Capturing Many-Body Correlations within the Nuclear *Ab initio* Framework

Alberto Scalesi

Chalmers University of Technology

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Outline

- *Ab initio* in nuclear physics
- Self-consistent Green's function method
- Strongly-correlated systems

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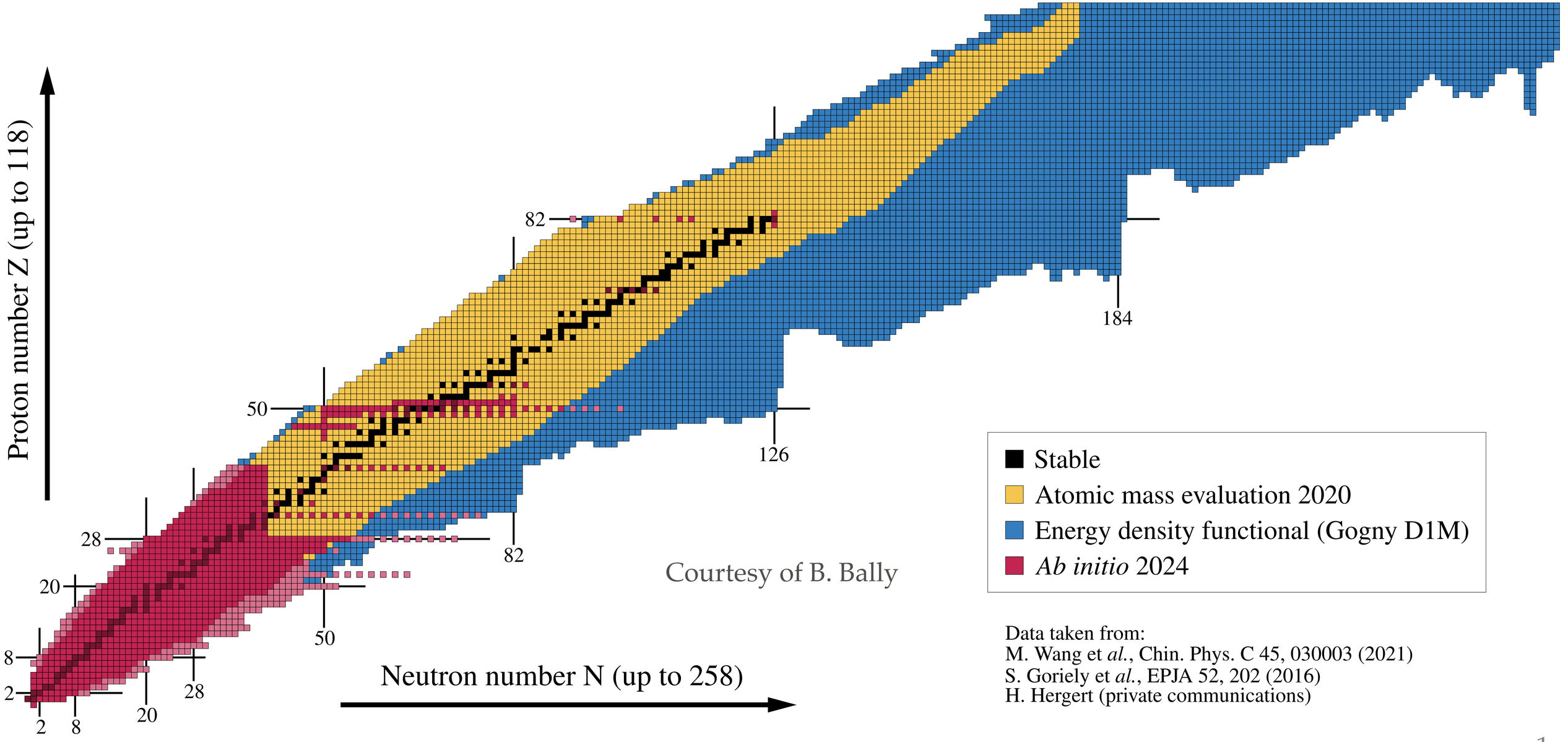
The Segrè chart



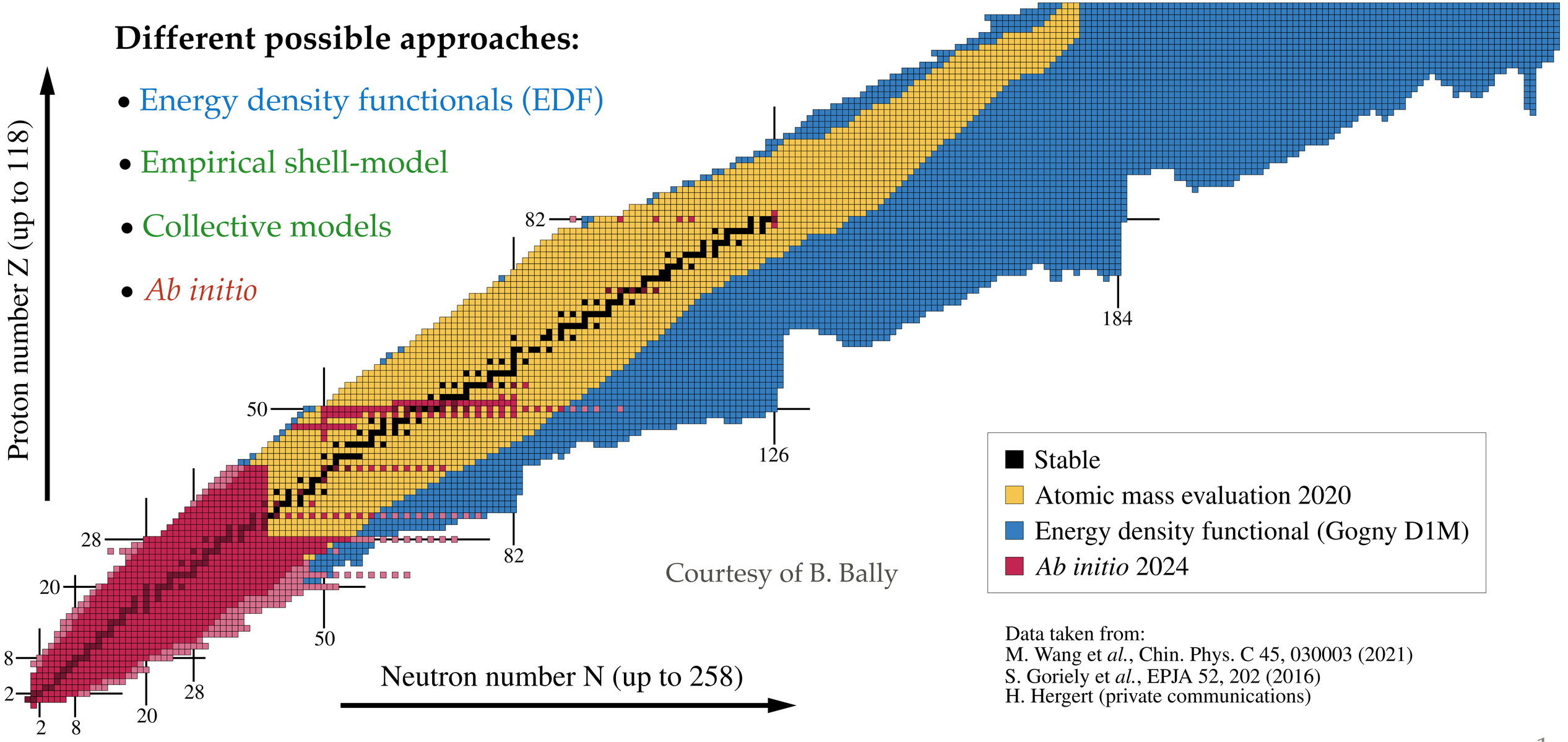
Courtesy of B. Bally

Data taken from:
M. Wang et *al.*, Chin. Phys. C 45, 030003 (2021)
S. Goriely et *al.*, EPJA 52, 202 (2016)
H. Hergert (private communications)

The Segrè chart

Different possible approaches:

- Energy density functionals (EDF)
- Empirical shell-model
- Collective models
- *Ab initio*



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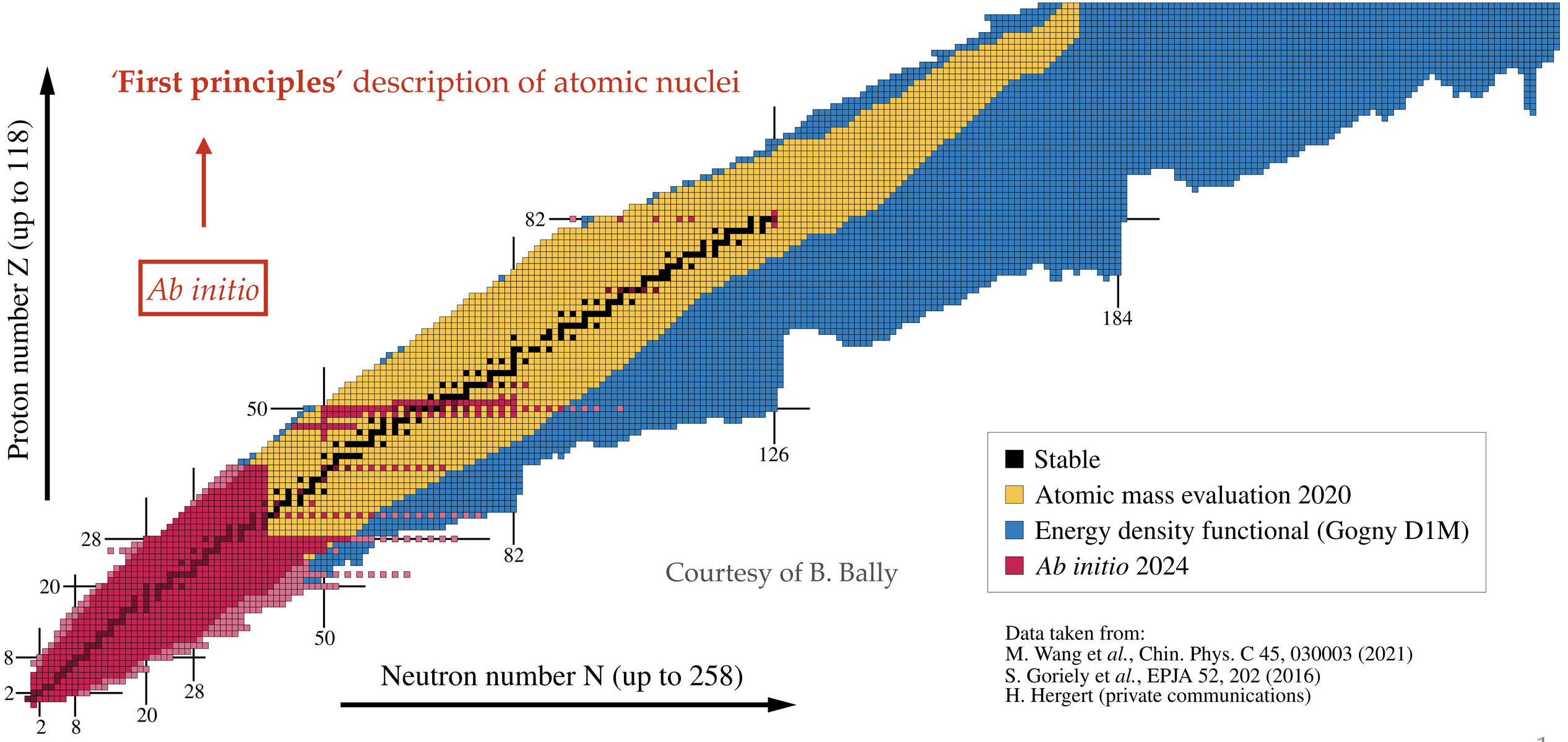

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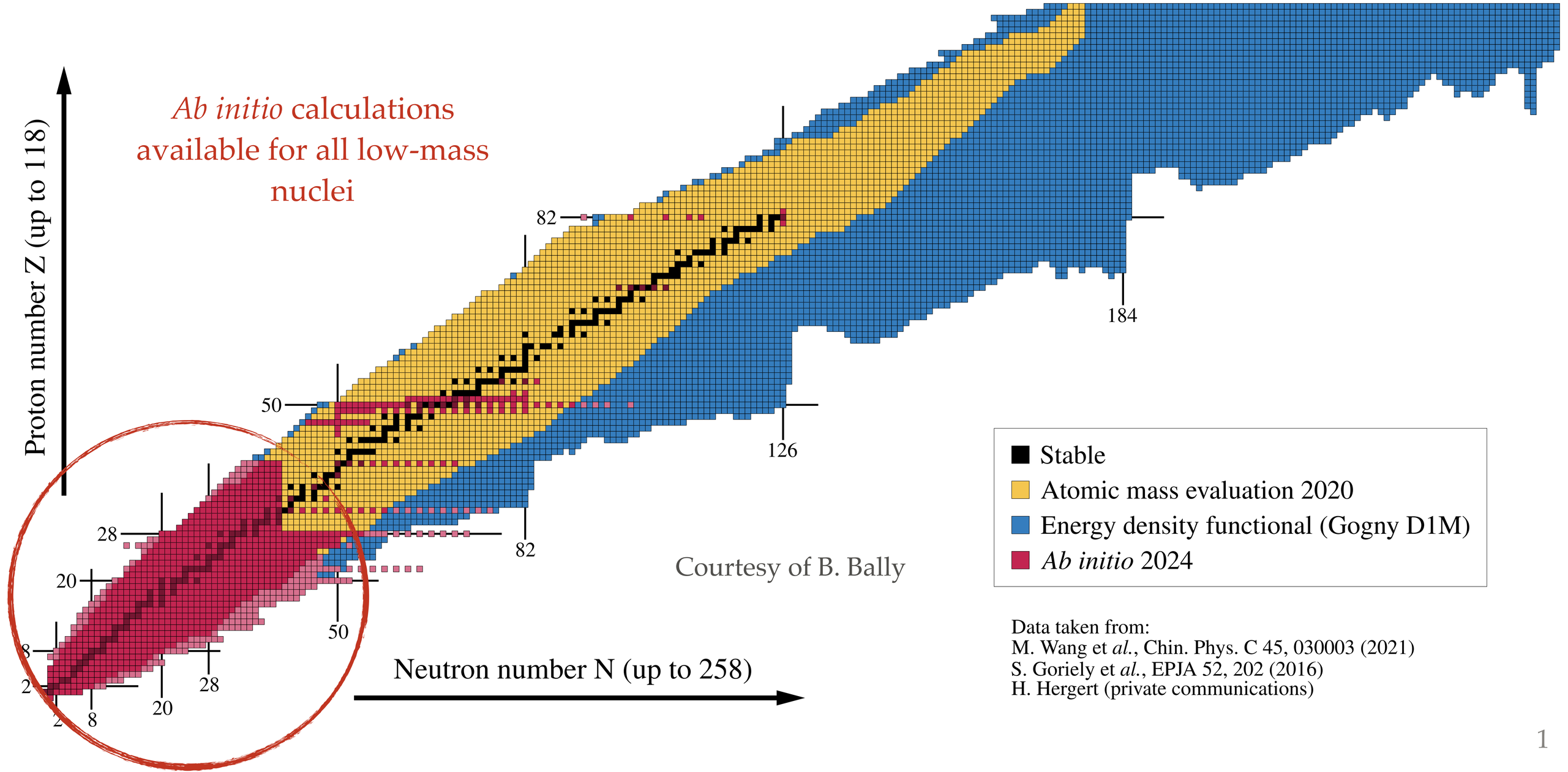

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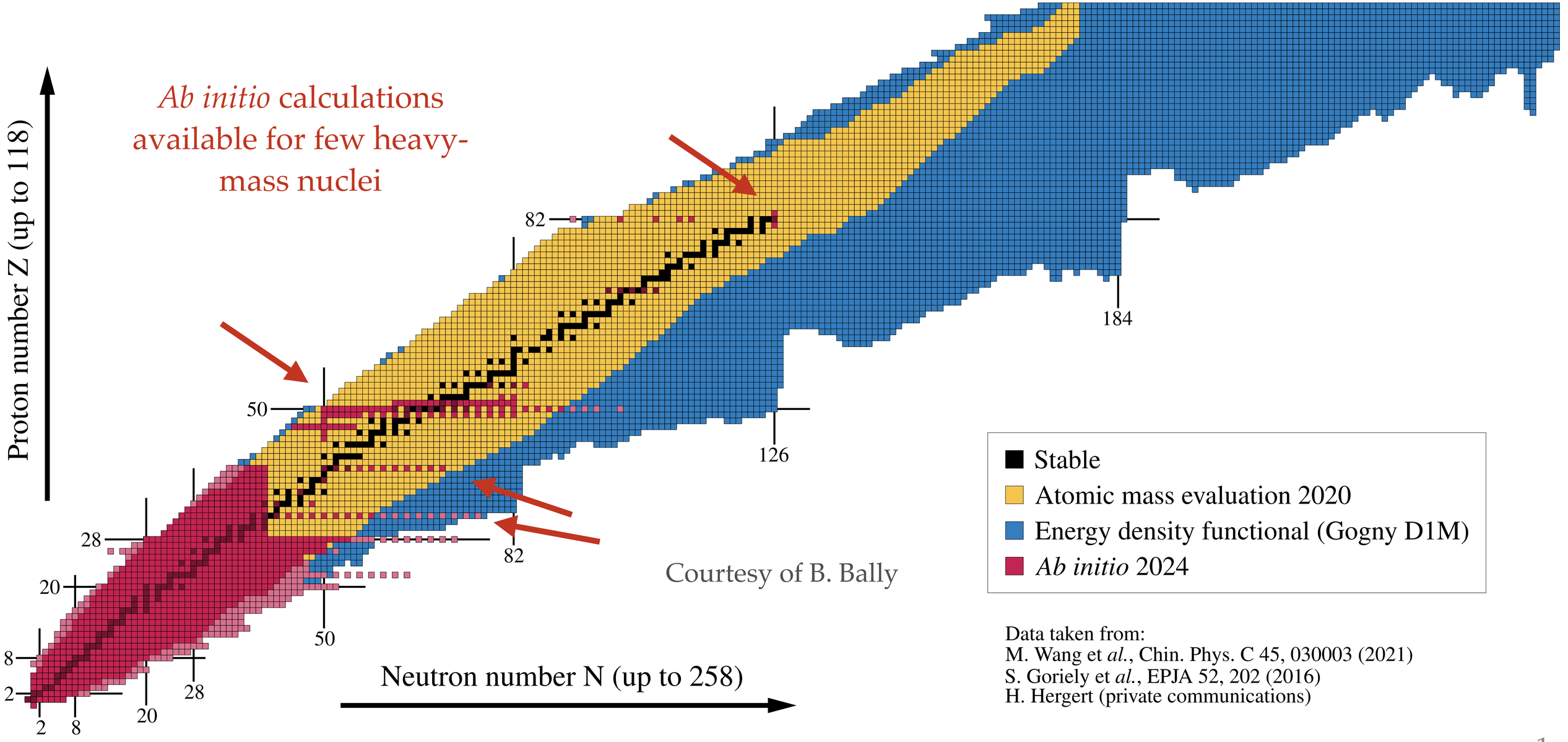

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Ab initio nuclear theory

- **Goal**: accurately describe atomic nuclei through systematically improvable methods
- **Dynamical equation** → non-relativistic many-body Schrödinger equation **(low-energy physics)**

$$H\,|\Psi_k^\sigma\rangle = E_k^\sigma\,|\Psi_k^\sigma\rangle$$

Total wave function

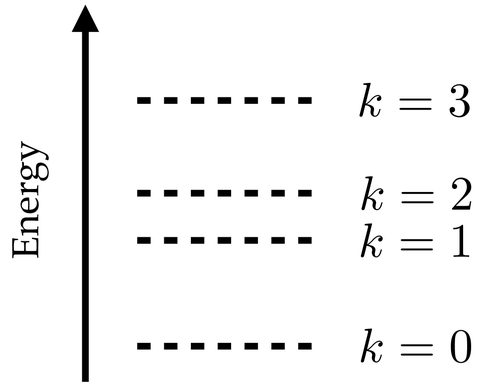
Total energy of the system

Hamiltonian operator: driving the equations of motion

- k runs over excited states of the system ($k = 0$ begin the ground-state)
- σ is the set of quantum number that characterizes the WF:

$$\sigma \equiv JM\Pi NZ$$

- J **total angular momentum**
- M **projection of** J
- Π **parity**
- N, Z **number of neutrons and protons**



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From **Chiral Effective Field Theory** (χEFT)

- Low-energy limit of QCD
- Nucleons and pions as effective d.o.f.
- Systematic expansion of H: NLO, N^{2}LO, N^{3}LO, …
- Set of symmetries: $[H, R(\theta)] = 0$

For **few-body systems** → exact solution

- Advantage: focus studies on H
- Drawback: techniques limited to low masses

For **many-body systems** → approximate solution

- Advantage: push calculations to $A \approx 200$
- Drawback: not applicable to every H

→ Non-trivial entanglement between H and $|\Psi_k^\sigma\rangle$ **interactions fit on MB systems**

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Systematically improvable approach

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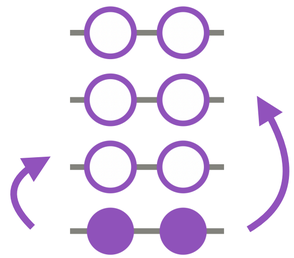
interactions fit on MB systems

Many-body *ab initio* methods

Correlation-expansion methods ⟶ CPU-scalable to heavy masses



Hamiltonian partitioning: $H = H_0 + H_1$

'easy'-to-handle — **'hard'-to-handle**

- Based on a mean-field approximation

↓

- Nucleons move independently in an average potential (**Hartree-Fock theory**)
- Delivers a reference state

$$H_0 \, |\Theta_k^{(0)}\rangle = E_k^{(0)} \, |\Theta_k^{(0)}\rangle$$

- Brings correlations on top of reference state
- Wave-operator expansion → **truncation**

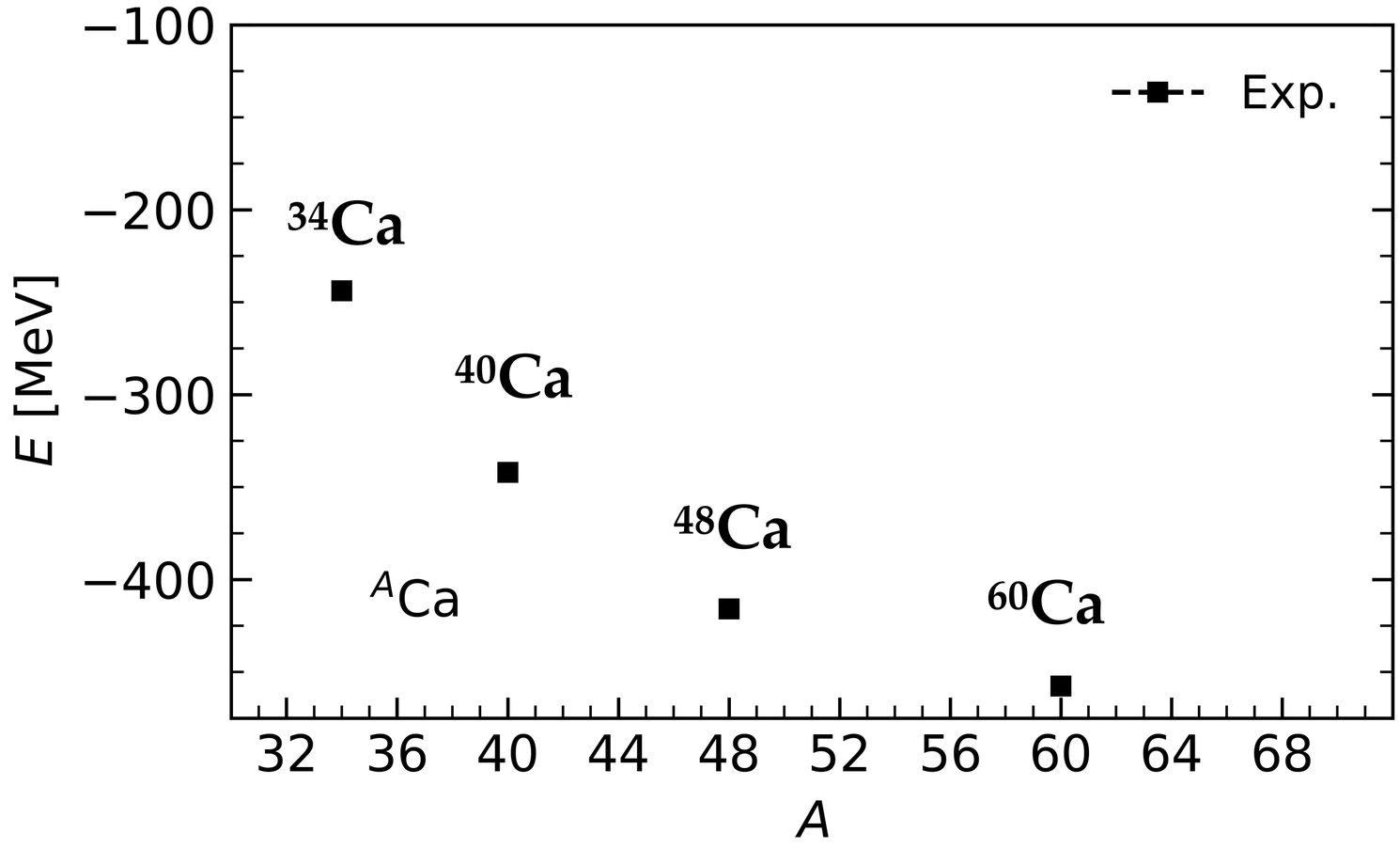
$$|\Psi_k^{\sigma}\rangle = \Omega_k \, |\Theta_k^{(0)}\rangle$$

- Beyond mean-field

Example of application: ground-state total energy

Calcium isotopic chain:

nuclei accessible with spherical methods



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Mean-field

- **HF** brings significant underbinding

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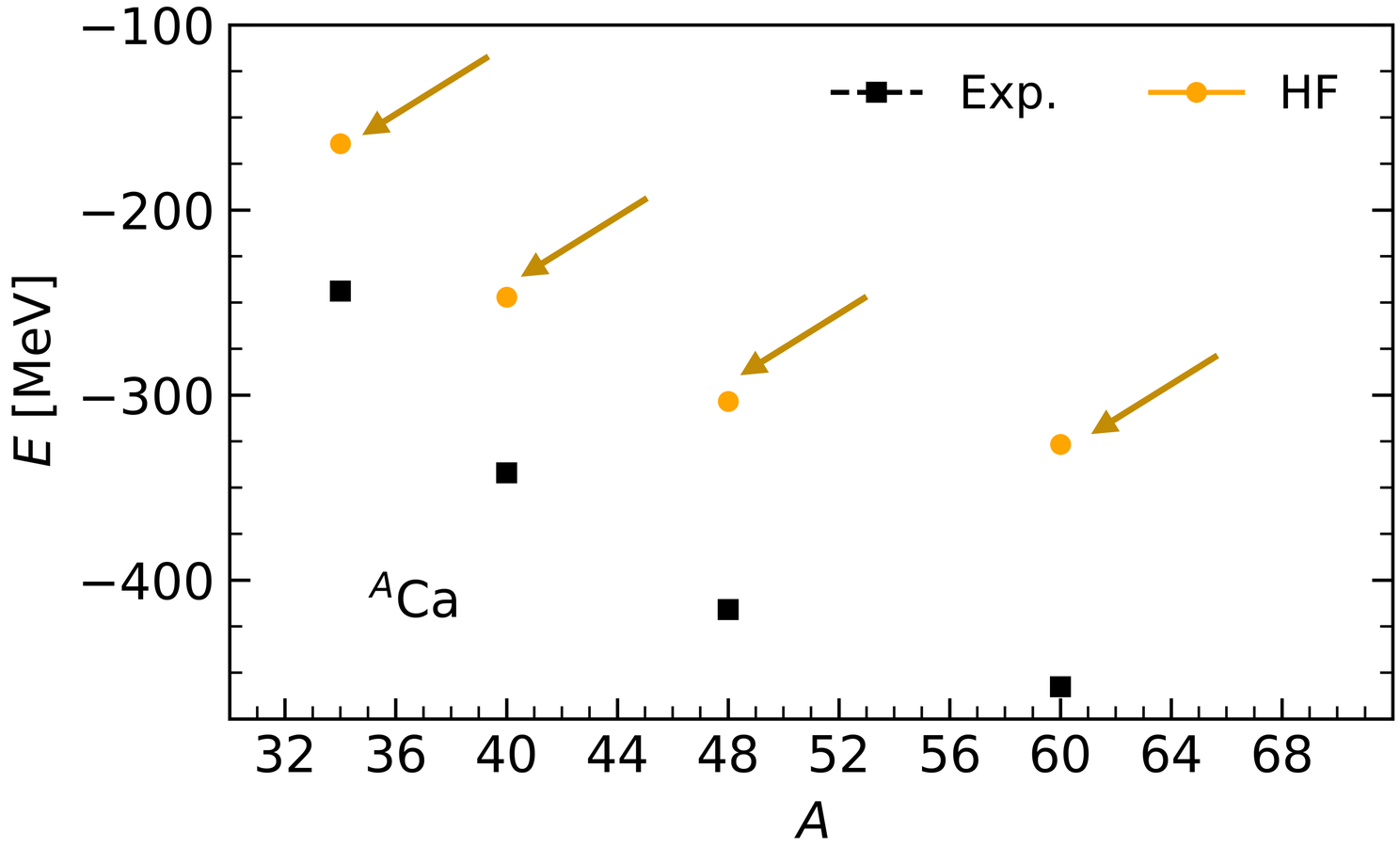

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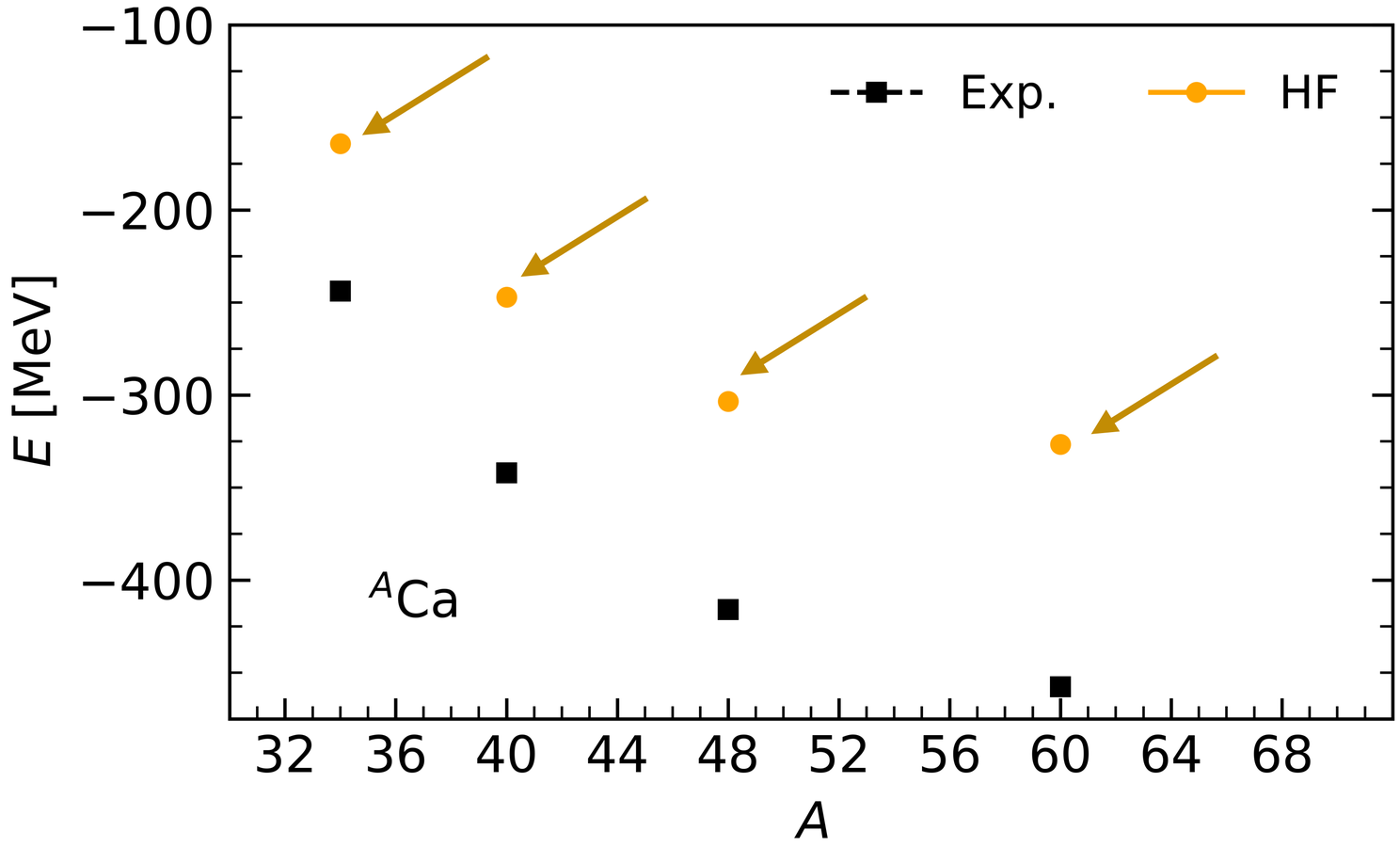

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- Perturbative expansion (Taylor-like)

  → Perturbation theory (**MBPT**)

- Non-perturbative expansion

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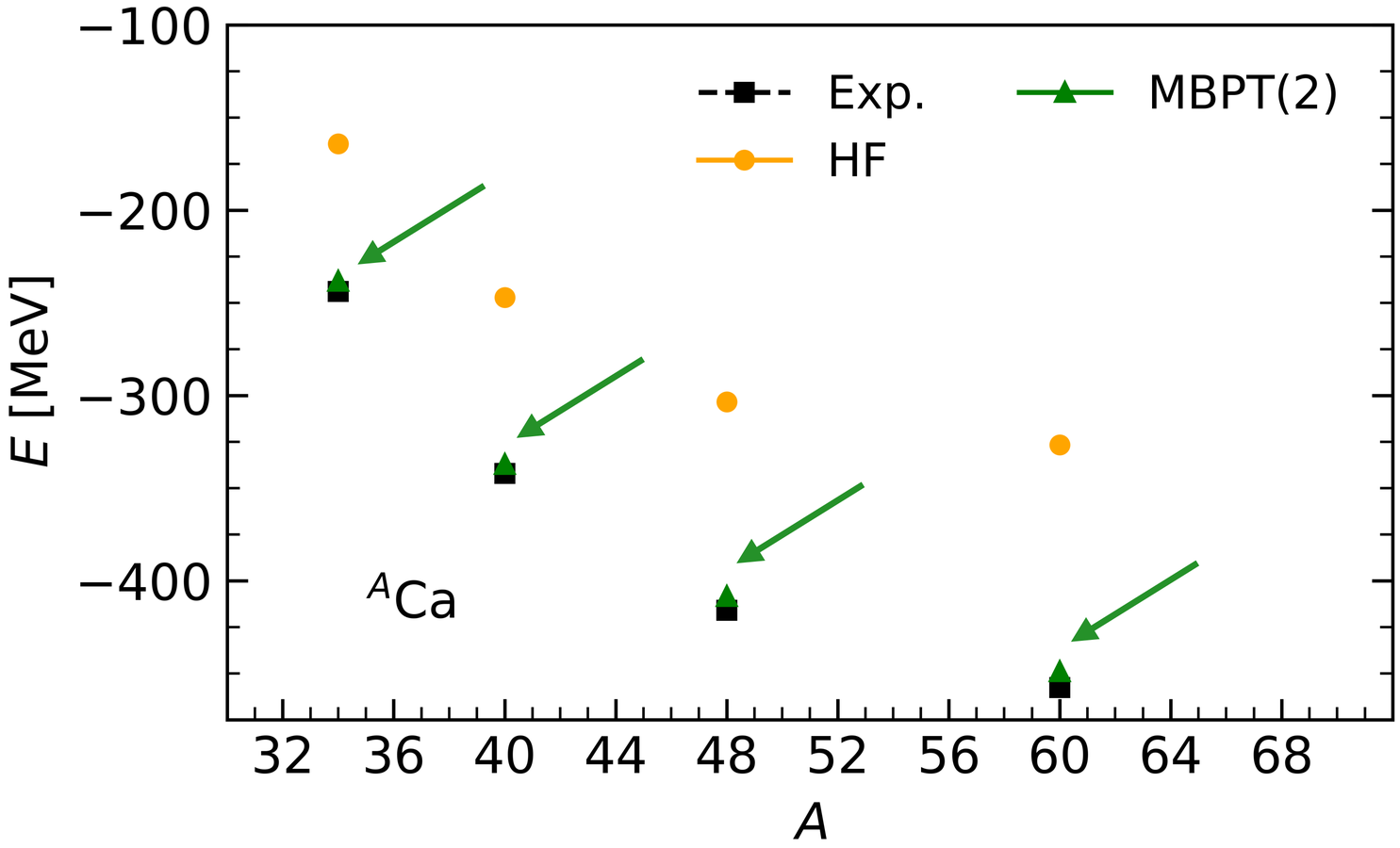

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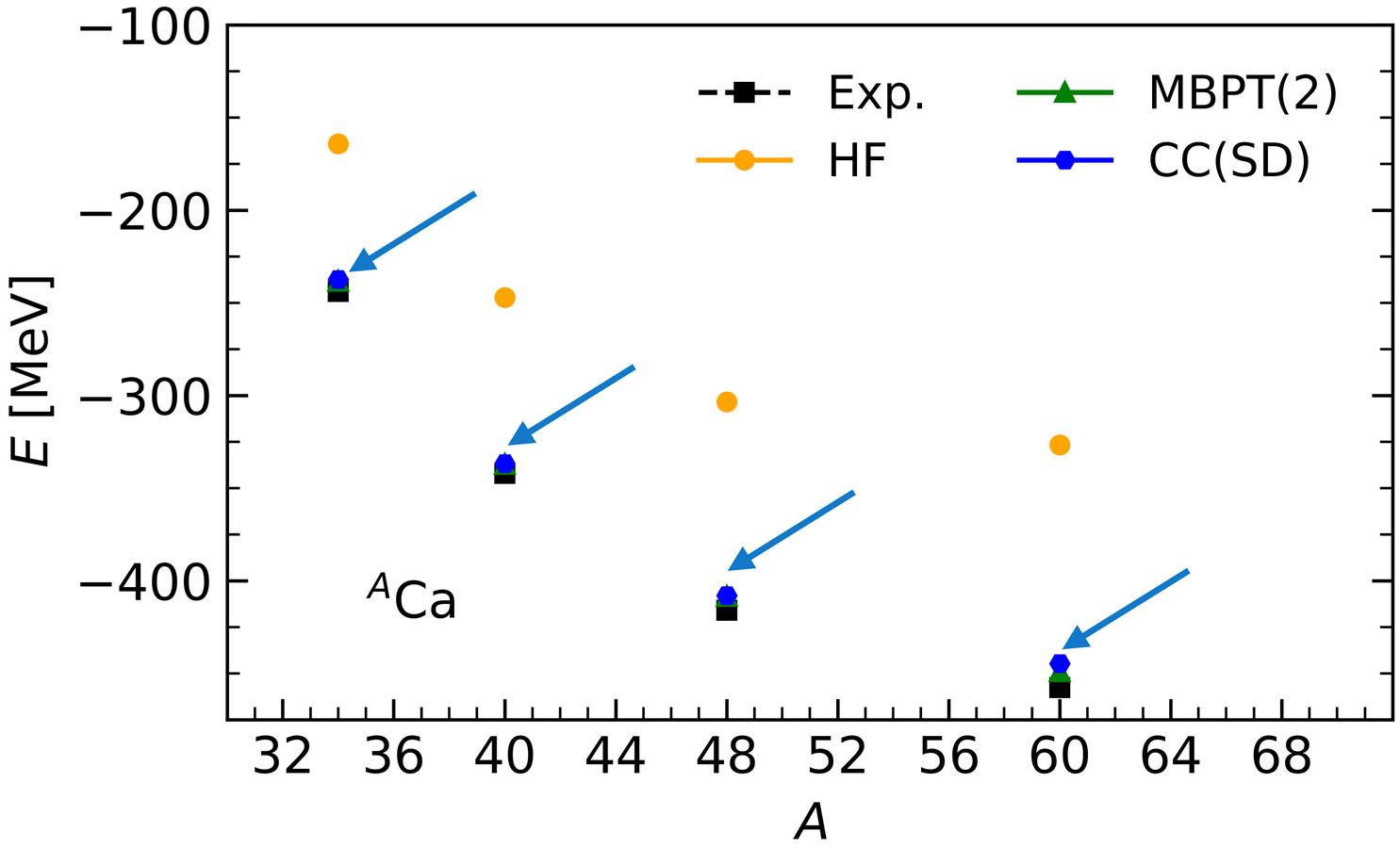

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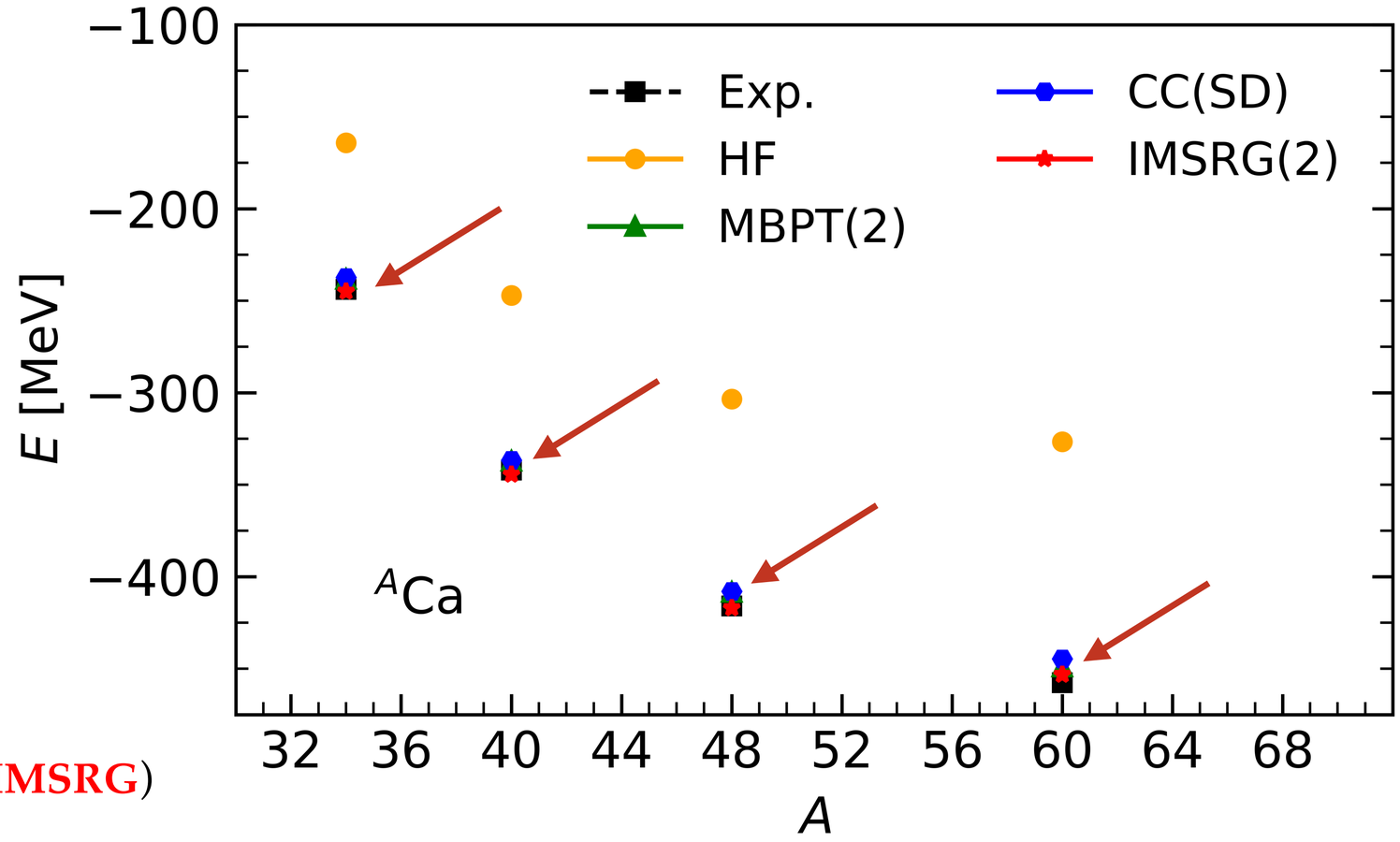

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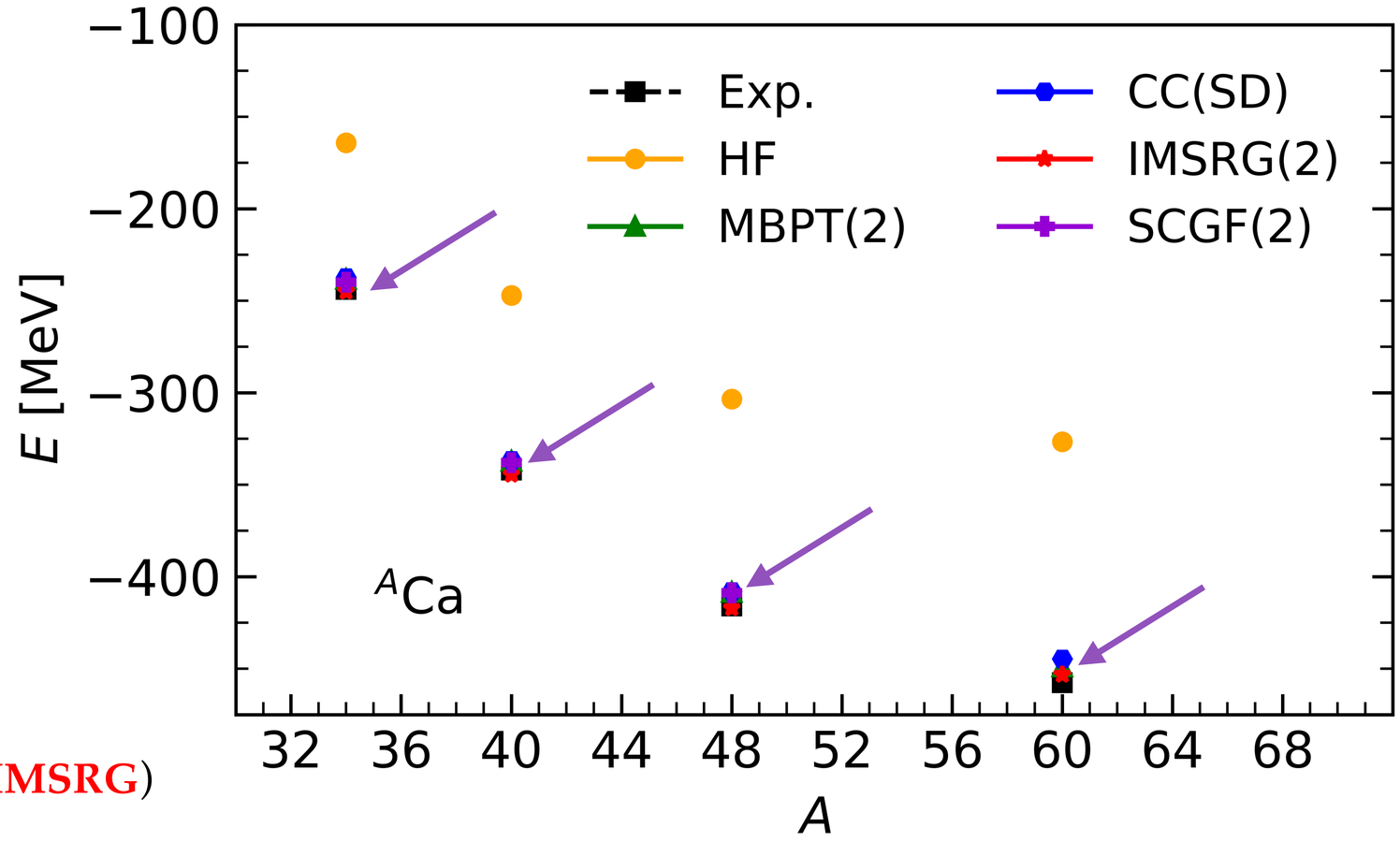

convergence of MB expansion

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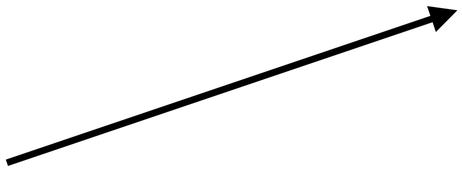

- Different methods are characterized by:
  - Resummation of different correlations
  - Differences in computational cost
  - Possible computation of different quantities

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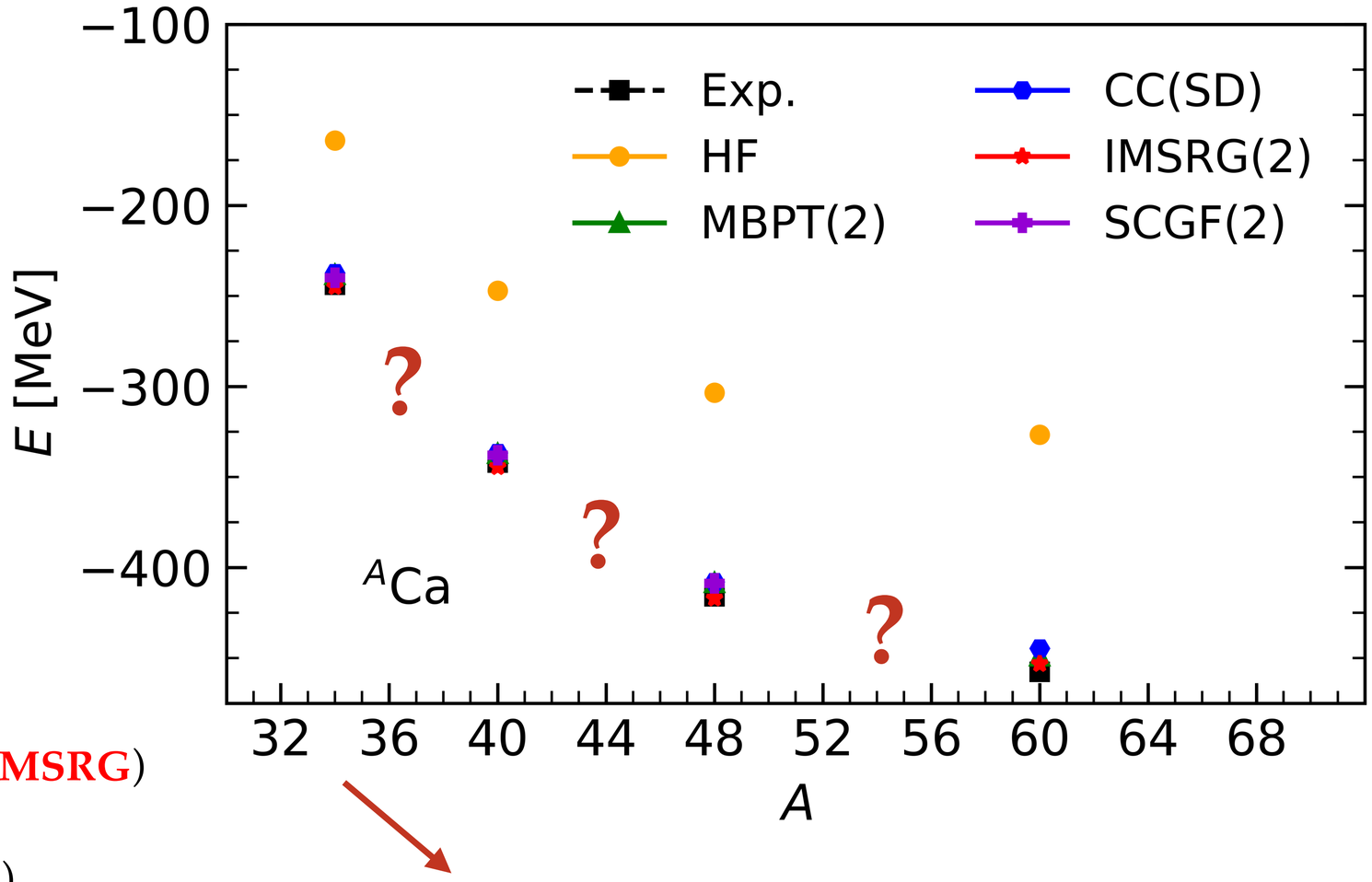

several points missing → odd nuclei

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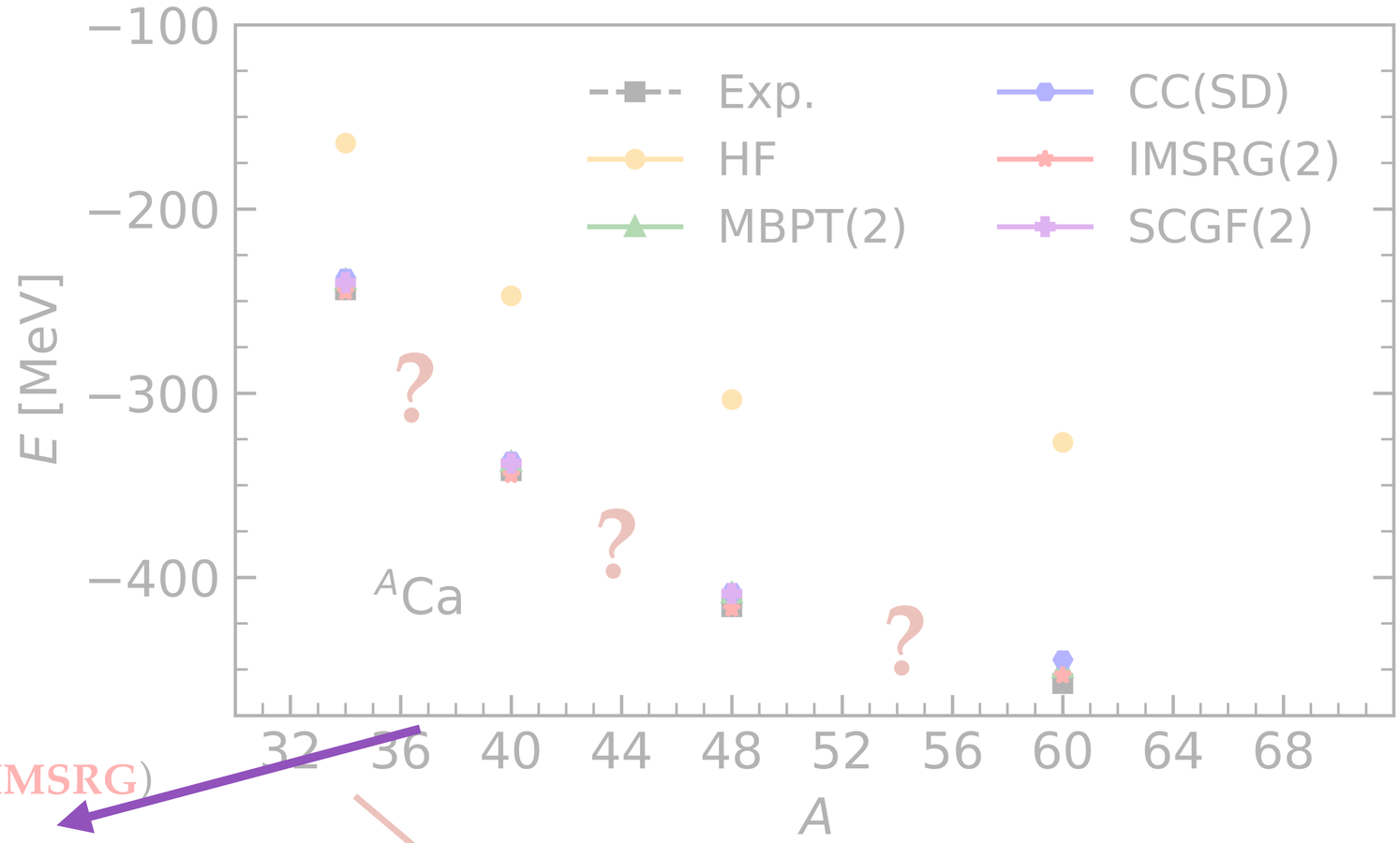

several points missing → open-shell systems

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Why choosing Green's function-based methods

- **Advantages**
  - Easy access to **odd-nuclei**
  - Access to **excited states**
  - Allow for computing **optical potentials** and one-nucleon scattering properties

- **Drawbacks**
  - Non-trivial formalism
  - **Increased computational cost** compared to other many-body *ab initio* methods

Spectral representation of the Green's function

$$g_{\alpha\beta}(\omega) = \sum_n \frac{(\mathcal{X}_\alpha^n)^* \mathcal{X}_\beta^n}{\omega - \varepsilon_n^+ + i\eta} + \sum_k \frac{\mathcal{Y}_\alpha^k (\mathcal{Y}_\beta^k)^*}{\omega - \varepsilon_k^- - i\eta}$$

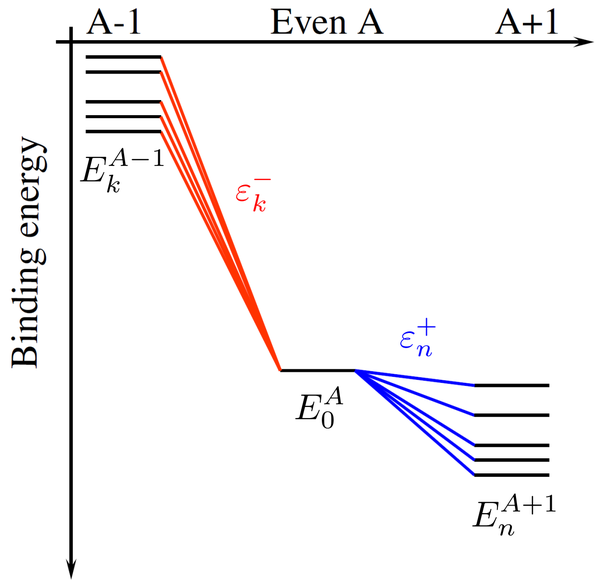
Separation energies

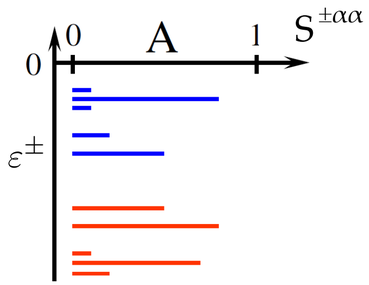
$$\varepsilon_n^+ = E_n^{A+1} - E_0^A$$
$$\varepsilon_k^- = E_0^A - E_k^{A-1}$$

Transition amplitudes

$$\mathcal{X}_\alpha^n = \langle \Psi_n^{\mathrm{A+1}} | a_\alpha^\dagger | \Psi_0^{\mathrm{A}} \rangle$$
$$\mathcal{Y}_\alpha^k = \langle \Psi_k^{\mathrm{A-1}} | a_\alpha | \Psi_0^{\mathrm{A}} \rangle$$

Numerator + denominator





Spectroscopic factors

$$SF_n^+ = \sum_{\alpha \in \mathcal{H}_1} |\mathcal{X}_\alpha^n|^2$$
$$SF_k^- = \sum_{\alpha \in \mathcal{H}_1} |\mathcal{Y}_\alpha^k|^2$$

Spectral strength distribution

$$\mathcal{S}(\omega) = \sum_{n \in \mathcal{H}_{A+1}} SF_n^+ \, \delta(\omega - \varepsilon_n^+) + \sum_{k \in \mathcal{H}_{A-1}} SF_k^- \, \delta(\omega - \varepsilon_k^-)$$

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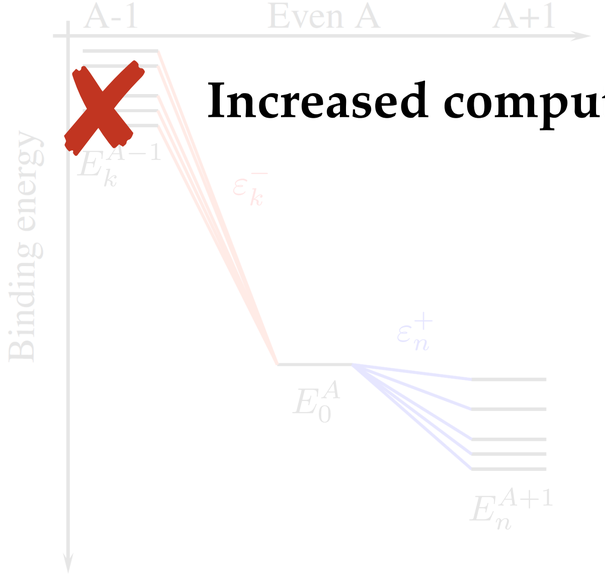

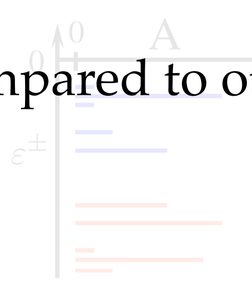

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- ✓ One single calculation delivers a wealth of information on **ground-state** and **excited states**
- ✗ **Increased computational cost** compared to other many-body *ab initio* methods

Basic ingredients of Self-Consistent Green's function

A-body wave function

$$|\Psi_k^A\rangle$$

A-body Schrödinger equation

$$H|\Psi_k^A\rangle = E_k^A|\Psi_k^A\rangle$$

Observables: expectation values

$$\mathrm{O} = \langle\Psi_0^A|O|\Psi_0^A\rangle$$

Green's functions

$$\mathrm{i}\, g_{\alpha\beta}(t_\alpha, t_\beta) \equiv \langle\Psi_0^A|\mathcal{T}[a_\alpha(t_\alpha)a_\beta^\dagger(t_\beta)]|\Psi_0^A\rangle$$

$$\mathrm{i}\, g^{4-\mathrm{pt}}_{\alpha\gamma\beta\delta}(t_\alpha, t_\gamma, t_\beta, t_\delta) \equiv \langle\Psi_0^A|\mathcal{T}[a_\gamma(t_\gamma)a_\alpha(t_\alpha)a_\beta^\dagger(t_\beta)a_\delta^\dagger(t_\delta)]|\Psi_0^A\rangle$$

$\dots$

Dyson equation

$$g_{\alpha\beta}(\omega) = g_{0\,\alpha\beta}(\omega) + \sum_{\gamma\delta} g_{0\,\alpha\gamma}(\omega)\, \Sigma^\star_{\gamma\delta}(\omega)\, g_{\delta\beta}(\omega)$$

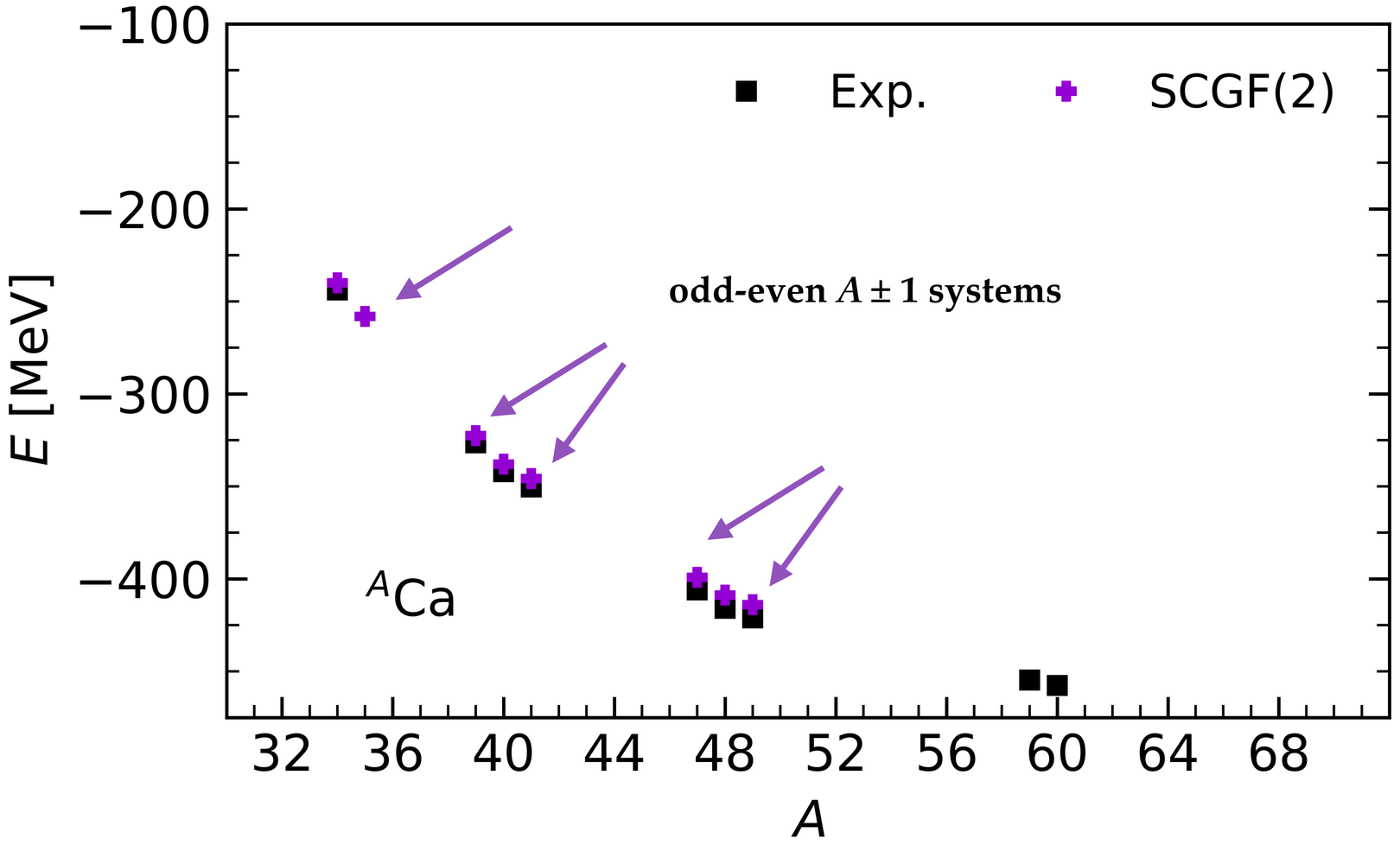
Self-energy expansion → Many-body approximation

Observables: convolutions with GFs

$$\langle\Psi_0^A\,|\,O^{1\mathrm{B}}\,|\,\Psi_0^A\rangle = \sum_{\alpha\beta}\int \frac{d\omega}{2\pi i}\, g_{\beta\alpha}(\omega)\, o_{\alpha\beta}$$

Ground-state energy of odd-even systems

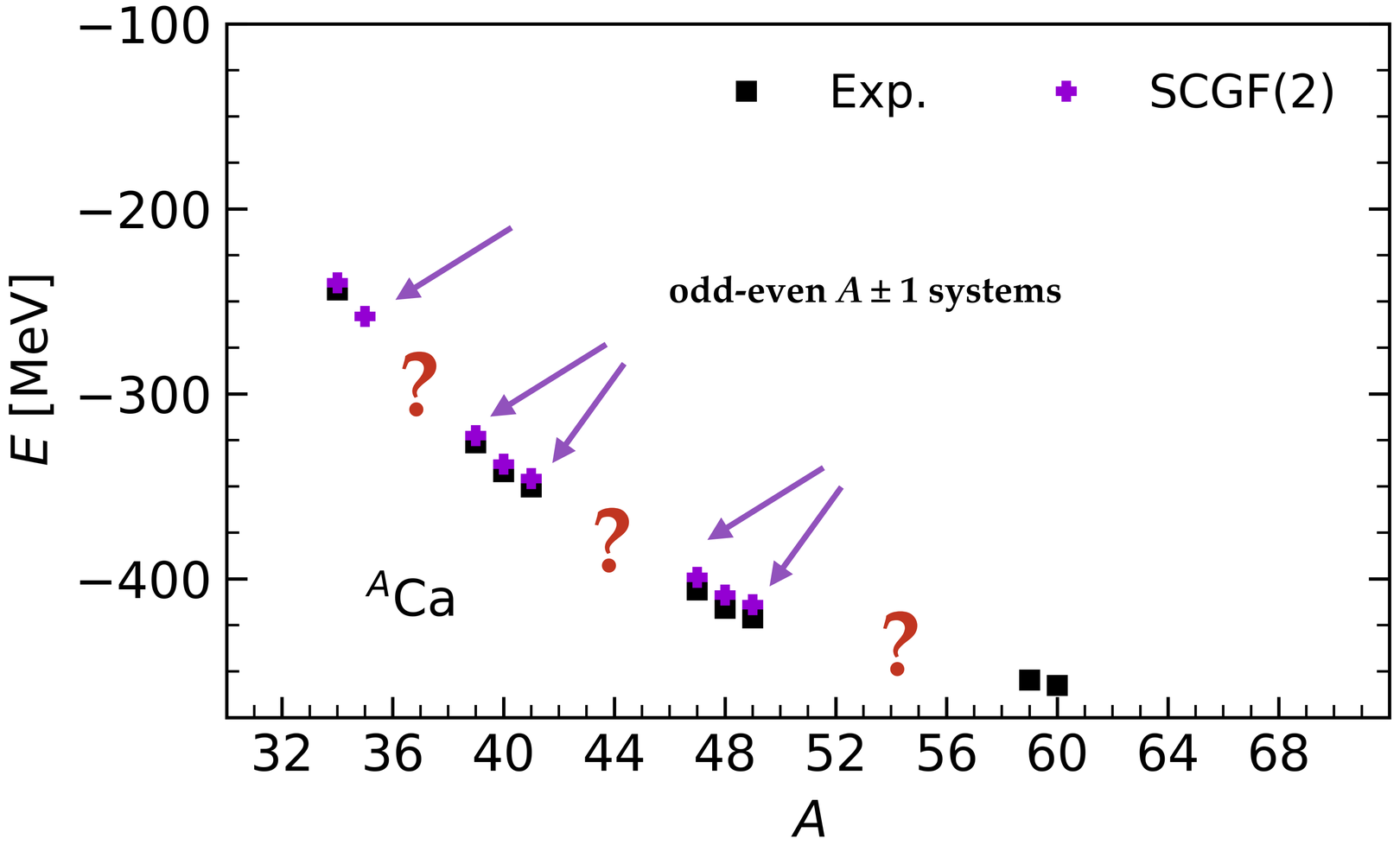
- A single calculation on a system with A particles delivers the ground-state energies of $A \pm 1$ systems



Ground-state energy of odd-even systems

A few missing points have been filled, but **the majority of them are still missing…**

open-shell systems



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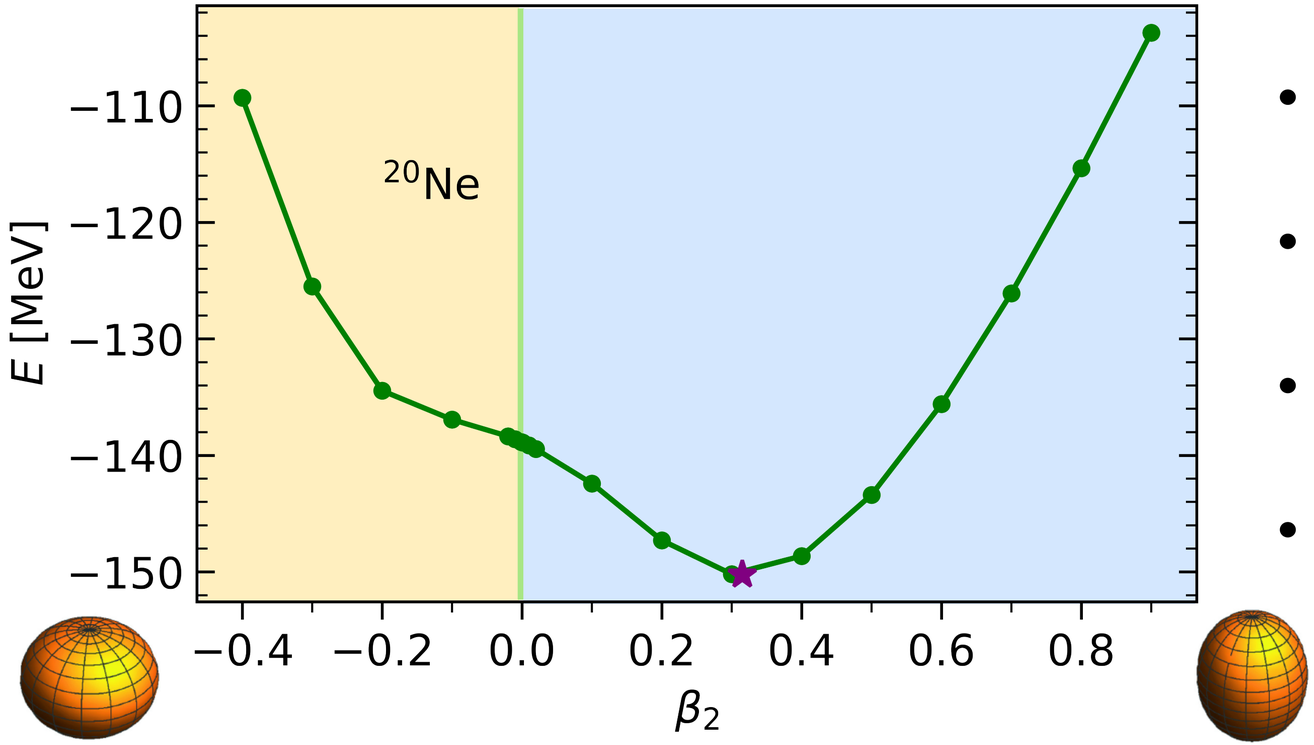
Strongly correlated systems: deformation

- Consider the breaking of rotational symmetry SU(2), which translates in the loss of good angular momentum J for $|\Psi_0^k\rangle$
- We can plot the ground-state energy as a function of the quadrupole deformation parameter β_2

Hartree-Fock method (delivering the reference state $|\Theta_k^{(0)}\rangle$)



- $\beta_2 = 0$ **spherical solution**
- $\beta_2 < 0$ **oblate solutions**
- $\beta_2 > 0$ **prolate solutions**
- ★ **global minimum**

- Deformation allows to explore a wider region of the Fock space
- Since HF is variational, this translates into a wider set of correlations when the solution $|\Theta_k^{(0)}\rangle$ is deformed

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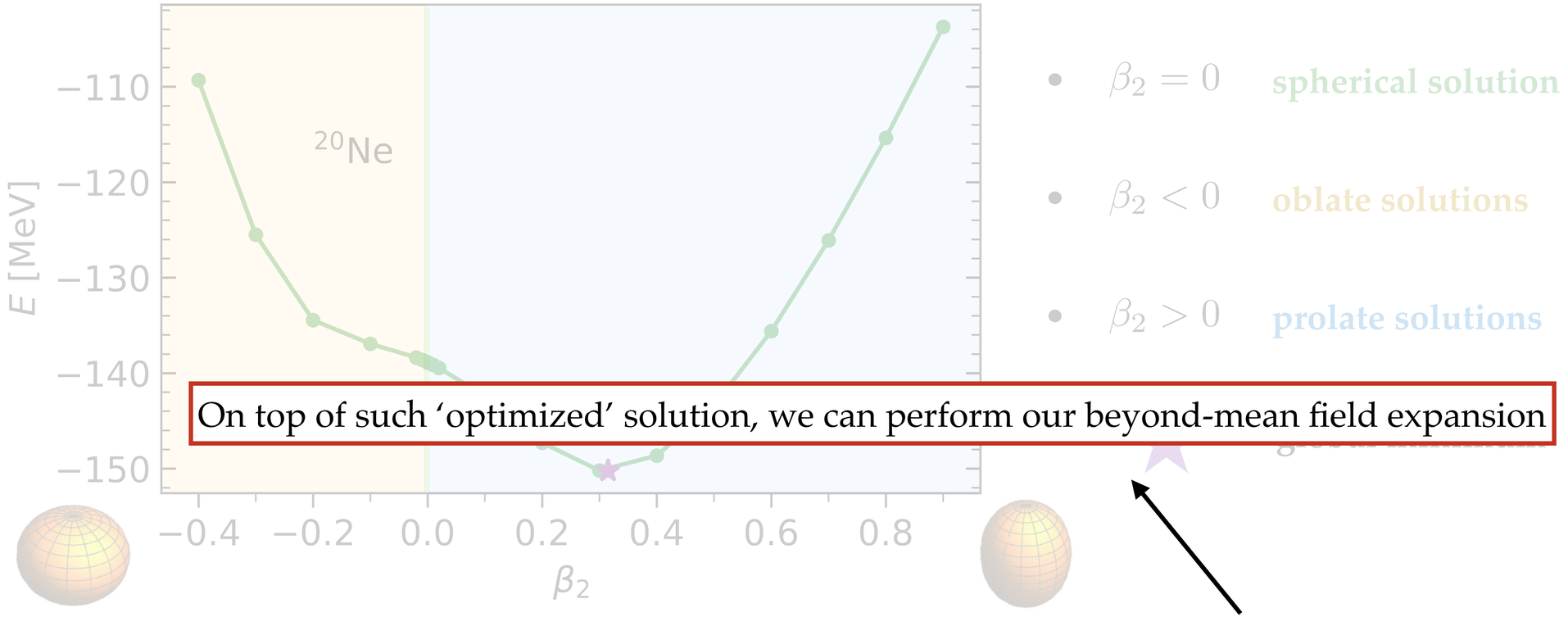

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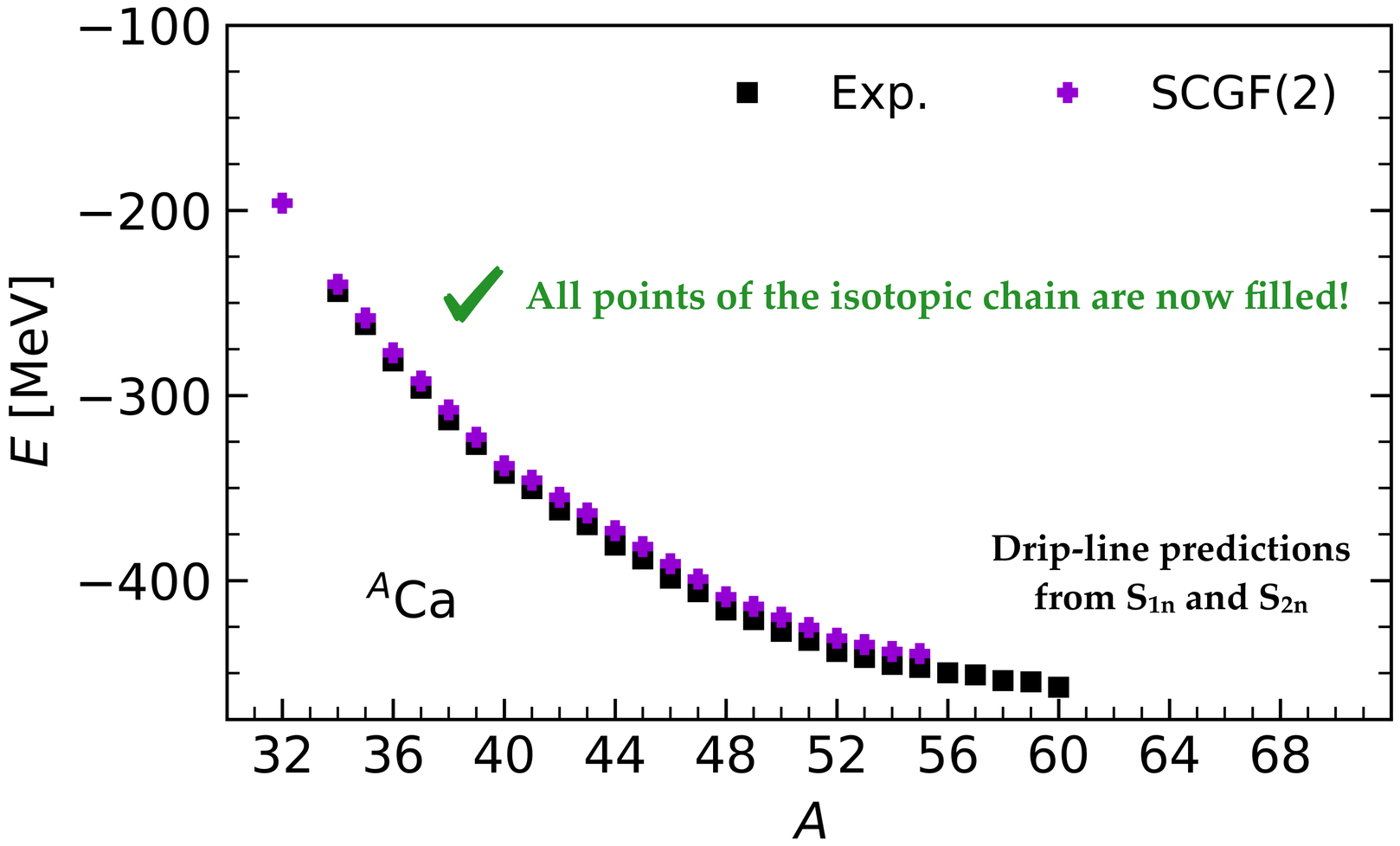
Ground-state energy of open-shell systems



Ab initio description of all nuclei … but there is no free lunch:

Deformed calculations → reduced number of symmetries → **increased computational cost**

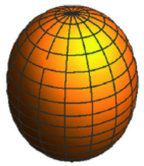
Extension to further symmetry breaking

So far **only axial symmetry** was considered ...

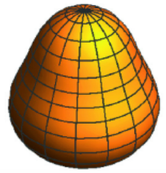
Breaking more symmetries allows to effectively enrich more the mean-field with correlations

Different types of deformation can be obtained by **breaking different symmetries**:

- **Axial** deformation $\rightarrow$ break total angular momentum J



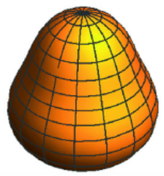
- **Ocupolar** deformation $\rightarrow$ break J and parity Π

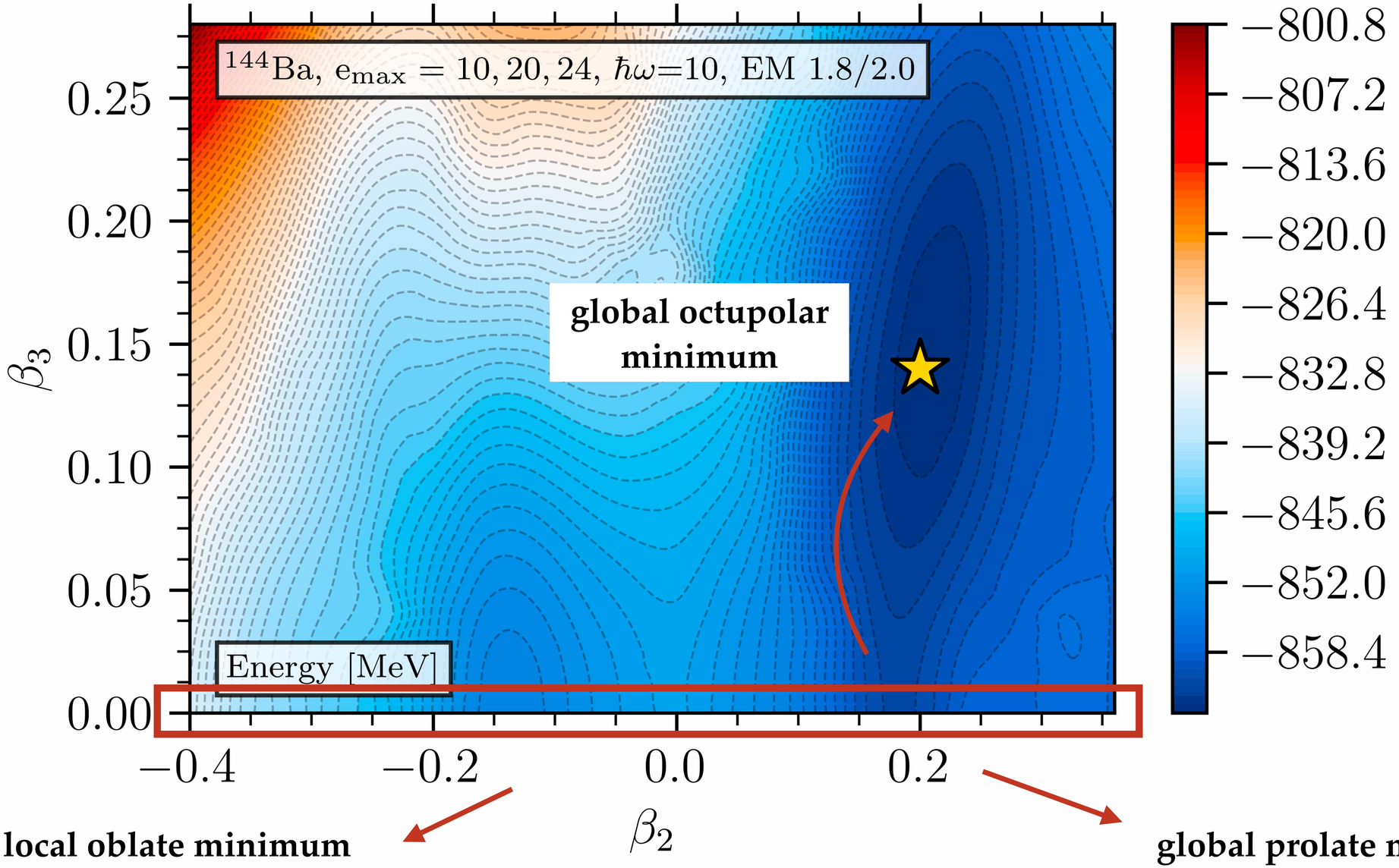


- **Triaxial** deformation $\rightarrow$ break J and its projection M along the quantization axis

- ...

Extension to further symmetry breaking

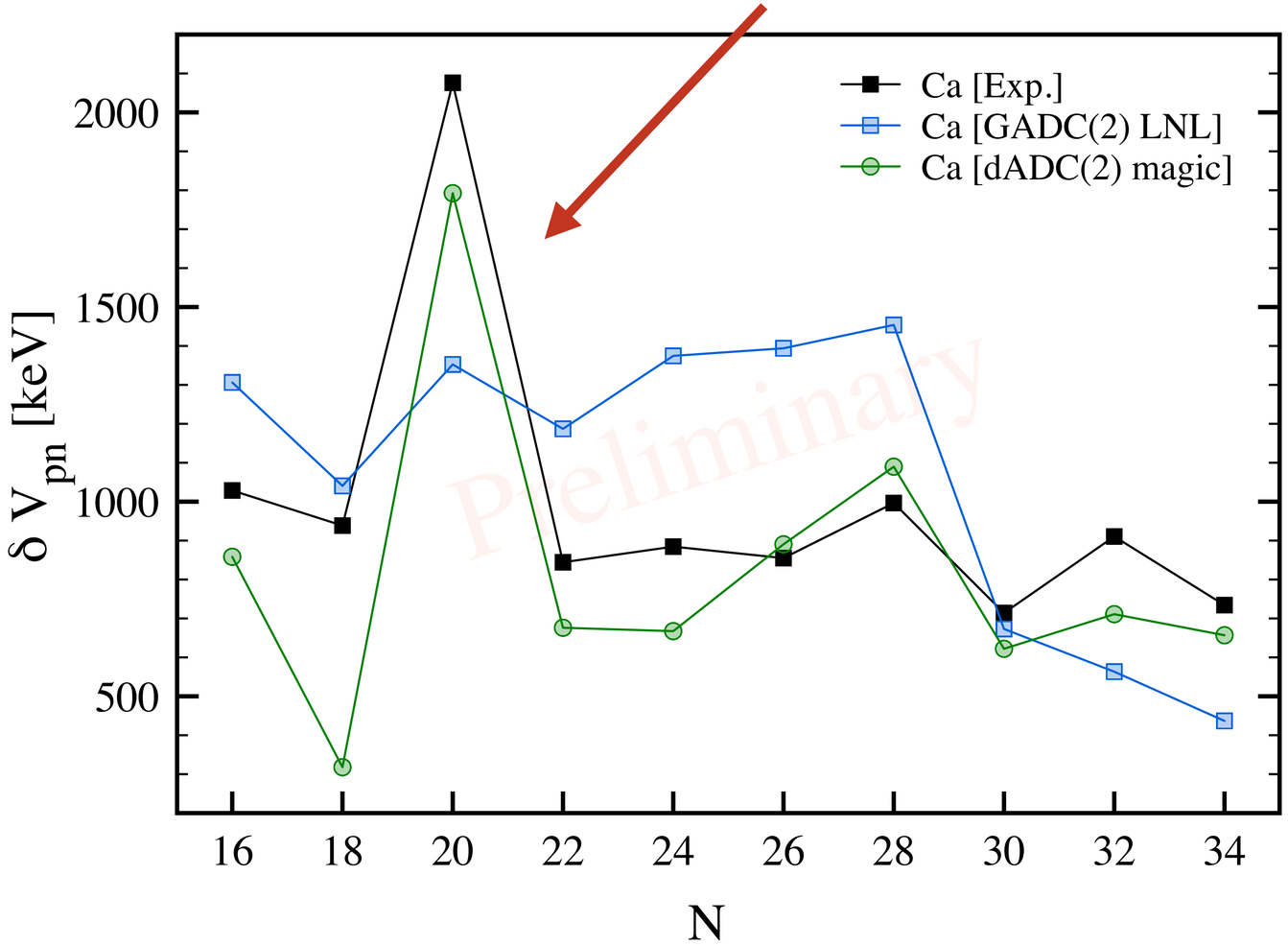




[A. Scalesi et al., *in preparation*]

Comparing spherical and deformed methods

Residual *pn* interaction: $\delta V_{pn} = \frac{1}{4}[B(N,Z) + B(N-2,Z-2) - B(N,Z-2) - B(N-2,Z)]$



- Computed for Calcium isotopes
- Peak when crossing **closed-shell configurations**
- Sensitive to **Argon deformations**
- $N = 20$ peak captured only with dDSCGF(2)

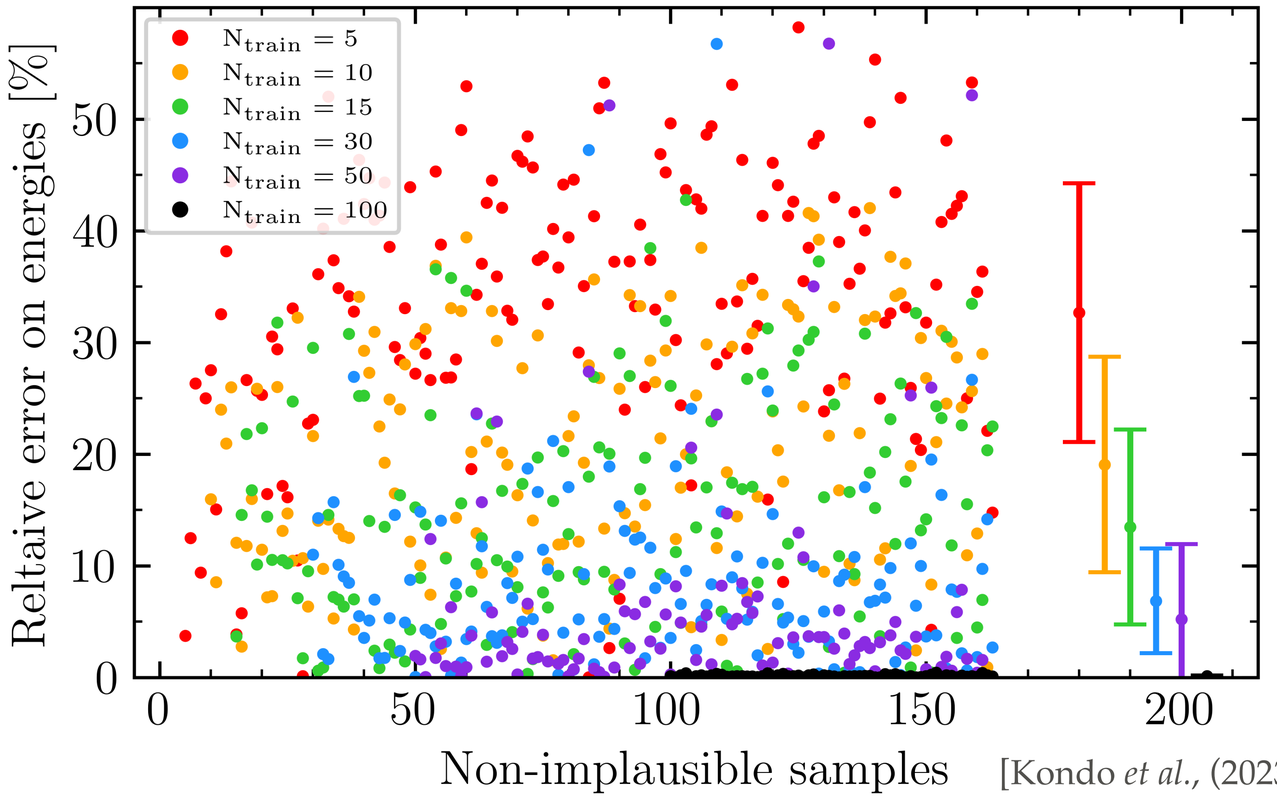
[Fu *et al., in preparation*] [Somà *et al.*, 2011]

Emulation of many-body calculations

Goal: reduce computational cost of MB calculations

- Parametric Matrix Models (PMM) [Cook *et al.*, (2025)]
- **Reduced-basis model** built with **machine learning**
- **Emulation** of HF ground-state energies

Emulation of many-body calculations



[Kondo *et al.*, (2023)]

- Parametric Matrix Models (PMM) [Cook *et al.*, (2025)]
- **Reduced-basis model** built with **machine learning**
- **Emulation** of HF ground-state energies

→ 3x3 matrices!

2.08 days for 100 training data

15.48 seconds for 1 Million emulations

vs

57 years for 1 Million calculations!

Conclusions

- *Ab initio* methods are a useful tool for a '**first principle**' description of atomic nuclei
- Many-body methods allow to access **high-masses**…

  … but constitute an **approximate solution** of the Schrödinger equation
- Spherical-symmetry - based approach limit the study to closed-shell nuclei
- Green's function approaches allow to extend the reach of many-body methods to **odd nuclei**
- Symmetry-breaking many-body methods allow for the description of **open-shell nuclei**
- **Emulators** can drastically reduced computational cost and can be used for interaction-sensitivity studies

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