Ab initio description of open-shell nuclei at polynomial cost

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Cutting-edge developments in nuclear structure physics

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Outline

- Open-shell nuclei at polynomial cost: necessity of deformation
- Deformed self-consistent Green's function
- Conclusions

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V. Somà, T. Duguet, M. Frosini

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

[A. Scalesi et al., Eur. Phys. J. A 60, 209 (2024)]

[A. Scalesi et al., Eur. Phys. J. A 61, 1 (2024)]

[E. M. Lykiardopoulou et al., Phys. Rev. Lett. 134, 052503 (2024)]

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NUMERICS

International PhD Program in Numerical Simulation at CEA

Outline

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

The Segrè chart

Different possible approaches:

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

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Solving the Schrödinger equation at polynomial cost

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

static correlations

$\downarrow$

included in ref. state through sym. break.

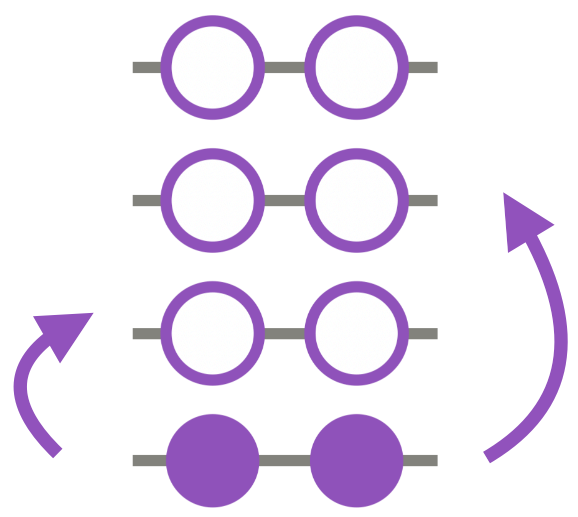
$\longrightarrow$ **Correlation-expansion methods**

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**: $H_0 \left|\Theta_k^{(0)}\right\rangle = E_k^{(0)} \left|\Theta_k^{(0)}\right\rangle$



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

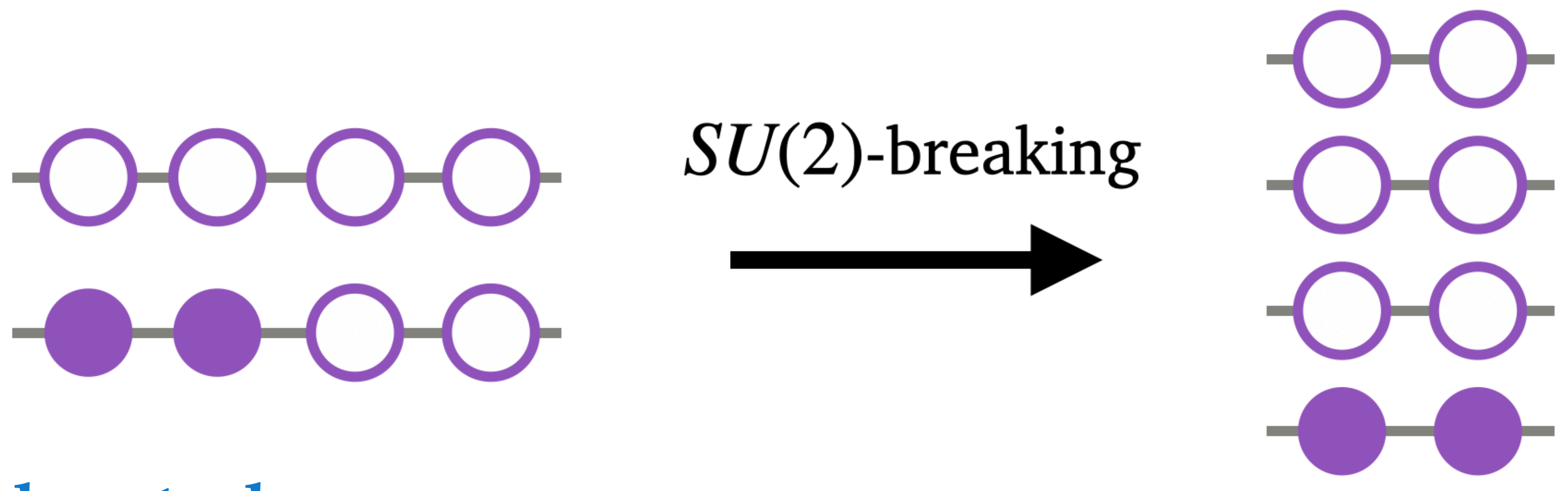
Wave-operator expansion: $\left|\Psi_k^\sigma\right\rangle = \Omega_k \left|\Theta_k^{(0)}\right\rangle$ $\longrightarrow$ **Resummation of dynamical correlations**

- **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**
Singly open-shell	2010 - 2020	**sHFB**
Doubly open-shell	2020 - …	**dHF(B)**

- 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)

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 sBMBPT(2) sBCCSD	dHFB dBMBPT(2)	[Tichai *et al.* 2020] [Frosini *et al.* 2021] [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)**

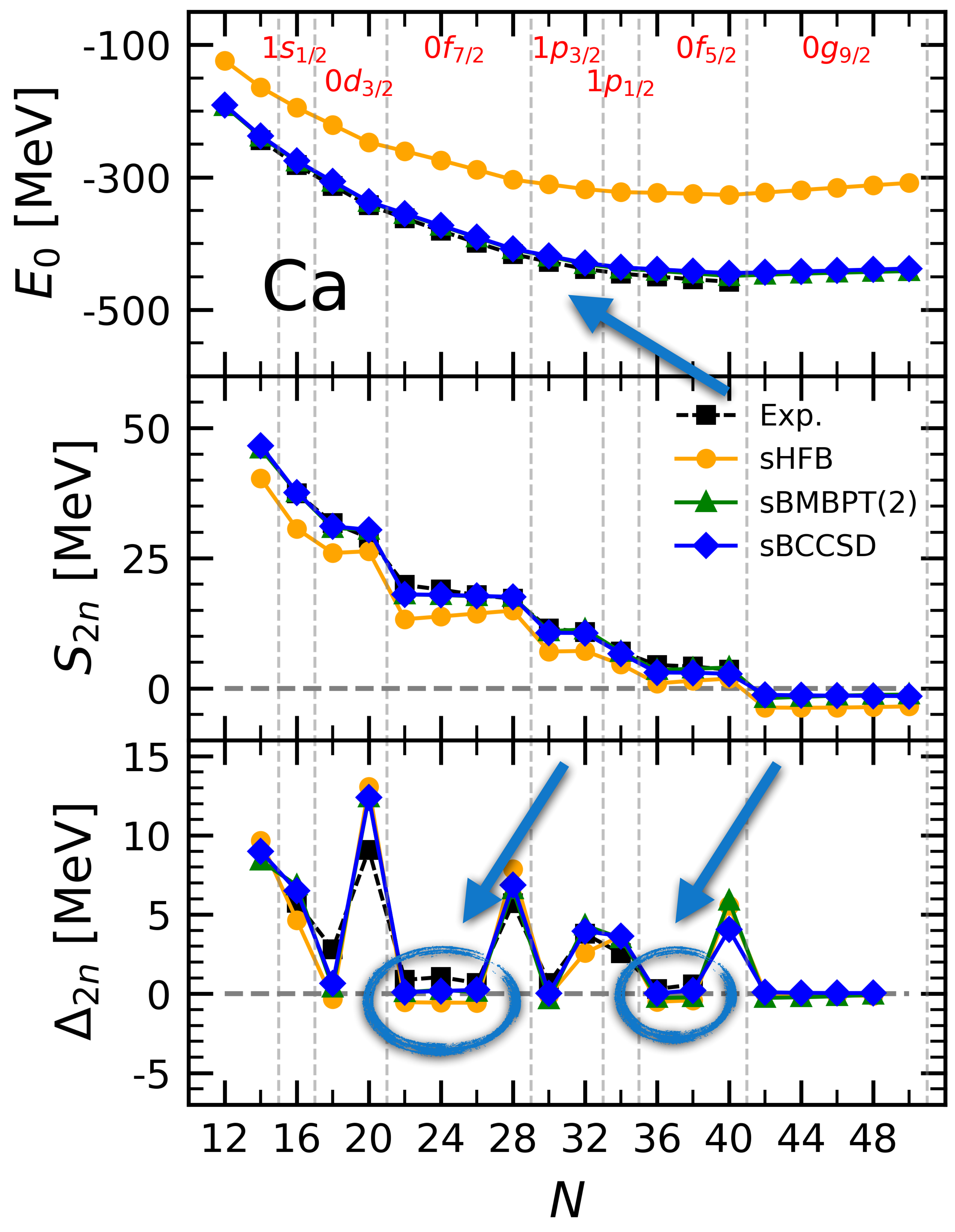
SU(2) Conserving vs **SU(2) Breaking**

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

SU(2)-conserving *ab initio* approaches



Singly open-shell

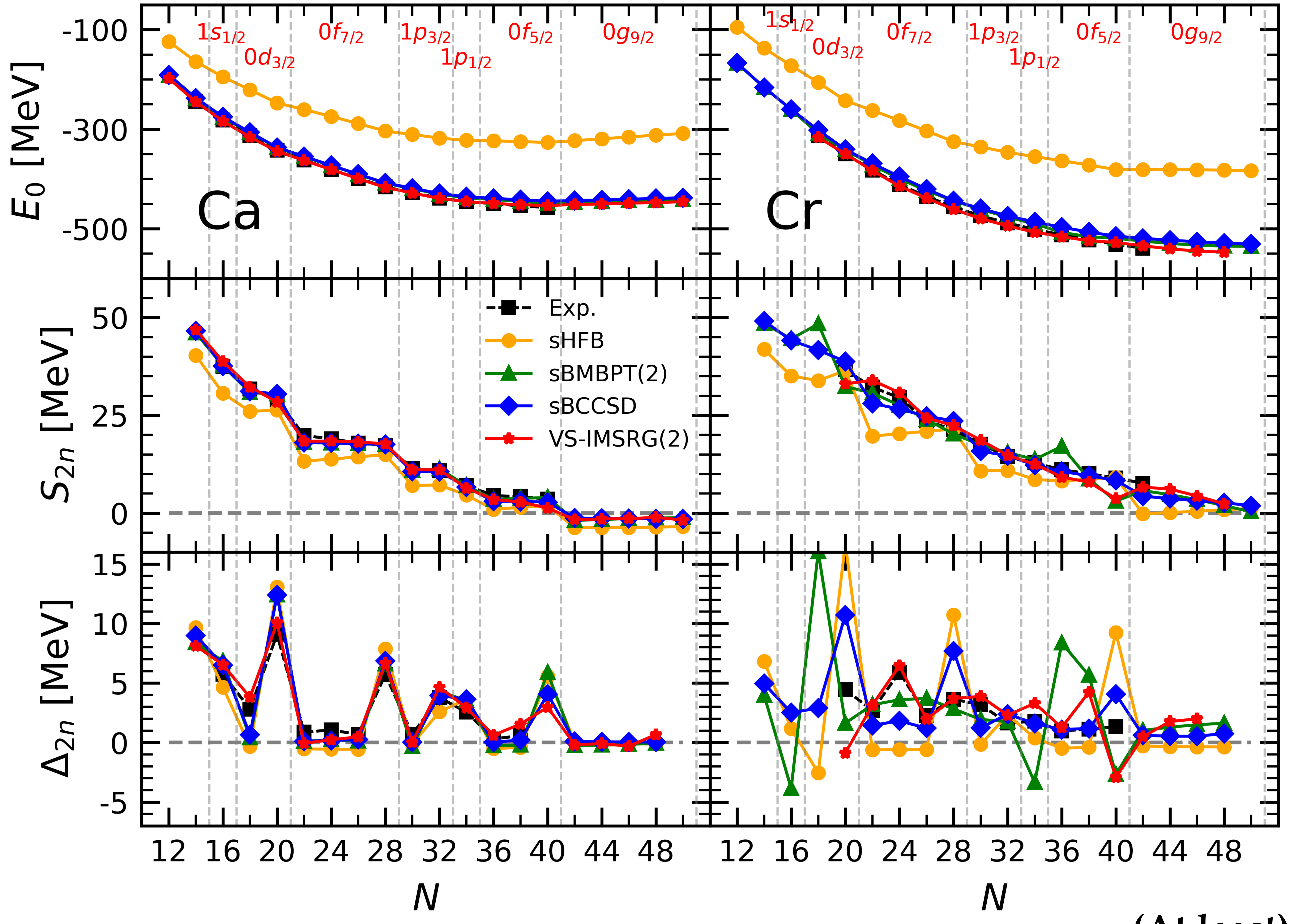
Spherical mean-field:

- **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**

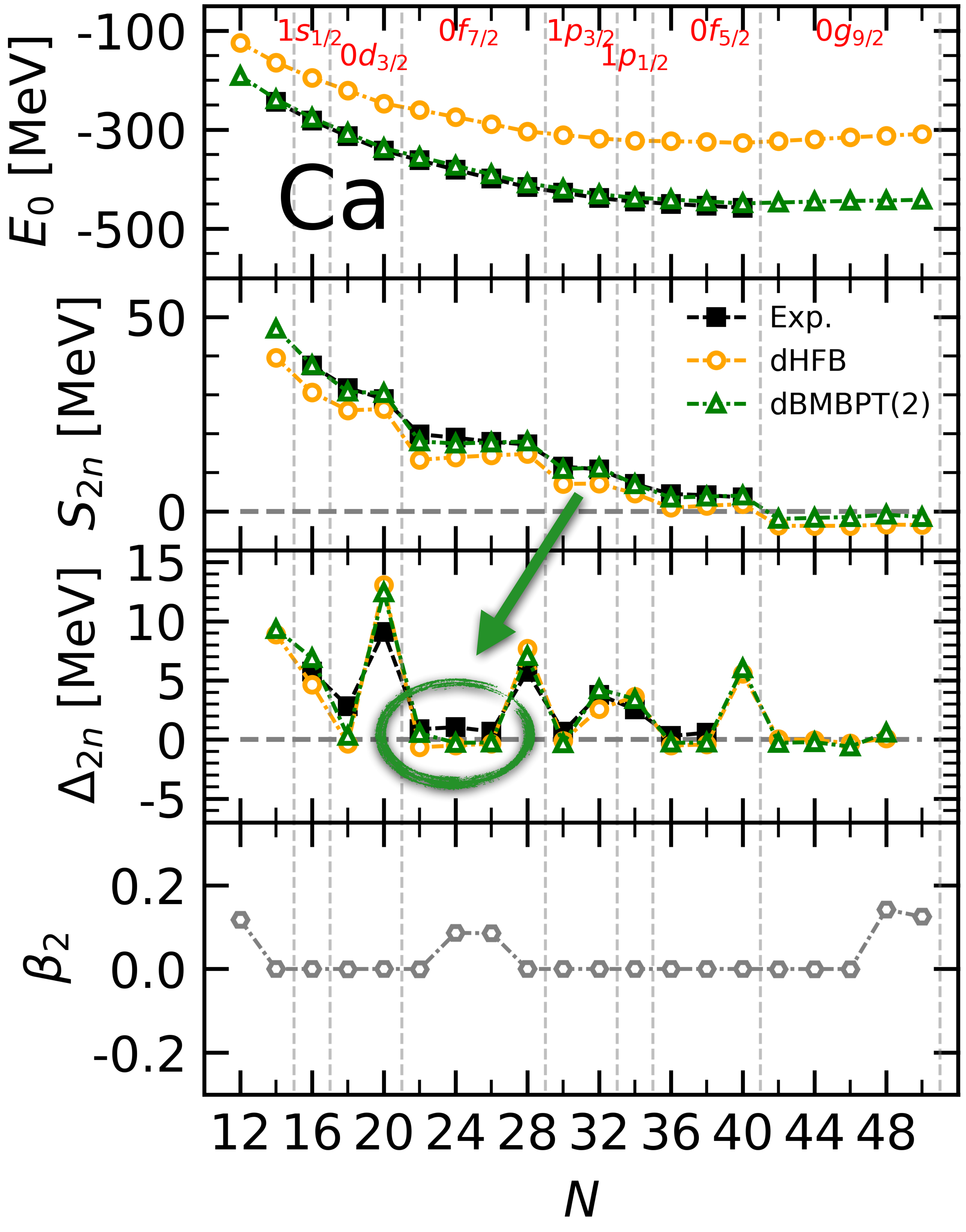
Non polynomial:

- 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

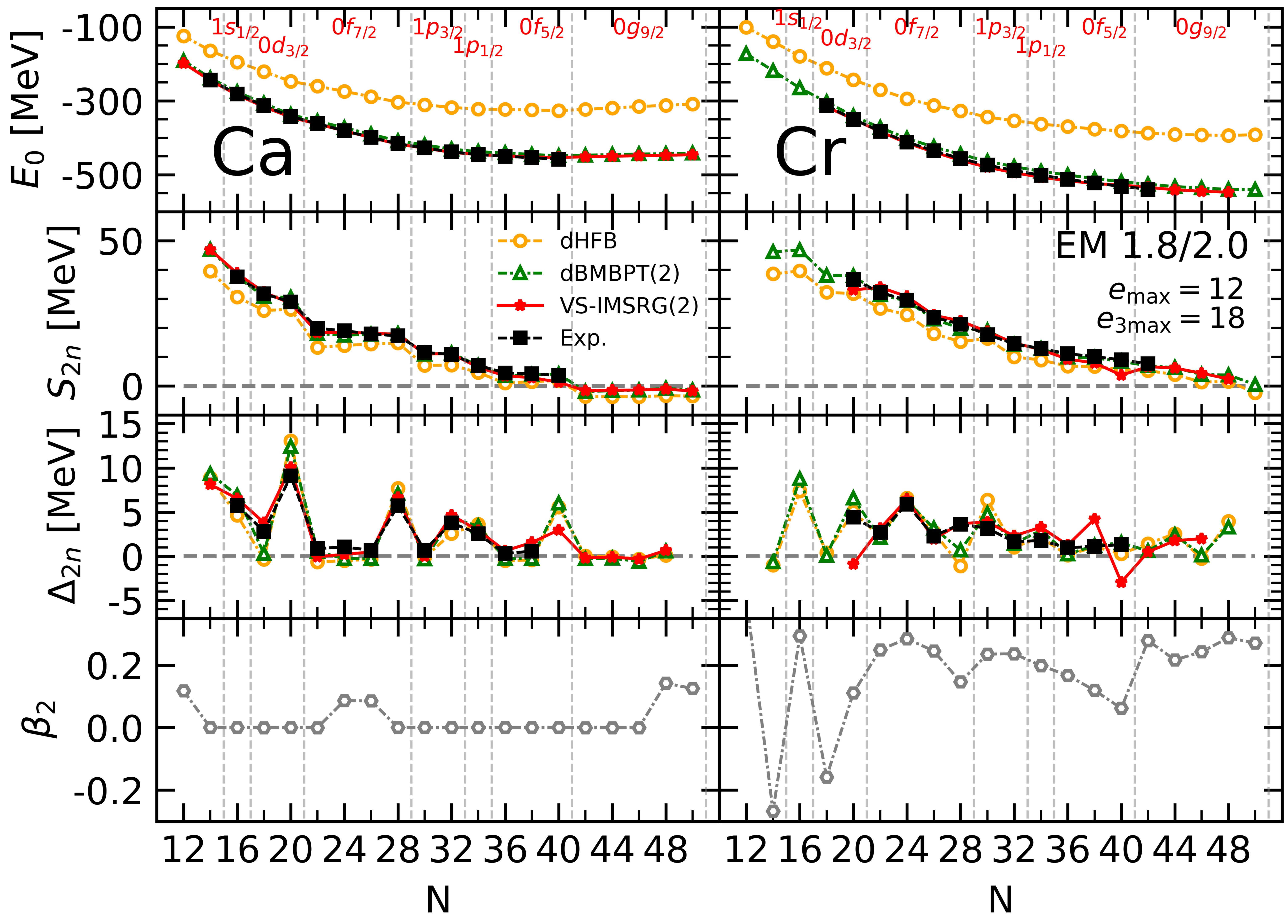
Deformed mean-field:

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

Low-order dynamical correlations:

- **Slightly improved** curvature

SU(2)-breaking *ab initio* approaches



Doubly open-shell

Deformed mean-field:

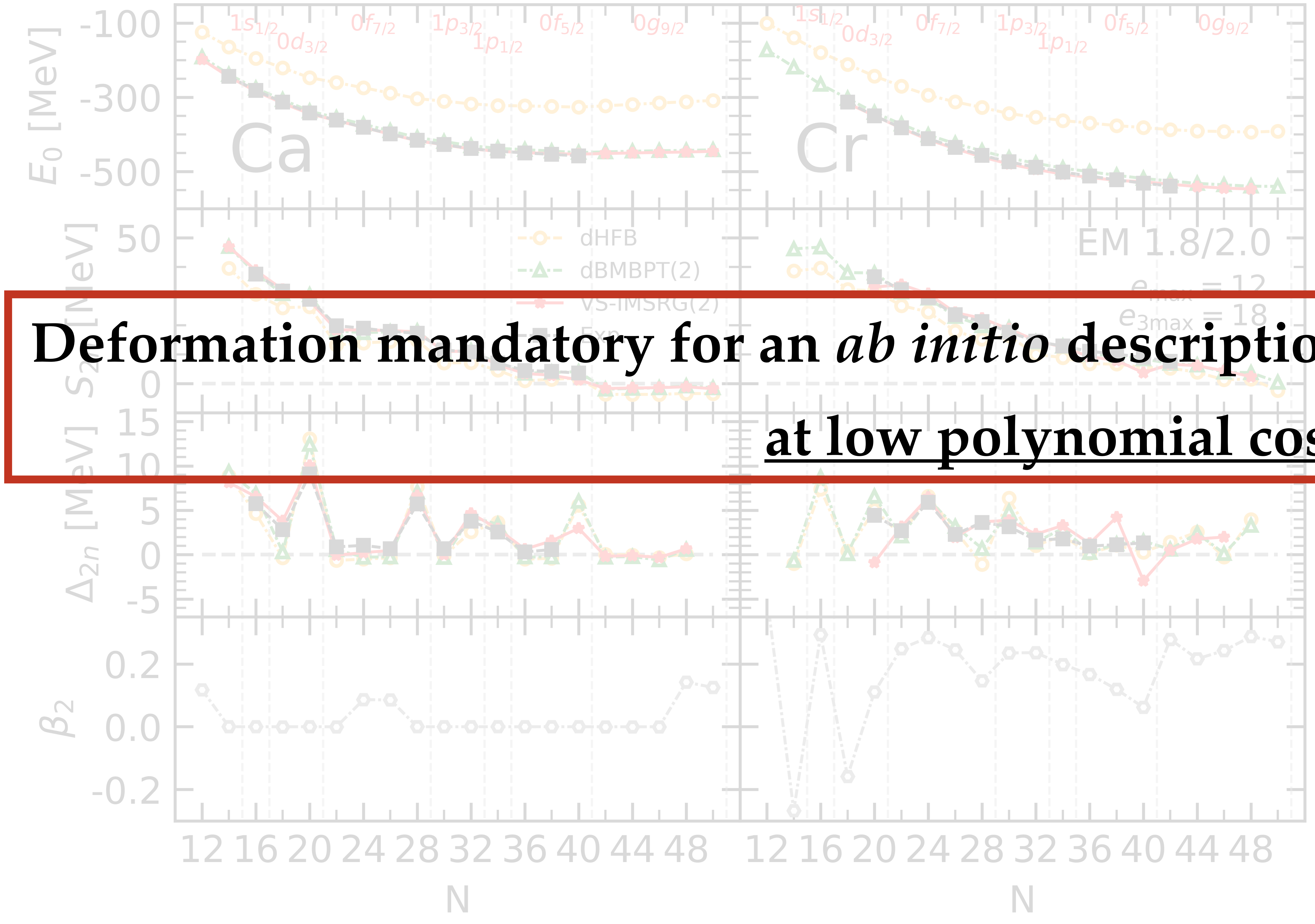
- **Underbinding** but **correct** curvature
- **Qualitatively** correct S_{2n}
- **Correct shell gaps**

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>

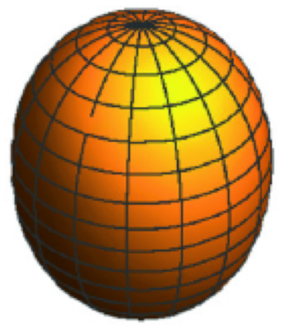
Extension to further symmetry breaking

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

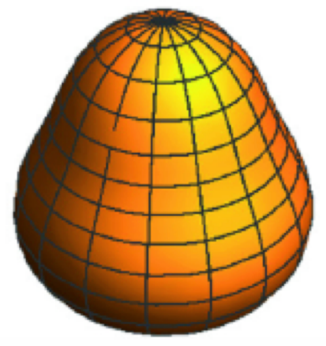
Breaking more symmetries allows to effectively enrich more the mean-field with correlations

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

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

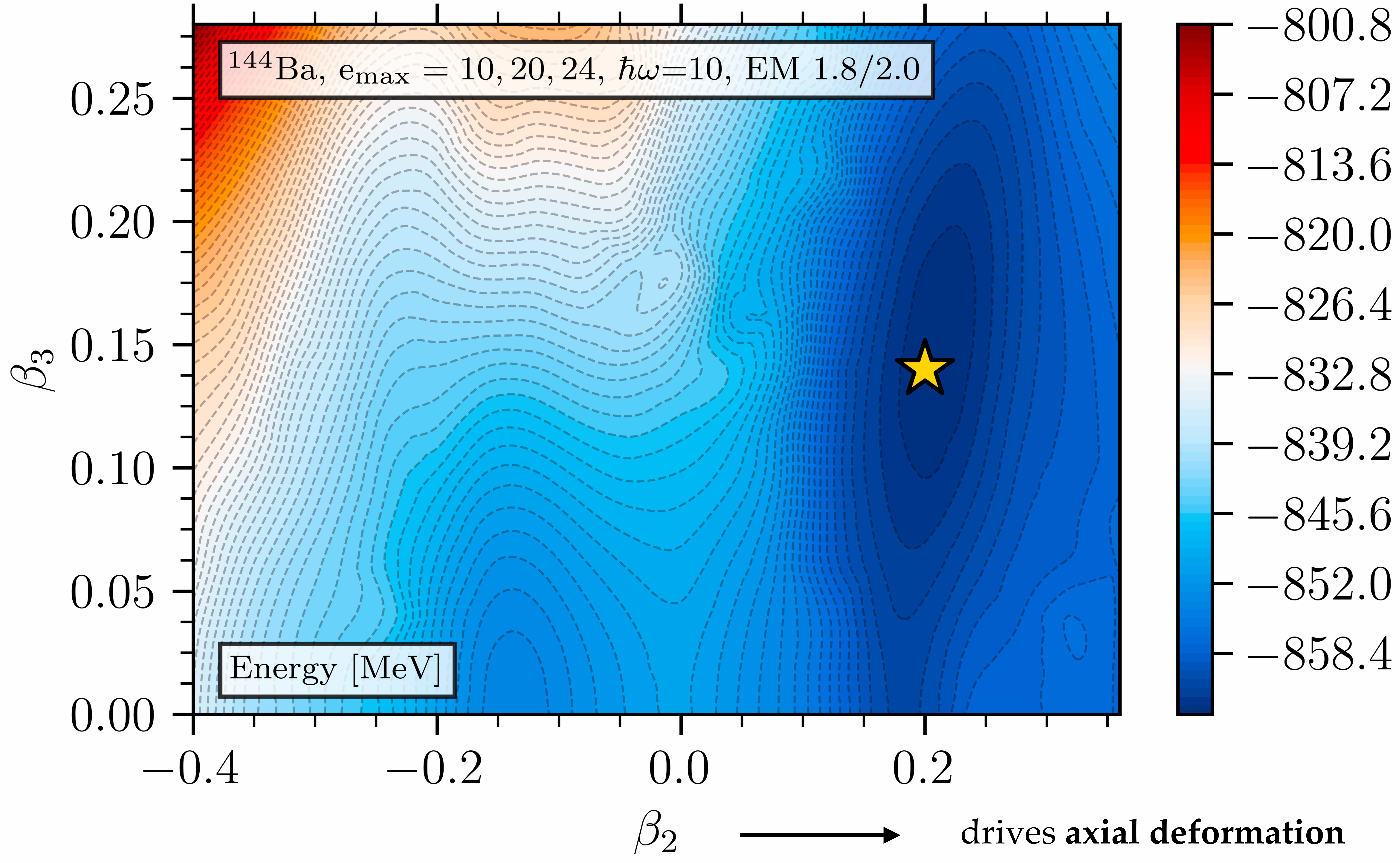


- **Ocupolar** deformation $\rightarrow$ break J and parity Π



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

Extension to further symmetry breaking

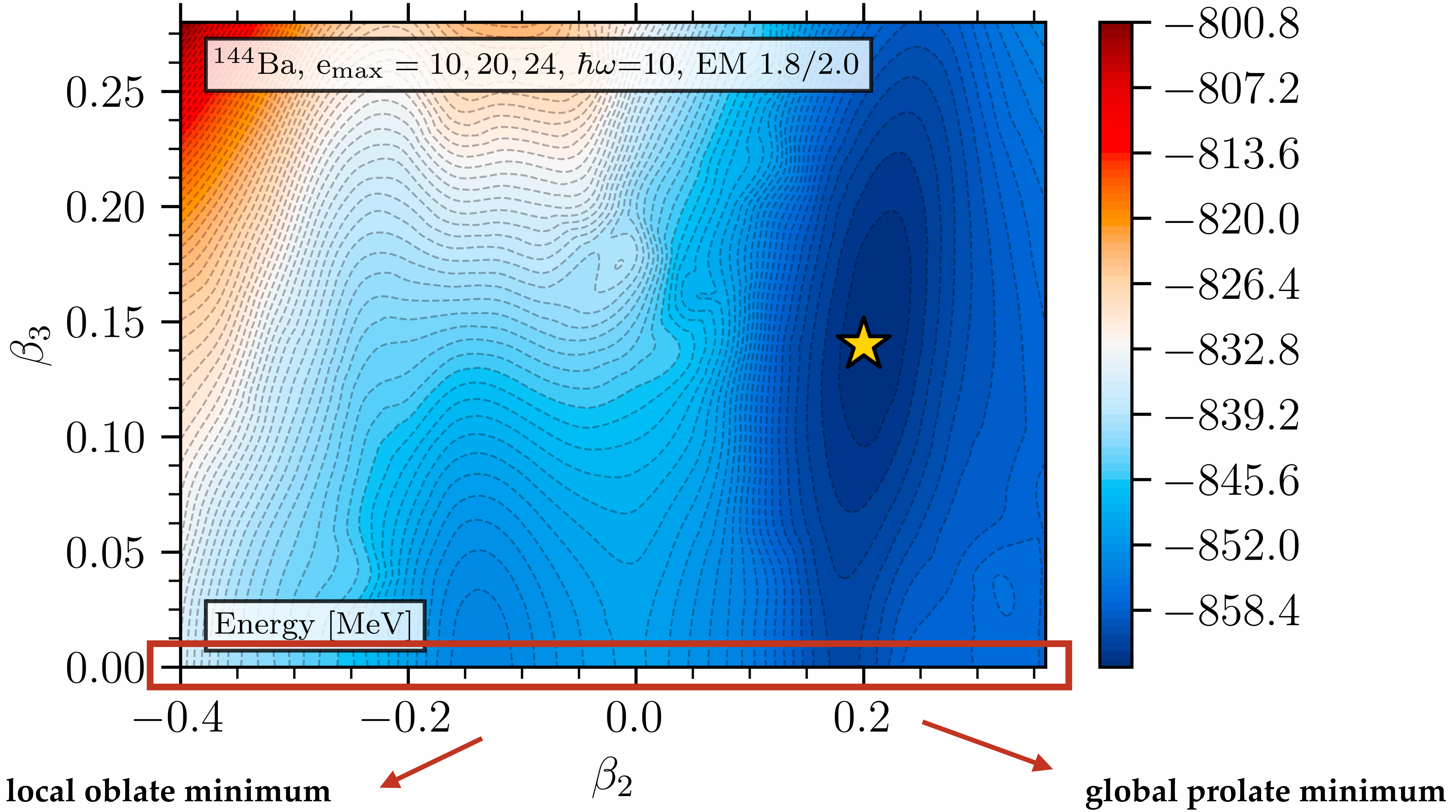


drives **octupolar deformation**

drives **axial deformation**

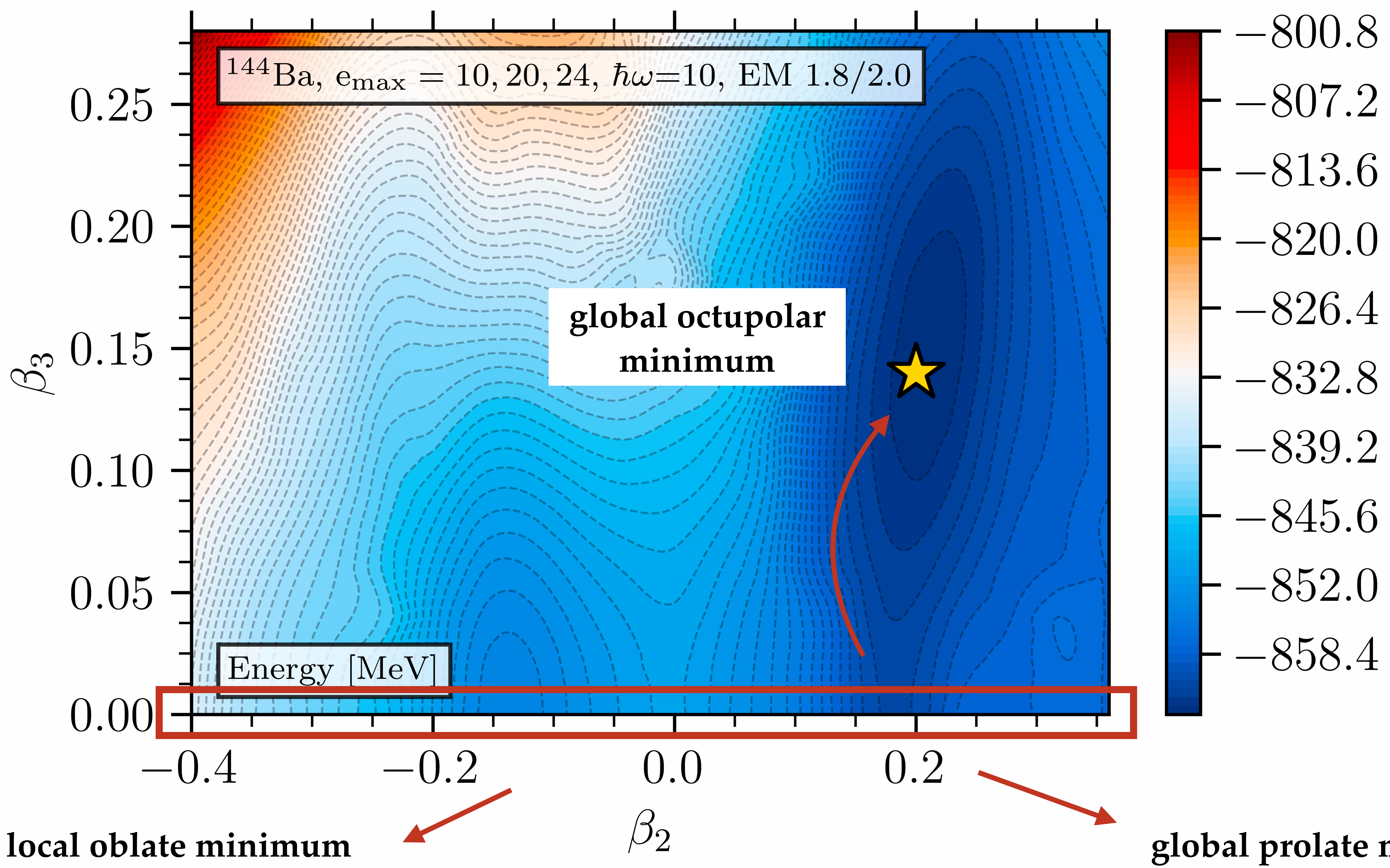
[A. Scalesi et al., *in preparation*]

Extension to further symmetry breaking



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

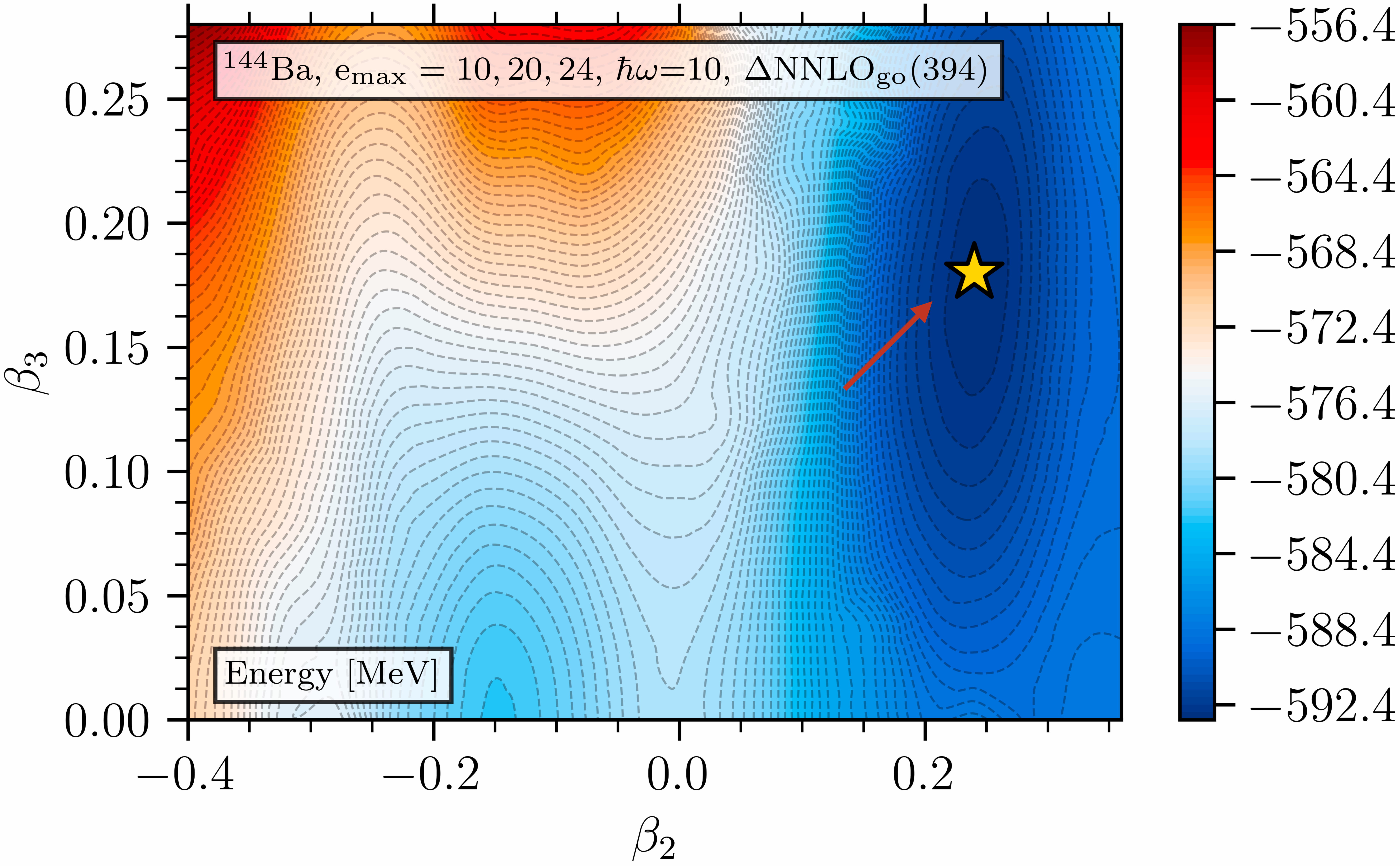
Extension to further symmetry breaking



local oblate minimum **global prolate minimum**

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

Extension to further symmetry breaking



→ **Stability w.r.t. nuclear interaction!**

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

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Basic ingredients

A-body wave function → Green's functions

$$|\Psi_k^A\rangle$$

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

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

$$\ldots$$

↓

A-body Schrödinger equation → Martin-Schwinger equations

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

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

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

$$\ldots$$

↓

Observables: expectation values

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

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

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

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

$$\dots$$

Martin-Schwinger equations

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

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$$\dots$$

Decouple via Σ

Basic ingredients

A-body wave function → Green's functions

$$|\Psi_k^A\rangle$$

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

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

$$\dots$$

↓

A-body Schrödinger equation → Dyson equation

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

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

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

$|\Psi_k^A\rangle$

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

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

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 → Many-body approximation

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

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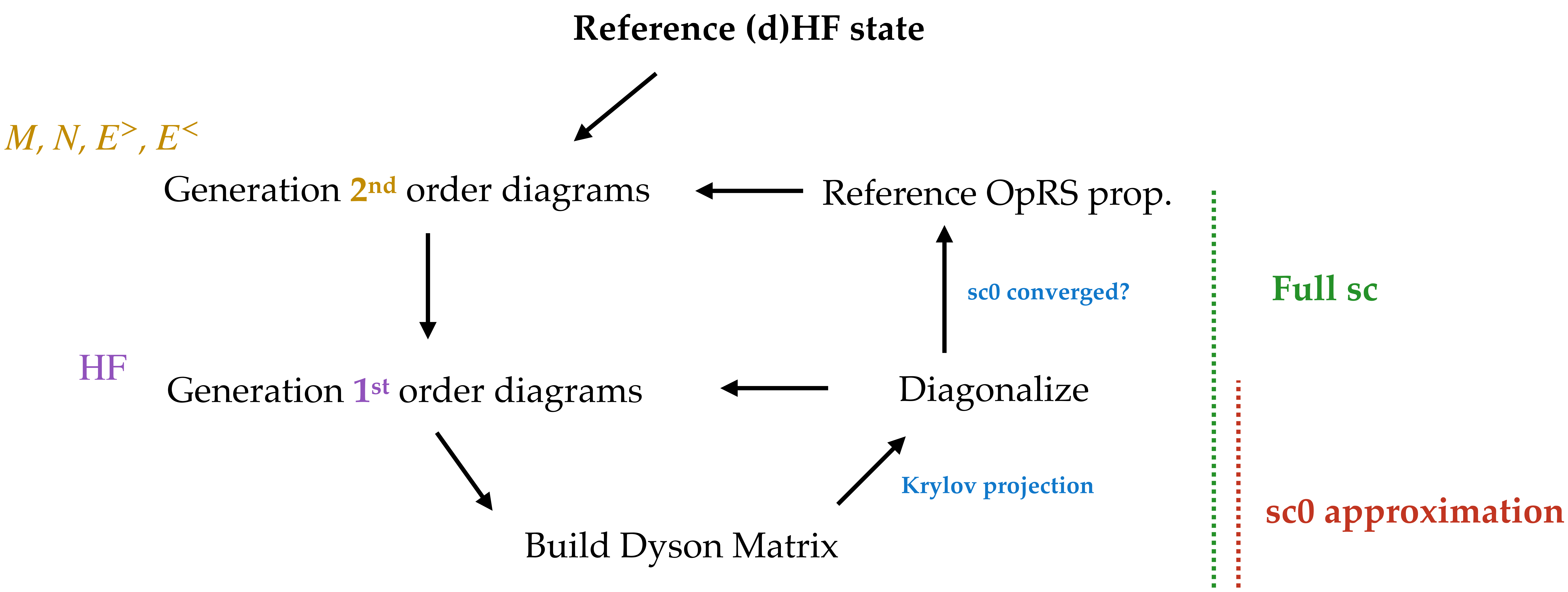
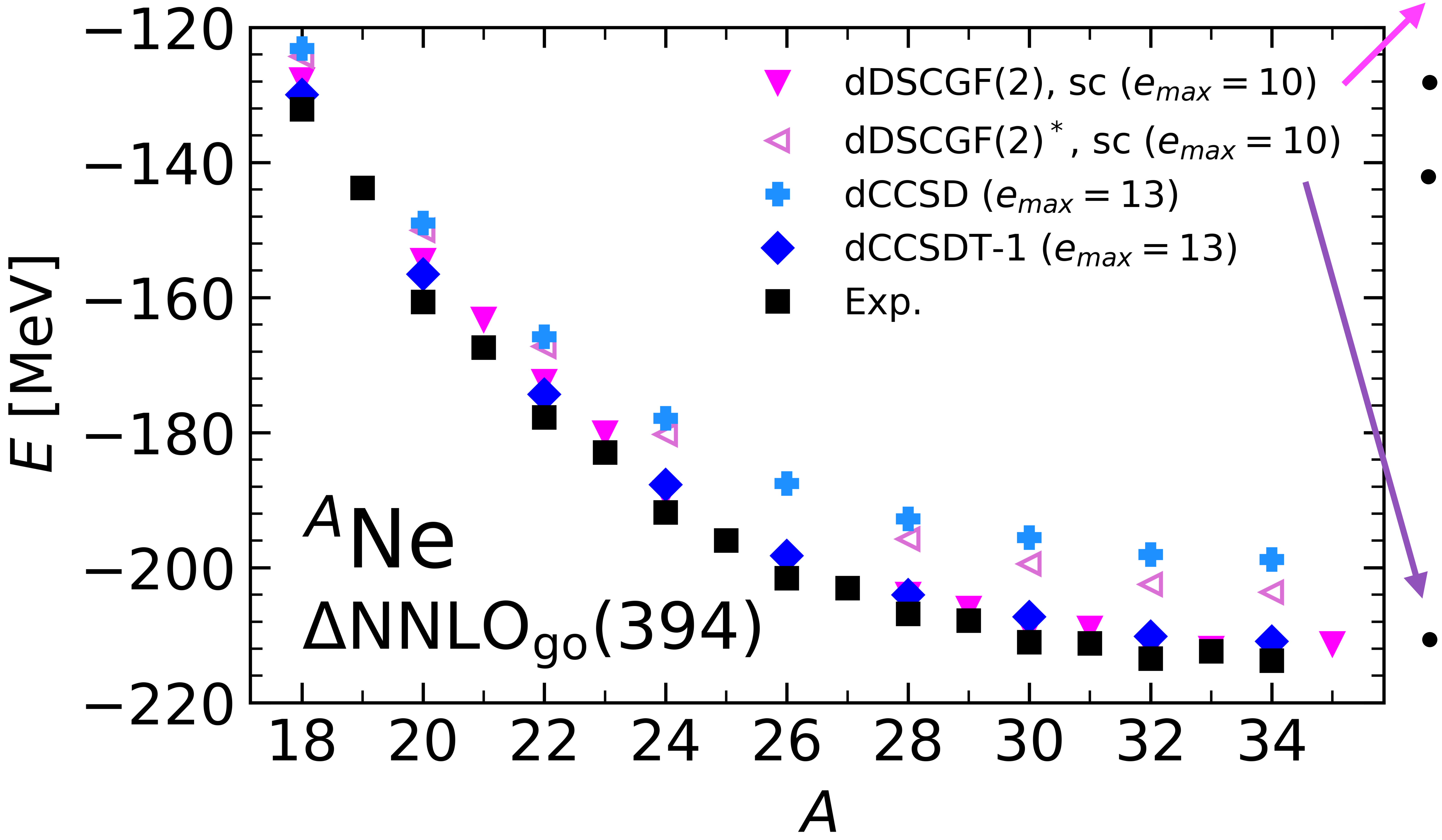
The self-consistent loop



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

↓

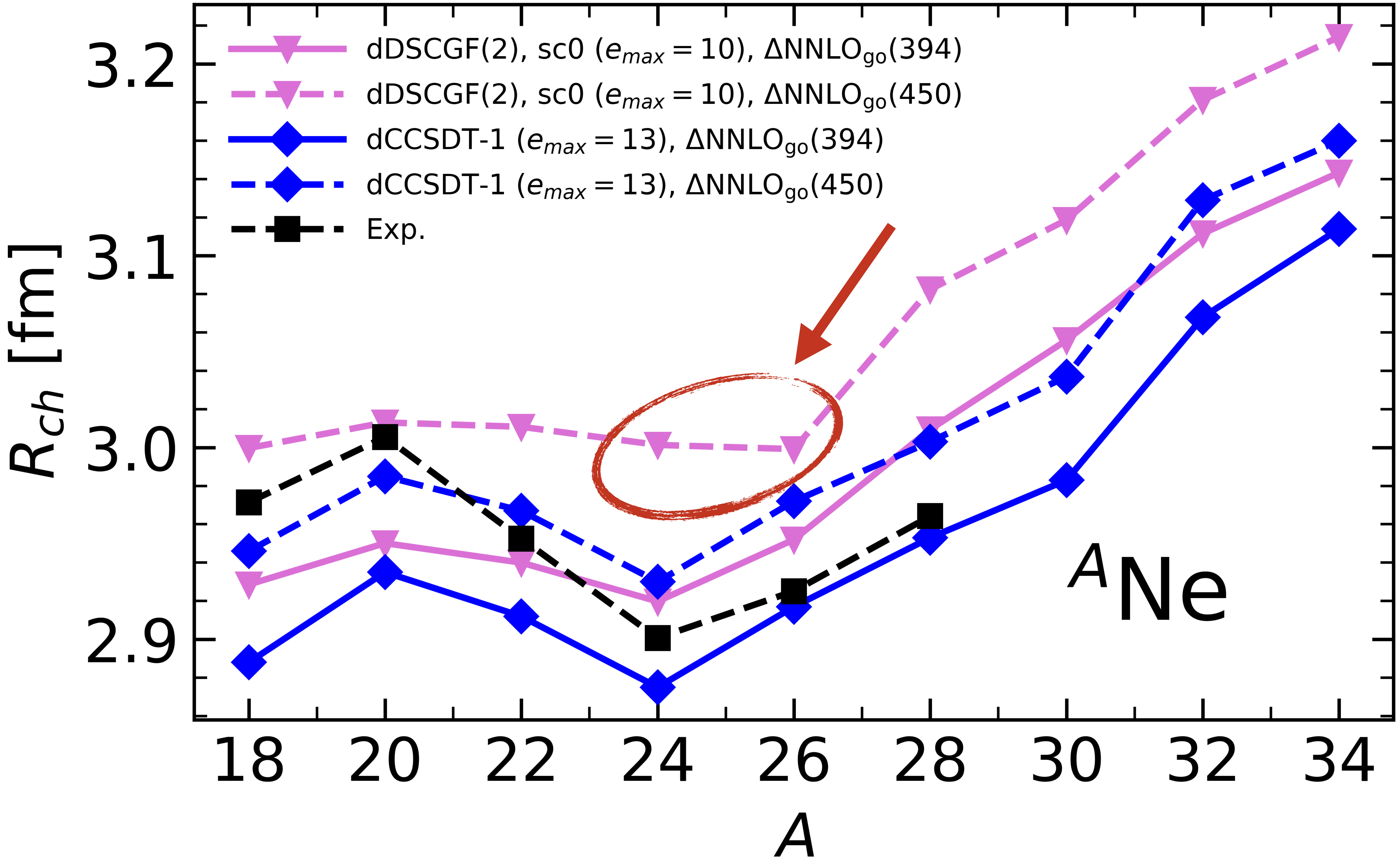
Need of a <u>particle adjustment</u>

- **Naïve rescaling** based on mass

↓

Energies compatible with **dCCSD**

Charge radii of Neon isotopes



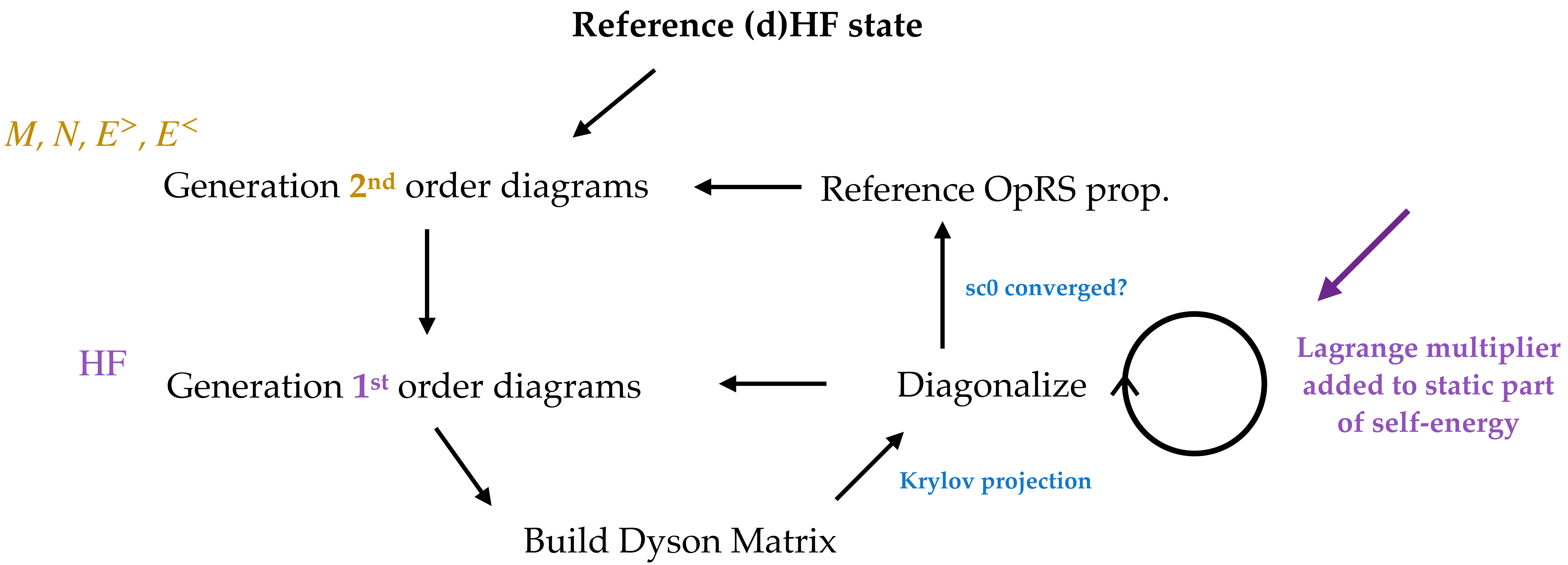
1B + 2B CoM corrections

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

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

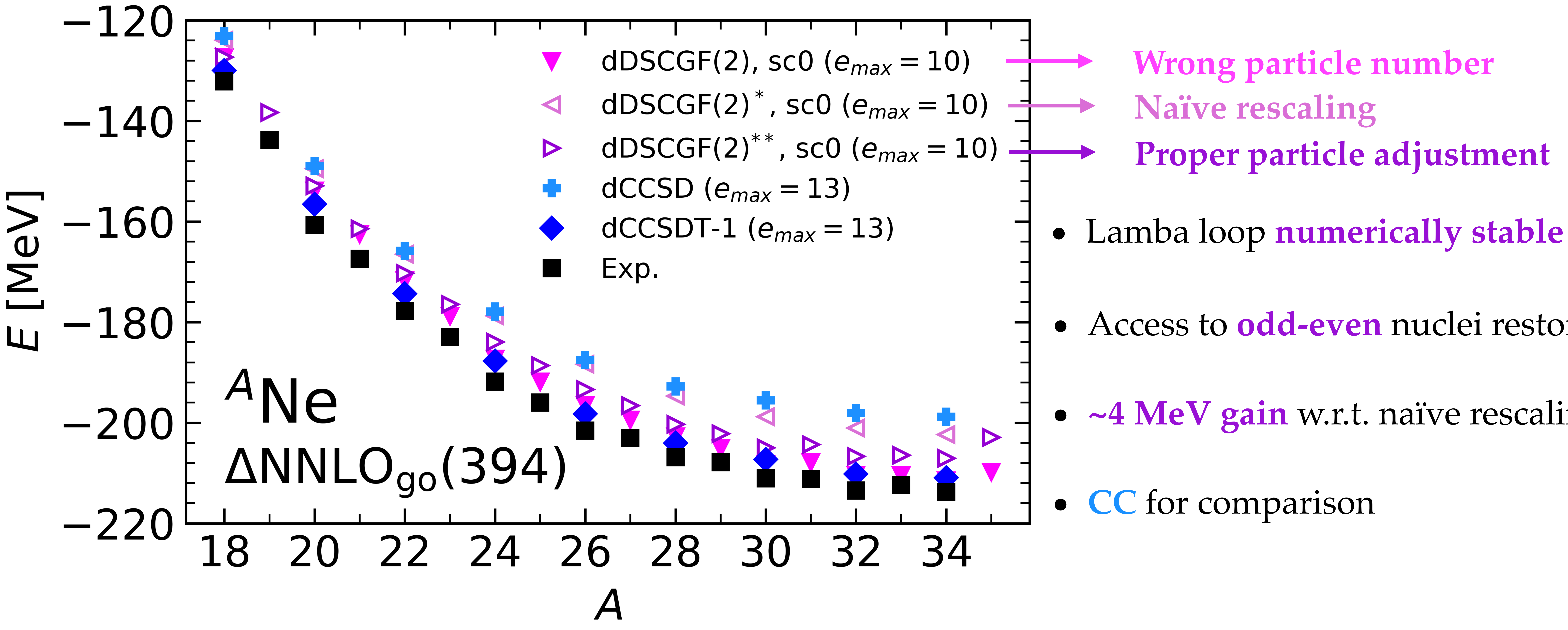
[Novario *et al.* 2020]

Particle adjustment: theoretical setup



→ **no additional computational cost!**

Particle adjustment: ground-state energy



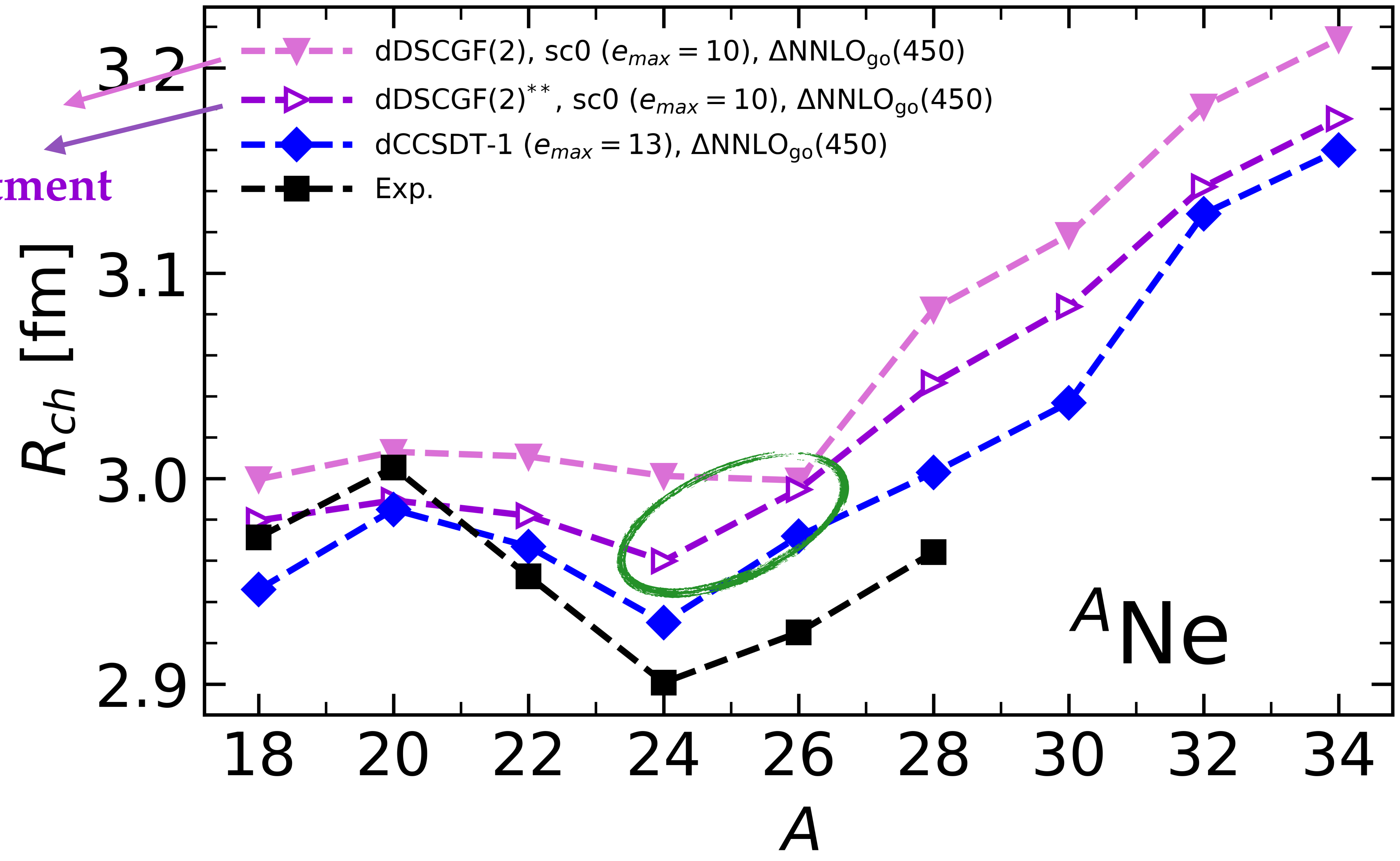
- Lamba loop **numerically stable**
- Access to **odd-even** nuclei restored
- **~4 MeV gain** w.r.t. naïve rescaling
- CC for comparison

Particle adjustment: charge radii

[Novario *et al.* 2020]

Standard sc0

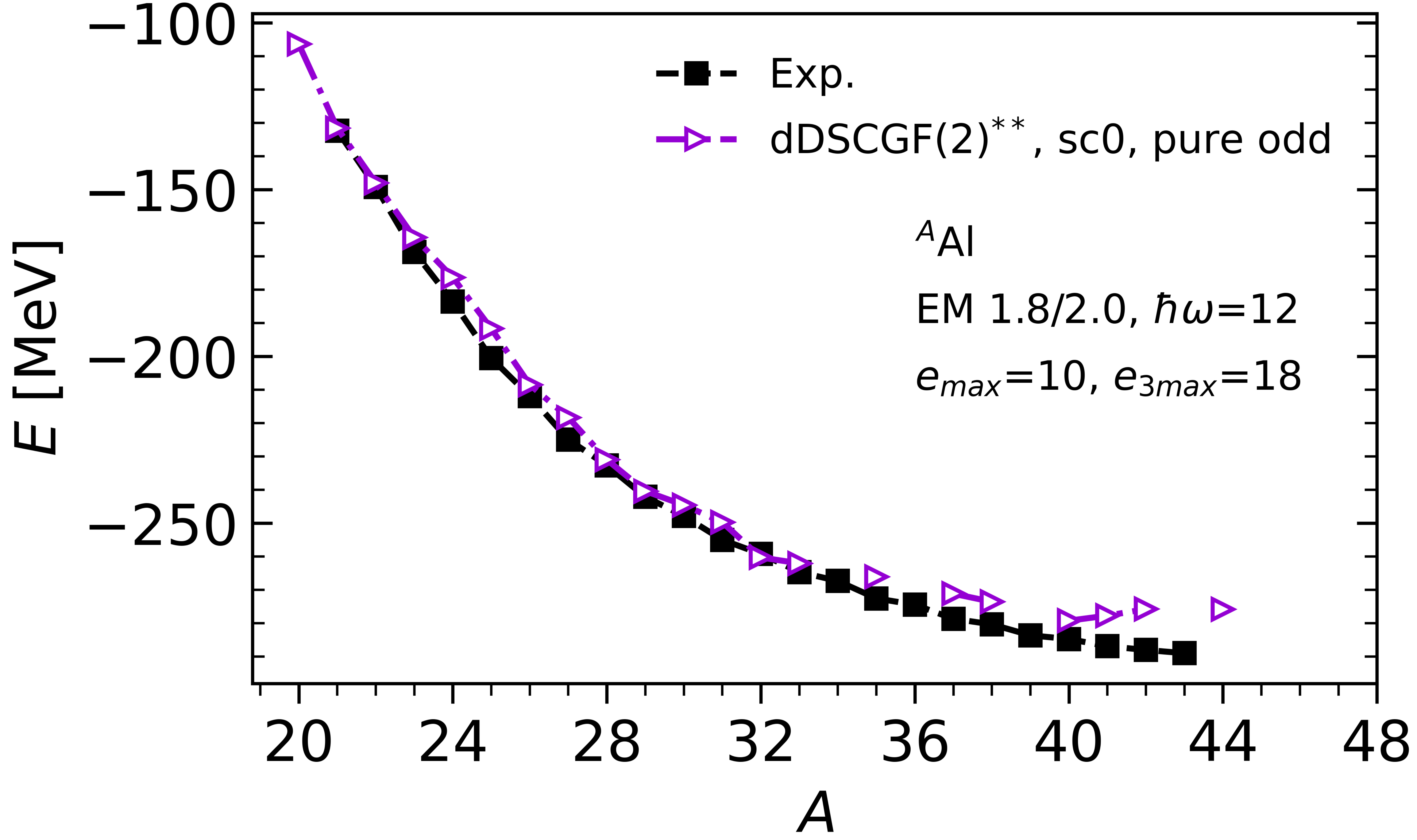
Proper particle adjustment



→ 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!

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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. dBMBPT(2) (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** [Sokolov *et al.*, 2018]

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

Collaborators

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