Ab initio perturbative and non-perturbative methods for open-shell nuclei



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Nuclear theory for astrophysics: bridging bound-state and continuum physics

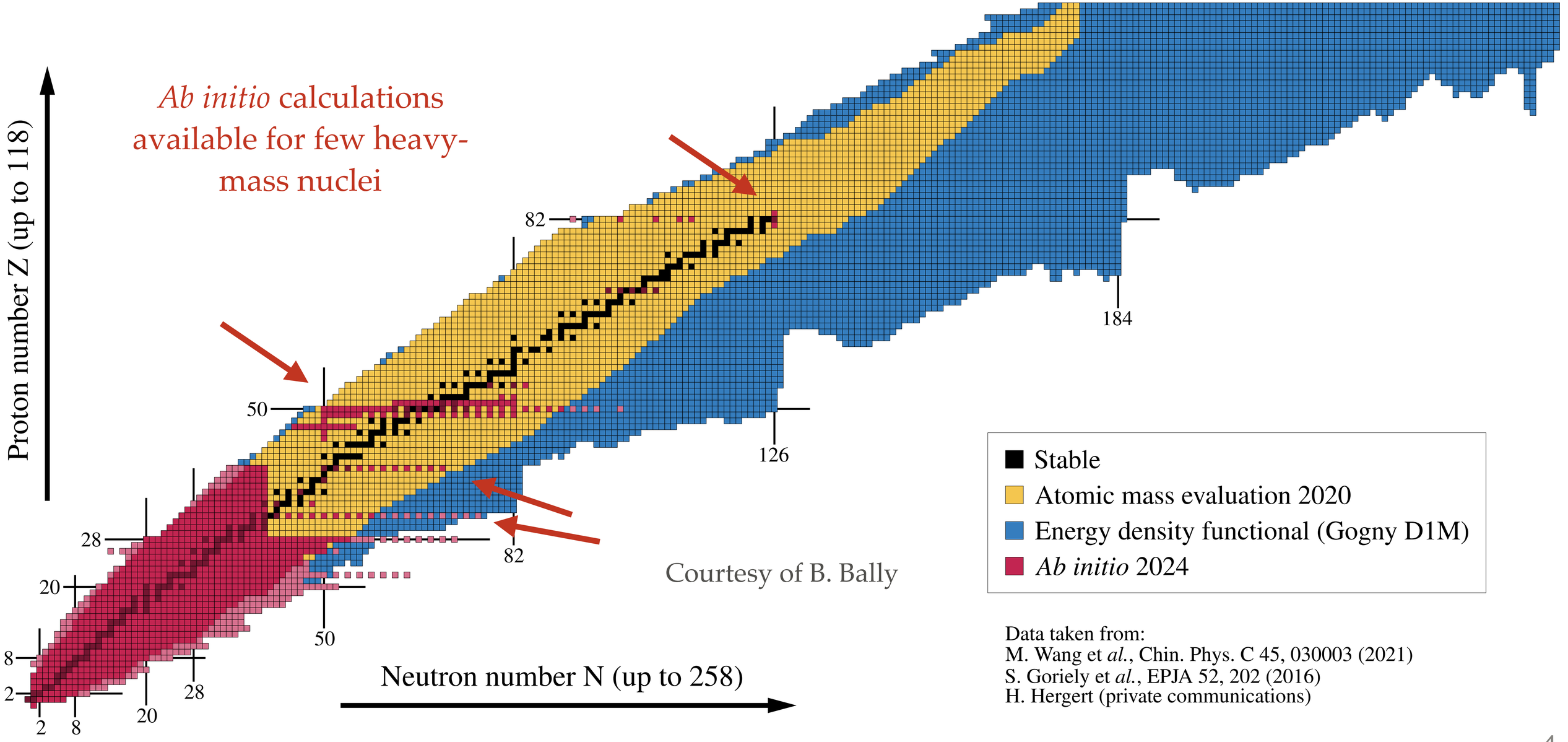
22nd May 2026, Trento

Outline

- Optimization of a*b initio* reference state by breaking symmetries
- The challenge in calcium isotopes
- Emulations
- Beyond the spherical Harmonic Oscillator basis
- Conclusions and current challenges

Optimization of a*b initio* reference state by breaking symmetries

The Segrè chart



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 dynamical equation

Dynamical equation → non-relativistic many-body Schrödinger equation **(low-energy physics)**

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

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**

Solving the Schrödinger equation at polynomial cost

Our choice: **polynomial methods with** A → CPU-scalable to heavy masses

static correlations

↓

included in ref. state through sym. break.

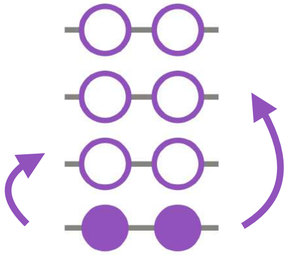
⟶ **Correlation-expansion methods**

Hamiltonian partitioning: $H = H_0 + H_1$

size of 1B Hilbert space

'easy'-to-handle ⟶ mean-field-like N^4

Eigenvalue equation for the **unperturbed state**: $H_0 \left|\Theta_k^{(0)}\right\rangle = E_k^{(0)} \left|\Theta_k^{(0)}\right\rangle$



'hard'-to-handle ⟶ beyond-mean-field N^p, $p > 4$

Wave-operator expansion: $\left|\Psi_k^\sigma\right\rangle = \Omega_k \left|\Theta_k^{(0)}\right\rangle$ ⟶ **Resummation of dynamical correlations**

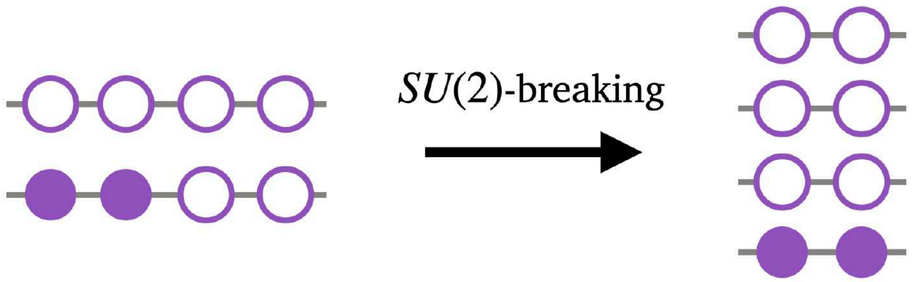
- **Perturbative** expansion: Taylor-like series, **BMBPT**
- **Non-perturbative** expansion: CC, **SCGF**, IMSRG

⟶ What is an optimal choice for the **reference state**?

The reference state

Symmetries of the reference state

- Chosen to lift particle-hole degeneracies:



- Chosen to include relevant static correlations for the **system under study**

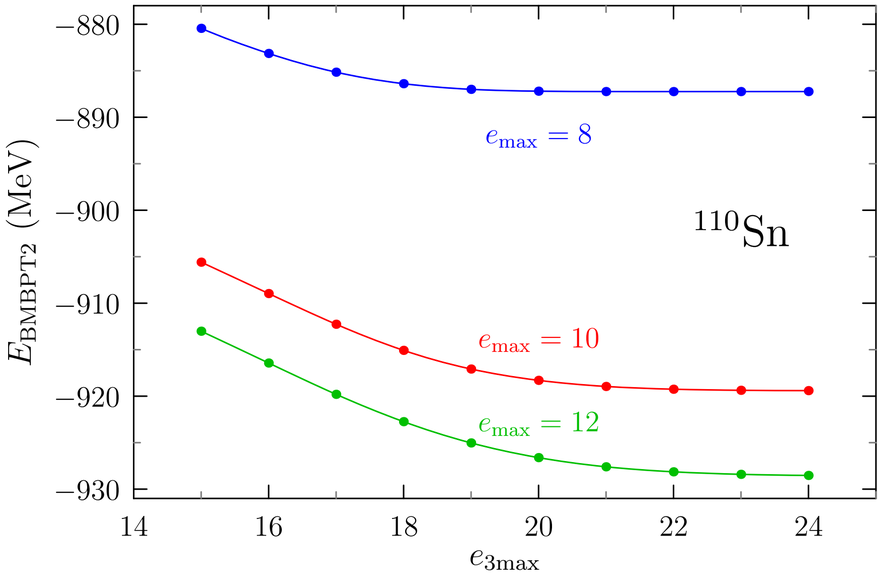
	Doubly closed-shell	~2010	**sHF**	[Barbieri, Bogner, Hagen, Hergert, …]
U(1)	**Singly open-shell**	2010 - 2020	**sHFB**	[Demol, Duguet, Hergert, Somà, Tichai, …]
SU(2)	**Doubly open-shell**	2020 - …	**dHF(B)**	[Duguet, Frosini, Hagen, …]

⟶ **Main focus on doubly open-shell nuclei, the most abundant ones!**

Many-body perturbation theory

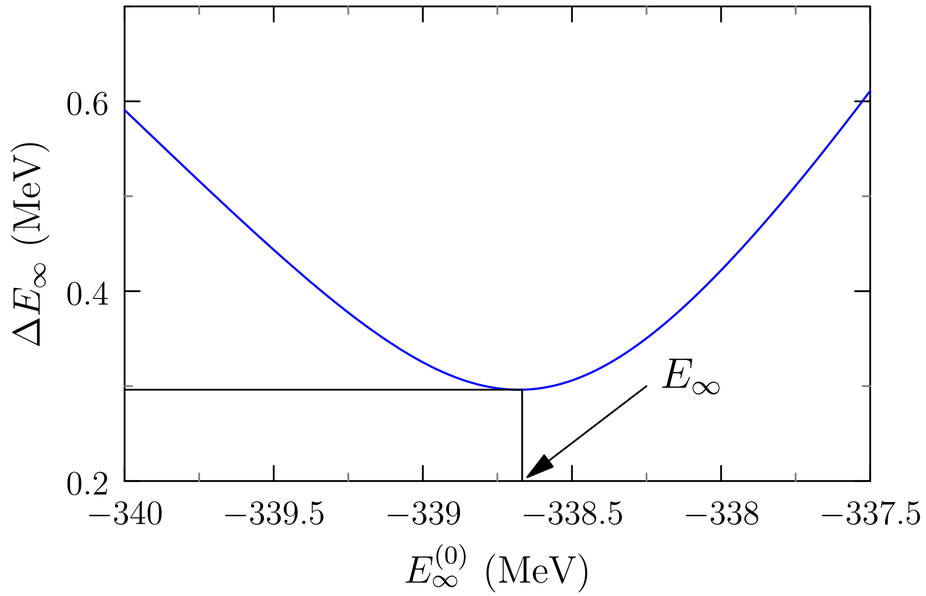
Perturbative methods: dBMBPT

- (deformed) [Bogoliubov] many-body perturbation theory (dBMBPT)
- Breaking of U(1) and SU(2) symmetries allowed at the same time
- Versatile tool for the description of singly and doubly open-shell nuclei



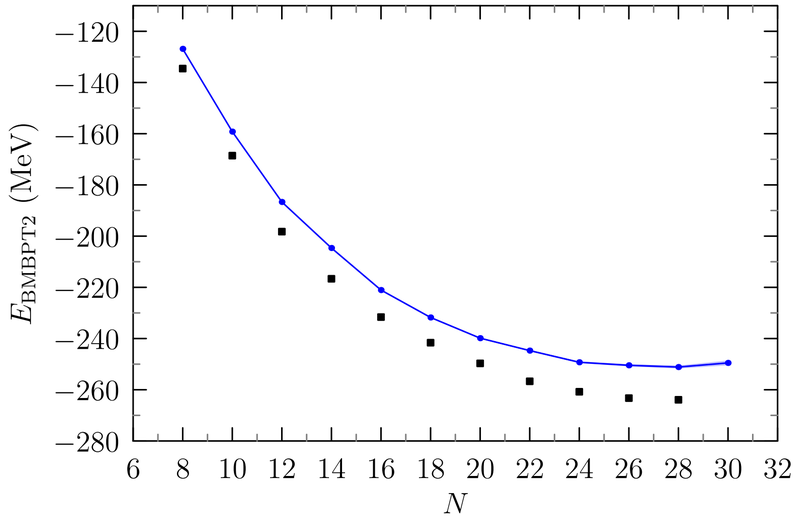
Large-scale calculations

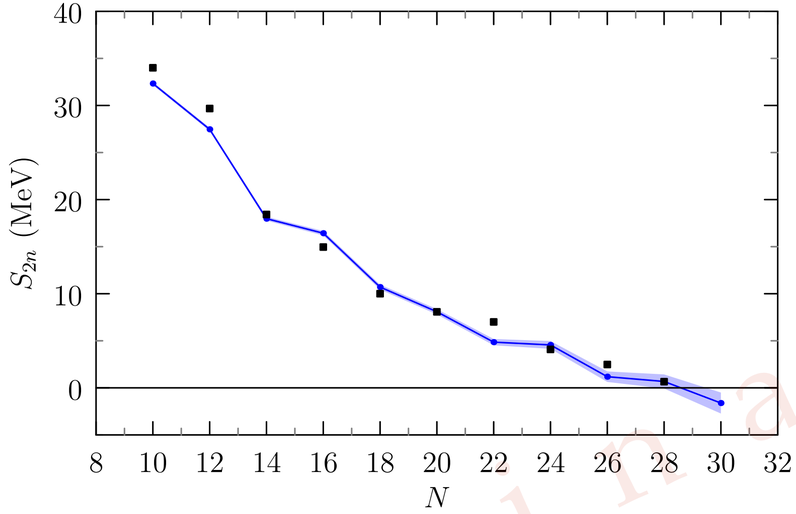
- Versatile tool for the description of singly and doubly open-shell nuclei
- **All even-even nuclei with $2 \leq Z \leq 50$** at **BMBPT2** level → ~ 520 isotopes
- Model space → e_{max} = 6-10, e_{3max} = 15-24, different $\hbar\omega$
- e_{max} and e_{3max} extrapolations under control
- **Evaluation of other uncertainties** ongoing (BMBPT3, symmetry breaking, …)

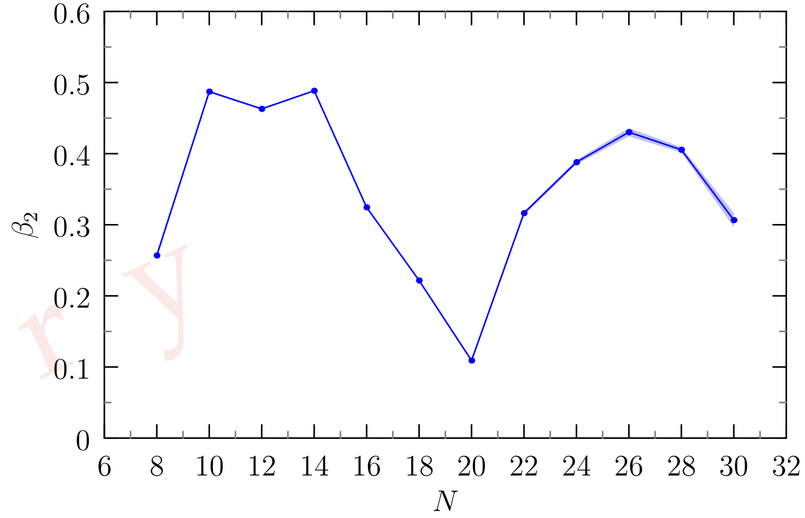


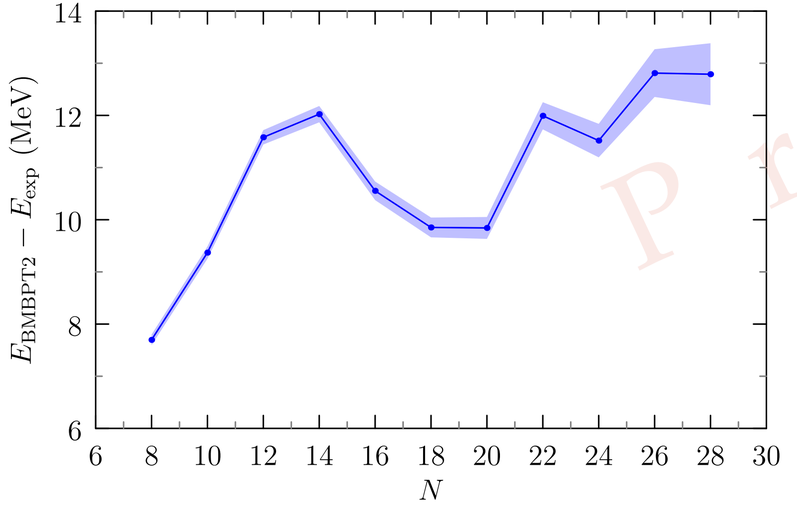
dBMBPT(2) systematics: Magnesium (Z=12)

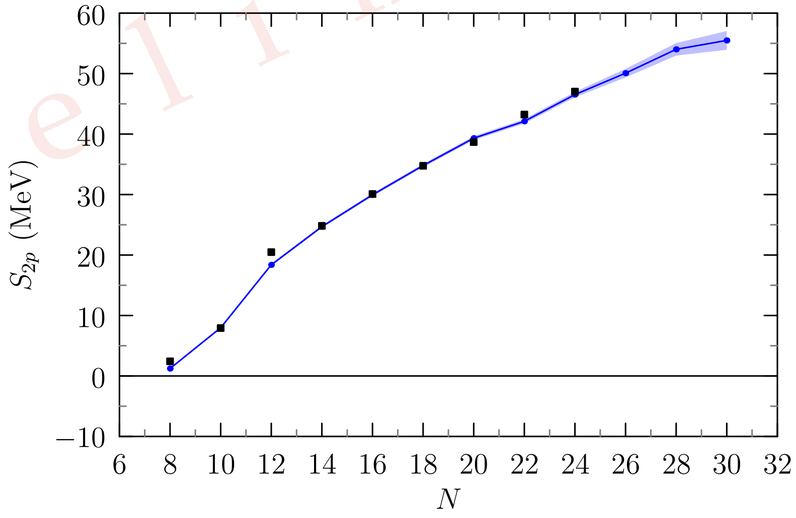
[Durel, AS *et al.*, in preparation]

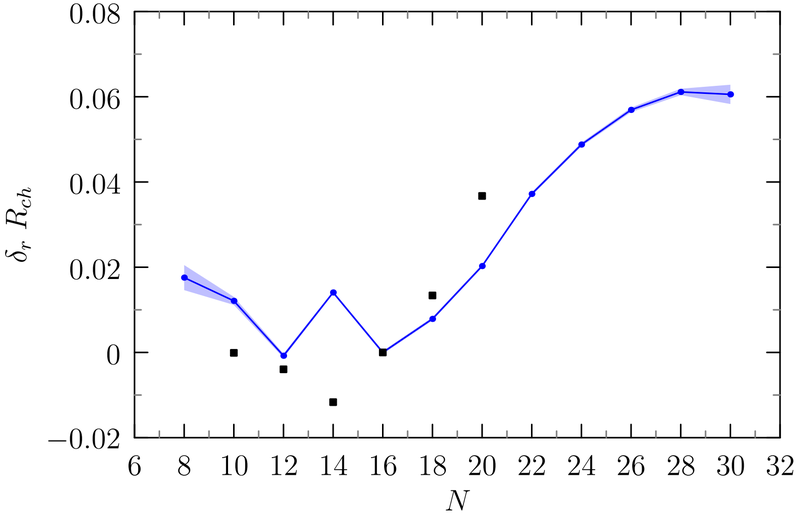








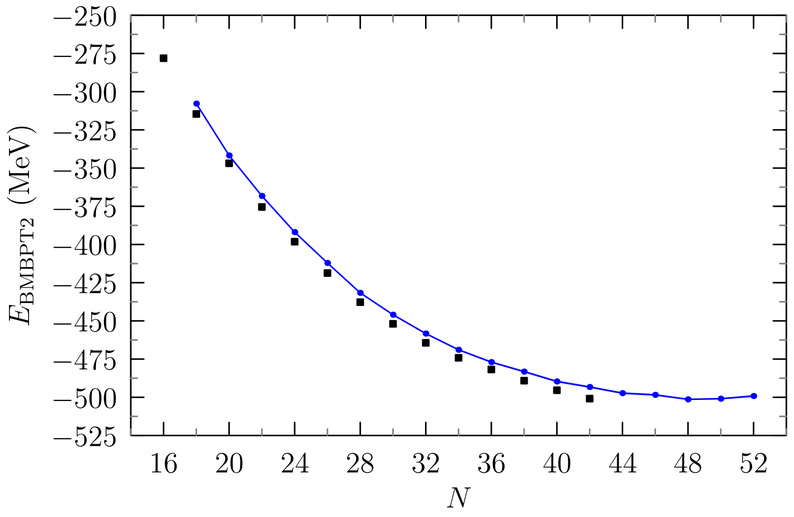


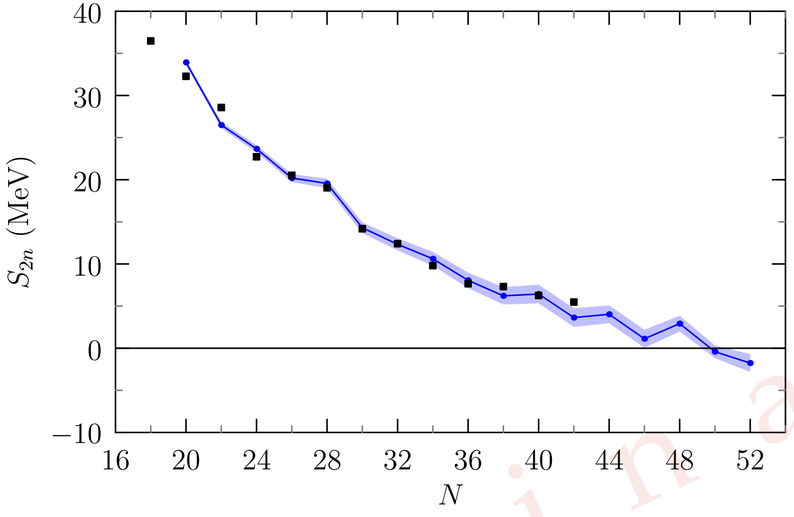


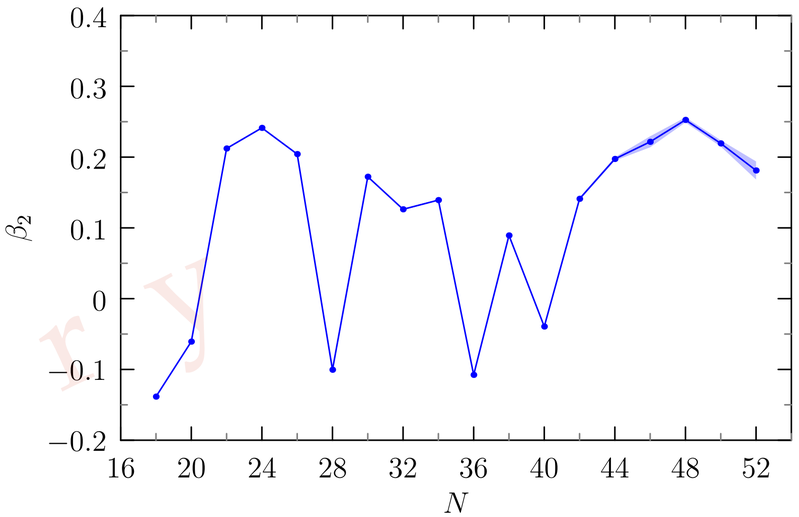
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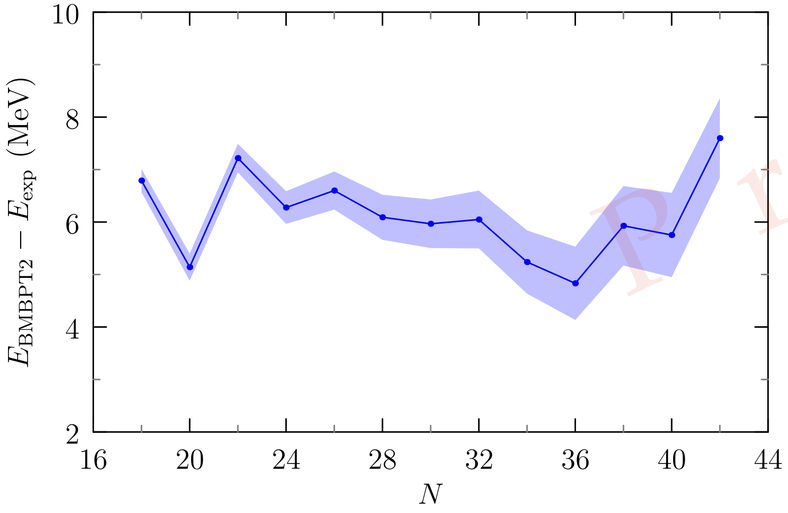
dBMBPT(2) systematics: Titanium (Z=22)

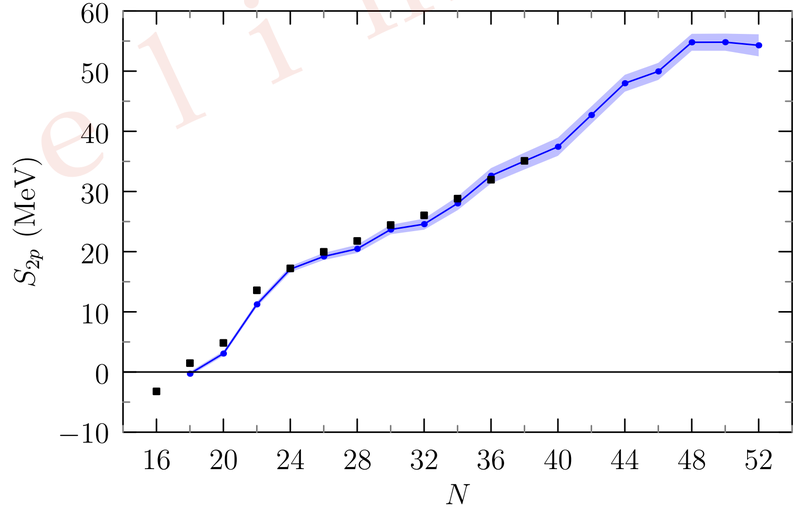
[Durel, AS *et al.*, in preparation]

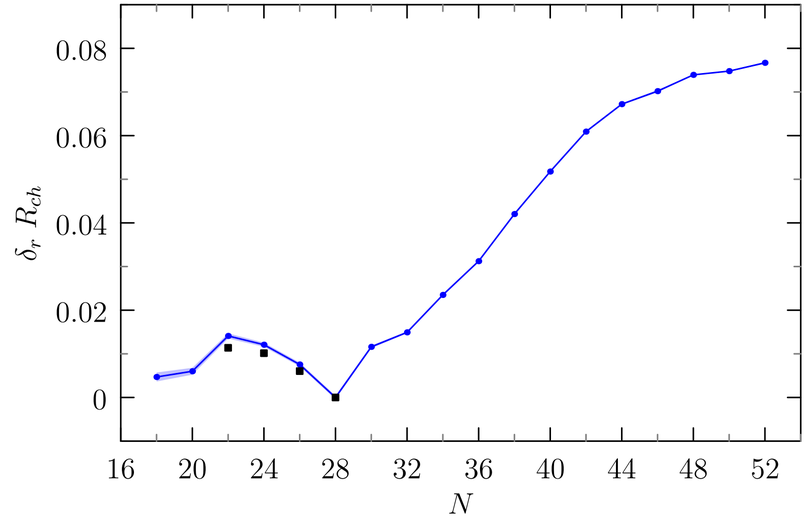








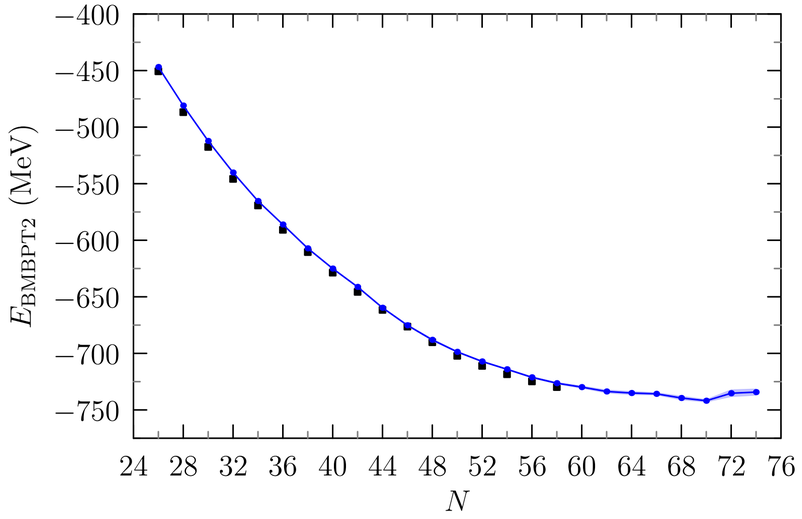


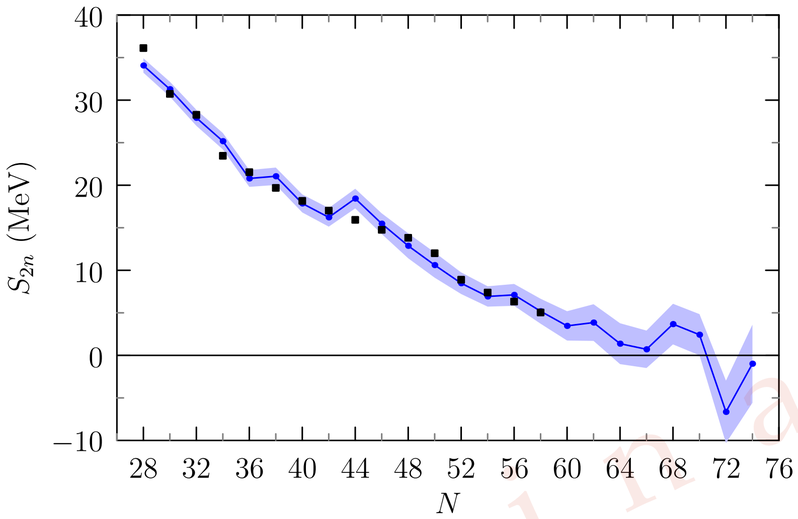


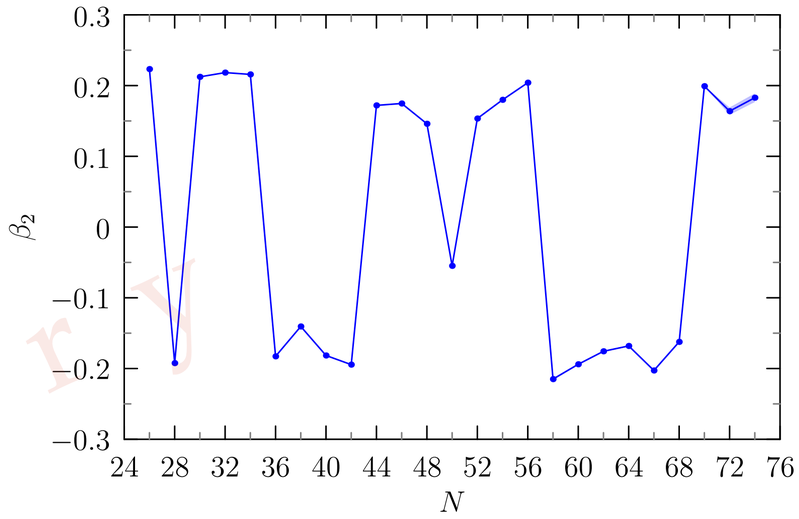
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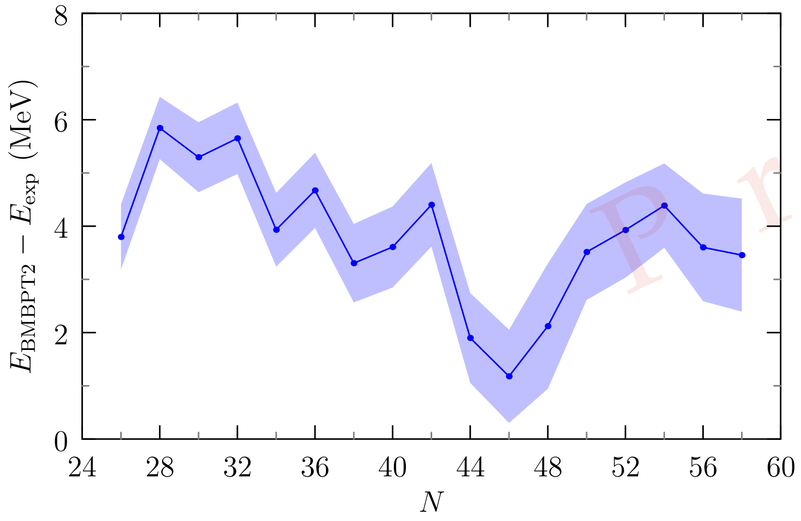
dBMBPT(2) systematics: Germanium (Z=32)

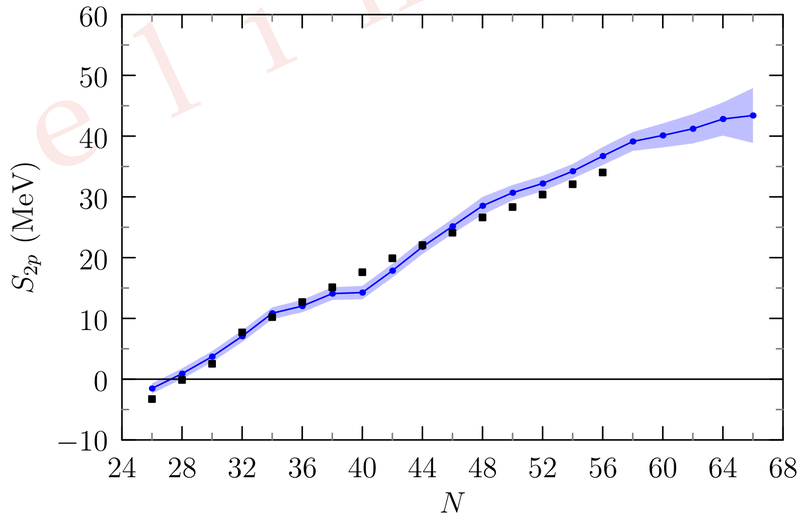
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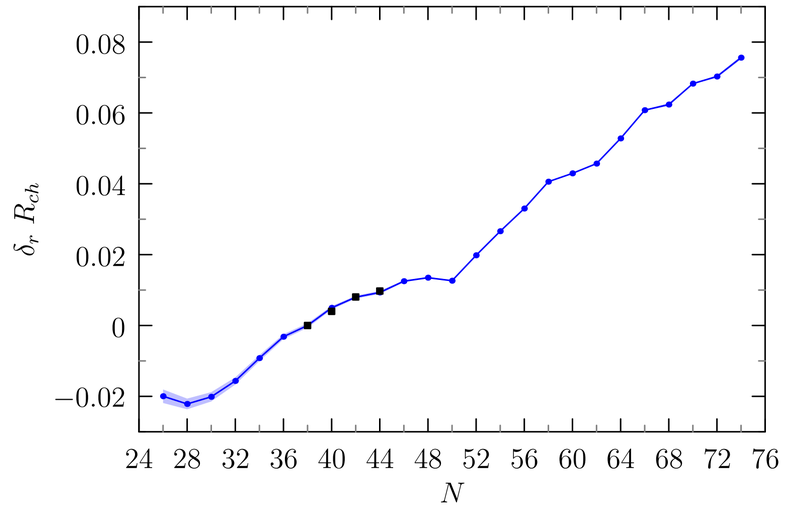








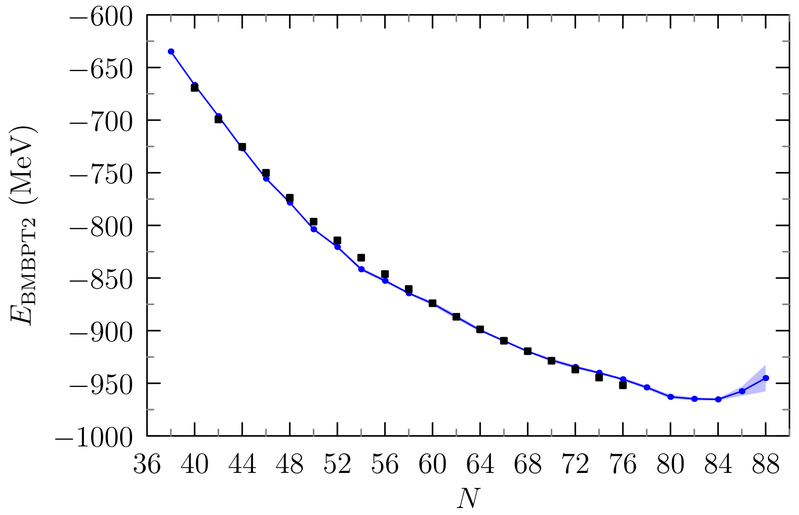


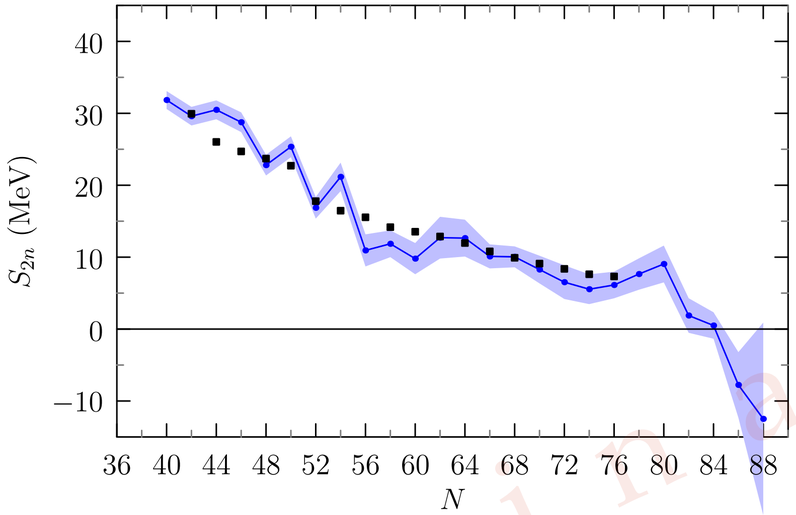


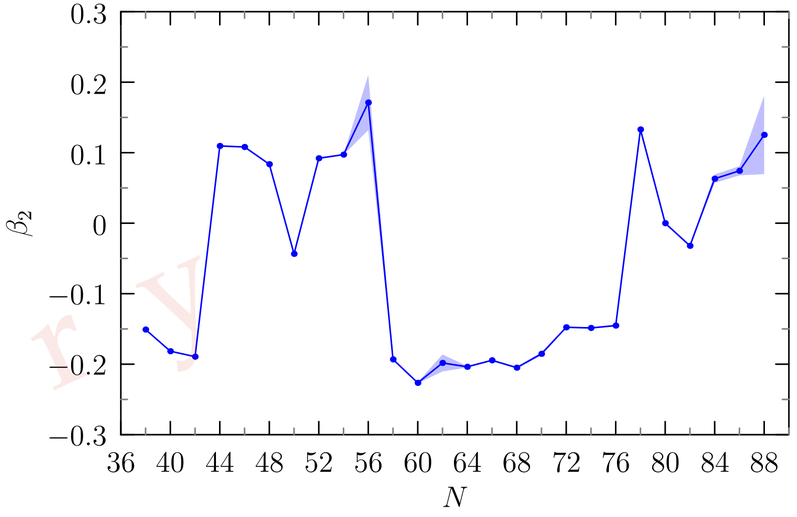
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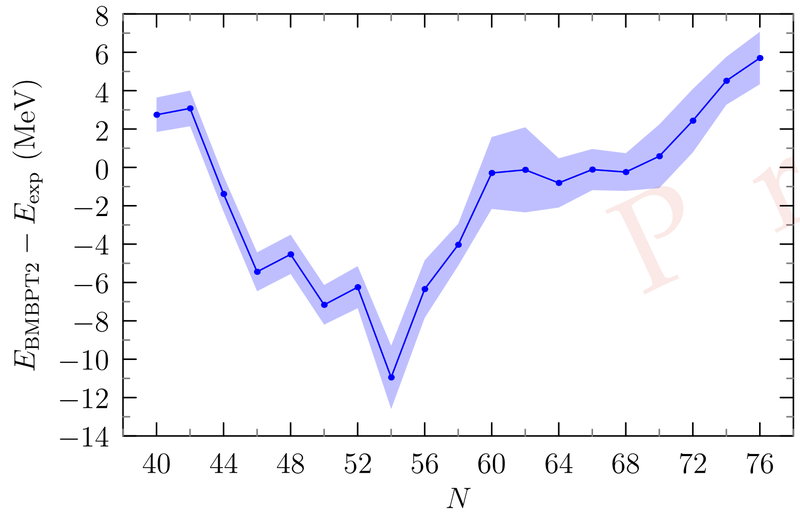
dBMBPT(2) systematics: Molybdenum (Z=42)

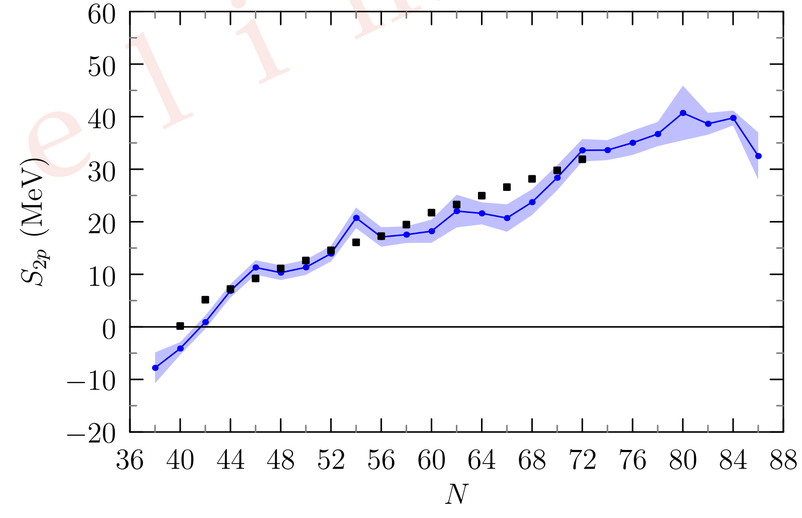
[Durel, AS *et al.*, in preparation]

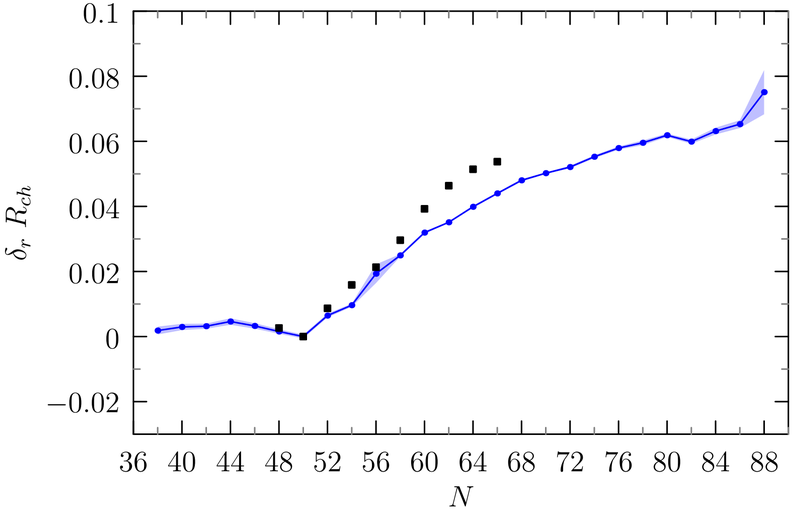






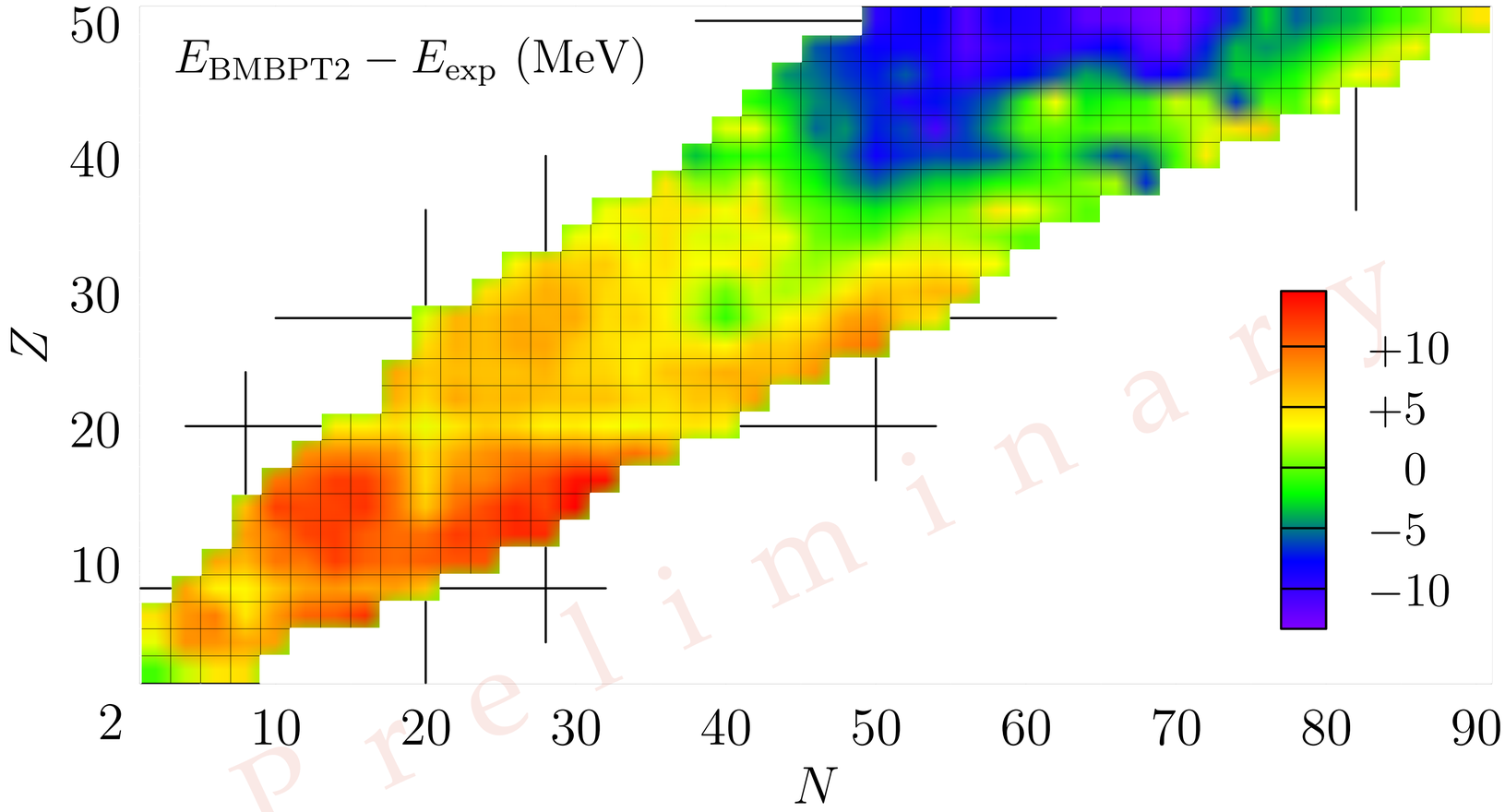






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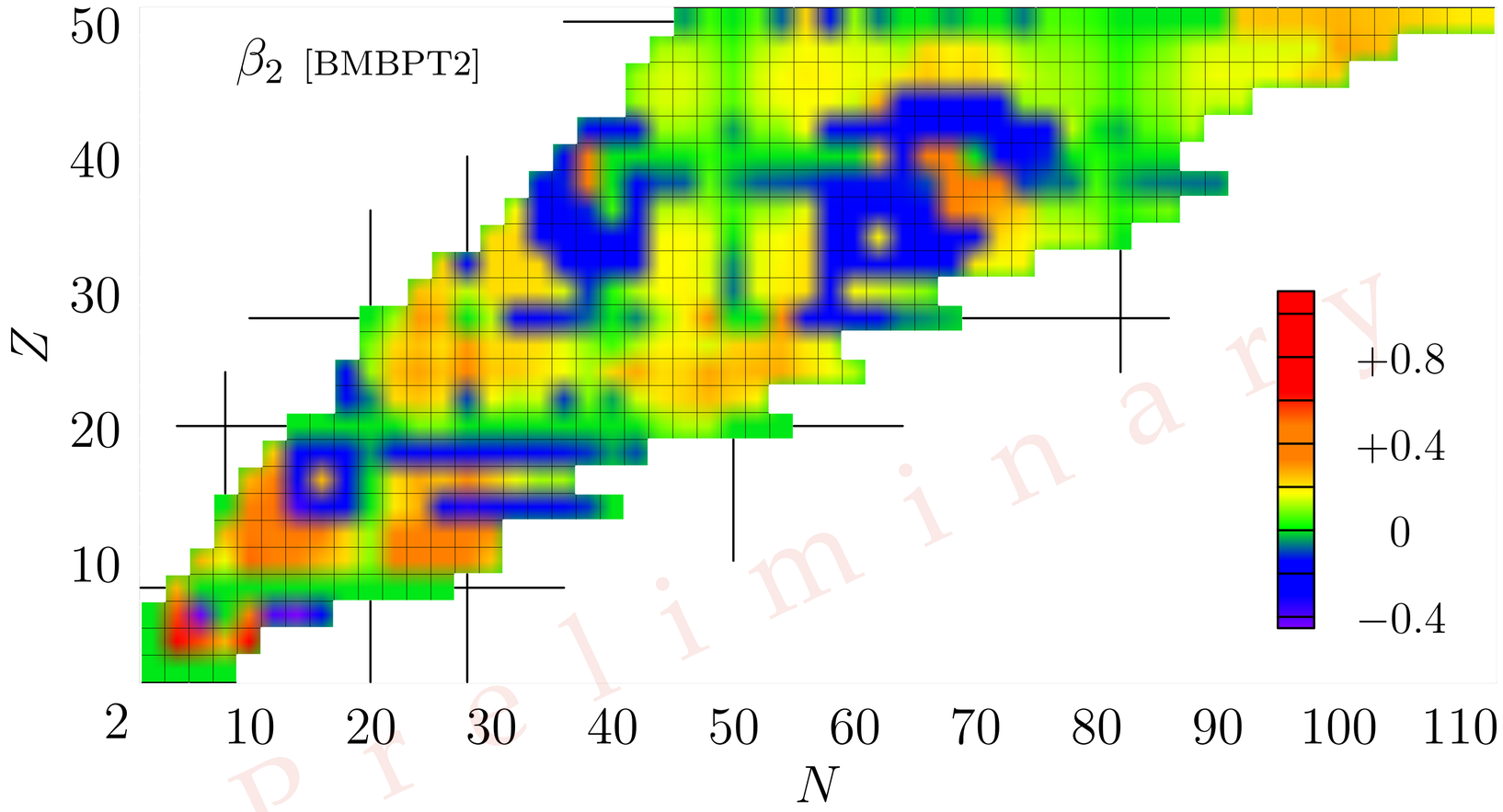
dBMBPT(2) systematics: deviation from data



[Durel, AS *et al.*, in preparation]
[V. Somà, INT (2026)]

- dBMBPT(2) **more bound** w.r.t. data as A increases → consistent with previous studies (e.g. Arthuis *et al.* 2024)
- For large Z, dBMBPT(2) **less bound** w.r.t. data for neutron-rich isotopes → cf. Hu *et al.* 2025
- Semi-magic chains systematically more bound by few MeV → **missing angular-momentum projection**?

dBMBPT(2) systematics: deformation map

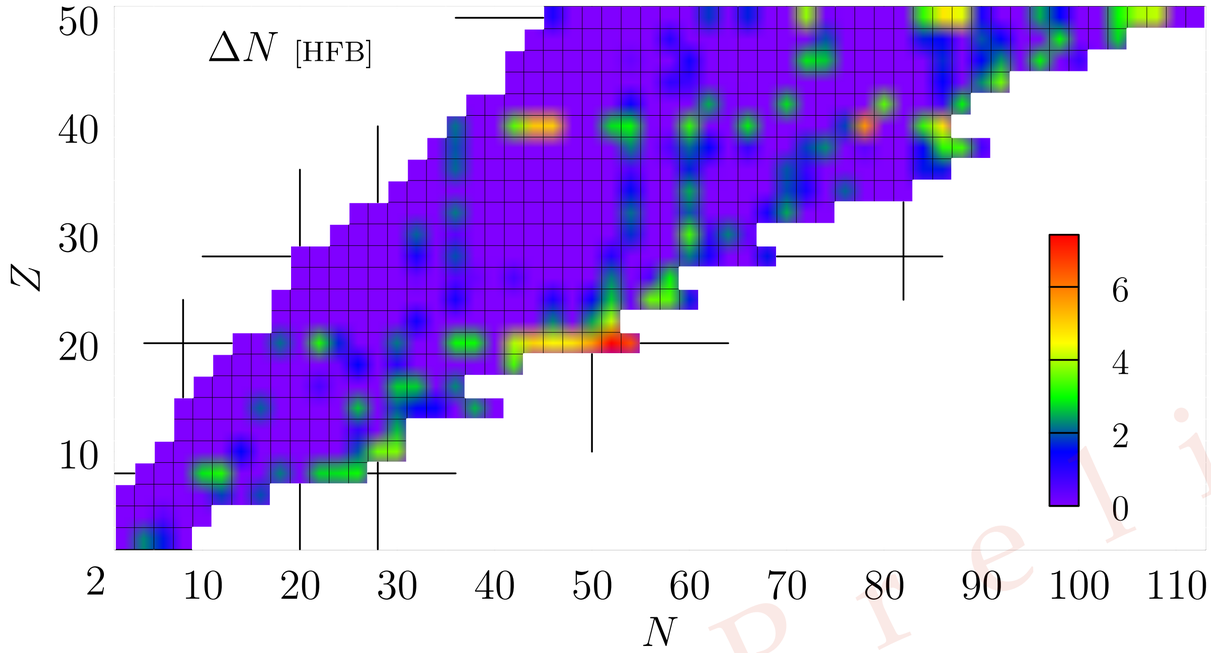


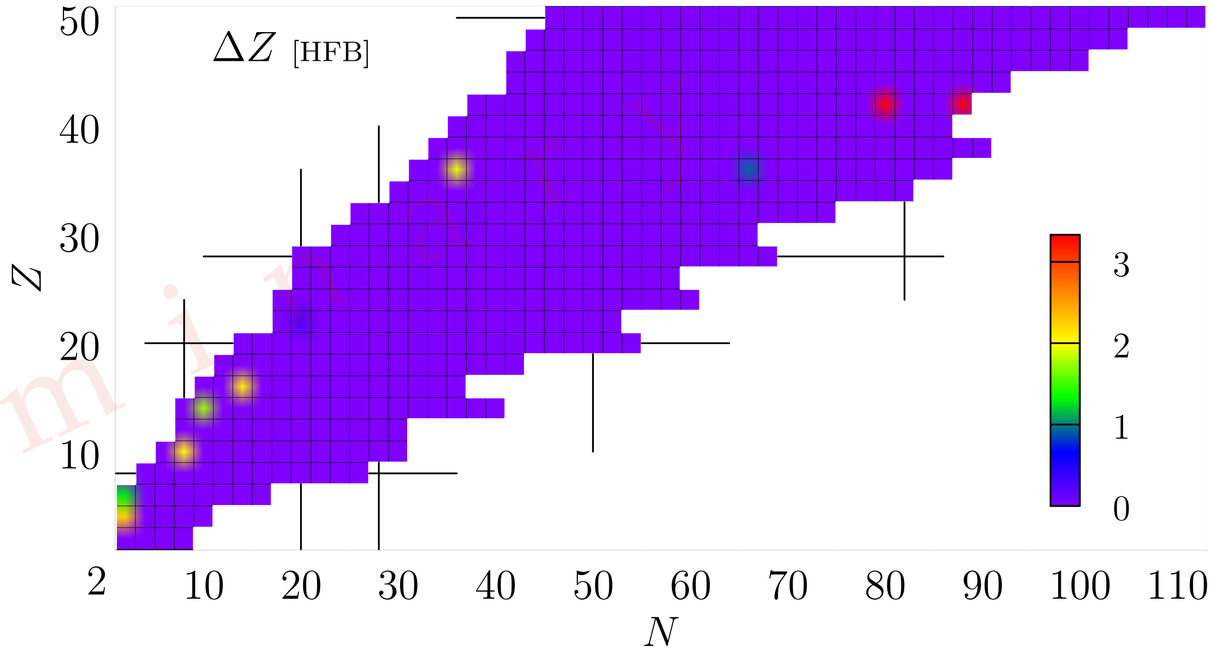
[Durel, AS *et al.*, in preparation]
[V. Somà, INT (2026)]

- Spherical solutions around **shell closures**
- **Known region of deformation** visible (e.g. “islands of inversion”)
- Qualitatively consistent with EDF systematics (e.g. Bender *et al.* 2006)

dBMBPT(2) systematics: pairing map

[Durel, AS *et al.*, in preparation]
[V. Somà, INT (2026)]





Preliminary

- **Deformation dominates** over pairing
- Confirms earlier indications that **ab initio Hamiltonians generate little pairing**
- **Neutron** pairing active mainly along some isotopic/isotonic chains
- **Proton** pairing almost absent

Deformed self-consistent Green's function

Why choosing Green's function-based methods

- **Advantages**
  - Direct access to **spectral information** and **odd-nuclei energies**
  - Access to **excited states**
  - The Green's function gives access to **density matrices** (radii)
  - 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
  - No access to the **many-body wave function**

Källén-Lehmann representation of the single-particle propagator

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

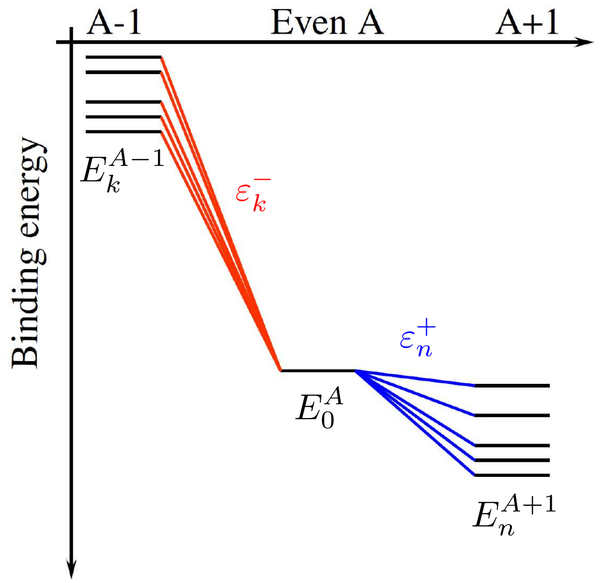
Separation energies

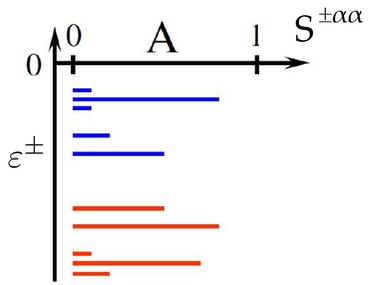
$$\varepsilon_n^+ = E_n^{A+1} - E_0^A$$
$$\varepsilon_k^- = E_0^A - E_k^{A-1}$$

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

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

Basic ingredients

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

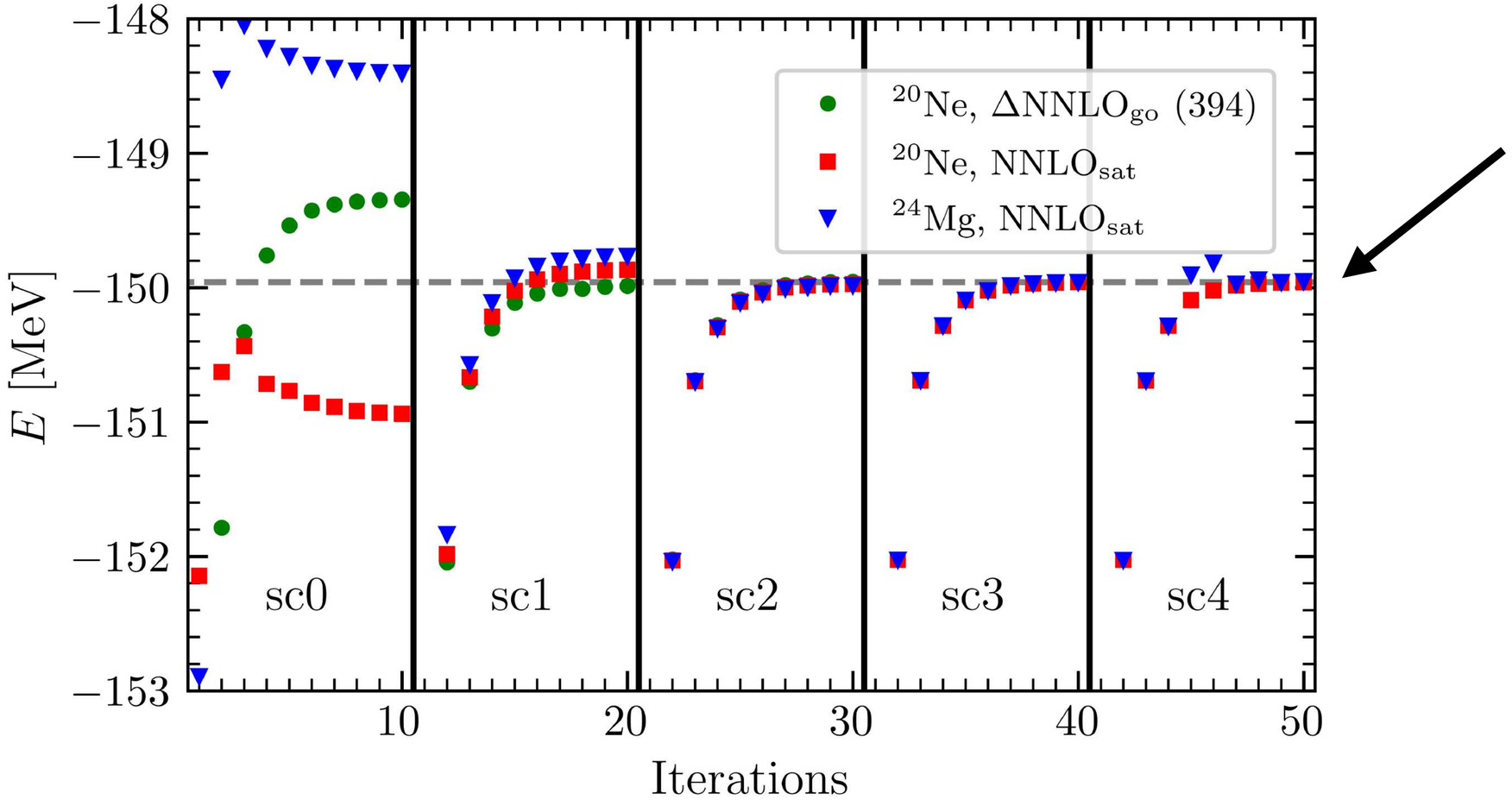
Observables: convolutions with GFs

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

+ Koltun sum rule

$$E_0 = \langle\Psi_0^A\,|\,H\,|\,\Psi_0^A\rangle = \frac{1}{2}\sum_{\alpha\beta}\int \frac{d\omega}{2\pi i}\, g_{\beta\alpha}(\omega)\, [t_{\alpha\beta} + \omega\,\delta_{\alpha\beta}]$$

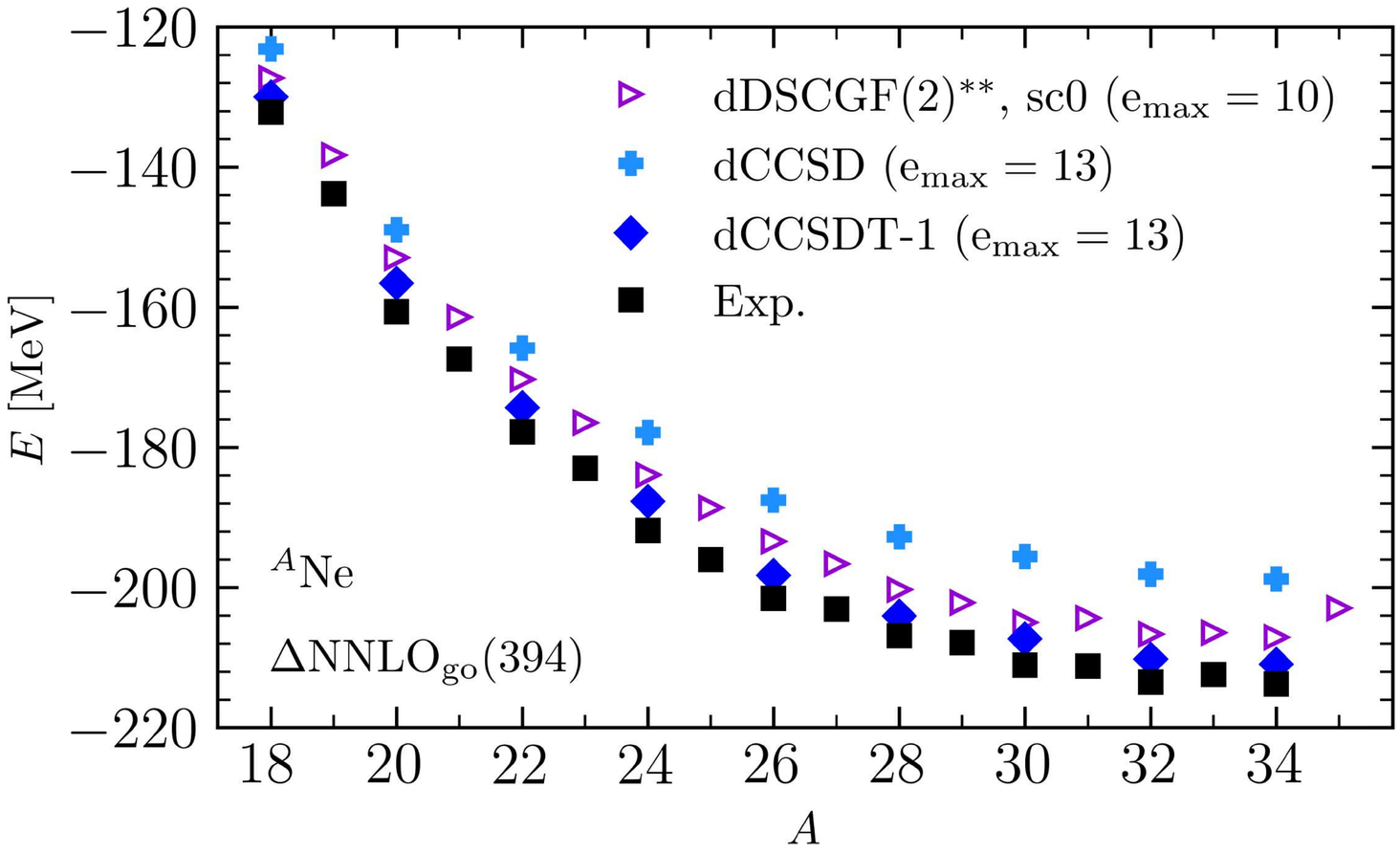
Self-consistency



→ Converged results independent on the reference state!

Ground-state energy of Neon isotopes

First tests on Neon isotopes where dCC results are available

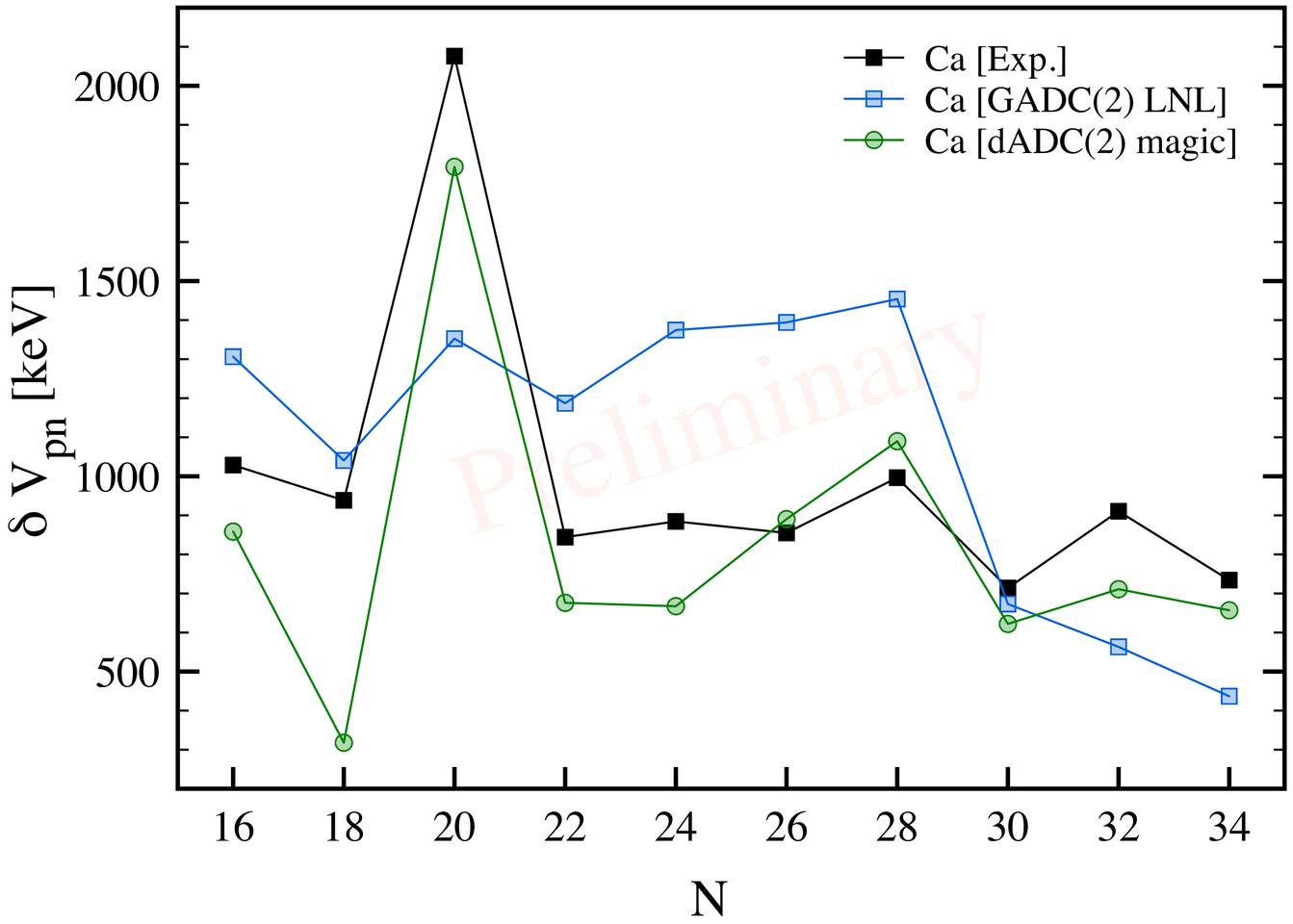


- Energies compatible with CC
- Access to **odd-even systems**
- Correct direction for odd-even staggering

[Novario *et al.* 2020]

Calcium isotopes - δV_{pn}

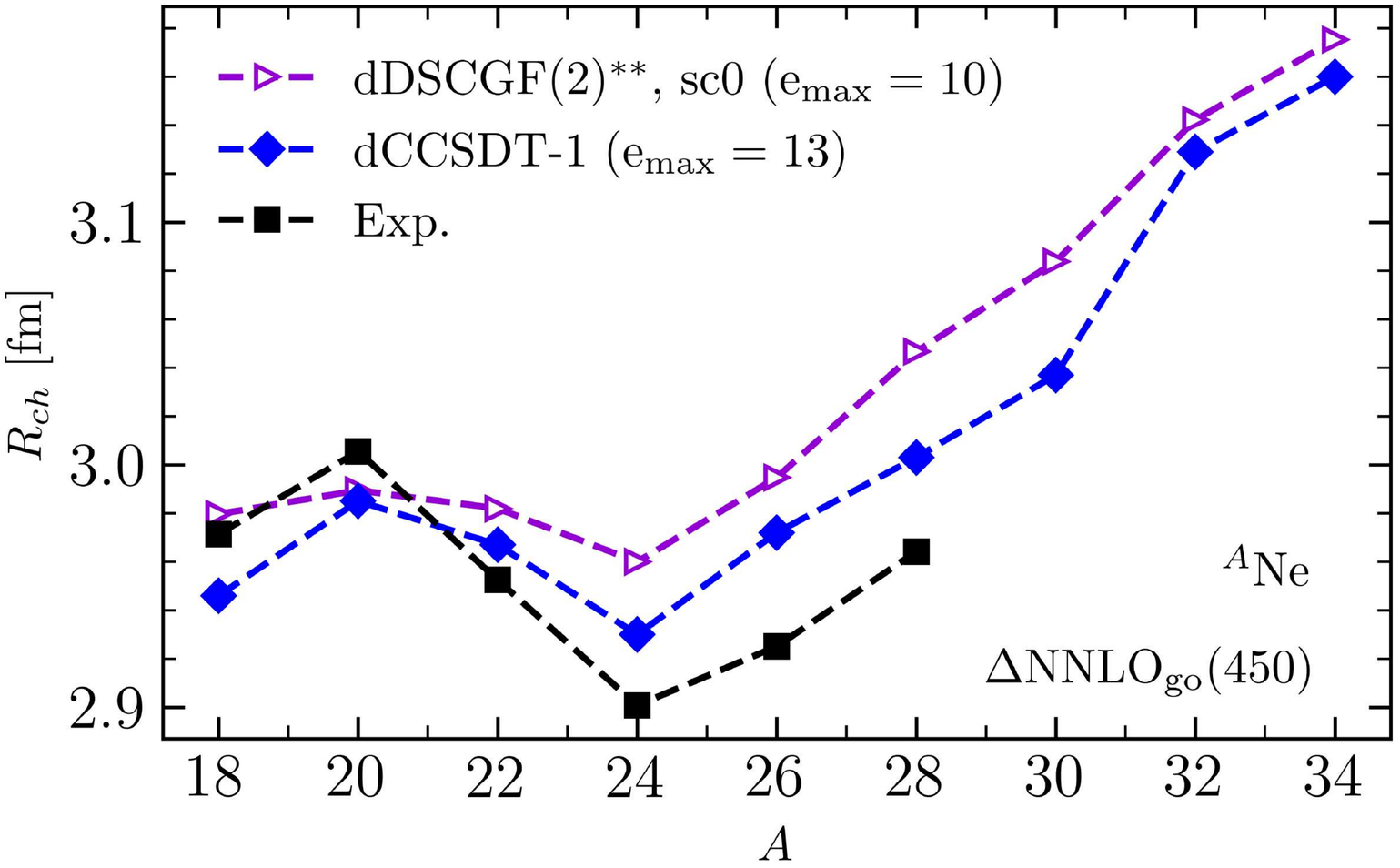
Residual *pn* interaction: $\delta V_{pn} = \frac{1}{4}[B(N,Z) + B(N-2,Z-2) - B(N,Z-2) - B(N-2,Z)]$



- Peak when crossing **closed-shell configurations**
- Sensitive to Argon deformations
- $N = 20$ peak captured only with dDSCGF(2)
- Good estimation of $0f_{7/2}$ **shell** with dDSCGF(2)

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

Charge radii of Neon isotopes



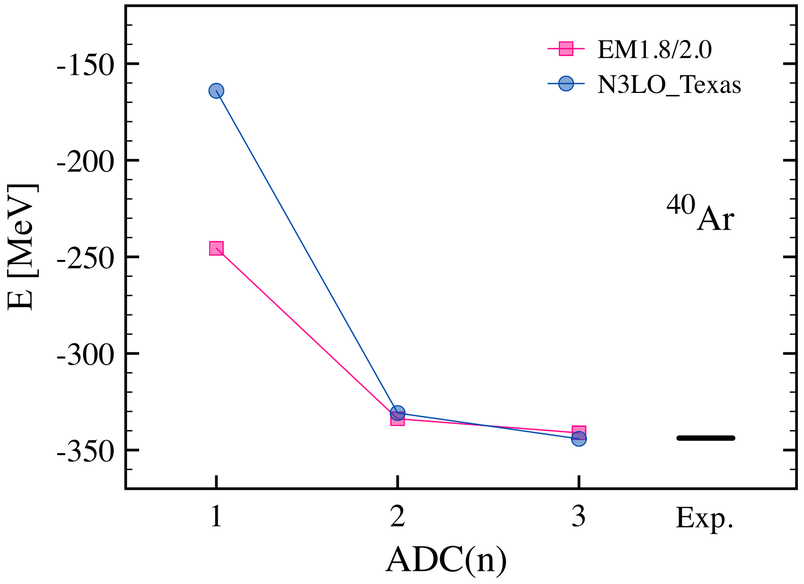
[Novario *et al.* 2020]

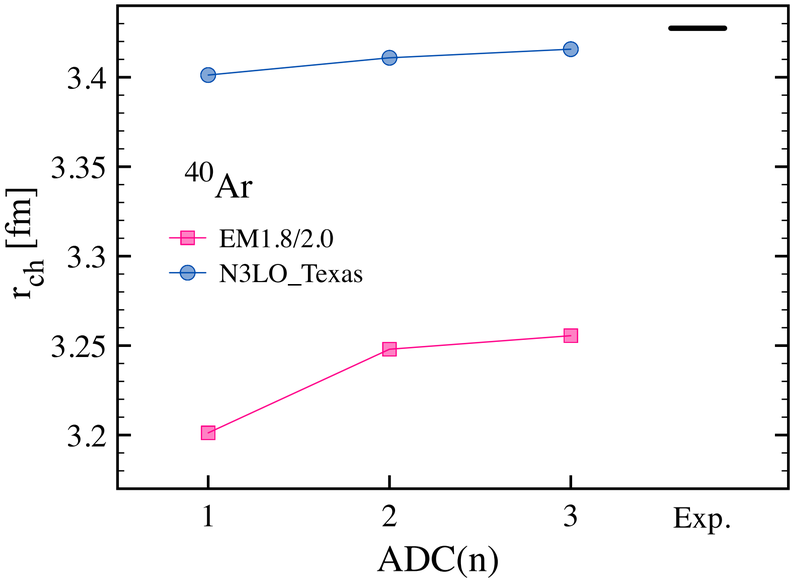
1B + 2B CoM corrections

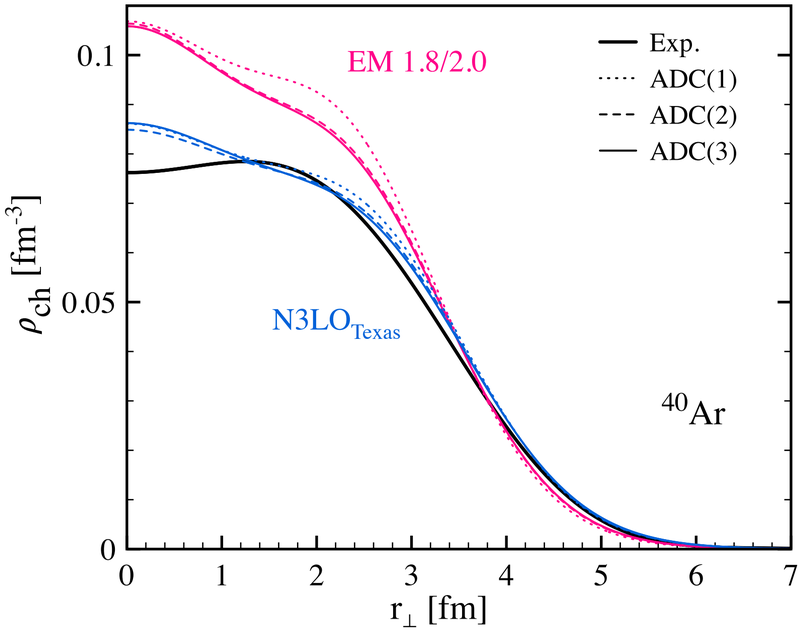
$$R_{ch}^2 = R_p^2 + \langle r_p^2 \rangle + \frac{N}{Z}\langle r_n^2 \rangle + \langle r_{\mathrm{DF}}^2 \rangle + \langle r_{\mathrm{SO}}^2 \rangle$$

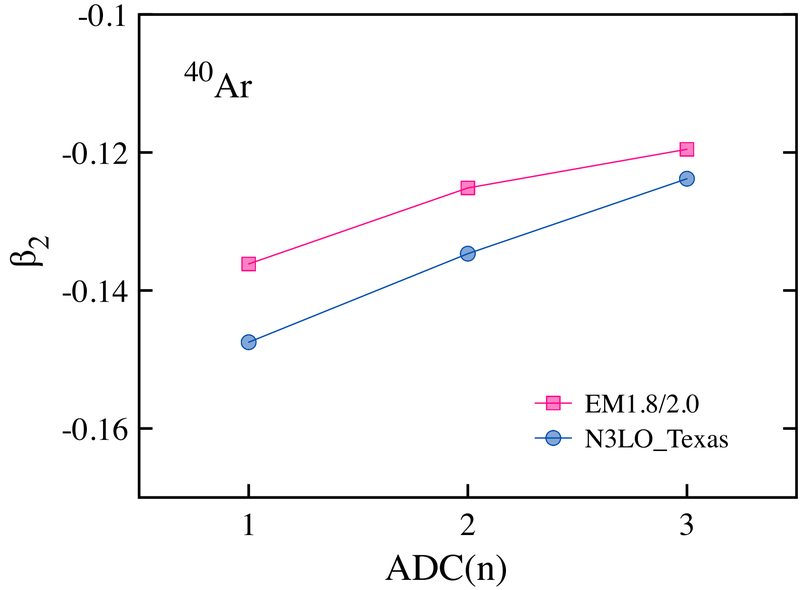
- Overall trend follows dCCSDT-1
- Shift prob. due to MB order and e_{max}

dDSCGF now available at 3rd order









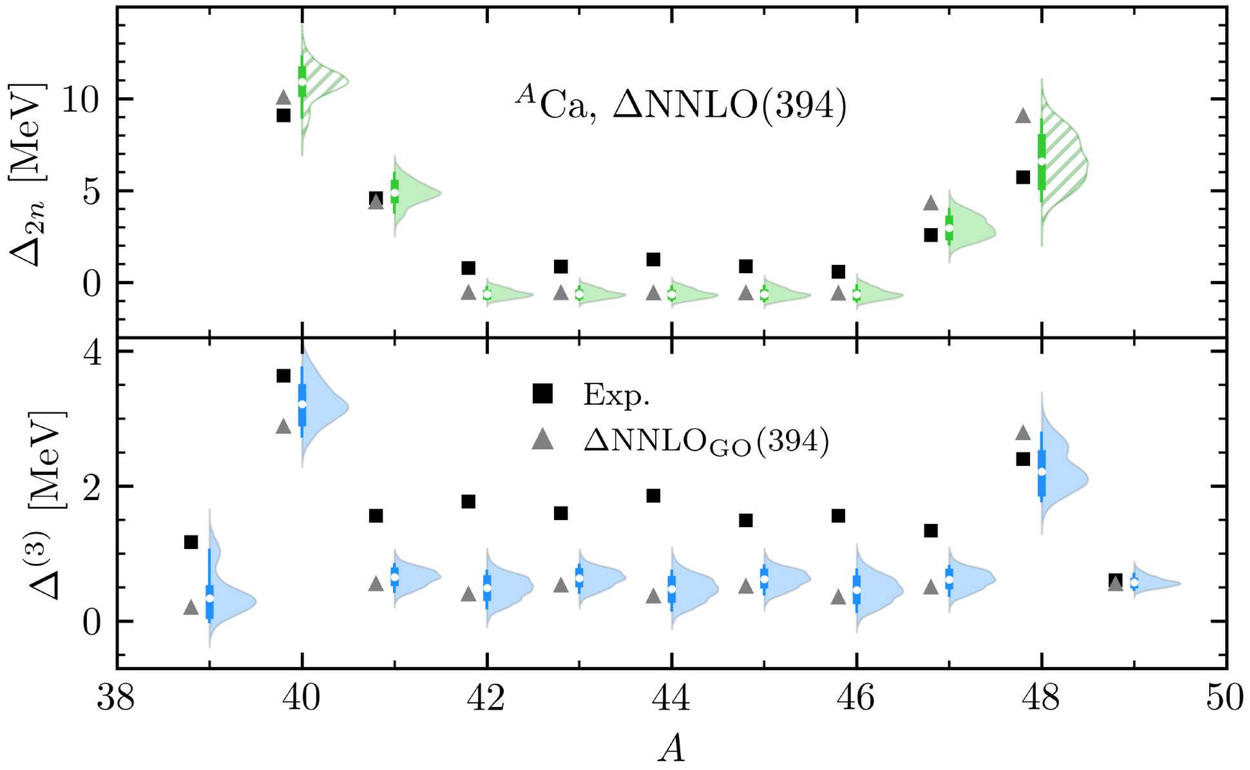
- Many-body convergence analogous to spherical case
- Deformation decreases as expected, but slowly

[V. Somà, INT (2026)]

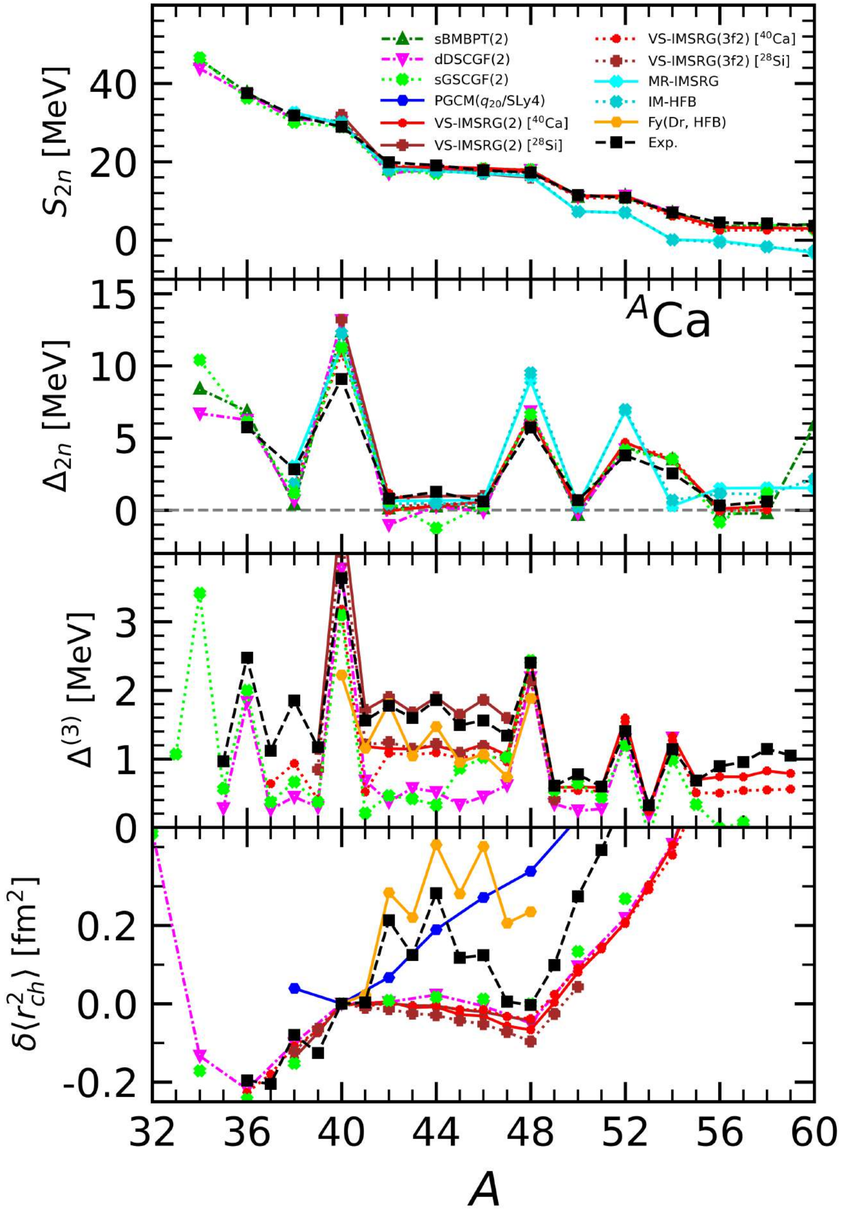
[Thanks to C. Barbieri for benchmarks]

The challenge in calcium isotopes

The challenge in calcium isotopes



[AS et al., Phys.Rev.C 113 (2026) 5, L051303]



Emulations

Emulation of many-body calculations

- **New general class of machine-learning algorithms** presented in for the first time in [P. Cook *et al.*, (2025)]

- Considering p.e. the one-parameter affine problem

$$H(c) = H_0 + cH_1$$

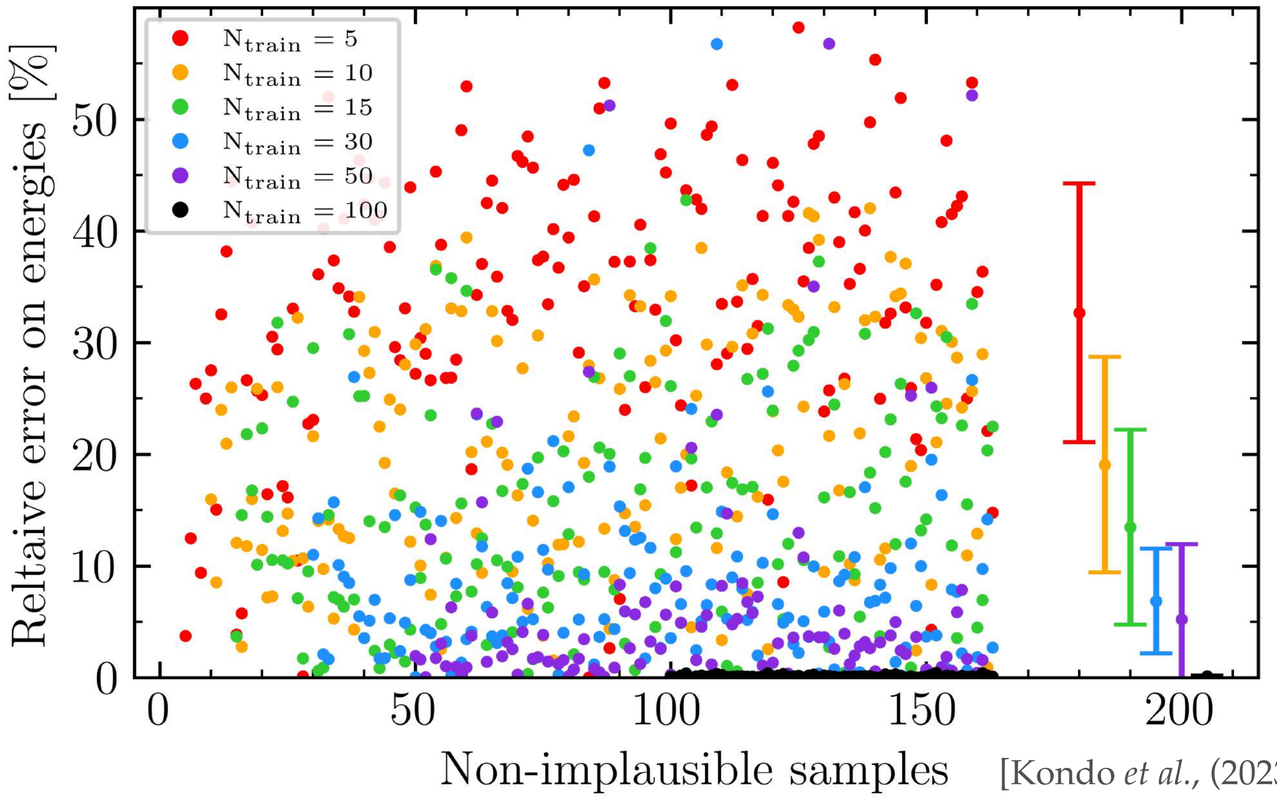
Eigenvector continuation (EC) with d training vectors corresponds to solve the new one-parameter affine problem

$$M(c) = M_0 + cM_1 \qquad \textbf{\textit{dxd} matrices}$$

- Suppose now that one has not access to the training vectors $\rightarrow$ it is the case for SCGF!

- The same $M(c)$ matrices can be **built to reproduce the eigenvalues** $E(c)$ through machine learning algorithms

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!

- ... but bigger sizes needed for beyond mean-field!

2.08 days for 100 training data

15.48 seconds for 1 Million emulations

vs **57 years** for 1 Million calculations!

Beyond the spherical Harmonic Oscillator basis

Beyond the spherical Harmonic Oscillator basis

Spherical Harmonic Oscillator basis

- **Advantages**:
  - optimal choice for well-bound closed-shell systems
  - exact separation of intrinsic and center-of-mass motion
  - Moshinsky coefficients diagonal in $2n + l$
  - isospin-independent (T-coupled matrix elements)

- **Drawbacks**:
  - neutron and proton sates expanded on the same basis
  - wrong asymptotic behavior
  - non-optimal for some classes of nuclei (weakly-bound, neutron rich, ...)

Expansion of MEs on generic single-particle basis

Transformation CoM to sp basis

Moshinsky brackets (**sHO**)

$$\langle nNlL;\lambda|n_1n_2(l_1l_2);\lambda\rangle$$

vs

Wong-Clement brackets (**generic basis**)

$$\langle pPlL;\lambda|n_1n_2(l_1l_2);\lambda\rangle$$

Generic spherical wave function:

$$\phi_{nlj\tau}(r) \quad \text{or} \quad \hat{\phi}_{nlj\tau}(k)$$

- explicit **spin**- and **isospin**-dependency
- **coordinate**- or **momentum**-space wave functions

$$H = \frac{\hat{A}}{\hat{A}-1}T^{lab} + \sum_{i<j}(V_{ij} - \tilde{T}^{cm}) + \sum_{i<j<k} W_{ijk}$$

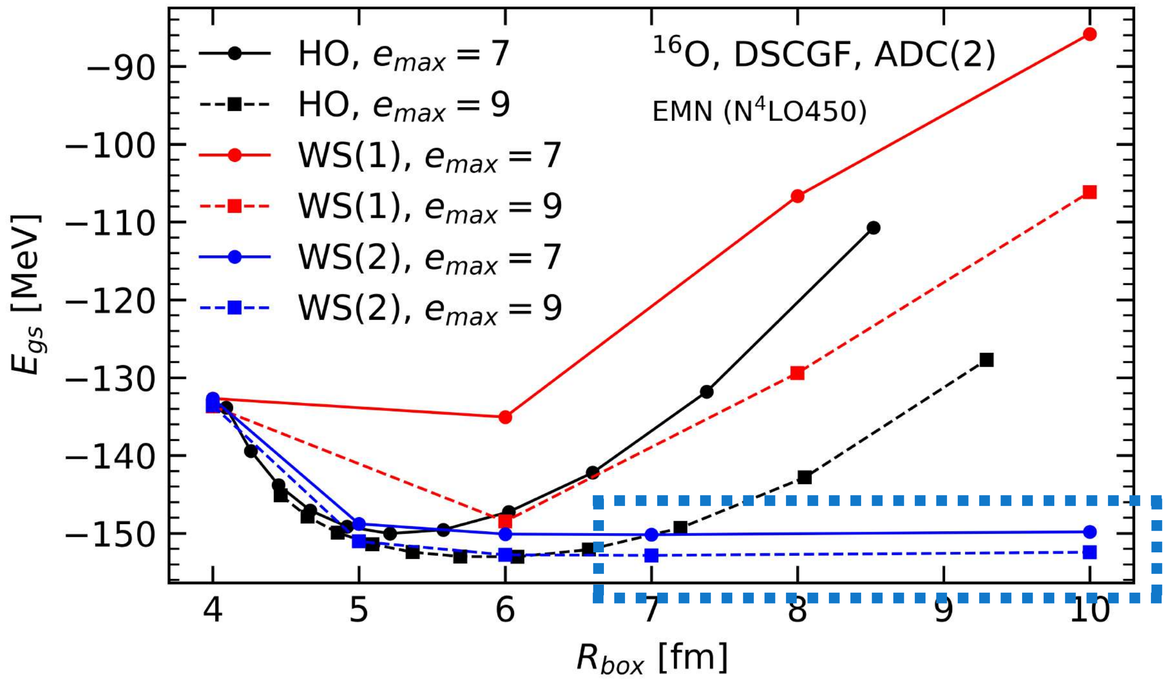
Goal of this work **+ CoM for radii**

- Expansion of **one**-, **two**- and **three**-body MEs on a generic spherical basis
- Development of a **machinery** to perform systematic calculations
- Sole requirement of **spherical symmetry** of the nuclear Hamiltonian

Works with **any generic spherical basis** read from file!

Alternative single-particle bases to sHO

- A few spherical bases implemented:
  - **standard HO** wave functions ⟶ **hard-wall spherical box** of radius R_{box} [Furnstahl *et al.* 2012]
  - **HO** wave functions with Dirichlet BC **in a box** in coordinate-space
  - **Spherical Bessel** wave functions in a box in coordinate-space
  - **Wood-Saxon** wave functions in a box in coordinate-space



- Preliminary tests on new bases
- **Two-body** only
- Carried out with **Dyson SCGF** method
- Modified IR behavior of **WS(2) basis**
- Further tests to find more optimal bases

Conclusions and current challenges

Conclusions and current challenges

→ **Deformed** *ab initio* methods provide an accurate description of open-shell nuclei

→ **Correlations** captured by dDSCGF bring visible results on observables w.r.t. GSCGF

→ **Emulators** critically lower the cost of MB calculations allowing for interaction-sensitivity studies

Challenges:

- dDSCGF with **good angular momentum** → Symmetry Restoration (yet to be formulated)
  → **MR-SCGF** [Sokolov *et al.*, 2018]

- **Emulation of SCGF calculations** for interaction-sensitivity studies
- Description of pairing and charge radii in **calcium** $0f_{7/2}$ **shell**
- Pushing many-body *ab initio* methods to **heavy deformed nuclei**

Collaborators



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