Capturing many-body correlations at polynomial cost

Alberto Scalesi

Chalmers University of Technology

Next generation *ab initio* nuclear theory workshop

17th July 2025, Trento

Outline

- *Ab initio* polynomially-scaling methods: why break symmetries?
- Deformed self-consistent Green's function
- Techniques to mitigate the 'curse of dimensionality'
- Conclusions

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- *Ab initio* polynomially-scaling methods: why break symmetries?

- Deformed self-consistent Green's function

- Techniques to mitigate the 'curse of dimensionality'

- Conclusions

UNIVERSITÀ DEGLI STUDI DI MILANO

C. Barbieri, E. Vigezzi

V. Somà, T. Duguet, M. Frosini

Based on the work carried out in Milan during my master and at CEA during my PhD!

[AS et al., *Annals Phys.* 467 (2024) 169688]

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

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

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NUMERICS

International PhD Program in Numerical Simulation at CEA

cea

Outline

- *Ab initio* polynomially-scaling methods: why break 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)

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**

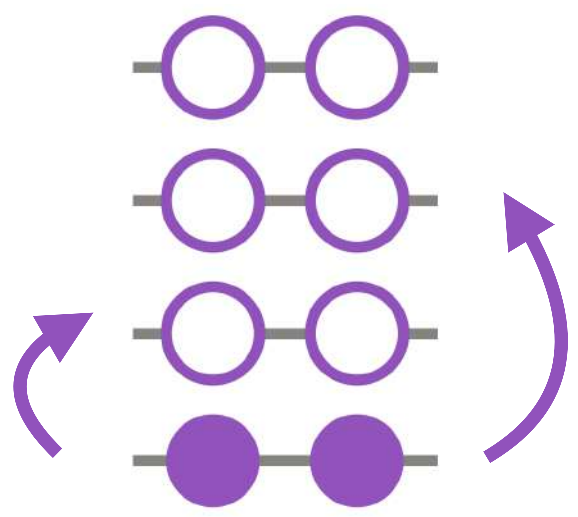
Hamiltonian partitioning: $H = \boxed{H_0} + \boxed{H_1}$

included in ref. state through sym. break.

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**

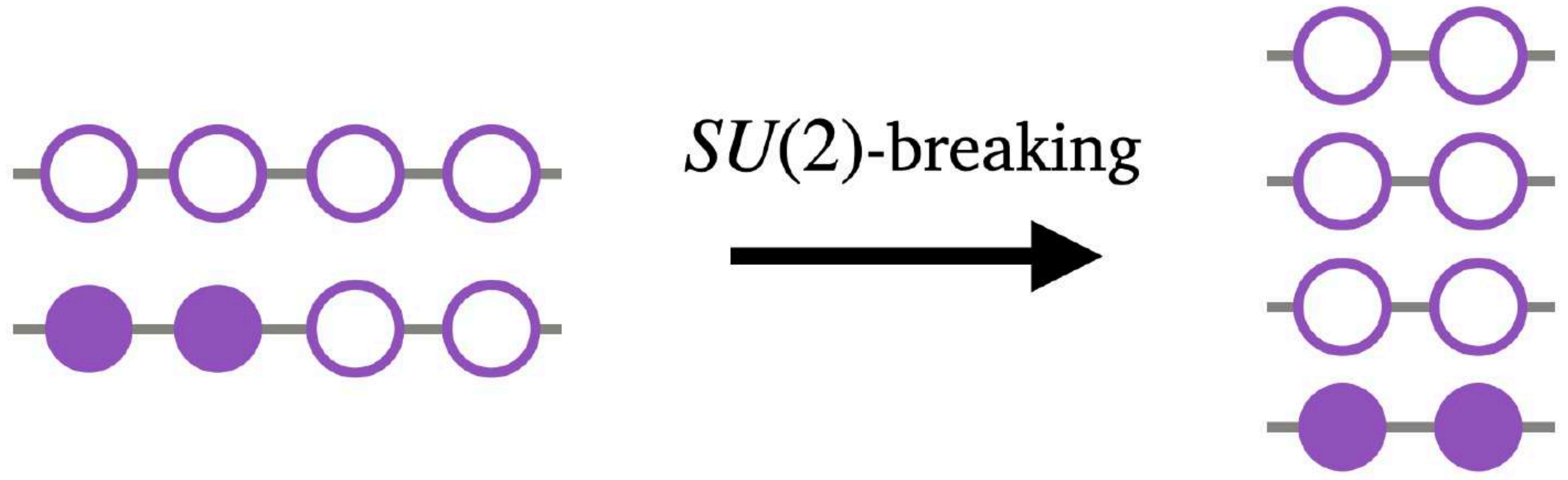
- **Perturbative** expansion: Taylor-like series
- **Non-perturbative** expansion: CC, SCGF, IMSRG

$\longrightarrow$ 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**	[Barbieri, Bogner, Hagen, Hergert, …]
Singly open-shell	2010 - 2020	**sHFB**	[Demol, Duguet, Hergert, Somà, Tichai, …]
Doubly open-shell	2020 - …	**dHF(B)**	[Duguet, Frosini, Hagen, …]

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

Impact of correlations on nuclear binding energies

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

	SU(2) conserving	SU(2) breaking	
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**

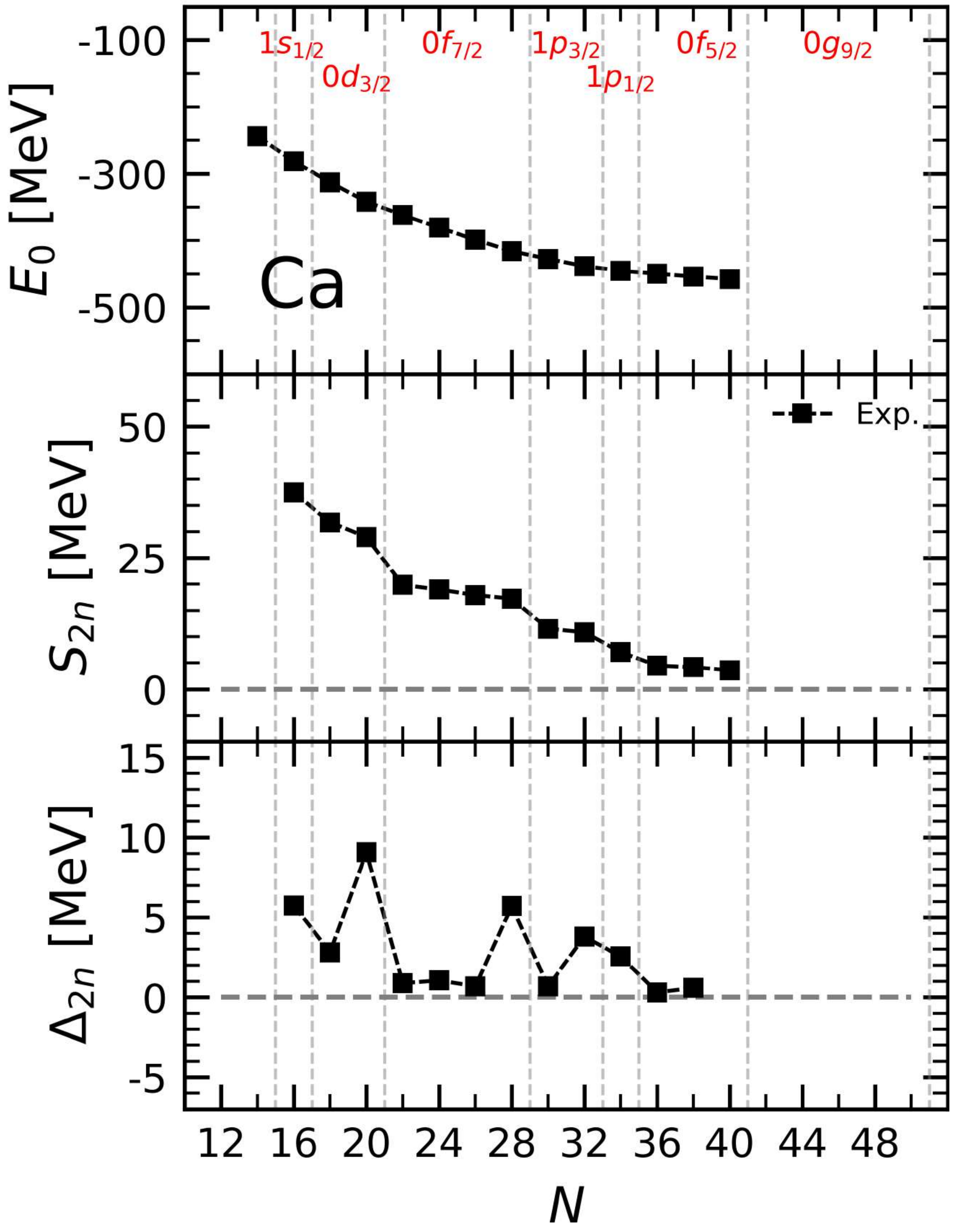
- Step-by-step study of the contribution of MB correlations to the **total energy** and **I-II derivatives**

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

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

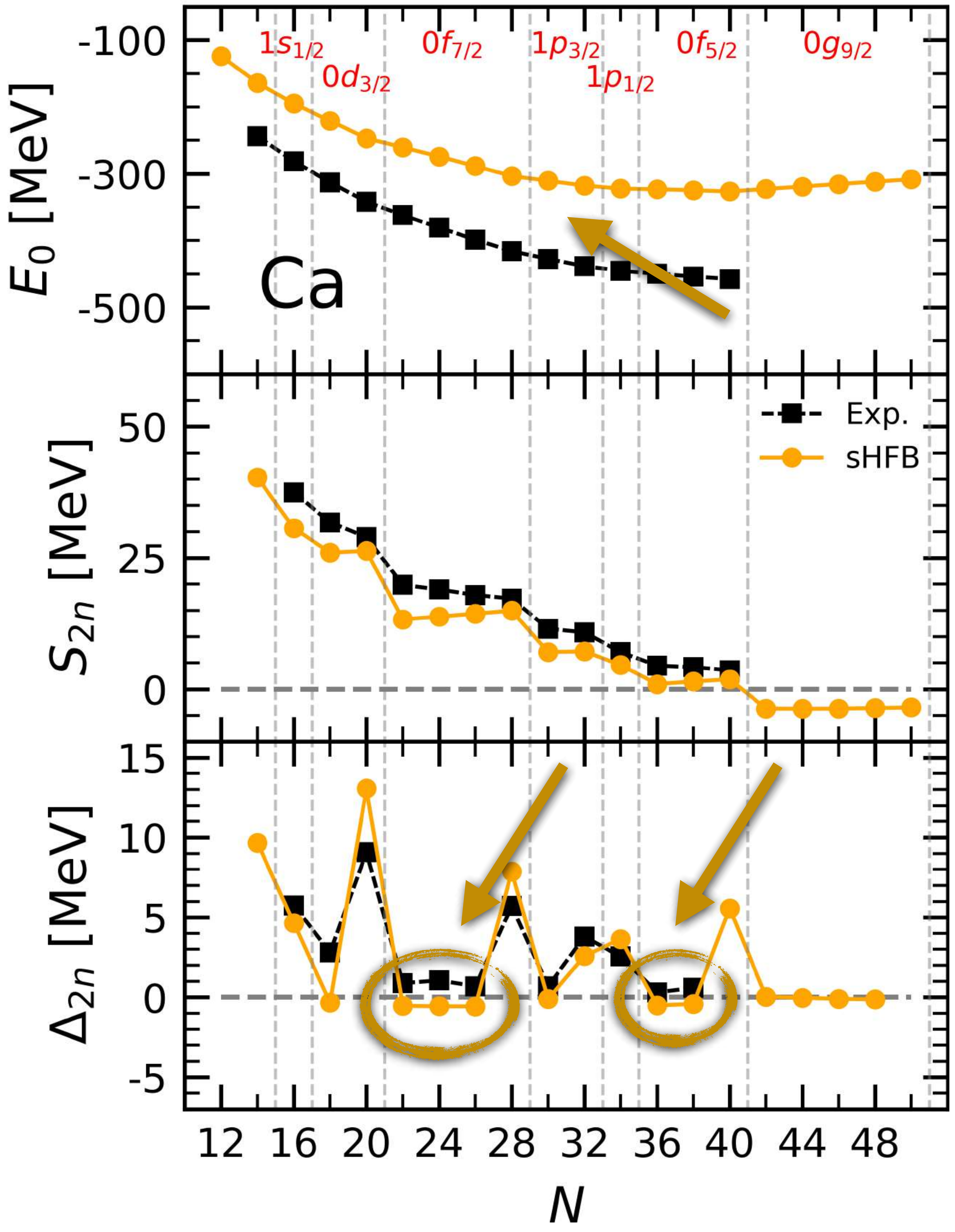
SU(2)-conserving *ab initio* approaches

SU(2)-conserving *ab initio* approaches



Singly open-shell

SU(2)-conserving *ab initio* approaches

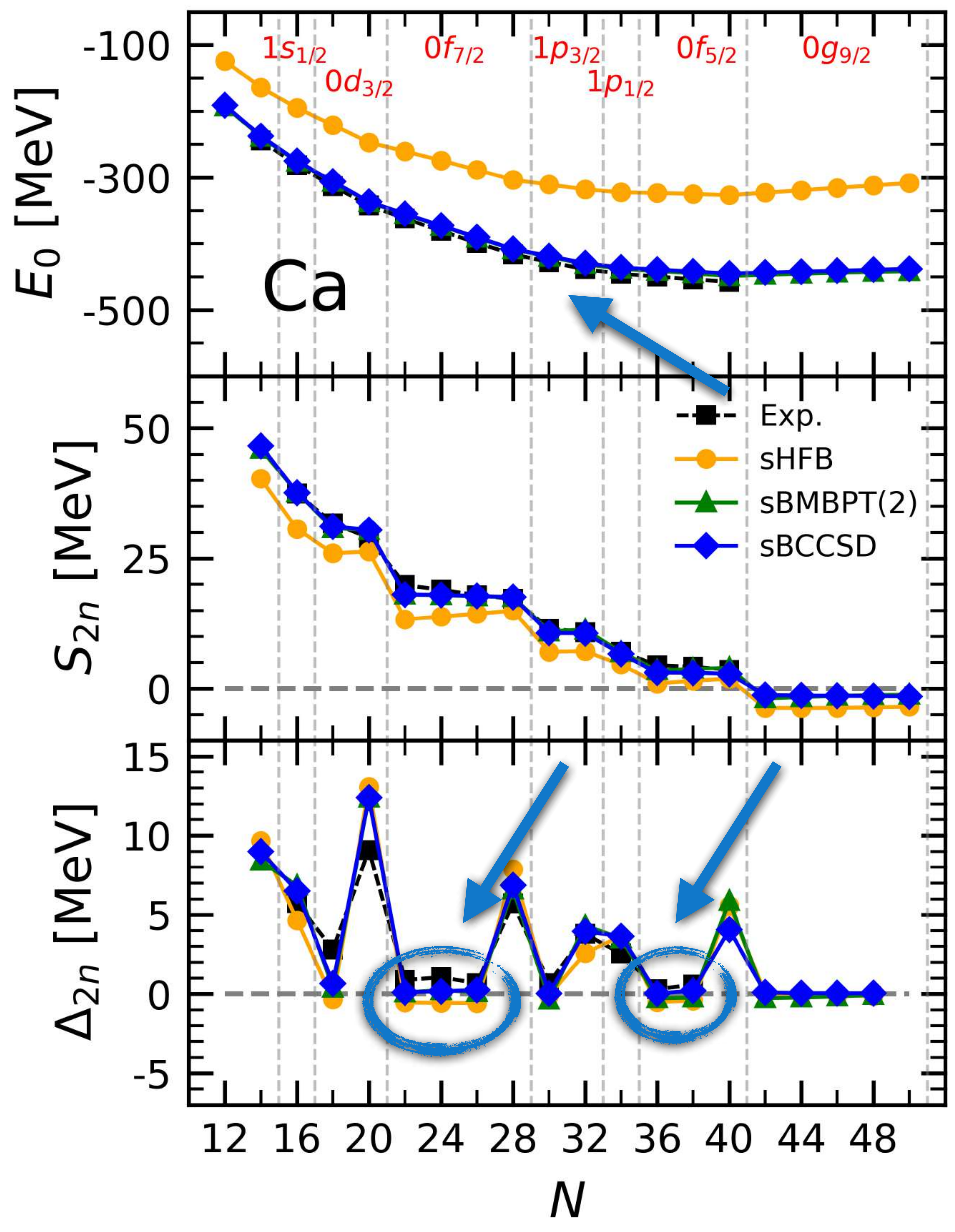


Singly open-shell

Spherical mean-field:

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

SU(2)-conserving *ab initio* approaches



Singly open-shell

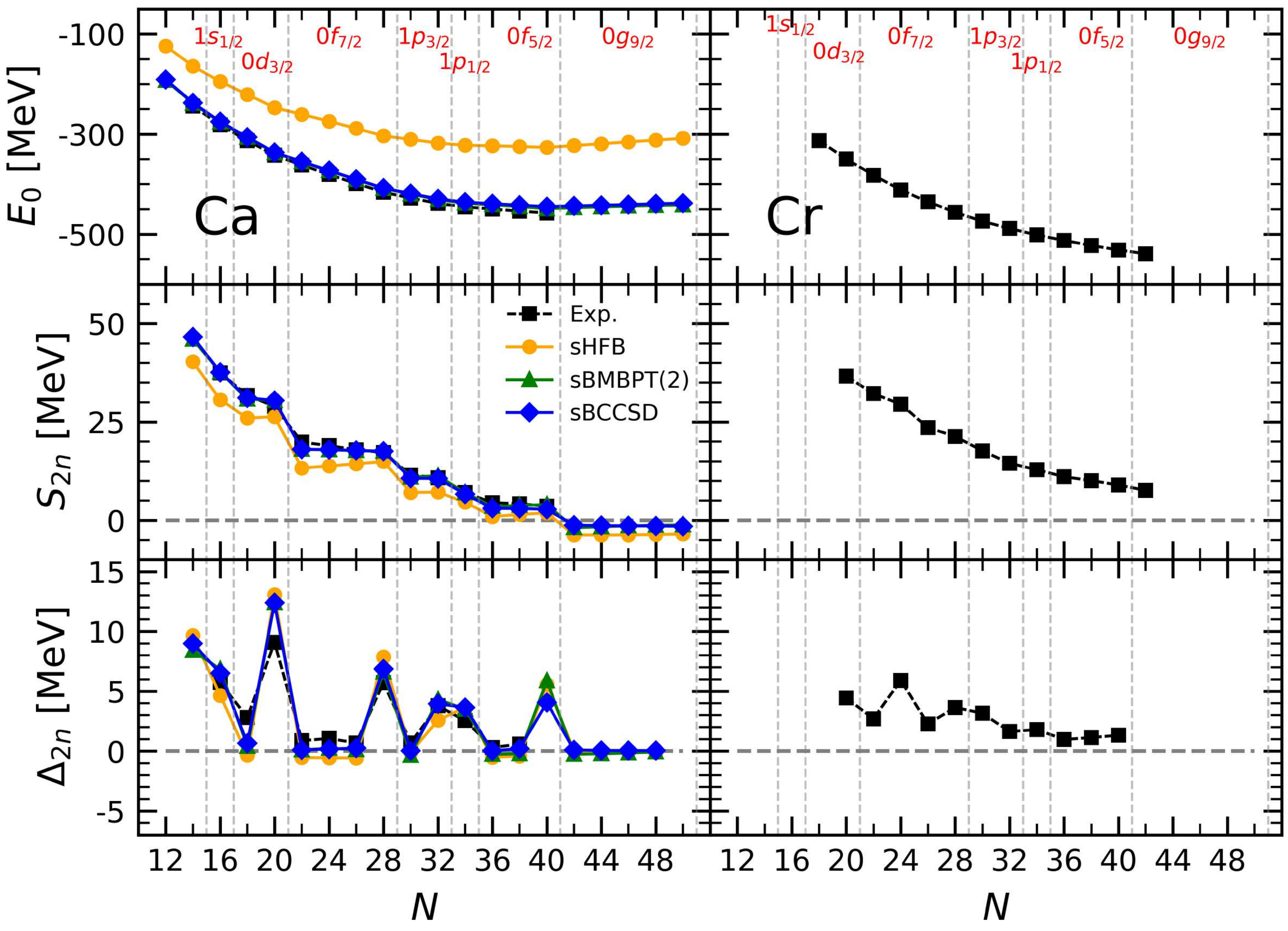
Spherical mean-field:

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

Low-order dynamical correlations:

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

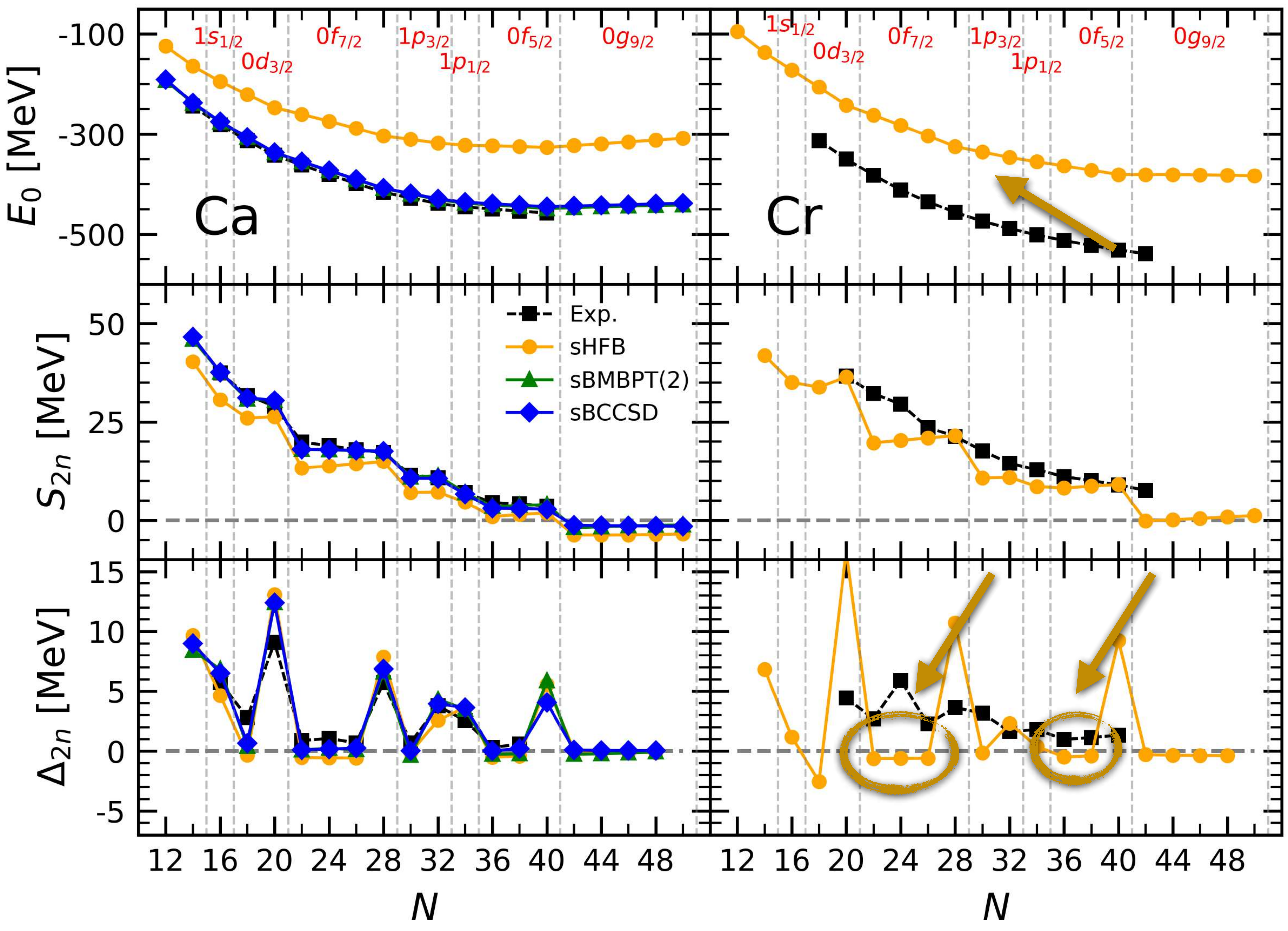
SU(2)-conserving *ab initio* approaches



Doubly open-shell

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

SU(2)-conserving *ab initio* approaches



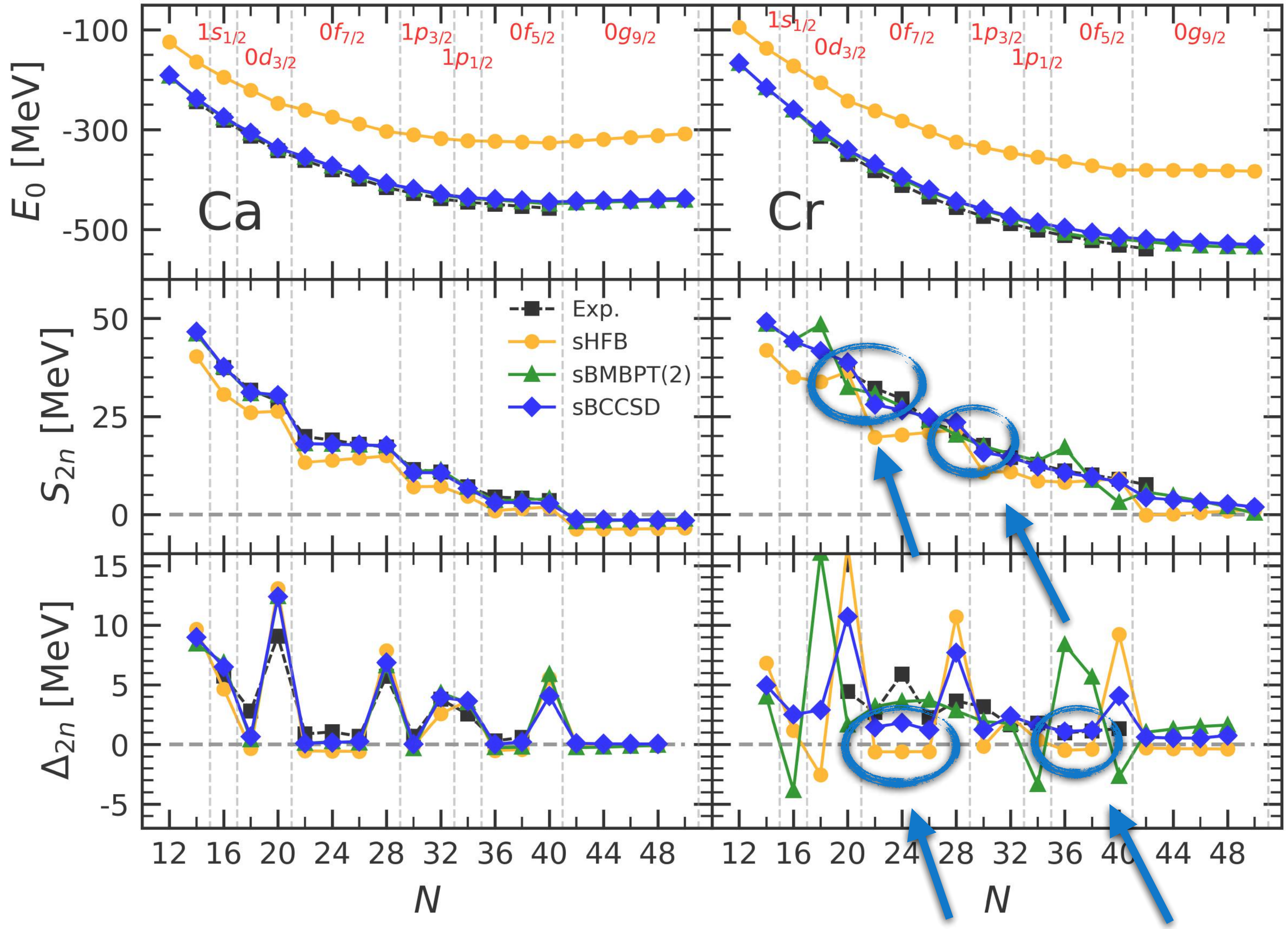
Doubly open-shell

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

Spherical mean-field:

- Defects even **more pronounced**

SU(2)-conserving *ab initio* approaches



Doubly open-shell

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

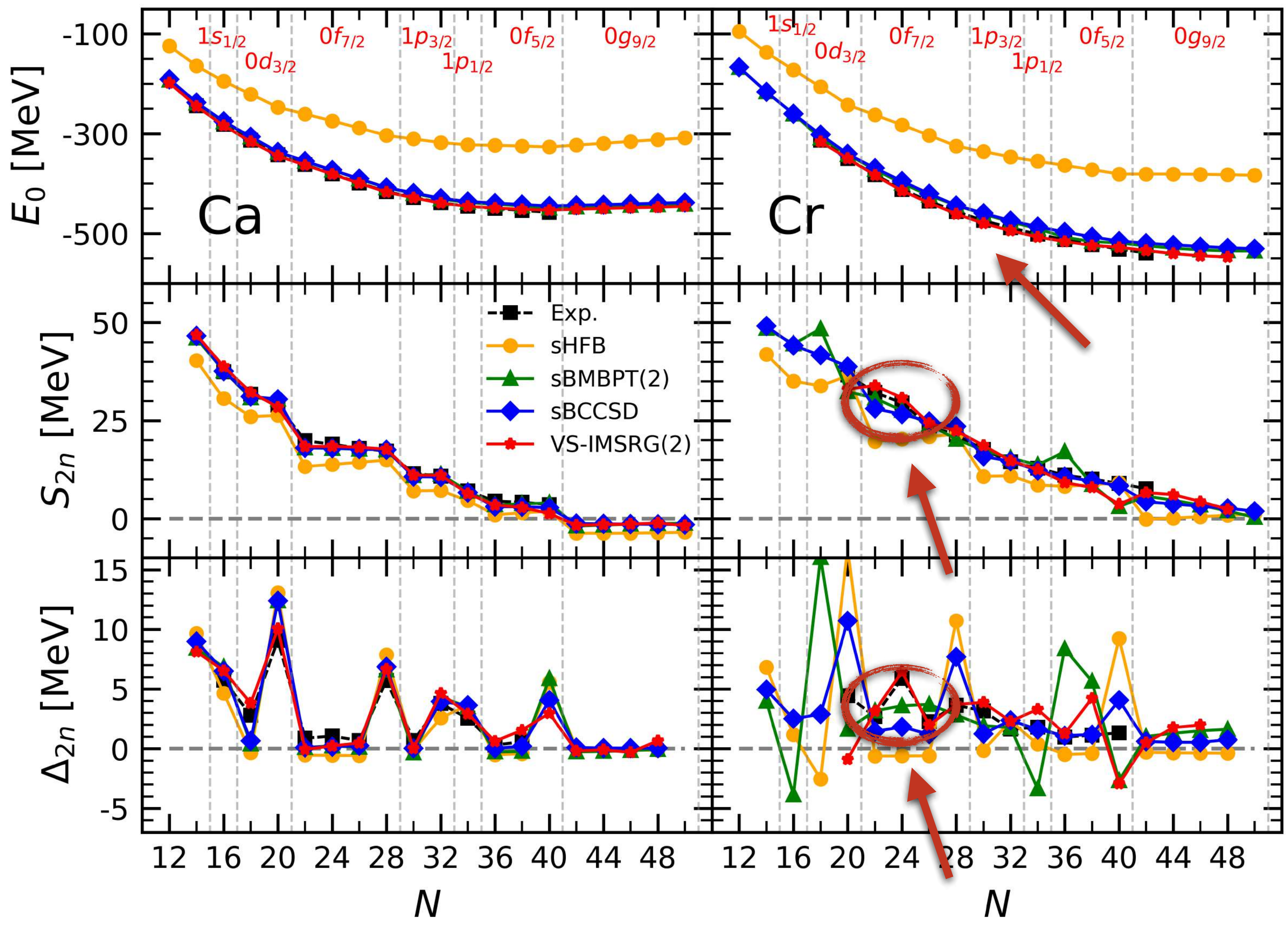
Spherical mean-field:

- Defects even **more pronounced**

Low-order dynamical correlations:

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

SU(2)-conserving *ab initio* approaches



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Spherical mean-field:

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Low-order dynamical correlations:

- Still **wrong curvature**
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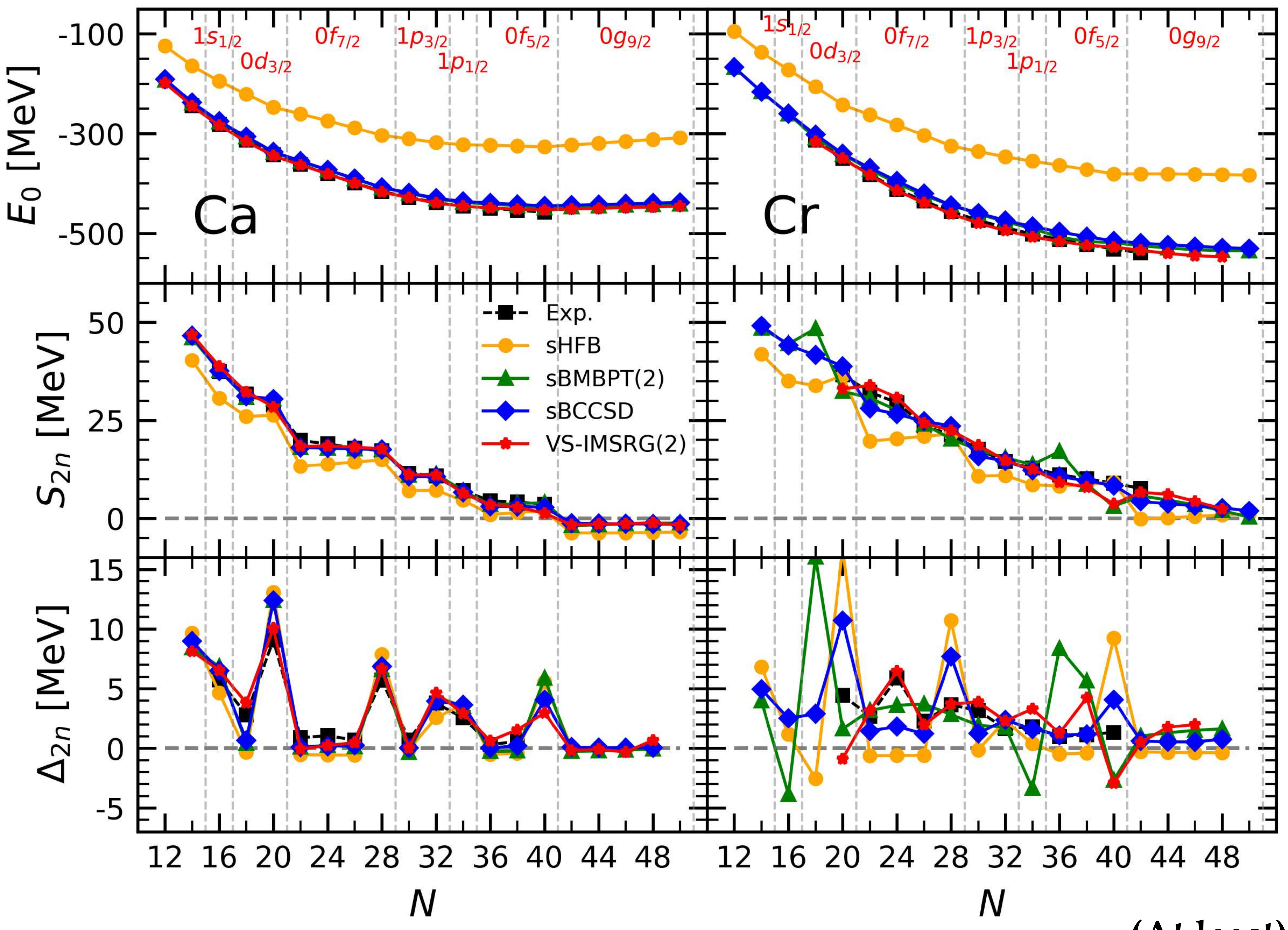
Non polynomial:

- Correct binding energy
- Correct shell gap
- Improved curvature

SU(2)-conserving *ab initio* approaches



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- Correct binding energy
- Correct shell gap
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(At least) high orders needed for SU(2)-cons. ref. state

SU(2)-breaking *ab initio* approaches

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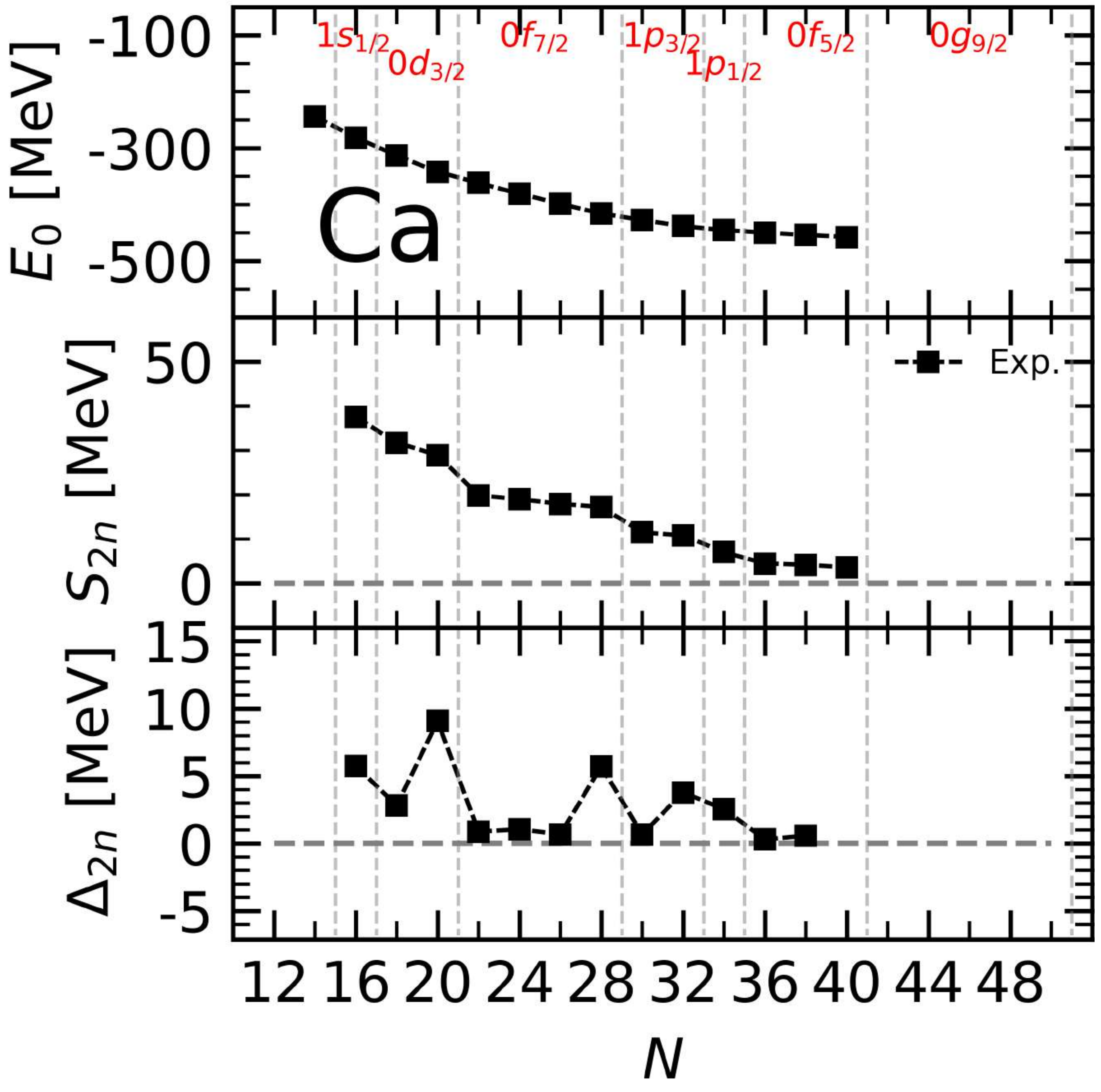
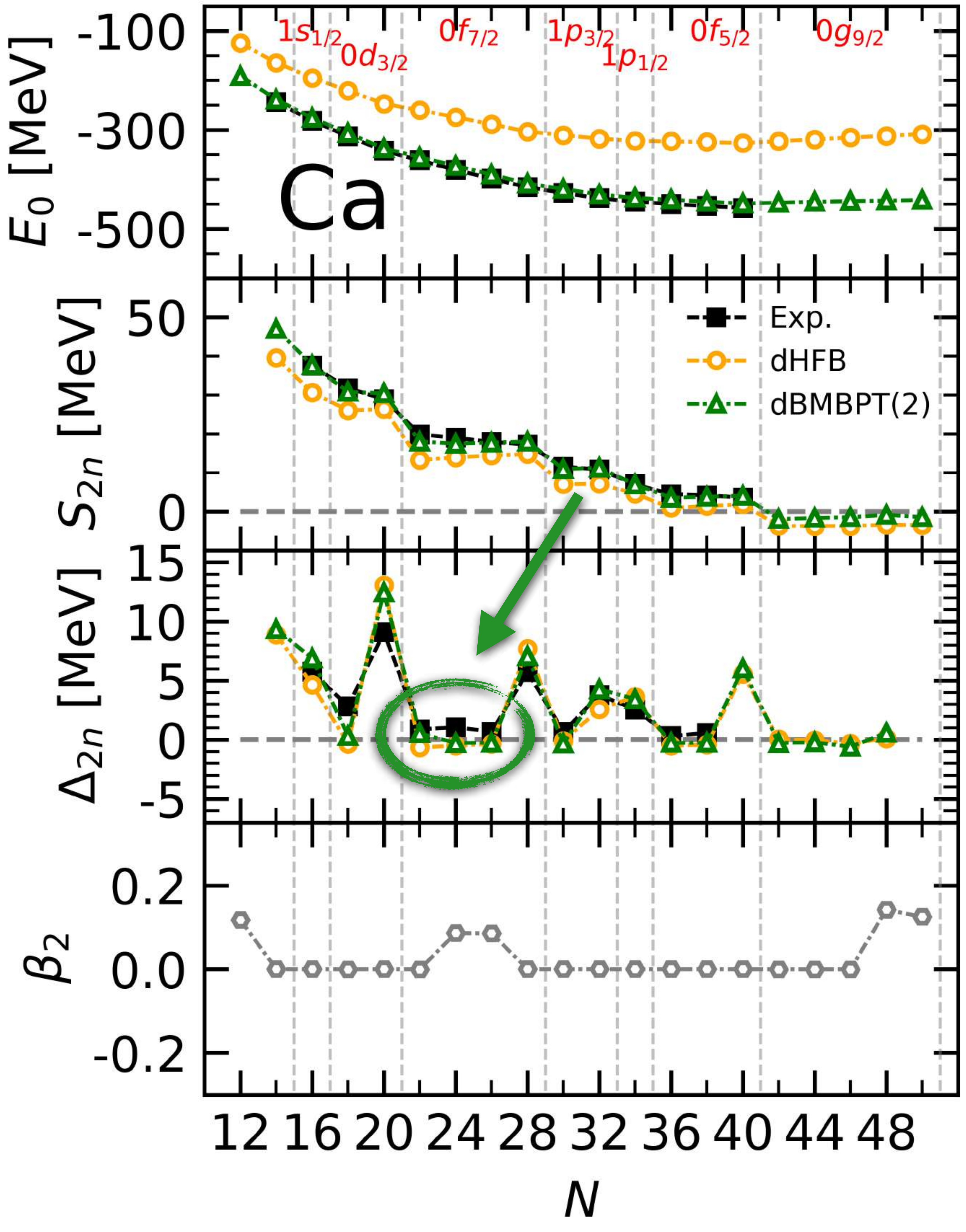


Singly open-shell

SU(2)-breaking *ab initio* approaches



Singly open-shell

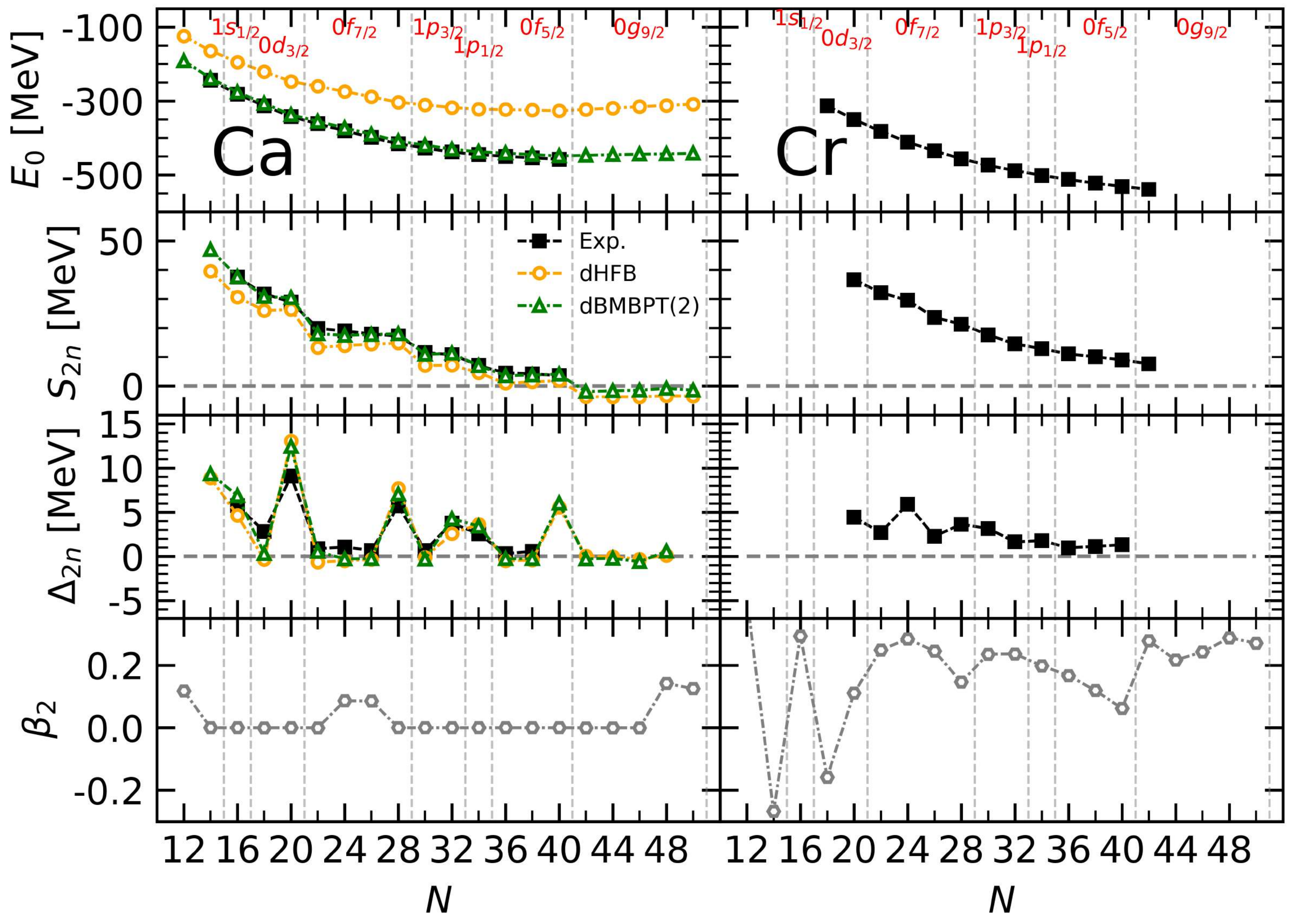
Deformed mean-field:

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

Low-order dynamical correlations:

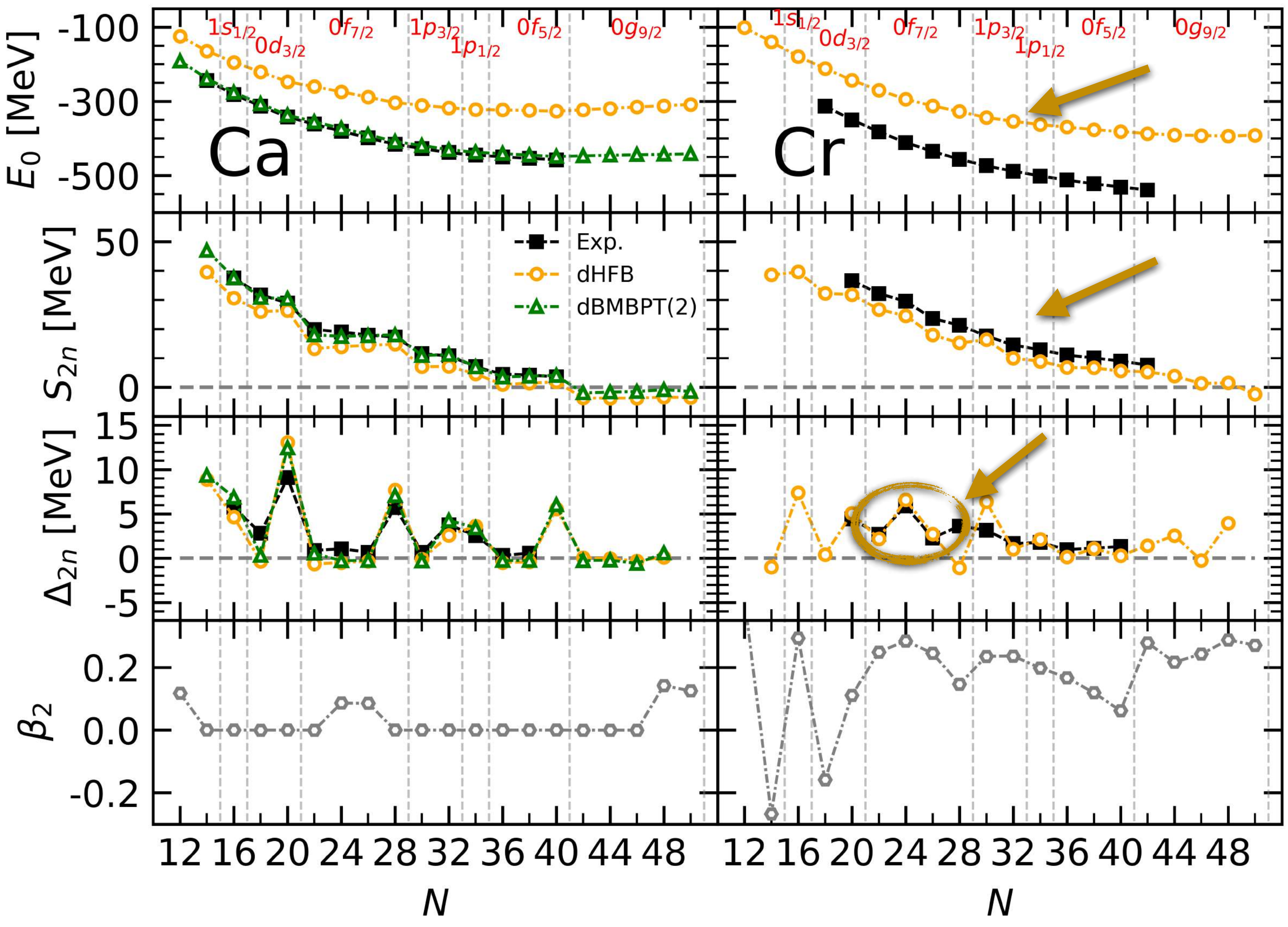
- **Slightly improved** curvature

SU(2)-breaking *ab initio* approaches



Doubly open-shell

SU(2)-breaking *ab initio* approaches

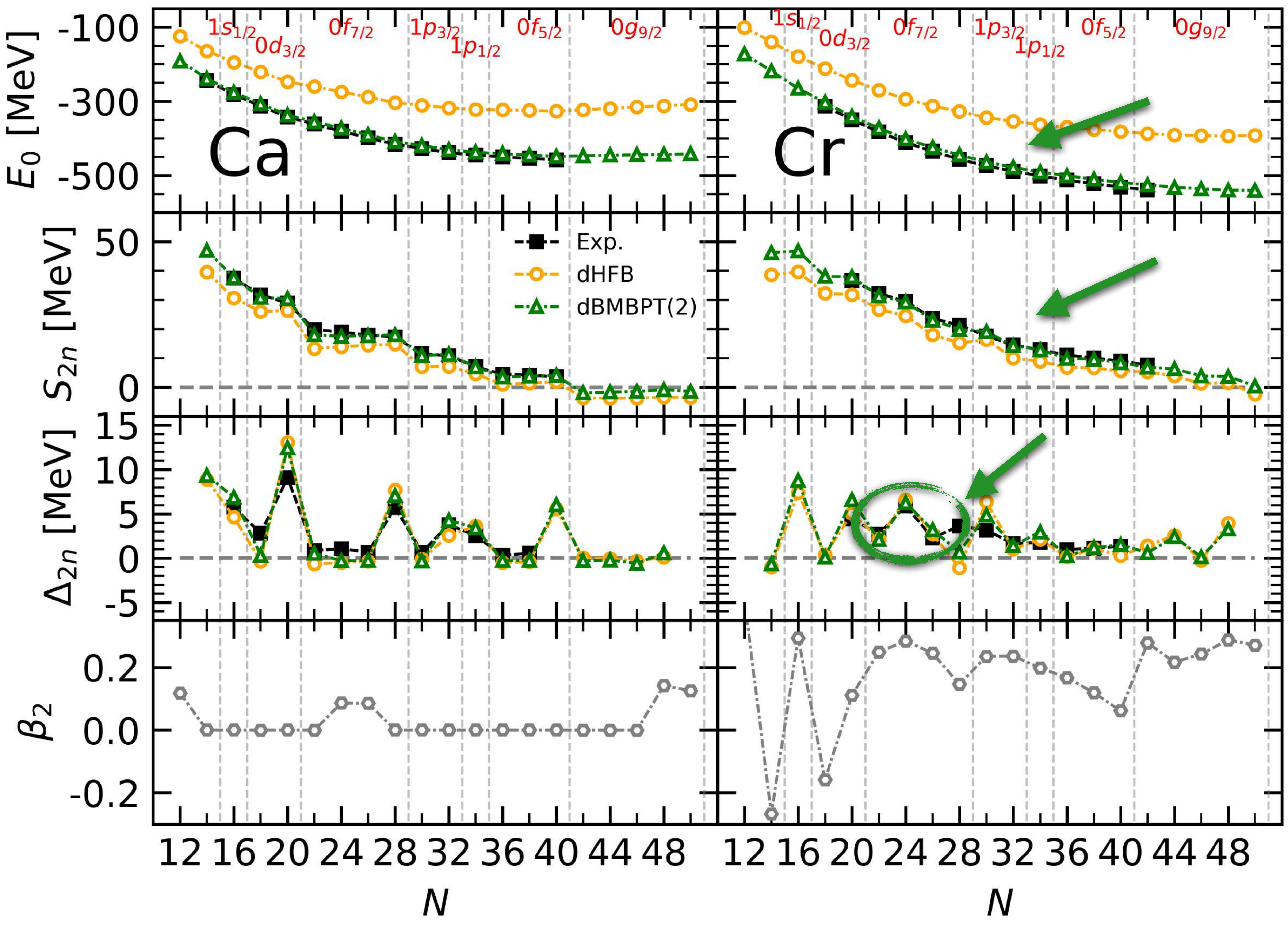


Doubly open-shell

Deformed mean-field:

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

SU(2)-breaking *ab initio* approaches



Doubly open-shell

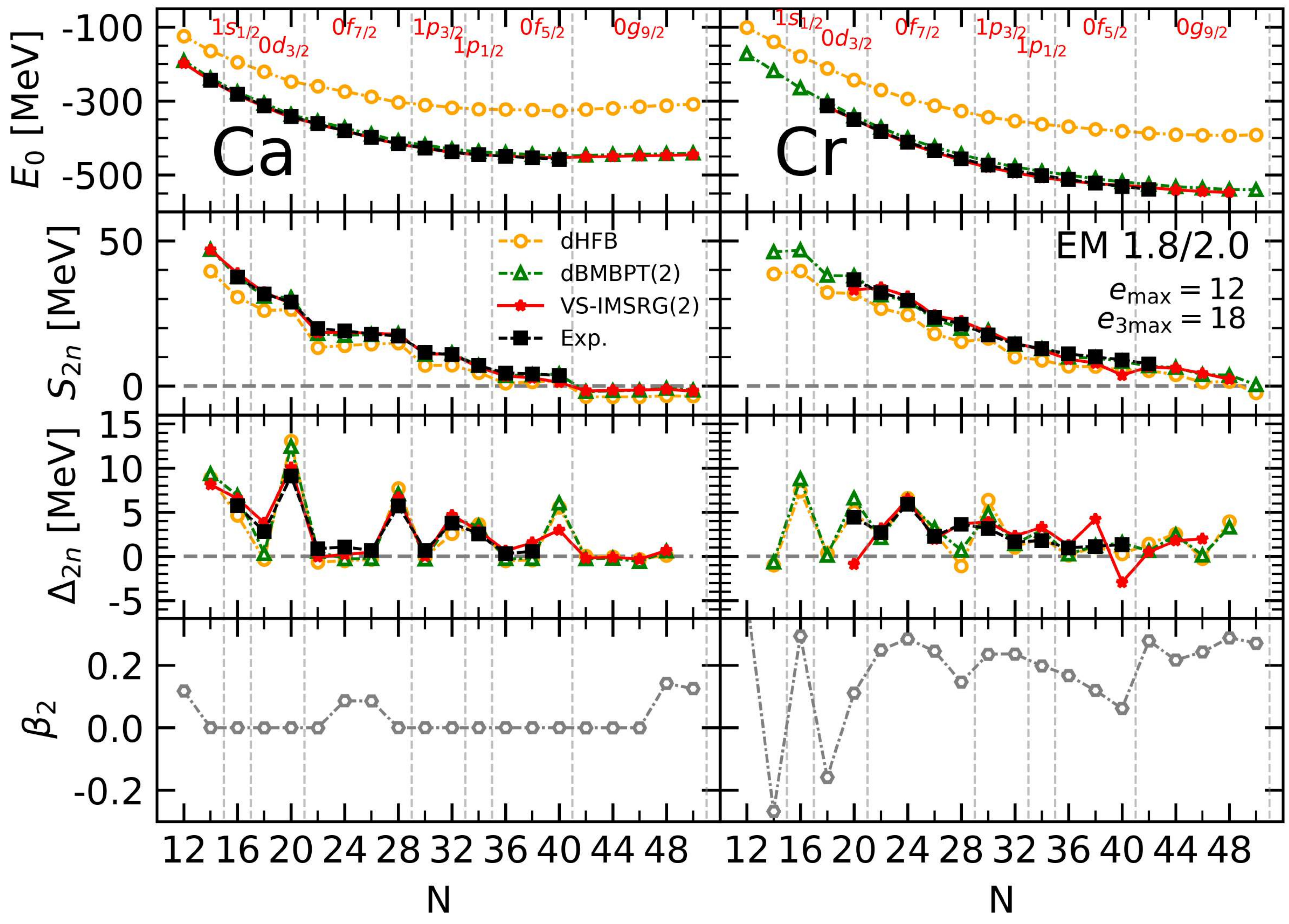
Deformed mean-field:

- **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**

SU(2)-breaking *ab initio* approaches



Doubly open-shell

Deformed mean-field:

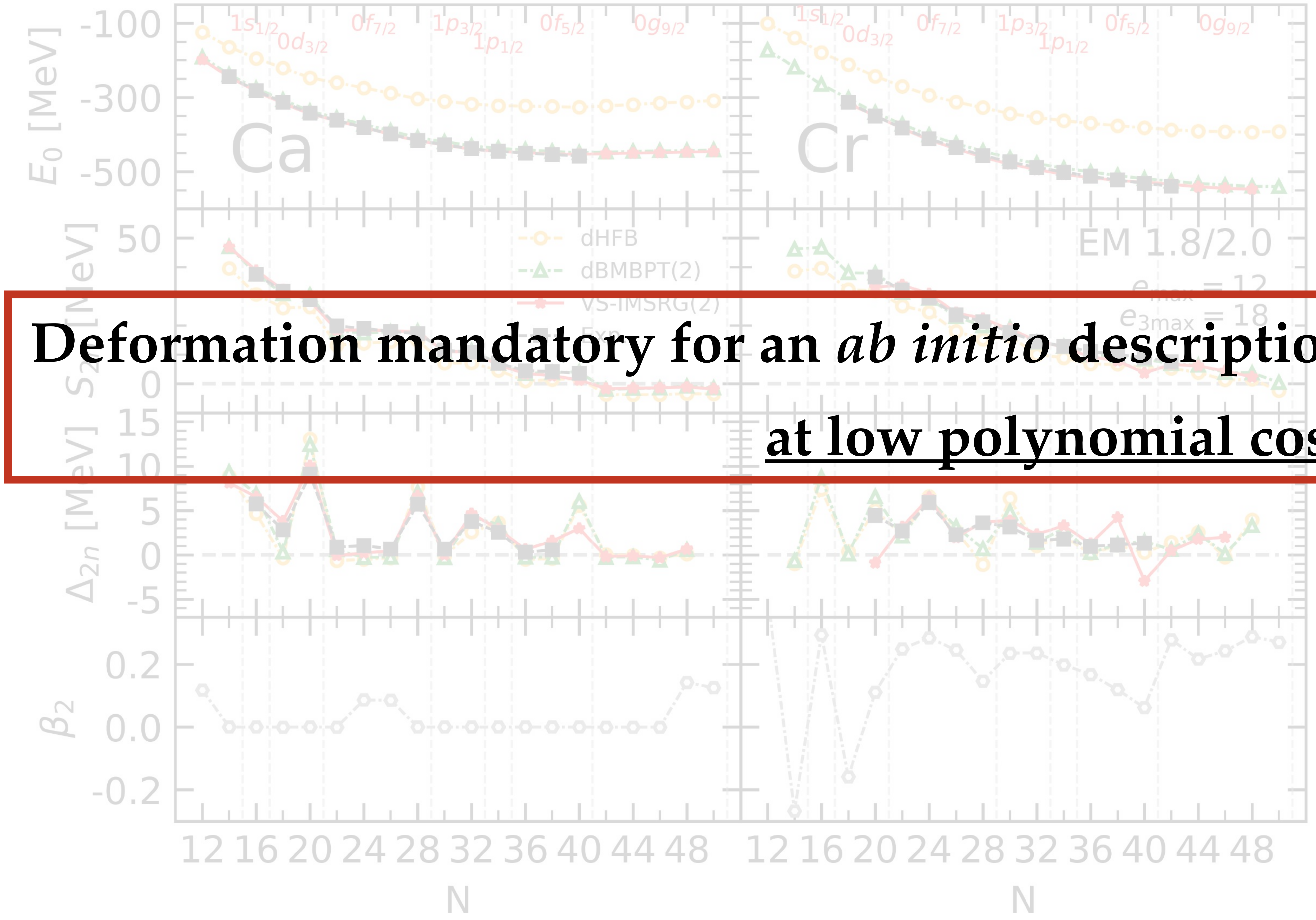
- **Underbinding** but **correct** curvature
- **Qualitatively** correct S_{2n}
- **Correct shell gaps**

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

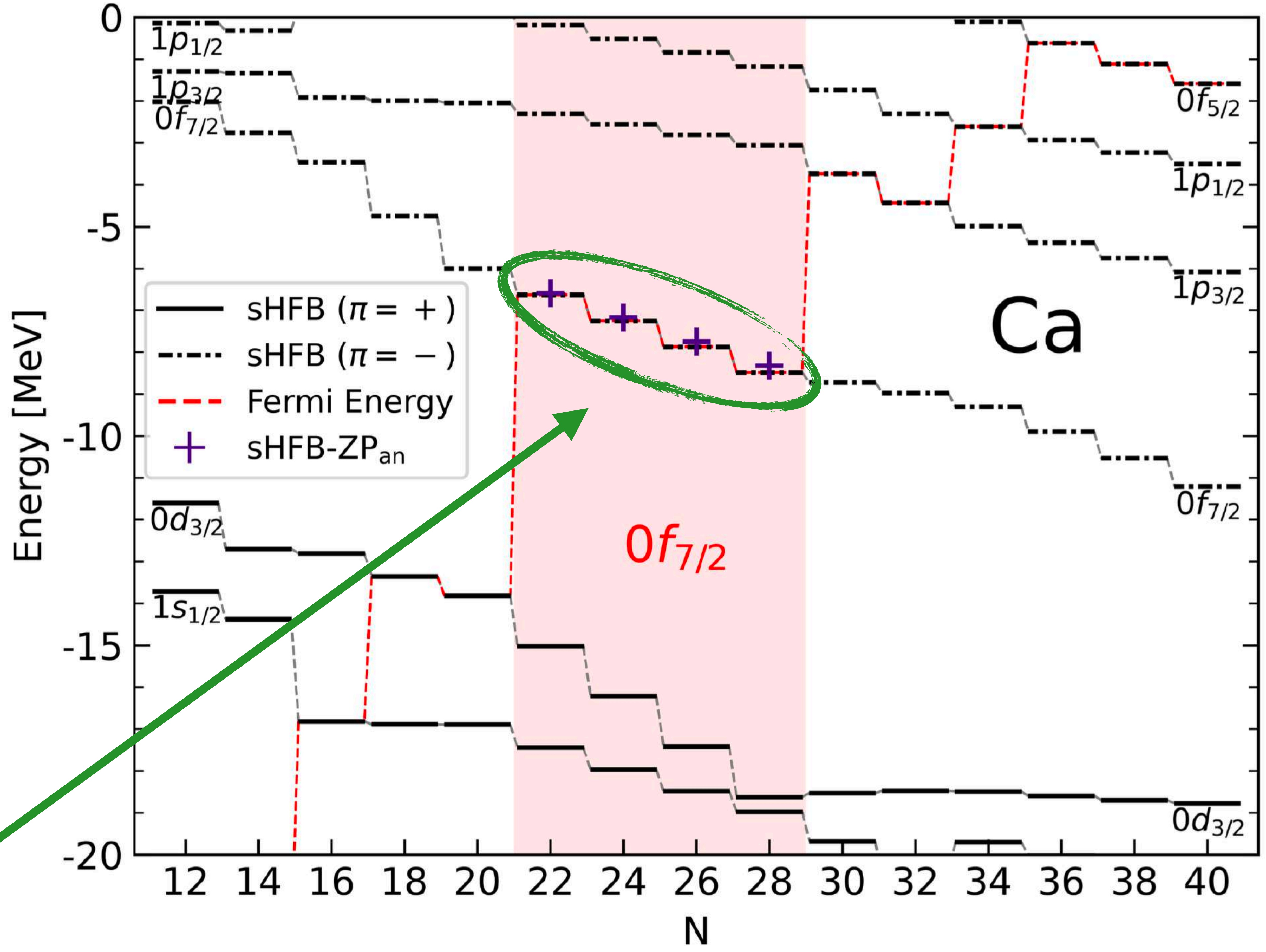
- Weak pairing in *ab initio* $\rightarrow$ sHF-EFA $\approx$ sHFB-ZP [Duguet *et al.* 2020]

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

- $\Delta_{2n}^{\text{sHF-EFA}}(a_v) = 4\beta_{\breve{v}}$, $\varepsilon_{\breve{v}}^{\text{sHF-EFA}}(a_v) = \varepsilon_{\breve{v}}^{\text{CS}} + \beta_{\breve{v}} a_v$

  concavity **ESPE**

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



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

Outline

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- Deformed self-consistent Green's function
-
-

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

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

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

$$\ldots$$

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

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

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$$\dots$$

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$$\dots$$

Decouple via Σ

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

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

A-body wave function → Green's functions

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

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

$$\cdots$$

A-body Schrödinger equation → 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

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

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

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

$$|\Psi_k^A\rangle$$

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

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

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 → Many-body approximation

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

Källén-Lehmann representation of the single-particle propagator

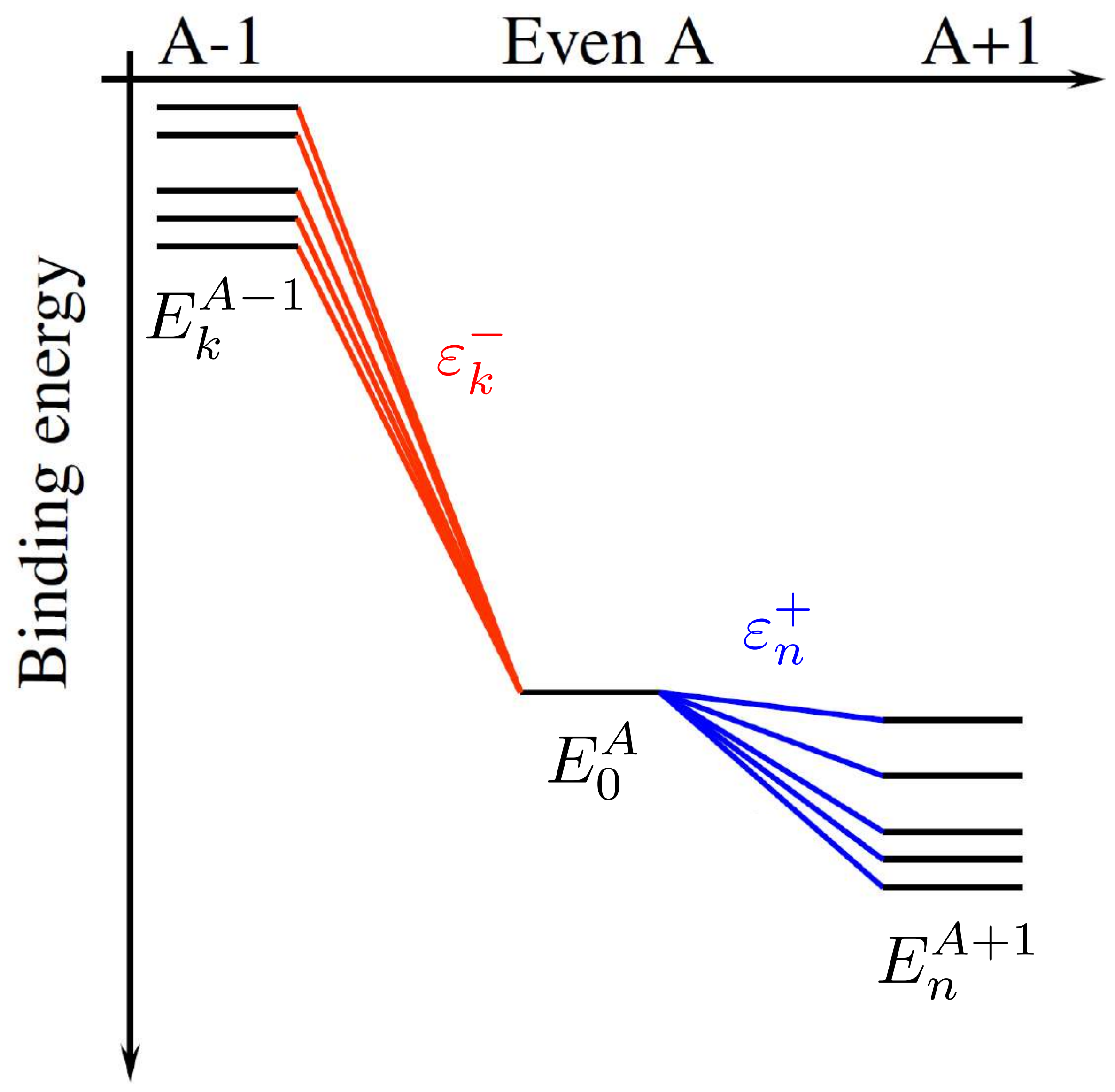
$$g_{\alpha\beta}(\omega) = \sum_n \frac{(\mathcal{X}^n_\alpha)^* \mathcal{X}^n_\beta}{\omega - \varepsilon^+_n + i\eta} + \sum_k \frac{\mathcal{Y}^k_\alpha (\mathcal{Y}^k_\beta)^*}{\omega - \varepsilon^-_k - i\eta}$$

Separation energies

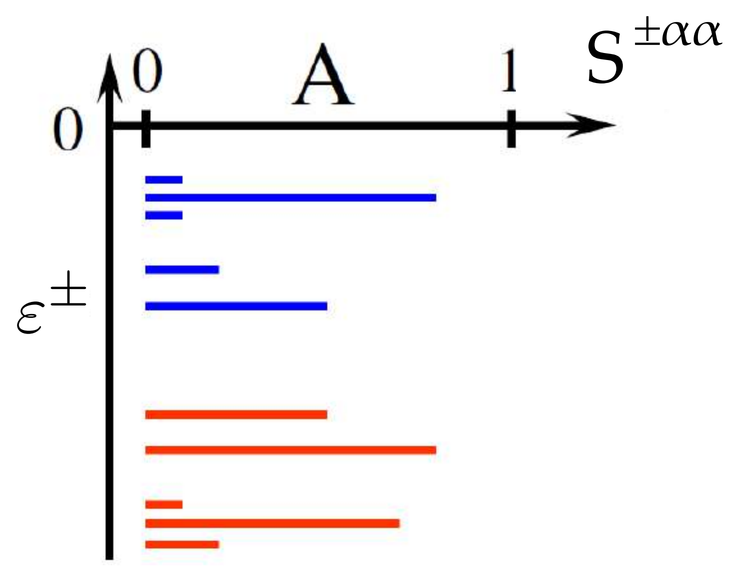
$$\varepsilon^+_n = E^{A+1}_n - E^A_0$$
$$\varepsilon^-_k = E^A_0 - E^{A-1}_k$$

Transition amplitudes

$$\mathcal{X}^n_\alpha = \langle \Psi^{\text{A+1}}_n | a^\dagger_\alpha | \Psi^{\text{A}}_0 \rangle$$
$$\mathcal{Y}^k_\alpha = \langle \Psi^{\text{A-1}}_k | a_\alpha | \Psi^{\text{A}}_0 \rangle$$



Numerator + denominator



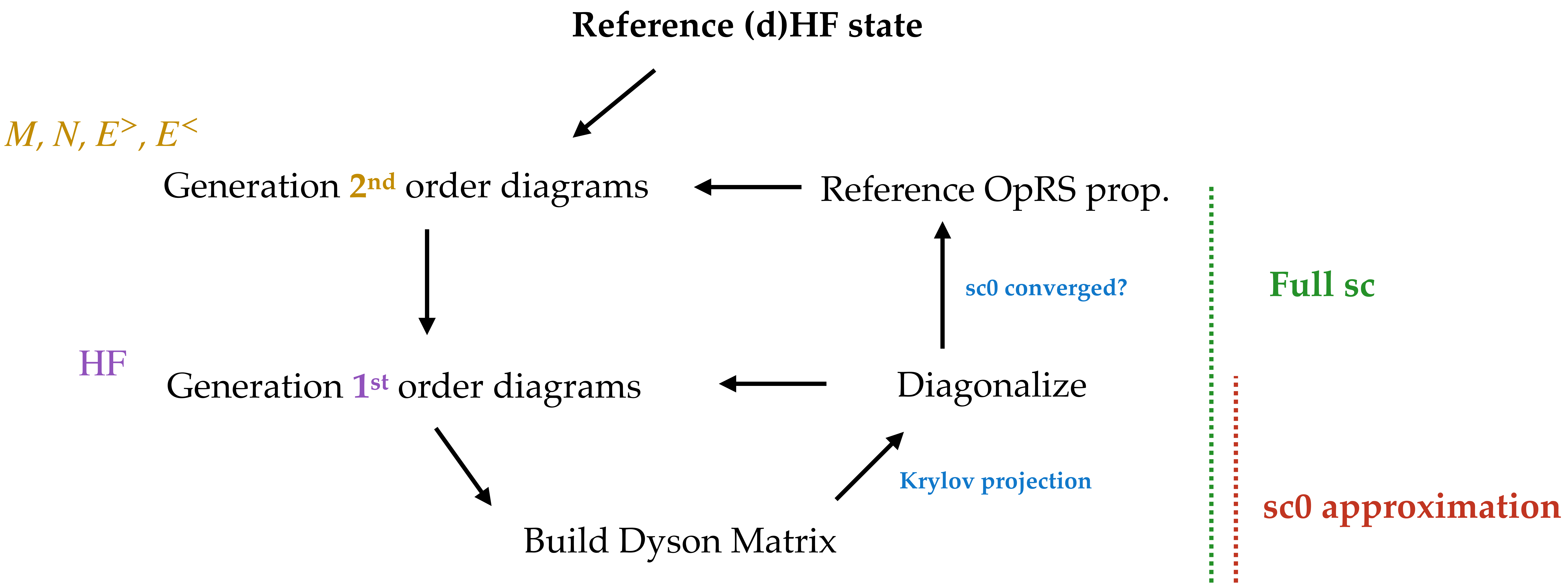
Spectroscopic factors

$$SF^+_n = \sum_{\alpha \in \mathcal{H}_1} |\mathcal{X}^n_\alpha|^2$$
$$SF^-_k = \sum_{\alpha \in \mathcal{H}_1} |\mathcal{Y}^k_\alpha|^2$$

Spectral strength distribution

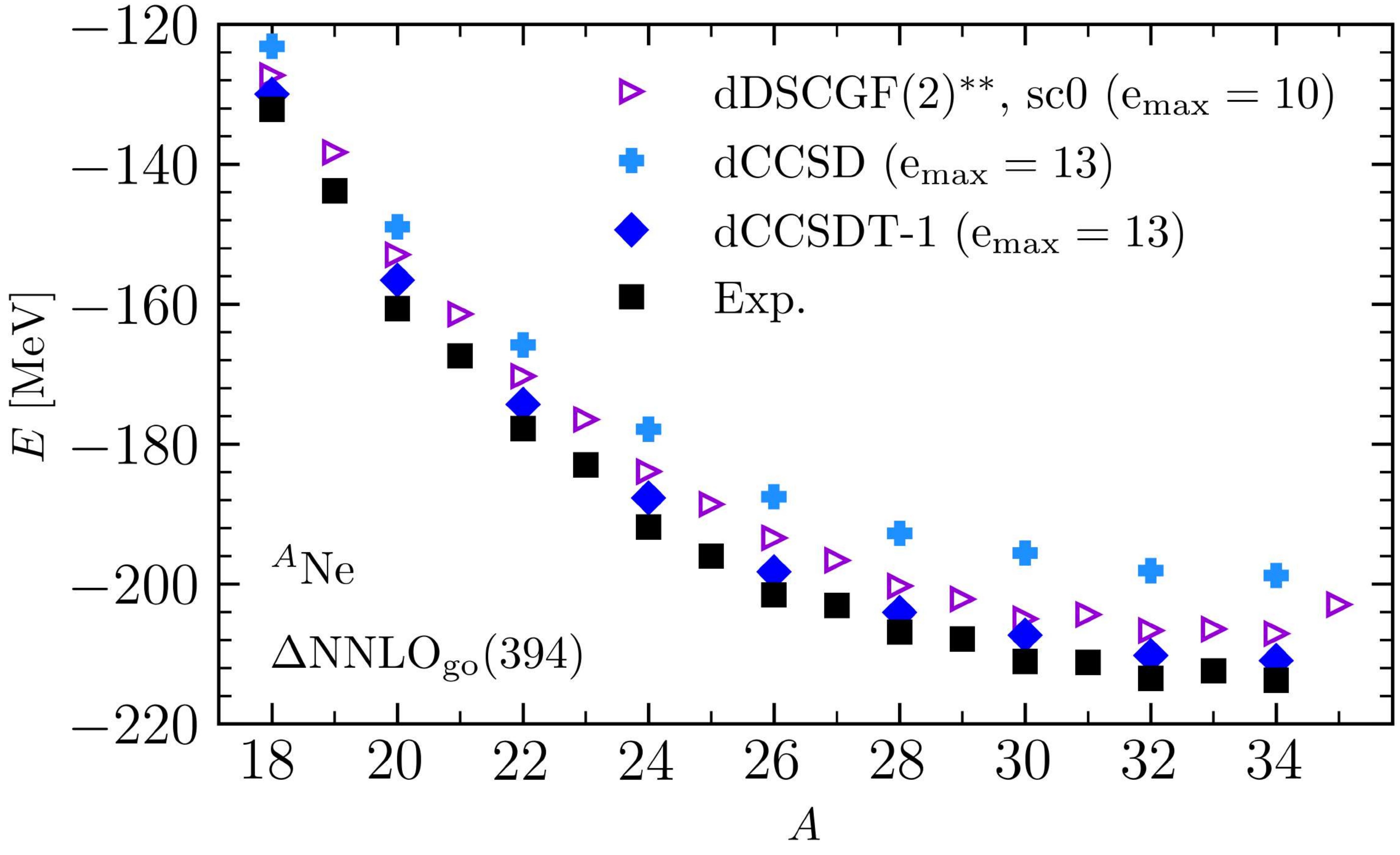
$$\mathcal{S}(\omega) = \sum_{n \in \mathcal{H}_{A+1}} SF^+_n \, \delta(\omega - \varepsilon^+_n) + \sum_{k \in \mathcal{H}_{A-1}} SF^-_k \, \delta(\omega - \varepsilon^-_k)$$

The self-consistent loop



Ground-state energy of Neon isotopes

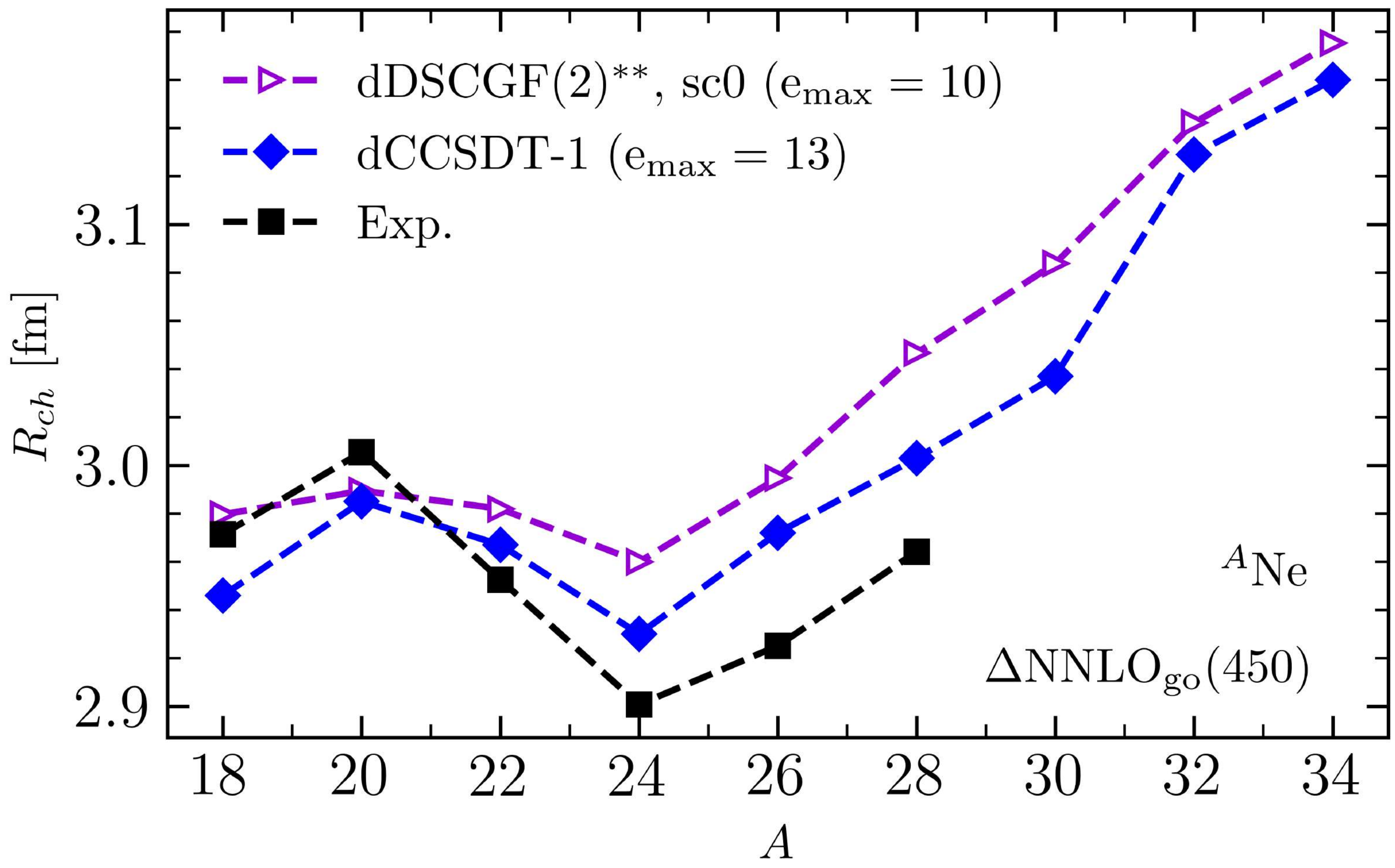
First tests on Neon isotopes where dCC results are available



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

[Novario *et al*. 2020]

Charge radii of Neon isotopes



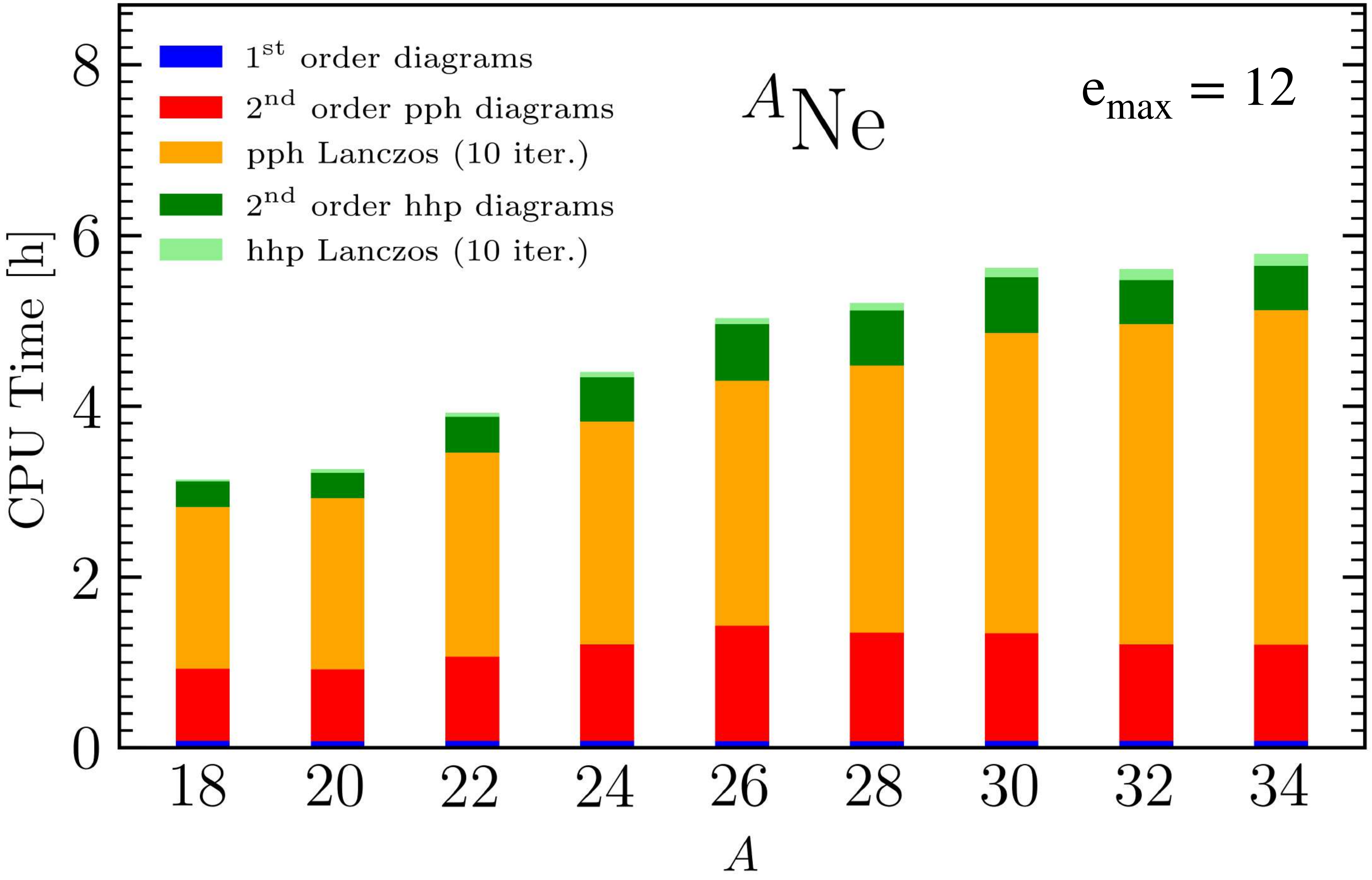
1B + 2B CoM corrections

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

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

[Novario *et al*. 2020]

CPU time for Neon isotopes



→ Increased computational cost with the mass of the system!

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Scaling of correlation-expansion methods

N^p

N

e_{max} \ Symmetry	Spherical (N^S)	Full (N)
0	1	2
1	3	8
2	6	20
3	10	40
4	15	70
5	21	112
6	28	168
7	36	240
8	45	330
9	55	440
10	66	572
11	78	728
12	91	910
13	105	1120
14	120	1360
15	136	1632

Opening SU(2) increases N

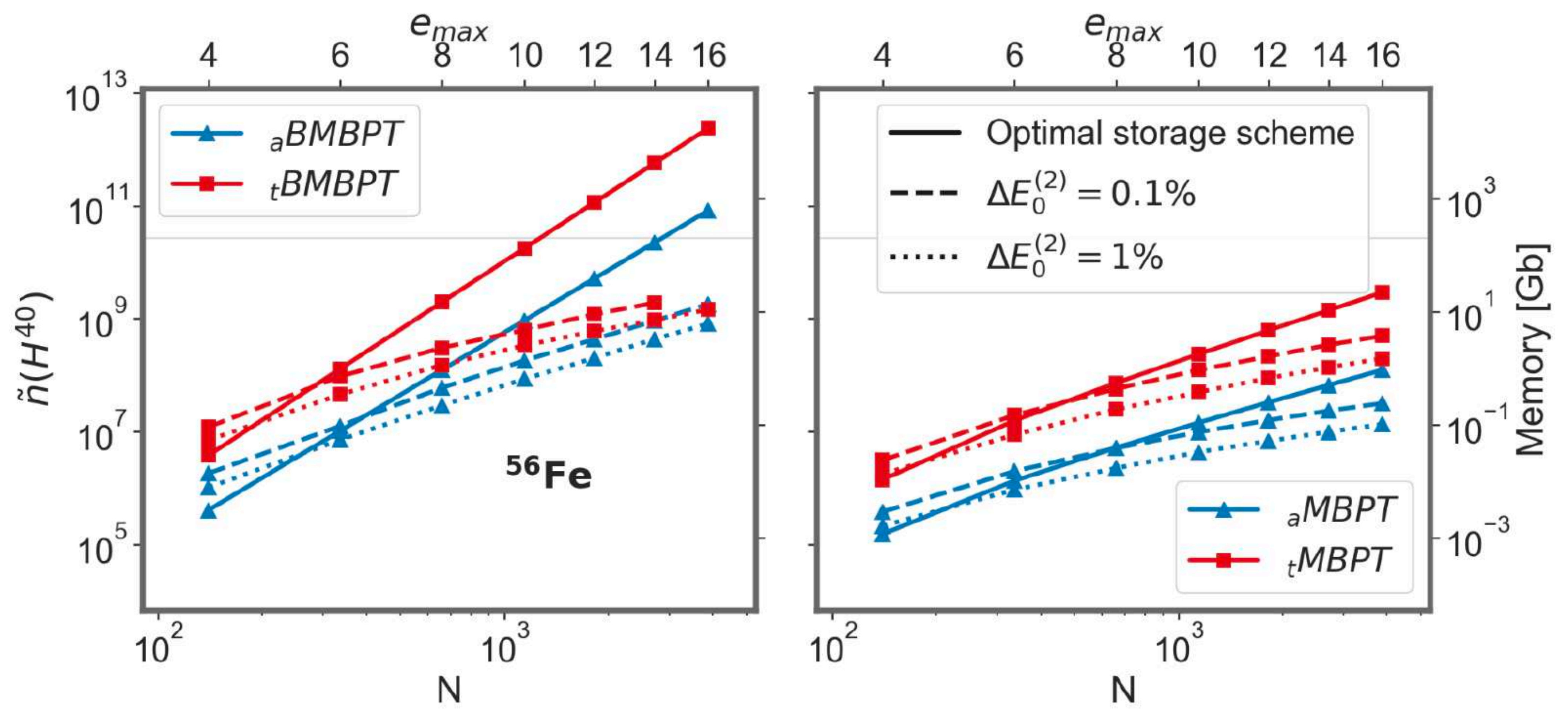
p

Truncation scheme	Scaling
(B)MBPT(2)	N^4
(B)MBPT(3)	N^5
(B)MBPT(4)	N^7
(B)CCSD	N^6
(B)CCSDT	N^8
IMSRG(2)	N^6
ADC(3)	N^6

p increases with the many-body truncation

→ **Increase computational cost and memory required!**

Techniques to mitigate the 'curse of dimensionality'



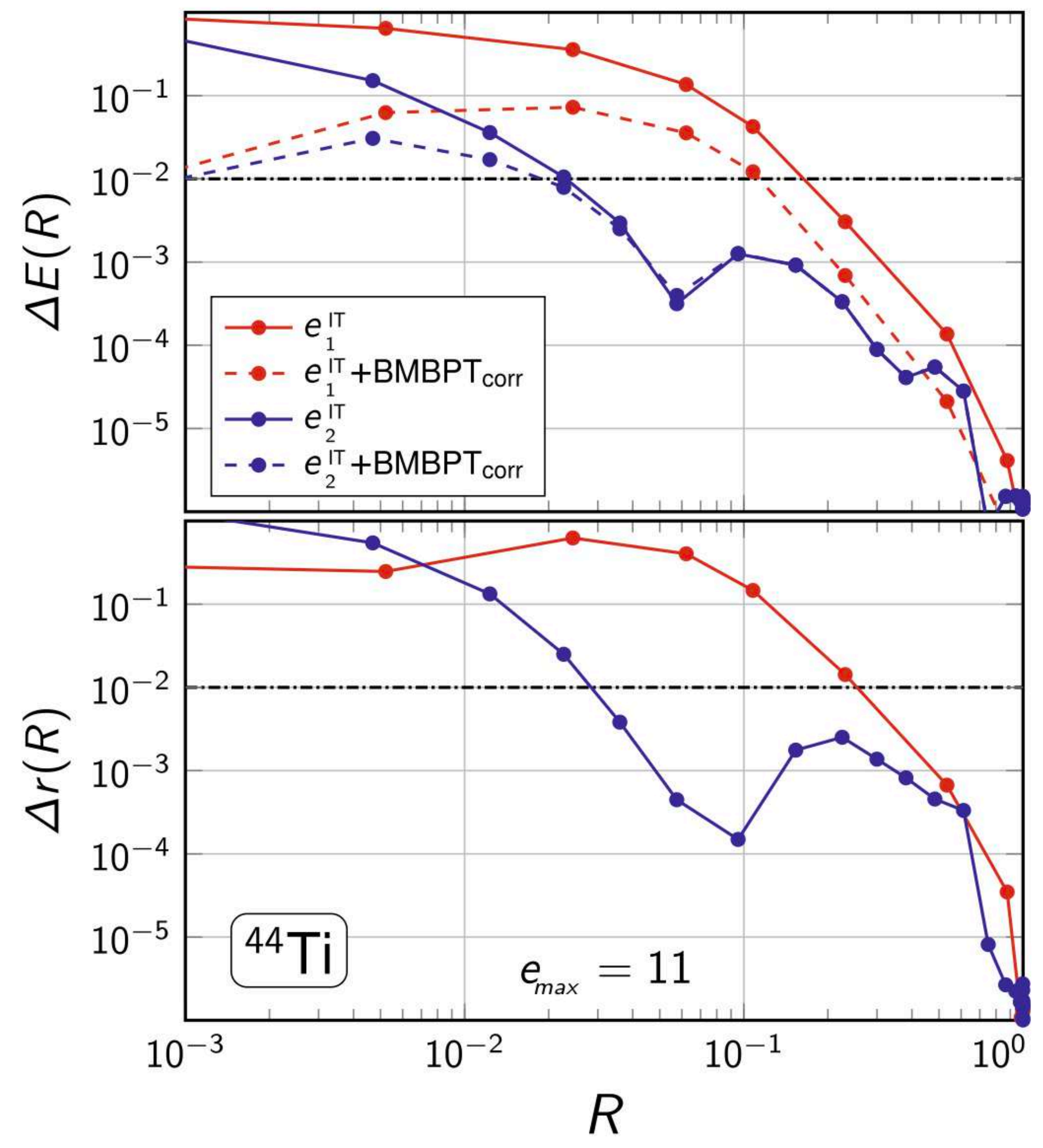
[Frosini *et al.* 2024]

Tensor factorization

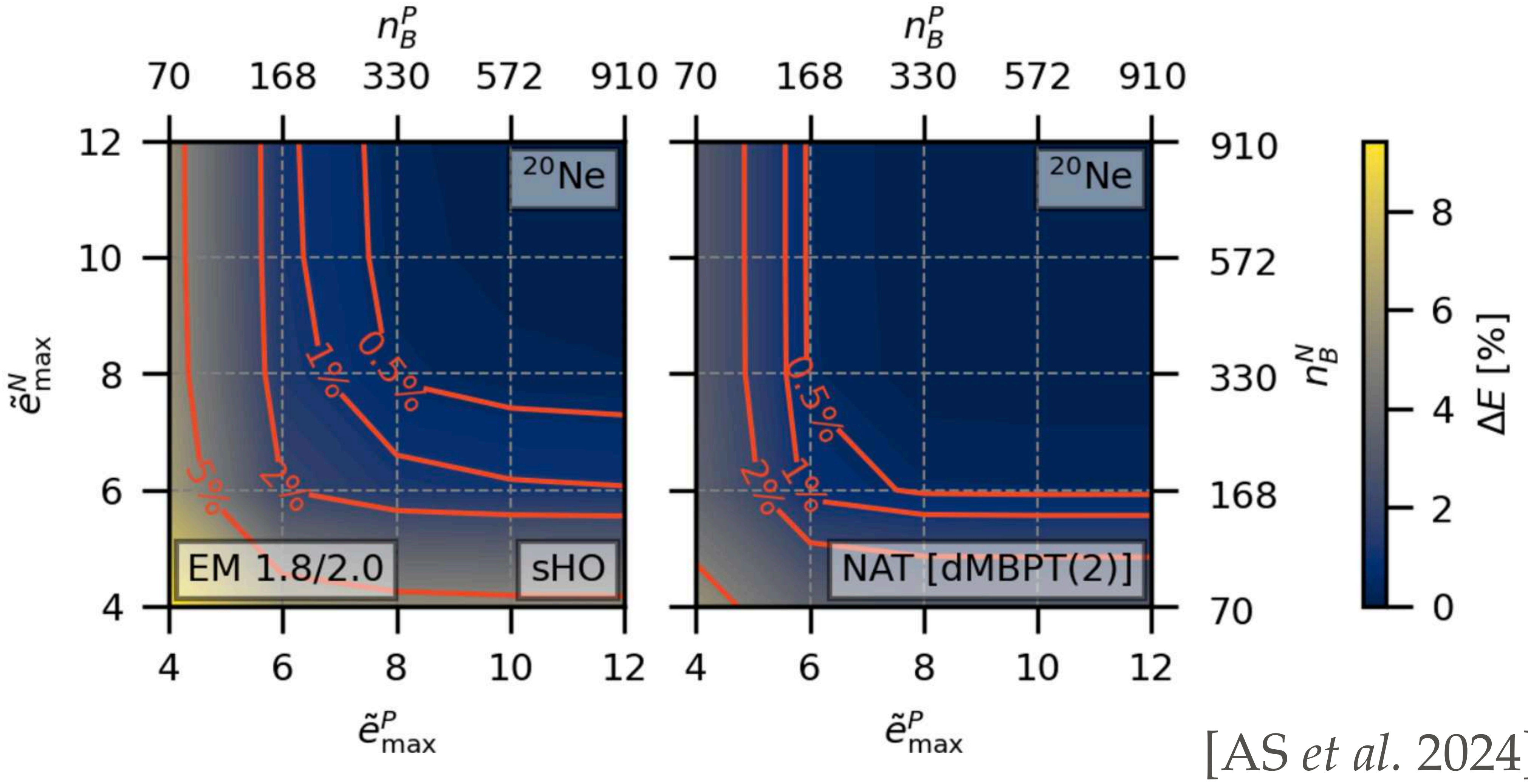
(see L. Zurek slides!)

Importance truncation

[Porro *et al.* 2021]

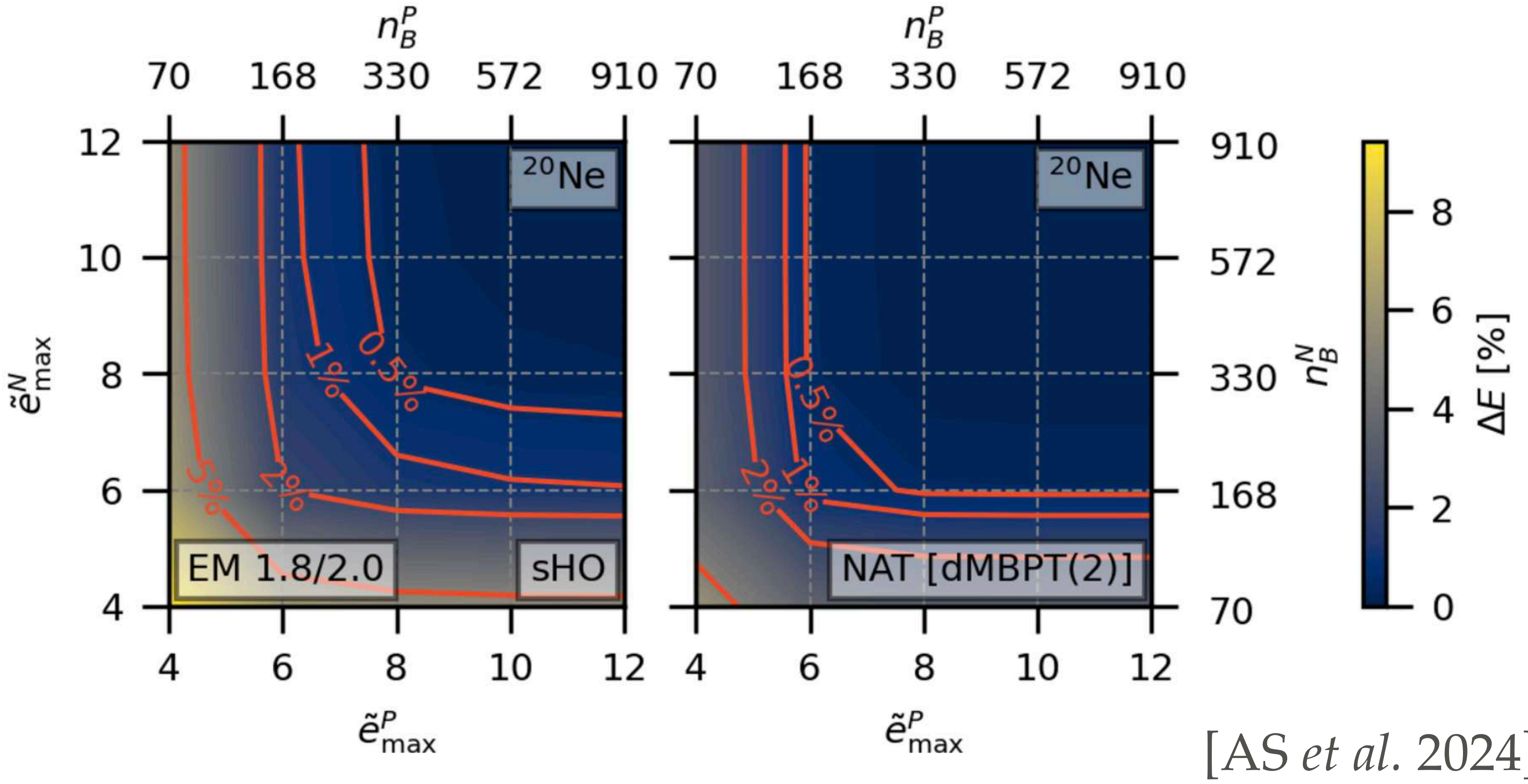


Alternative single-particle bases to sHO



[AS *et al.* 2024]

Techniques to mitigate the 'curse of dimensionality'



Alternative single-particle bases to sHO

[AS *et al.* 2024]

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

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

+ CoM for radii

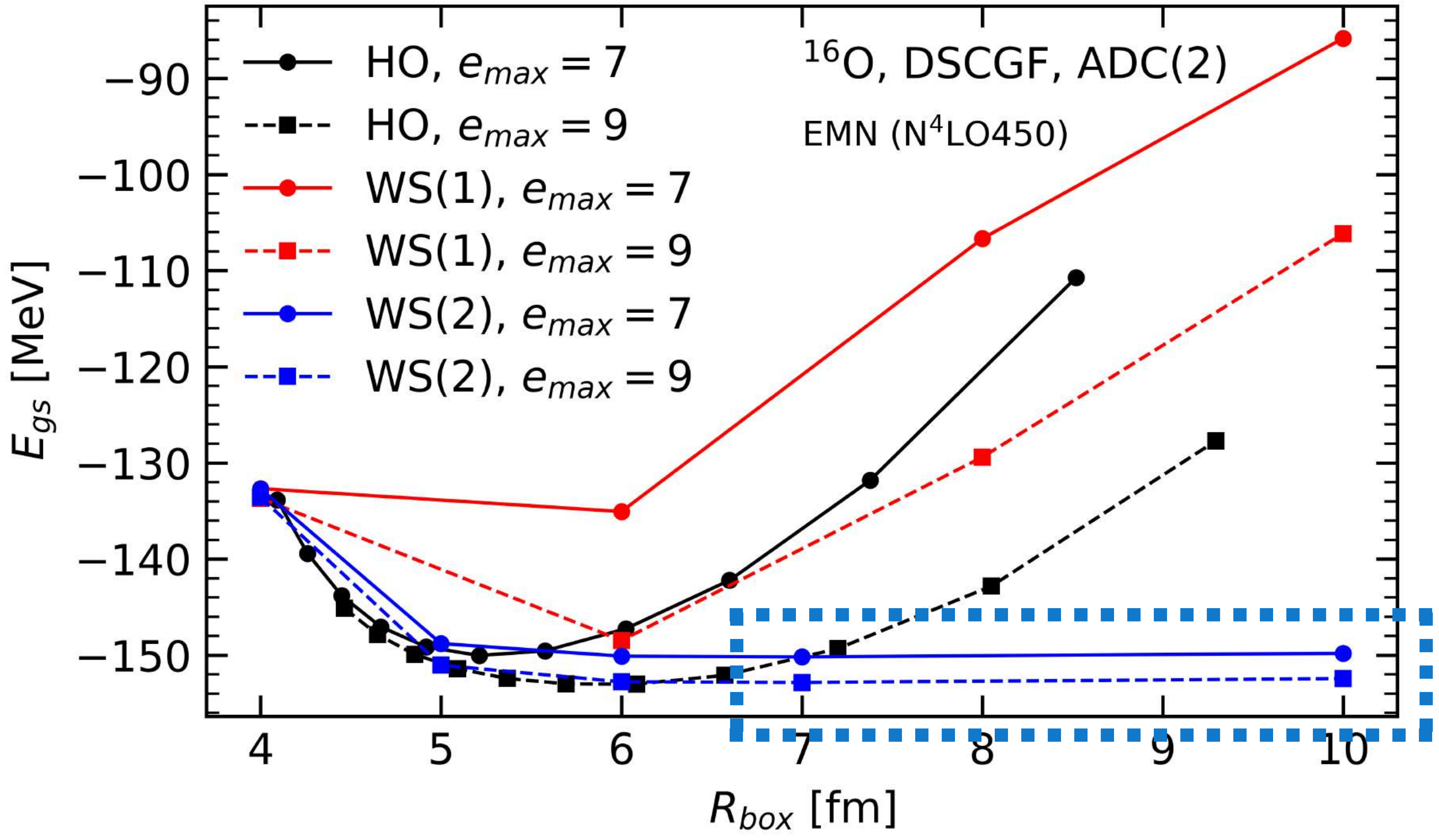
Goal of this work

- 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

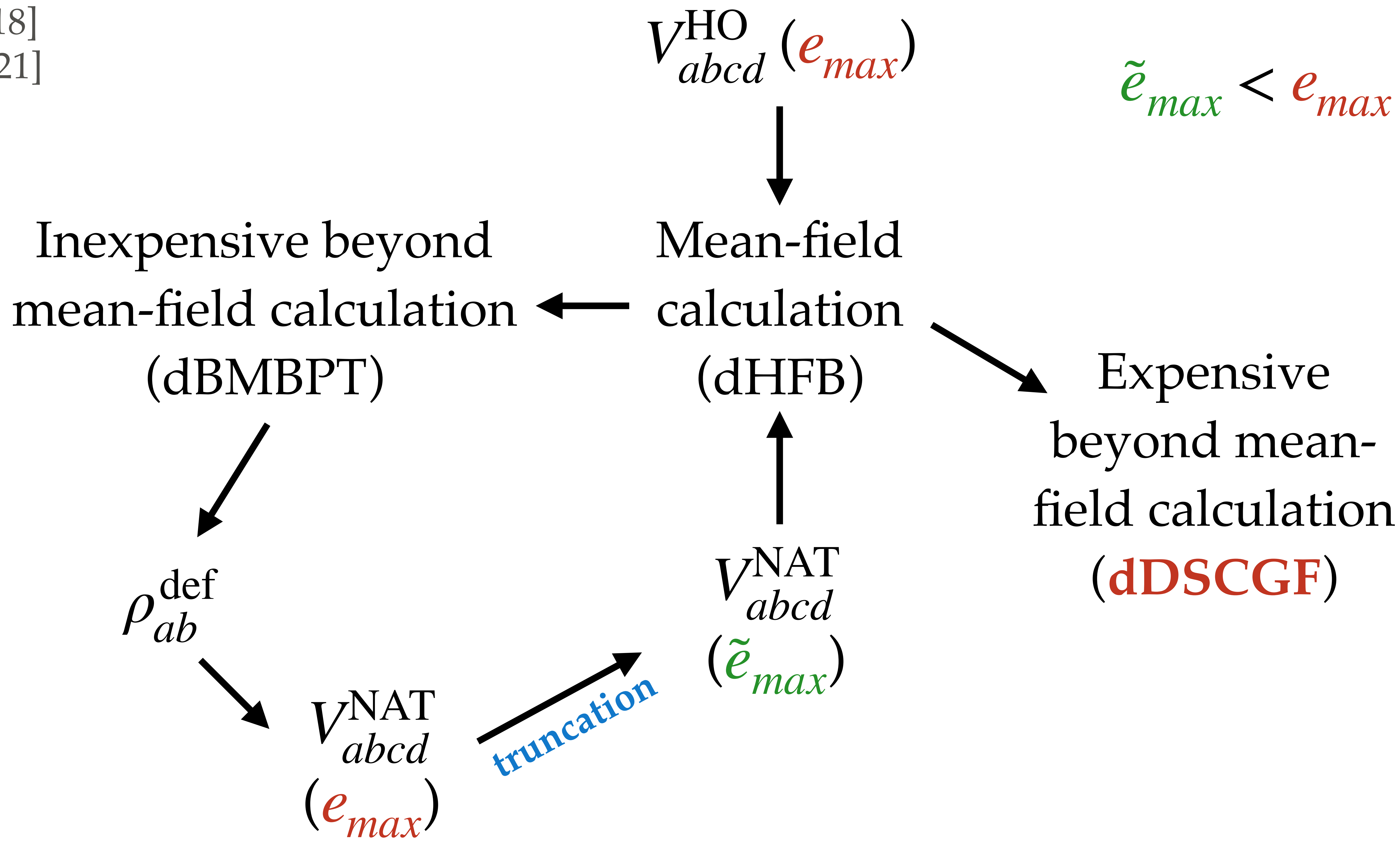


- Preliminary tests on new bases
- **Two-body** only
- Carried out with **Dyson SCGF** method
- Modified IR behavior of **WS(2) basis**
- Further tests to find more optimal bases

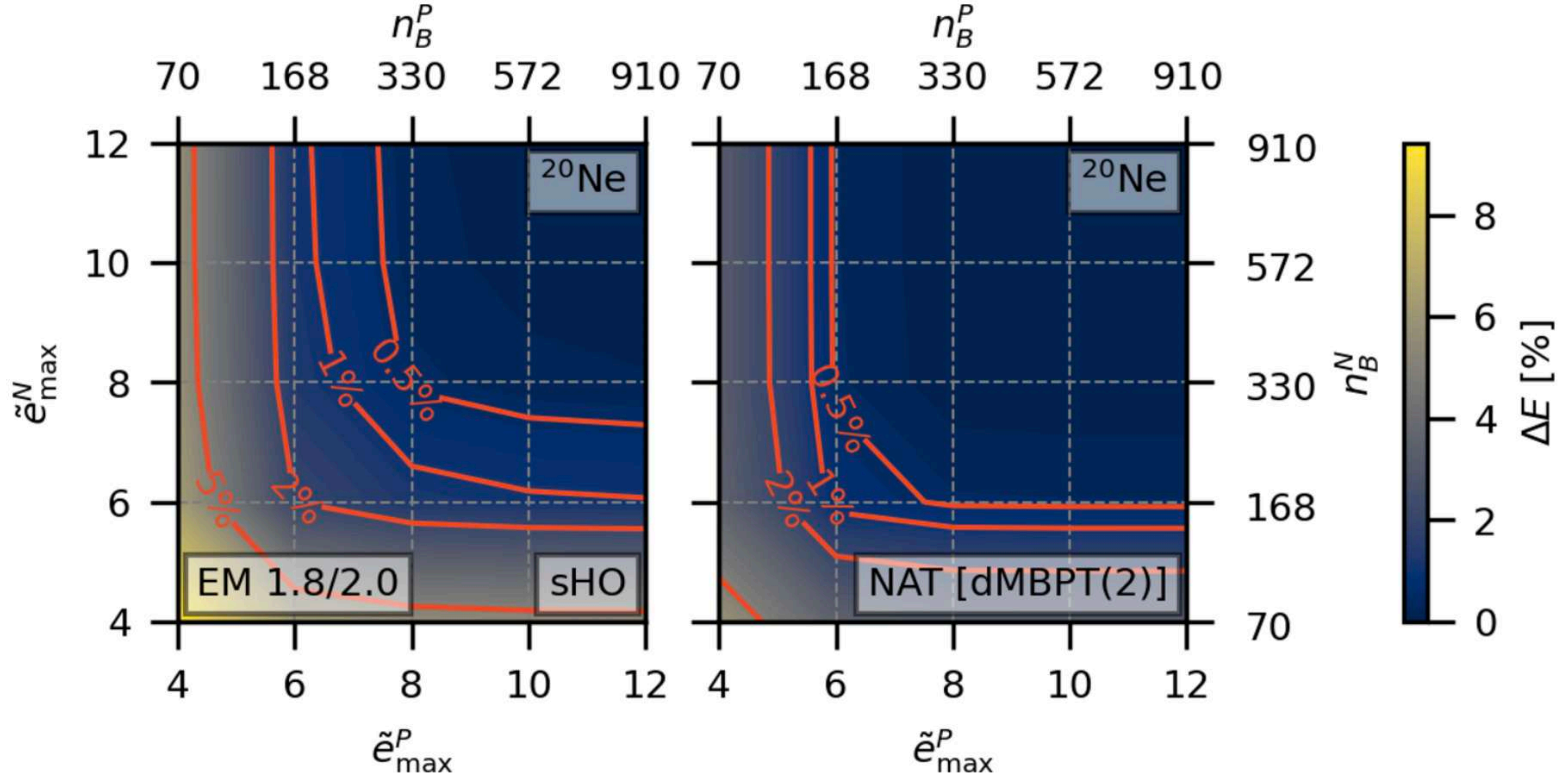
Deformed Natural Orbitals

- Main objective: reduce the cost of an expensive calculation
- How it can be done: via an **auxiliary cheaper calculation**

[Tichai *et al.* 2018]
[Hoppe *et al.* 2021]



Deformed Natural Orbitals



check out [*Eur.Phys.J.A* 61 (2025) 1, 1] for more details on deformed NAT!

Outline

- *Ab initio* polynomially-scaling methods: why break symmetries?
- Deformed self-consistent Green's function
- Techniques to mitigate the 'curse of dimensionality'

Outline

- *Ab initio* polynomially-scaling methods: why break symmetries?
- Deformed self-consistent Green's function
- Techniques to mitigate the 'curse of dimensionality'
- Conclusions

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

→ **Generic bases** can help to lighten the cost of beyond mean-field calculations

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
- Exploration of new **generic spherical bases**

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