State-of-the-art calculations for large nuclei

Benjamin Bally

INT - Seattle - 25/01/2023

Outline of the presentation

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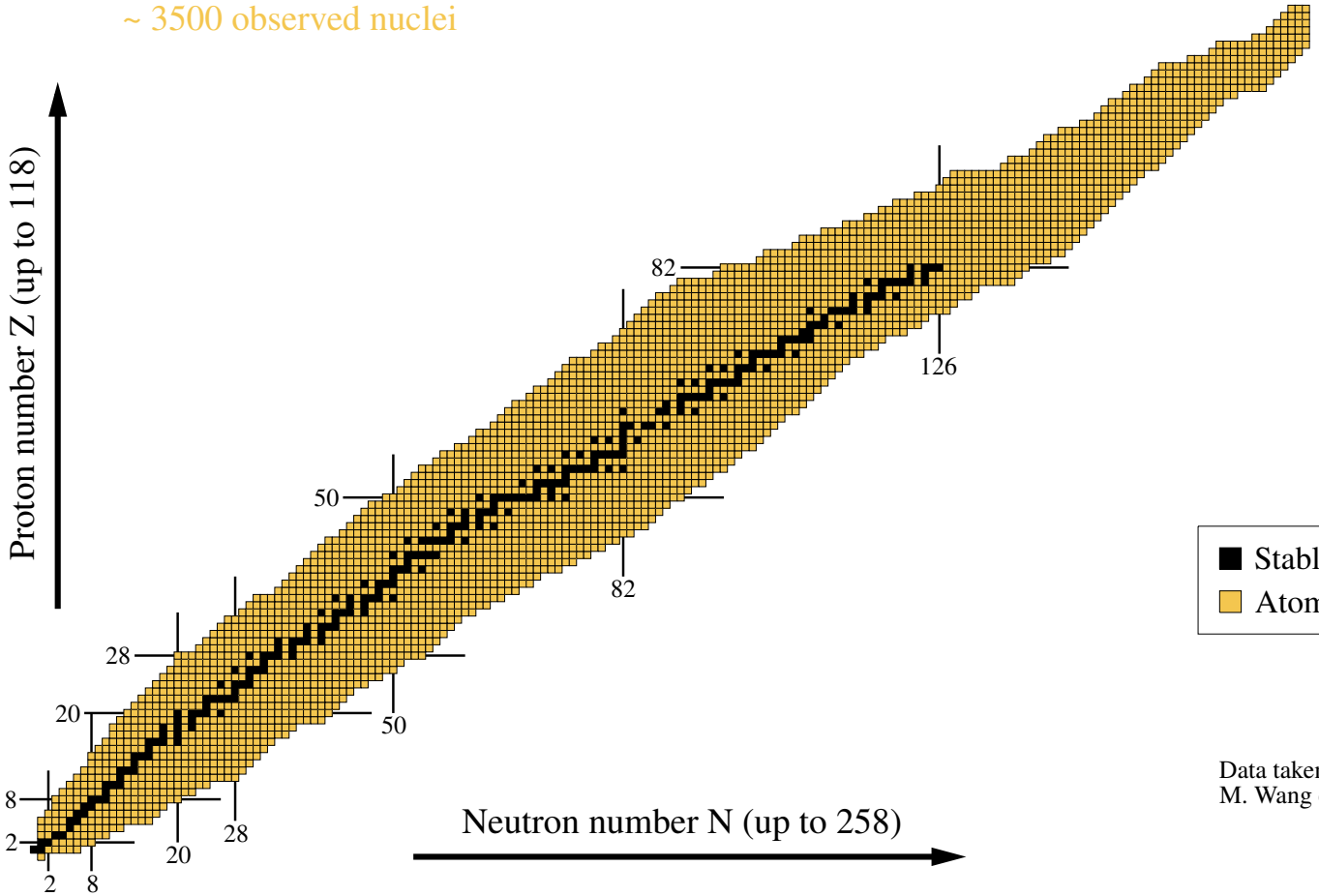
Nuclear chart: available data

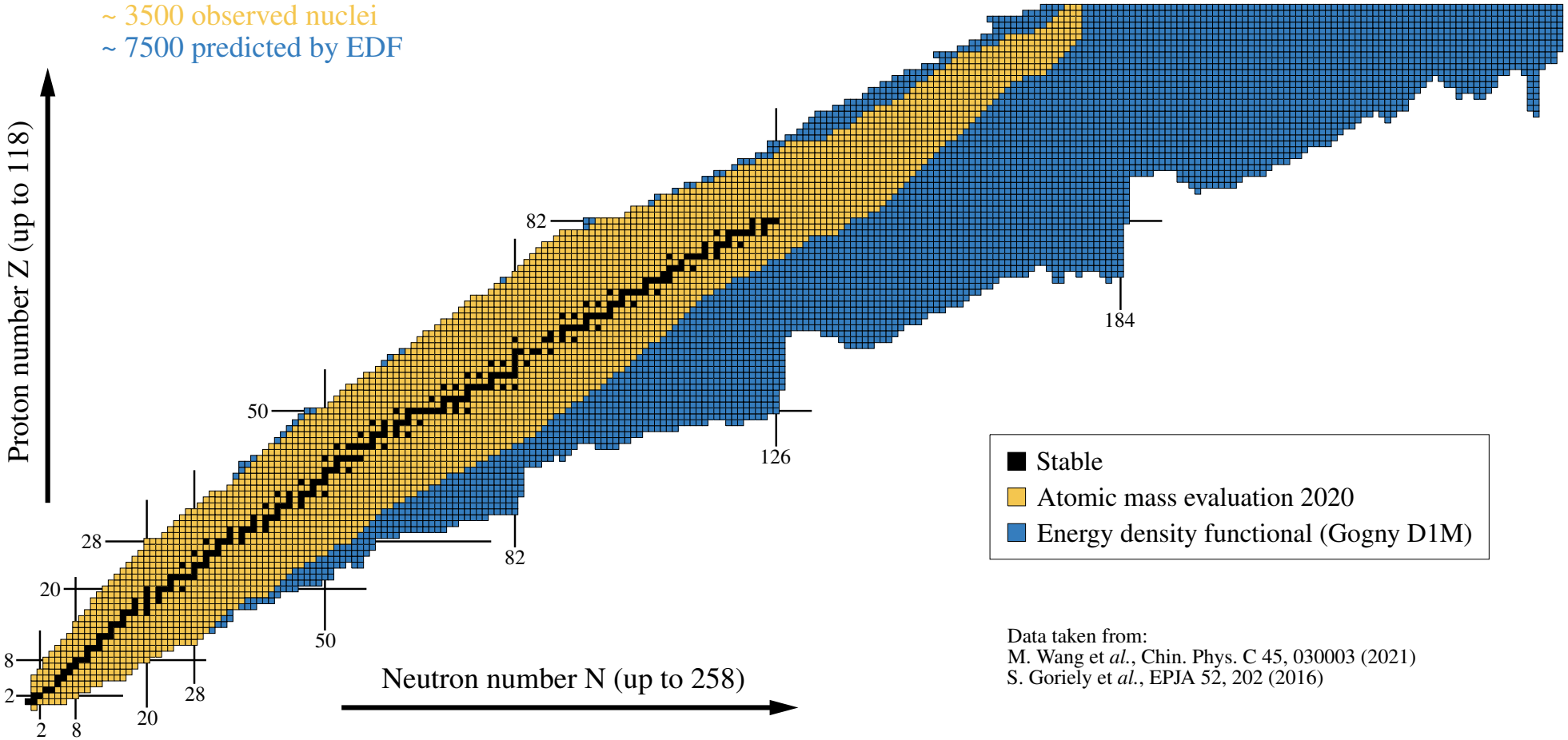
~ 3500 observed nuclei



Data taken from:
M. Wang et *al.*, Chin. Phys. C 45, 030003 (2021)

Nuclear chart: global EDF calculations

~ 3500 observed nuclei
~ 7500 predicted by EDF



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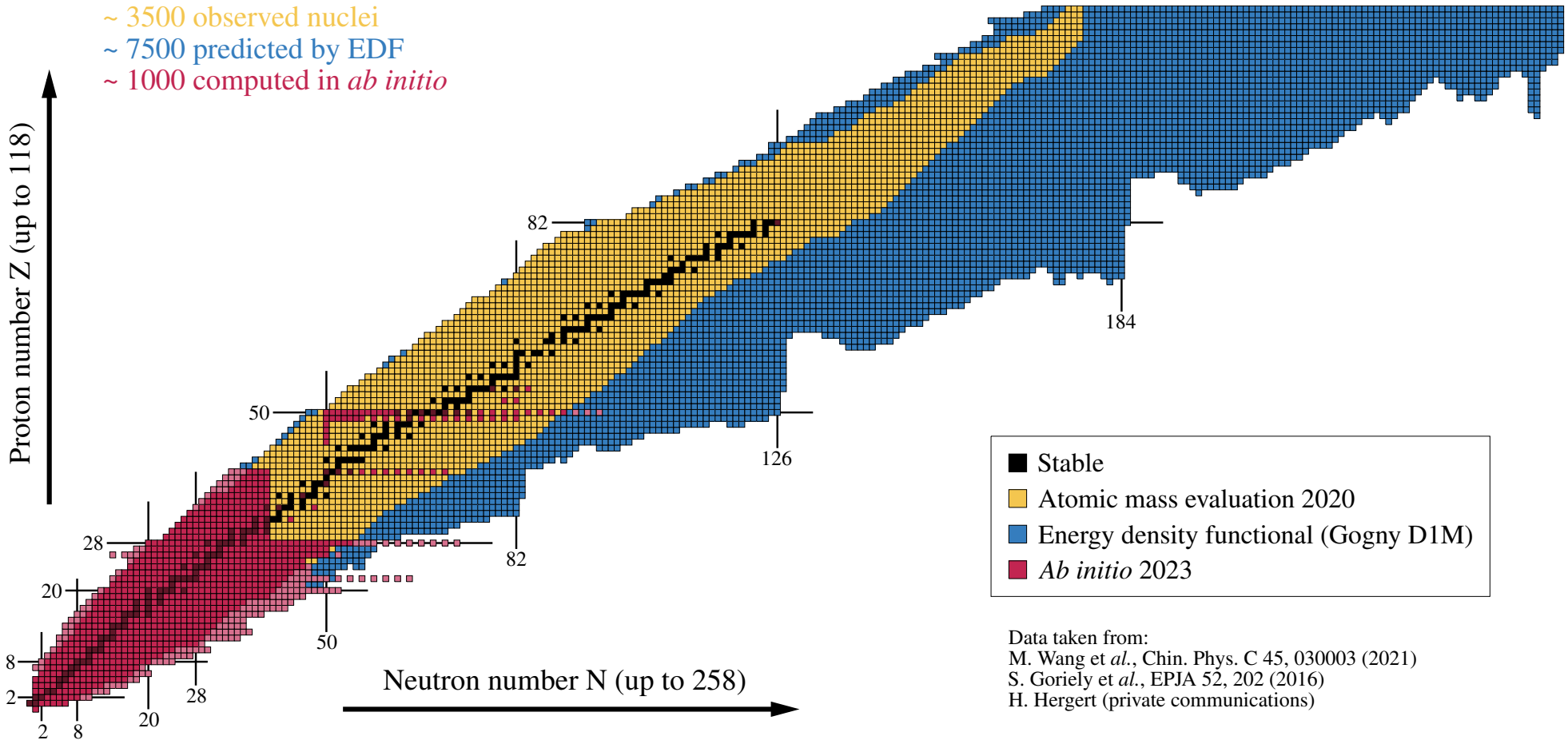
Nuclear chart: reach of *ab initio* methods



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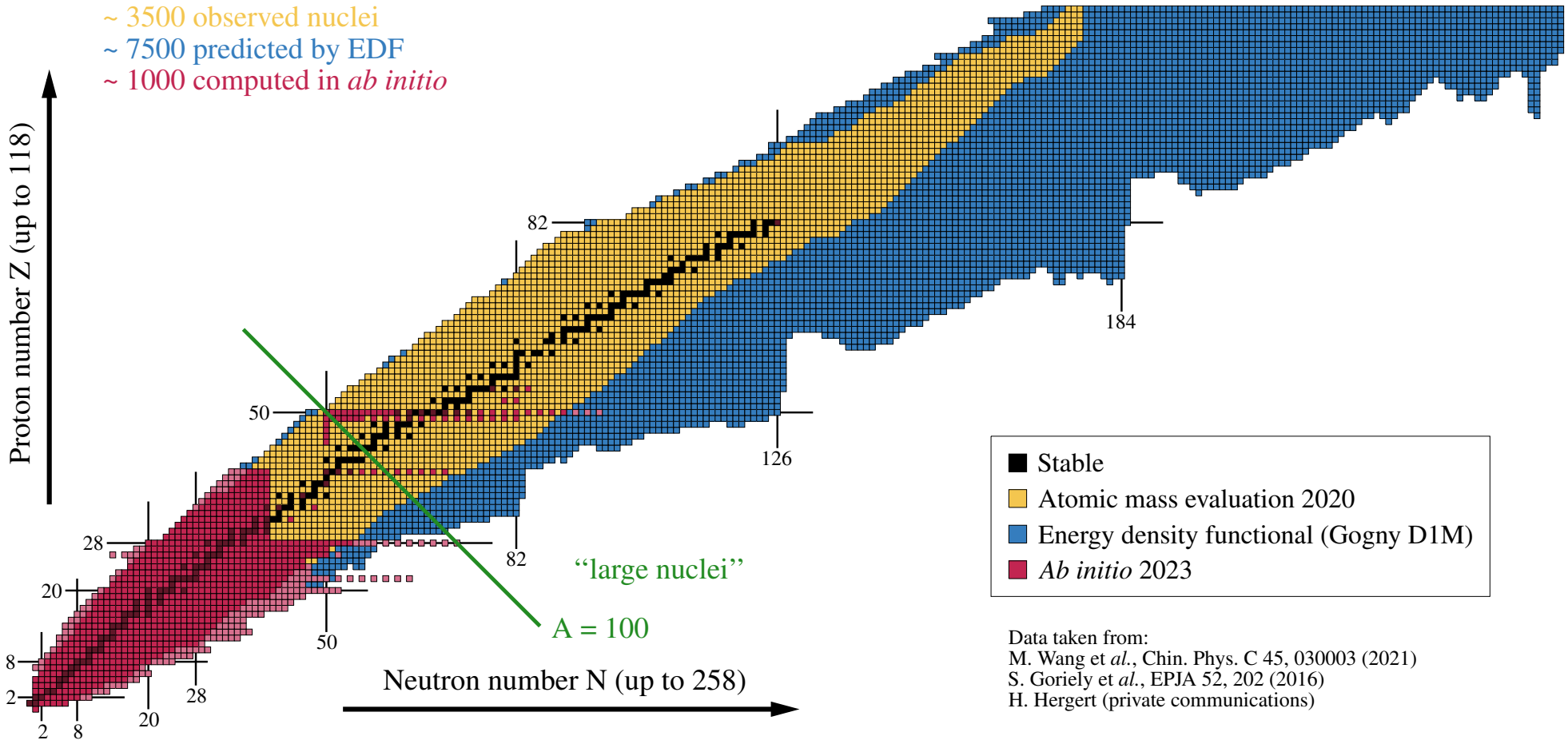
H. Hergert (private communications)

Nuclear chart: "large nuclei"



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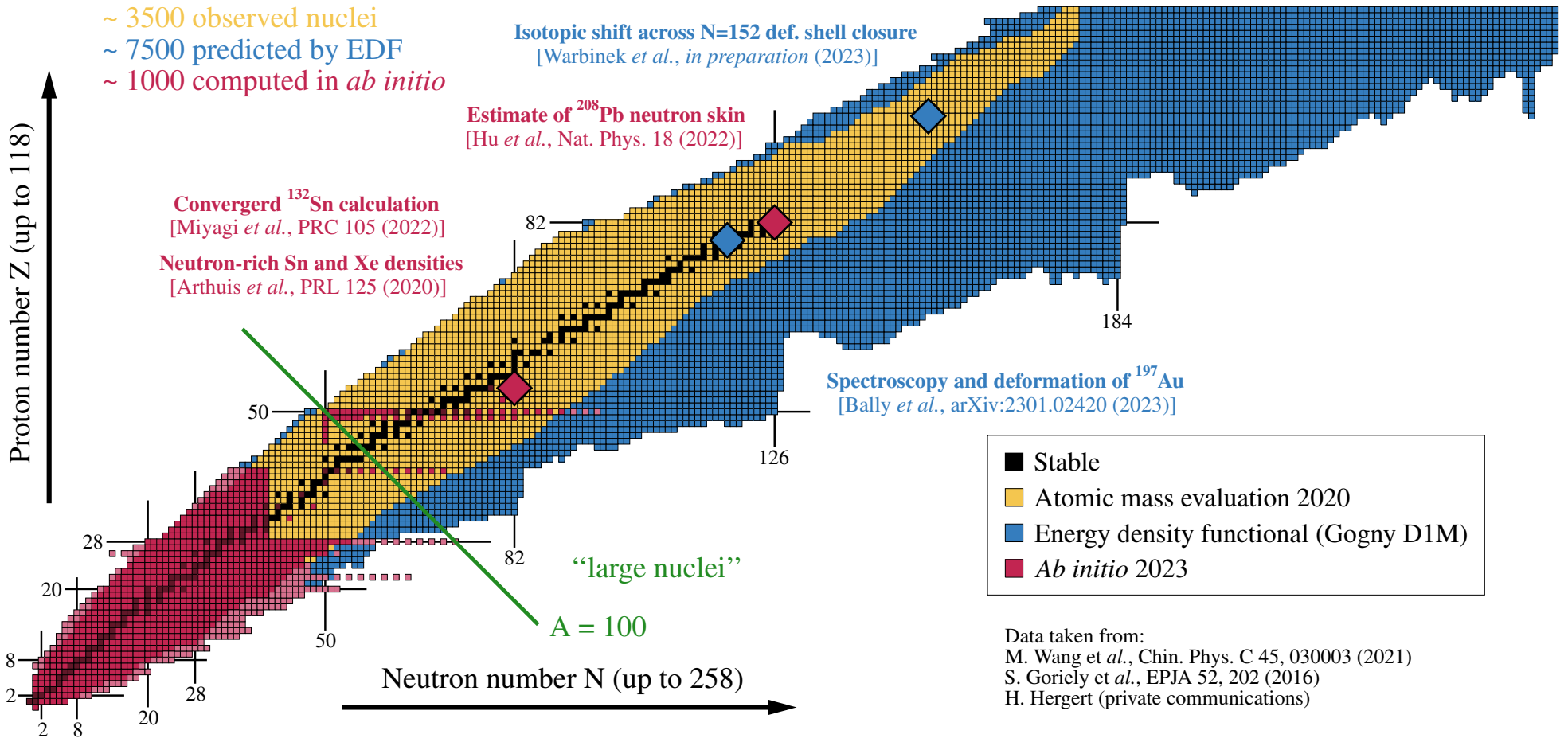
Nuclear chart: highlights



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State-of-the art methods for large nuclei

- *Ab initio* and EFT
  - Several approaches but mainly for "spherical" nuclei and still limited in A

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- Nuclear shell model (but probably less relevant in our context)
  - Monte Carlo Shell Model
    (talk of T. Otsuka, EMMI, Heidelberg 10/2022)

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Short introduction to nuclear *ab initio* methods

- Main principles:
  - Consider Z protons and N neutrons interacting
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- Many theoretical frameworks exist:
  - Coupled Cluster (CC)
  - Self-Consistent Green's Functions (SCGF)
  - No-Core Shell Model (NCSM)
  - In-Medium Similarity Renormalization Group (IMSRG)
  - Valence-Space IMSRG (VS-IMSRG)
  - Nuclear Lattice Effective Field Theory (NLEFT)
  - Projected Generator Coordinate Method + Perturbation Theory (PGCM-PT)
  - ...

Nuclear Hamiltonian

- In second quantization:

$$H = h^{(0)} + \sum_{ij} h^{(1)}_{ij} c^\dagger_i c_j + \frac{1}{(2!)^2} \sum_{ijkl} \overline{h}^{(2)}_{ijkl} c^\dagger_i c^\dagger_j c_l c_k + \frac{1}{(3!)^2} \sum_{ijklmn} \overline{h}^{(3)}_{ijklmn} c^\dagger_i c^\dagger_j c^\dagger_k c_n c_m c_l + \dots$$

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- "Bare" Hamiltonian

$$\begin{aligned} h^{(0)} &= 0 \\ h^{(1)} &= T^{(1)} \\ \overline{h}^{(2)} &= V^{(2)} \\ \overline{h}^{(3)} &= W^{(3)} \\ \overline{h}^{(n>3)} &= 0 \end{aligned}$$

Rank reduction of the Hamiltonian

- Consider an effective 2-body nuclear Hamiltonian

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  Frosini *et al.*, EPJA 58, 63 (2022)

  Reference state $|\Phi\rangle$ with one-body density: $\rho_{ij} = \langle\Phi|a^\dagger_j a_i|\Phi\rangle$

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  (Example: $\left[W^{(3)} \cdot \rho\right]_{ijln} = \sum_{kn} W^{(3)}_{ijklmn} \rho_{nk}$)

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- Error $< 3\%$ for excitation energies

Choice of basis: Spherical Harmonic Oscillator

- SHO basis: $|a\rangle \equiv |n_a, l_a, s_a = \frac{1}{2}, j_a, m_{j_a}, t_a = \frac{1}{2}, m_{t_a}\rangle$

  with $m_{j_a} \in [\![-j_a, j_a]\!]$ and $m_{t_a} \in [\![-t_a, t_a]\!]$

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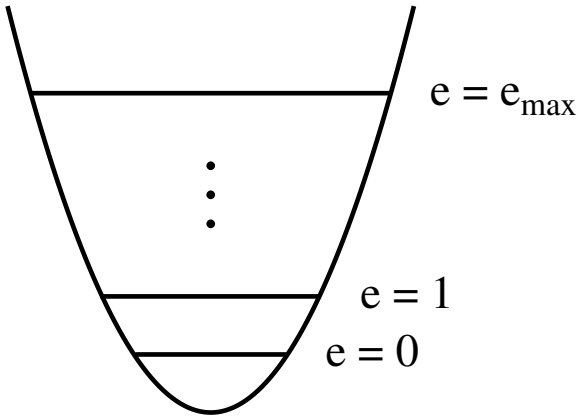
- Principal quantum number: $e_a = 2n_a + l_a$

- Limit for single-particle states $|a\rangle$: $\forall a,\ e_a \leq e_{\max}$



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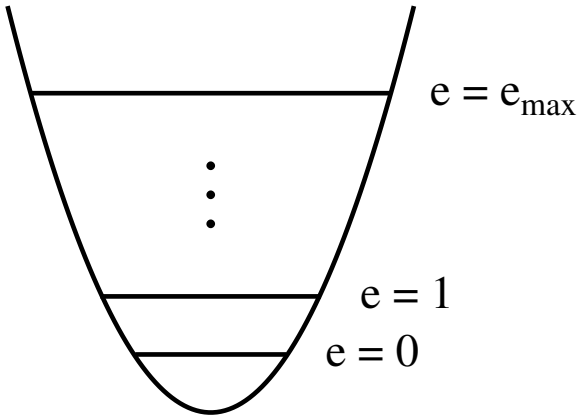

- Limit for two-particle states $|ab\rangle$: $\forall a, b,\ e_a + e_b \leq e_{2\text{max}} \underbrace{= 2e_{\text{max}}}_{\text{generally}}$

  $\Rightarrow$ all elements $V_{abcd} = \langle ab|V^{(2)}|cd\rangle$ taken into account

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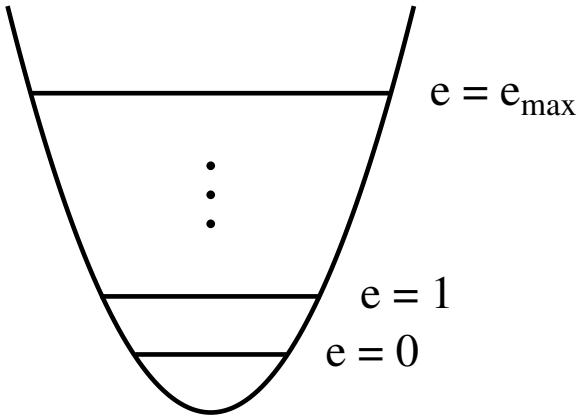

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- Limit for three-particle states $|abc\rangle$: $\forall a, b, c,\ e_a + e_b + e_c \leq e_{3\max} \underbrace{< 3e_{\max}}_{\text{generally}}$

  $\Rightarrow$ not all elements $W_{abcdef} = \langle abc|W^{(3)}|def\rangle$ taken into account

Scaling of V_{ijkl} with the basis size

- 4 octets/matrix element

e_{max}	N_{sp}
0	4
1	16
2	40
3	80
4	140
5	224
6	336
7	480
8	660
9	880
10	1144
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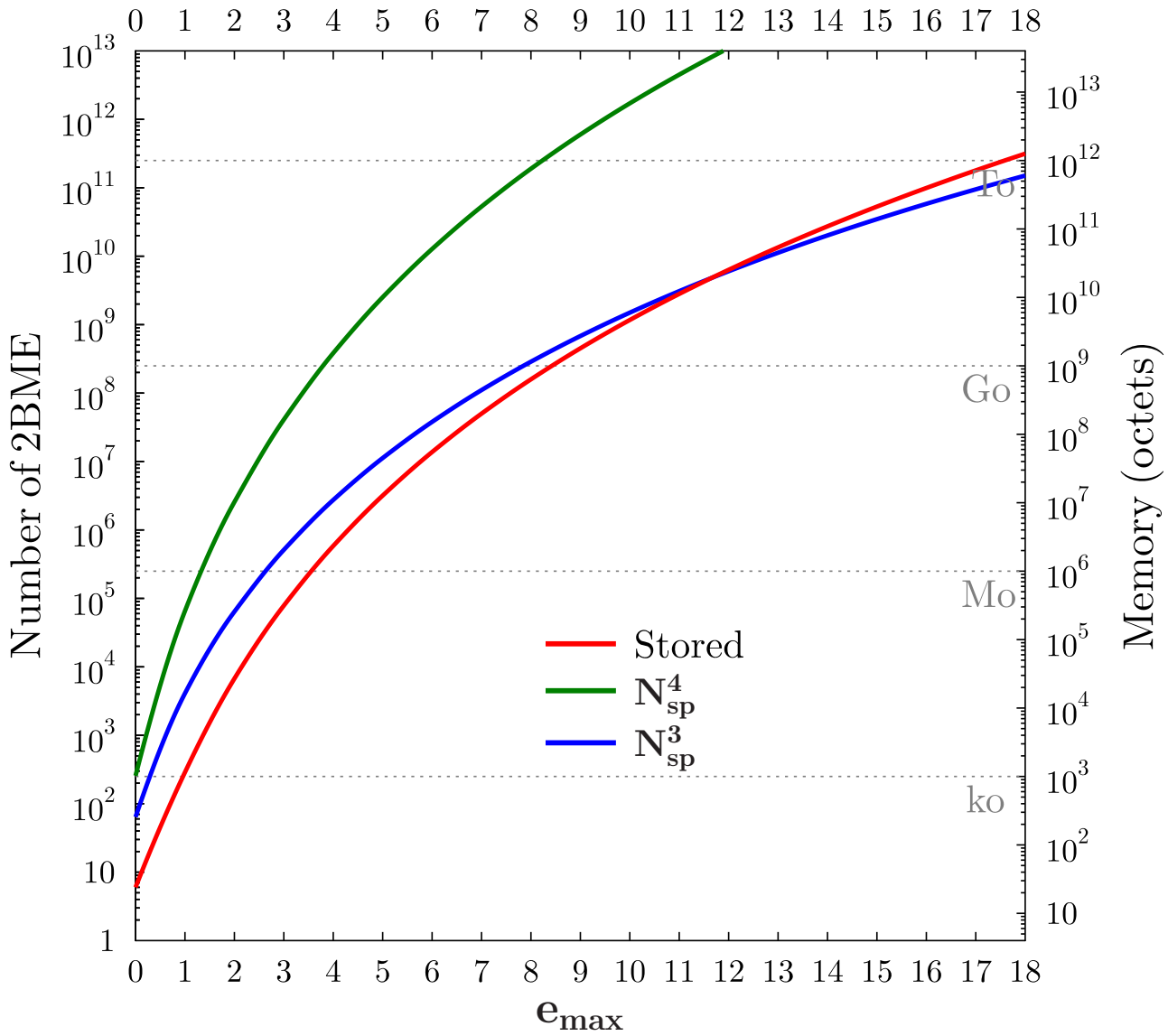

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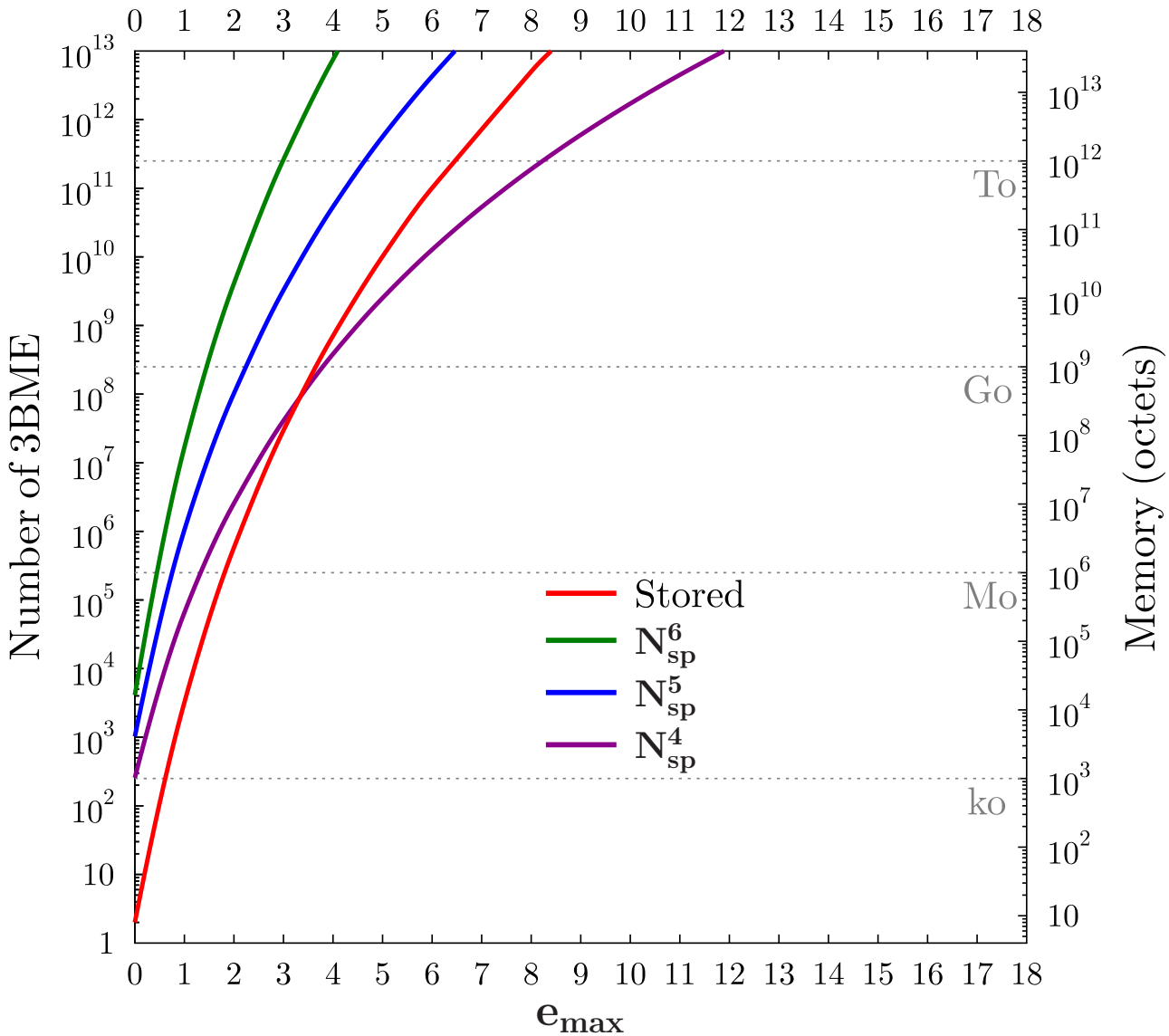

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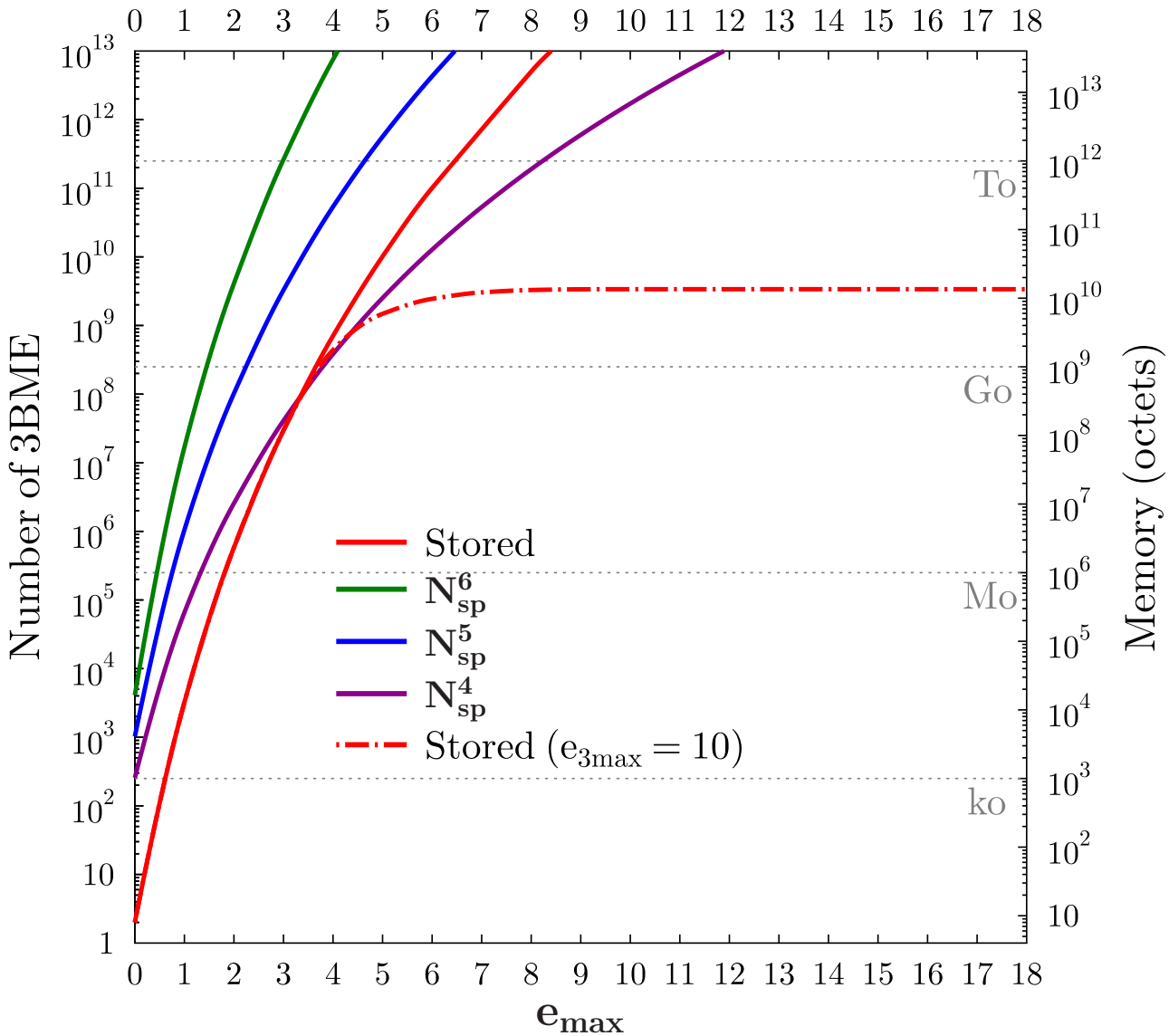
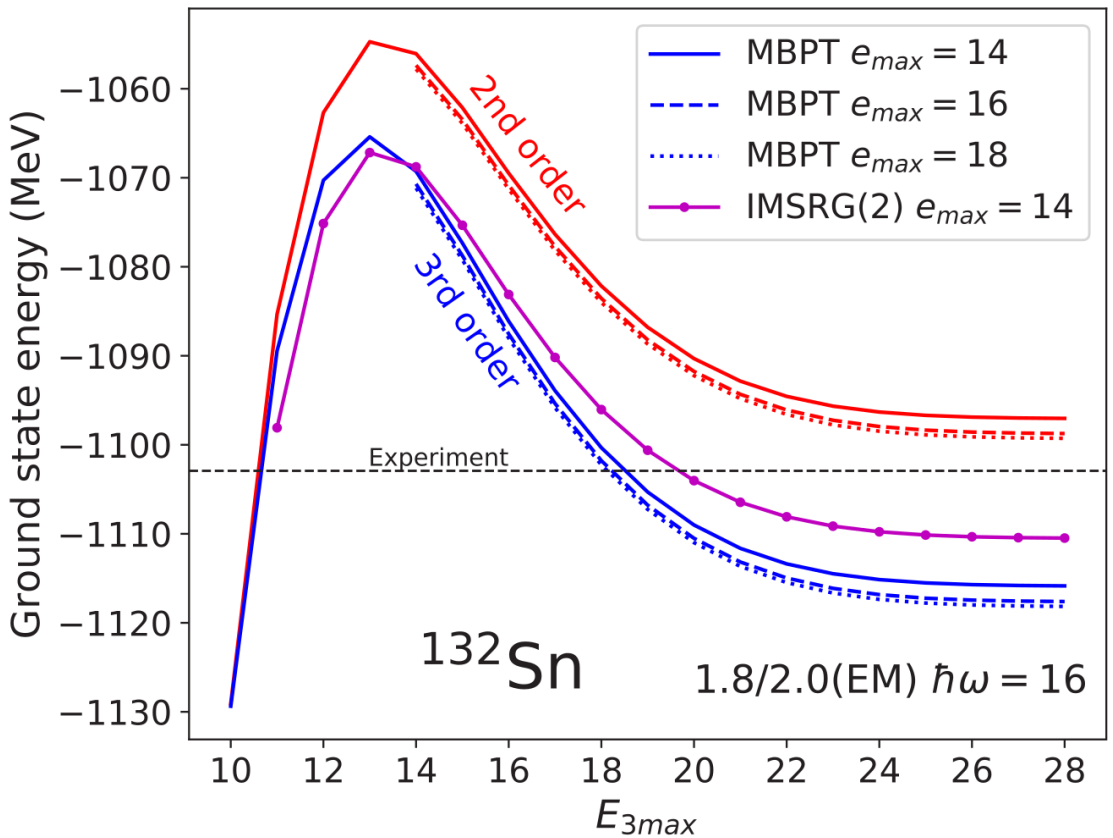


Breakthrough: large e_{3max} now possible

- Store only required linear combinations of matrix elements

  Miyagi *et al.*, PRC 105, 014302 (2022)



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Mean-field (MF) and symmetry-unrestricted calc.

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- Capture strong collective correlations keeping the simple one-body picture

Constrained calculations

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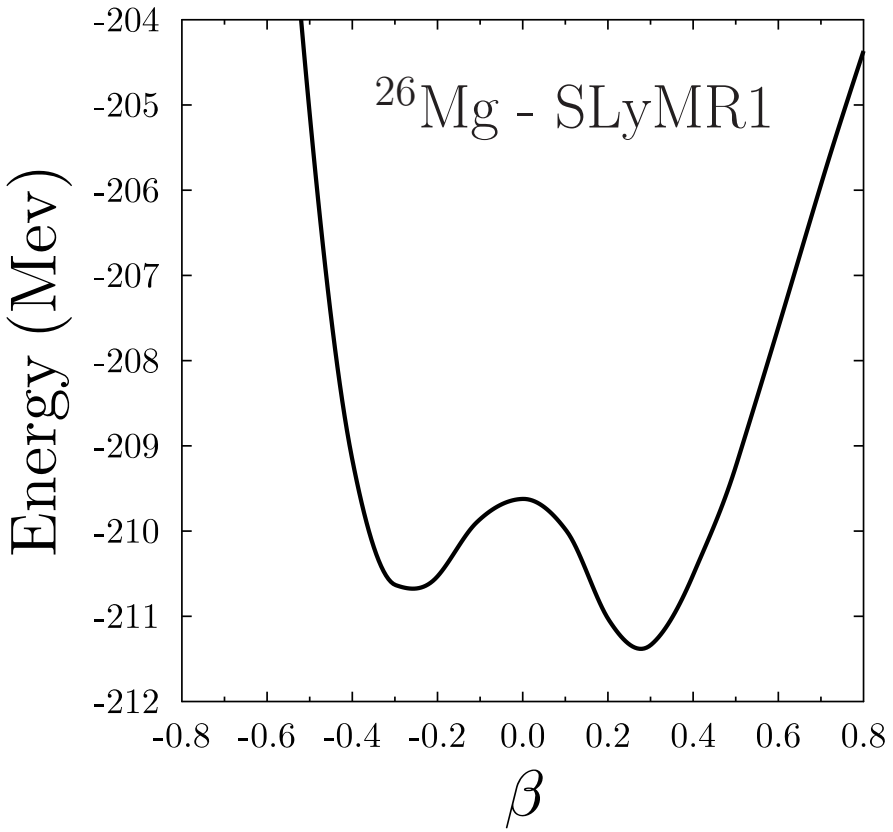

Symmetry-breaking and quantum numbers

- Deformed solutions break the symmetries of H

$$|\Phi(q_i)\rangle = \sum_{ZNJM\pi} \sum_{\epsilon} c_{\epsilon}^{ZNJM\pi}(q_i)|\Theta_{\epsilon}^{ZNJM\pi}(q_i)\rangle \quad \Rightarrow \text{ unphysical in nuclei}$$

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  - ◇ Break symmetries at MF level ⇒ explore larger variational space
  - ◇ Restore symmetries at BMF level ⇒ get good quantum numbers

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  - ◇ Break symmetries at MF level $\Rightarrow$ explore larger variational space
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  - ◇ Symmetry-breaking MF $\xrightarrow{\text{reference states}}$ Symmetry-restored BMF

Symmetry-breaking and quantum numbers

- Projection operators from Group Theory

$$P^Z P^N \equiv \text{proton and neutron numbers}$$

$$P^J_{MK} \equiv \text{angular momentum}$$

$$P^\pi \equiv \text{parity}$$

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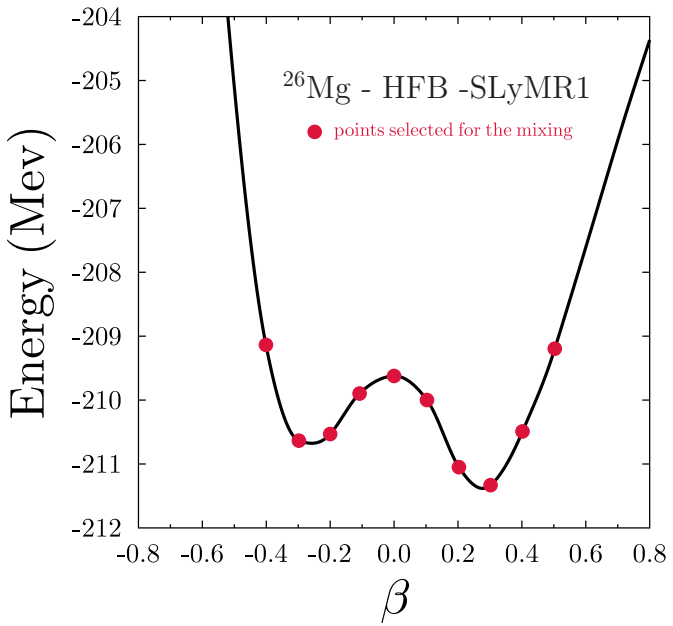
- Projected Generator Coodinate Method

$$|\Theta^{ZNJM\pi}_\sigma\rangle \equiv \sum_{q_i,K} f^{ZNJM\pi}_\sigma(q_i,K)\, P^Z P^N P^J_{MK} P^\pi |\Phi(q_i)\rangle$$

$$\delta \frac{\langle\Theta^{ZNJM\pi}_\sigma|H|\Theta^{ZNJM\pi}_\sigma\rangle}{\langle\Theta^{ZNJM\pi}_\sigma|\Theta^{ZNJM\pi}_\sigma\rangle} = 0$$



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Energy Density Functional (EDF)

- The energy is represented as a functional of one-body densities

$$\langle\Phi|H|\Phi\rangle \equiv E[\rho,\kappa,\kappa^*] \text{ with } \begin{cases} \rho_{ij} = \langle\Phi|a_j^\dagger a_i|\Phi\rangle \\ \kappa_{ij} = \langle\Phi|a_j a_i|\Phi\rangle \\ \kappa_{ij}^* = \langle\Phi|a_i^\dagger a_j^\dagger|\Phi\rangle \end{cases}$$

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- But EDF philosophy goes further
  - Form of $E[\rho,\kappa,\kappa^*]$ is general (e.g. ρ^α with $\alpha \notin \mathbb{N}$)
  - Parameters of $E[\rho,\kappa,\kappa^*]$ fitted to experimental data

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  - Not much progress in recent years

Example: structure of ^{197}Au

- SLyMR1 parametrization

  R. Jodon, PhD Thesis, tel-01158085, Sadoudi *et al.*, PRC 88, 064326 (2013)

  - no density dependence → three-body with gradients
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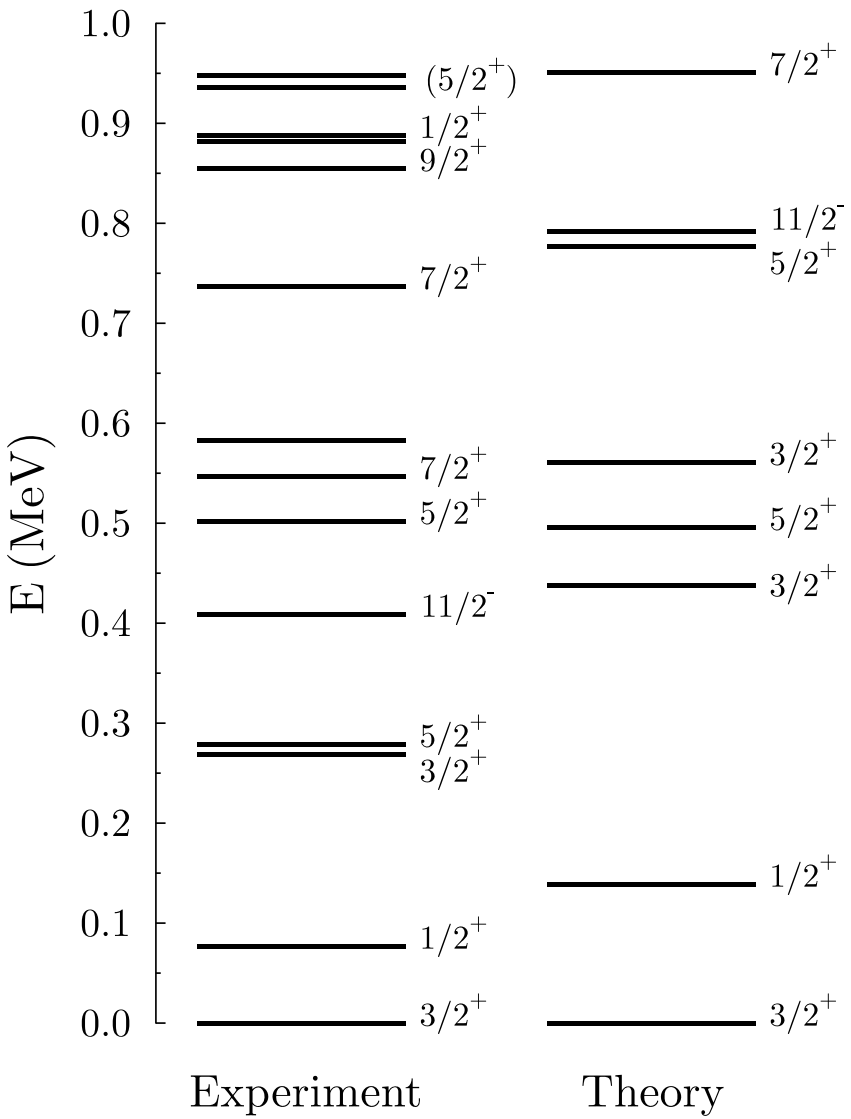
- MR-EDF calculations with
  - Projection on Z, N, J, M_J (P conserved)
  - Exporing explicitly: β, γ, 1qp

Low-energy spectrum

- Correct J^π for the g.s.
- Ordering reasonable
- Too spread in energy



Spectroscopic quantities

Quantity	Experiment	Theory
$E(3/2_1^+)$	-1559.384	-1556.044
$r_{\text{rms}}(3/2_1^+)$	5.4371(38)	5.389
$\mu(1/2_1^+)$	+0.416(3)	+0.01
$\mu(3/2_1^+)$	+0.1452(2)	-0.38
$\mu(5/2_1^+)$	+0.74(6)	+0.15
$\mu(5/2_2^+)$	+3.0(5)	+0.14
$\mu(7/2_1^+)$	+0.84(7)	+0.51
$\mu(9/2_1^+)$	+1.5(5)	+0.81
$\mu(11/2_1^-)$	(+)5.96(9)	+6.87
$Q_s(3/2_1^+)$	+0.547(16)	+0.65
$Q_s(11/2_1^-)$	+1.68(5)	+2.05

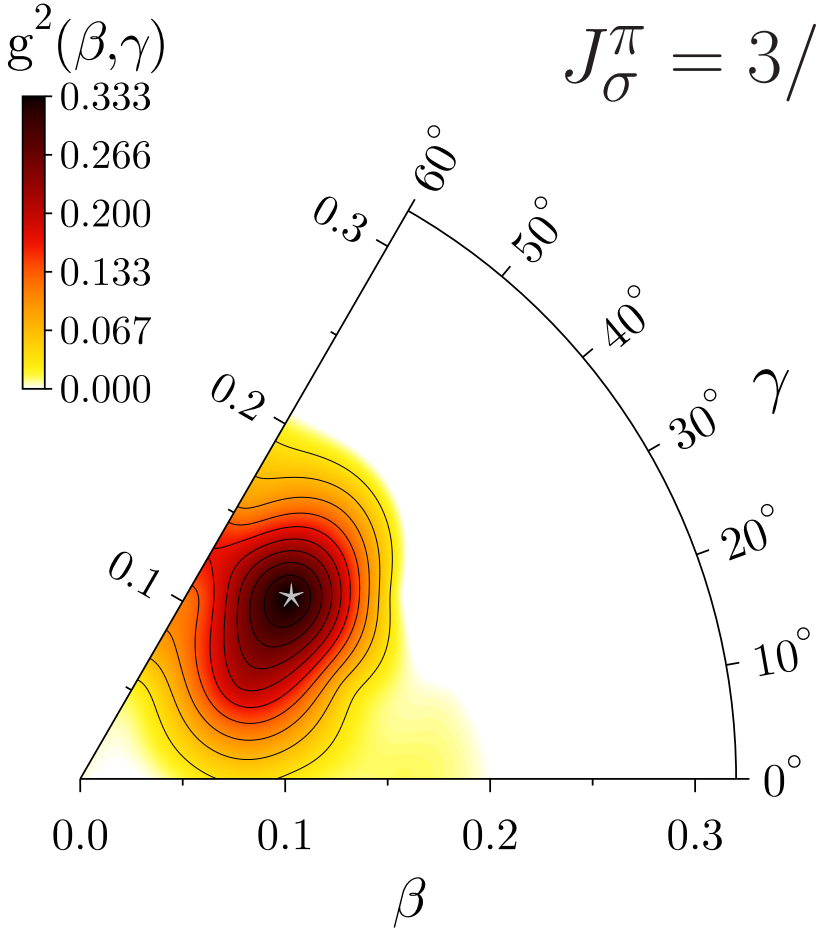
Table: Total energy E (MeV), root-mean-square charge radius r_{rms} (fm), magnetic dipole moments μ (μ_N), and spectroscopic quadrupole moments Q_s (eb).

Electromagnetic transitions

Transition	Type	Experiment	Theory
$1/2^+_1 \to 3/2^+_1$	E2	35(3)	45
	M1	0.004	0.019
$3/2^+_2 \to 1/2^+_1$	E2	18(3)	6
	M1	0.089(9)	0.048
$3/2^+_3 \to 1/2^+_1$	E2		9
$3/2^+_2 \to 3/2^+_1$	E2	18.5(19)	0.4
$5/2^+_1 \to 1/2^+_1$	E2	14.4(17)	12
$5/2^+_1 \to 3/2^+_1$	E2	26(6)	30
	M1	0.034(4)	0.065
$5/2^+_2 \to 1/2^+_1$	E2	7.6(23)	8
$5/2^+_2 \to 3/2^+_1$	E2	7(6)	0.4
	M1	0.083(10)	< 0.001
$7/2^+_1 \to 5/2^+_1$	E2	0.18(7)	1
	M1	0.012(1)	0.106
$7/2^+_1 \to 3/2^+_1$	E2	33(3)	38
$7/2^+_1 \to 3/2^+_2$	E2	6.8(20)	0.3
$7/2^+_2 \to 3/2^+_2$	E2	6(4)	22
$7/2^+_2 \to 5/2^+_1$	E2	21(6)	13
	M1	0.175(23)	0.010
$9/2^+_1 \to 7/2^+_1$	E2	10(7)	10
$9/2^+_1 \to 5/2^+_1$	E2	41(5)	43

Table: Reduced transition probabilities in Weisskopf units.

Average deformation



- Average deformations

$$\bar{\beta} = \sum_q g^2(q)\,\beta(q)$$

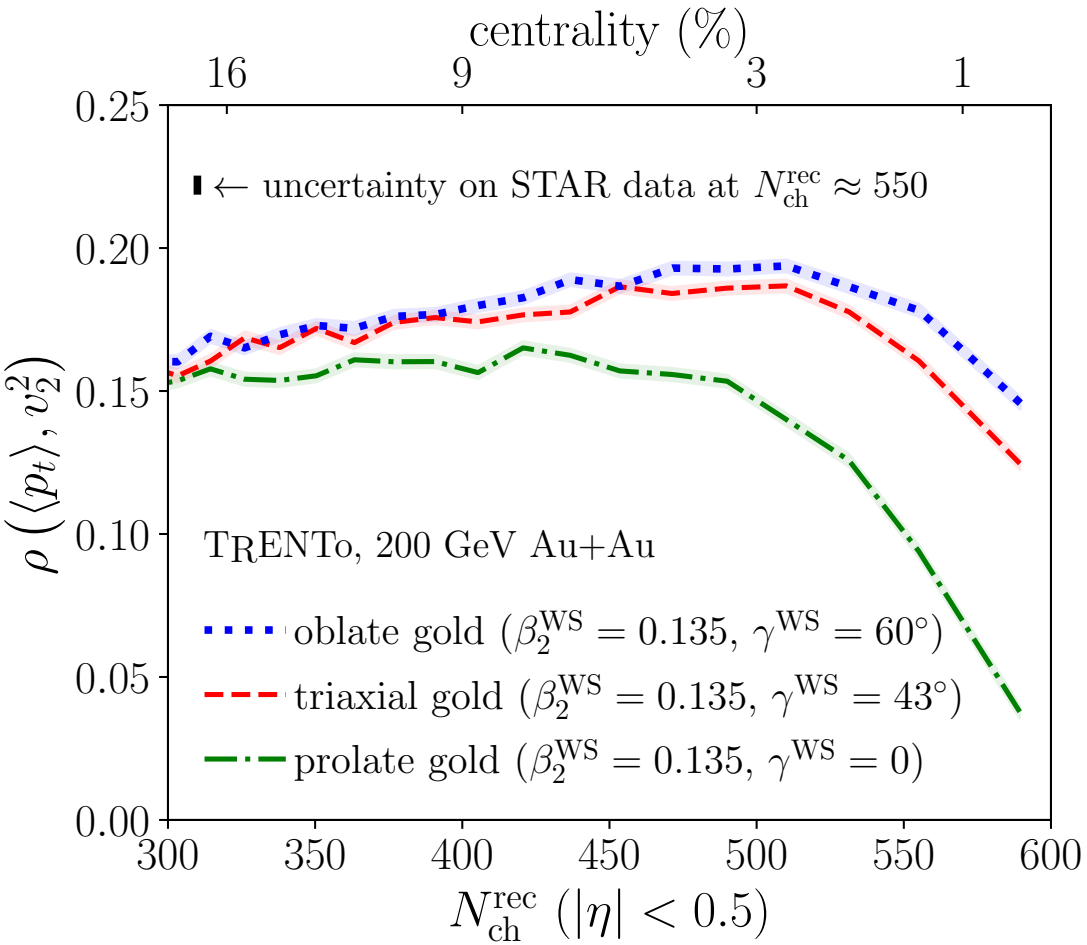
$$\bar{\gamma} = \sum_q g^2(q)\,\gamma(q)$$

- For ^{197}Au

$$\bar{\beta} = 0.13$$

$$\bar{\gamma} = 40°$$

Effects of triaxiality



- Nuclear structure input: $\langle \Phi(\bar{\beta}, \bar{\gamma}) | a_r^\dagger a_r | \Phi(\bar{\beta}, \bar{\gamma}) \rangle \rightarrow$ WS fit

Bally *et al.*, PRL 128, 082301 (2022)

Neutron skin

- Definition: $\Delta r_{np} = \langle r_n^2 \rangle^{1/2} - \langle r_p^2 \rangle^{1/2}$

- Good agreement between calculations and high-energy data

  STAR Collaboration, Sci. Adv. 9, eabq3903 (2023)

$$\Delta r_{np}[\mathrm{MREDF}] = 0.17 \text{ fm}$$

$$\Delta r_{np}[\mathrm{STAR}] = 0.17 \pm 0.03 \text{ (stat.)} \pm 0.08 \text{ (syst.) fm}$$

Other similar calculations

- ^{129}Xe and ^{208}Pb

  Bally *et al.*, PRL 128, 082301 (2022)

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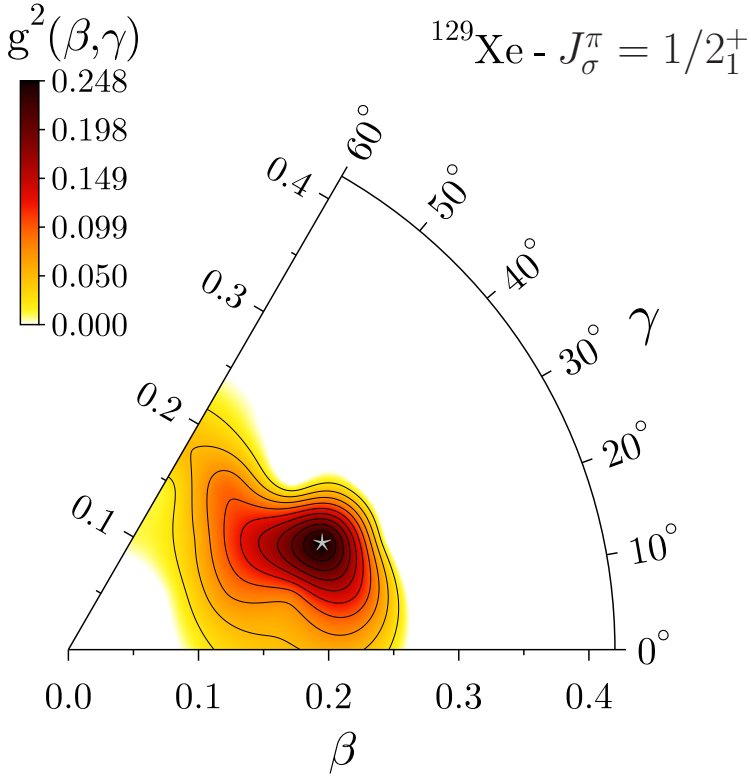

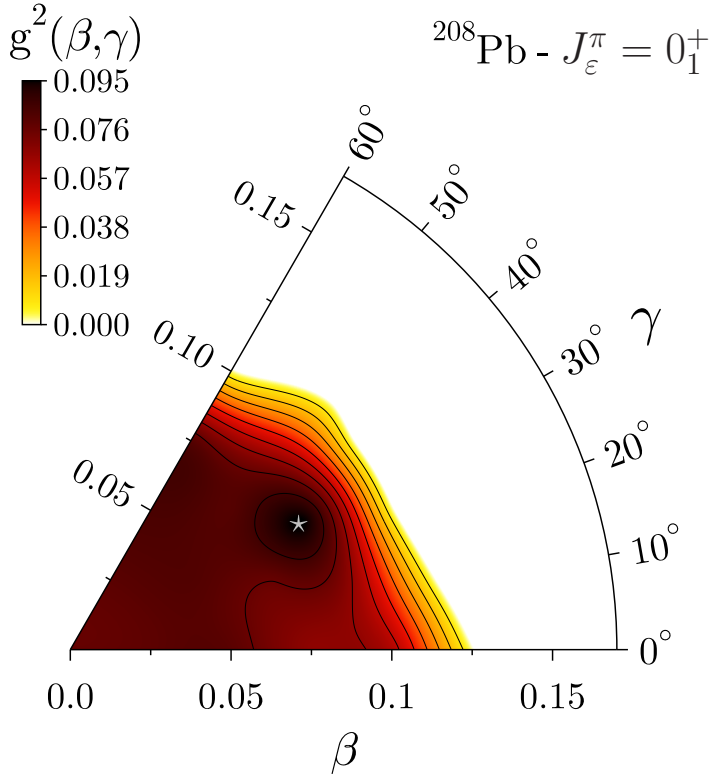

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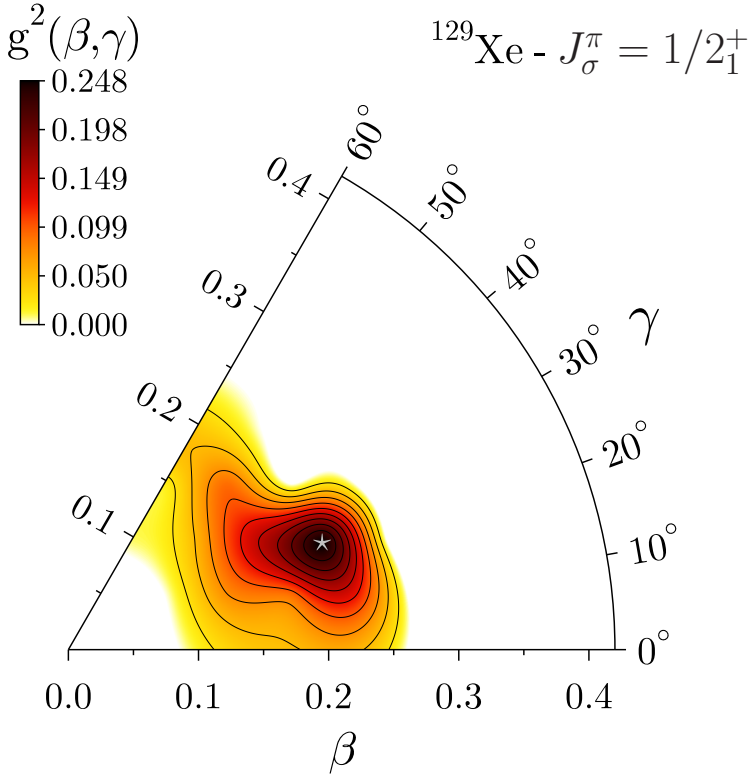

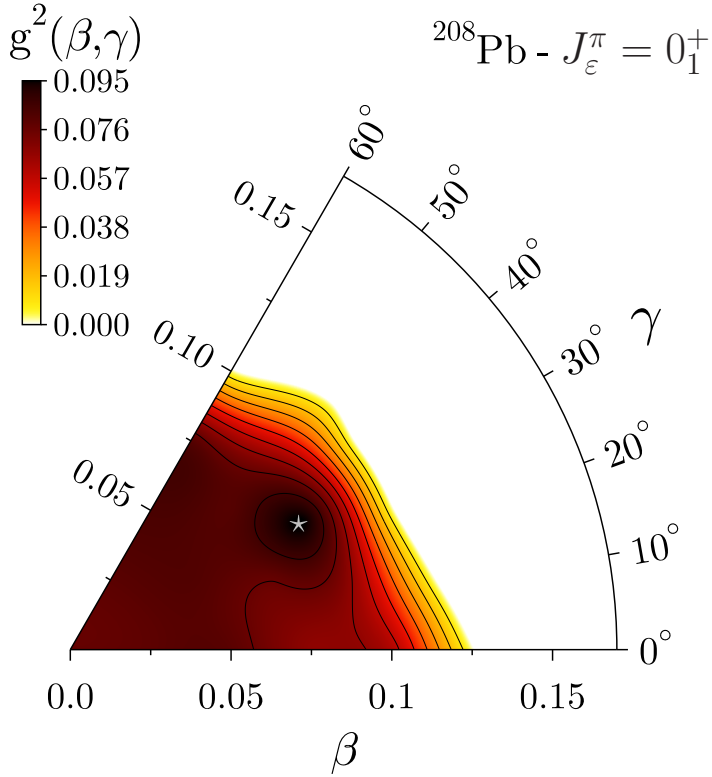

- ^{238}U → too deformed with SLyMR1

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  - Biggest problem: quality of the functionals
    But there people are still working!
    Ph. da Costa, PhD Thesis, Univ. Lyon (2022)