In-Medium SRG for Deformed Nuclei and Other New Developments

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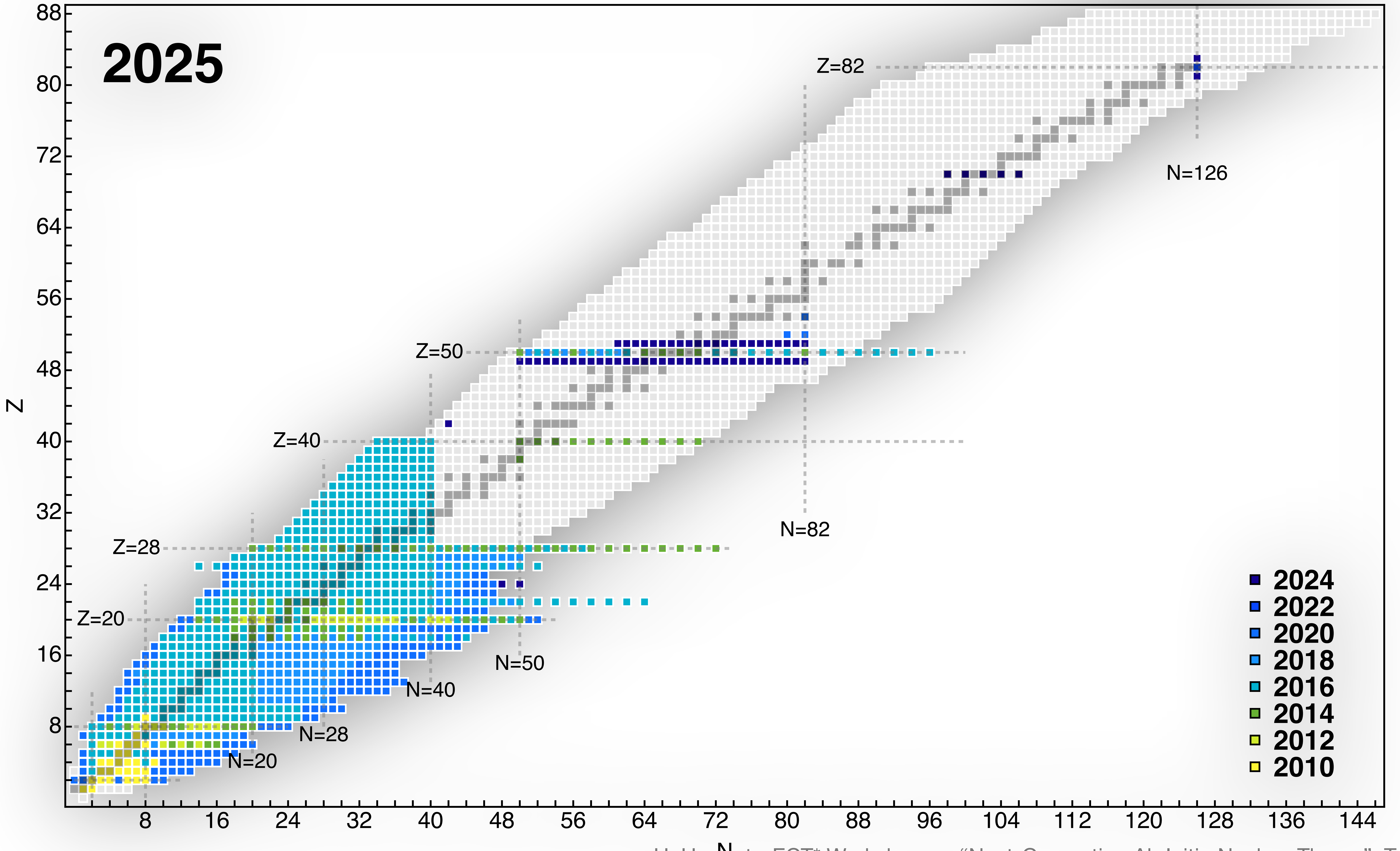
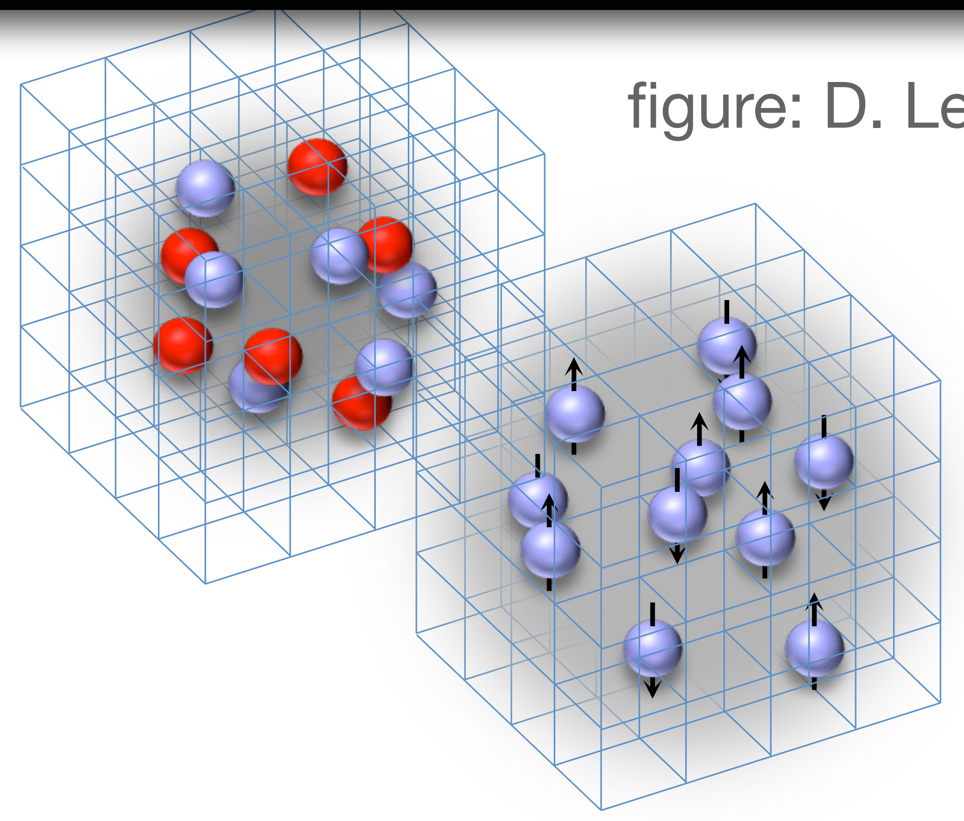
Progress in *Ab Initio* Calculations

[cf. HH, Front. Phys. **8**, 379 (2020)]

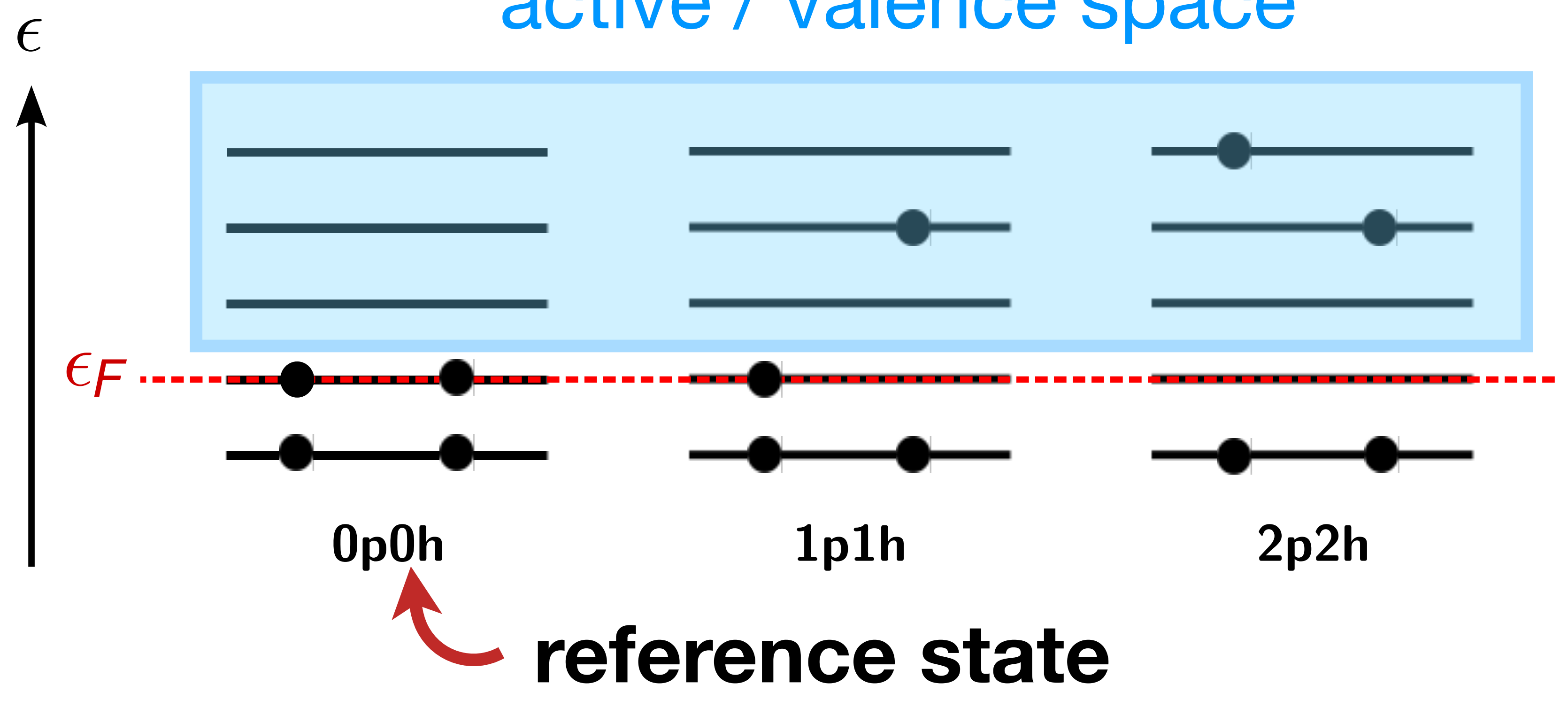


Many-Body Methods: Paradigms

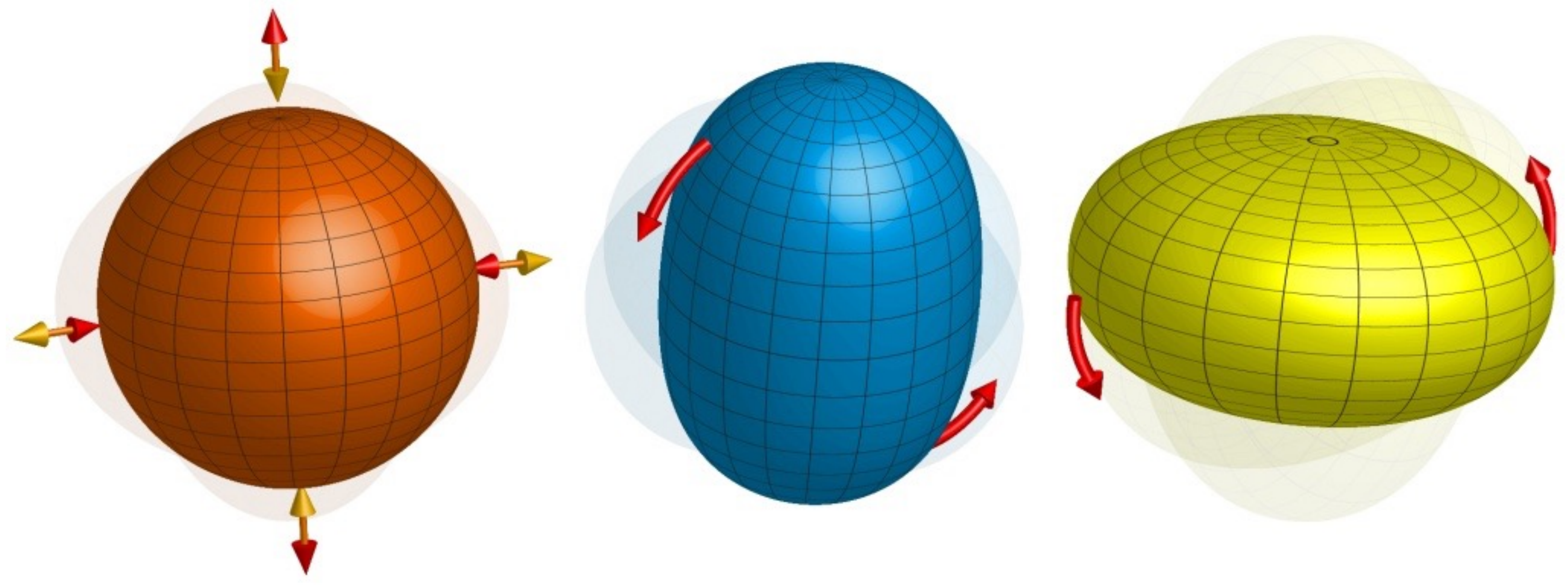
- **Coordinate Space**
  - Quantum Monte Carlo
  - Lattice EFT



- **Configuration Space: Particle-Hole Expansions**
  - Many-Body Perturbation Theory (MBPT)
  - (No-Core) Configuration Interaction (aka Shell Model, (NC)SM)
  - Coupled Cluster (CC)
  - In-Medium Similarity Renormalization Group (IMSRG)
  - Self-Consistent Green's Functions (SCGF / ADC)



- **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

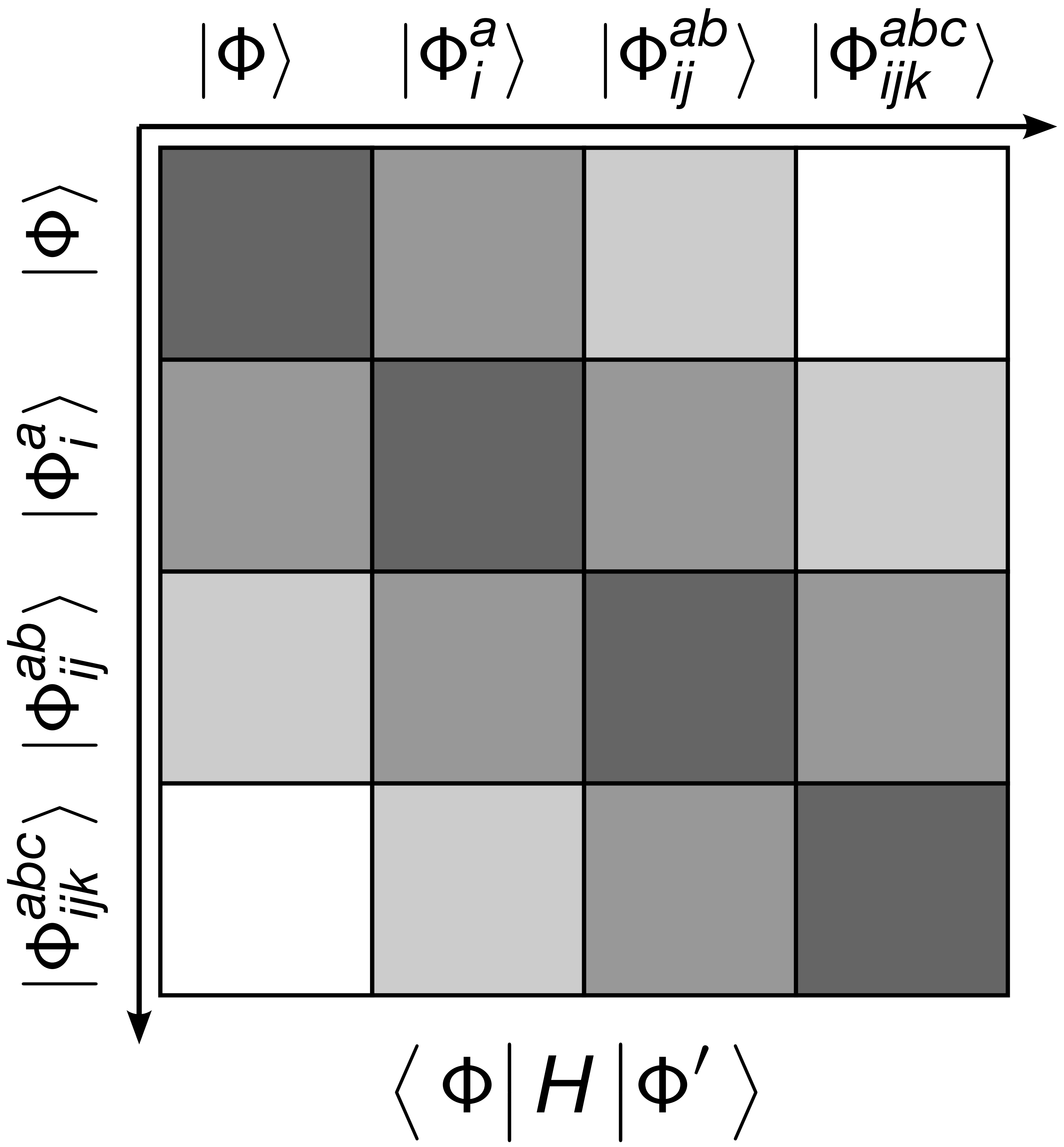
Recent(-ish) Reviews:
HH, Front. Phys. **8**, 379 (2020)
S. Gandolfi, D. Lonardoni, A. Lovato and M. Piarulli, Front. Phys. **8**, 117 (2020)
D. Lee, Front. Phys. **8**, 174 (2020)
V. Somà, Front. Phys. **8**, 340 (2020)

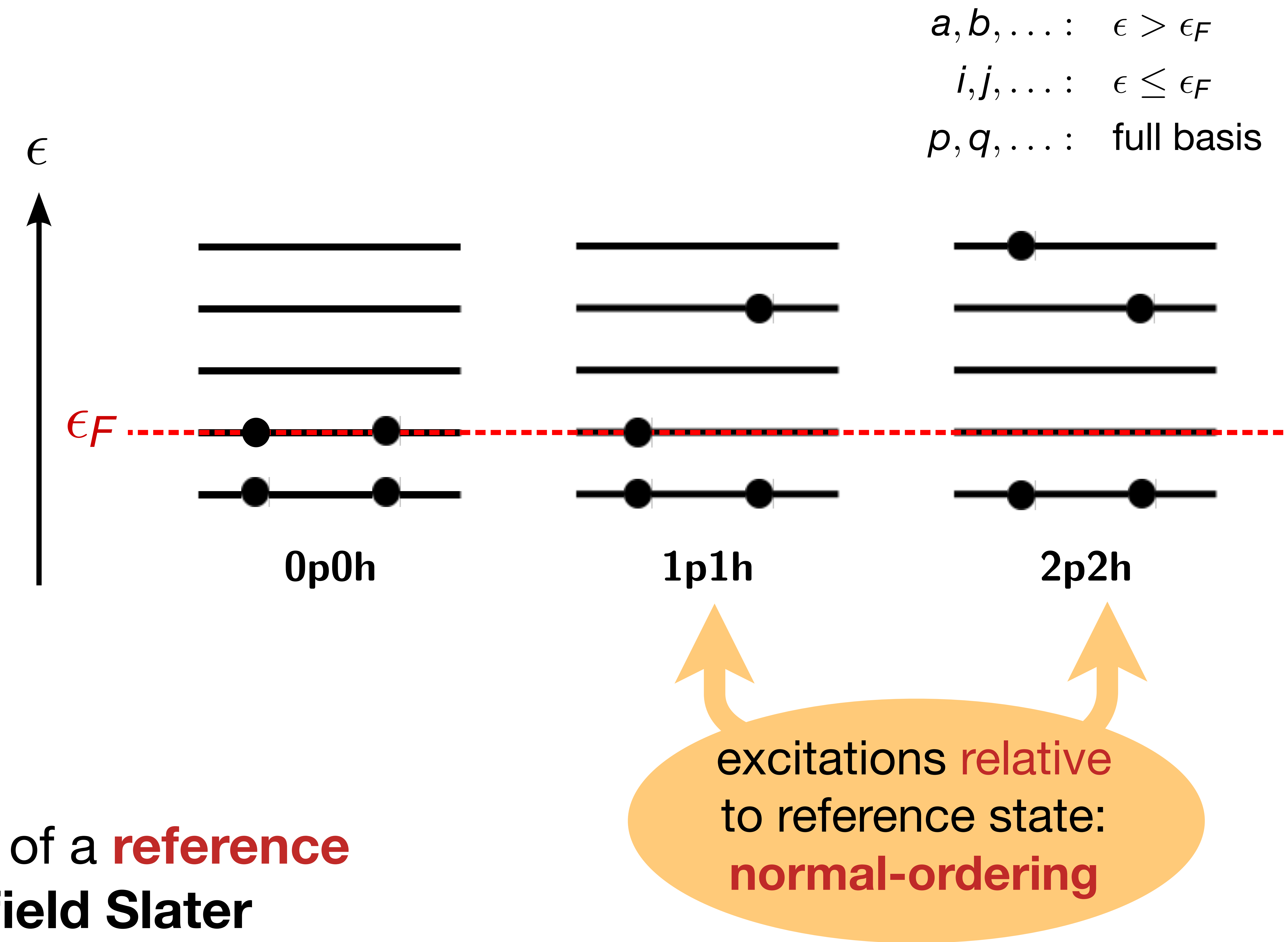
also see
“What is *ab initio* in nuclear theory?”, A. Ekström, C. Forssén, G. Hagen, G. R. Jansen, W. Jiang, T. Papenbrock, Front. Phys. **11**, 1129094 (2023)

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

In-Medium SRG Methods for Deformed Nuclei

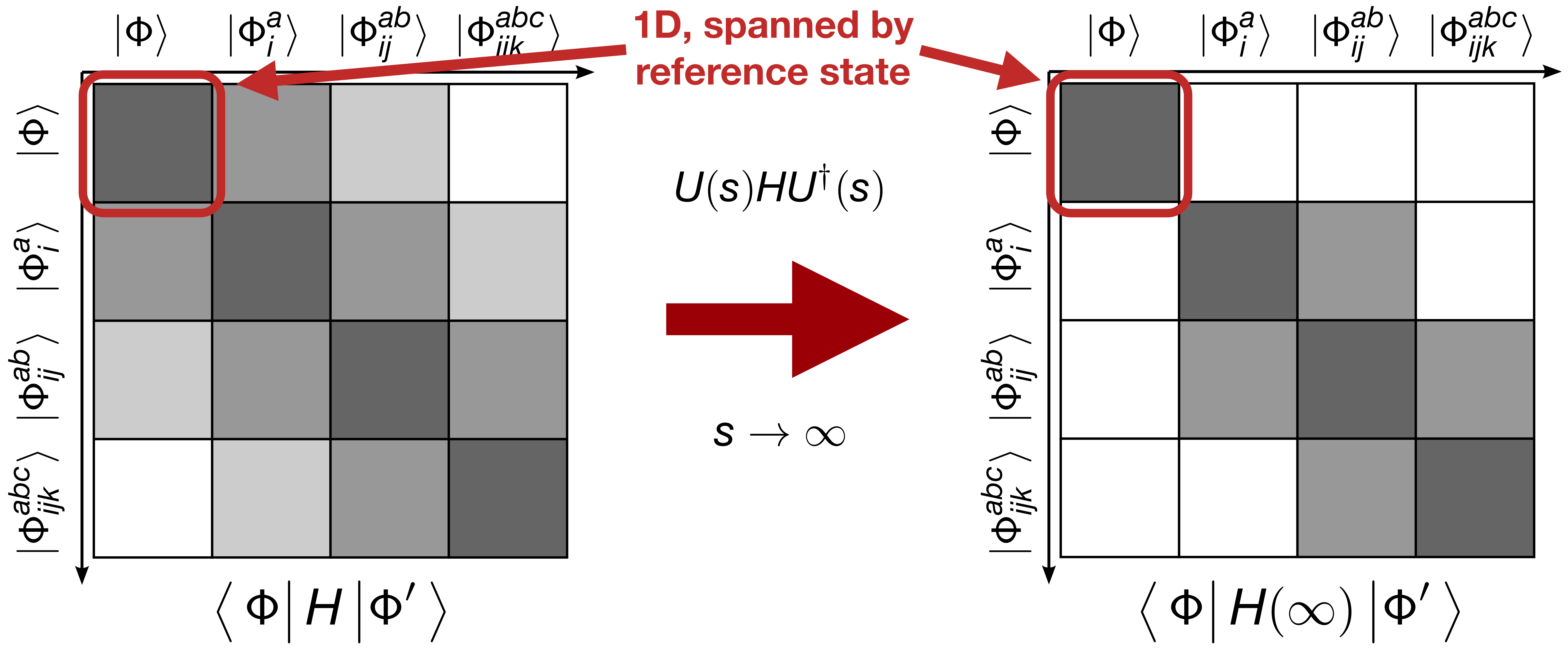
Many-Body Methods: Configuration Space





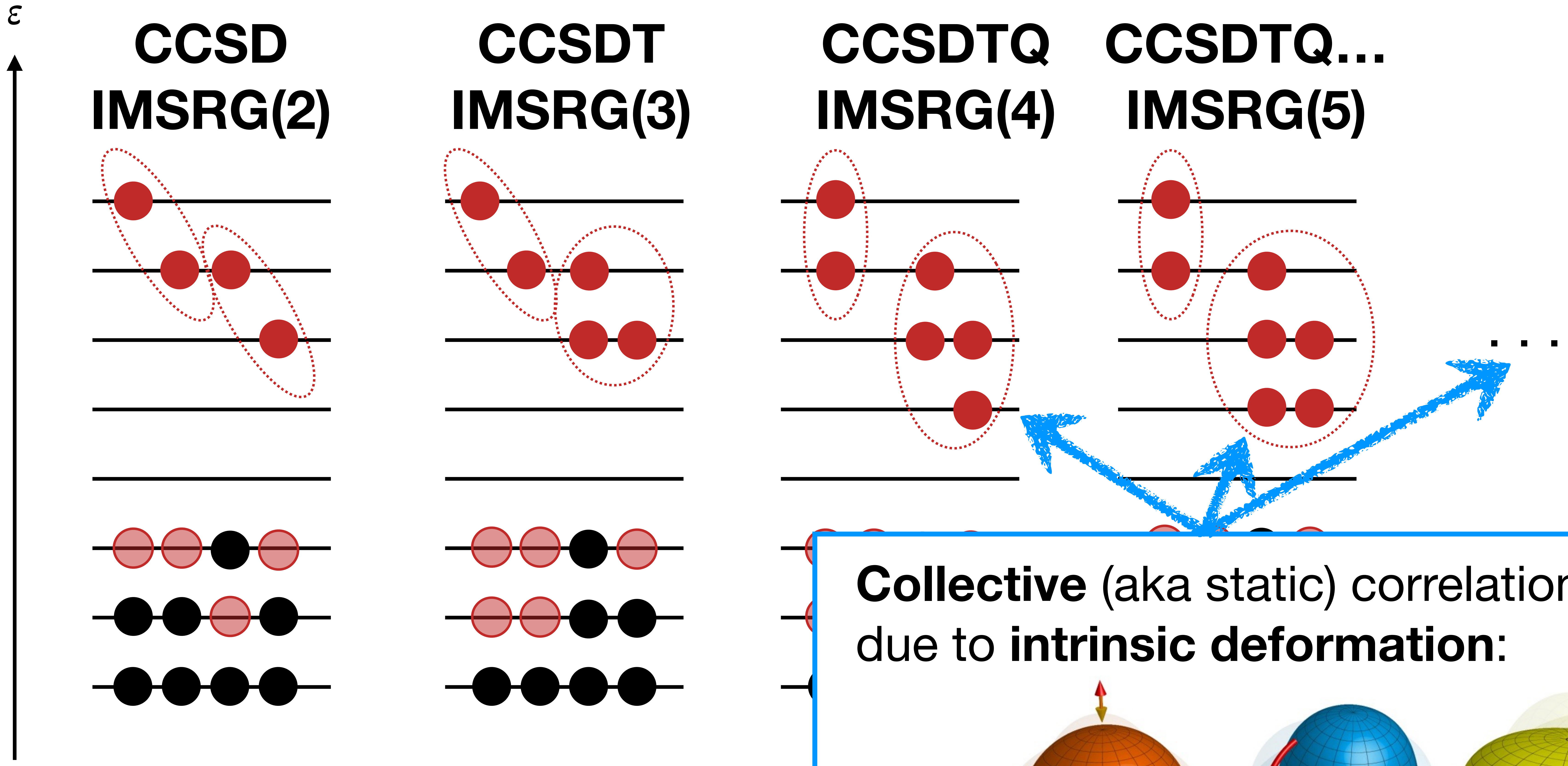
construct **particle-hole excitations** of a **reference state - ** usually an optimized **mean-field Slater determinant**

Decoupling in A-Body Space

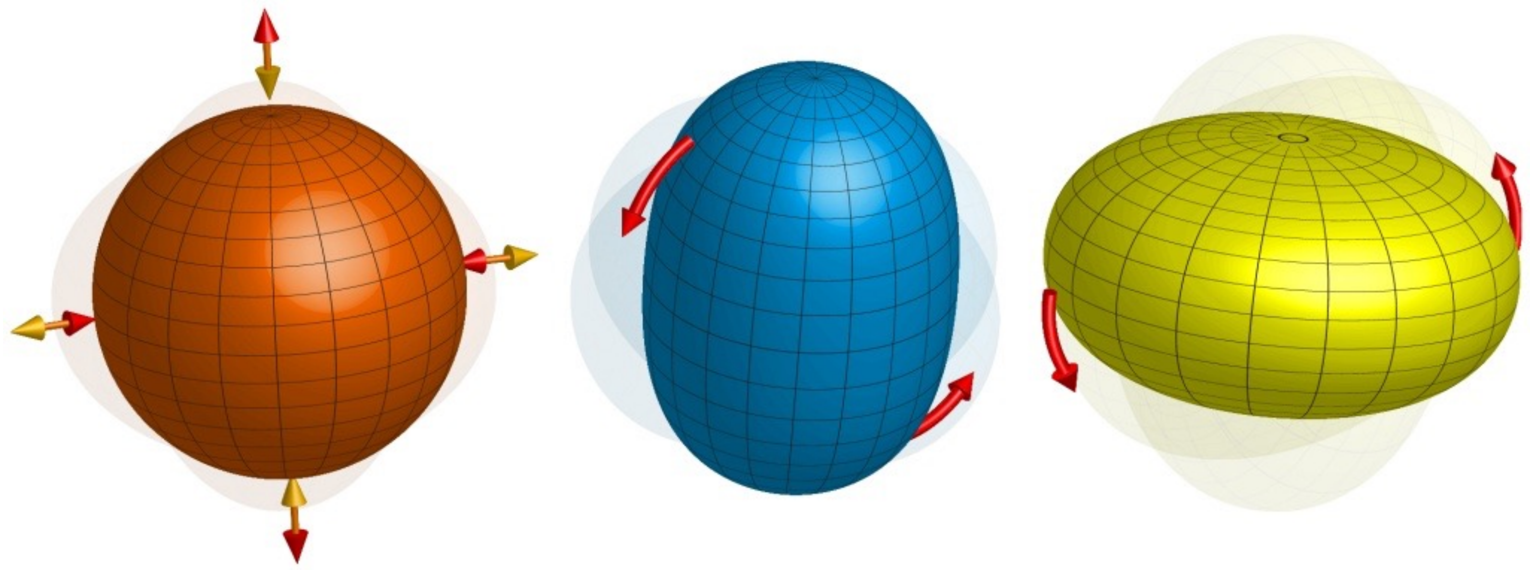


- **identify** the parts of the **operator *H*** which **couple reference state to excitations**
- **eliminate** them with unitary (**IMSRG**) or general similarity transformations (**CC**)
- **efficient: polynomial scaling,** no need to construct matrix !

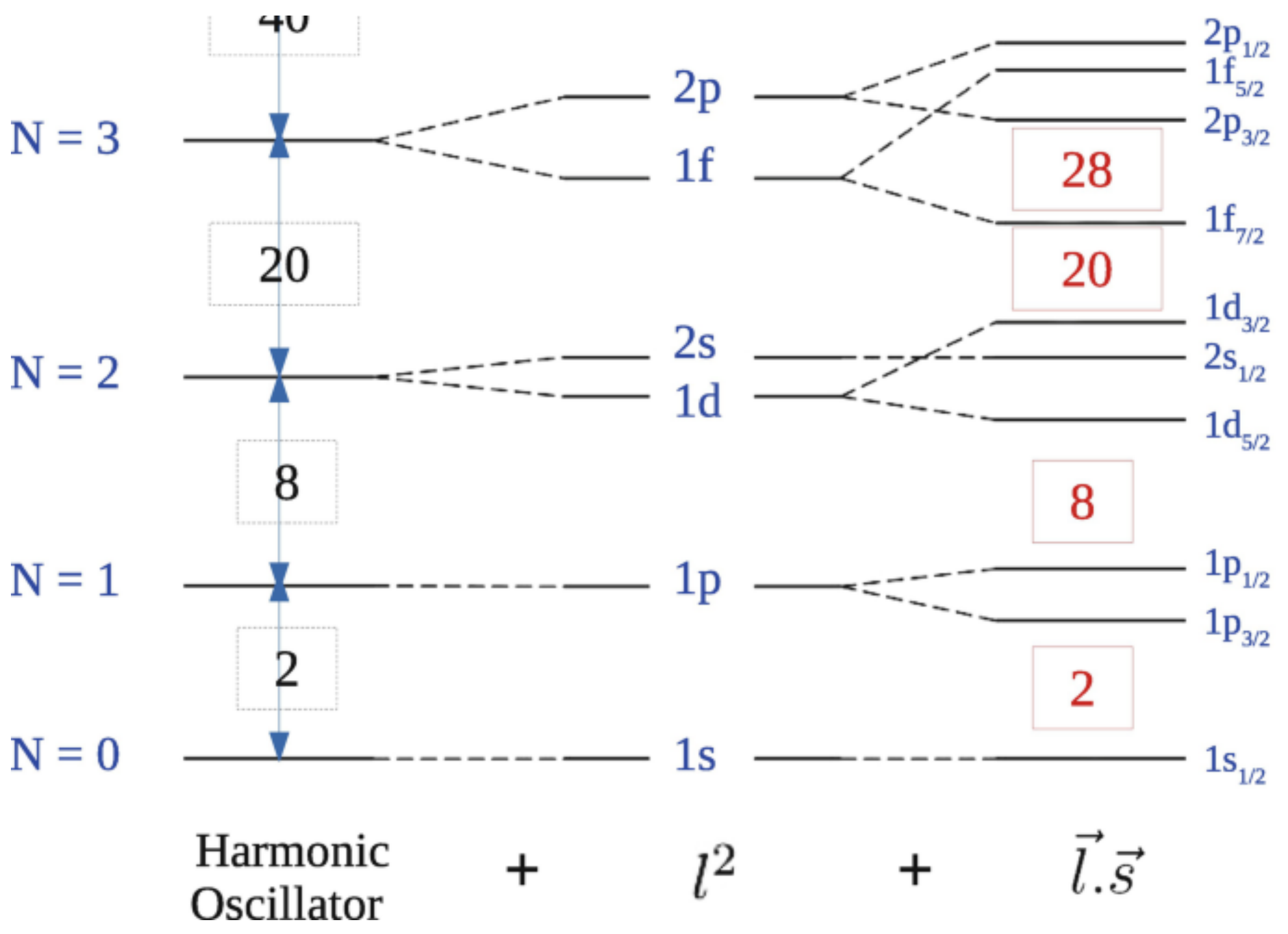
Correlations in Nuclei

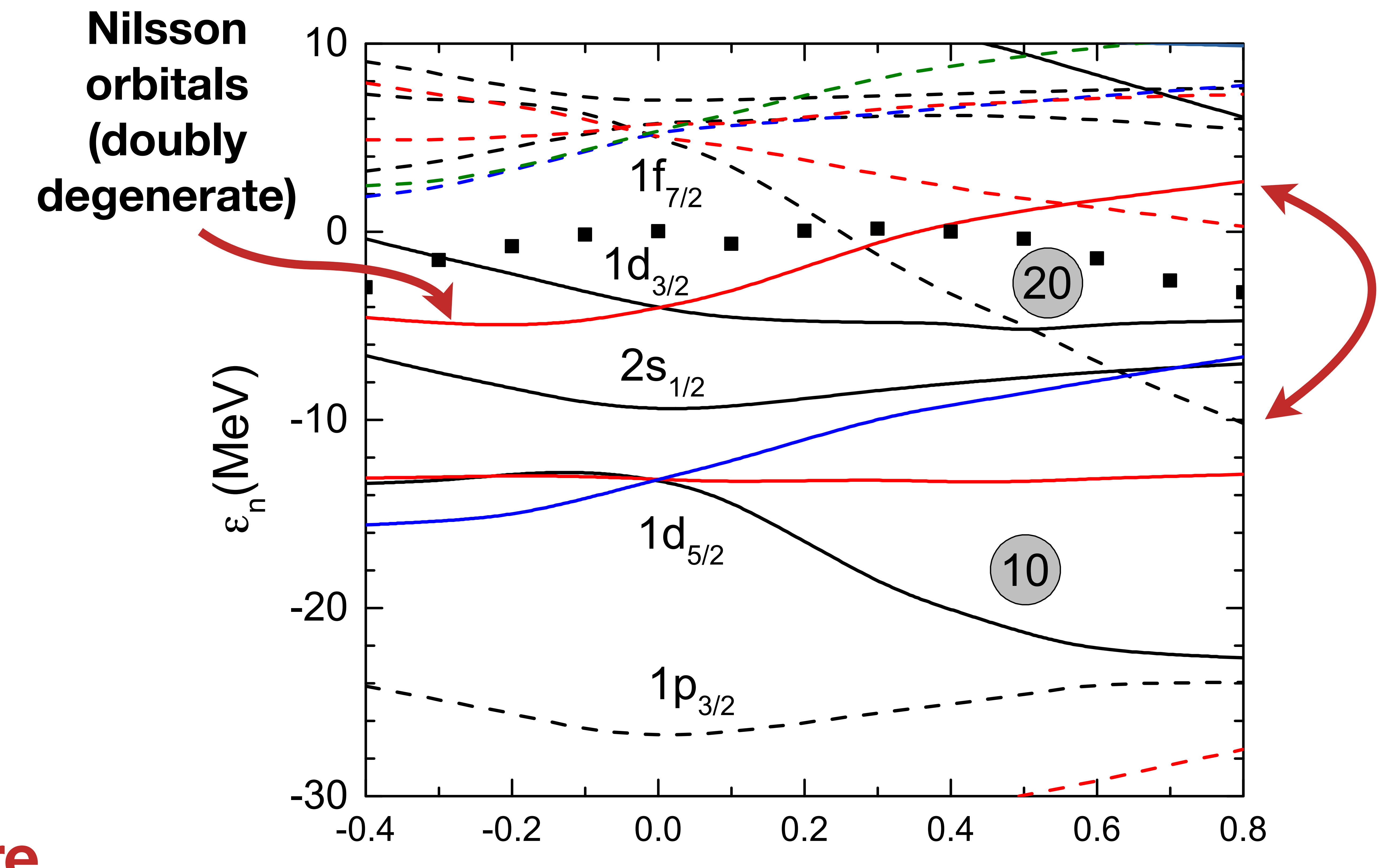


Collective (aka static) correlations, e.g. due to **intrinsic deformation**:



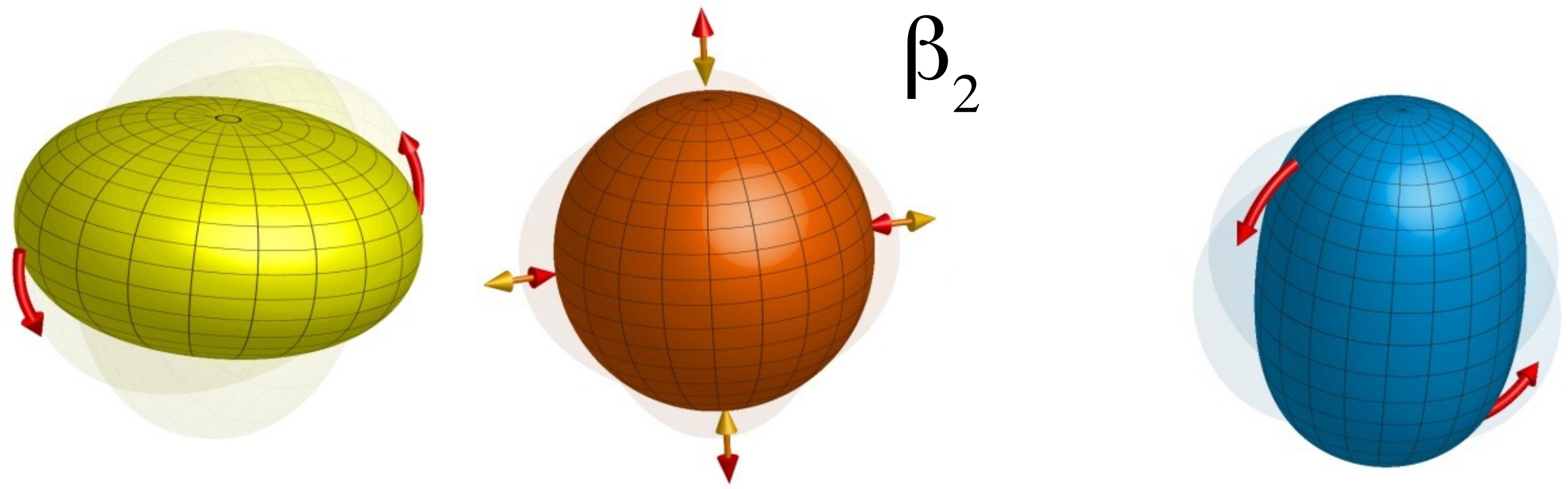
Symmetry Breaking and Restoration





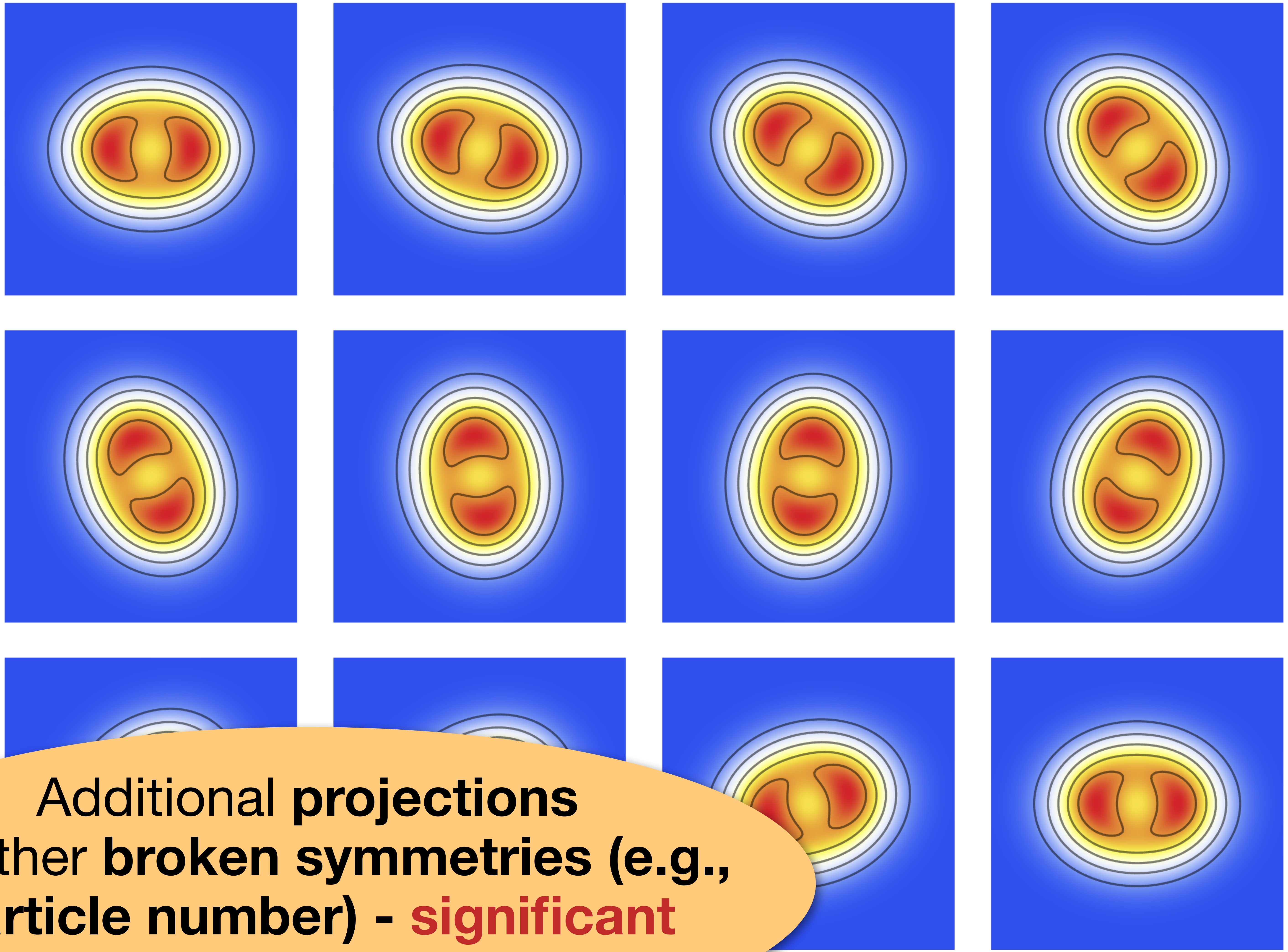
- **break spherical symmetry** to **capture static correlation** from deformation

- **restore symmetry** by constructing **(specific) superpositions** of **all rotations** of intrinsic state (aka **projection**)

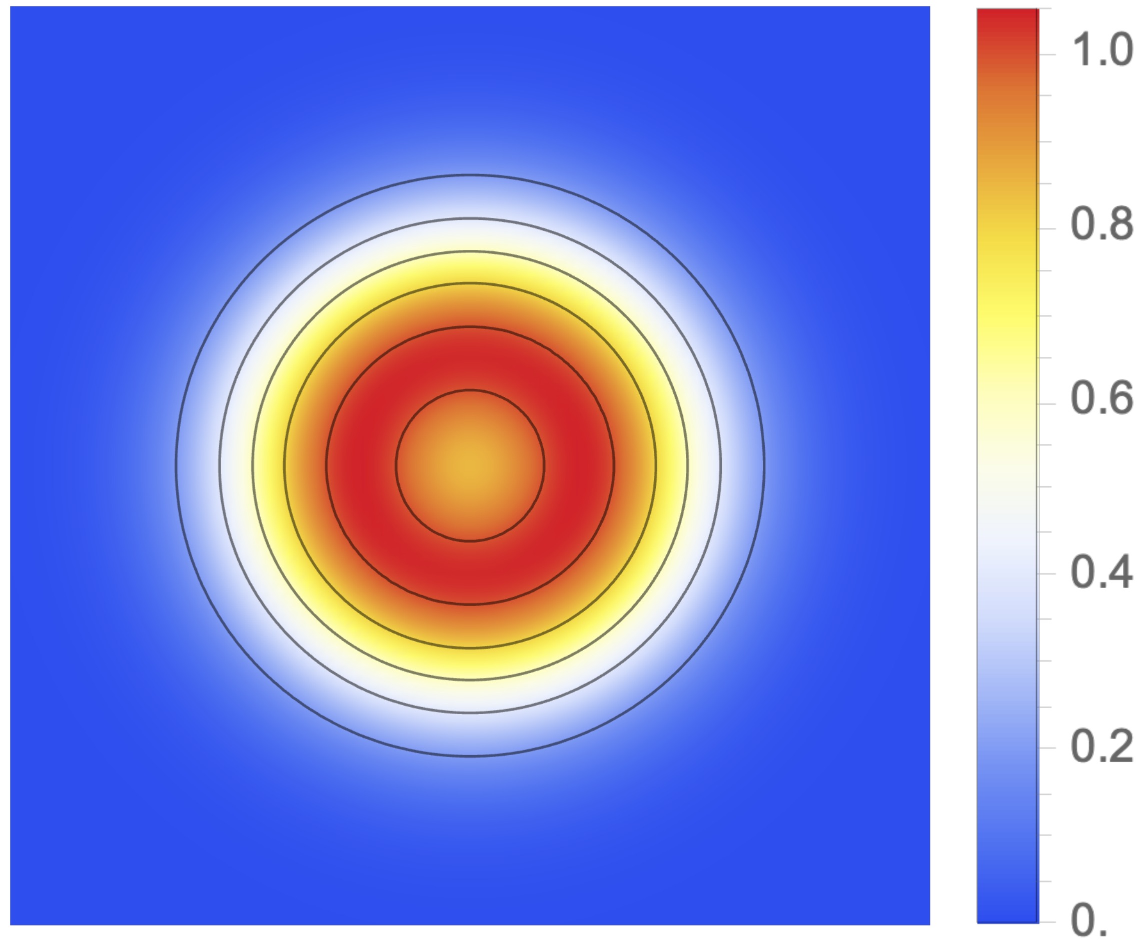


Symmetry Breaking and Restoration

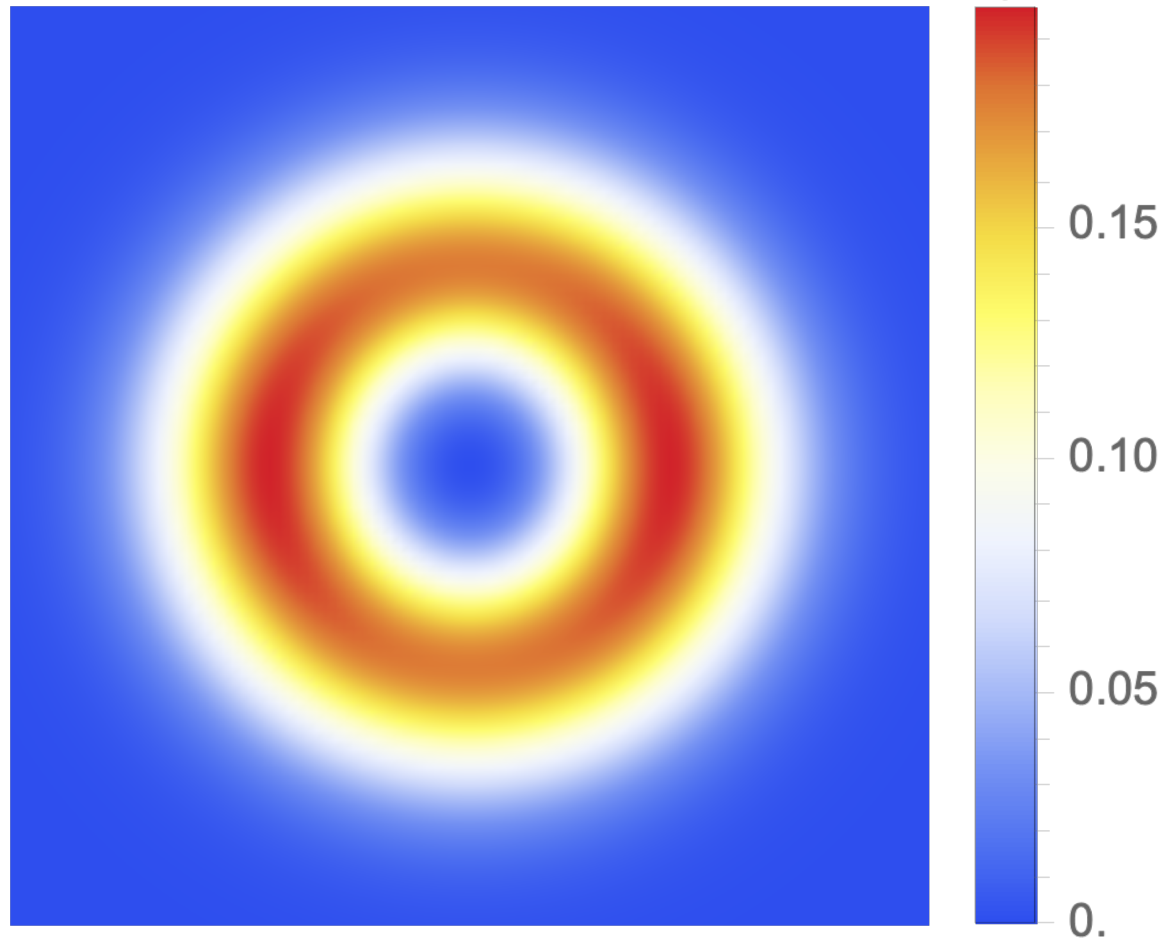
deformed configurations



projected w.f.

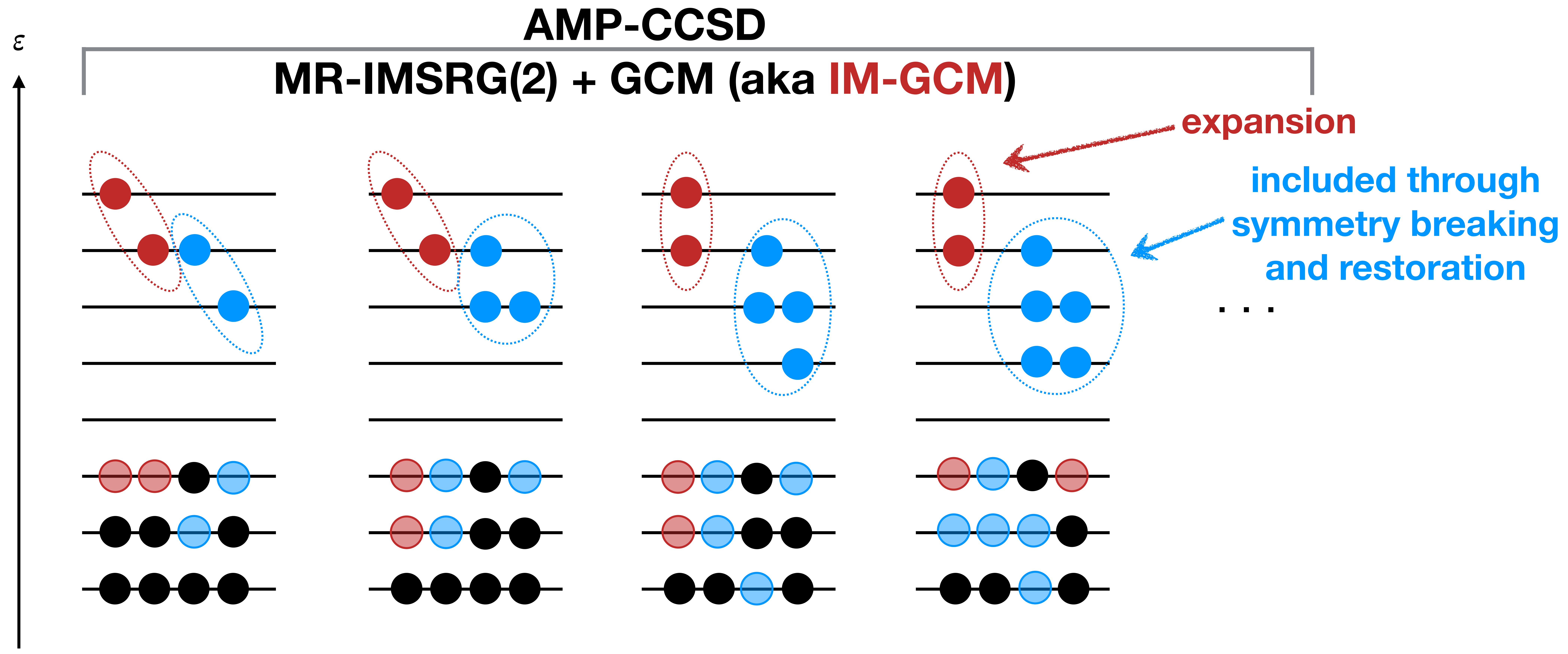


difference from spherical w.f. with same basis size /length scale



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

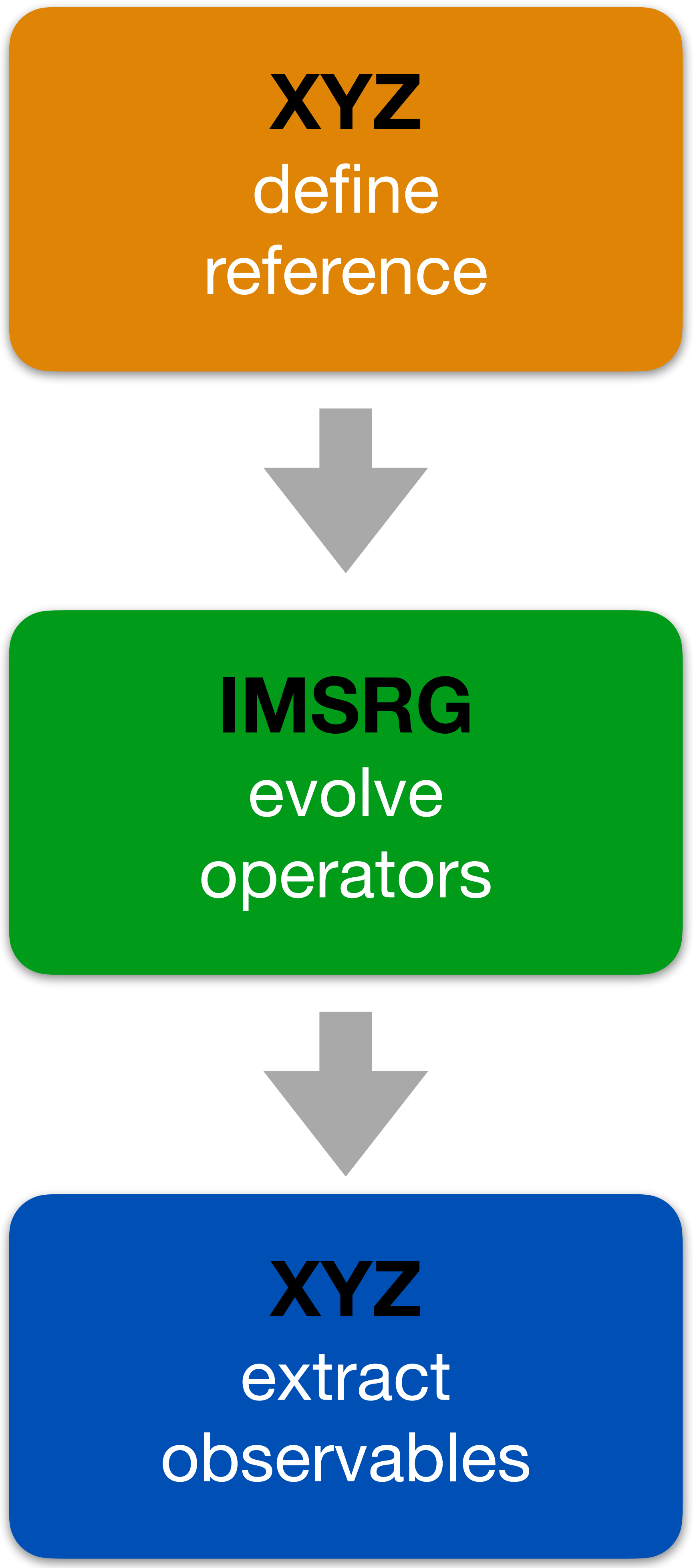
Correlations in Nuclei



In-Medium Similarity Renormalization Group

HH et al., Phys. Rept 621, 165; Phys. Scr. 92, 023002
*S. R. Stroberg et al., Ann. Rev. Nucl. Part. Sci, **69**, 307*
*J. M. Yao et al., PRC **98**, 054311; PRL **124**, 232501*

- IMSRG can be used to build specific types of correlations into **RG-improved interactions** and **operators**
  - ideally, 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)

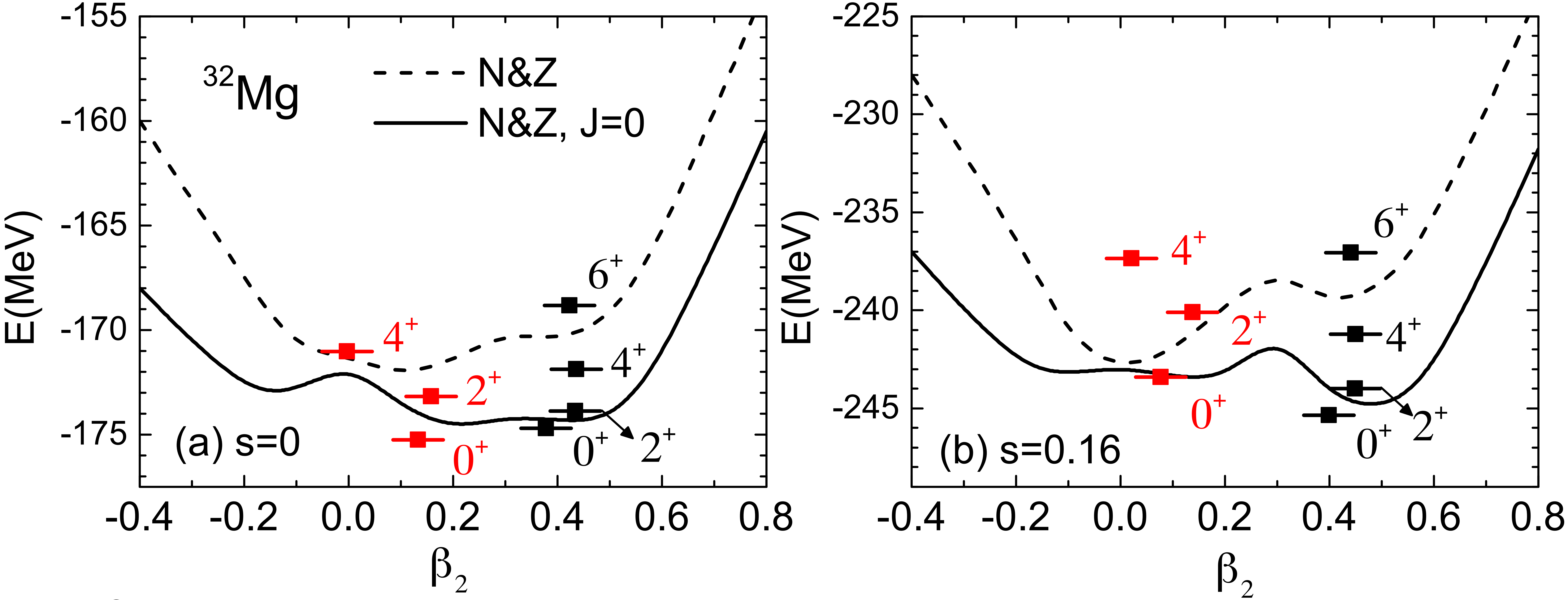


Selected Applications

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

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

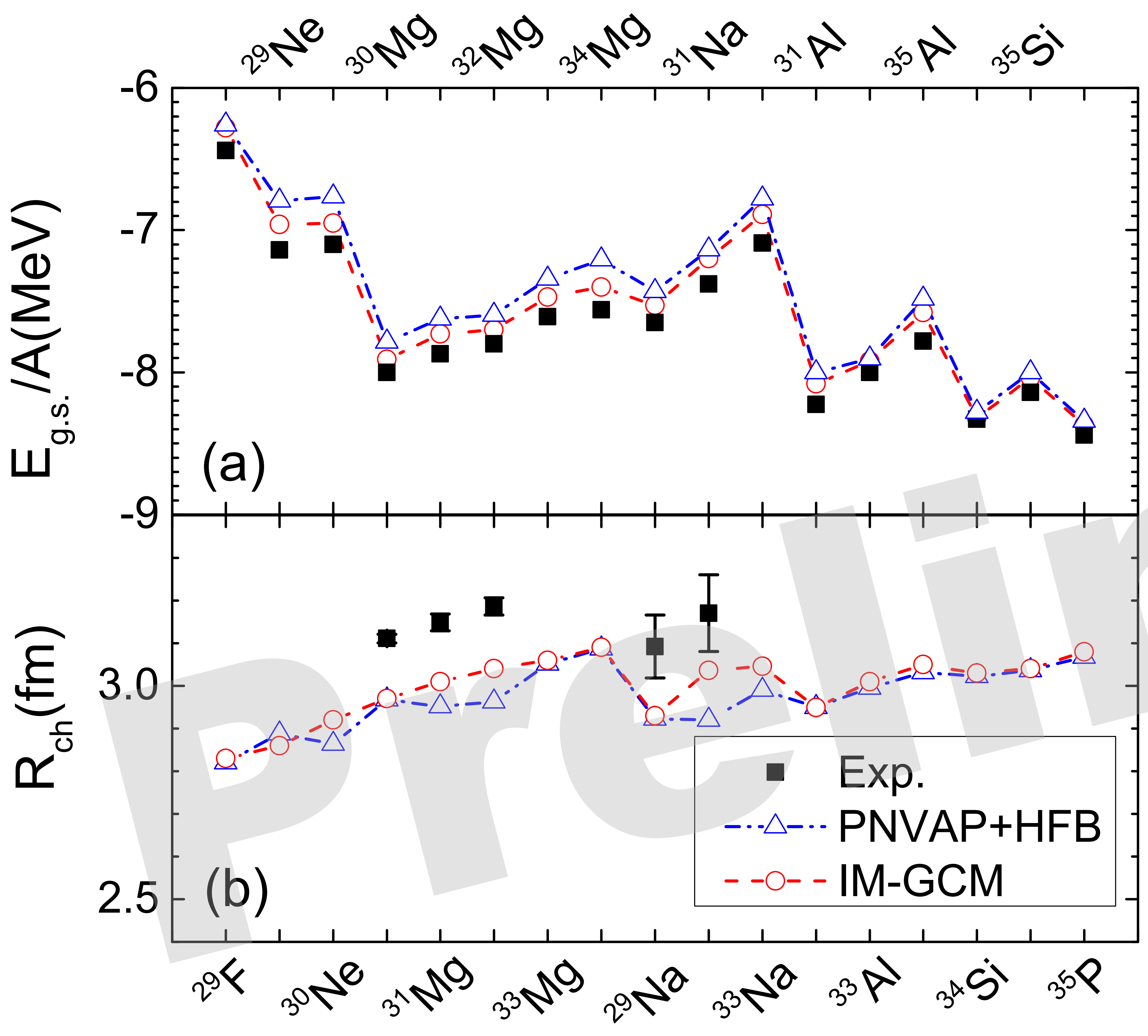
EM1.8/2.0, $\hbar\omega = 12\,\mathrm{MeV}, e_{max} = 8$

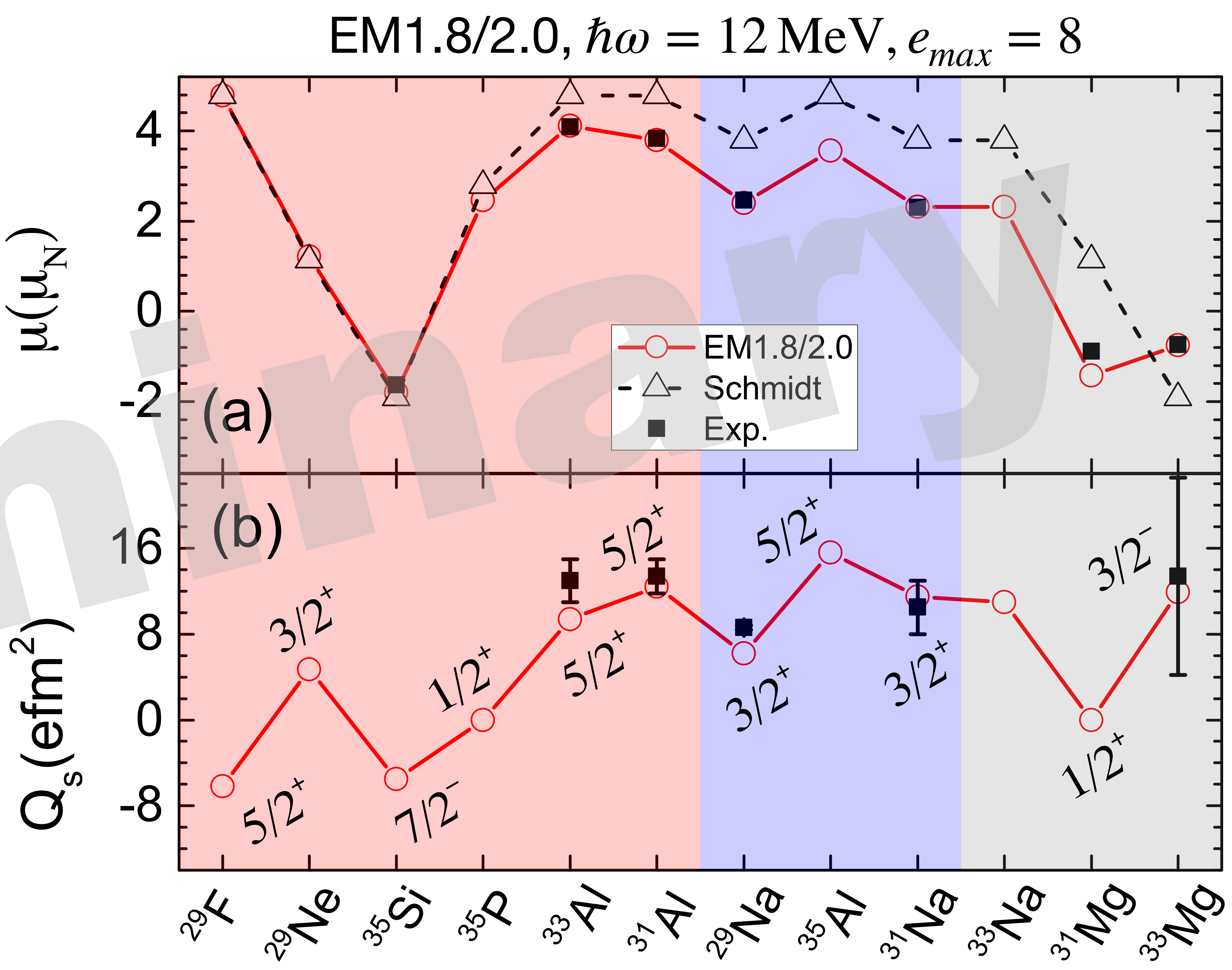


- **Dynamic correlations** captured by IMSRG…
  - bring **absolute energies** close to experiment (E=-249.7 MeV (AME) vs. -249.5 MeV (extrapolated theory))
  - reveal prominent **prolate deformation** of the **ground state**

N=20 Island of Inversion Region

E. F. Zhou et al., arXiv:250x.xxxx

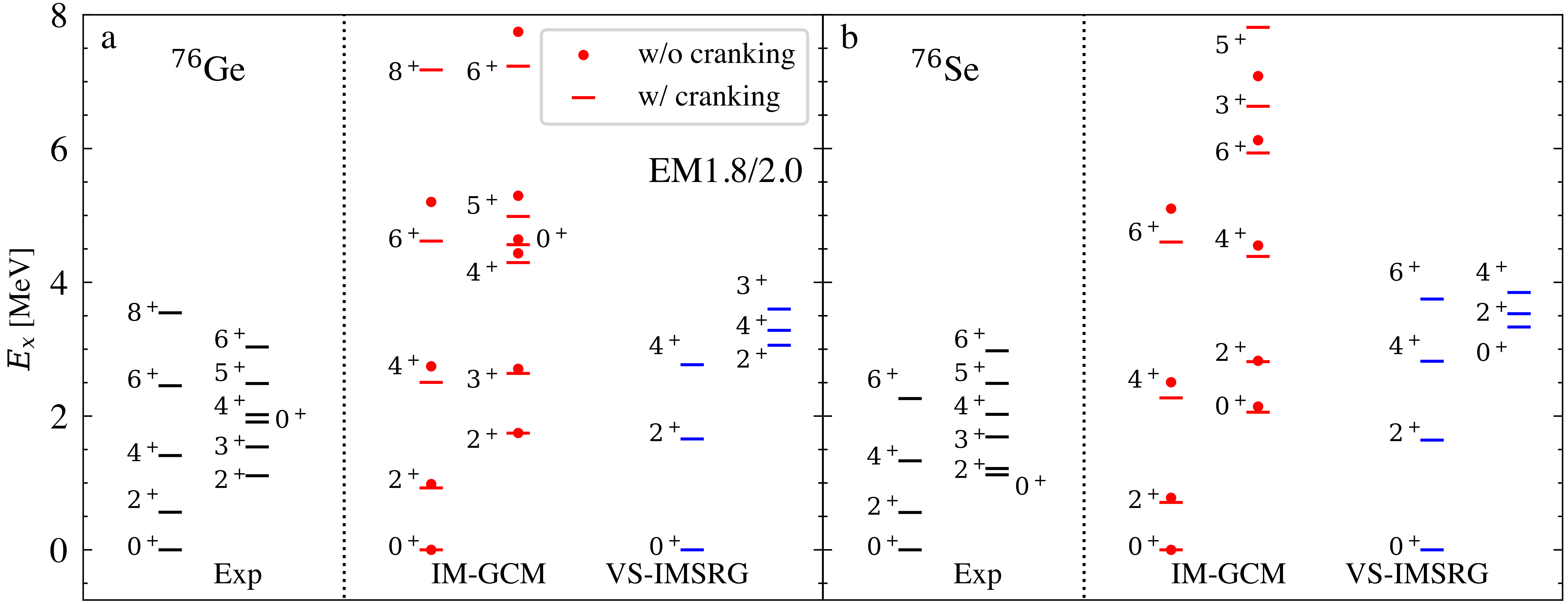


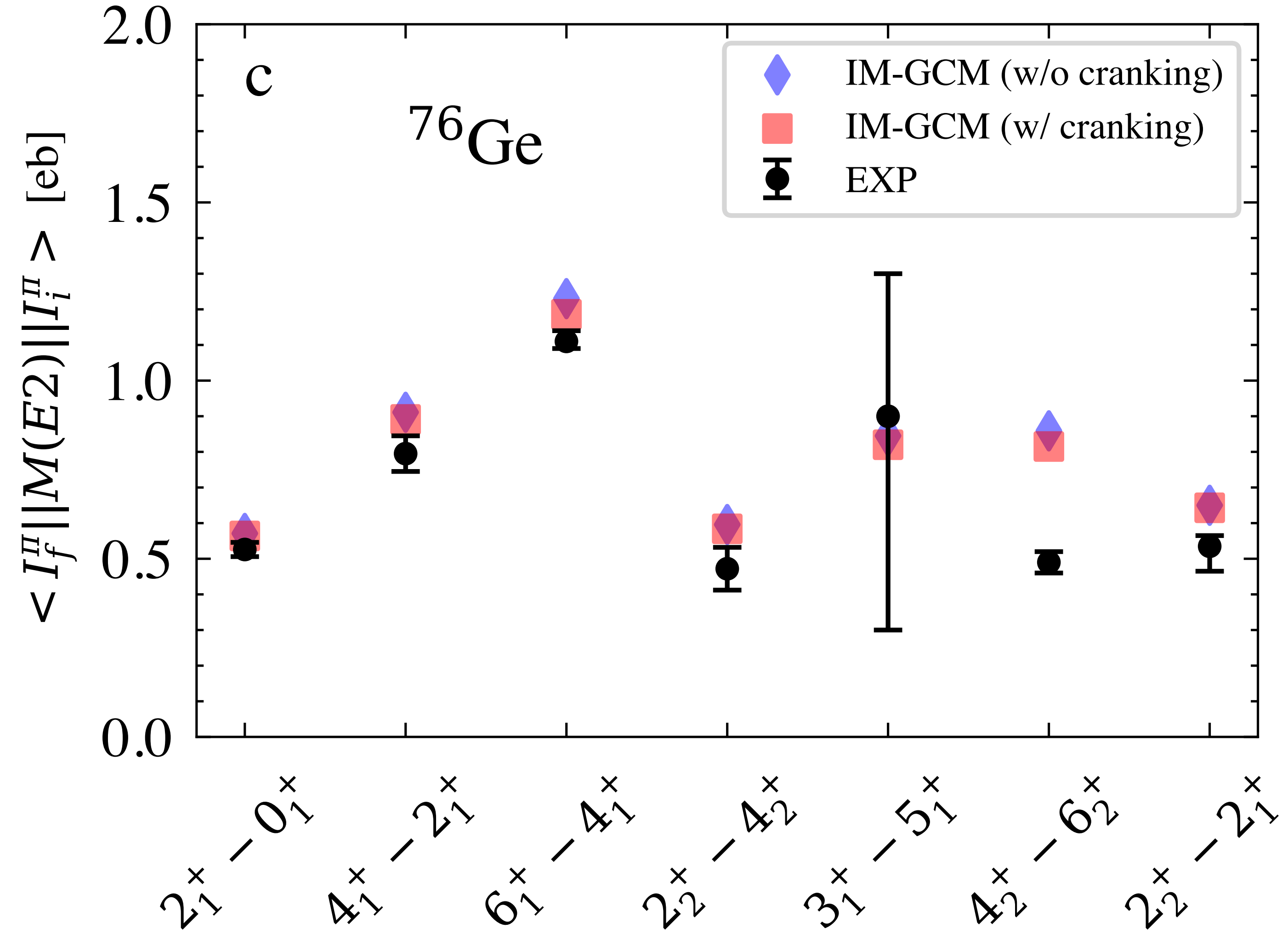


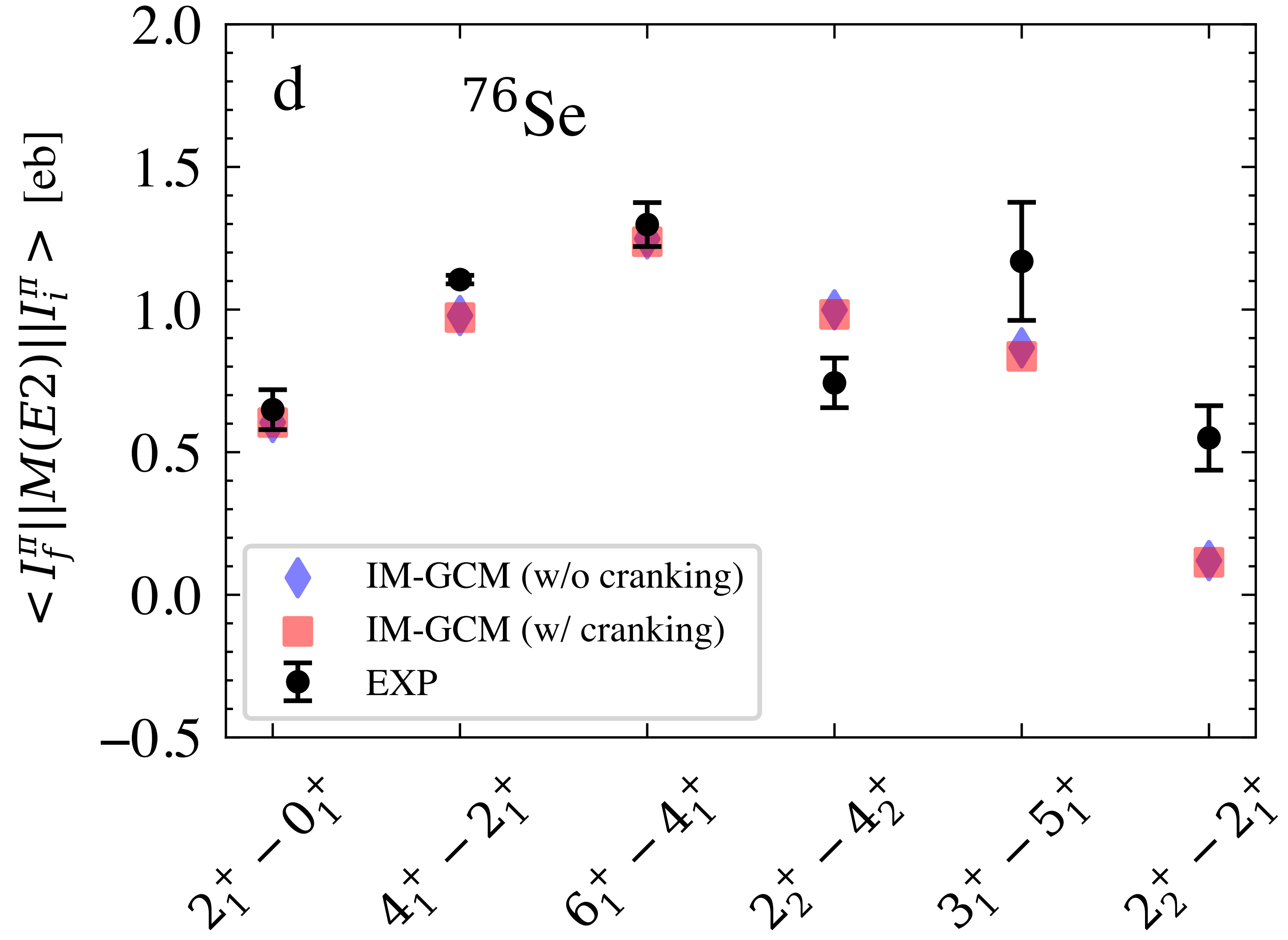
IM-GCM survey in progress

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

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





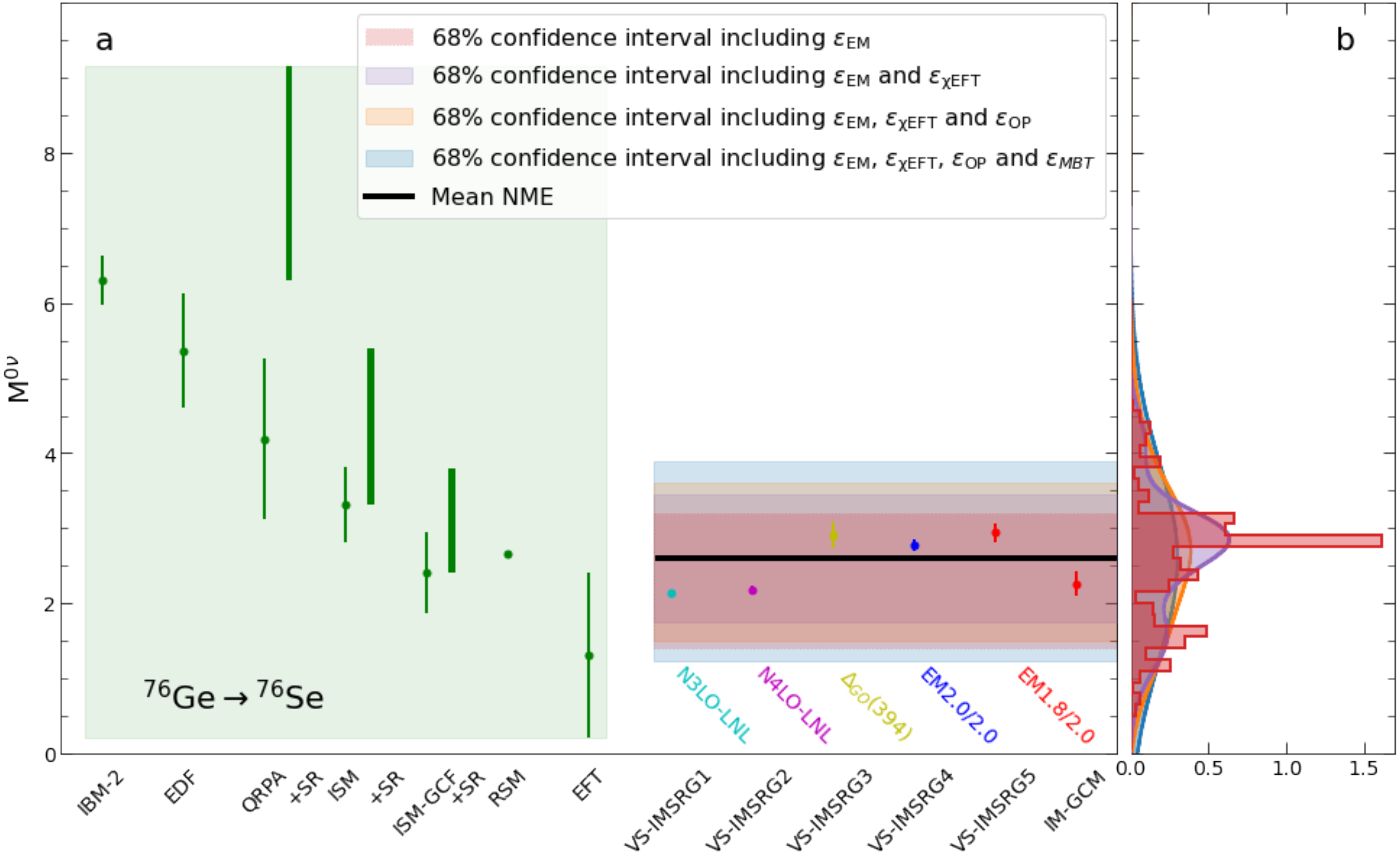


EM1.8/2.0 NN+3N interaction, $\hbar\omega = 12\,\mathrm{MeV}, e_{max} = 10$

- 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**

^{76}Ge: Neutrinoless Double Beta Decay

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

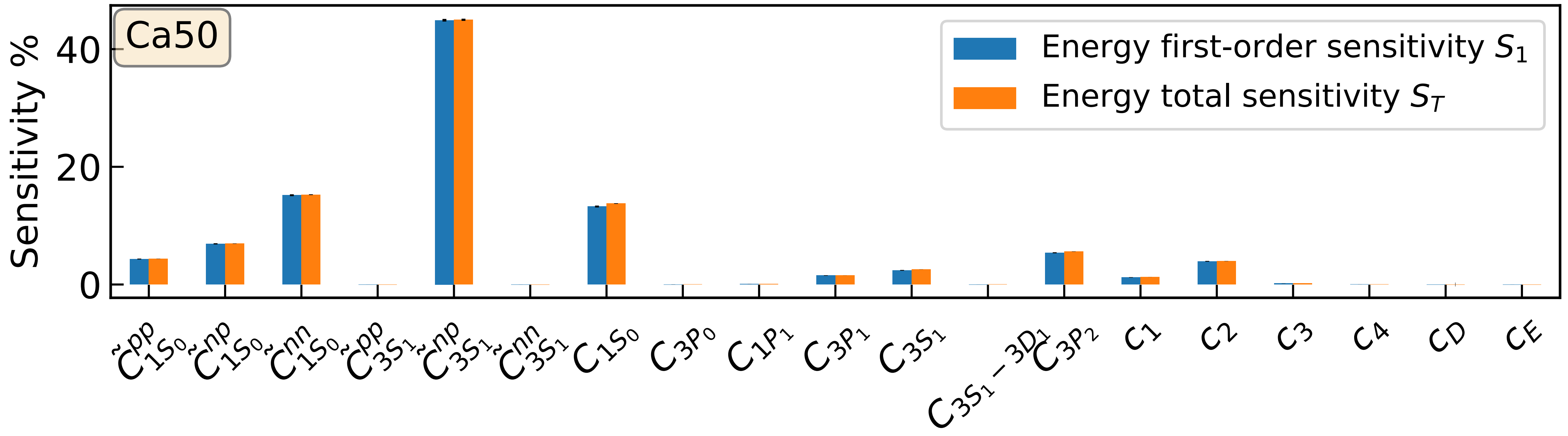


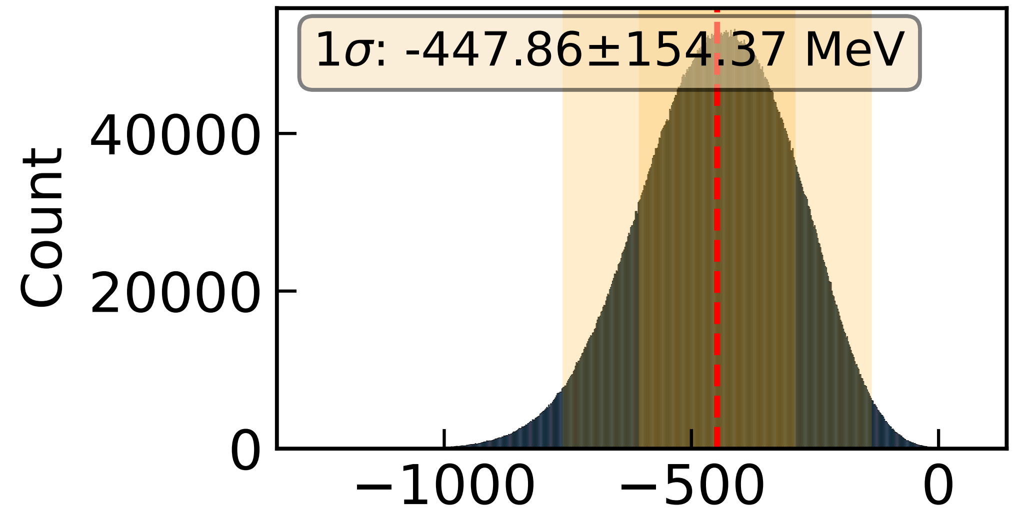
- **state of the art** study
- **complementary methods:** IM-GCM & VS-IMSRG
- explores interactions, many-body and EFT truncations, contact term, …
- leverages **novel emulators**
- identifies **main drivers** of uncertainty and what to improve next

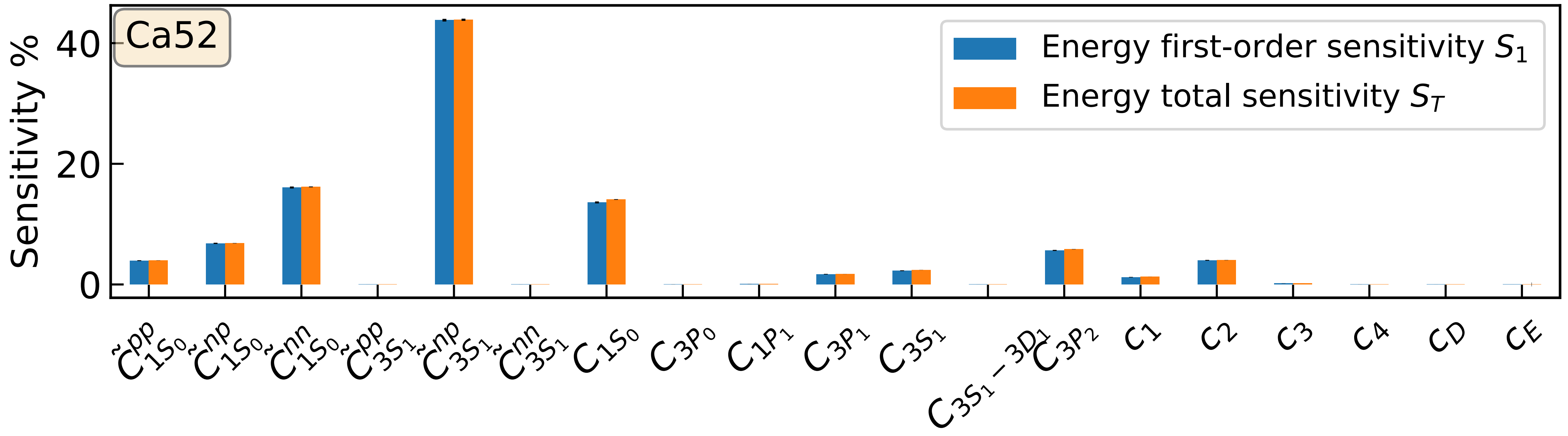
IMSRG Emulators

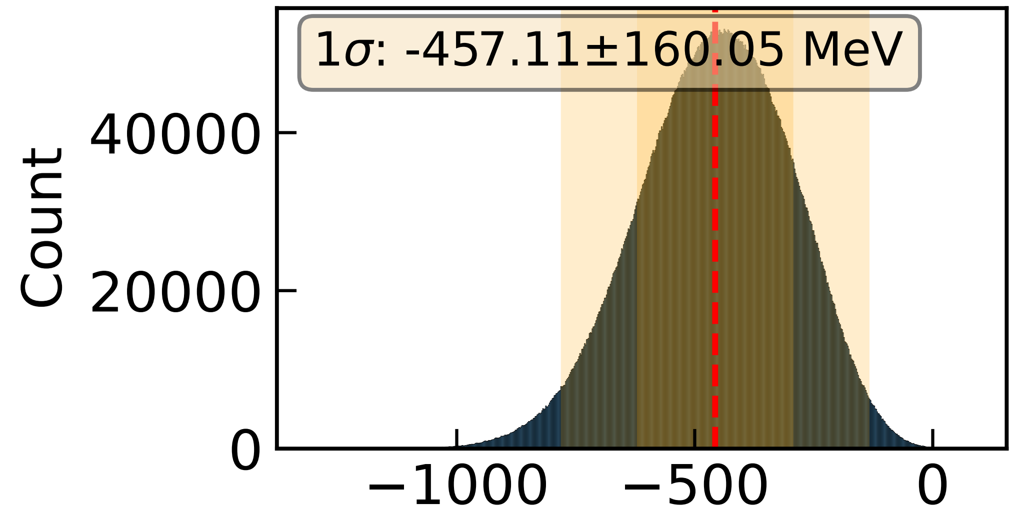
IMSRG Emulators

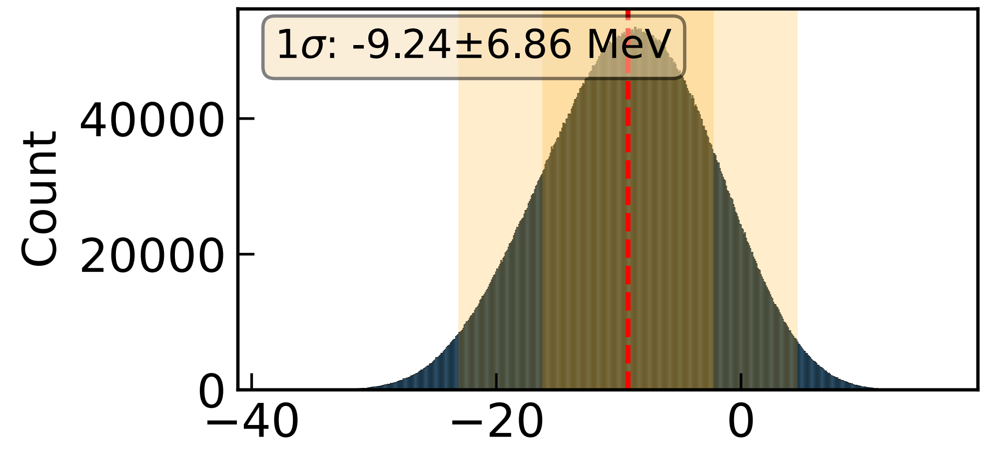
J. A. Davison et al., arXiv:250x.xxxx









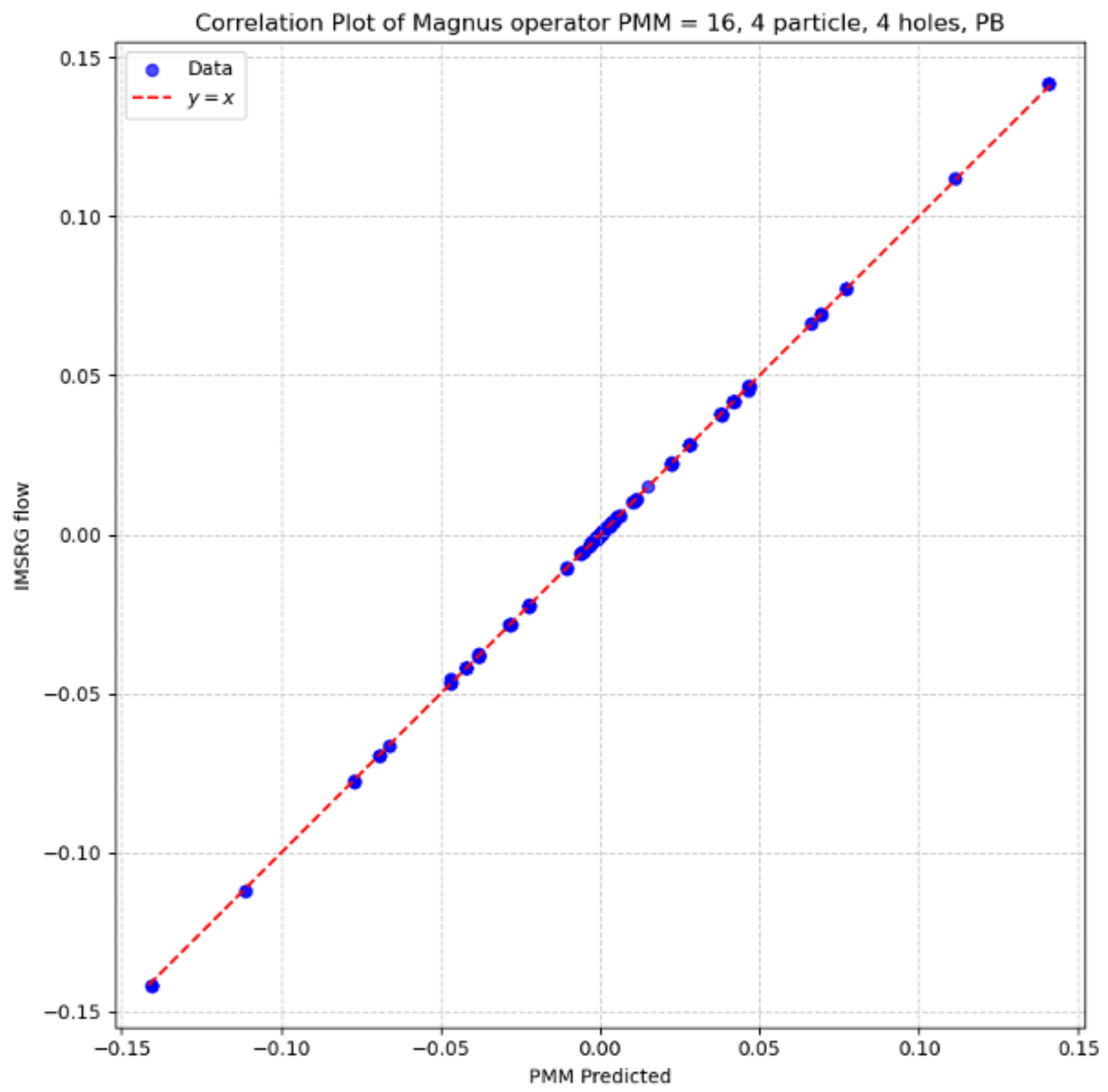


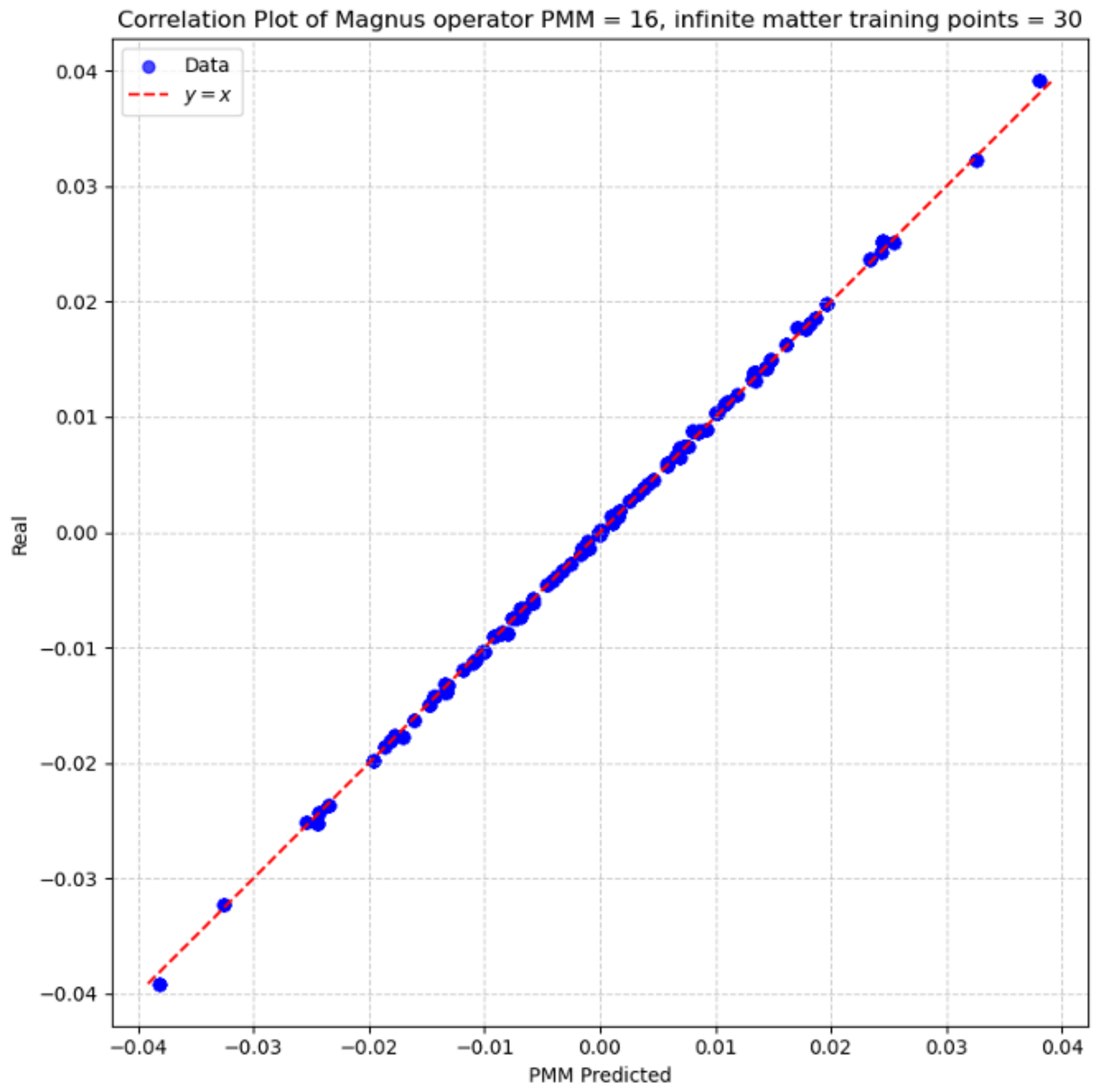
VS-IMSRG
with emulated Hamiltonians
(in progress)

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

Parametric Matrix Models

B. Clark et al., in progress

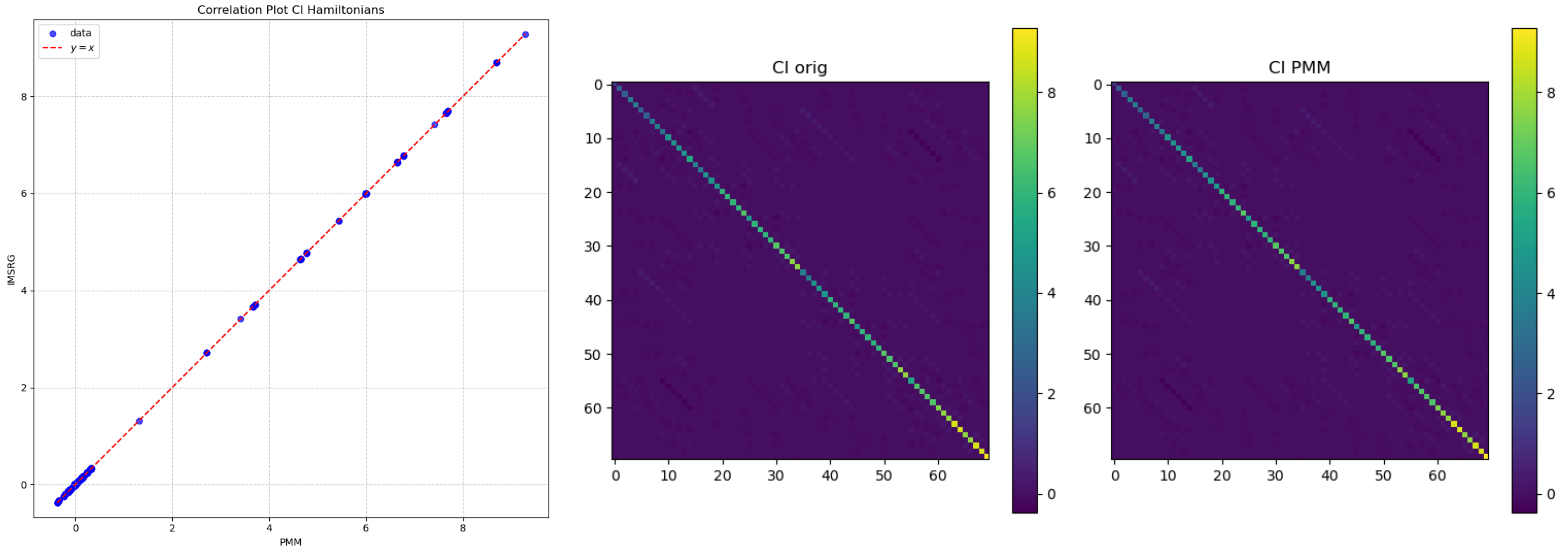




- DMD fails to emulate $\Omega(s)$ unless training is done at large s, **but PMMs work**
- **promising** first results for **parametric emulation** (schematic models, neutron matter @N3LO)

Parametric Matrix Models

B. Clark et al., in progress



- **PMM-emulated Hamiltonians** in hybrid approaches (VS-IMSRG, IM-NCSM, IM-GCM, …)

Emulating Observables

B. Clark et al., in progress

- **Two strategies available:**
  - emulate Magnus operators $\Omega(s)$
  - use reduced-order model for $H(s)$ to construct $\eta(s)$ at arbitrary flow parameters and "trotterize" the unitary transformation:

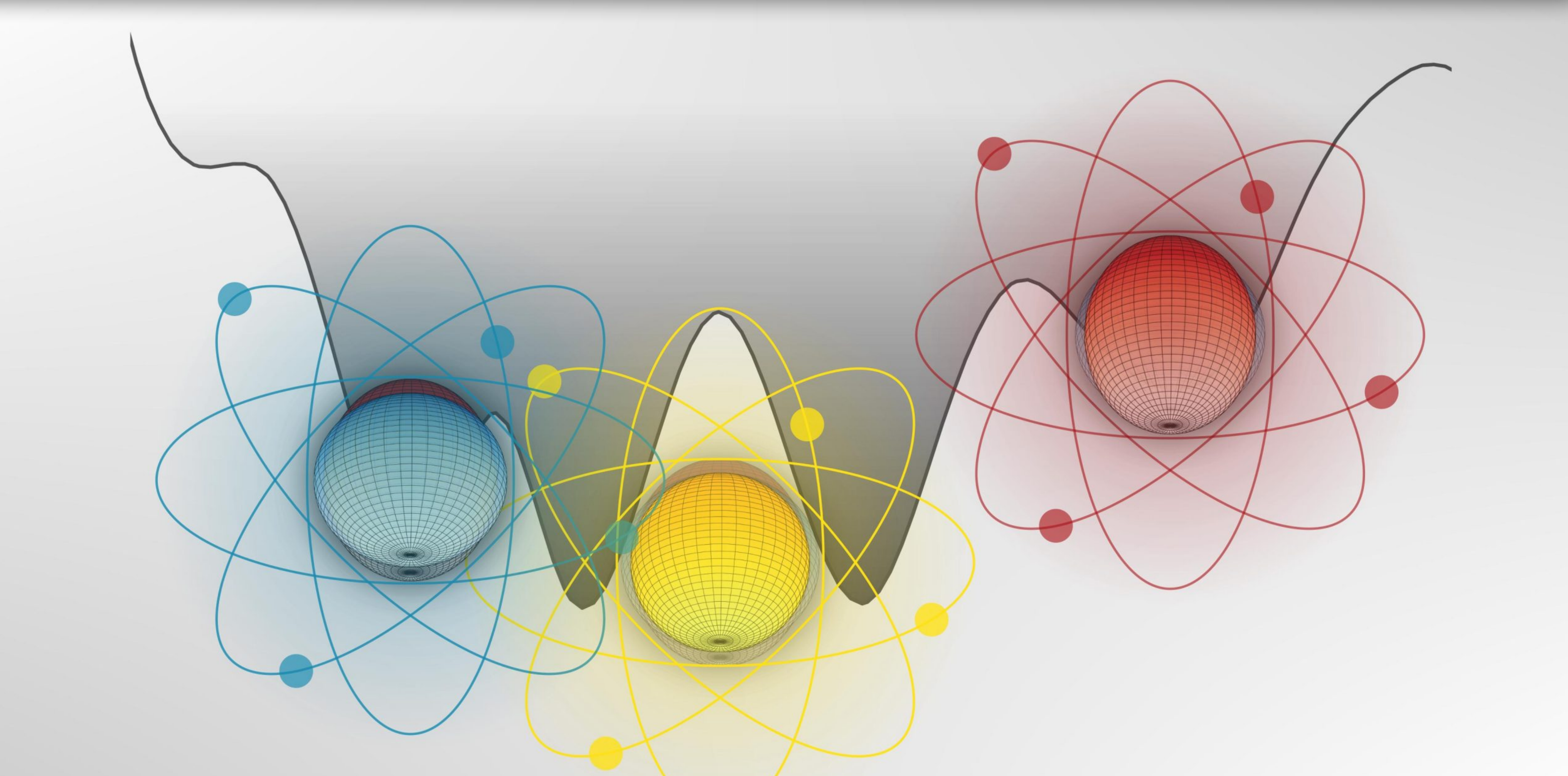
$$U(s) = \lim_{n\to\infty} \prod_n e^{\eta(s_n)}$$

S^2	CI	IMSRG	IMSRG DMD	Magnus	Magnus PMM
ground state no pair breaking	0	0	0	0.000856	0.00085<u>4</u>
ground state with pair breaking	0	0	0	0.001356	0.00135<u>7</u>
1st excited state no pair breaking	2	2	2	2.000002	2.000002
1st excited state with pair breaking	2	1.999461	1.999<u>787</u>	1.99928	1.99928

Challenges and Opportunities

Challenges and Opportunities

- **Asks: ab initio results for nuclear structure, reactions, astrophysics**
  - structure calculations (shape coexistence, isomerism, …) for multiple experimental groups
  - inputs for nuclear astrophysics: masses, beta decay rates, **finite temperature effects**
  - nuclear observables relevant for **BSM physics**: beta decays for CKM unitarity, Schiff moments, …)
  - **differential quantities (often) converge more rapidly,** ab initio results play a role, e.g., in **describing isotopic trends** in excitation spectra, charge radii, magnetic moments, …
- **Asks: Precision, Quantified Uncertainties, Experimental Design**



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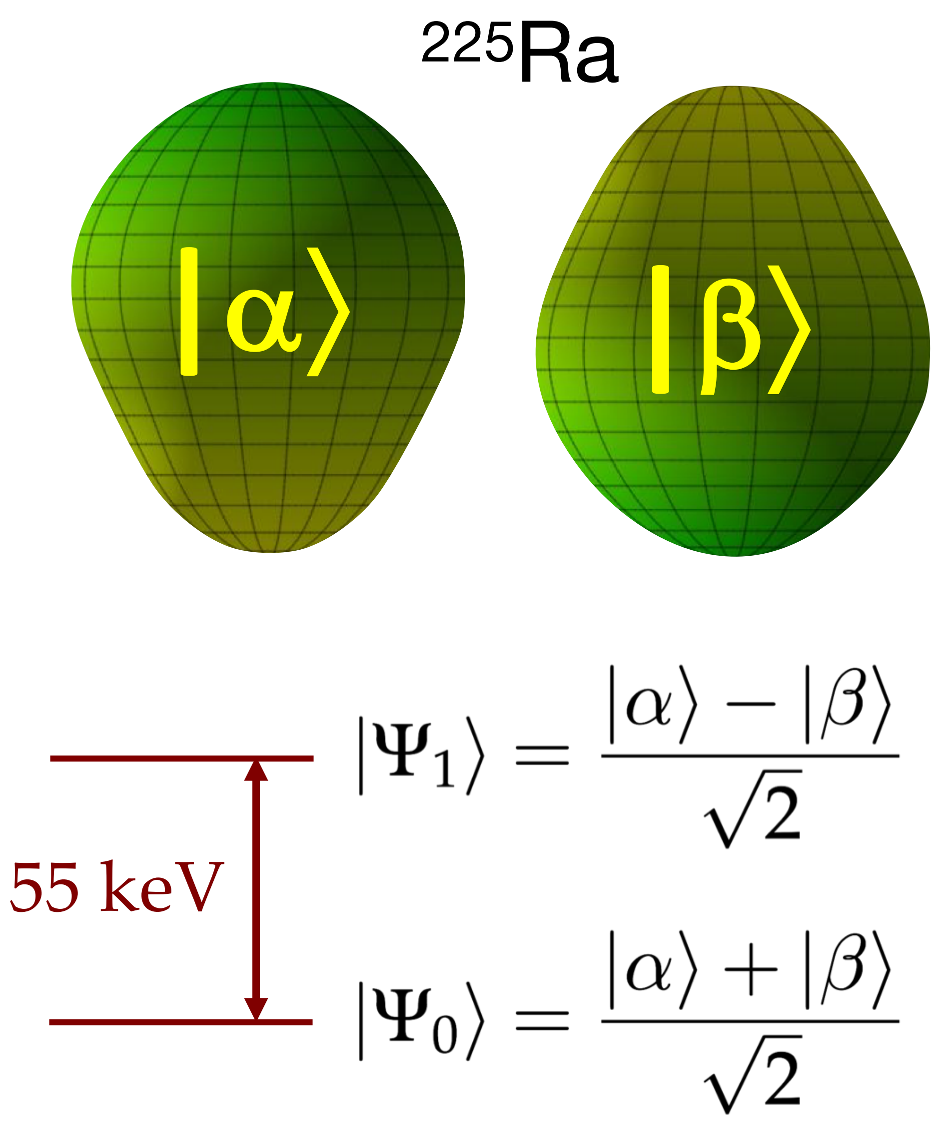


image credit: J. Singh

Challenges and Opportunities

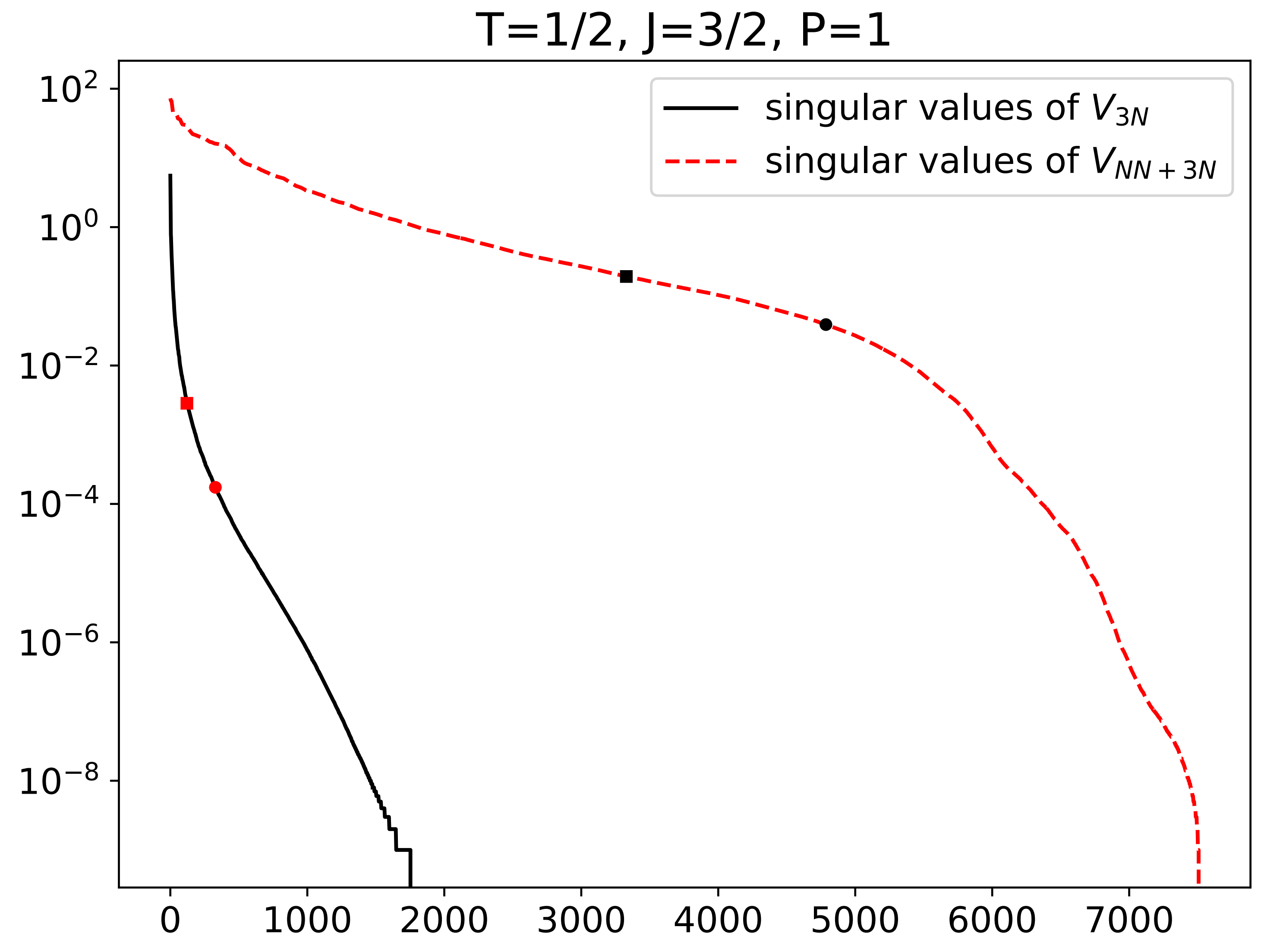
- **Need improved truncations** for **Hilbert space & many-body expansion:**
  - **approximate (MR-)IMSRG(3)** (or more), e.g,. through **factorization** (He & Stroberg)
  - full MR-IMSRG(3) is worked out, but scaling is prohibitive for everyday use (and implementation would require automation)
  - **tailored operator bases?**

- **Need emulators** for **uncertainty quantification / sensitivity analysis**
  - **efficient DMD and PMM emulators** for (MR-)IMSRG evolution
  - operators are **no longer linear in original LECs**, which is key for **“offline” pre-computation** in **reduced-basis methods** (eigenvector continuation, ….)
  - Can we tackle this with Discrete Empirical Interpolation Method (DEIM), PMMs, … ?

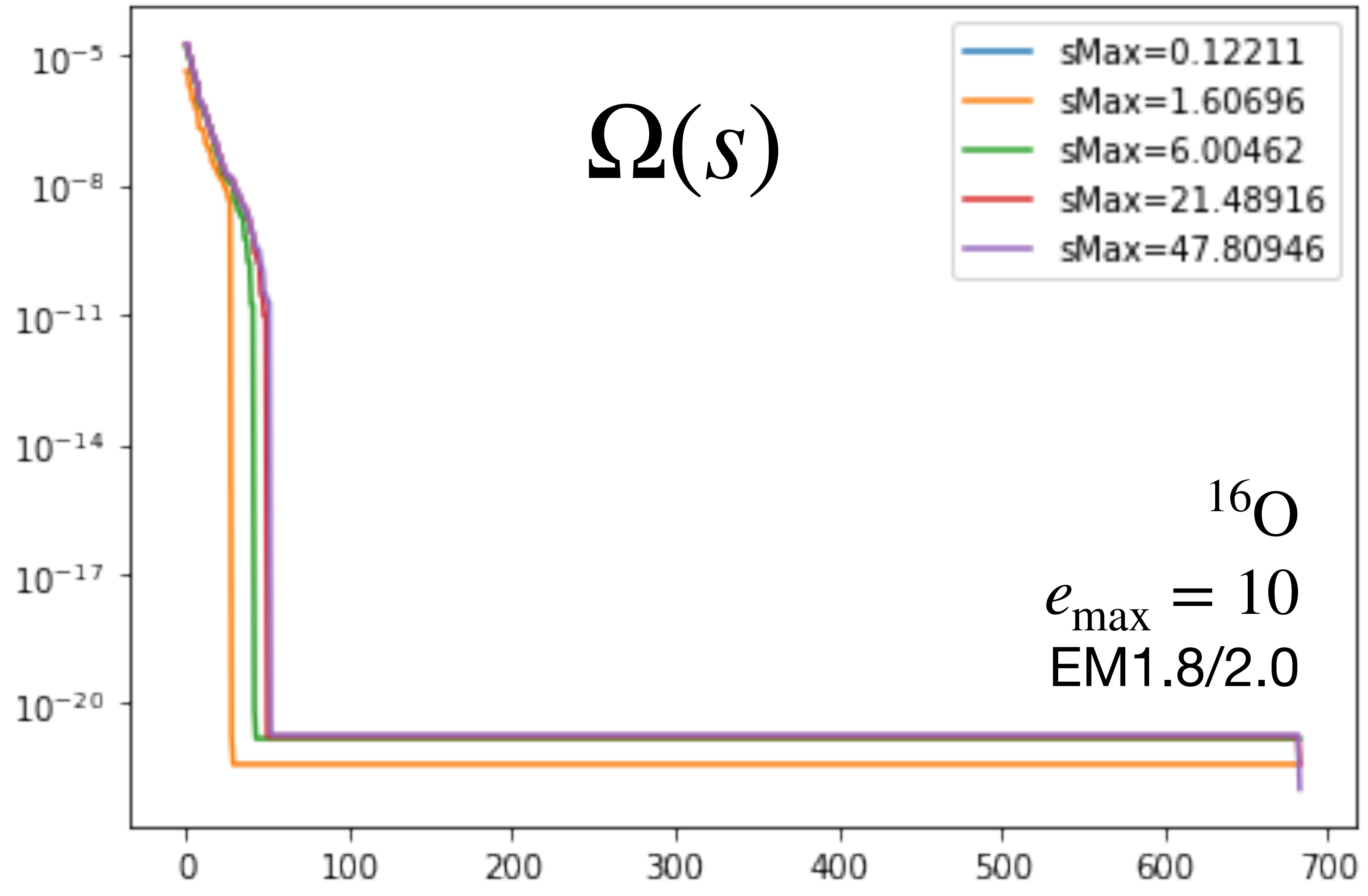
Challenges and Opportunities

- Can we compress interactions / Hamiltonians?
- **interactions** are low-rank in Jacobi NN / 3N representation, but this is **spoiled by SRG and transformation to lab frame**
- **working equations** may still allow rank reduction, e.g.,
  - IMSRG: generator η_{abij}, Magnus operator (less obvious), irreducible densities λ_{pqrs} etc.
  - CC: cluster operator T
- SVD, cross interpolation / CUR, **tensor networks, ...**
  - **symmetries can be an obstacle**
  - IMSRG can act as a **disentangler**

cf. talk by **L. Zurek**



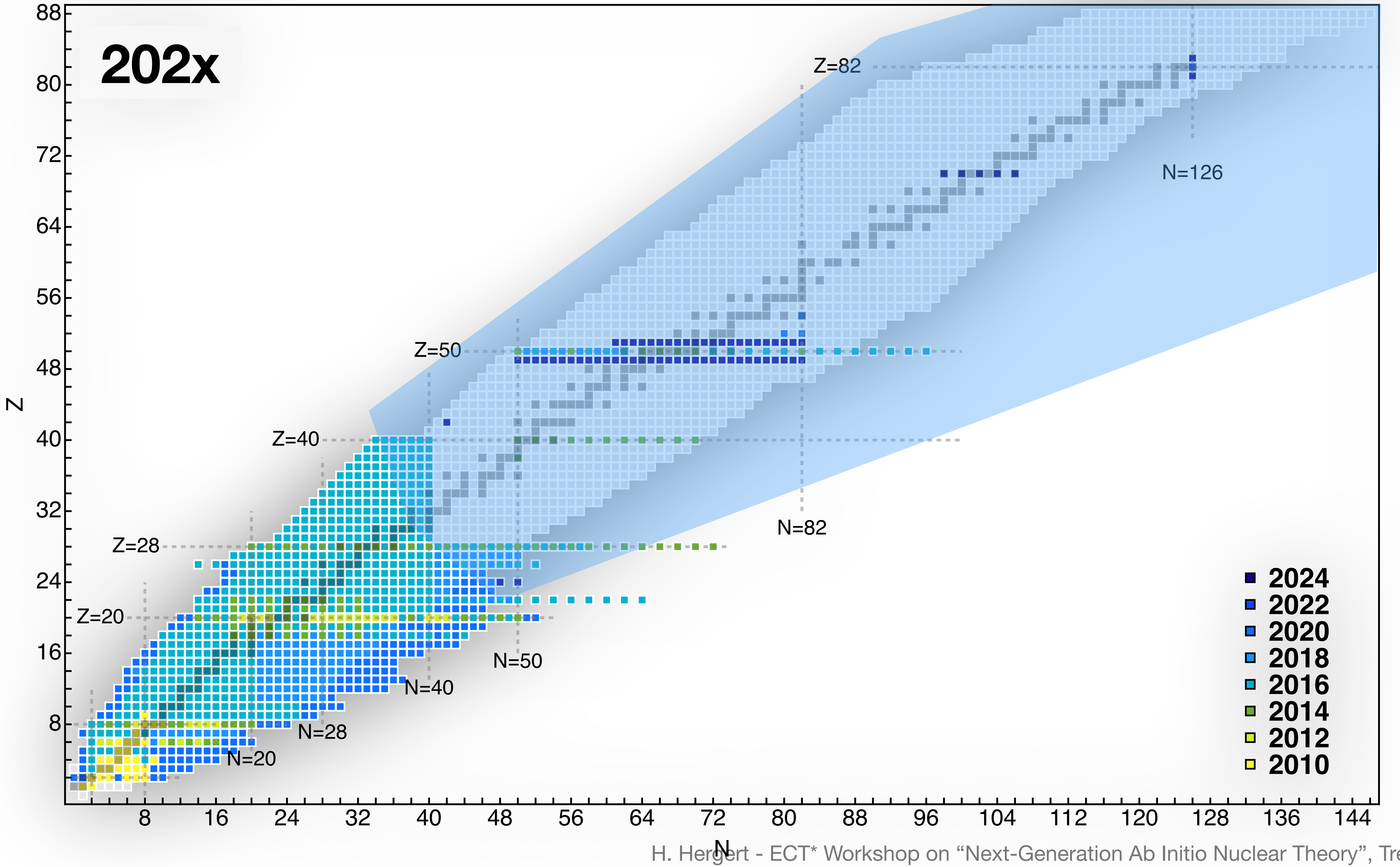
Jacobi 3N - pre SRG



Magnus IMSRG

Outlook

[cf. HH, Front. Phys. **8**, 379 (2020)]



Acknowledgments

T. S. Blade, S. K. Bogner, B. Clark, P. Cook, M. Gajdosik, P. Gysbers, M. Hjorth-Jensen, D. Lee
FRIB, Michigan State University

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Institute for Nuclear Theory, Seattle

S. Gandolfi, E. Mereghetti
Los Alamos National Laboratory

M. Heinz
Oak Ridge National Laboratory

S. Yoshida
Utsunomiya University

S. König
North Carolina State University

K. Fossez
Florida State University

and many more…

NUCLEI
Nuclear Computational Low-Energy Initiative

@NDB

NTNP Topical Collaboration

NERSC

ICER

Support: US DOE-SC **DE-SC0023516, DE-SC0023175** (SciDAC NUCLEI Collaboration), **DE-SC0023663** (NTNP Topical Collaboration), NSF **PHY-2402275** (@NDBD Fundamental Research Hub)

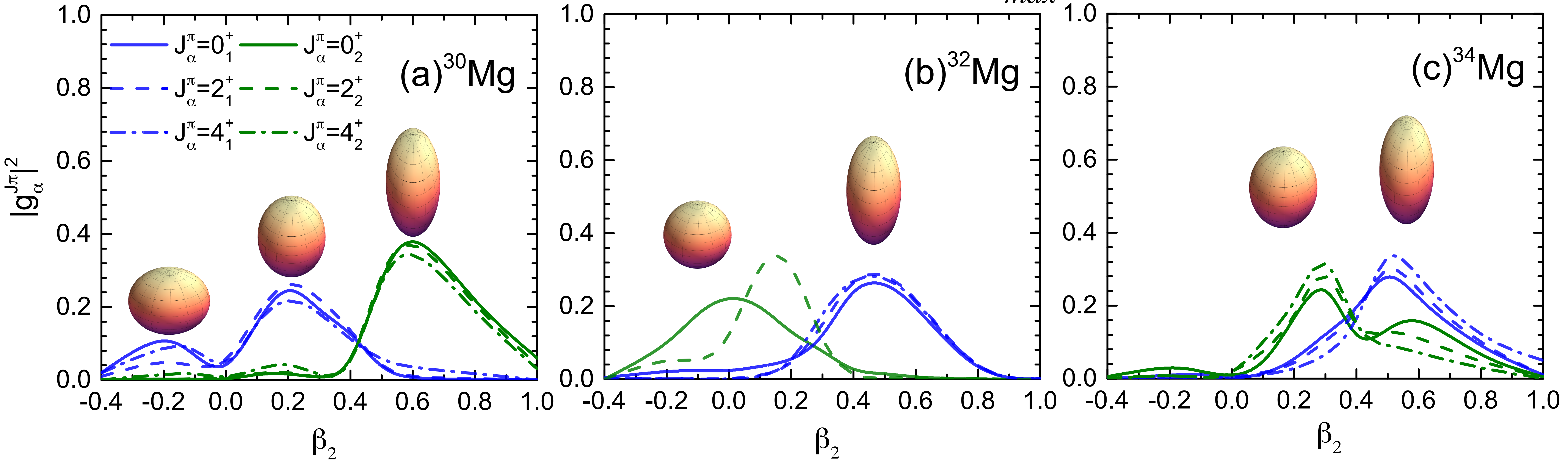
Thank you for your attention!

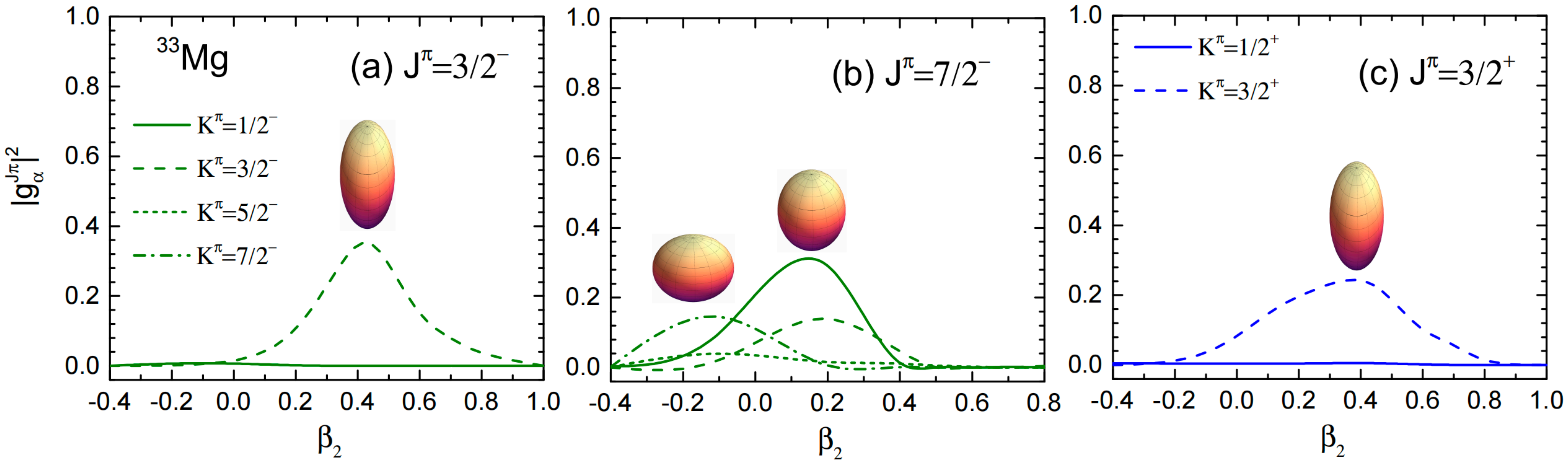
Supplements

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

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

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

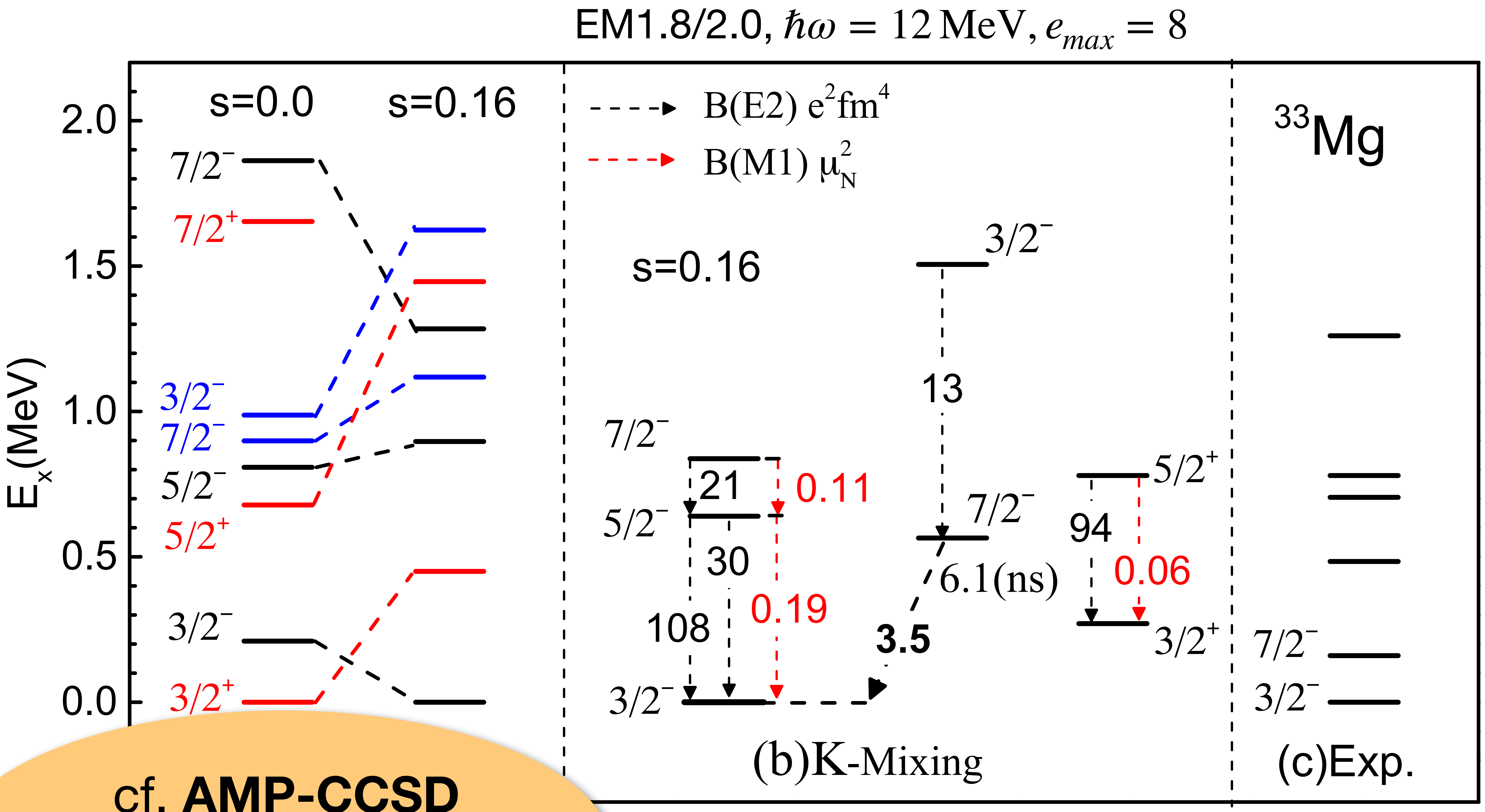




- **shape coexistence** comes with **shape mixing**
- **caveat:** wave function components are not observable - **compare with care**!

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

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



cf. **AMP-CCSD**

Z. H. Sun et al., arXiv:2409.02279 & PRX 15, 011028; G. Hagen et al., PRC 105, 064311

- **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]

(Multireference) EOM-IMSRG

cf. N. M. Parzuchowski et al., PRC95, 044304 (2017)

- 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**):

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

$$Q_k^\dagger(s) = \sum_{p} \left(Q_k^{(k)}\right)_{p}(s) : a_p^\dagger : + \frac{1}{4} \sum_{pqr} \left(Q^{(k)}\right)_{pqr}(s) : a_p^\dagger a_q^\dagger a_r : + \ldots$$

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

Reshuffling of Correlations

Benefit:
collective correlations are captured in **much simpler states** (even mean field)

Cost:
deformed **s.p. basis is 10+ times bigger**, symmetry **projection is expensive**