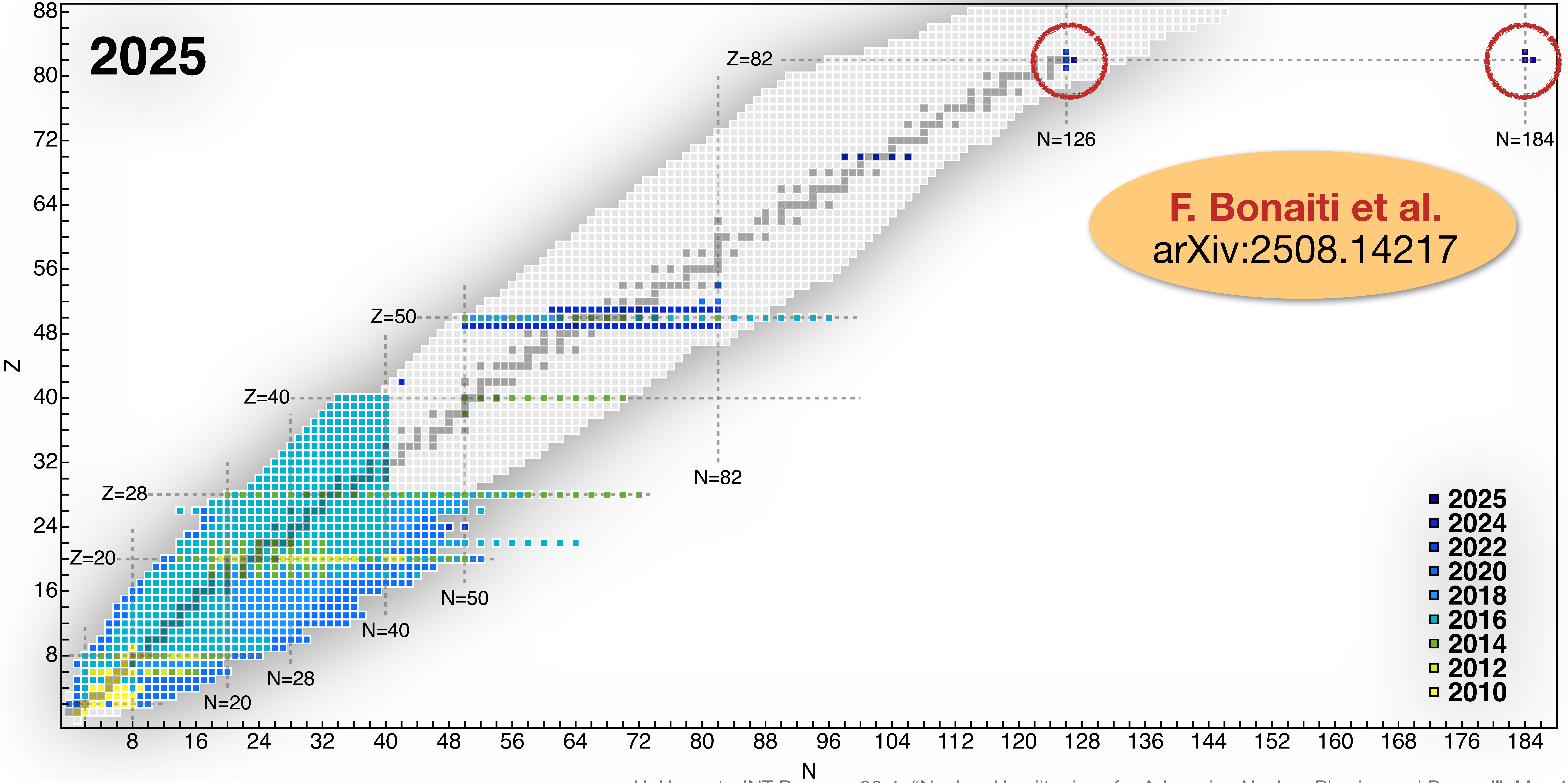
In-Medium Similarity Renormalization Group for Deformed Nuclei

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

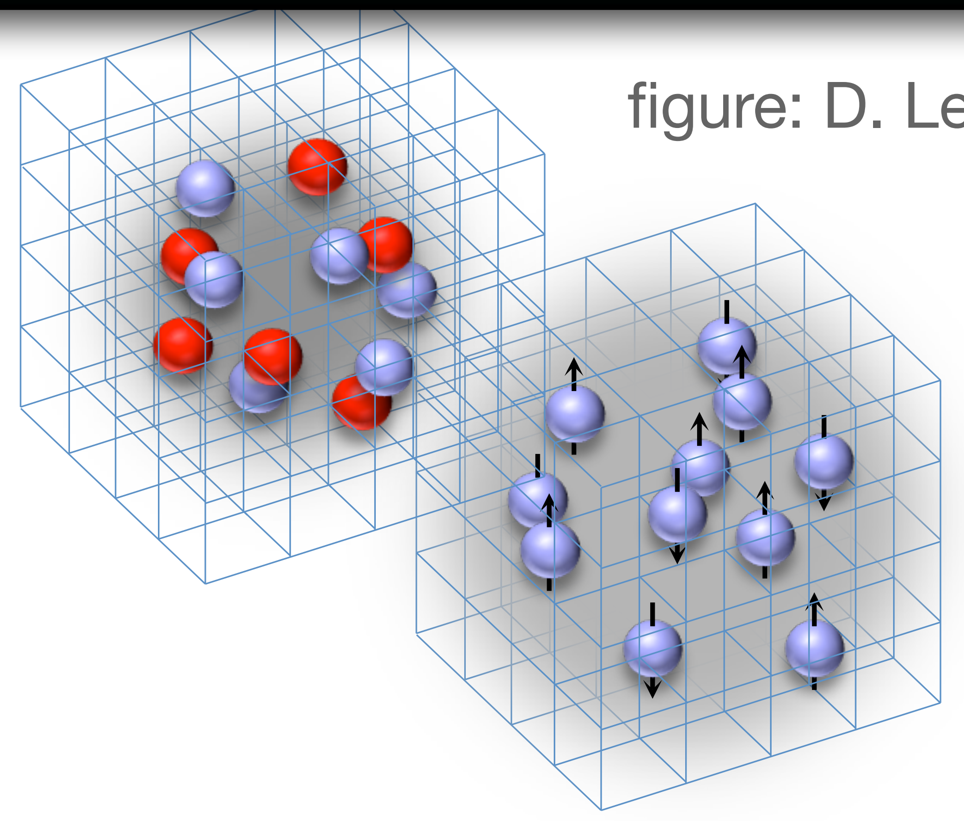
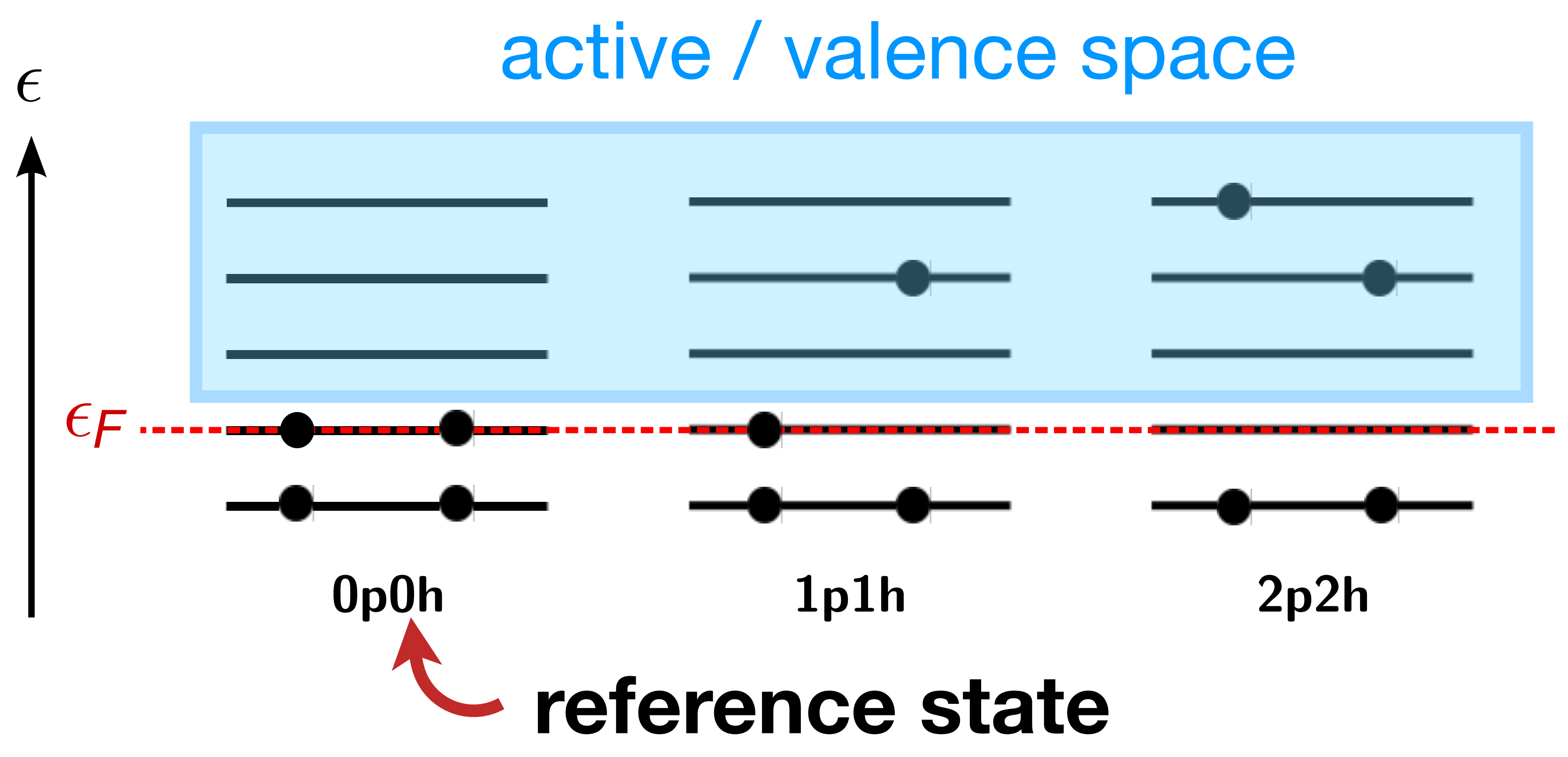
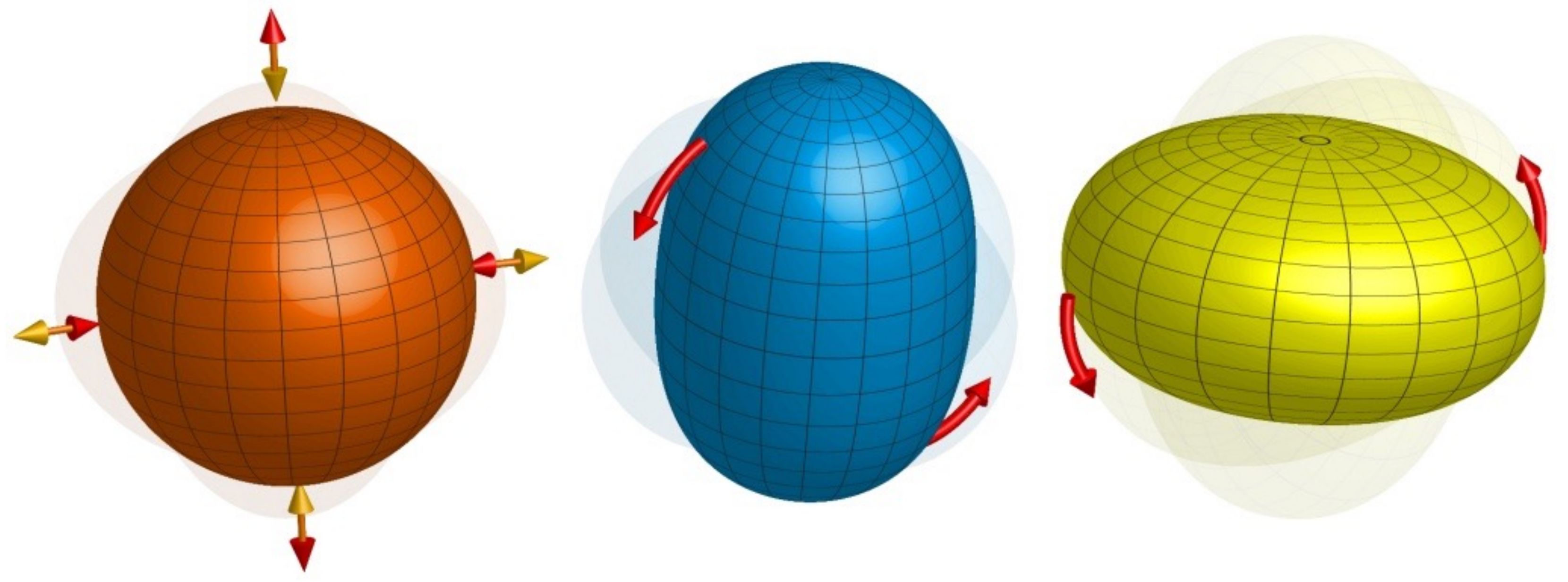


figure: D. Lee





Many-Body Methods: Paradigms

- **Coordinate Space**
  - Quantum Monte Carlo

figure: D. Lee

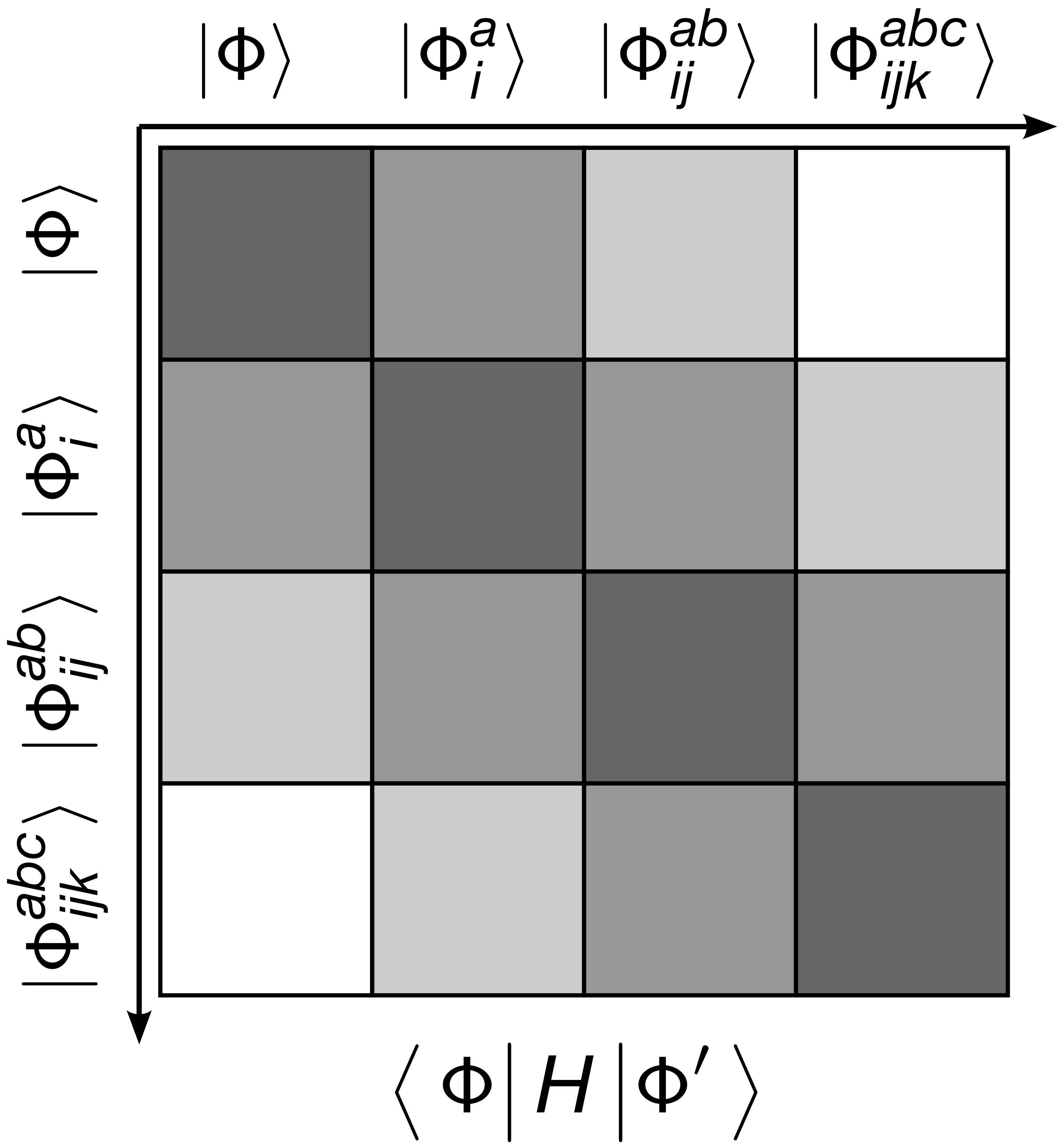
Recent(-ish) Reviews:
HH, Front. Phys. **8**, 379 (2020)
S. Gandolfi, D. Lonardoni, A. Lovato and M. Piarulli, Front. Phys. **8**, 117 (2020)
D. Lee, Front. Phys. **8**, 174 (2020)
V. Somà, Front. Phys. **8**, 340 (2020)

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

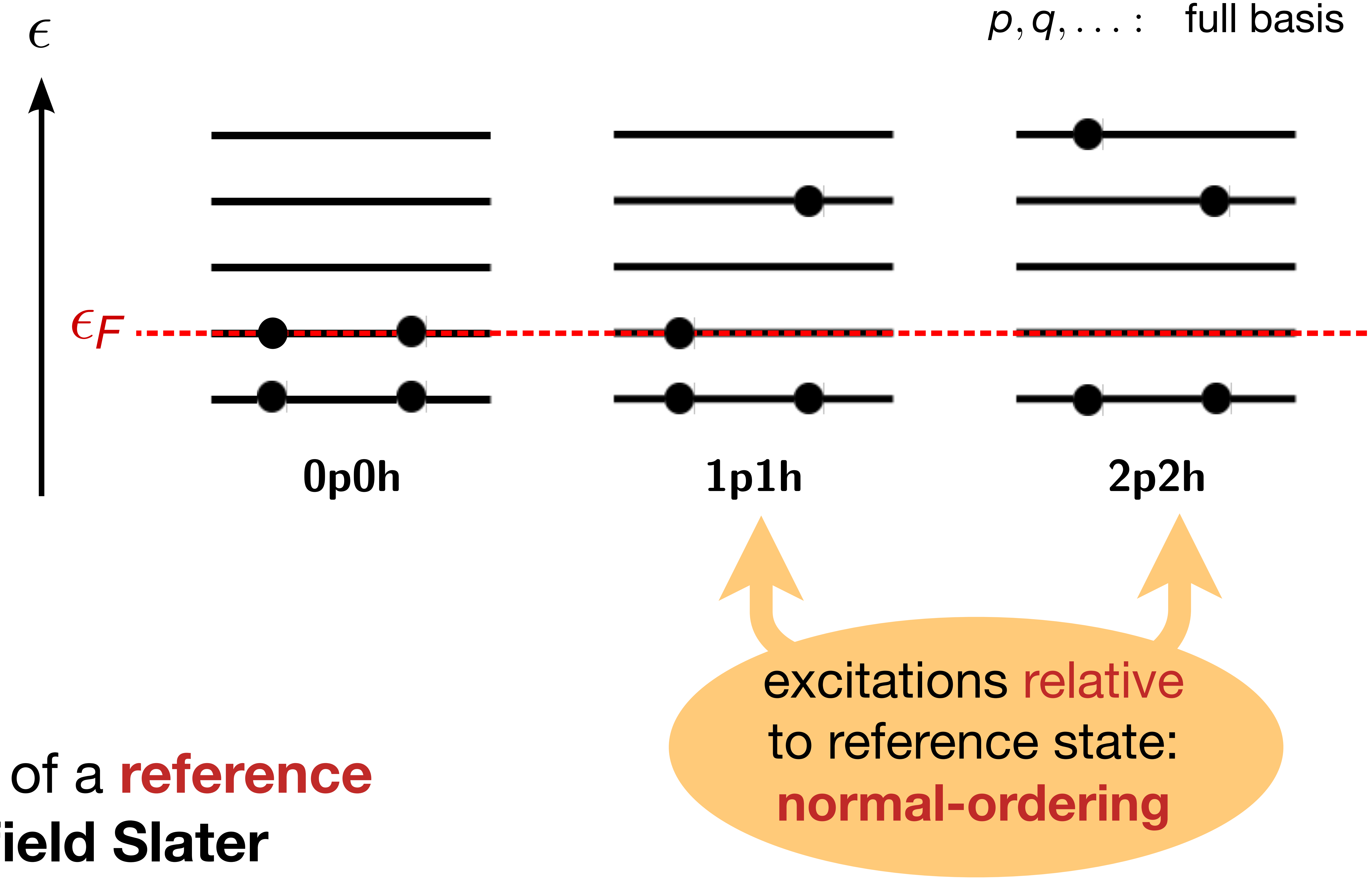
Many-Body Methods: Configuration Space



$a, b, \ldots : \quad \epsilon > \epsilon_F$

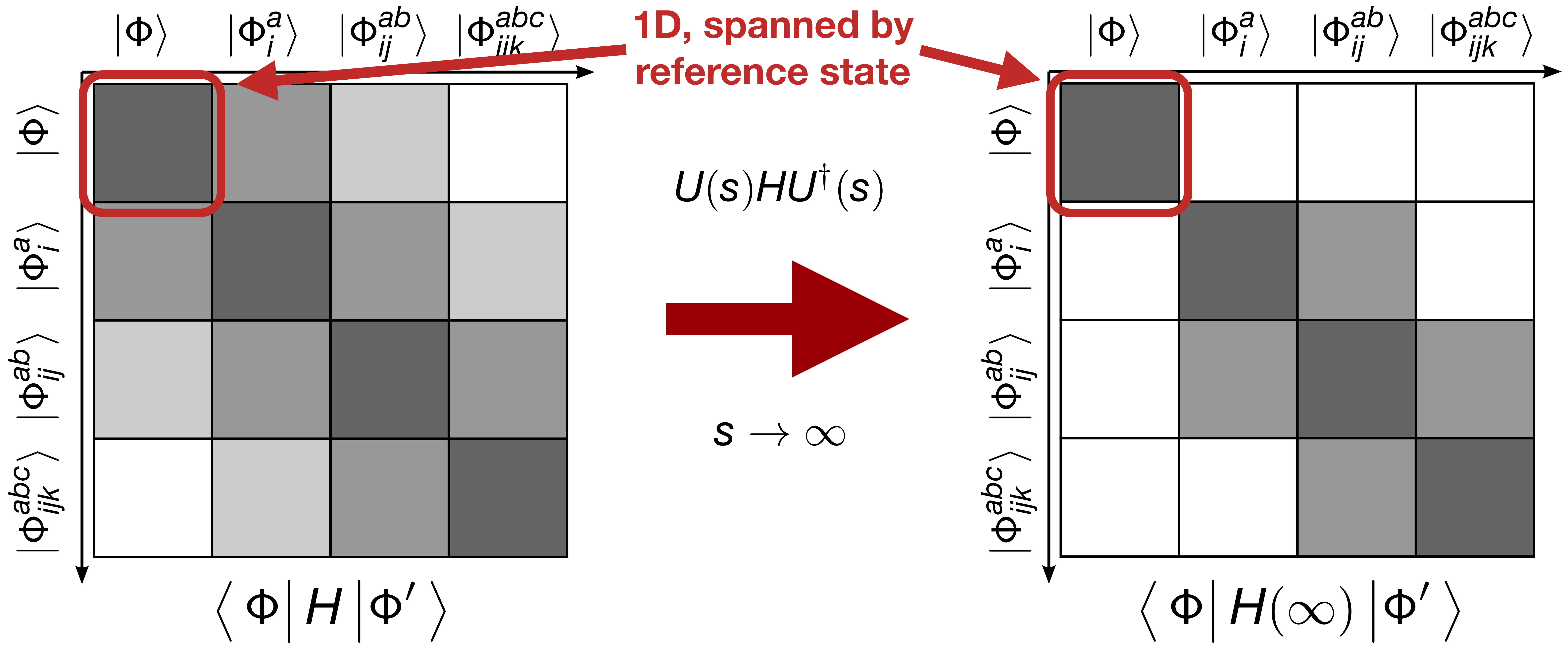
$i, j, \ldots : \quad \epsilon \leq \epsilon_F$

$p, q, \ldots :$ full basis



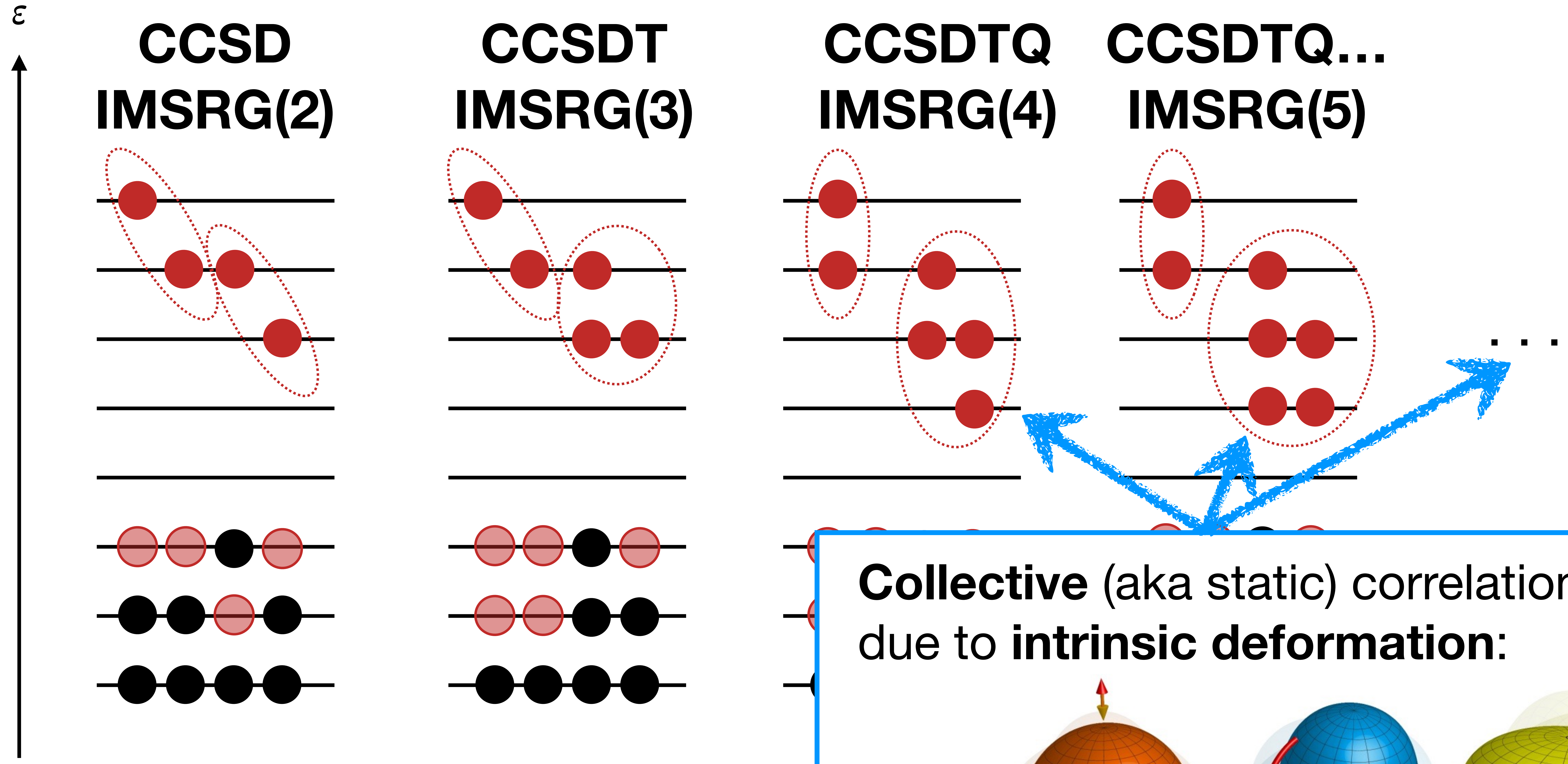
construct **particle-hole excitations** of a **reference state** - usually an optimized **mean-field Slater determinant**

Decoupling in A-Body Space

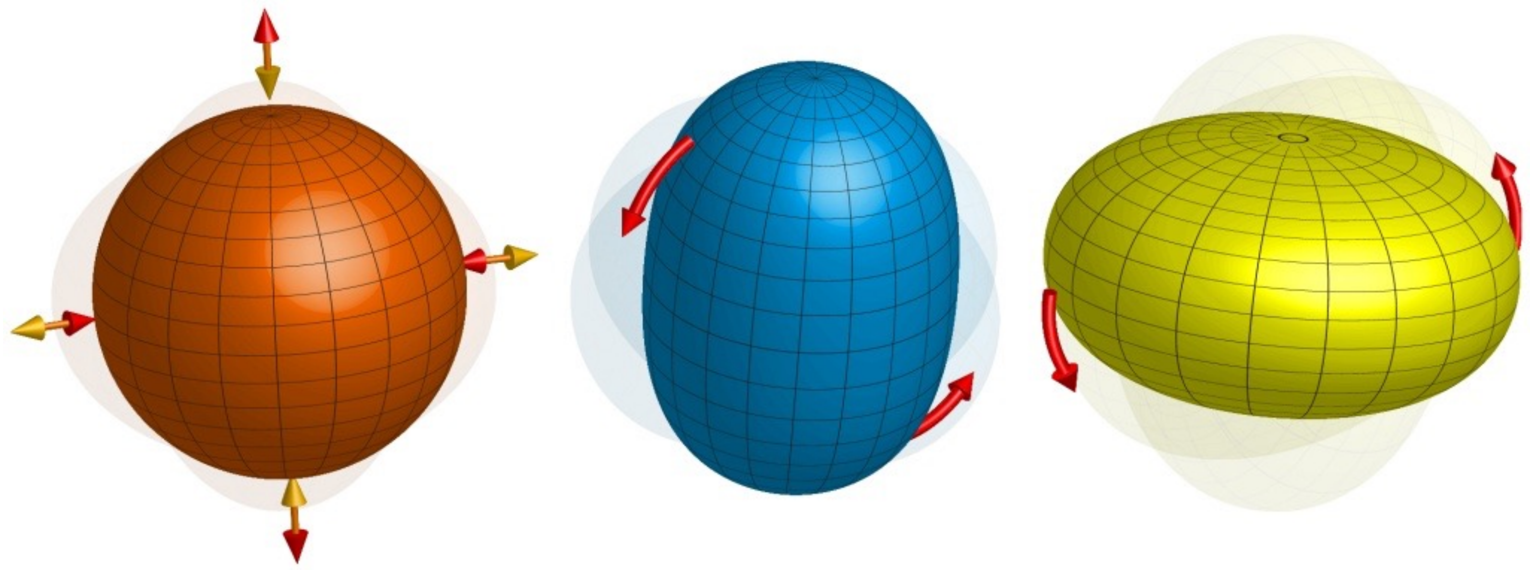


- **identify** the parts of the **operator *H*** which **couple reference state to excitations**
- **eliminate** them with unitary (**IMSRG**) or general similarity transformations (**CC**)
- **efficient: polynomial scaling,** no need to construct matrix !

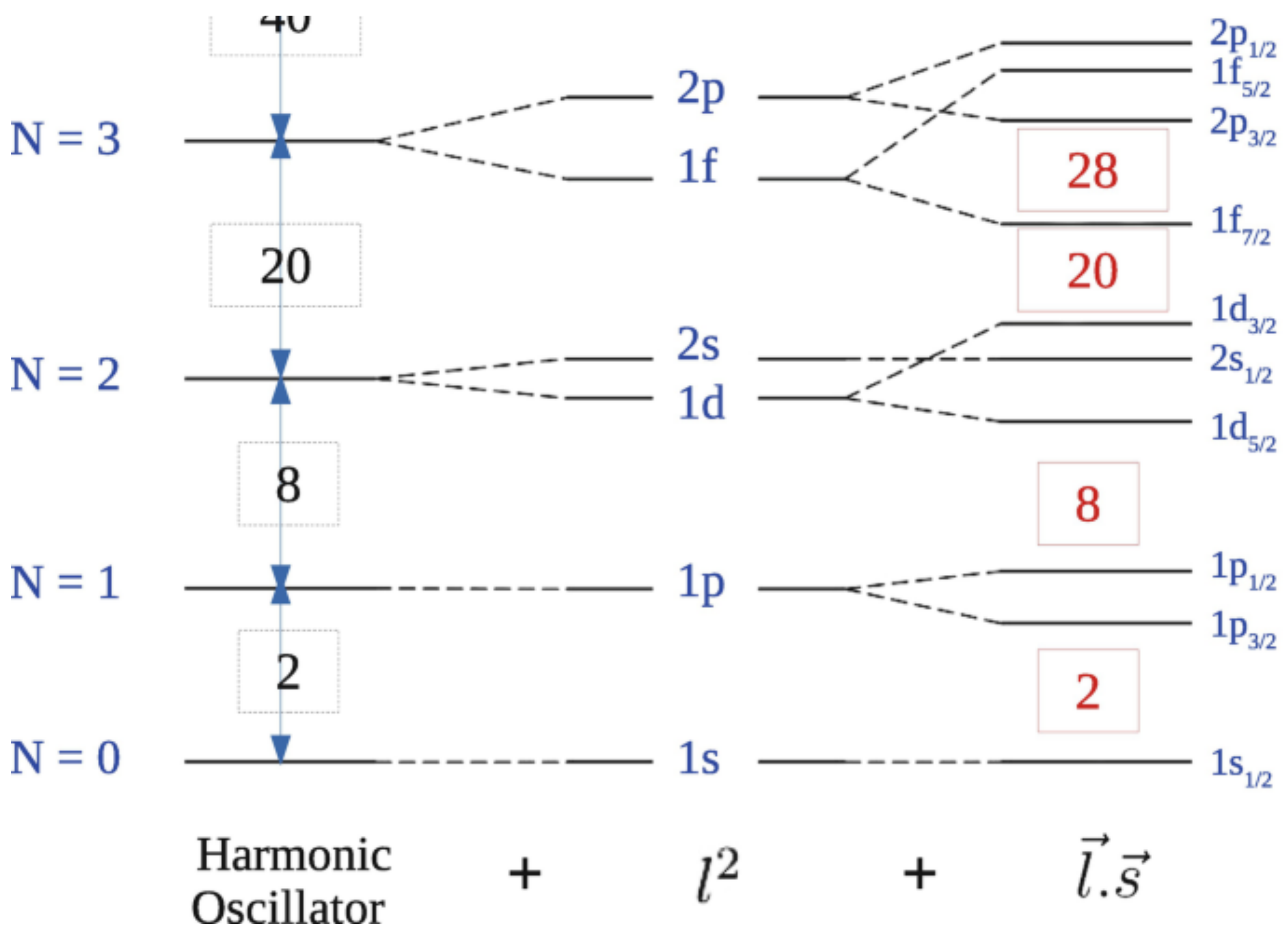
Correlations in Nuclei

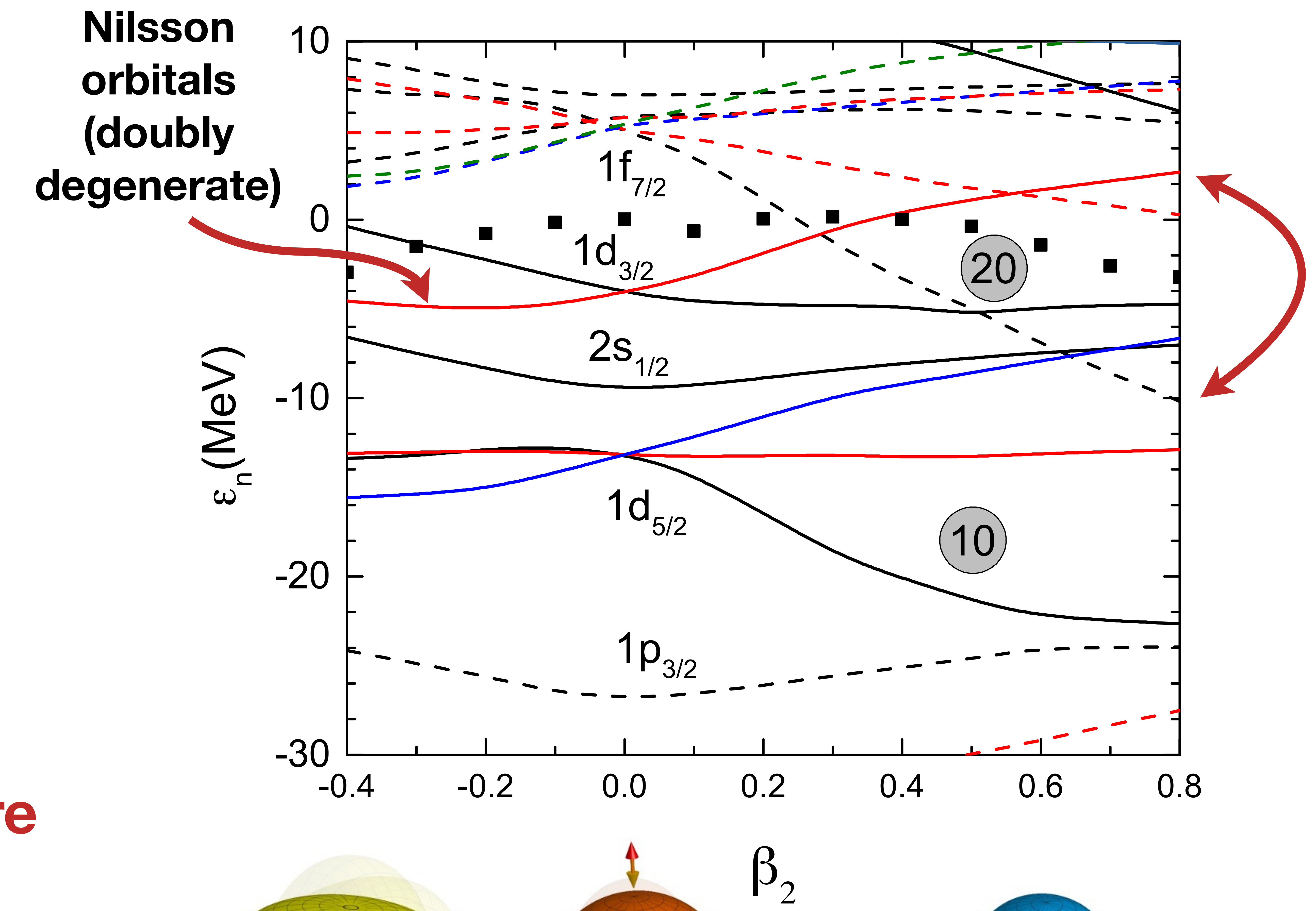


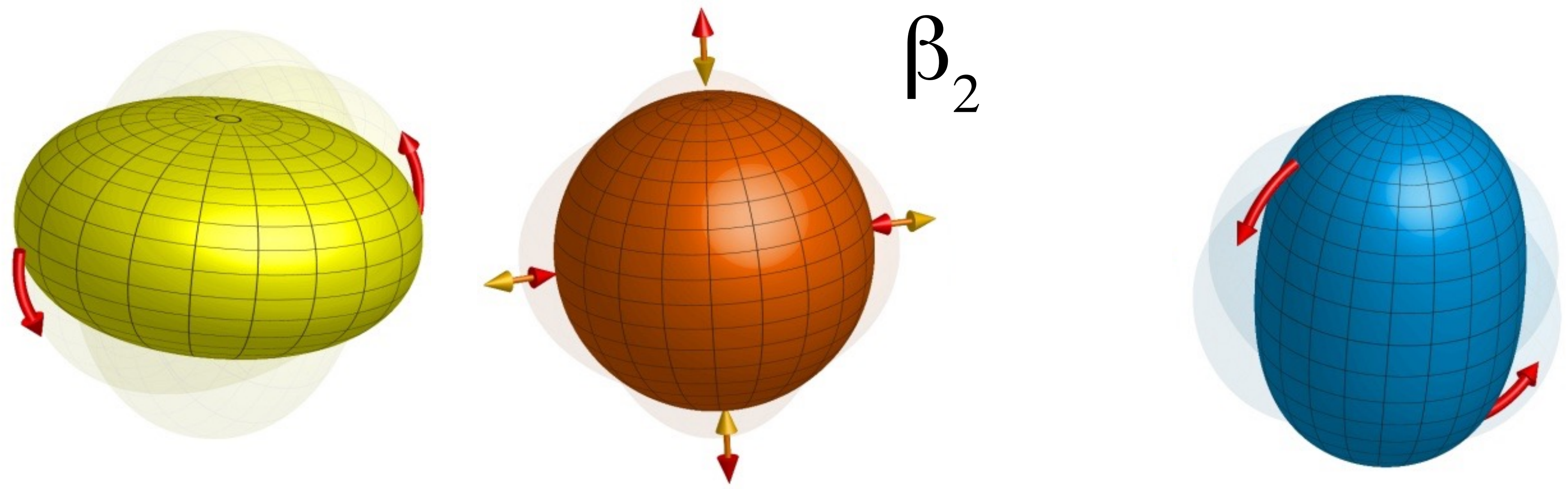
Collective (aka static) correlations, e.g. due to **intrinsic deformation**:



Symmetry Breaking and Restoration



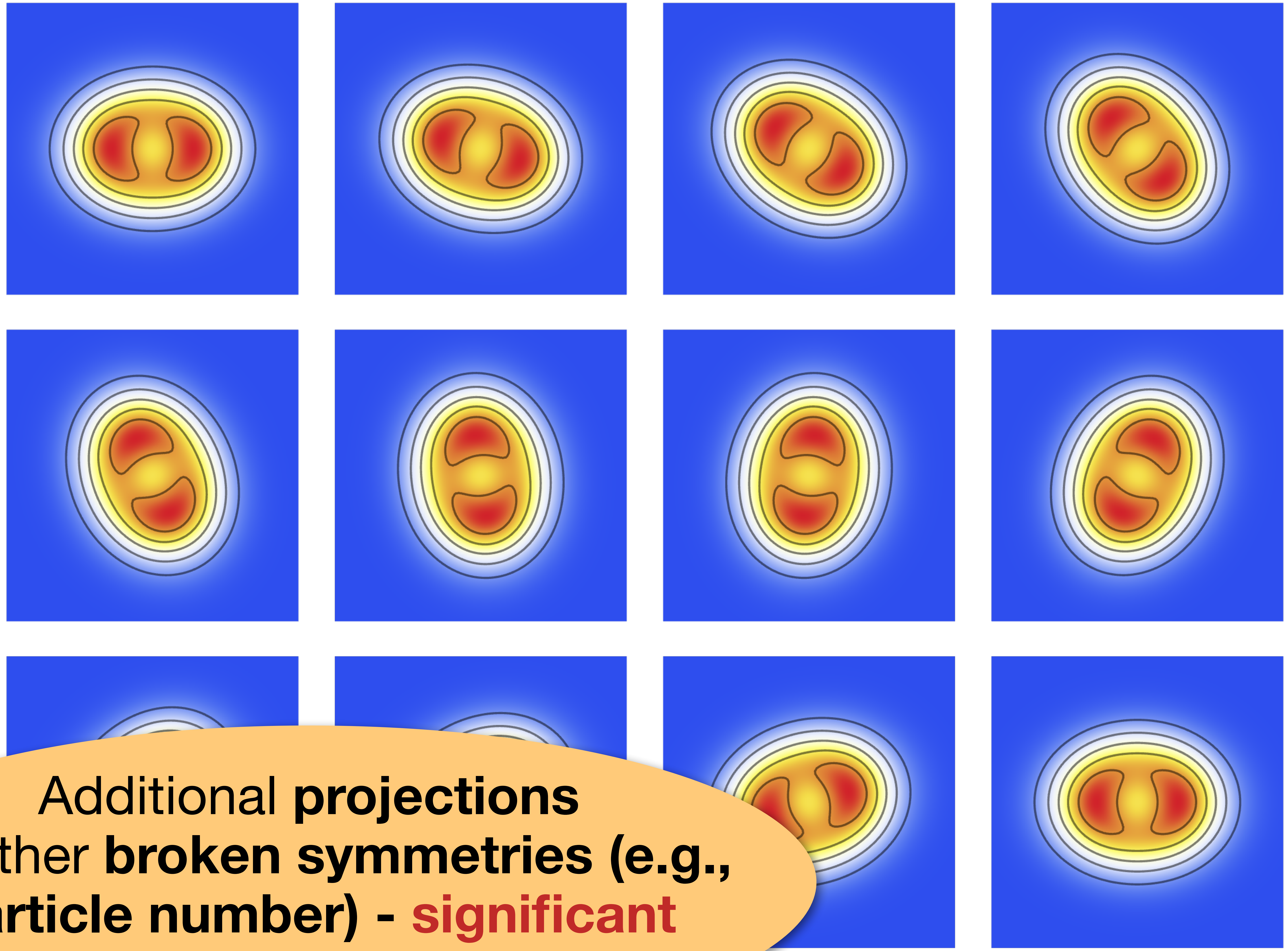




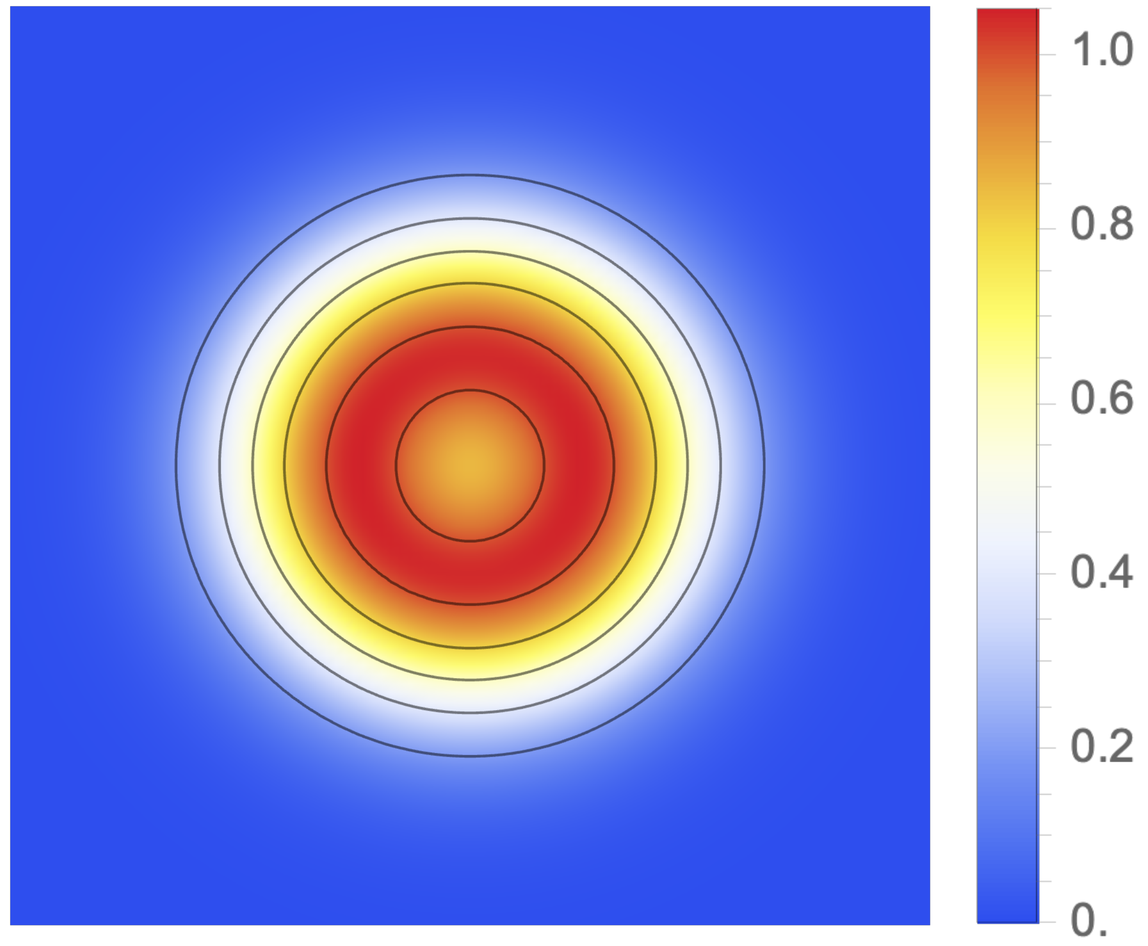
- **break spherical symmetry** to **capture static correlation** from deformation
- **restore symmetry** by constructing **(specific) superpositions** of **all rotations** of intrinsic state (aka **projection**)

Symmetry Breaking and Restoration

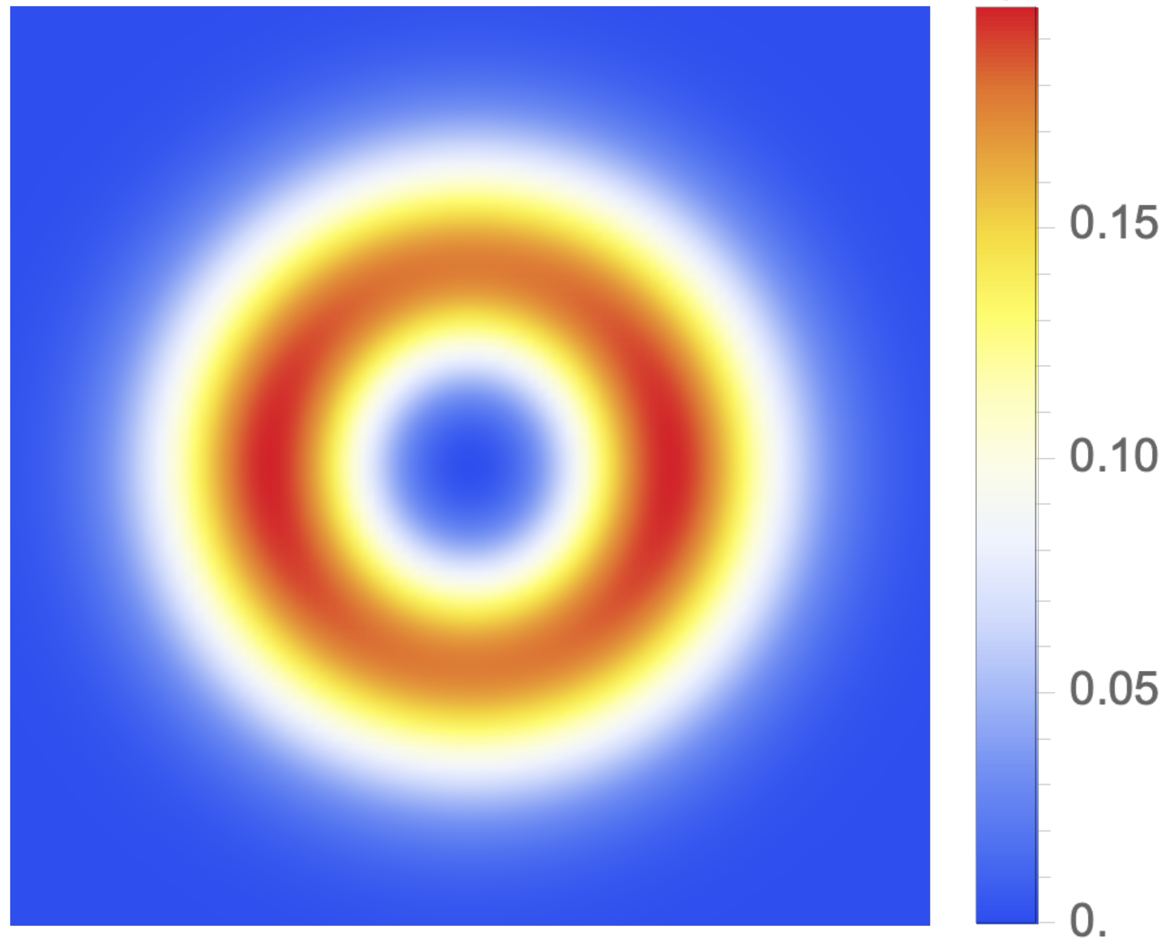
deformed configurations (not a real nucleus)



projected w.f.

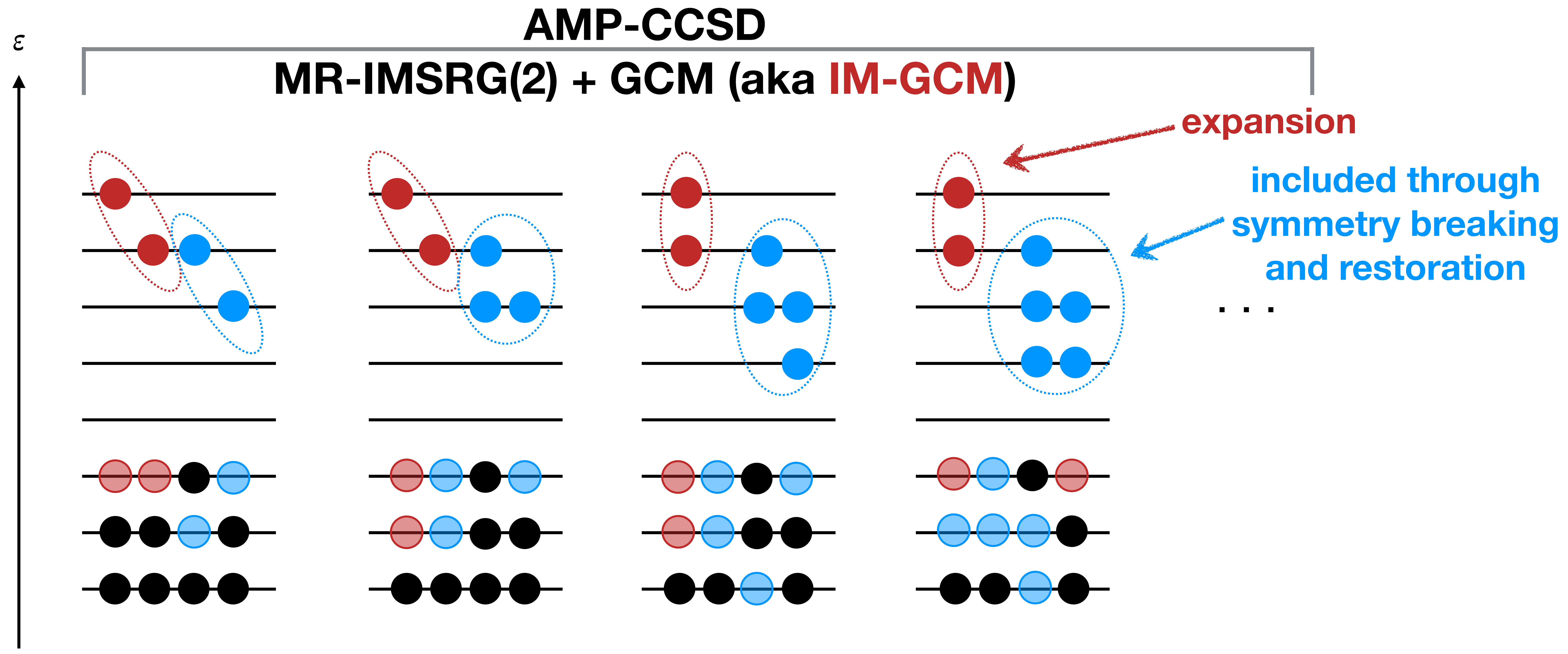


difference from spherical w.f. with same basis size /length scale



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

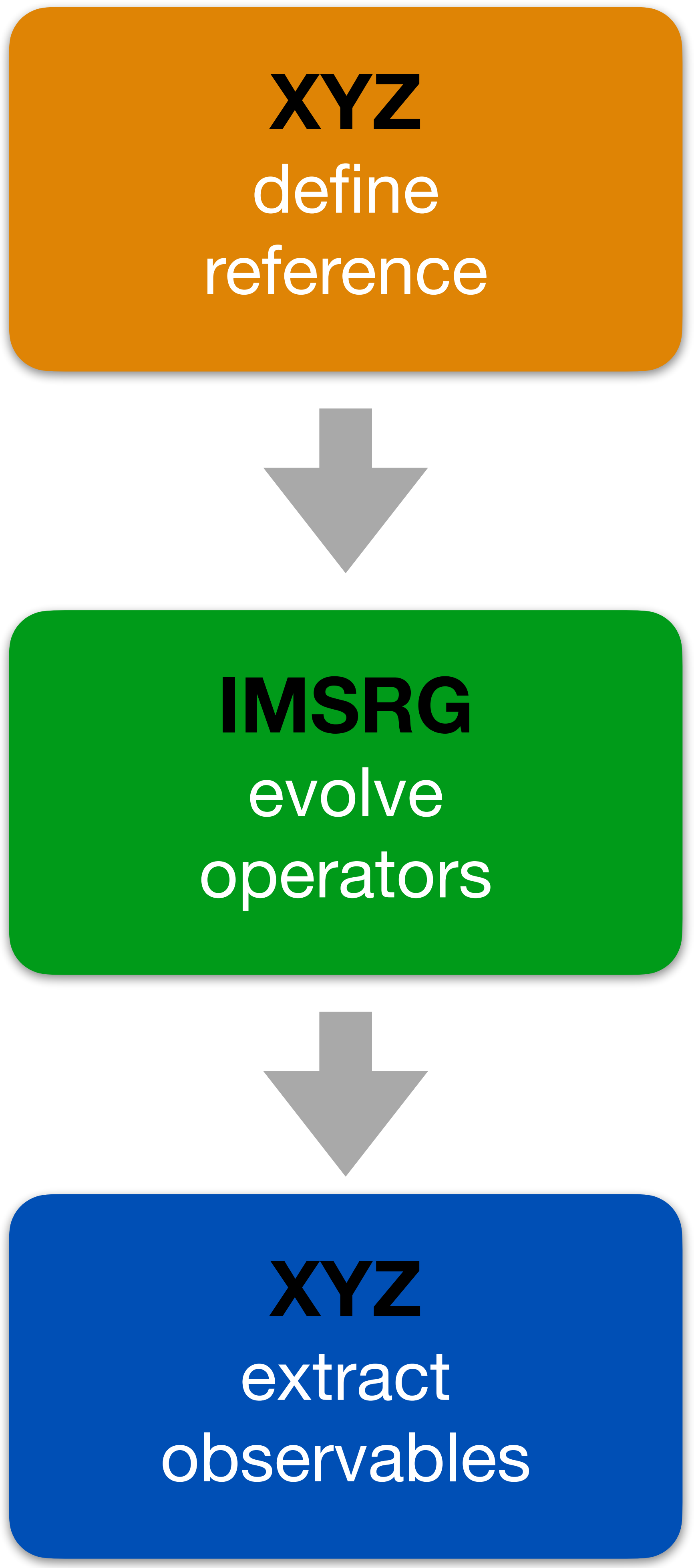
Correlations in Nuclei



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)

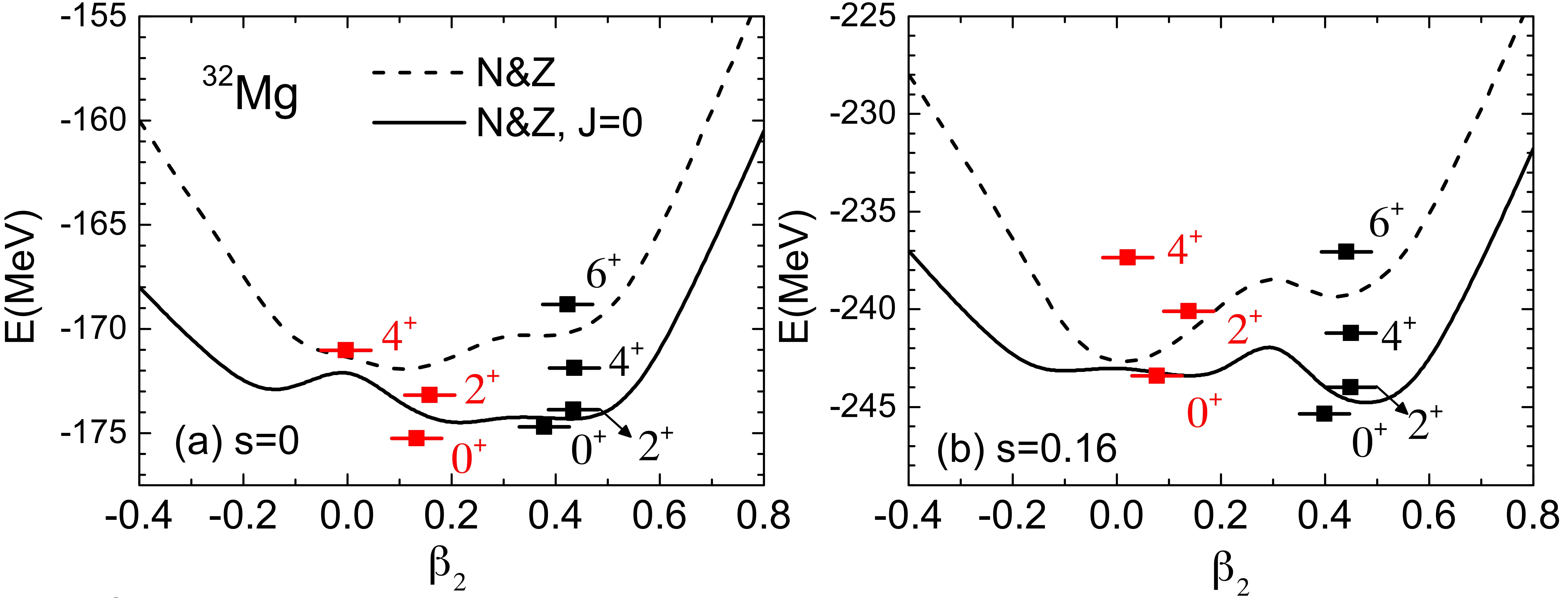


Selected Applications

Shape Coexistence: ^{32}Mg

E. F. Zhou et al., PLB 865, 139464 (2025) & arXiv:2603.07363

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

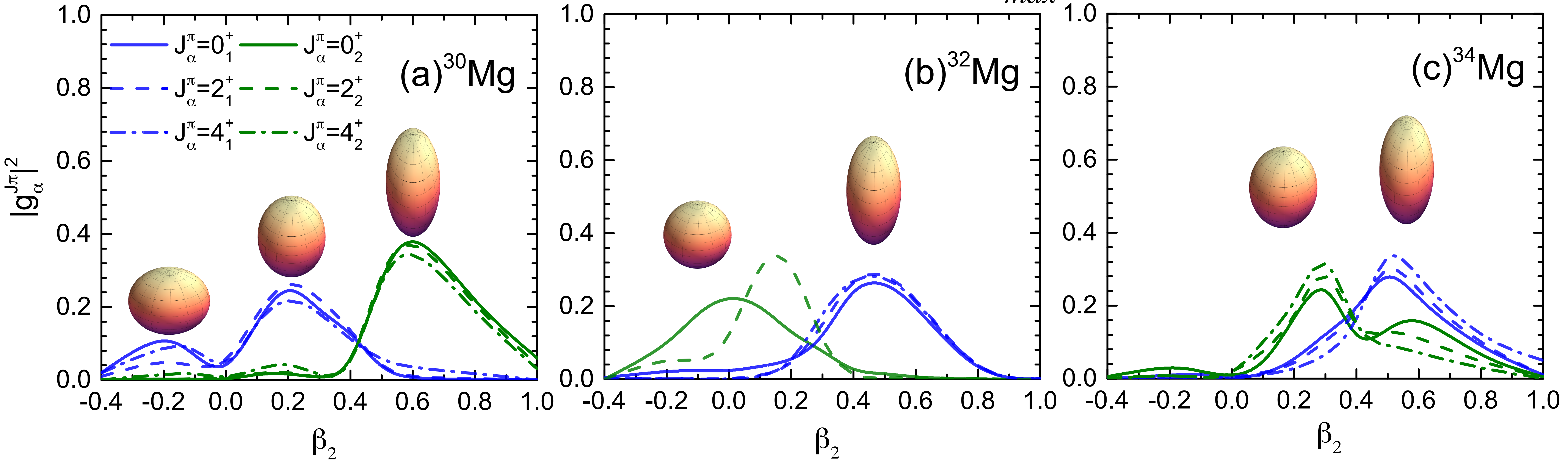


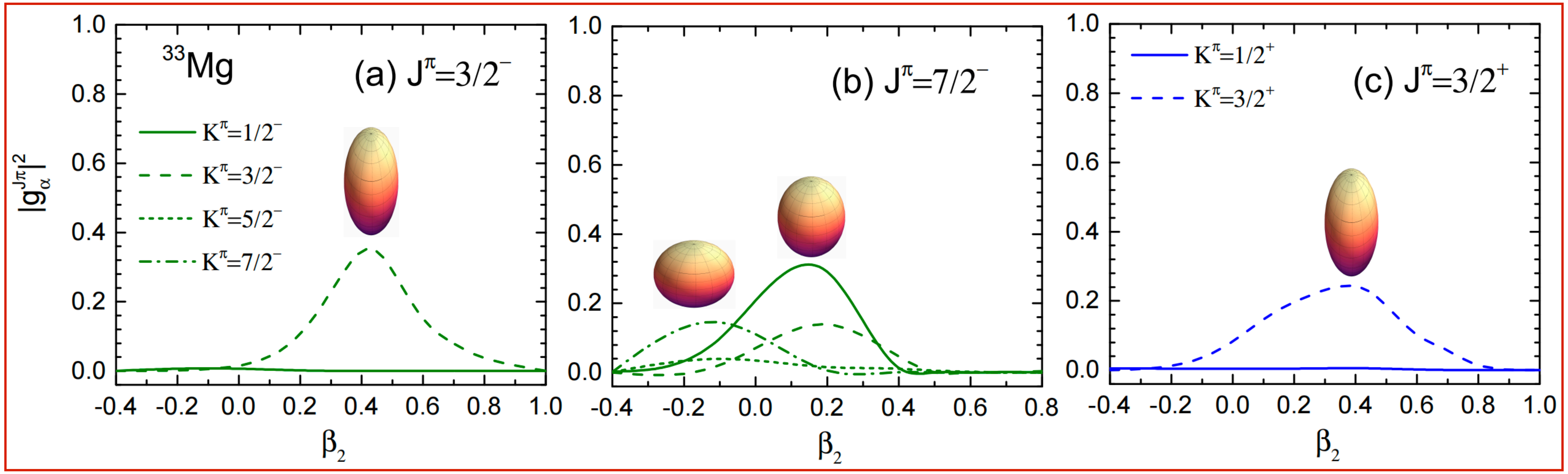
- **Dynamic correlations** captured by IMSRG…
  - bring **absolute energies** close to experiment (E=-249.7 MeV (AME) vs. -249.5 MeV (extrapolated theory))
  - reveal prominent **prolate deformation** of the **ground state**

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

E. F. Zhou et al., PLB 865, 139464 (2025) & arXiv:2603.07363

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

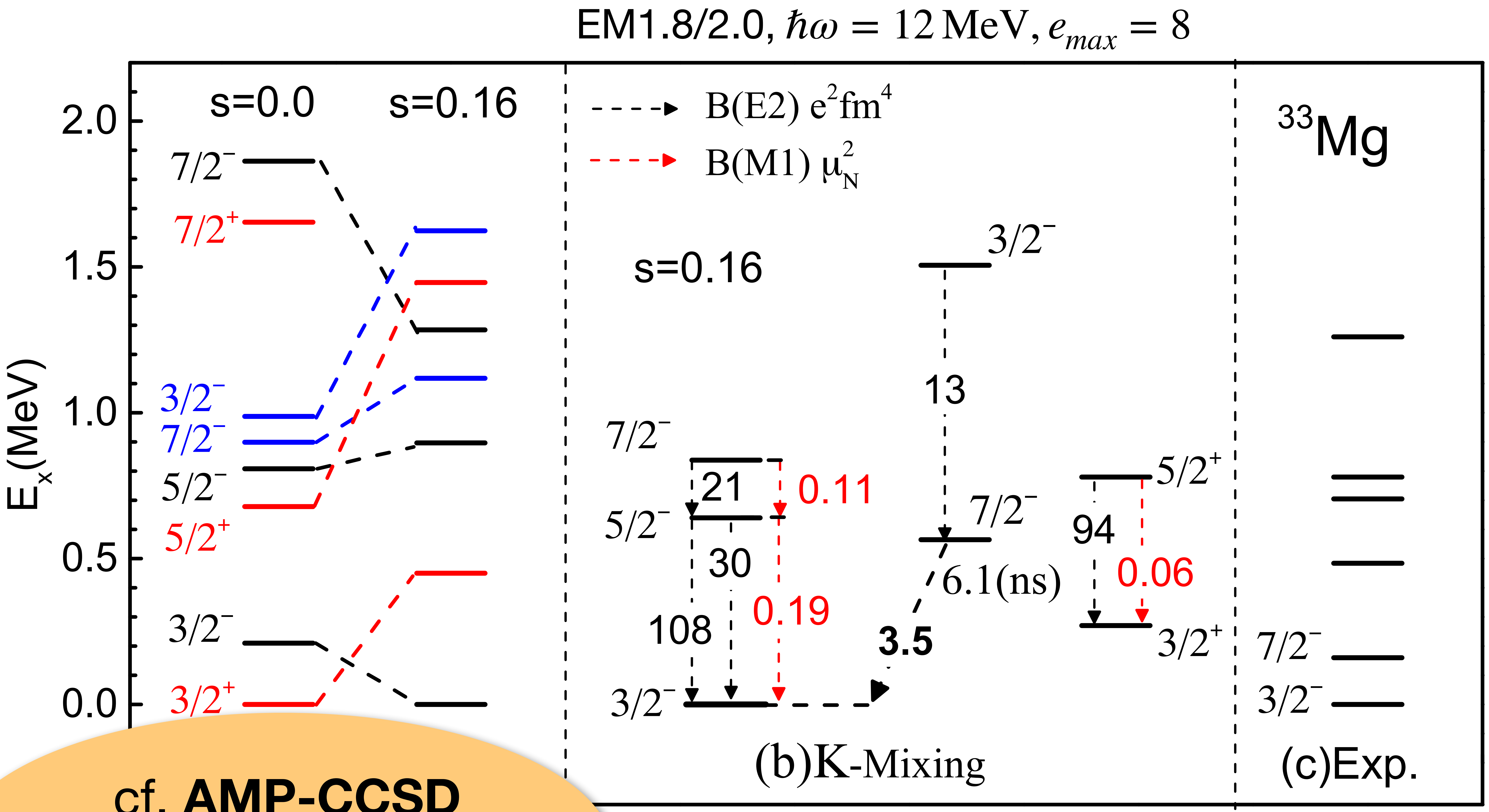




- **shape coexistence** comes with **shape mixing**
- **caveat:** (collective) wave functions are not observable - **compare with care**!

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

E. F. Zhou et al., PLB 865, 139464 (2025) & arXiv:2603.07363

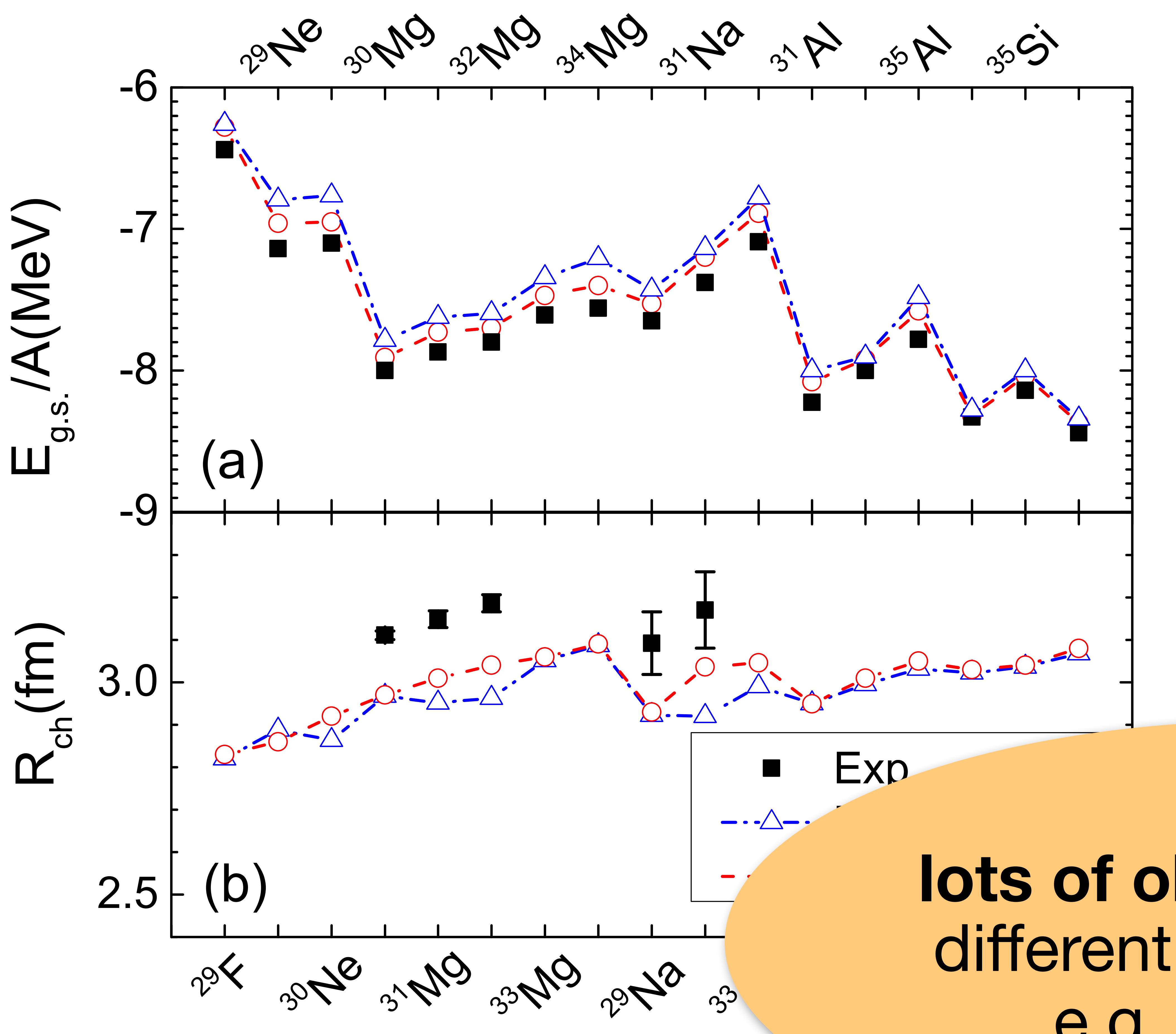


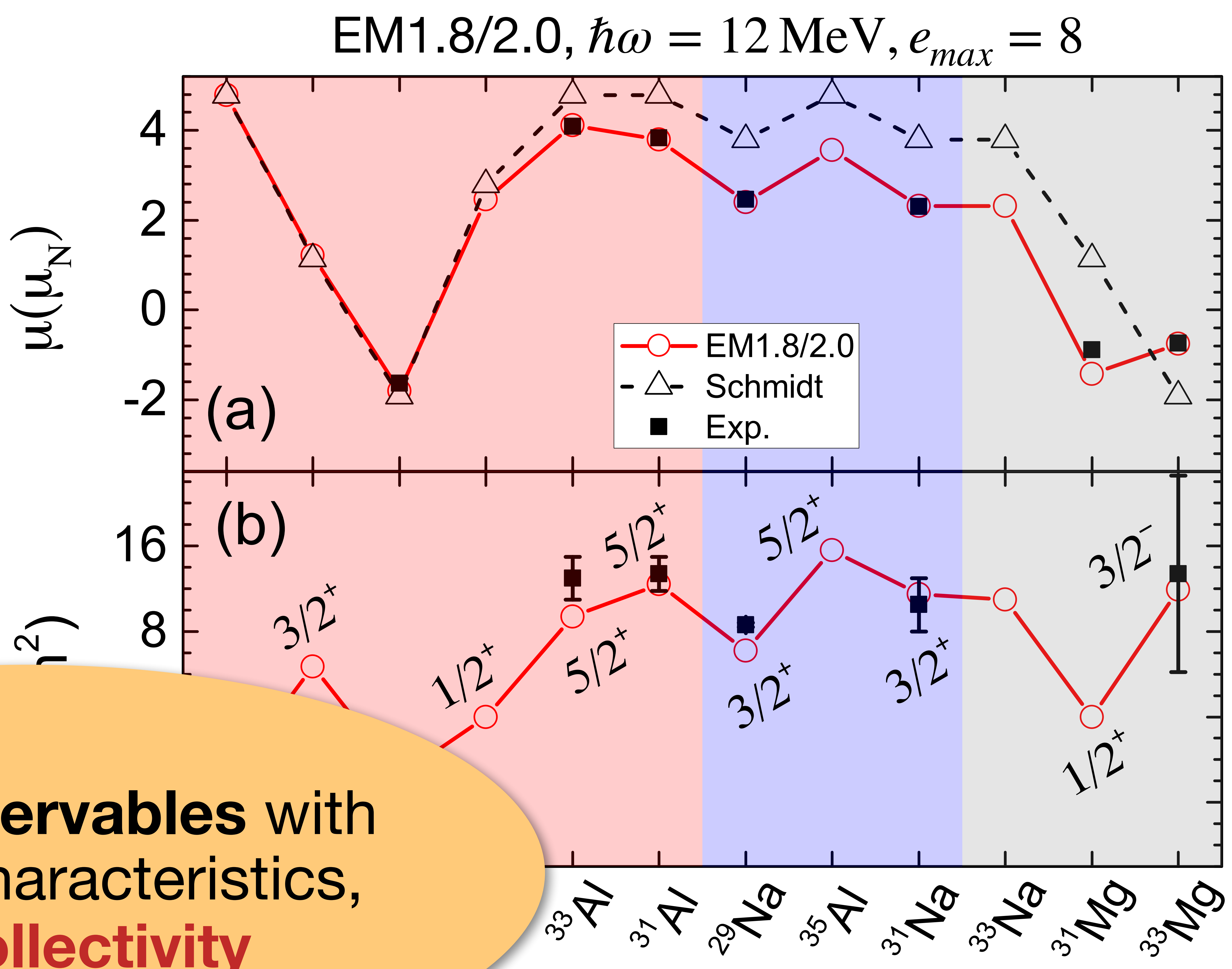
- **shape and K mixing have** notable impact on ^{33}Mg spectrum
- **boosts** lifetime of $\frac{7}{2}^-$ state - **predicted to be a shape isomer**
- related to ^{32}Na shape isomer measured at FDSi in 2023 ?
  [Gray et al., PRL 130, 132501]

cf. **AMP-CCSD**
Z. H. Sun et al., 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:2603.07363

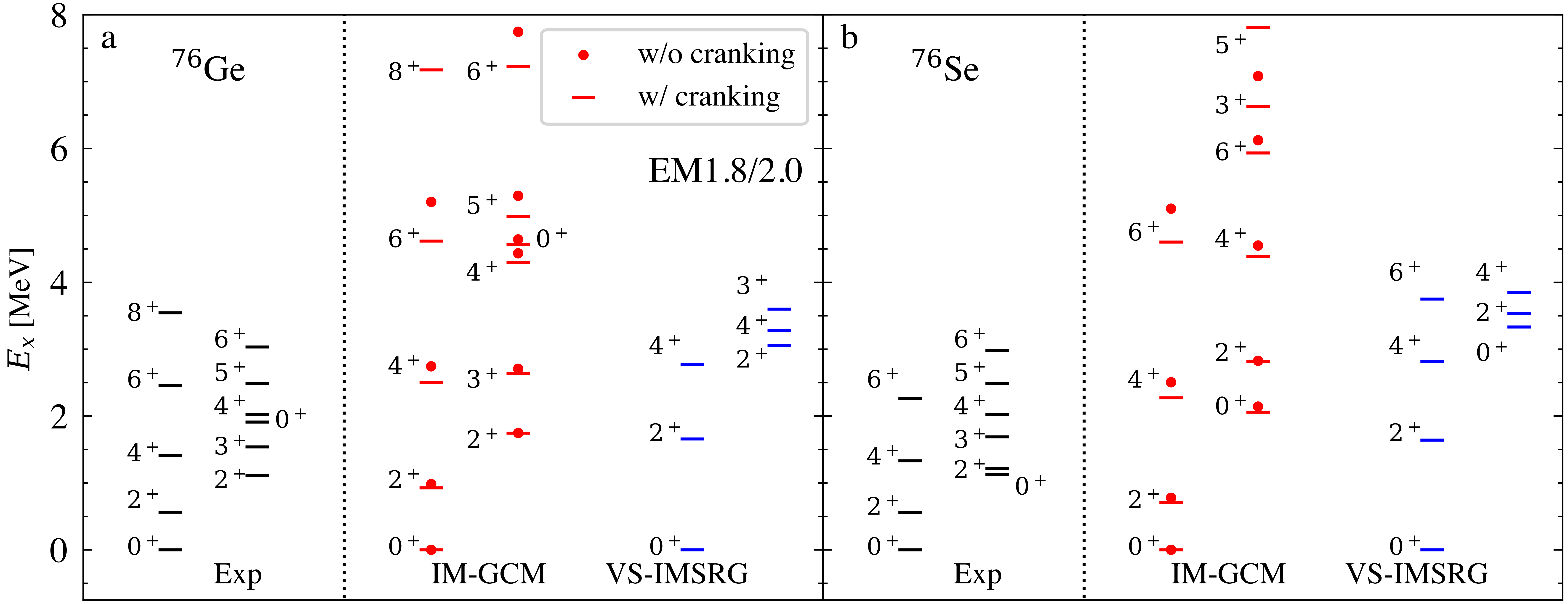


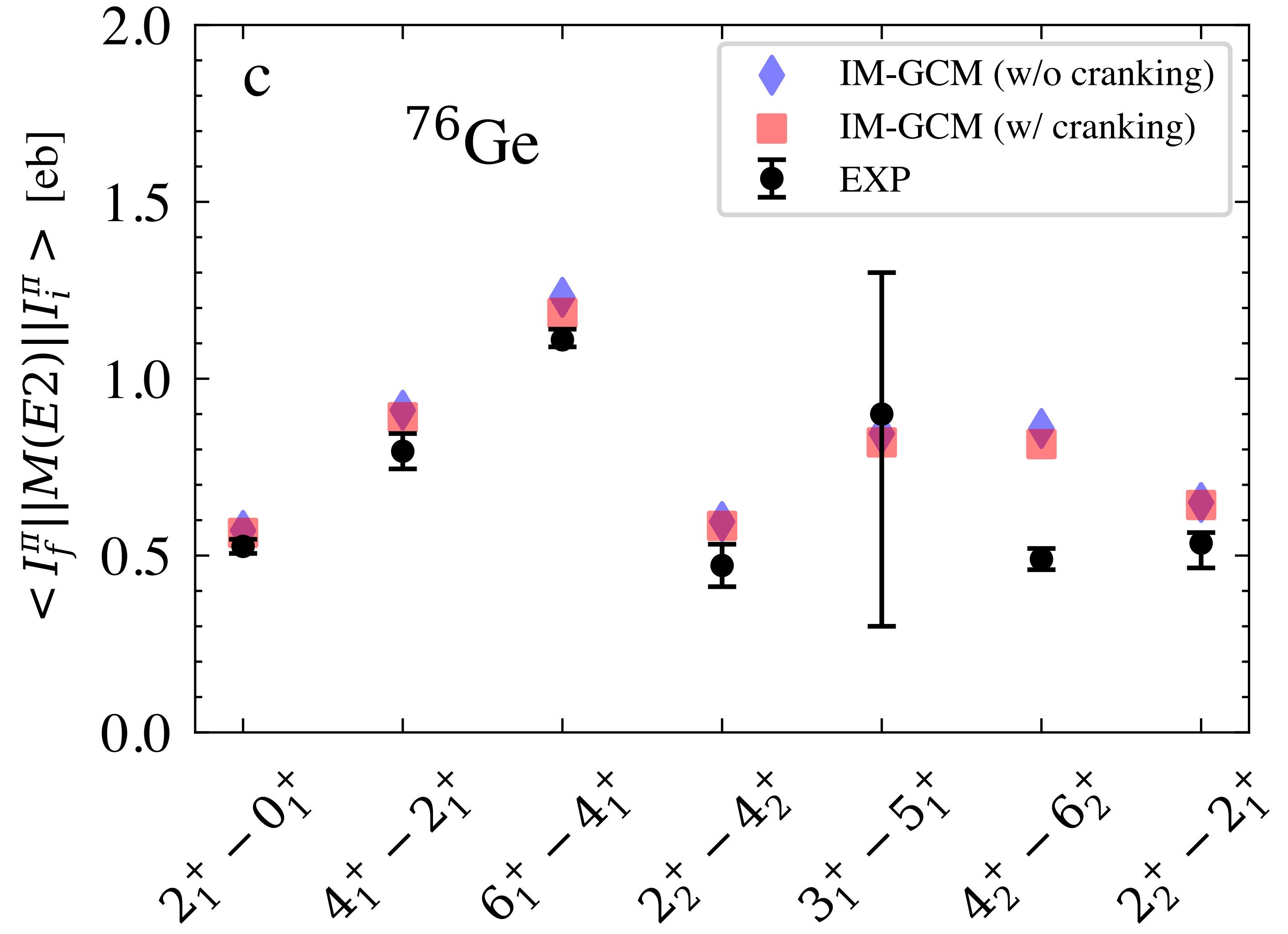


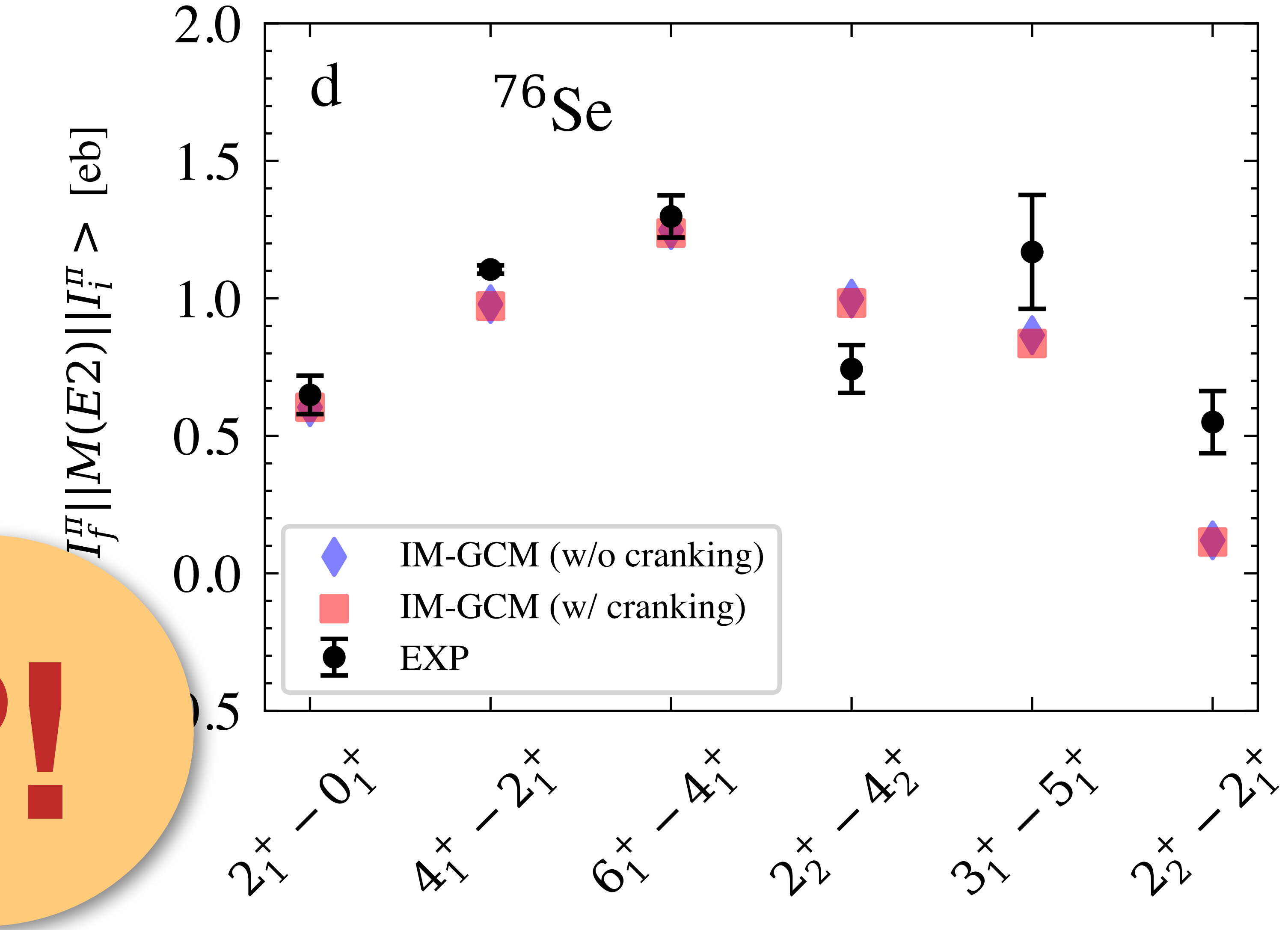
lots of observables with different characteristics, e.g. **collectivity**

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

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







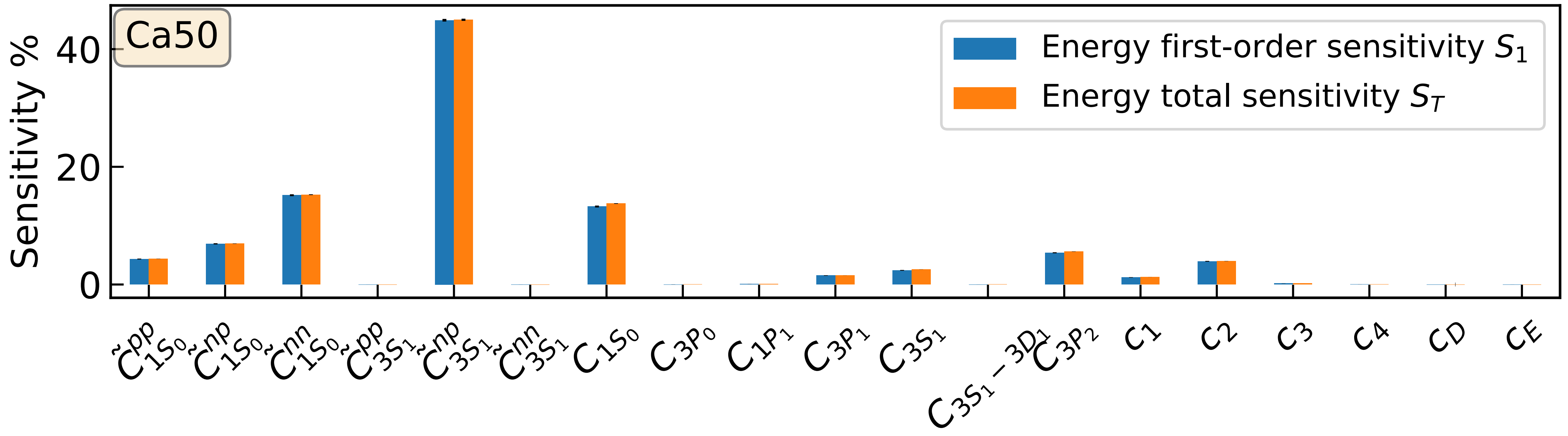
EM1.8/2.0 NN+3N interaction, $\hbar\omega = 12\,\mathrm{MeV}, e_{max} = 10$

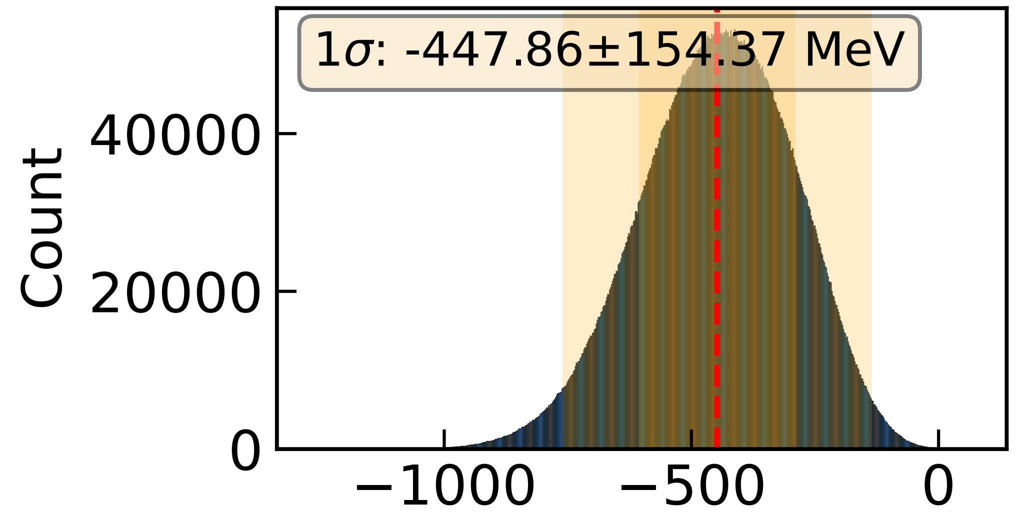
- IM-GCM spectra too extended (common)
- E2 transitions (and static moments) in **excellent agreement with experiment…**
- …although EM1.8/2.0 underpredicts **radii by a few percent**

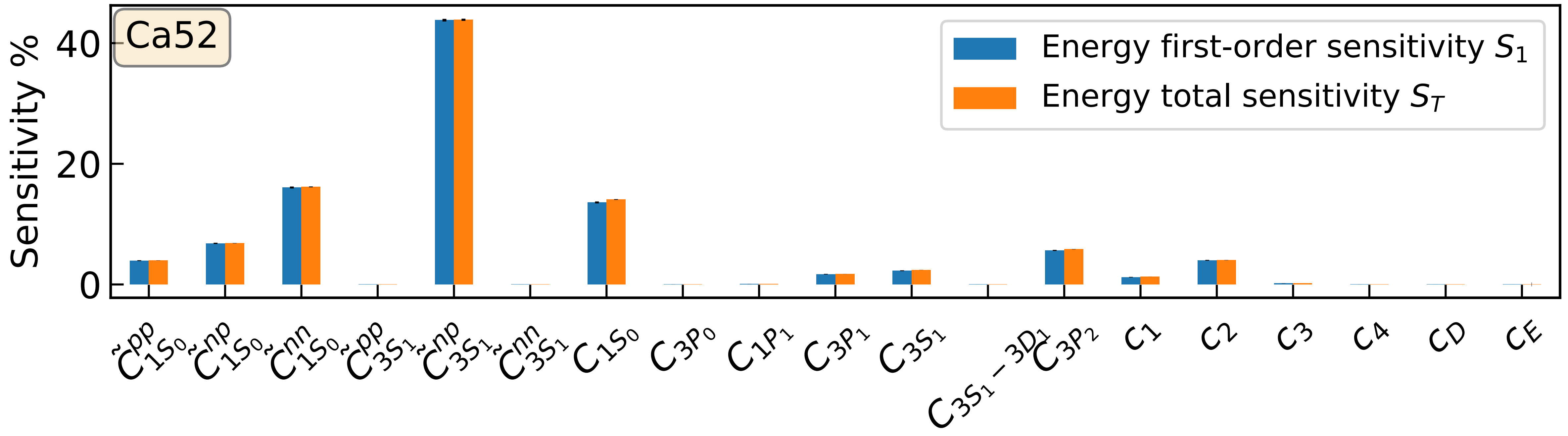
?!

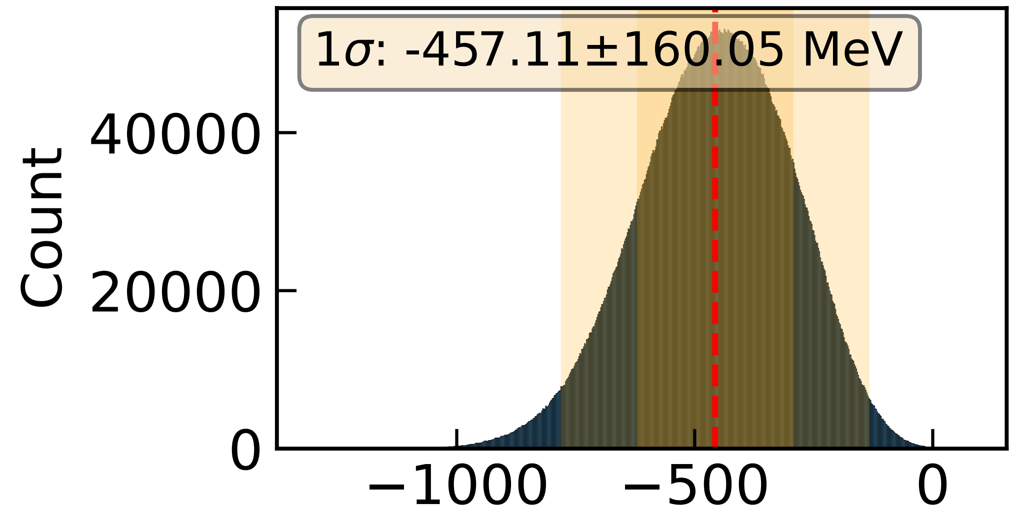
IMSRG Emulators

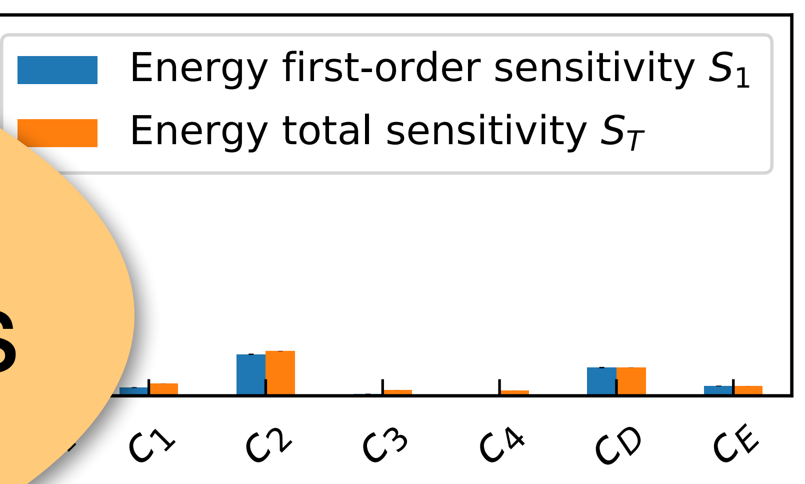
J. A. Davison et al., in prep.

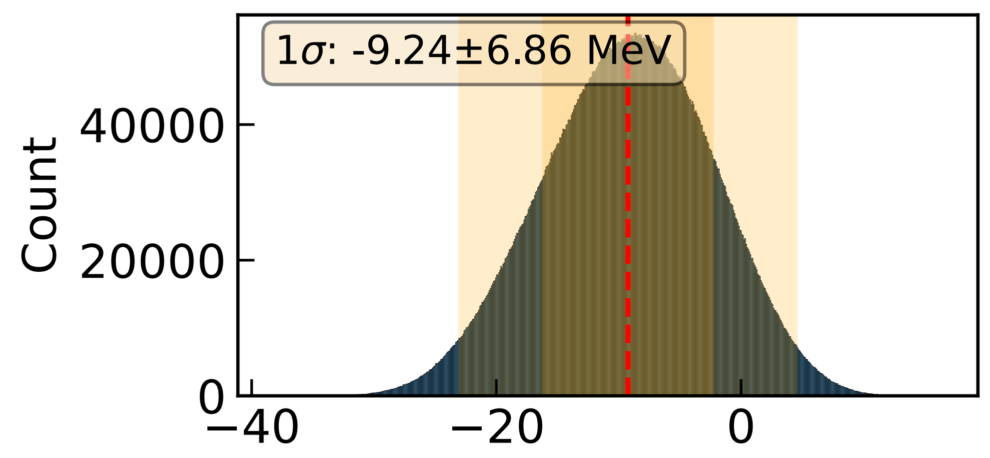










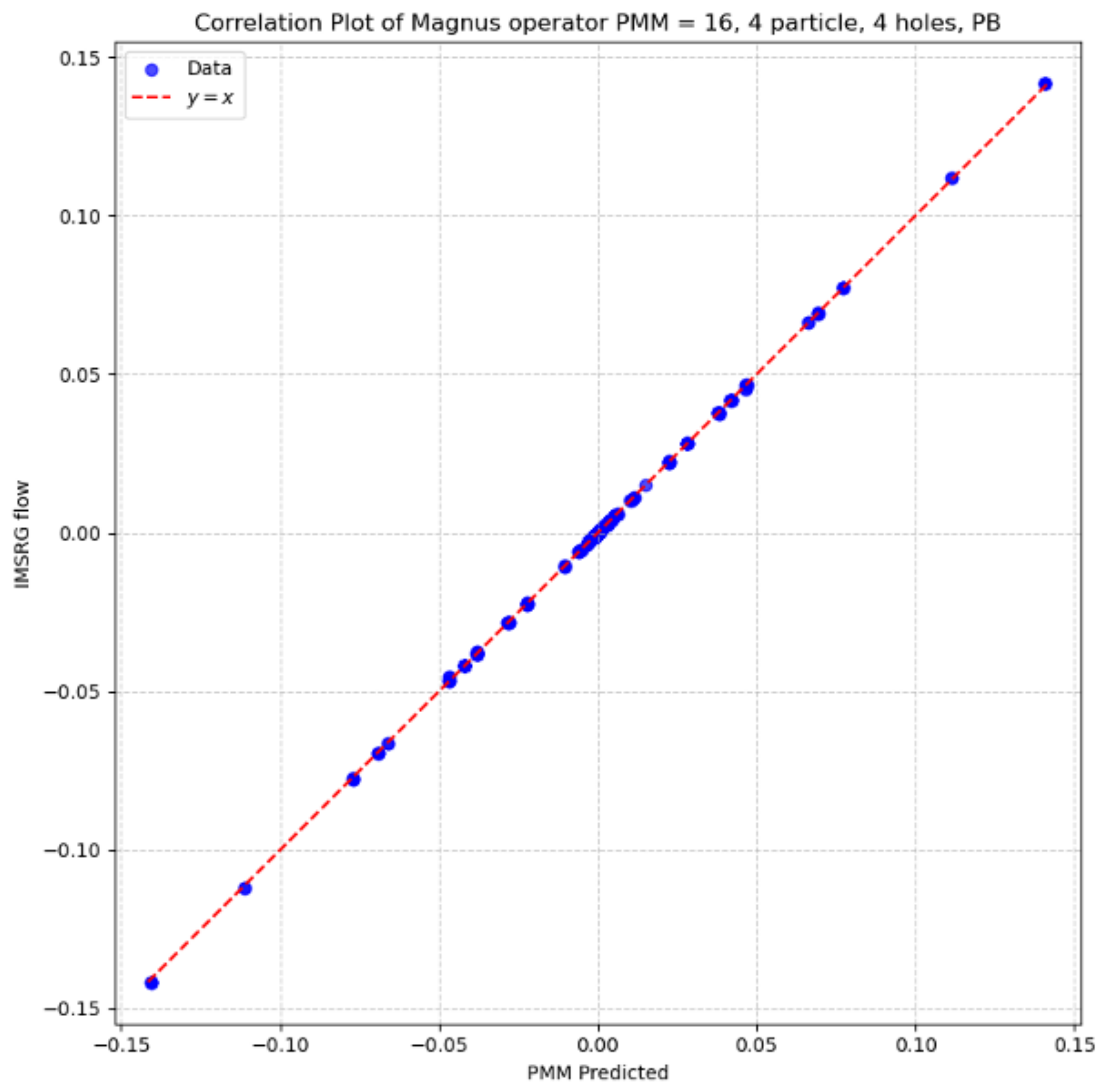


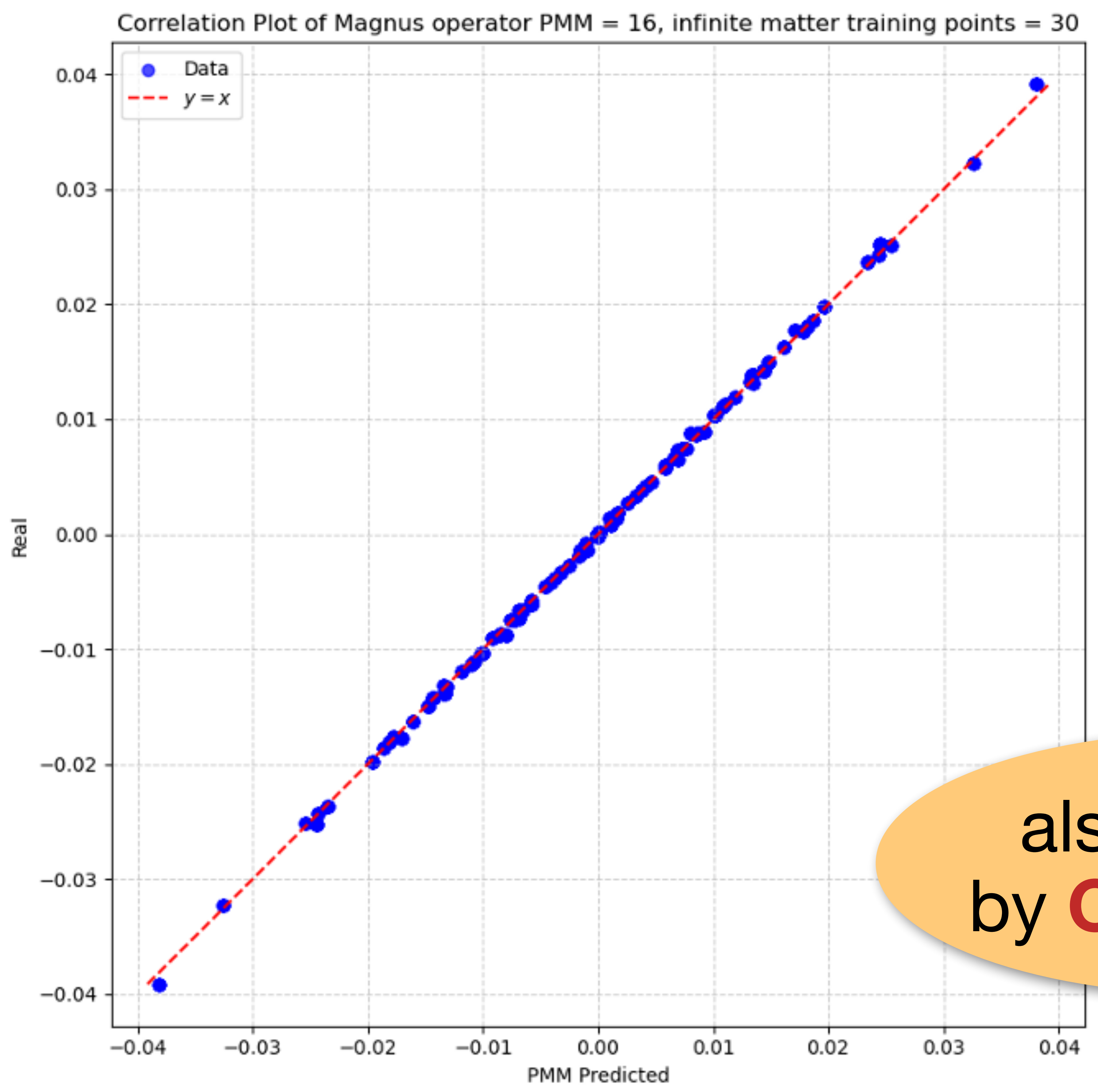
(ambitious) goal: emulate
full $H(s)$ or $\Omega(s)$ from snapshots
(O(10-100M) coefficients)

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

Parametric Matrix Models

B. Clark et al., in progress





also see talk by **C. Drischler**

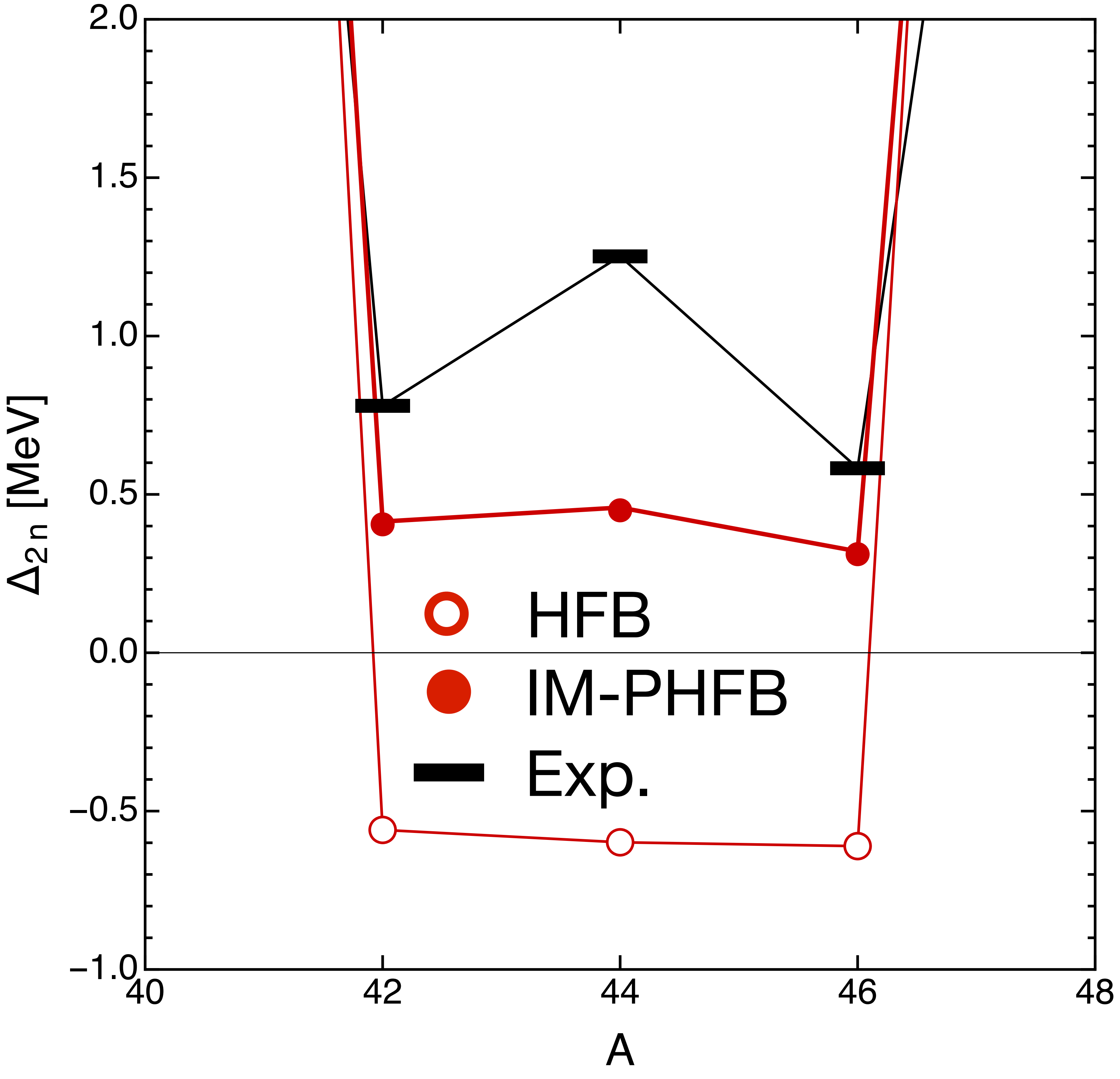
- DMD fails to emulate $\Omega(s)$ unless training is done at large s, **but PMMs work**
- **promising** first results for **parametric emulation** (schematic models, neutron matter @N3LO)

Epilogue

Questions, Thoughts, Caveats

- pragmatic perspective: experimental impact (currently) hinges on accuracy more so than precision (?)
  - fine to have accurate, fine-tuned interactions among or alongside families of non-implausible ones
- What observables should we get right **first**?
  - **Is that even the right question to ask?**
  - phase shifts within truncation uncertainties (non-collective)
  - beta decays: non-collective, expansion impacted by symmetry, …
  - **collectivity not fully controlled in medium-mass & heavy nuclei**
- **scales of A-body system may not cleanly separate few-/many-body physics**
  - related to previous item - scales associated with emerging collectivity
  - we conflate them if we use input from many-body system and truncated many-body methods (model space, many-body expansion) - **need to be careful**

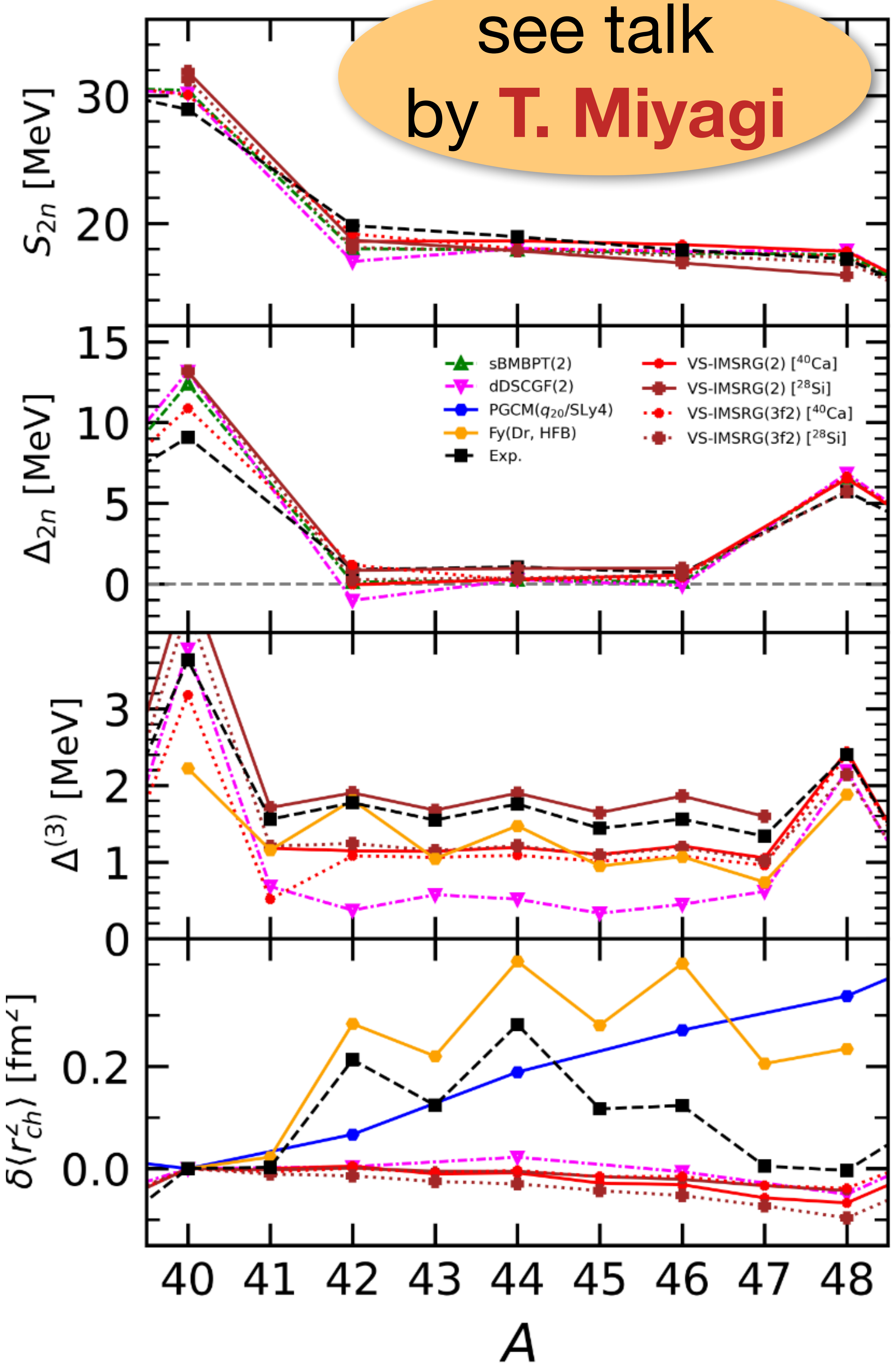
Questions, Thoughts, Caveats



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

also cf. A. Scalesi et al., EPJA **60**, 209 (2024)

see talk by **T. Miyagi**

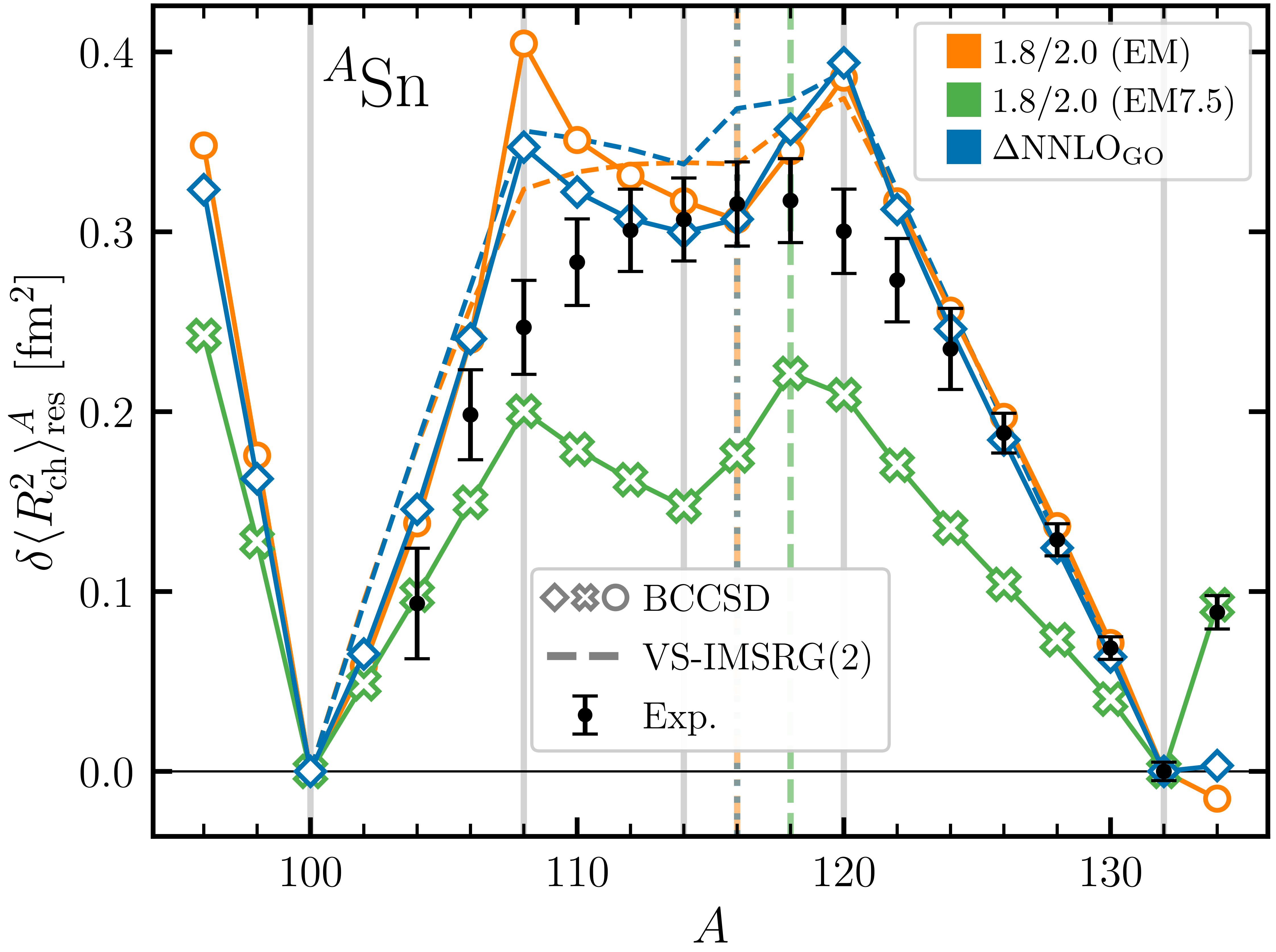


Calcium chain:
Current **(truncated!)** many-body methods **miss trends** in

- "pairing gap" / three-point energy diffs.
- charge radii (inverted parabola)
- B(E2)s **(not shown)**
- **points to collective correlations**

Questions, Thoughts, Caveats

P. Demol et al., arXiv:2602.22030



Similar features are seen in heavier nuclei, e.g., tin chain

- artificial features (shell structure exaggerated/pairing hindered?)
- EM7.5 produces increase in charge radius in ^{134}Sn…
- … but by "warping" the shell structure, as shown by Demol et al.

What's Next?

- **improved truncations:** (MR-)IMSRG(3) + factorized approximations, tailored operator bases
- several hybrid approaches: IM-GCM, IM-NCSM, IM-DMRG / VS-DMRG, …
- **(MR-)Equation of Motion IMSRG**
  - replicating closed-shell results (EM & charge changing) of Parzuchowski et al. with new code
  - response functions (incl. Lorentz integral transform)
  - next: correlated reference states, particle attachment/removal
- **finite temperature**
- **model reduction, compression & tensor factorization for IMSRG, EOM & IM-GCM**
  - **DMD and PMM emulators for uncertainty quantification / sensitivity analysis**
- **applications**
  - IM-GCM (+enhancements) for multiple experiments
  - nuclear observables for BSM physics (beta decays for CKM unitarity, Schiff moments, …)

Acknowledgments

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S. König
North Carolina State University

K. Fossez, A. Sedhirovic
Florida State University

and many more…

Thank you for your attention!

NUCLEI
Nuclear Computational Low-Energy Initiative

@NDB

NTNP Topical Collaboration

NERSC

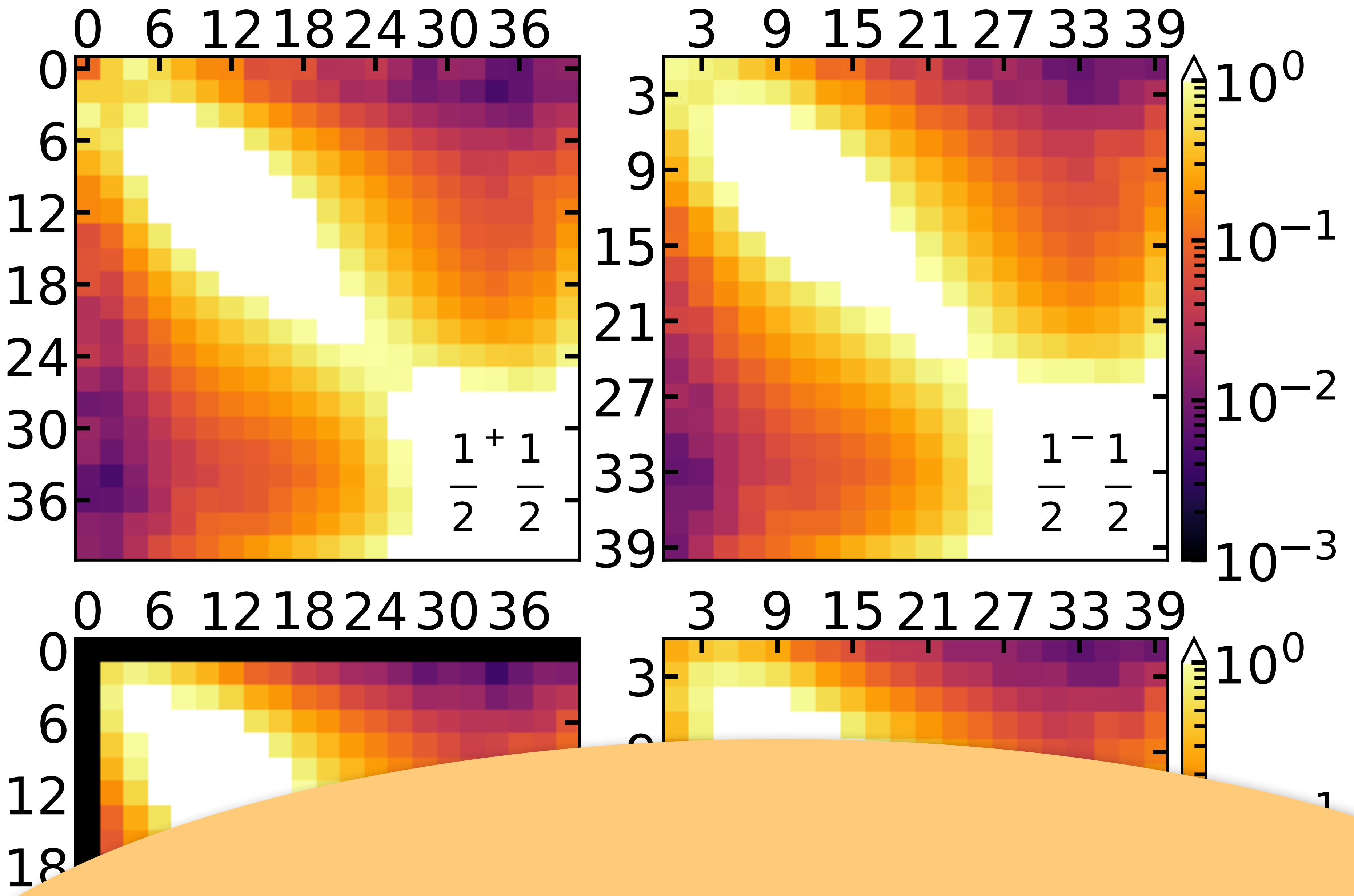
ICER

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

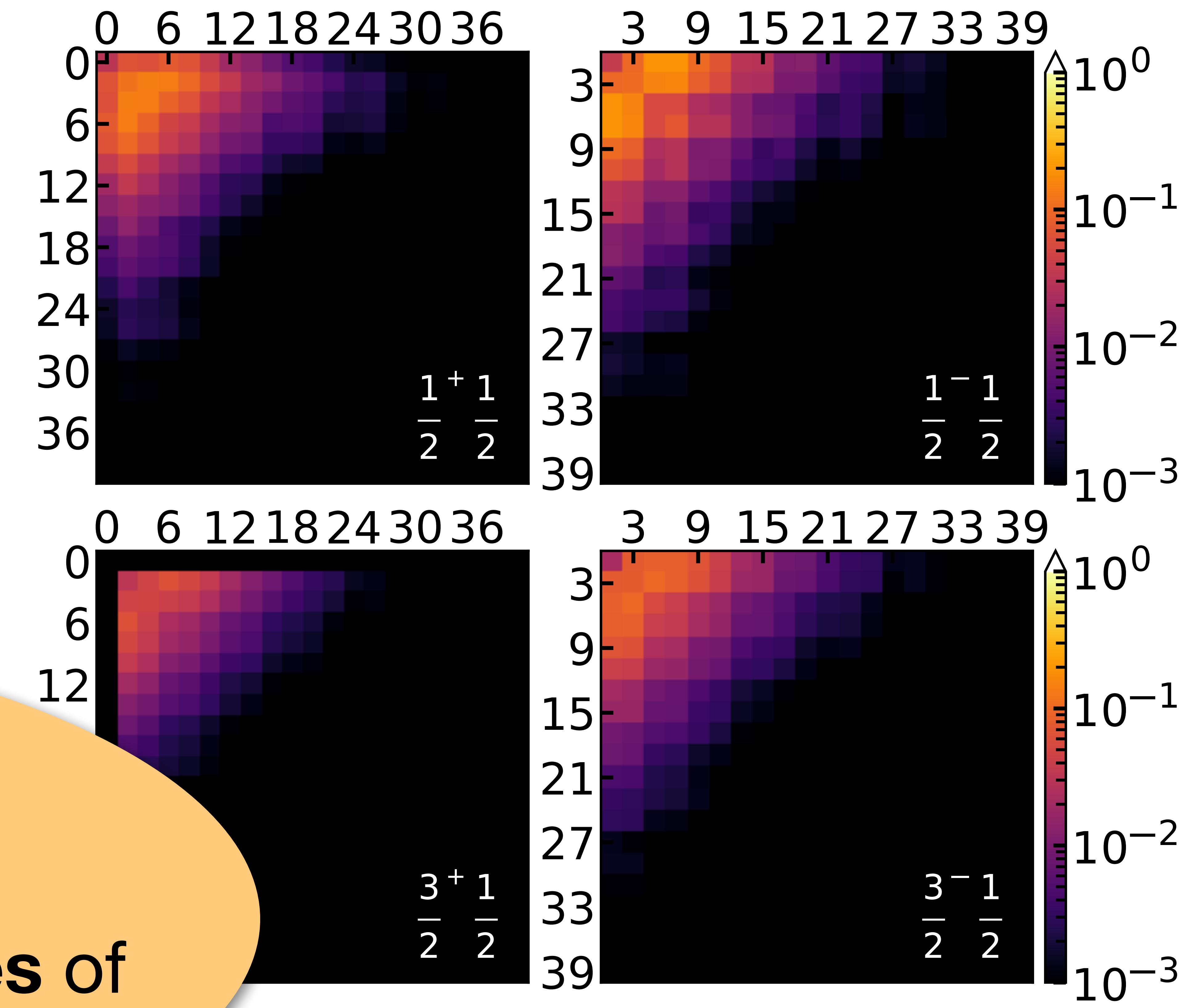
Supplements

Questions, Thoughts, Caveats

$$|\langle EJ^\pi T | V_{2\to3} | E'J^\pi T\rangle|$$



$$|\langle EJ^\pi T | V_{3\to3} | E'J^\pi T\rangle|$$



Even if **full RG invariance is elusive**: can we use **(S)RG diagnostics to understand features** of magic / pragmatic interactions?

Free-space SRG

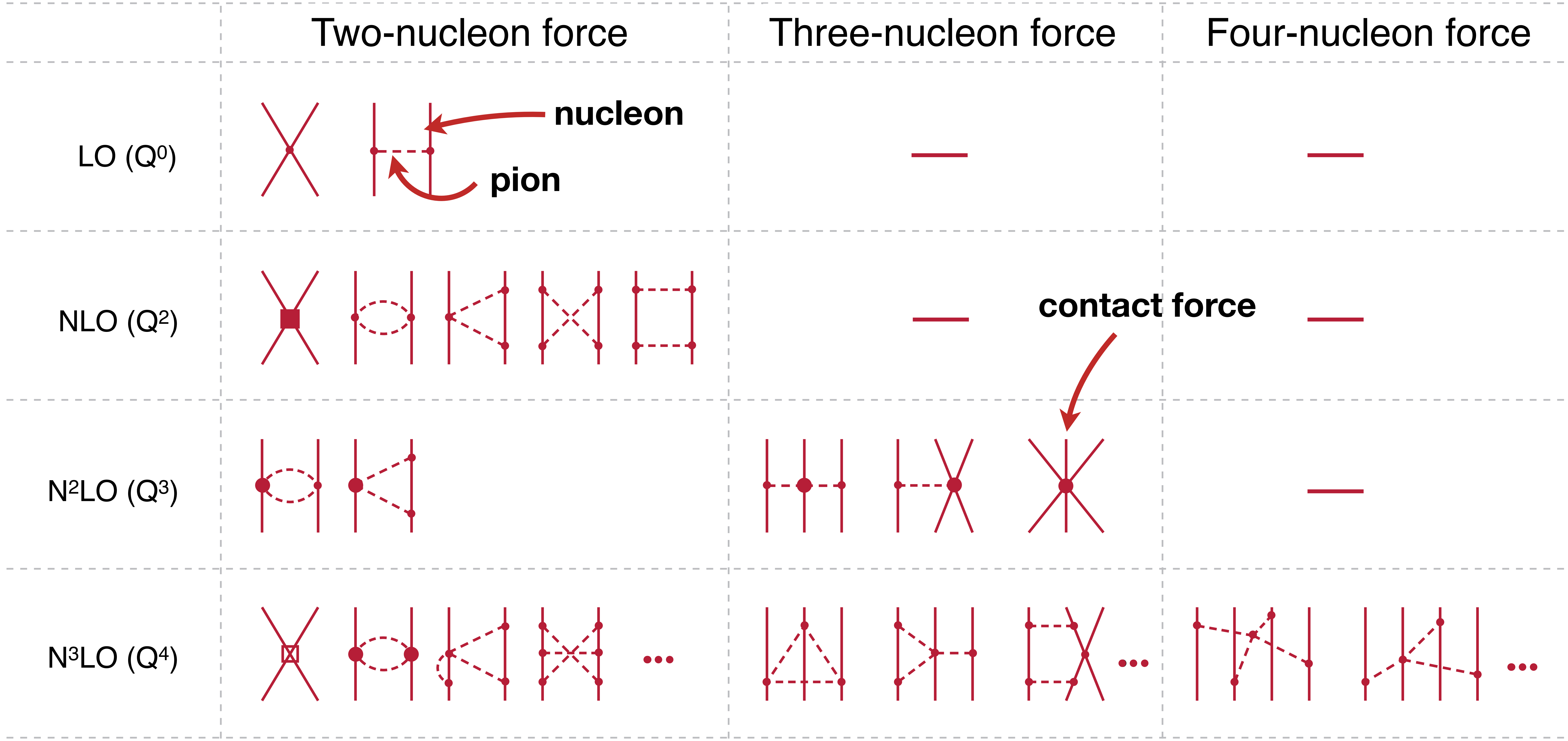
$V_{2\to3}$

- contributions from **all energies** (up to model space truncation)
- **dominant diagonal**
- **different from N²LO topologies**

$V_{3\to3}$

- shape is similar to initial 3N force
- **weak** compared to $V_{2\to3}$

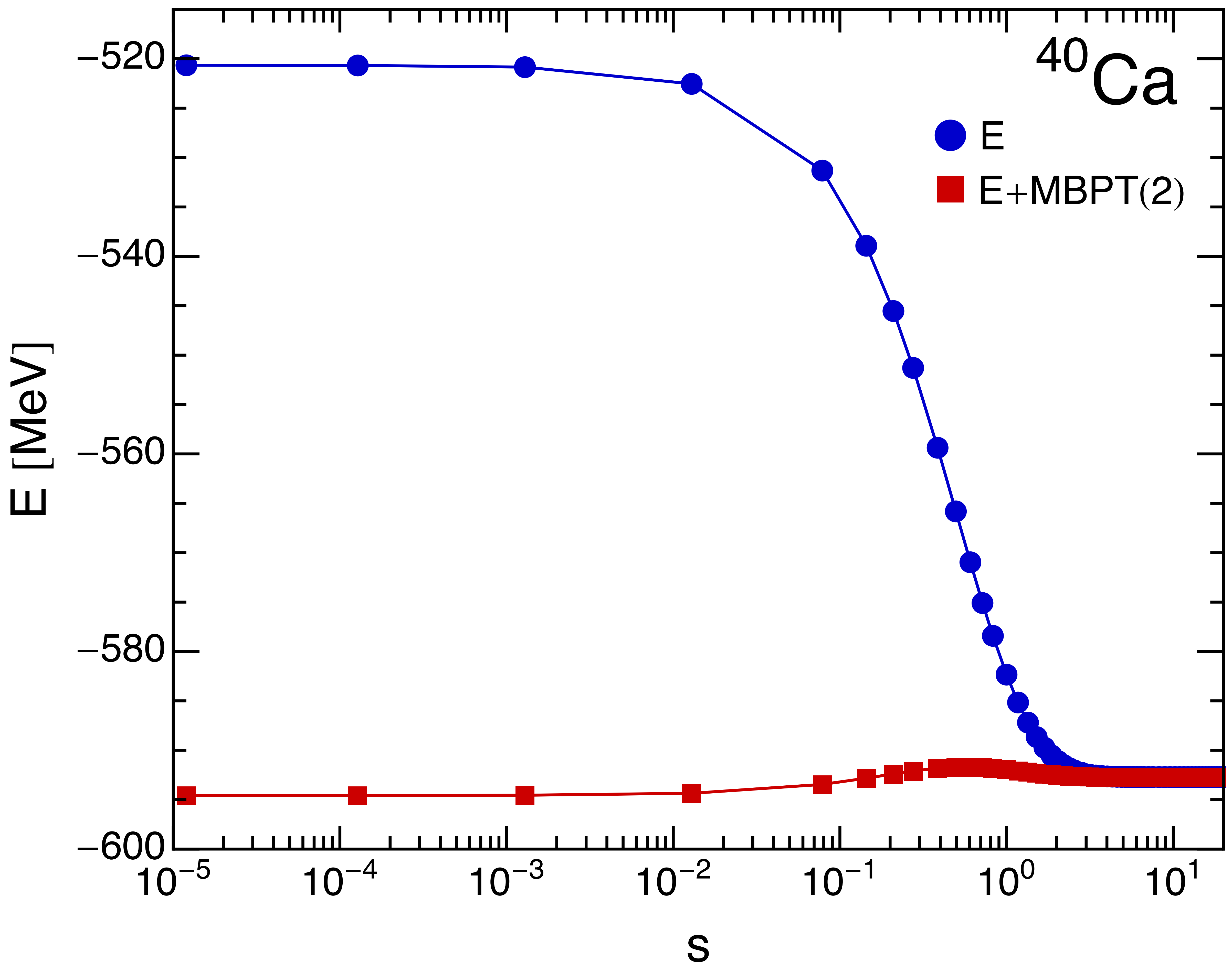
Chiral Effective Field Theory

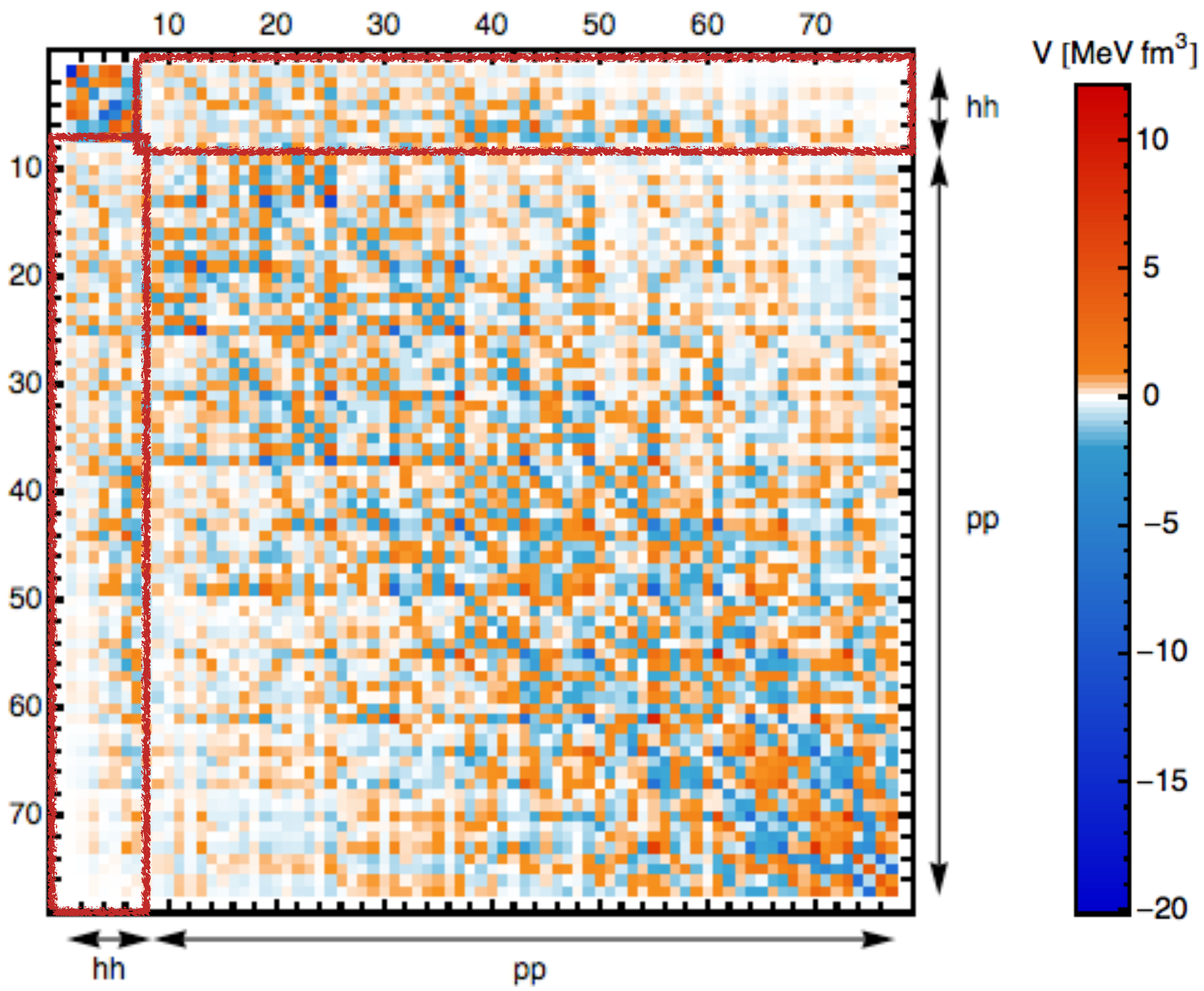


[figure by H. Krebs]

- 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

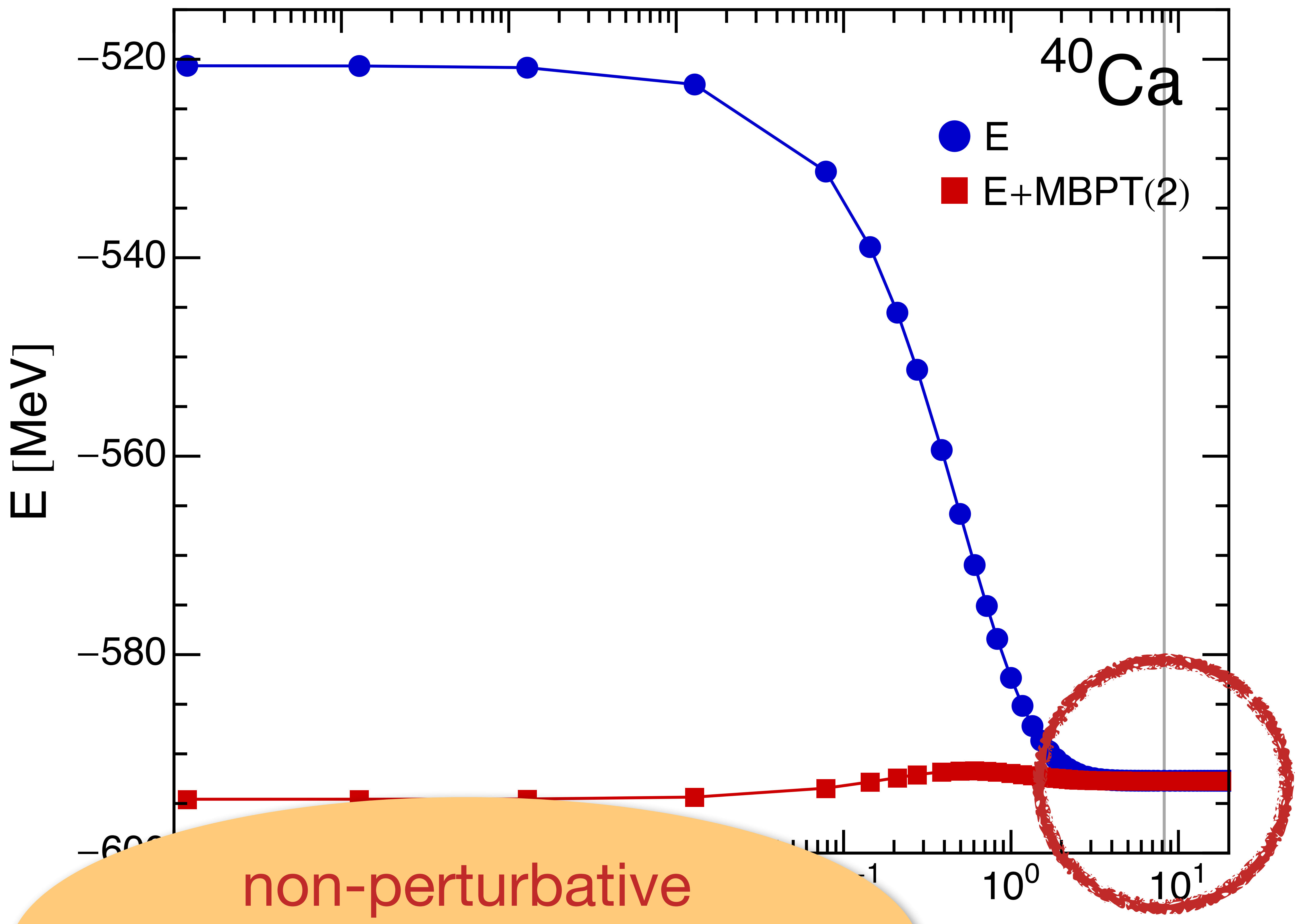
Decoupling

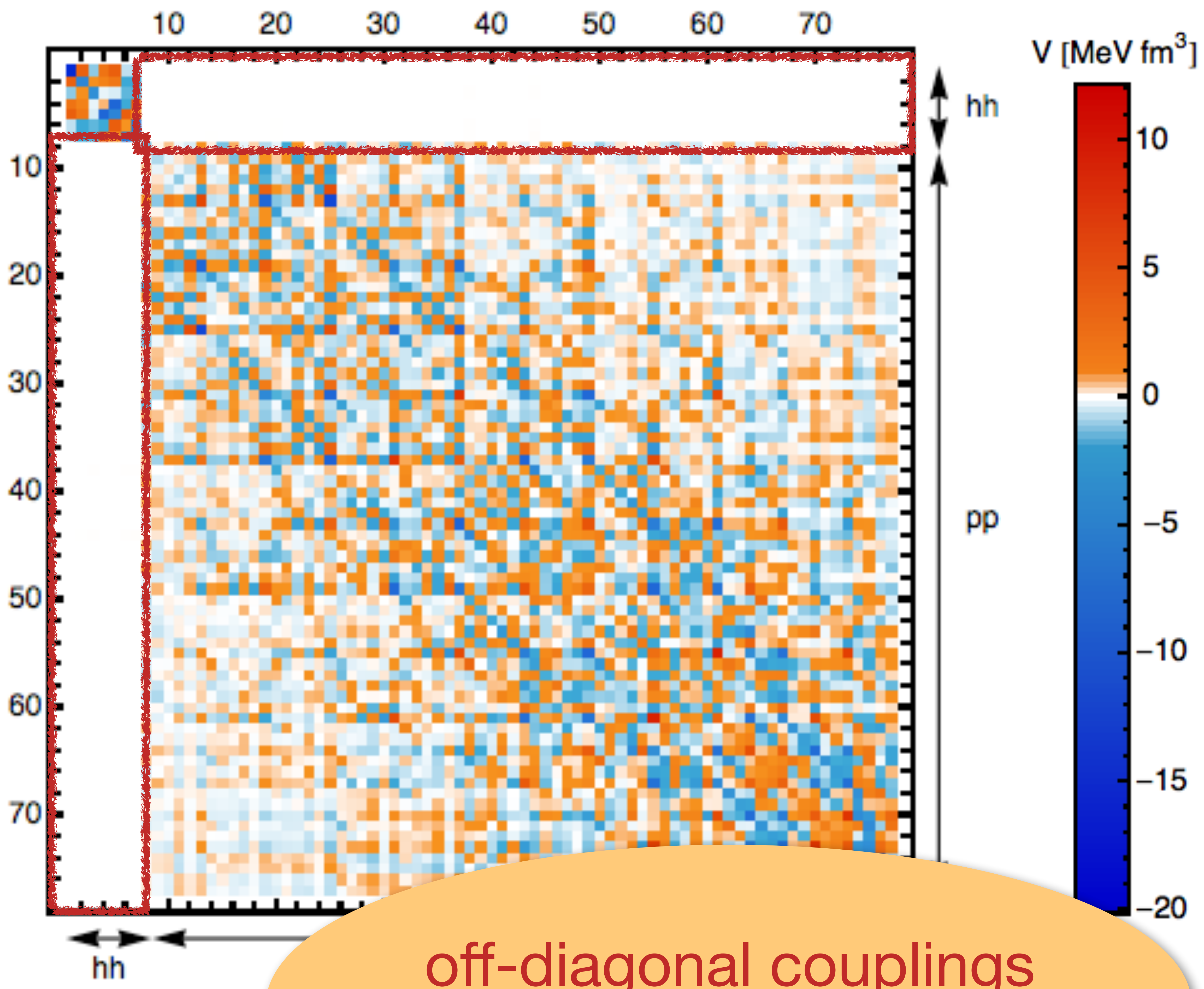




Entem-Machleidt N³LO, $\lambda = 2.0\,\mathrm{fm}^{-1}$, $e_{\mathrm{Max}} = 8$

Decoupling



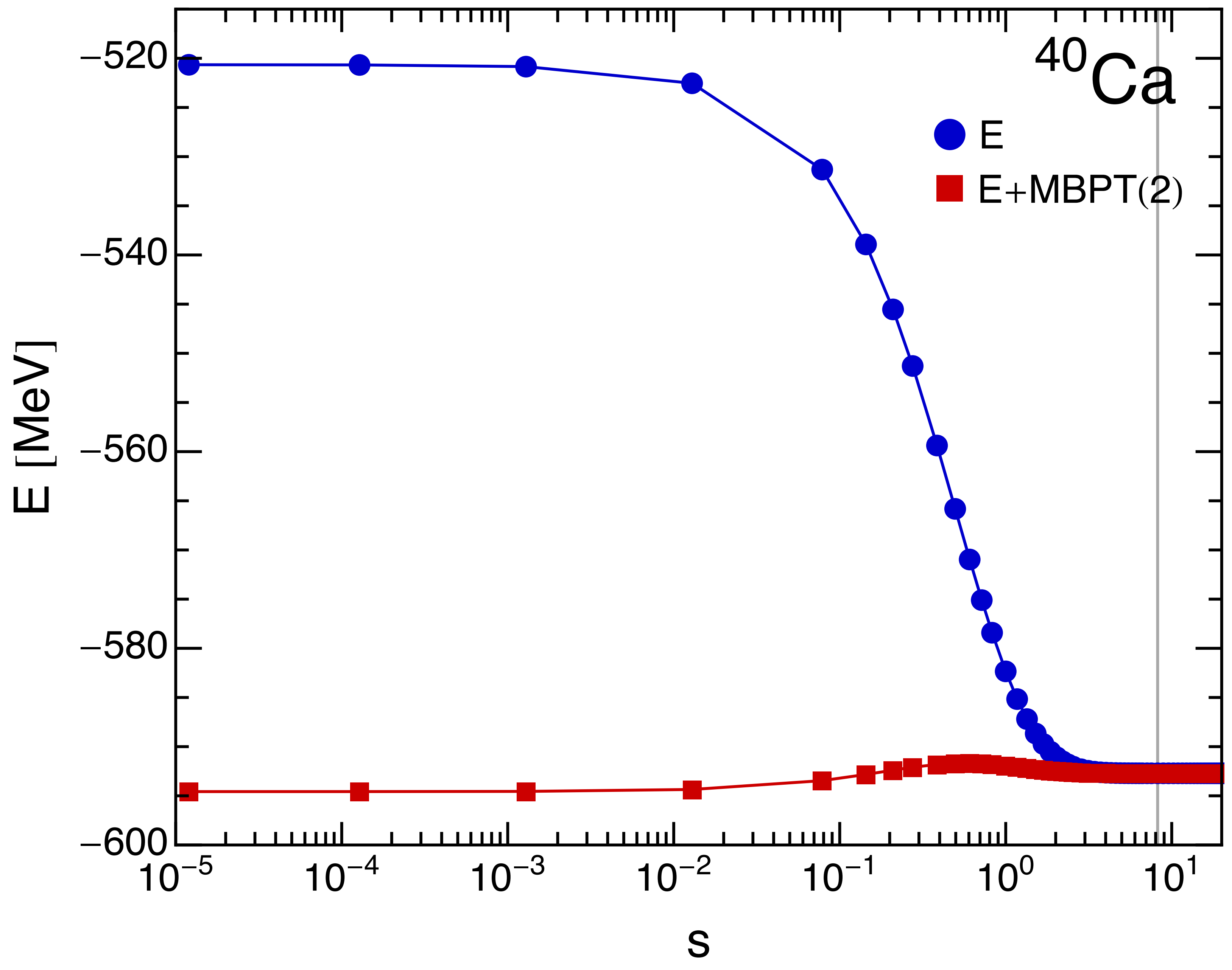


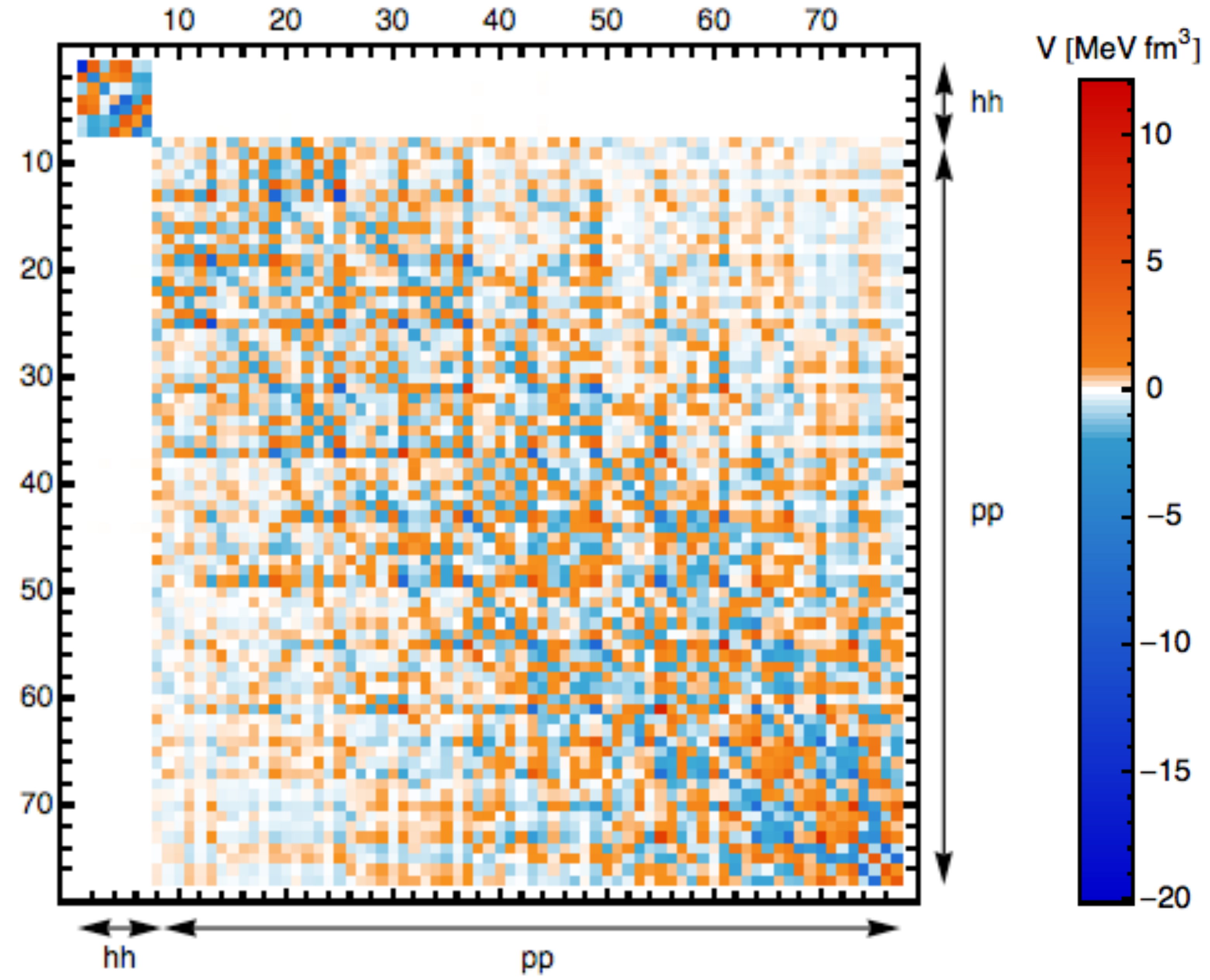
non-perturbative resummation of MBPT series **(correlations)**

Machleidt N³LO, $\lambda = 2.0\,\mathrm{fm}^{-1}$,

off-diagonal couplings are rapidly driven to zero

Decoupling





Entem-Machleidt N³LO, $\lambda = 2.0\,\mathrm{fm}^{-1}$, $e_{\mathrm{Max}} = 8$

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

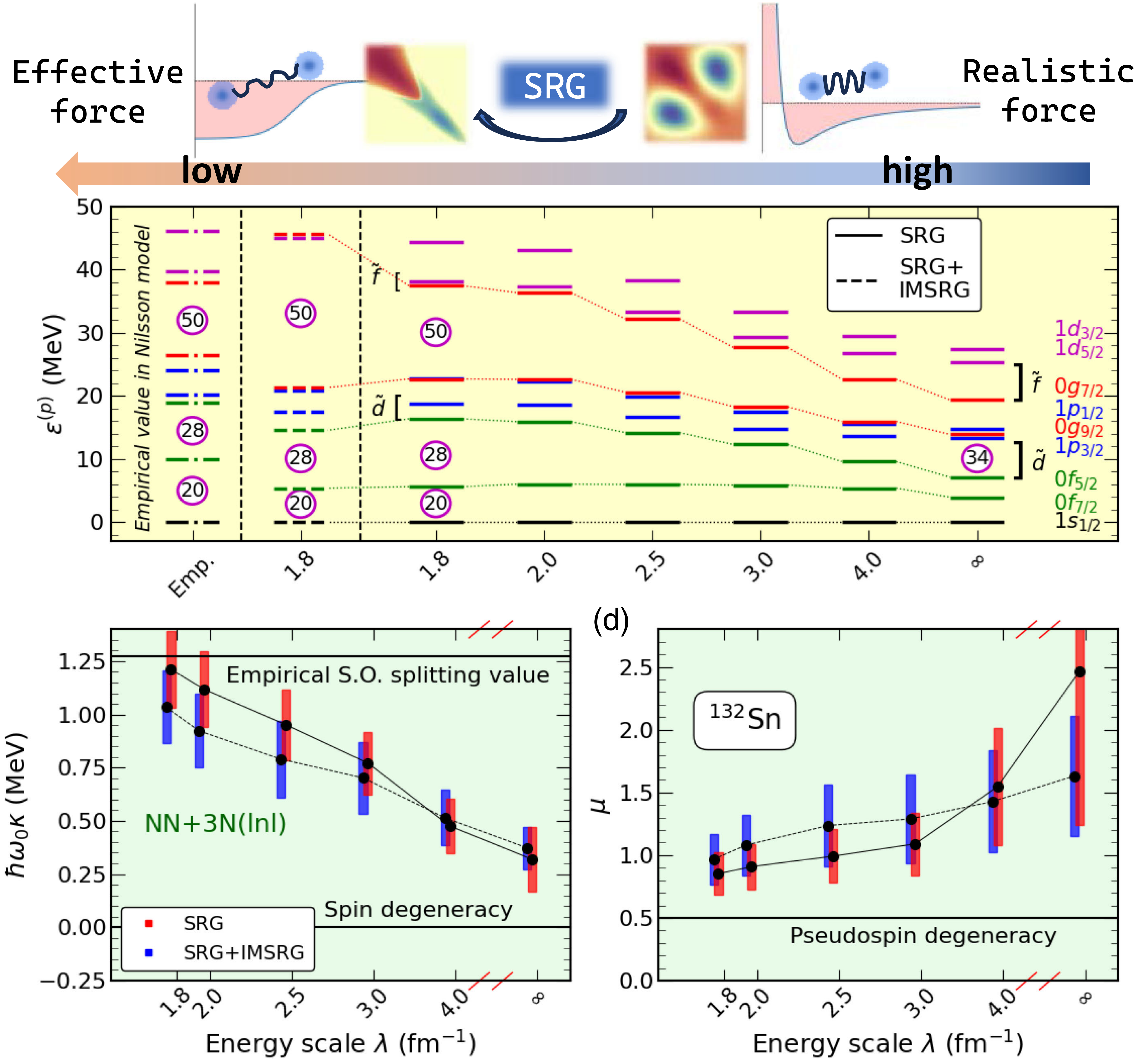
$$U(s)HU^{\dagger}(s)U(s)|\Psi_n\rangle = E_n U(s)|\Psi_n\rangle$$

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

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

Evolution of Effective Single-Particle Energies

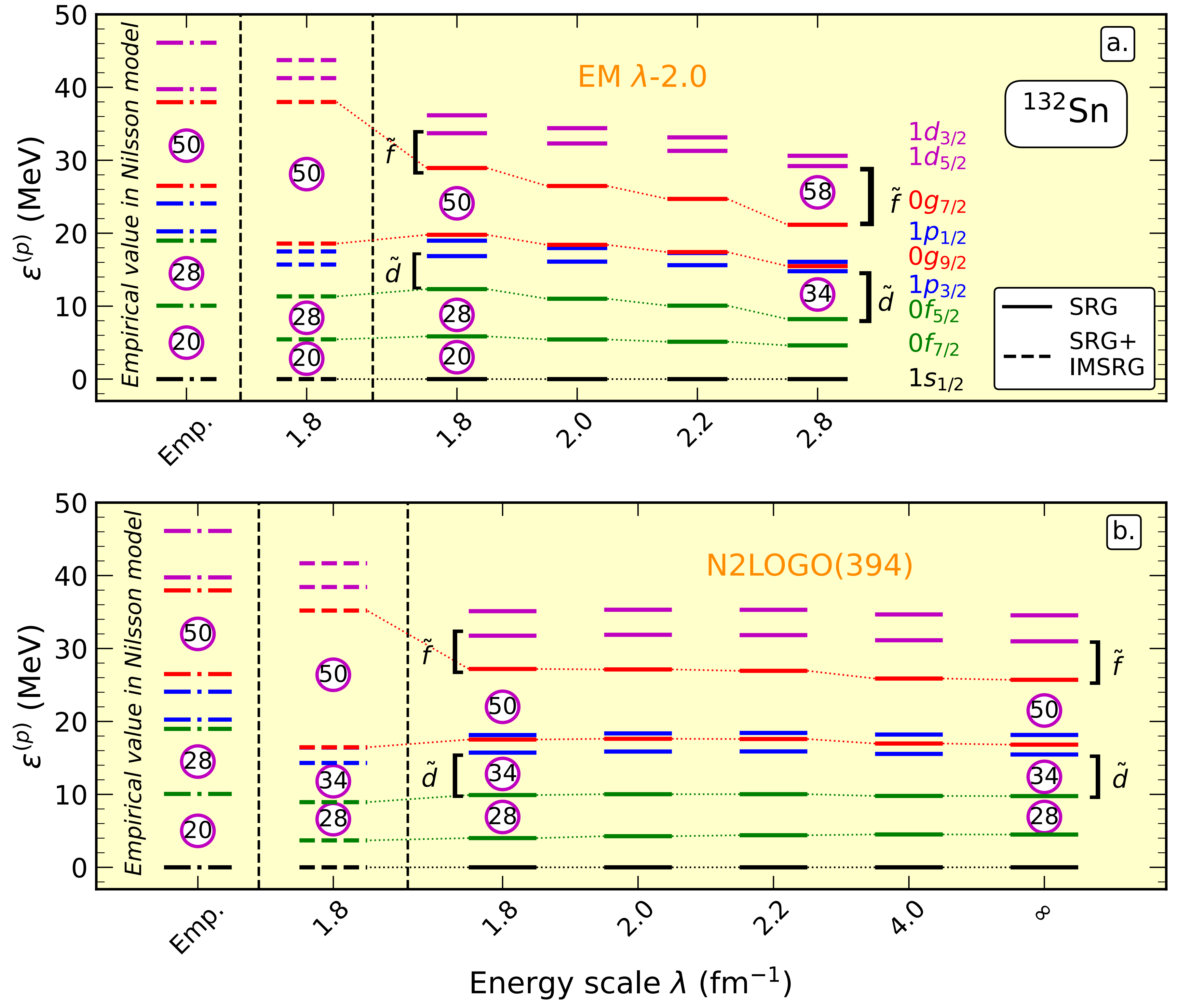
C. R. Ding et al., PRL 136, 052501 (2026)

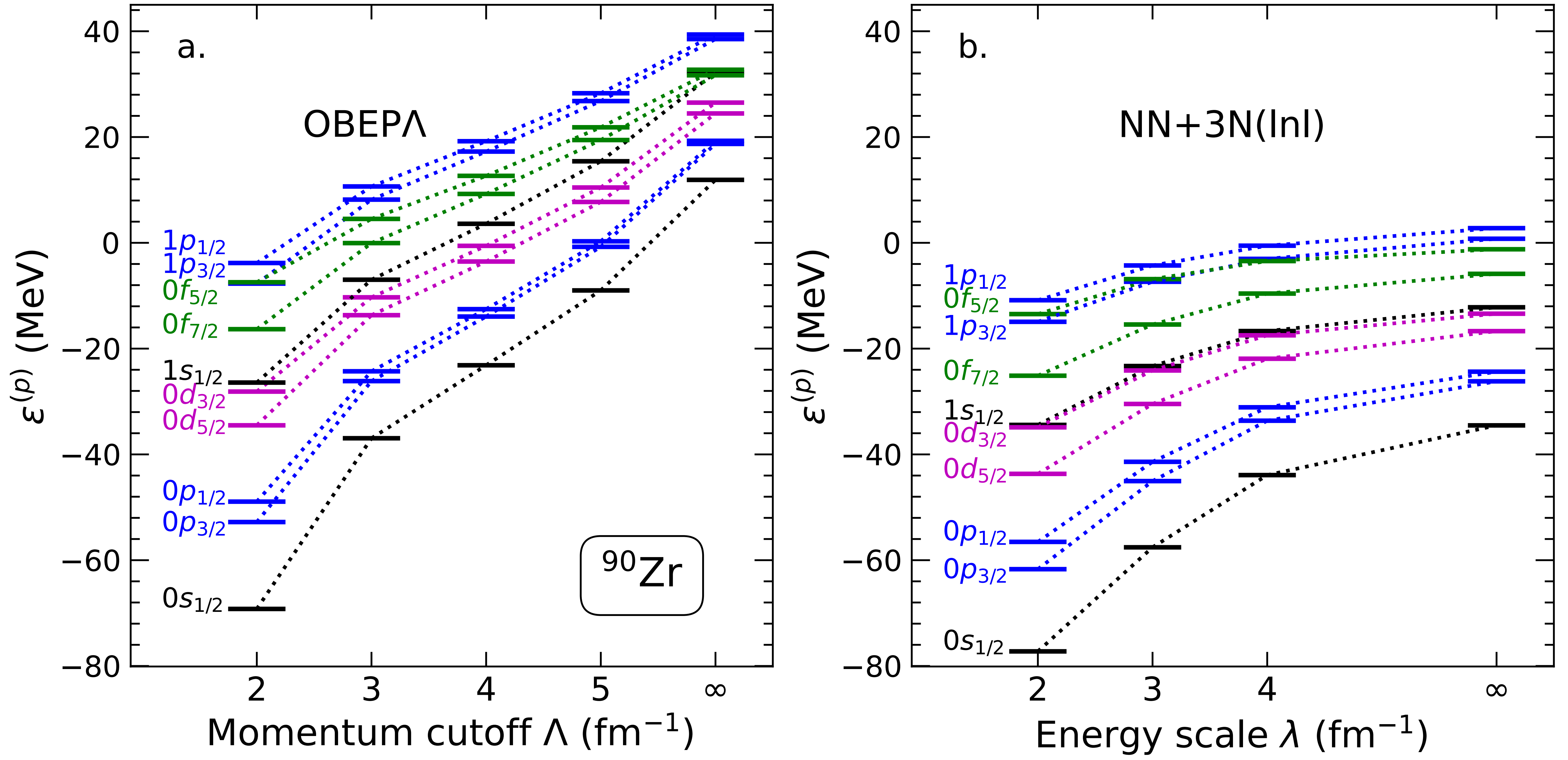


- **Mean-field / Shell model** is inherently a **low-momentum picture**
- empirical density functionals/ Shell model interactions are **“effective” parameterizations of low-resolution nuclear forces (+ correlations)**
- SRG + IMSRG can be used to **quantitatively bridge** high- and low-resolution descriptions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

Evolution of Effective Single-Particle Energies

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





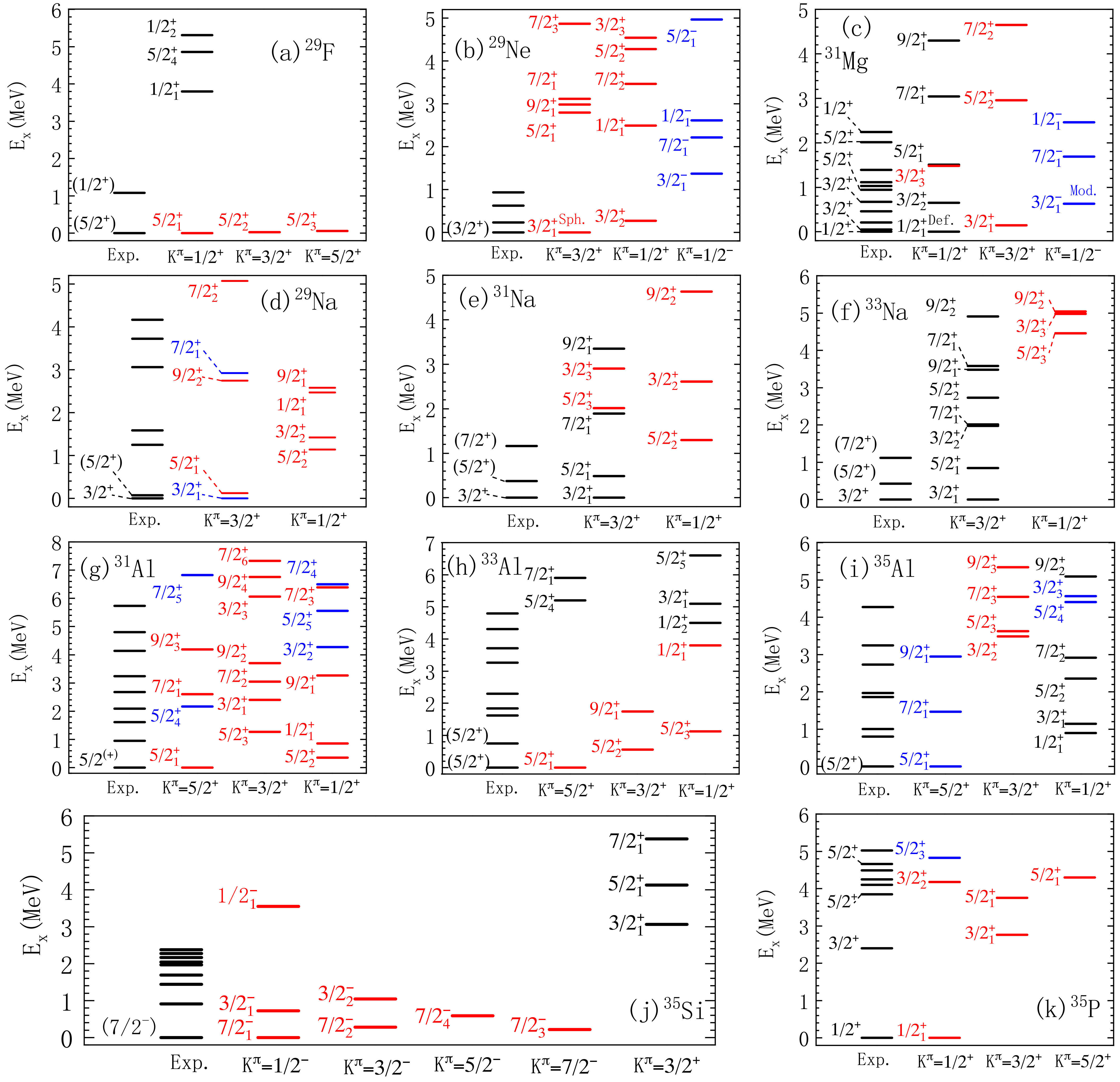
- **low-resolution interactions** already exhibit much o[…] **symmetries** at the mean-field level
- behavior is **consistent** in **non-relativistic and relativ**[…]

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: N=20 Island of Inversion Region

FRIB

E. F. Zhou et al., arXiv:2603.07363

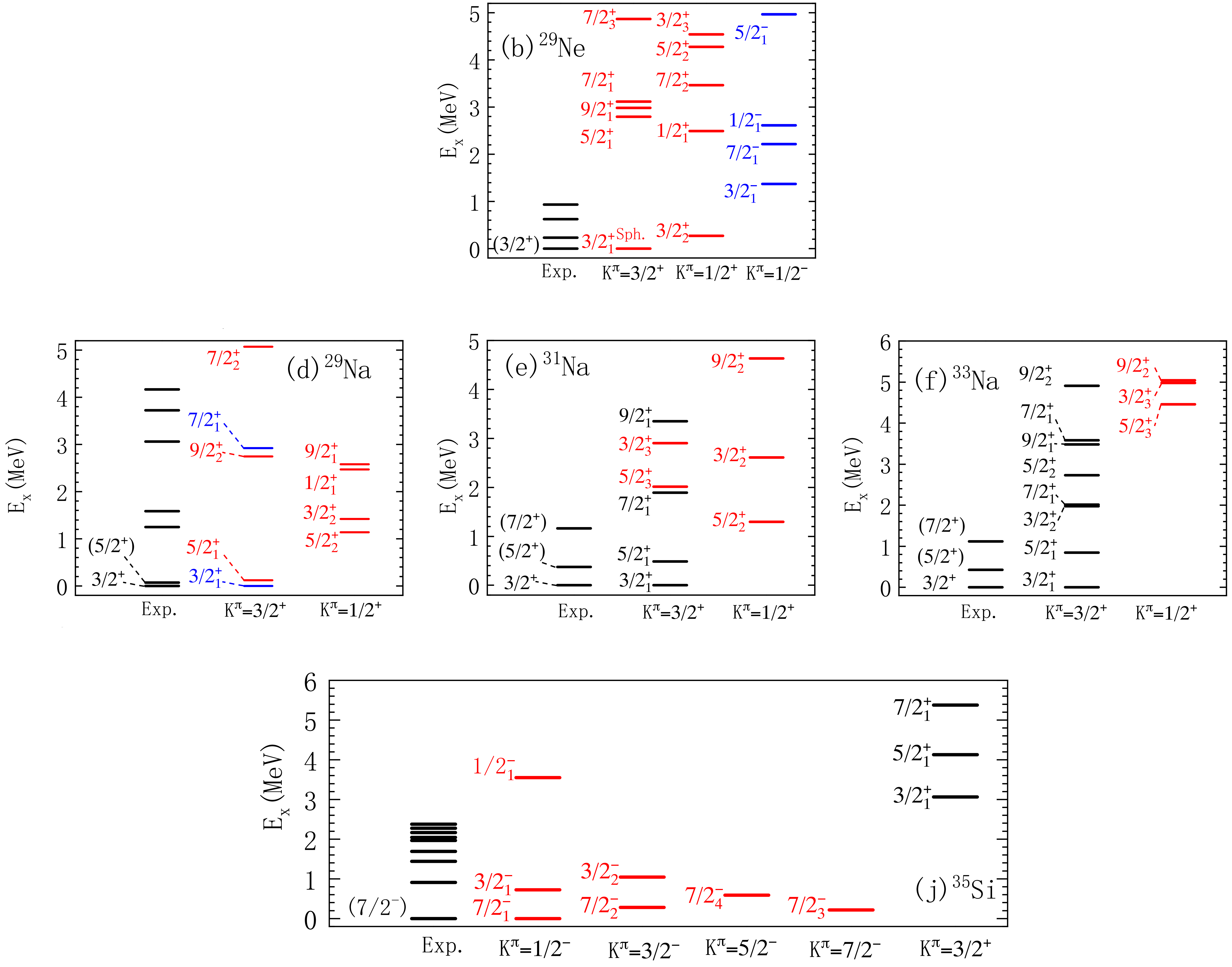


IM-GCM survey of the **island-of-inversion region**

- **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:2603.07363

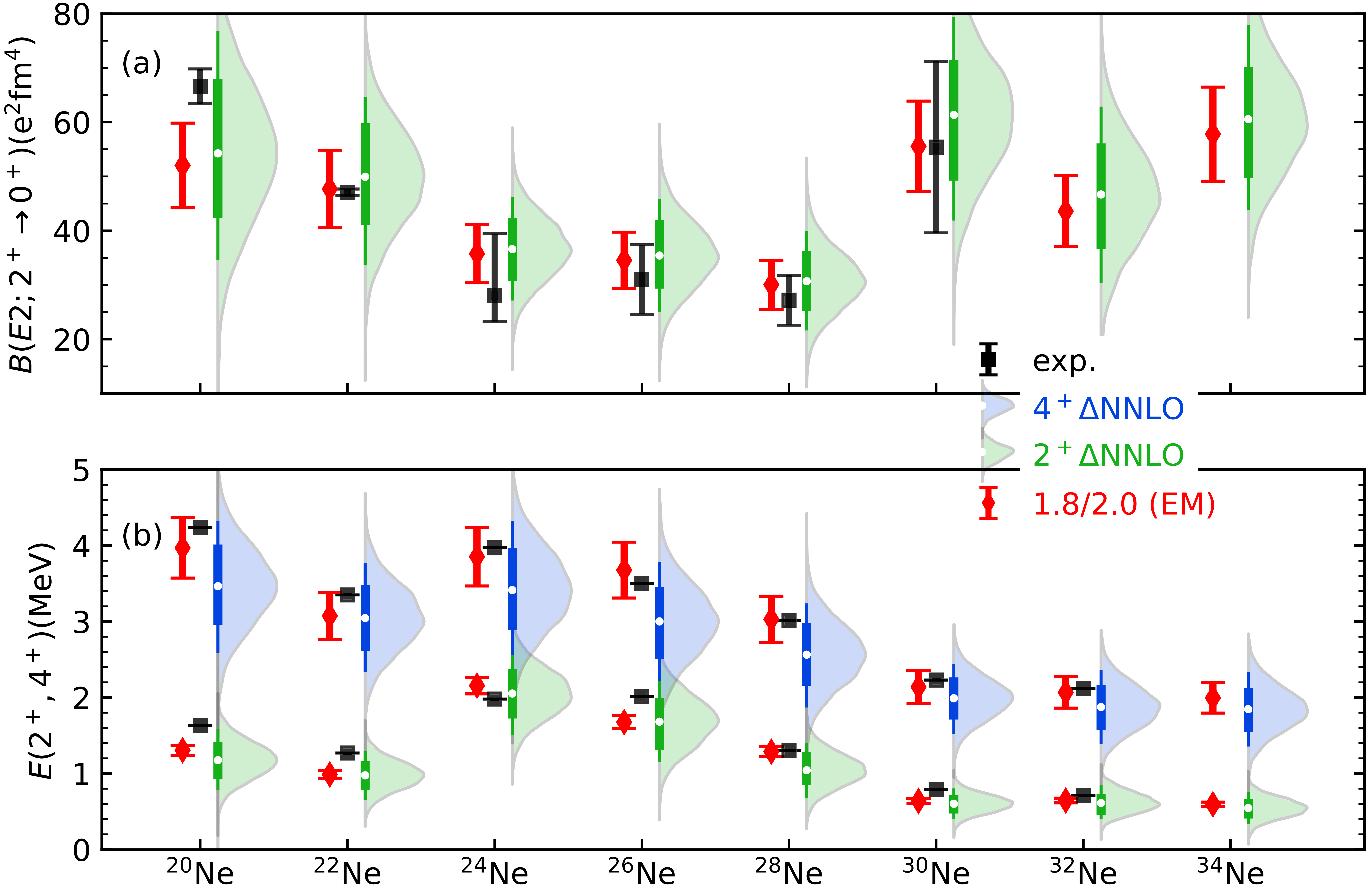


IM-GCM survey of the **island-of-inversion region**

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

AMP-CCSD: Ne, Na, Mg Isotopes

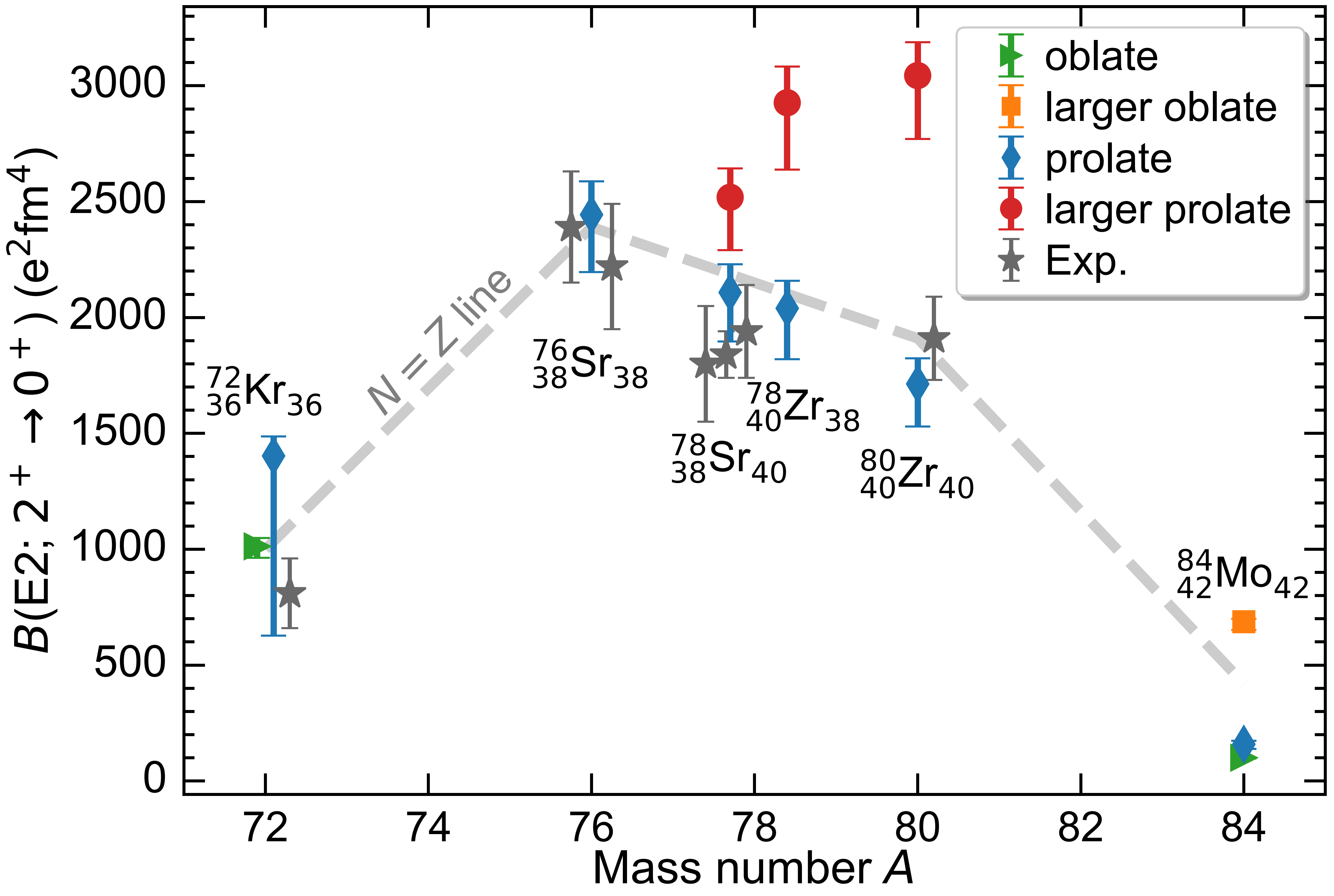
*Z. H. Sun et al., PRX **15**, 011028 (2025)*
Z. H. Sun et al., arXiv:2409.02279

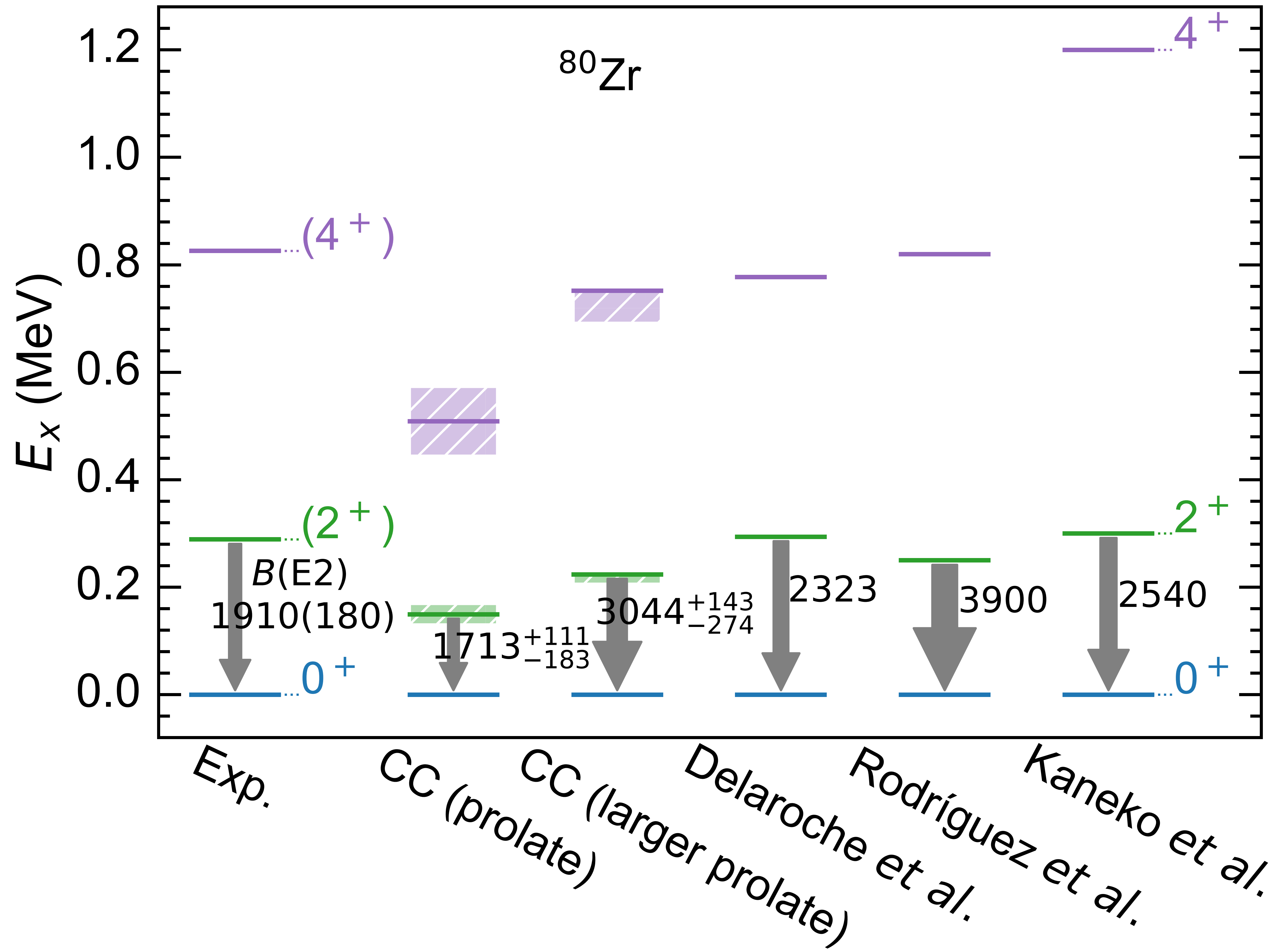


- AMP-CCSD for **even and odd Ne, Na, Mg** isotopes
- **emulators for UQ**
- rotational bands and $B(E2, 2^+ \to 0^+)$ values in **very good agreement** with data
- **consistent results** for EM1.8/2.0 and a family of 8000+ ΔN2LO interactions

AMP-CCSD: Z~80 Region

B.S. Hu et al., PRC **110**, L011302 (2024)

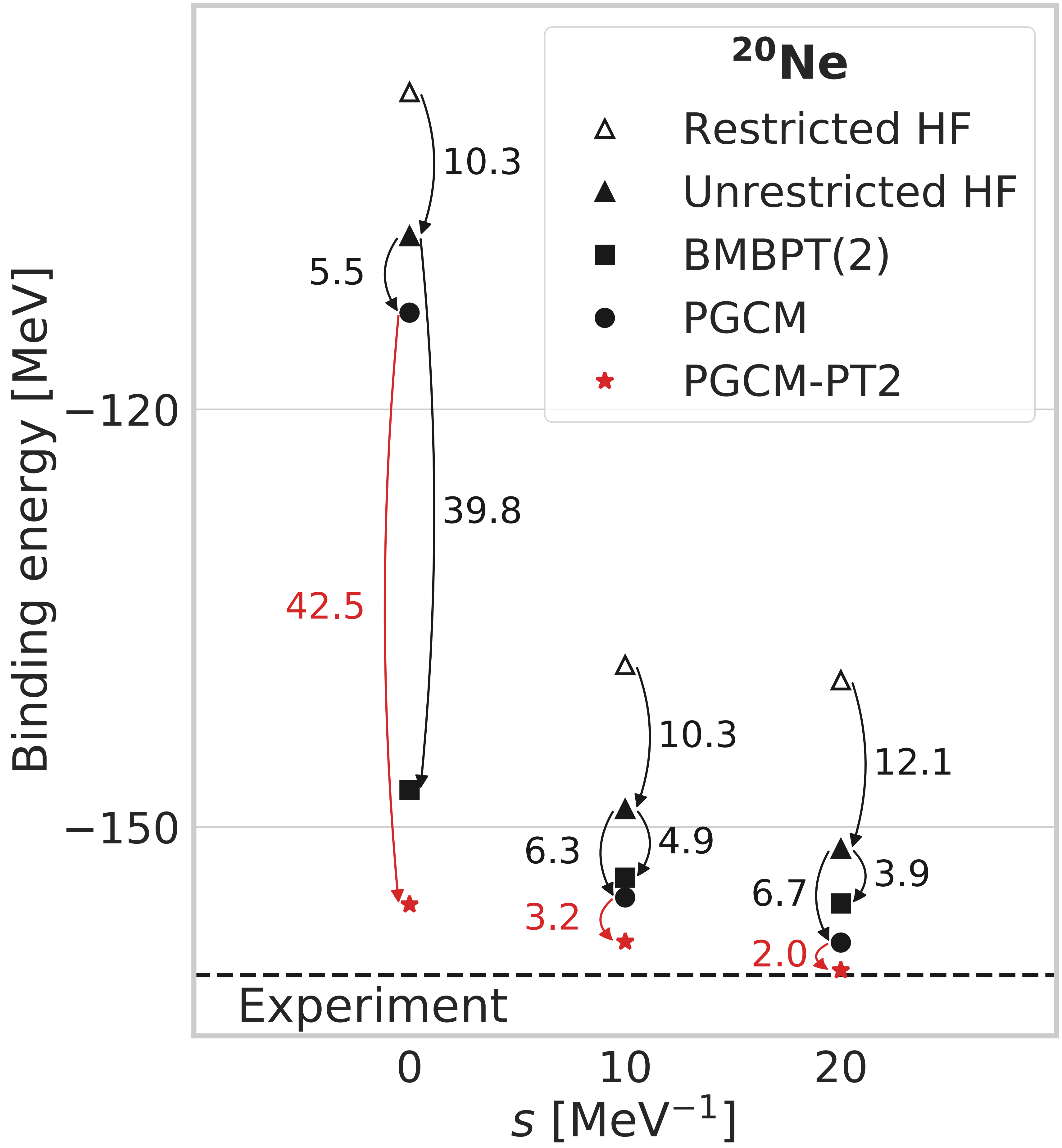


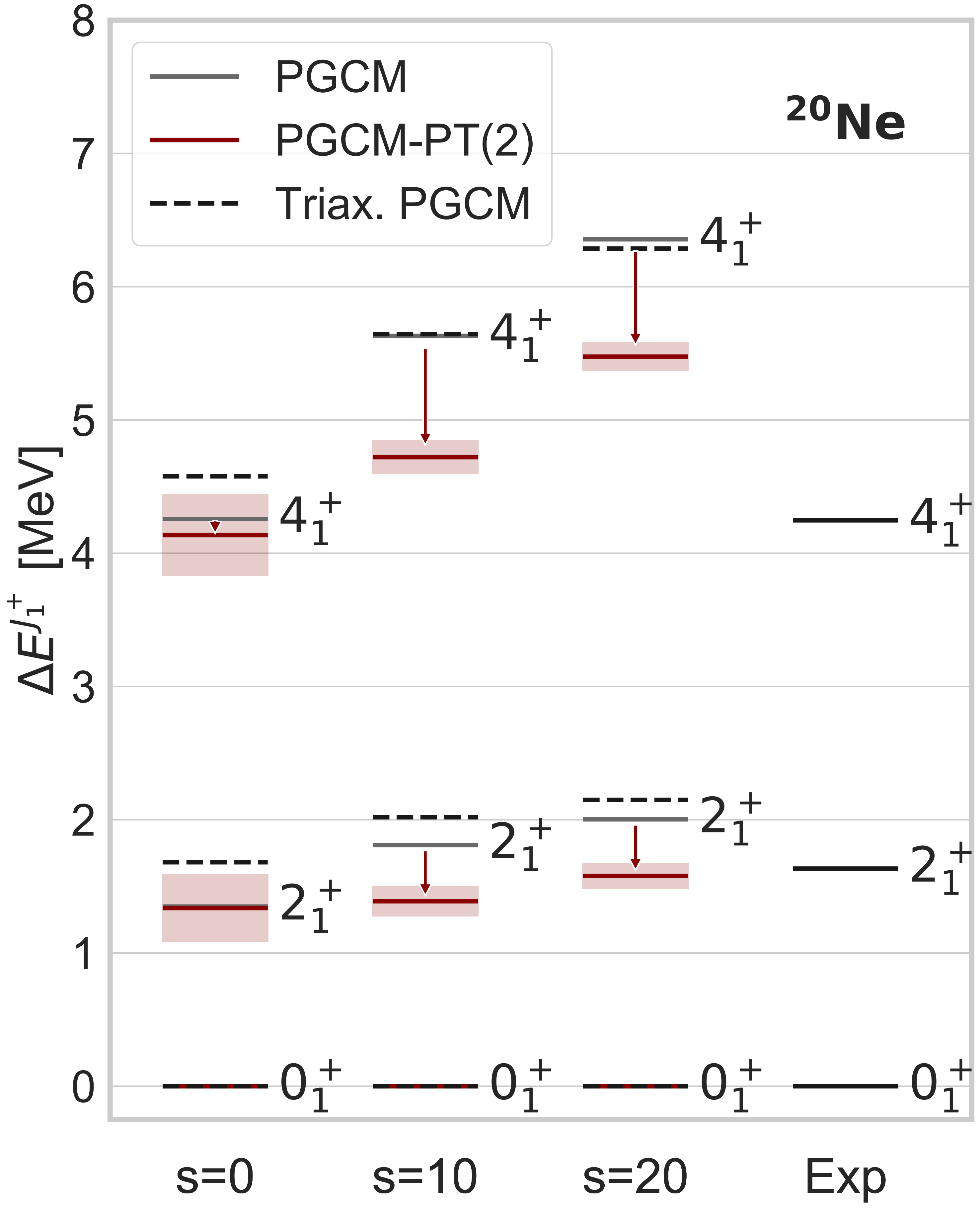


- *ab initio* calculations poised to offer insight into **rich shape coexistence phenomena** in N=Z nuclei near ^{80}Zr
- **challenges:** computational cost restricts model size, effects of **shape mixing**, …

IM-GCM: Reshuffling of Correlations

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

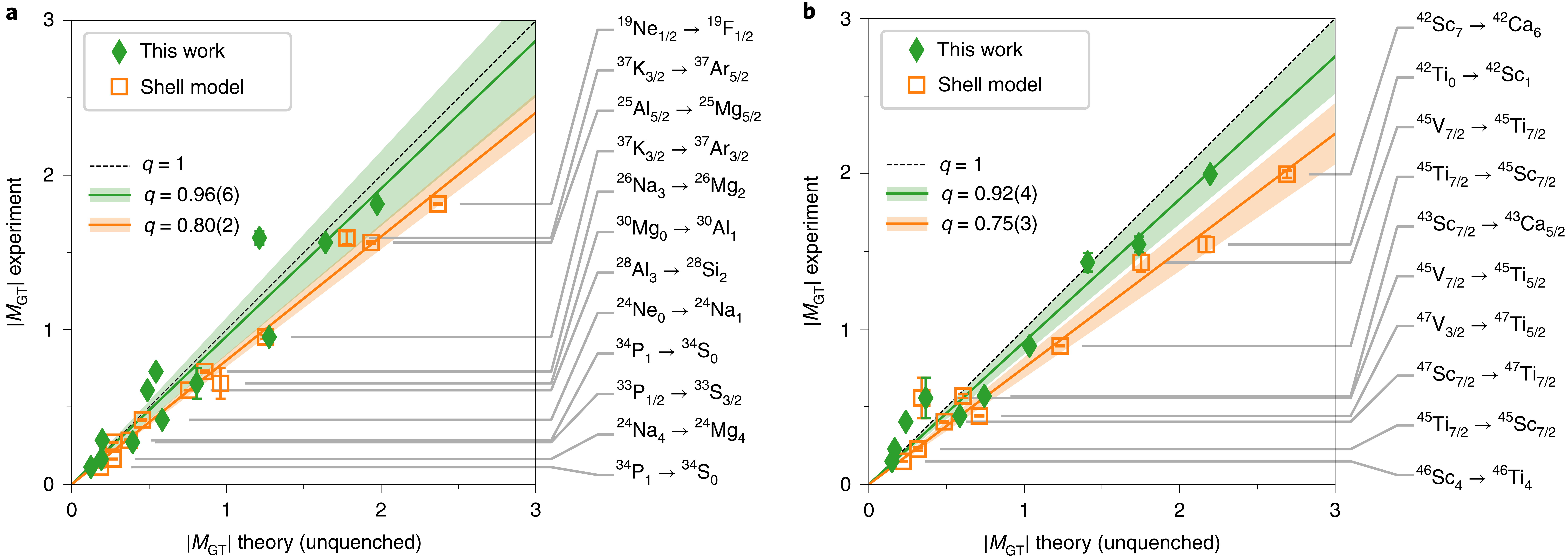




- s-dependence is a **built-in diagnostic tool** for IM-GCM **(not available in phenomenological GCM)**
  - if operator and wave function offer sufficient degrees of freedom, **evolution of observables is unitary**
- need **richer references and/or IMSRG(3)** for certain observables

Quenching of Gamow-Teller Decays

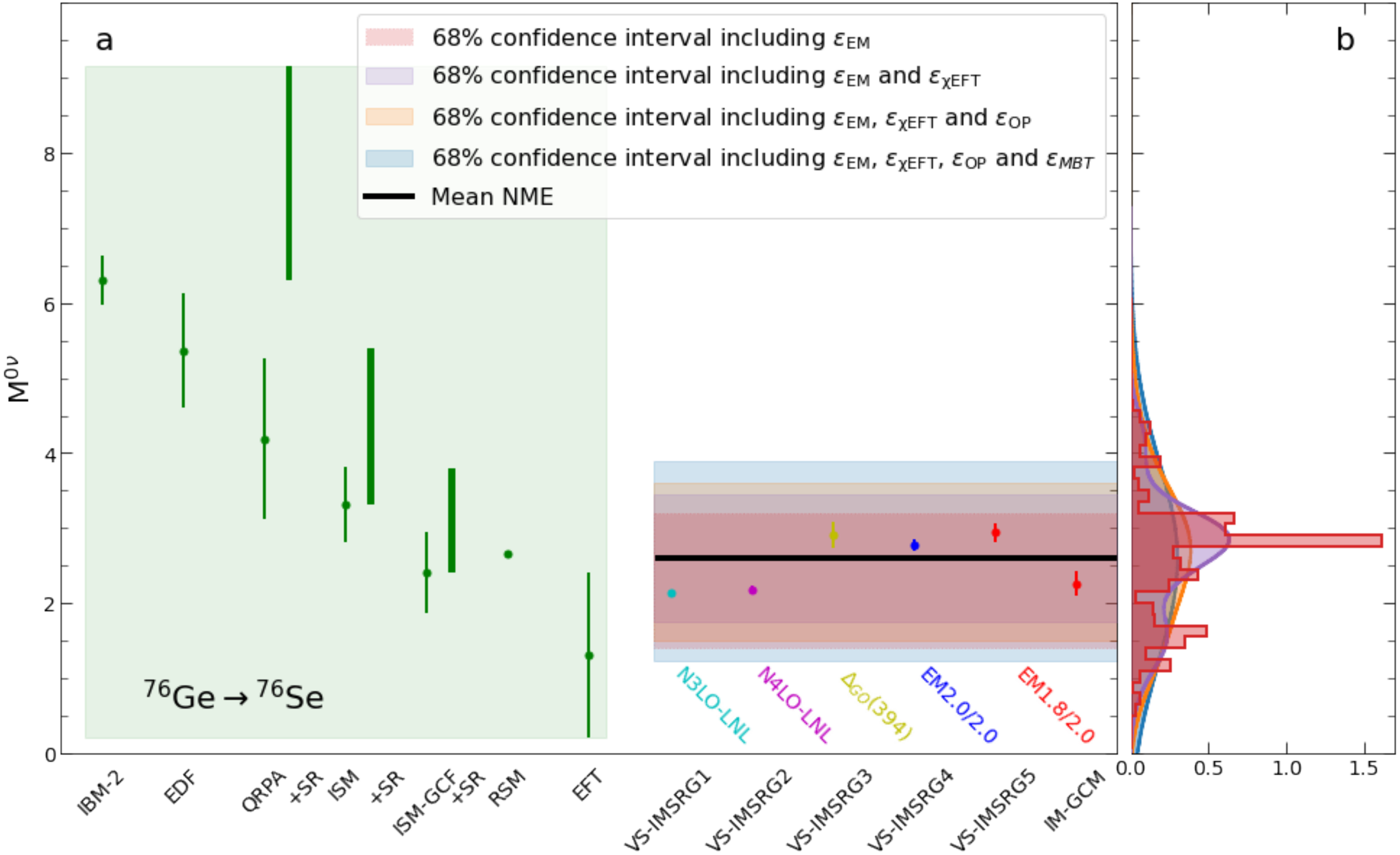
P. Gysbers et al., Nature Physics 15, 428 (2019)



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

^{76}Ge: Neutrinoless Double Beta Decay

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

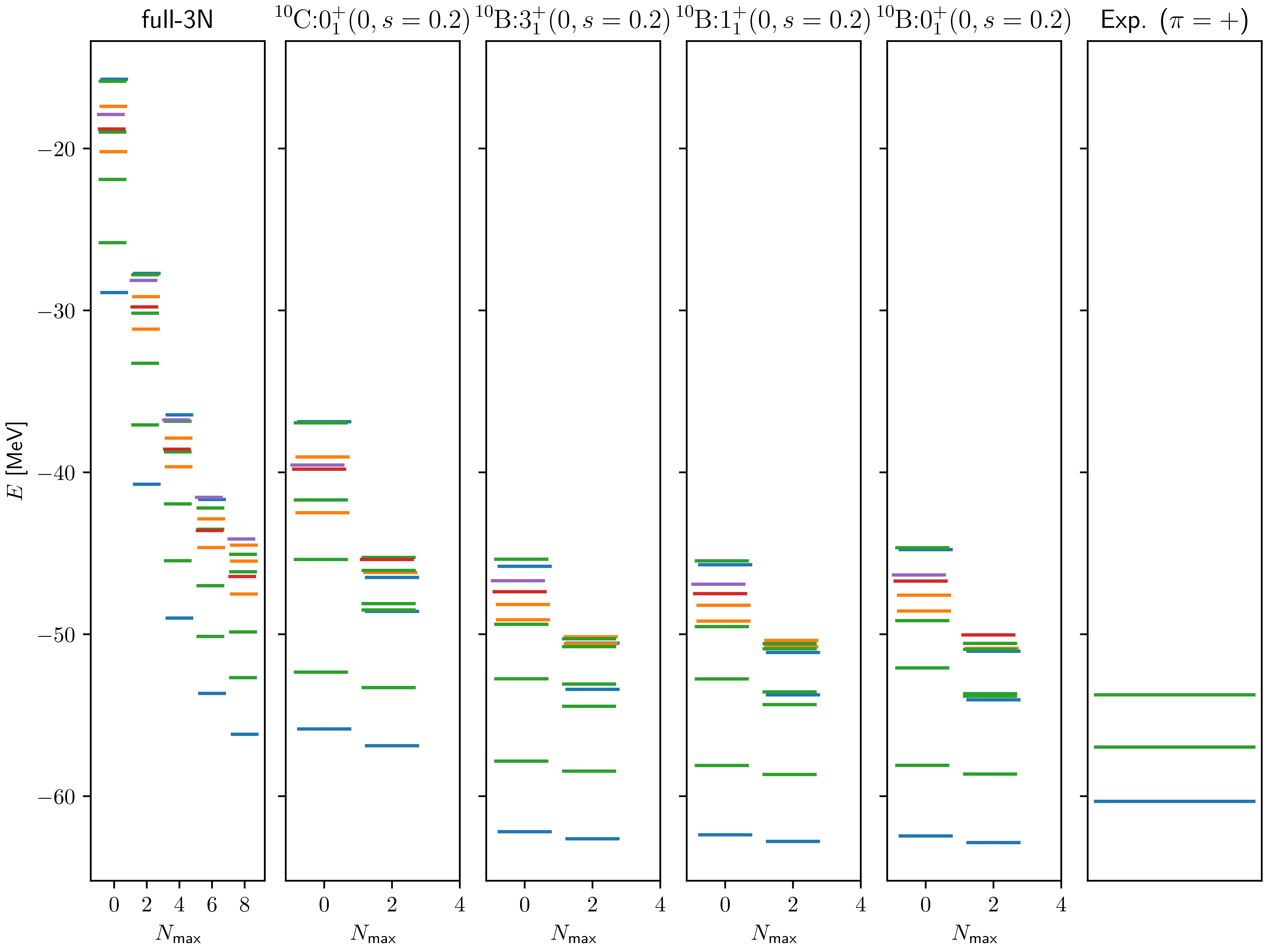


- **state of the art** study
- **complementary methods:** IM-GCM & VS-IMSRG
- explores interactions, many-body and EFT truncations, contact term, …
- leverages **novel emulators**
- identifies **main drivers** of uncertainty and what to improve next

(IM-)NCSM for Super-Allowed Decays

^{10}C

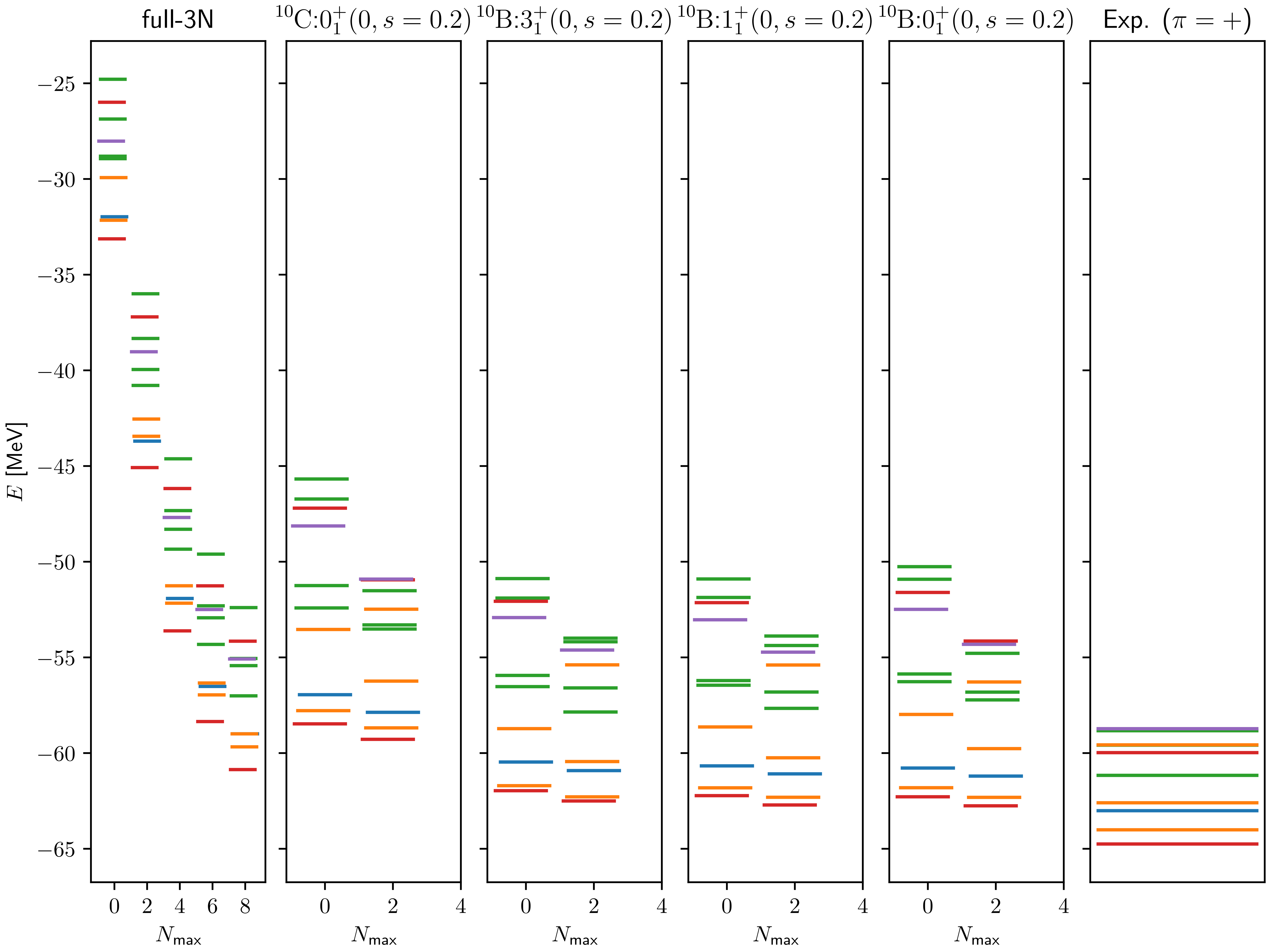
N_{max}	Dim.
0	51
2	10111
4	430137
6	9213794
8	129149891



Eta: ImTime
Int: n4lo500-3NlnlE7
e_{max} = 8
$\hbar\Omega$ = 18MeV

(IM-)NCSM for Super-Allowed Decays

^{10}B



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

Eta: ImTime
Int: n4lo500-3NlnlE7
e_{max} = 8
$\hbar\Omega$ = 18MeV

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: δ_C and δ_{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}Mg, ^{26m}Al, …
- benchmarks for CC, IM-GCM, VS-IMSRG, …
- test exact sum over intermediate states vs. new EFT approach

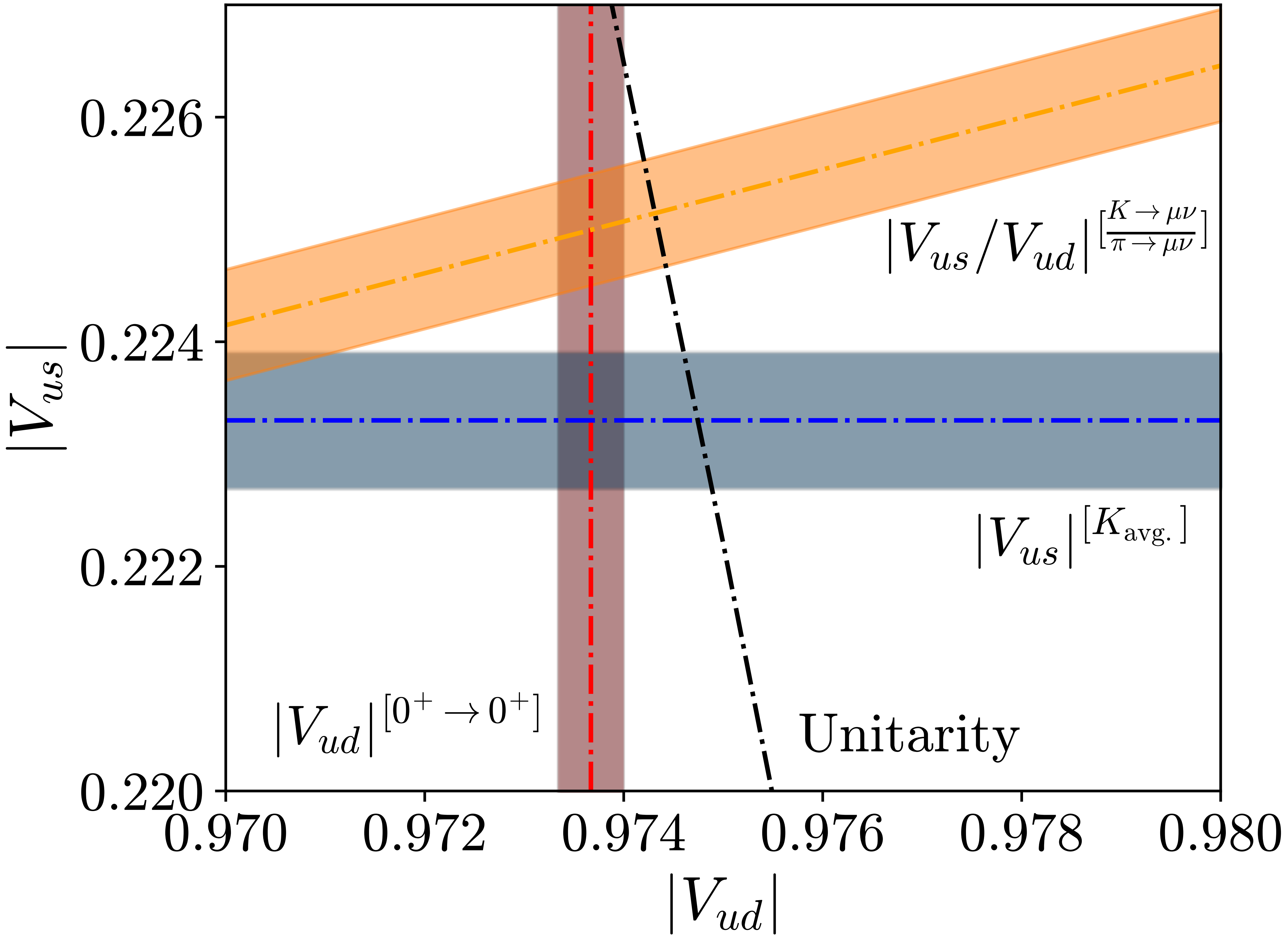
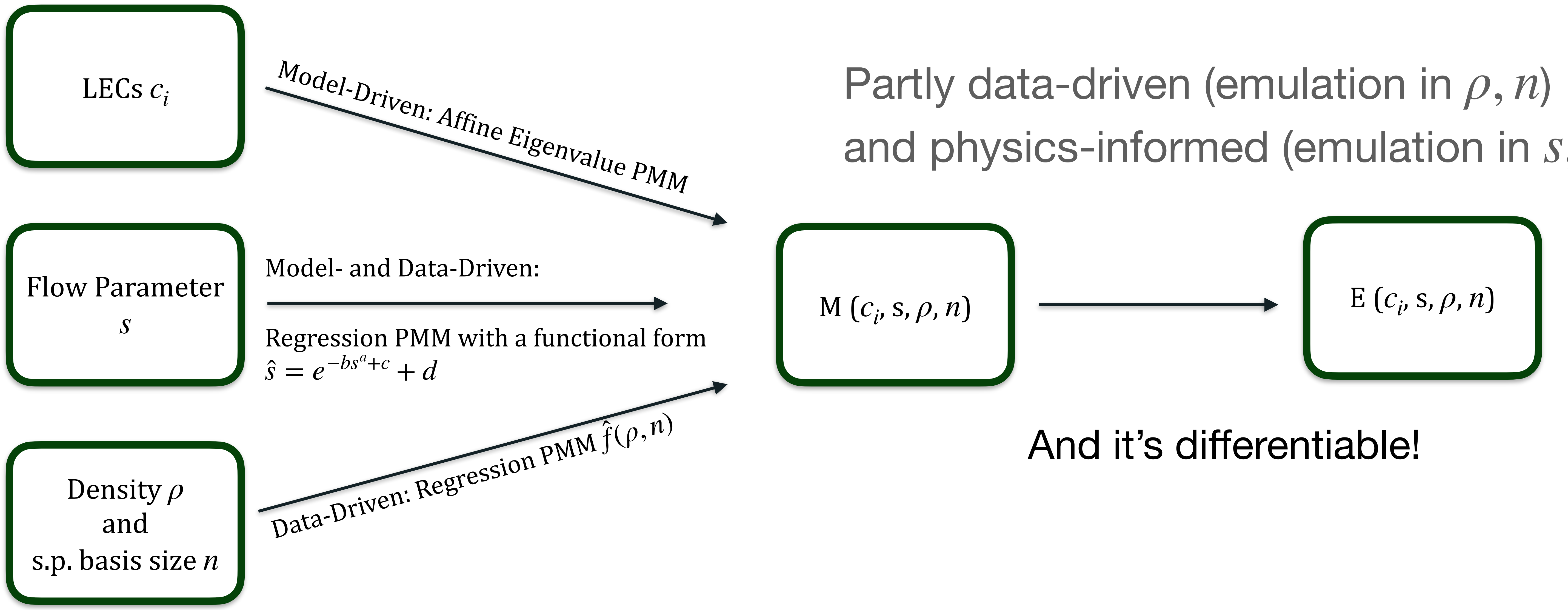


image credit: M. Gennari

PMMs for IMSRG Equation of State Calculations

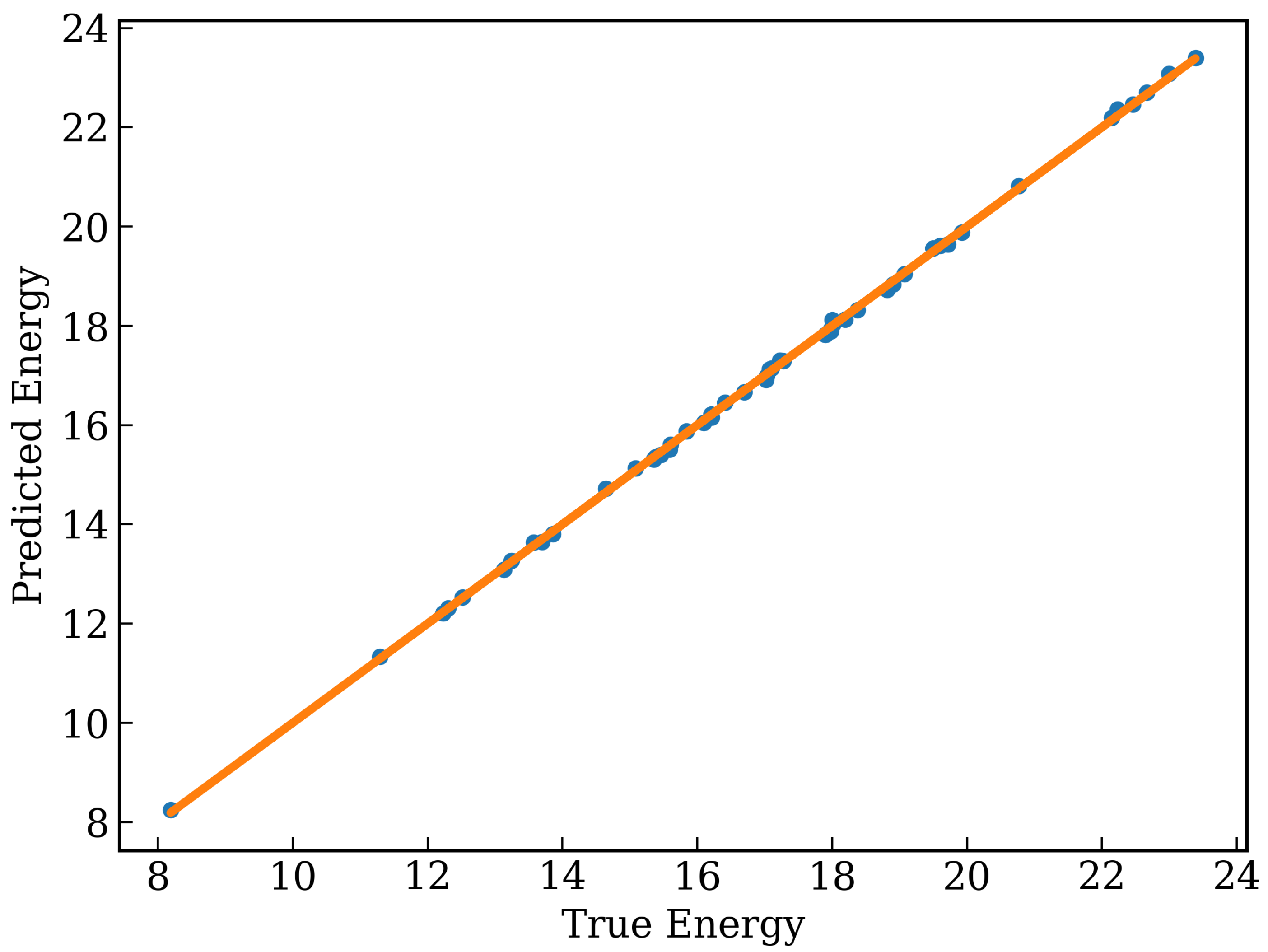


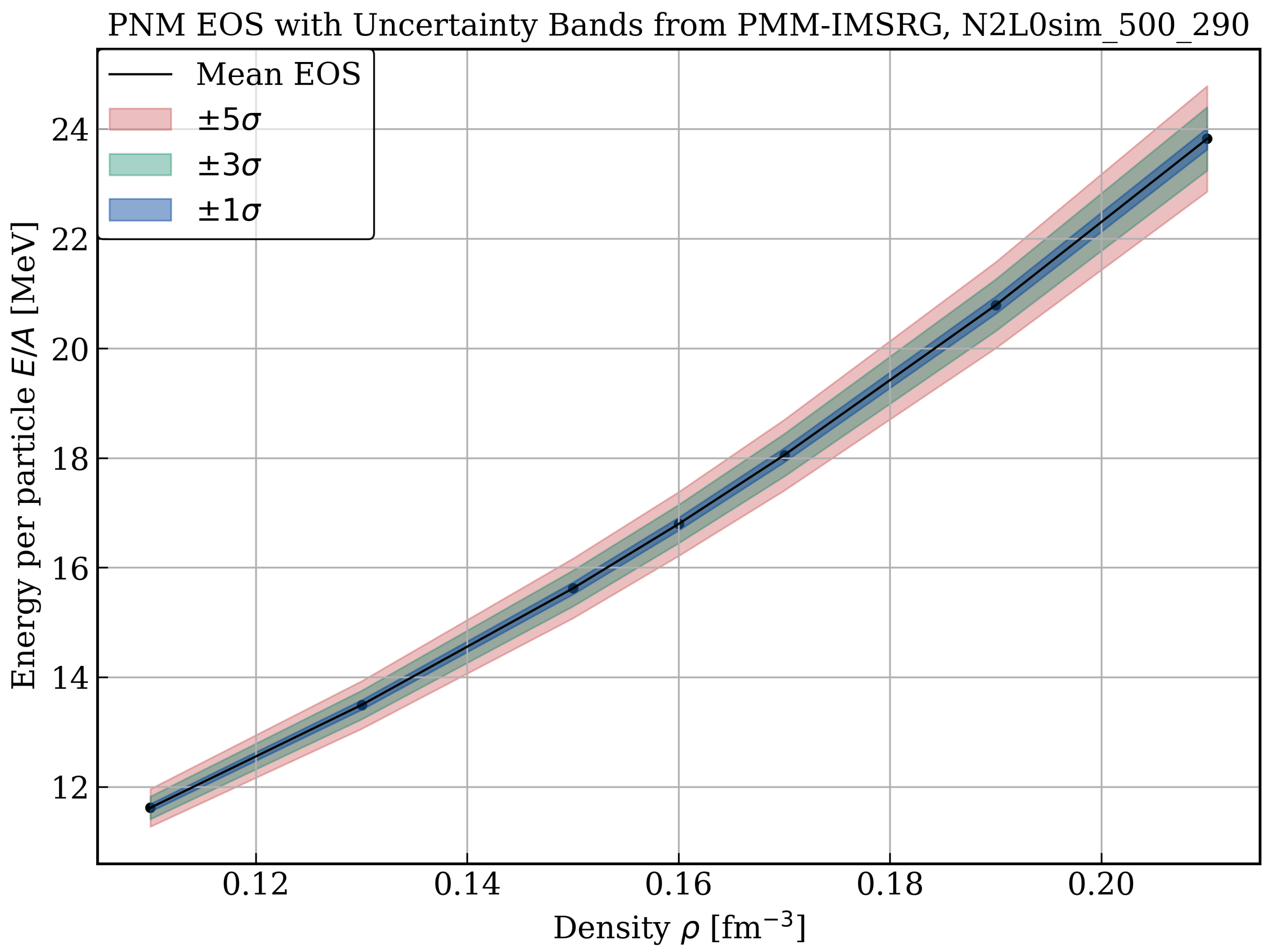
Partly data-driven (emulation in ρ, n) and physics-informed (emulation in s, c_i)

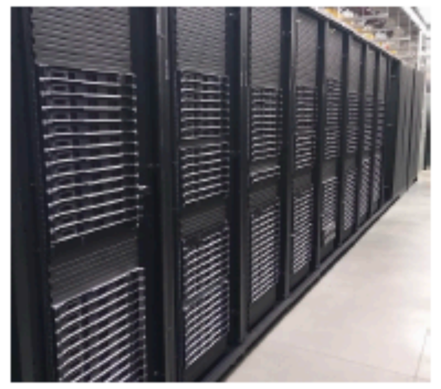
And it's differentiable!

Patrick Cook **Kang Yu**

+ Scott Bogner, Christian Drischler

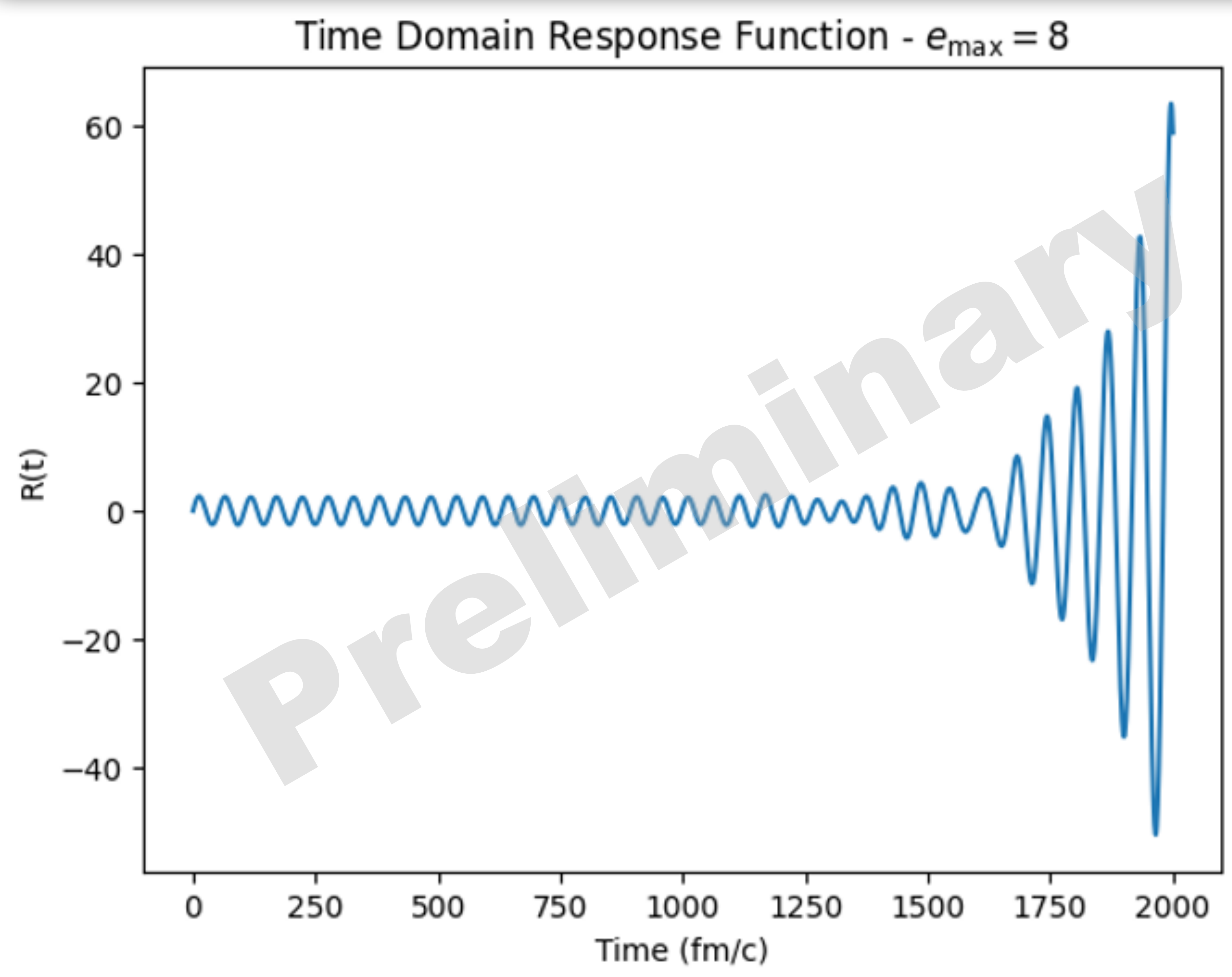


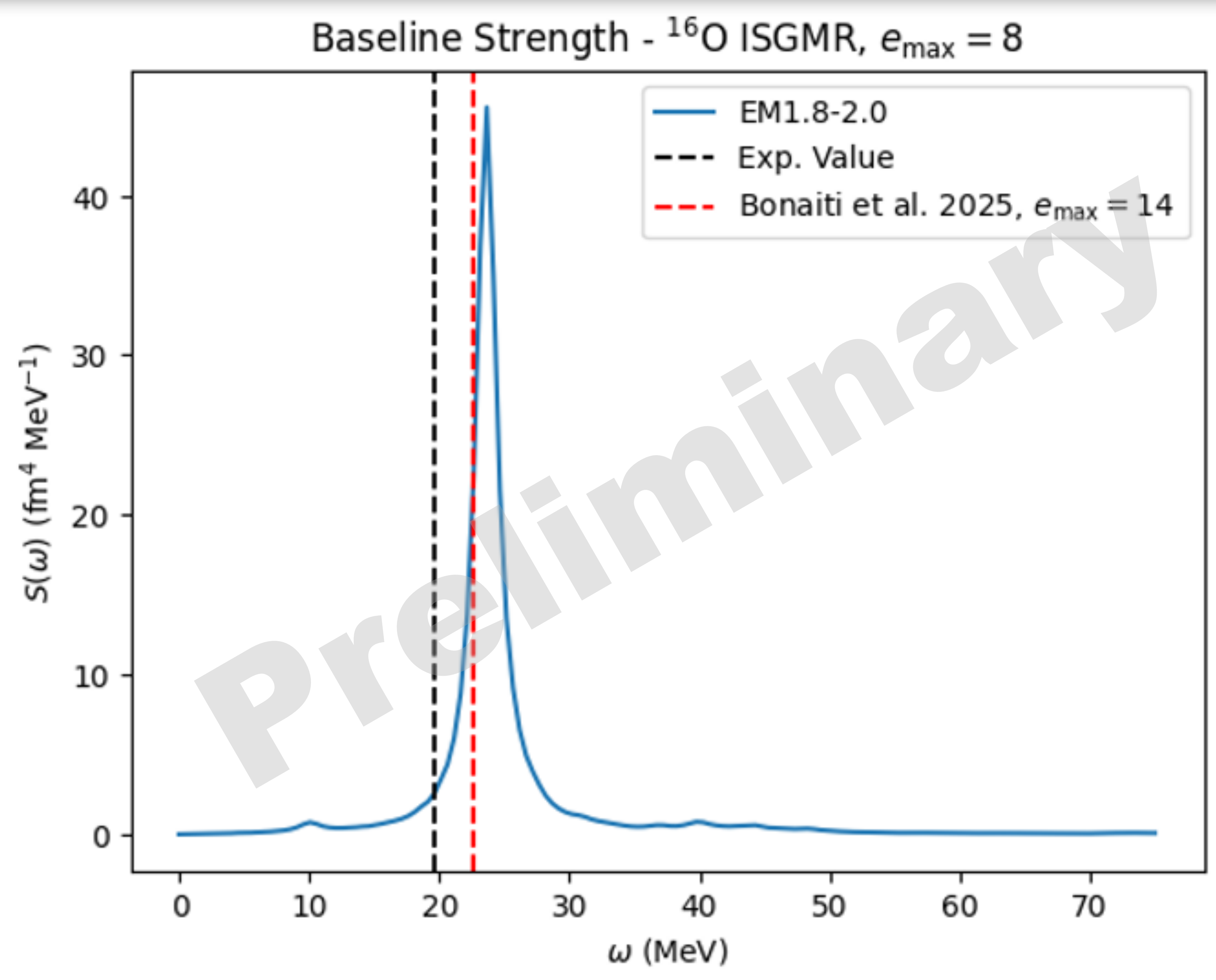




	IMSRG		**PMM**	
Hardware	AMD EPYC 7763 Server $> \$10,000$ per, plus infrastructure		PC with Nvidia RTX A2000 12GB $< \$1,000$	
Energy	*All Runs*	~ 965 kWh $\sim \$174$	*Train*	< 6 kWh $< \$1.08$
	Single Run	10^{-4} to 7.5 kWh $\$10^{-5}$ to $1.34	*Inference*	$< 10^{-6}$ kWh $< \$4 \times 10^{-7}$
xPU-Time	CPU		GPU	
	All Runs	> 17.5 years	*Train*	1 day
	Single Run	100 sec to 50 days	*Inference*	< 1 s
Real-Time	*All Runs*	> 1 week	*Train*	1 day
	Single Run	18 sec to 2 days	*Inference*	< 1 s
Memory	Peak 600 GB		Peak < 12 GB	

Time-Dependent Response from the IMSRG





Aryan Vaidya
+ Scott Bogner, Jon Engel, …

- 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

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