How to describe all nuclei at polynomial cost in the *ab initio* framework

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Recent Progress in Many-Body Theories

23-27 September 2024, Tsukuba

The Segrè chart

Nuclear structure approaches

- **Energy density functionals**
- Empirical shell model
- **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)

The nuclear *ab initio* endeavour

A systematic approach to describe nuclei

$$H\,|\Psi_k^\sigma\rangle = E_k^{\tilde{\sigma}}\,|\Psi_k^\sigma\rangle$$

Hamiltonian from chiral effective field theory

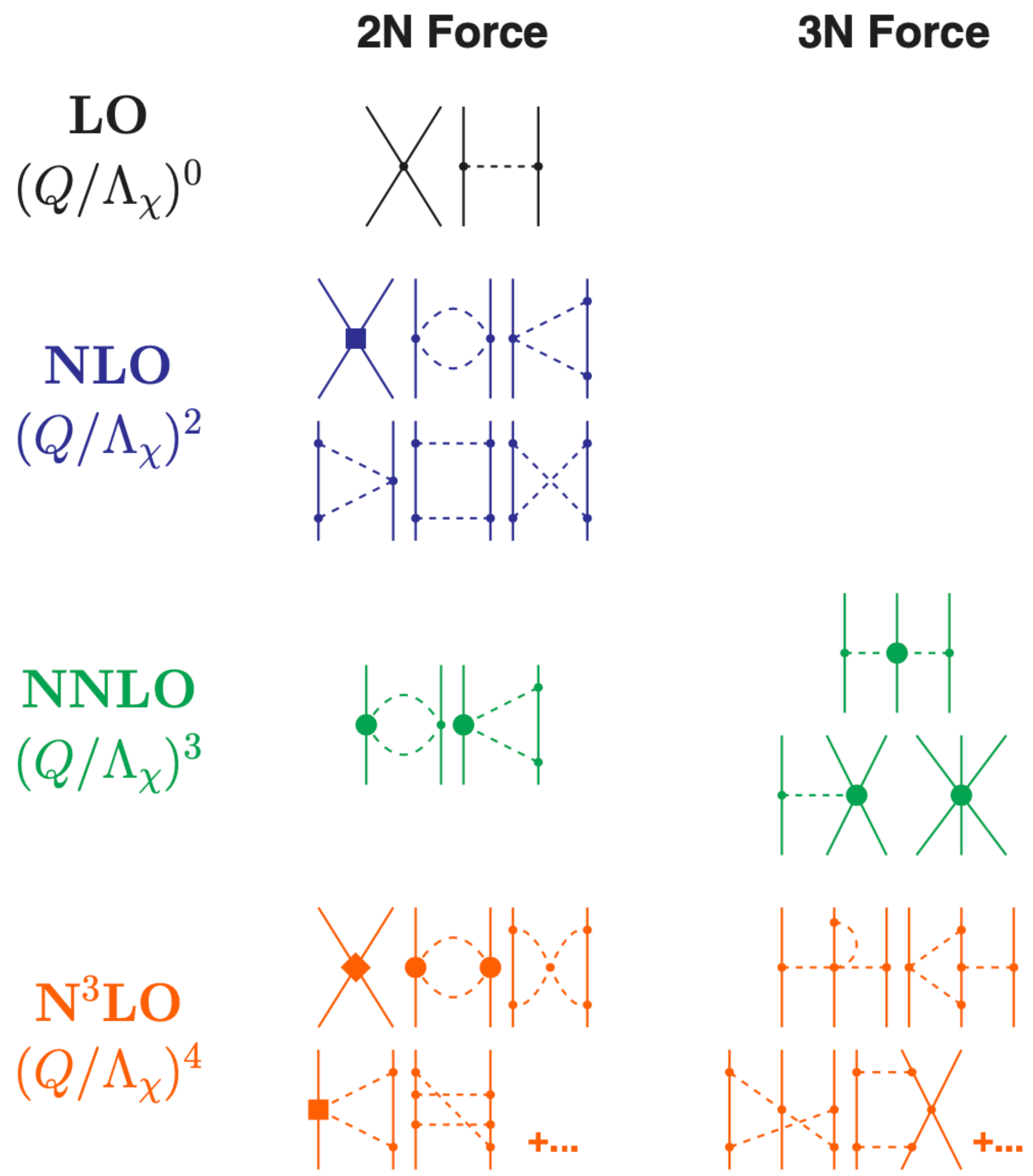
- ○ Low-energy limit of QCD
- ○ Nucleons and pions as d.o.f.
- ○ Power counting → expansion of H

Set of quantum numbers

$$\sigma \equiv JM\Pi NZ \equiv \tilde{\sigma} M$$

Set of symmetries

$$[H, R(\theta)] = 0$$



1) Exact solutions have factorial or exponential scaling → limited to light nuclei

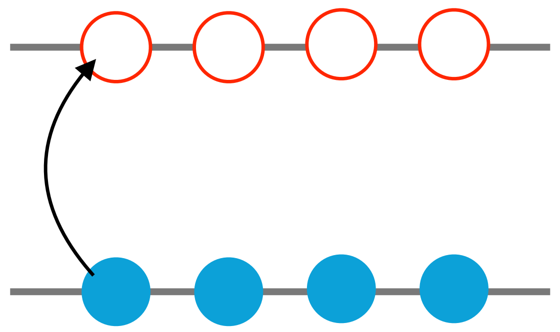
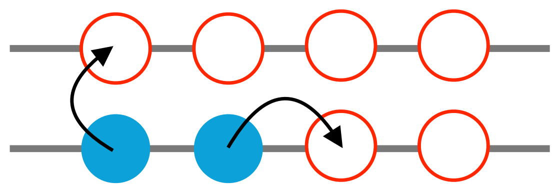
2) Correlation-expansion methods to achieve **polynomial** scaling → CPU-scalable to **heavy masses**

- ○ Hamiltonian partitioning $H = H_0 + H_1$
- ○ Reference state $H_0\,|\Theta_k^{(0)}\rangle = E_k^{(0)}\,|\Theta_k^{(0)}\rangle$ → scaling n^4
- ○ Wave-operator expansion $|\Psi_k^\sigma\rangle = \Omega_k\,|\Theta_k^{(0)}\rangle$ → scaling n^α with $\alpha > 4$

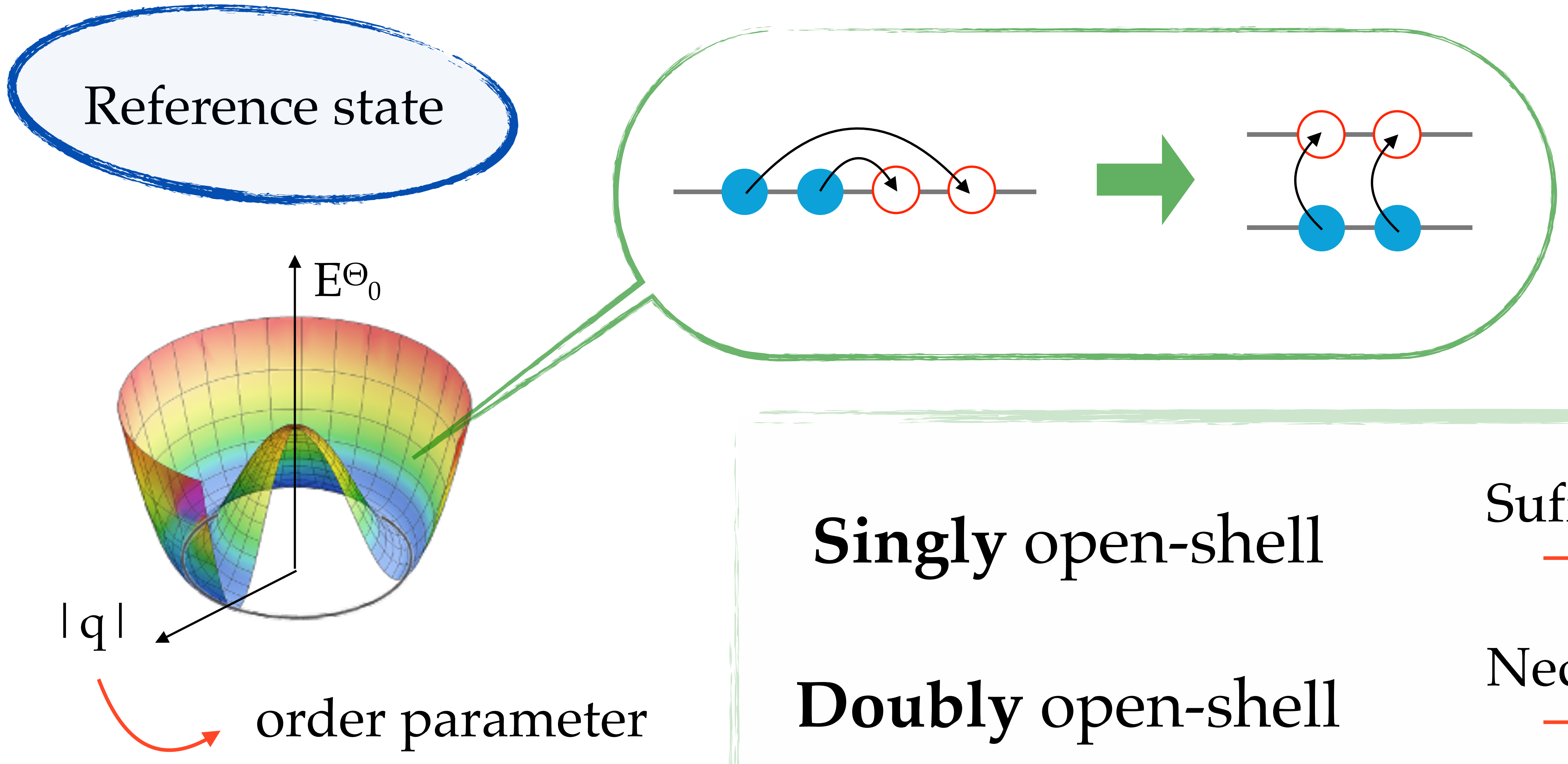
MBPT, CC, SCGF, IM-SRG, …

Closed- and open-shells, symmetry breaking

○ Reference state varies with Z & N

Closed-shell		Weakly correlated	*ph* expansion well defined	5%
Open-shell		Strongly correlated	*ph* expansion breaks down	95%

○ Exploit **symmetry breaking** to lift *ph* degeneracy



1) Incorporate **static** correlations into reference state

2) Account for **dynamical** correlations via *ph* excitation

→ Symmetries must be eventually **restored**

Singly open-shell	Sufficient to break →	$U(1)_N \times U(1)_Z$	Superfluidity
Doubly open-shell	Necessary to break →	$SU(2)$	Deformation

Outline

1) **Perturbative** calculations (proof that deformation is mandatory)

2) Strategy #1: **expand, then project**

3) Strategy #2: **project, then expand**

Study on the necessity of deformation

- **Goal**: prove that deformation is mandatory for describing doubly open-shell nuclei at a polynomial cost

- **Physical case**:

  → **Singly open-shell** calcium chain (Z=20)

  → **Doubly open-shell** chromium chain (Z=24)

- **Many-body approaches**:

  → U(1)-breaking & SU(2)-conserving / -breaking many-body perturbation theory (**sBMBPT** / **dBMBPT**)

- **Observables**:

  → Total binding energies $E(N, Z)$

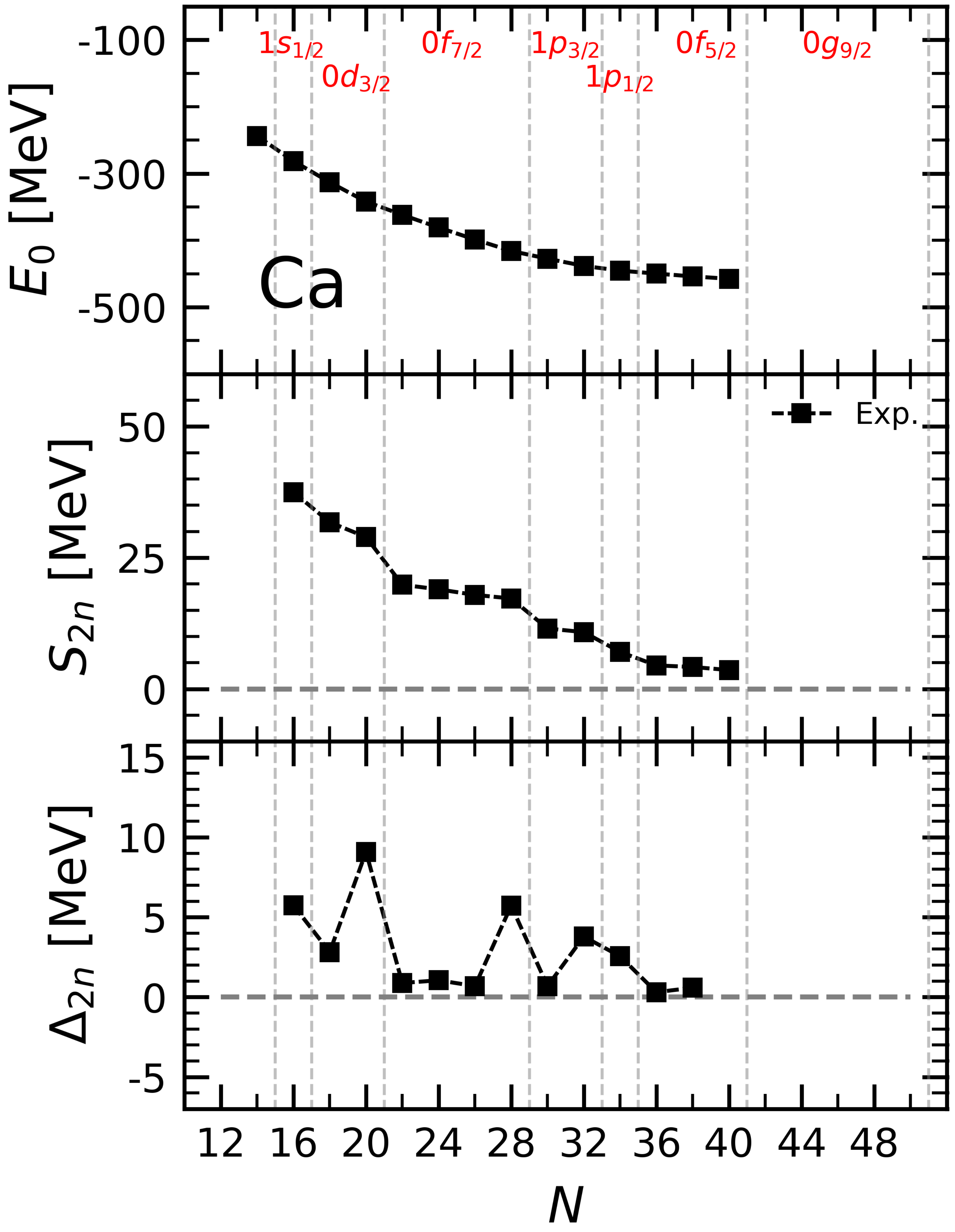
  → Two-neutron separation energies $S_{2n}(N,Z) \equiv E(N-2,Z) - E(N,Z)$

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

- **Hamiltonian**: empirically optimal (to disentangle H & many-body expansion)

  → EM 1.8/2.0 [Hebeler *et al.* 2011]

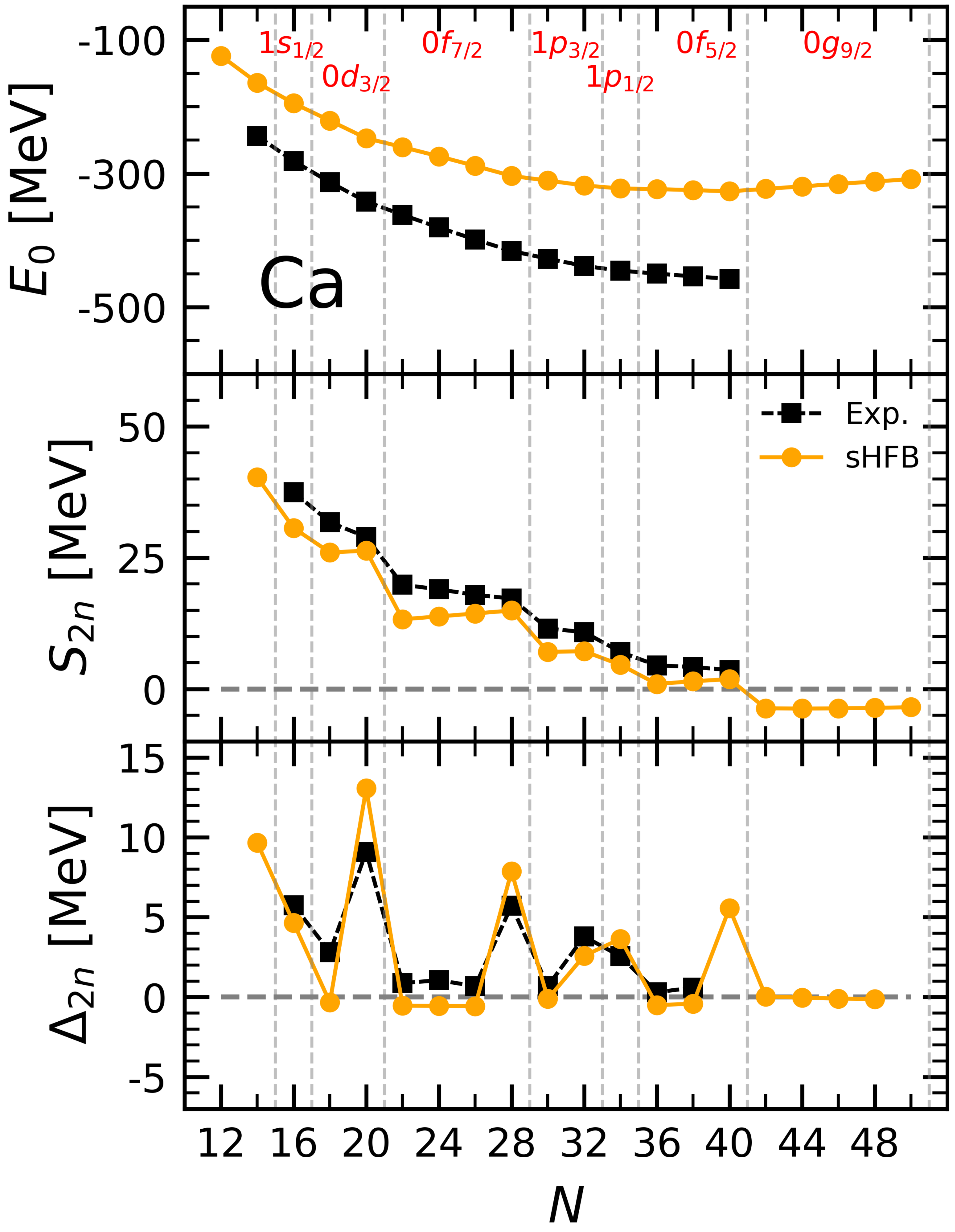
SU(2)-conserving approach



Singly open-shell

[Scalesi *et al*. 2024]

SU(2)-conserving approach



[Scalesi *et al*. 2024]

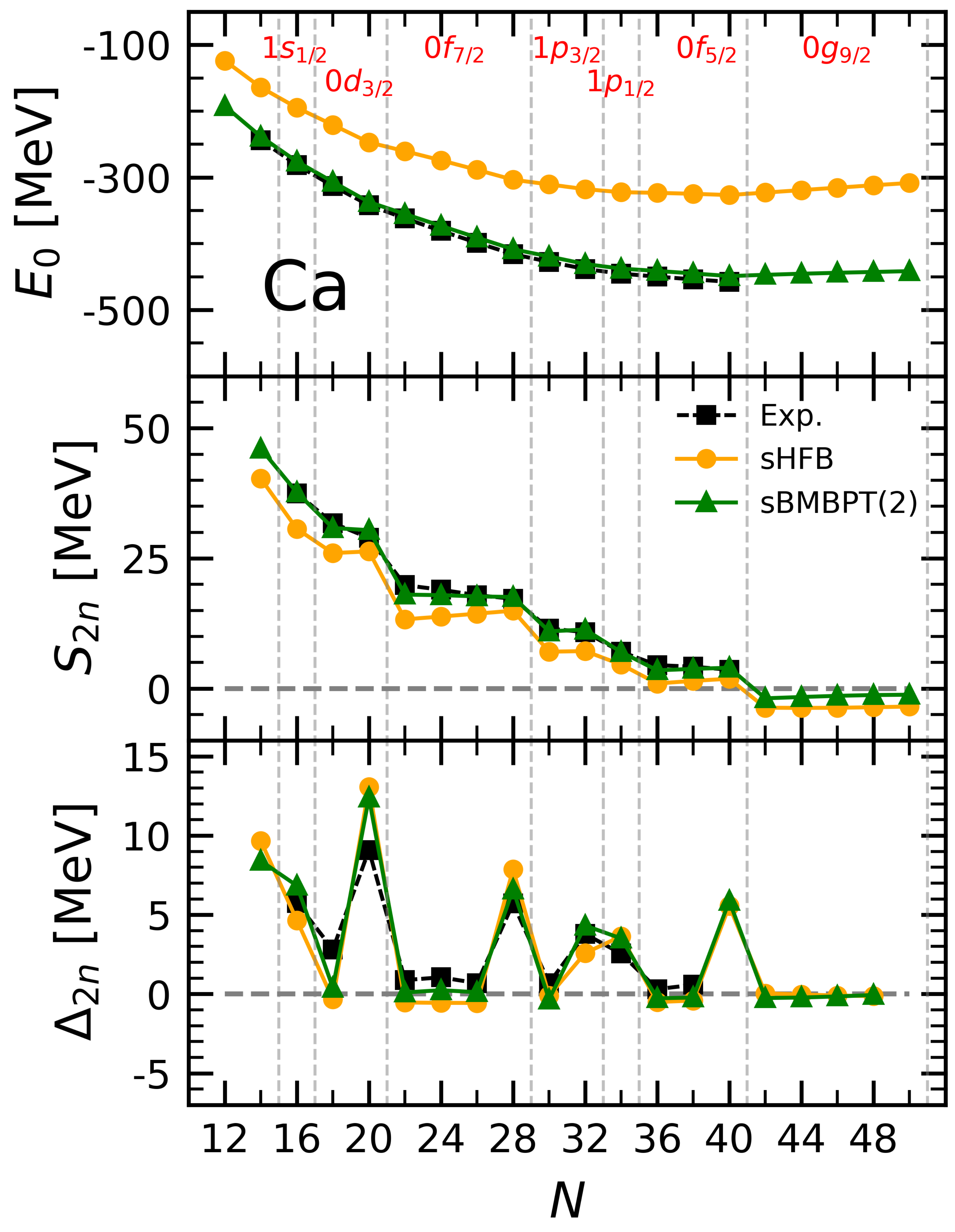
Singly open-shell

Spherical mean field

○ Underbinding

○ Wrong curvature

SU(2)-conserving approach



[Scalesi *et al*. 2024]

Singly open-shell

Spherical mean field

○ Underbinding

○ Wrong curvature

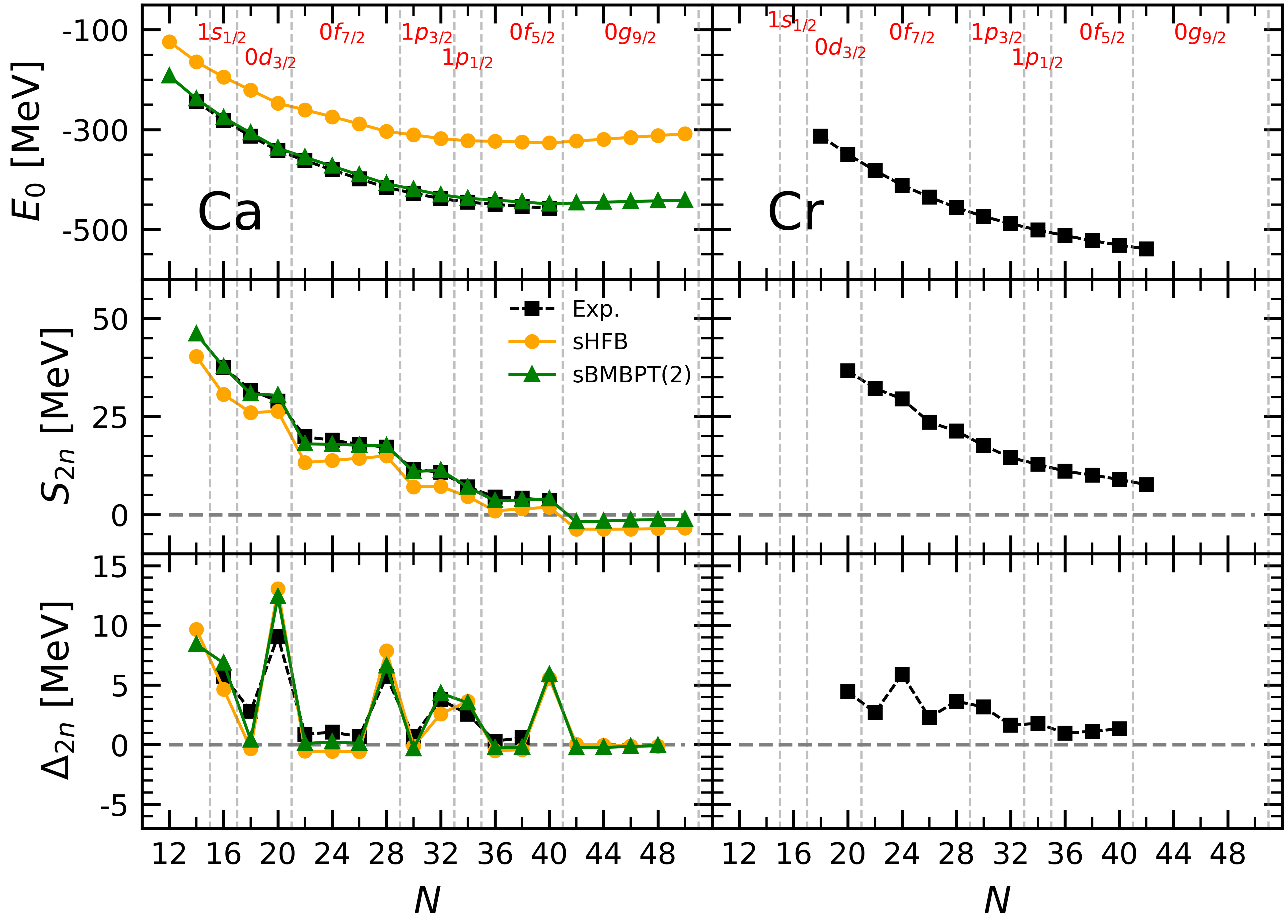
Low-order dynamical correlations

○ Correct binding

○ Improved curvature

→ **Low-order sufficient**

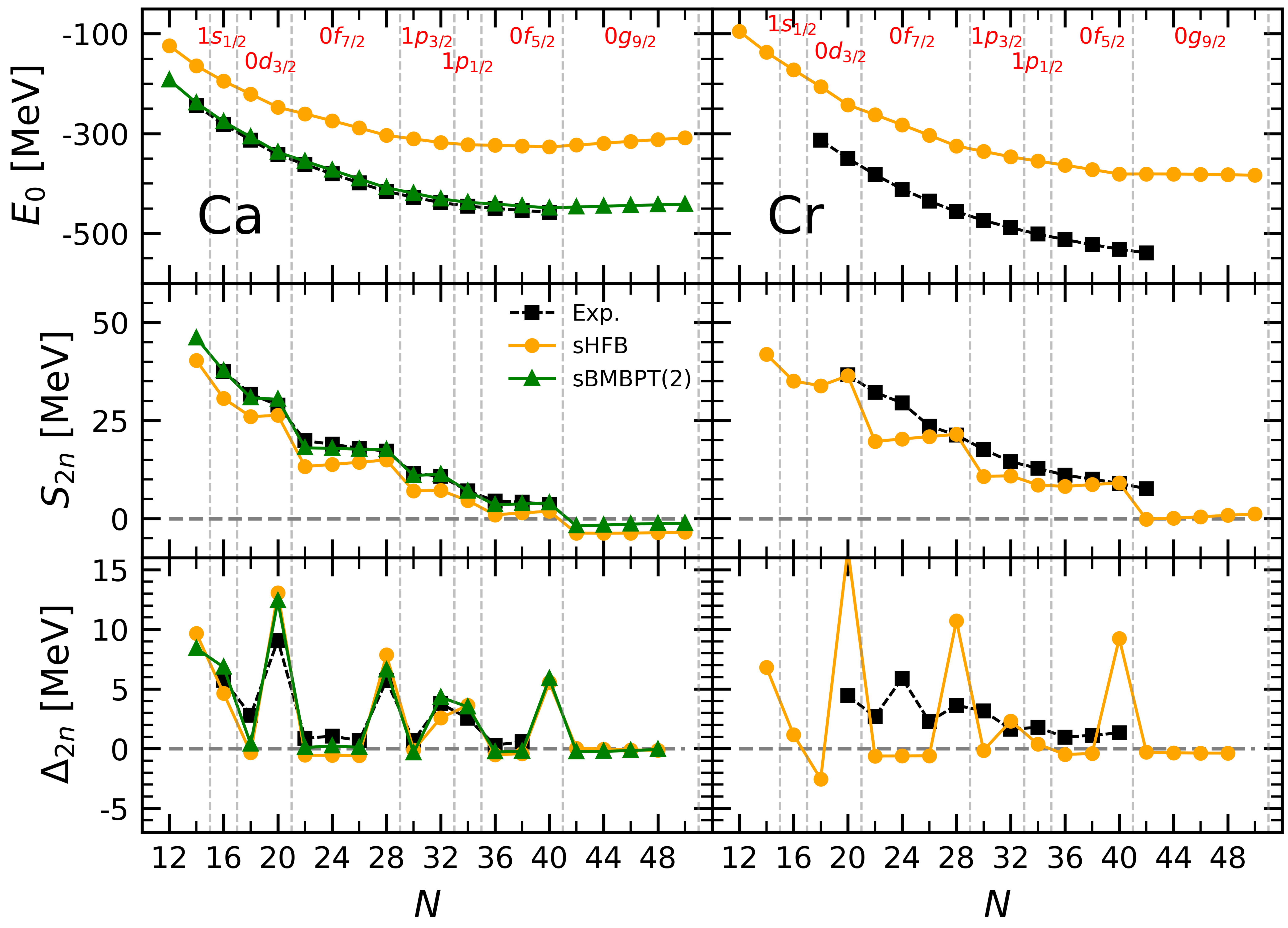
SU(2)-conserving approach



Doubly open-shell

[Scalesi *et al*. 2024]

SU(2)-conserving approach



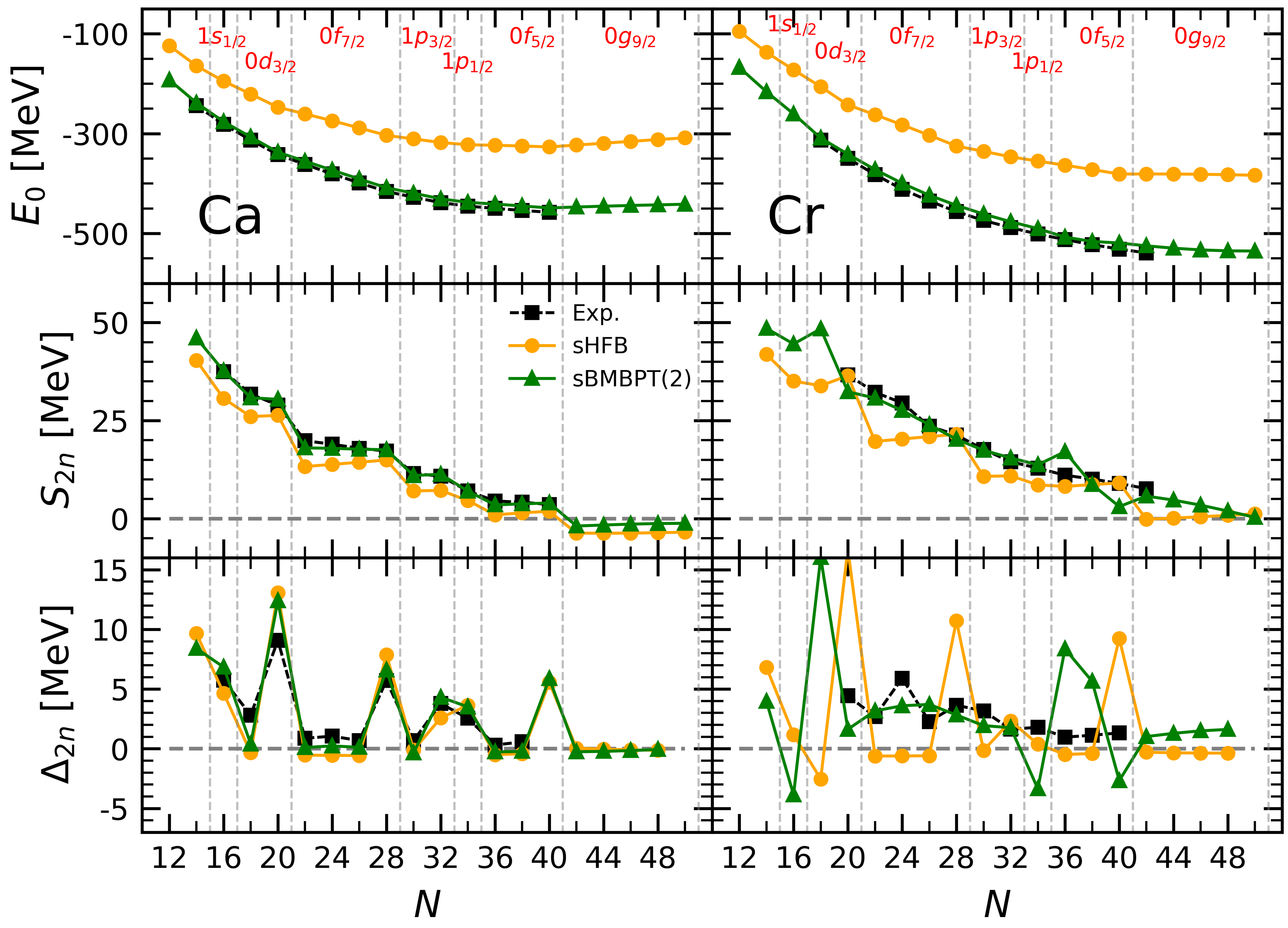
Doubly open-shell

Spherical mean field

- Defects even more pronounced

[Scalesi *et al*. 2024]

SU(2)-conserving approach



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Doubly open-shell

Spherical mean field

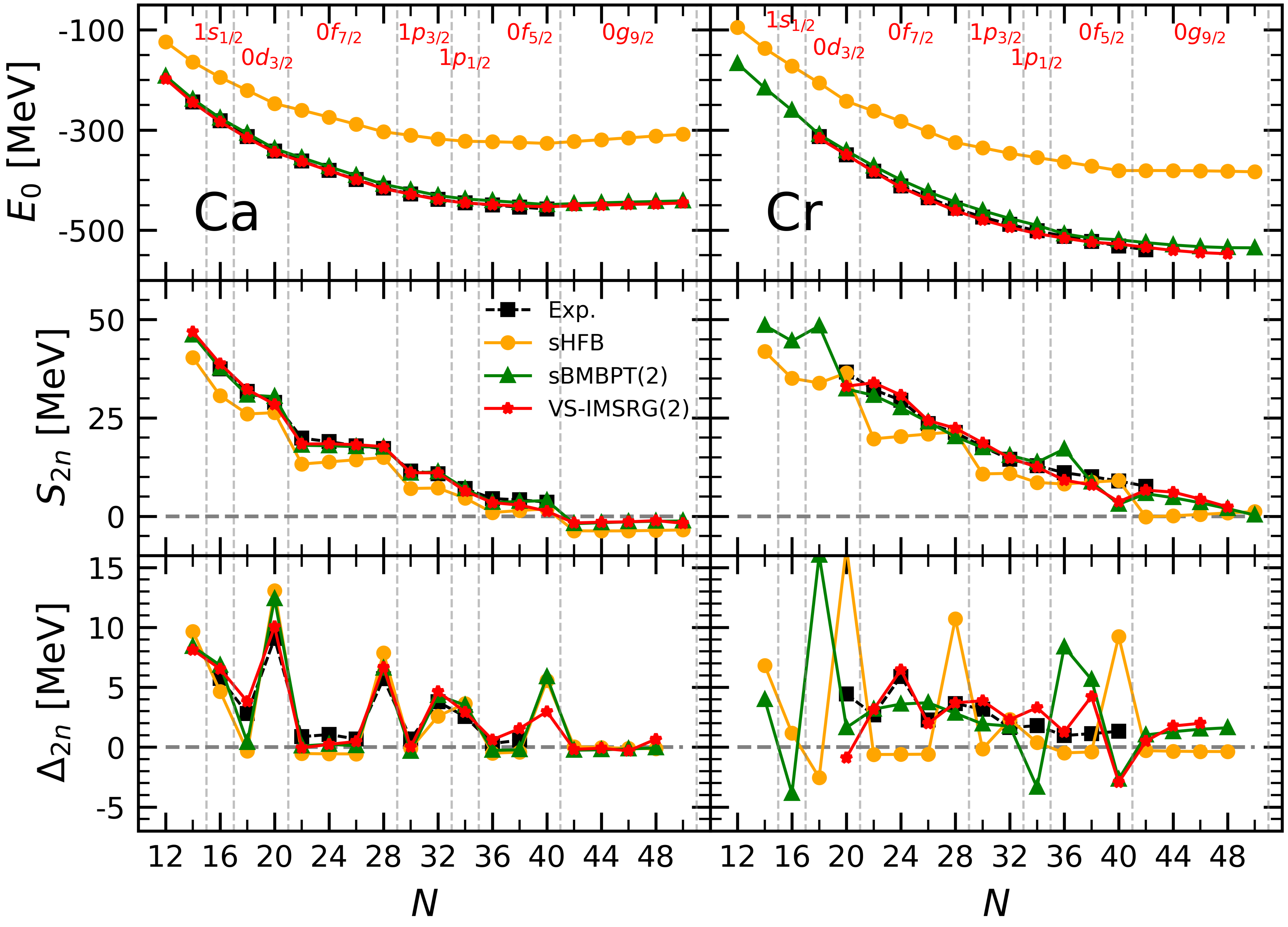
○ Defects even more pronounced

Low-order dynamical correlations

○ Improved curvature

○ Wrong shell gaps

SU(2)-conserving approach



Doubly open-shell

Spherical mean field

○ Defects even more pronounced

Low-order dynamical correlations

○ Improved curvature

○ Wrong shell gaps

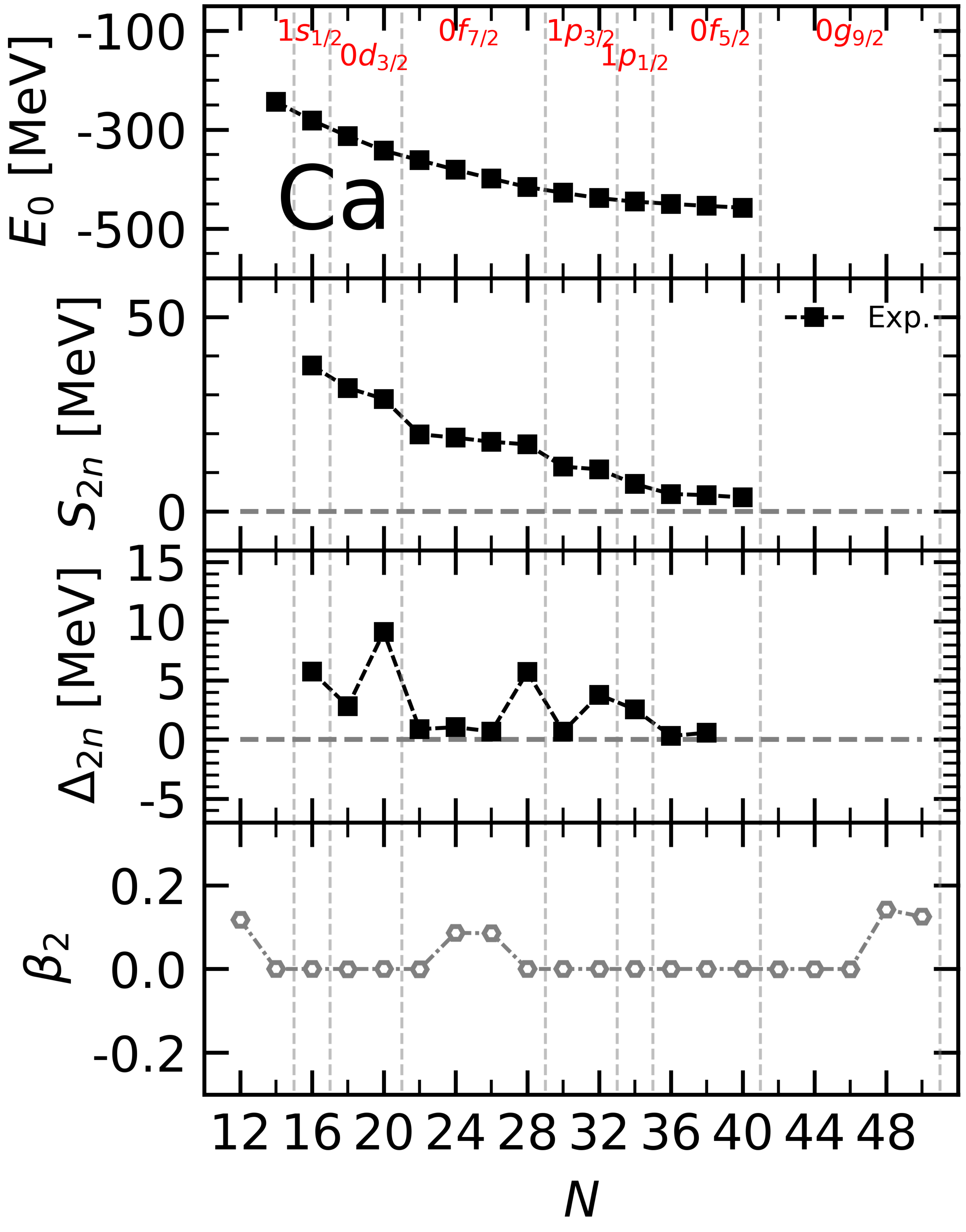
Non-polynomial (diagonalisation)

○ Correct E_0, S_{2n} and gaps

→ **At least high orders needed**

[Scalesi *et al*. 2024]

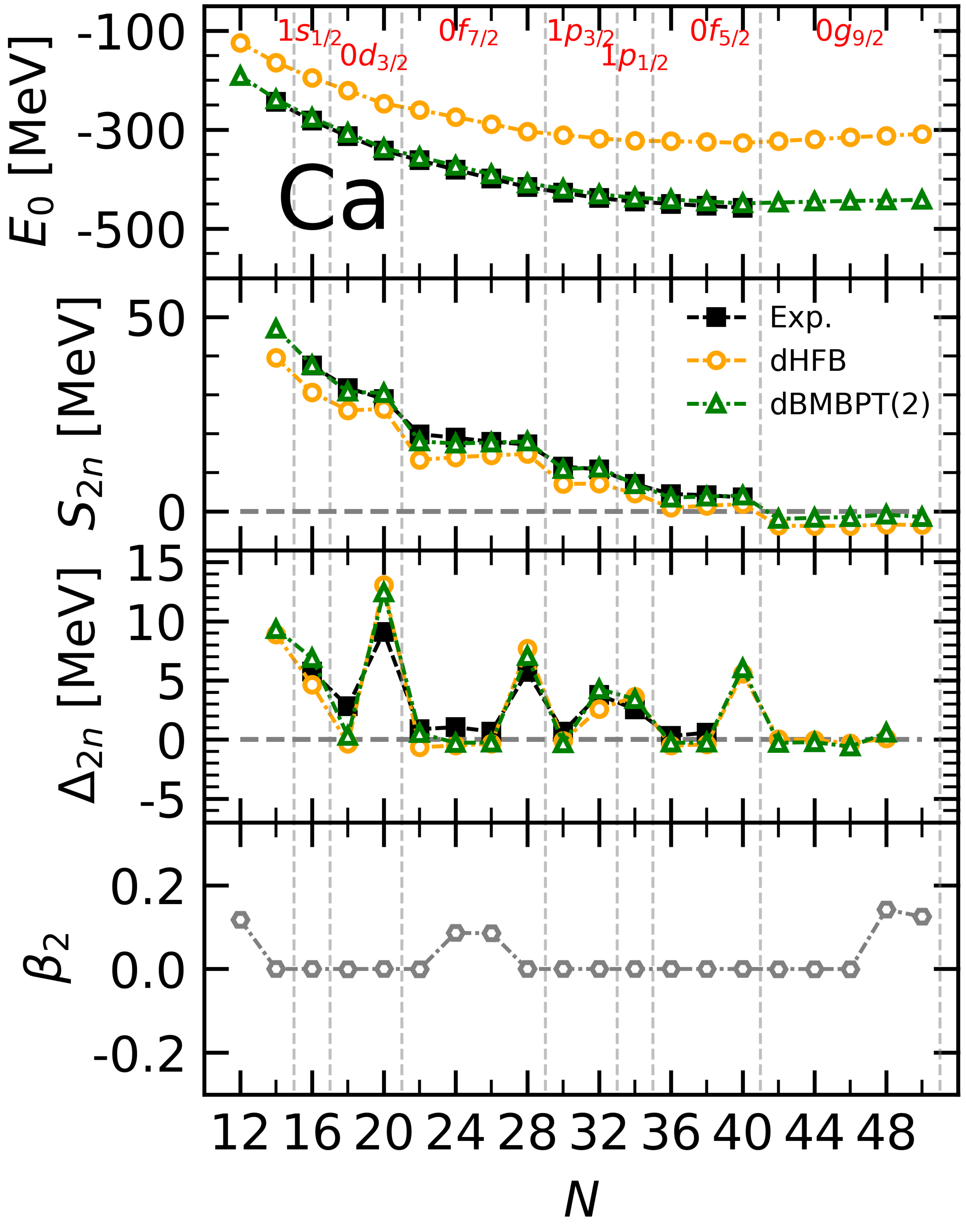
SU(2)-breaking approach



Singly open-shell

[Scalesi *et al*. 2024]

SU(2)-breaking approach



[Scalesi *et al*. 2024]

Singly open-shell

Deformed mean field

○ Underbinding

○ Wrong curvature

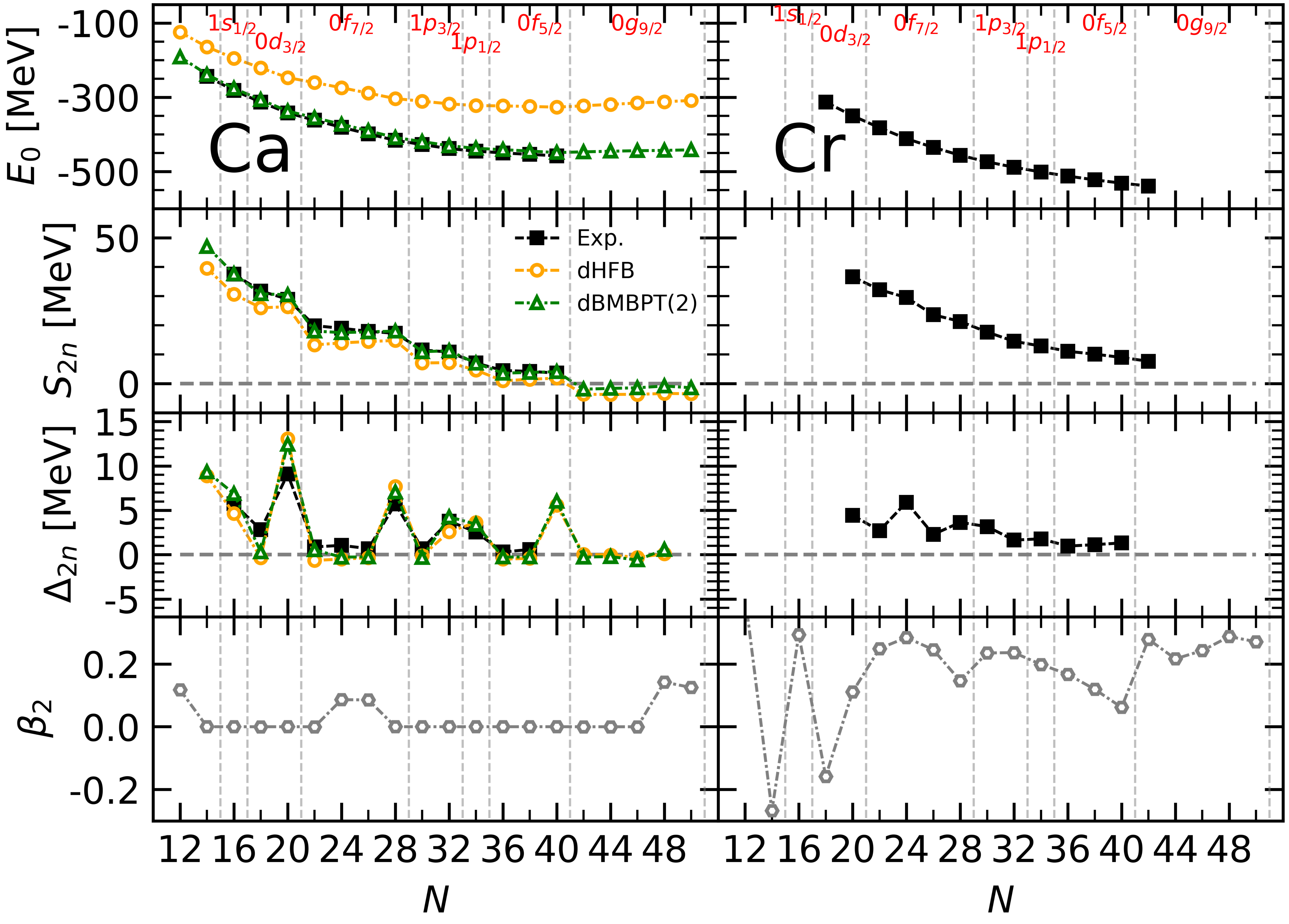
Low-order dynamical correlations

○ Binding energy now fine

○ Improved curvature

→ **Low-order sufficient**

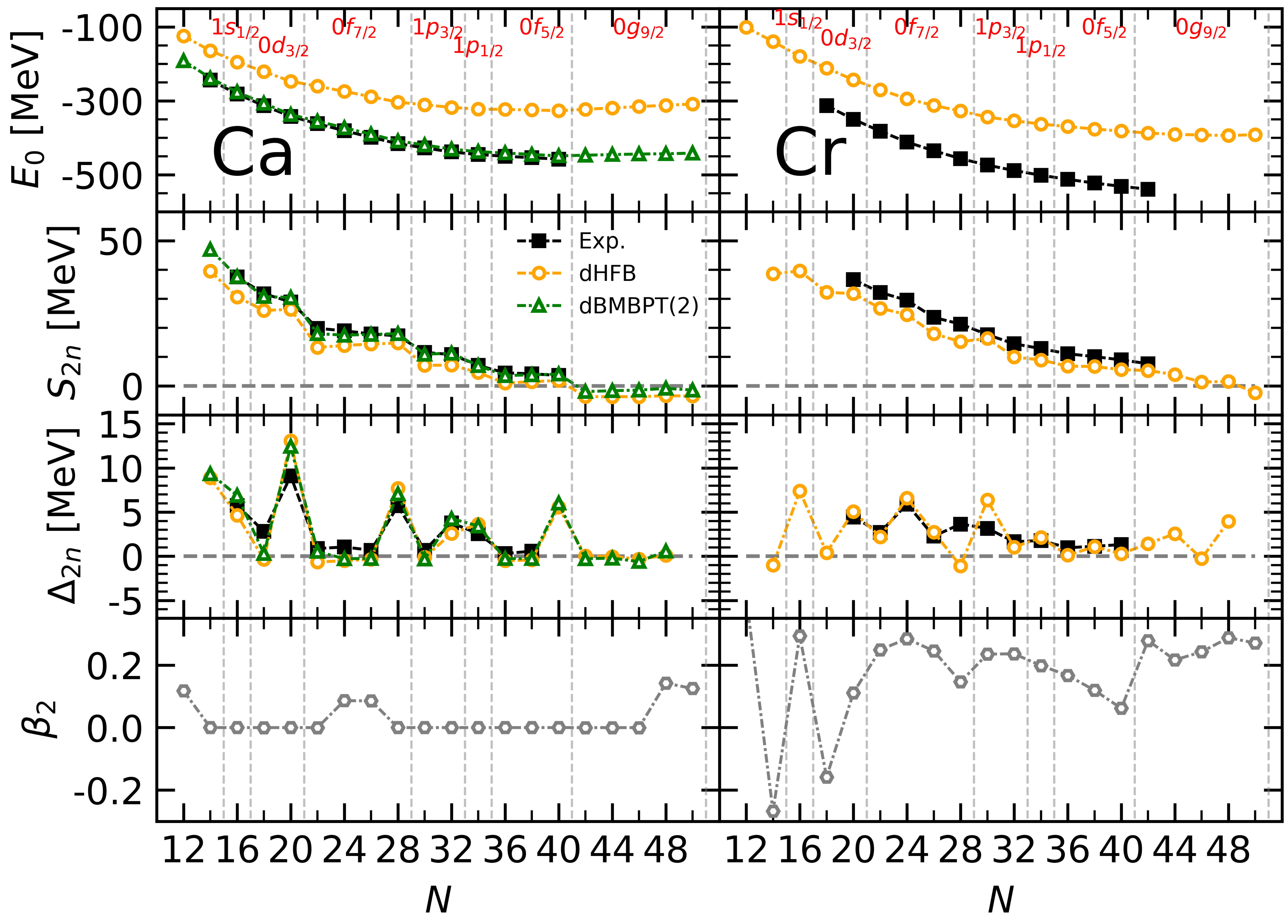
SU(2)-breaking approach



Doubly open-shell

[Scalesi *et al.* 2024]

SU(2)-breaking approach



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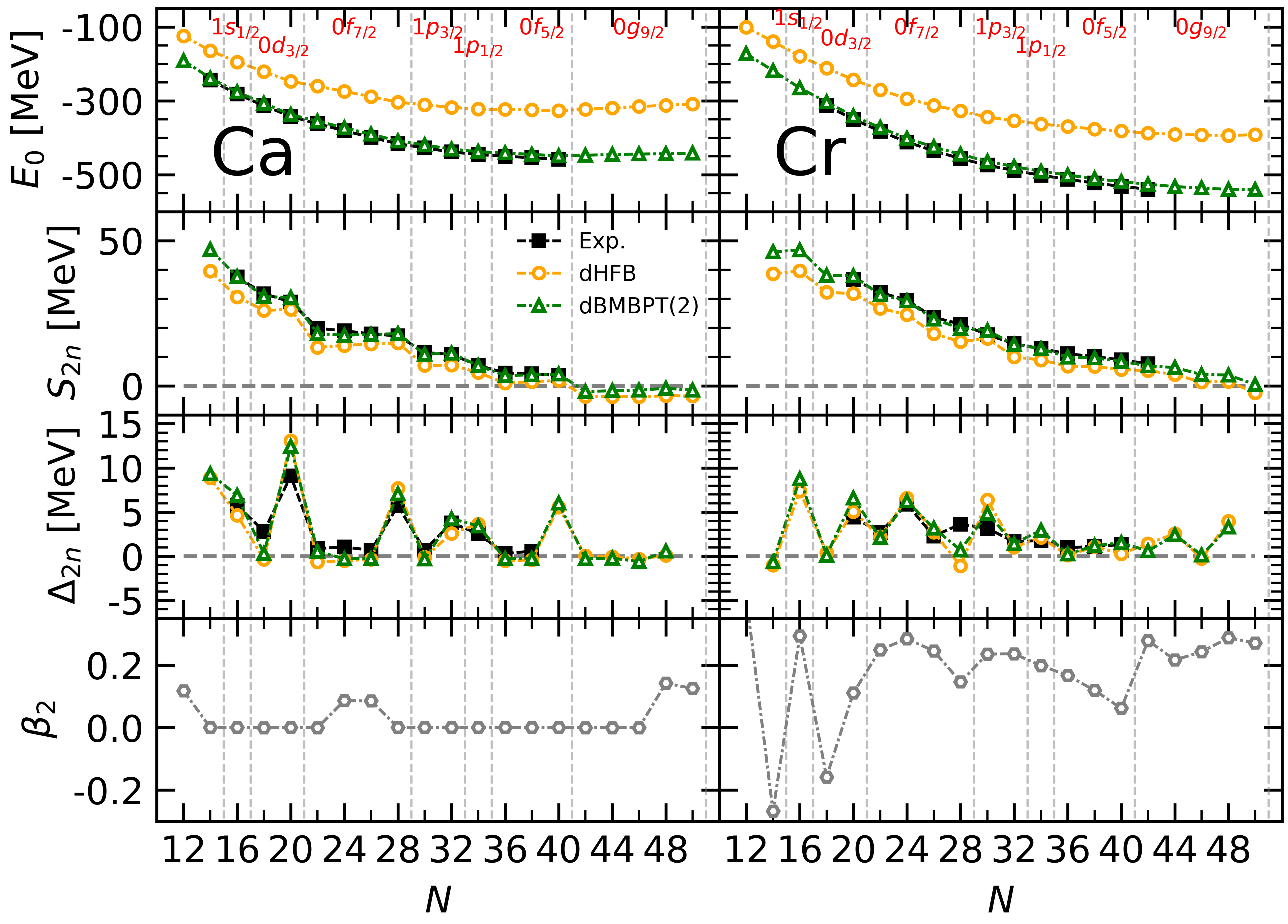
Doubly open-shell

Deformed mean field

- Underbinding
- Improved curvature

SU(2)-breaking approach



Doubly open-shell

Deformed mean field

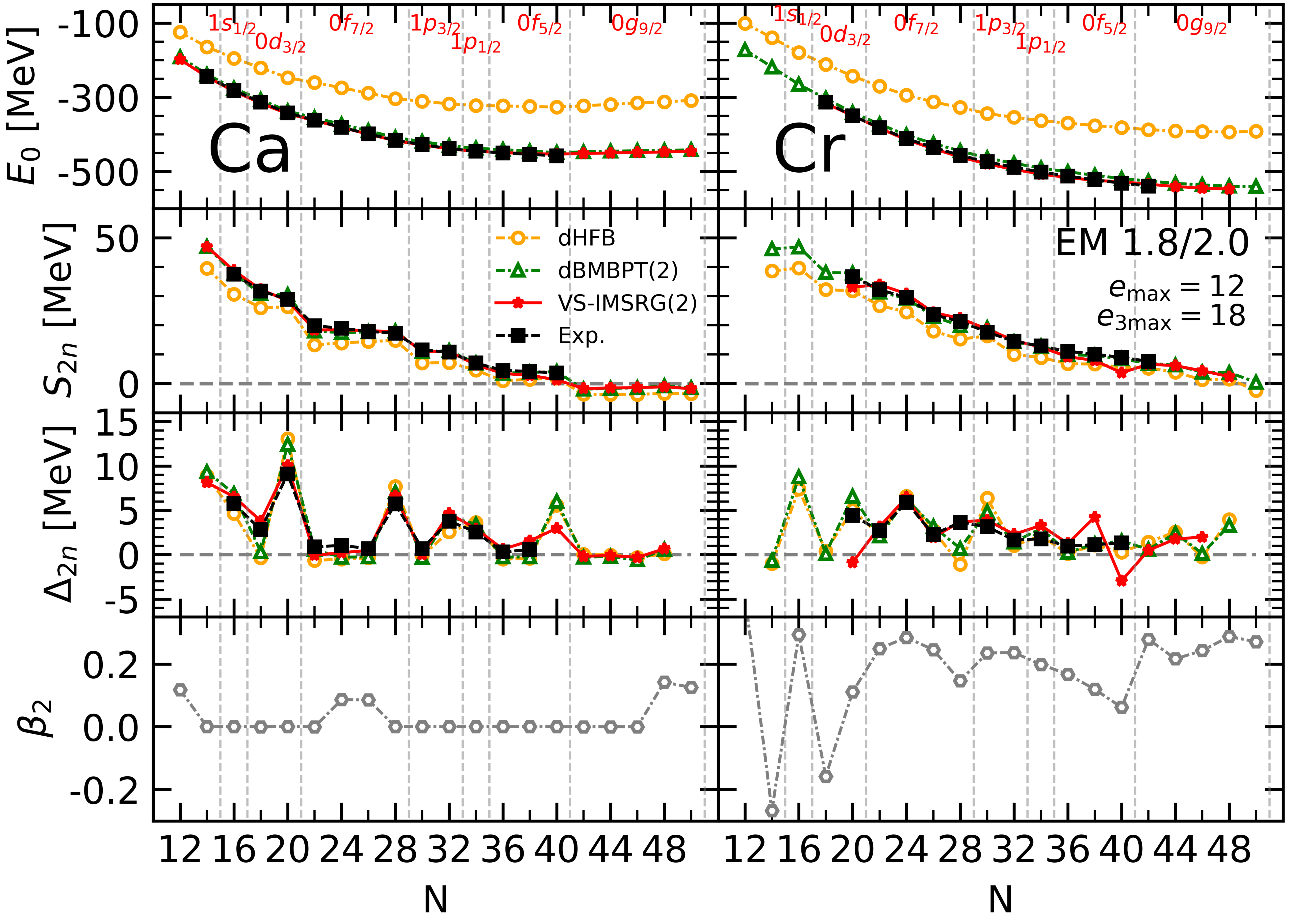
- Underbinding
- Improved curvature

Low-order dynamical correlations

- Correct binding
- Correct curvature
- Improved gaps

[Scalesi *et al*. 2024]

SU(2)-breaking approach



[Scalesi *et al*. 2024]

Doubly open-shell

Deformed mean field

- Underbinding
- Improved curvature

Low-order dynamical correlations

- Correct binding
- Correct curvature
- Improved gaps

Non-polynomial (diagonalisation)

- Correct E_0, S_{2n} and gaps

→ **Low-order sufficient**

→ **Deformation necessary**

Superfluid self-consistent Green's functions

Gorkov self-consistent Green's functions

[Gorkov 1958]

Normal & anomalous propagators

$$\mathrm{i}\, g^{11}_{\alpha\beta}(t-t') \equiv \langle\Psi_0|\, T[a_\alpha(t) a^\dagger_\beta(t')]\, |\Psi_0\rangle$$
$$\mathrm{i}\, g^{12}_{\alpha\beta}(t-t') \equiv \langle\Psi_0|\, T[a_\alpha(t) \bar{a}_\beta(t')]\, |\Psi_0\rangle$$
$$\mathrm{i}\, g^{21}_{\alpha\beta}(t-t') \equiv \langle\Psi_0|\, T[\bar{a}^\dagger_\alpha(t) a^\dagger_\beta(t')]\, |\Psi_0\rangle$$
$$\mathrm{i}\, g^{22}_{\alpha\beta}(t-t') \equiv \langle\Psi_0|\, T[\bar{a}^\dagger_\alpha(t) \bar{a}_\beta(t')]\, |\Psi_0\rangle$$

Nambu notation

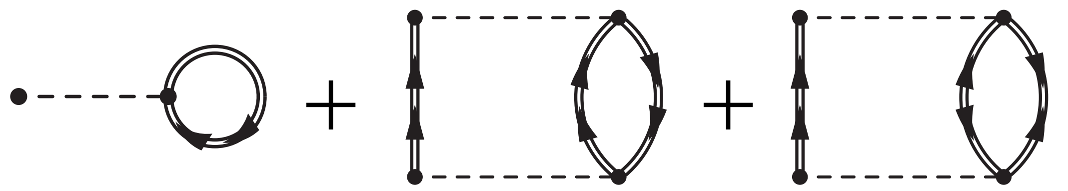
$$\mathrm{i}\,\mathbf{g}_{\alpha\beta}(t-t') \equiv \langle\Psi_0| T\left\{\mathbf{A}_\alpha(t)\mathbf{A}^\dagger_\beta(t')\right\}|\Psi_0\rangle = \mathrm{i}\begin{pmatrix} g^{11}_{\alpha\beta}(t-t') & g^{12}_{\alpha\beta}(t-t') \\ g^{21}_{\alpha\beta}(t-t') & g^{22}_{\alpha\beta}(t-t') \end{pmatrix}$$

Generalised spectral representation

$$\mathbf{g}_{\alpha\beta}(\omega) = \sum_k \left\{ \frac{\mathbf{X}^k_\alpha\, \mathbf{X}^{k\dagger}_\beta}{\omega - \omega_k + \mathrm{i}\eta} + \frac{\mathbf{Y}^k_\alpha\, \mathbf{Y}^{k\dagger}_\beta}{\omega + \omega_k - \mathrm{i}\eta} \right\}$$

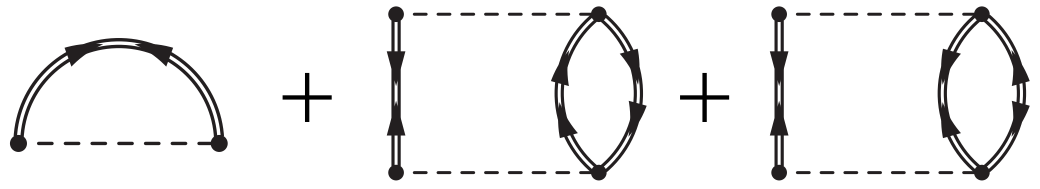
Self-energy expansion

$\Sigma^{\star\,11}_{\alpha\beta}(\omega) =$



$+ \ldots$

$\Sigma^{\star\,21}_{\alpha\beta}(\omega) =$



$+ \ldots$

$$\boldsymbol{\Sigma}^\star_{\alpha\beta}(\omega) \equiv \begin{pmatrix} \Sigma^{\star\,11}_{\alpha\beta}(\omega) & \Sigma^{\star\,12}_{\alpha\beta}(\omega) \\ \Sigma^{\star\,21}_{\alpha\beta}(\omega) & \Sigma^{\star\,22}_{\alpha\beta}(\omega) \end{pmatrix}$$

Generalised Dyson equation

$$\mathbf{g}_{\alpha\beta}(\omega) = \mathbf{g}_{0\,\alpha\beta}(\omega) + \sum_{\gamma\,\delta} \mathbf{g}_{0\,\alpha\gamma}(\omega)\, \boldsymbol{\Sigma}^\star_{\gamma\delta}(\omega)\, \mathbf{g}_{\gamma\beta}(\omega)$$

Superfluid self-consistent Green's functions

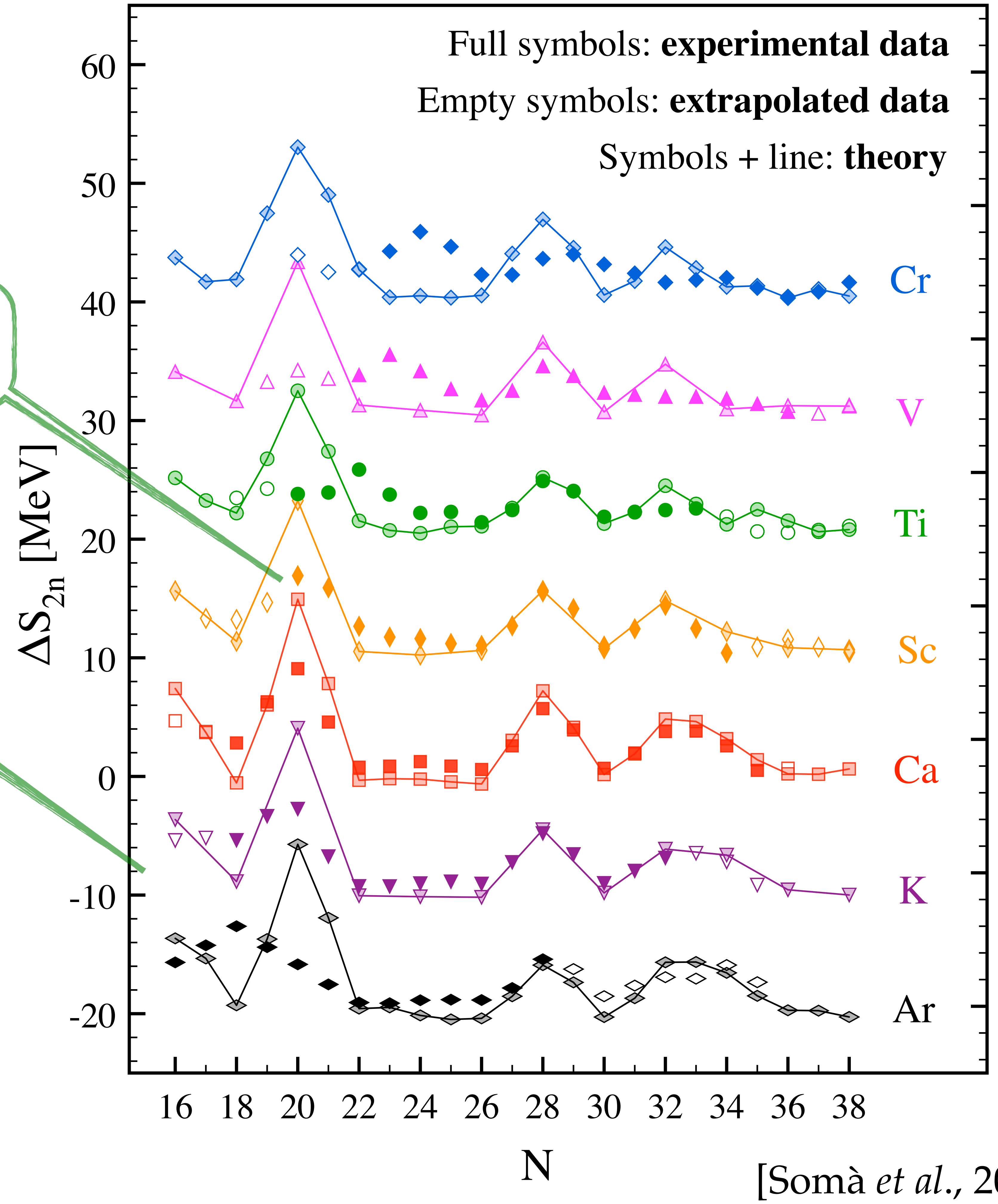
Gorkov self-consistent Green's functions

→ Algebraic diagrammatic construction [Schirmer 1982]

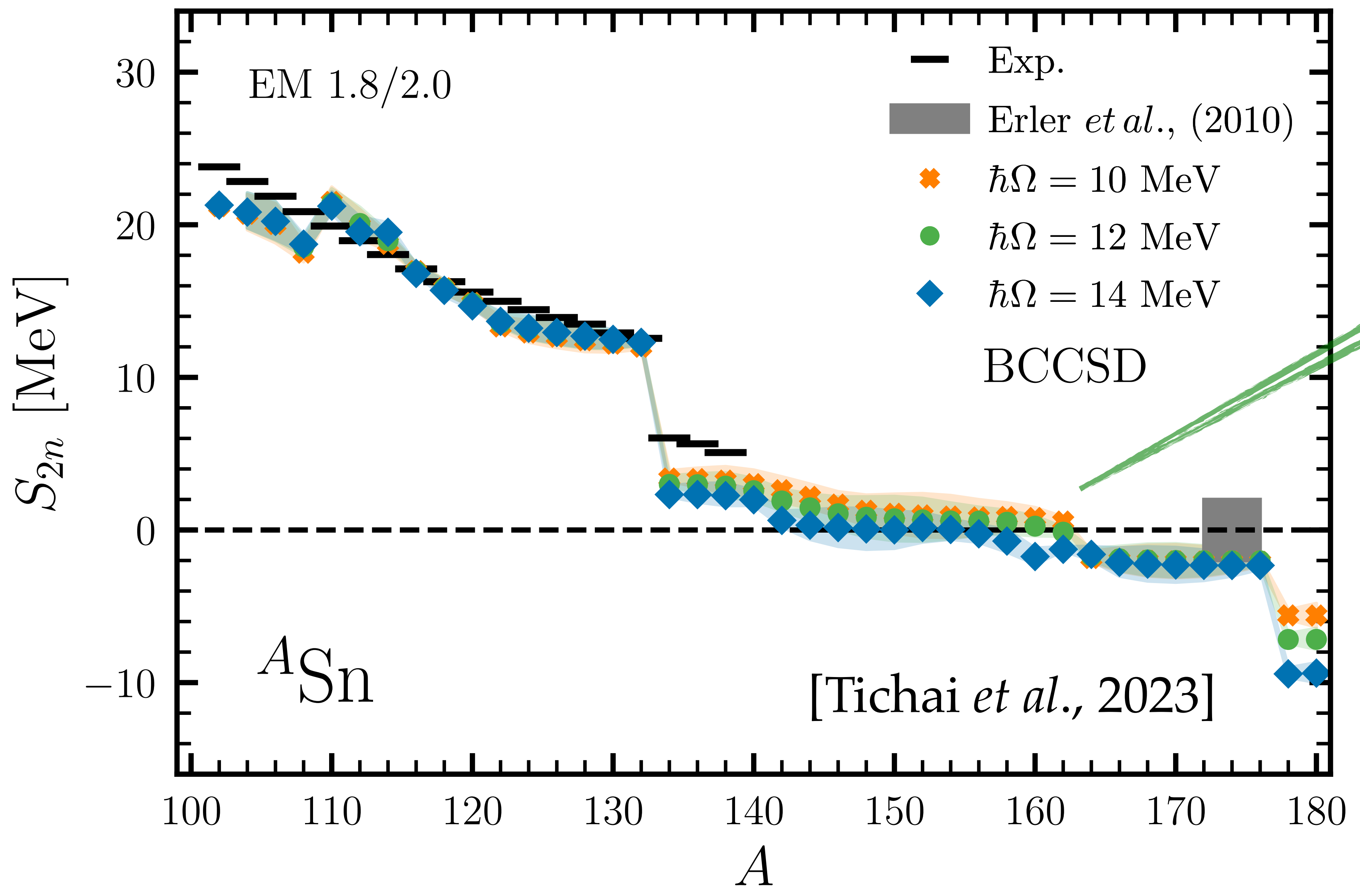
- ○ ADC(2) implemented [Somà *et al.* 2011]
- ○ ADC(3) derived [Barbieri *et al.* 2023]

Magic numbers emerge "ab initio"

○ Accuracy degrades away from semi-magic Ca
○ Correlation with nuclear deformation
→ Calls for explicit inclusion of deformation



[Somà *et al.*, 2021]



Drip line predicted

Bogolyubov coupled-cluster

- ○ BCCSD implemented [Tichai *et al.*, 2023]
- ○ BCCSD(T) in progress [Vernik *et al.*, in preparation]

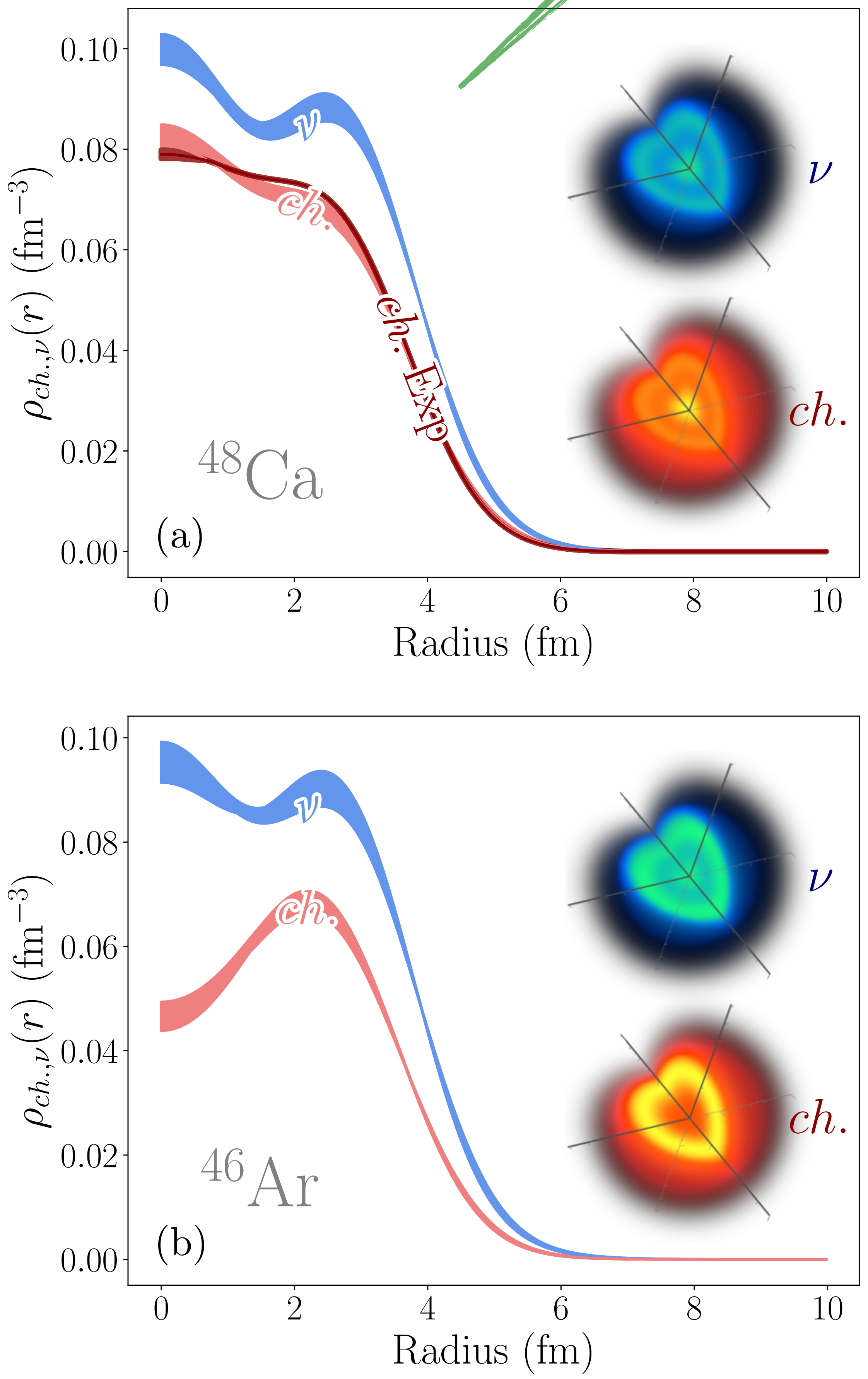
Superfluid self-consistent Green's functions

SCGF provide easy access to several **other observables**

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

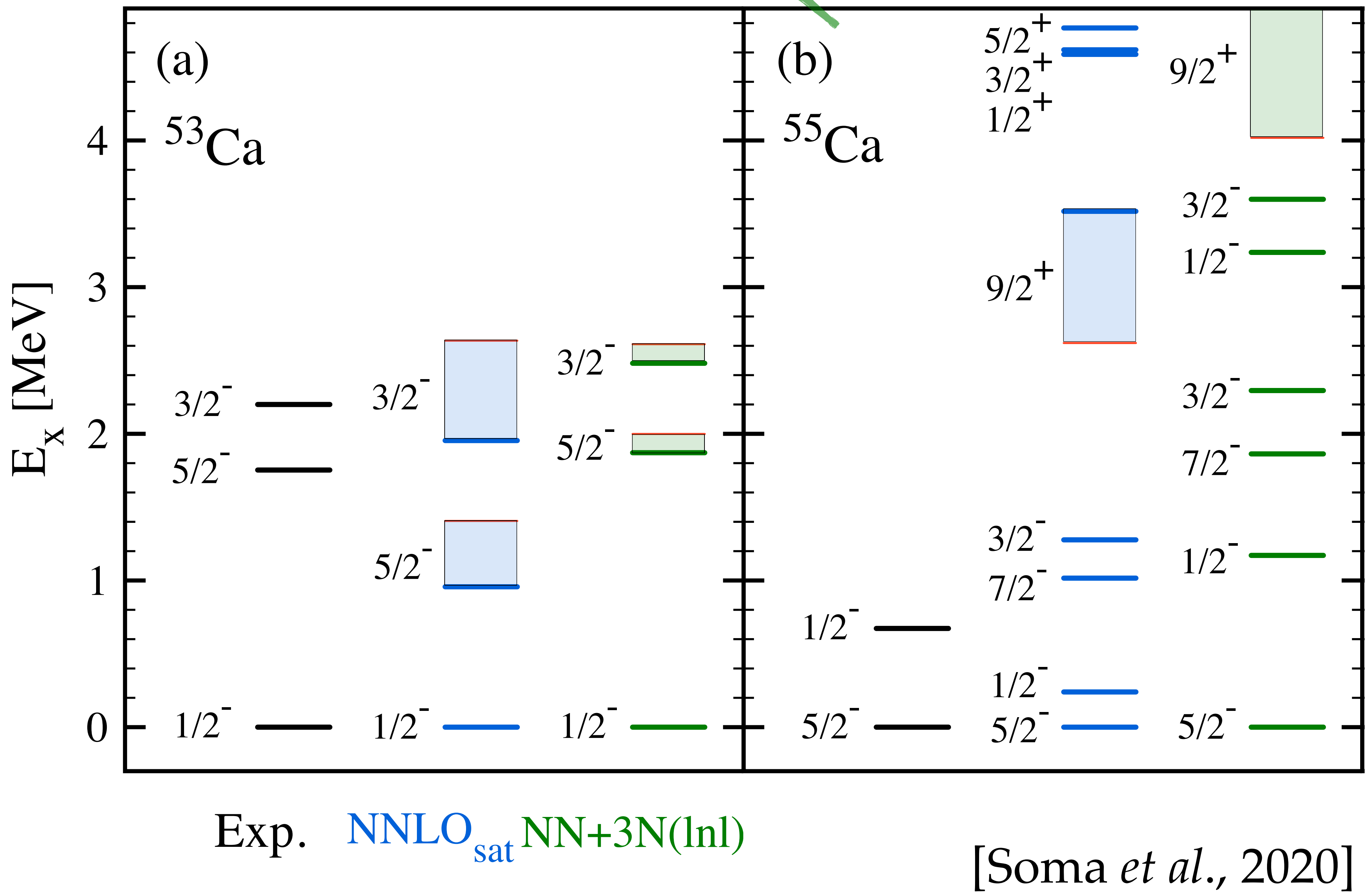
Lehmann representation

Density distributions



[Brugnara *et al.*, submitted]

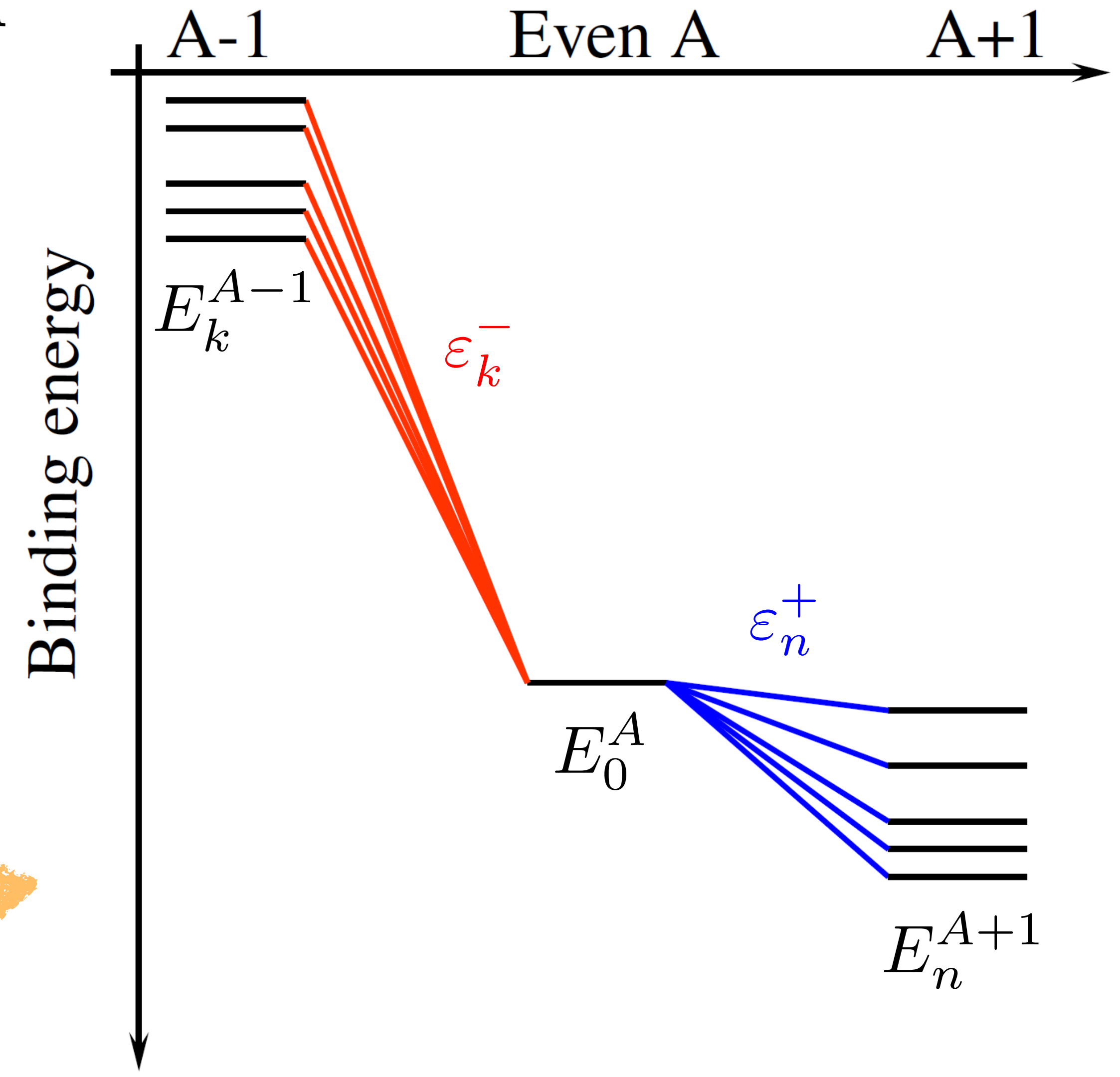
Spectroscopy of A±1



[Soma *et al.*, 2020]

Separation energies

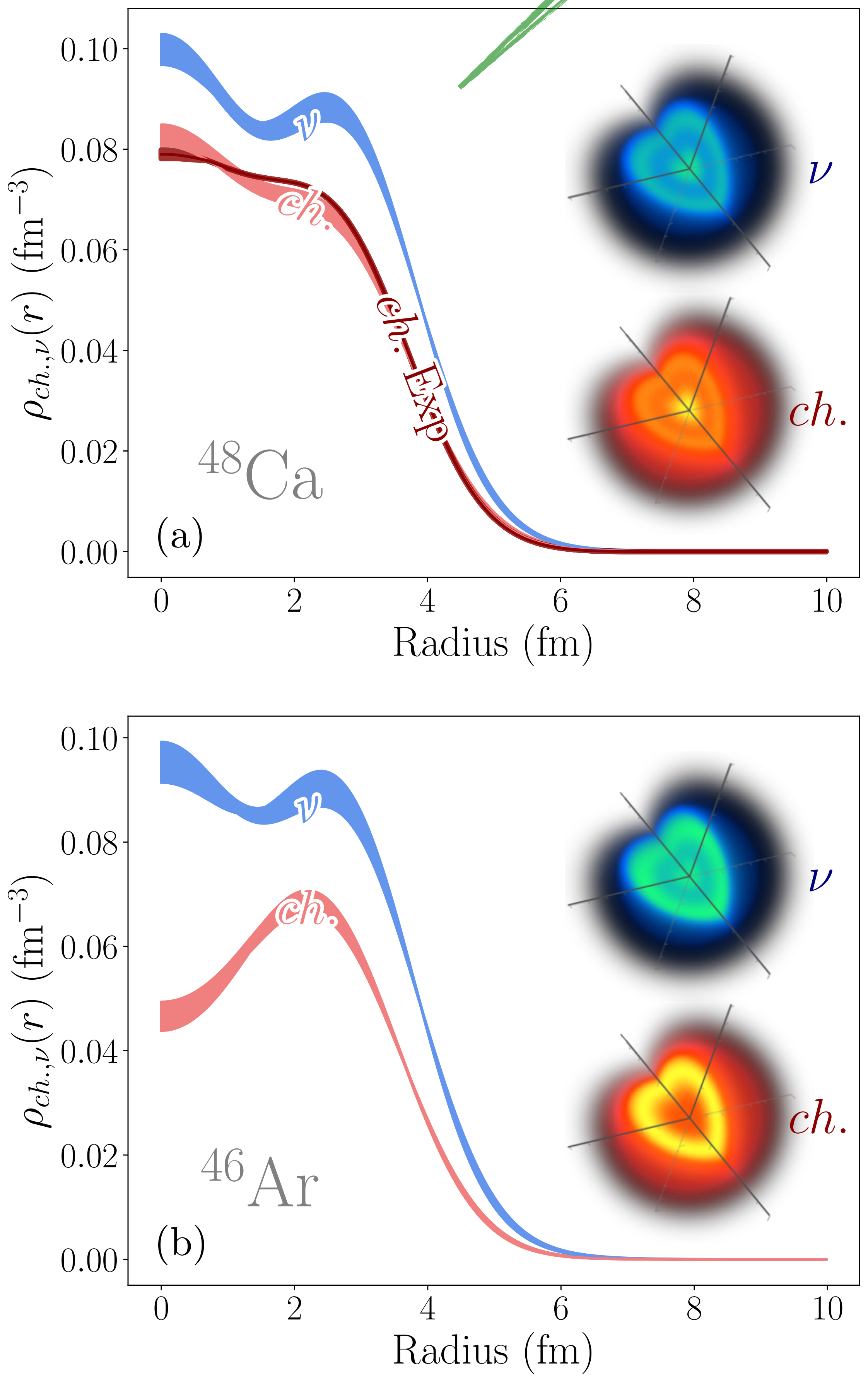
$$\varepsilon^+_n = E^{A+1}_n - E^A_0$$
$$\varepsilon^-_k = E^A_0 - E^{A-1}_k$$



Superfluid self-consistent Green's functions

SCGF provide easy access to several **other observables**

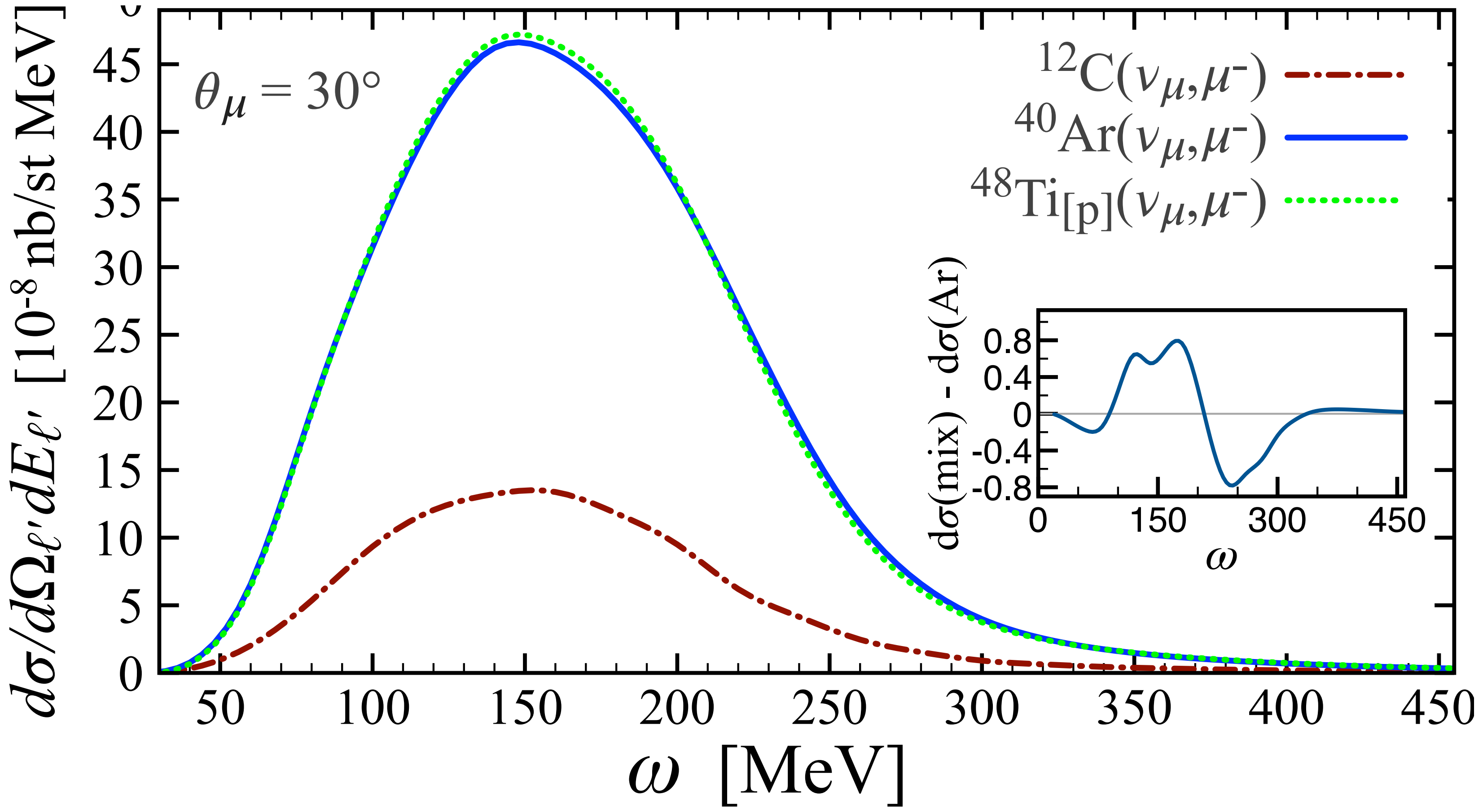
Density distributions



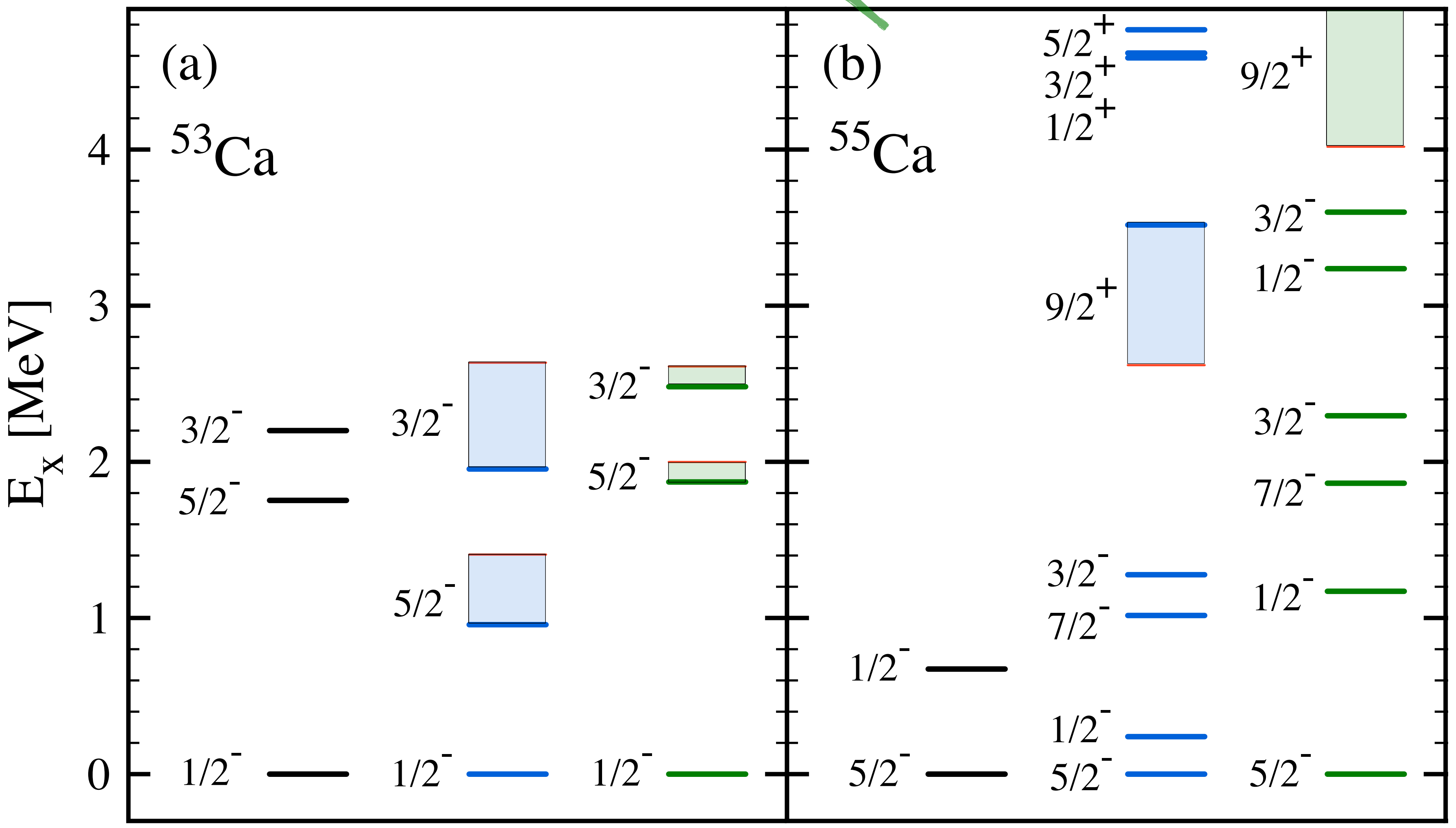
[Brugnara *et al.*, submitted]

ν-nucleus scattering

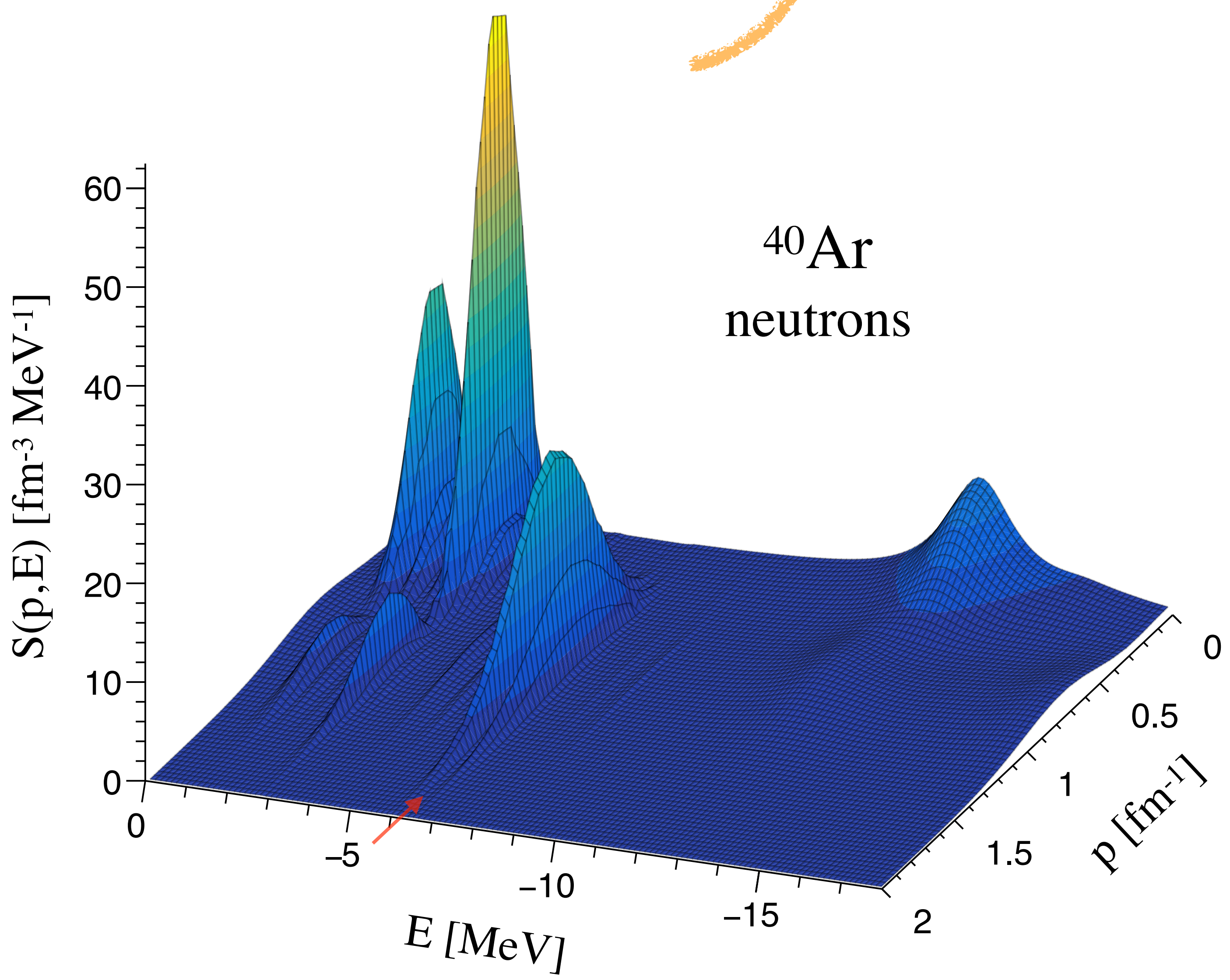
[Barbieri *et al.*, 2019]



Spectroscopy of A±1



[Soma *et al.*, 2020]

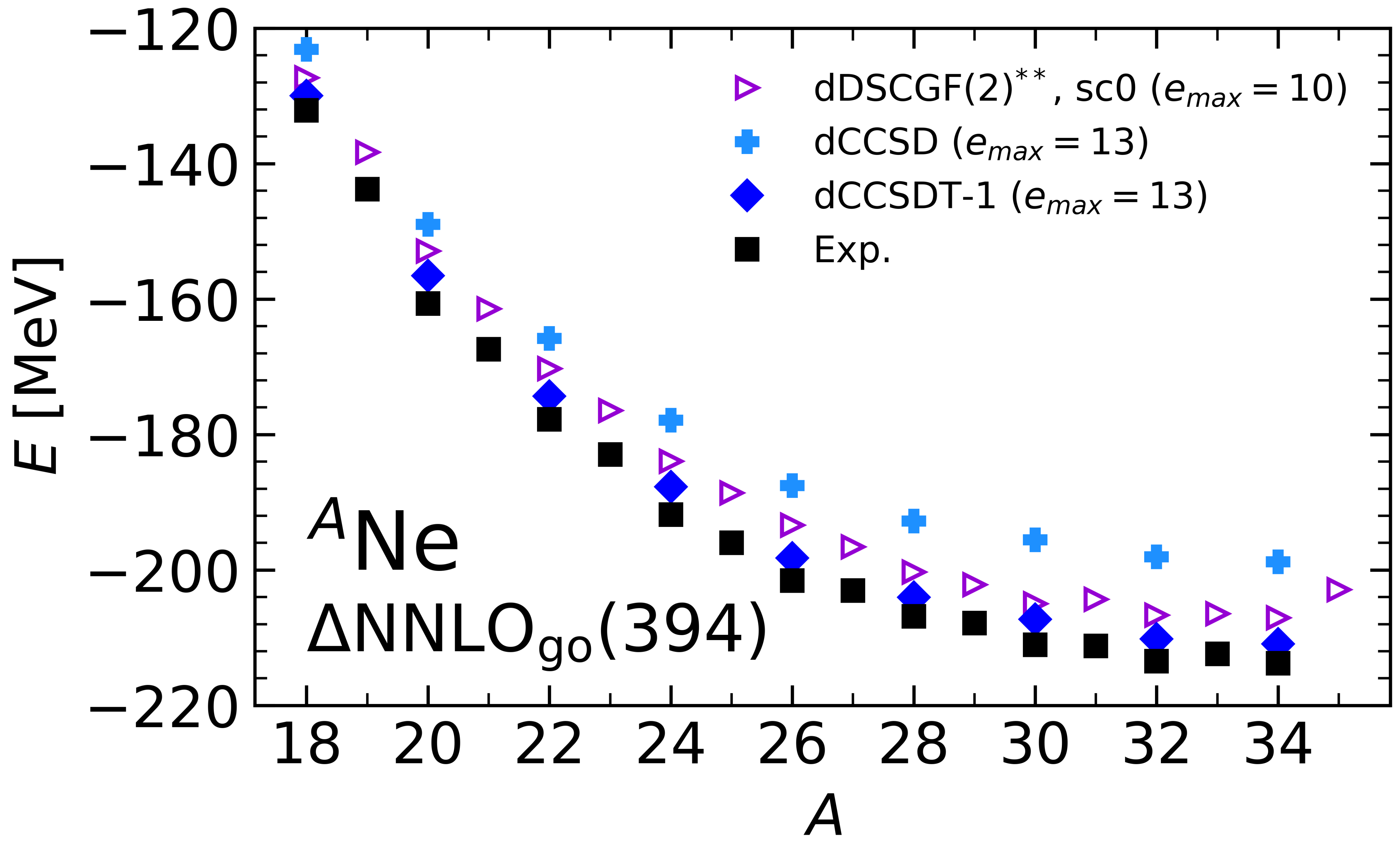


Deformed self-consistent Green's functions

Extension of SCGF to **SU(2)-breaking** framework

- Deformed HF reference state
- ADC(2) truncation

[Scalesi *et al.* in preparation]



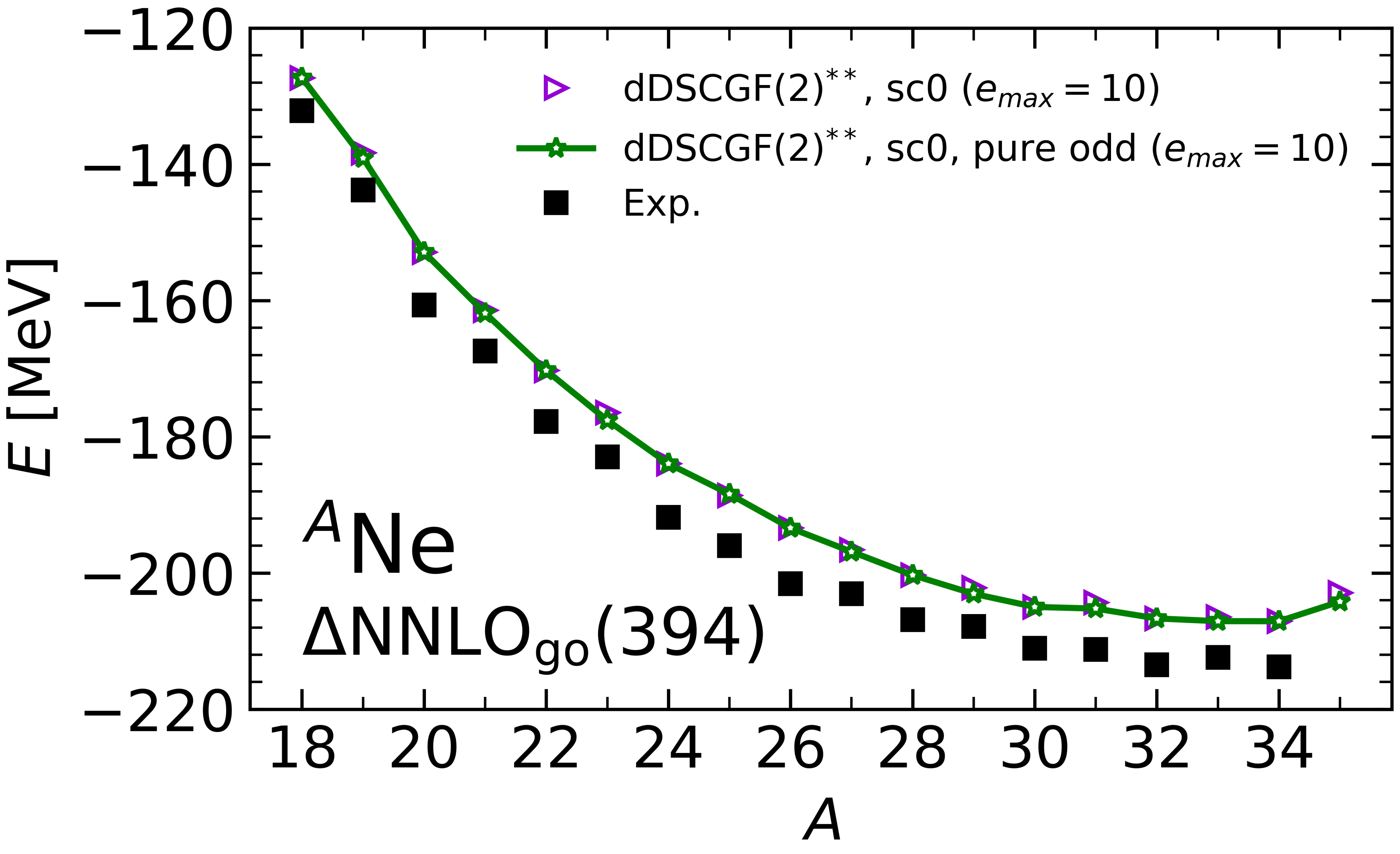
- Trend consistent with CC results

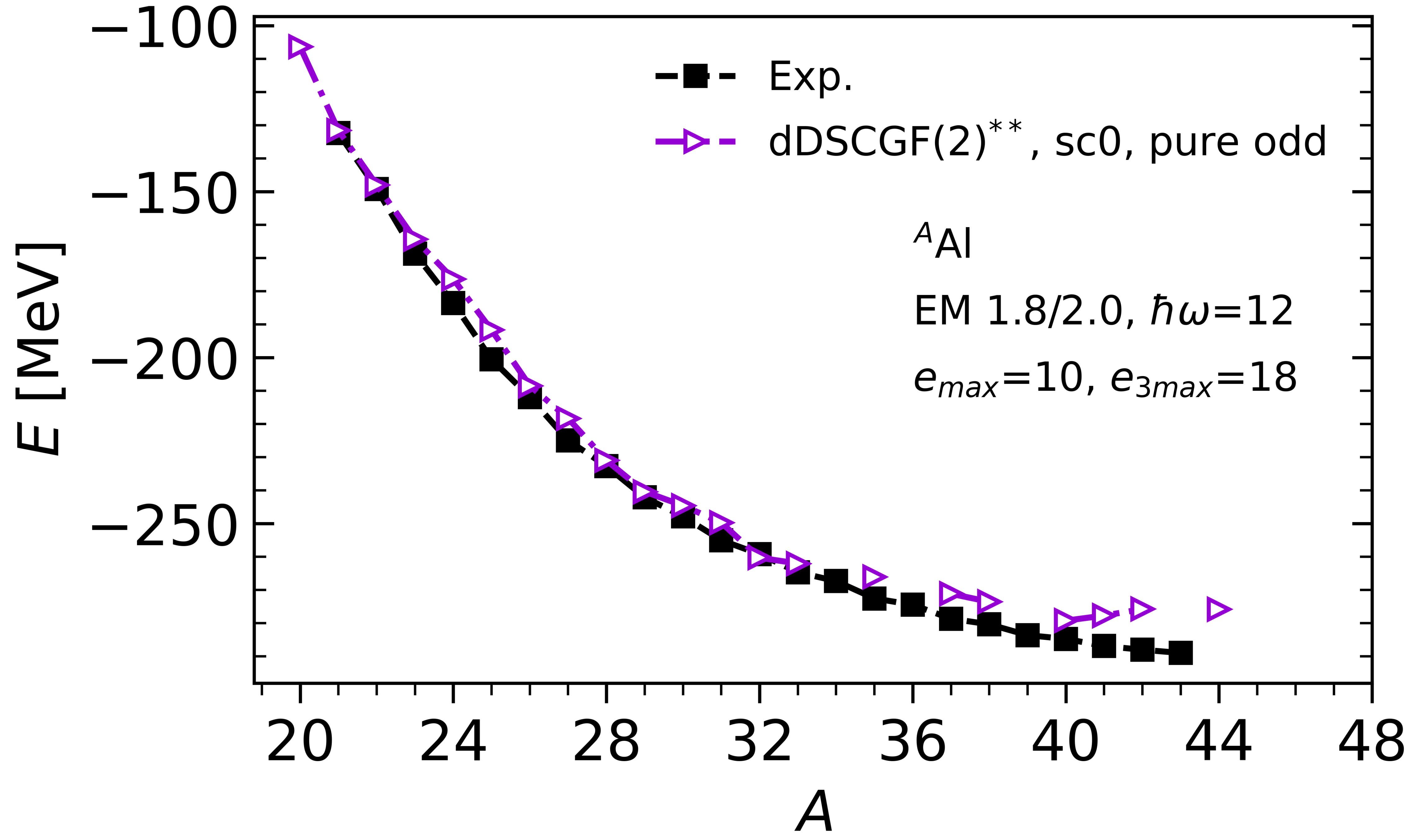
Deformed self-consistent Green's functions

Extension of SCGF to **SU(2)-breaking** framework

- Deformed HF reference state
- ADC(2) truncation
- Opens the possibility of targeting **odd systems**

[Scalesi *et al*. in preparation]





- Trend consistent with CC results
- Successful benchmark in odd-even isotopes
- Preliminary test in odd-Z chain promising

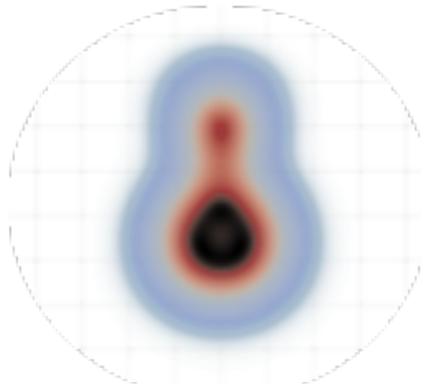
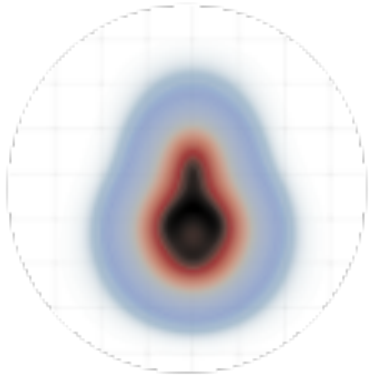
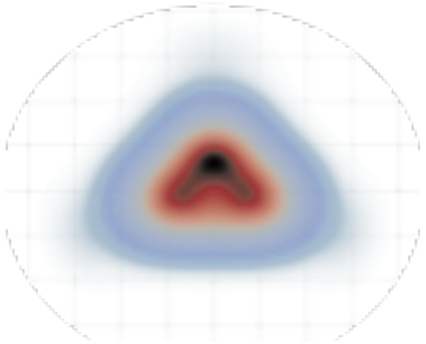
  → **First odd-odd calculations** with expansion methods!
- **Absence of symmetry restoration** problematic

PGCM

Alternative strategy: break symmetries, project, then expand

- Construction of the unperturbed state via **projected generator coordinate method** (PGCM)
- Low-dimensional linear combination of *non-orthogonal* projected Bogolyubov product states (← EDF)

Def. vacua

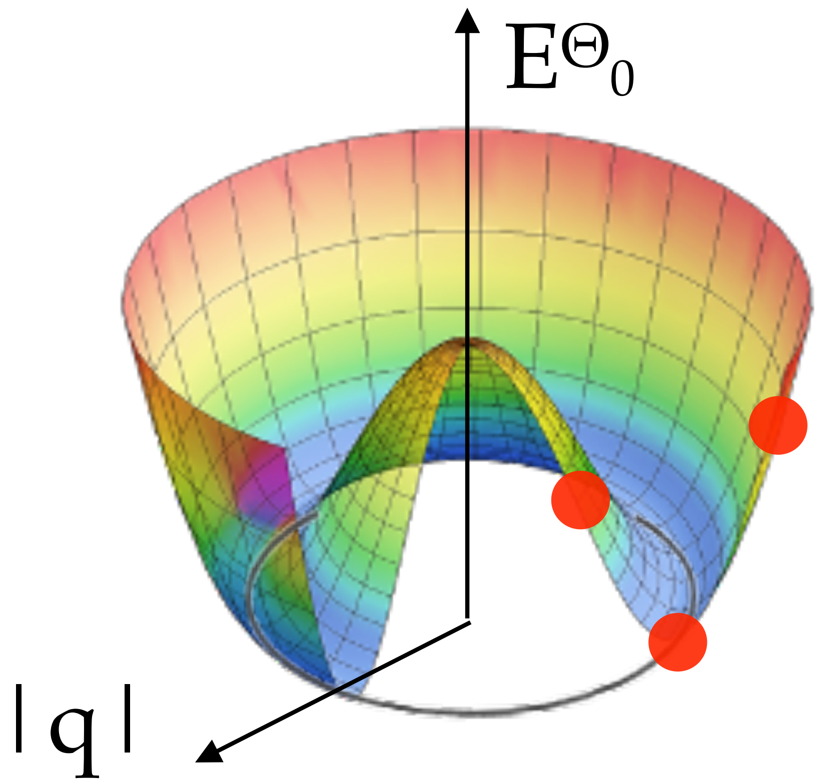




$|\Phi(q_1)\rangle$ $|\Phi(q_2)\rangle$ $|\Phi(q_3)\rangle$

Projection

$\tilde{\sigma} \equiv (J^{\Pi}, N, Z)$

$P^{\tilde{\sigma}}|\Phi(q_1)\rangle$ $P^{\tilde{\sigma}}|\Phi(q_2)\rangle$ $P^{\tilde{\sigma}}|\Phi(q_3)\rangle$ → *Rotational modes*



Shape mixing

$$|\Theta^{\tilde{\sigma}}_{\mu}\rangle = \sum_q f^{\tilde{\sigma}}_{\mu}(q)\, P^{\tilde{\sigma}}\, |\Phi(q)\rangle$$

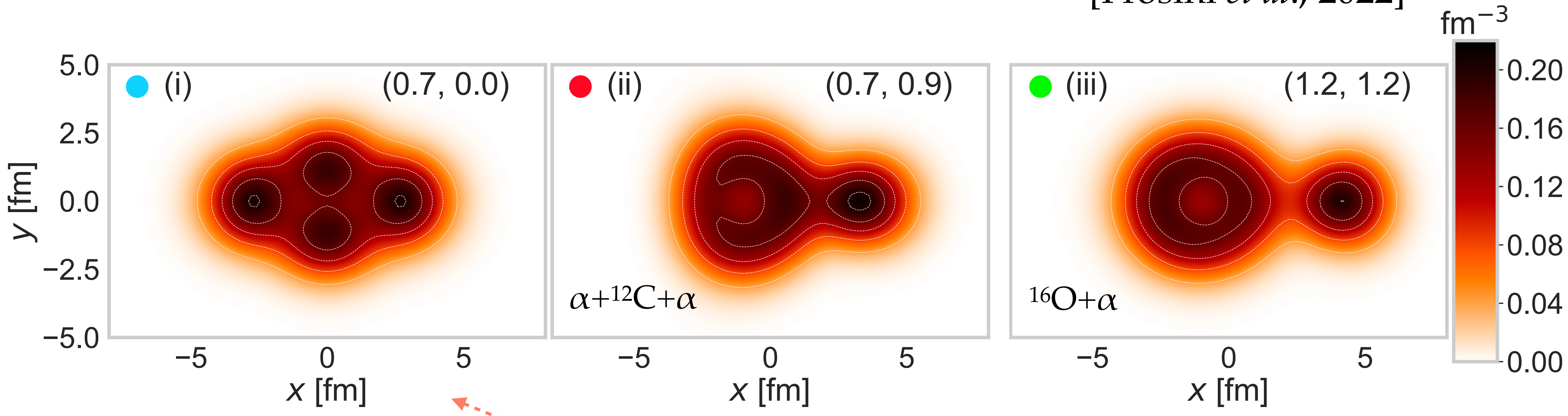
→ *Vibrational modes*

Variational principle → **Hill-Wheeler-Griffin equation**

$$\sum_q H^{\tilde{\sigma}}_{qp} f^{\tilde{\sigma}}_{\mu}(q) = \epsilon^{\tilde{\sigma}}_{\mu} \sum_q N^{\tilde{\sigma}}_{qp} f^{\tilde{\sigma}}_{\mu}(q)$$

PGCM

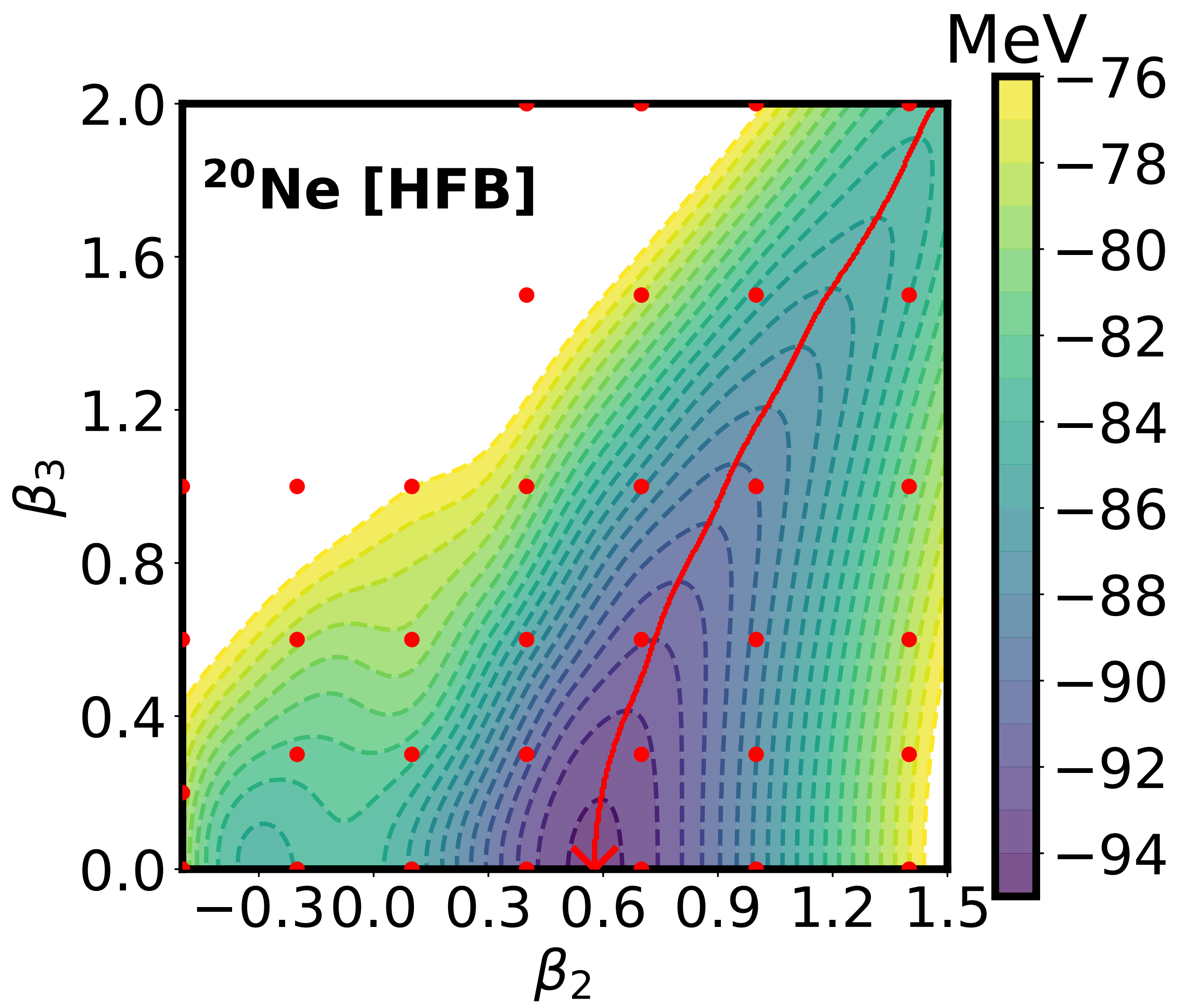
[Frosini *et al.*, 2022]



Example: doubly open-shell Neon-20

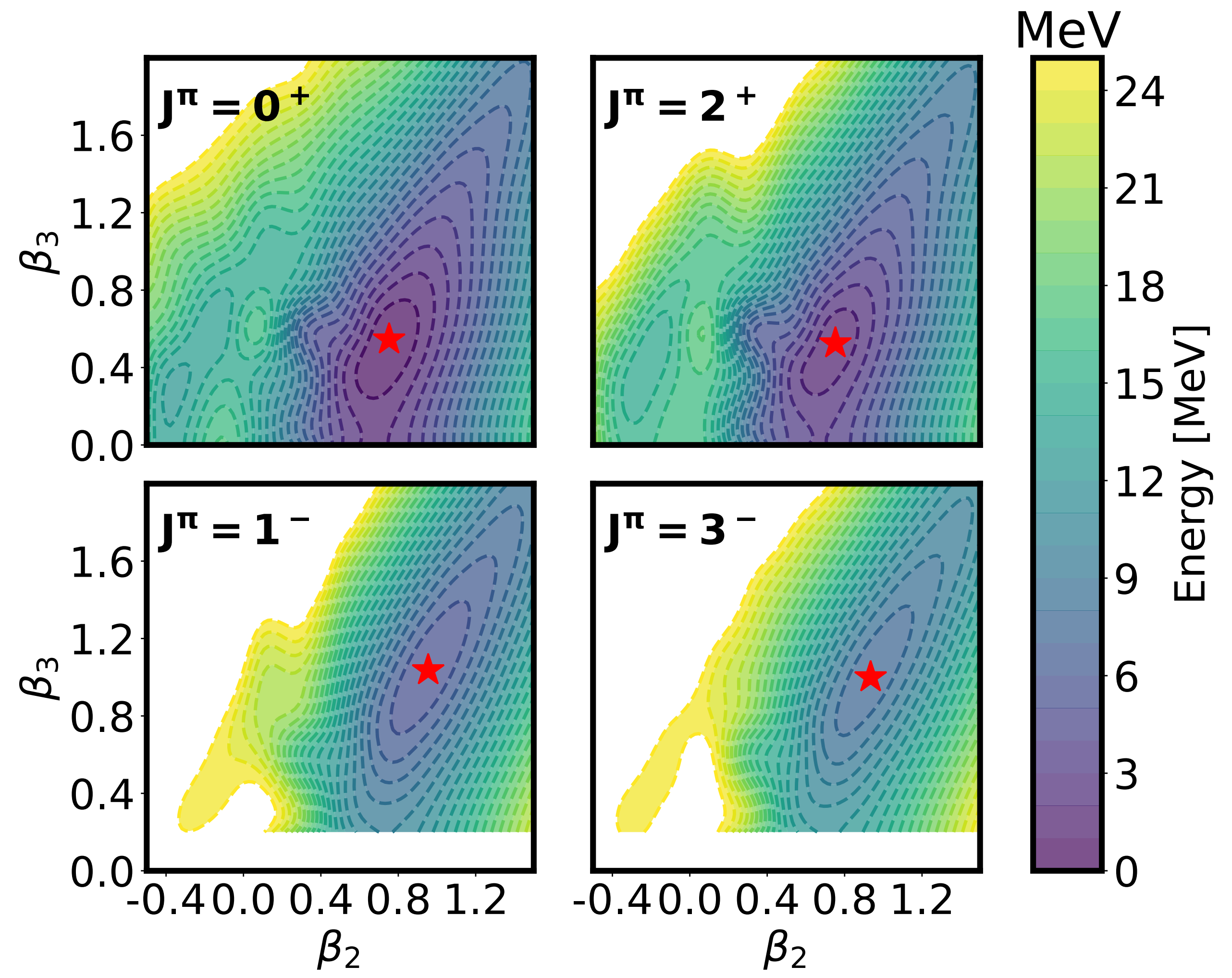
- ○ Static correlations play important role
- ○ Well-studied experimentally
- ○ GC: quadrupole (β_2) and octupole (β_3) deform.

1. Constrained HFB



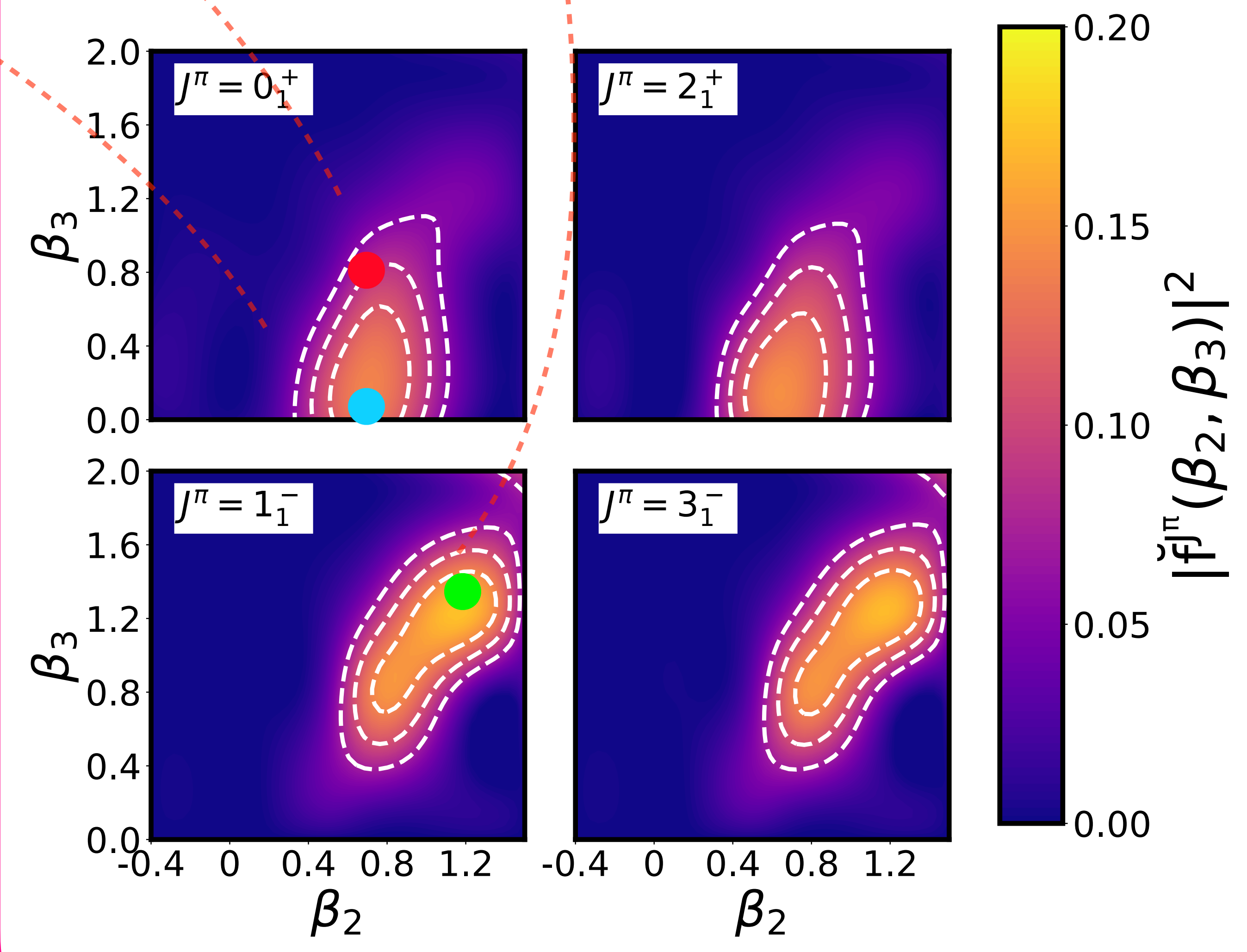
- ○ Maps total energy surface (TES)
- ○ Strongly deformed minimum

2. Projected HFB



- ○ Projections favour deformation
- ○ Provide input for PGCM

3. PGCM



- ○ Collective w.f. ≈ probability distr.
- ○ Significant shape fluctuations

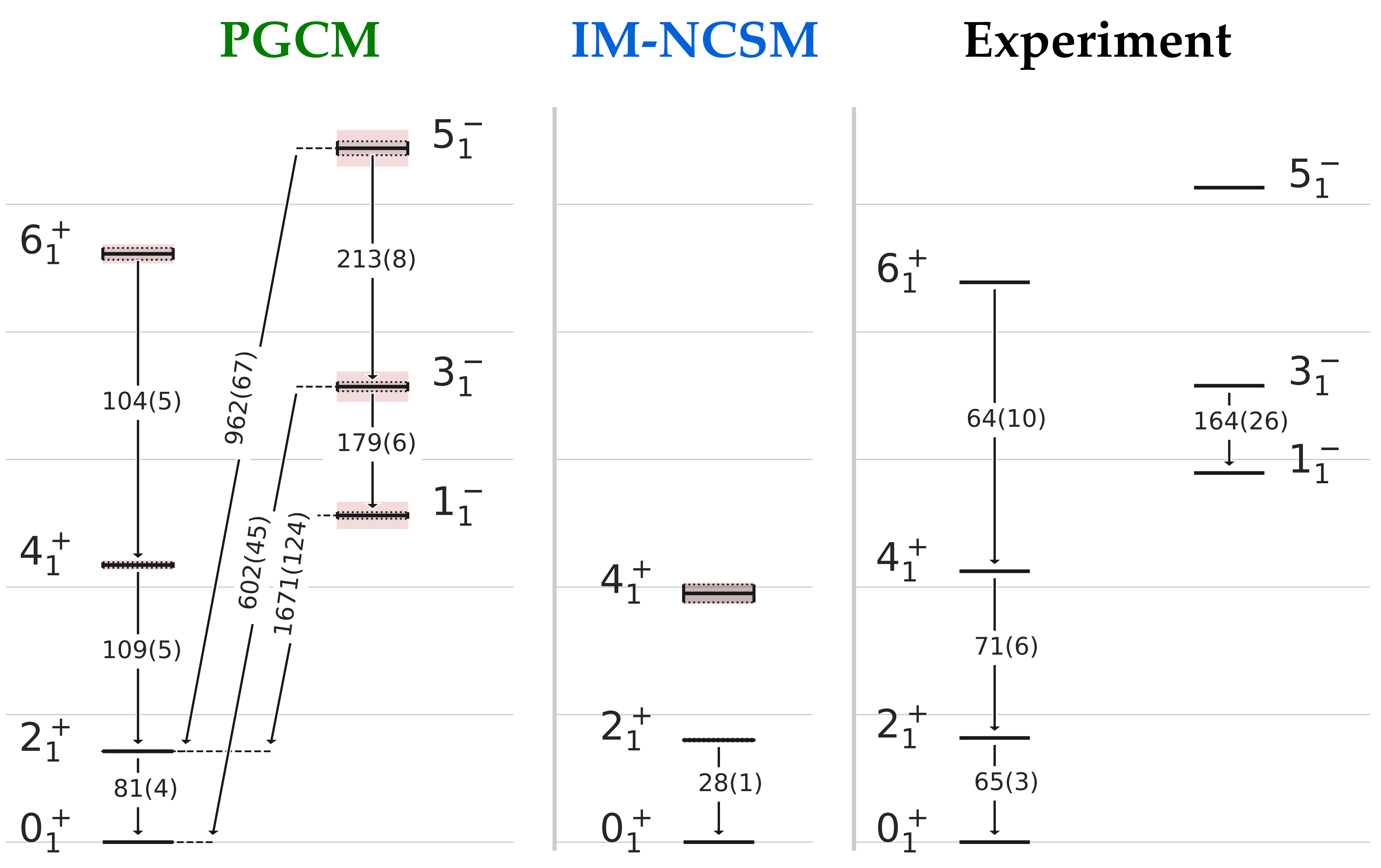
PGCM & PGCM-PT

PGCM excitation spectrum

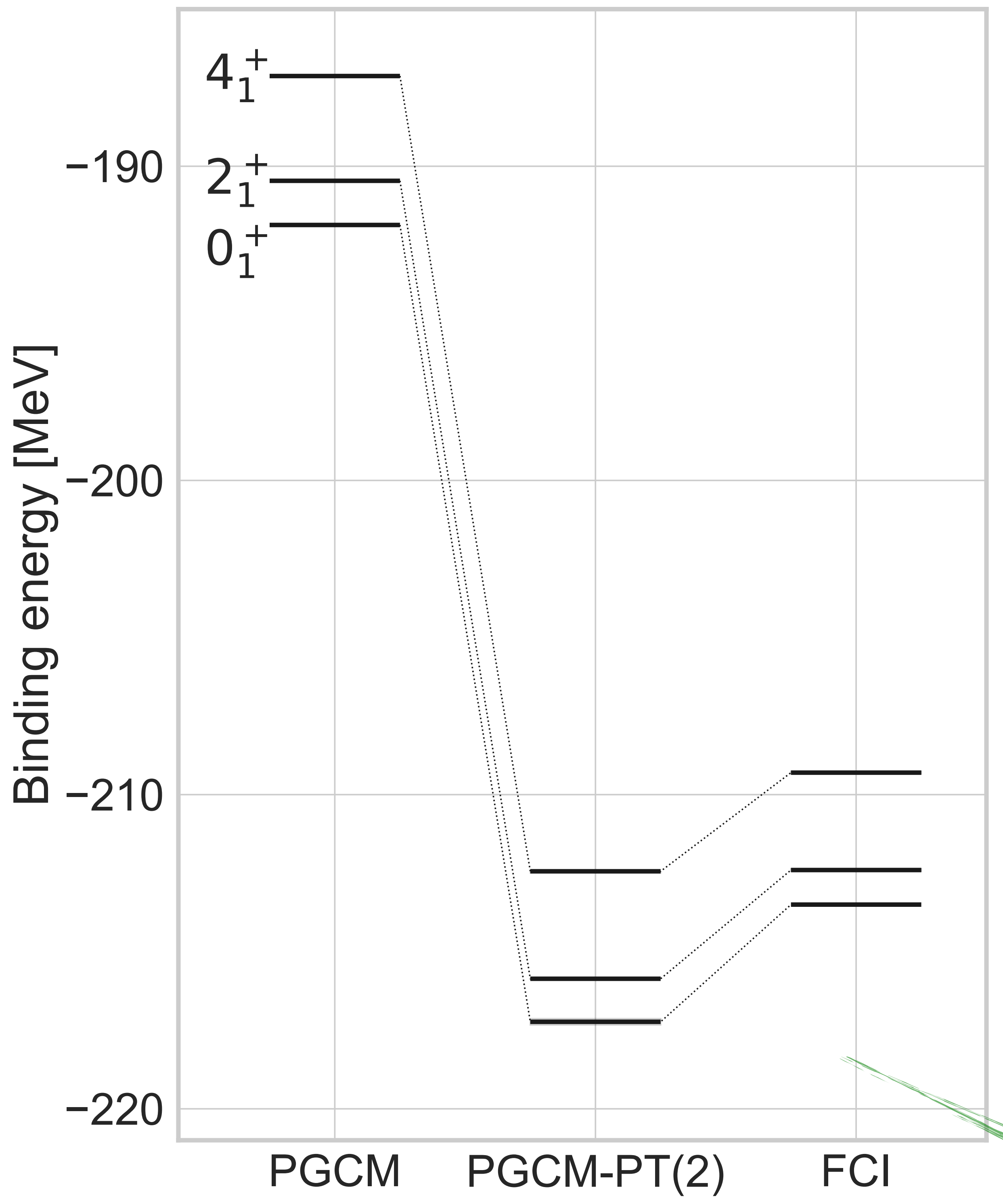
○ Good agreement with experiment and (quasi-)exact IM-NCSM

→ Essential **static correlations** captured by PGCM

[Frosini *et al.*, 2022]



Dynamical correlations?



Perturbative expansion on top of PGCM state (PGCM-PT)

○ Non-orthogonal PT: only one eigenstate of H_0 is known

○ No well-defined Hilbert-space partitioning

○ Rigorous PT formalised only recently [Burton & Thom 2020]

Dynamical correlations **cancel out** to a large extent in relative energies

Conclusions and perspectives

Symmetry breaking

- Deformation [SU(2) breaking] **mandatory** for describing (**doubly open-shell**) nuclei at **polynomial** cost
- Superfluidity [U(1)-breaking] sufficient if one targets singly open-shell systems

Symmetry restoration

- Formulated for MBPT and CC [Duguet 2015, Duguet & Signoracci 2017, Qiu *et al.*, 2017, …] & recently applied [Hagen *et al.*, 2022, …]
- To be formulated for SCGF

Numerical cost

- Symmetry breaking (and restoration) come with **extra cost**
  - → Larger number of basis states needed for deformed calculations (n~2000 compared to n~200 in spherical)
  - → PGCM: remains mean-field-like, n^4, but acquires large prefactor (~hundreds)
  - → PGCM-PT: second order already scales as n^8 (compared to n^5 for standard MBPT)
- Techniques needed to **reduce costs**
  - → Natural orbitals, importance truncation, tensor factorisation, ….

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○ Recent developments

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