New Extensions and Applications of the IMSRG

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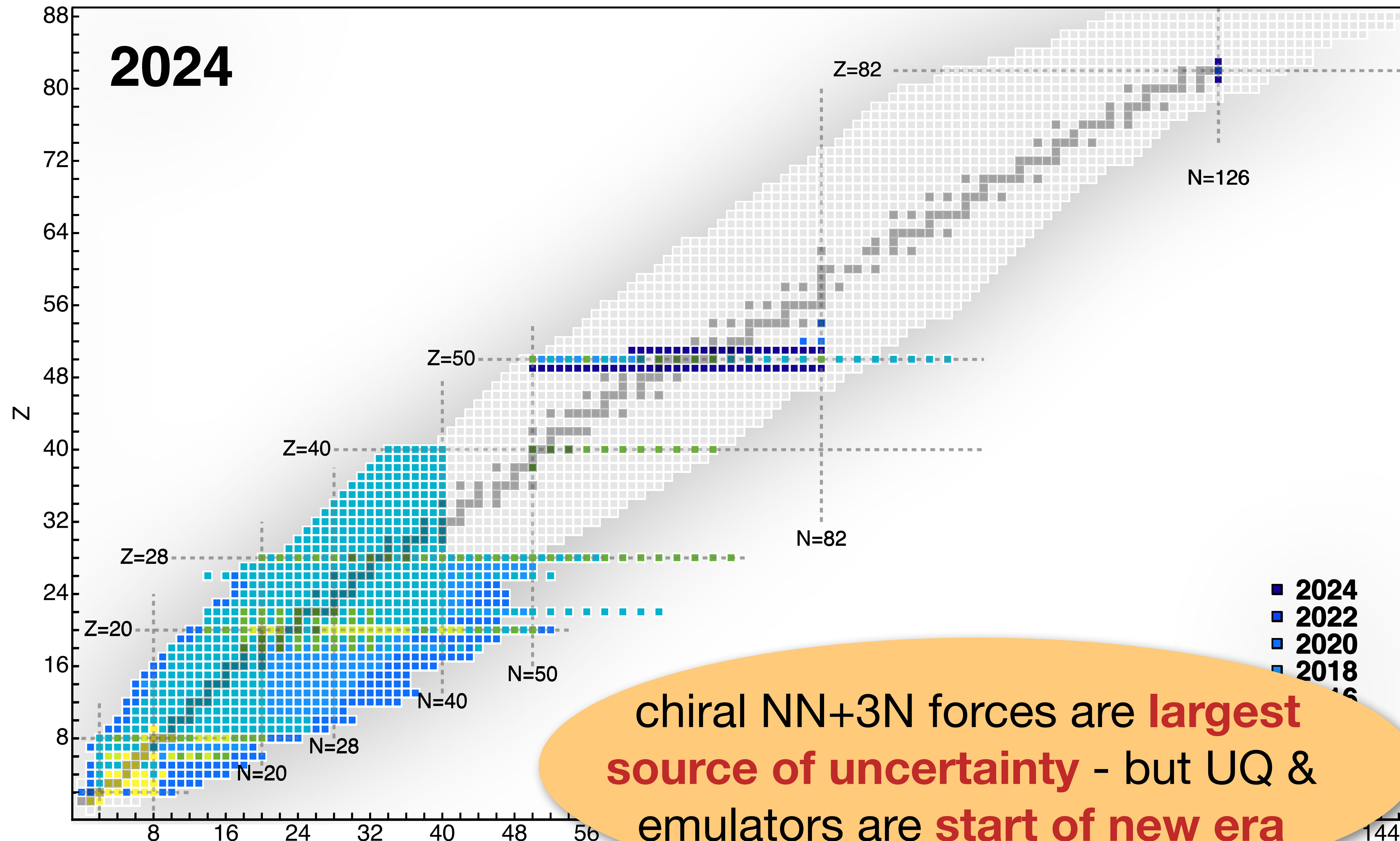
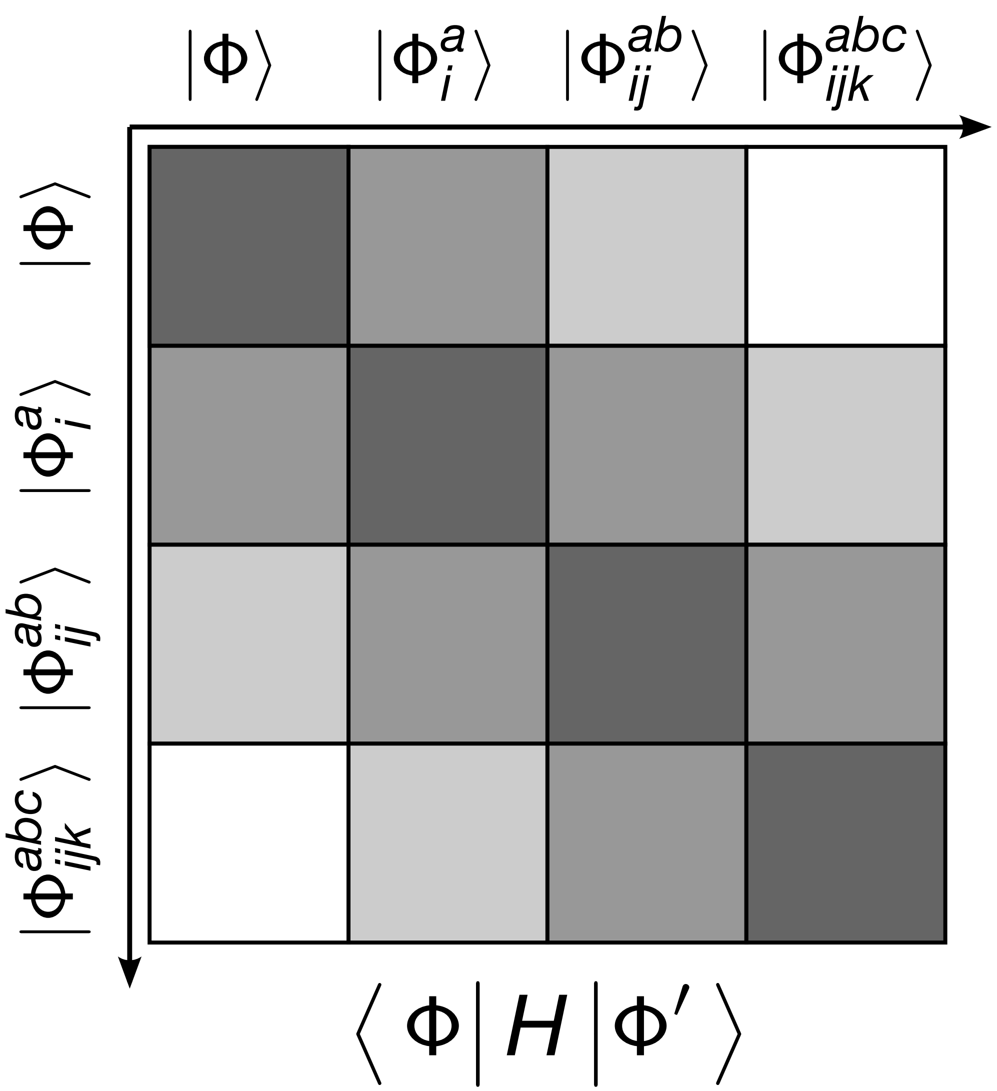
Progress in *Ab Initio* Calculations

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



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

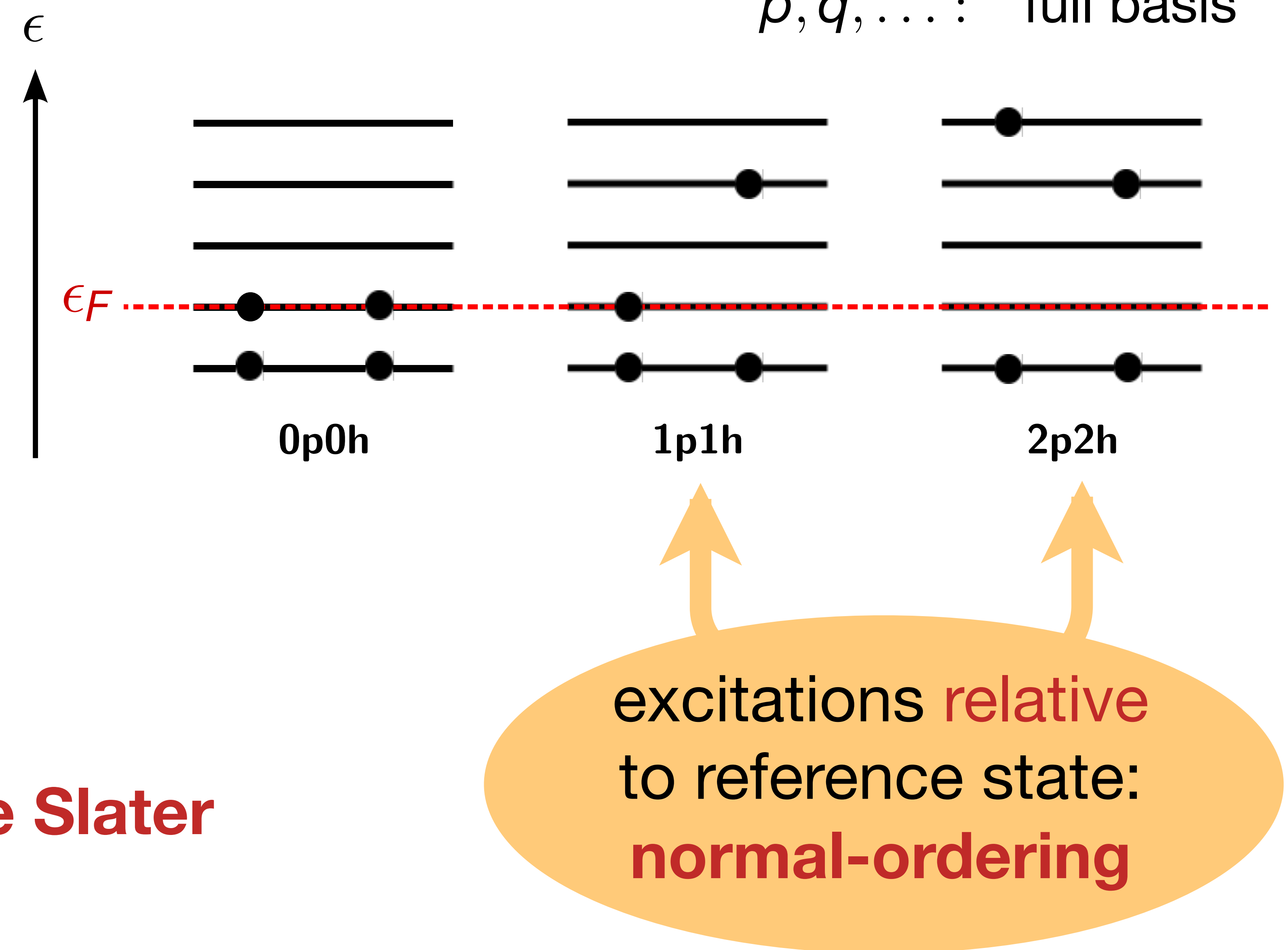
Transforming the Hamiltonian



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

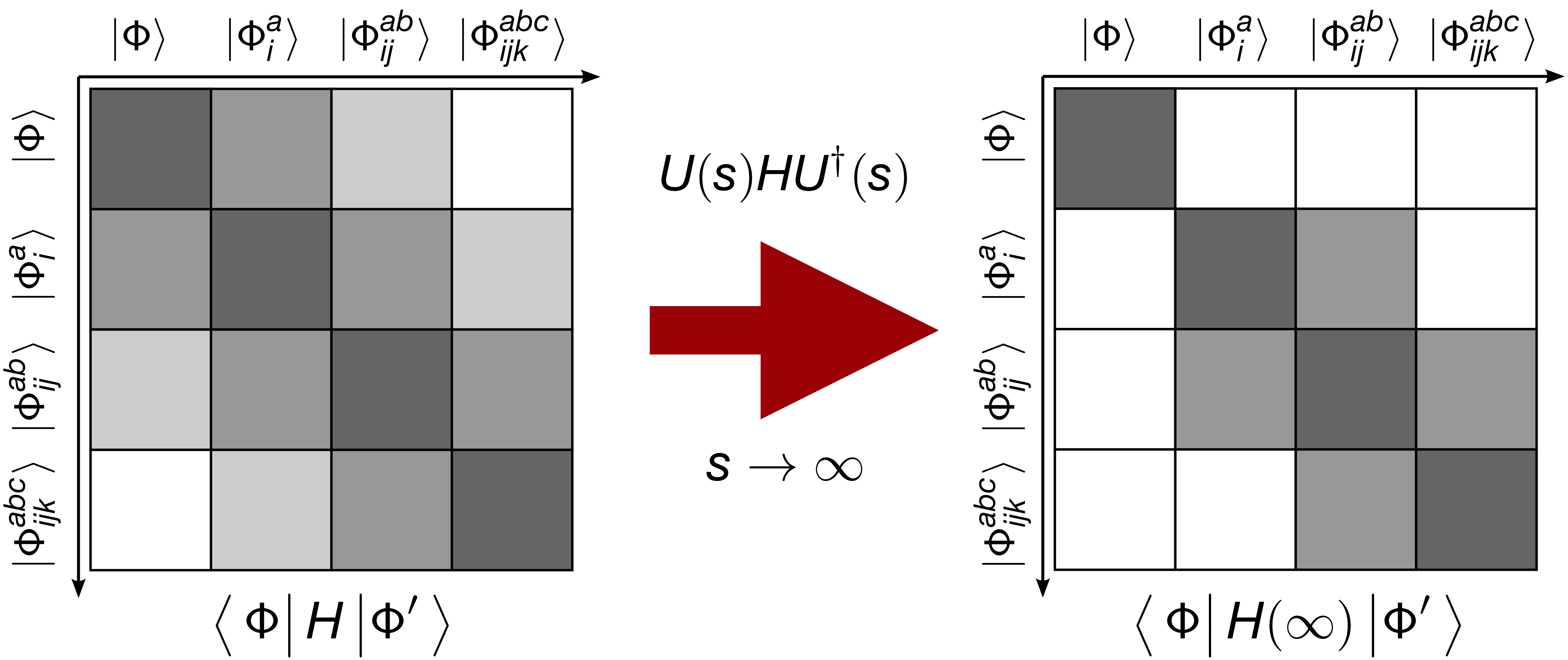
$i, j, \ldots : \quad \epsilon \leq \epsilon_F$

$p, q, \ldots :$ full basis



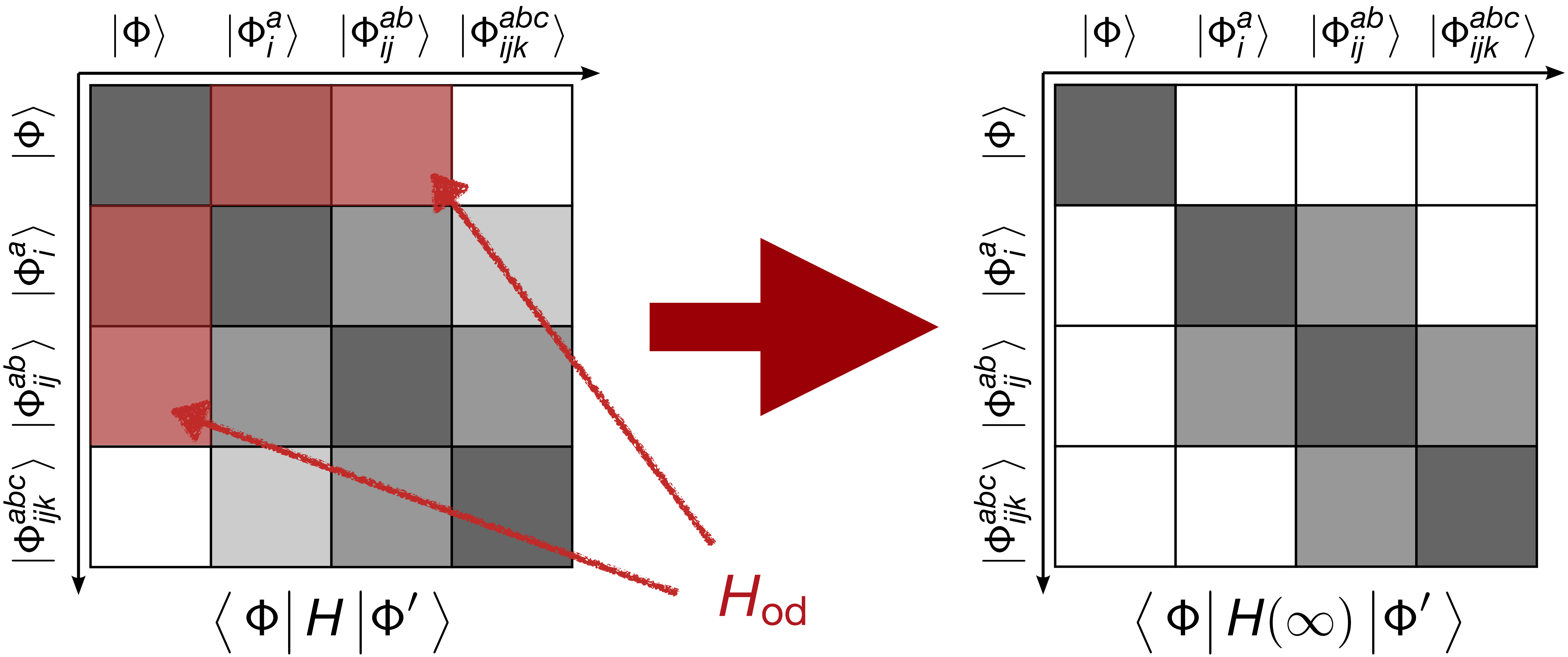
- reference state: **single Slater determinant**

Decoupling in A-Body Space



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

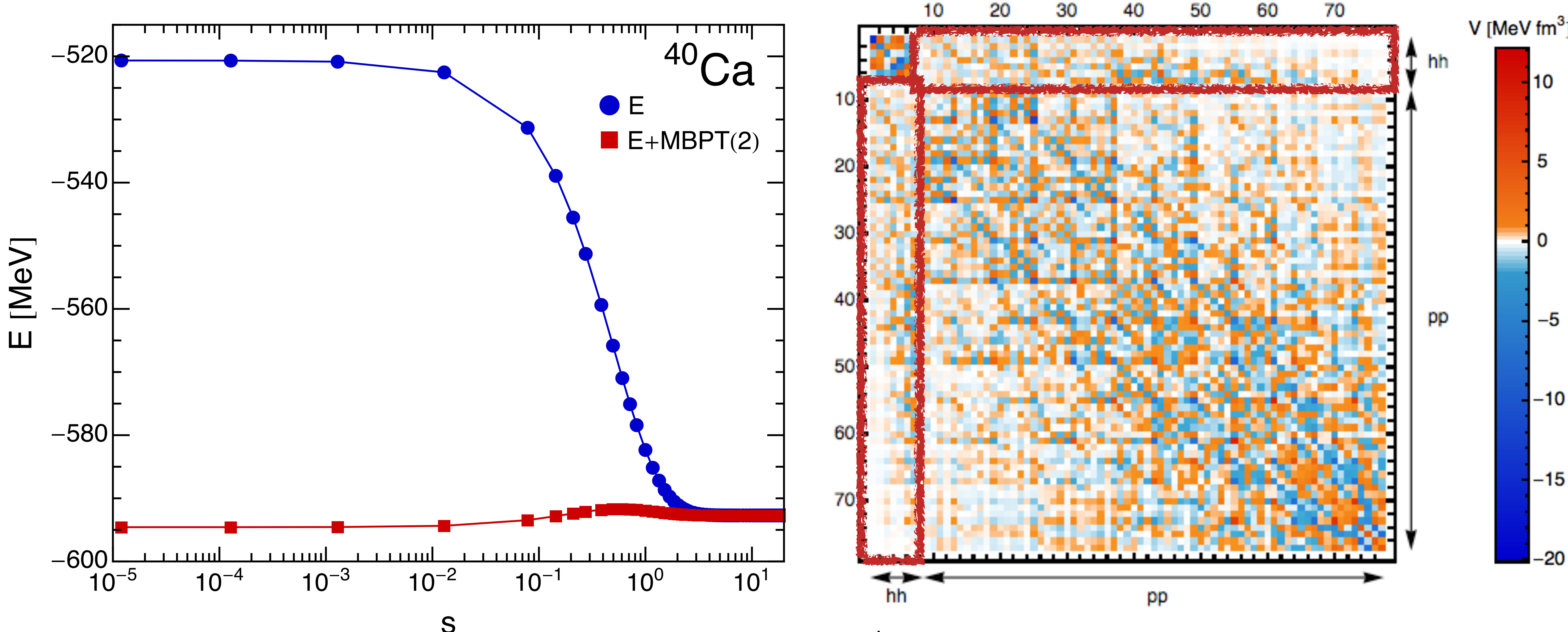
Flow Equation



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

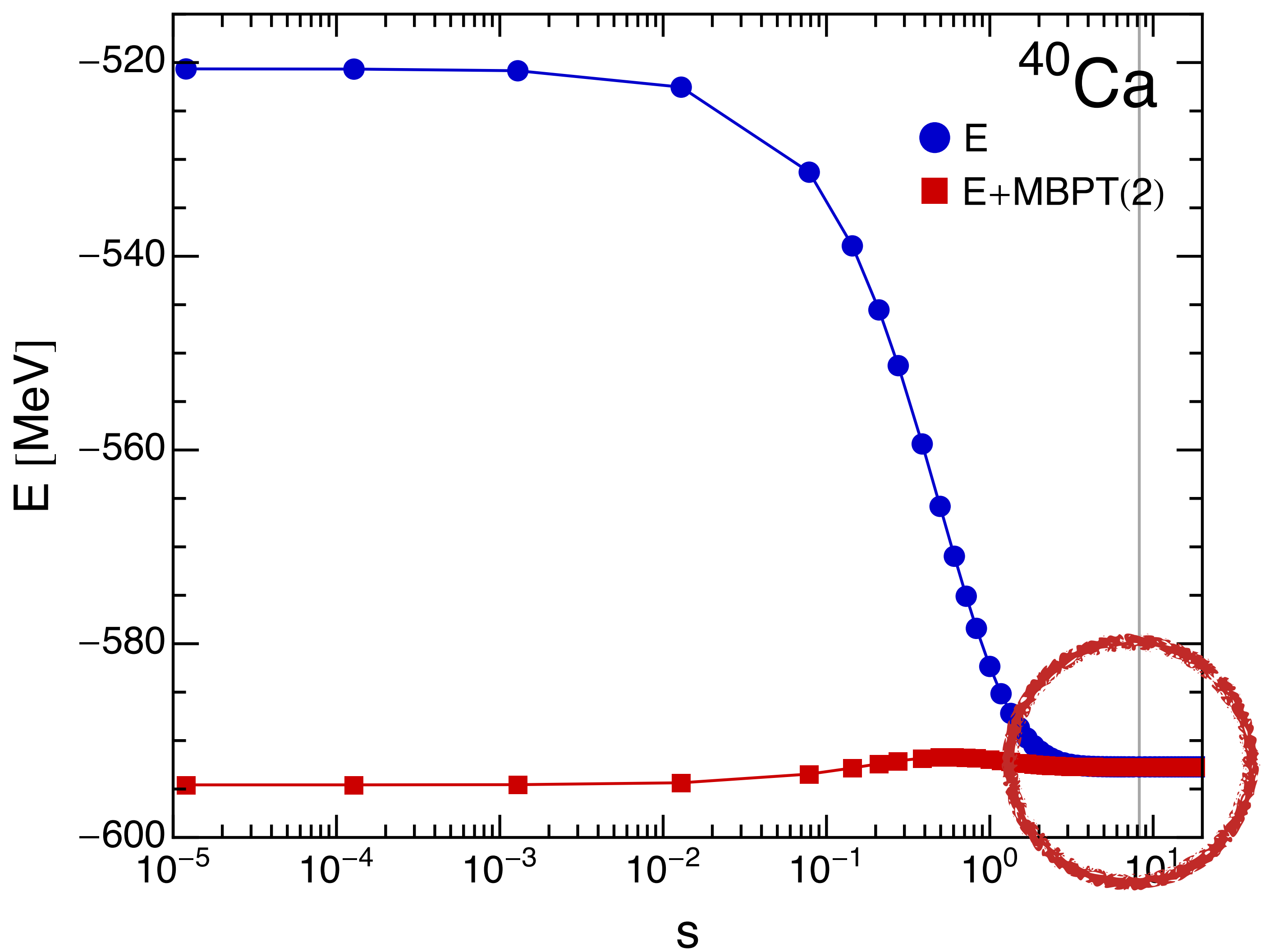
Operators
truncated at **two-body level** -
matrix is never constructed explicitly!

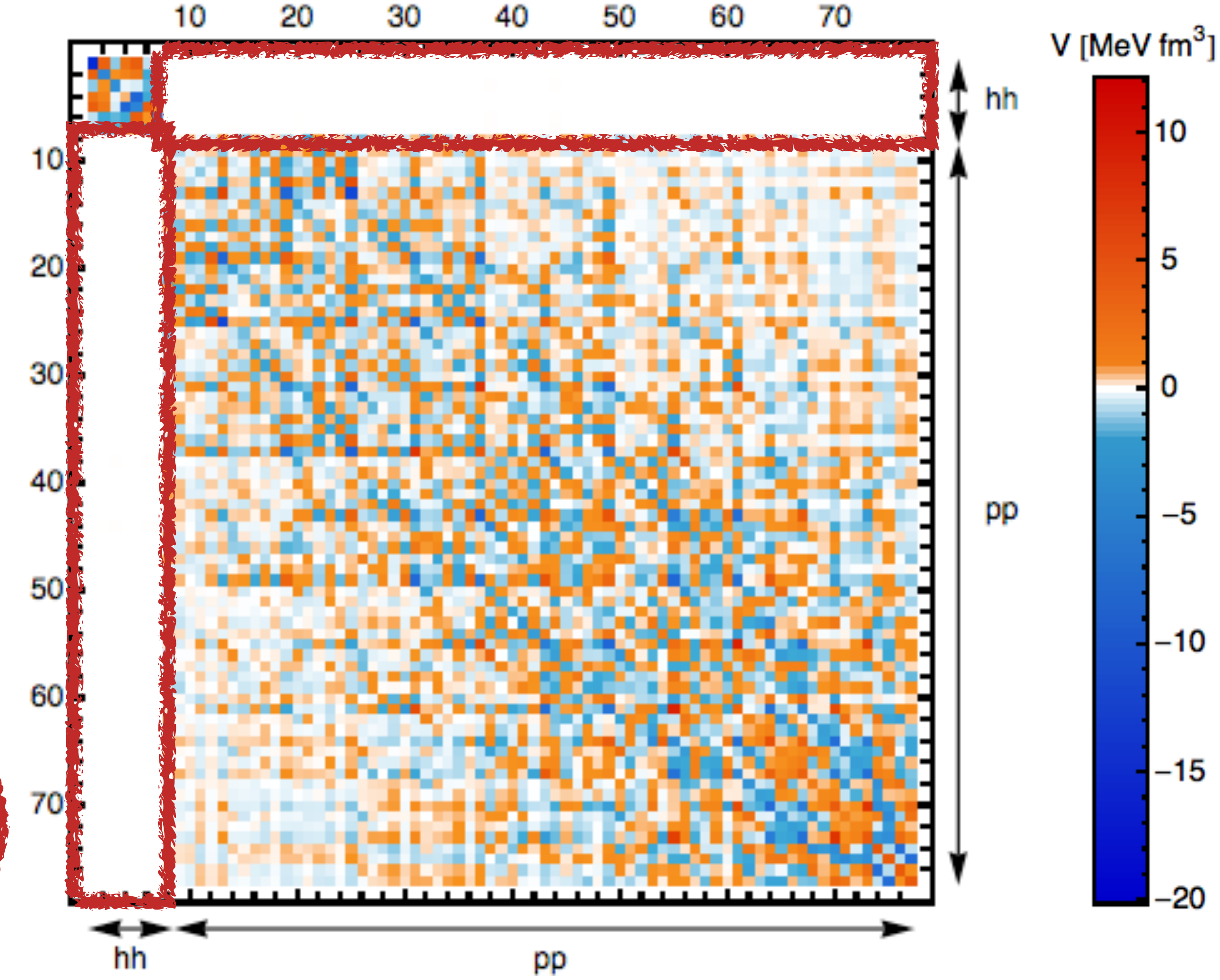
Decoupling



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

Decoupling



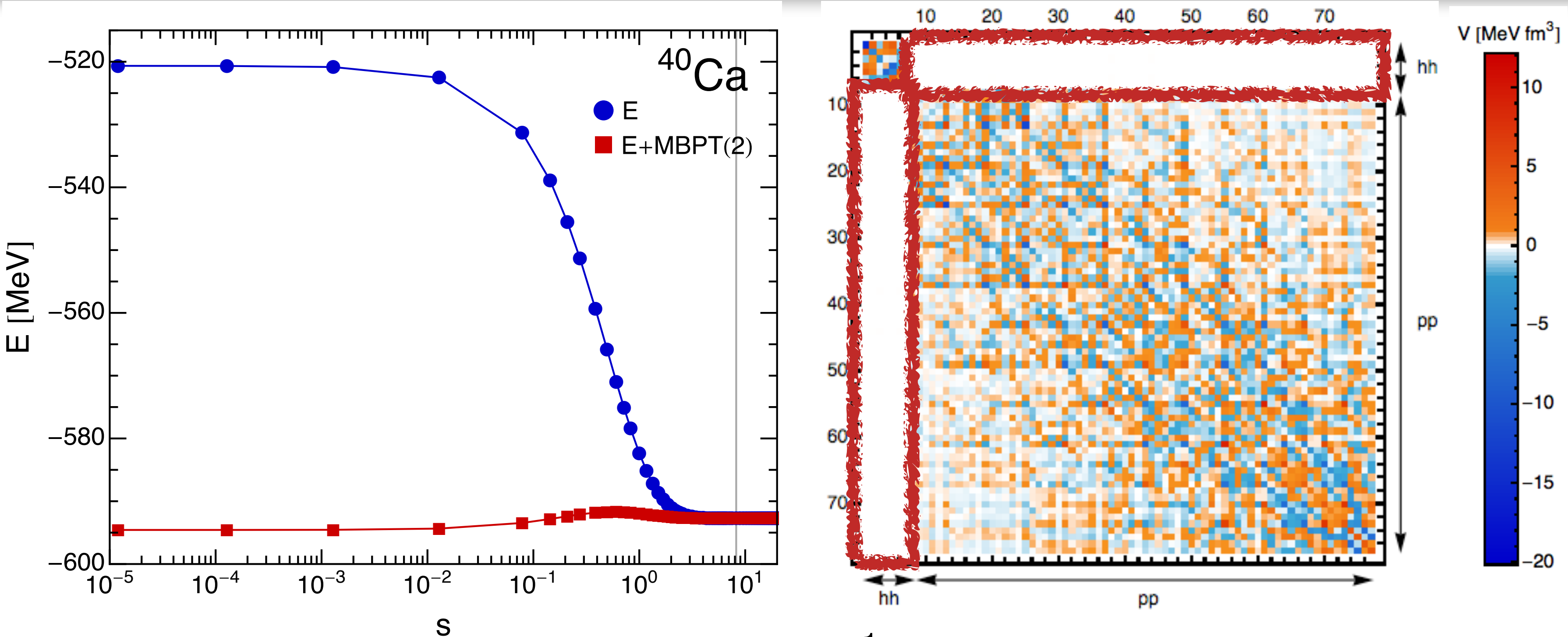


N3LO, $\lambda = 2.0\ \mathrm{fm}^{-1}, e_{\mathrm{Max}} = 8$

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

off-diagonal couplings are rapidly driven to zero

Decoupling



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

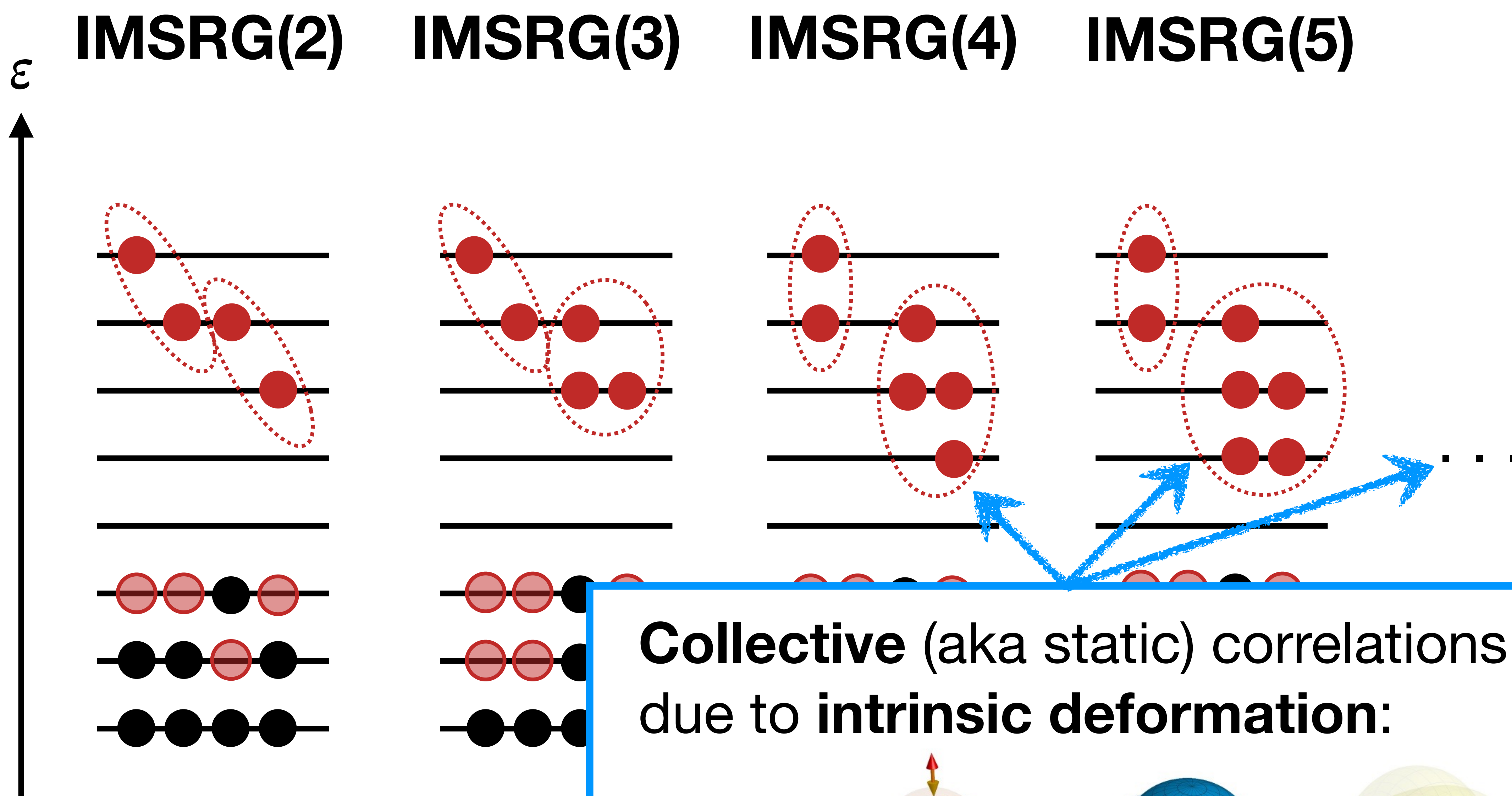
- absorb correlations into **RG-improved Hamiltonian**

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

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

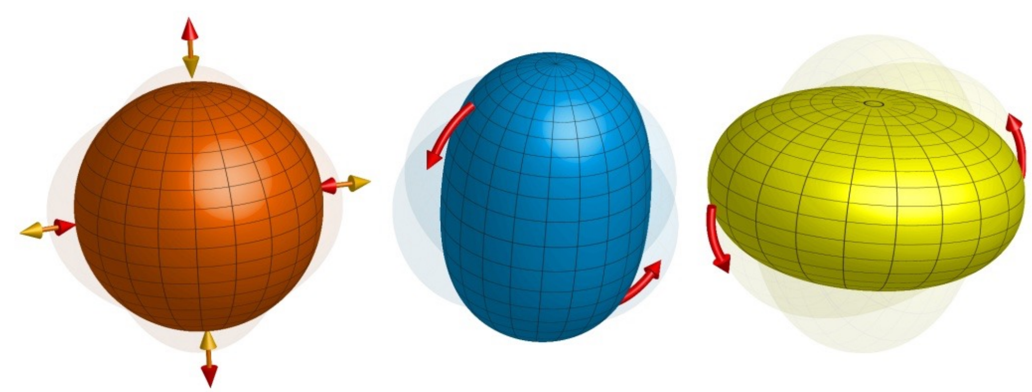
$$U(s)\left|\Psi_n\right\rangle \stackrel{!}{=} \left|\Phi\right\rangle$$

Correlated Reference States

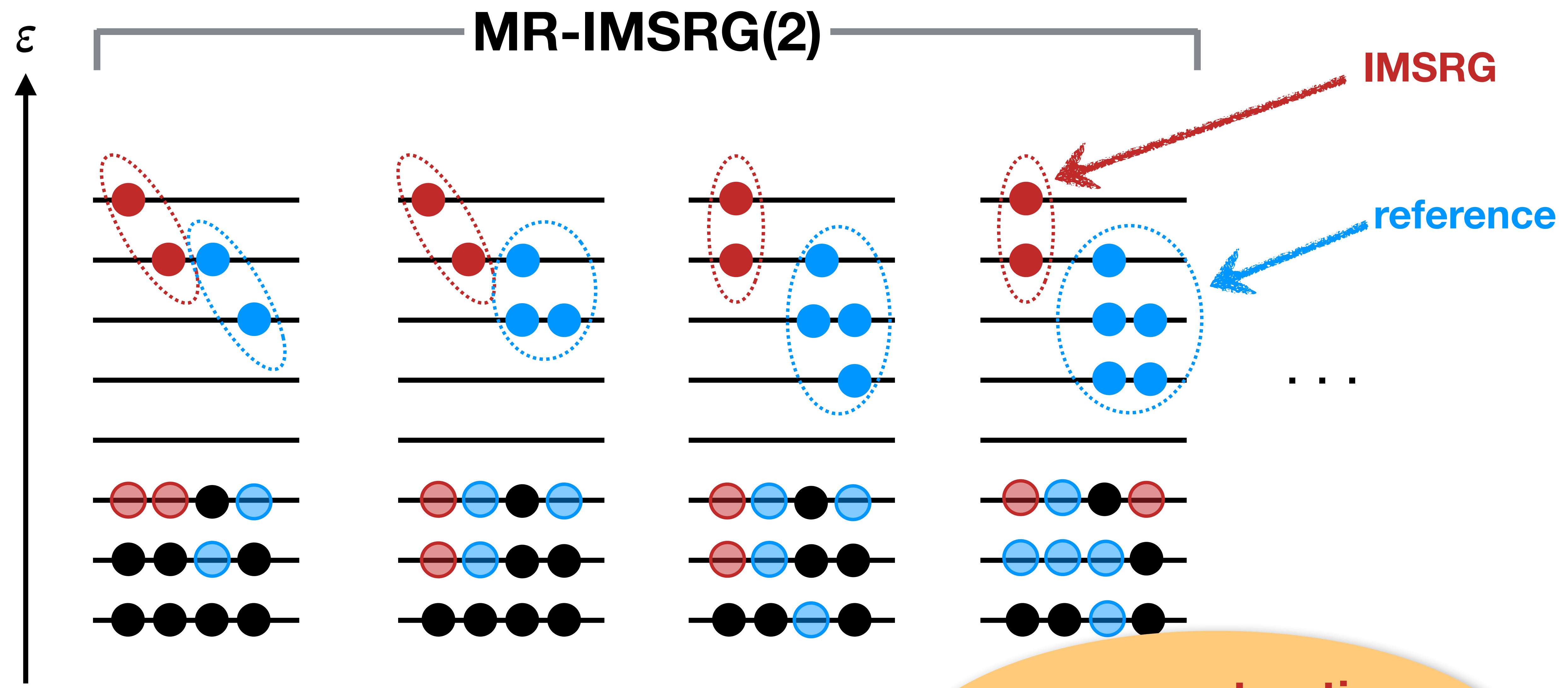


“standard” IMS
Slater determinan

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



Correlated Reference States

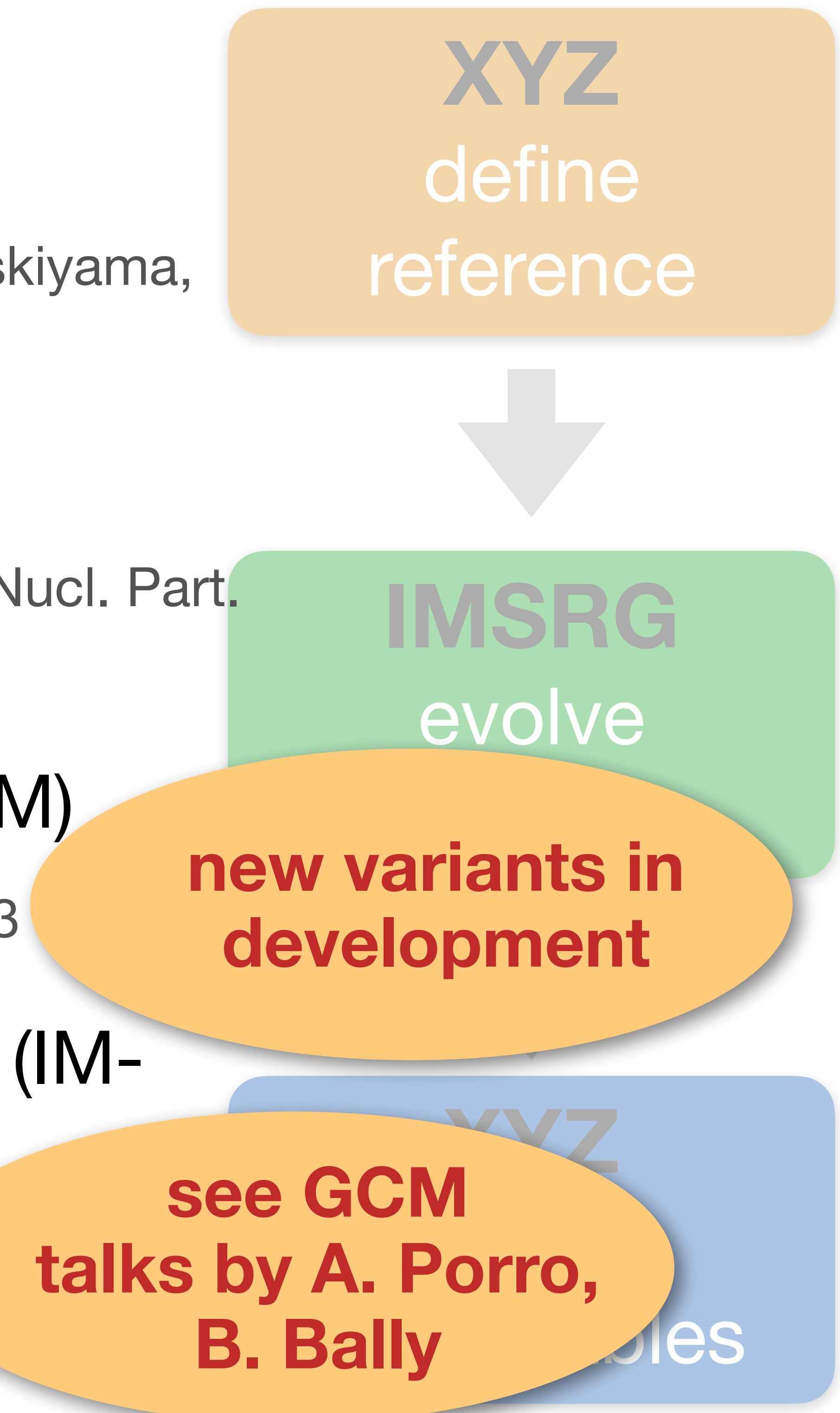


MR-IMSRG: build correlations on top of **already correlated** state (e.g., from a method that describes static correlation well)

new contractions (two-body and higher densities), but **scaling remains unchanged**

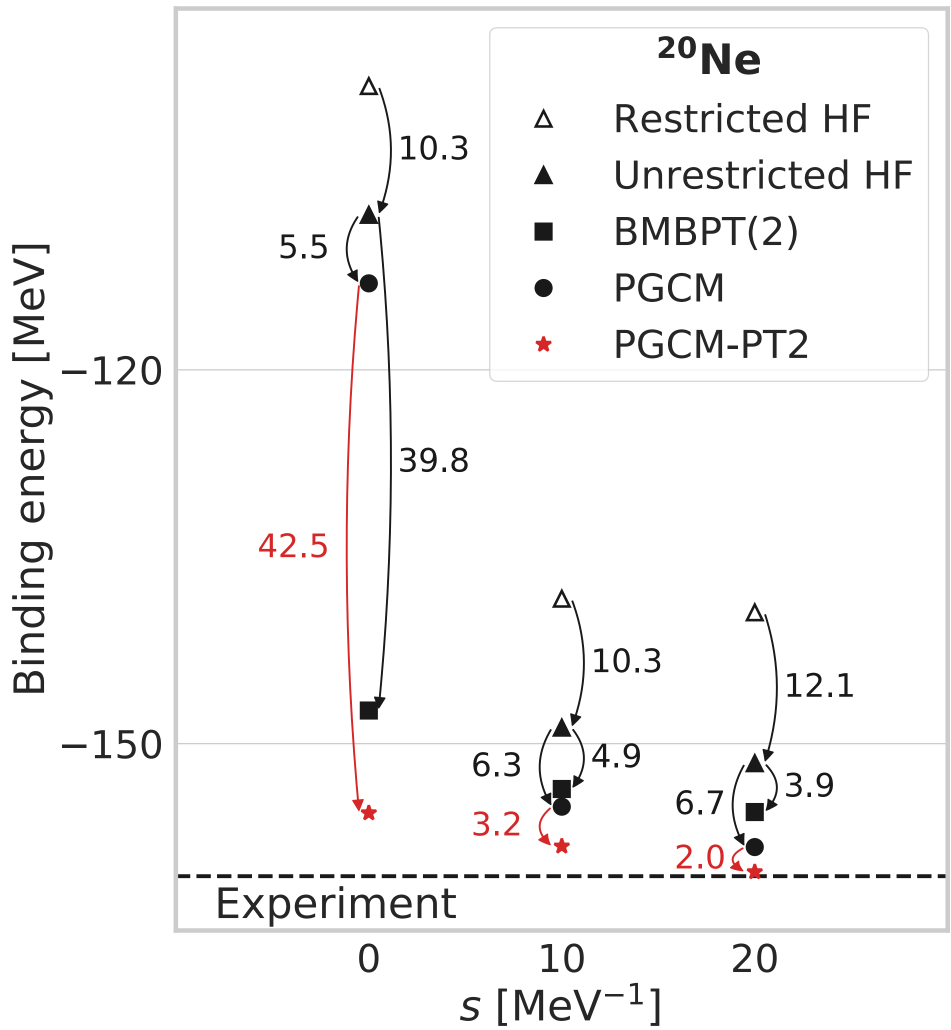
IMSRG-Improved Methods

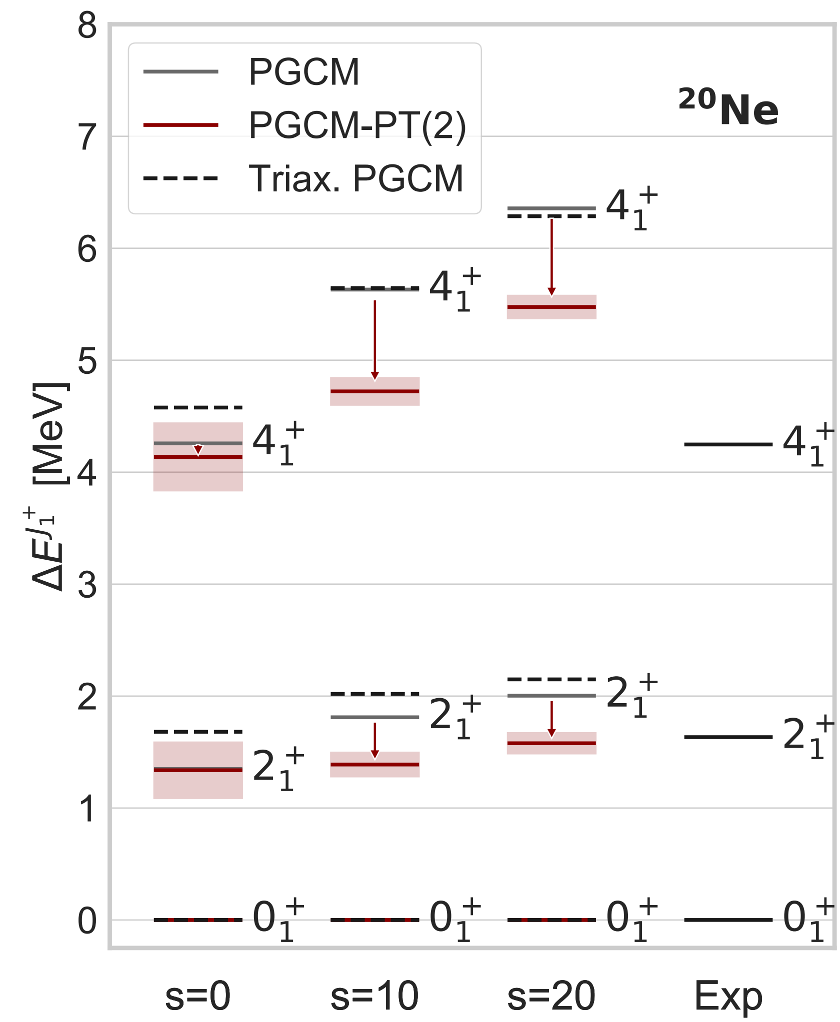
- IMSRG for closed and open-shell nuclei: IM-HF and IM-PHFB
  - HH, Phys. Scripta, Phys. Scripta 92, 023002 (2017)
  - HH, S. K. Bogner, T. D. Morris, A. Schwenk, and K. Tuskiyama, Phys. Rept. 621, 165 (2016)
- Valence-Space IMSRG (VS-IMSRG)
  - S. R. Stroberg, HH, S. K. Bogner, J. D. Holt, Ann. Rev. 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 (2018)
  - J. M. Yao et al., PRL 124, 232501 (2020)



Perturbative Enhancement of IM-GCM

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



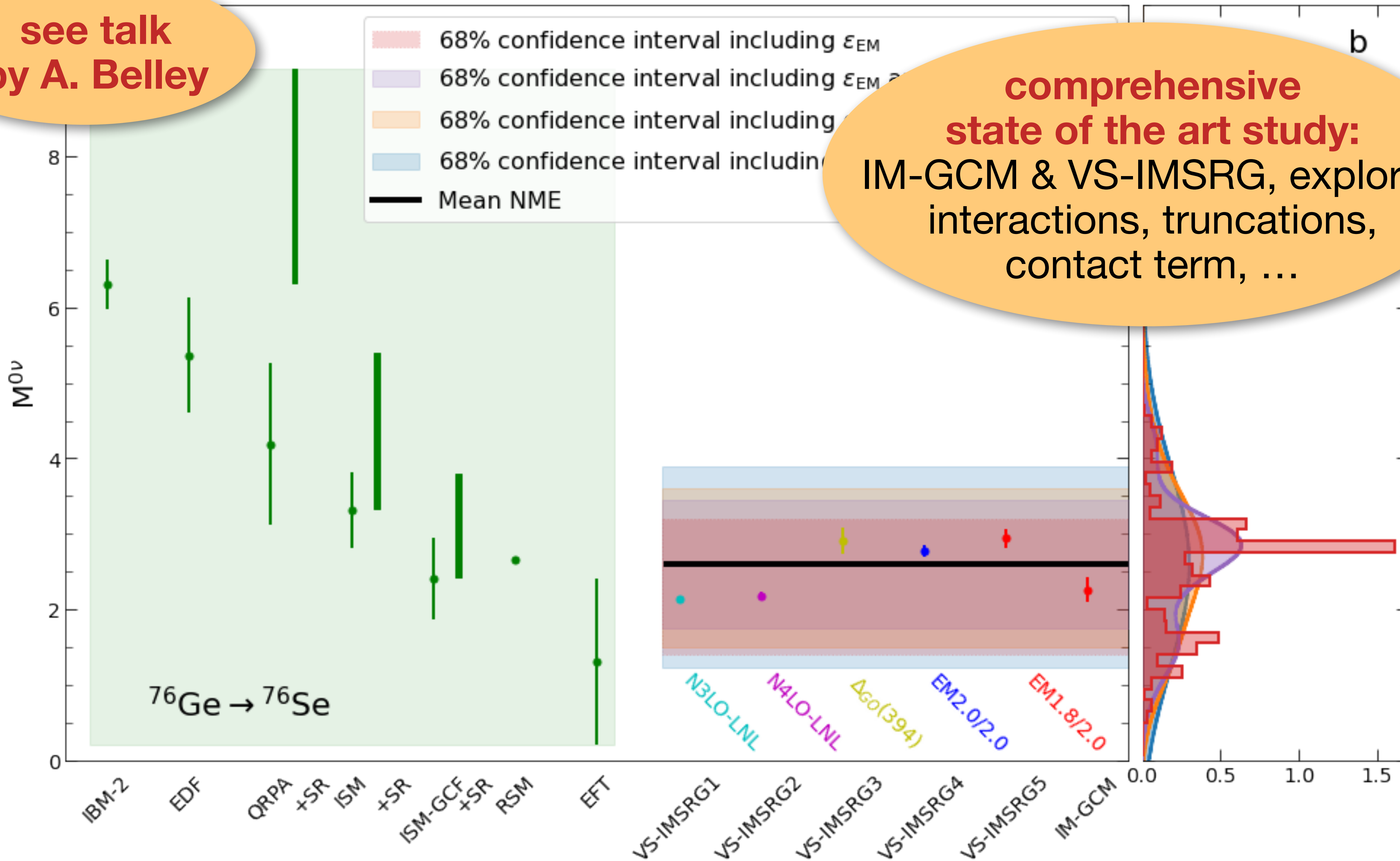


- s-dependence is a **built-in diagnostic tool** for IM-GCM **(not available in phenomenological GCM)**
    - if operator and wave function offer sufficient degrees of freedom, evolution of observables is unitary
- need **richer references and/or IMSRG(3)** for certain observables

^{76}Ge

A. Belley et al., arXiv:2308.15643 (**v2**)

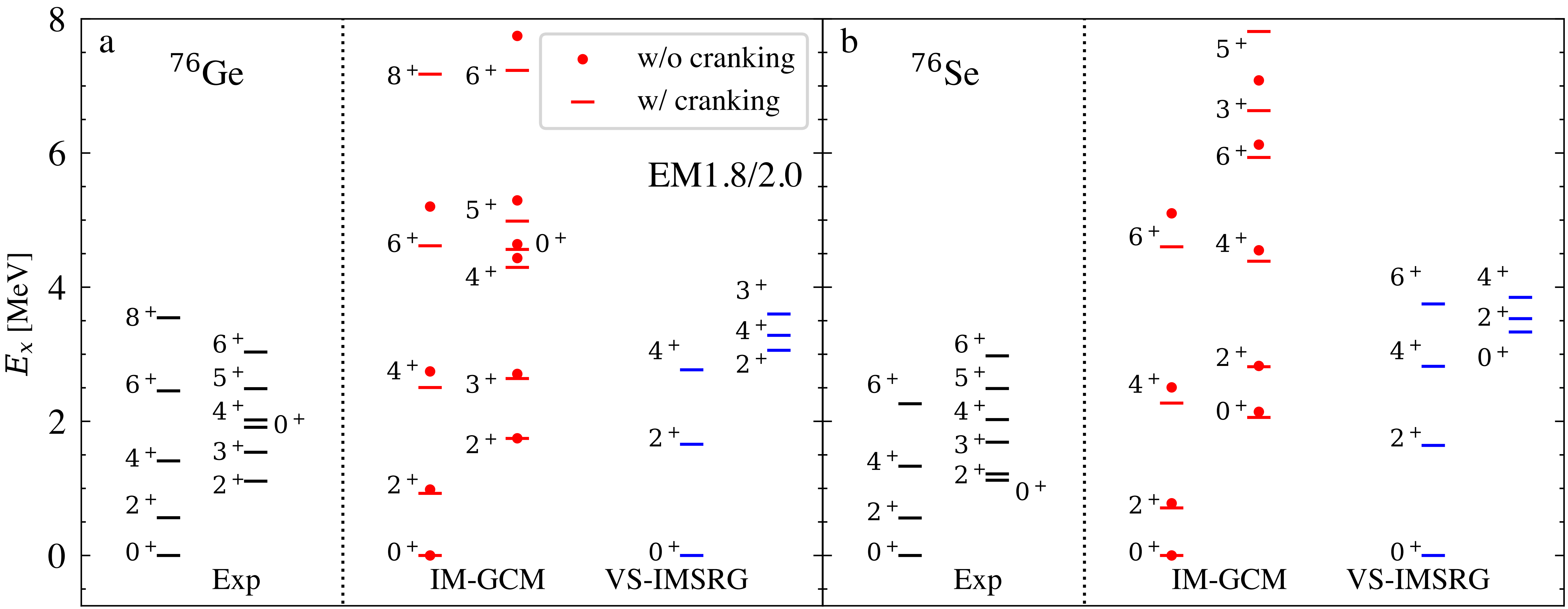
see talk by A. Belley



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

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

*A. Belley et al., arXiv:2308.15643 (**v2**)*



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

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

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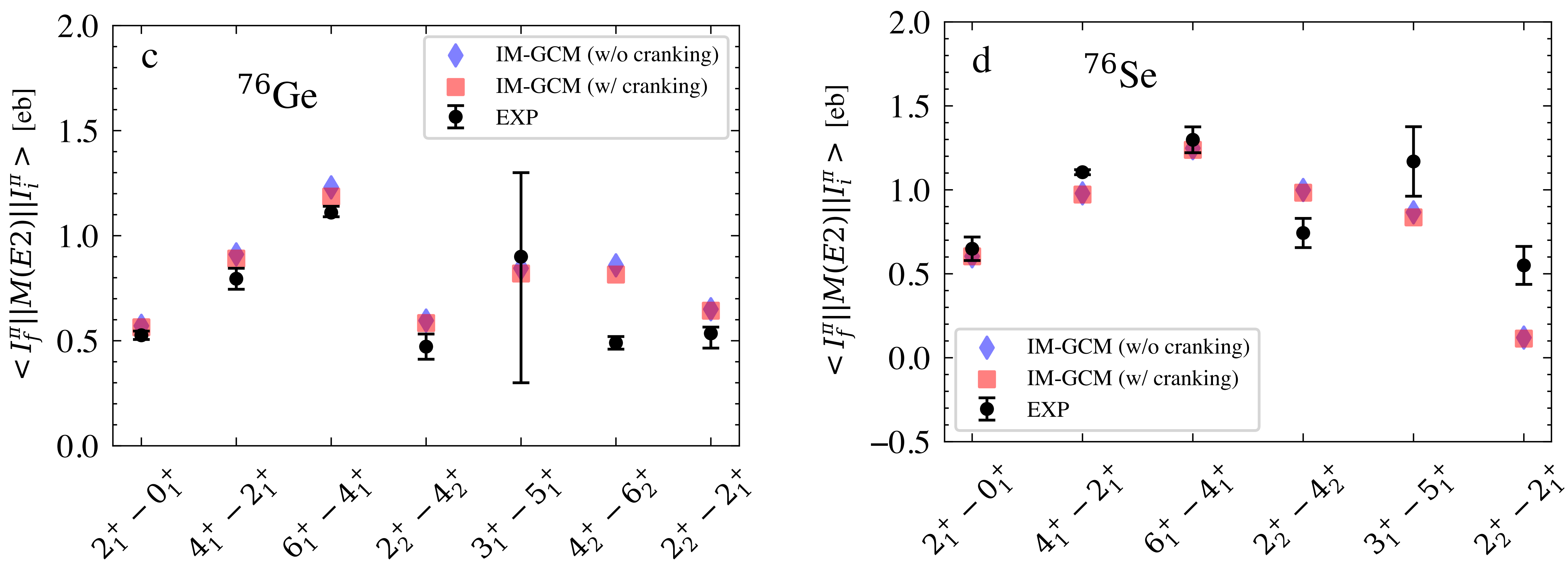
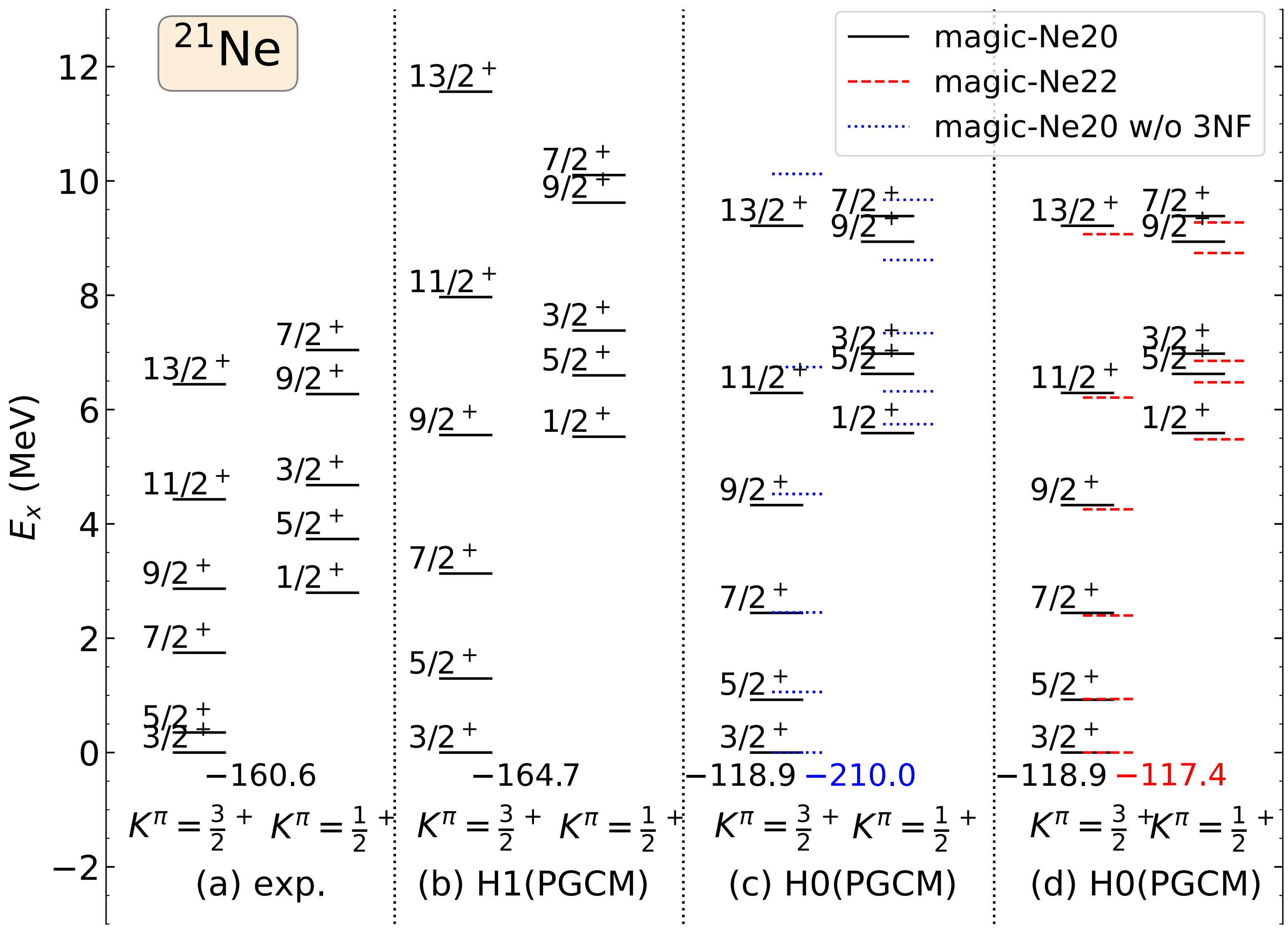


EM1.8/2.0 NN+3N interaction, $\hbar\omega = 12\,\text{MeV}, e_{max} = 10$

caveat: EM1.8/2.0 gives radii that are a few percent too small

IM-GCM for Odd Nuclei

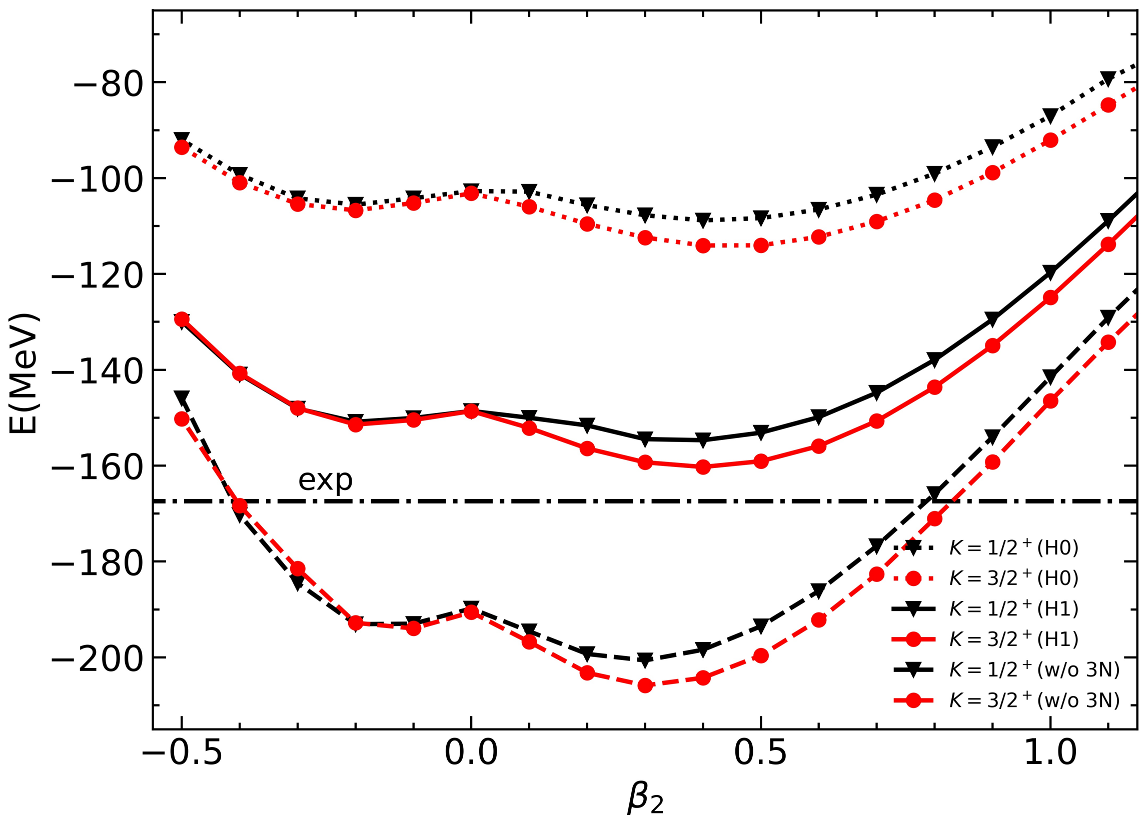
W. Lin, J. M. Yao, E. F. Zhou, HH, in preparation

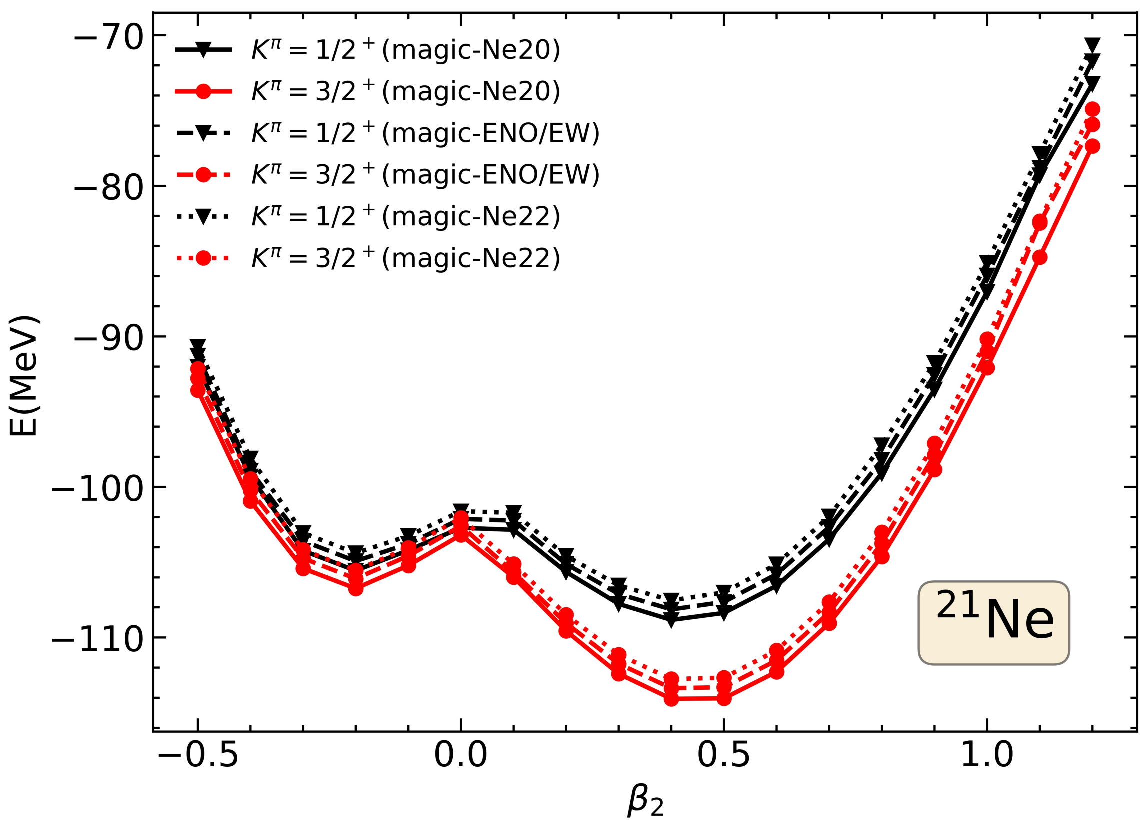


- IMSRG evolution improves **absolute energies**
- working to understand how/why evolution increases **spread of spectrum**: reshaping of PES, tailoring to g.s.
- **weak sensitivity to choice of reference** (even neighbors, ensemble, …)

IM-GCM for Odd Nuclei

W. Lin, J. M. Yao, E. F. Zhou, HH, in preparation





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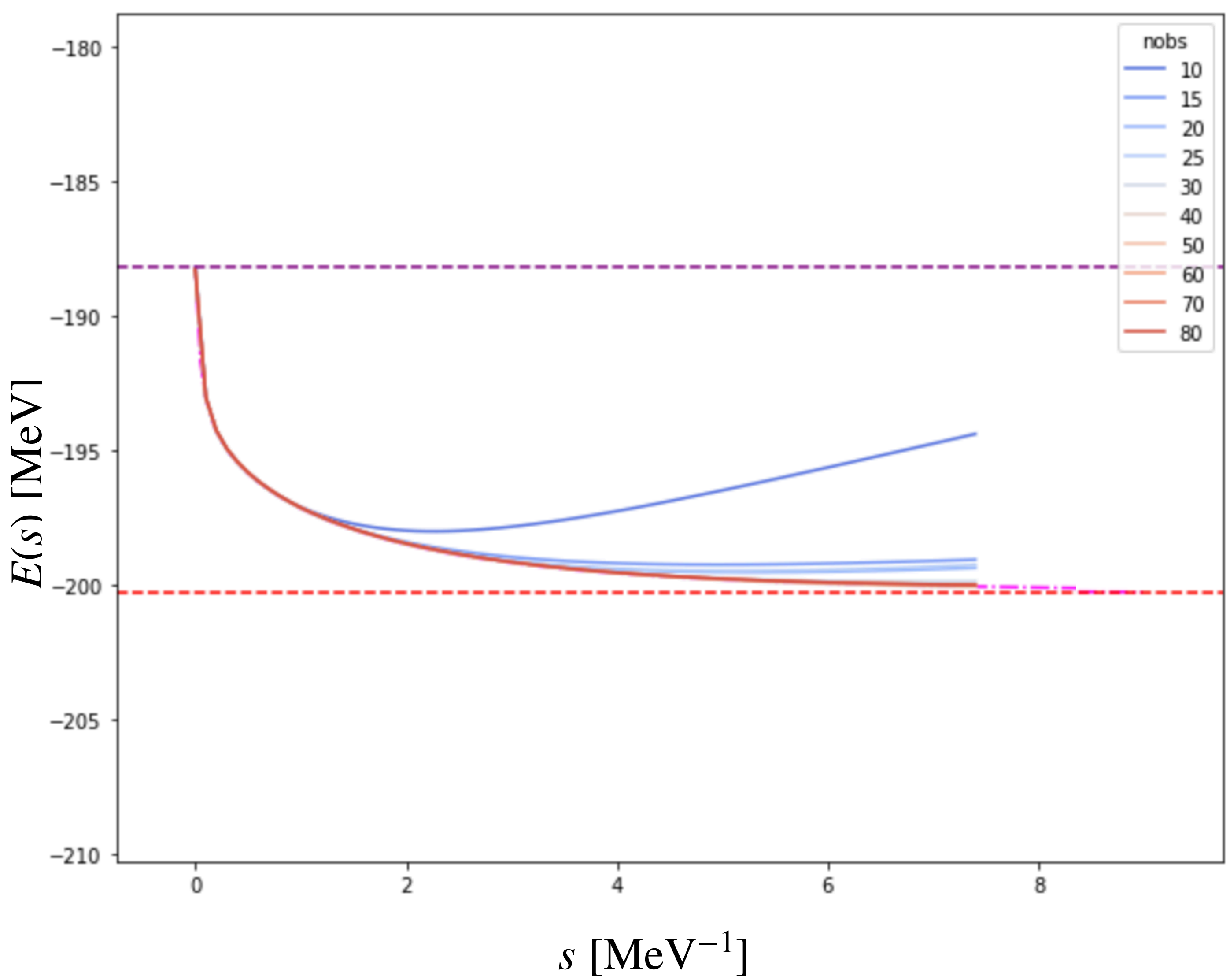
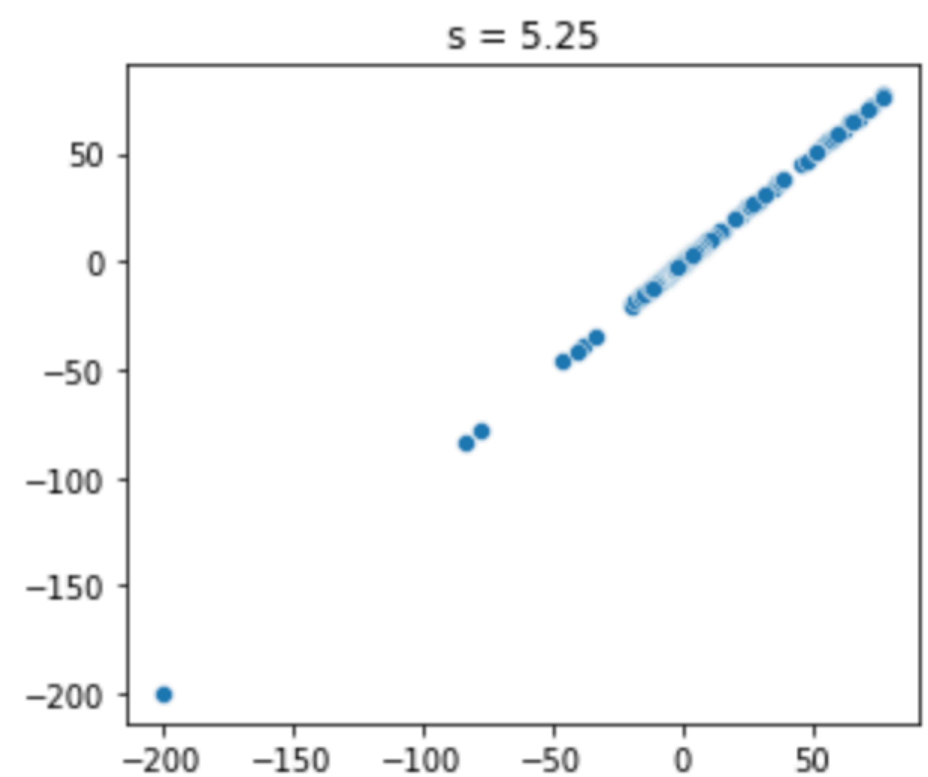
Emulating IMSRG Flows

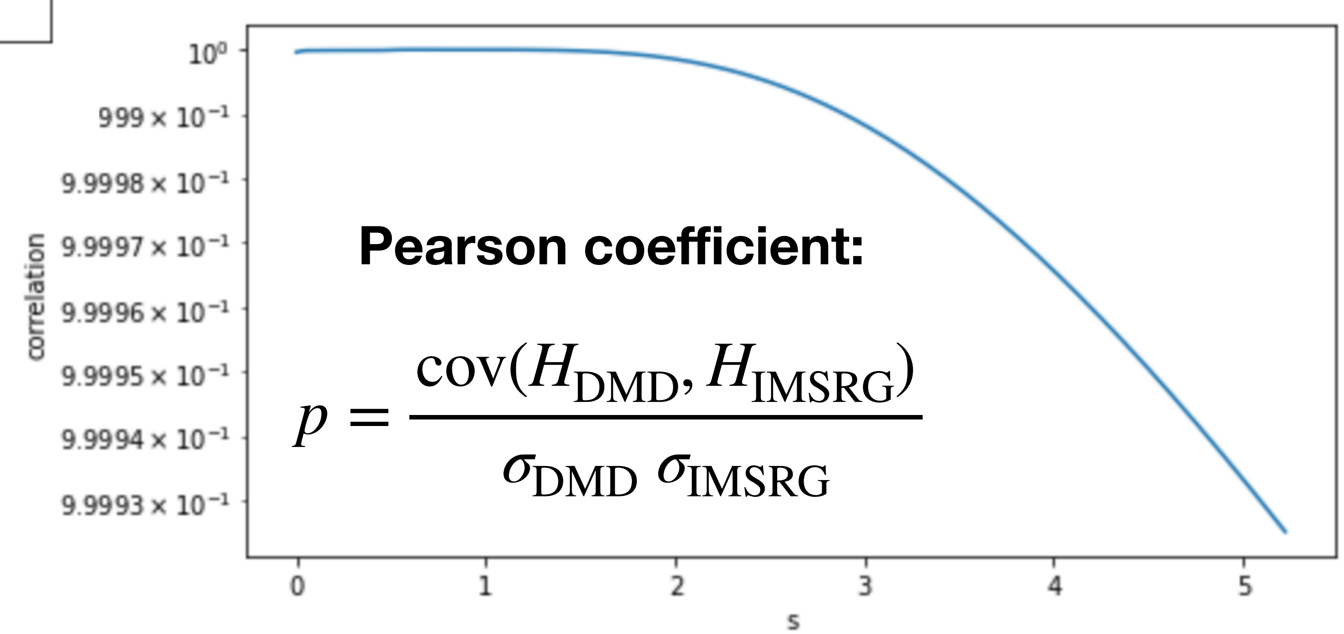
***J. Davison, HH,** J. Crawford, S. Bogner, in preparation*

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



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





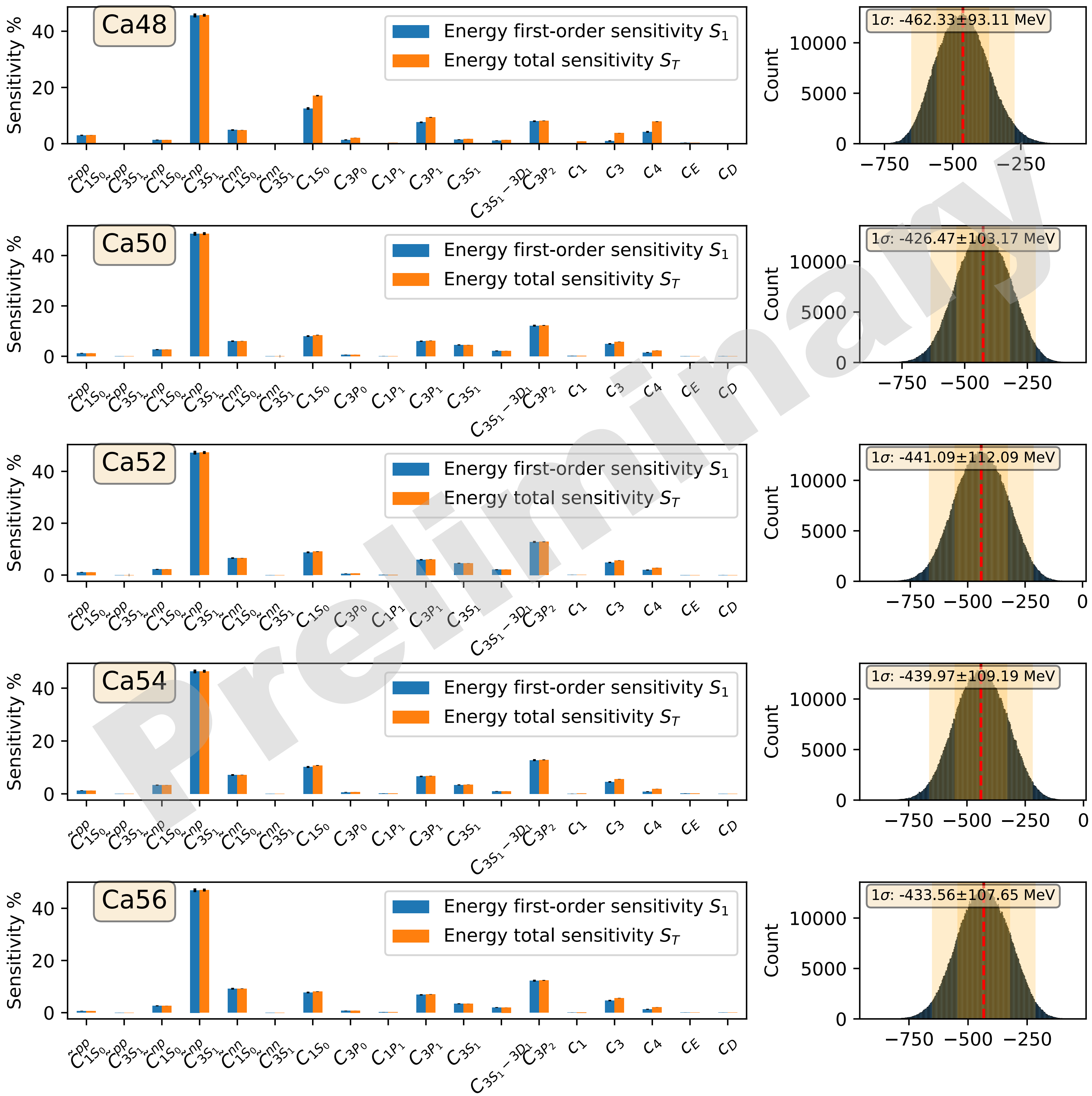
Pearson coefficient:

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

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

Emulation for Operators (IMSRG)

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



- 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**

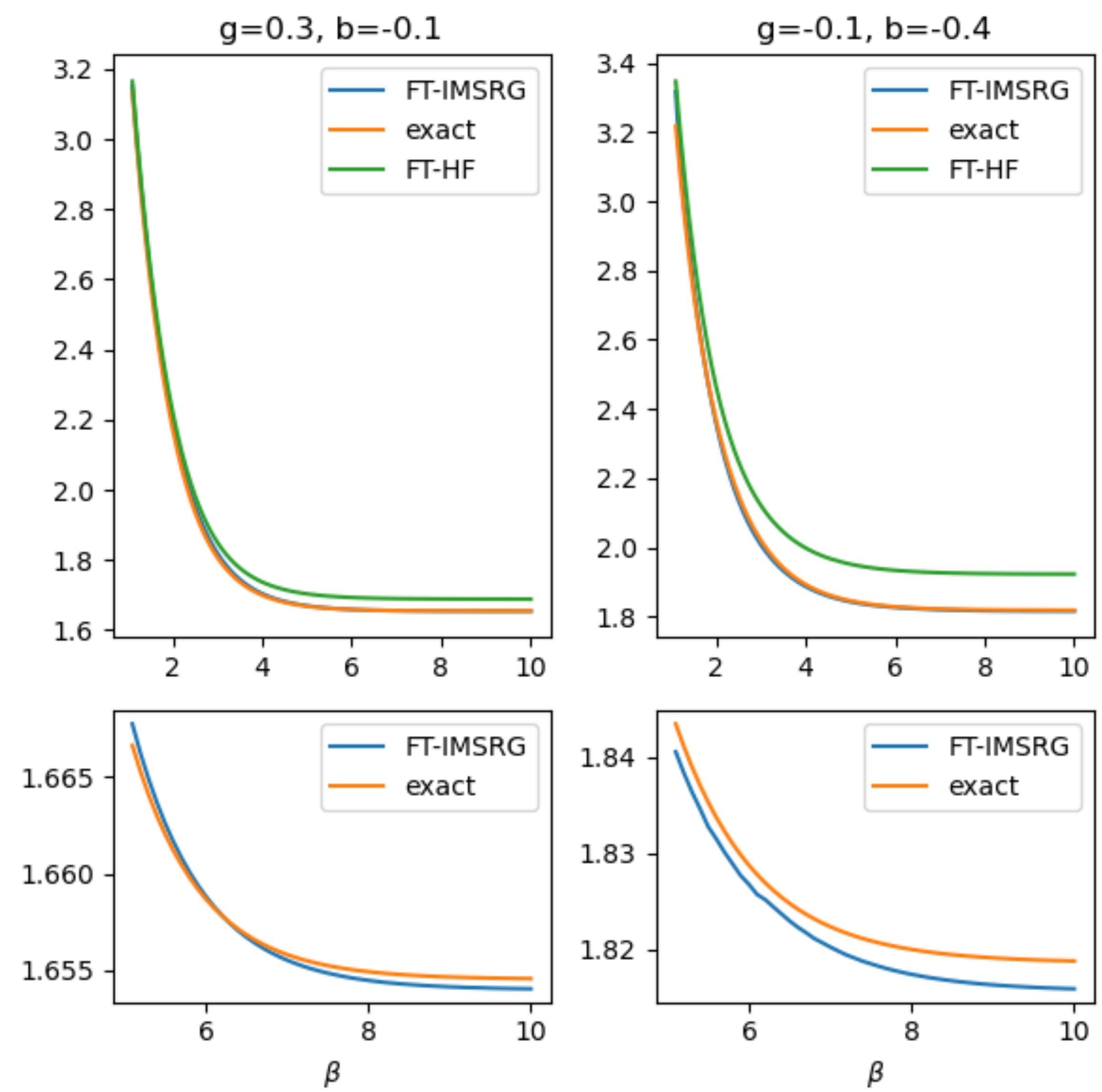
Preview: Finite-Temperature IMSRG

- formalism and benchmark paper **out soon**
- implementation for **realistic nuclei and chiral interactions** complete, under validation
- expect first **applications to structure, beta decays** within next 1-2 years

The In-Medium Similarity Renormalization Group at Finite Temperature

Isaac G. Smith, Heiko Hergert, Scott K. Bogner
Facility for Rare Isotope Beams, Department of Physics and Astronomy, Michigan State University, East Lansing, MI 48824

The study of nuclei at finite-temperature is of immense interest in nuclear astrophysics. Many *ab initio* methods for determining properties of nuclei at zero-temperature have been developed over the past few decades. We expand one such method, the In-Medium Similarity Renormalization Group (IMSRG), to finite temperature. The implementation of the finite-temperature IMSRG (FT-IMSRG), including the implementation of finite-temperature Hartree-Fock, is detailed. Using an exactly-solvable toy model, we show that the FT-IMSRG can accurately determine the energetics of nuclei at finite temperature. The effect of model parameters on the FT-IMSRG's accuracy is



What Else Is There?

- **improved truncations:** IMSRG(3), tailored operator bases
  [also cf. talks by M. Heinz, R. Stroberg]
- **accelerate IMSRG & IM-GCM**
  - GPUs, factorization, Machine Learning, …
  - (random) **compression & tensor factorization**
- **Uncertainty Quantification / Sensitivity Analysis**
  - emulators for GCM (wave function / Galerkin methods)
  - **emulation workflow based on (IM)SRG ROMs ?**

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R. J. Furnstahl
The Ohio State University

and everyone I forgot to list…

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Supplements

Similarity Renormalization Group

Basic Idea

continuous unitary transformation of the Hamiltonian to band-diagonal form w.r.t. a given "uncorrelated" many-body basis

- flow equation for Hamiltonian $H(s) = U(s)HU^\dagger(s)$:

$$\frac{d}{ds}H(s) = \left[\eta(s), H(s)\right], \quad \eta(s) = \frac{dU(s)}{ds}U^\dagger(s) = -\eta^\dagger(s)$$

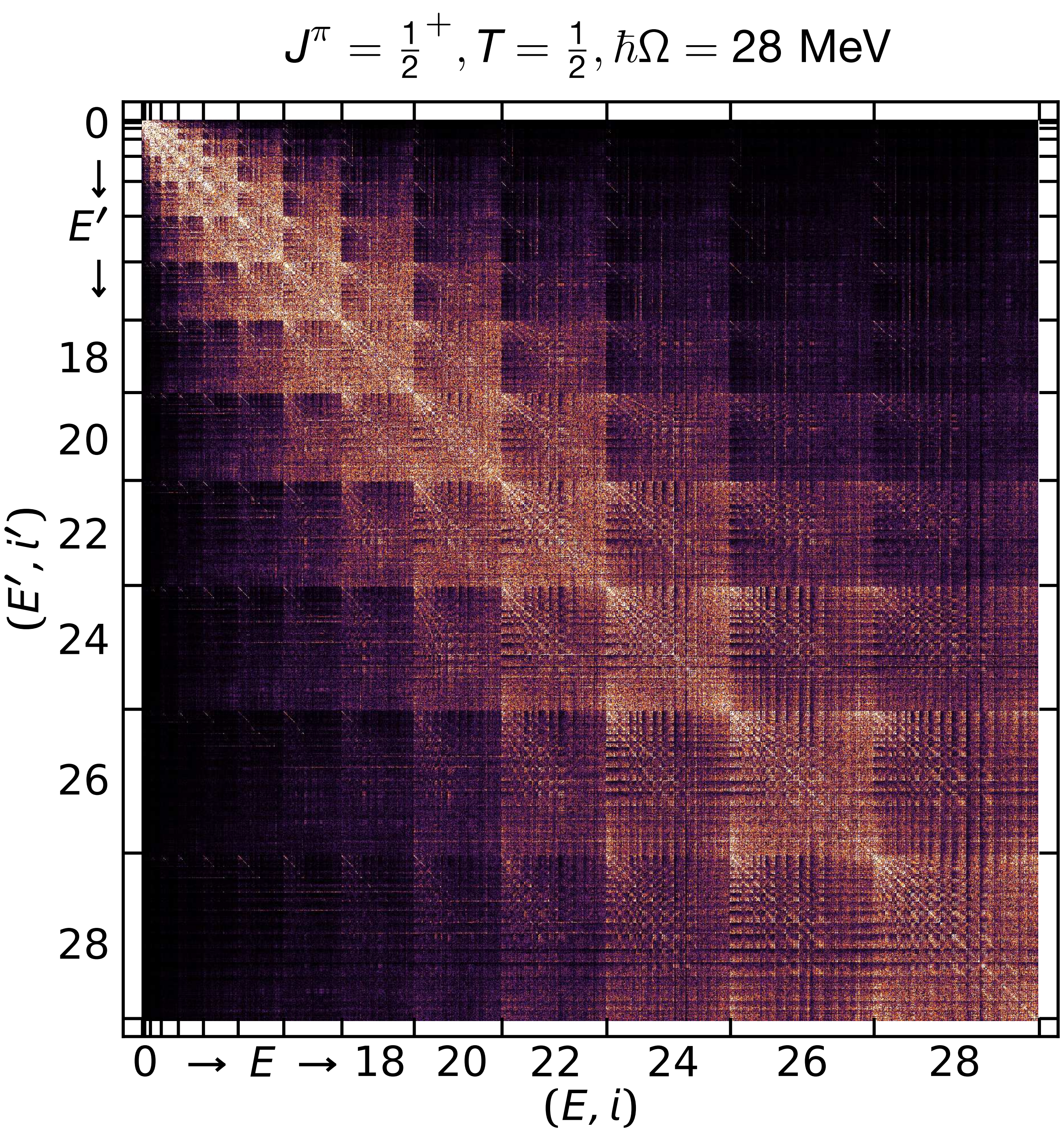
- choose $\eta(s)$ to achieve desired behavior, e.g.,

$$\eta(s) = \left[H_d(s), H_{od}(s)\right]$$

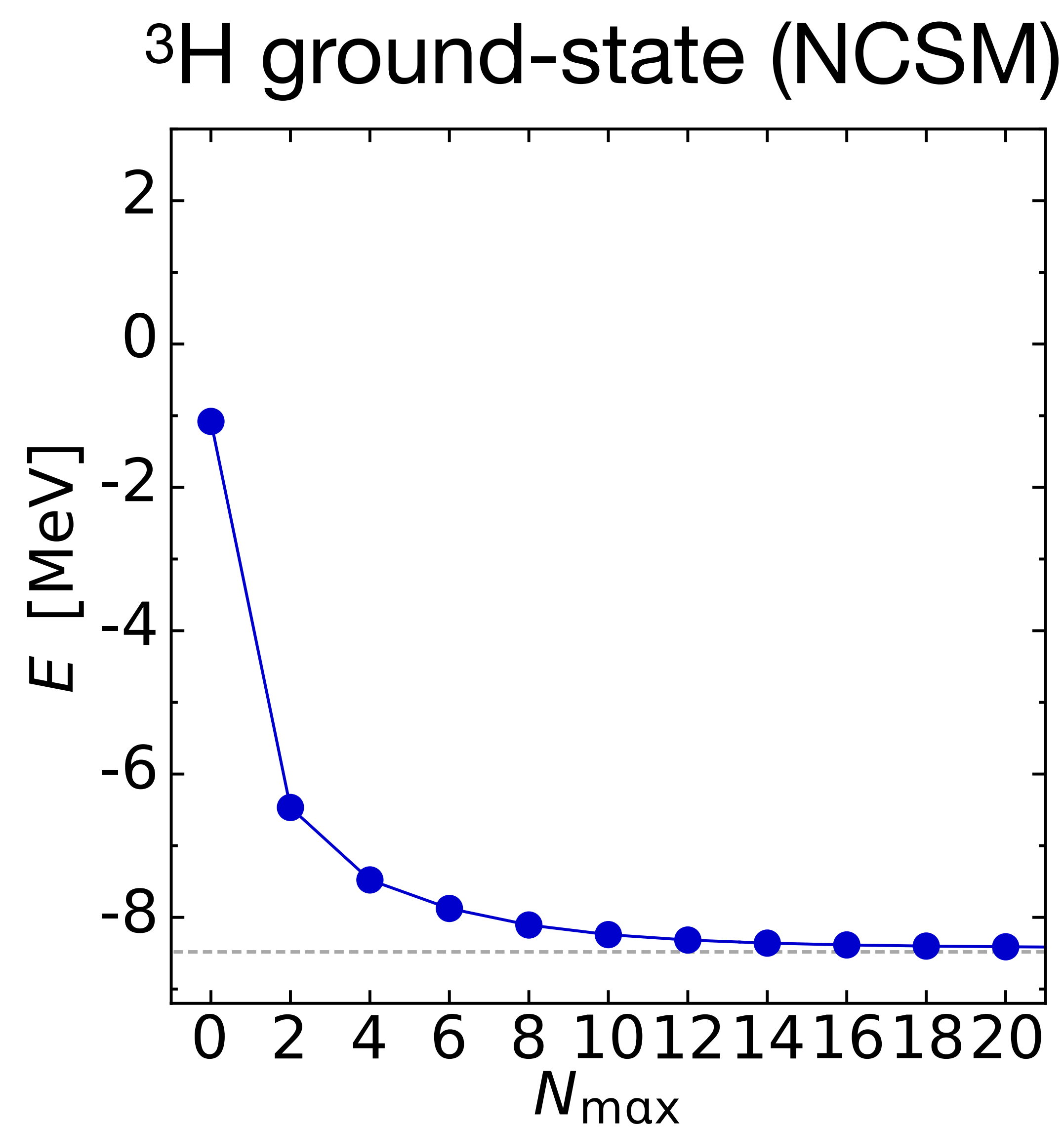
to suppress (suitably defined) off-diagonal Hamiltonian

- consistent evolution for all observables of interest

SRG in Three-Body Space



λ = 1.33 fm⁻¹



[figures courtesy of A. Calci and R. Roth]

Operator Bases for the IMSRG

- choose a **basis of operators** to represent the flow (make an educated guess about physics):

$$H(s) = \sum_i c_i(s) O_i\,, \quad \eta(s) = \sum_i f_i(\{c(s)\}) O_i$$

- **close algebra by truncation,** if necessary:

$$[O_i, O_j] = \sum_k g_{ijk} O_k$$

- **flow equations** for the coefficient (**coupling constants**):

$$\frac{d}{ds} c_k = \sum_{ij} g_{ijk}\, f_i(\{c\})\, c_j$$

- “obvious” choice for many-body problems:

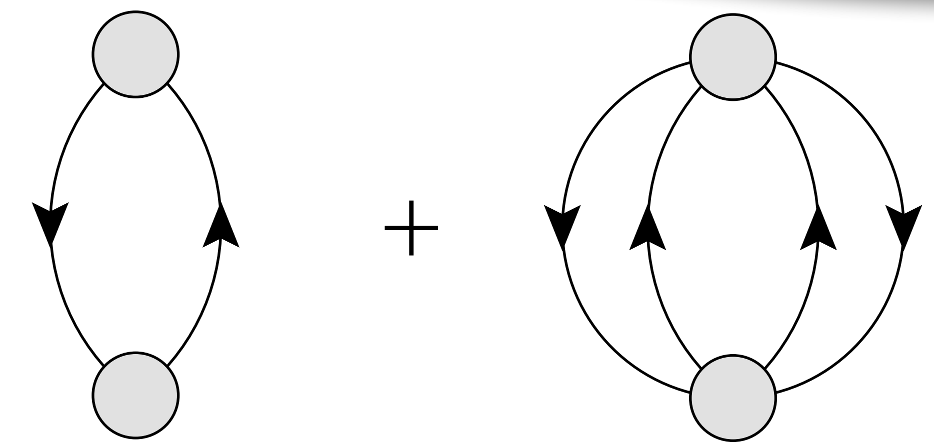
$$\{O_{pq}, O_{pqrs}, \dots\} = \{a^\dagger_p a_q, a^\dagger_p a^\dagger_q a_s a_r, \dots\}$$

Standard IMSRG(2) Flow Equations

0-body Flow

~ 2nd order MBPT for *H(s)*

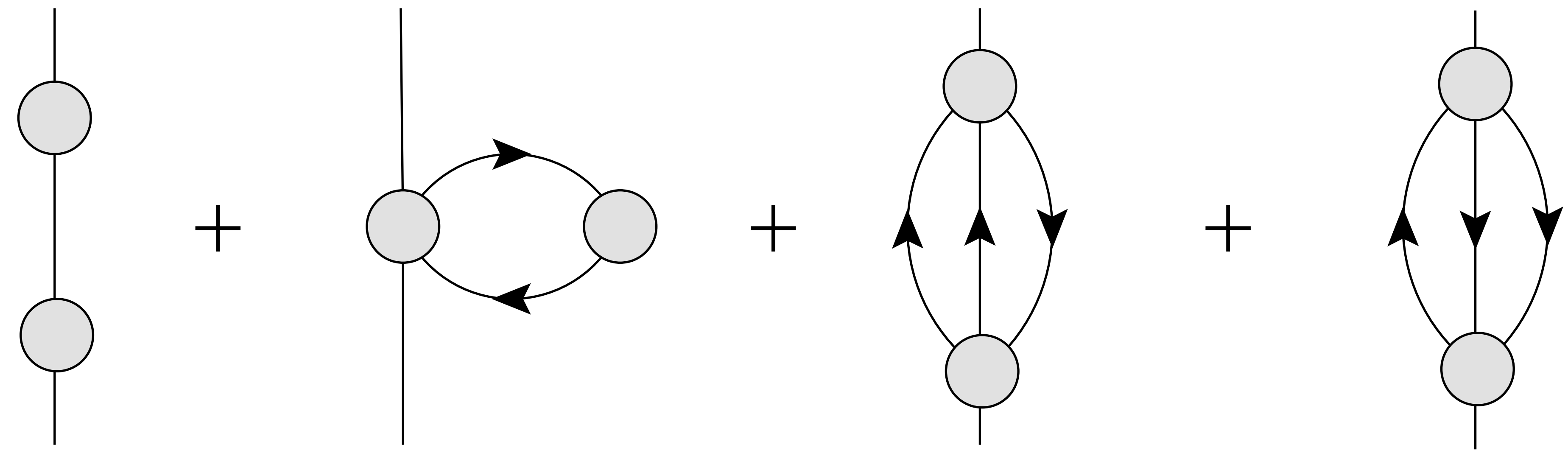
$$\frac{dE}{ds} =$$



1-body Flow

coefficients (couplings) of H(s)

$$\frac{df}{ds} =$$



Standard IMSRG(2) Flow Equations

O(N⁶) scaling
(before particle/hole distinction)

2-body Flow

$$\frac{d\Gamma}{ds} =$$