

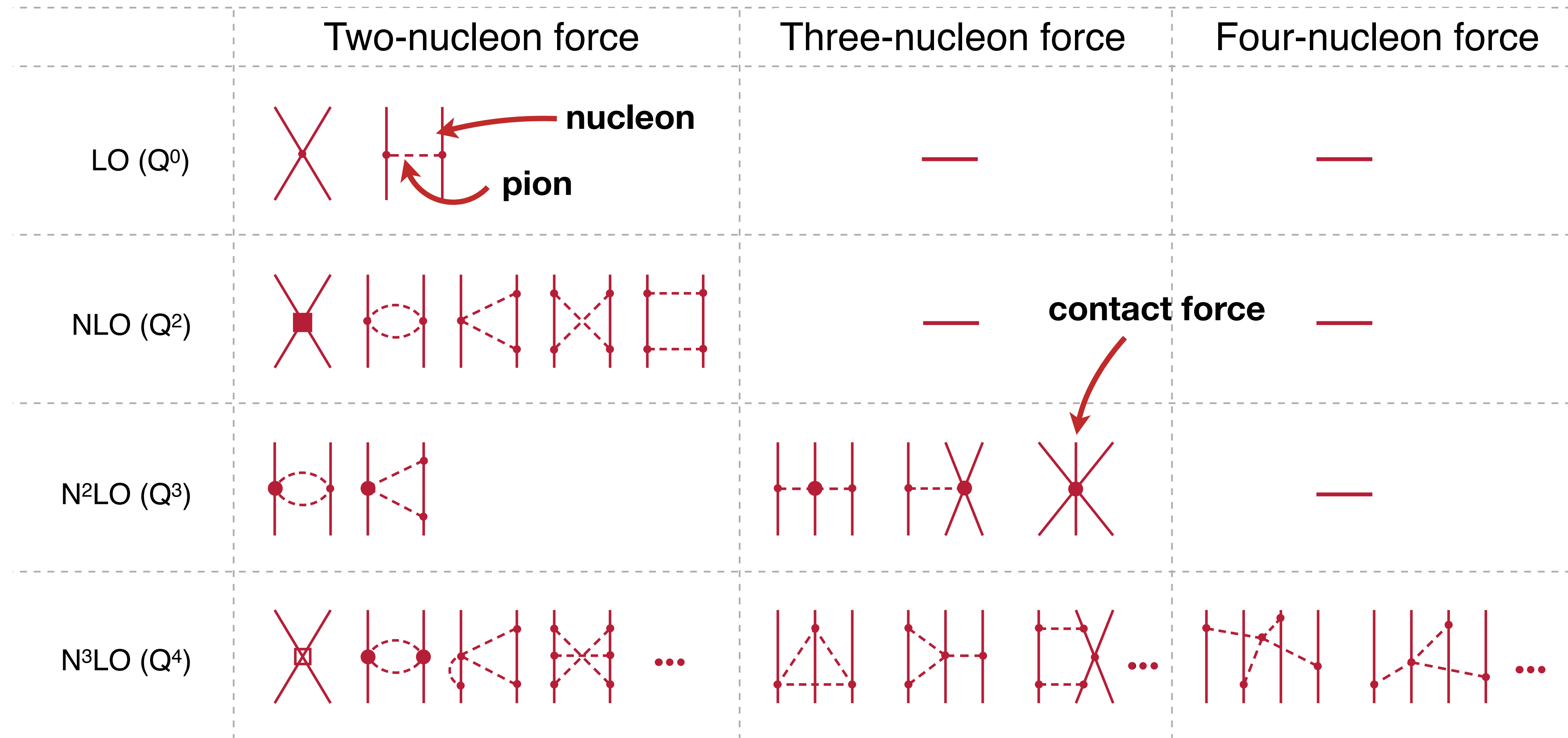
Pairing in Multi-Reference IMSRG Calculations

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Facility for Rare Isotope Beams
& Department of Physics and Astronomy
Michigan State University



Ingredients

Chiral Effective Field Theory

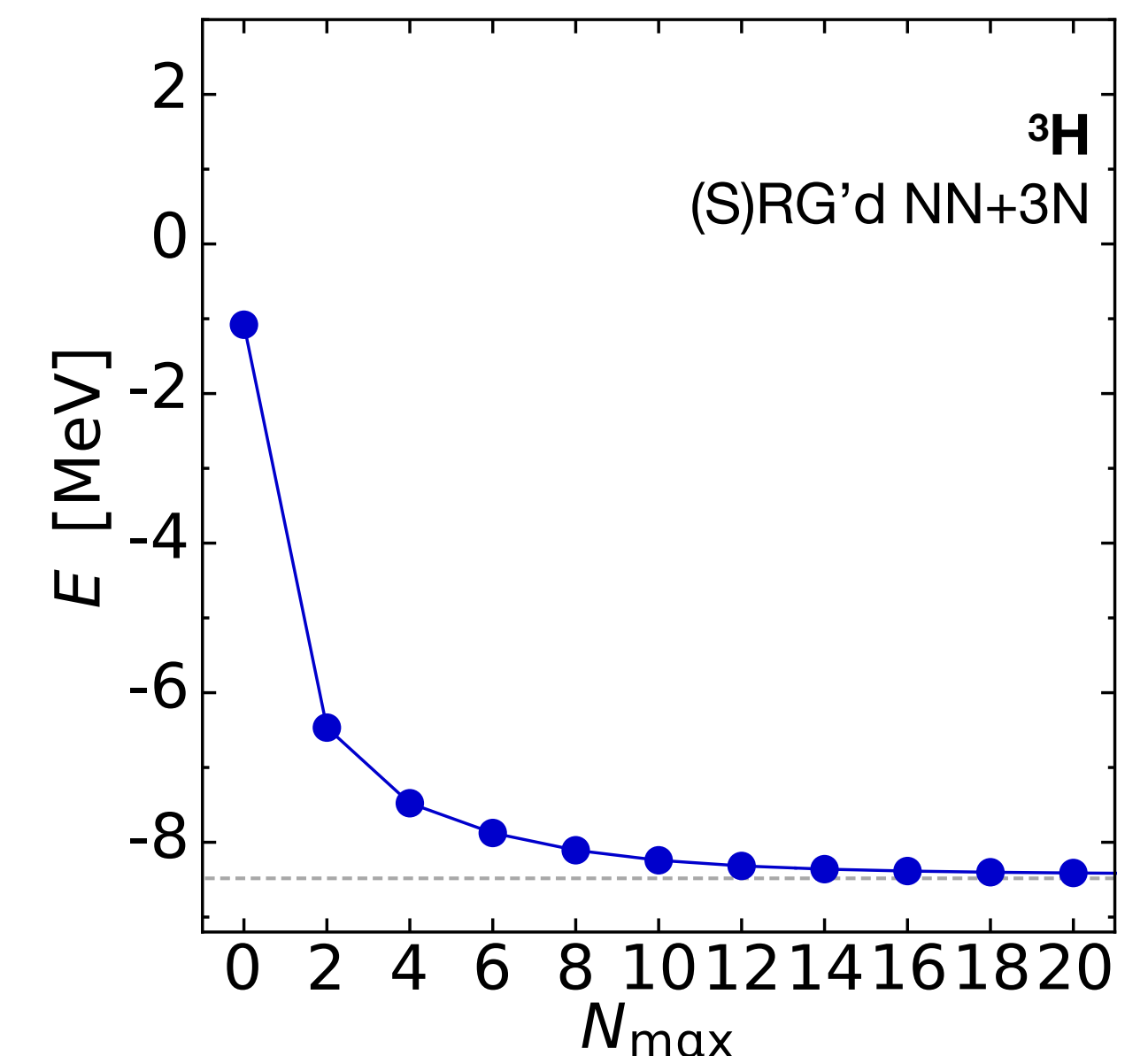
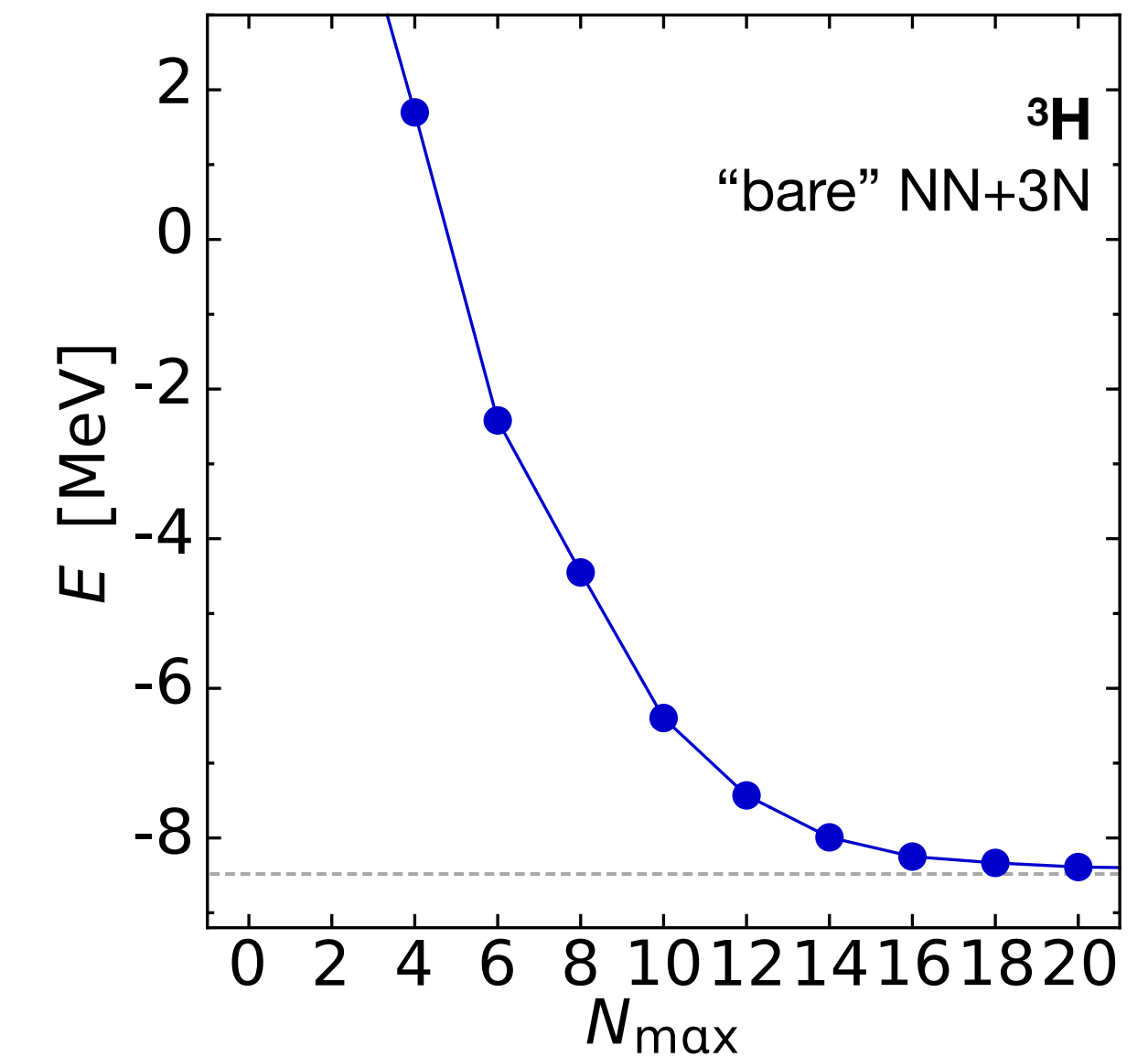


[figure by H. Krebs]

- organization in powers $(Q/\Lambda_\chi)^n$ allows **systematic improvement**
- low-energy constants **fit to NN, 3N data** (future: from Lattice QCD (??))
- **consistent** NN, 3N, ... interactions & transition operators by coupling to gauge fields

Renormalization of Inputs

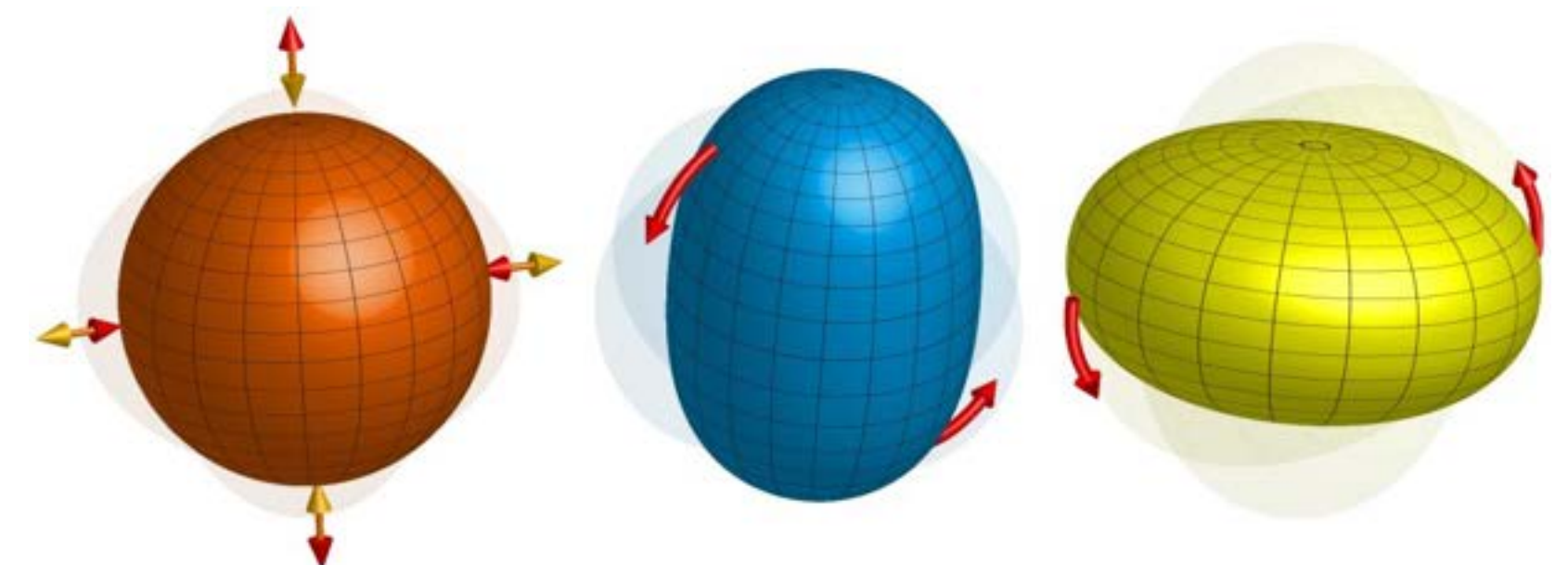
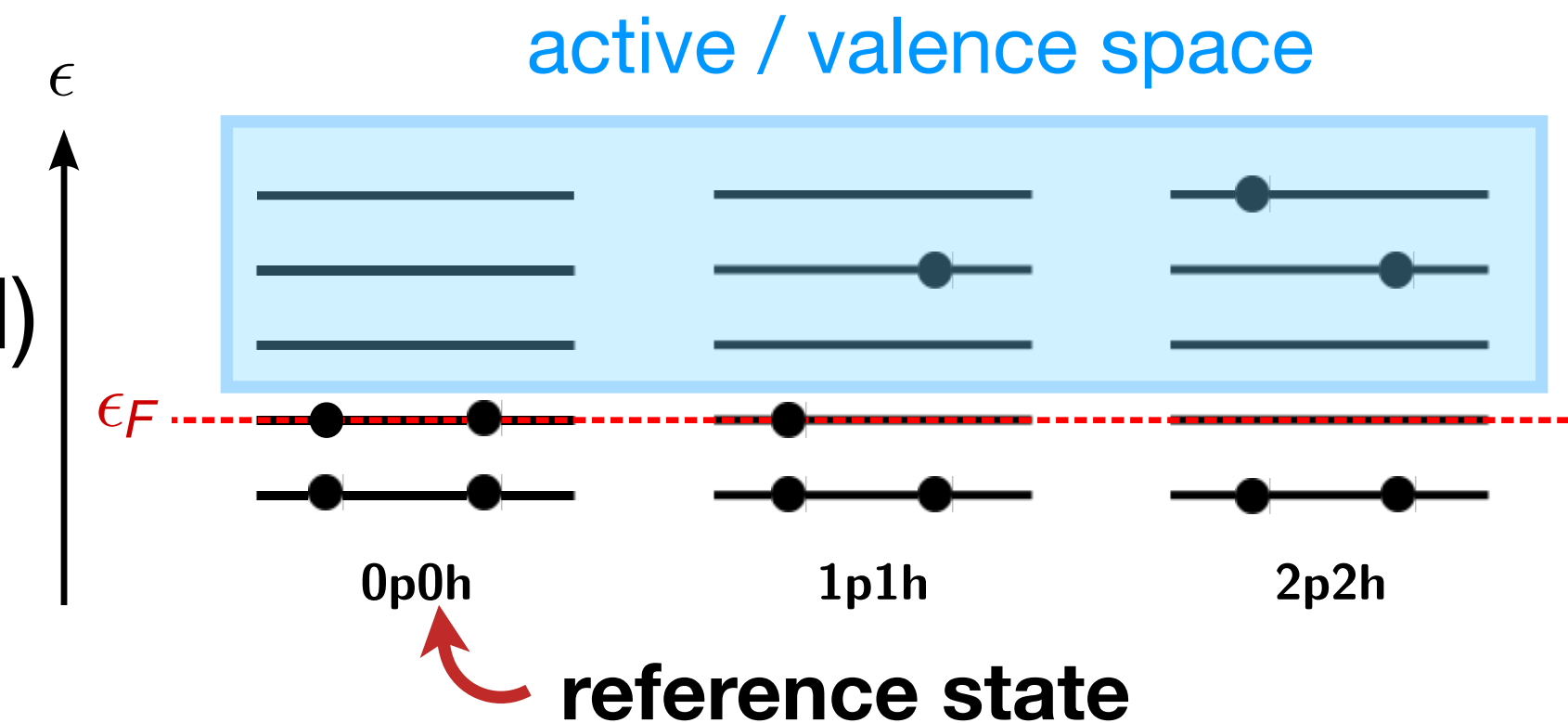
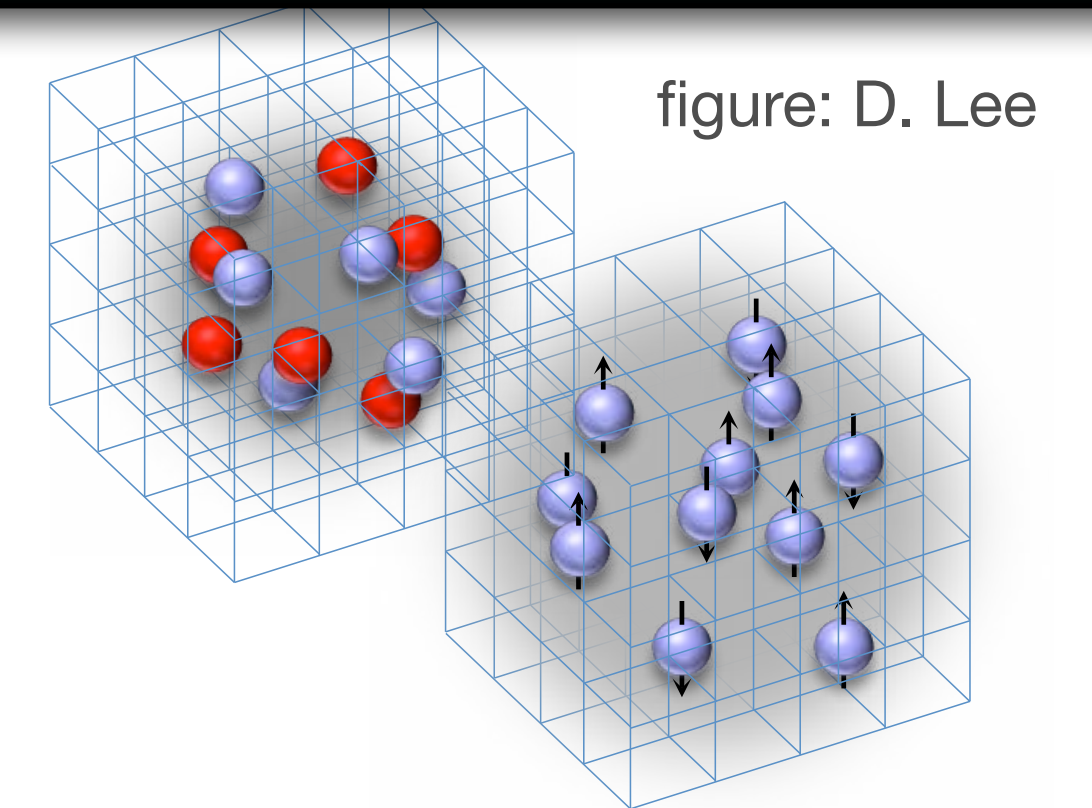
- EFT degrees of freedom (nucleons with a **specific resolution scale**) might not be “optimal” for many-body calculations
- tune **resolution scale** of a theory in **systematic fashion** with **Renormalization Group** methods
- **conserve relevant information** in low-resolution theory
- renormalization reduces effort by **orders of magnitude**, allows many-body methods to **reach heavier nuclei**
- **example:** ^3H ground-state energy from exact diagonalization
- **must be applied consistently to all observables**



Many-Body Methods

Many-Body Methods: Paradigms

- **Coordinate Space**
 - Quantum Monte Carlo
 - Lattice EFT
- **Configuration Space: Particle-Hole Expansions**
 - Many-Body Perturbation Theory (MBPT)
 - Self-Consistent Green's Functions
 - (No-Core) Configuration Interaction (aka Shell Model, (NC)SM)
 - Coupled Cluster (CC)
 - In-Medium Similarity Renormalization Group (IMSRG)
- **Configuration Space / Coordinate Space: Geometric Expansions**
 - deformed HF(B) + projection
 - projected Generator Coordinate Method (PGCM)
 - symmetry-adapted NCSM



Many-Body Methods: Paradigms

- **Coordinate Space**

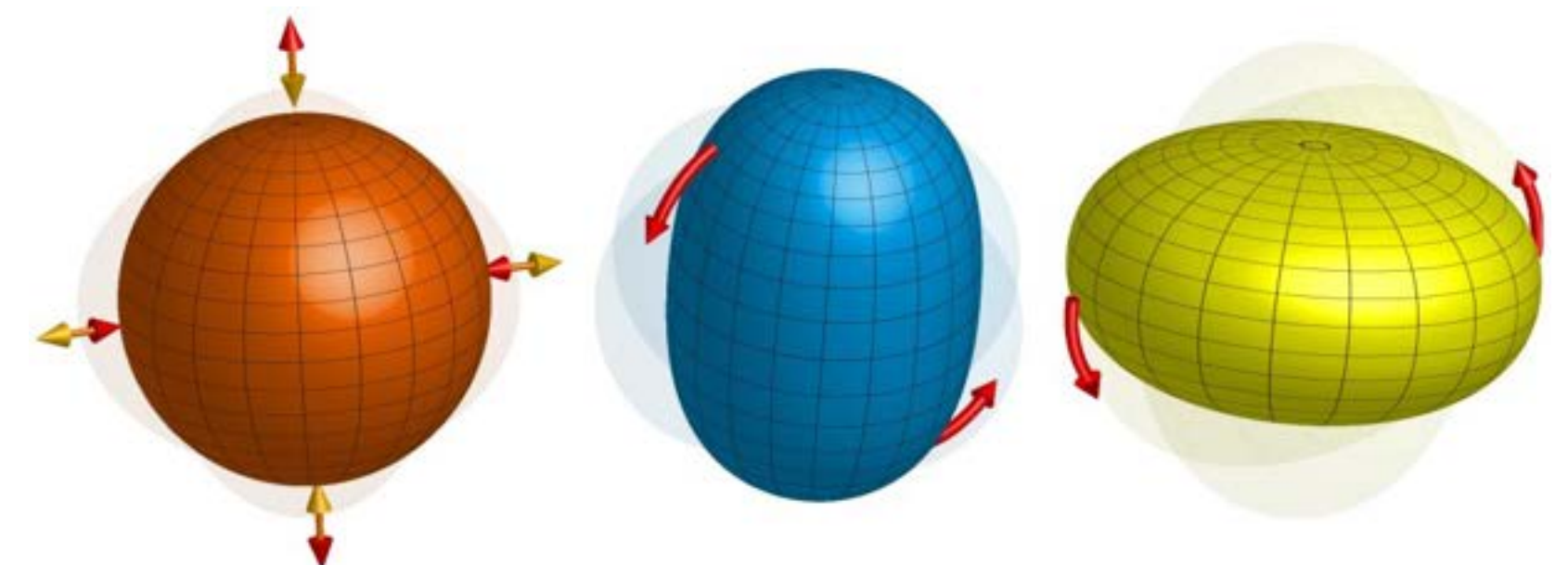
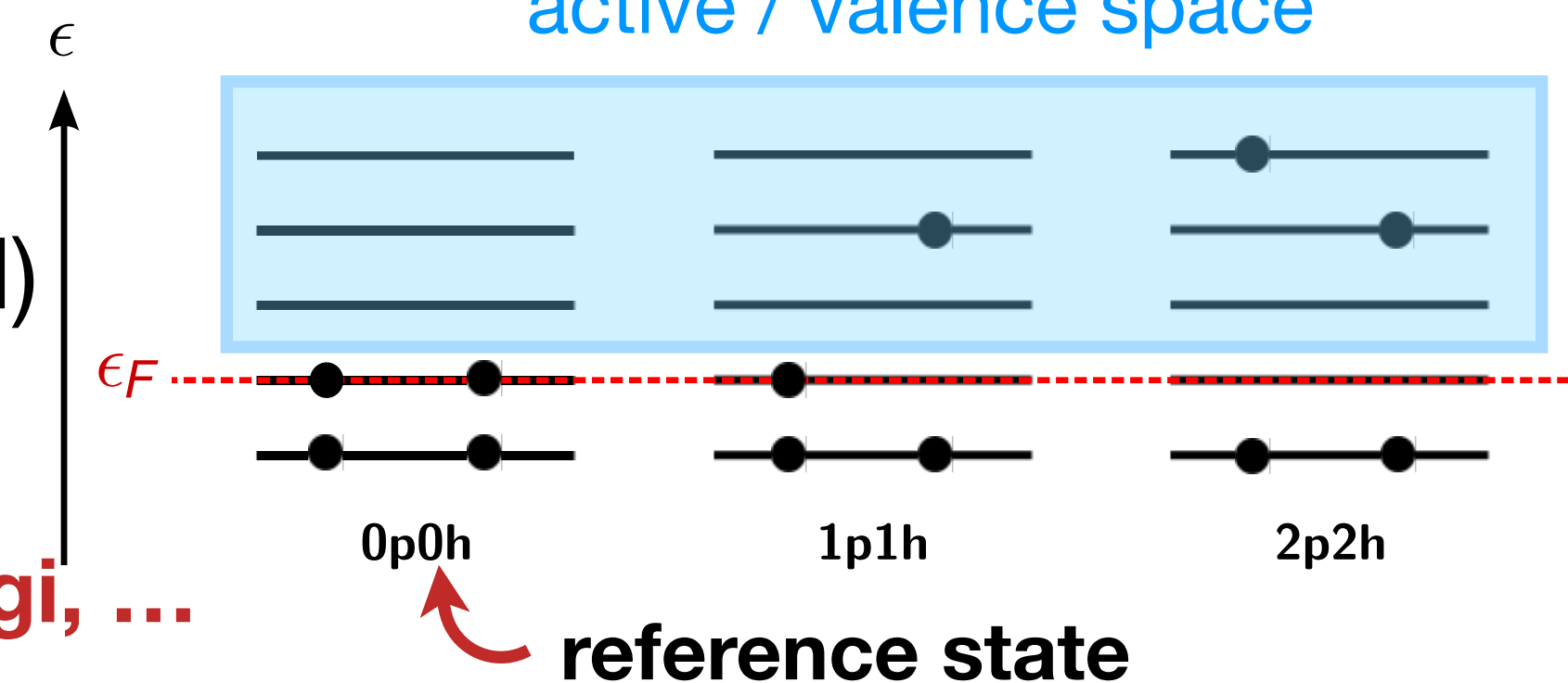
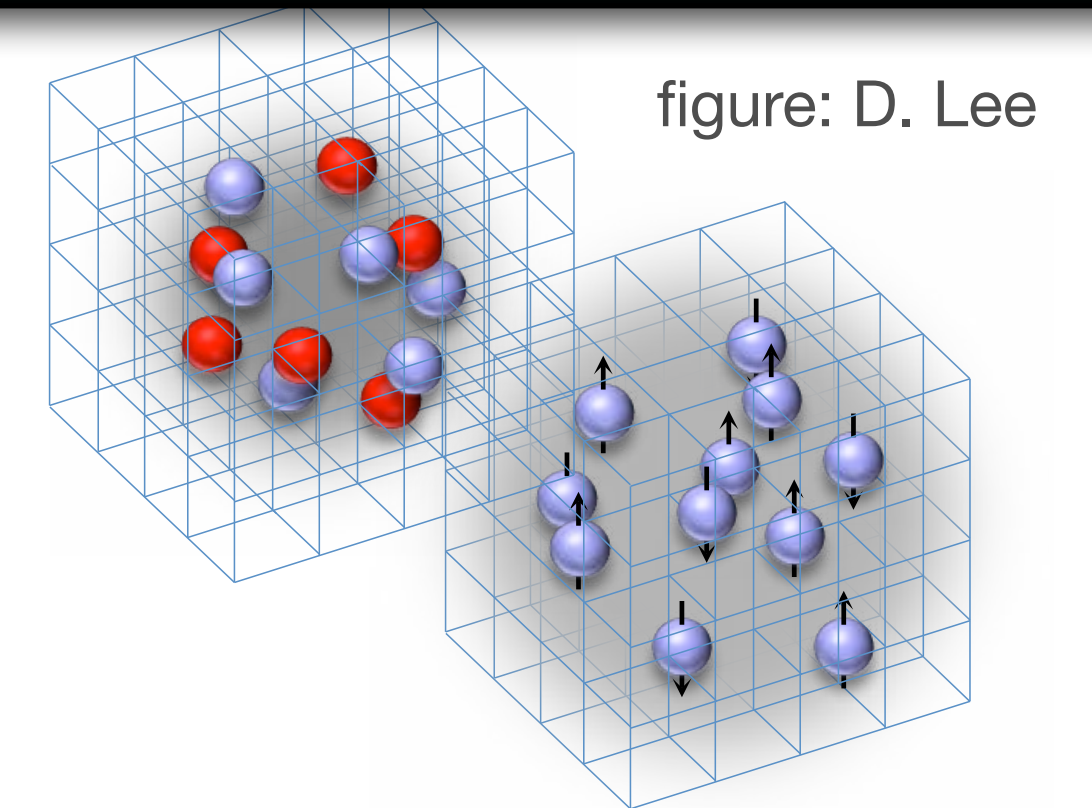
- Quantum Monte Carlo **A. Gezerlis, G. Palkanoglou**
- Lattice EFT **D. Lee**

- **Configuration Space: Particle-Hole Expansions**

- Many-Body Perturbation Theory (MBPT)
- Self-Consistent Green's Functions **A. Rios, V. Somà, ...**
- (No-Core) Configuration Interaction (aka Shell Model, (NC)SM)
- Coupled Cluster (CC) **G. Hagen, P. Demol, ...**
- In-Medium Similarity Renormalization Group (IMSRG) **T. Miyagi, ...**

- **Configuration Space / Coordinate Space: Geometric Expansions**

- deformed HF(B) + projection **B. Bally, A. Porro, ...**
- projected Generator Coordinate Method (PGCM)
- symmetry-adapted NCSM



Many-Body Methods: Paradigms



- **Coordinate Space**
 - Quantum Monte Carlo



Recent(-ish) Reviews:

HH, Front. Phys. **8**, 379 (2020)

S. Gandolfi, D. Lonardoni, A. Lovato and M. Piarulli, Front. Phys. **8**, 117 (2020)

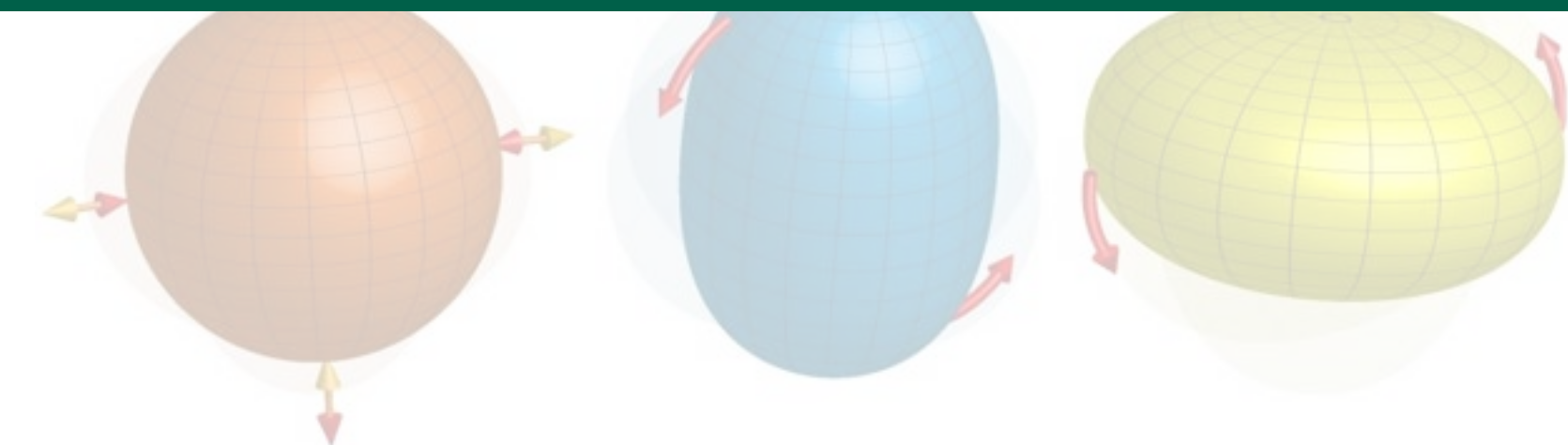
D. Lee, Front. Phys. **8**, 174 (2020)

V. Somà, Front. Phys. **8**, 340 (2020)

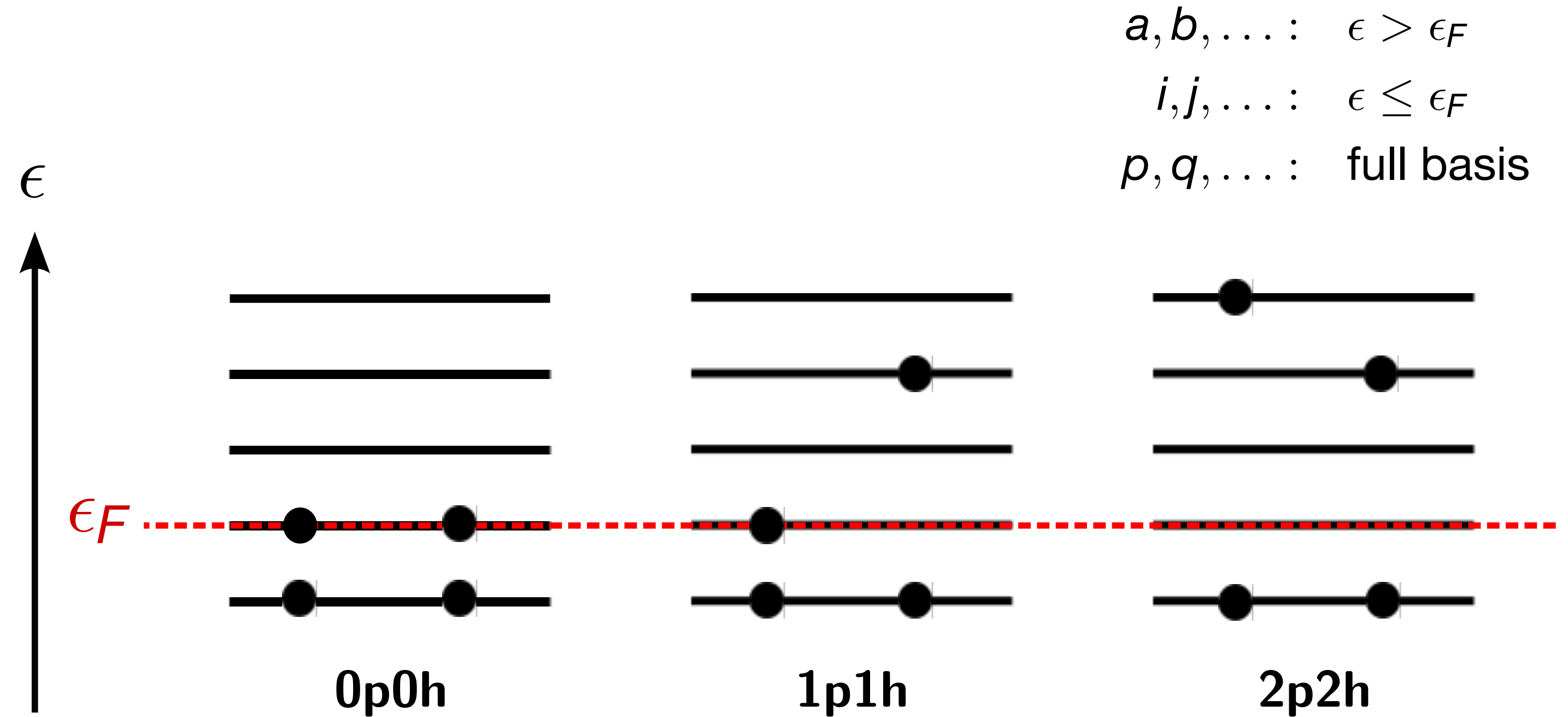
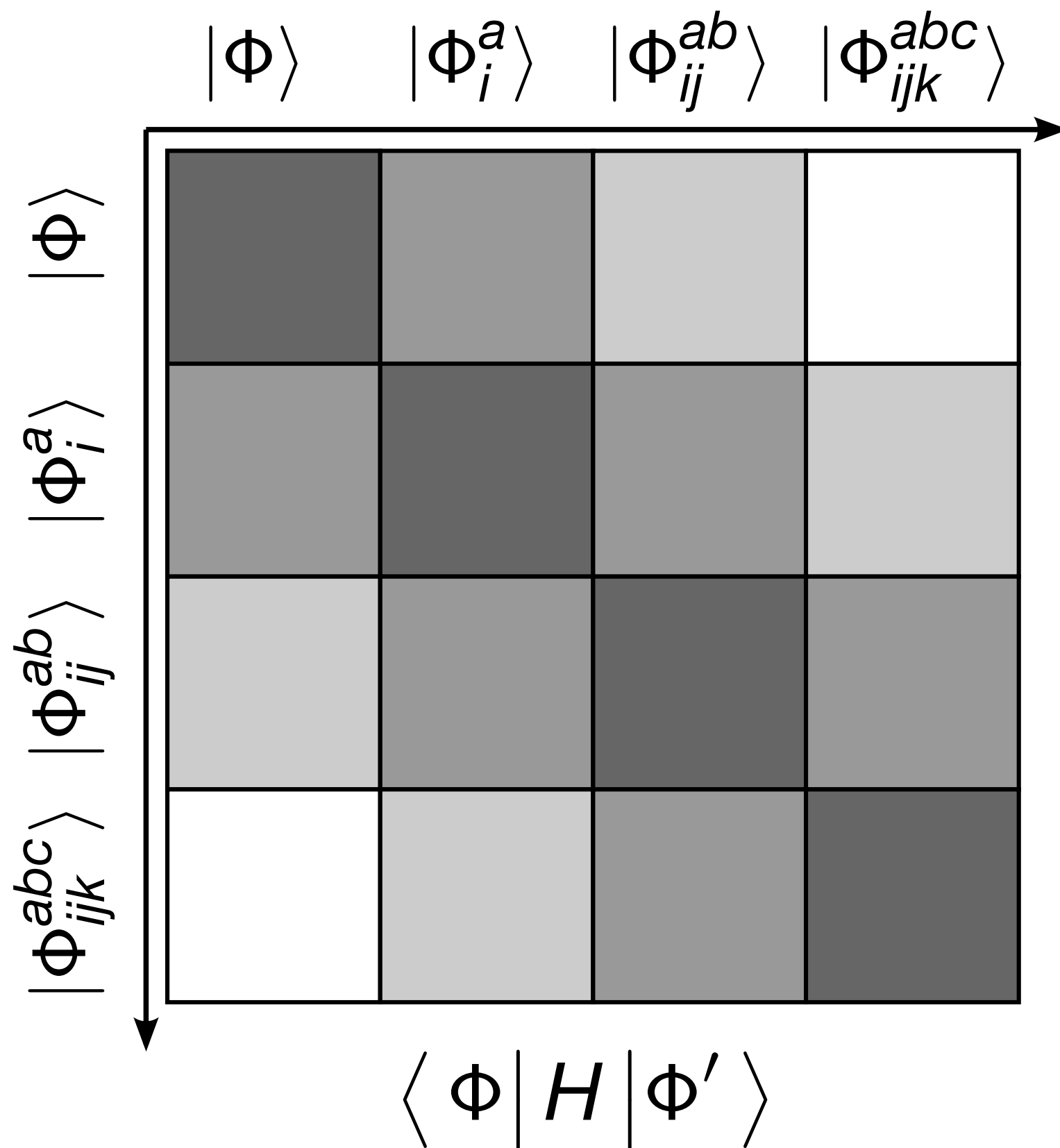
also see

“What is *ab initio* in nuclear theory?”, A. Ekström, C. Forssén, G. Hagen, G. R. Jansen, W. Jiang, T. Papenbrock, Front. Phys. **11**, 1129094 (2023)

- deformed HF(B) + projection
- projected Generator Coordinate Method (PGCM)
- symmetry-adapted NCSM



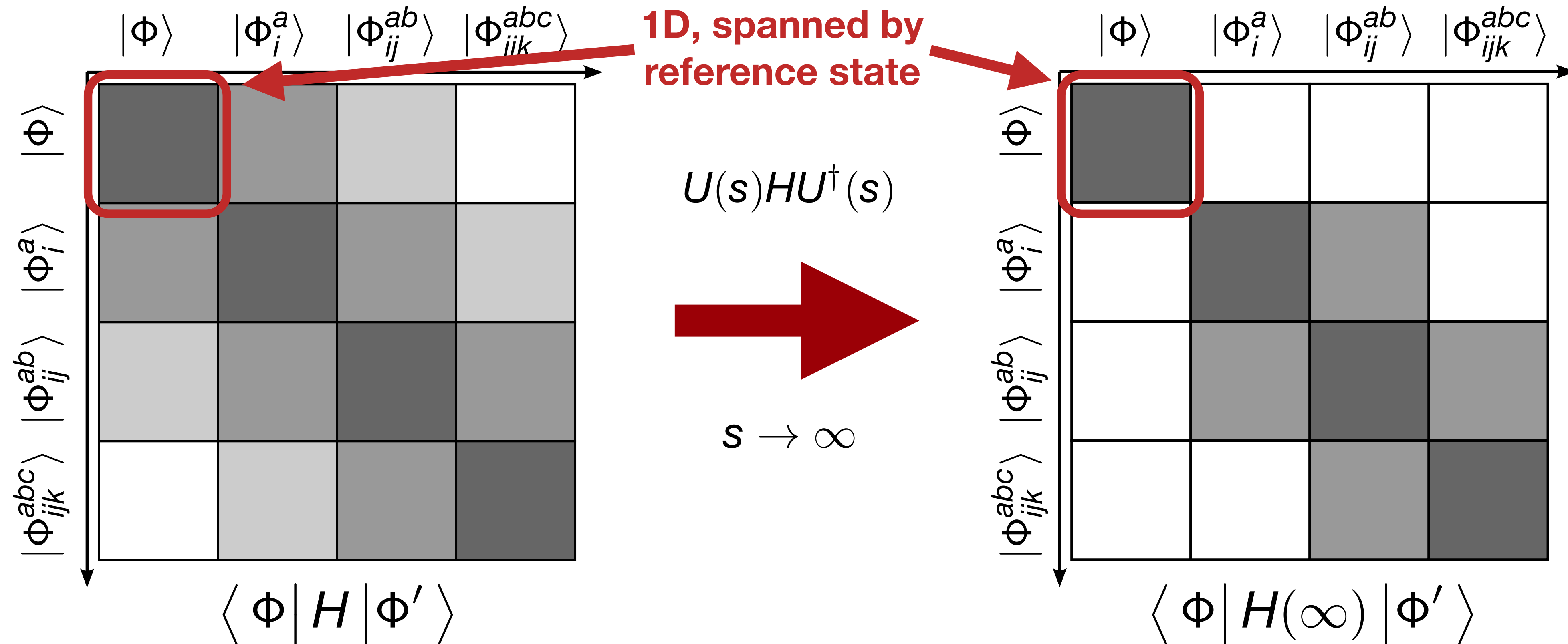
Many-Body Methods: Configuration Space



construct **particle-hole excitations** of a **reference state** - usually an optimized **mean-field Slater determinant**

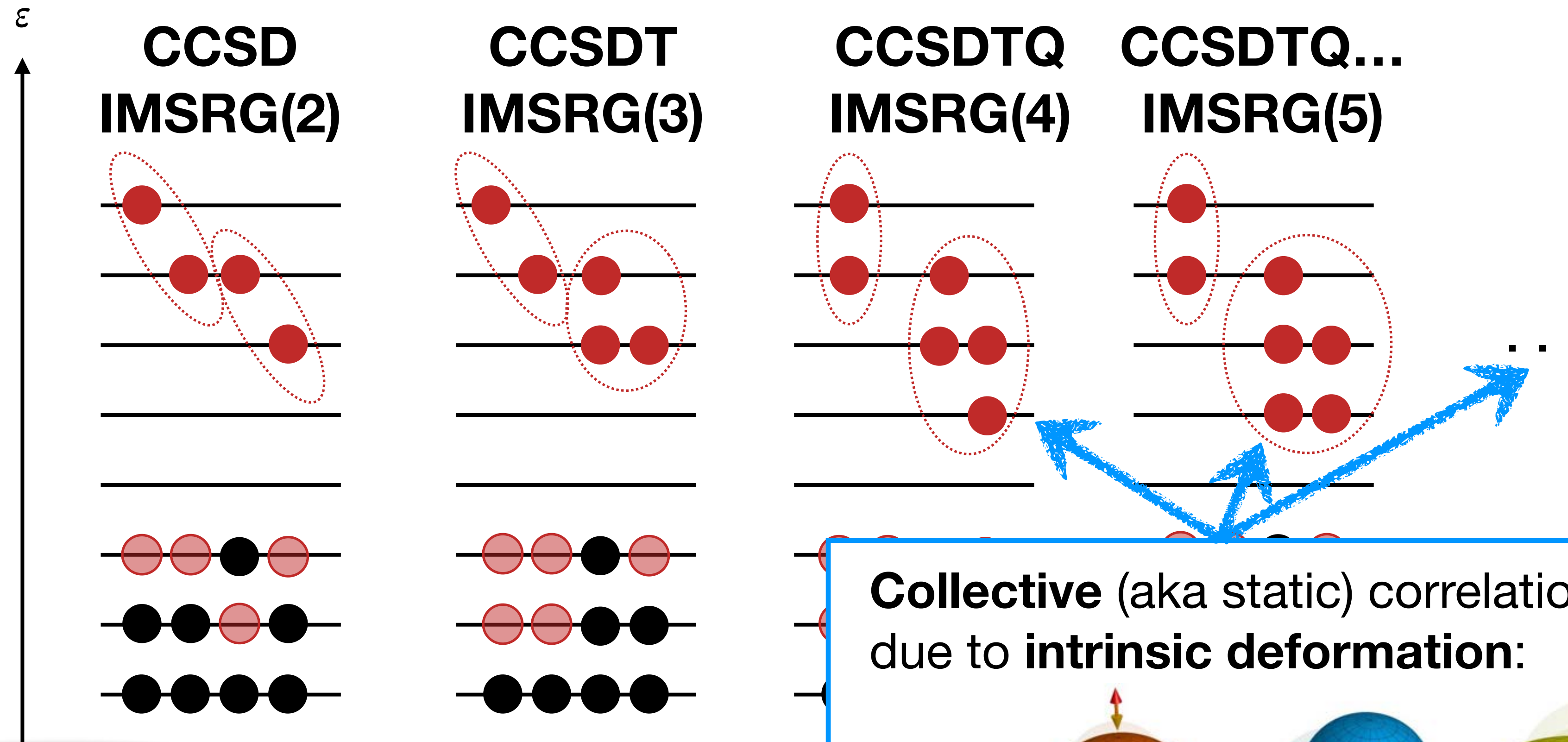
excitations **relative** to reference state:
normal-ordering

Decoupling in A-Body Space

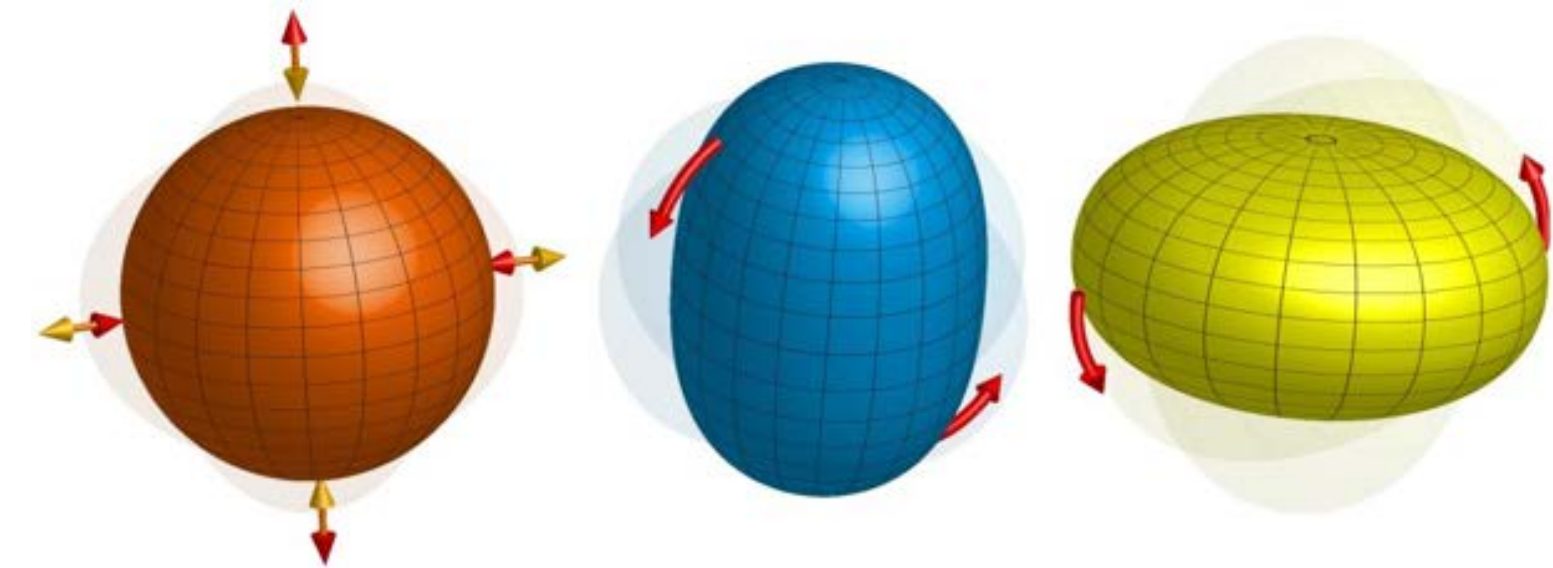


- **identify** the parts of the **operator H** which **couple reference state to excitations**
- **eliminate** them with unitary (**IMSRG**) or general similarity transformations (**CC**)
- **efficient: polynomial scaling**, no need to construct matrix !

Correlations in Nuclei

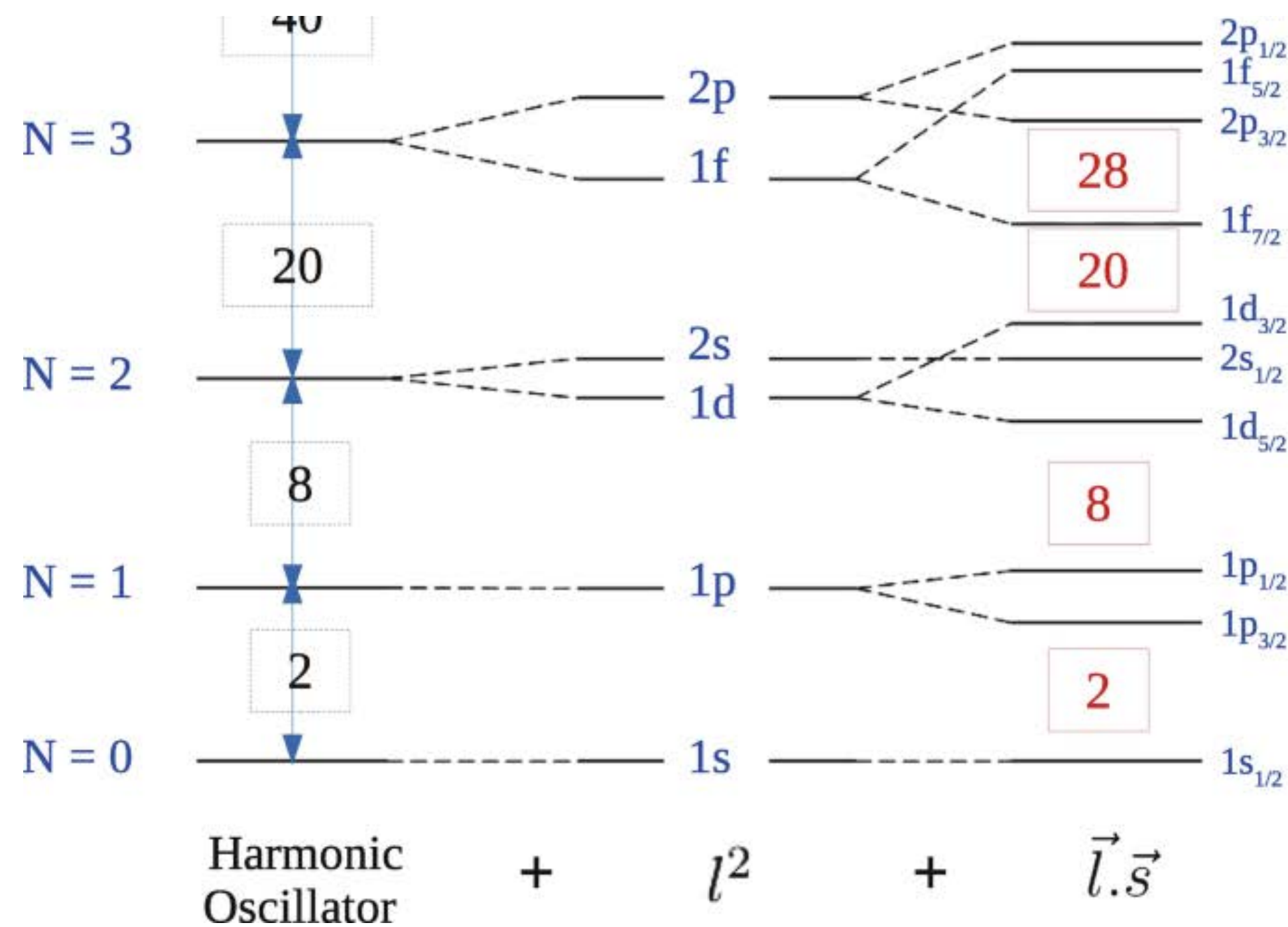


Collective (aka static) correlations, e.g. due to **intrinsic deformation**:

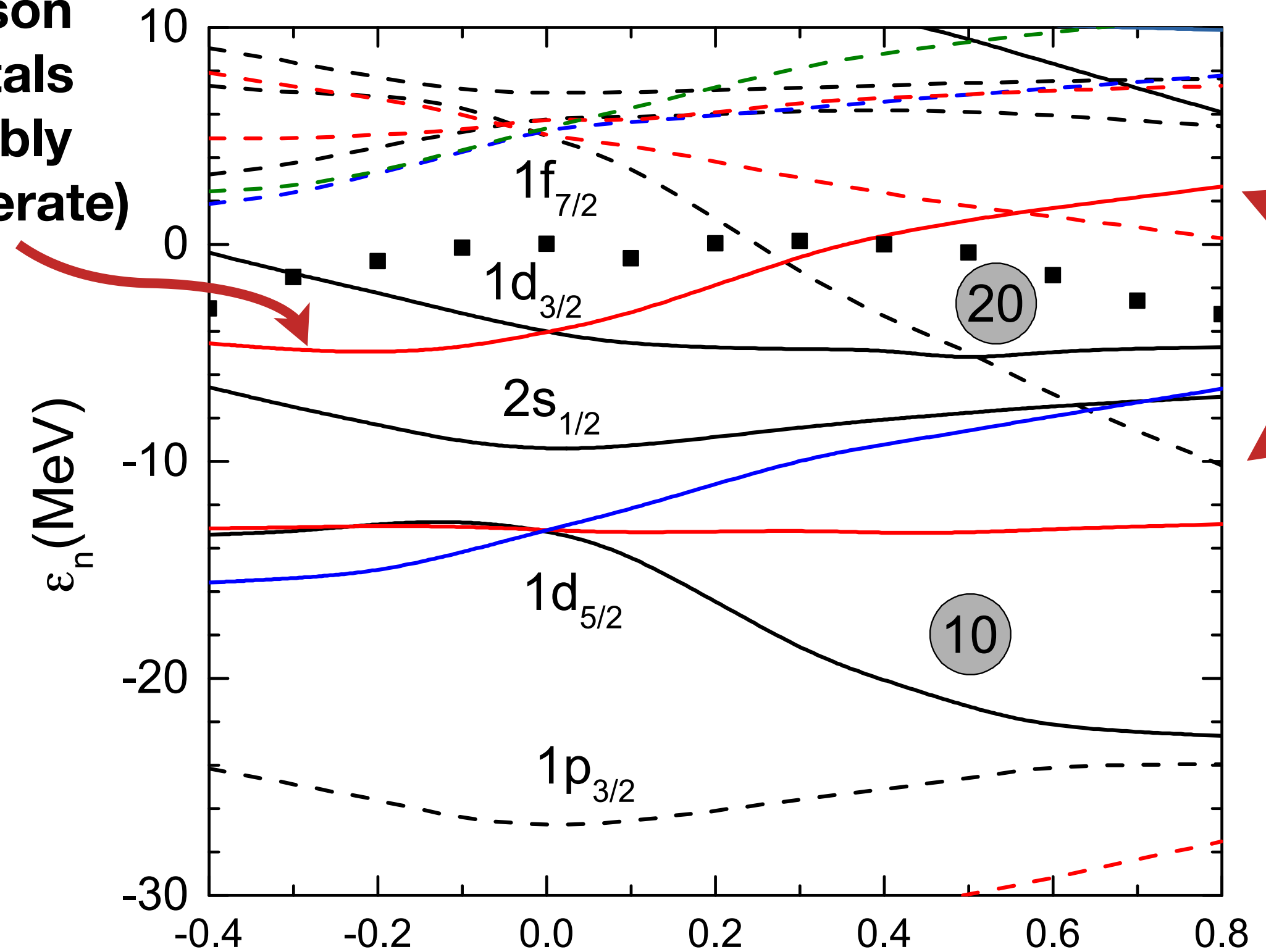


Important for rare transitions
($0\nu\beta\beta$ decay, ...): Other decays
impeded by energy differences and
wave function overlaps!

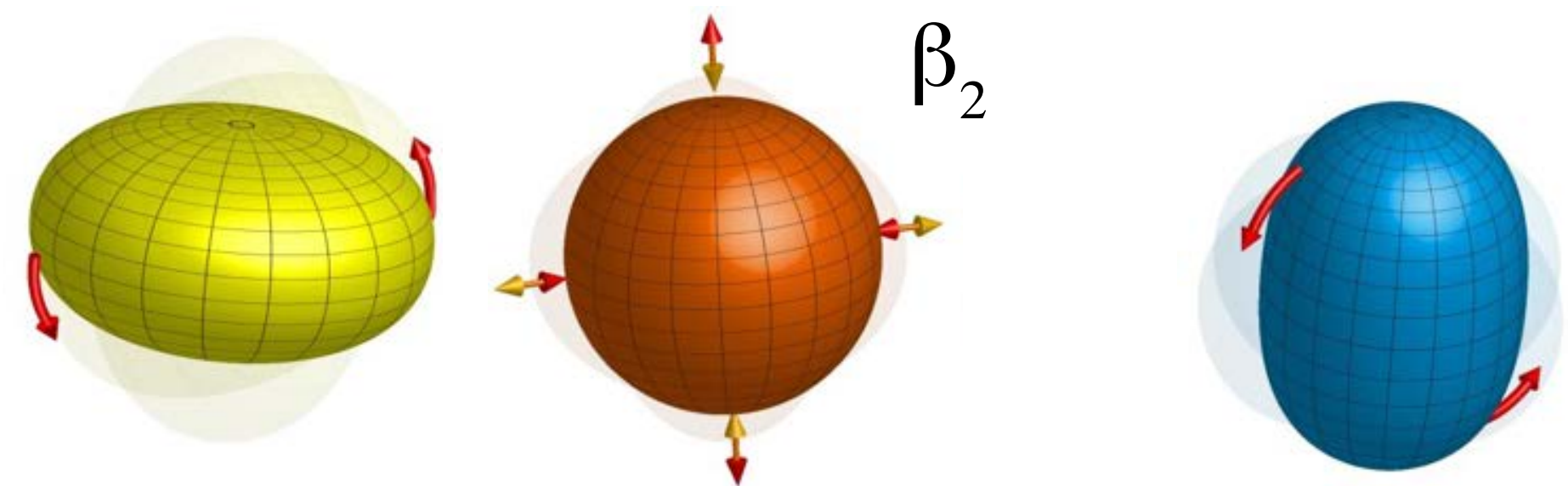
Symmetry Breaking and Restoration



Nilsson orbitals (doubly degenerate)

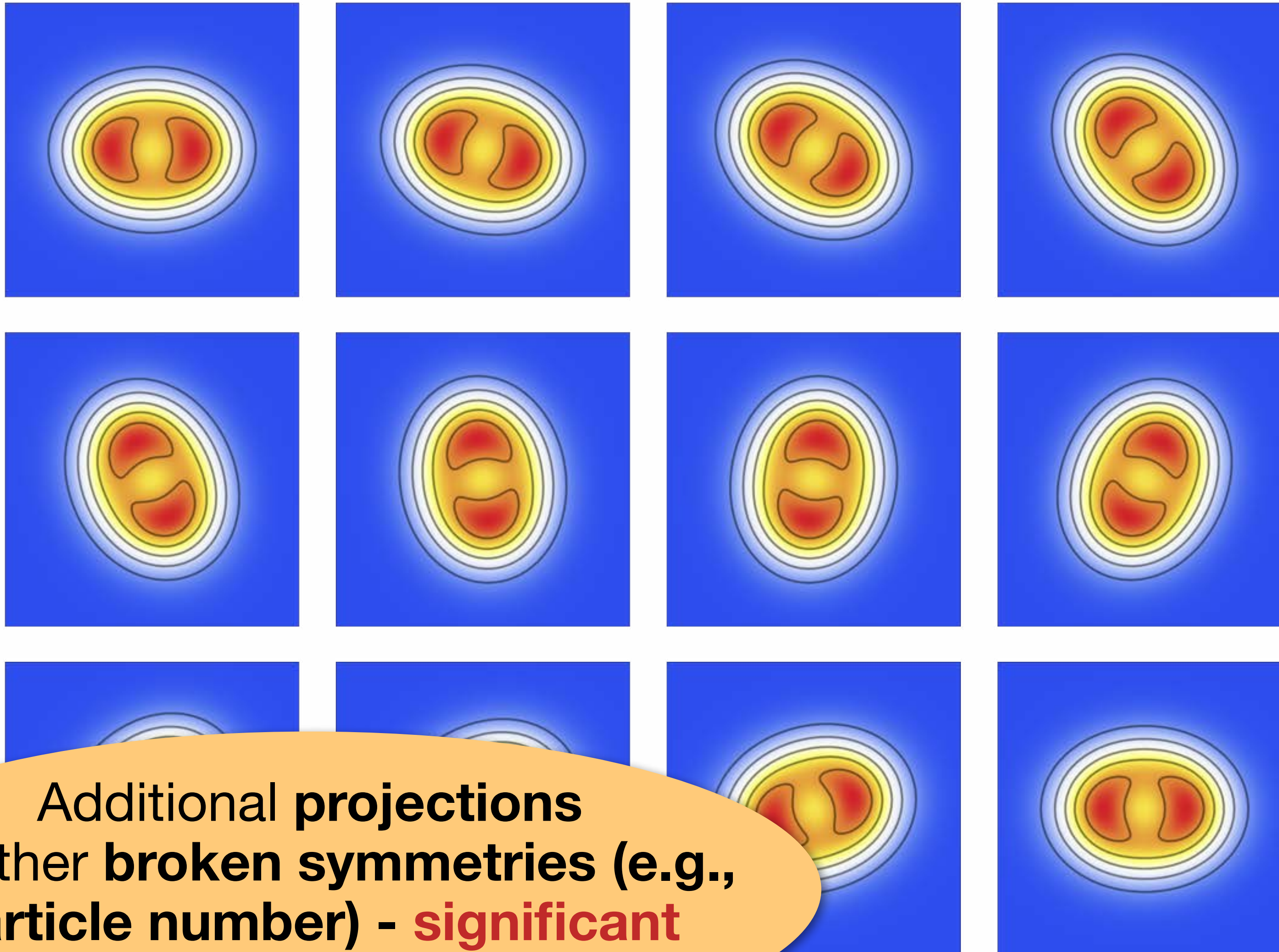


- **break spherical symmetry** to **capture static correlation** from deformation
- **restore symmetry** by constructing **(specific) superpositions of all rotations** of intrinsic state (aka **projection**)



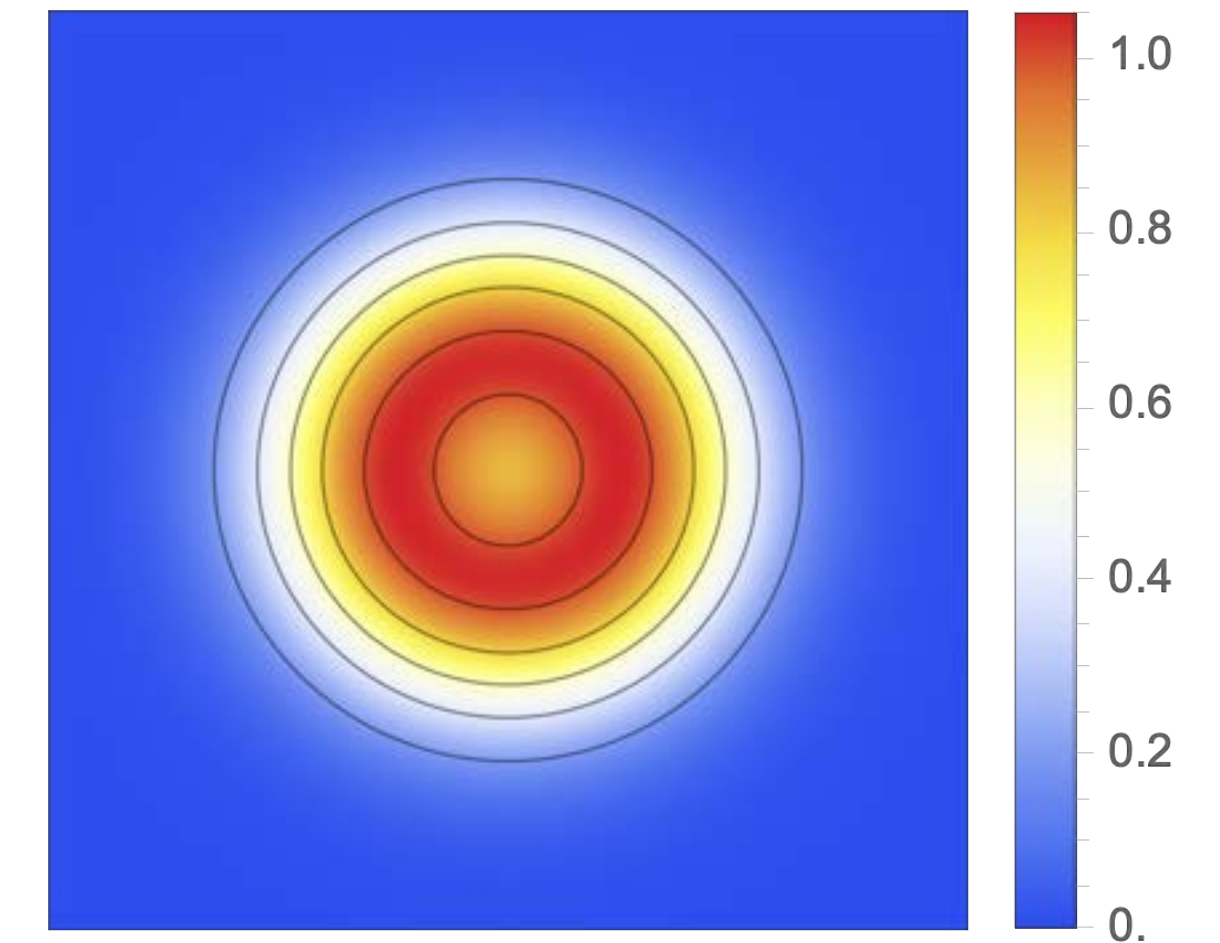
Symmetry Breaking and Restoration

deformed configurations

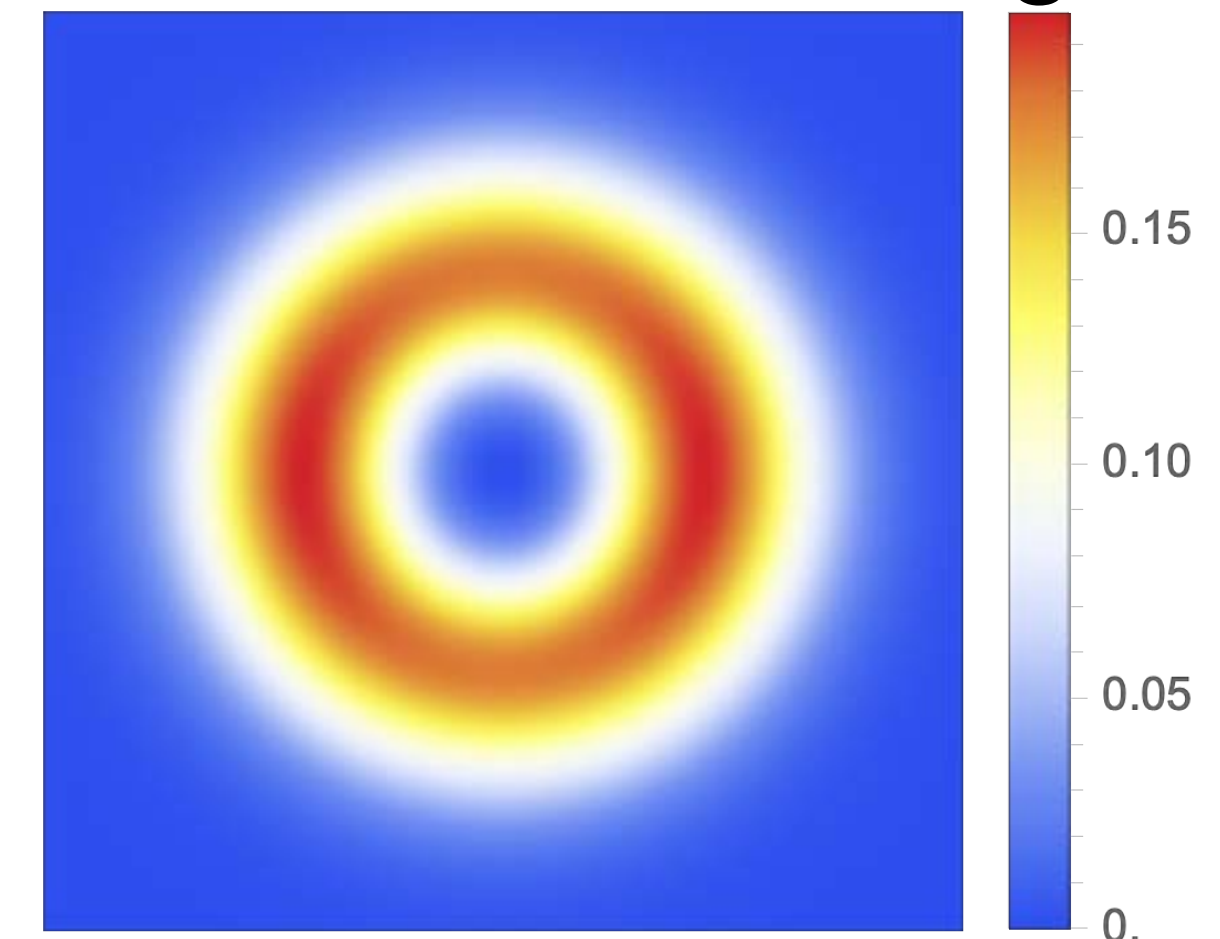


Additional **projections**
for other **broken symmetries** (e.g.,
particle number) - **significant**
overhead!

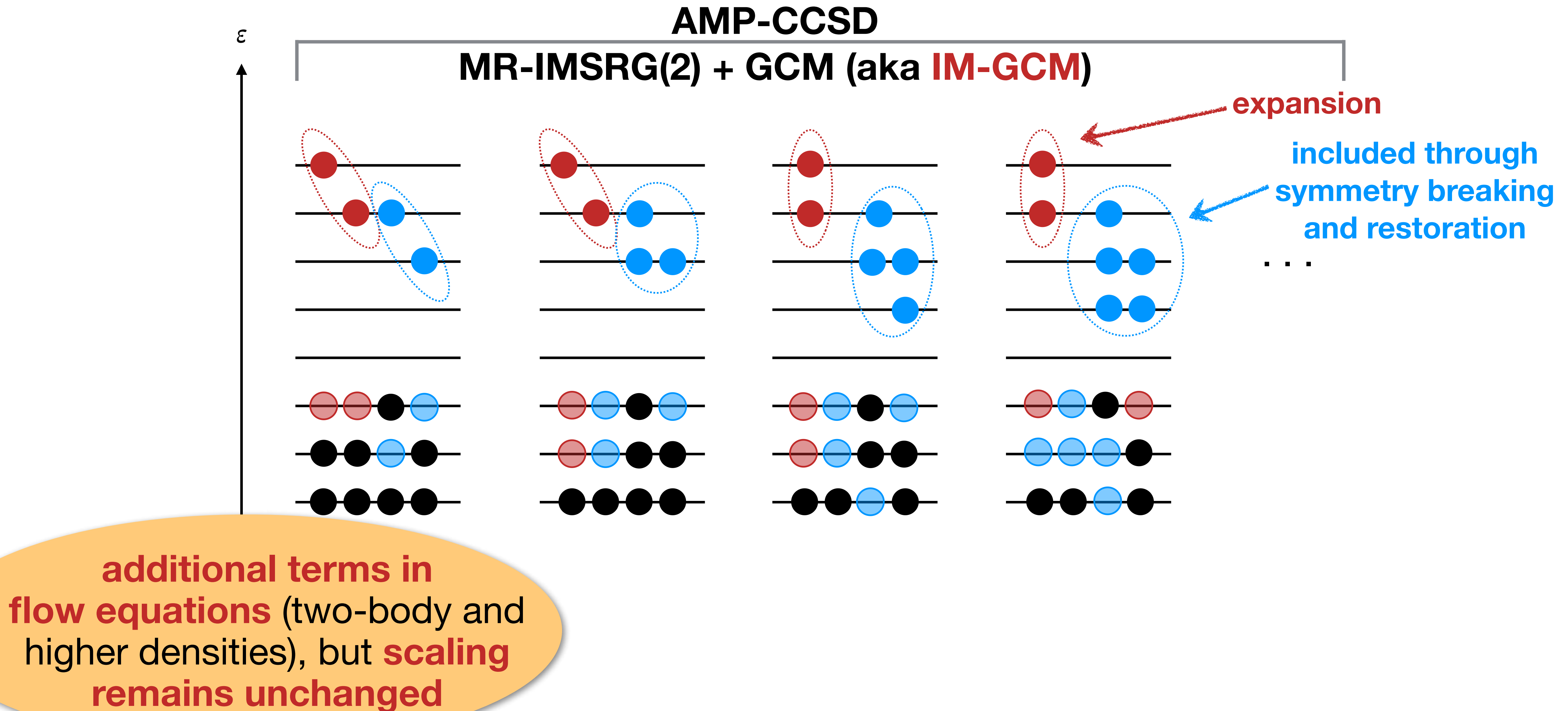
projected w.f.



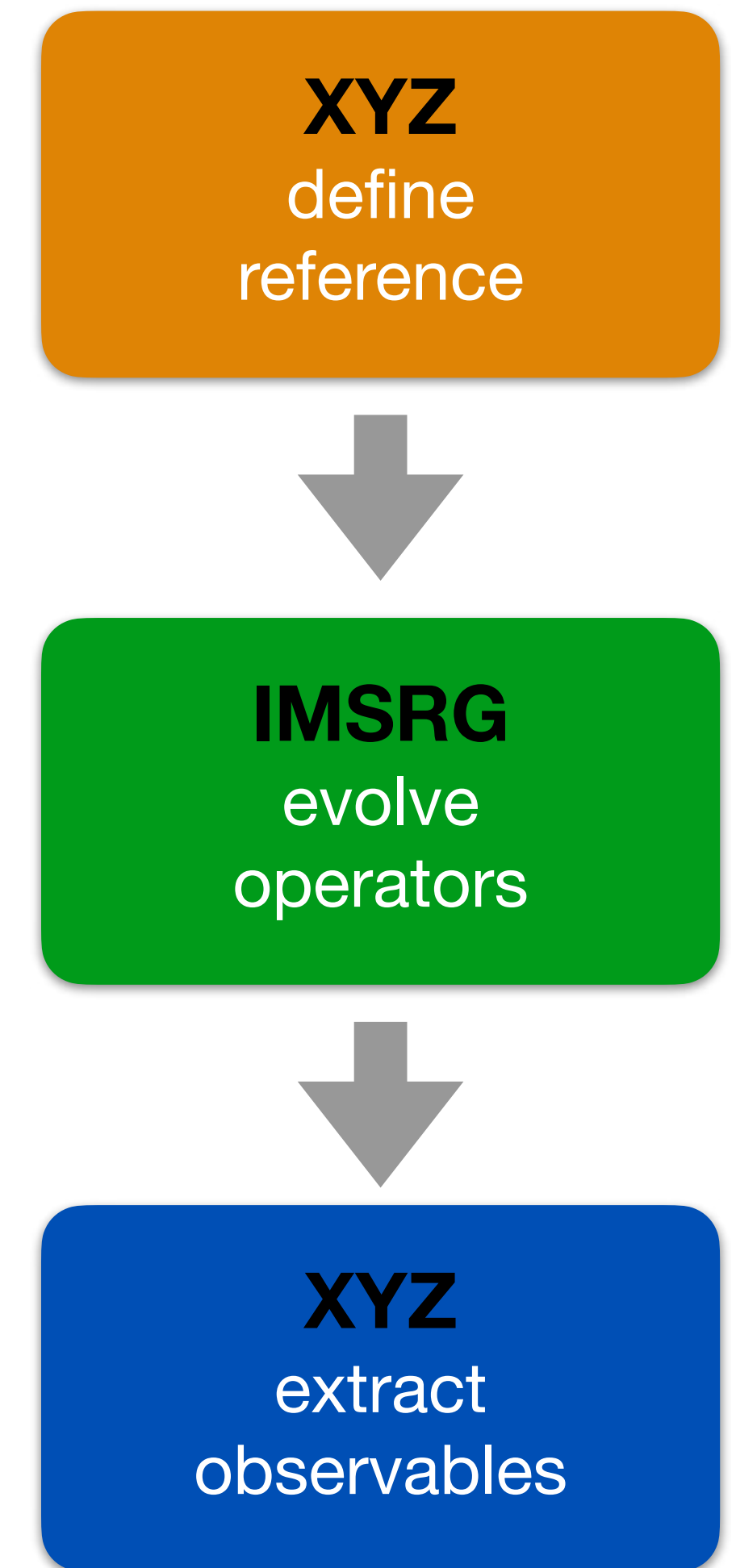
difference from spherical w.f.
with same basis size /length scale



Correlations in Nuclei

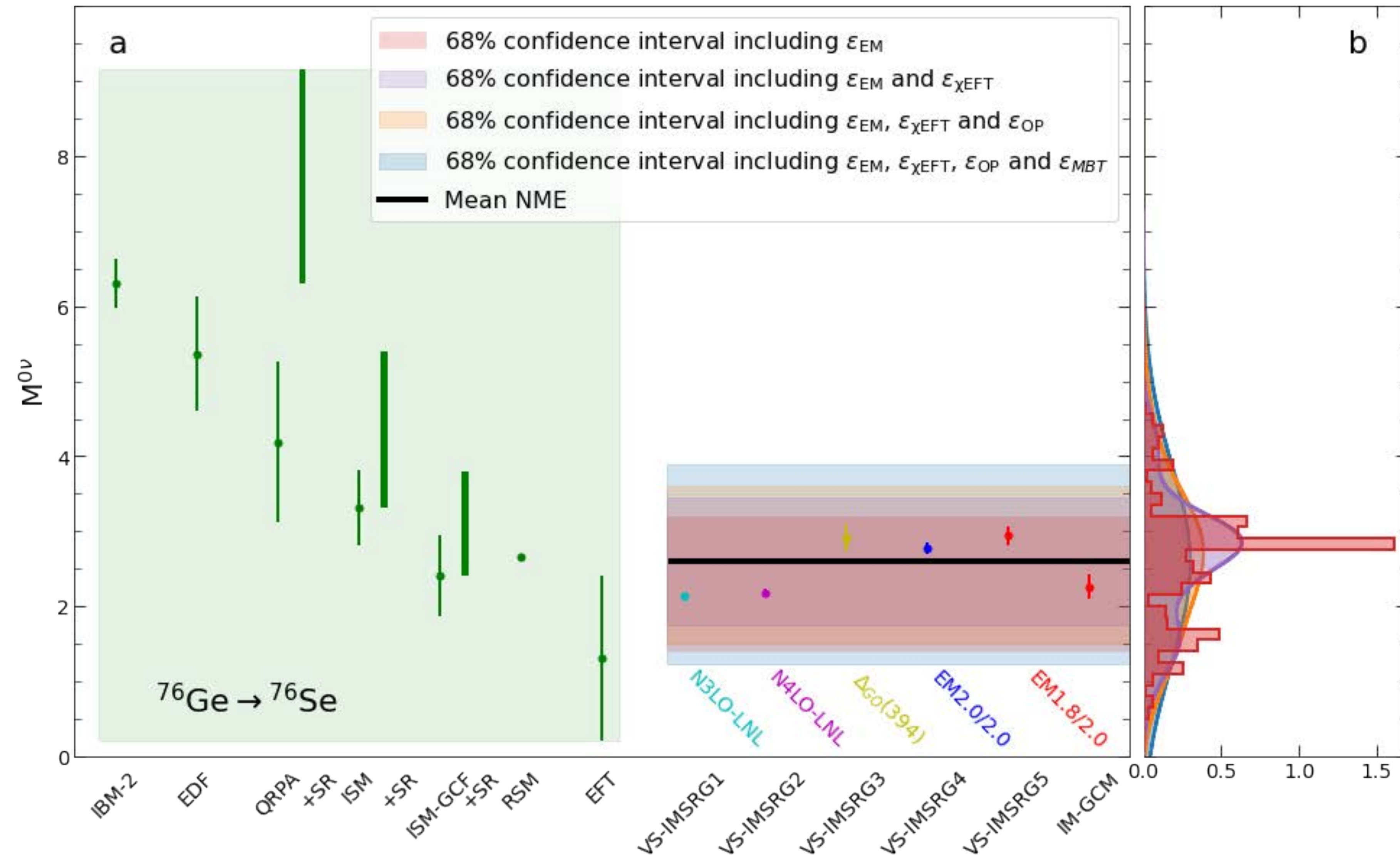


- IMSRG can be used to build specific types of correlations into **RG-improved interactions** and **operators**
- IMSRG captures correlations that are **complementary** to target method
- mean-field or **correlated reference state(s)** for a specific nucleus
define(s) **operator basis** for IMSRG evolution
- **diagnostic:** flow is unitary if all **relevant operators** are included
- **examples:**
 - (MR-)IMSRG(2) aka In-Medium HF / PHFB
 - Valence-Space IMSRG for Shell model / VS-CI
 - In-Medium No-Core Shell Model / NC-CI
 - In-Medium Generator Coordinate Method (IM-GCM)



Selected Results

^{76}Ge : Neutrinoless Double Beta Decay

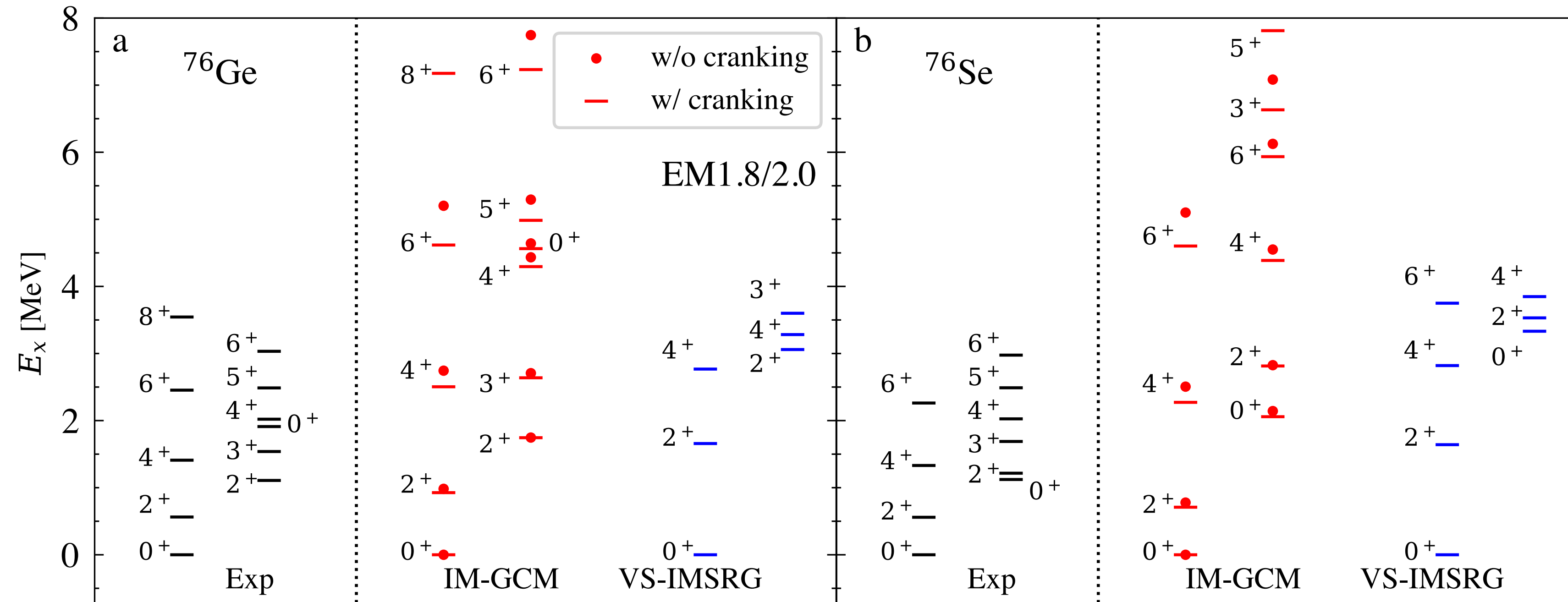


- **state of the art** study
- **complementary methods:** IM-GCM & VS-IMSRG
- explores interactions, many-body and EFT truncations, contact term, ...
- leverages **novel emulators**
- identifies **main drivers** of uncertainty and what to improve next

^{76}Ge / ^{76}Se Structure

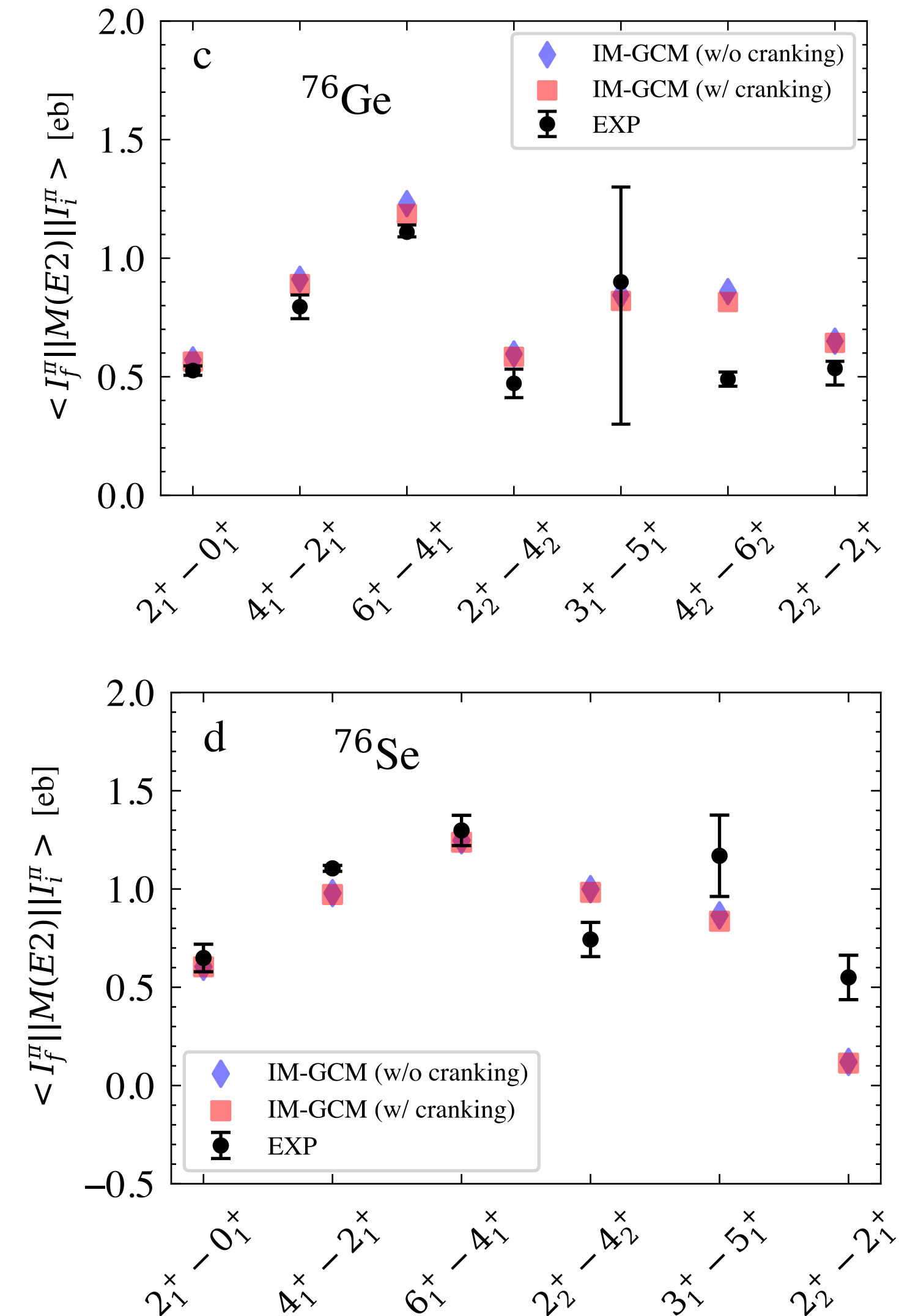


A. Belley et al., PRL **132**, 182502 (2024)

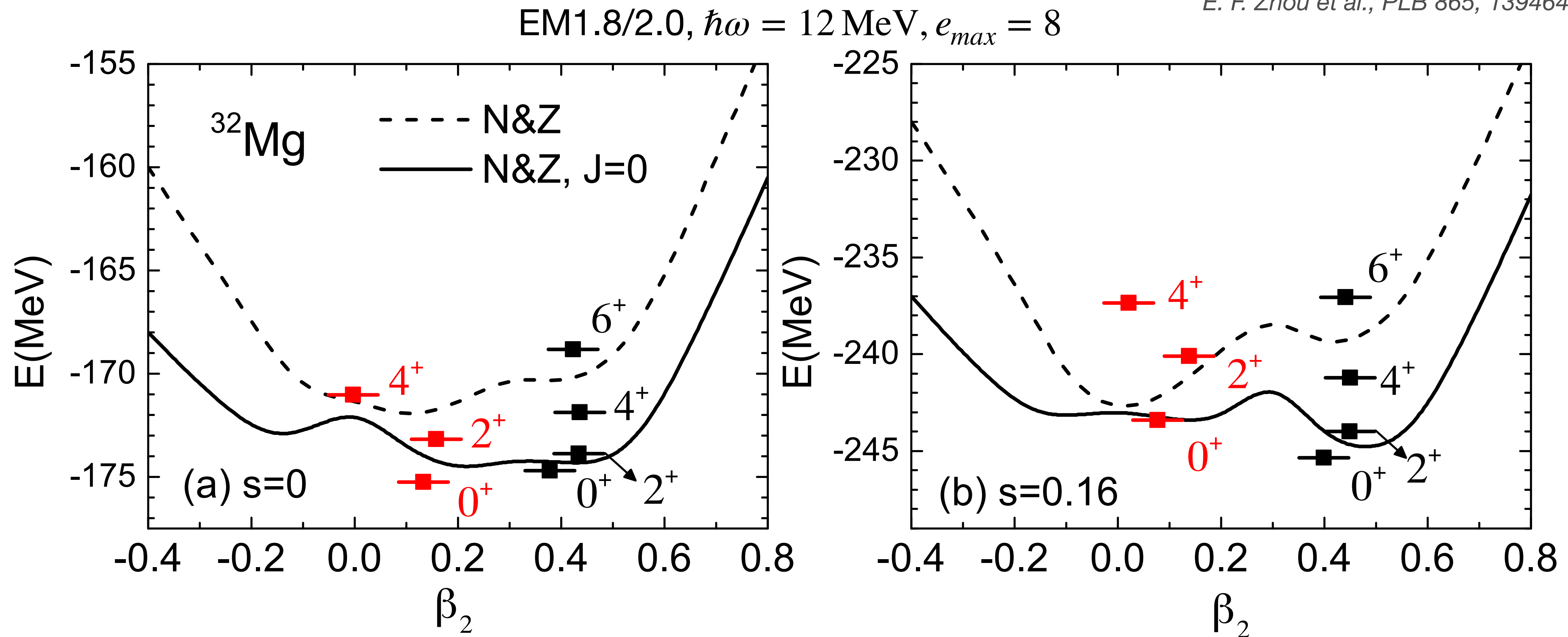


EM1.8/2.0 NN+3N interaction, $\hbar\omega = 12 \text{ MeV}$, $e_{max} = 10$

- IM-GCM spectra too extended (common)
- E2 transitions (and static moments) in **excellent agreement with experiment...**
- ...although EM1.8/2.0 **underpredicts radii by a few percent**



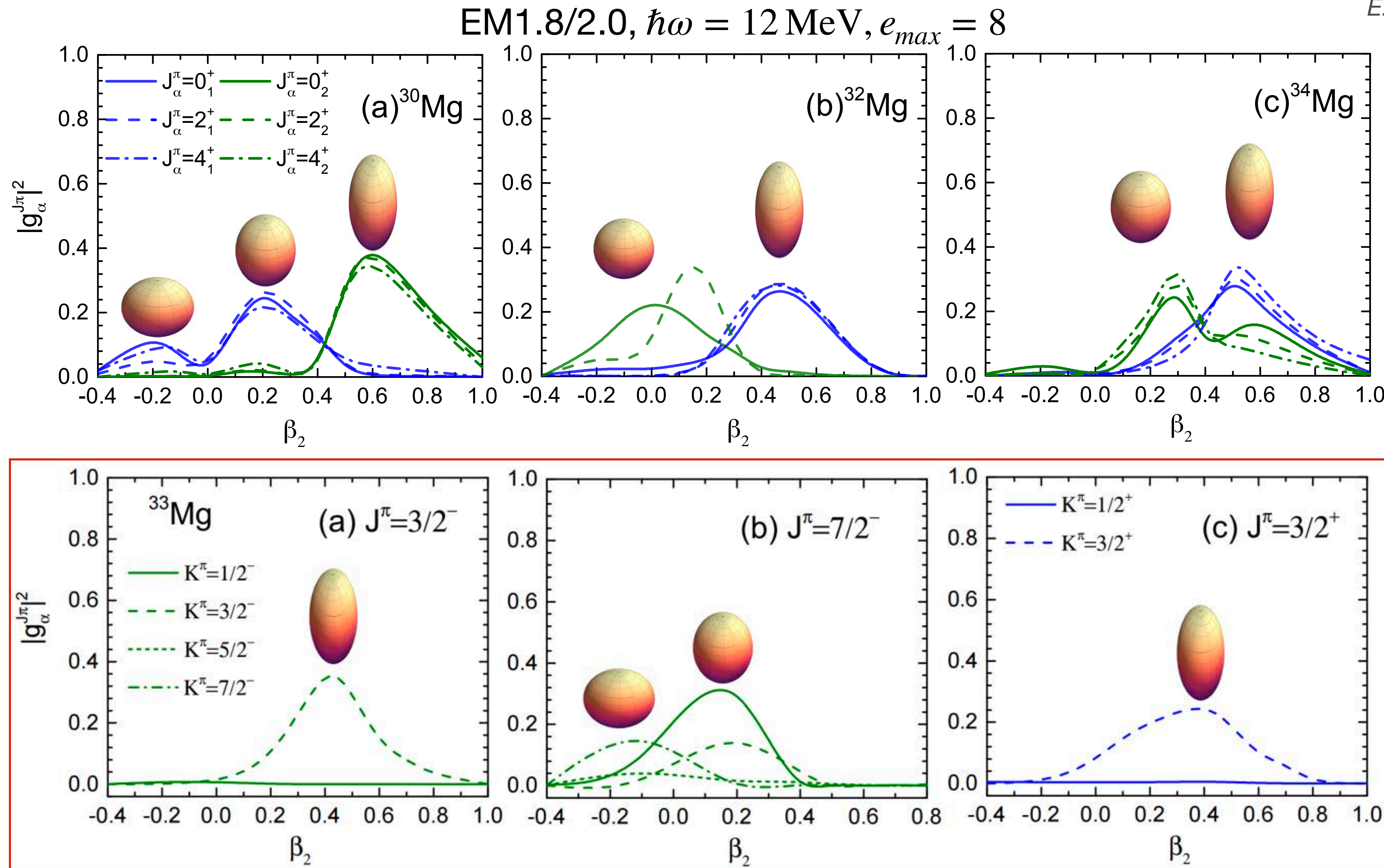
N=20 Island of Inversion: ^{32}Mg



- **Dynamic correlations** captured by IMSRG...
- bring **absolute energies** close to experiment ($E = -249.7 \text{ MeV}$ (AME) vs. -249.5 MeV (extrapolated theory))
- reveal prominent **prolate deformation** of the **ground state**

N=20 Island of Inversion: $^{32-34}\text{Mg}$

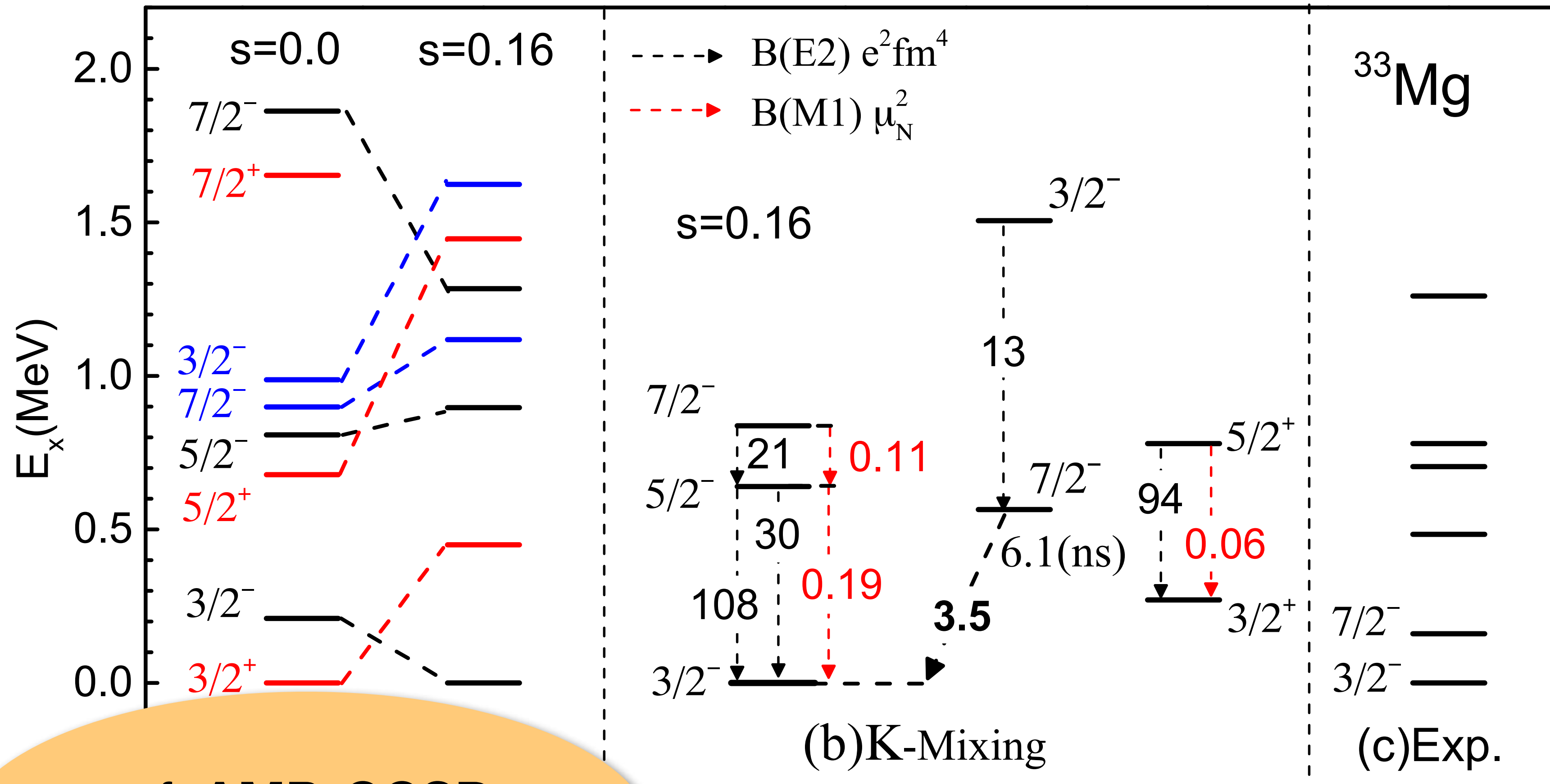
E. F. Zhou et al., PLB 865, 139464 (2025) & in prep.



- **shape coexistence** comes with **shape mixing**
- **caveat:** wave function components are not observable - **compare with care!**
- **odd nuclei** described with **projected (multiply) blocked HFB vacua**

N=20 Island of Inversion: ^{33}Mg

EM1.8/2.0, $\hbar\omega = 12 \text{ MeV}$, $e_{\max} = 8$

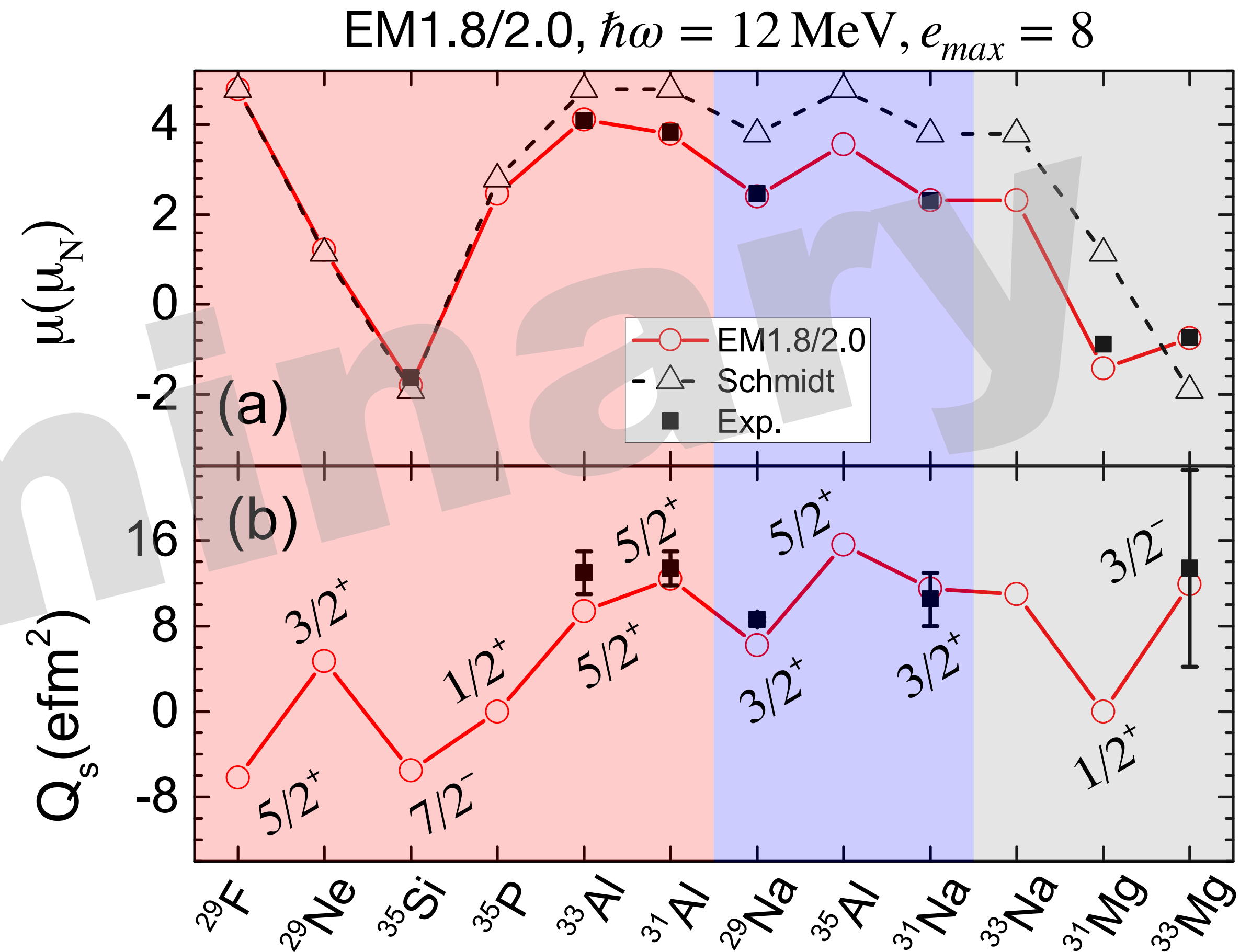
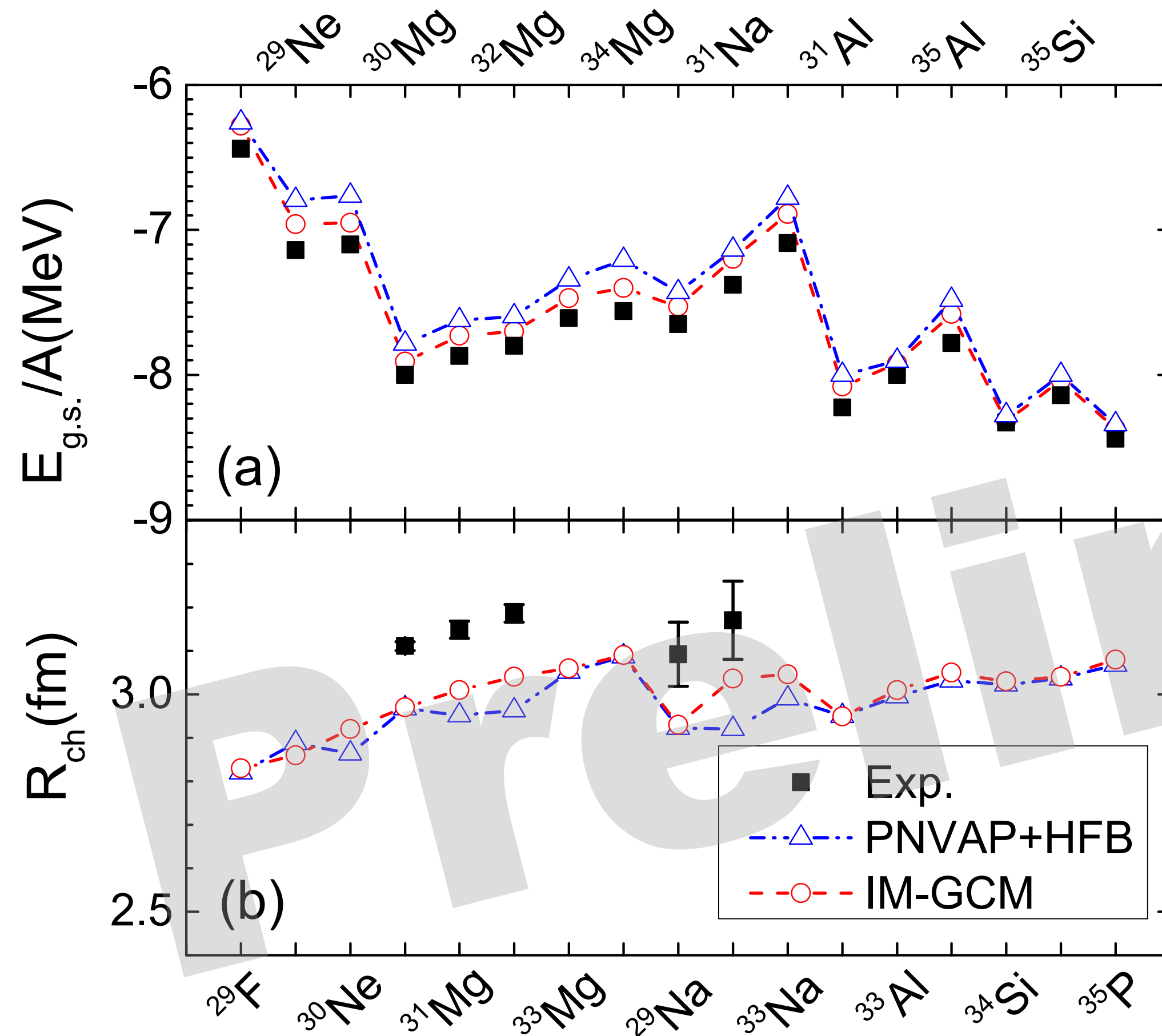


- **shape and K mixing** have notable impact on ^{33}Mg spectrum
- **boosts** lifetime of $\frac{7}{2}^-$ state - **predicted to be a shape isomer**
- related to ^{32}Na shape isomer measured at FDSi in 2023 ?
[Gray et al., PRL 130, 132501]

cf. **AMP-CCSD**

Z. H. Sun et al., PRC 111, 044304 & PRX 15, 011028

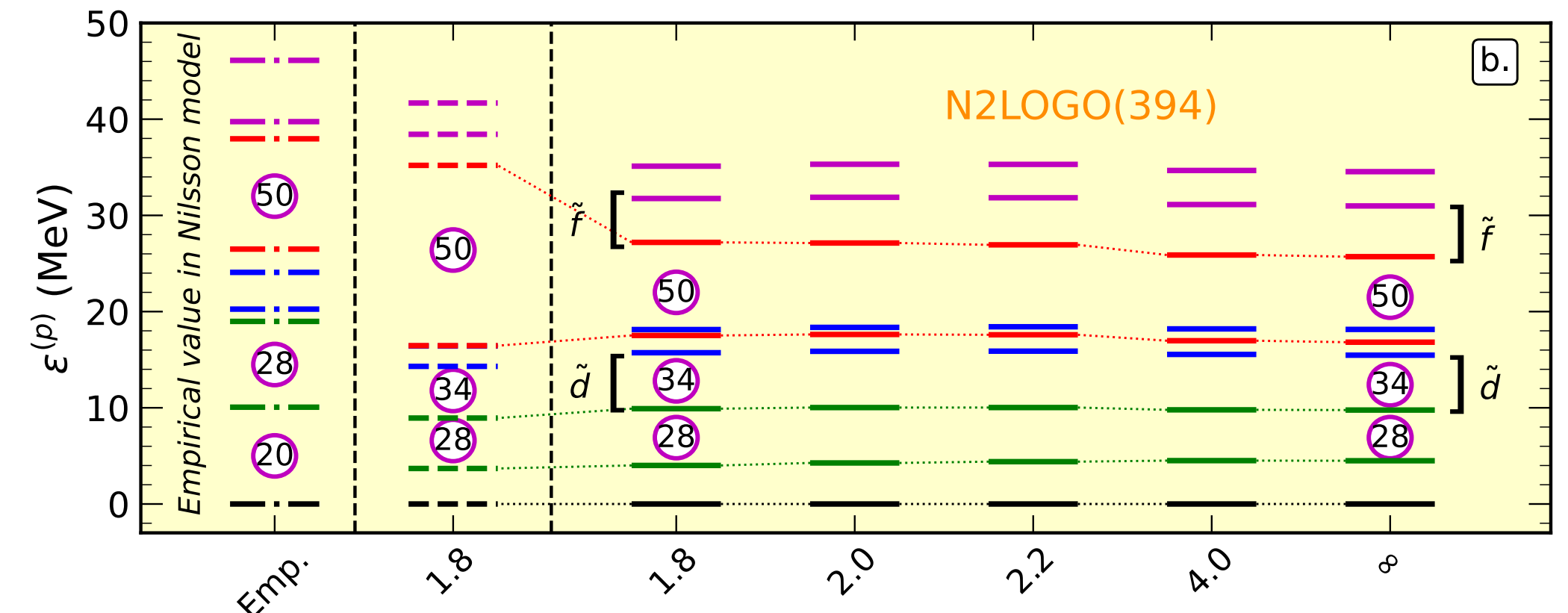
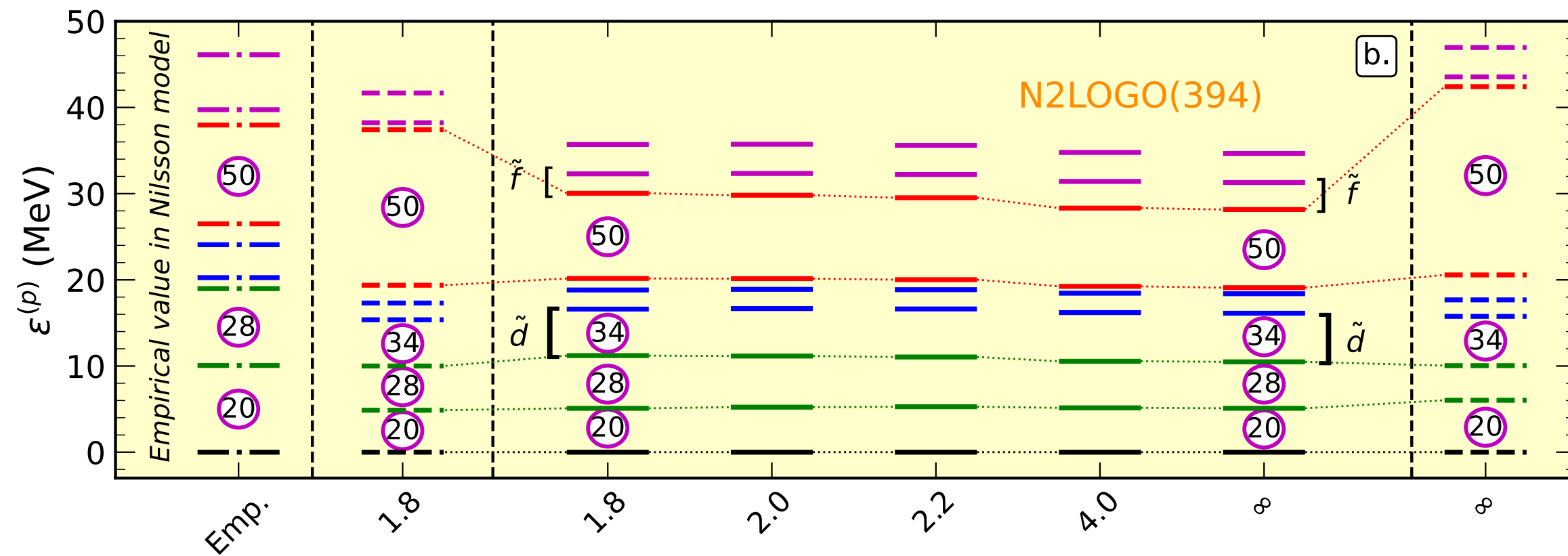
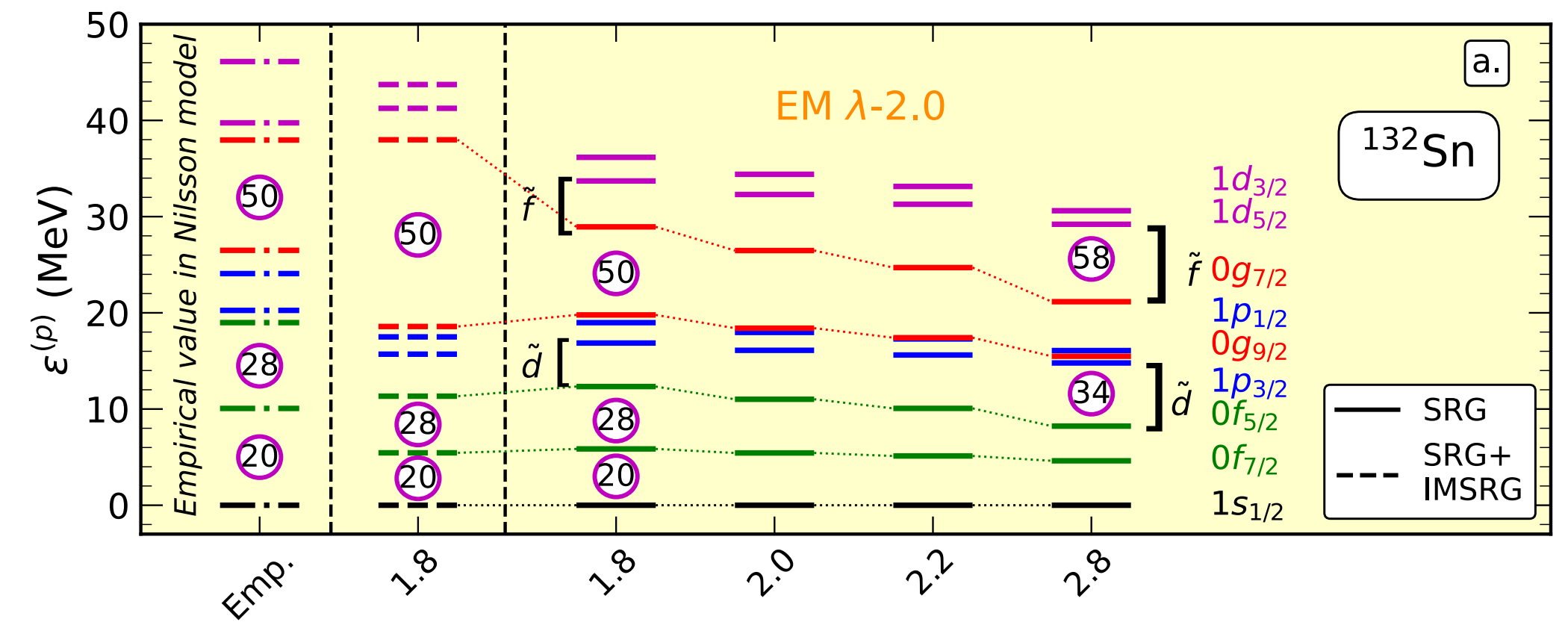
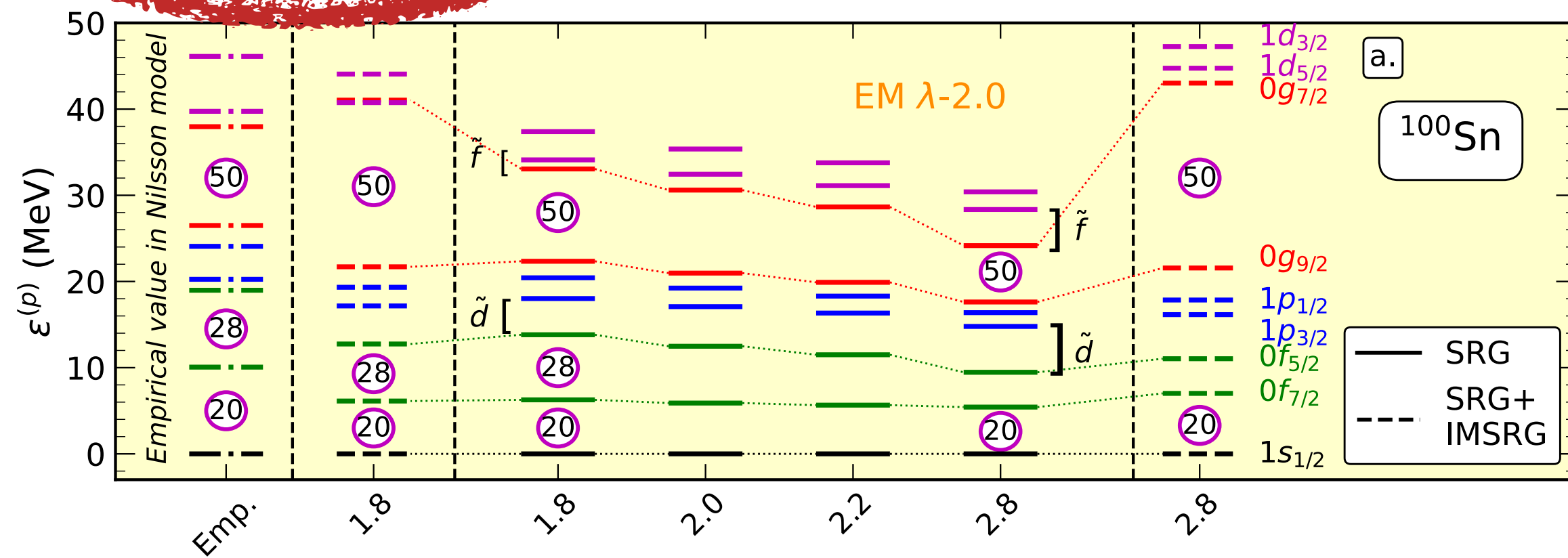
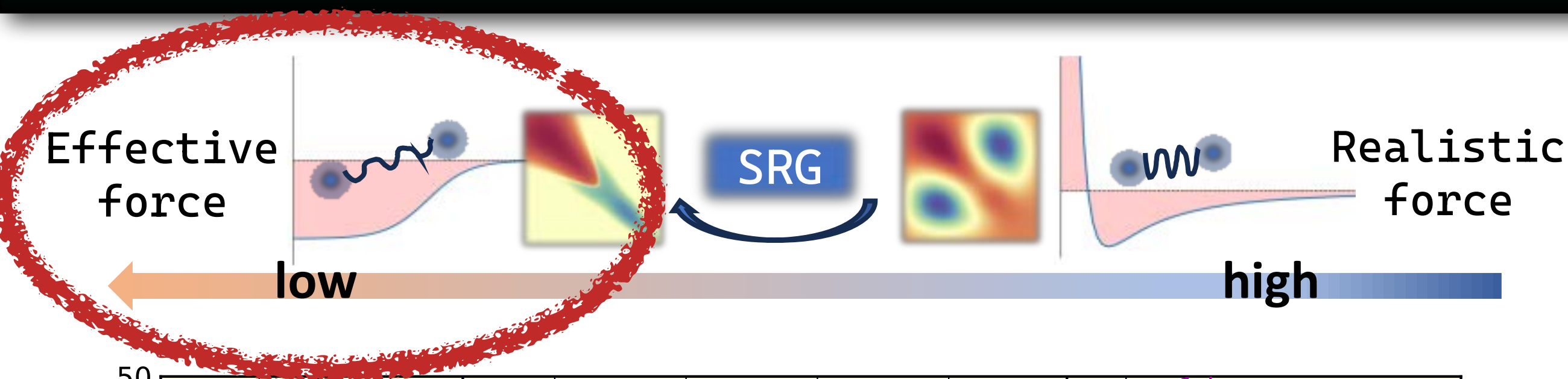
N=20 Island of Inversion Region



IM-GCM survey in progress

Pairing

Evolution of Effective Single-Particle Energies



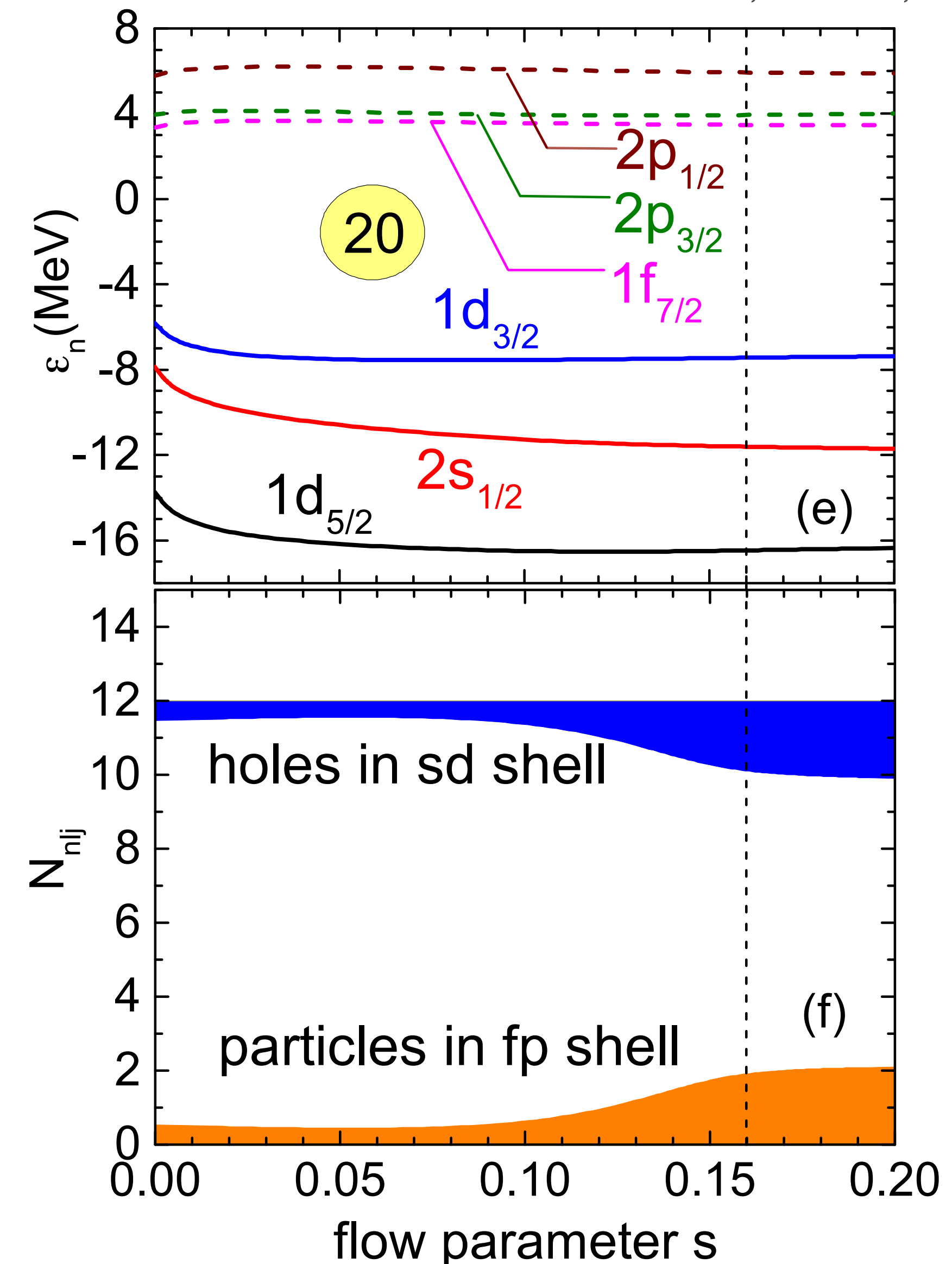
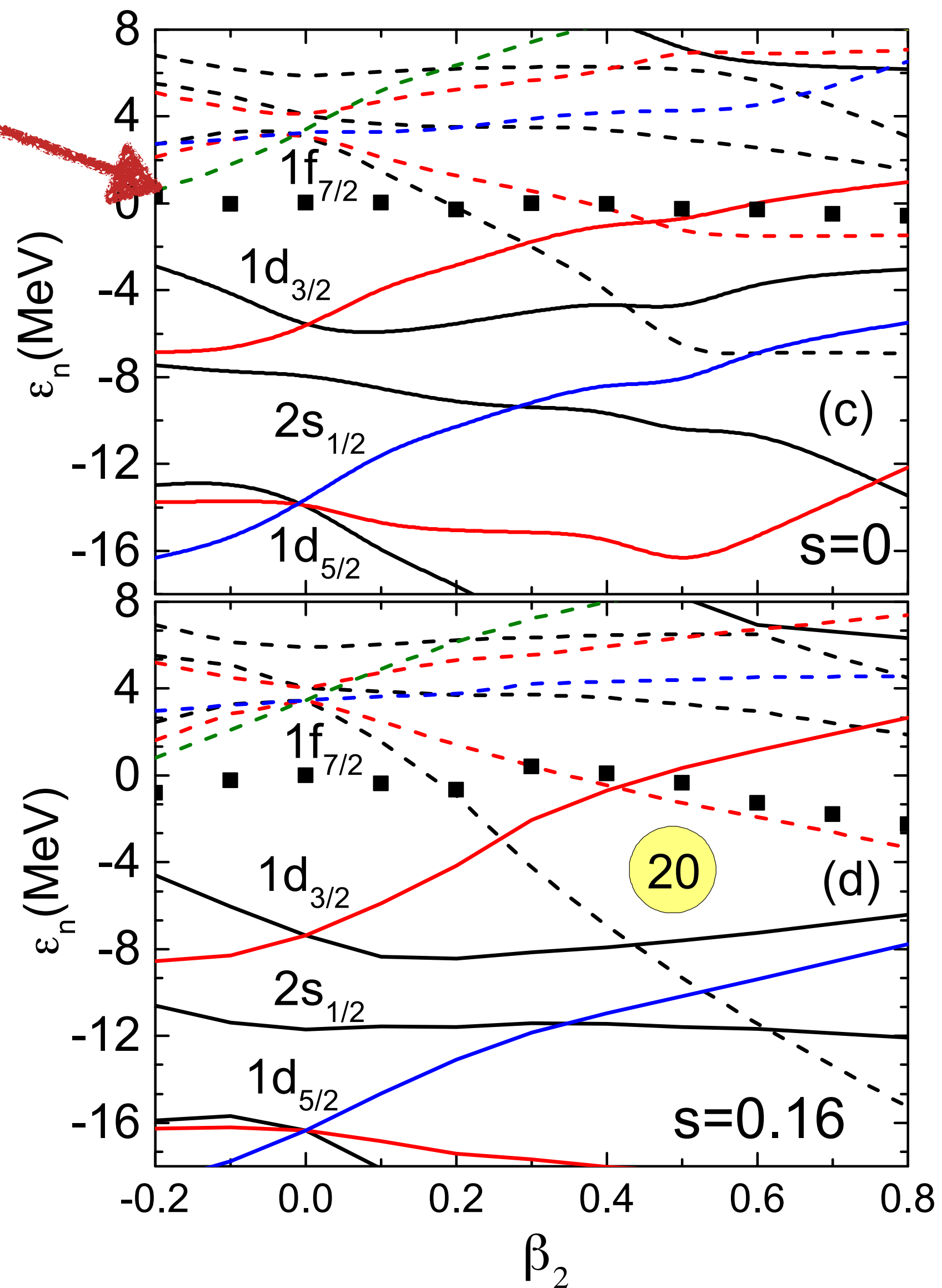
Energy scale λ (fm^{-1})

Energy scale λ (fm^{-1})

Evolution of Single-Particle Energies

E. F. Zhou et al., PLB 865, 139464 (2025) & in prep.

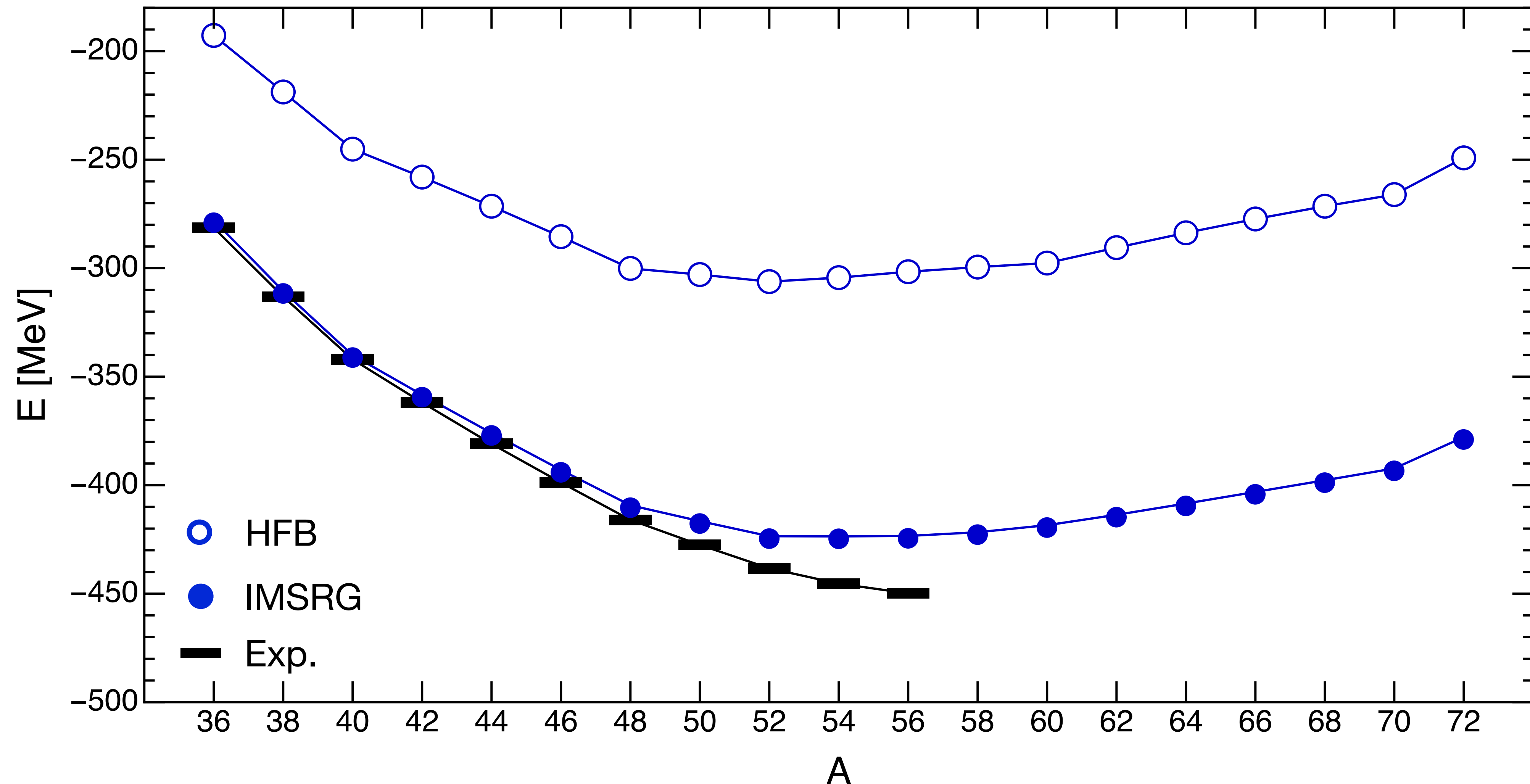
Fermi
energies



Calcium Isotopes: Ground-State Energies



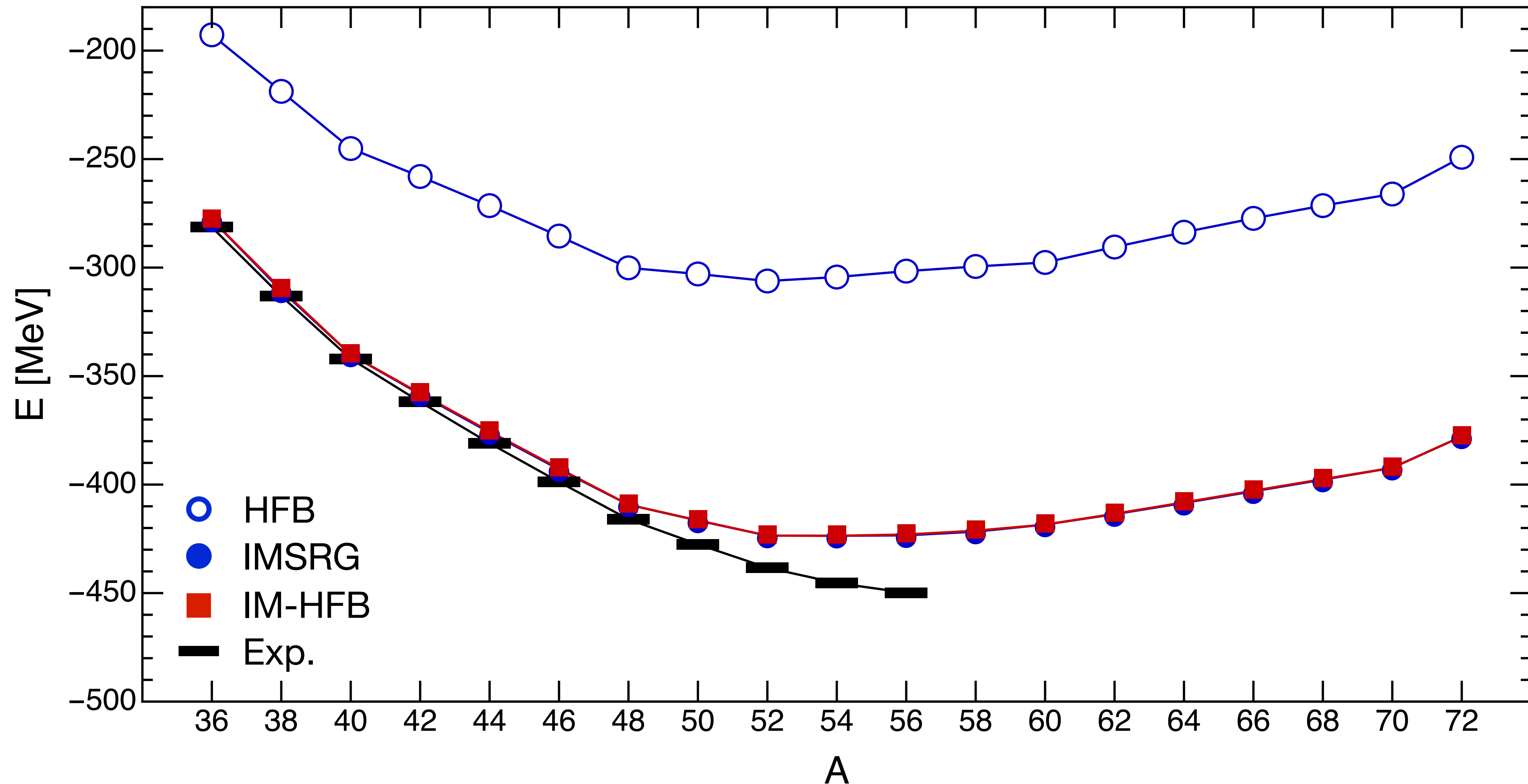
EM1.8-2.0, $e_{\text{Max}} = 8$, $E_{3\text{Max}} = 14$, $\hbar\omega = 20 \text{ MeV}$



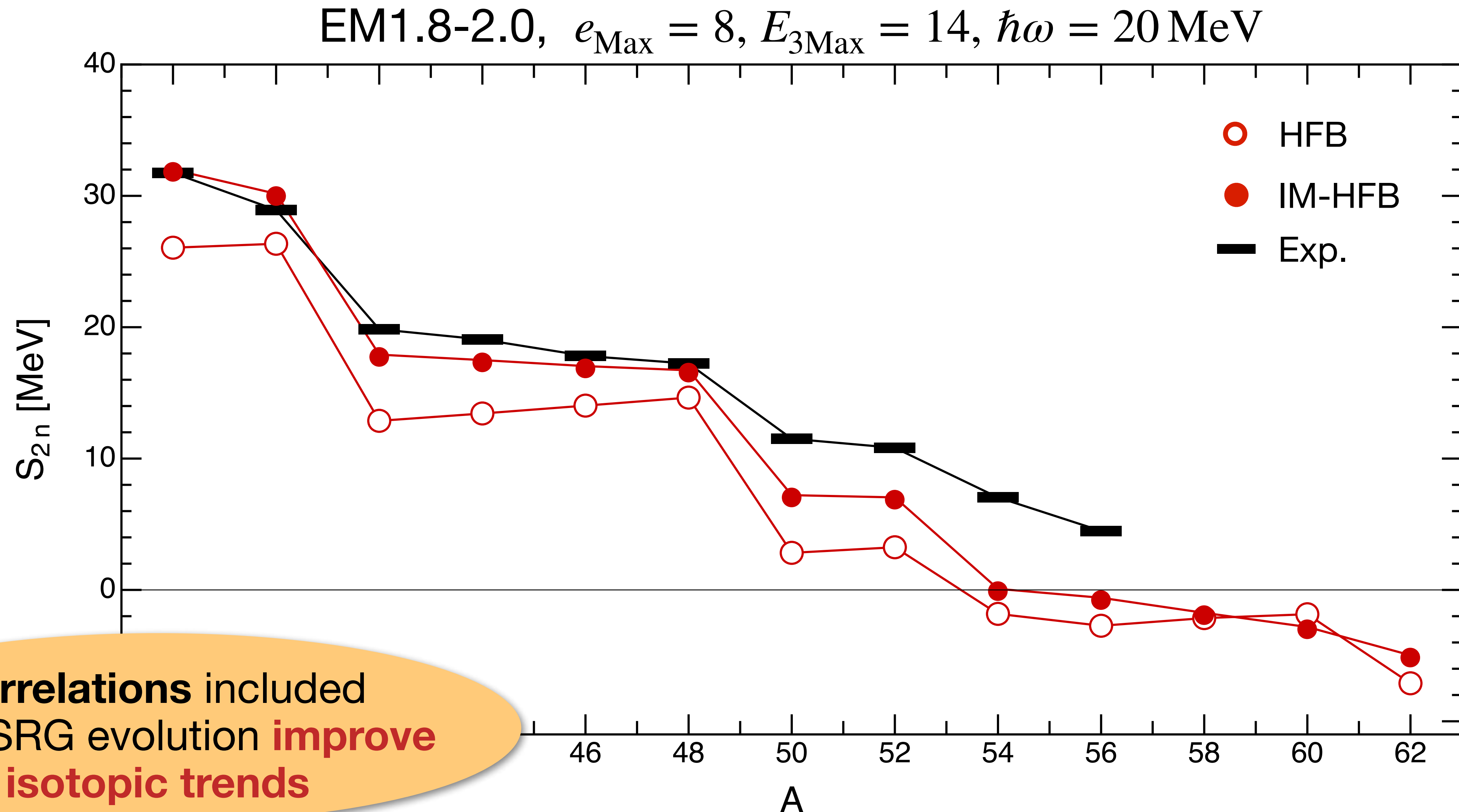
Calcium Isotopes: Ground-State Energies



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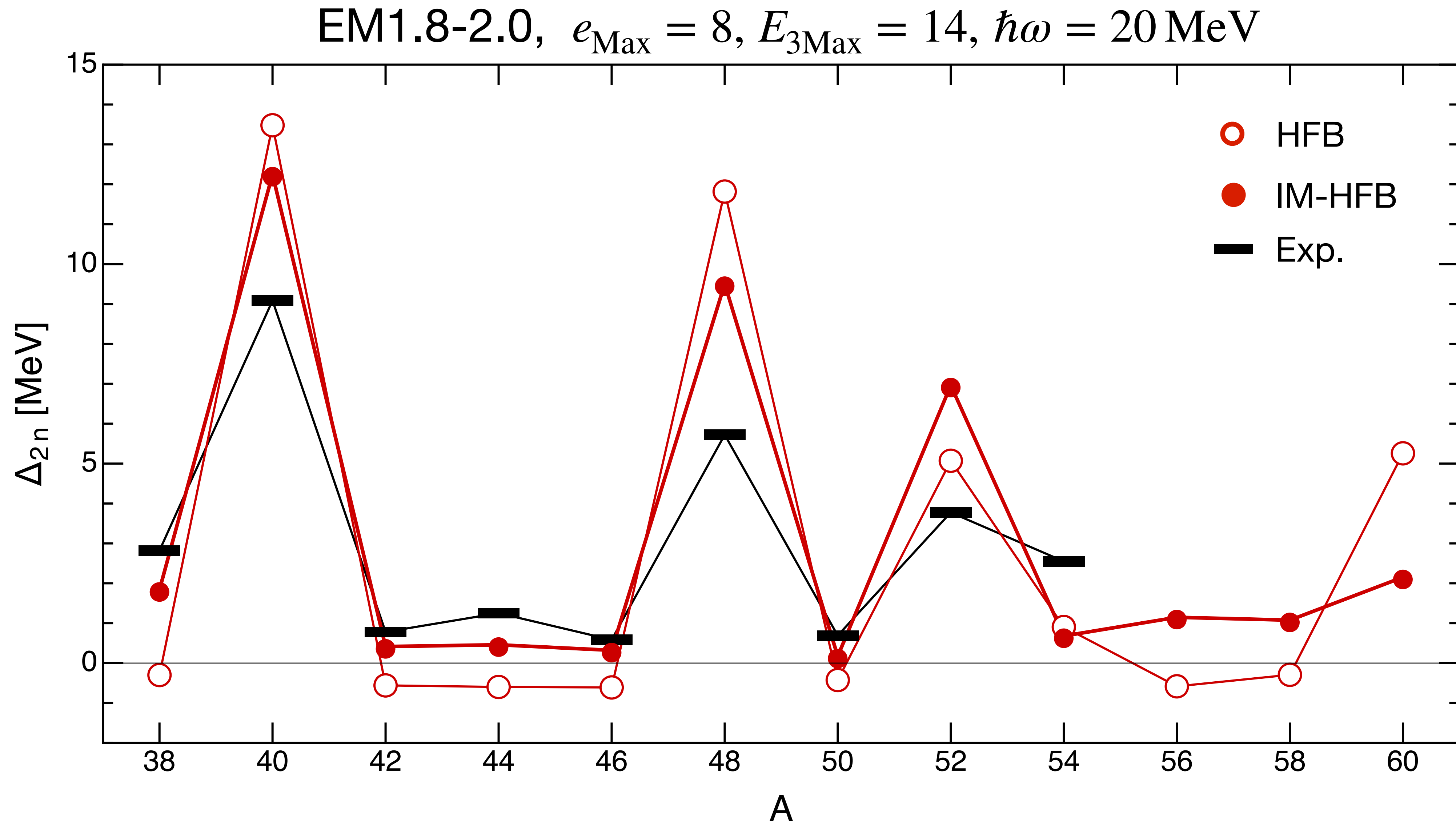


Calcium Isotopes: Two-Neutron Separation Energies



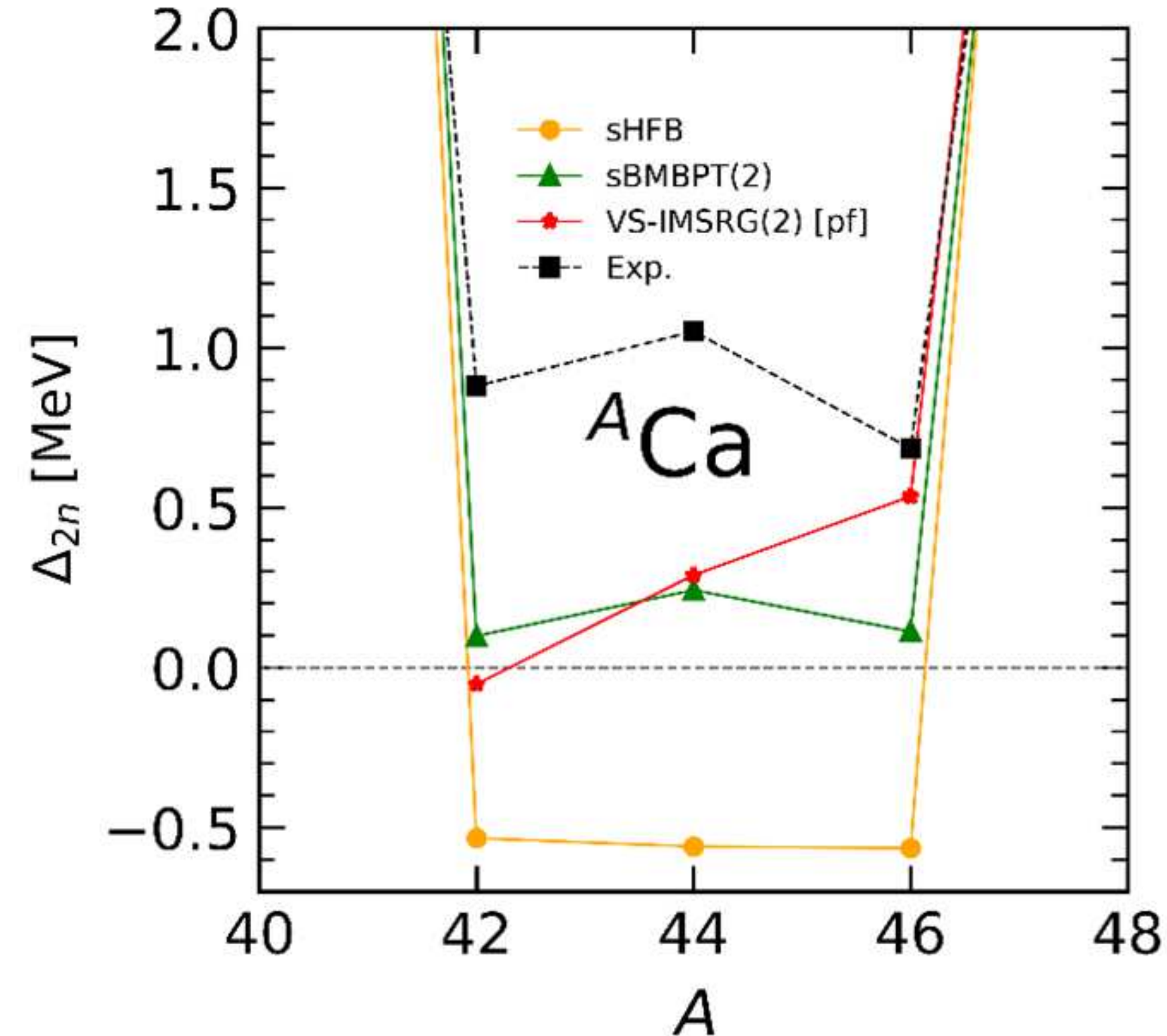
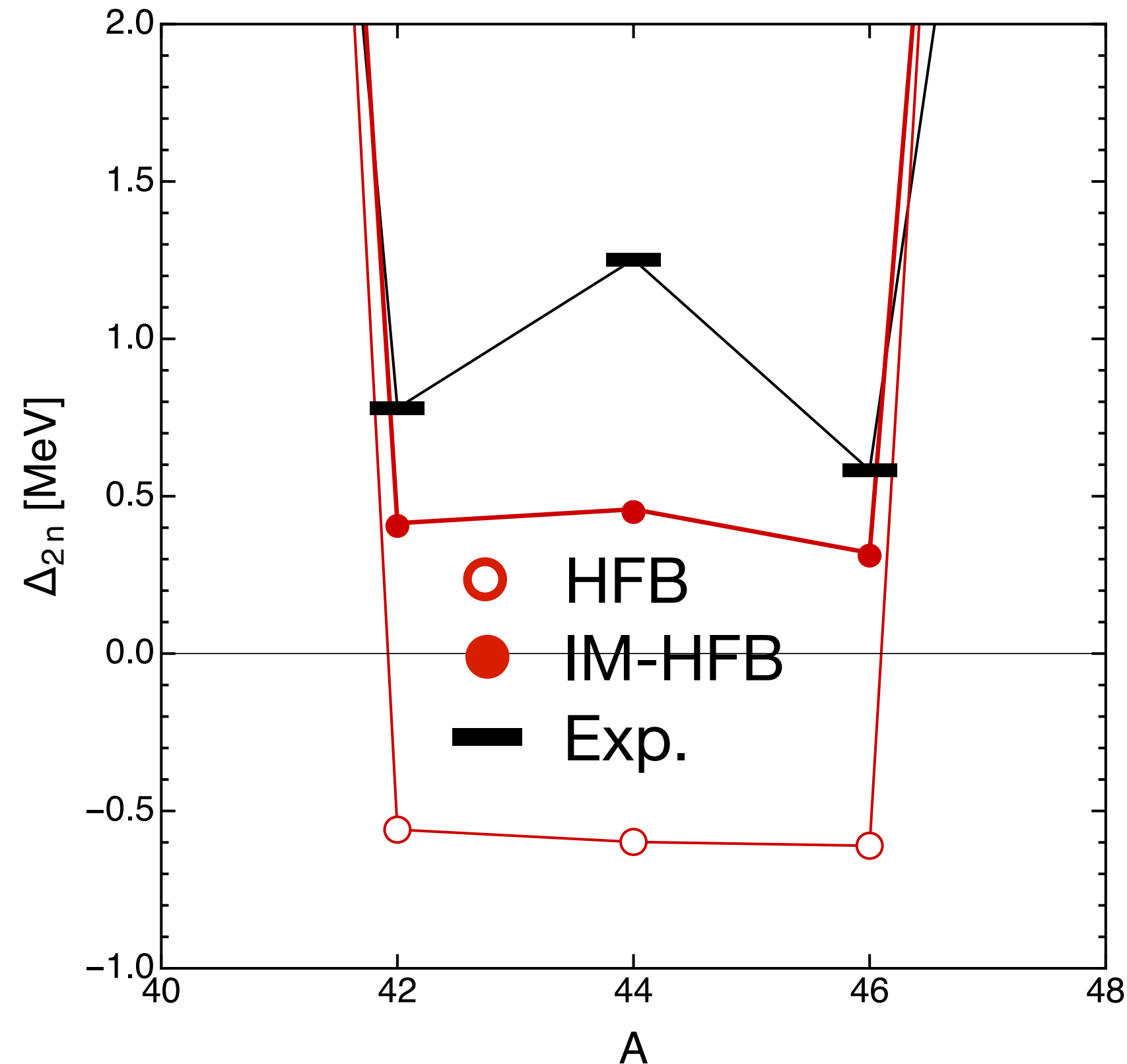
correlations included
by IMSRG evolution **improve**
isotopic trends

Calcium Isotopes: Two-Neutron Gap



Calcium Isotopes: Two-Neutron Gap

EM1.8-2.0, $e_{\text{Max}} = 8$, $E_{3\text{Max}} = 14$, $\hbar\omega = 20$ MeV

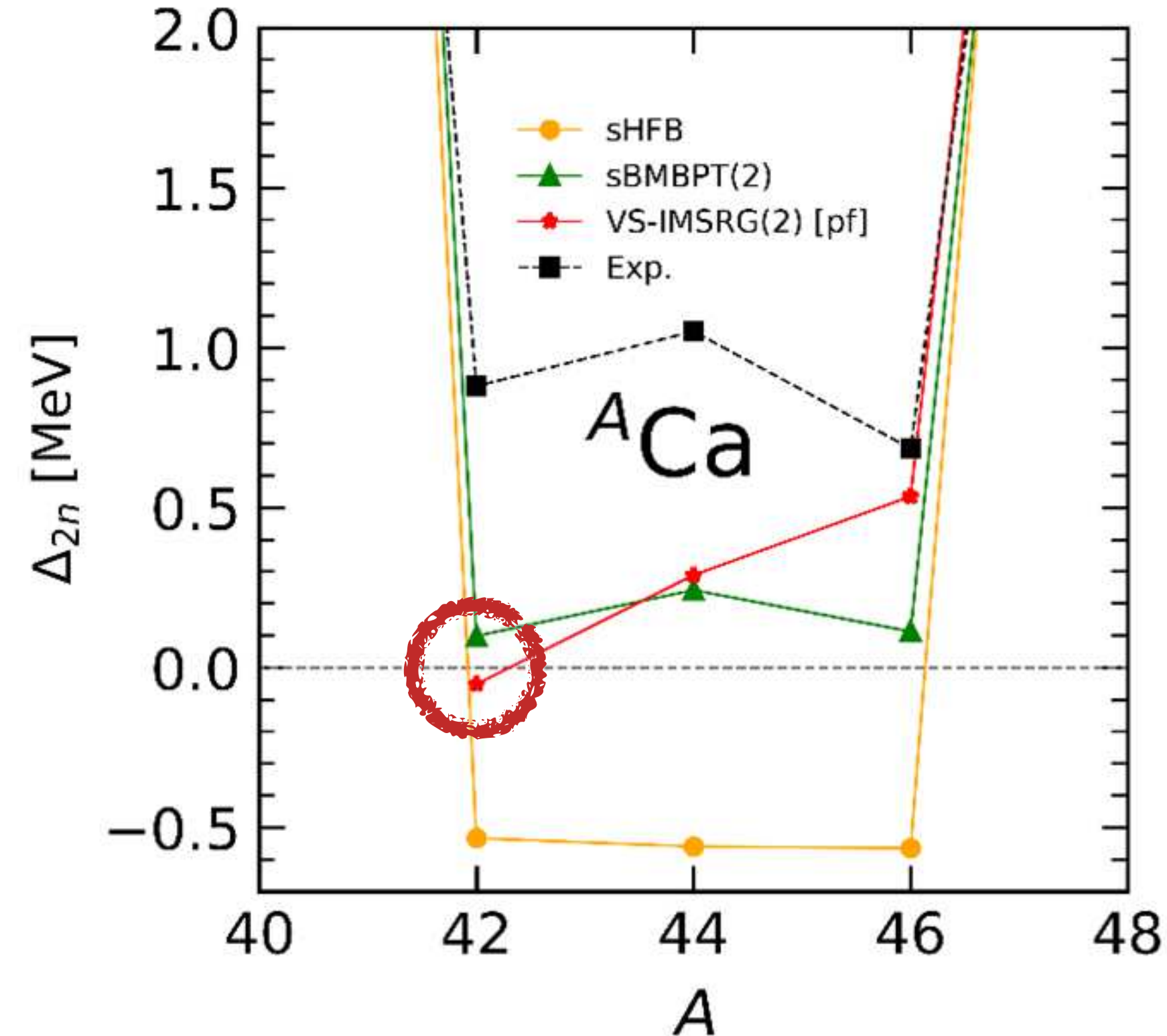
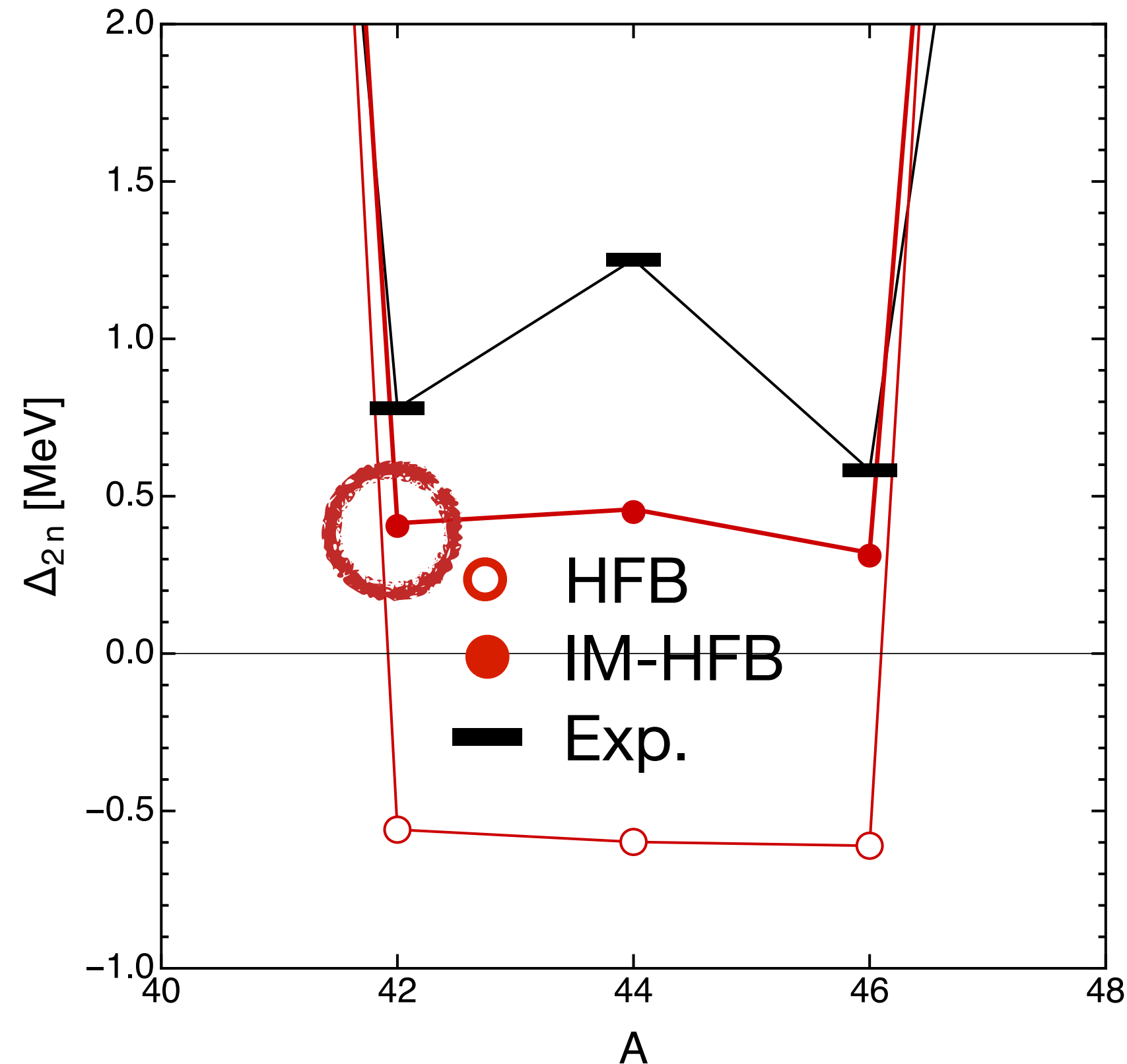


cf. talk by **T. Duguet**
and
A. Scalesi et al., EPJA
60, 209 (2024)

- IMSRG evolution gives positive Δ_{2n} , but not enough curvature
- IM-HFB calculation: no collapse of Δ_{2n} near N=20

Calcium Isotopes: Two-Neutron Gap

EM1.8-2.0, $e_{\text{Max}} = 8$, $E_{3\text{Max}} = 14$, $\hbar\omega = 20$ MeV

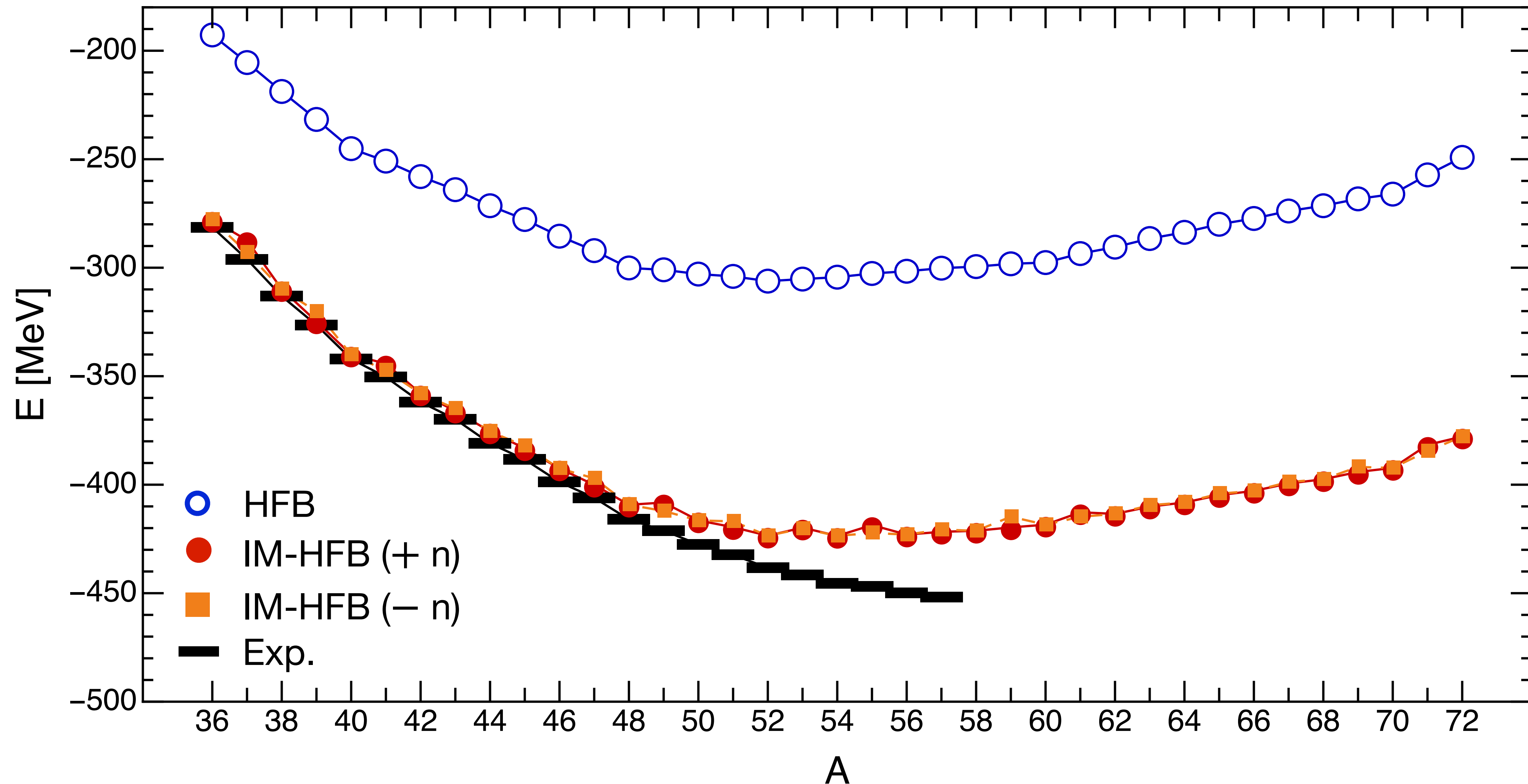


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Calcium Isotopes: Adding Odd Isotopes

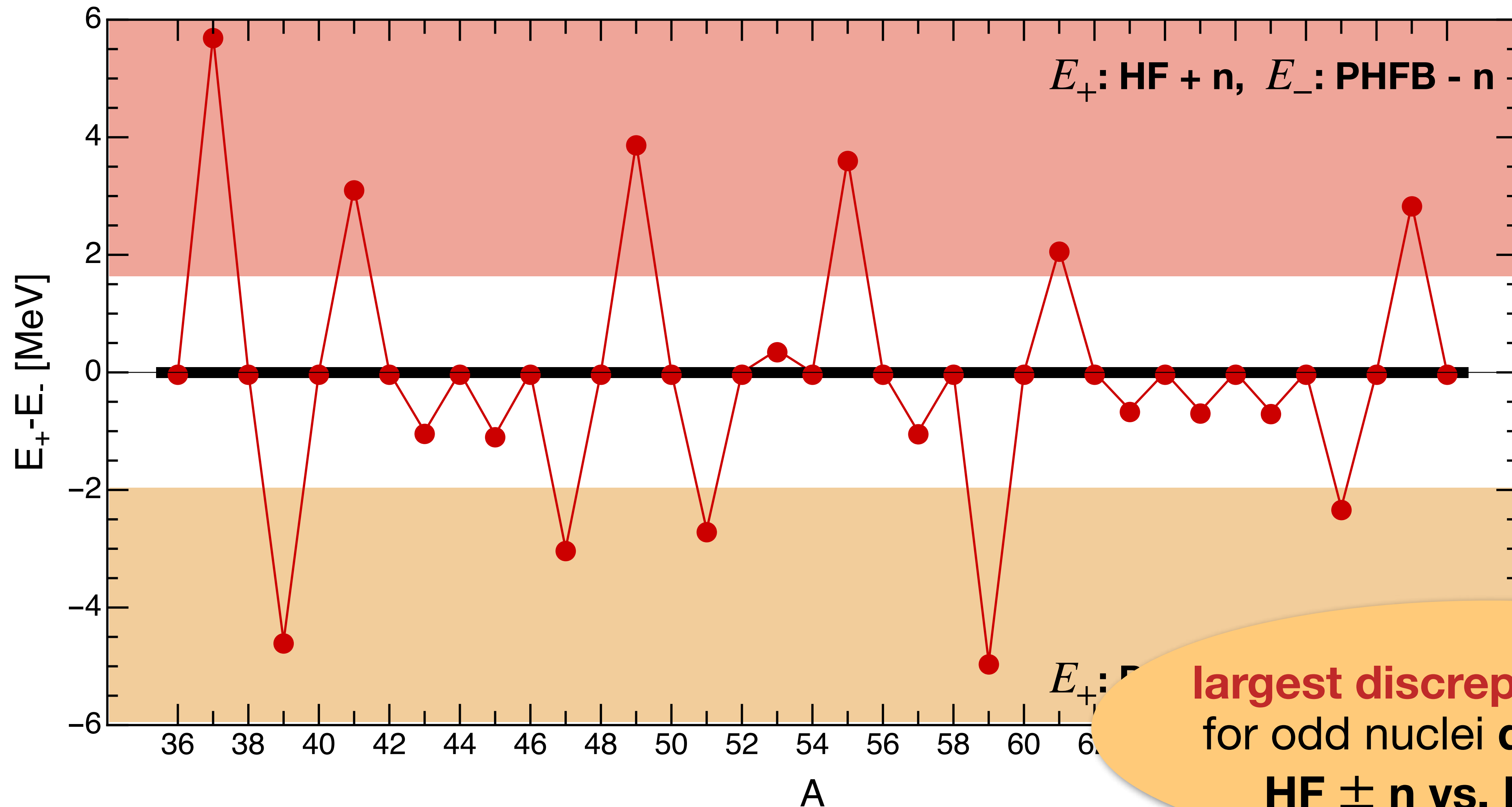
EM1.8-2.0, $e_{\text{Max}} = 8$, $E_{3\text{Max}} = 14$, $\hbar\omega = 20$ MeV



Calcium Isotopes: IM-HFB with HF vs. PHFB Reference

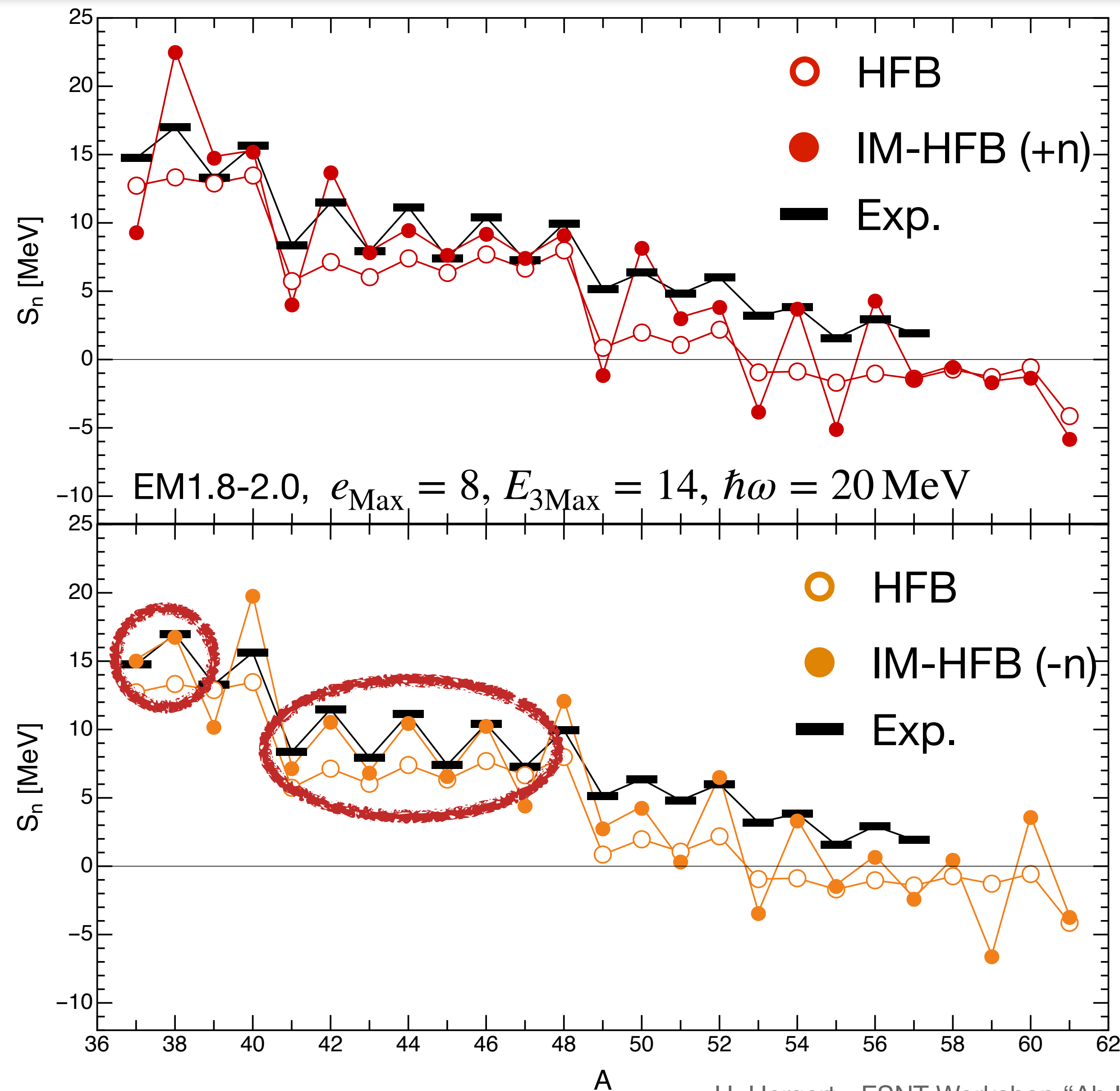


EM1.8-2.0, $e_{\text{Max}} = 8$, $E_{3\text{Max}} = 14$, $\hbar\omega = 20$ MeV



largest discrepancies occur
for odd nuclei described as
HF \pm n vs. PHFB \mp n

Calcium Isotopes: Neutron Separation Energies

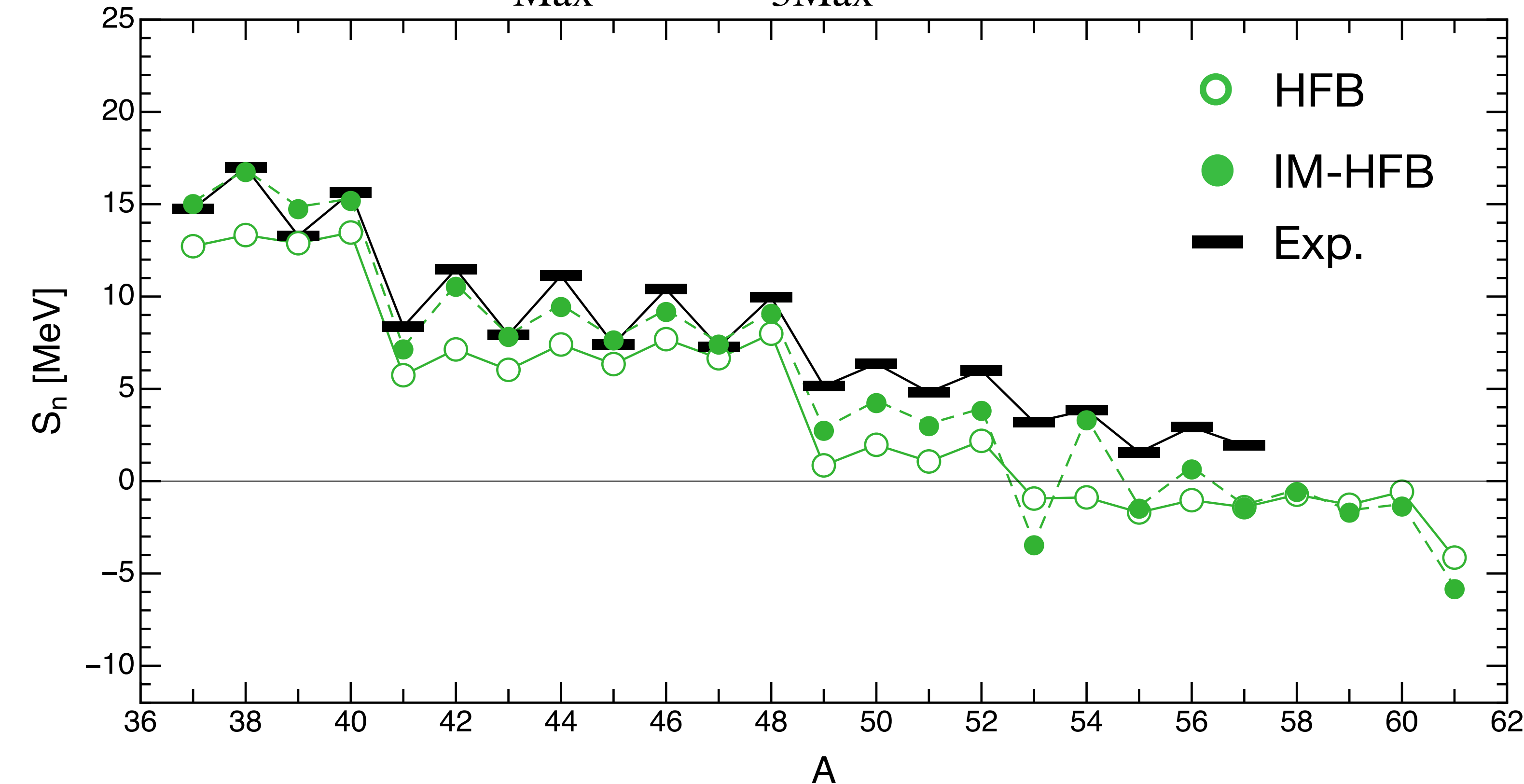


- IMSRG evolution **enhances odd-even staggering** of S_n
- largest jumps occur when combining IM-HFB based on HF and PNP references
- local description can be (surprisingly) good - in particular for IM-HFB (-n)
- no good explanation (yet)

Calcium Isotopes: Neutron Separation Energies

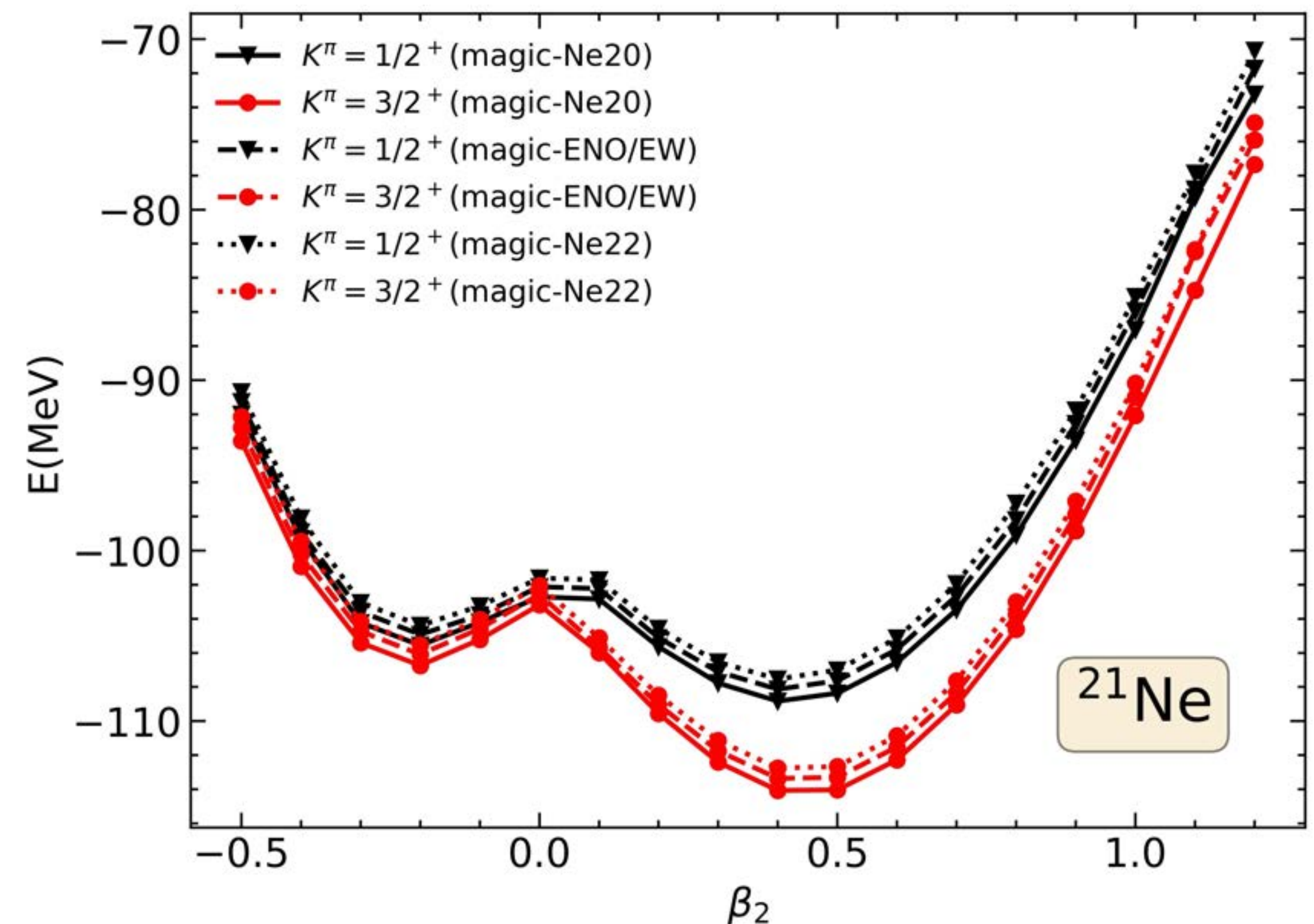
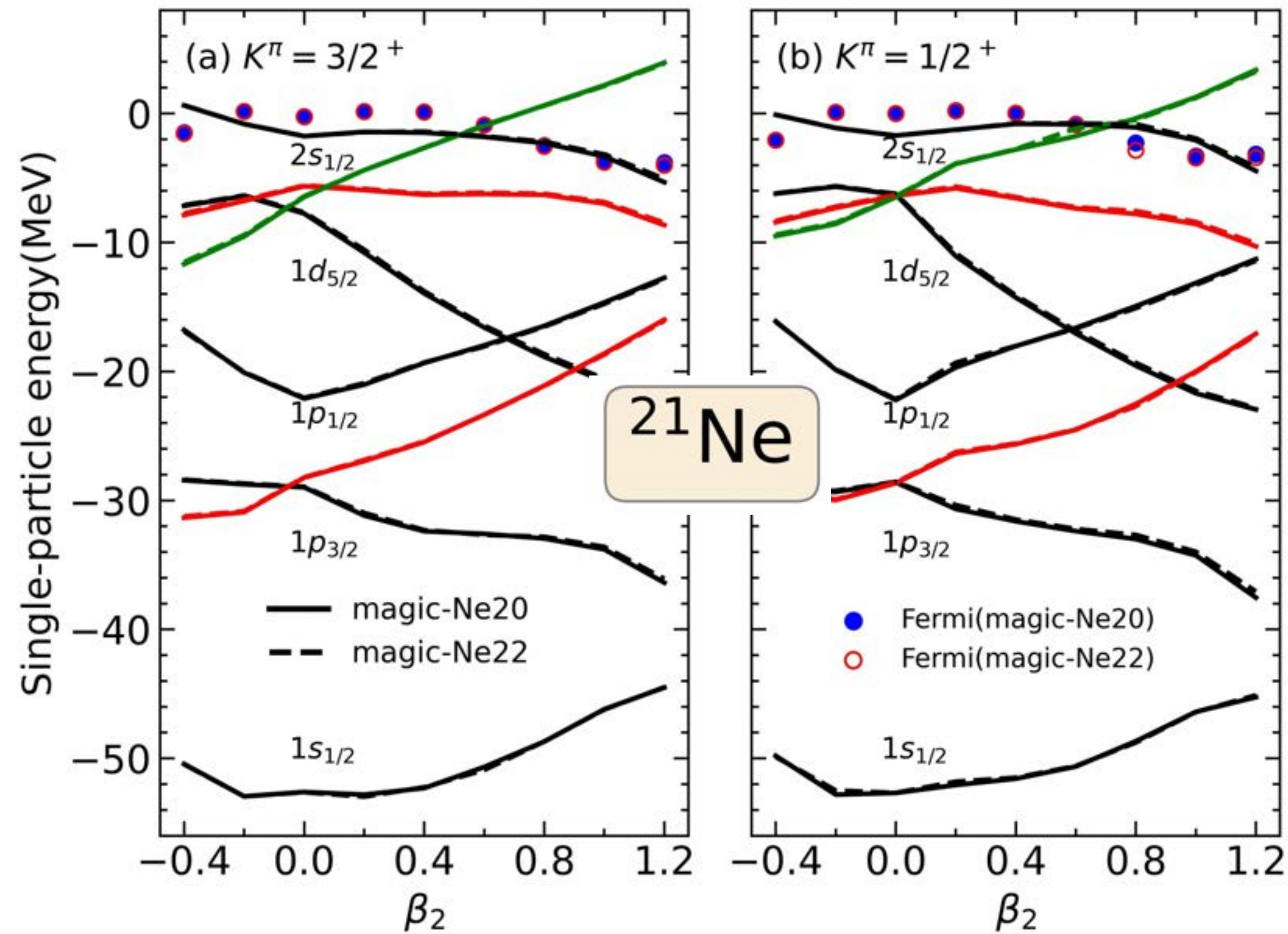


EM1.8-2.0, $e_{\text{Max}} = 8$, $E_{3\text{Max}} = 14$, $\hbar\omega = 20$ MeV



- use evolved Hamiltonian constructed with **open-shell PHFB reference**
- possible for all nuclei except ^{53}Ca
- **usually gives minimal energy in IM-HFB** (always true?)
- **next:** use spherical HFB / EFA + PNP as reference

Extension to Deformed Odd Nuclei



- perform **IMSRG evolution** using even-even $J^\pi = 0$ neighbors of odd nuclei as references and use evolved Hamiltonian to study properties (incl. pairing)
- energies, transition, PES, typically agree **within < 1% for different** neighboring references (because **equal filling approximation is avoided?**)

- describe “excited” states based on reference state $|\Phi_k\rangle = Q_k^\dagger |\Phi_0\rangle$
- **(MR-)IMSRG effective Hamiltonian** in EOM approach:

$$[H(s), Q_k^\dagger(s)] |\Phi_0\rangle = \omega_k(s) Q_k^\dagger(s) |\Phi_0\rangle, \quad \omega_k(s) \equiv E_k(s) - E_0(s)$$

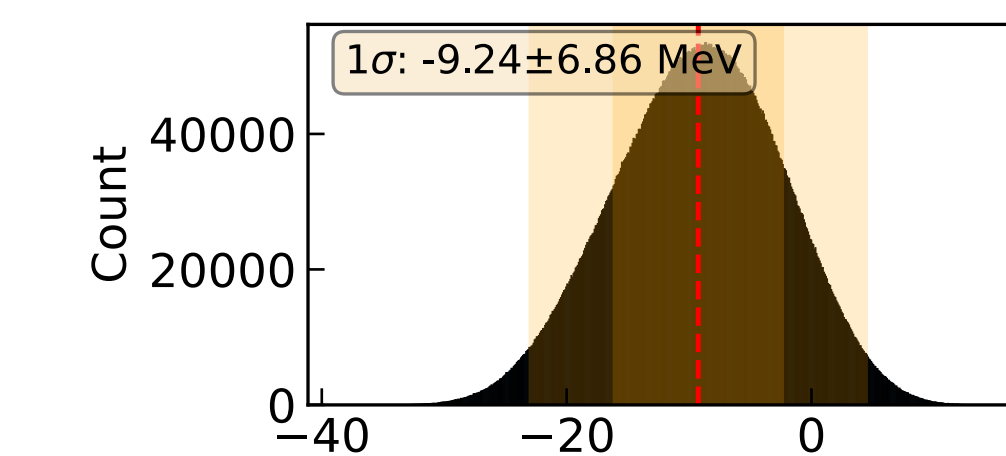
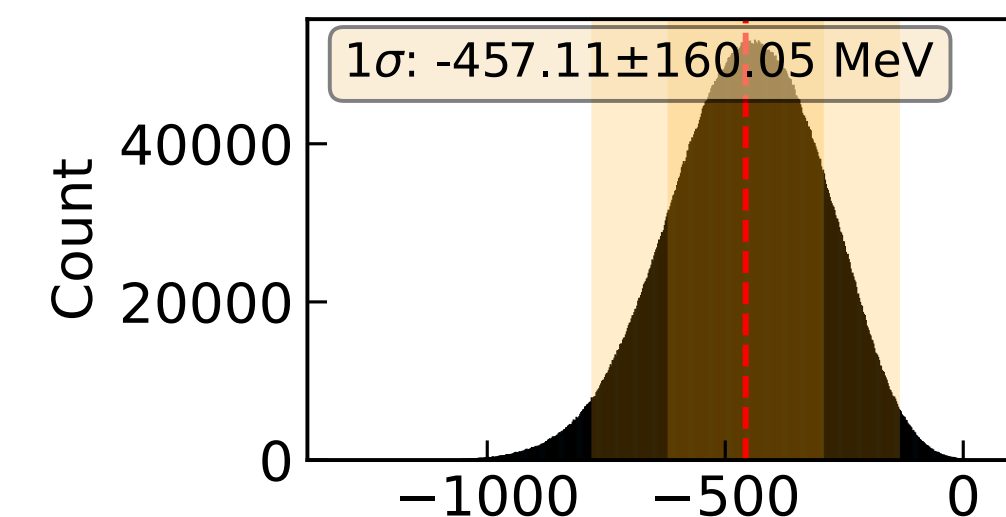
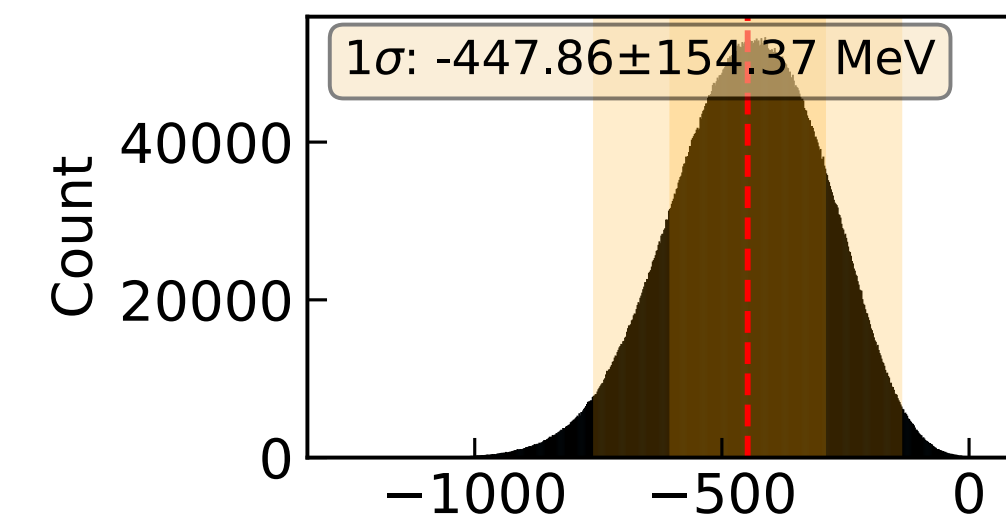
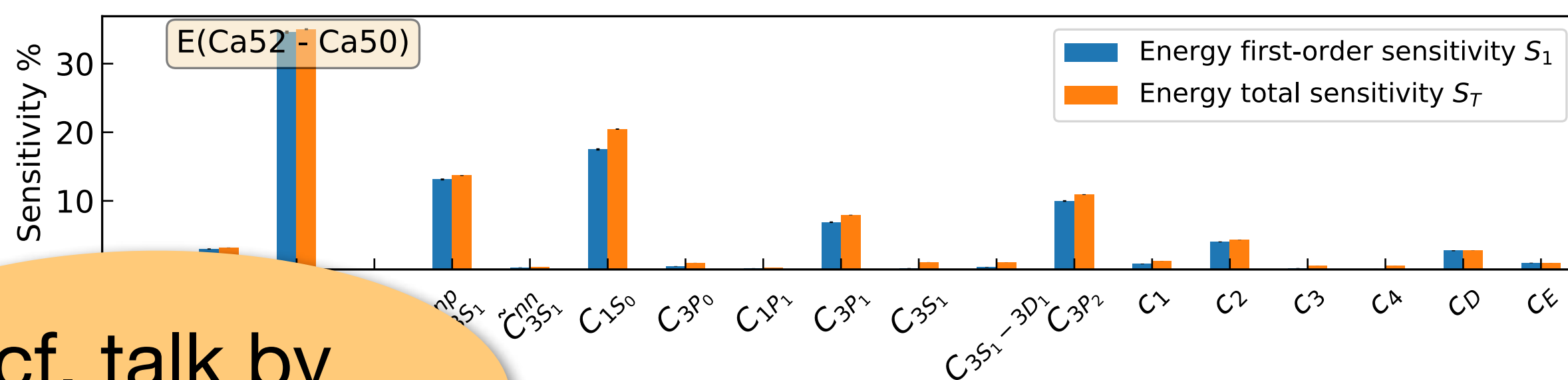
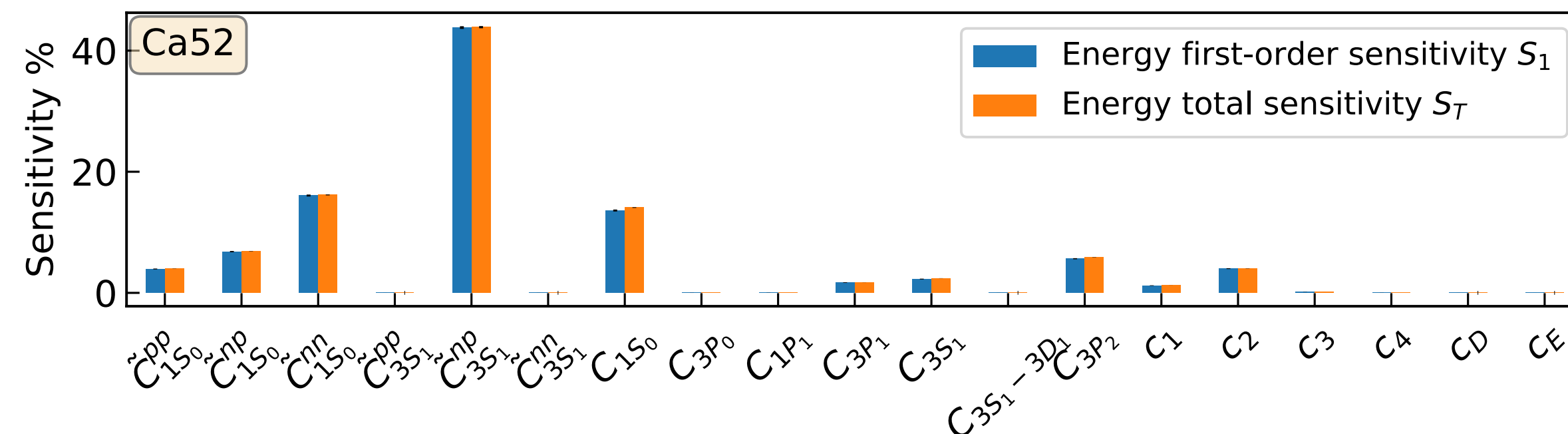
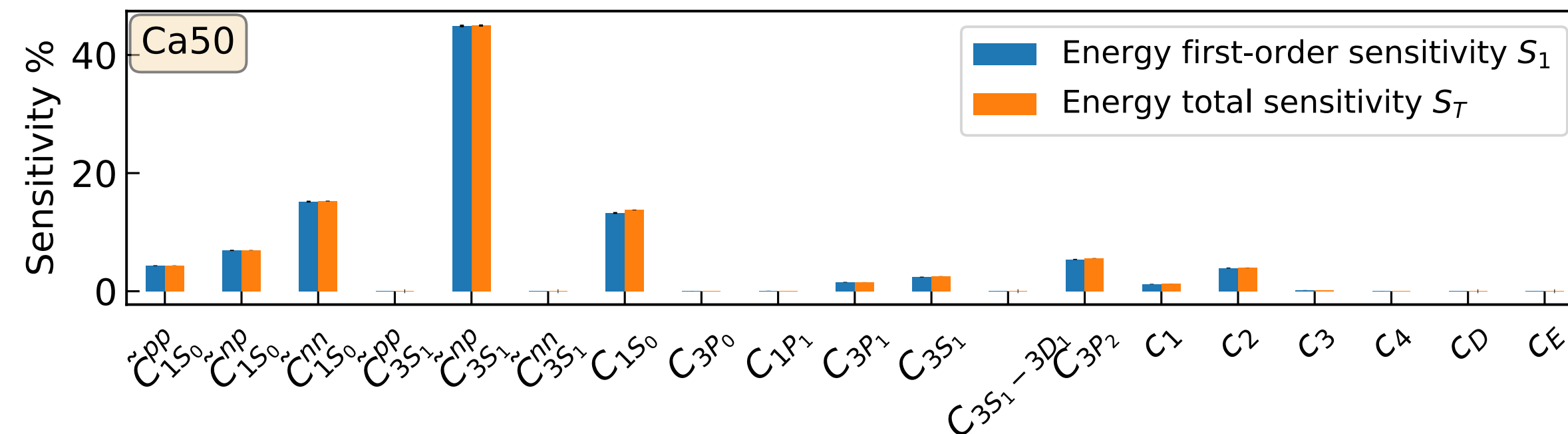
- **approximations** make $\omega_k(s)$ **s-dependent**
- ansätze for excitation operators (**g.s. correlations built into Hamiltonian**):

$$Q_k^\dagger(s) = \sum_{pq} (Q^{(k)})_{pq}(s) : a_p^\dagger a_q : + \frac{1}{4} \sum_{pqrs} (Q^{(k)})_{pqrs}(s) : a_p^\dagger a_q^\dagger a_s a_r : + \dots$$

$$Q_k^\dagger(s) = \sum_p (Q_k^{(k)})_p(s) : a_p^\dagger : + \frac{1}{4} \sum_{pqr} (Q^{(k)})_{pqr}(s) : a_p^\dagger a_q^\dagger a_r : + \dots$$

- **polynomial** effort, commutator formulation **identical to flow equations**

Outlook: IMSRG Emulators



- non-invasive **ROM** emulator based on **Dynamic Mode Decomposition**
- $\Delta\text{NNLO}_{\text{GO}}$, NN+3N,
 $e_{\text{max}} = 12$,
 $E_{3\text{max}} = 14$
- O(10M) samples
- **computational effort reduced by 5+ orders of magnitude**

cf. talk by
A. Ekström

Summary

- **improved truncations:** (MR-)IMSRG(3) + factorized approximations, tailored operator bases
 - full MR-IMSRG(3) is worked out, but scaling is prohibitive for everyday use (and implementation would require automation)
- **accelerate IMSRG & IM-GCM**
 - **compression & tensor factorization**
 - model reduction for **projection / GCM kernels**
- **uncertainty quantification / sensitivity analysis**
 - emulator development: DMD, POD, Parametric Matrix Models, ...
- **applications**
 - working on requests from multiple experimental groups
 - nuclear observables relevant for BSM physics (beta decays for CKM unitarity, Schiff moments, ...)

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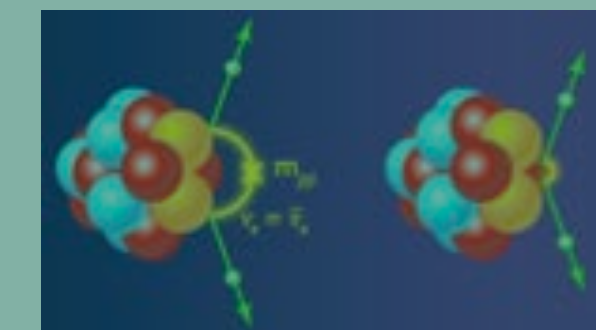
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and many more...

Thank you for your attention!



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