Update on IMSRG Developments

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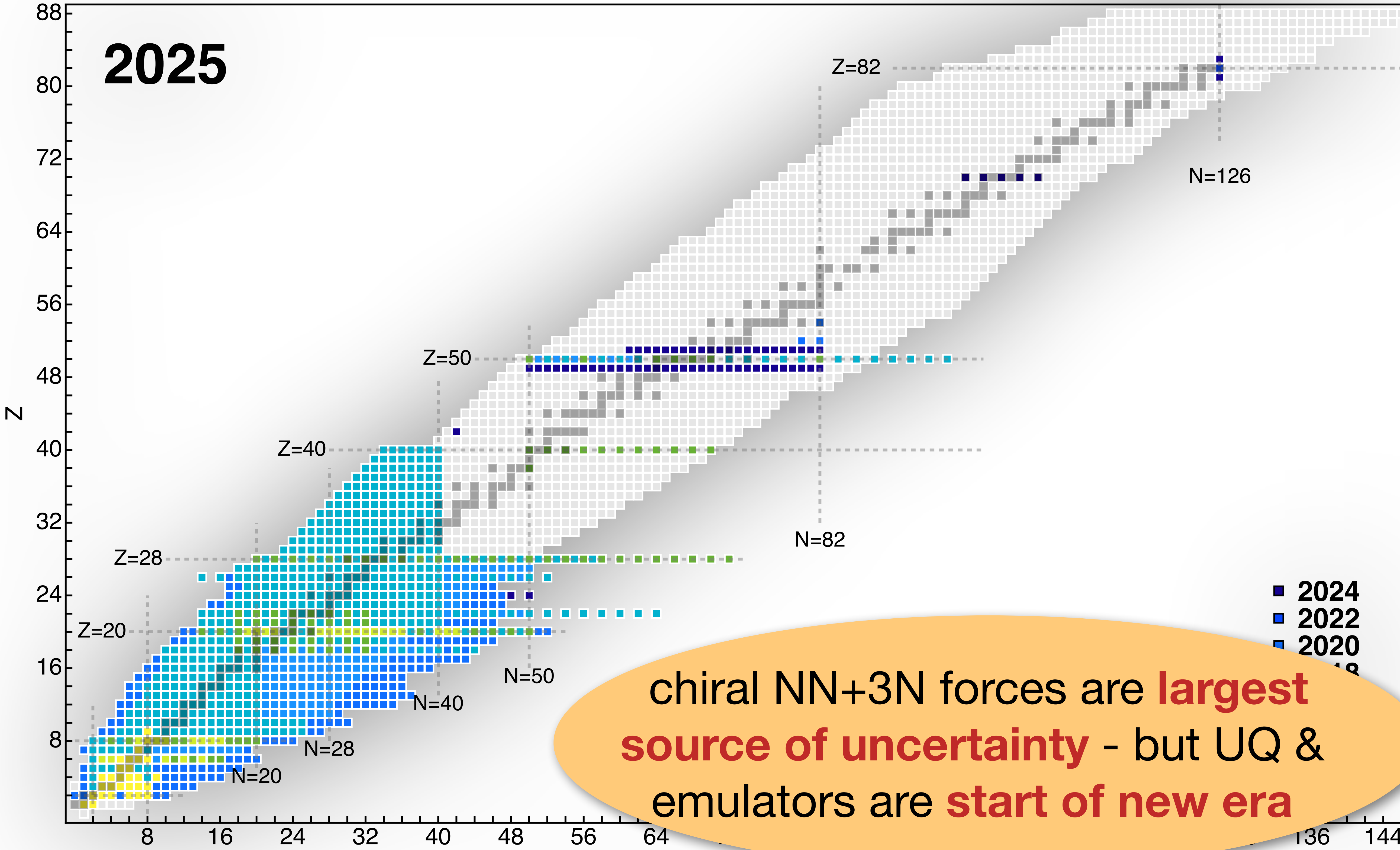
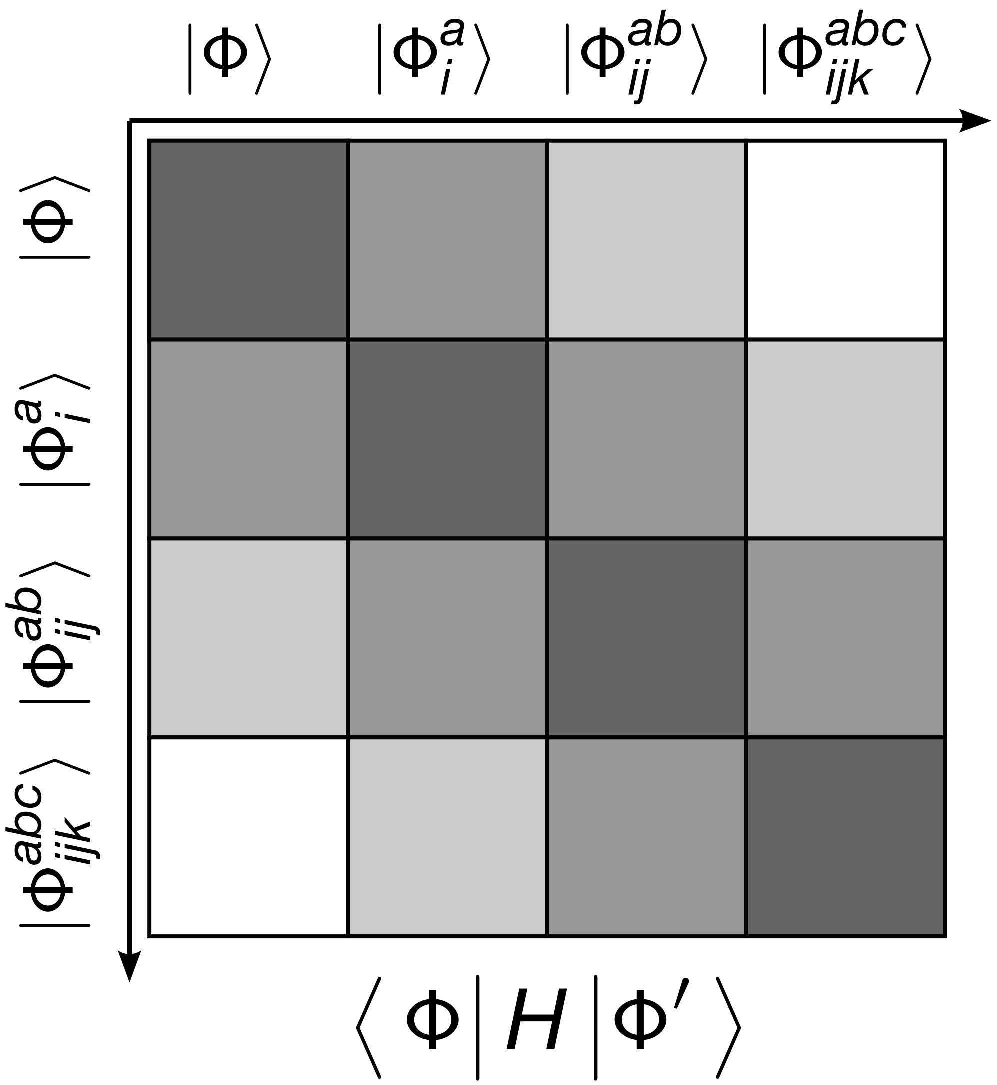
Progress in *Ab Initio* Calculations

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

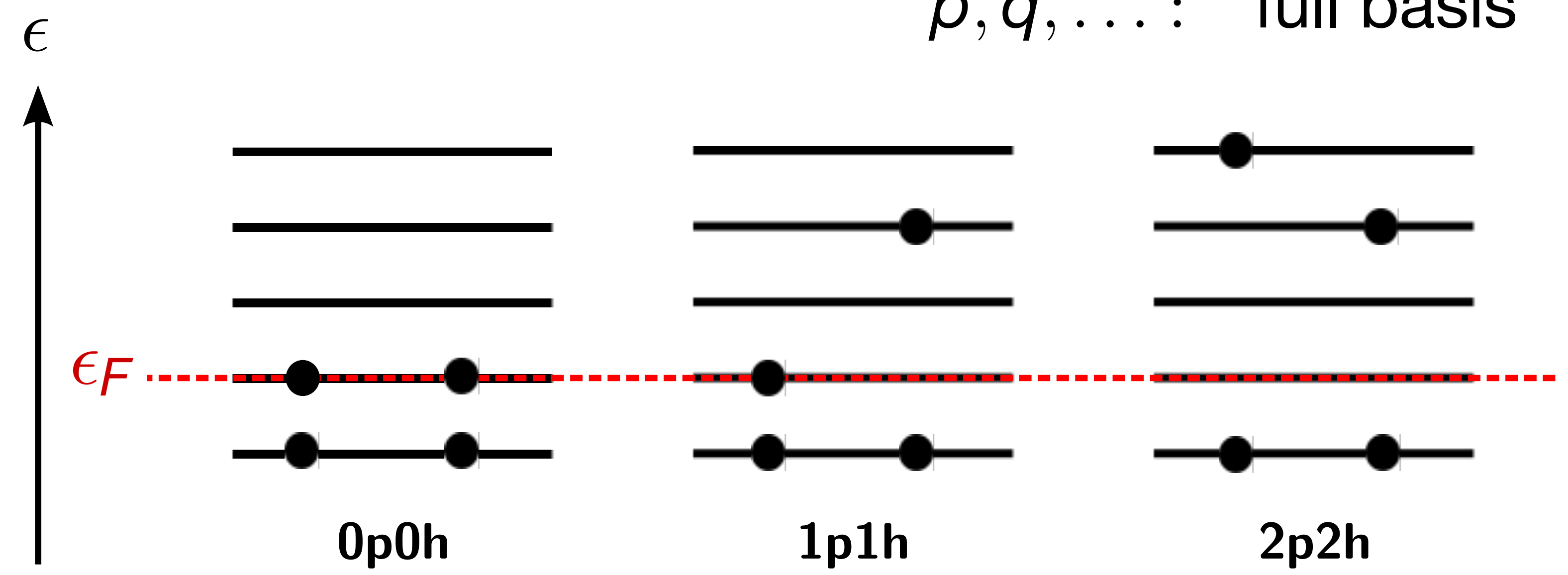


chiral NN+3N forces are **largest source of uncertainty** - but UQ & emulators are **start of new era**

Transforming the Hamiltonian



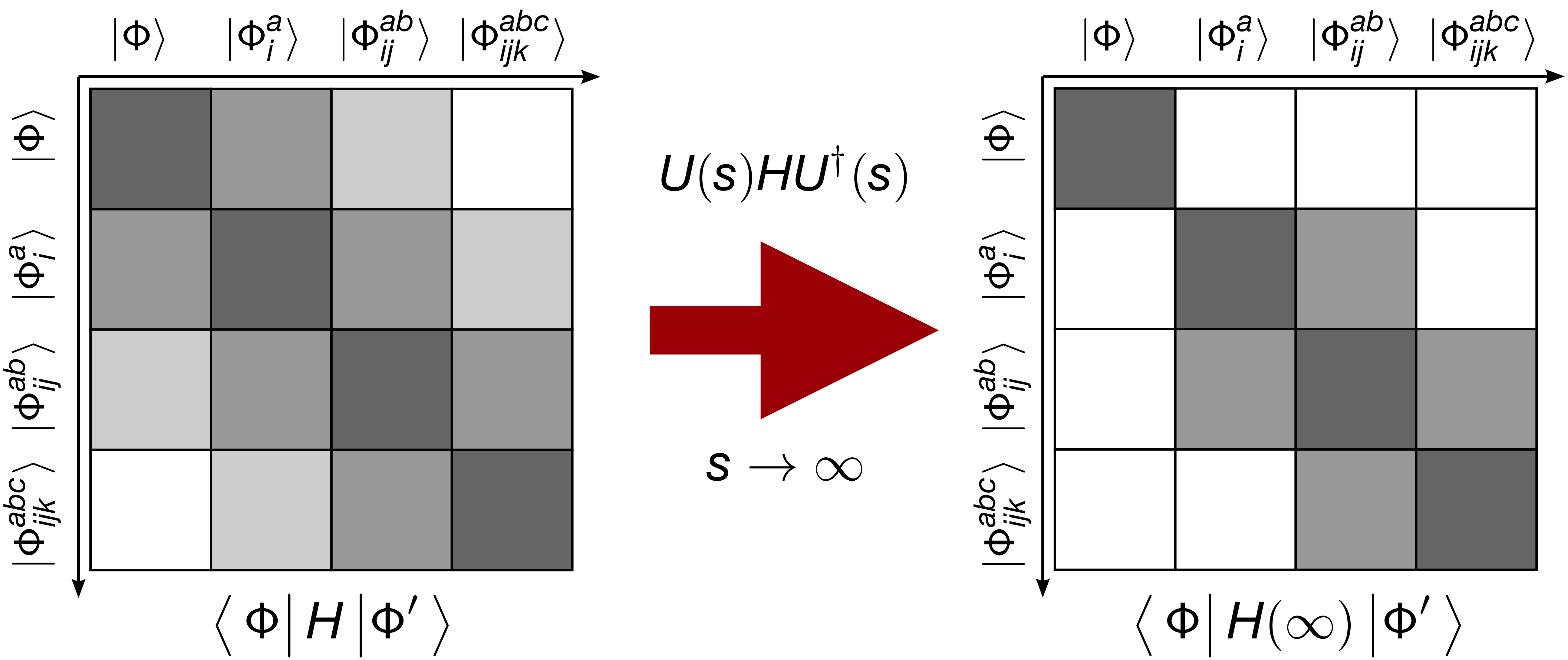
$a, b, \ldots : \quad \epsilon > \epsilon_F$
$i, j, \ldots : \quad \epsilon \leq \epsilon_F$
$p, q, \ldots : \quad$ full basis



- reference state: **single Slater determinant**

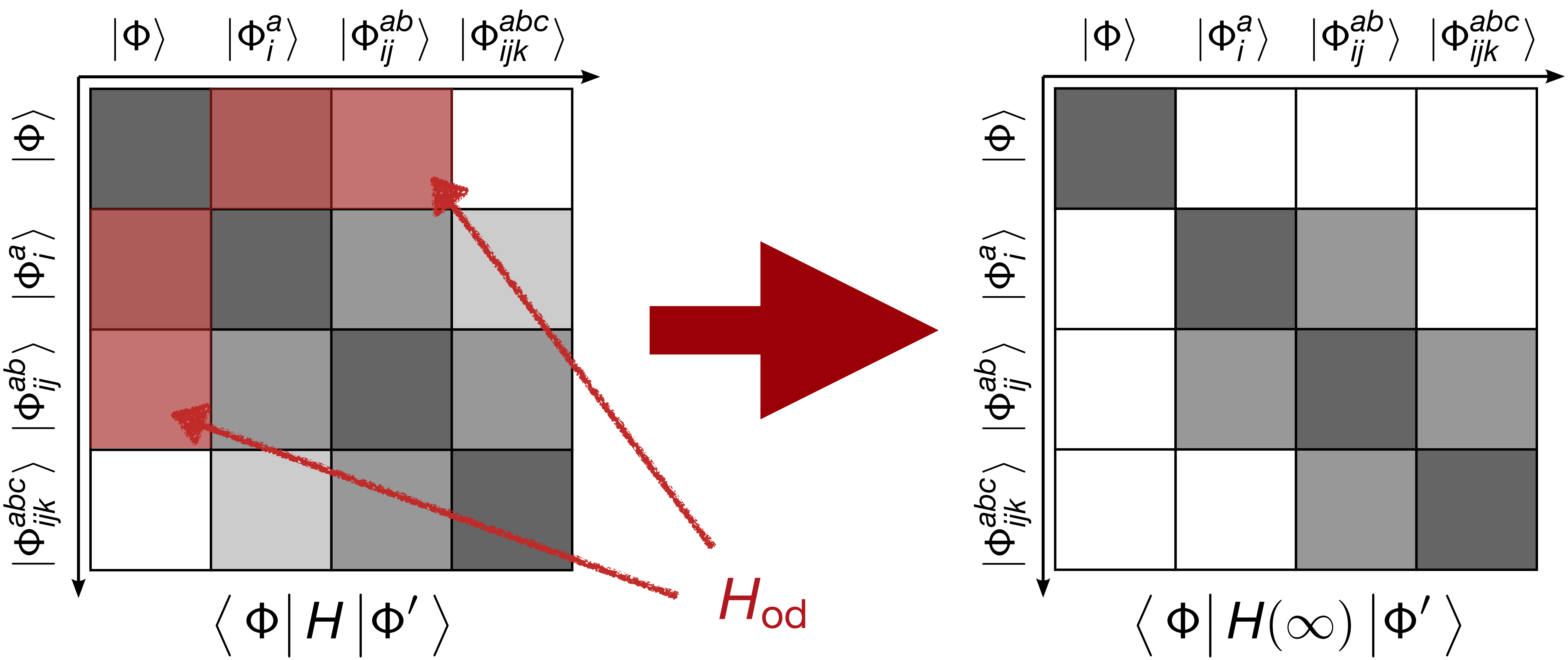
excitations relative to reference state: **normal-ordering**

Decoupling in A-Body Space



goal: decouple reference state $|\Phi\rangle$ from excitations

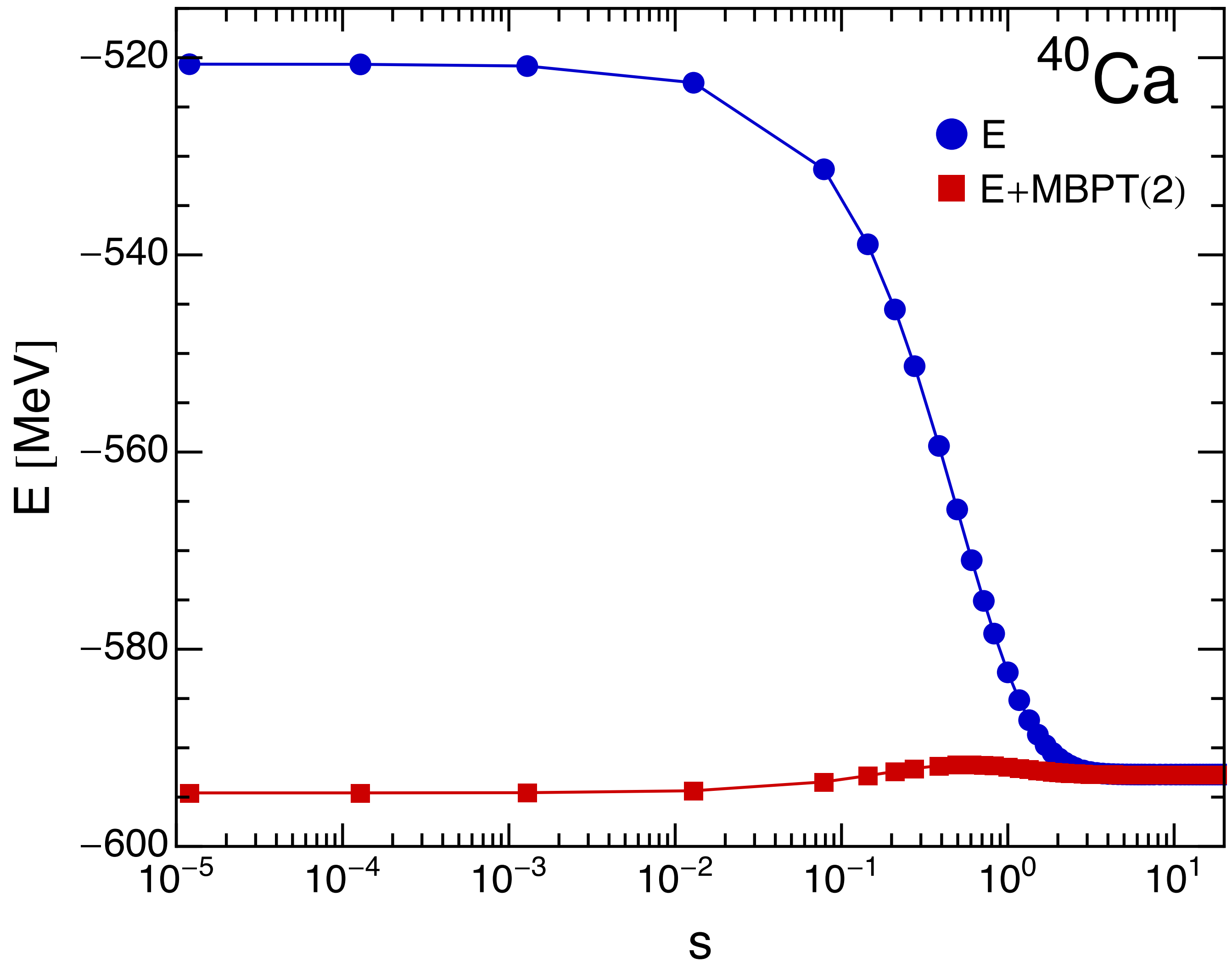
Flow Equation

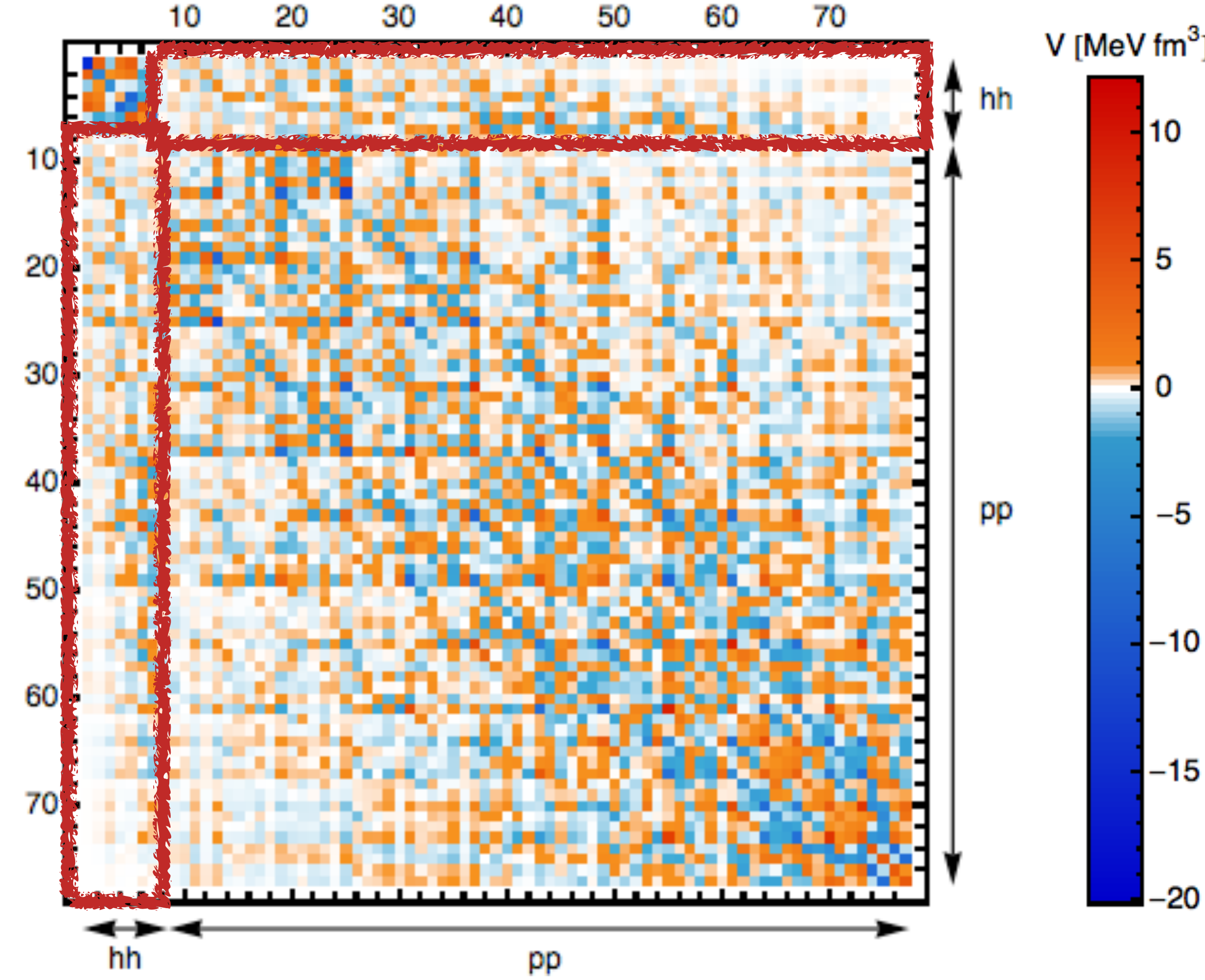


$$\frac{d}{ds}H(s) = \left[\eta(s), H(s)\right],$$

Operators
truncated at **two-body level** -
matrix is never constructed explicitly!

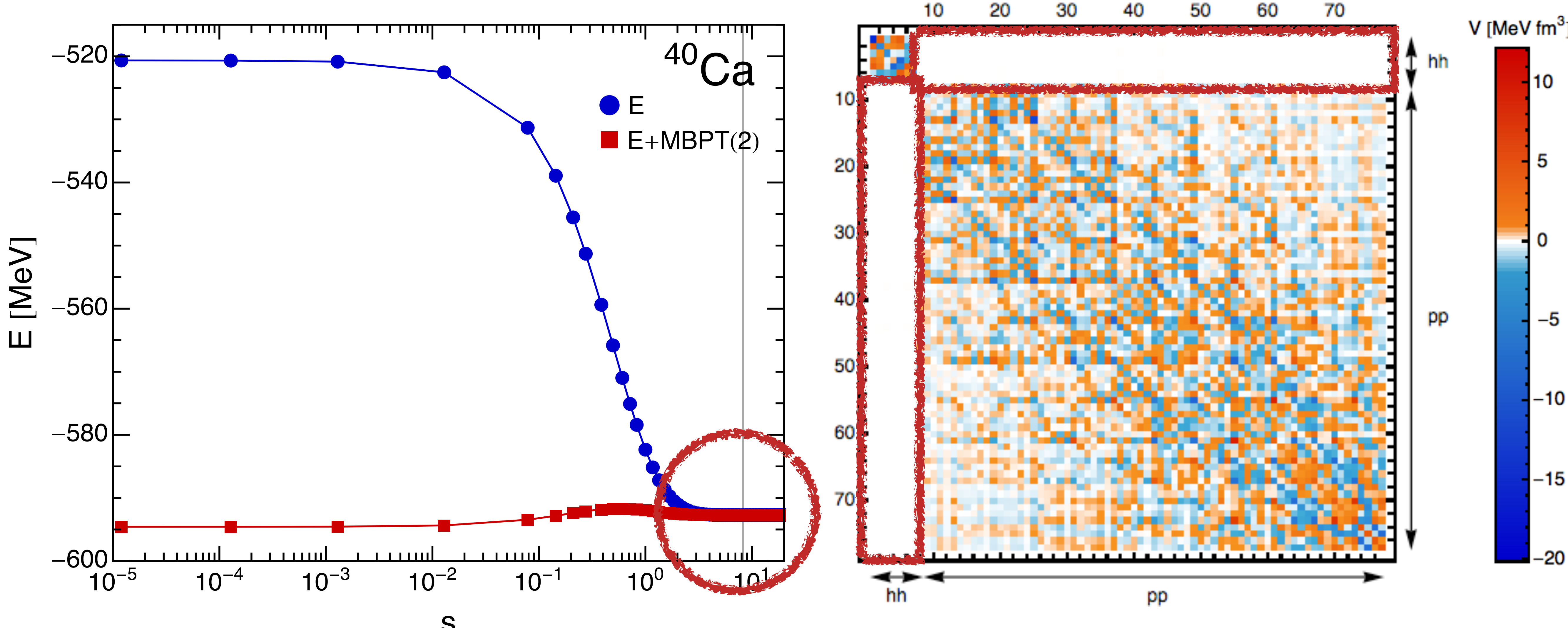
Decoupling





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

Decoupling

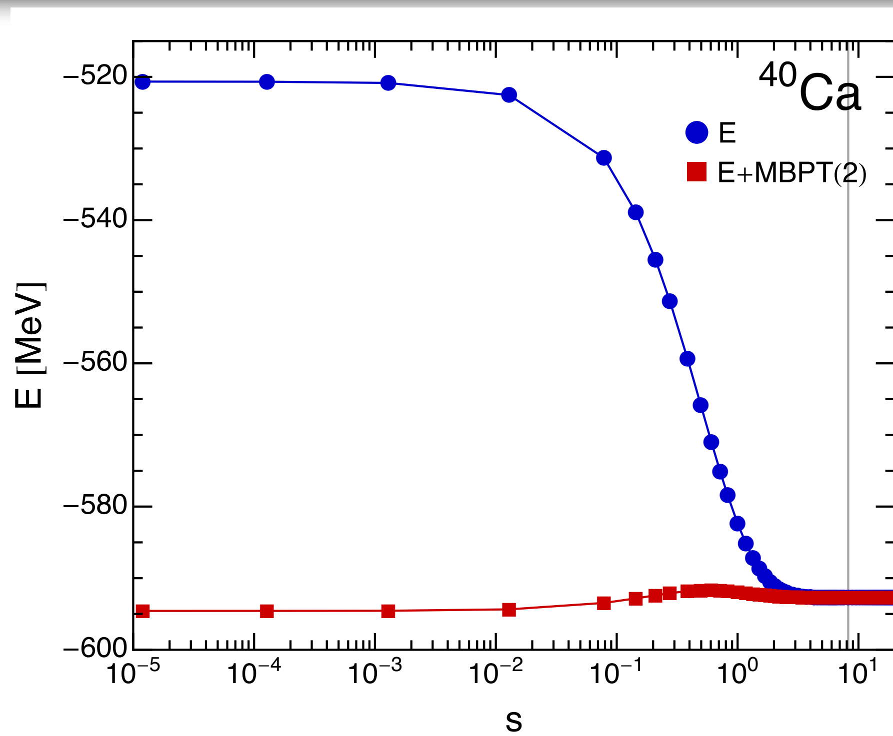


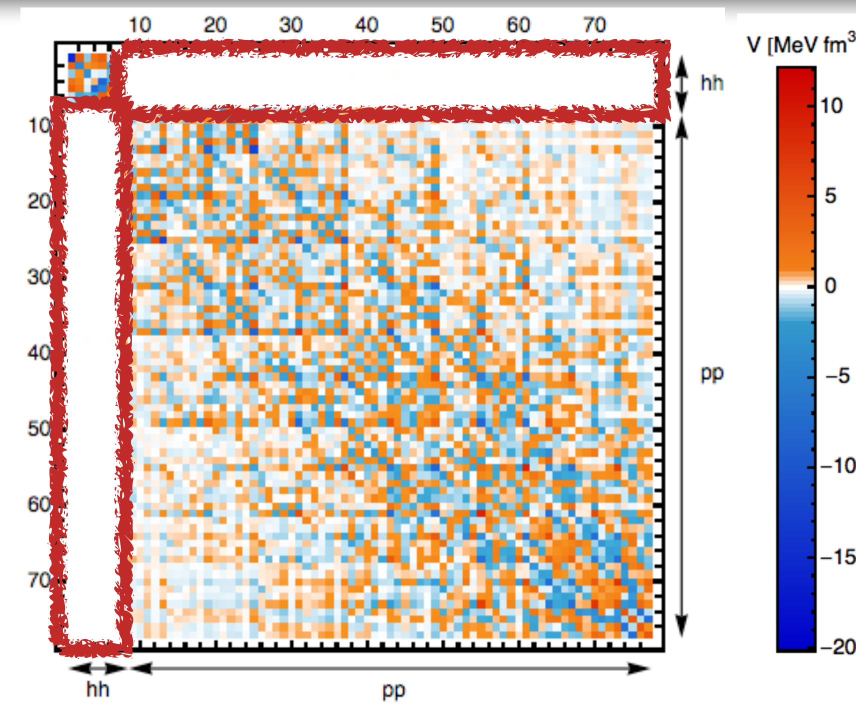
N3LO, $\lambda = 2.0\ \mathrm{fm}^{-1}, e_{\mathrm{Max}} = 8$

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

off-diagonal couplings are rapidly driven to zero

Decoupling





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

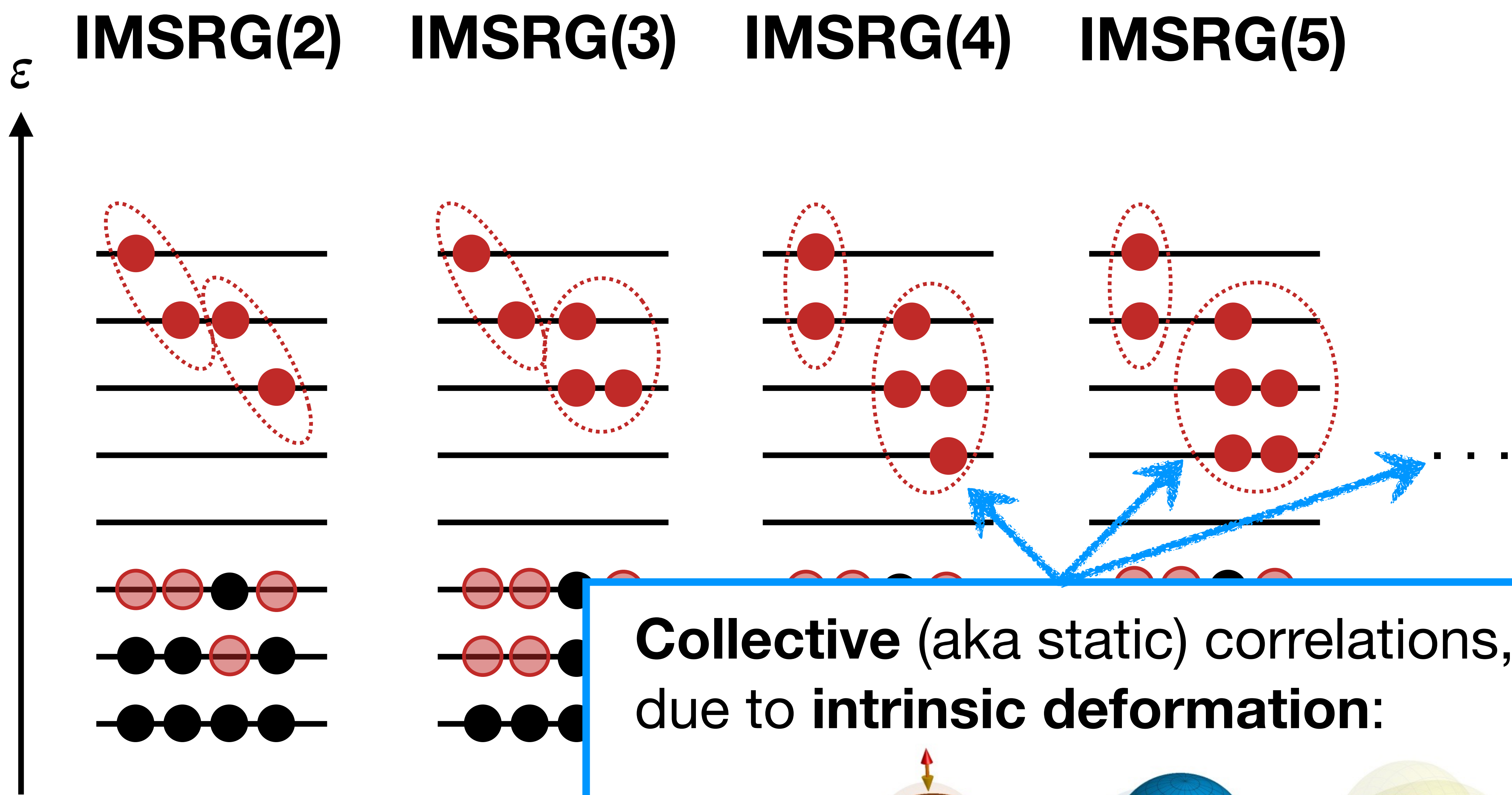
- absorb correlations into **RG-improved Hamiltonian**

$$U(s)HU^\dagger(s)U(s)\left|\Psi_n\right\rangle = E_n U(s)\left|\Psi_n\right\rangle$$

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

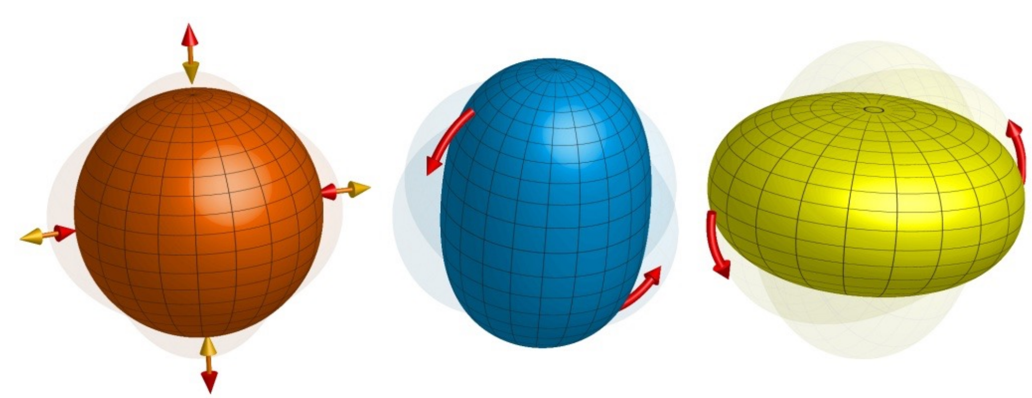
$$U(s)\left|\Psi_n\right\rangle \stackrel{!}{=} \left|\Phi\right\rangle$$

Correlated Reference States

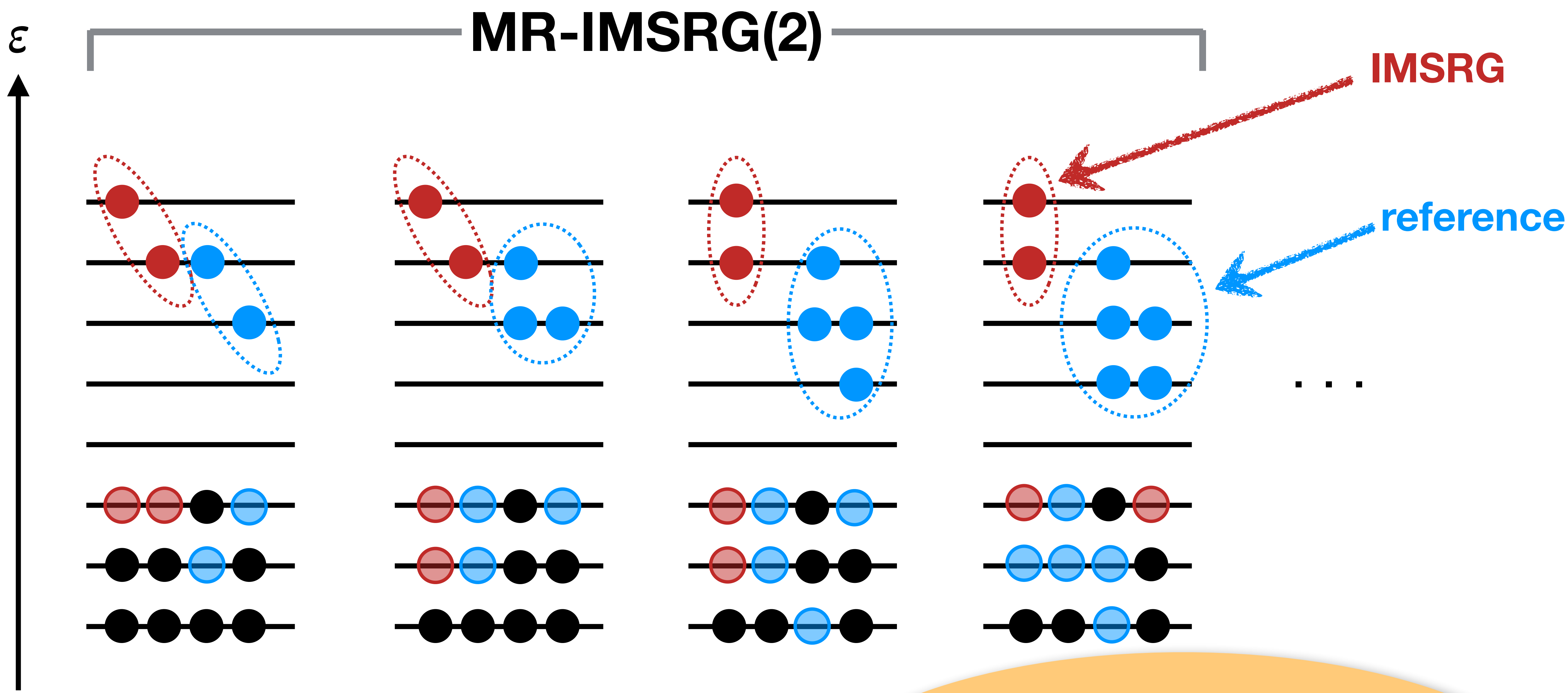


“standard” IMS
Slater determinan

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



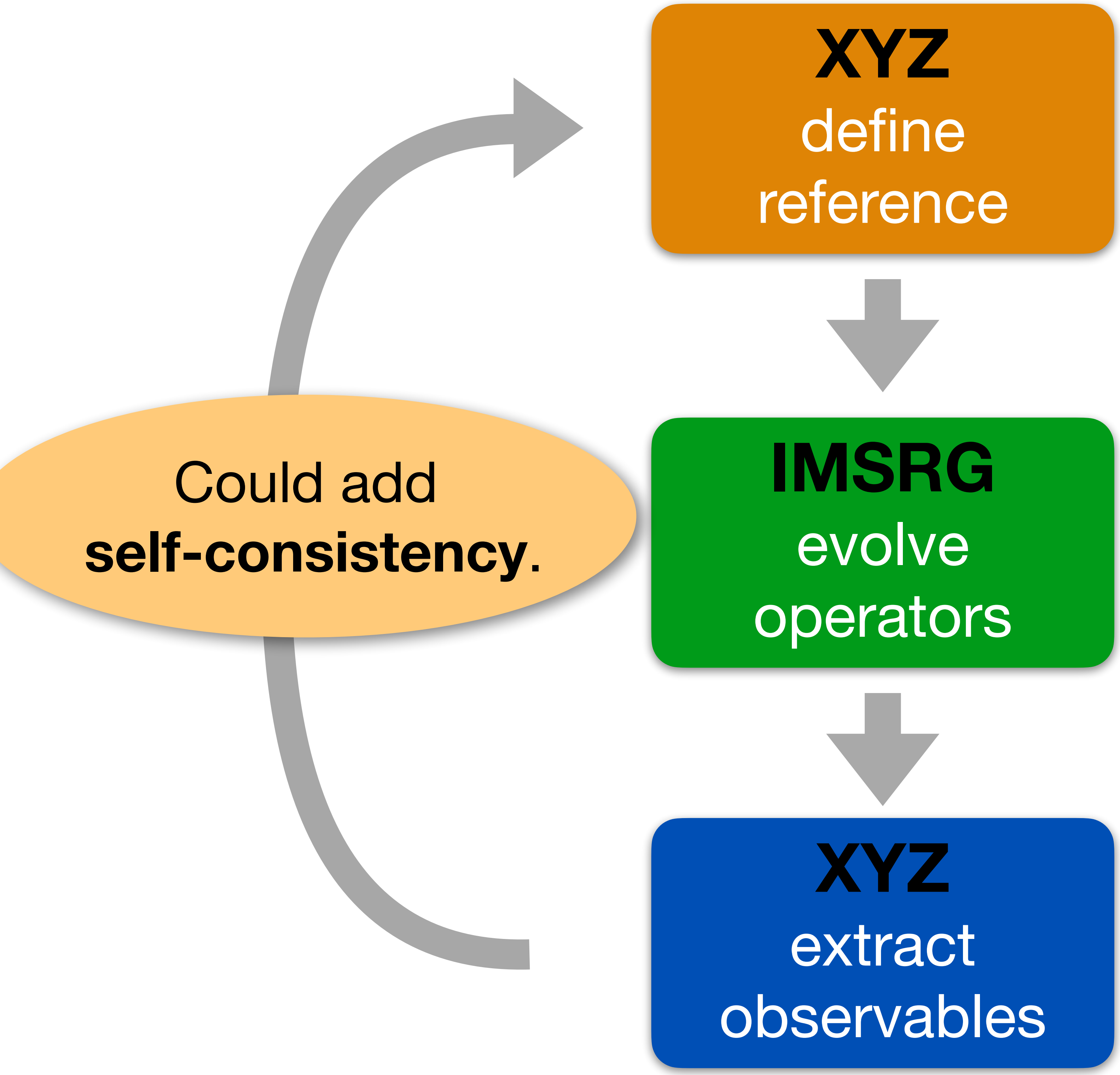
Correlated Reference States



MR-IMSRG: build correla[…]
already correlated state (e.g[…]
describes static cor[…]

additional terms in flow equations (two-body and higher densities), but **scaling remains unchanged**

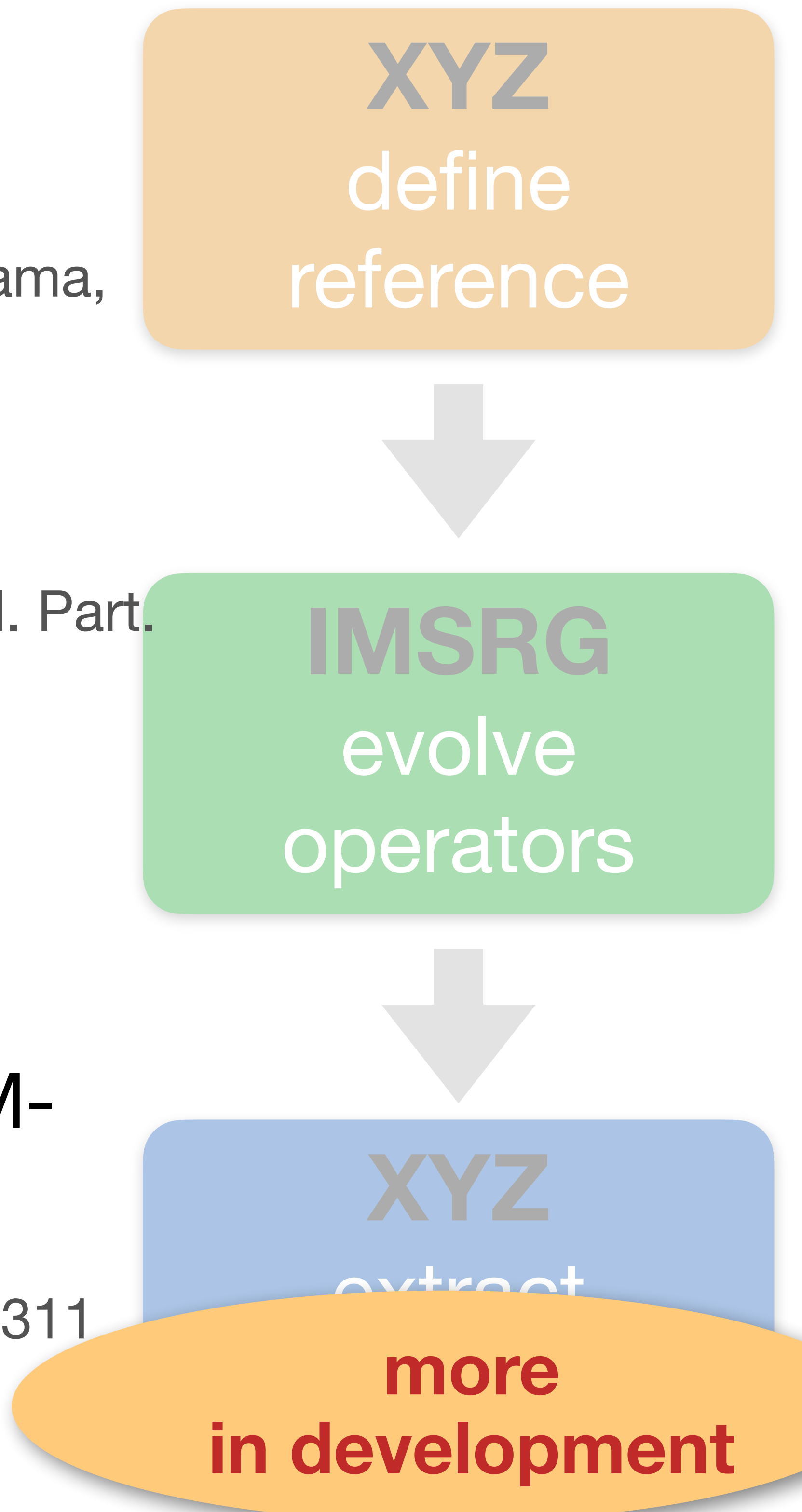
IMSRG-Improved Methods



* mean field or
explicitly correlated

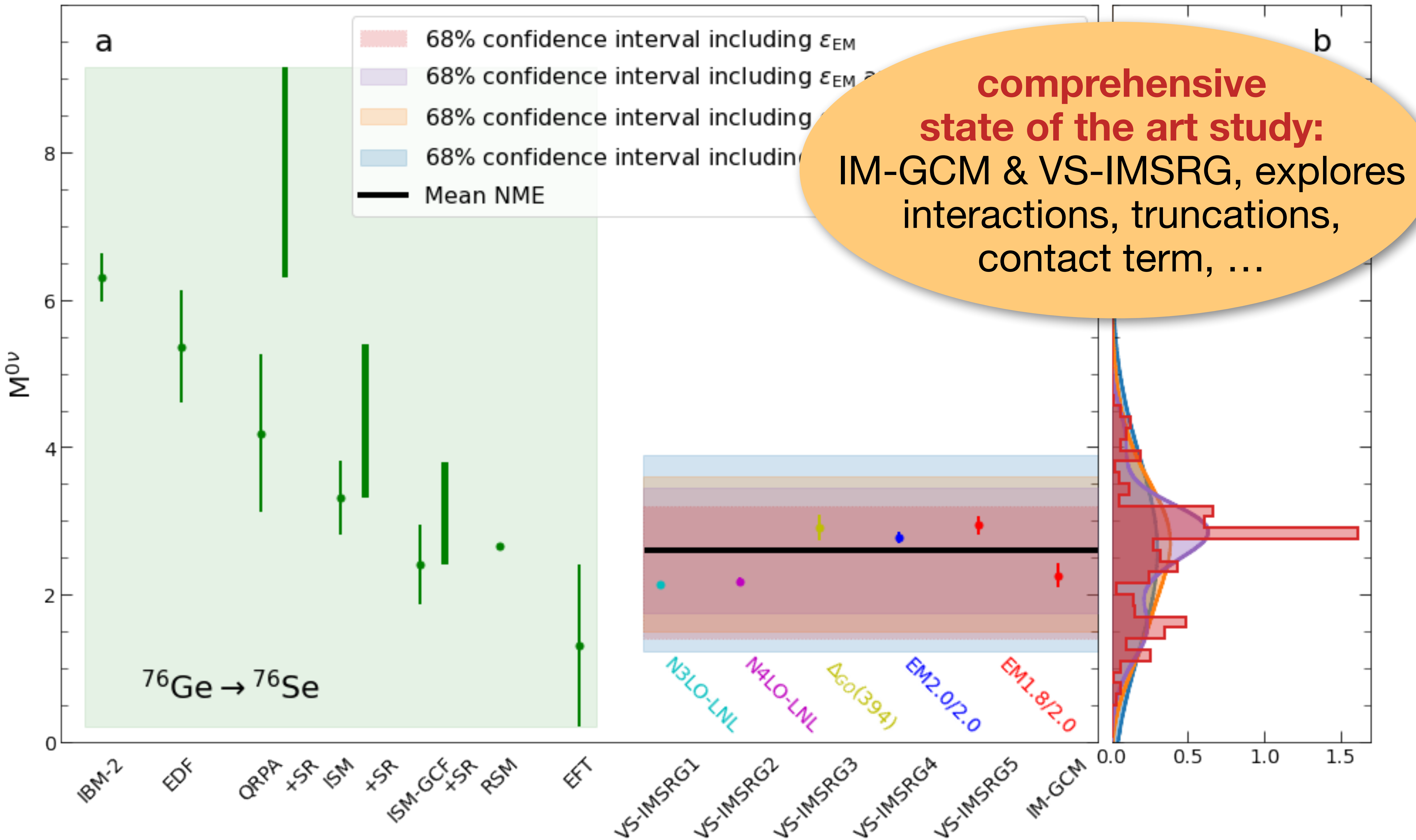
IMSRG-Improved Methods

- IMSRG for closed and open-shell nuclei: IM-HF and IM-PHFB
  - HH, Phys. Scripta, Phys. Scripta 92, 023002 (2017)
  - HH, S. K. Bogner, T. D. Morris, A. Schwenk, and K. Tuskiyama, Phys. Rept. 621, 165 (2016)
- Valence-Space IMSRG (VS-IMSRG)
  - S. R. Stroberg, HH, S. K. Bogner, J. D. Holt, Ann. Rev. Nucl. Part. Sci. **69**, 165
- In-Medium No Core Shell Model (IM-NCSM)
  - E. Gebrerufael, K. Vobig, HH, R. Roth, PRL **118**, 152503
- In-Medium Generator Coordinate Method (IM-GCM)
  - J. M. Yao, J. Engel, L. J. Wang, C. F. Jiao, HH PRC 98, 054311 (2018)
  - J. M. Yao et al.. PRL 124. 232501 (2020)



^{76}Ge

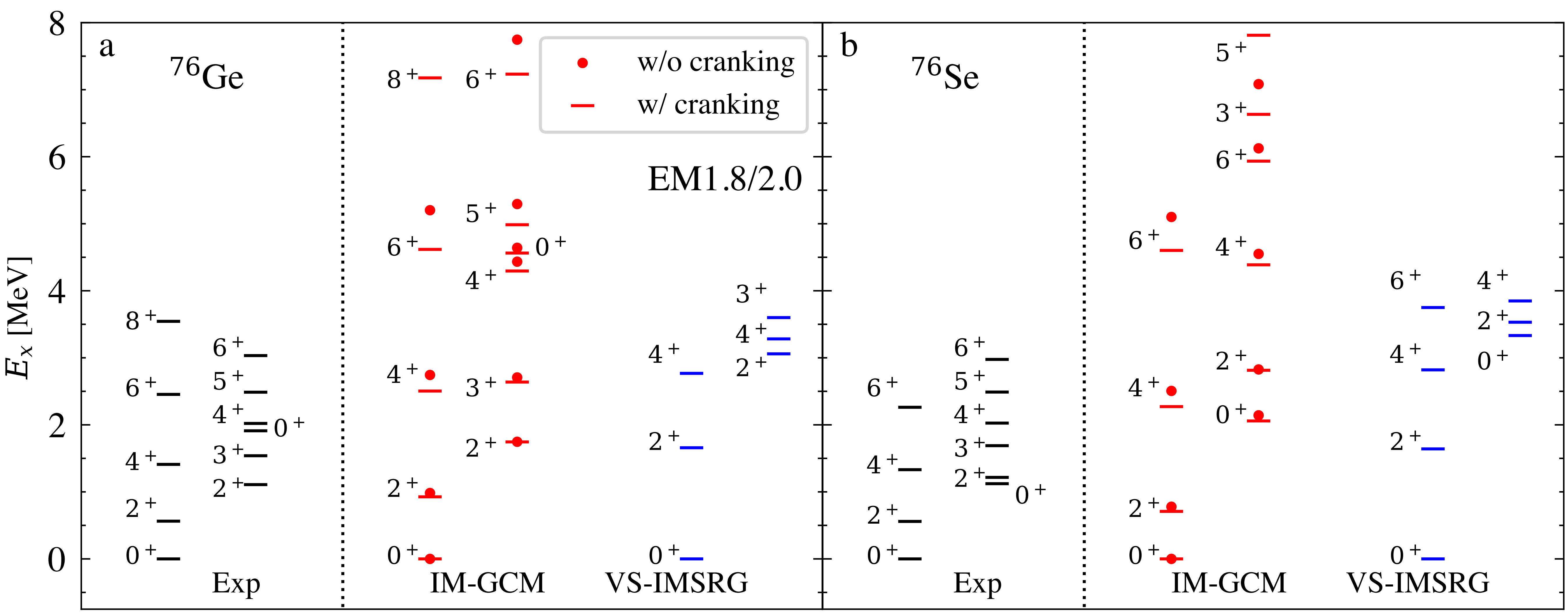
*A. Belley et al., PRL **132**, 182502 (2024)*



comprehensive state of the art study:
IM-GCM & VS-IMSRG, explores interactions, truncations, contact term, …

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

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

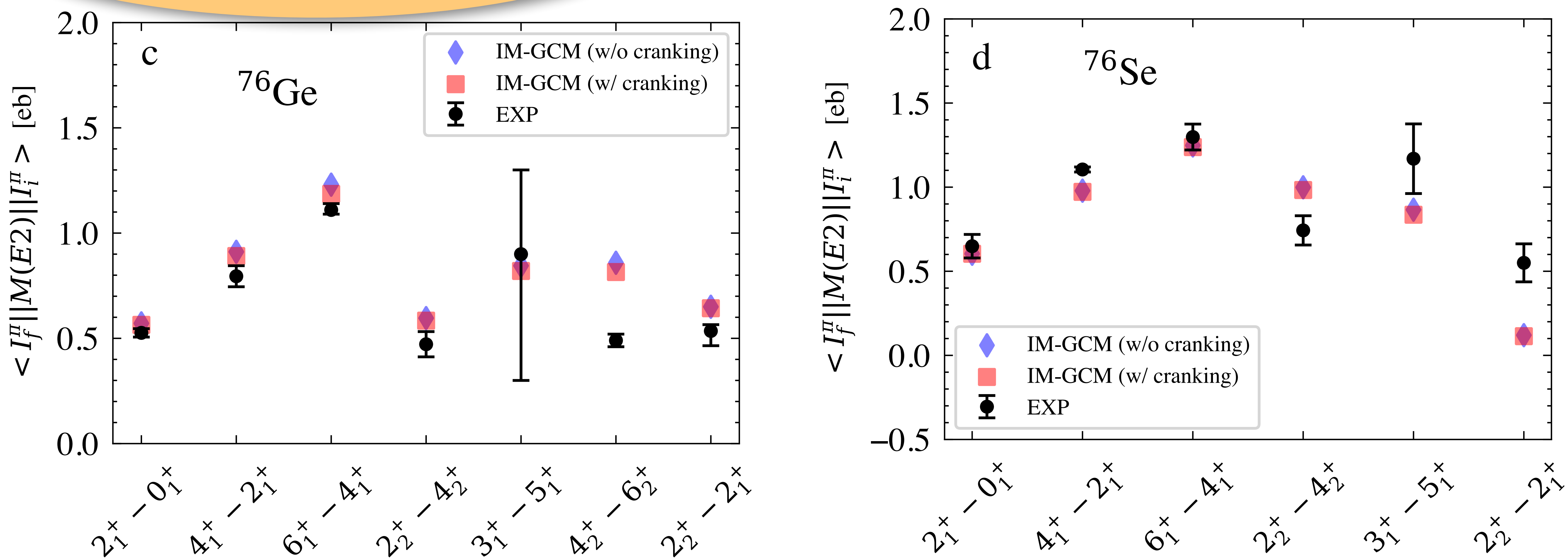


EM1.8/2.0 NN+3N interaction, $\hbar\omega = 12\,\mathrm{MeV}$, $e_{max} = 10$

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

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

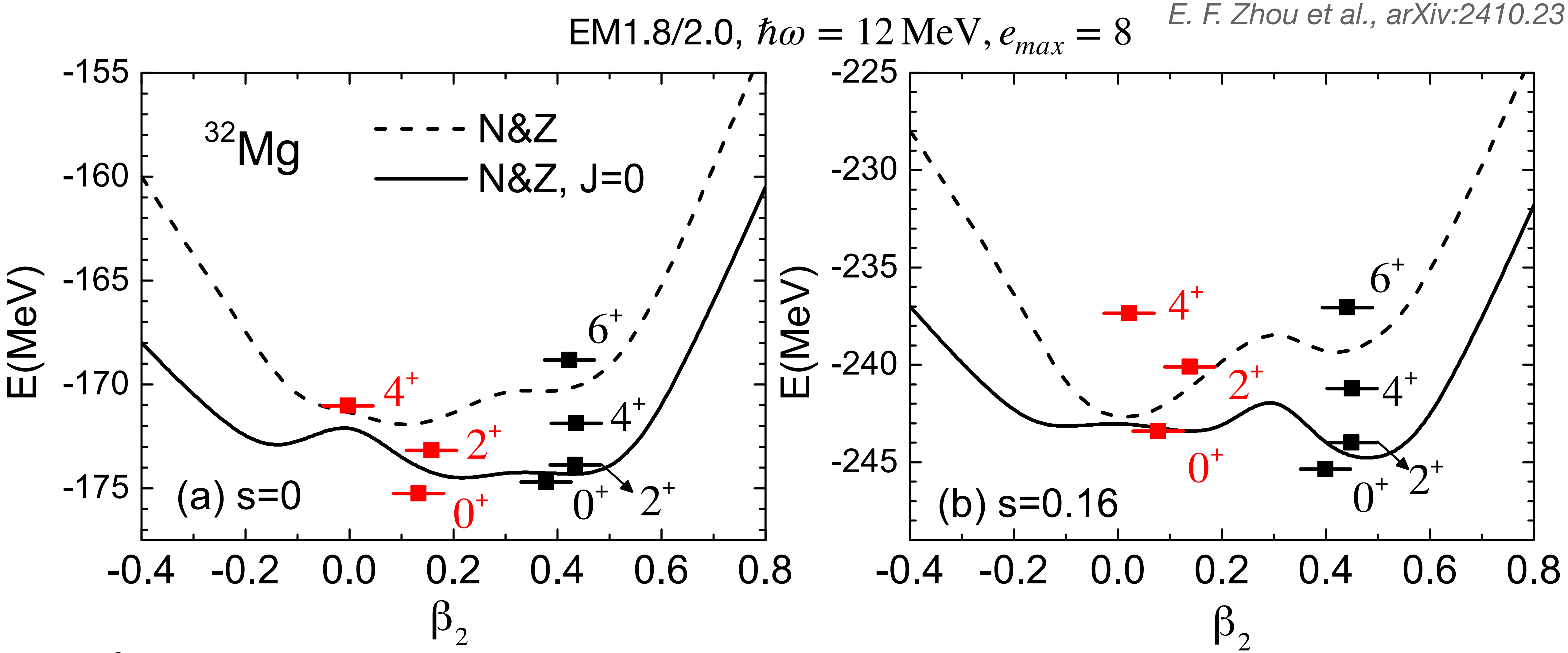
compatible with
A~80 results from AMP-CCSD
[B.S. Hu et al., PRC110, L011302]



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

N=20 Island of Inversion

E. F. Zhou et al., arXiv:2410.23113

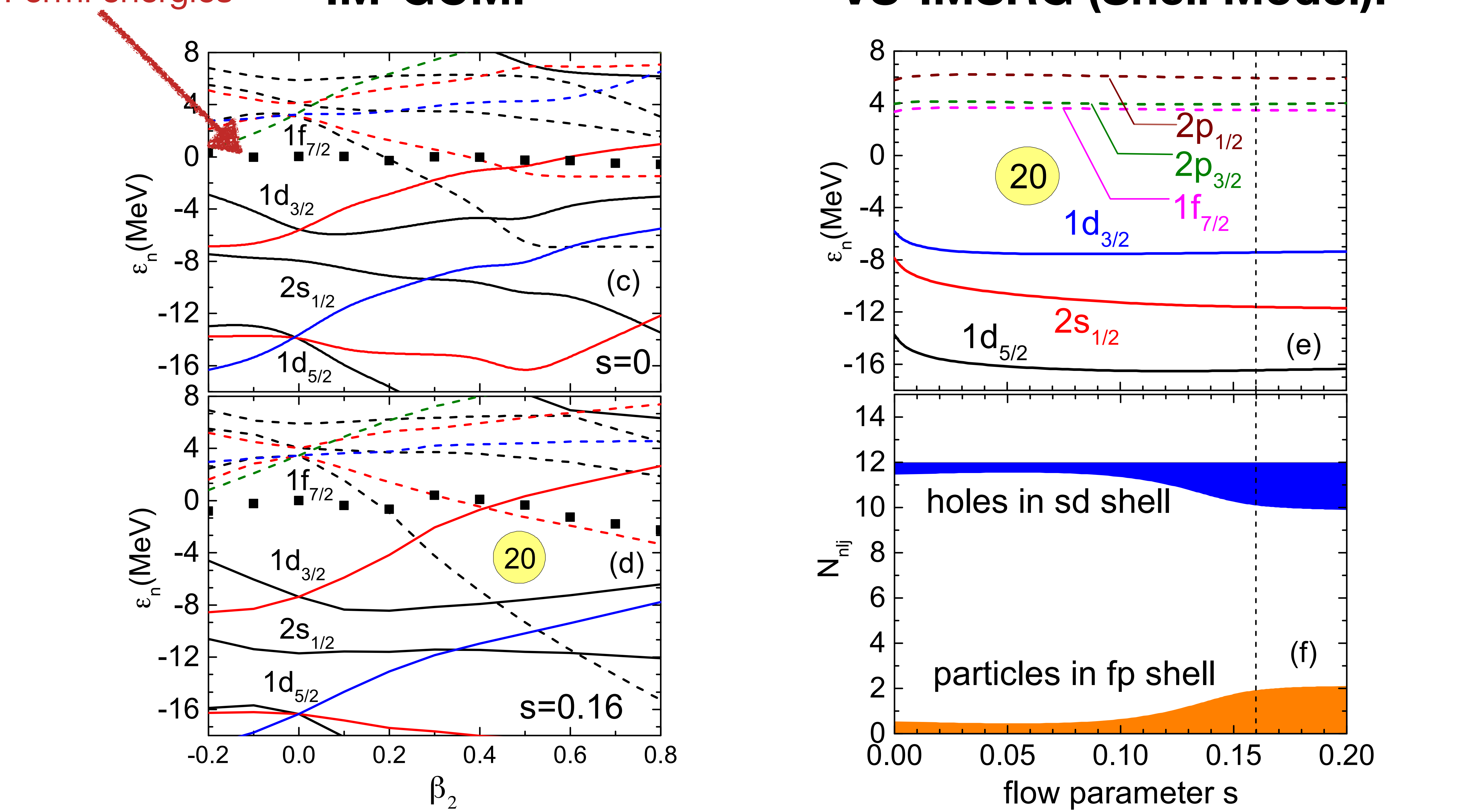


- **Dynamic correlations** captured by IMSRG…
  - bring **absolute energies** close to experiment (E=-249.7 MeV (AME) vs. -249.5 MeV (extrapolated theory))
  - reveal prominent **prolate deformation** of the **ground state**

N=20 Island of Inversion

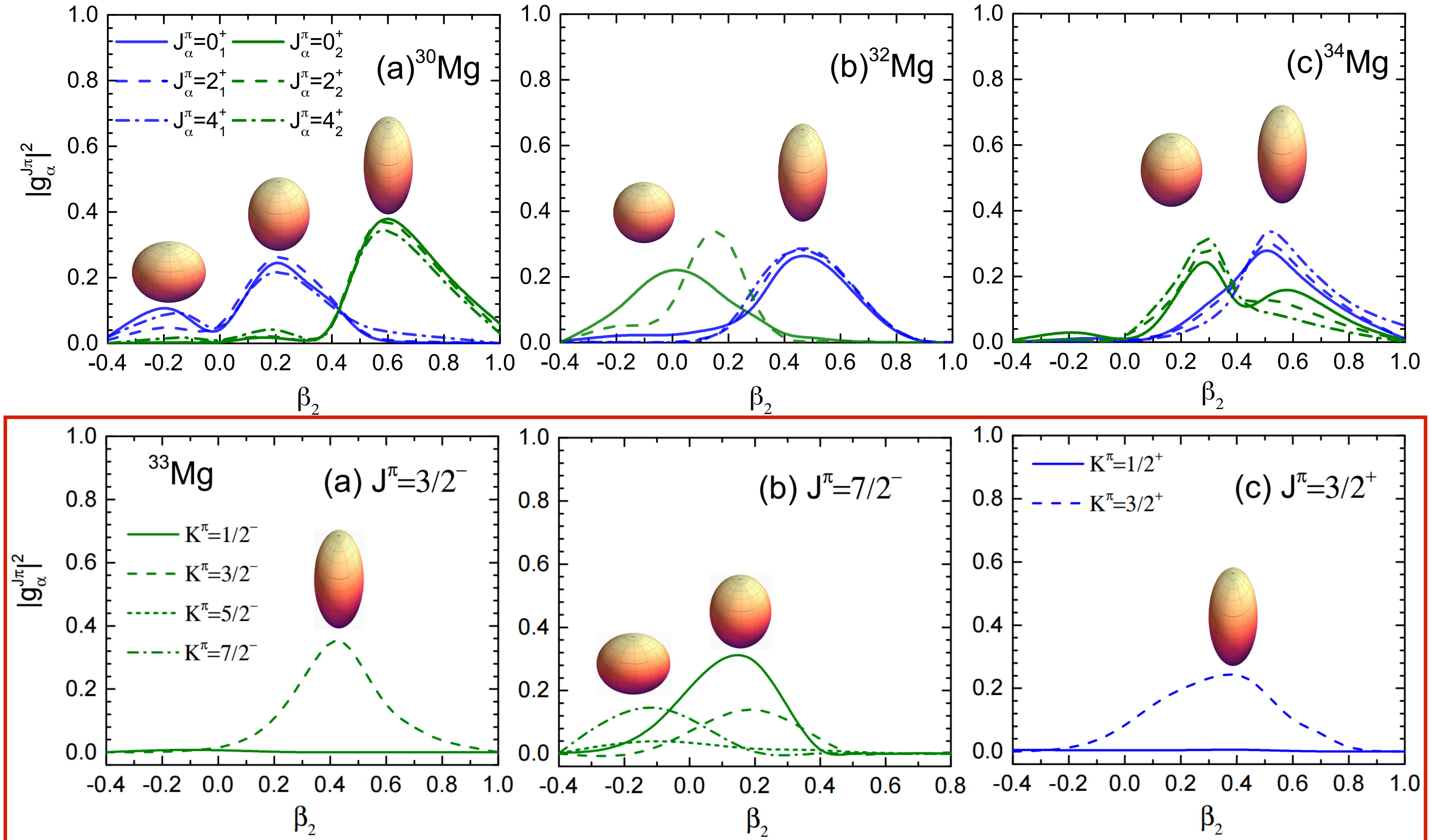
E. F. Zhou et al., arXiv:2410.23113

IM-GCM: **VS-IMSRG (Shell Model):**



Shape Mixing

E. F. Zhou et al., arXiv:2410.23113

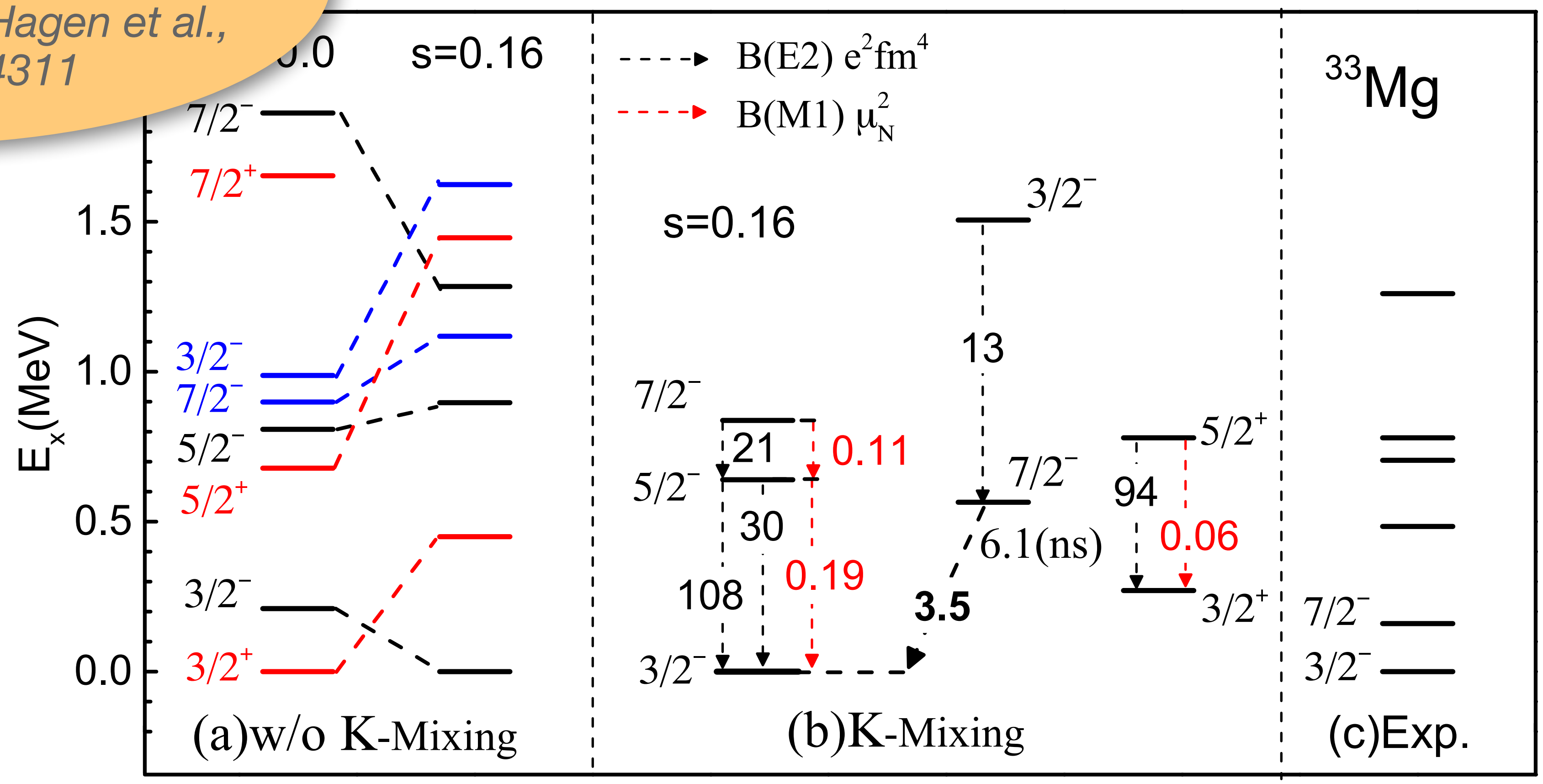


- **shape coexistence** can come with **shape mixing**
- **(but keep in mind:** wave function components are not observable)

N=20 Island of Inversion

E. F. Zhou et al., arXiv:2410.23113

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



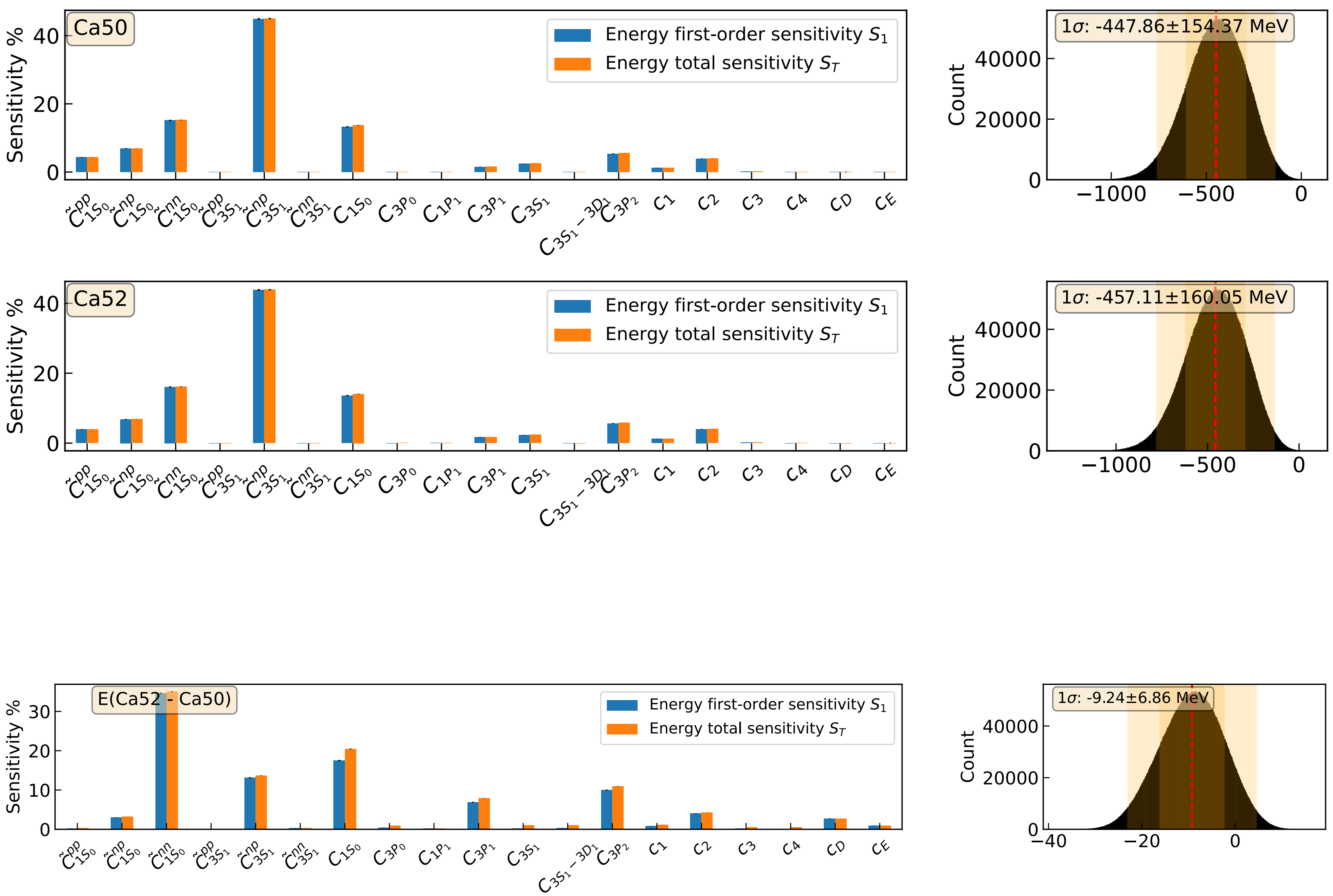
- **shape and K mixing have** notable impact on ^{33}Mg spectrum
- **boosts** lifetime of $\frac{7}{2}^{-}$ state - **predicted to be a shape isomer**
- related to ^{32}Na shape isomer measured at FDSi in 2023 ?
  [Gray et al., PRL 130, 132501]

Modern Uncertainty Quantification

- treat **model parameters** as **probability distributions** rather than just numbers
  - condition, calibrate, and validate with data
- **predictions for observables** become **probability distributions** as well
  - allows characterization of likelihood, standard deviations (=error bars), correlations, parameter sensitivity, …
- **challenge:** need **lots** of **expensive** many-body calculations
- **solution:** construct **emulators** for costly simulations - can reduce computational effort by **many orders of magnitude** (but still need **training data**)

Emulators for the IMSRG

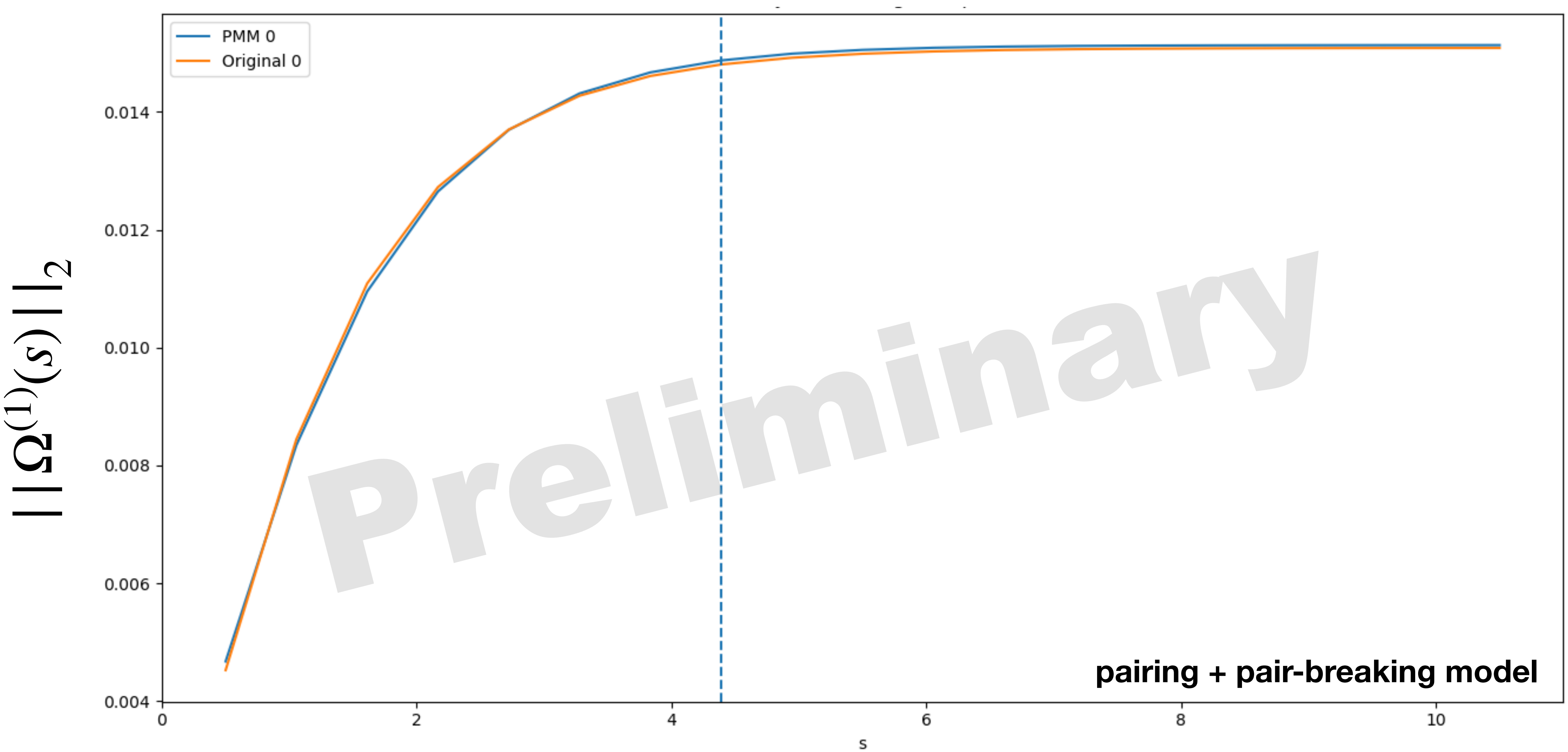
J. Davison, HH, J. Crawford, S. Bogner, arXiv:2503.xxxx



- 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 Model Emulators

B. Clark, P. Cook, …
also see: S. Yoshida, Particles 2025, 8



- DMD fails for Magnus operator if snapshots are taken during initial stages of flow…
- … but PMMs seem to work

Parametric Matrix Model Emulators

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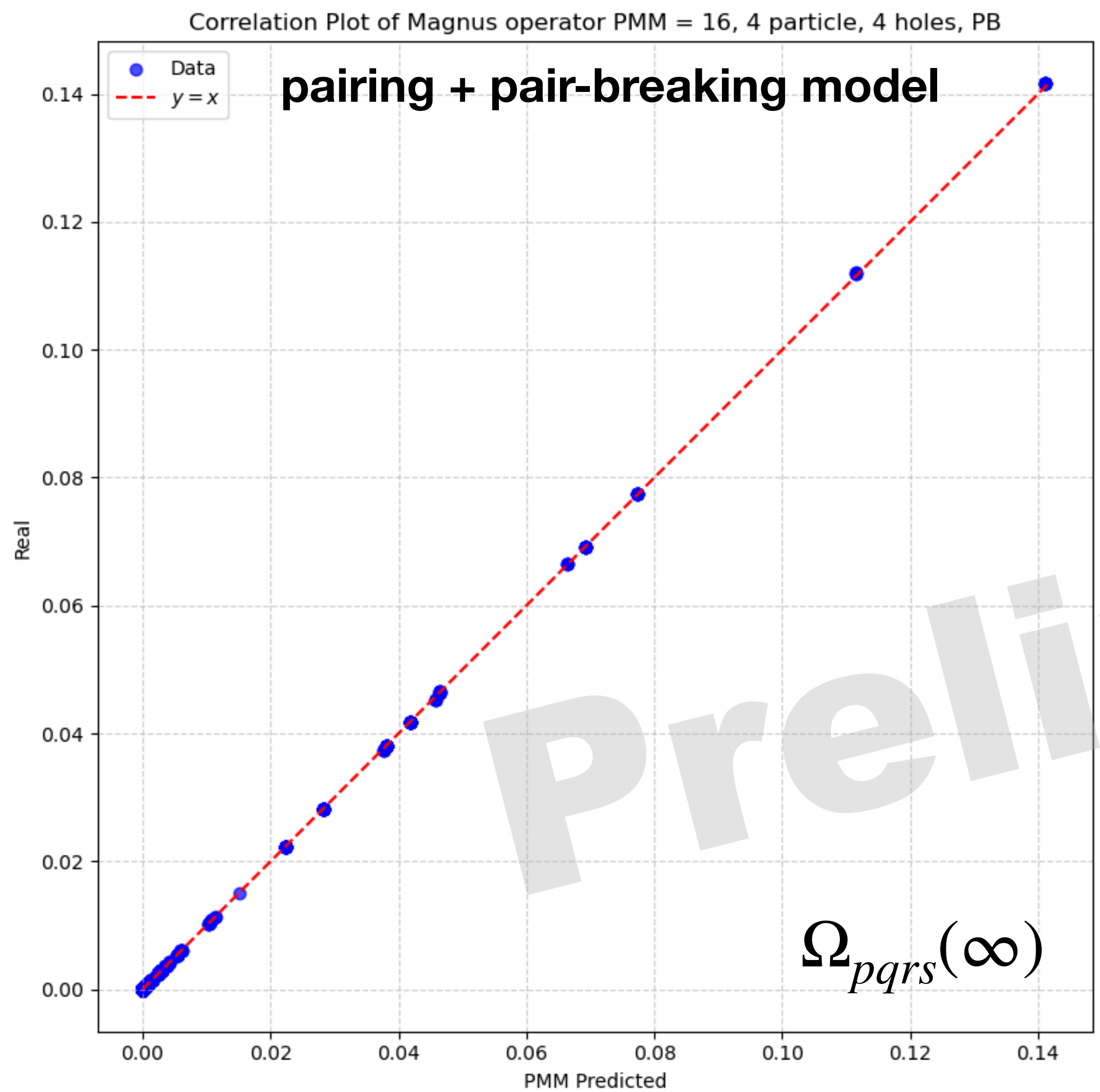
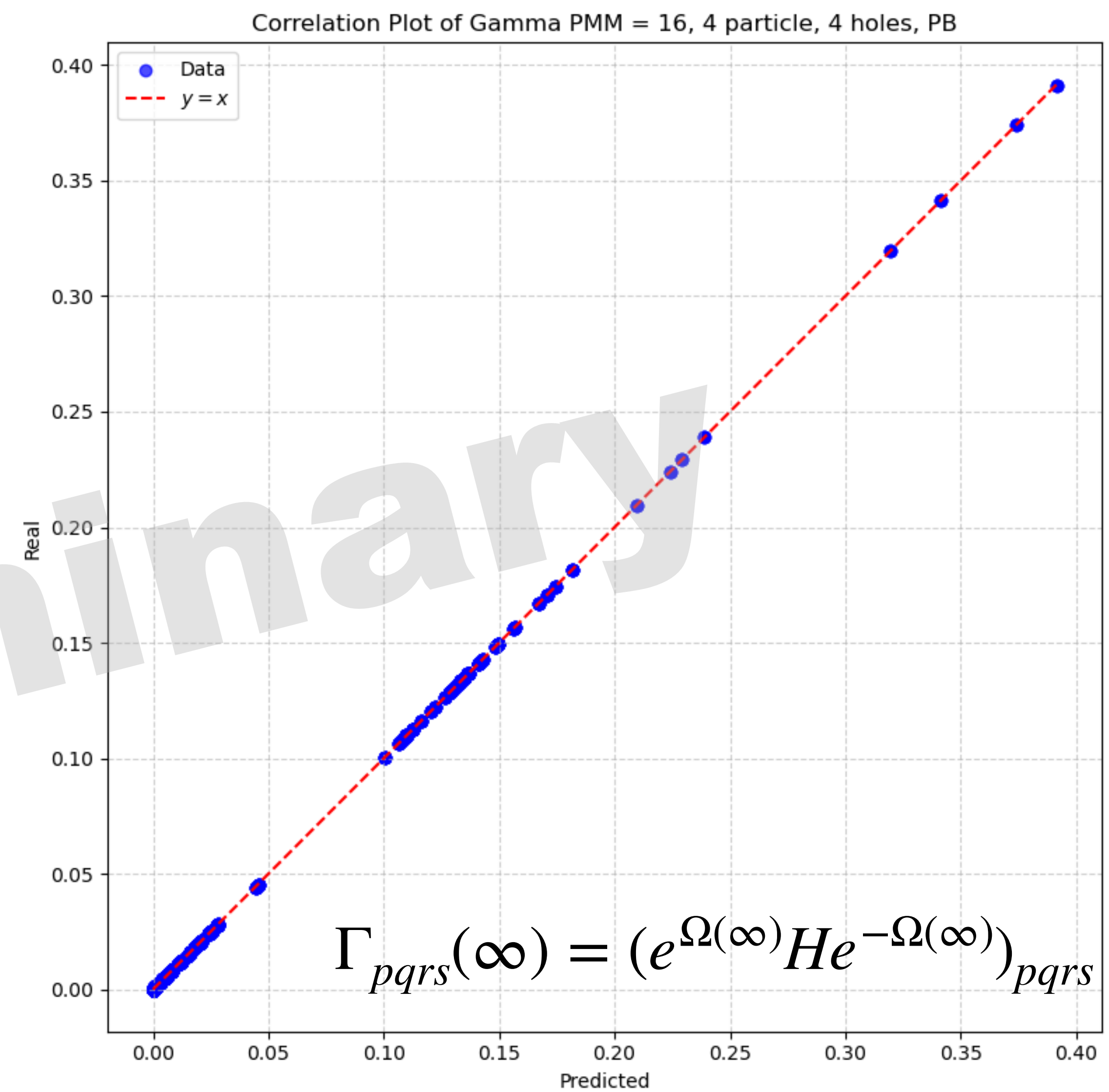




- DMD fails for Magnus operator if snapshots are taken during initial stages of flow…
- … but PMMs seem to work

Where Do We Go From Here?

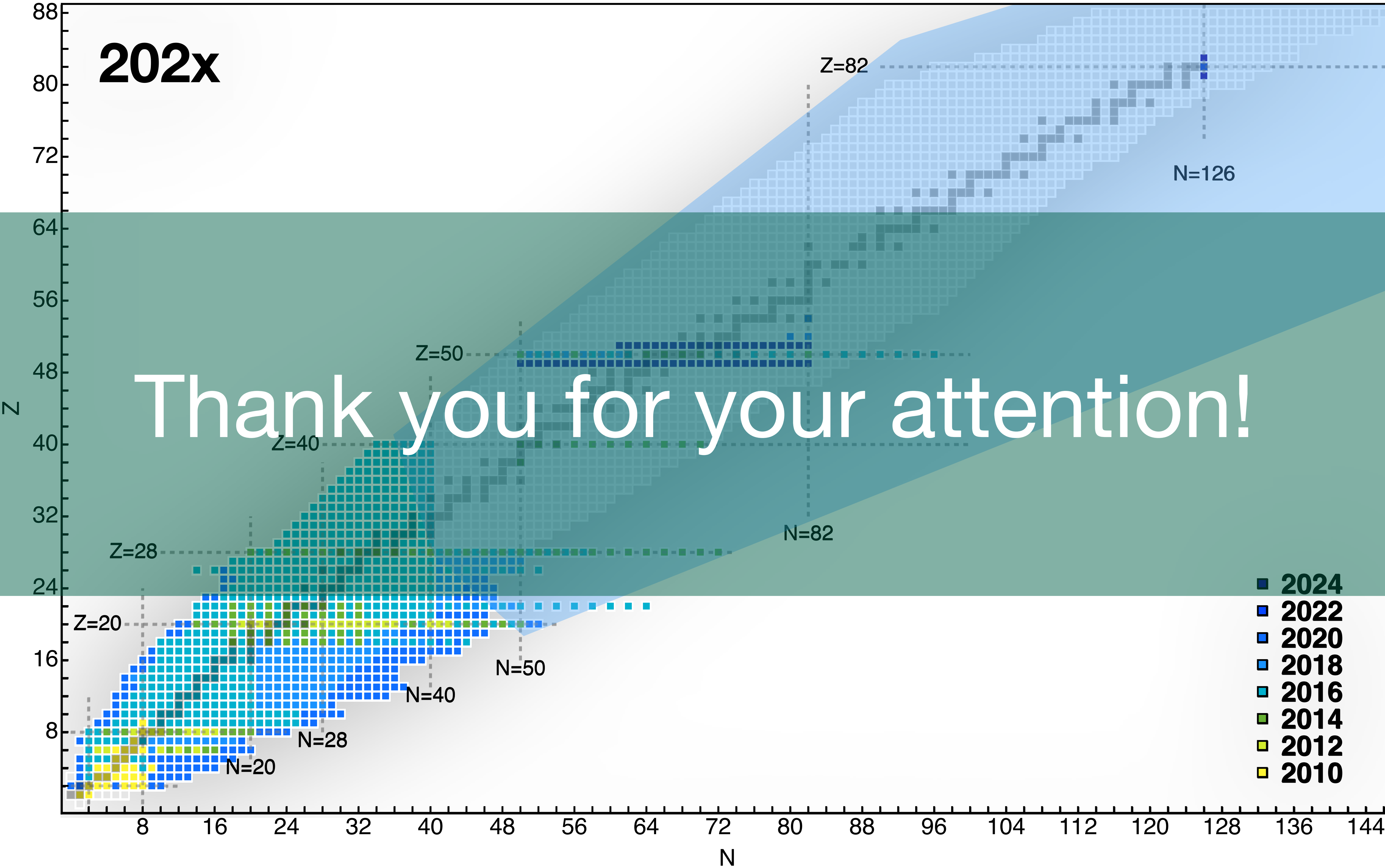
What Is Next?

- **improved truncations:** (MR-)IMSRG(3) + factorized approximations, tailored operator bases
- **accelerate IMSRG & IM-GCM**
  - (random) **compression & tensor factorization**
  - model reduction for **projection / GCM kernels ?**
- **uncertainty quantification / sensitivity analysis**
  - emulator development, Parametric Matrix Models, …
- **applications**
  - working on requests from multiple experimental groups
  - …lear observables relevant for BSM physics (beta … for CKM unitarity, Schiff moments, …)

also see talk
by P. Geysers

Progress in *Ab Initio* Calculations

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



Thank you for your attention!

Acknowledgments

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and many more…

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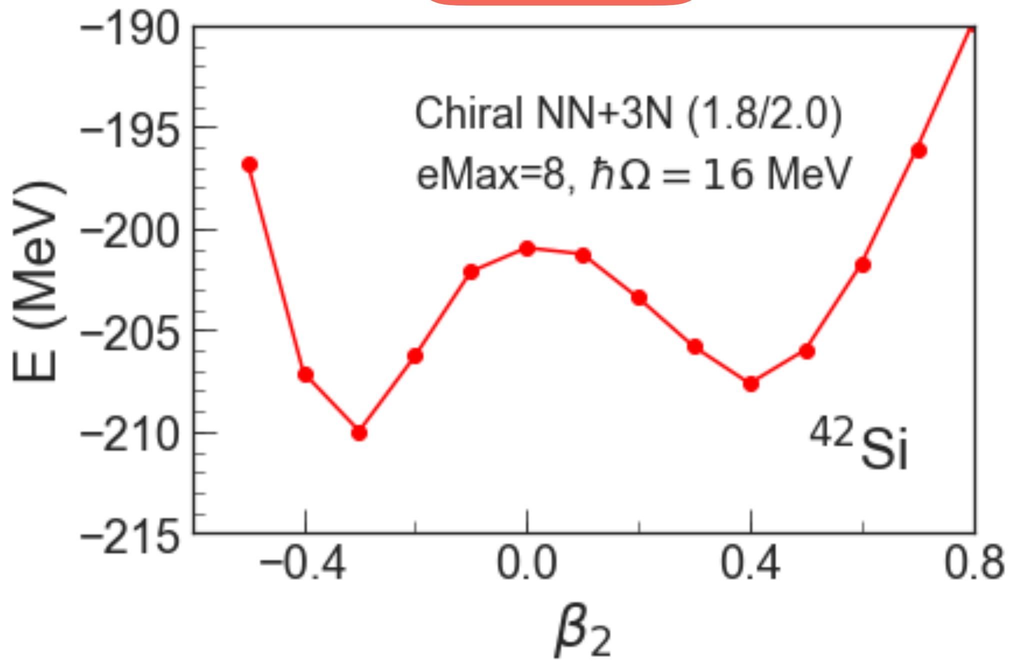
NUCLEI Nuclear Computational Low-Energy Initiative NERSC ICER

Supplements

Projected GCM

HFB
Generate reference state



Take into account static correlations (pairing, deformation) via symmetry breaking.

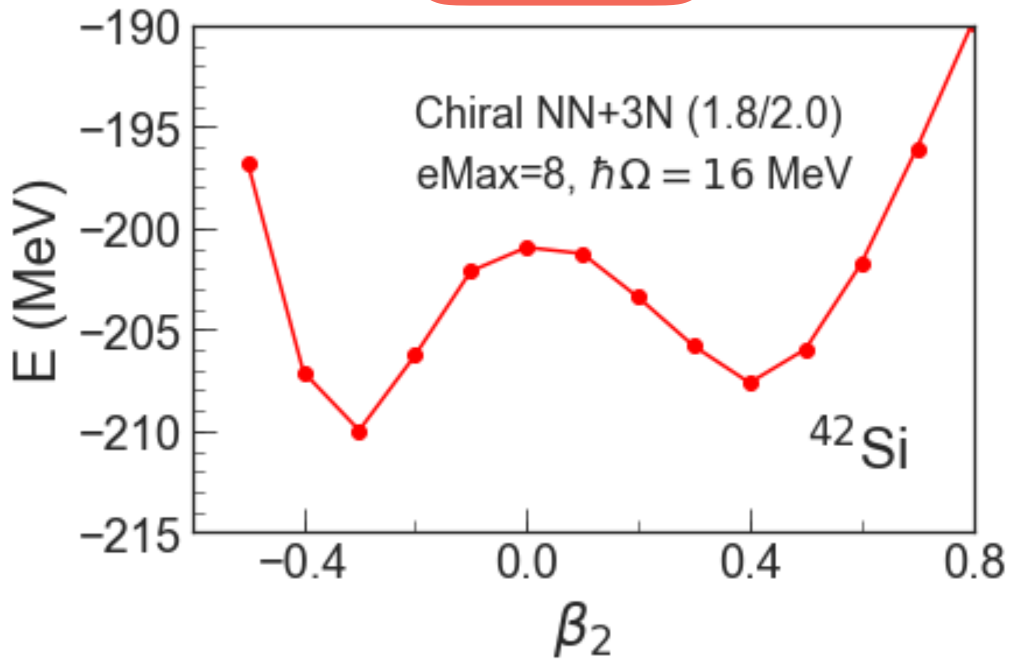
$$\frac{\langle \mathrm{HFB}(\mathbf{q})|\hat{H}|\mathrm{HFB}(\mathbf{q})\rangle}{\langle \mathrm{HFB}(\mathbf{q})|\mathrm{HFB}(\mathbf{q})\rangle}$$

Potential Energy Surface

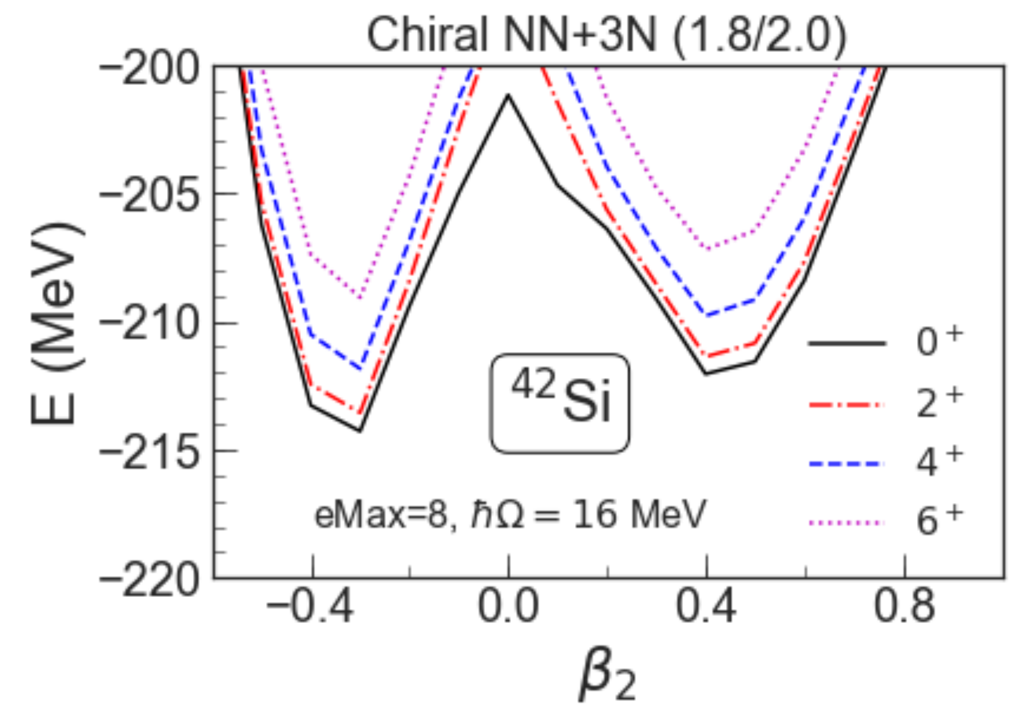
[slides by **J. M. Yao**]

Projected GCM

HFB
Generate reference state

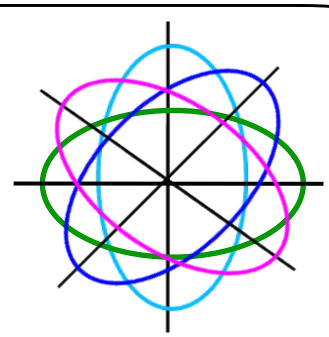


Projection
Compute different kernels



particle-number projector

$$\hat{P}_{N_0} = \frac{1}{2\pi}\int_0^{2\pi} d\phi_N \underbrace{e^{-i\phi_N N_0}}_{\text{weight}} \overbrace{e^{i\phi_N \hat{N}}}^{\text{rotation in gauge space}}$$



angular-momentum restoration operator

$$\hat{P}^J_{MK} = \frac{2J+1}{16\pi^2}\int_0^{4\pi} d\alpha \int_0^{\pi} d\beta \,\sin(\beta) \int_0^{2\pi} d\gamma \underbrace{\mathcal{D}^{*J}_{MK}(\alpha,\beta,\gamma)}_{\text{Wigner function}} \overbrace{\hat{R}(\alpha,\beta,\gamma)}^{\text{rotation in real space}}$$

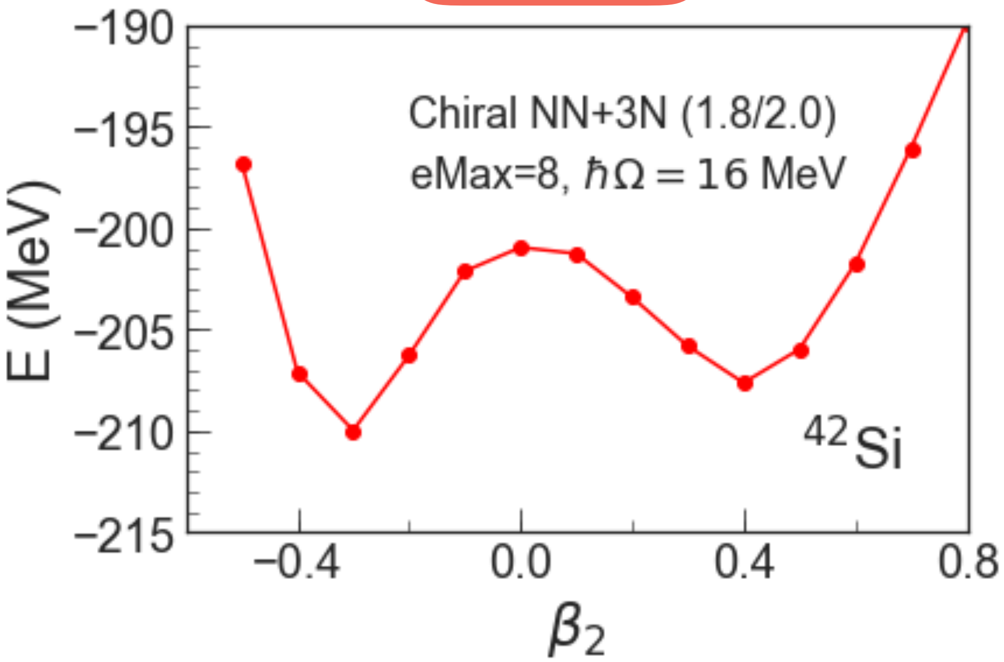
$$|\Phi^{JNZ}(\mathbf{q})\rangle = \hat{P}^J_{MK}\hat{P}_{N_0}\hat{P}_{Z_0}|\mathbf{q}\rangle$$

$$\frac{\langle\Phi^{JNZ}(\mathbf{q})|\hat{H}|\Phi^{JNZ}(\mathbf{q})\rangle}{\langle\Phi^{JNZ}(\mathbf{q})|\Phi^{JNZ}(\mathbf{q})\rangle}$$

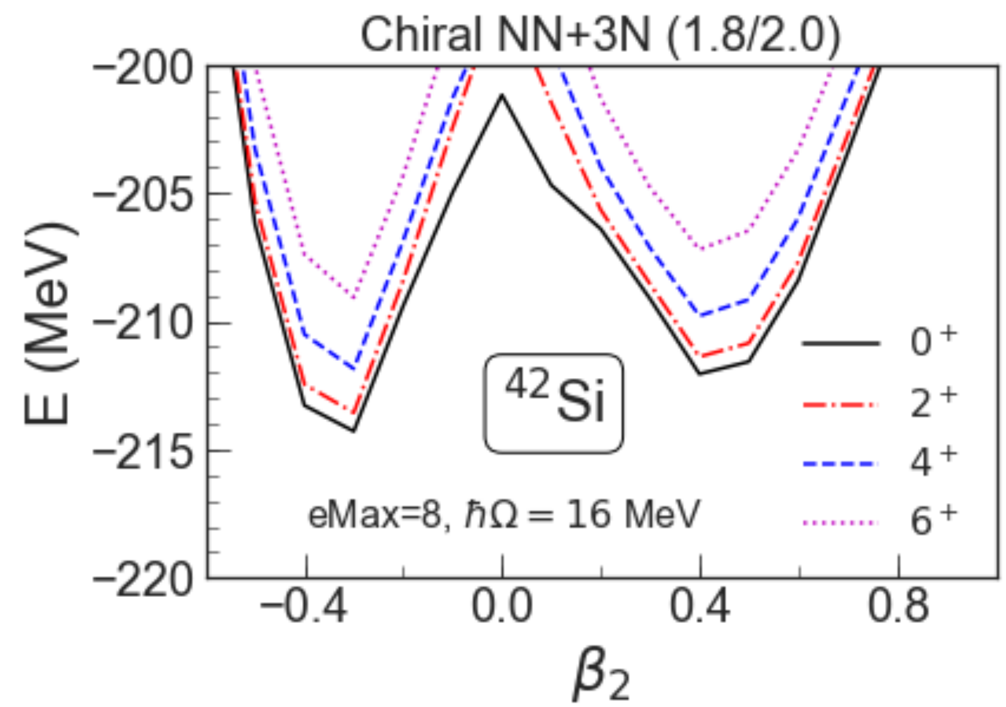
[slides by **J. M. Yao**]

Projected GCM

HFB
Generate reference state



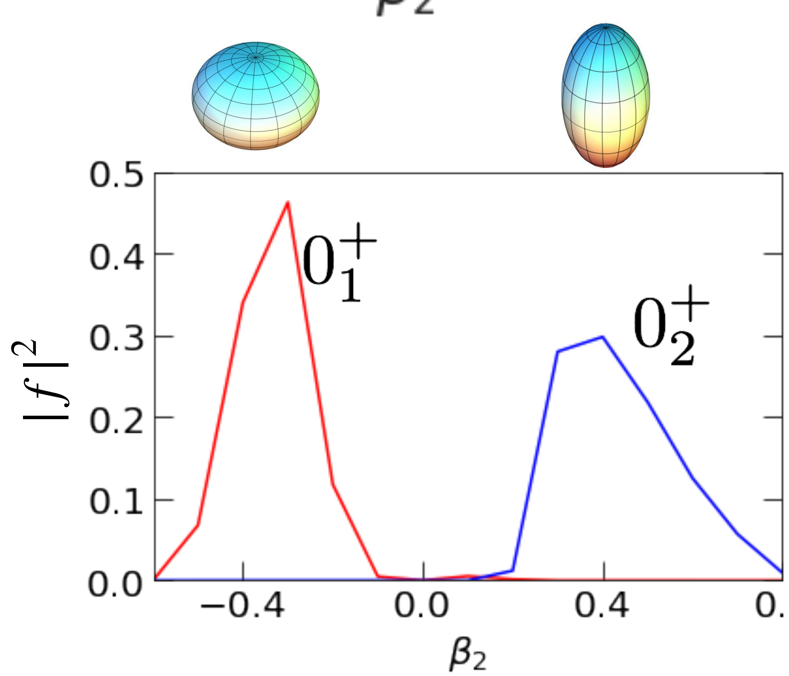
Projection
Compute different kernels



$$|\Phi\rangle = \sum_{\mathbf{q}} f^J(\mathbf{q})|\Phi^{JNZ}(\mathbf{q})\rangle$$

$$\sum_{\mathbf{q}_b} \left[\mathscr{H}^J_{\mathbf{q}_a,\mathbf{q}_b} - E^J_\alpha \mathscr{N}^J_{\mathbf{q}_a,\mathbf{q}_b}\right] f^J_\alpha(\mathbf{q}_b) = 0$$

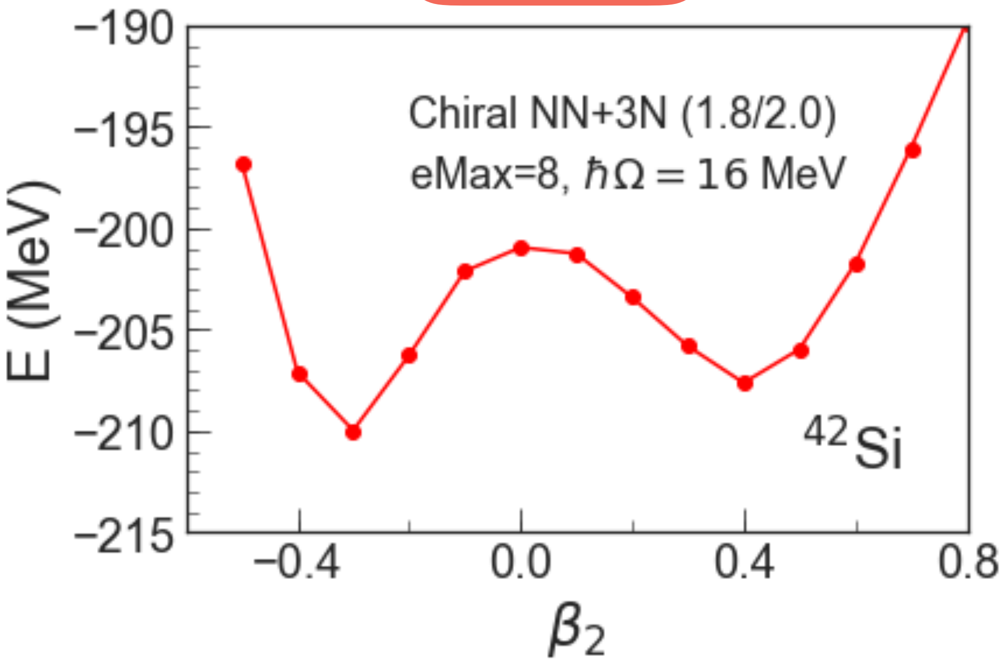
GCM
Solve
Hill-Wheeler equation



[slides by **J. M. Yao**]

Projected GCM

HFB
Generate reference state



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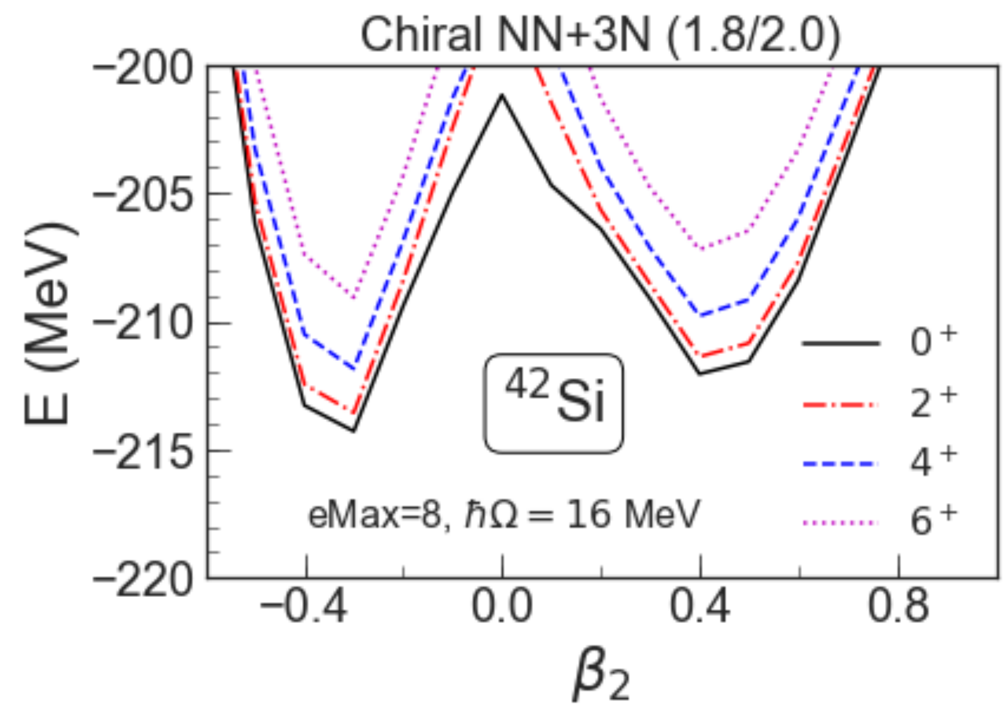
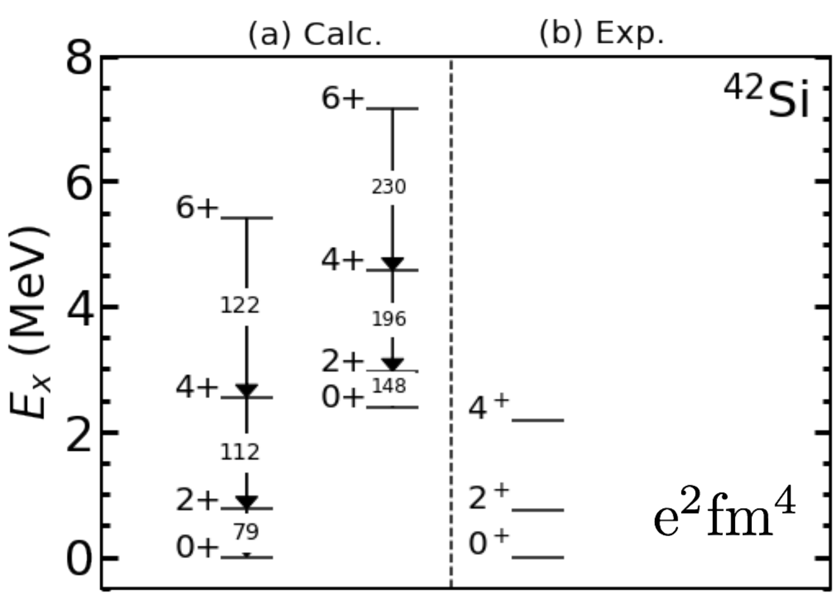
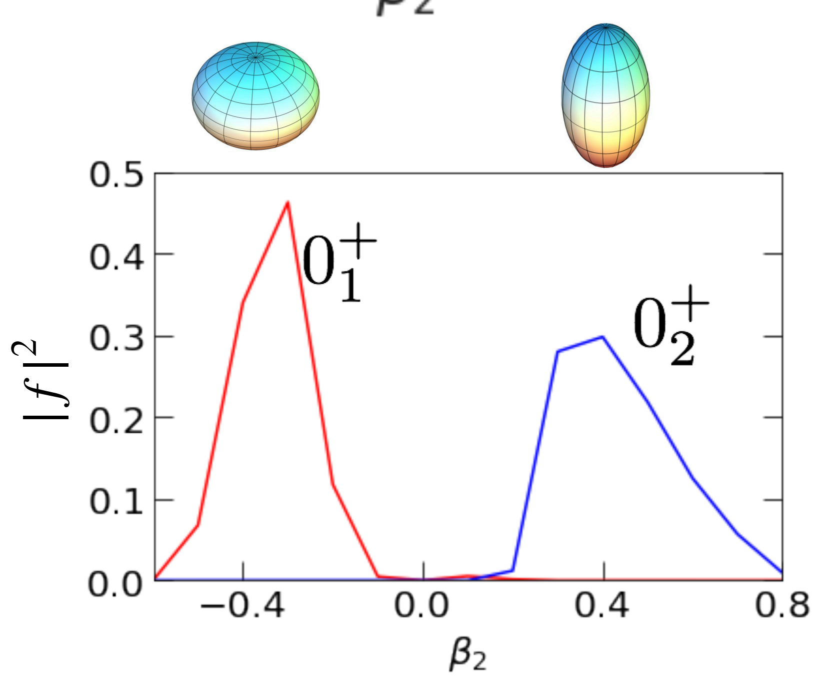


GCM
Solve Hill-Wheeler equation

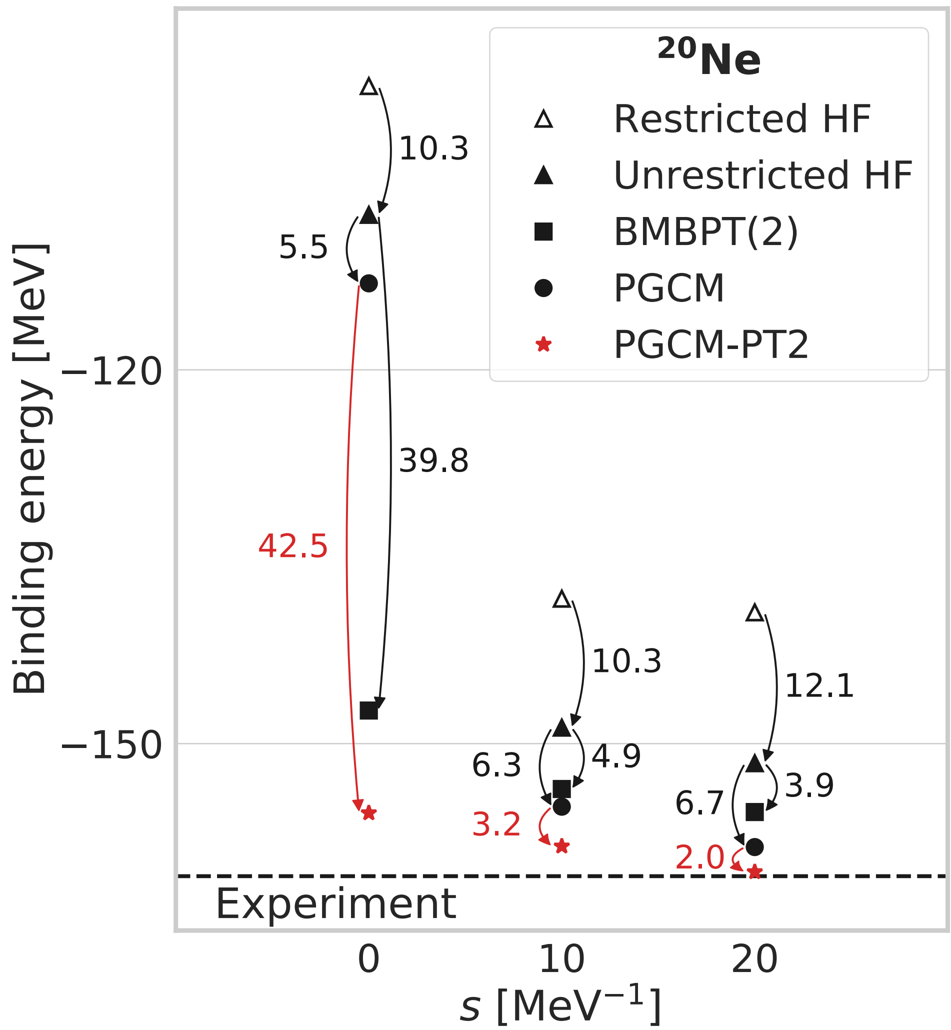


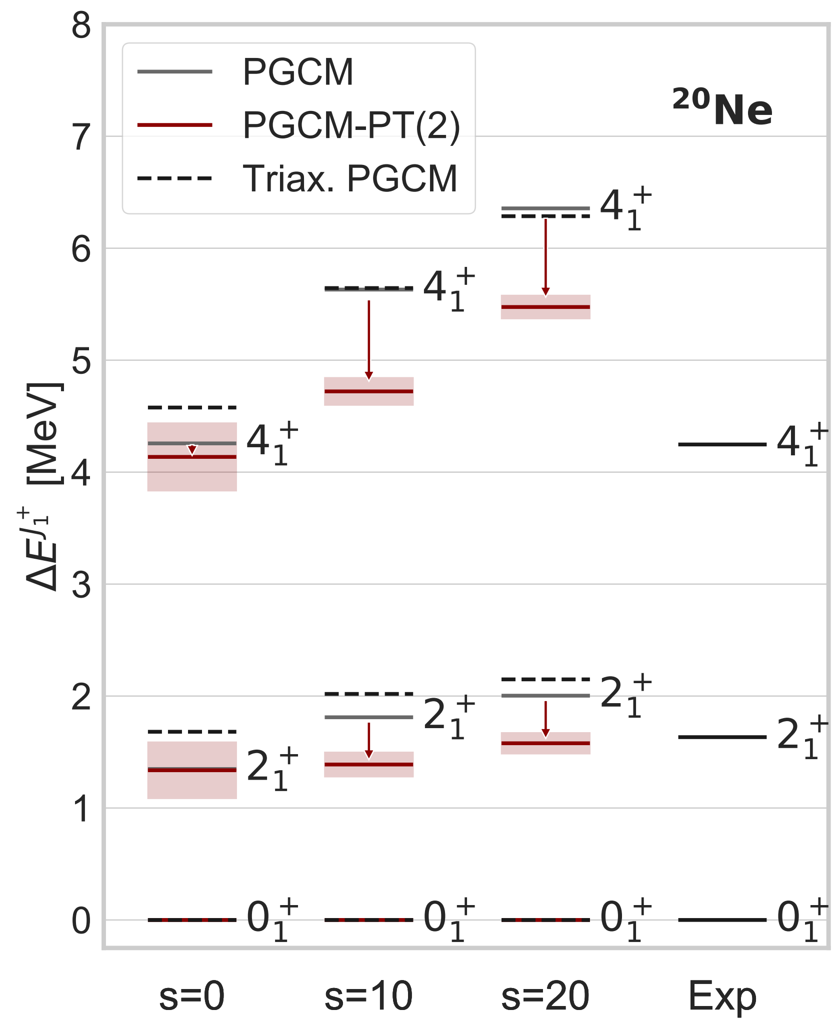


[slides by **J. M. Yao**]

Perturbative Enhancement of IM-GCM

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

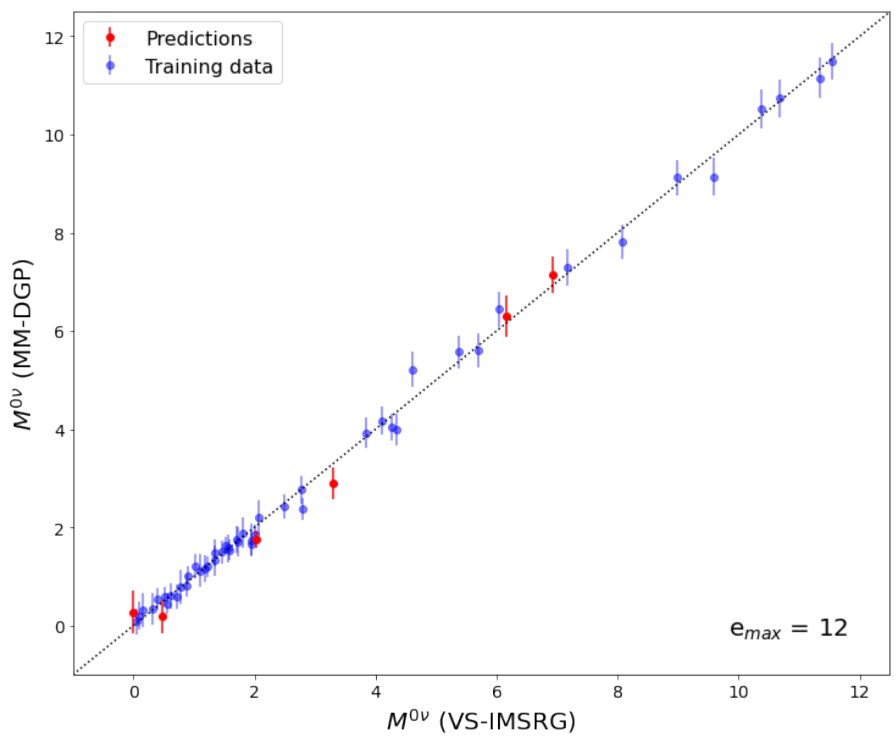


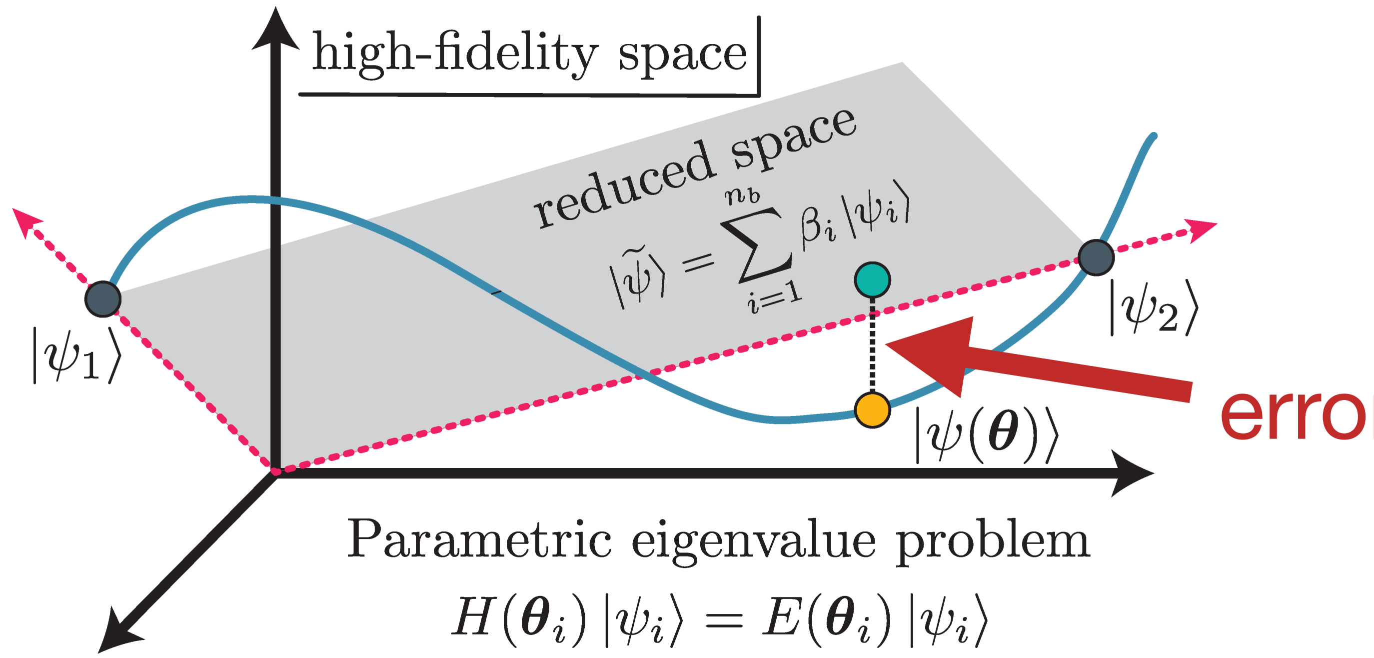


- s-dependence is a **built-in diagnostic tool** for IM-GCM **(not available in phenomenological GCM)**
    - if operator and wave function offer sufficient degrees of freedom, evolution of observables is unitary
- need **richer references and/or IMSRG(3)** for certain observables

Emulators

J. Melendez et al., JPG 49, 102001 (2022), C. Drischler et al., Front. Phys. 10, 1092931 (2023)
E. Bonilla et al., PRC 106, 054322 (2022), P. Giuliani et al., Front. Phys. 10, 1054524 (2023)
J. Pitcher, A. Belley et al., in preparation, A. Belley et al., arXiv:2308.15643 (v2)



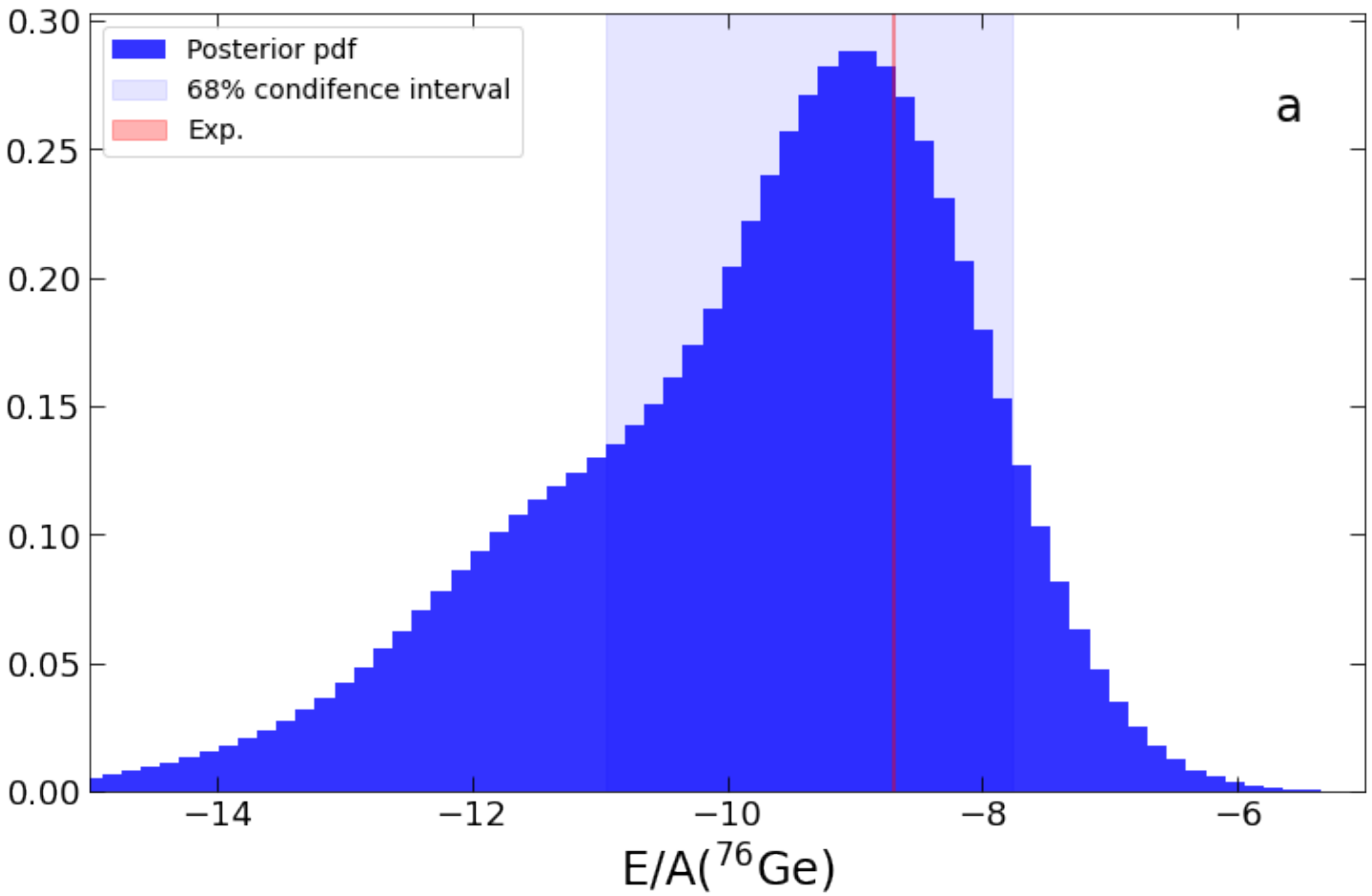


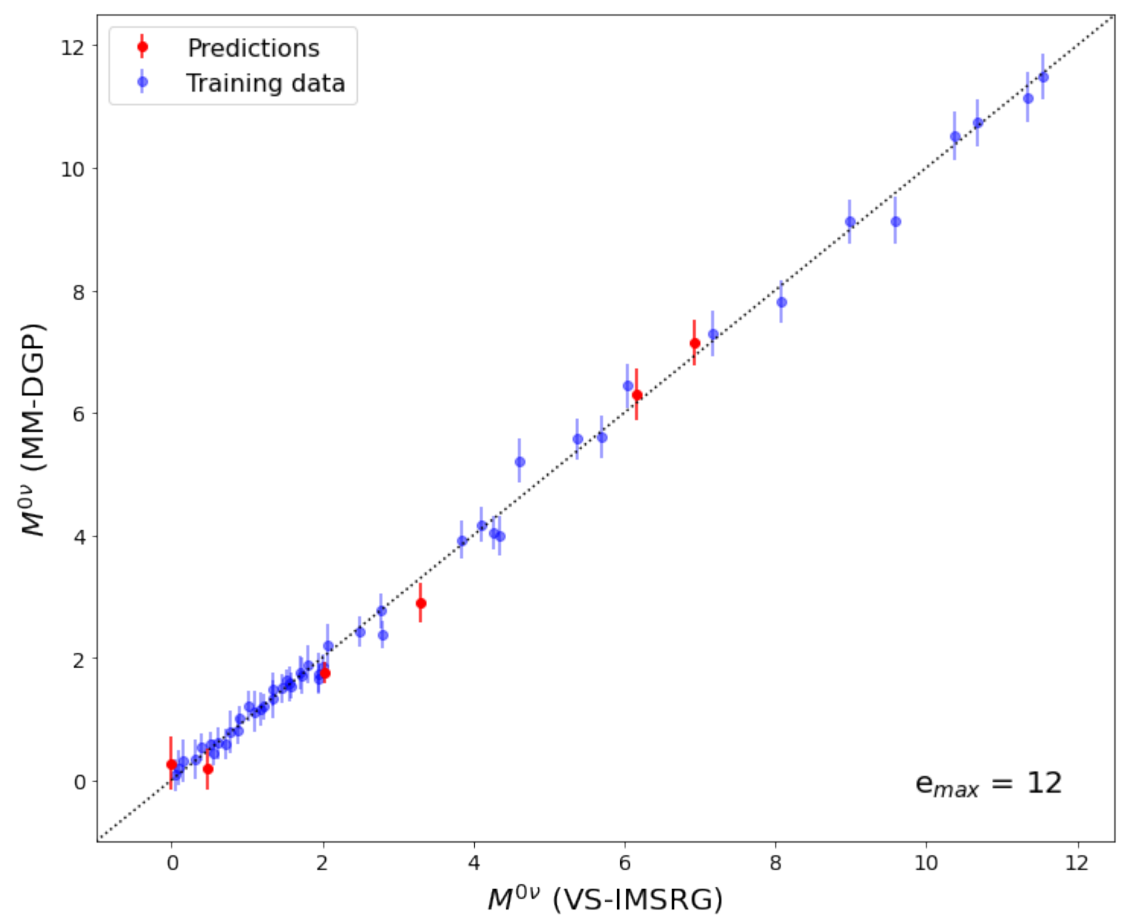
- **Data driven** (only expectation values)
- E.g. Multi-output, Multi-fidelity **Deep Gaussian Processes** (MM-DGP)

- **Physics driven** reduced-order models (ROMs)
- E.g., **Galerkin projection** for bound-state or scattering wave functions

Emulating Data (^{76}Ge NMEs)

J. Pitcher, A. Belley et al., in preparation
A. Belley et al., arXiv:2308.15643



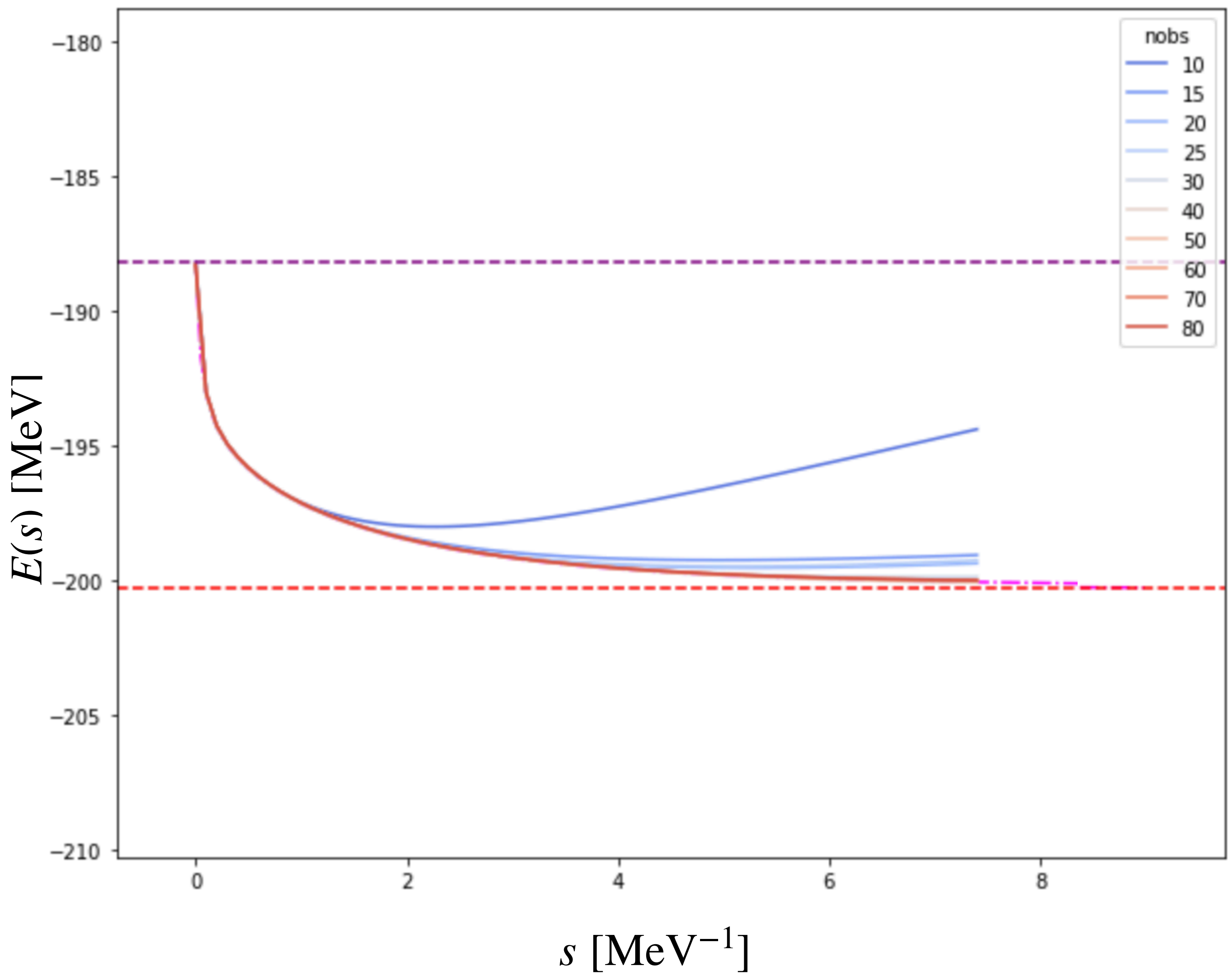


- **Deep Gaussian Process** emulator for observables (**purely data-driven**)
- 8818 **non-implausible** Δ-full NNLO NN+3N interactions (cf. neutron skin study) + EM1.8/2.0 & family, ΔNNLO$_{GO}$, …

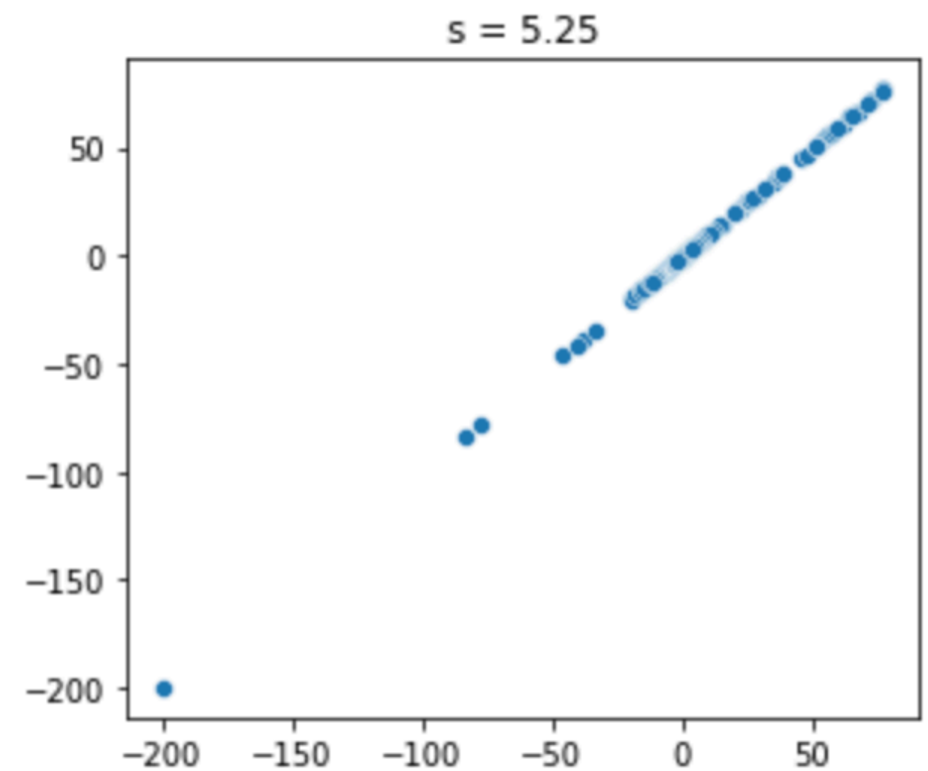
Emulating IMSRG Flows

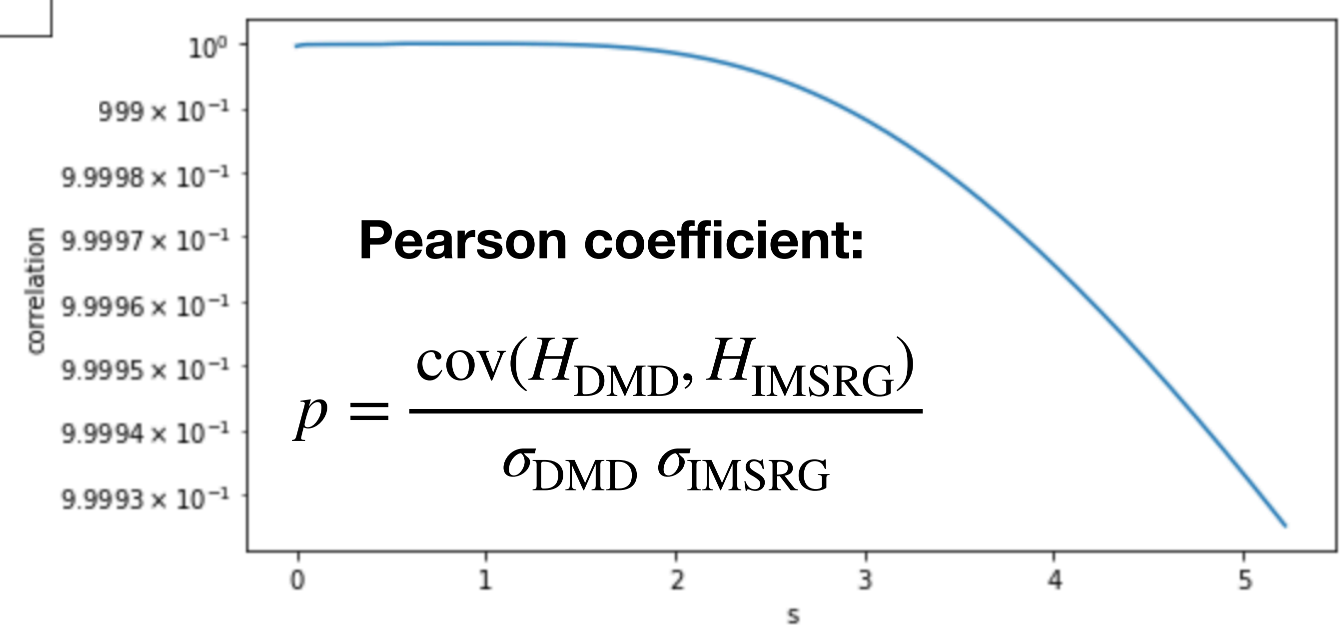
J. Davison, HH, J. Crawford, S. Bogner, in preparation

EM(500) N³LO, $\lambda = 2.0\,\mathrm{fm}^{-1}$



$H_{\mathrm{DMD}}(s)$ vs. $H_{\mathrm{IMSRG}}(s)$





Pearson coefficient:

$$p = \frac{\mathrm{cov}(H_{\mathrm{DMD}}, H_{\mathrm{IMSRG}})}{\sigma_{\mathrm{DMD}}\ \sigma_{\mathrm{IMSRG}}}$$

Dynamic Mode Decomposition **emulator** "learns" **all flowing operator coefficients** from snapshots!