

# IMSRG Developments for Deformed Nuclei, Excitations and Response

(with a Dash of Emulation)

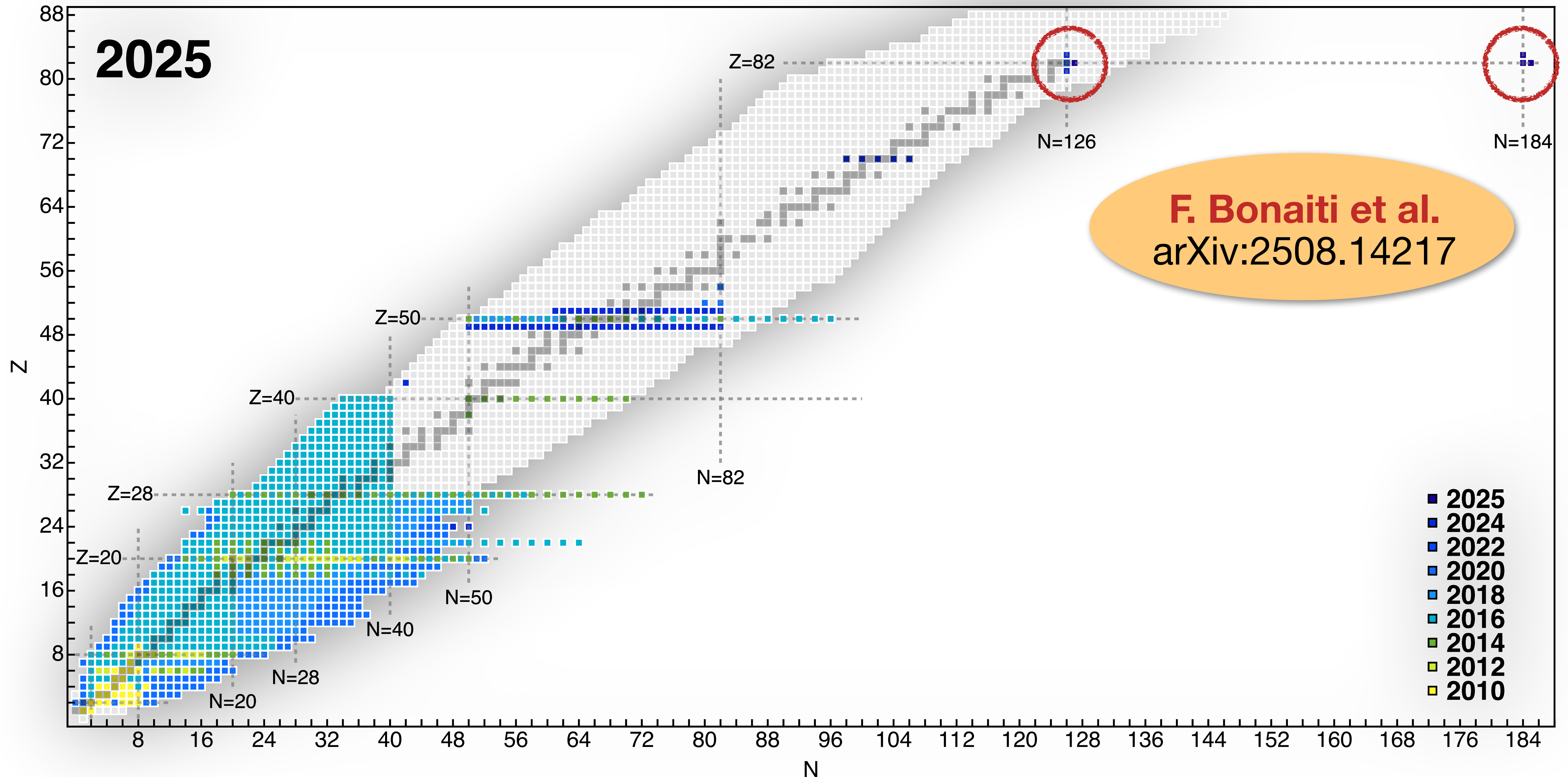
Heiko Hergert  
Facility for Rare Isotope Beams  
& Department of Physics and Astronomy  
Michigan State University



# Progress in *Ab Initio* Calculations



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



# Many-Body Methods: Paradigms



- **Coordinate Space**

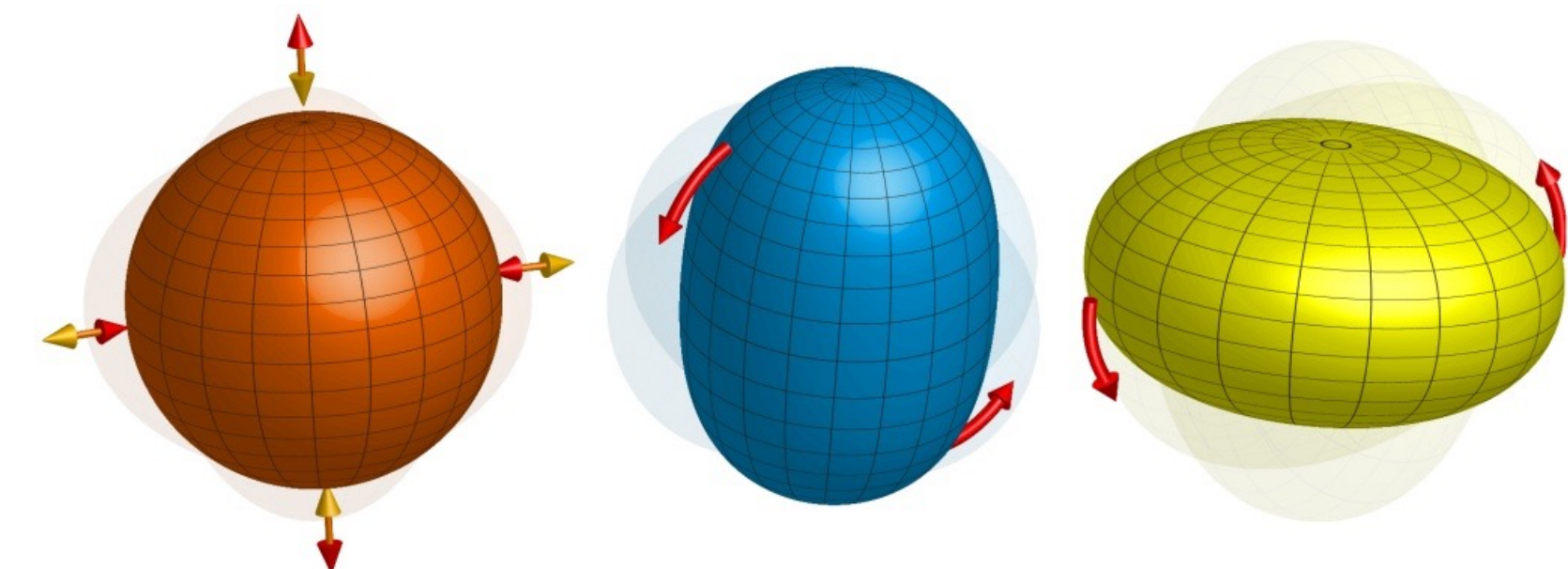
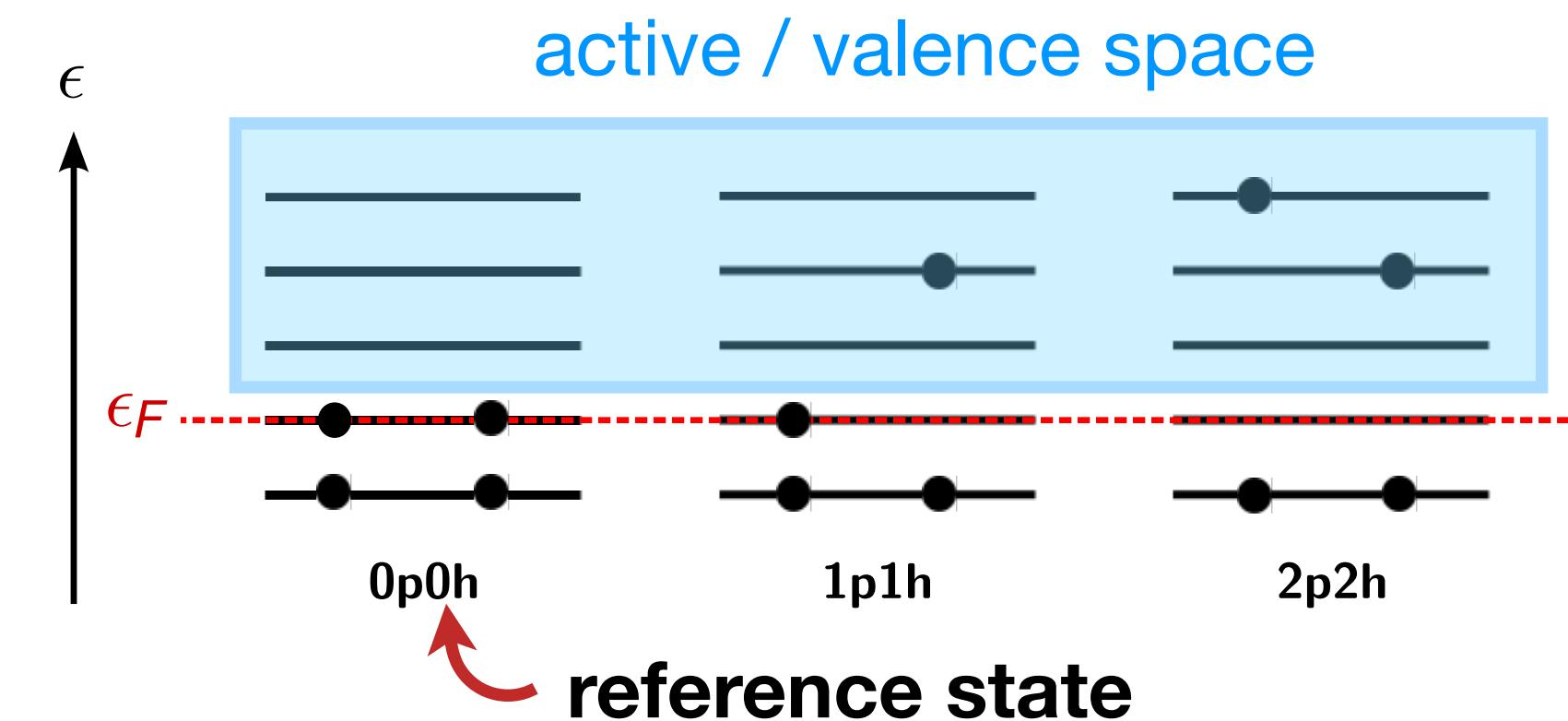
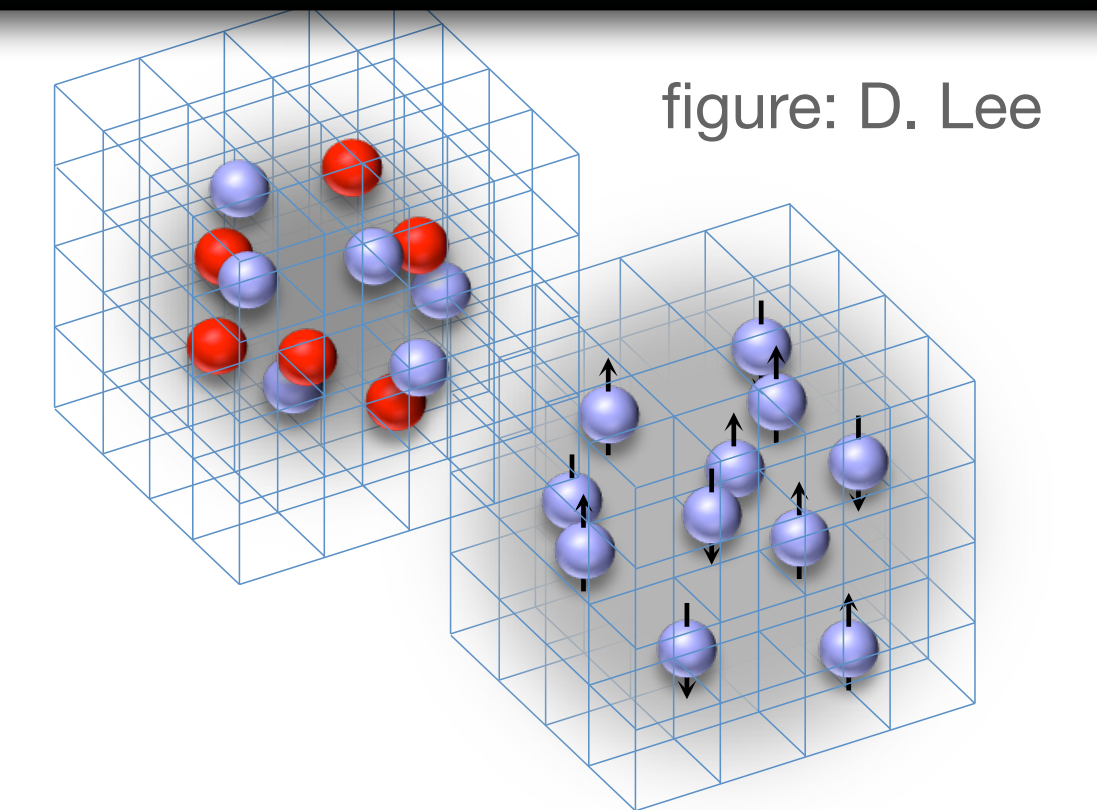
- Quantum Monte Carlo
- Lattice EFT

- **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**

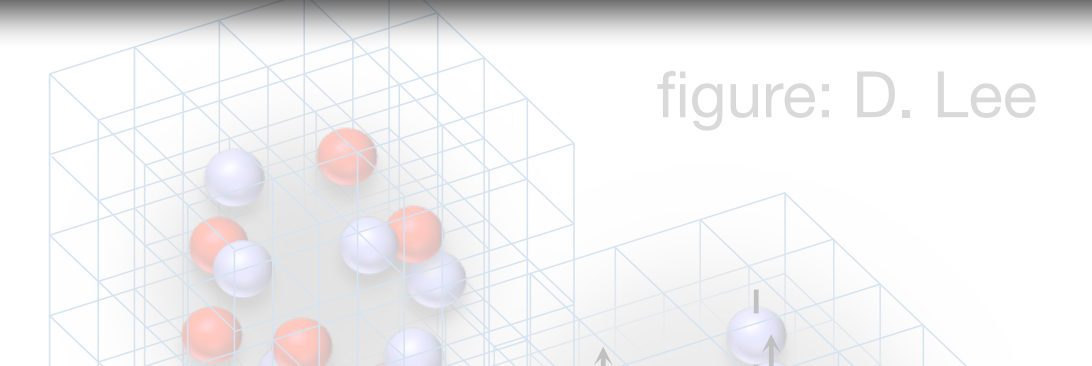
- deformed HF(B) + projection
- projected Generator Coordinate Method (PGCM)
- symmetry-adapted NCSM



# Many-Body Methods: Paradigms



- **Coordinate Space**
  - Quantum Monte Carlo



## Recent(-ish) Reviews:

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

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

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

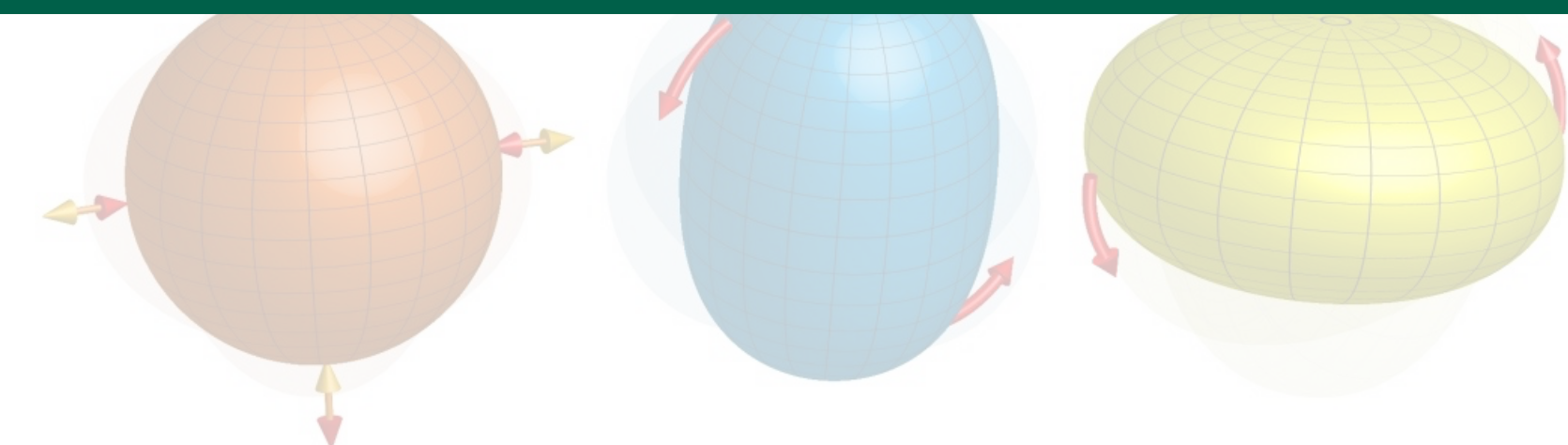
V. Somà, *Front. Phys.* **8**, 340 (2020)

## 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)

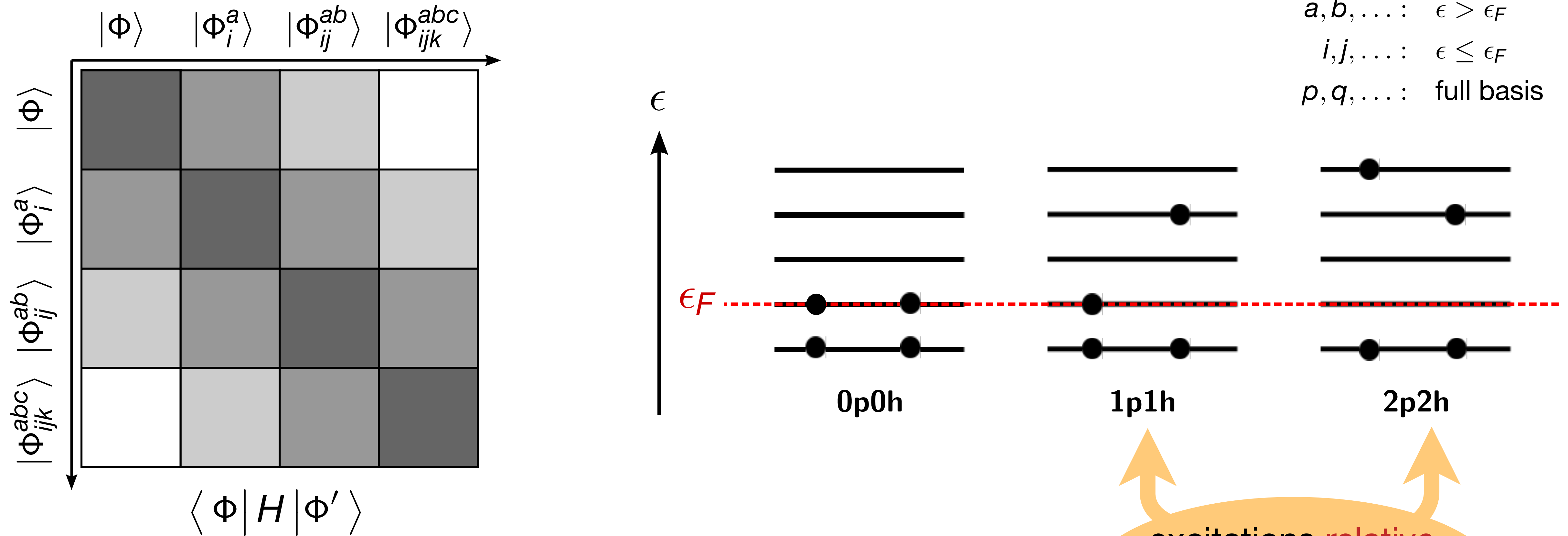
## Expansions

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



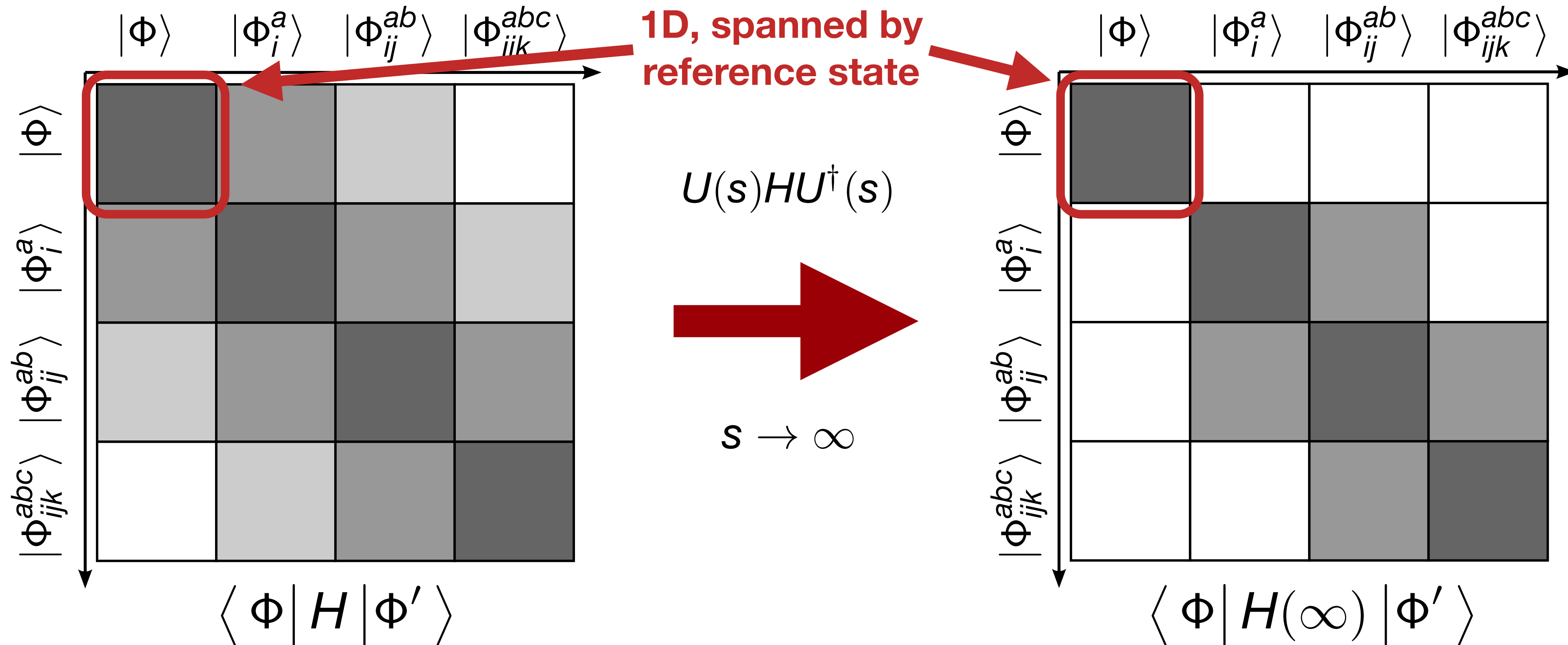
# In-Medium SRG Methods

# Many-Body Methods: Configuration Space



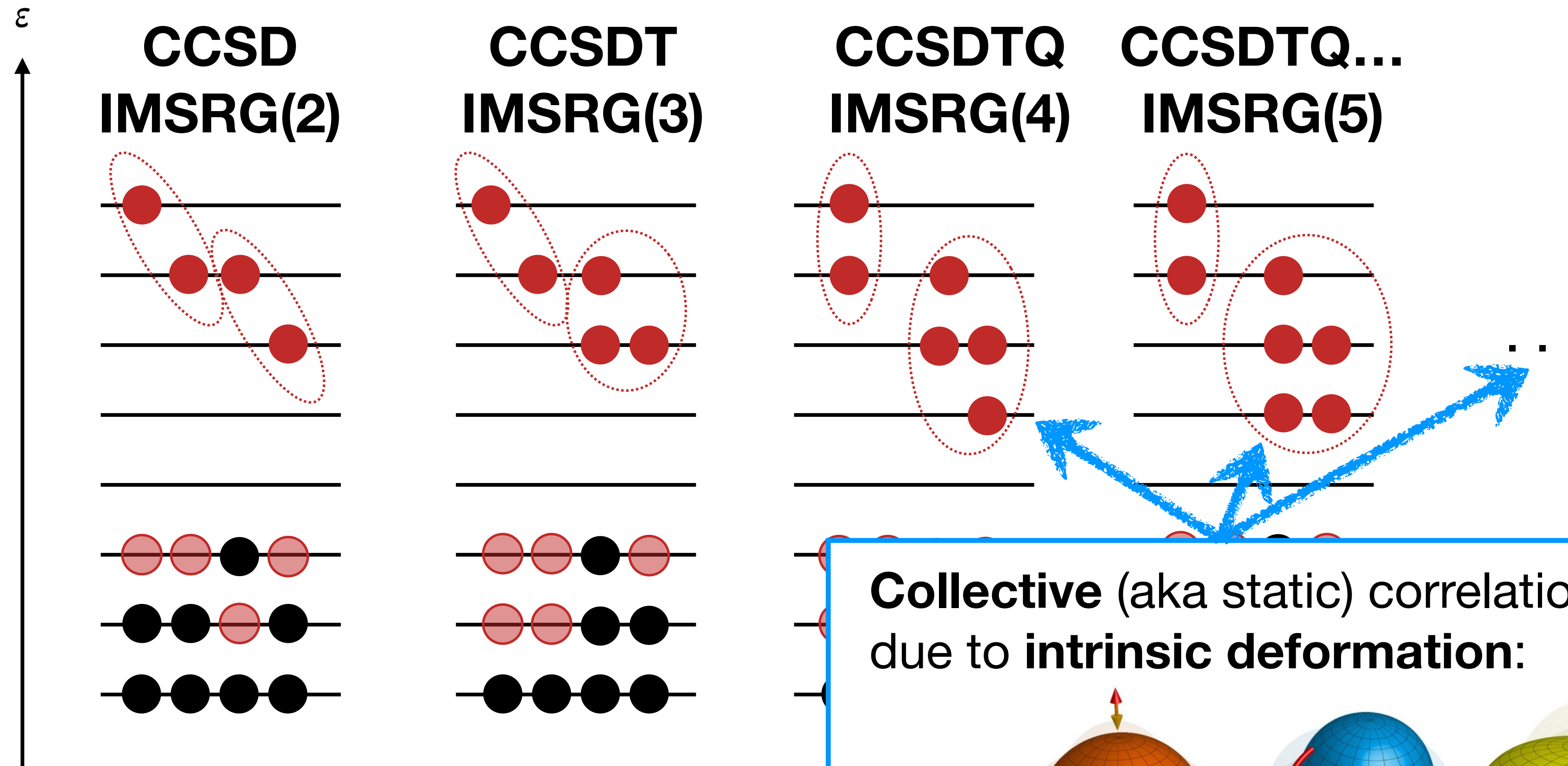
construct **particle-hole excitations** of a **reference state** - usually an optimized **mean-field Slater determinant**

# Decoupling in A-Body Space

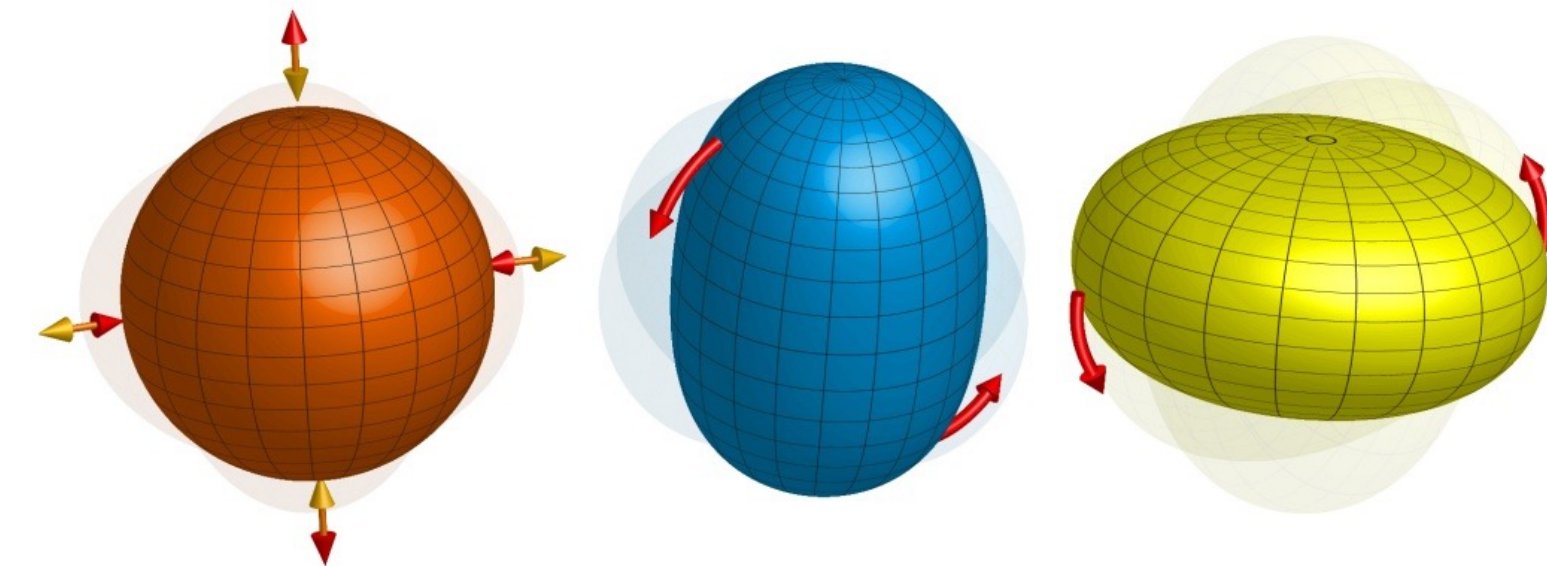


- **identify** the parts of the **operator  $H$**  which **couple reference state to excitations**
- **eliminate** them with unitary (**IMSRG**) or general similarity transformations (**CC**)
- **efficient: polynomial scaling**, no need to construct matrix !

# Correlations in Nuclei

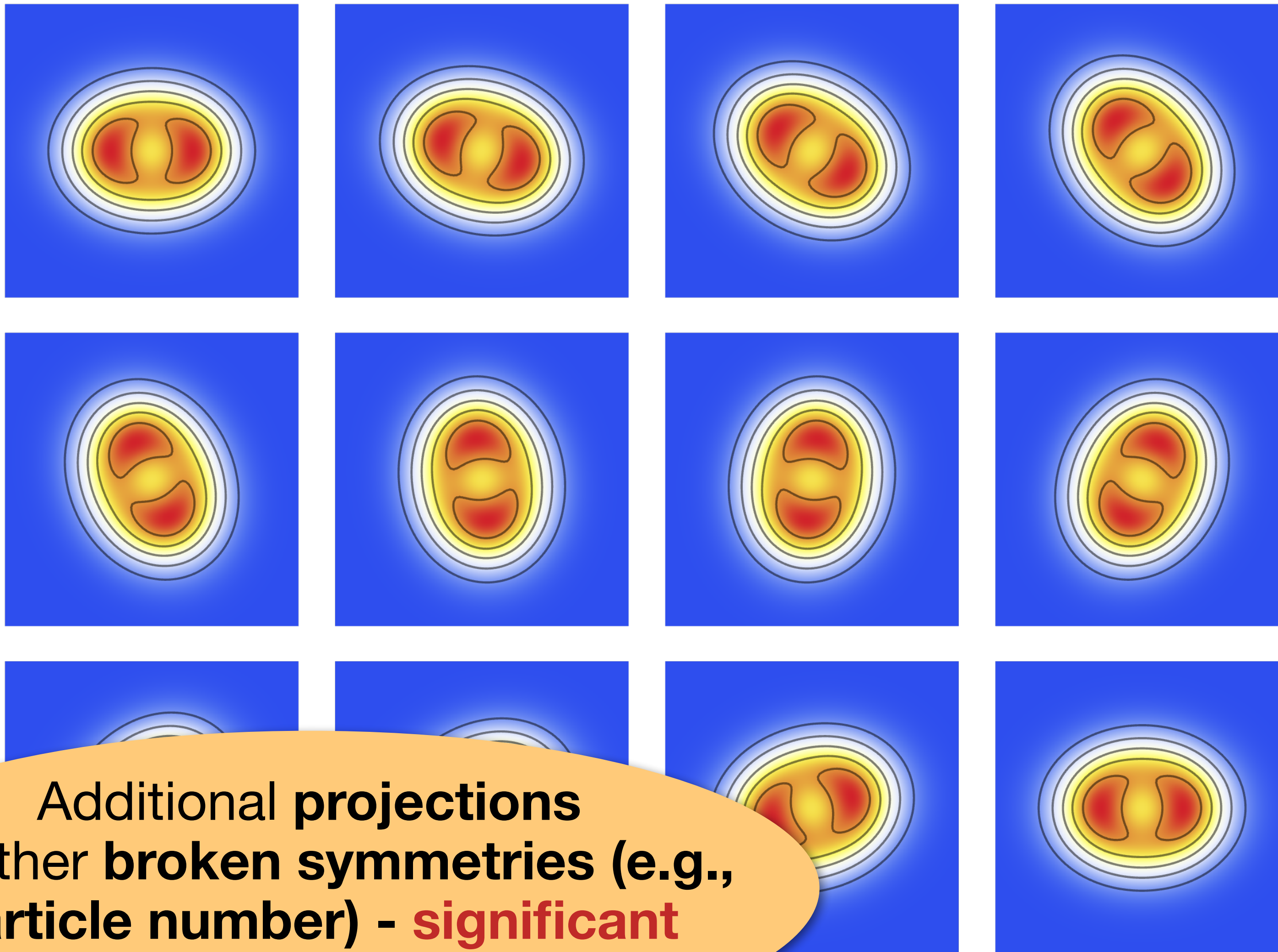


**Collective** (aka static) correlations, e.g. due to **intrinsic deformation**:

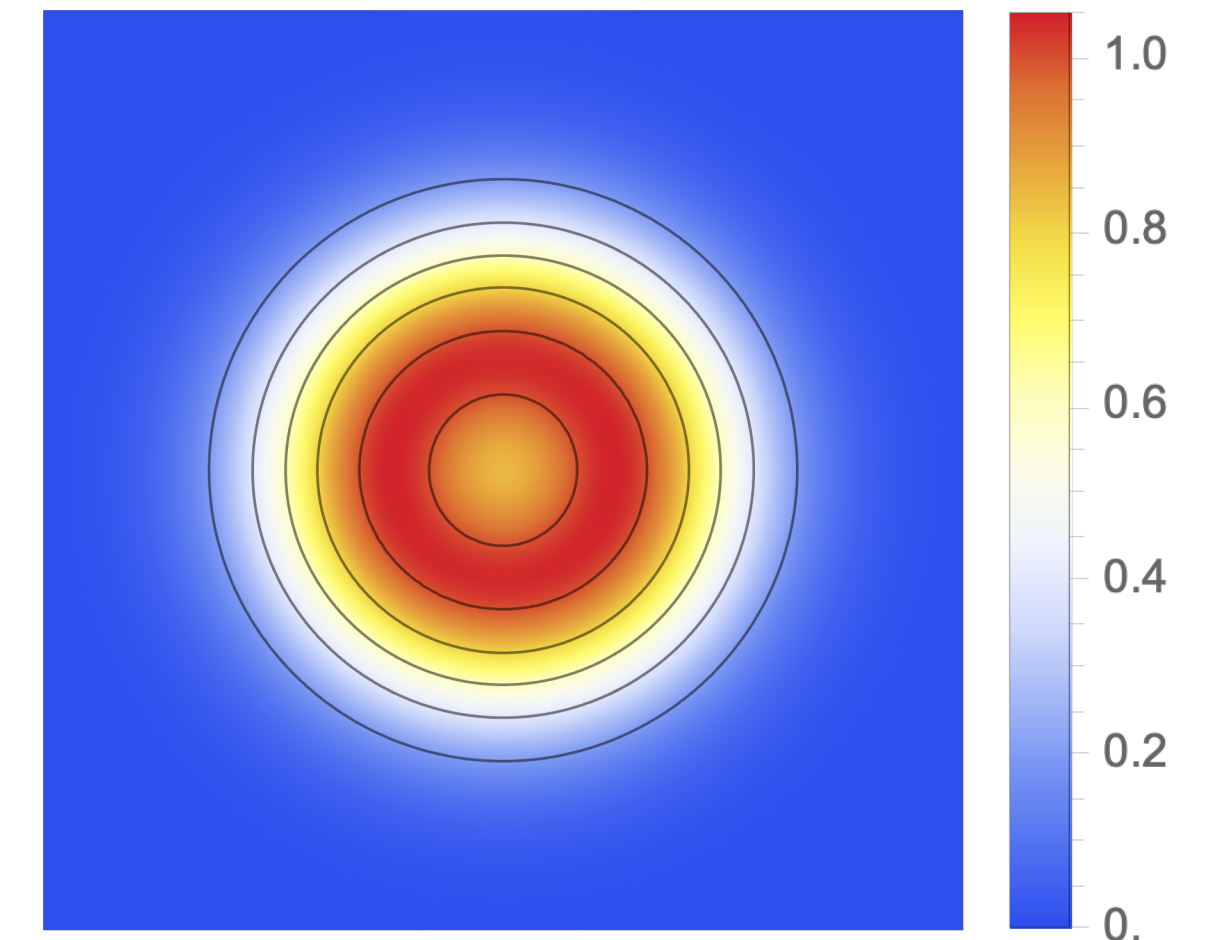


# Symmetry Breaking and Restoration

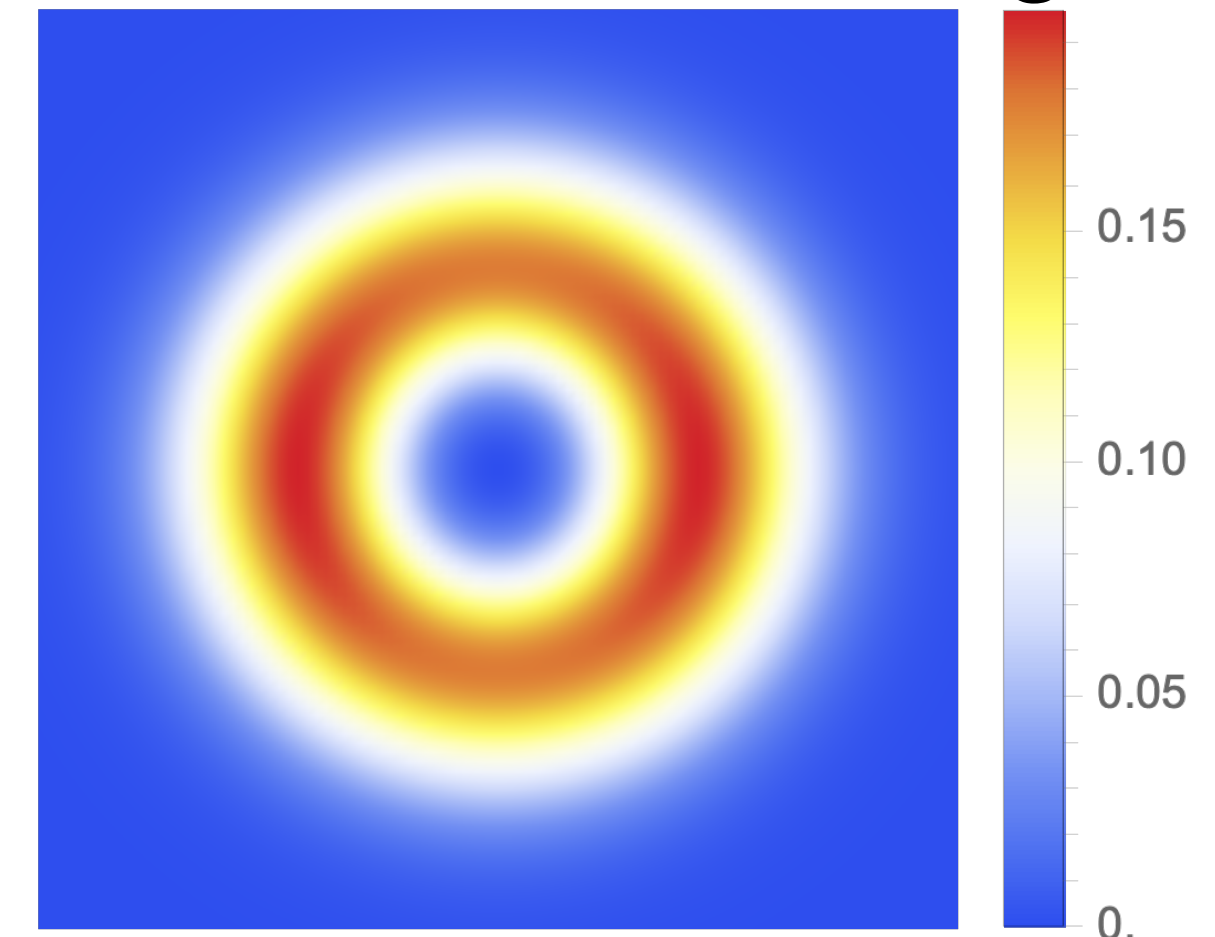
deformed configurations



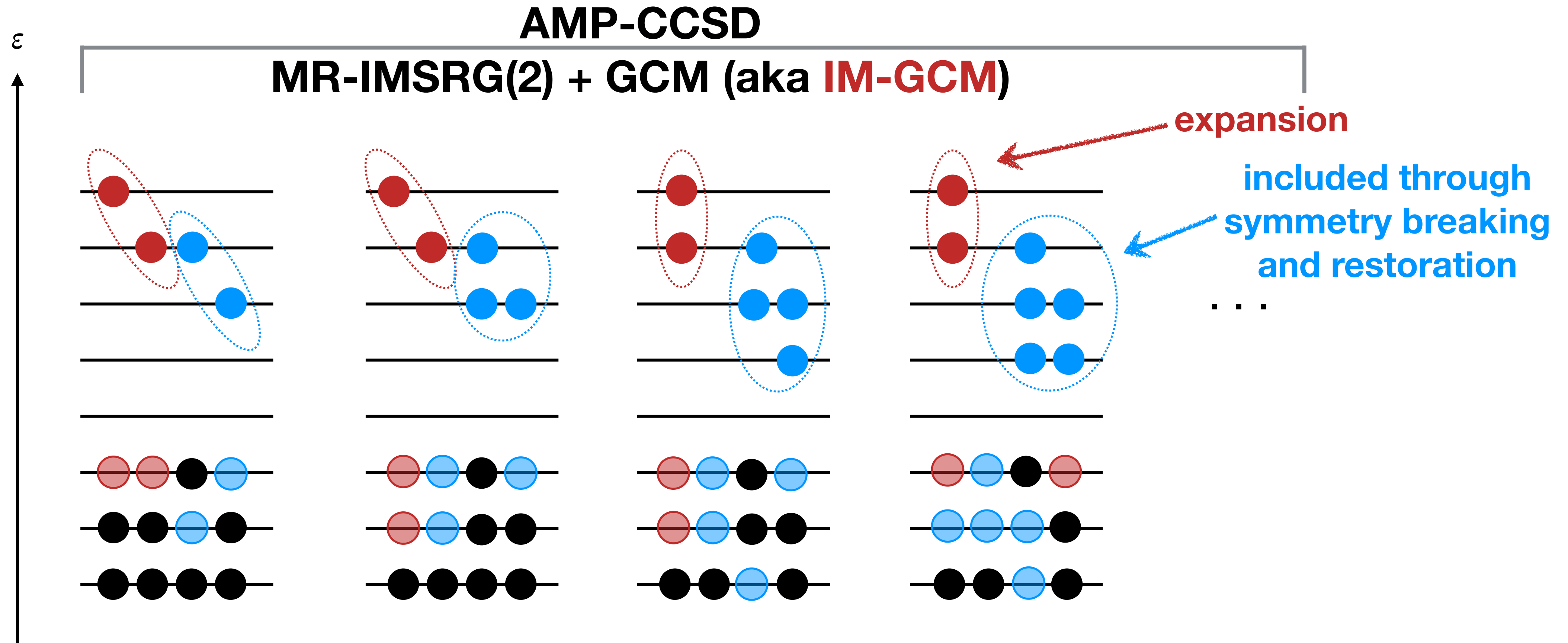
projected w.f.



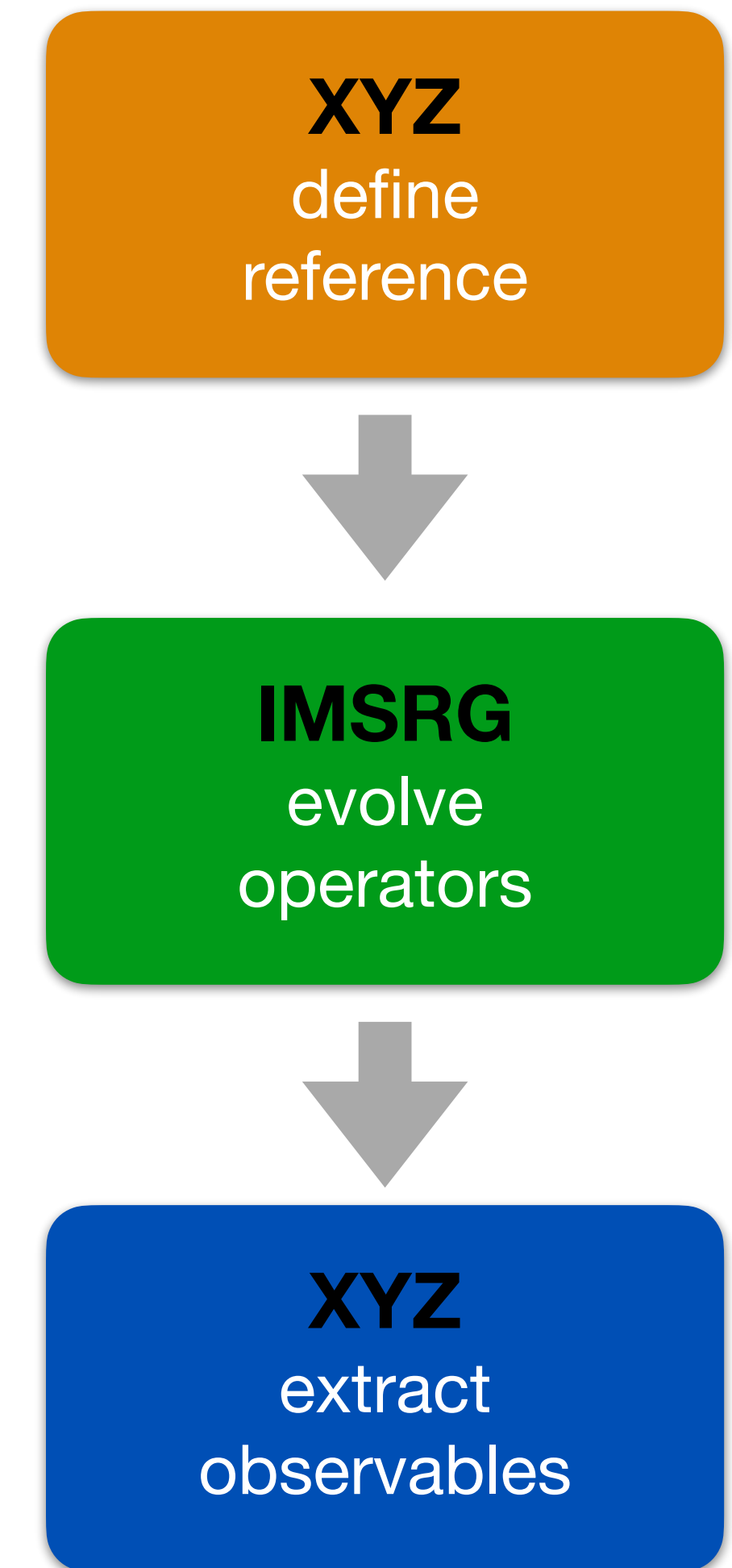
difference from spherical w.f.  
with same basis size /length scale



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

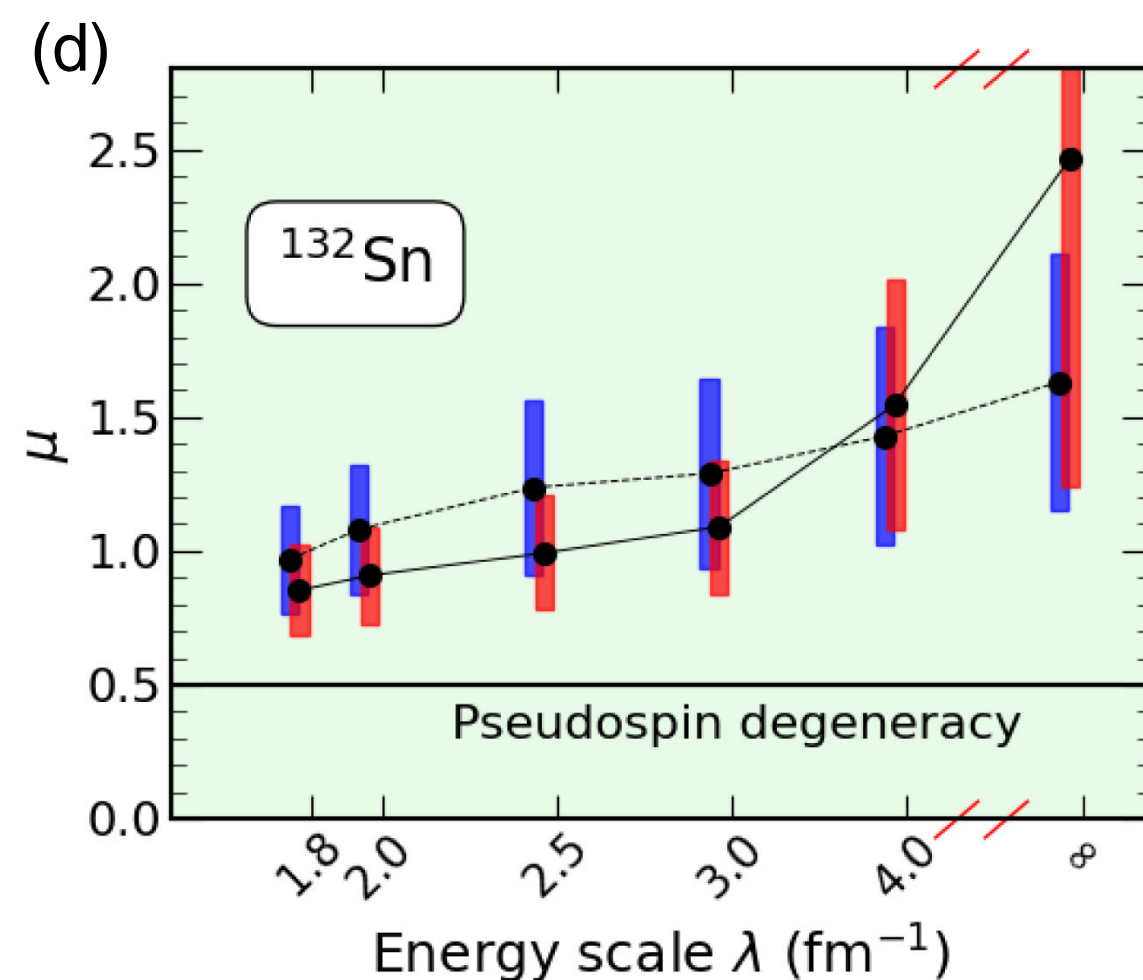
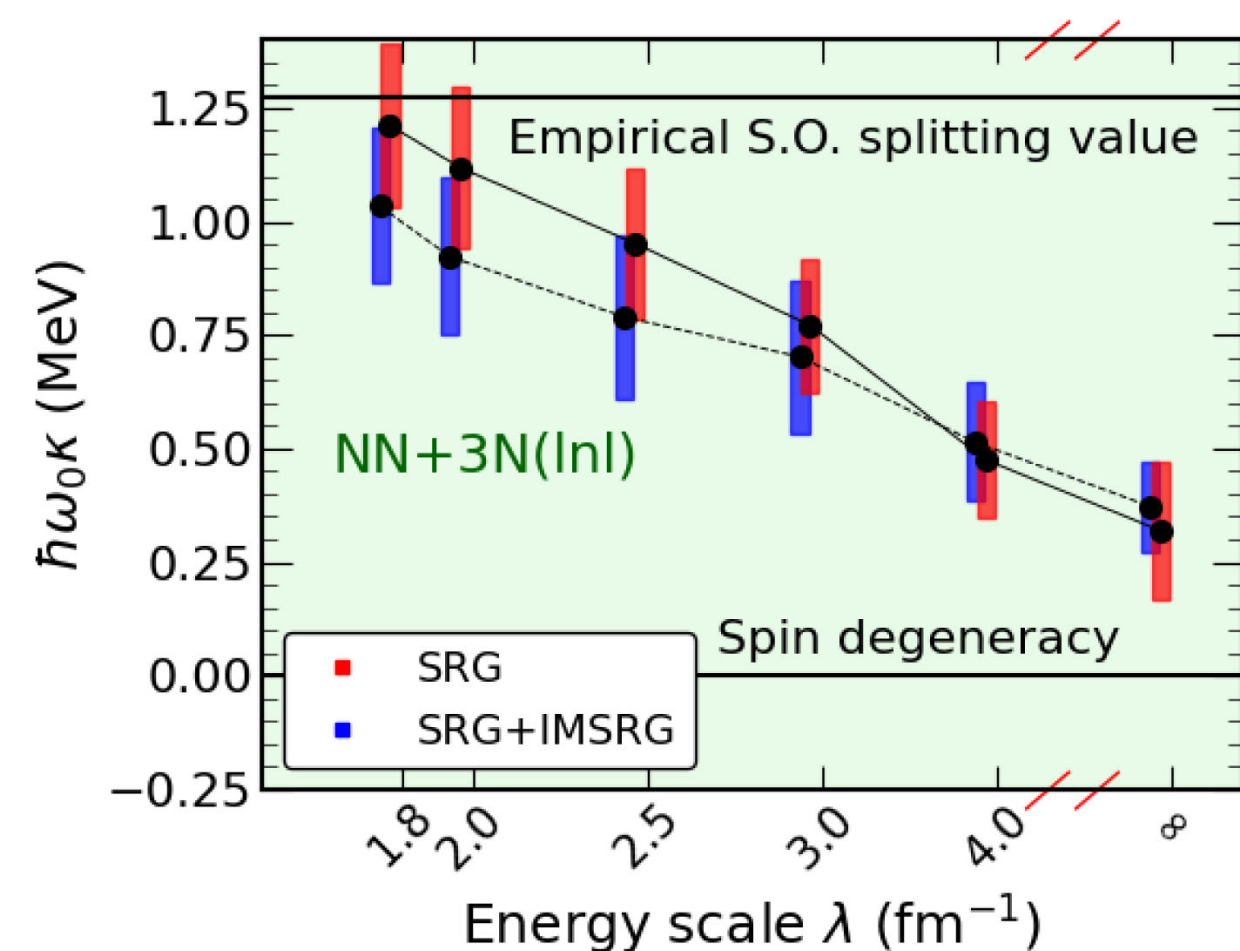
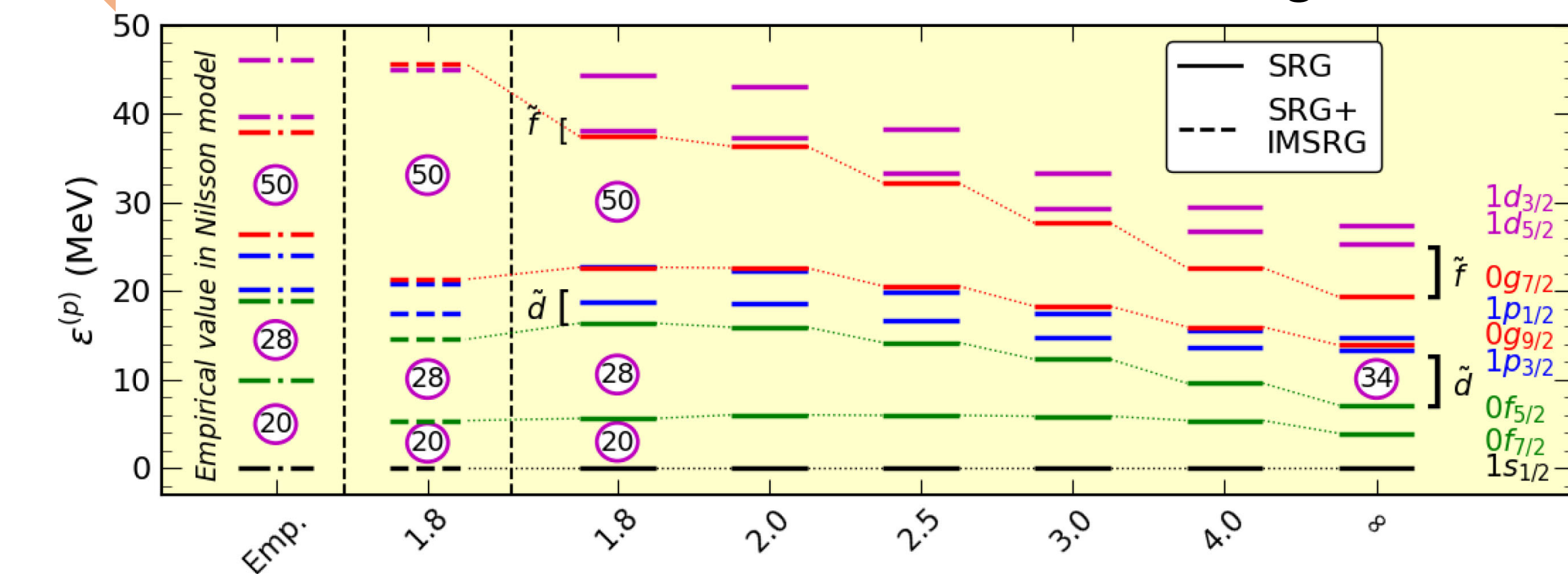
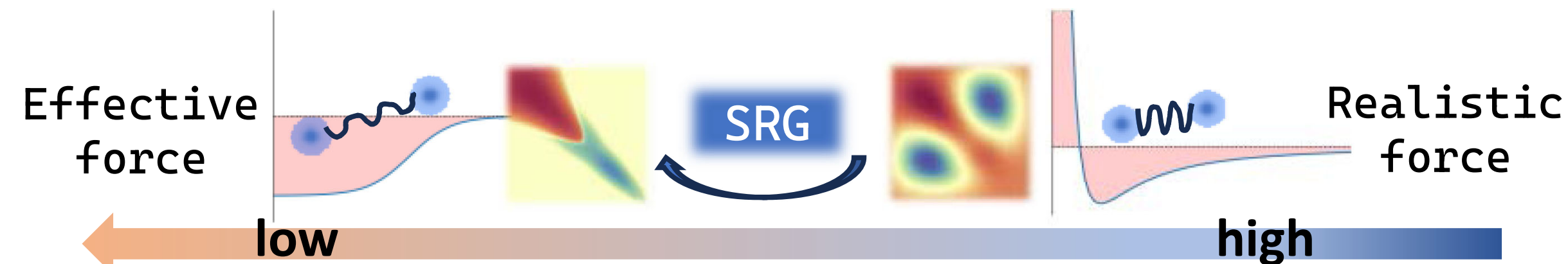


- IMSRG can be used to build specific types of correlations into **RG-improved interactions and operators**
  - ideally, IMSRG captures correlations that are **complementary** to target method
  - mean-field or **correlated reference state(s)** for a specific nucleus  
define(s) **operator basis** for 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

# Evolution of Effective Single-Particle Energies

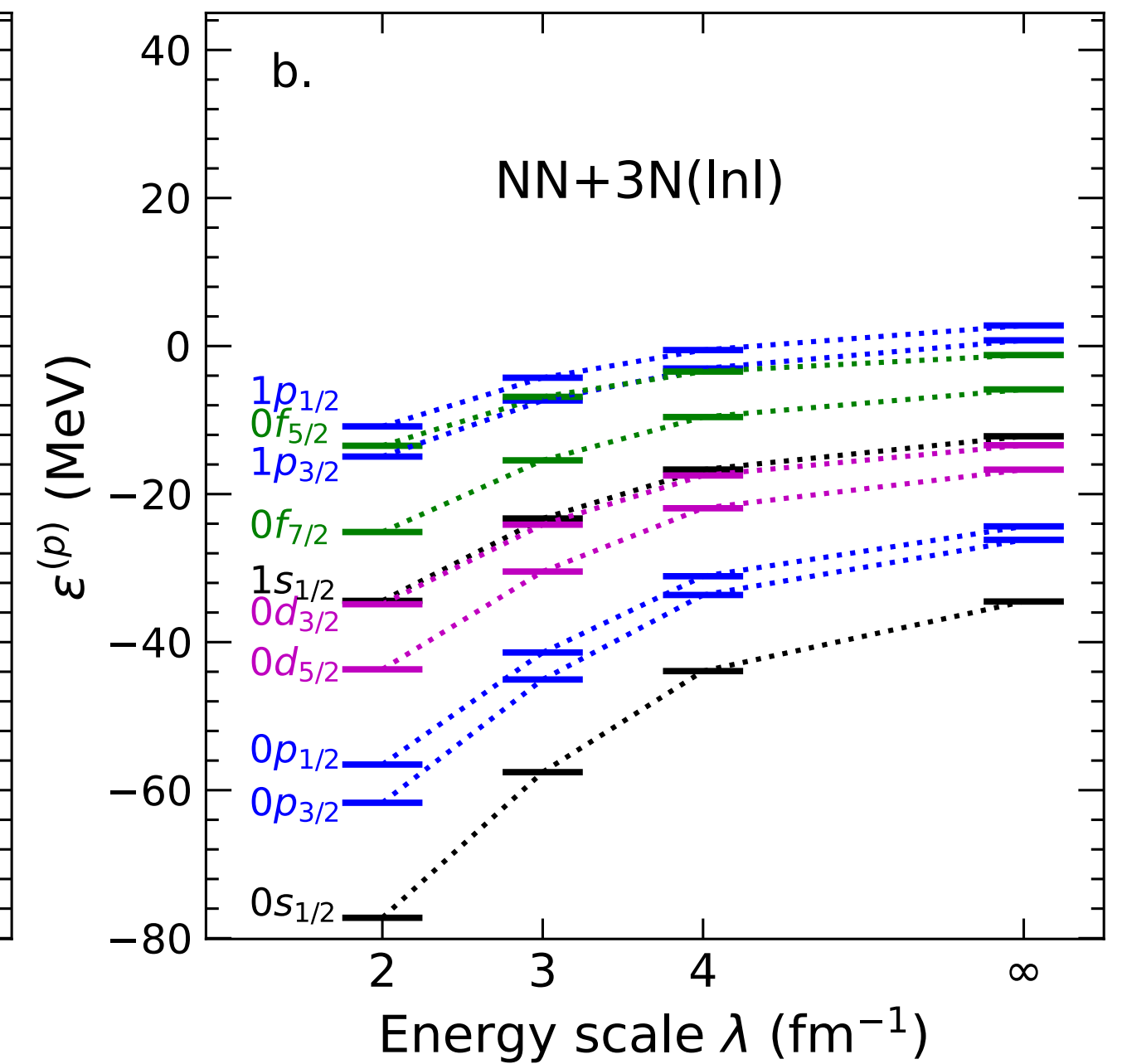
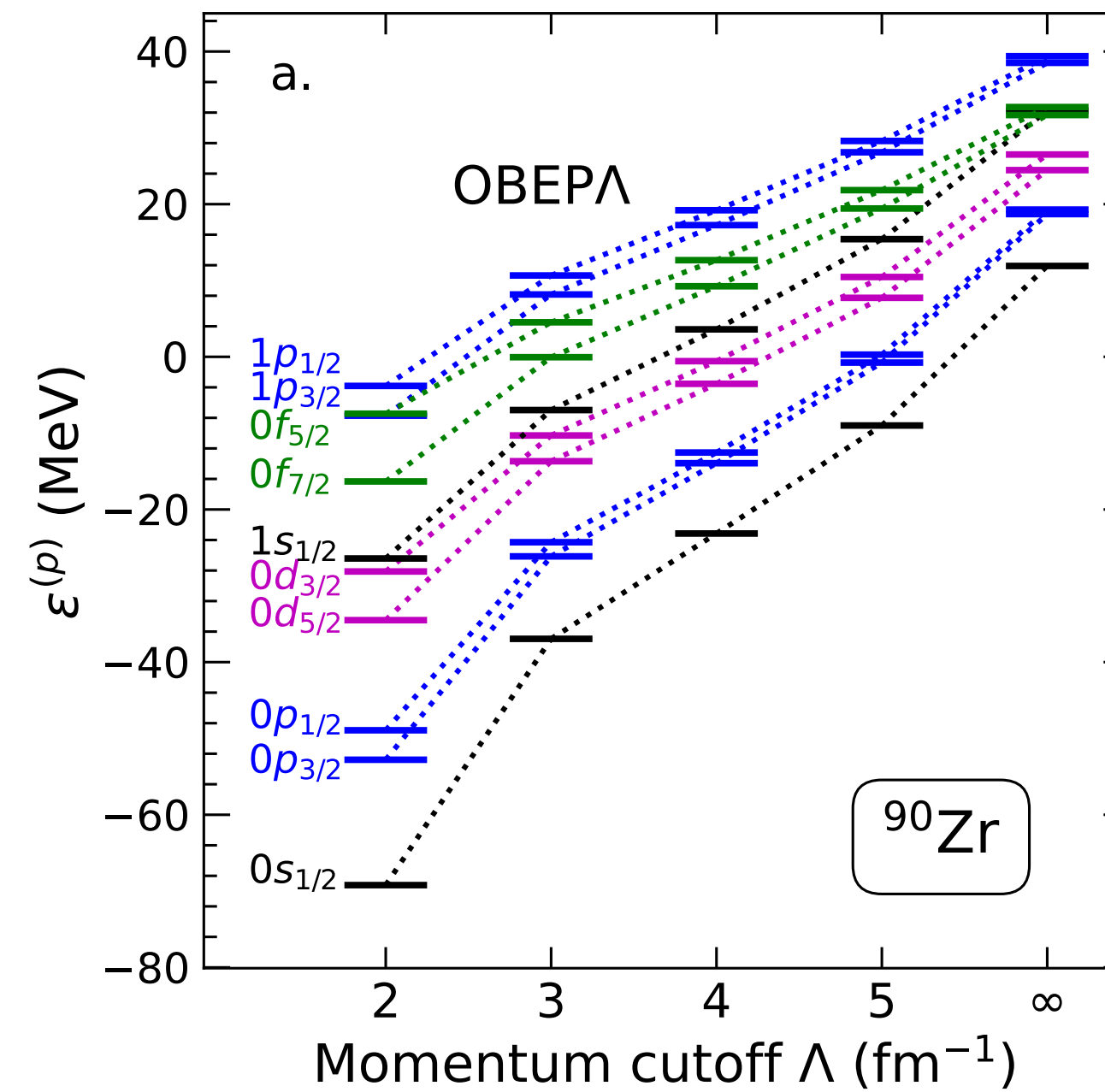
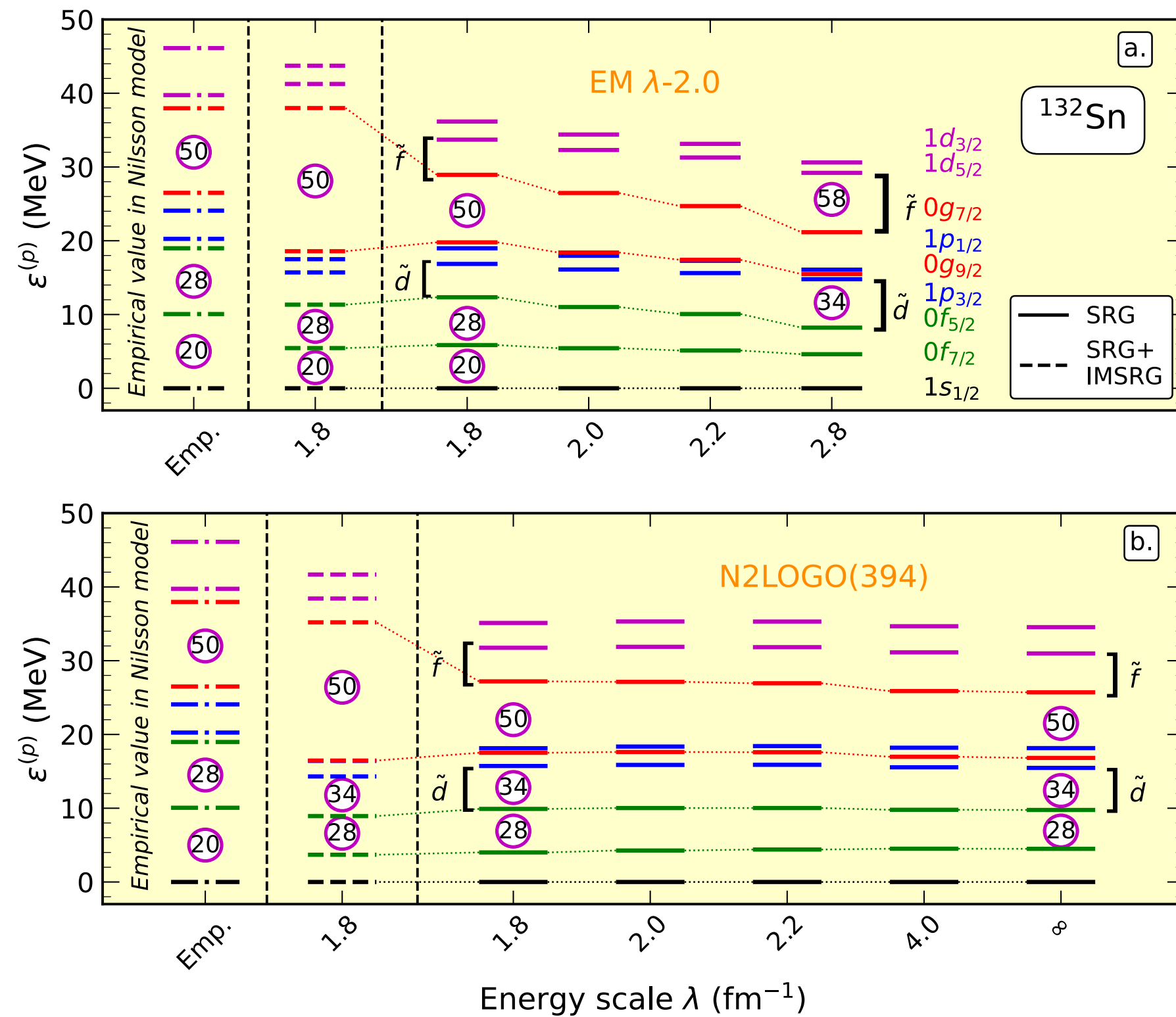


- **Mean-field / Shell model is inherently a low-momentum picture**
- empirical density functionals/ Shell model interactions are **“effective” parameterizations of low-resolution nuclear forces (+ correlations)**
- SRG + IMSRG can be used to **quantitatively bridge** high- and low-resolution descriptions of nuclear forces **and correlations**

# Evolution of Effective Single-Particle Energies



C. R. Ding et al., PRL 136, 052501 (2026)



- **low-resolution interactions** already exhibit much of the **symmetries** at the mean-field level
- behavior is **consistent in non-relativistic and relativistic** frameworks

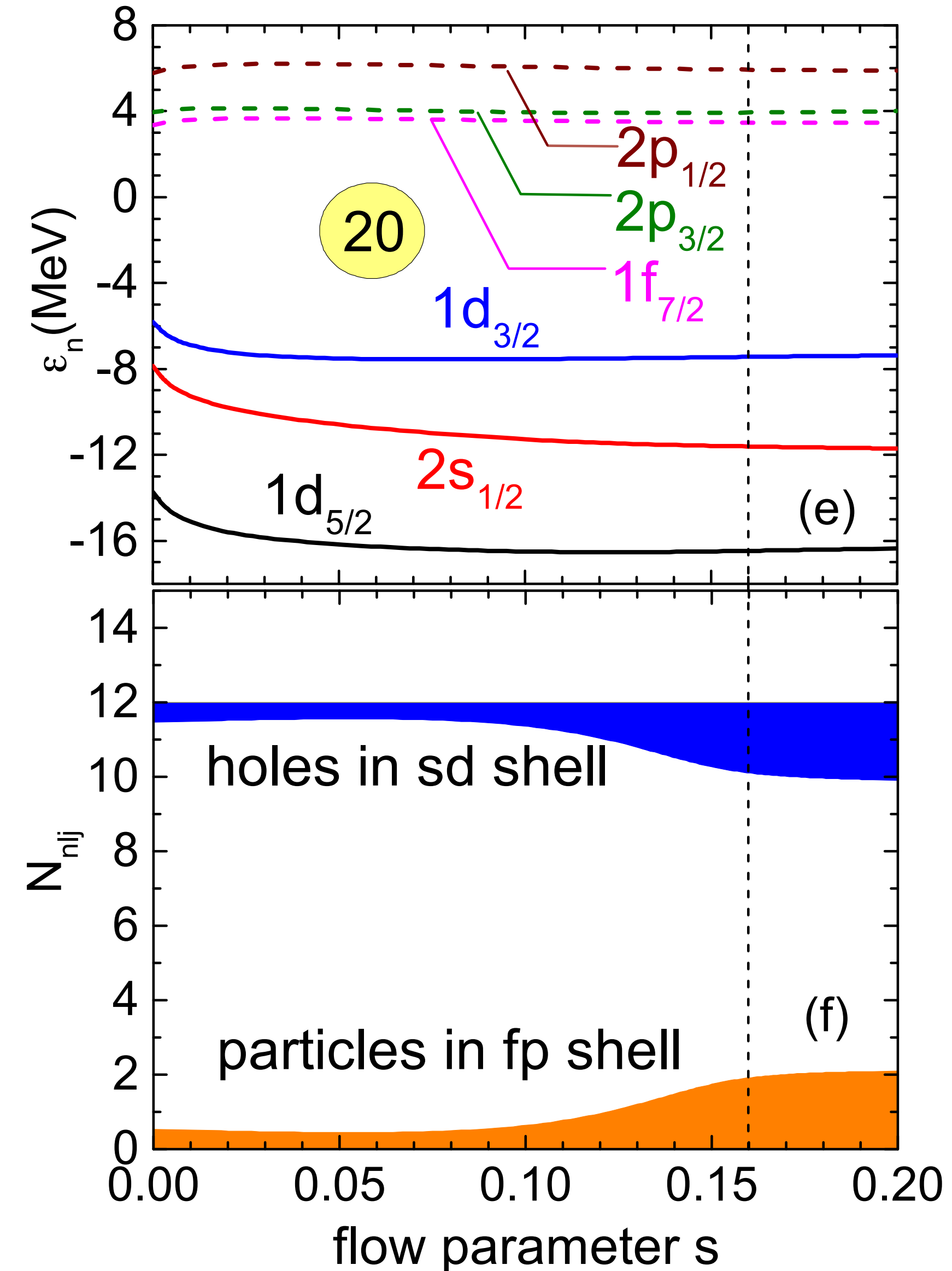
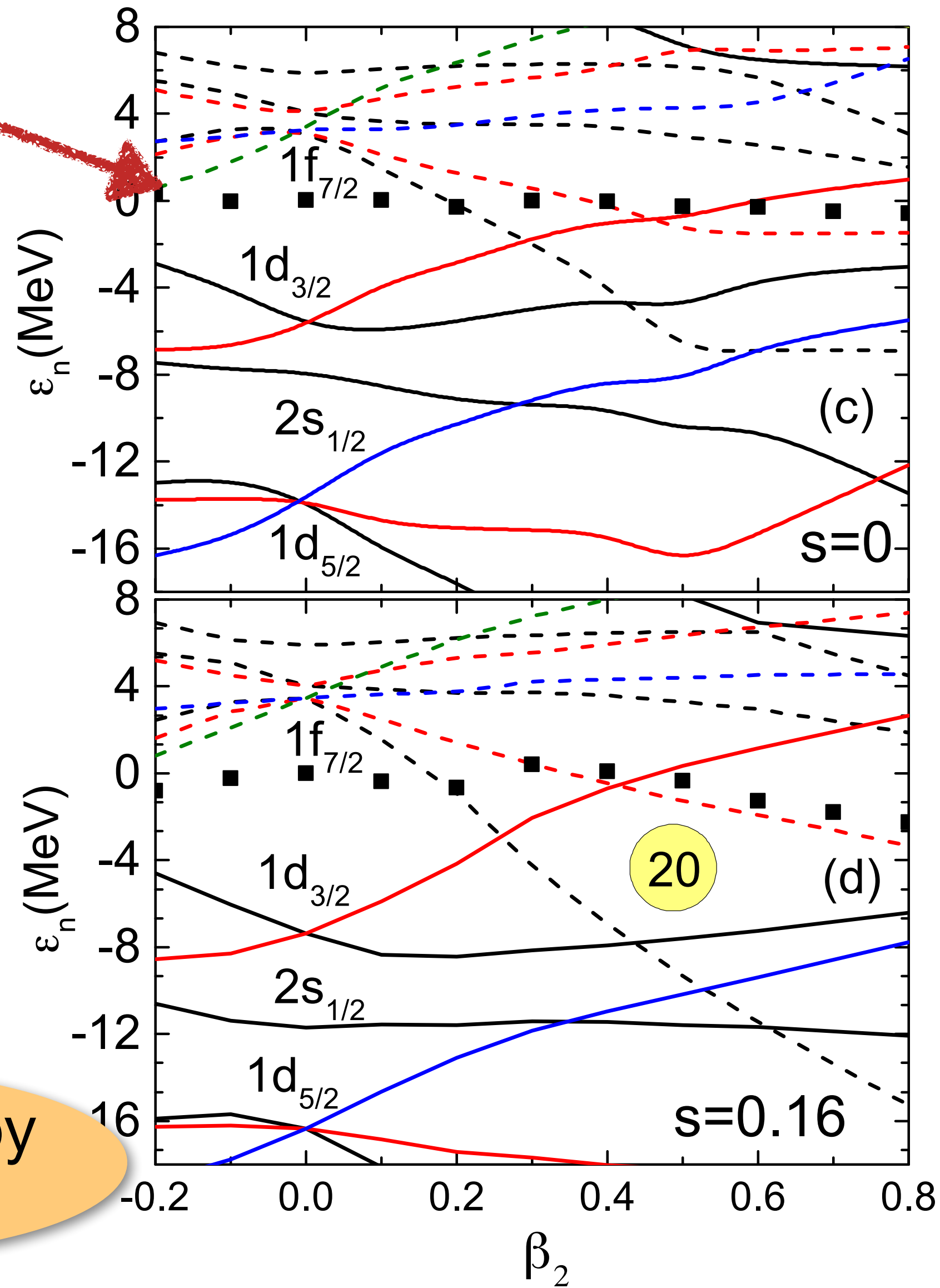
cf.  $g_A$  **quenching**,  
 [P. Gysbers et al., Nat. Phys. 15, 428]  
**emergence of rotational bands**,  
 [M. Caprio et al., PLB 719, 179;  
 Z. H. Sun et al., PRX 15, 011028]  
**etc.**

# Shape Coexistence: $^{32}\text{Mg}$



*E. F. Zhou et al., PLB 865, 139464 (2025) & 2603.xxxx*

Fermi energies

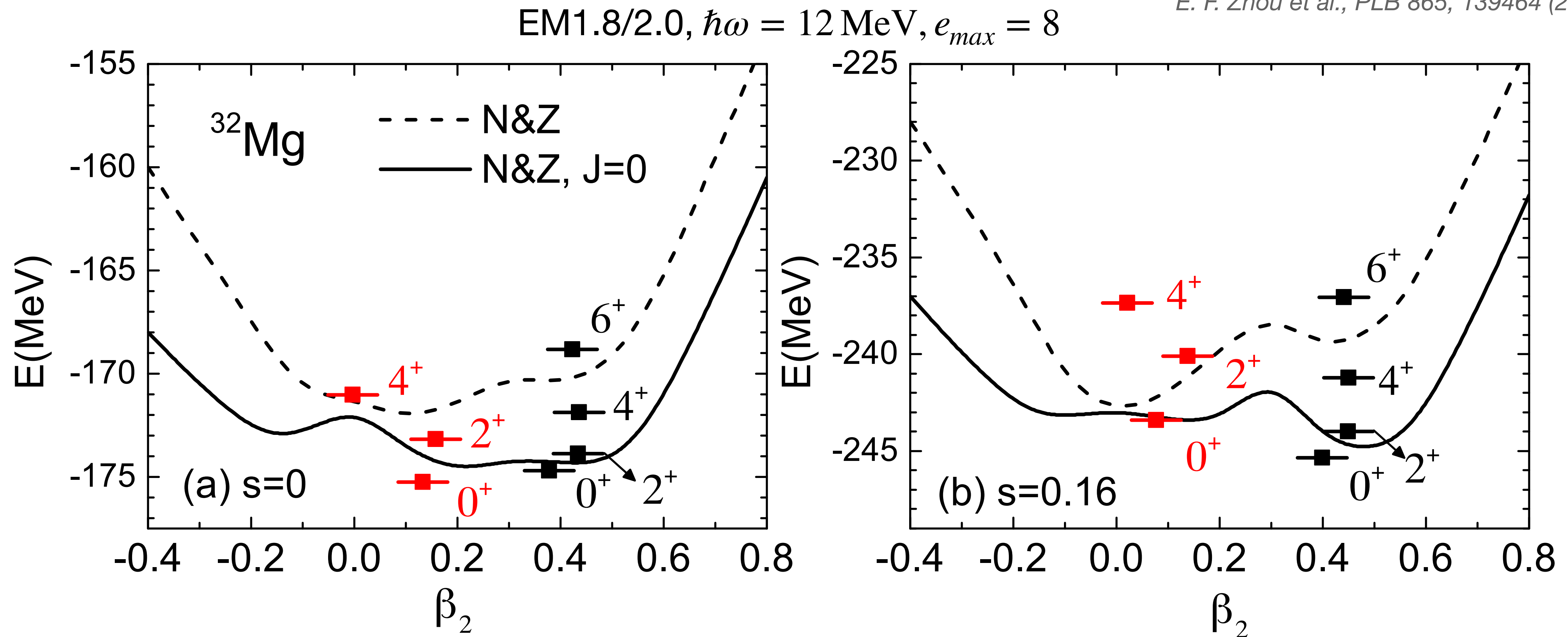


see poster by  
**S. Blade**

# Shape Coexistence: $^{32}\text{Mg}$



*E. F. Zhou et al., PLB 865, 139464 (2025) & 2603.xxxx*

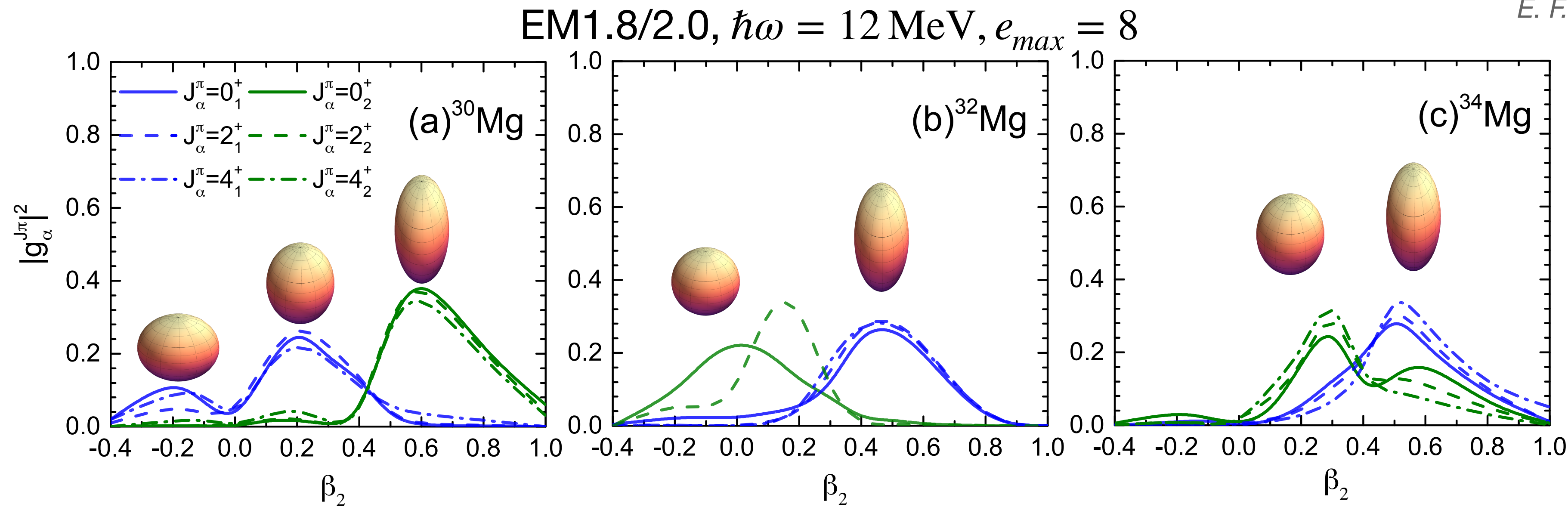


- **Dynamic correlations** captured by IMSRG...
  - bring **absolute energies** close to experiment ( $E = -249.7 \text{ MeV}$  (AME) vs.  $-249.5 \text{ MeV}$  (extrapolated theory))
  - reveal prominent **prolate deformation** of the **ground state**

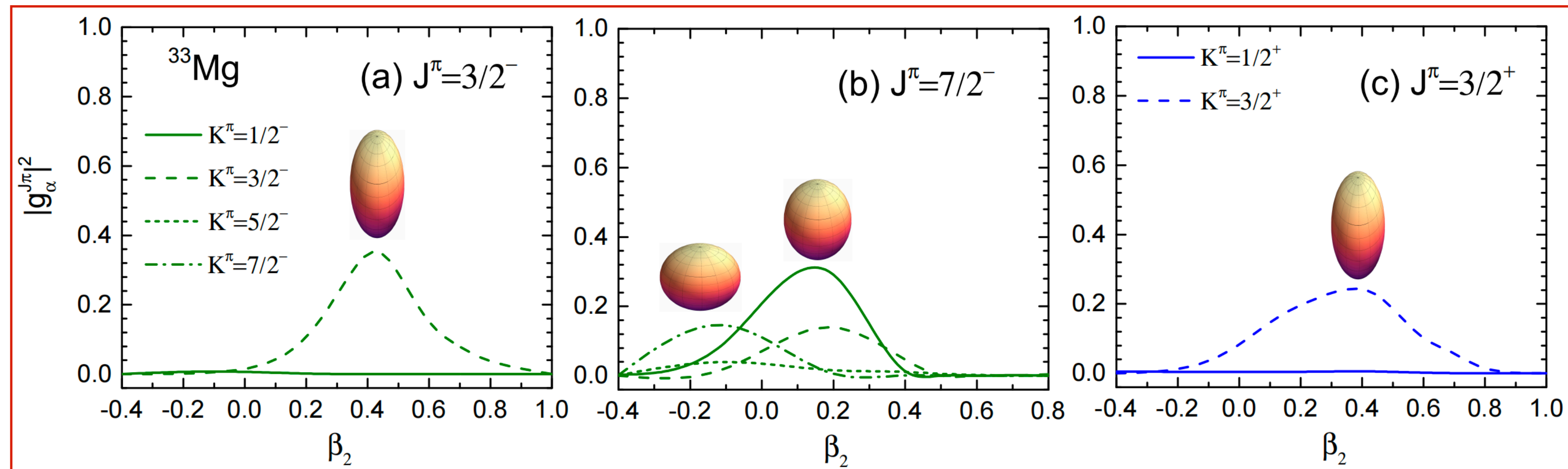
# N=20 Island of Inversion: $^{32-34}\text{Mg}$



*E. F. Zhou et al., PLB 865, 139464 (2025) & 2603.xxxx*



- **shape coexistence** comes with **shape mixing**



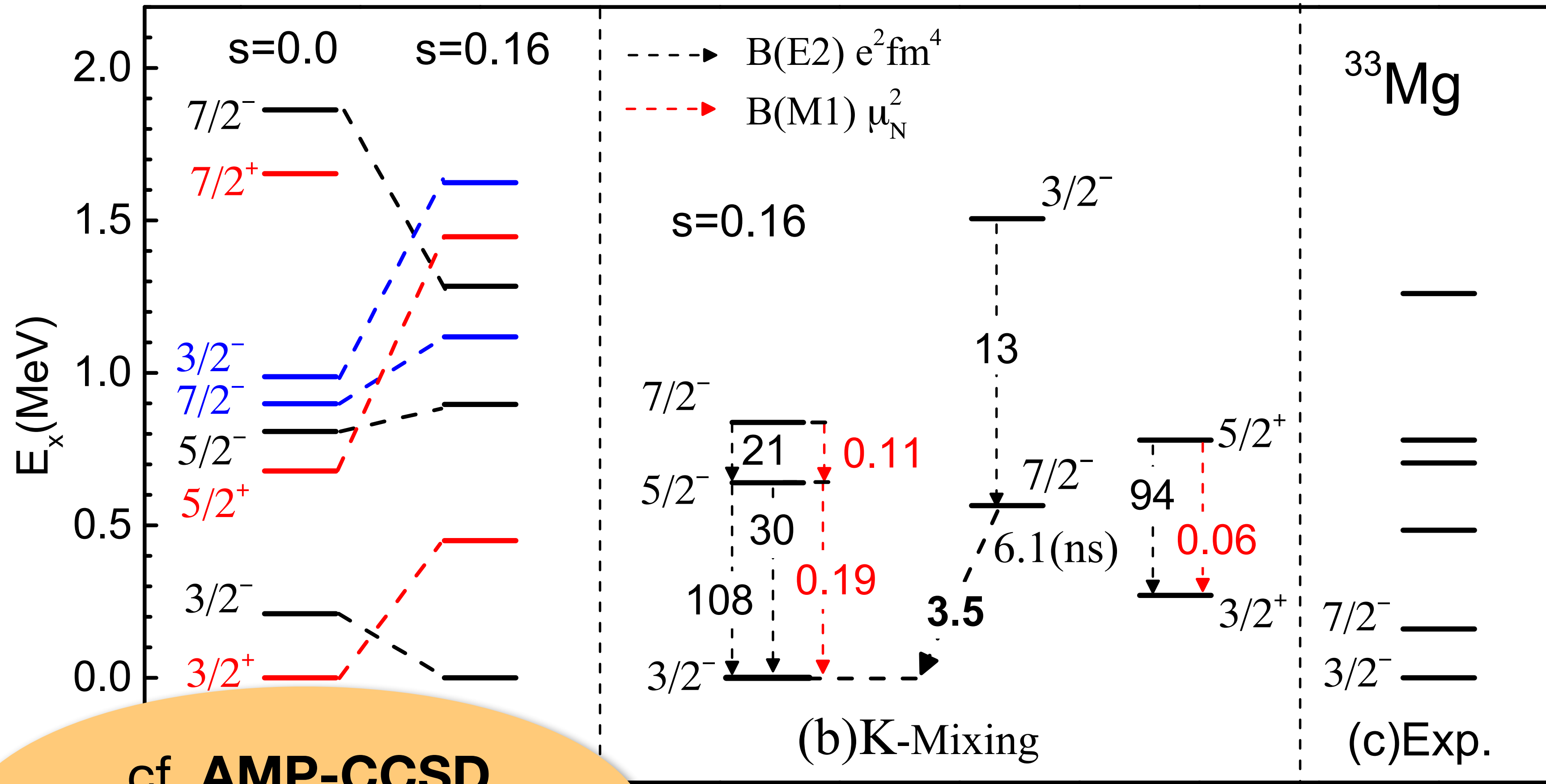
- **caveat:** (collective) wave functions are not observable - **compare with care!**

# N=20 Island of Inversion: $^{33}\text{Mg}$



E. F. Zhou et al., PLB 865, 139464 (2025) & in 2603.xxxx

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



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

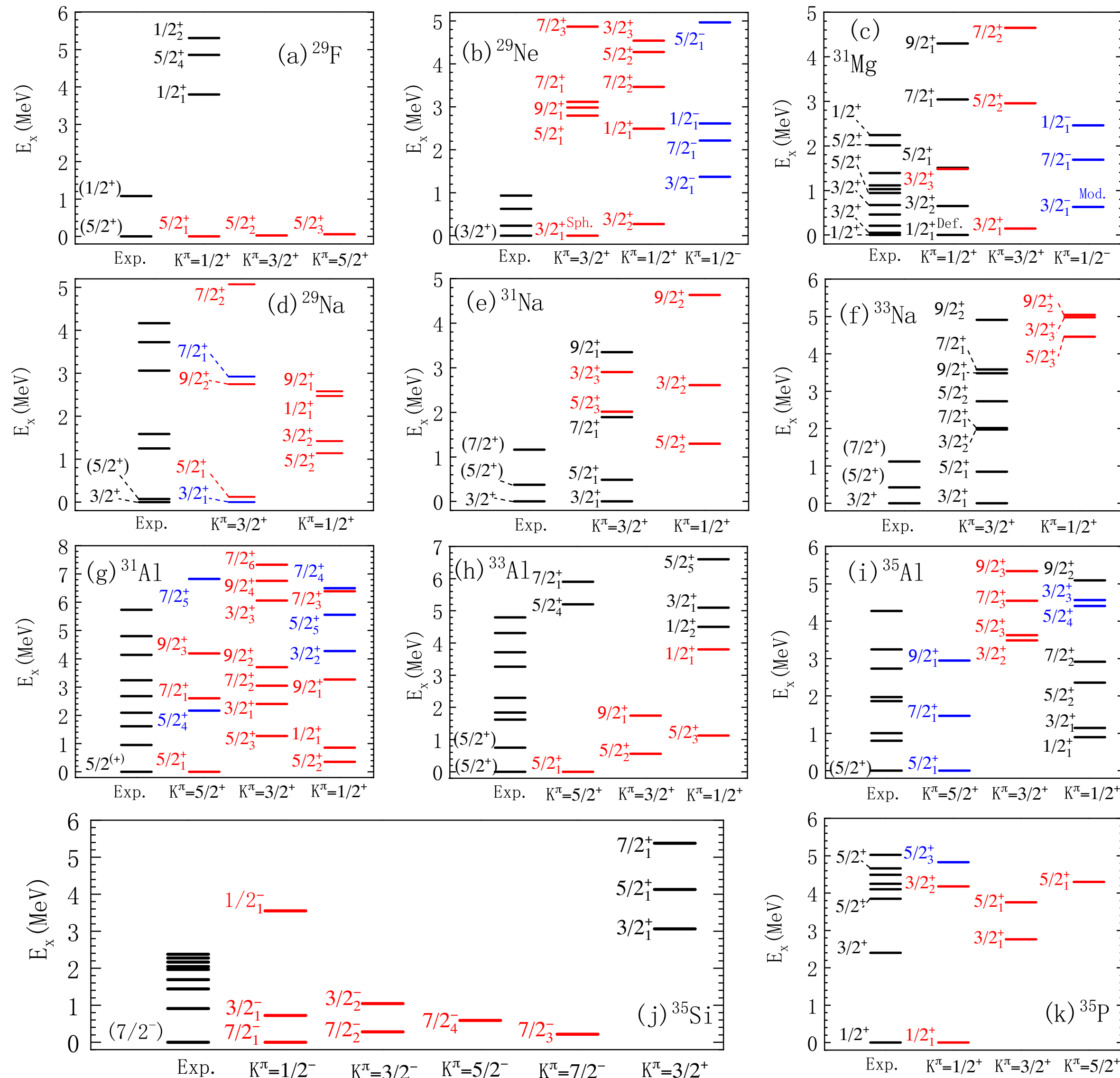
cf. **AMP-CCSD**

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

# Shape Coexistence: N=20 Island of Inversion Region



E. F. Zhou et al., arXiv:2603.xxxx



## IM-GCM survey of the **island-of-inversion region**

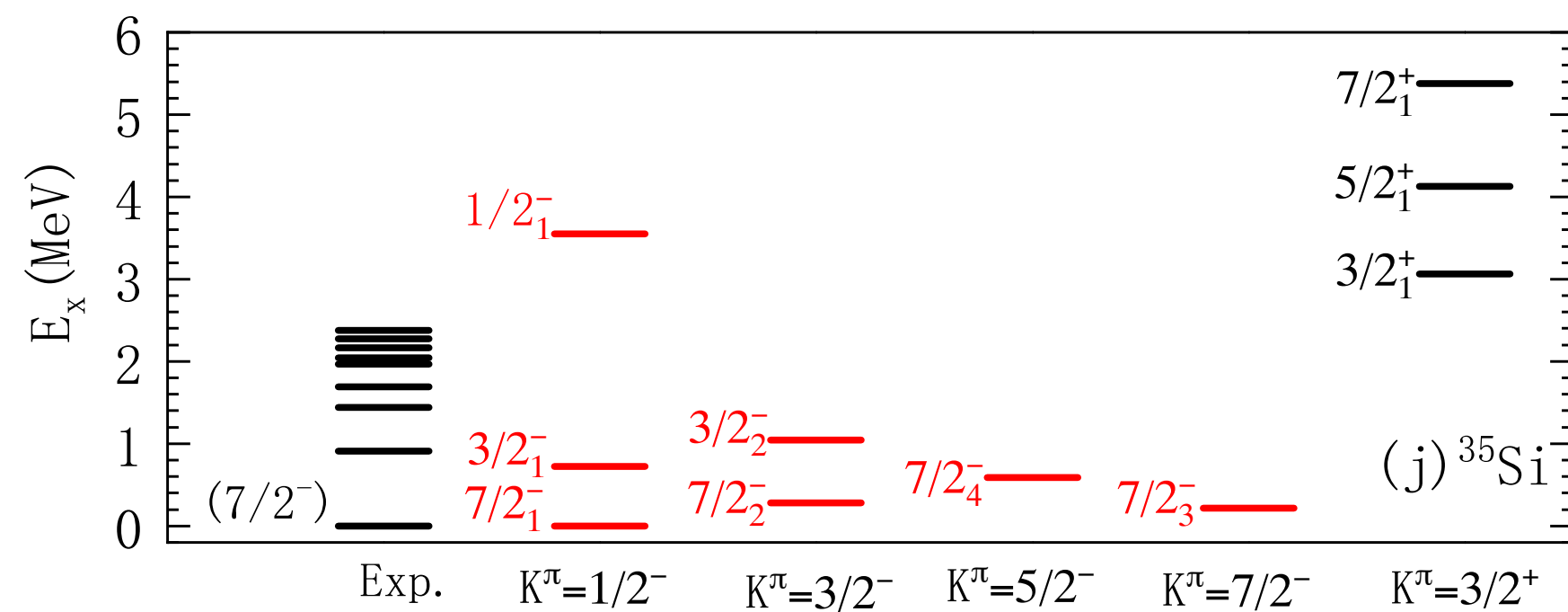
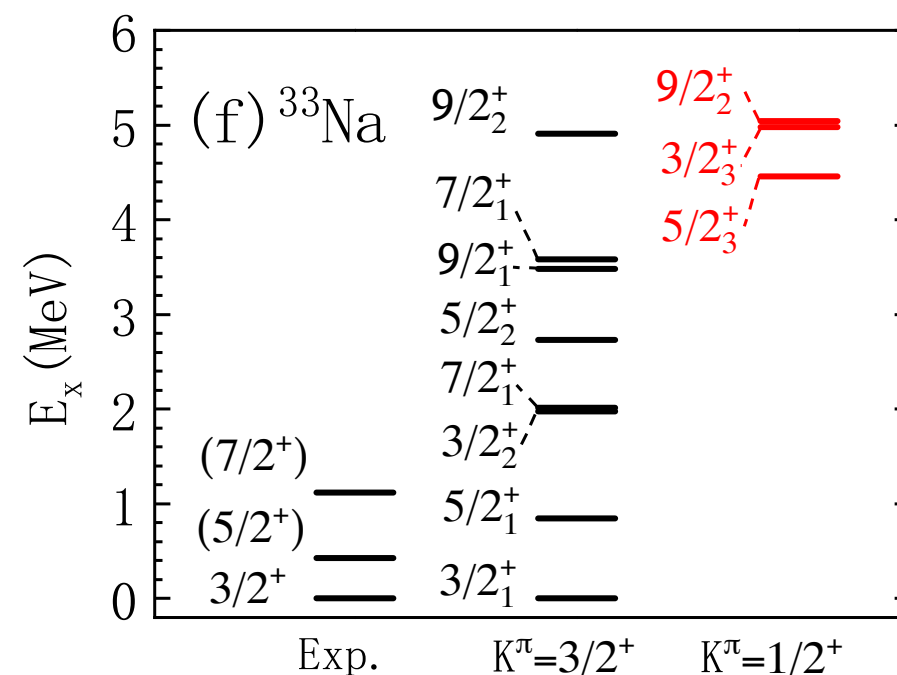
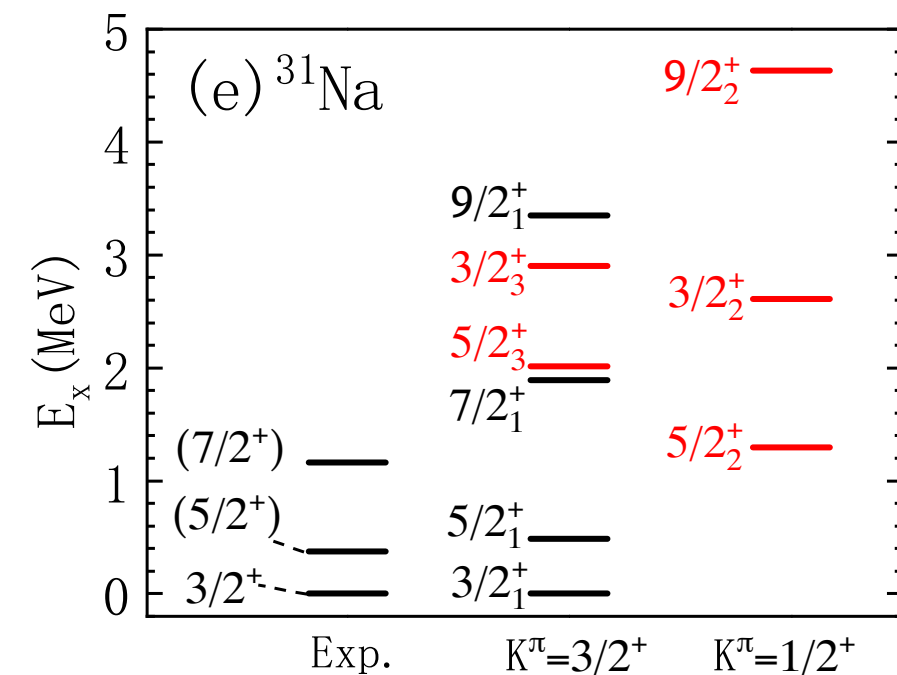
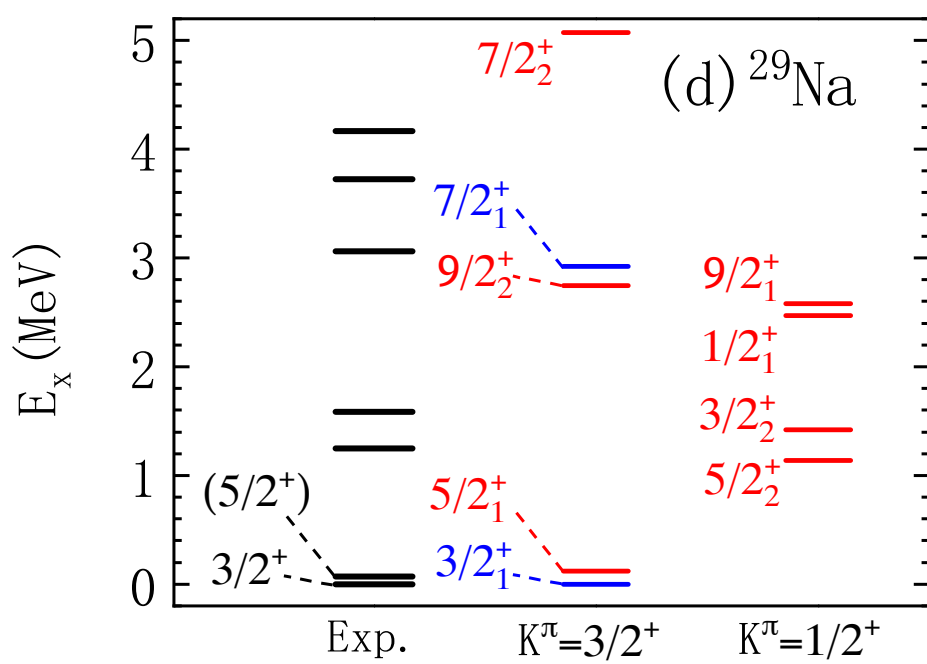
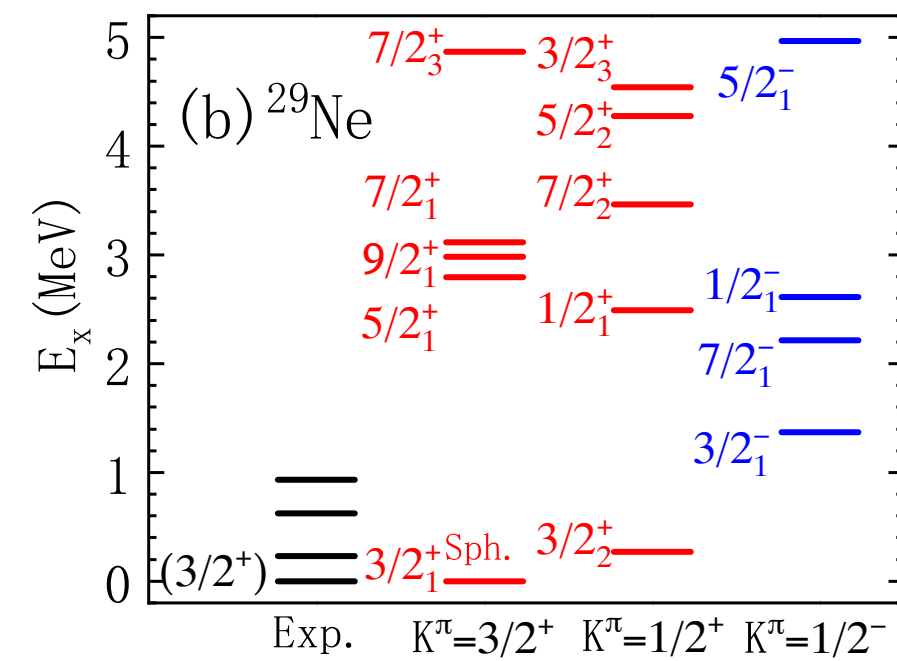
- **even-even and odd-A - odd-odd nuclei** now also possible
- IM-GCM spectra are **spread too wide**, but this will (at least in part) be addressed through
  - improved IMSRG (working on MR-IMSRG(3) variants)
  - more degrees of freedom in GCM: cranking, full triaxiality, explicit quasiparticle excitations, ...

# Shape Coexistence: N=20 Island of Inversion Region



E. F. Zhou et al., arXiv:2603.xxxx

## IM-GCM survey of the **island-of-inversion region**

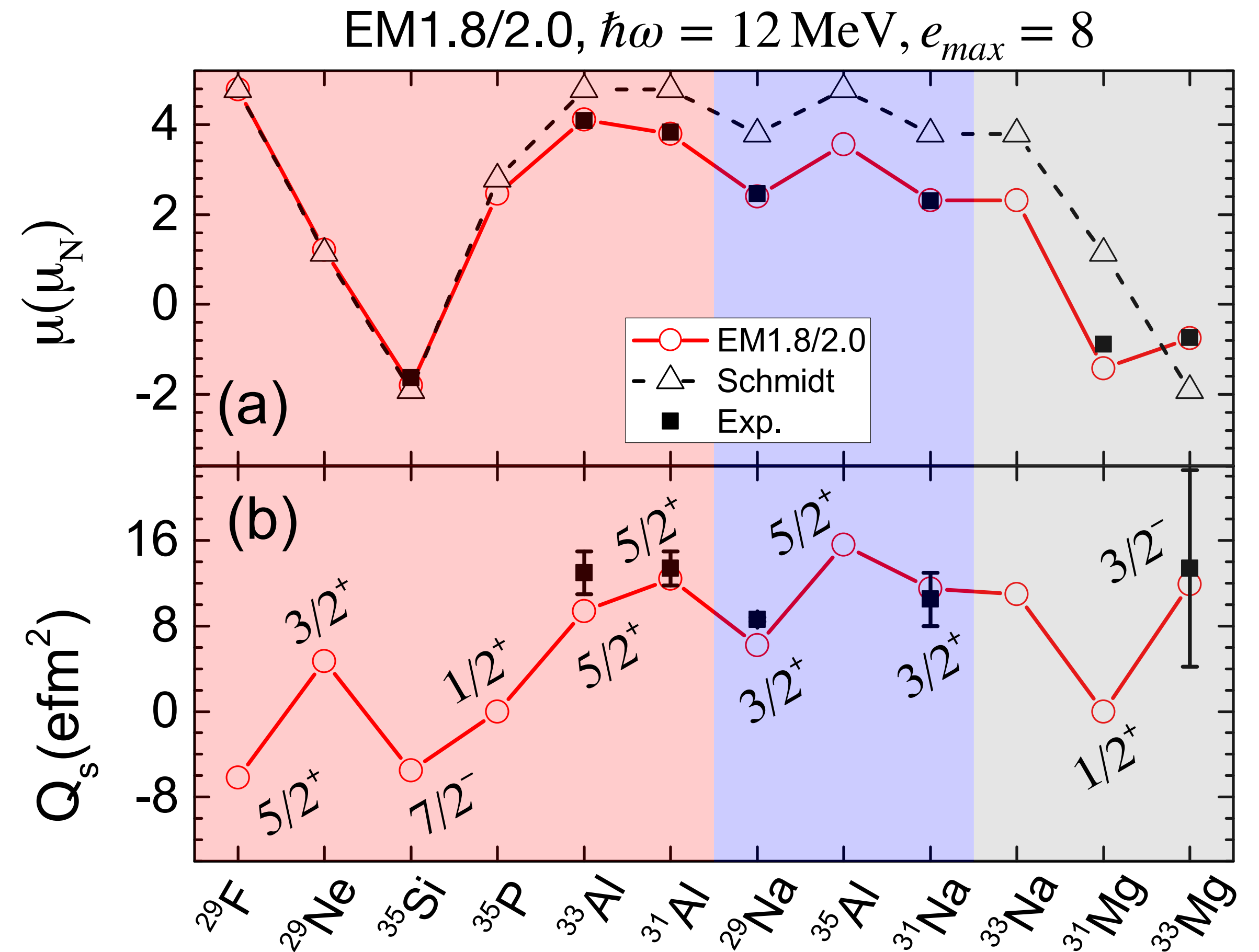
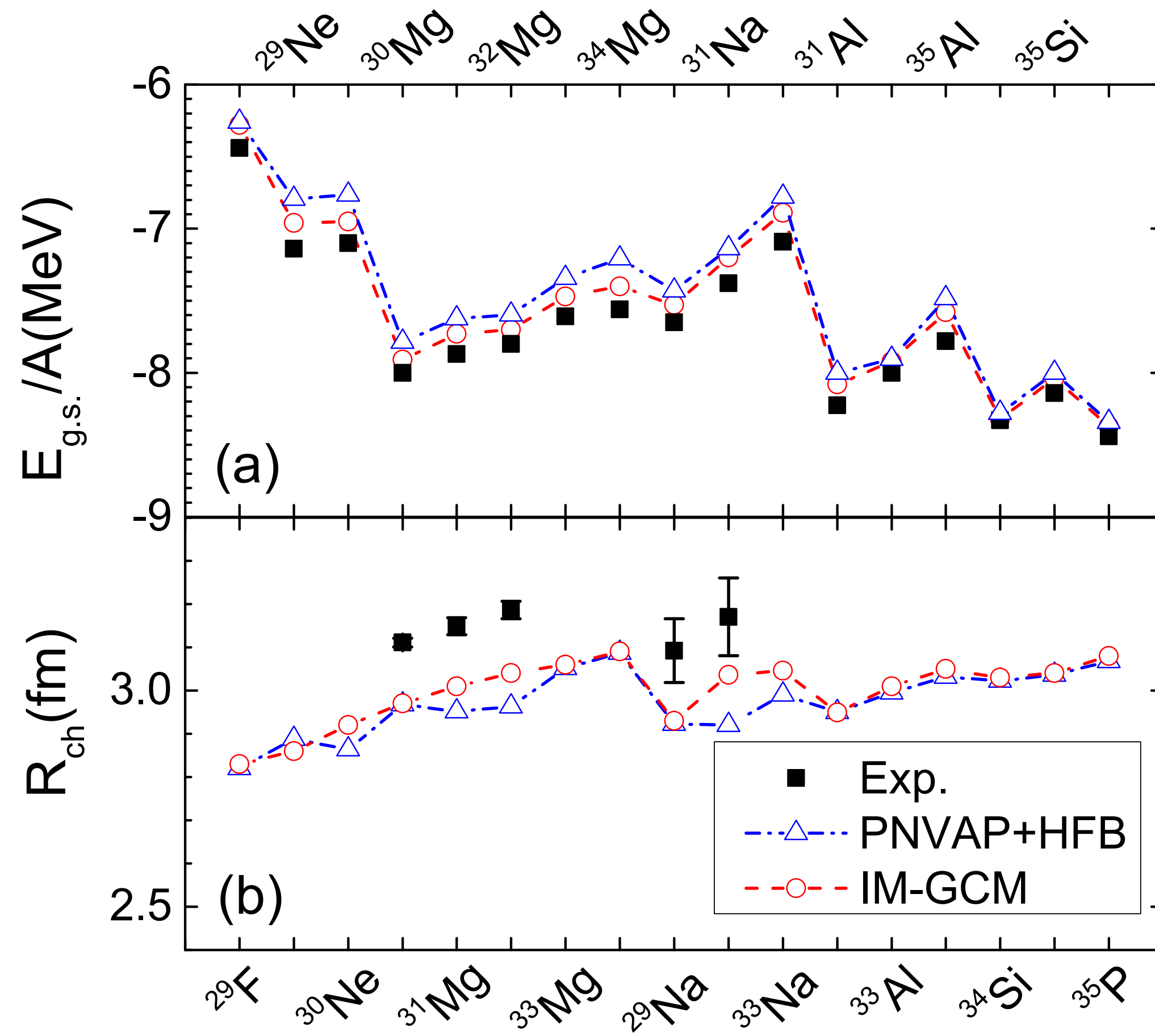


support **state identification**  
and offer *ab initio* insights into  
**intrinsic shapes**

# Shape Coexistence: N=20 Island of Inversion Region



E. F. Zhou et al., arXiv:2603.xxxx

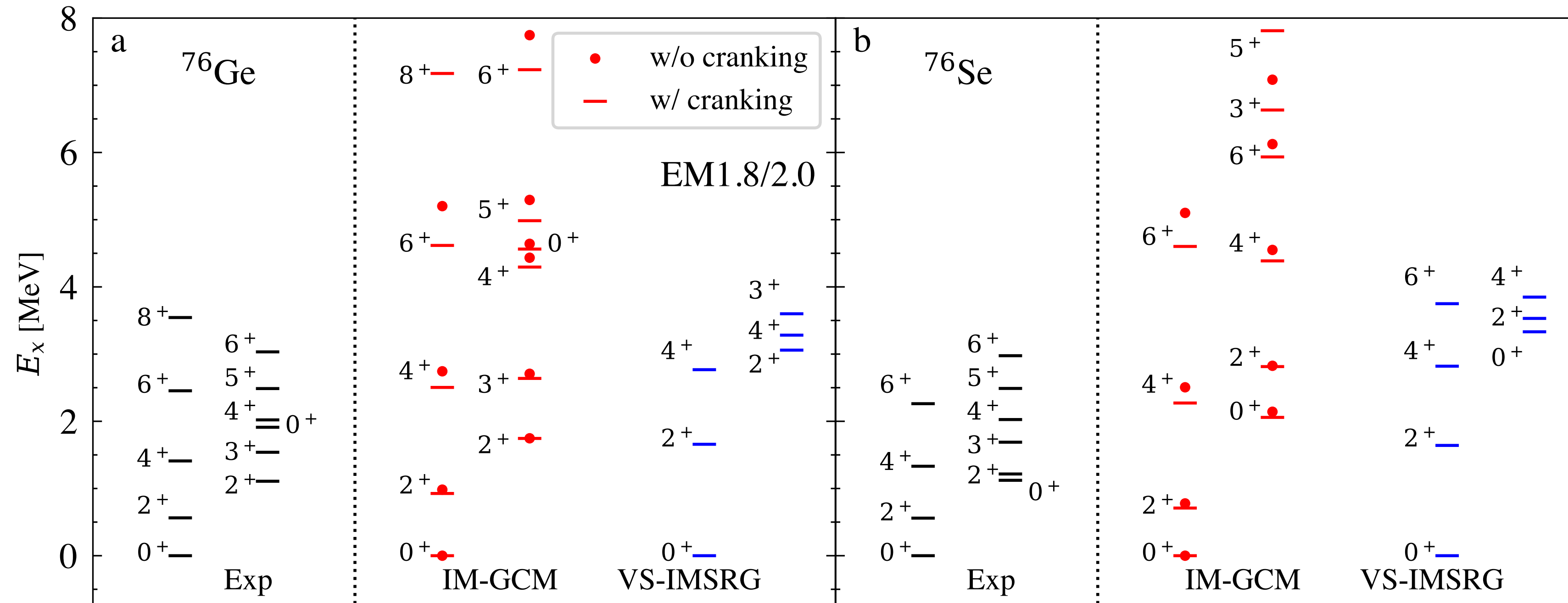


**IM-GCM survey completed, will be submitted within next couple of weeks**

# $^{76}\text{Ge}$ / $^{76}\text{Se}$ Structure

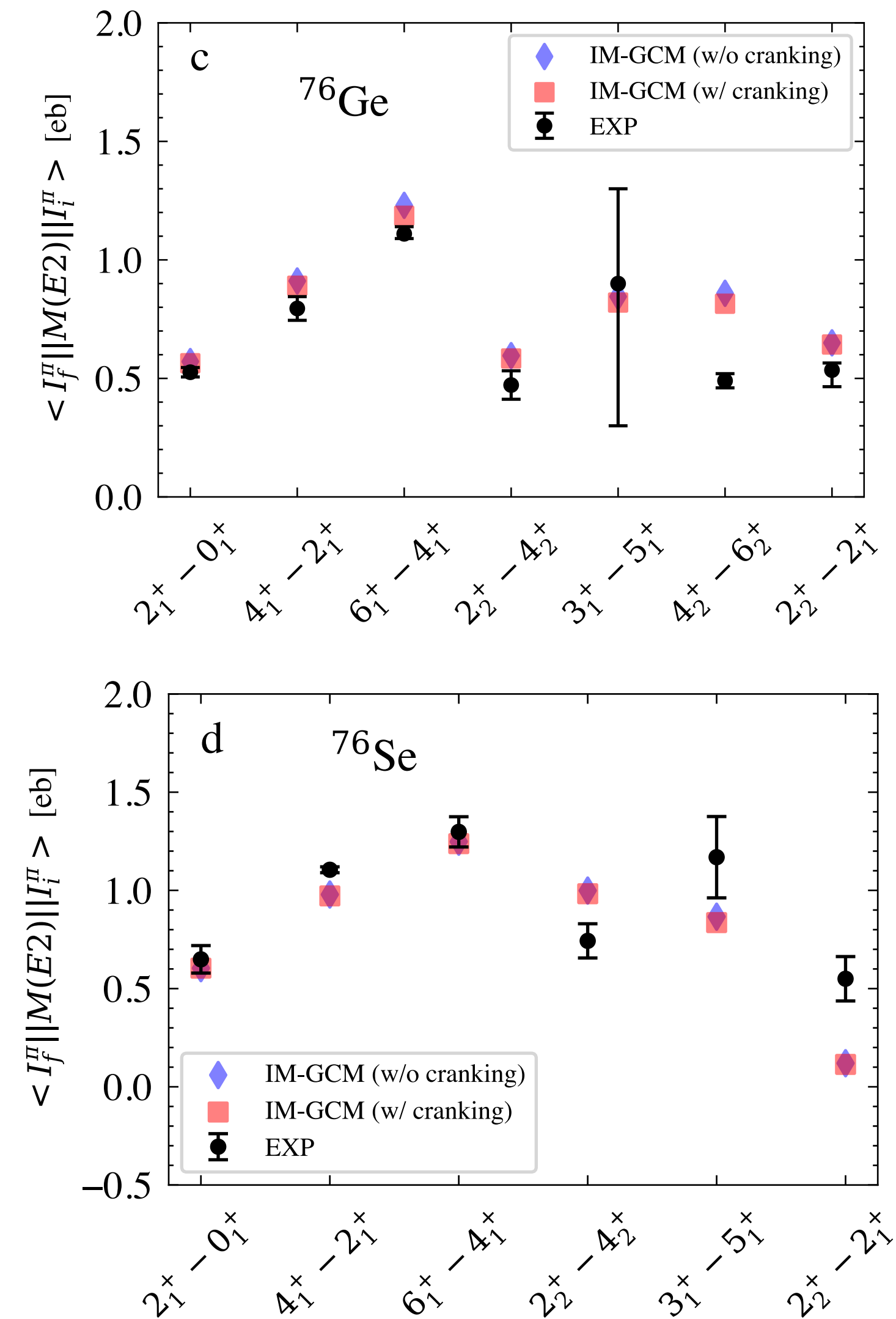


A. Belley et al., PRL 132, 182502 (2024)



EM1.8/2.0 NN+3N interaction,  $\hbar\omega = 12$  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**

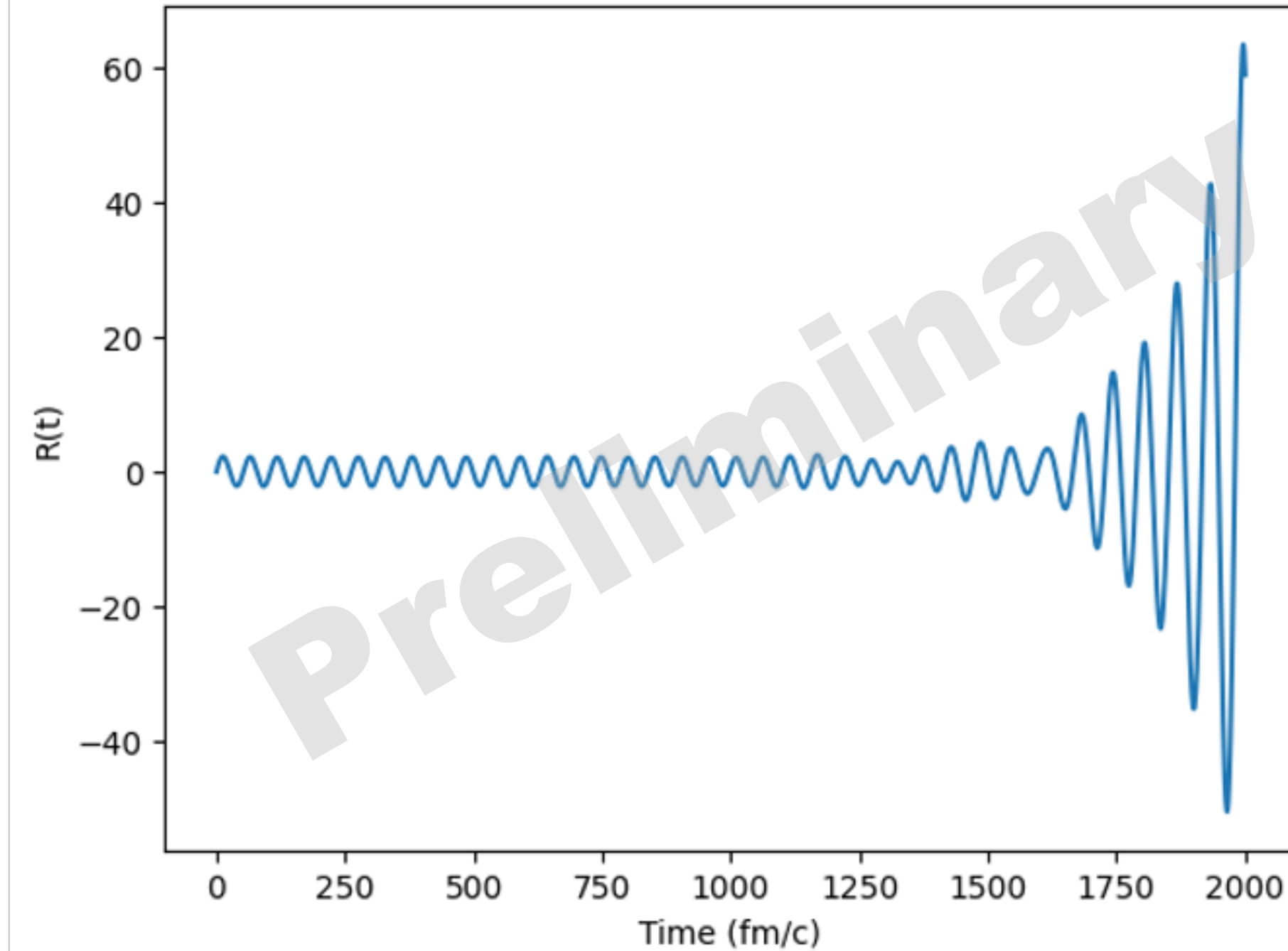


# Time-Dependent Response from the IMSRG

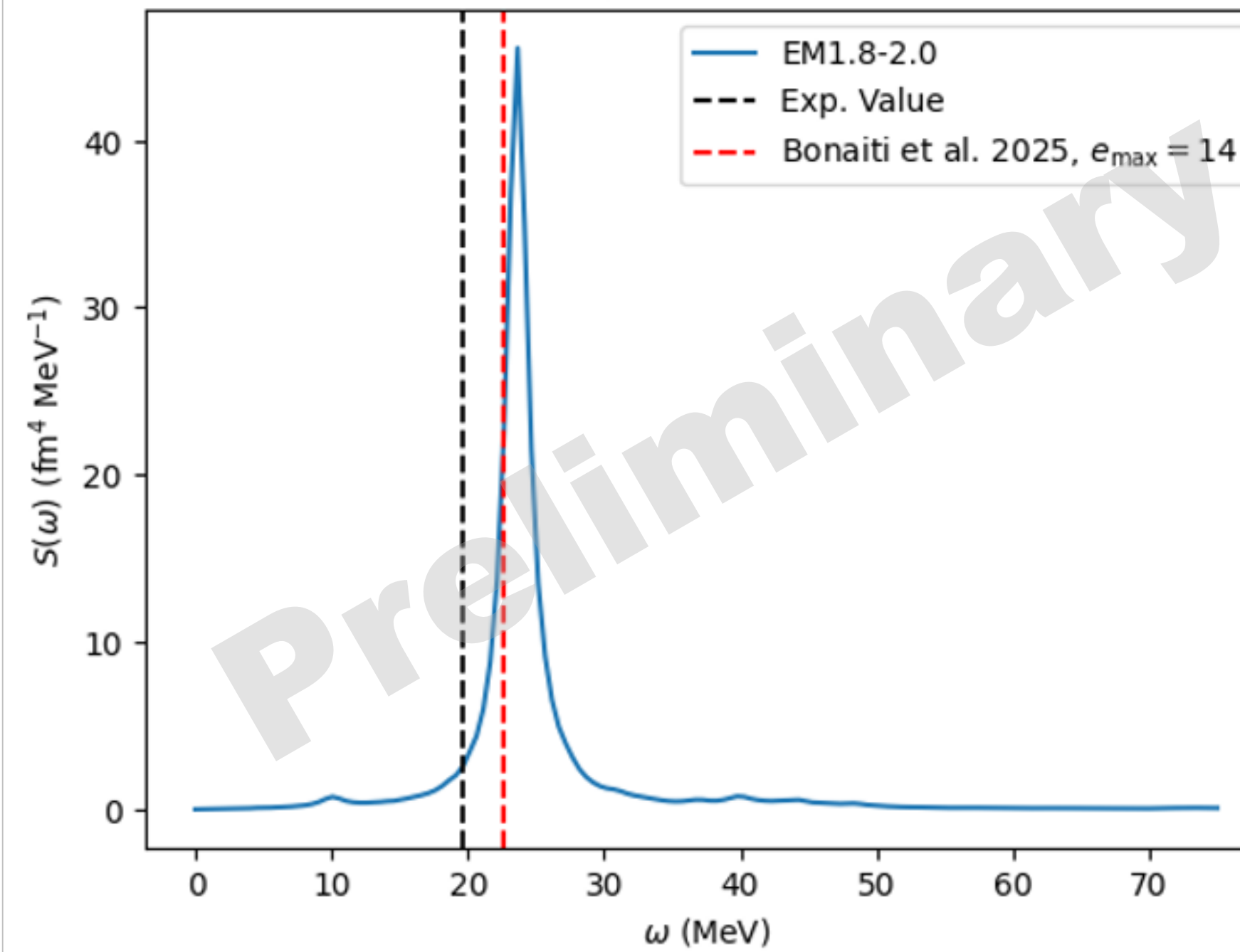


Aryan Vaidya  
+ Scott Bogner, Jon Engel, ...

Time Domain Response Function -  $e_{\max} = 8$



Baseline Strength -  $^{16}\text{O}$  ISGMR,  $e_{\max} = 8$

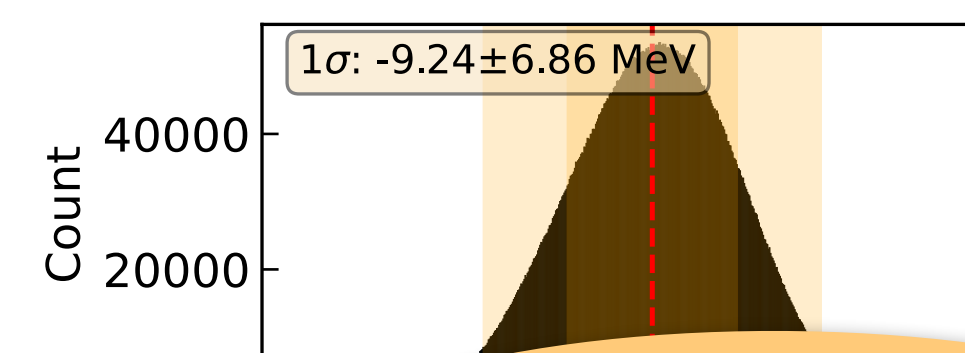
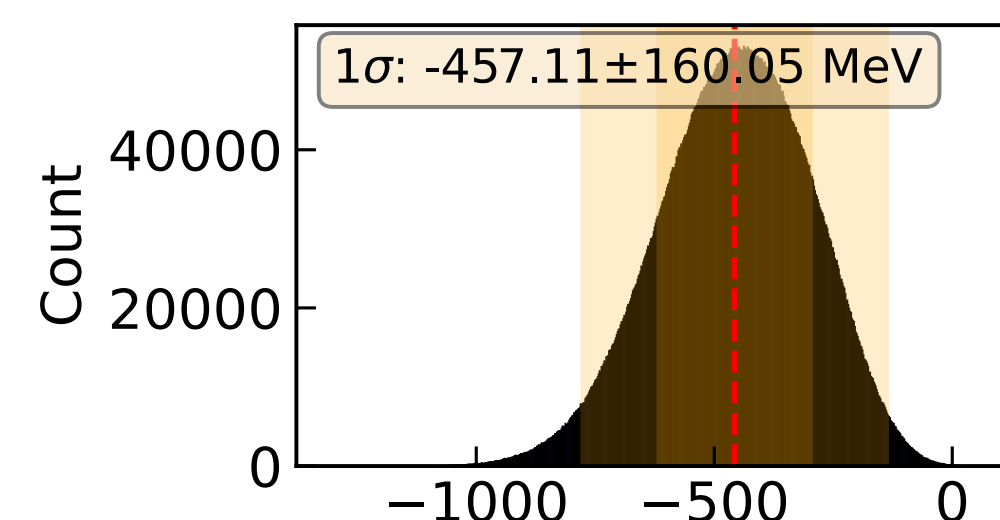
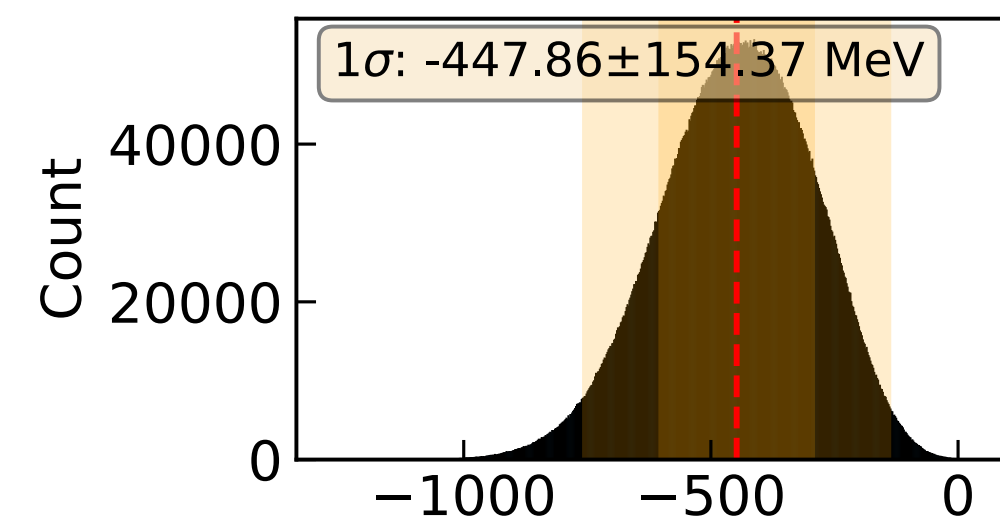
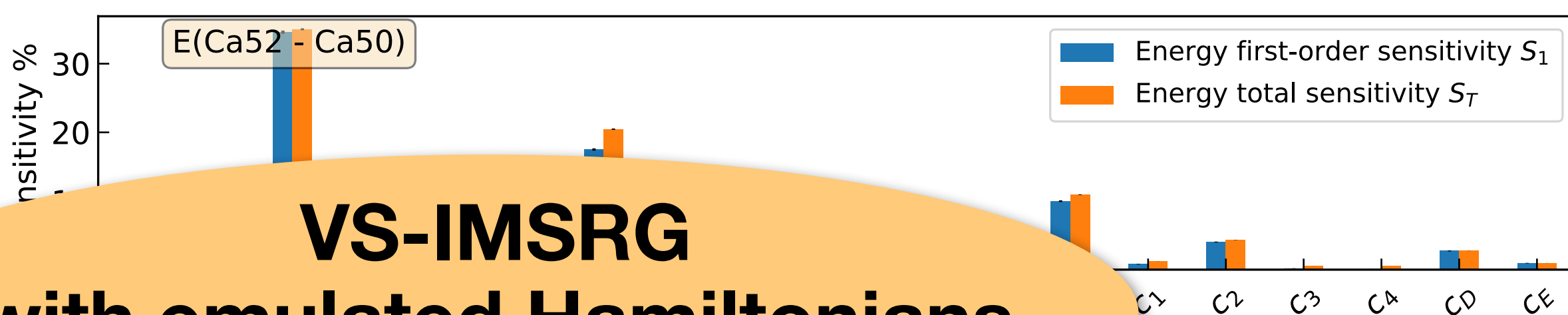
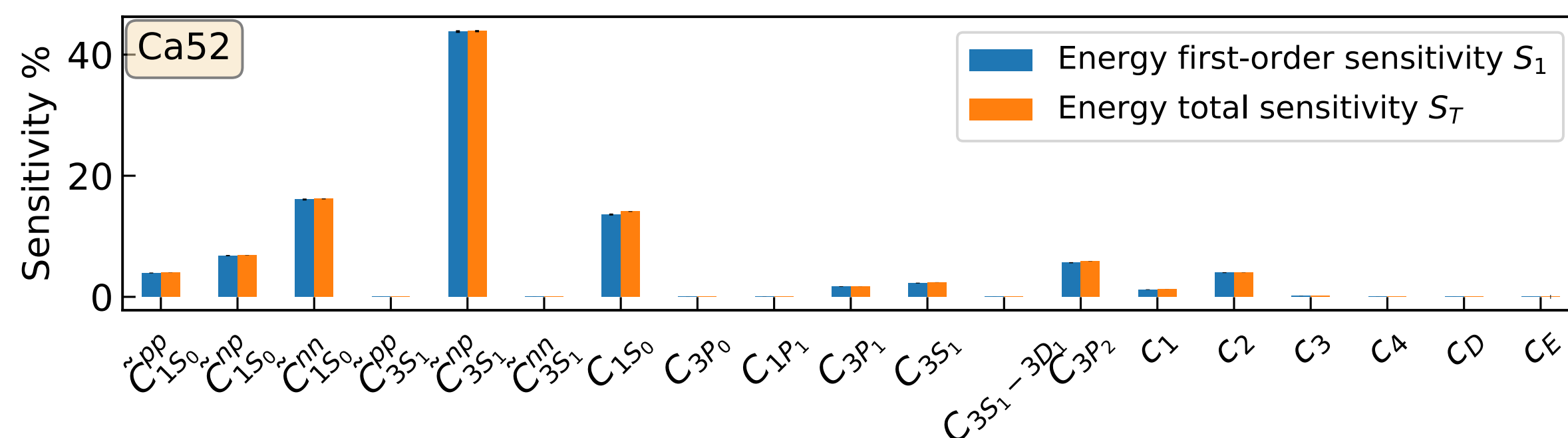
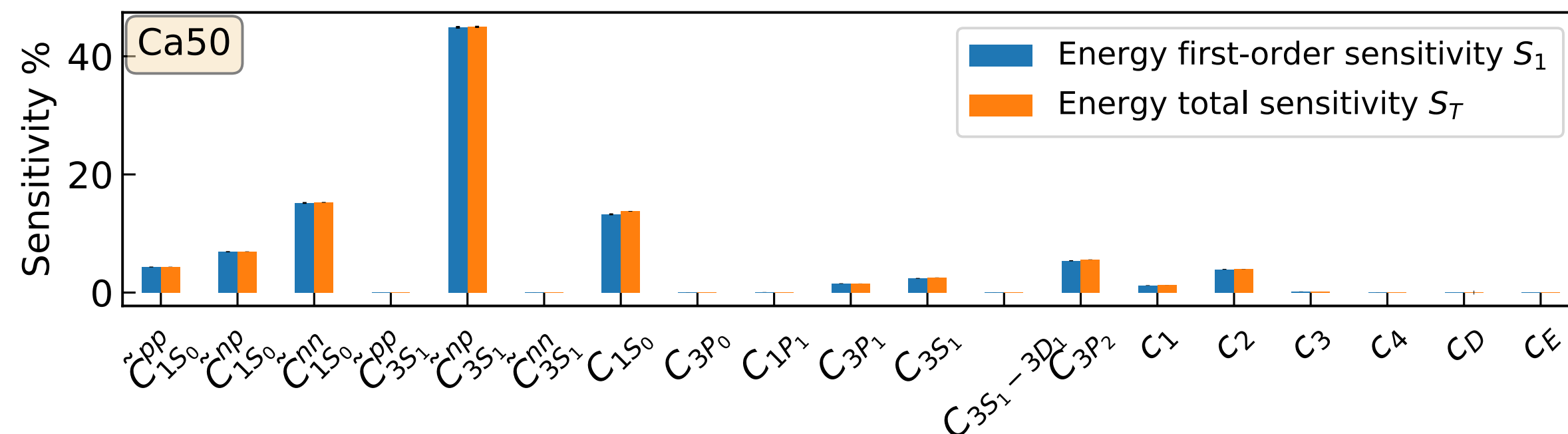


- Linear response of  $A$  to a perturbation  $B$ , with IMSRG improvement ( $U = U(s)$ ):

$$R_{AB}(t, t') = \langle \Psi_0 | [A(t), B(t')] | \Psi_0 \rangle = \langle \Phi_0 | UA(t)U^\dagger, UB(t')U^\dagger | \Phi_0 \rangle$$

- fix  $t' = 0$ , expand time-dependence (=time evolution due to  $H(s)$ ) & Fourier transform

$$R_{AB}(t) = \sum_m (2 - \delta_{m0}) i^{m+1} J_m(2at) \mu_m, \quad \mu_m \equiv \langle \Phi_0 | \left[ [UHU^\dagger, UAU^\dagger]^{(n)}, UBU^\dagger \right] | \Phi_0 \rangle$$

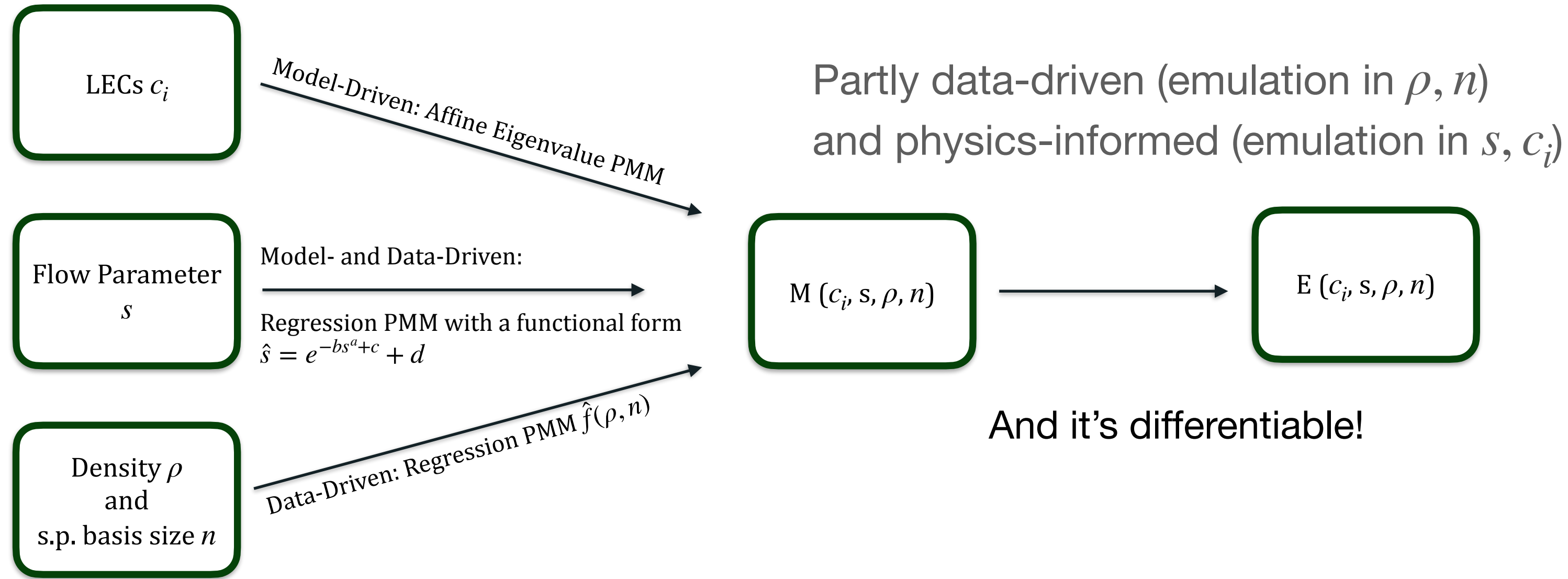


- non-invasive **ROM emulator** based on **Dynamic Mode Decomposition**
- $\Delta$ NNLO<sub>GO</sub>, NN+3N,  $e_{max} = 12, E_{3max} = 14$
- O(10M) samples
- **effort reduced by  $\sim O(10^5)$**
- **DMD doesn't work well for Magnus formulation - switch to PMMs**
- access to H(s) may allow workaround

**VS-IMSRG with emulated Hamiltonians (in progress)**

see poster by **B. Clark**

# PMMs for IMSRG Equation of State Calculations



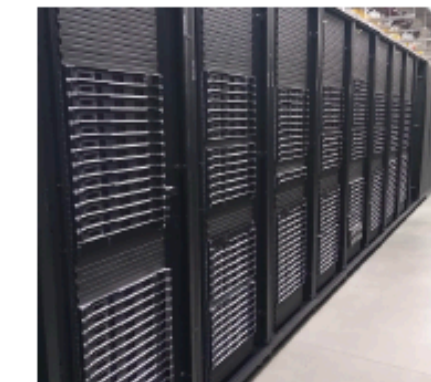
Patrick Cook



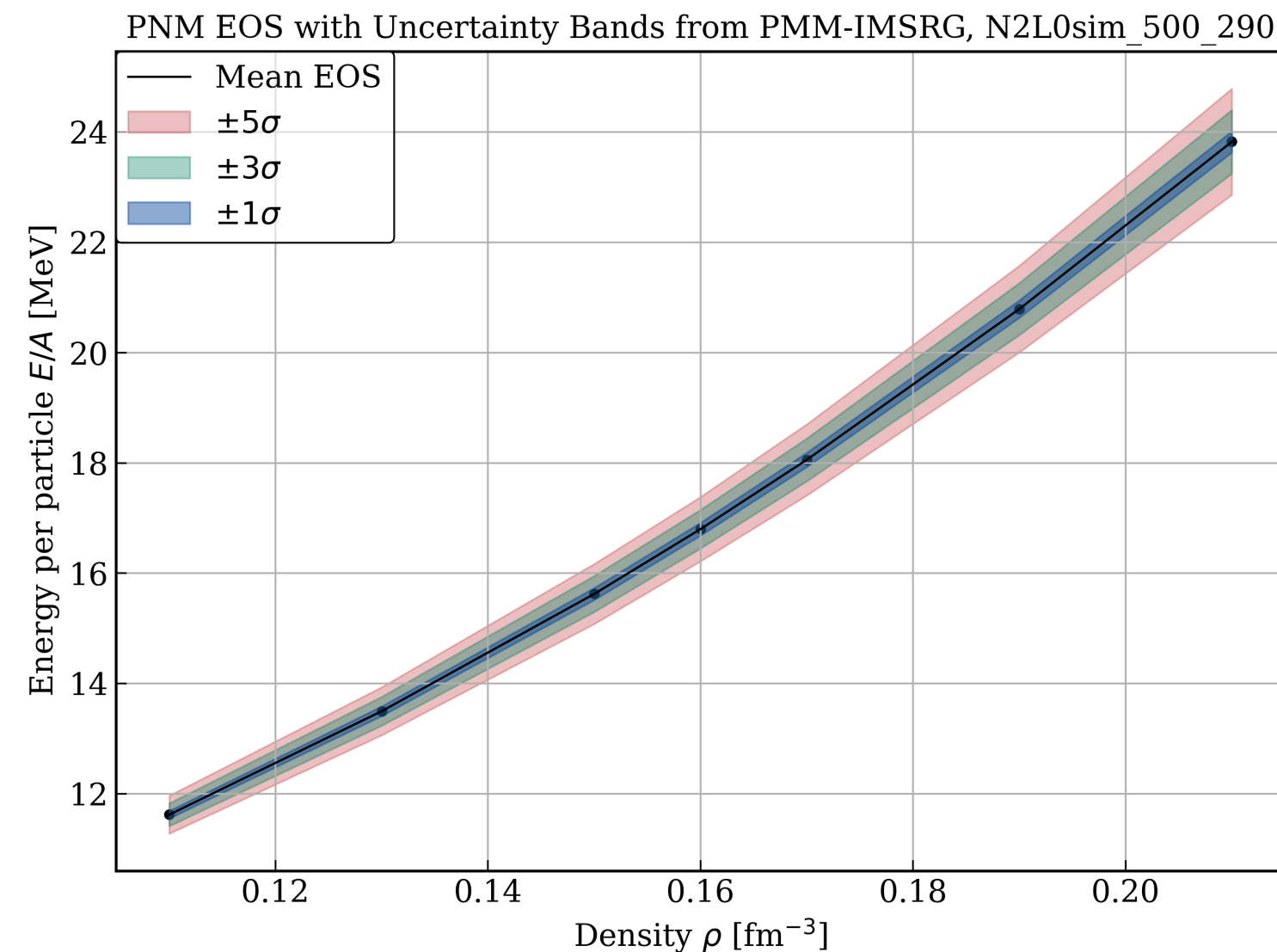
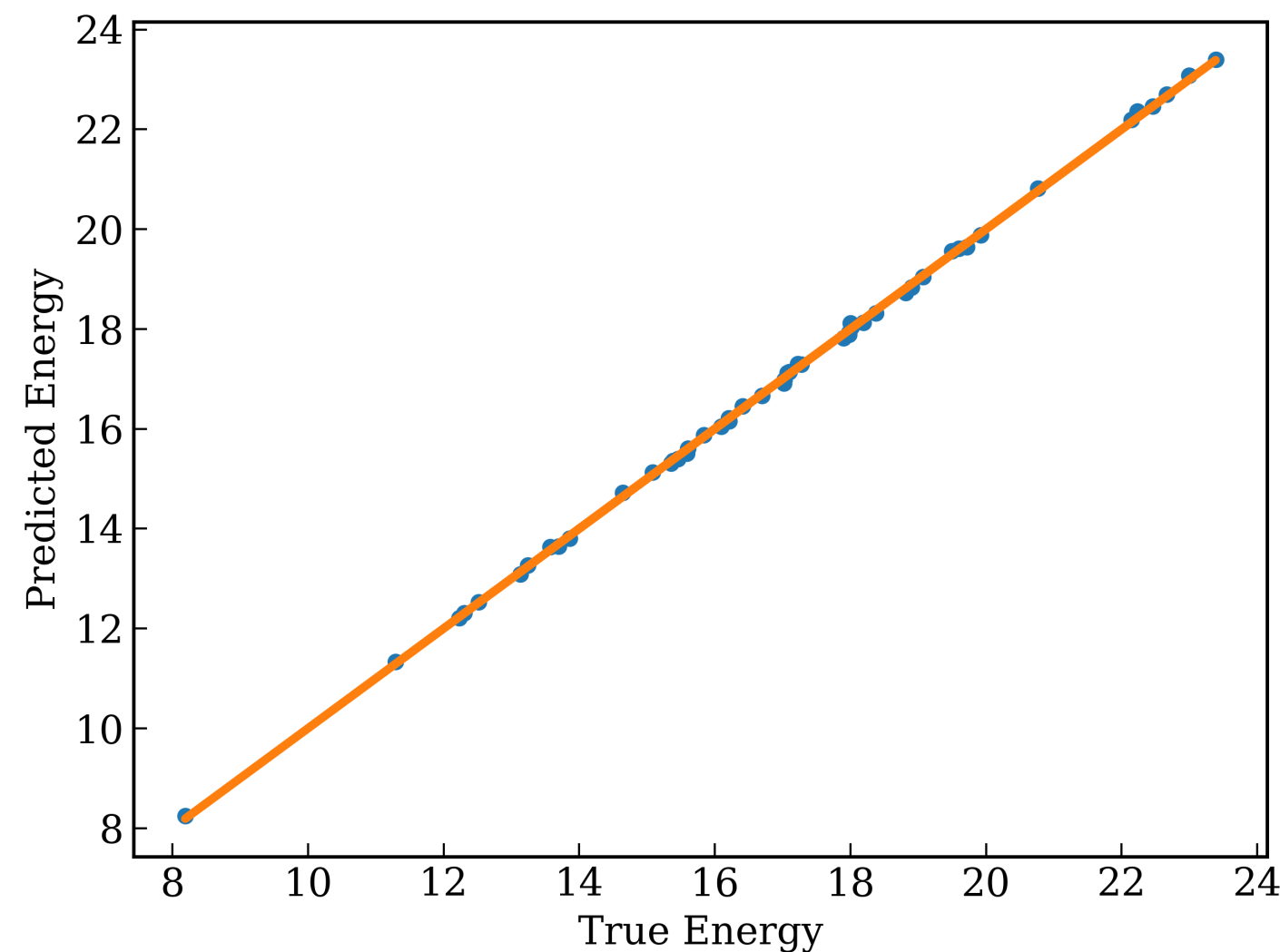
Kang Yu

+ Scott Bogner, Christian Drischler

IMSRG



PMM



Hardware	AMD EPYC 7763 Server	PC with Nvidia RTX A2000 12GB
	> \$10,000 per, plus infrastructure	< \$1,000
Energy	All Runs	Train
	Single Run	Inference
xPU-Time	All Runs	Train
	Single Run	Inference
Real-Time	All Runs	Train
	Single Run	Inference
Memory	Peak 600 GB	Peak < 12 GB

# Outlook

- **improved truncations:** (MR-)IMSRG(3) + factorized approximations, tailored operator bases
  - full MR-IMSRG(3) worked out, but scaling is prohibitive at present
- **IM-NCSM** (see talk by **P. Gysbers**)
- **(MR-)Equation of Motion IMSRG** (see poster by **M. Gajdosik**)
  - replicating closed-shell results (EM & charge changing) of Parzuchowski et al. with new code
  - next: response, correlated reference states, particle attachment/removal
- **model reduction, compression & tensor factorization for IMSRG, EOM & IM-GCM** (see poster by **B. Clark**)
  - **DMD and PMM emulators for uncertainty quantification / sensitivity analysis**
- **applications**
  - IM-GCM (+enhancements) for multiple experiments (see poster by **S. Blade**)
  - nuclear observables for BSM physics (beta decays for CKM unitarity, Schiff moments, ...)

# Acknowledgments



T. S. Blade, S. K. Bogner, B. Clark, P. Cook, M. Gajdosik, P. Gysbers, D. Lee, B. Lem, A. Vaidya  
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T. R. Rodríguez  
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M. Frosini  
CEA Cadarache

T. Miyagi  
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Institute for Nuclear Theory, Seattle

S. Gandolfi, E. Mereghetti  
Los Alamos National Laboratory

M. Heinz  
Oak Ridge National Laboratory

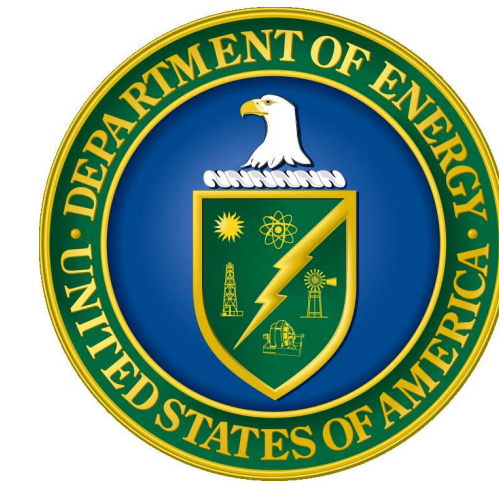
C.-Y. Seng  
University of Tennessee-Knoxville

S. König  
North Carolina State University

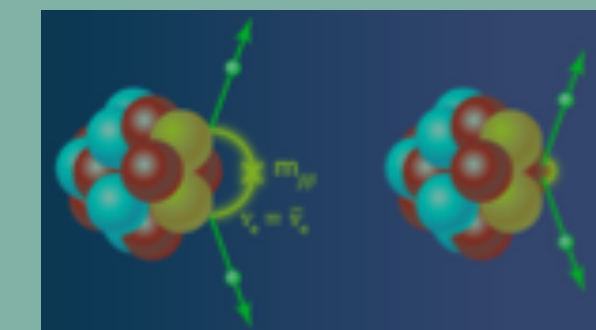
K. Fosse, A. Sedhirovic  
Florida State University

**and many more...**

## Thank you for your attention!



**NUCLEI**  
Nuclear Computational Low-Energy Initiative



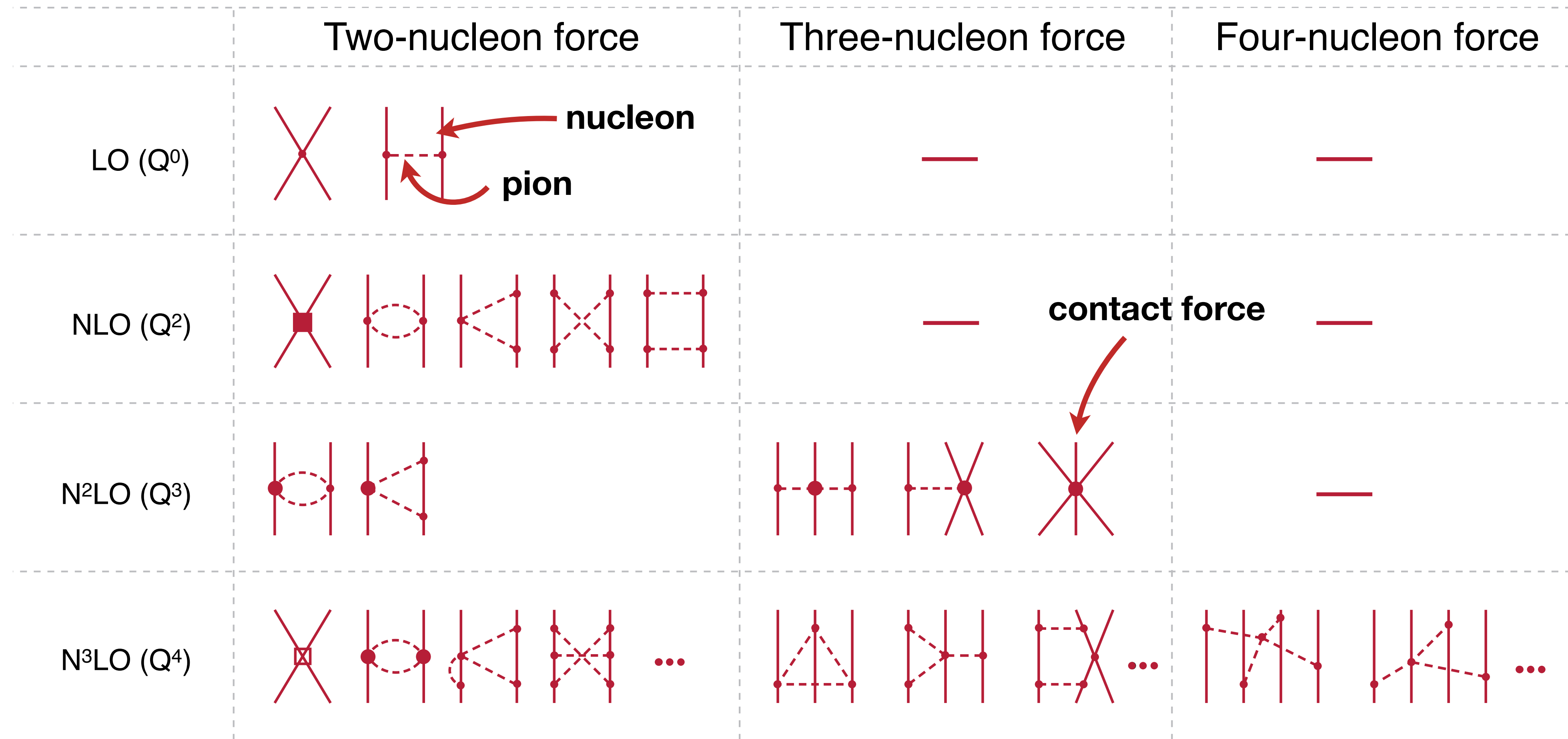
@NDB

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



# Supplements

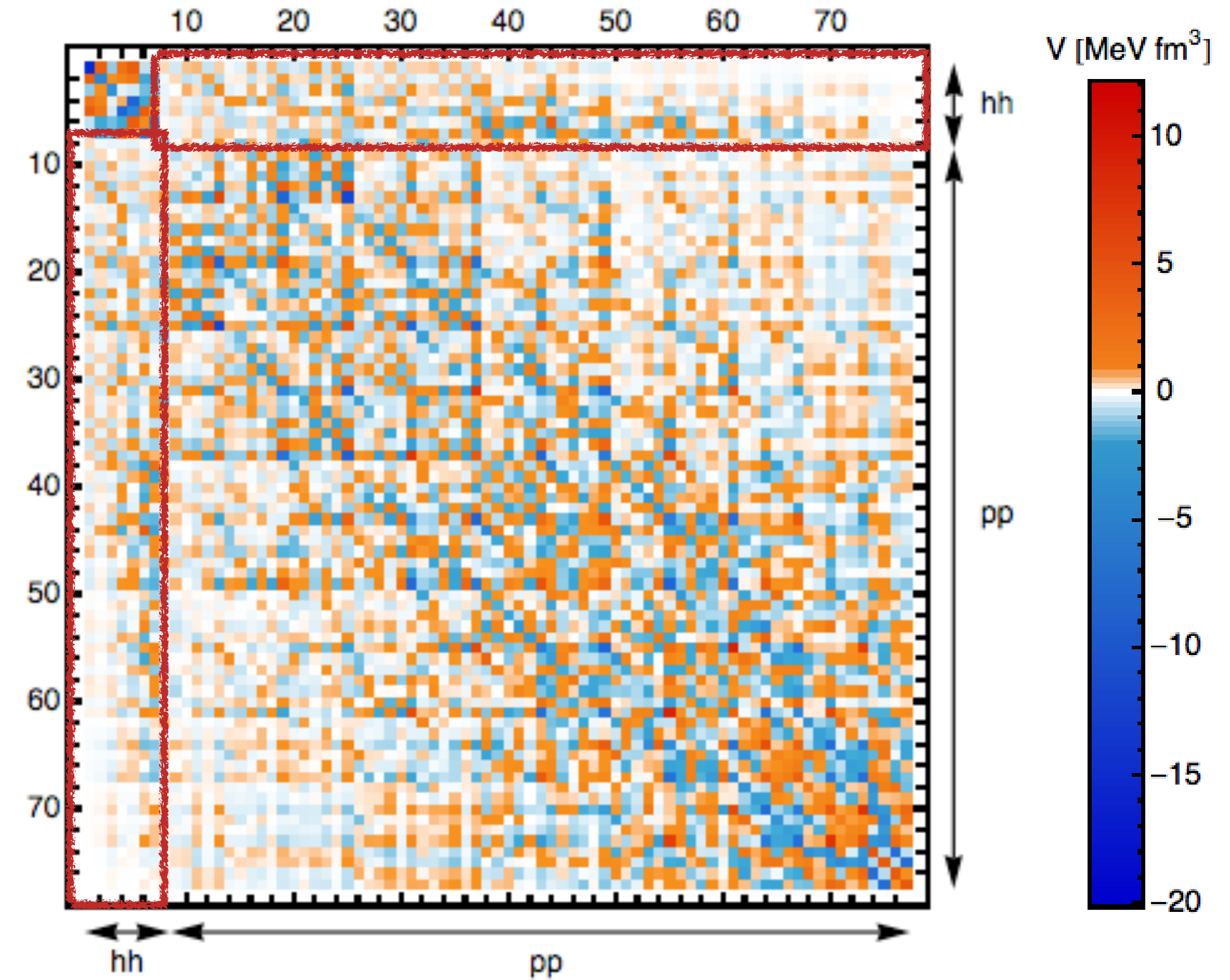
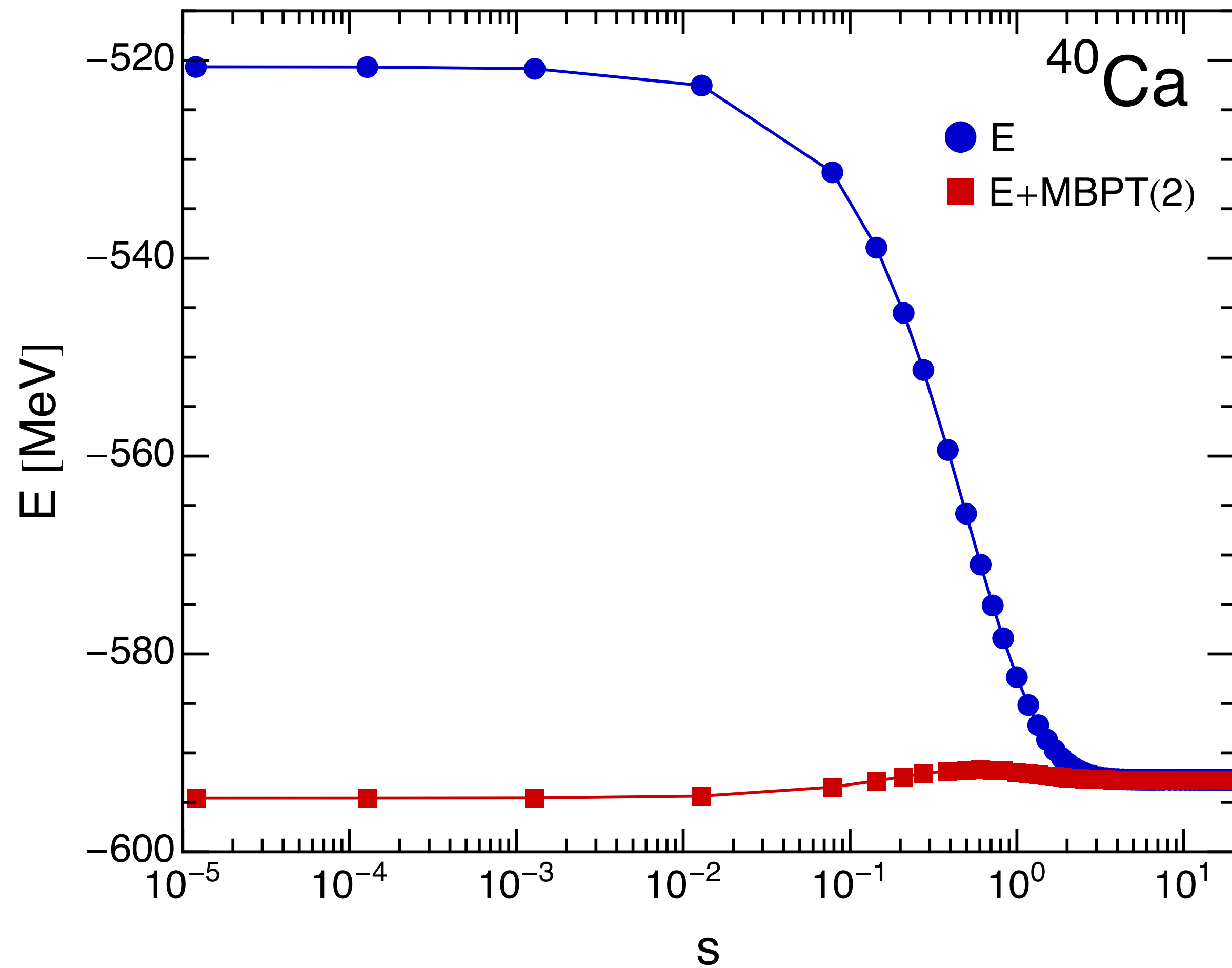
# Chiral Effective Field Theory



[figure by H. Krebs]

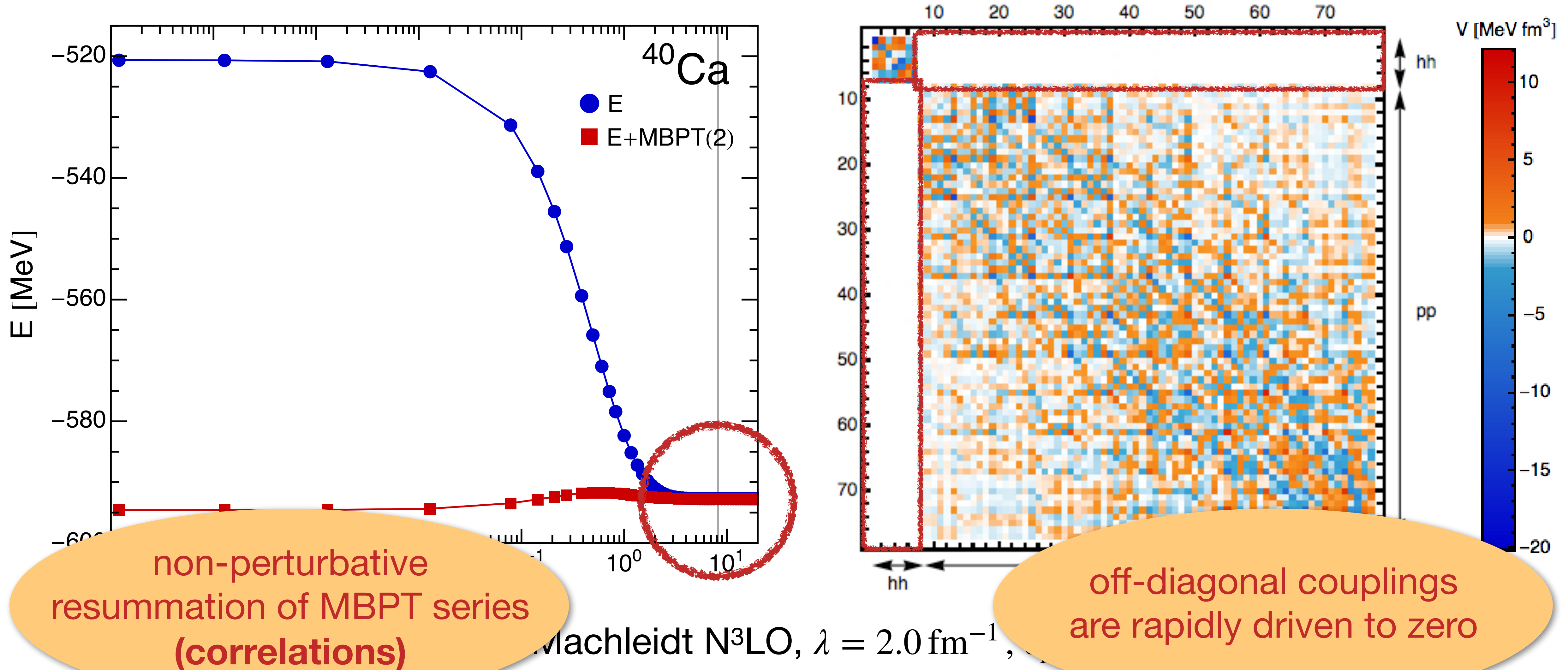
- organization in powers  $(Q/\Lambda_\chi)^n$  allows **systematic improvement**
- low-energy constants **fit to NN, 3N data** (future: from Lattice QCD (??))
- **consistent** NN, 3N, ... interactions & transition operators by coupling to gauge fields

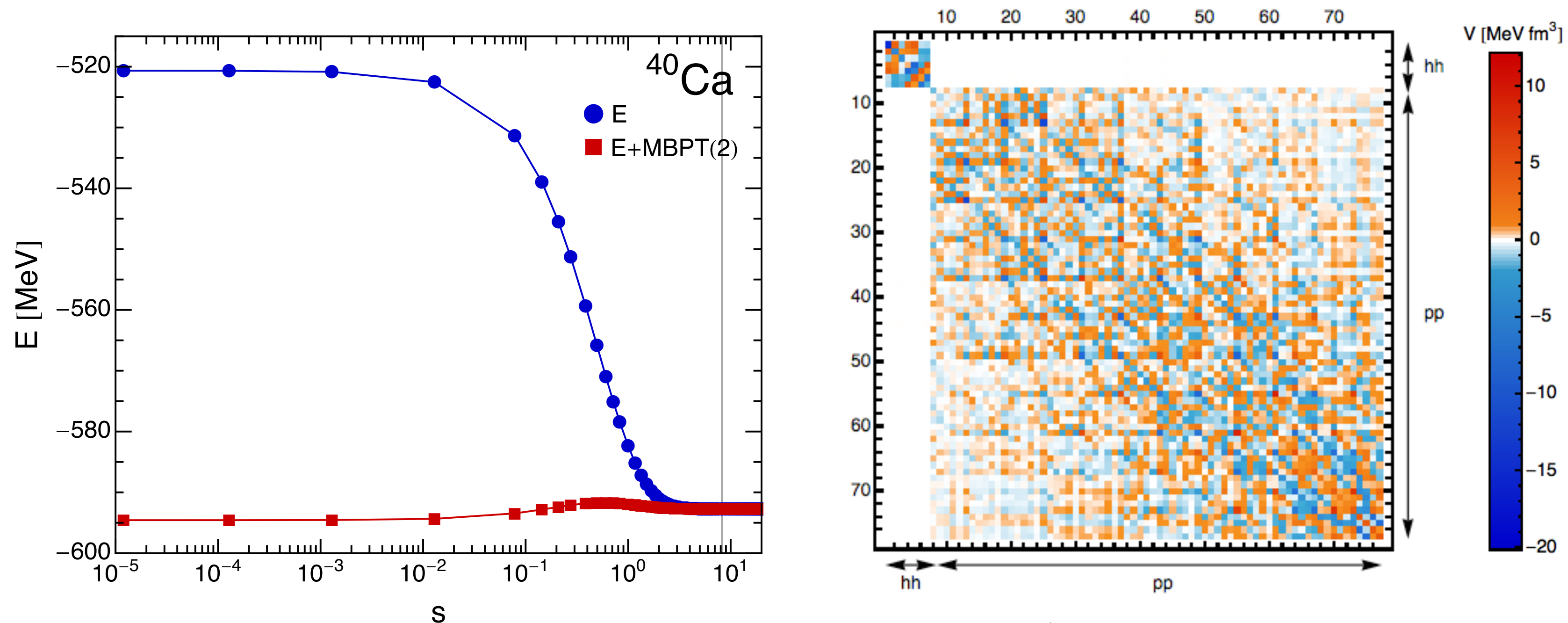
# Decoupling



Entem-Machleidt N<sup>3</sup>LO,  $\lambda = 2.0 \text{ fm}^{-1}$ ,  $e_{\text{Max}} = 8$

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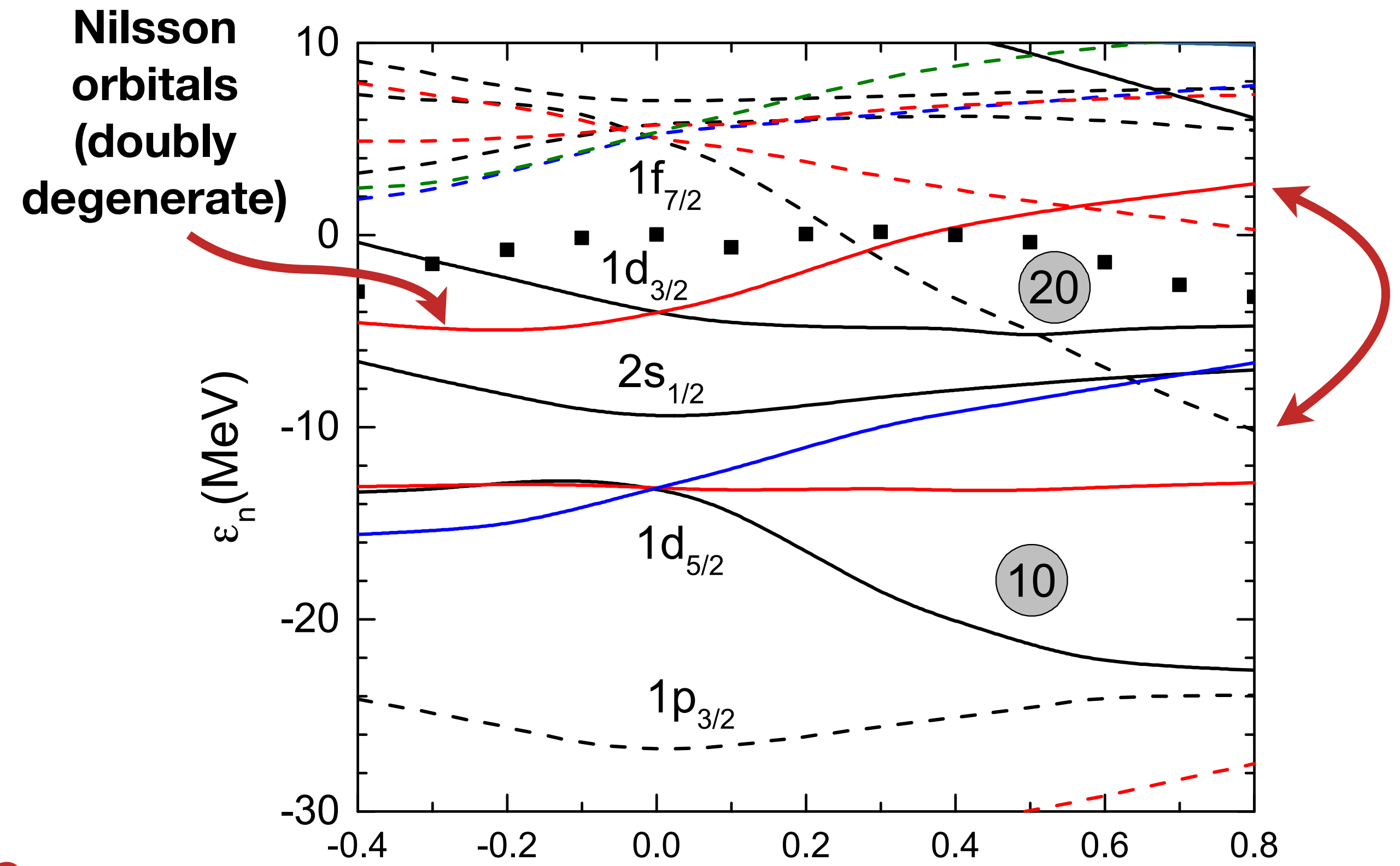
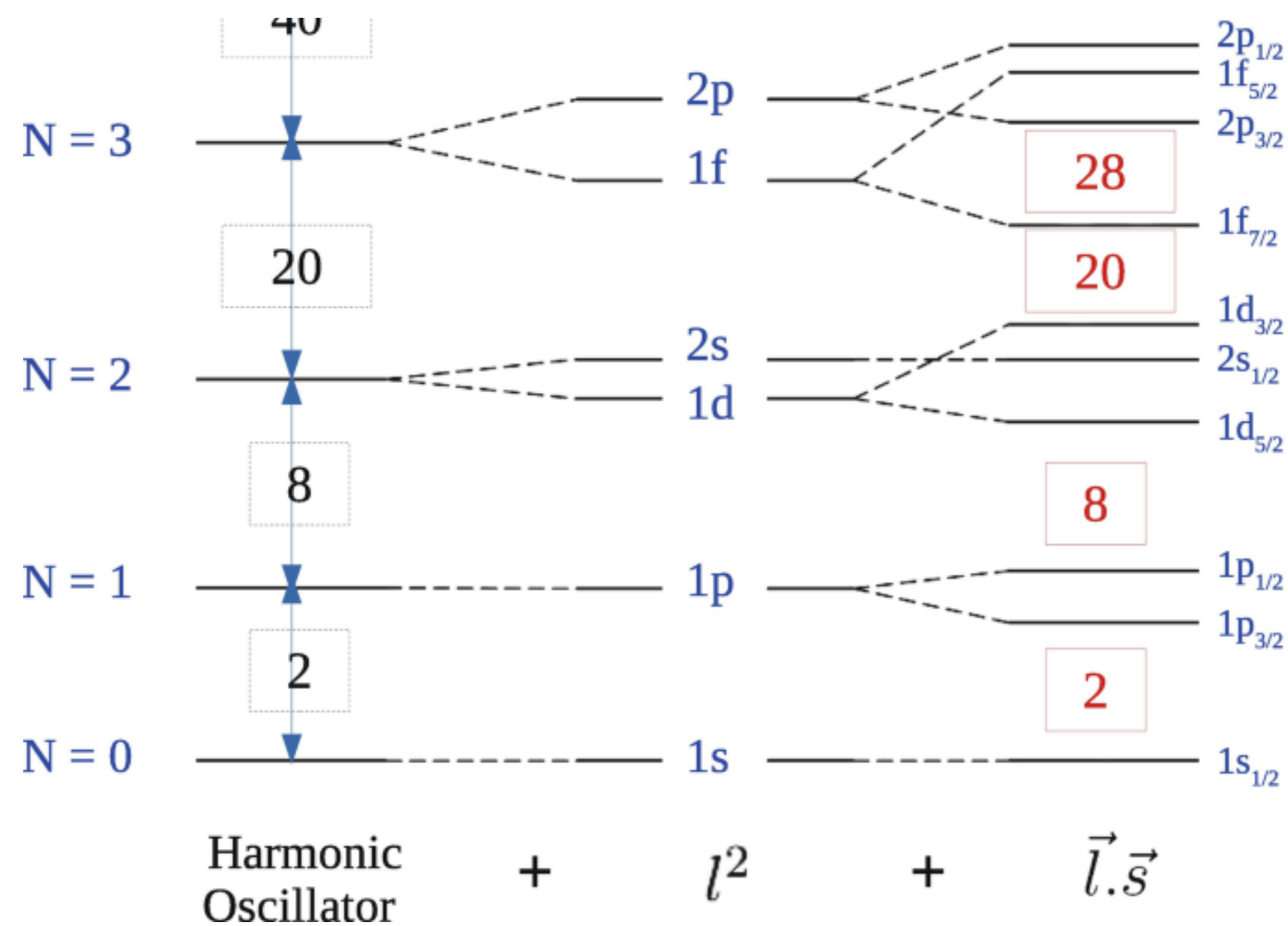
- absorb correlations into **RG-improved Hamiltonian**:

$$U(s) H U^\dagger(s) U(s) |\Psi_n\rangle = E_n U(s) |\Psi_n\rangle$$

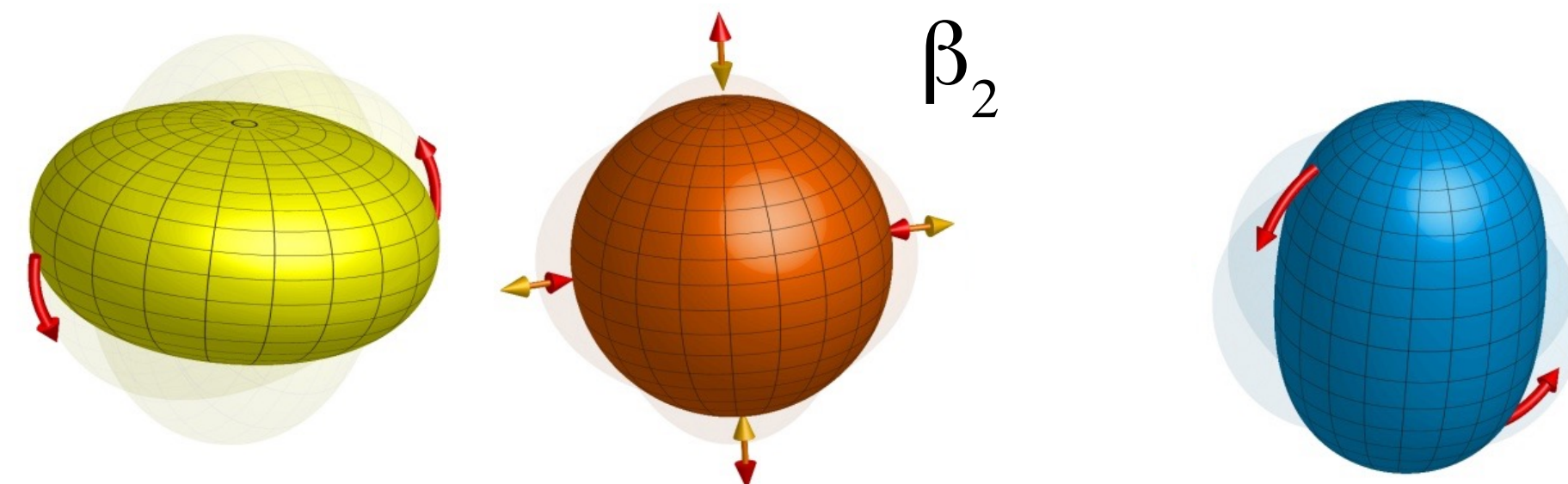
- reference state is ansatz for transformed, **less correlated** reference state:

$$U(s) |\Psi_n\rangle \stackrel{!}{=} |\Phi\rangle$$

# Symmetry Breaking and Restoration



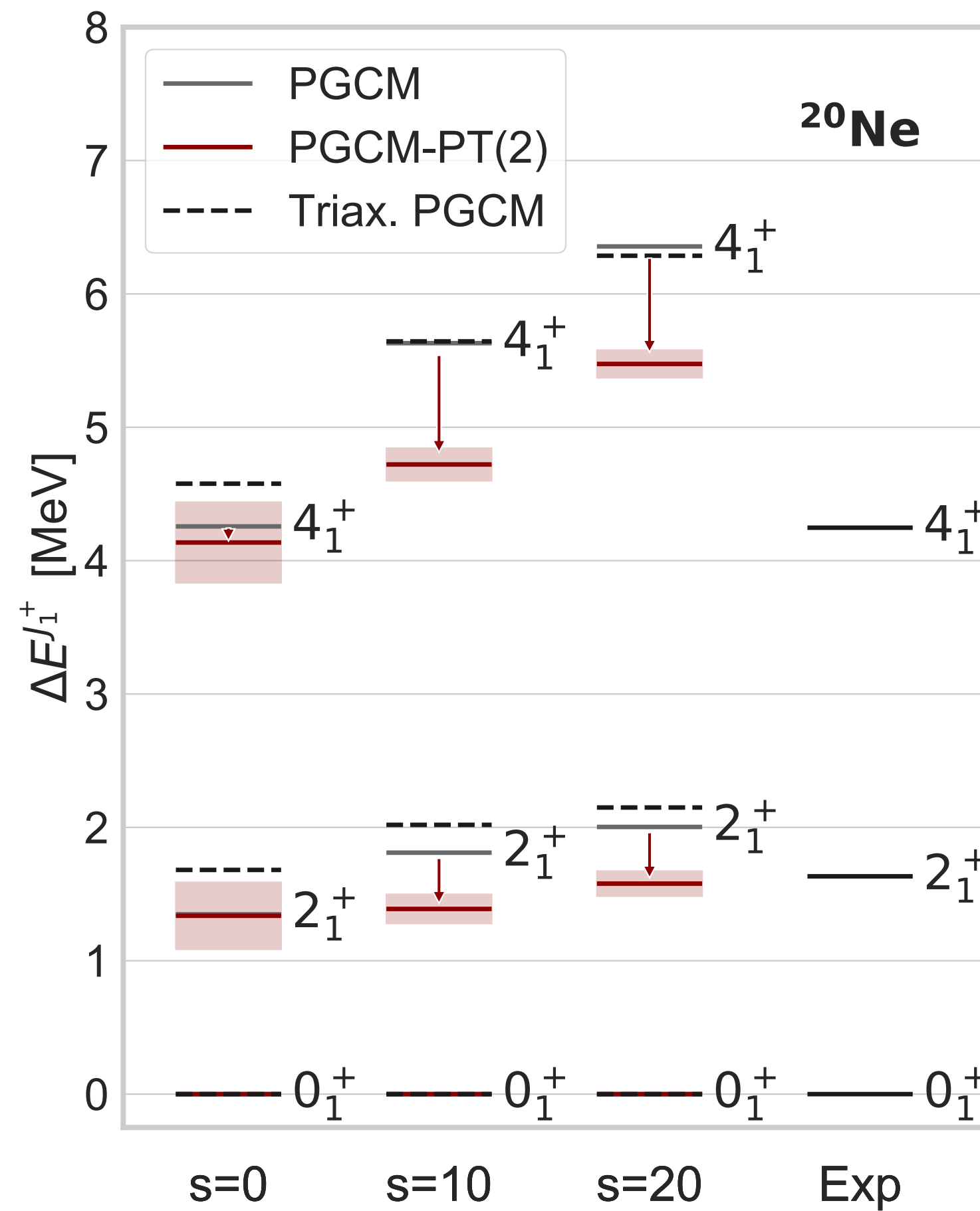
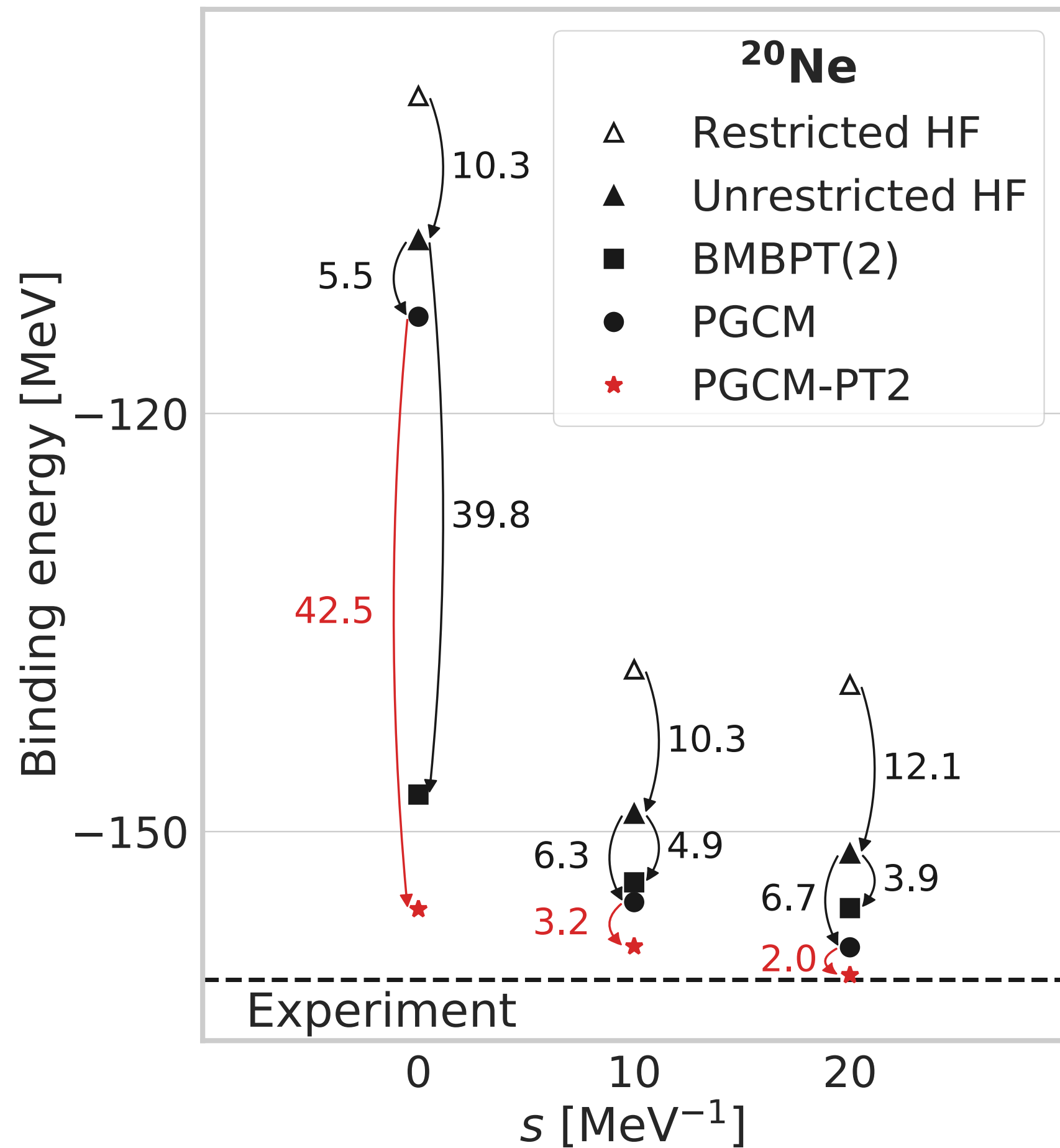
- **break spherical symmetry** to **capture static correlation** from deformation
- **restore symmetry** by constructing **(specific) superpositions of all rotations** of intrinsic state (aka **projection**)



# IM-GCM: Reshuffling of Correlations



M. Frosini et al., EPJA 58, 64 (2022)

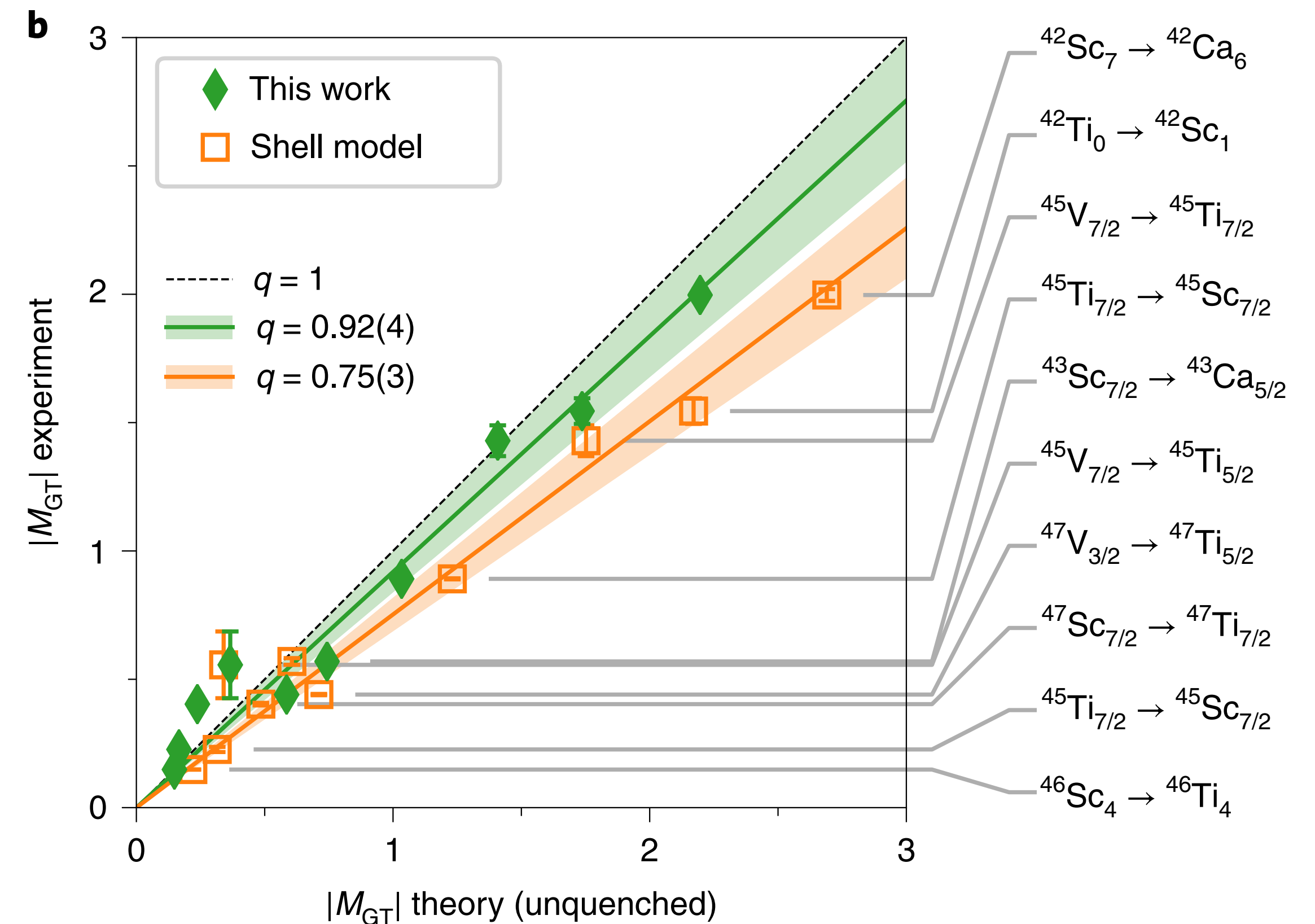
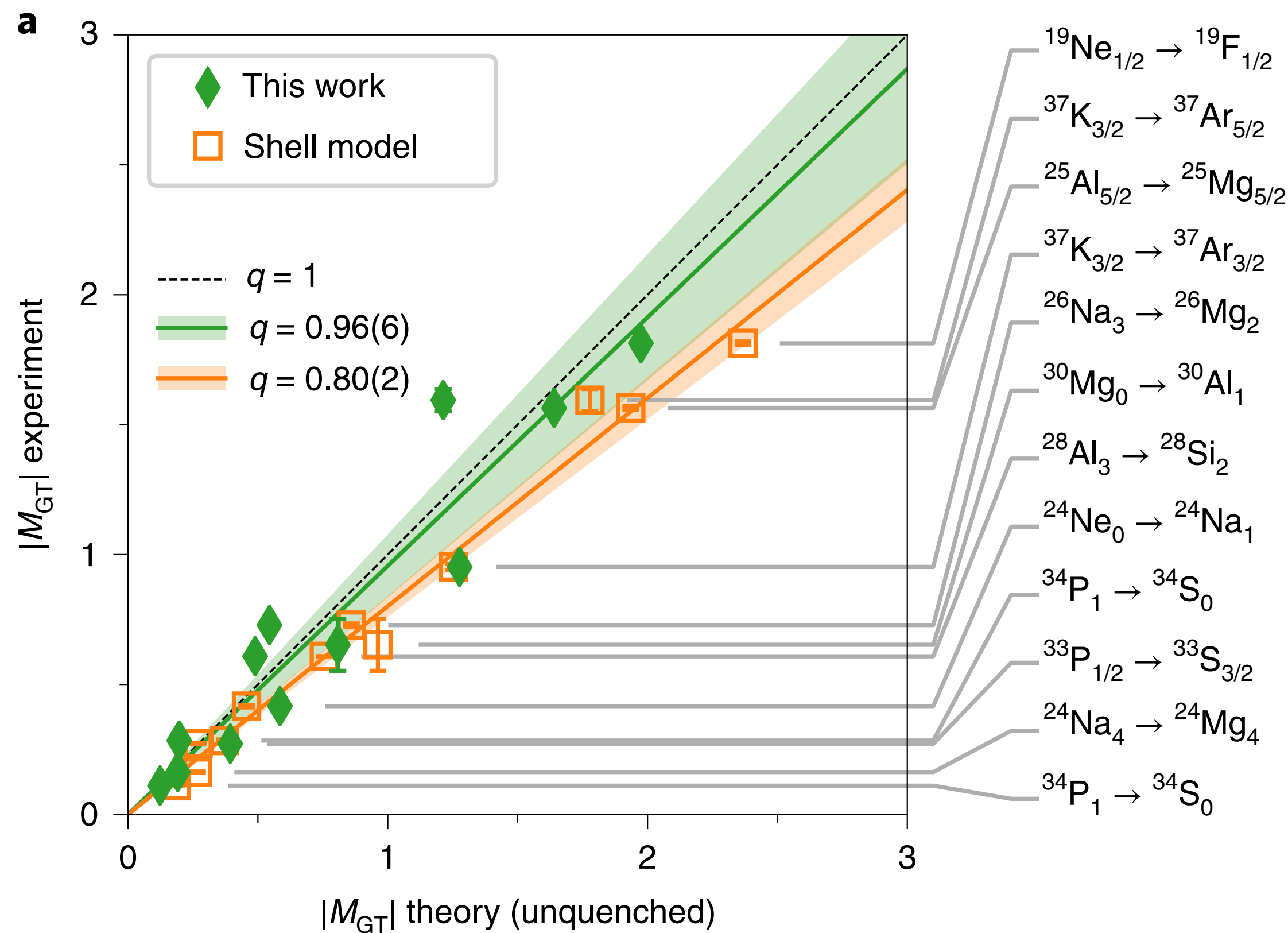


- s-dependence is a **built-in diagnostic tool** for IM-GCM (**not available in phenomenological GCM**)
- if operator and wave function offer sufficient degrees of freedom, **evolution of observables is unitary**
- need **richer references and/or IMSRG(3)** for certain observables

# Quenching of Gamow-Teller Decays



*P. Gysbers et al., Nature Physics 15, 428 (2019)*



- **empirical Shell model** calculations require **quenching factors** of the weak axial-vector coupling  $g_A$
- **VS-IMSRG** explains this through consistent **renormalization** of transition operator, incl. **two-body currents**

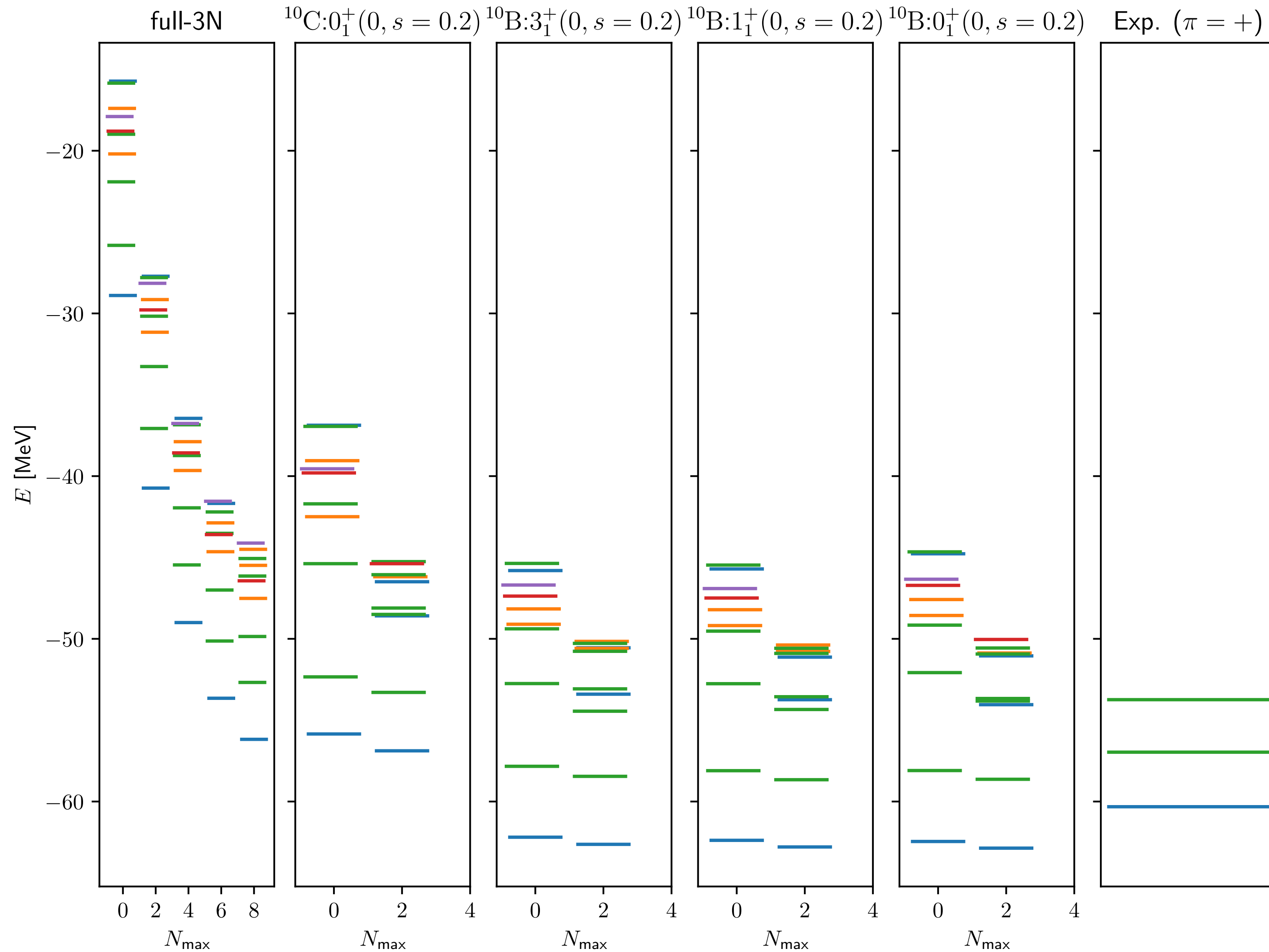
# (IM-)NCSM for Super-Allowed Decays



# <sup>10</sup>C

see talk by  
**P. Gysbers**

$N_{\max}$	Dim.
0	51
2	10111
4	430137
6	9213794
8	129149891



Eta: ImTime  
Int: n4lo500-3NinIE7  
 $e_{\max} = 8$   
 $\hbar\Omega = 18\text{MeV}$

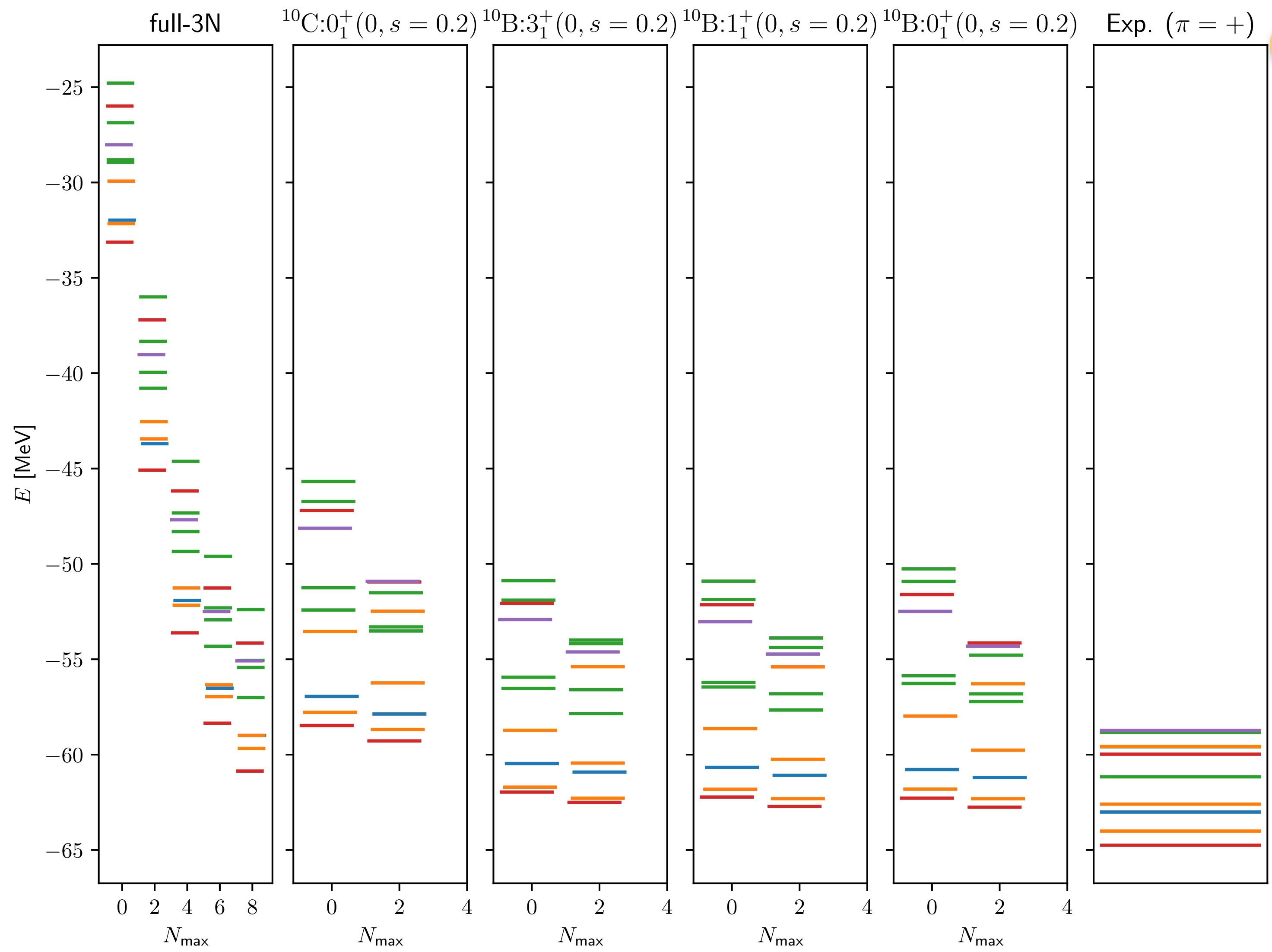
# (IM-)NCSM for Super-Allowed Decays



## $^{10}\text{B}$

see talk by  
**P. Gysbers**

$N_{\text{max}}$	Dim.
0	84
2	12502
4	581740
6	12060706
8	165613656



Eta: ImTime  
Int: n4lo500-3NinIE7  
 $e_{\text{max}} = 8$   
 $\hbar\Omega = 18\text{MeV}$

# Super-Allowed Beta Decays



- **Super-allowed beta decays constrain  $|V_{ud}|$  in the CKM matrix**
- **Precision treatment requires radiative corrections** that are sensitive to **nuclear structure**:  $\delta_C$  and  $\delta_{NS}$
- *ab initio* calculations of  $A = 10, 14$  decays in **light nuclei** using NCSM and QMC [Gennari et al., PRL 134, 012501; Cirigliano et al., PRC 110, 055502; King et al., arXiv:2509.07310]
- use **IM-NCSM** to extend mass range  $^{22}\text{Mg}$ ,  $^{26m}\text{Al}$ , ...
- benchmarks for CC, IM-GCM, VS-IMSRG, ...
- test exact sum over intermediate states vs. new EFT approach

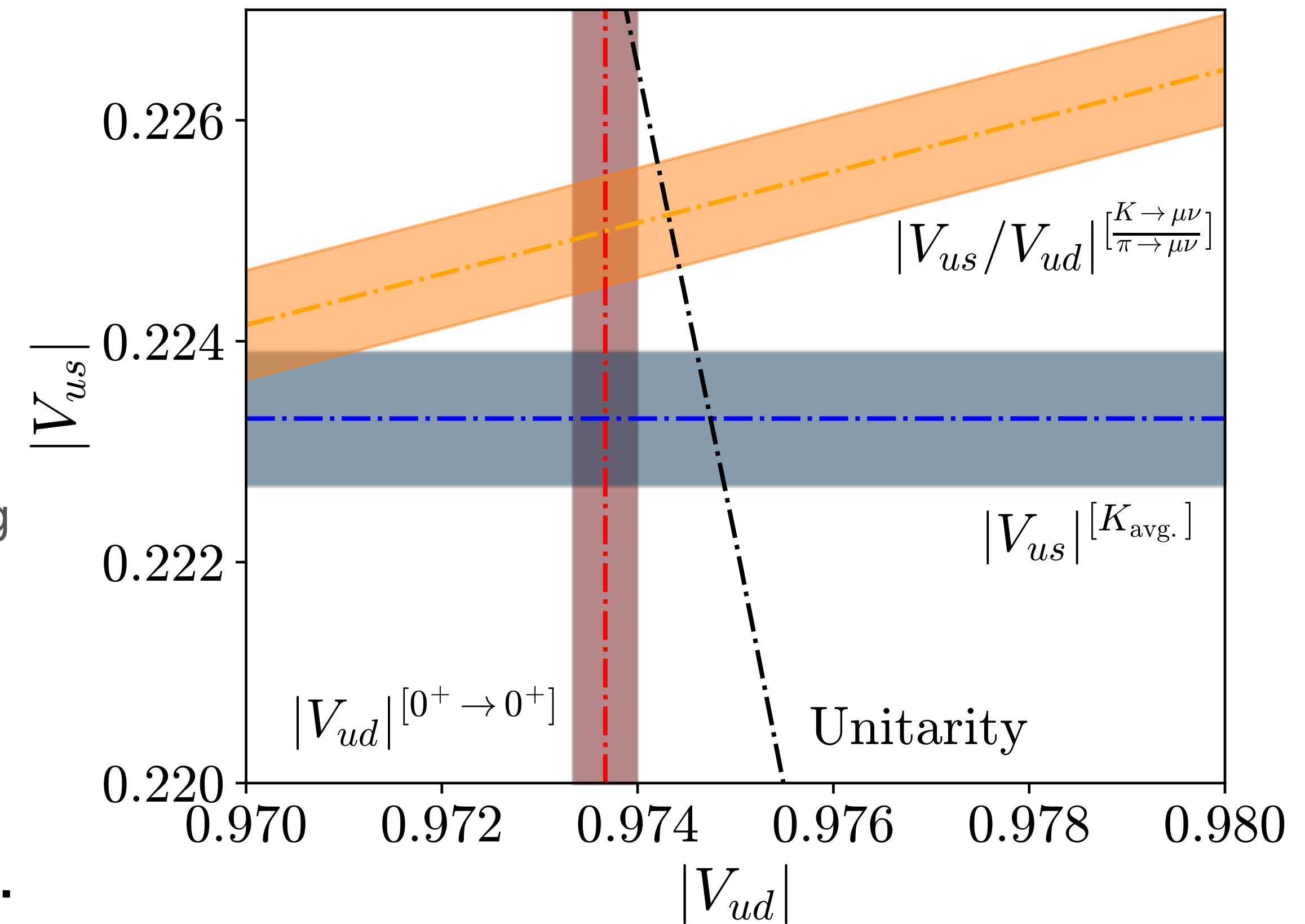


image credit: M. Gennari