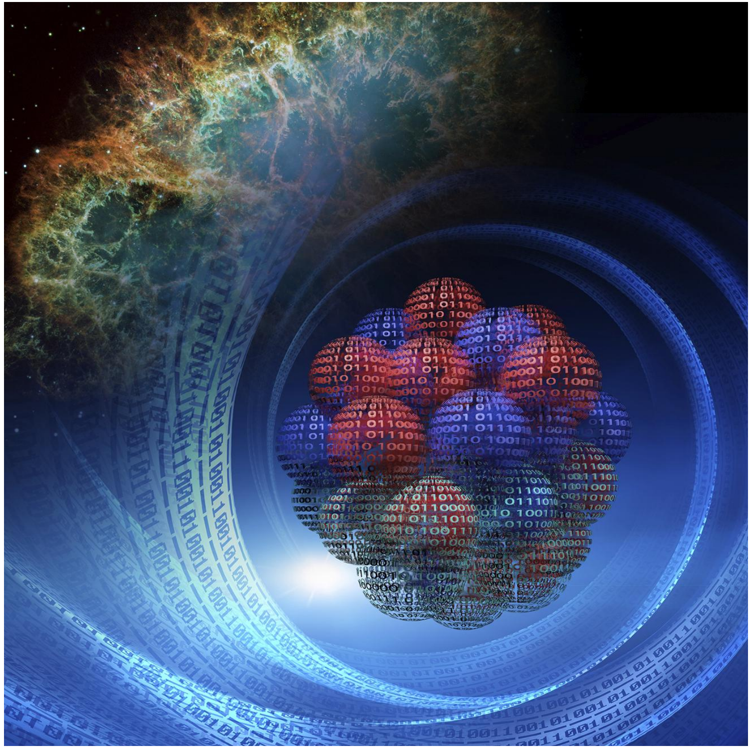

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- Homework will put all of this in practice for U isotopes!

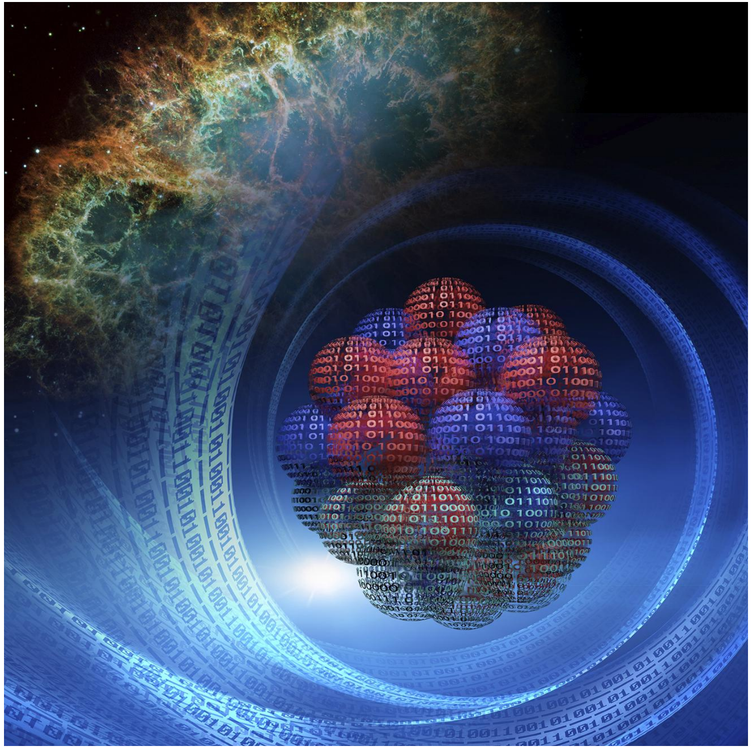

Image credit: Andy Sproles, ORNL

References & Additional reading

Important references for today:

- P. Bonche, H. Flocard, and P. H. Heenen, Comp. Phys. Comm. **171**, 49 (2005).
- W. Ryssens, V. Hellemans, M. Bender, and P.-H. Heenen, Comp. Phys. Comm. **187**, 175 (2015).

Additional reading, in order of rising complexity:

- D. Lacroix, *Review of mean-field theory*, EJC 2011 course (https://ejc2011.sciencesconf.org).
- N. Schunck et al., *Energy Density Functional Methods for Atomic Nuclei* (IOP Publishing, 2019).
- P. Ring and P. Schuck, *The nuclear many-body problem* (Springer Verlag, 1980).
- M. Bender, P.-H. Heenen, and P.-G. Reinhard, Rev. Mod. Phys. 75, 121 (2003).