Capturing many-body correlations at polynomial cost

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PAINT2025 - Workshop on Progress in Ab Initio Nuclear Theory

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Outline

- Open-shell nuclei at polynomial cost: necessity of deformation

- Deformed self-consistent Green's function

- Conclusions

V. Somà, T. Duguet, M. Frosini

Based on the work carried out at CEA during my PhD!

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NUMERICS International PhD Program in Numerical Simulation at CEA

The Segrè chart

Ab initio limited to:

- medium-light region
- doubly/singly close shell

→ **how to extend the reach of *ab initio*?**

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)

Solving the Schrödinger equation at polynomial cost

Our choice: **polynomial methods with A** $\rightarrow$ CPU-scalable to heavy masses

static correlations

$\longrightarrow$ **Correlation-expansion methods**

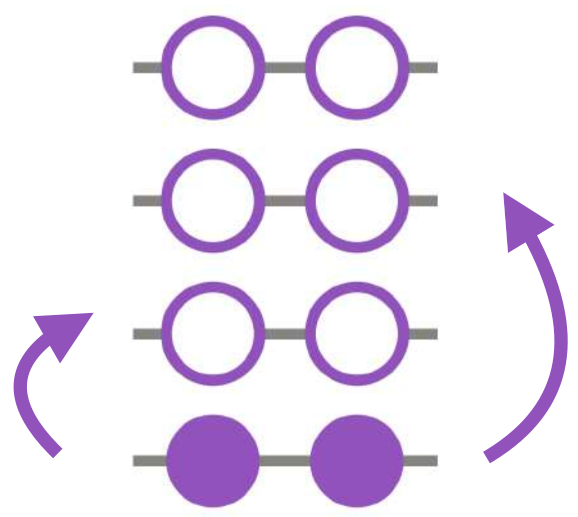
included in ref. state through sym. break.

Hamiltonian partitioning: $H = \boxed{H_0} + \boxed{H_1}$

size of 1B Hilbert space

'easy'-to-handle $\longrightarrow$ mean-field-like N^4

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



'hard'-to-handle $\longrightarrow$ beyond-mean-field $N^p, \;\; p > 4$

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

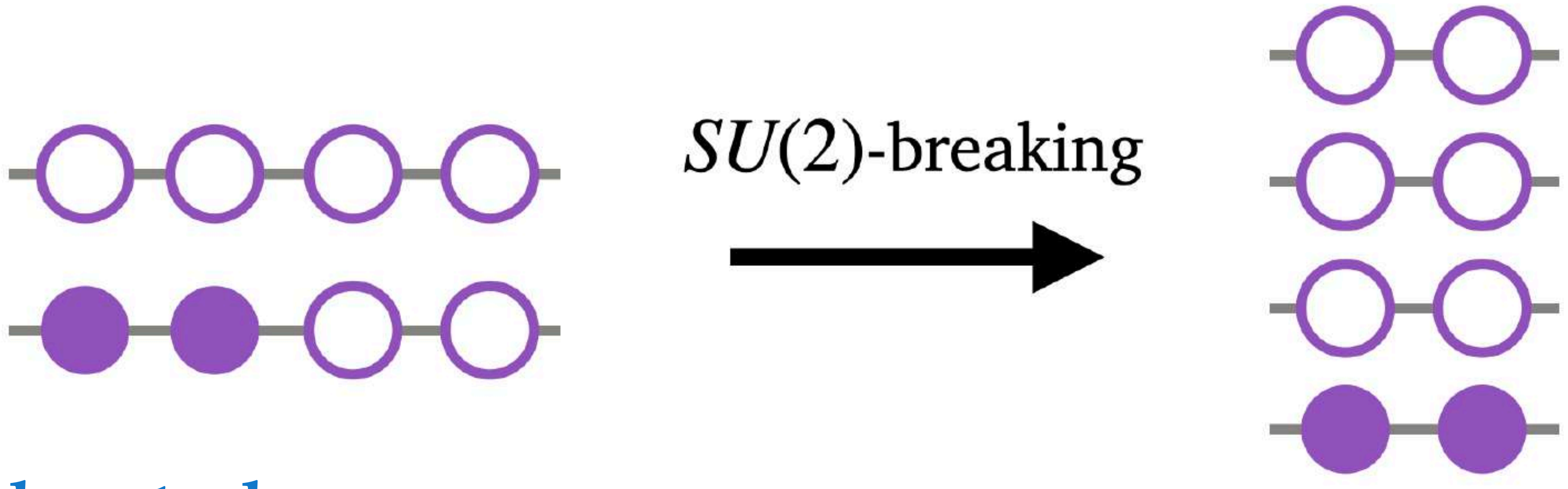
- **Perturbative** expansion: Taylor-like series
- **Non-perturbative** expansion: CC, SCGF, IMSRG

$\longrightarrow$ 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**	sMBPT, sIMSRG, sCC, sDSCGF	[Barbieri, Bogner, Hagen, Hergert, …]
Singly open-shell	2010 - 2020	**sHFB**	sBMBPT, sBCC, sIMSRG, sGSCGF	[Demol, Duguet, Hergert, Somà, Tichai, …]
Doubly open-shell	2020 - …	**dHF(B)**	d(B)MBPT, (P)dCC, PGCM-PT, **dDSCGF** IMSRG	[Duguet, Frosini, Hagen, …]

- Opening SU(2) keeps polynomial cost but **increases** N → Techniques to moderate cost:

[Scalesi *et al.* 2025] [Tichai *et al.* 2018]
[Hoppe *et al.* 2021]
[Porro *et al.* 2021]
[Frosini *et al.* 2024]

- **Natural Orbitals (NAT)**
- **Importance Truncation (IT)**
- **Tensor Factorization (TF)** (see L. Zurek talk)

The reference state

Eur. Phys. J. A (2025) 61:1
https://doi.org/10.1140/epja/s10050-024-01466-5

THE EUROPEAN PHYSICAL JOURNAL A

Check for updates

Regular Article - Theoretical Physics

Deformed natural orbitals for ab initio calculations

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- <u>Natural Orbitals</u> (NAT)

→ **check out** *Eur. Phys. J. A 61, 1* **(2025)**

The reference state

Focus of this talk!

Investigate the necessity of breaking SU(2) to study doubly open-shell at polynomial cost

Develop a new SU(2)-breaking non-perturbative method

Impact of correlations on nuclear binding energies

- Goal: proof that deformation is mandatory for an *ab initio* description at polynomial cost

Polynomial:	sHFB	dHFB	[Tichai *et al.* 2020]
	sBMBPT(2)	dBMBPT(2)	[Frosini *et al.* 2021]
	sBCCSD		[Tichai, Demol, Duguet 2024]
Non-polynomial:	sVS-IMSRG(2)		[Stroberg *et al.* 2022]

- Computational setting: e_{max}=12, e_{3max}=18, EM 1.8/2.0 [Hebeler *et al.* 2011]

- Systems under study: **singly open-shell** (**Ca**) and **doubly open-shell** (**Cr**)

SU(2) Conserving vs **SU(2) Breaking**

- Step-by-step study of the contribution of MB correlations to the **total energy** and **I-II derivatives**

Two-neutron separation energy: $S_{2n}(N,Z) \equiv E(N-2,Z) - E(N,Z)$

Two-neutron shell gap: $\Delta_{2n}(N,Z) \equiv S_{2n}(N,Z) - S_{2n}(N+2,Z)$

Impact of correlations on nuclear binding energies

Eur. Phys. J. A (2024) 60:209
https://doi.org/10.1140/epja/s10050-024-01424-1

THE EUROPEAN PHYSICAL JOURNAL A

Check for updates

Regular Article - Theoretical Physics

Impact of correlations on nuclear binding energies

Ab initio calculations of singly and doubly open-shell nuclei

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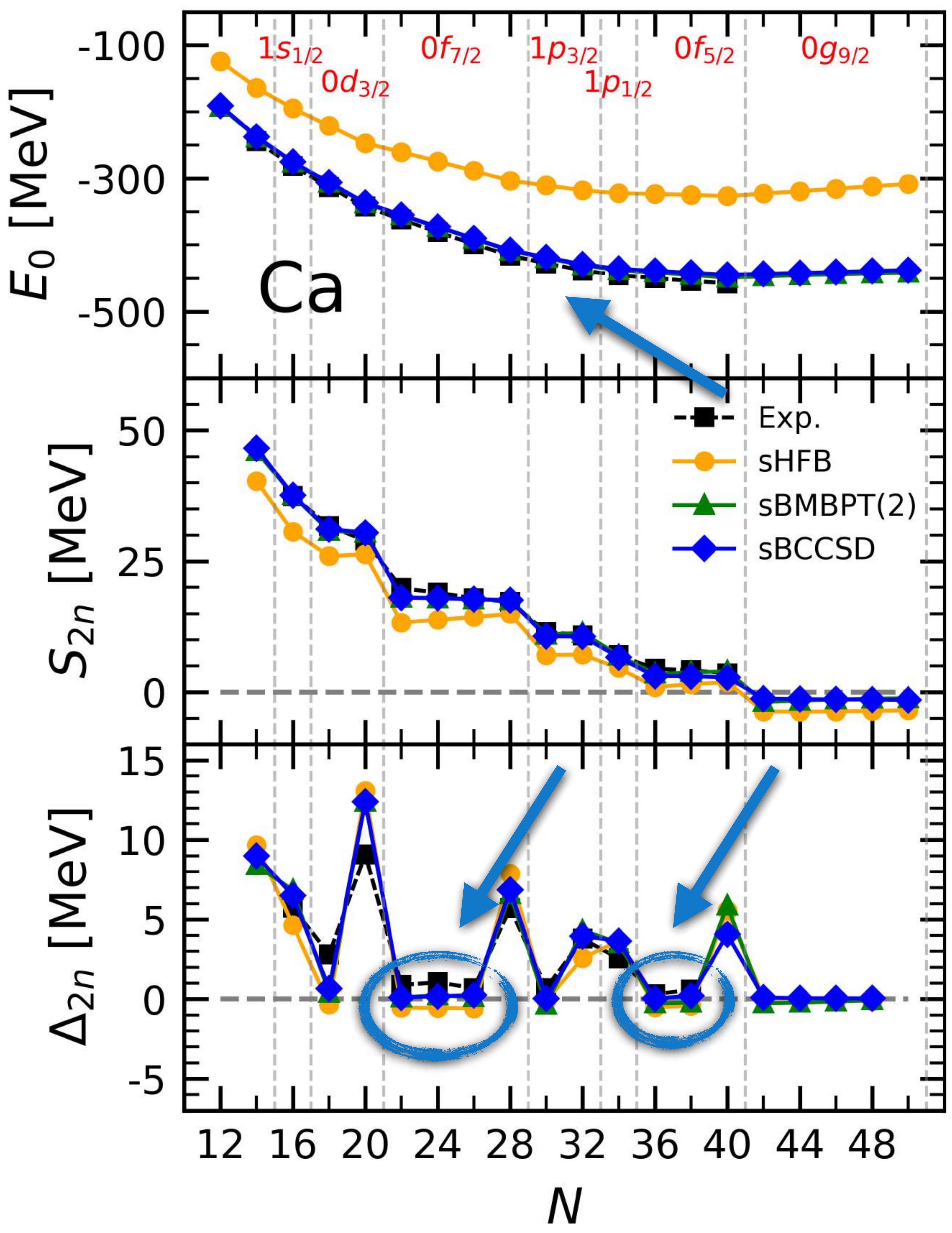
→ **check out** *Eur. Phys. J. A 60, 209* **(2024)**

$$S_{2n}(N,Z) \equiv E(N-2,Z) - E(N,Z)$$

$$\Delta_{2n}(N,Z) \equiv S_{2n}(N,Z) - S_{2n}(N+2,Z)$$

SU(2)-conserving *ab initio* approaches



Singly open-shell

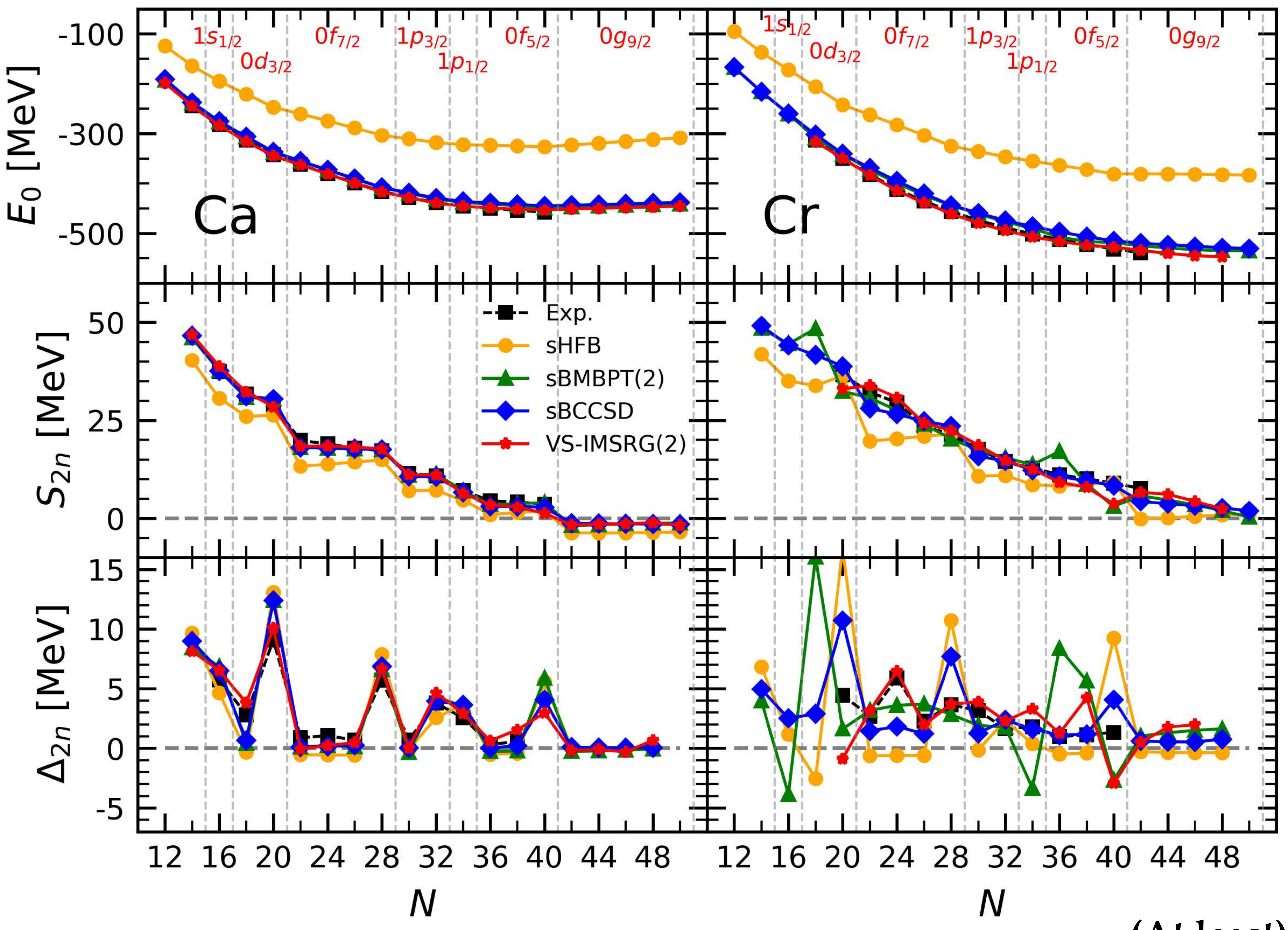
Spherical mean-field:

- **Quantitative** defect: **underbinding**
- **Qualitative** defect: **wrong curvature**

Low-order dynamical correlations:

- **Binding energy** corrected
- **Improved curvature** (not fully quant.)

SU(2)-conserving *ab initio* approaches



Doubly open-shell

- No presence of magicity in **Exp. data**

Spherical mean-field:

- Defects even **more pronounced**

Low-order dynamical correlations:

- Still **wrong curvature**
- **Wrong shell gaps**

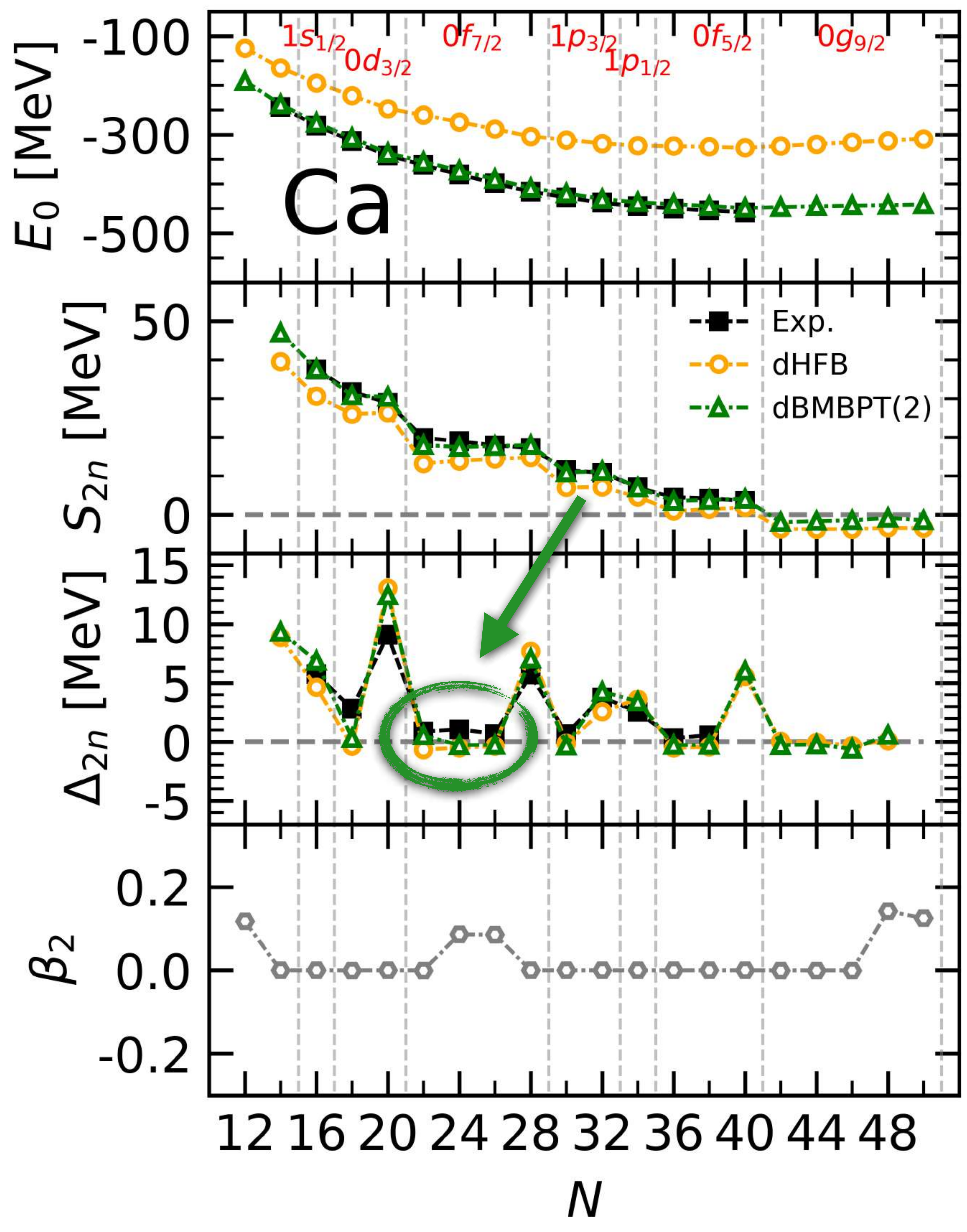
Non polynomial:

- **Correct binding energy**
- **Correct shell gap**
- **Improved curvature**

↓

(At least) high orders needed for SU(2)-cons. ref. state

SU(2)-breaking *ab initio* approaches



Singly open-shell

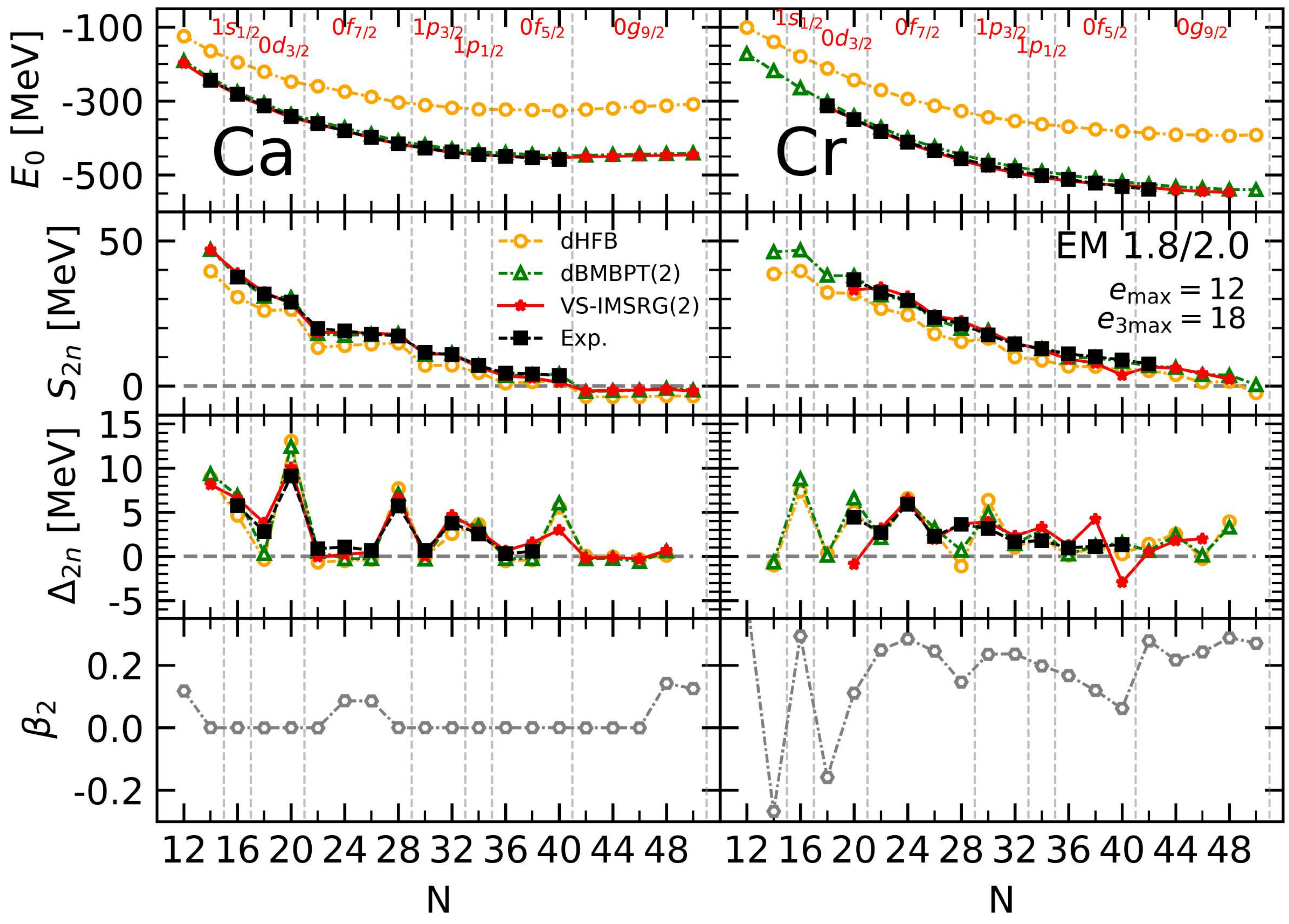
Deformed mean-field:

- **Underbinding** and **wrong** curvature

Low-order dynamical correlations:

- **Slightly improved** curvature

SU(2)-breaking *ab initio* approaches



Doubly open-shell

Deformed mean-field:

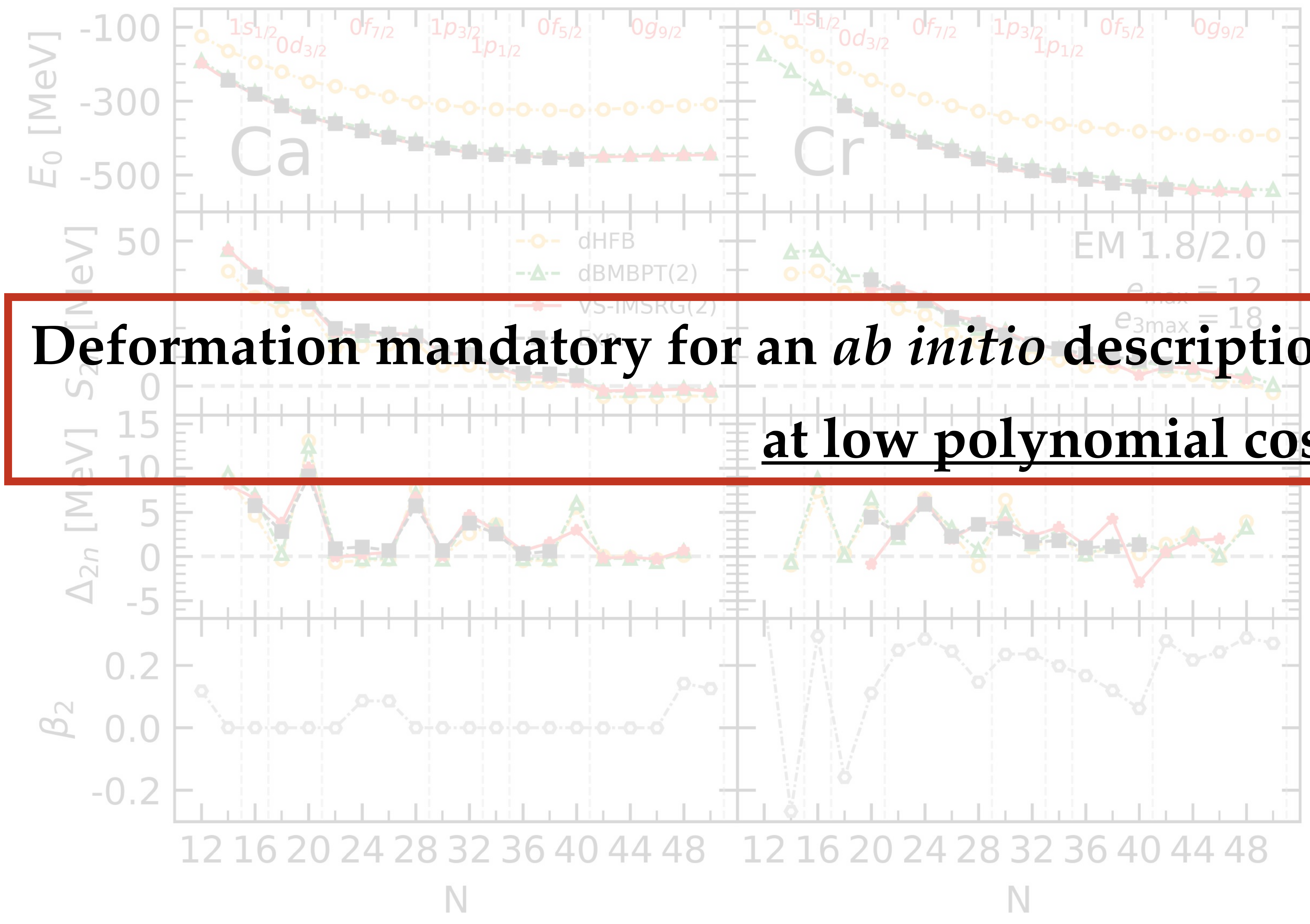
- **Underbinding** but **correct** curvature
- **Qualitatively** correct S_{2n}
- **Correct shell gaps**

Low-order dynamical correlations:

- **Correct** curvature
- Underbinding **corrected**
- **Quantitatively** correct S_{2n}
- **Correct shell gaps**

Non polynomial for reference

SU(2)-breaking *ab initio* approaches



Deformation mandatory for an *ab initio* description of doubly open-shell nuclei

<u>at low polynomial cost</u>

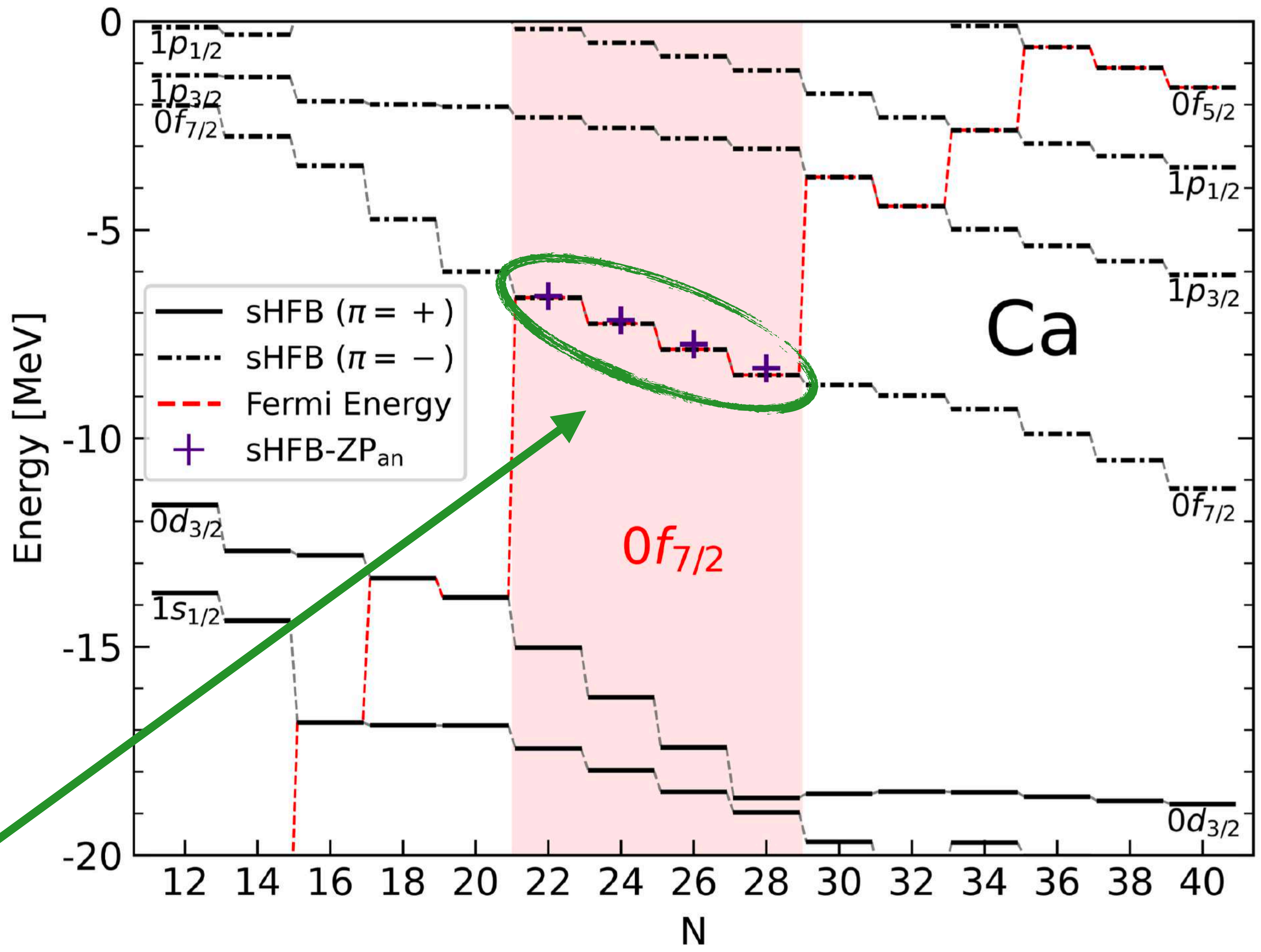
Analytical analysis of wrong curvature in spherical HFB

- Weak pairing in *ab initio* $\rightarrow$ sHF-EFA $\approx$ sHFB-ZP [Duguet *et al.* 2020]

- $$\Delta E^{\text{sHF-EFA}}(a_v) \equiv \alpha_{\breve{v}} a_v + \frac{\beta_{\breve{v}}}{2} a_v^2$$
  - a_v number of nucleons in the open shell
  - $\alpha_{\breve{v}} = \varepsilon^{\text{CS}}_{\breve{v}}$
  - $\beta_{\breve{v}} \equiv \frac{1}{d_{\breve{v}}} \sum_{m_{v'}}^{d_v} \bar{\boldsymbol{v}}_{vv'vv'}$ → **monopole valence-shell ME**

- $\Delta^{\text{sHF-EFA}}_{2n}(a_v) = 4\beta_{\breve{v}}$ → **concavity**, $\varepsilon^{\text{sHF-EFA}}_{\breve{v}}(a_v) = \varepsilon^{\text{CS}}_{\breve{v}} + \beta_{\breve{v}} a_v$ → **ESPE**

- $\beta_{\breve{v}}$ **negative**
  - → **concave** binding energy ✗
  - → **decreasing** ESPE ✓



- Conclusions tested to be stable w.r.t. interaction (LECs, Chiral Order, SRG)

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

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

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

$$\ldots$$

Martin-Schwinger equations

$$g_{\alpha\beta}(\omega) = g_{0\,\alpha\beta}(\omega) - \sum_{\gamma\delta} g_{0\,\alpha\gamma}(\omega)\, u_{\gamma\delta}\, g_{\delta\beta}(\omega)$$

$$\int \frac{d\omega_1}{2\pi} \int \frac{d\omega_2}{2\pi}\, g_{\delta\mu,\beta\epsilon}^{4-\mathrm{pt}}(\omega_1, \omega_2; \omega, \omega_1 + \omega_2 - \omega)$$

$$\ldots$$

Decouple via Σ

Basic ingredients

A-body wave function ⇢ Green's functions

$$|\Psi_k^A\rangle$$

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

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

$$\cdots$$

↓

A-body Schrödinger equation ⇢ Dyson equation

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

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

Self-energy expansion → Many-body approximation

↓

Observables: expectation values ⇢ Observables: convolutions with GFs

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

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

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

Basic ingredients

$$|\Psi_k^A\rangle$$

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

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

Algebraic Diagrammatic Construction (ADC)
Employed here at 2nd order (ADC(2))

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

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

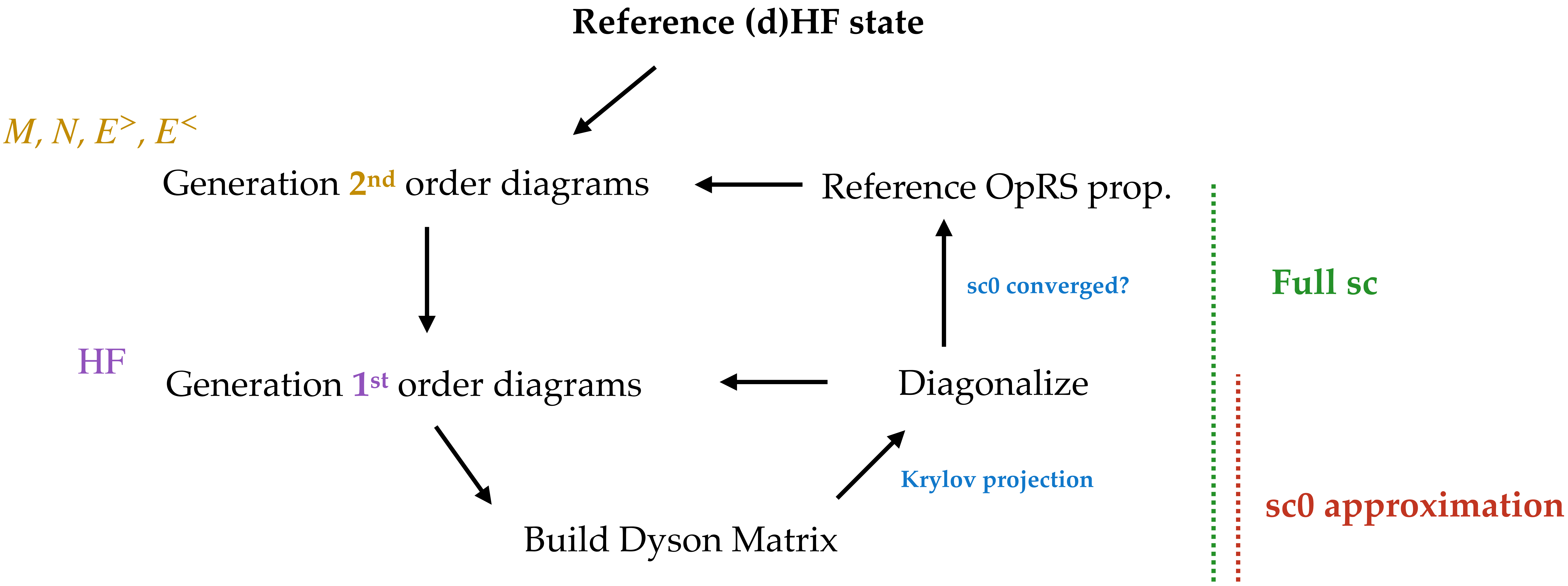
Self-energy expansion $\rightarrow$ Many-body approximation

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

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

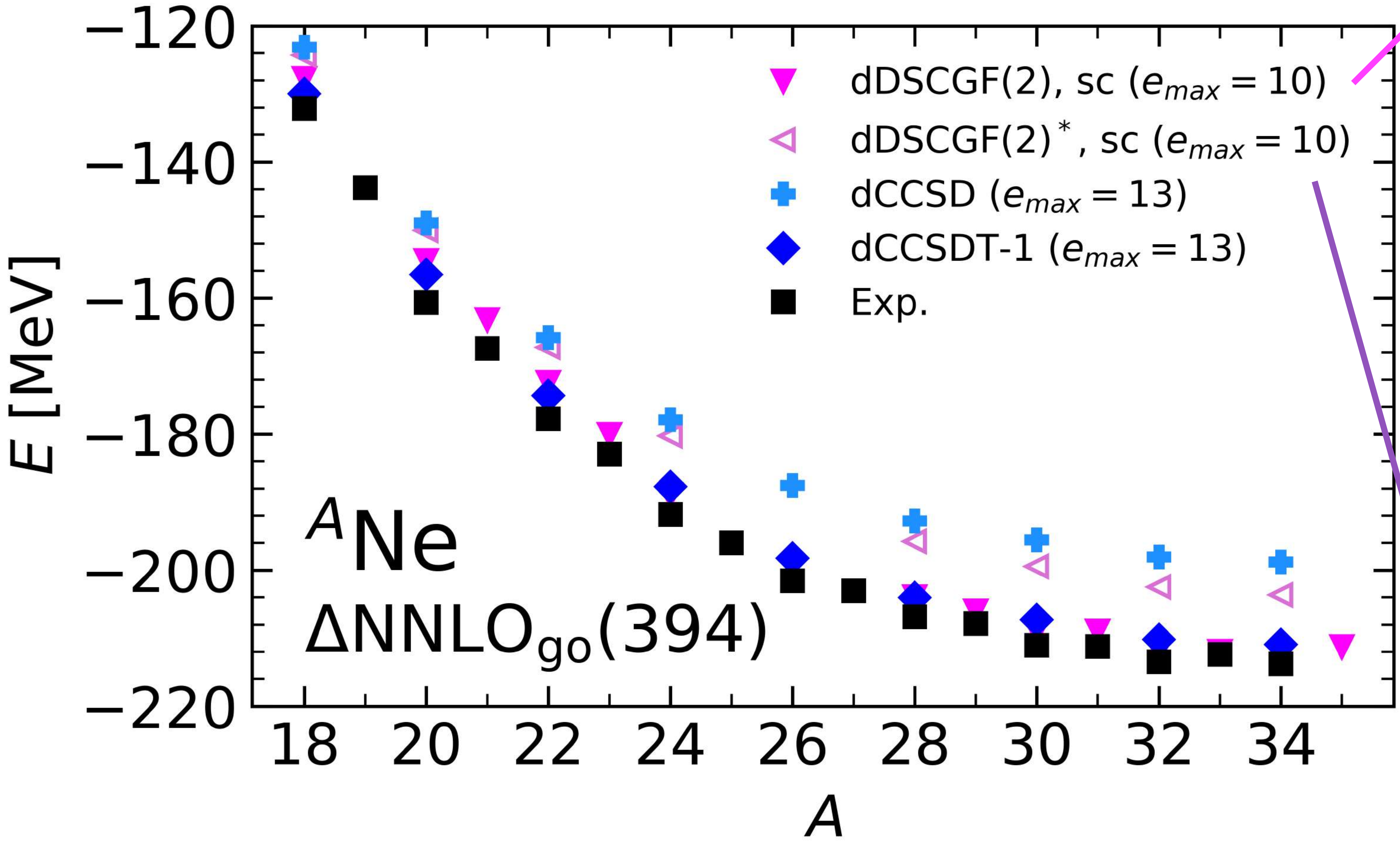
$$E_0 = \langle \Psi_0^A \,|\, H \,|\, \Psi_0^A \rangle = \frac{1}{2} \sum_{\alpha\beta} \int \frac{d\omega}{2\pi i}\, g_{\beta\alpha}(\omega)\, [t_{\alpha\beta} + \omega\, \delta_{\alpha\beta}]$$

The self-consistent loop



Ground-state energy of Neon isotopes

First tests on Neon isotopes where dCC results are available



[Novario *et al*. 2020]

- **dDSCGF** trend in line with CC and Exp.
- Access to **odd-even systems**
- **dDSCGF** results deliver wrong part. num.

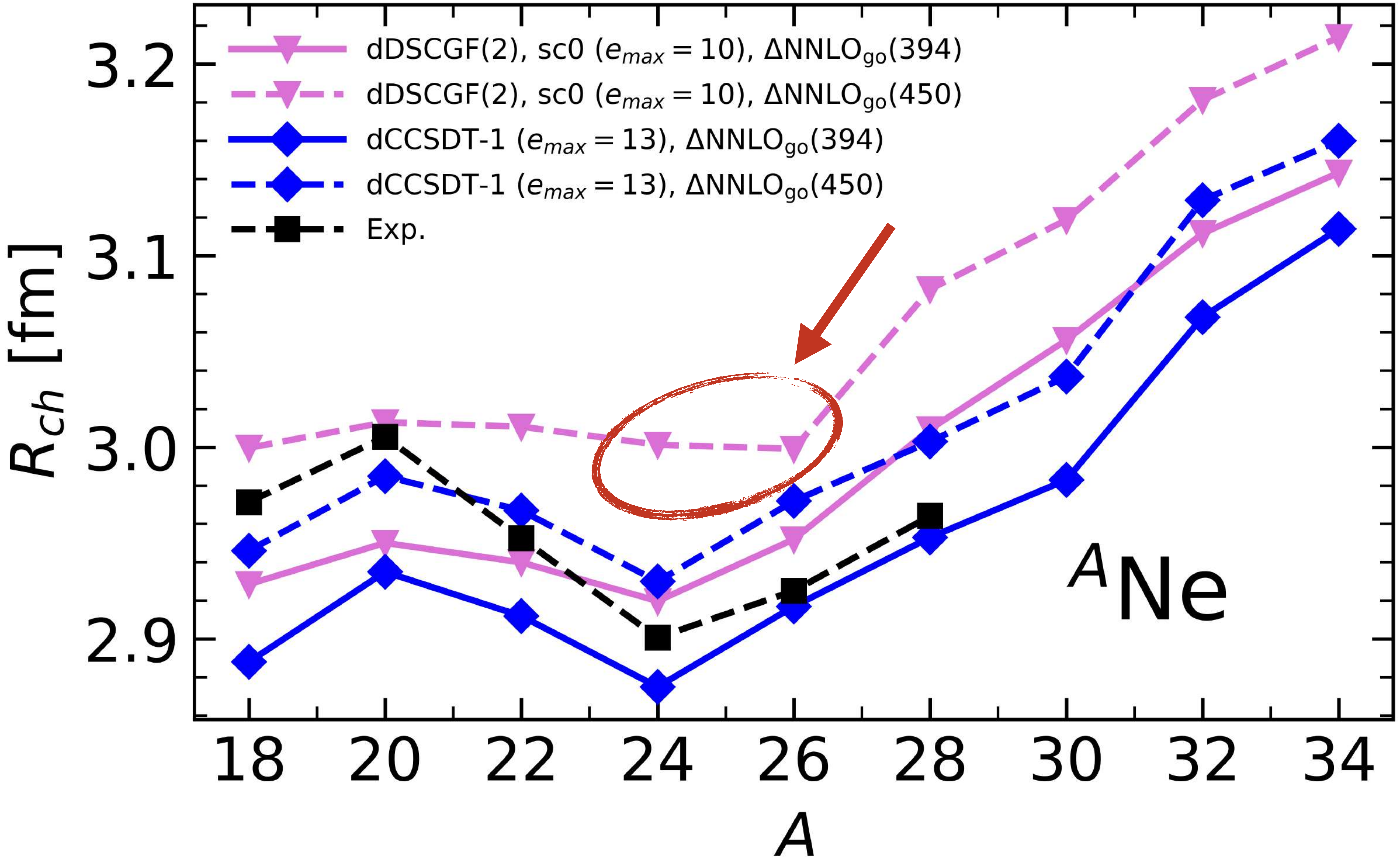
overbinding

Need of a <u>particle adjustment</u>

- **Naïve rescaling** based on mass

Energies compatible with **dCCSD**

Charge radii of Neon isotopes



1B + 2B CoM corrections

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

- Overall trend follows dCCSDT-1
- Shift prob. due to MB order and e_{max}
- **Wrong trend** for $^{24\text{-}26}$Ne

[Novario *et al.* 2020]

dDSCGF(2) vs sGSCGF(2) in Argon isotopes

(2021)

Moving away from singly-magic nuclei with Gorkov Green's function theory

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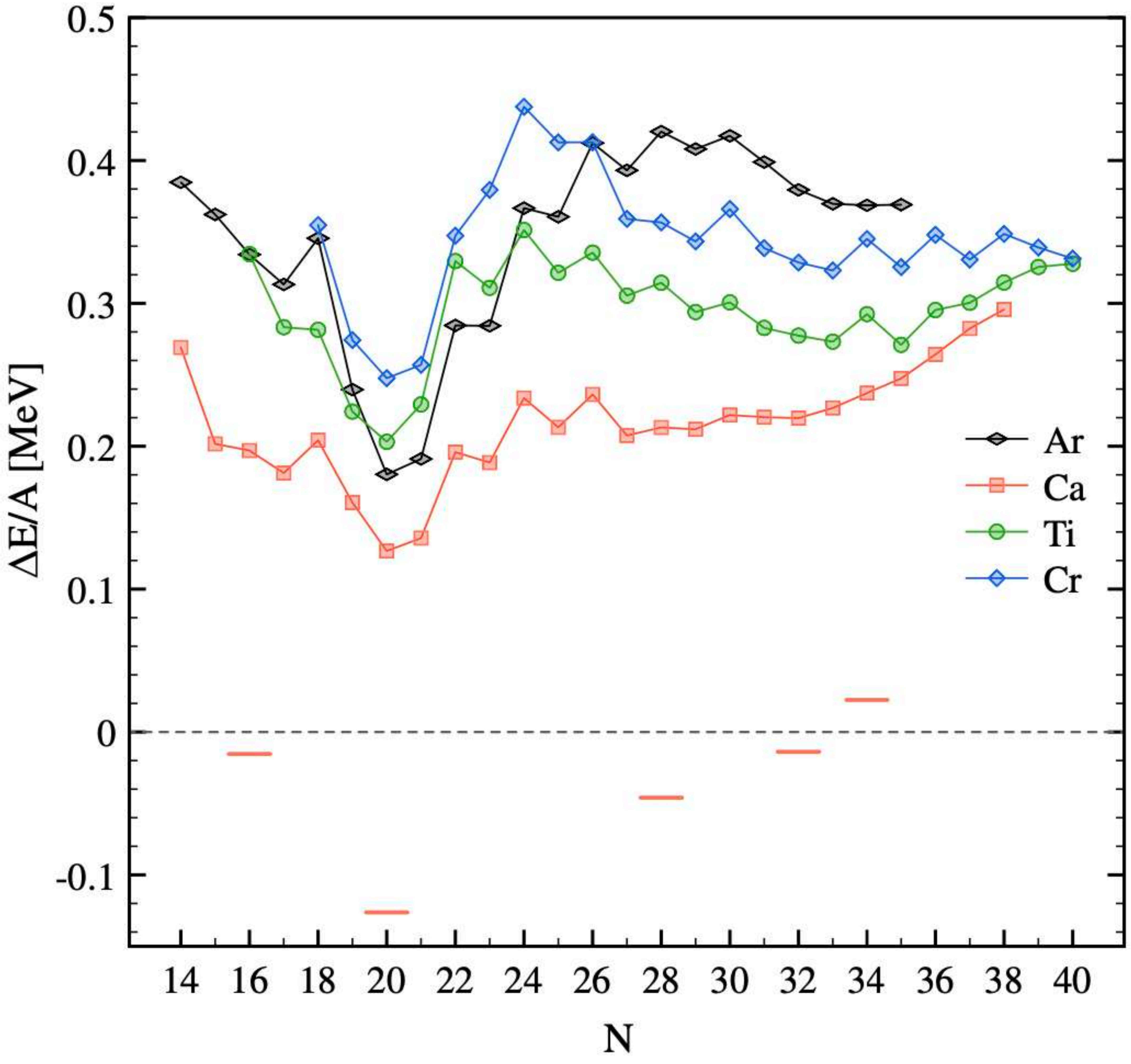
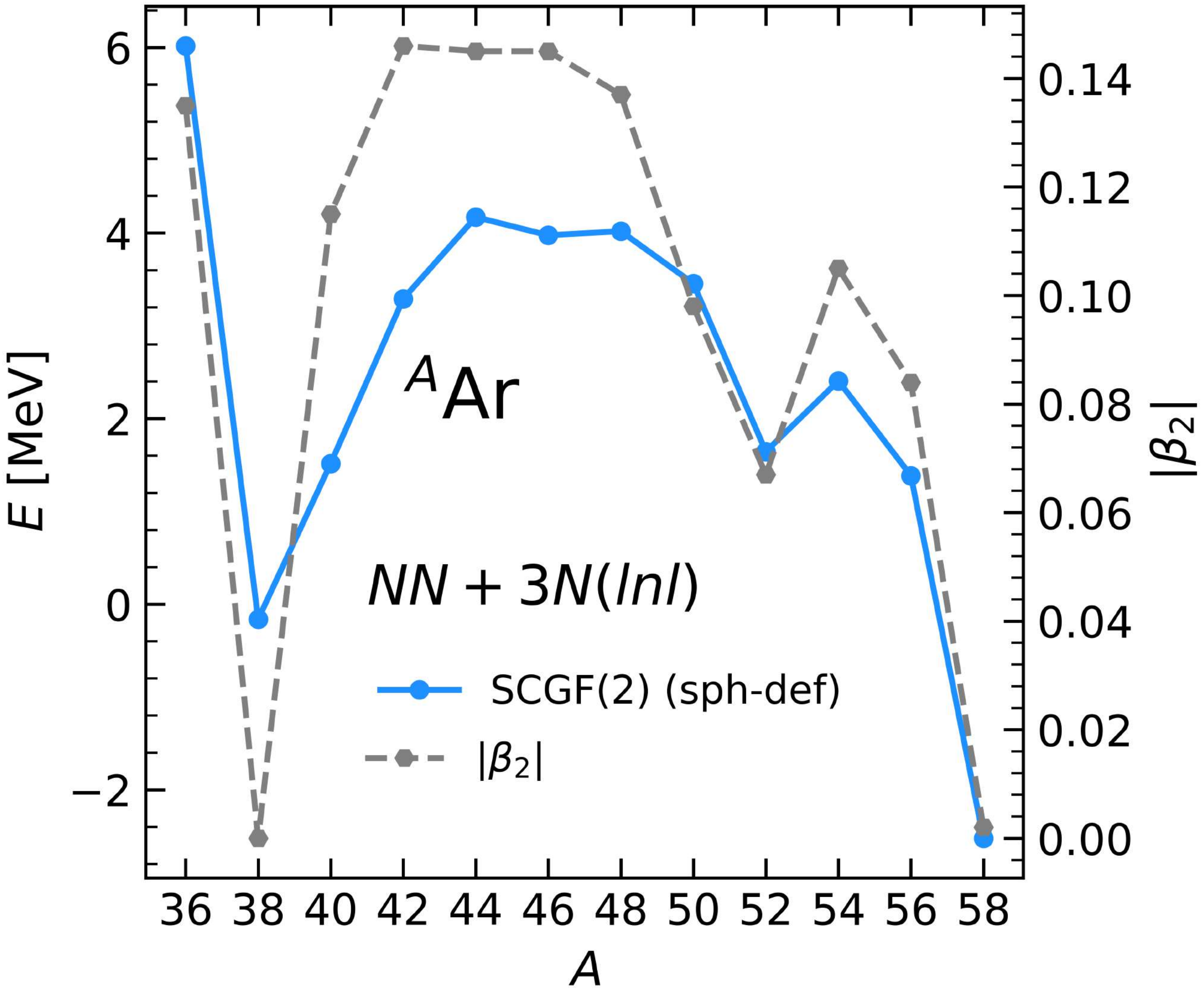
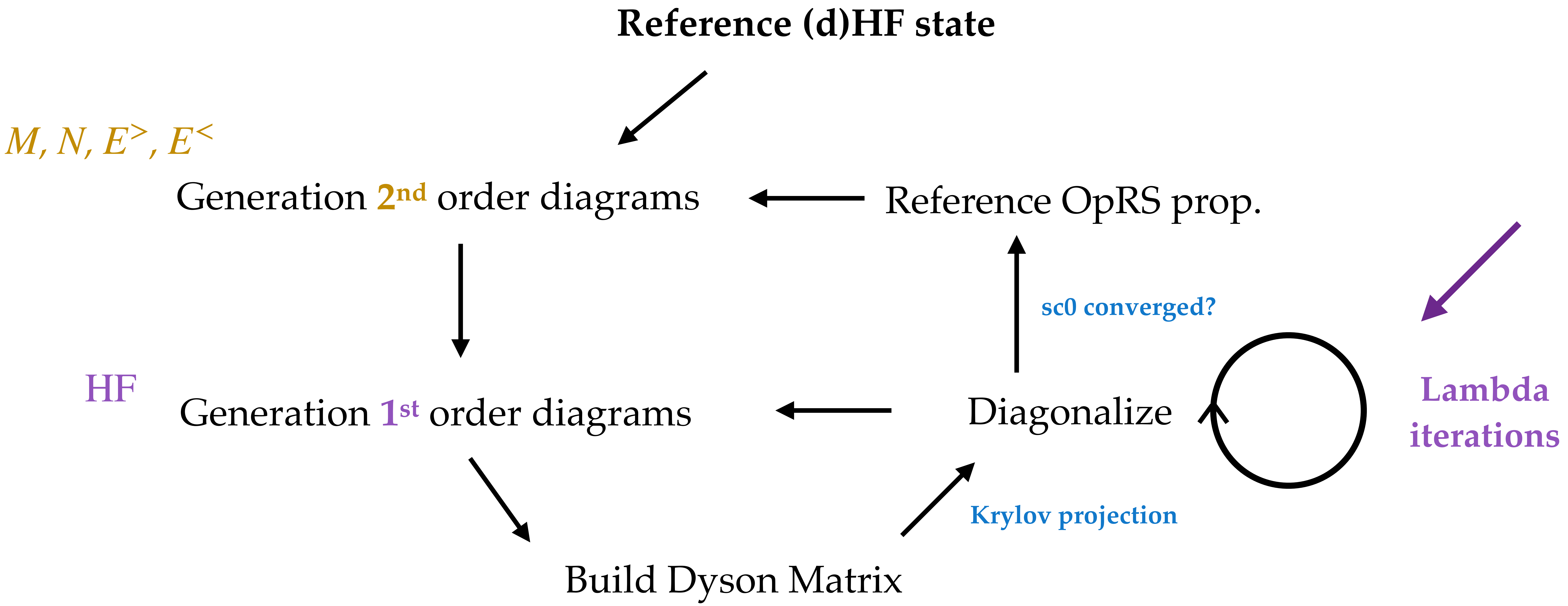


dDSCGF(2) vs sGSCGF(2) in Argon isotopes



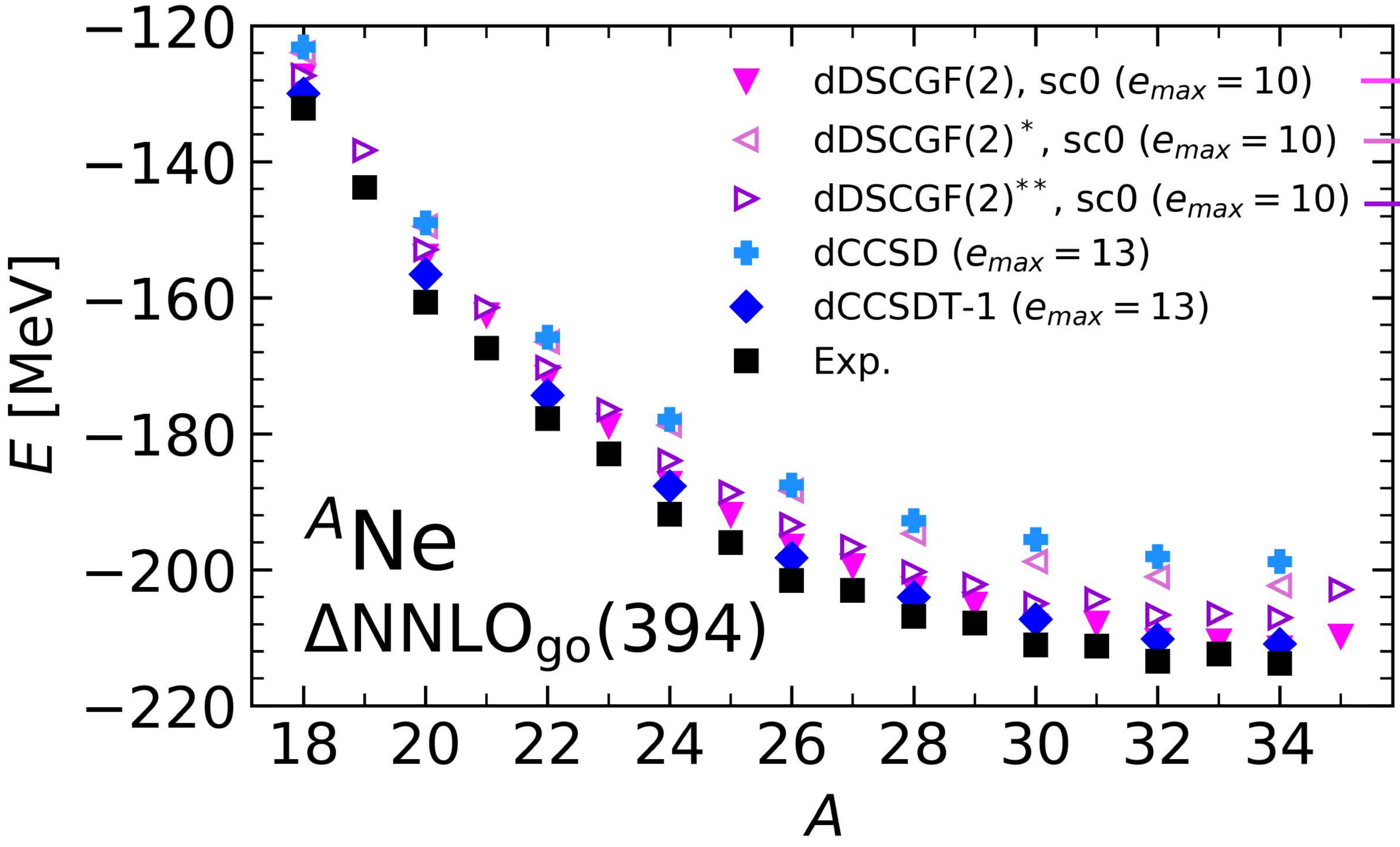
- Comparison with **spherical Gorkov** calc.
- **Oblate** isotopic chain
- **Correlation** of difference **w.r.t. def.**
- **Improved description** of collectivity
- **Necessity of deformation**

Particle adjustment: theoretical setup



→ **no additional computational cost!**

Particle adjustment: ground-state energy



→ **Wrong particle number**

→ **Naïve rescaling**

→ **Proper particle adjustment**

- Lamba loop **numerically stable** for sc0
- Access to **odd-even** nuclei restored
- **~4 MeV gain** w.r.t. naïve rescaling
- CC for comparison

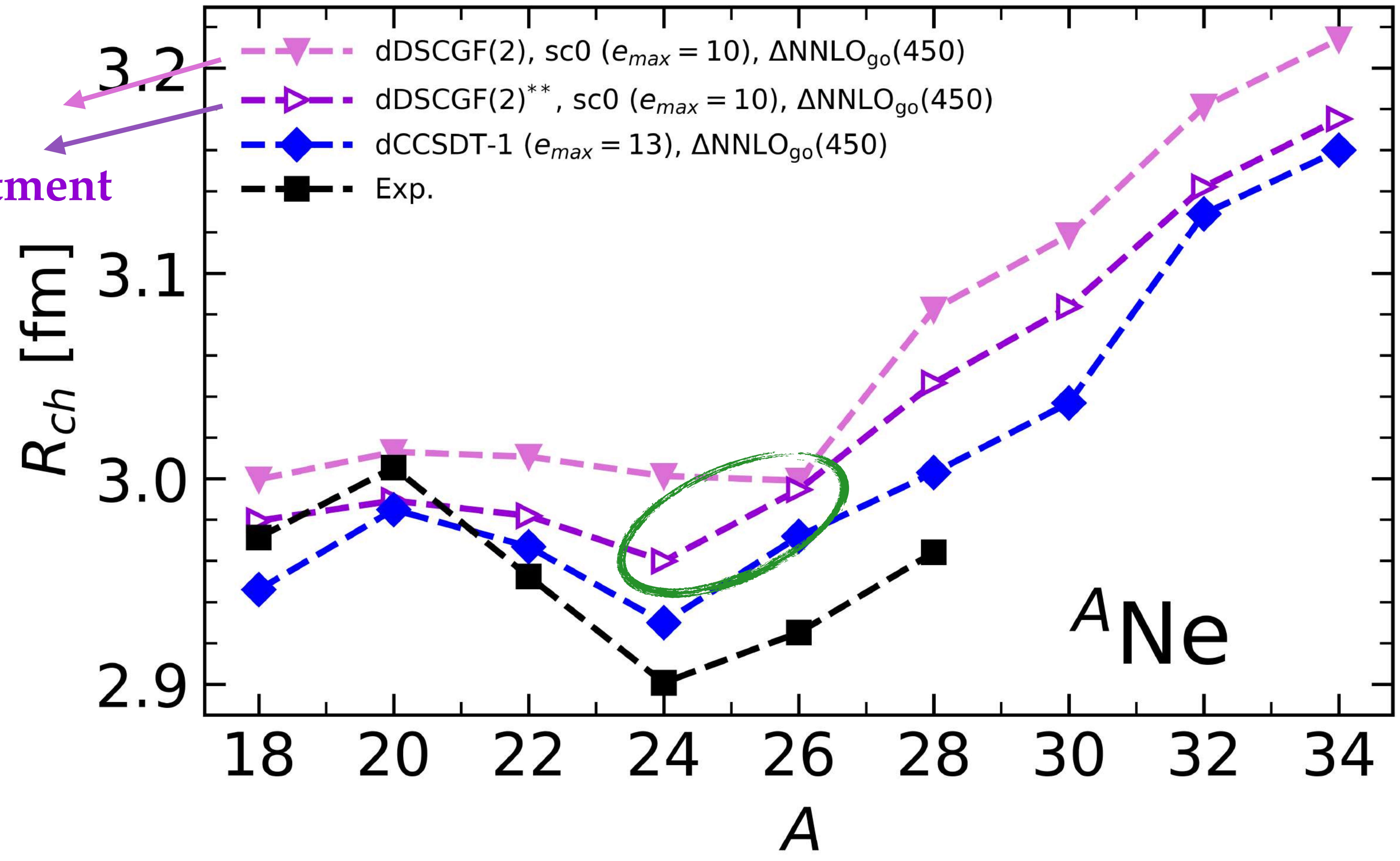
→ **Self-consistent** loop also numerically stable with particle adjustment!

Particle adjustment: charge radii

[Novario *et al.* 2020]

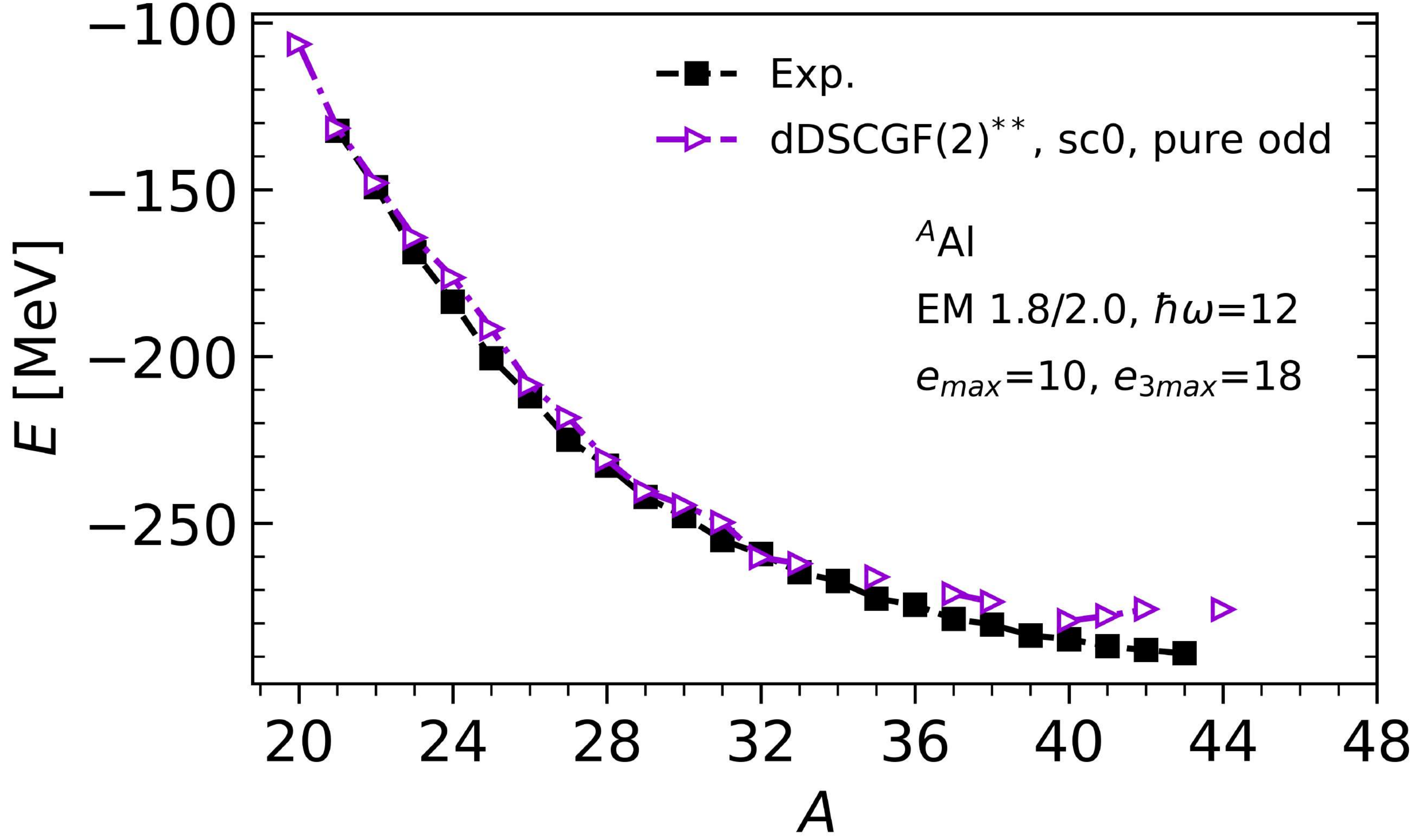
Standard sc0

Proper particle adjustment



→ Results **closer** to dCCSDT-1 and Exp. → **Correct trend** for $^{24\text{-}26}$Ne

Direct calculation of odd systems



Super-preliminary calculation of Aluminium isotopes!

Conclusions

⟶ **Deformation** is mandatory for the *ab initio* description of open-shell nuclei with polynomial scaling

⟶ **Correlations** captured by dDSCGF bring visible results on observables w.r.t. dBMBPT2 (and sGSCGF)

Future perspectives:

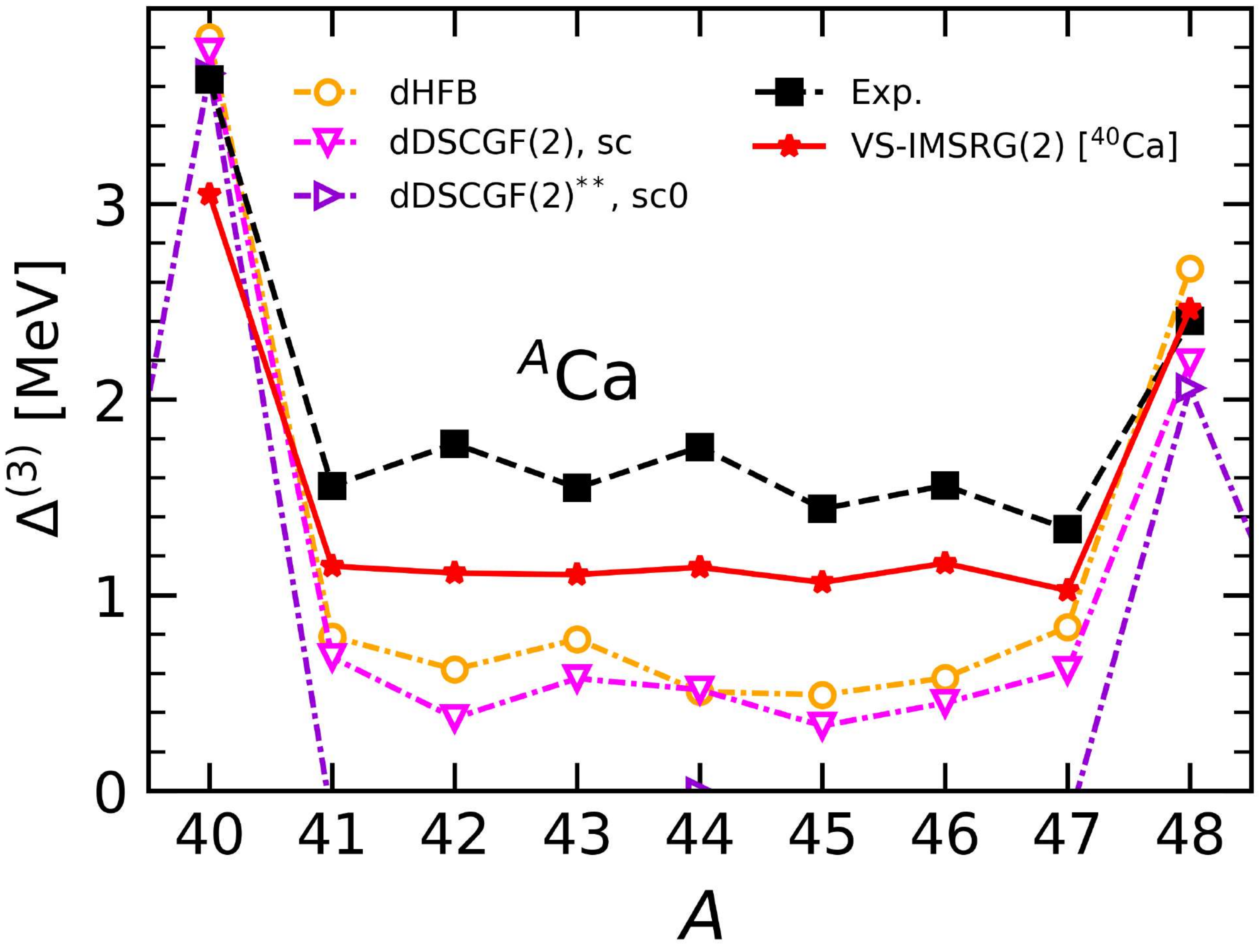
- Beyond ADC(2): extended ADC(2) and **ADC(3)** ⟶ Numerical optimization code (MPI)

- Generalize to more general symmetry breakings: **triaxial** and **octupolar** deformations

- dDSCGF with **good angular momentum** ⟶ Symmetry Restoration (yet to be formulated)
  ⟶ **MR-SCGF**

- First application: **optical potentials** in open-shell nuclei

Upcoming project on nuclear superfluidity



- **Nuclear superfluidity** → three-point mass formula

$$\Delta^{(3)}(N) \equiv \frac{(-1)^N}{2}[E(N+1) - 2E(N) + E(N-1)]$$

- Many-body correlations go in the right direction

[*Paper in preparation*]

- Results for EM 1.8/2.0 interaction

⟶ Upcoming sensitivity study on impact of LECs on superfluidity

[*Influence of chiral forces on nuclear pairing*. AS, A. Ekström, C. Forssén. *In preparation*]

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