Progress in *Ab Initio* Nuclear Theory for Deformed Nuclei

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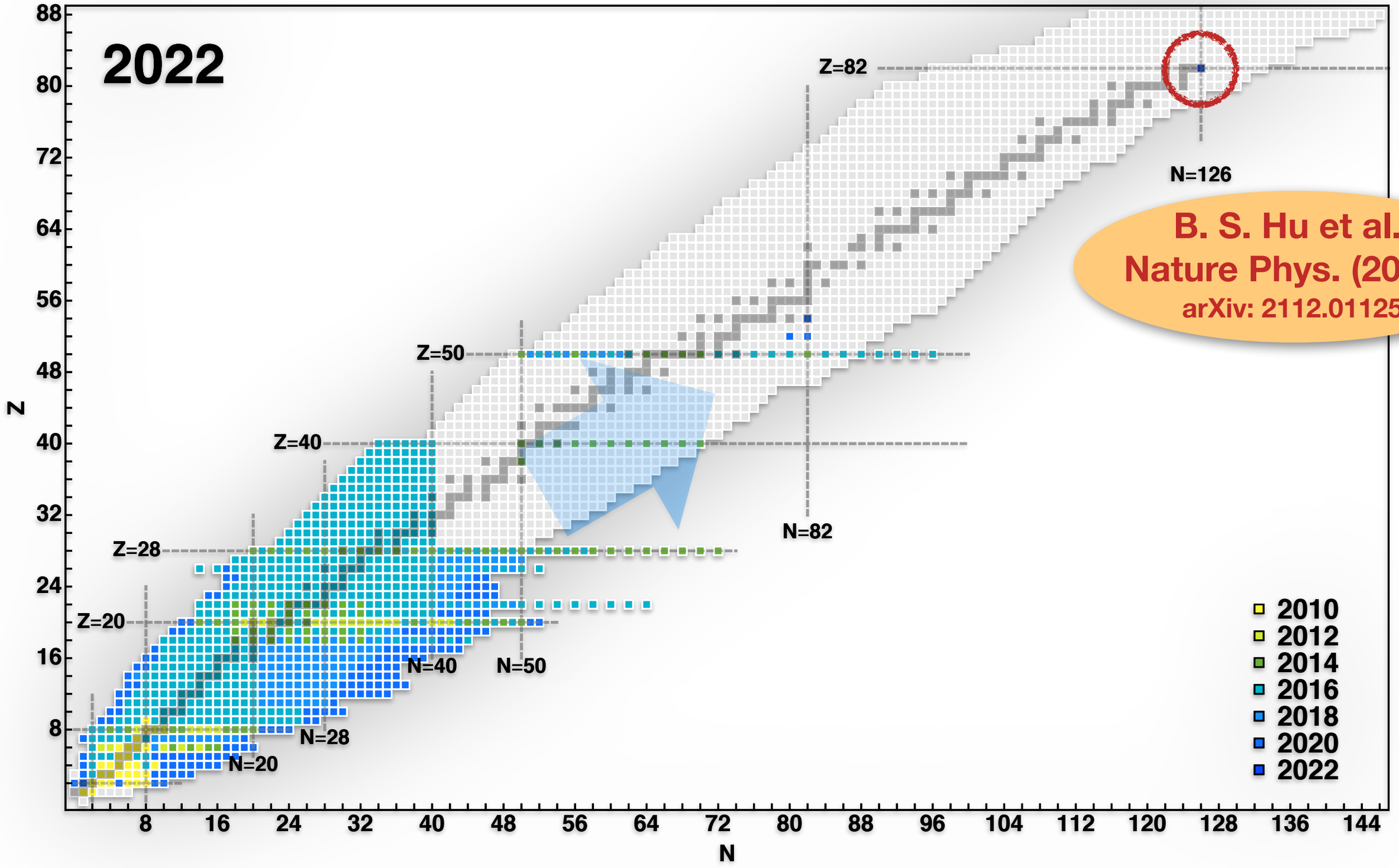
Progress in *Ab Initio* Calculations

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



(Multi-Reference) In-Medium Similarity Renormalization Group

HH, Phys. Scripta **92**, 023002 (2017)

HH, S. K. Bogner, T. D. Morris, A. Schwenk, and K. Tuskiyama, Phys. Rept. **621**, 165 (2016)

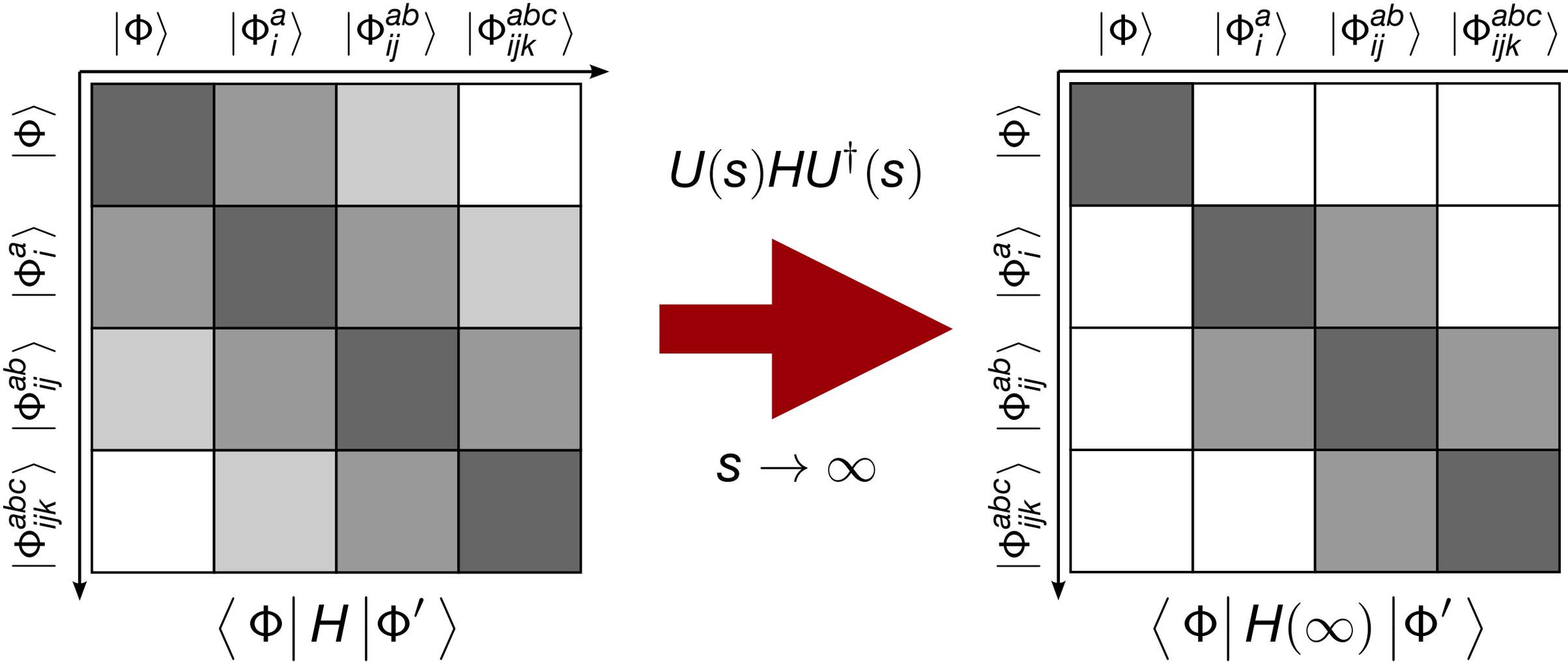
HH, S. K. Bogner, T. Morris, S. Binder, A. Calci, J. Langhammer, R. Roth, Phys. Rev. C **90**, 041302 (2014)

HH, S. Binder, A. Calci, J. Langhammer, and R. Roth, Phys. Rev. Lett **110**, 242501 (2013)

K. Tsukiyama, S. K. Bogner, A. Schwenk, PRL **106**, 222502 (2011)

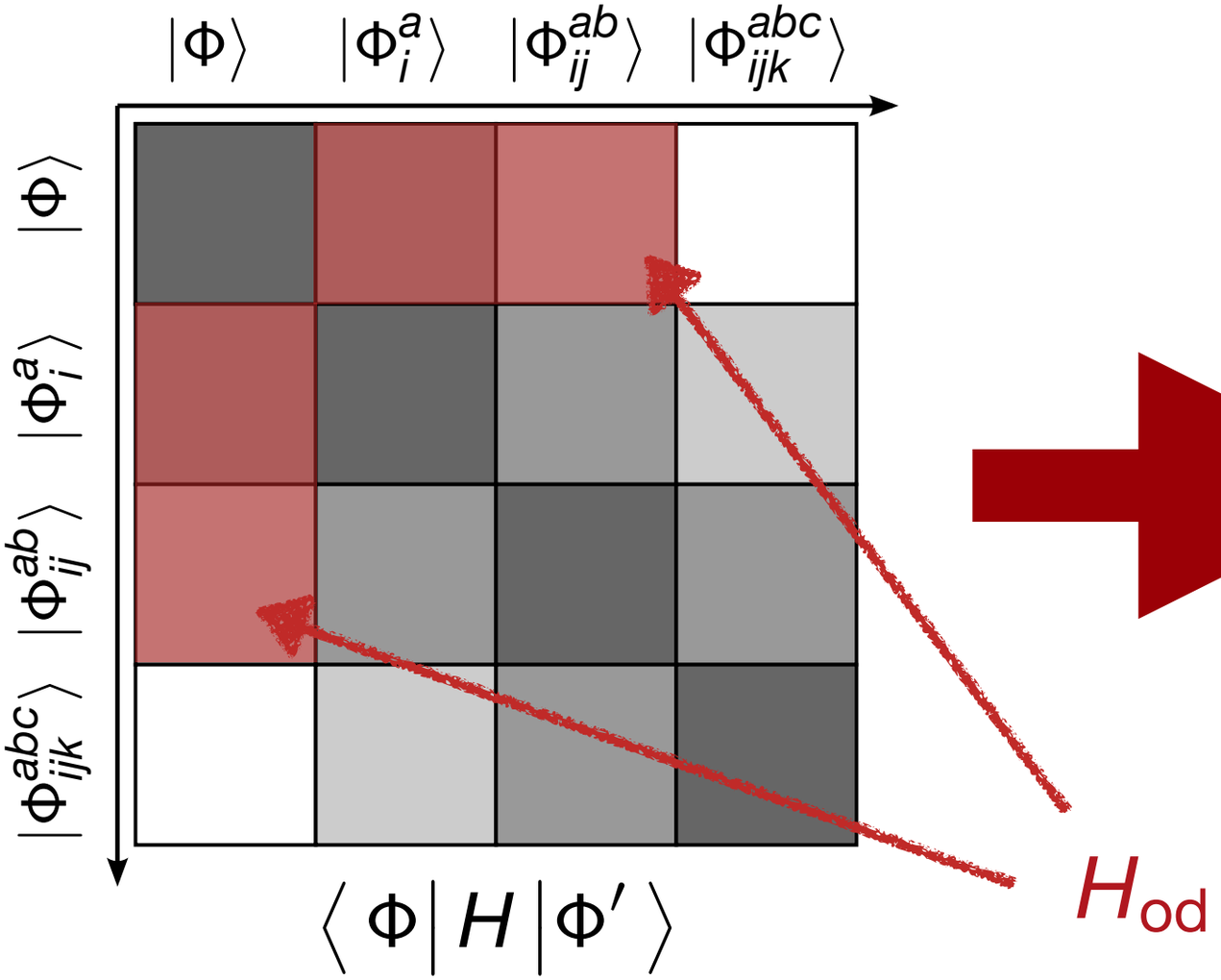
S. K. Bogner, R. J. Furnstahl, and A. Schwenk, Prog. Part. Nucl. Phys. **65**, 94

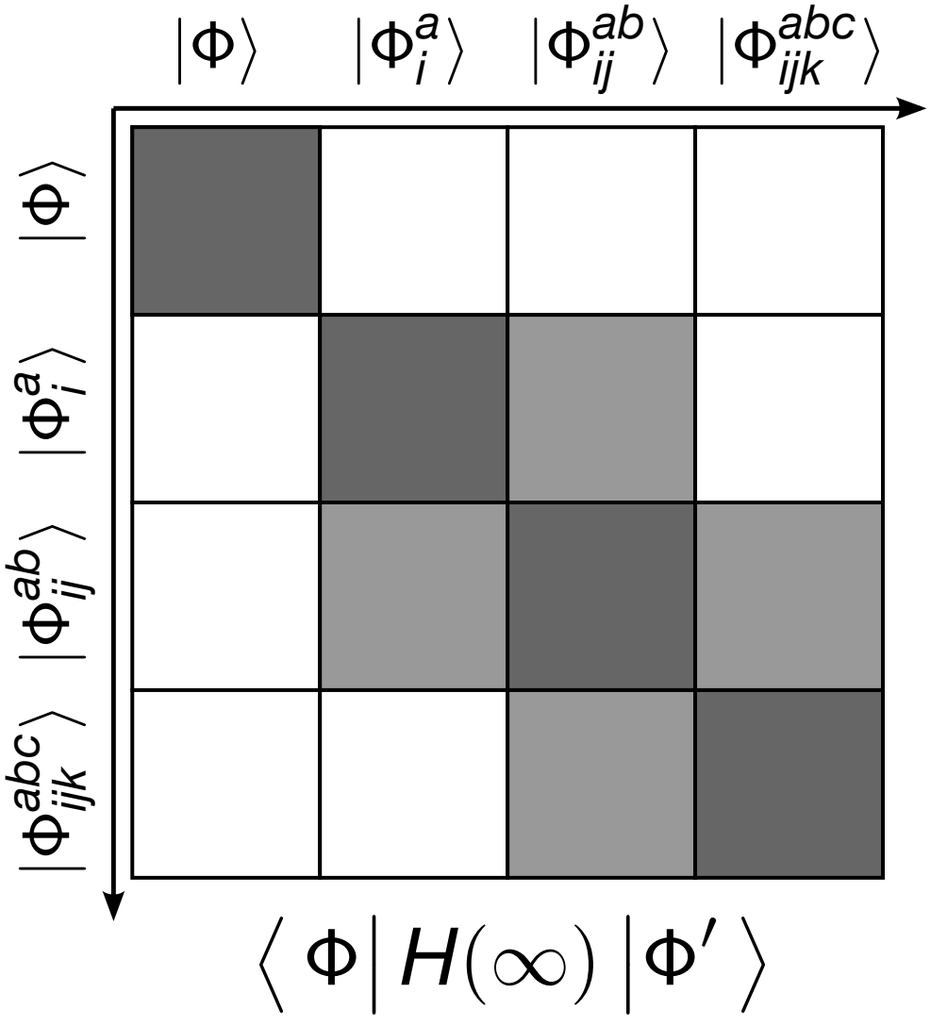
Decoupling in A-Body Space



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

Flow Equation

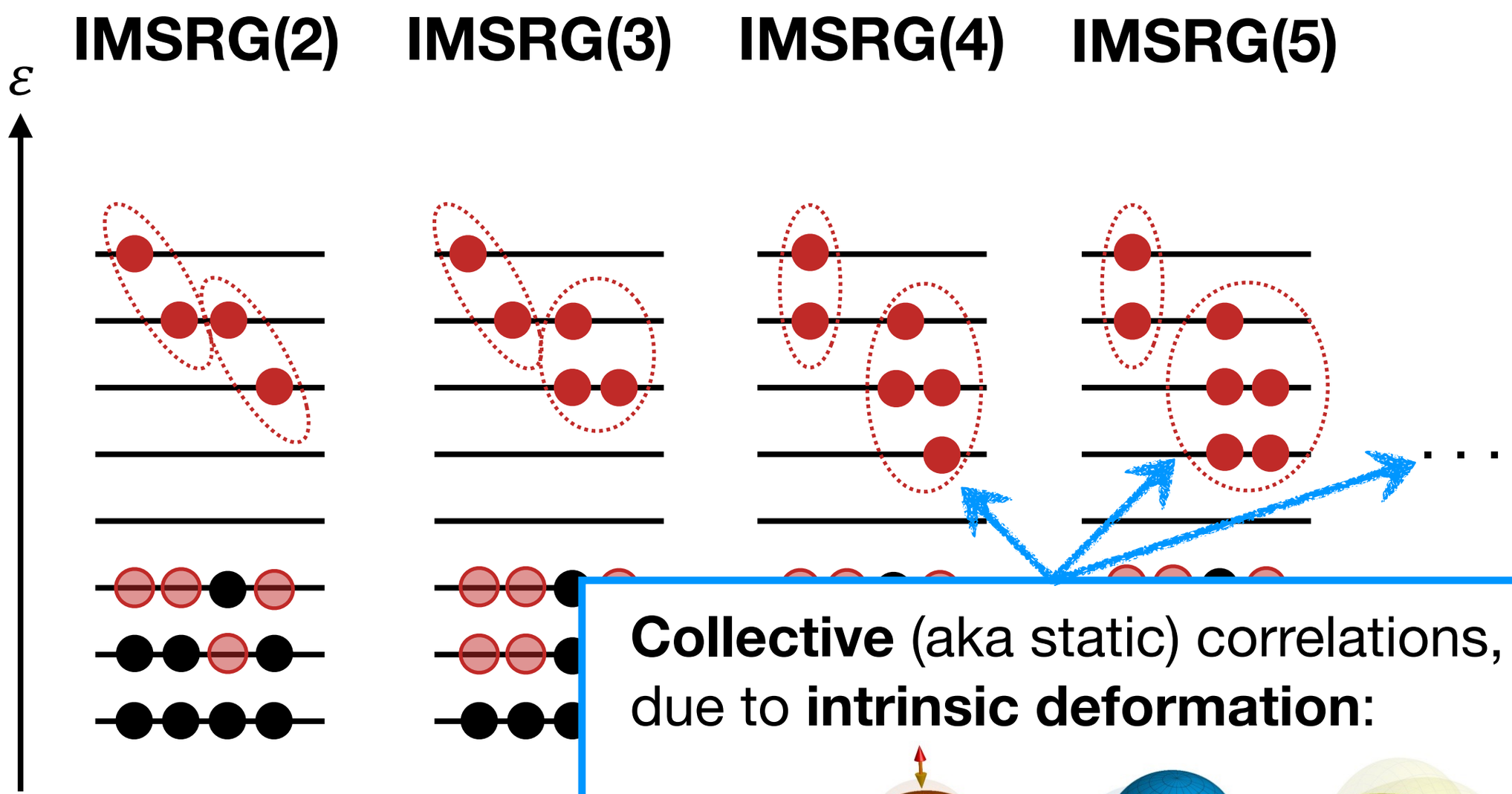




$$\frac{d}{ds}H(s) = \left[\eta(s), H(s)\right],$$

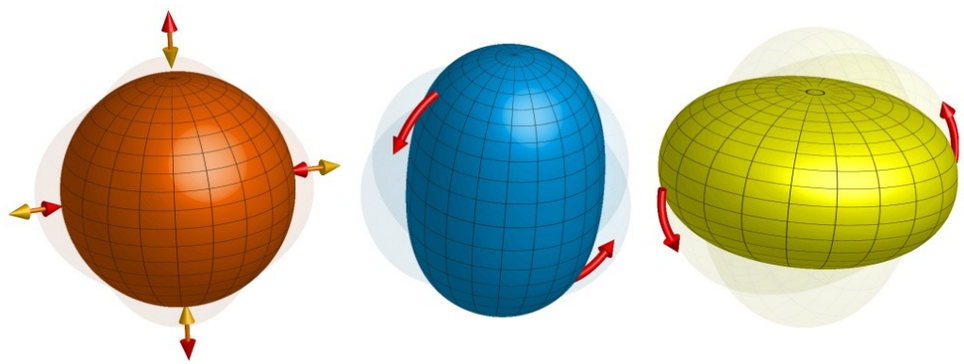
Operators
truncated at **two-body level** -
matrix is never constructed explicitly!

Correlated Reference States

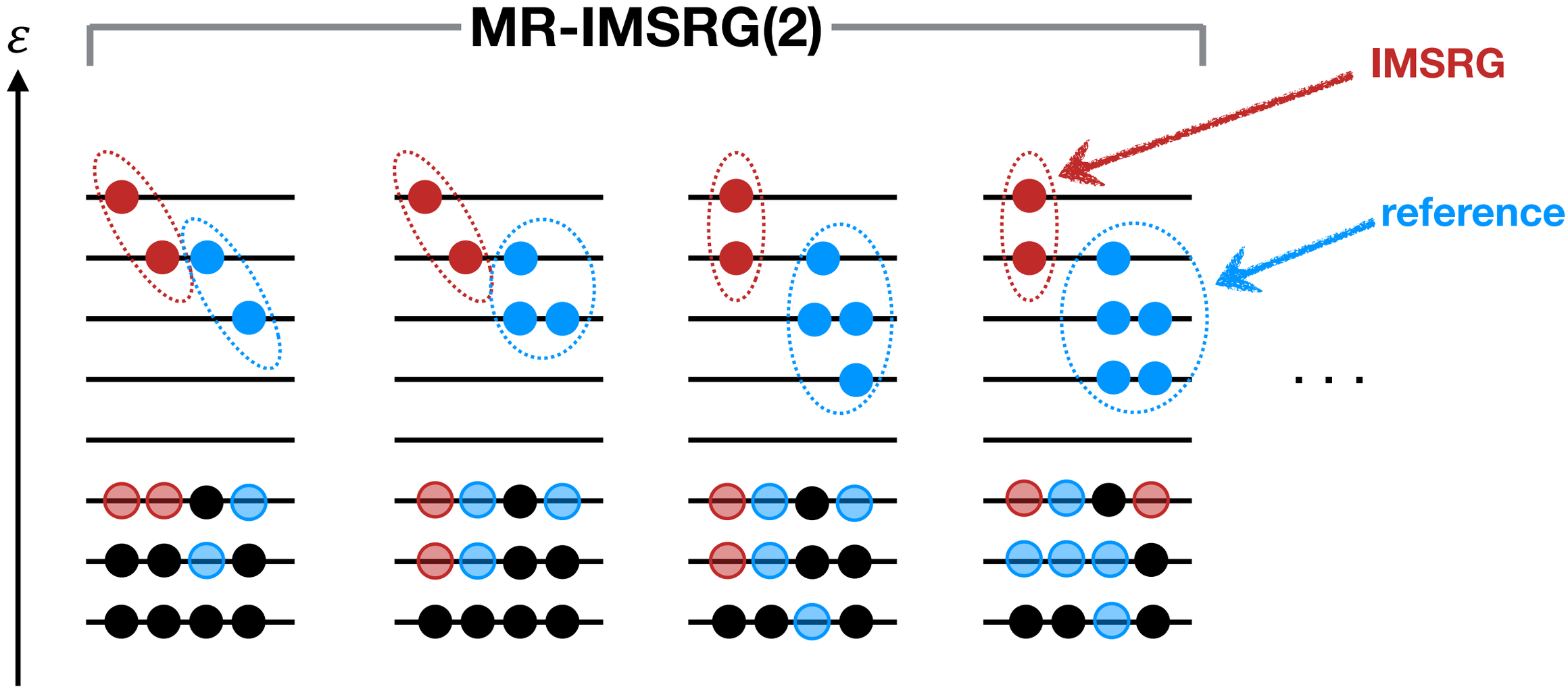


“standard” IMS
Slater determinar

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

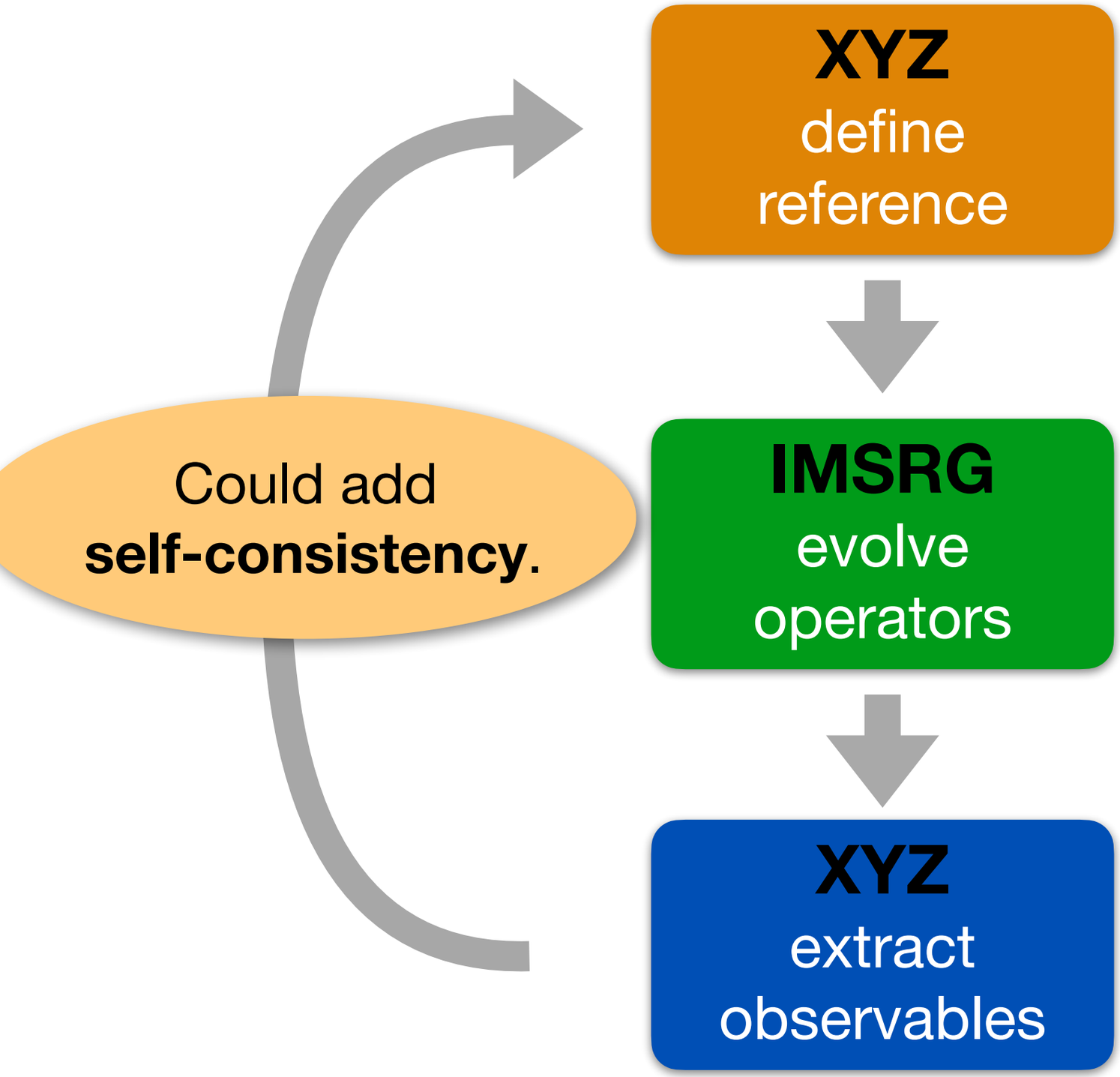


Correlated Reference States



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

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)

XYZ define reference

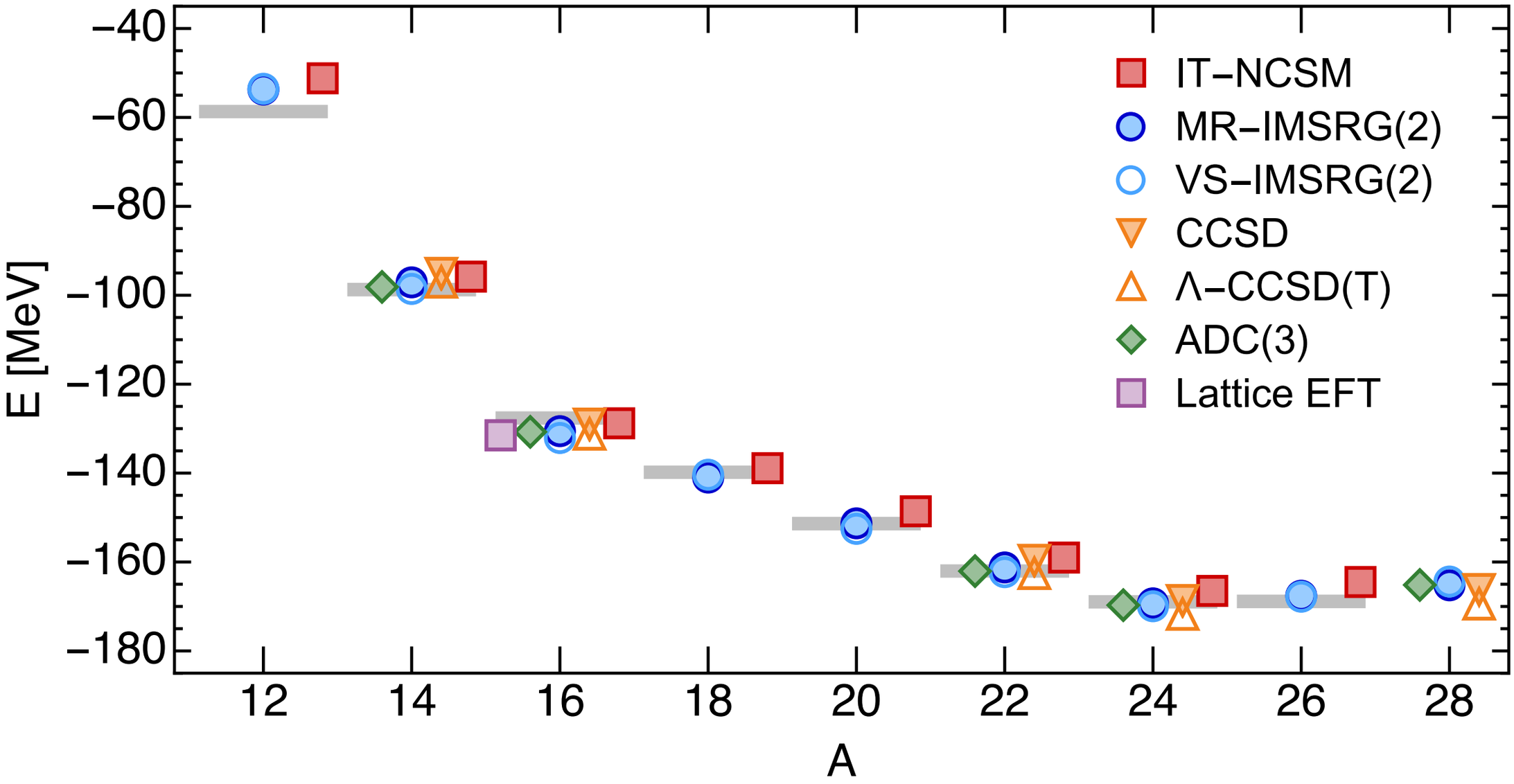
cf. talk by Jason Holt

IMSRG evolve operators

XYZ extract observables

Oxygen Isotope

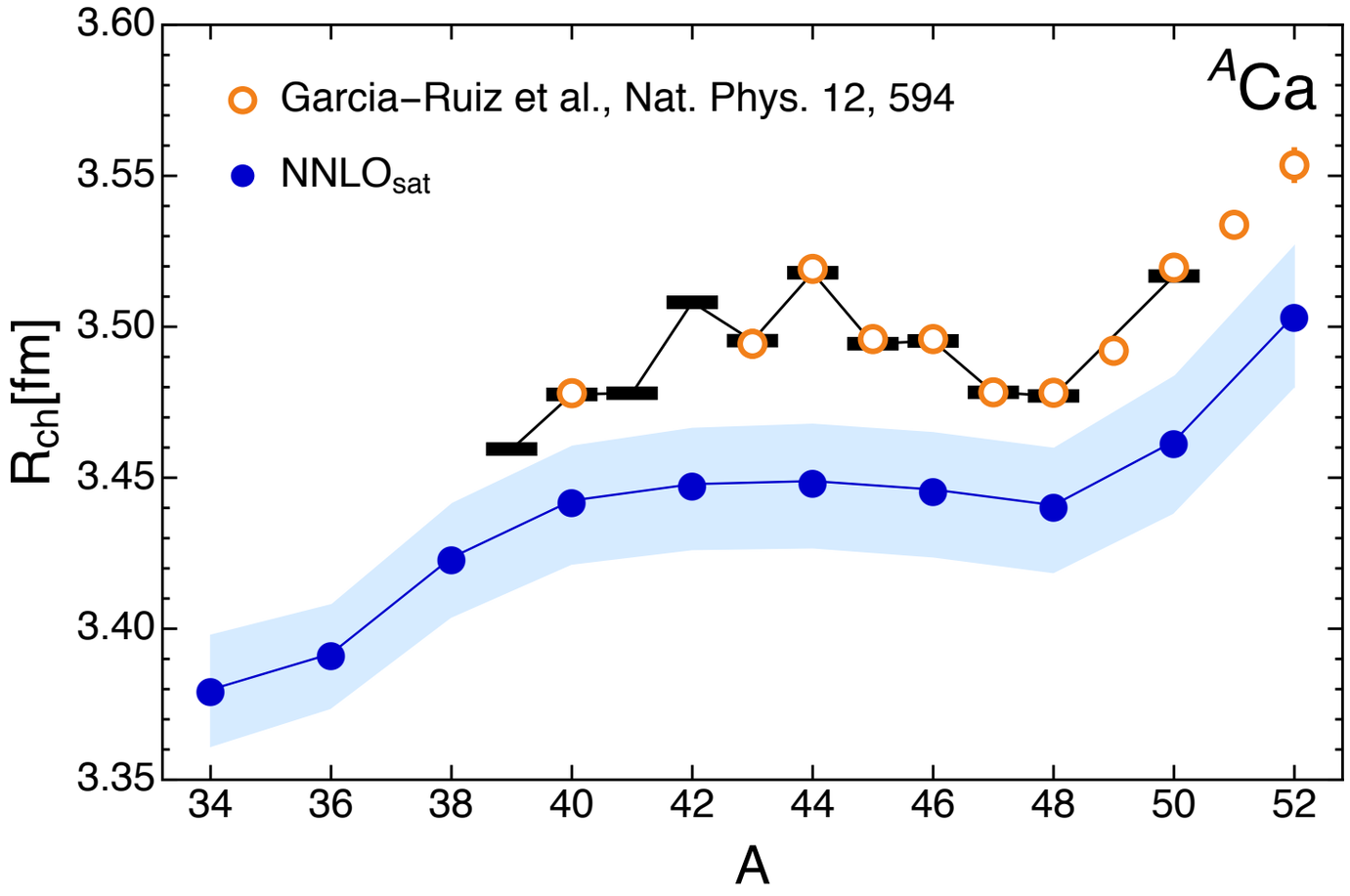
HH, Front. Phys. ***8****, 379 (2020)*

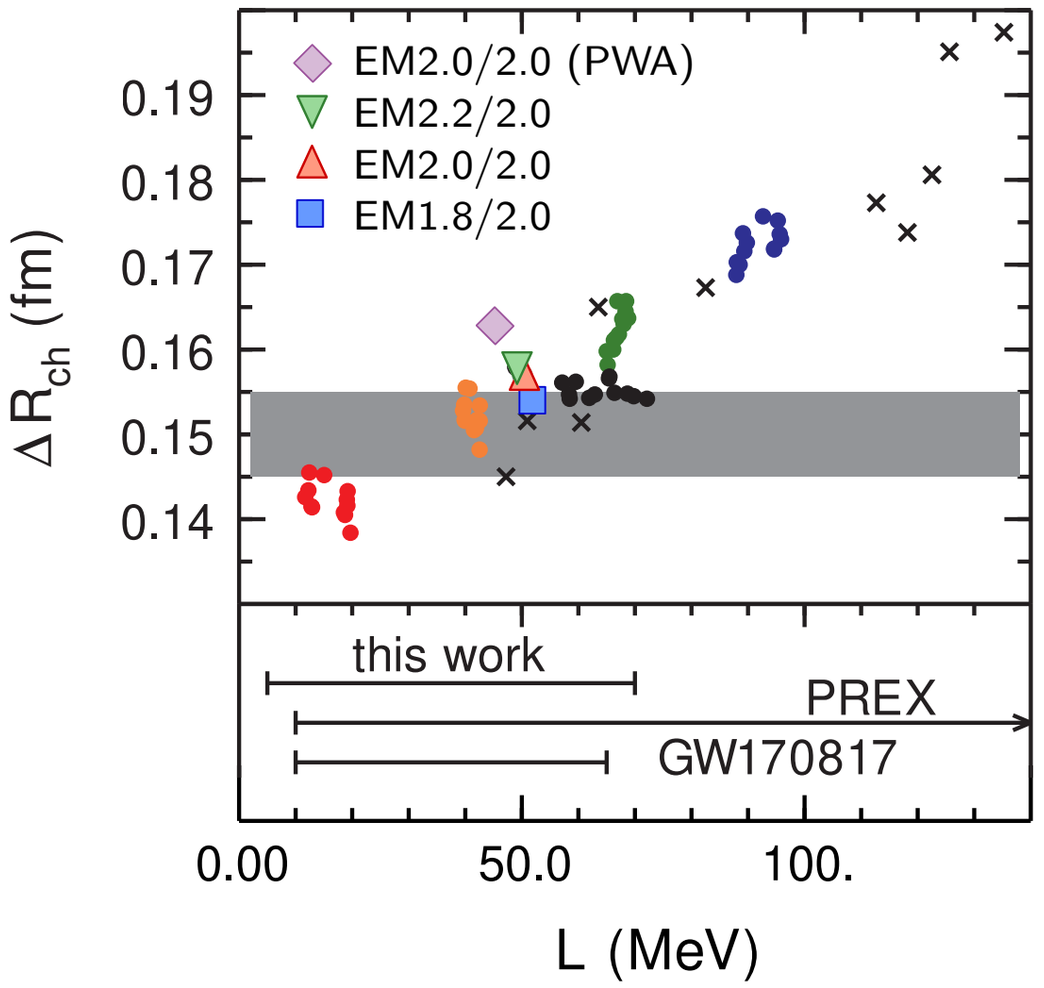


consistent ground-state energies for the **same interaction**
(and comparable Lattice EFT action)

Calcium Charge Radii

*HH, Front. Phys. **8**, 379 (2020)*
*B. A. Brown et al., PRR **2**, 022305(R) (2020)*



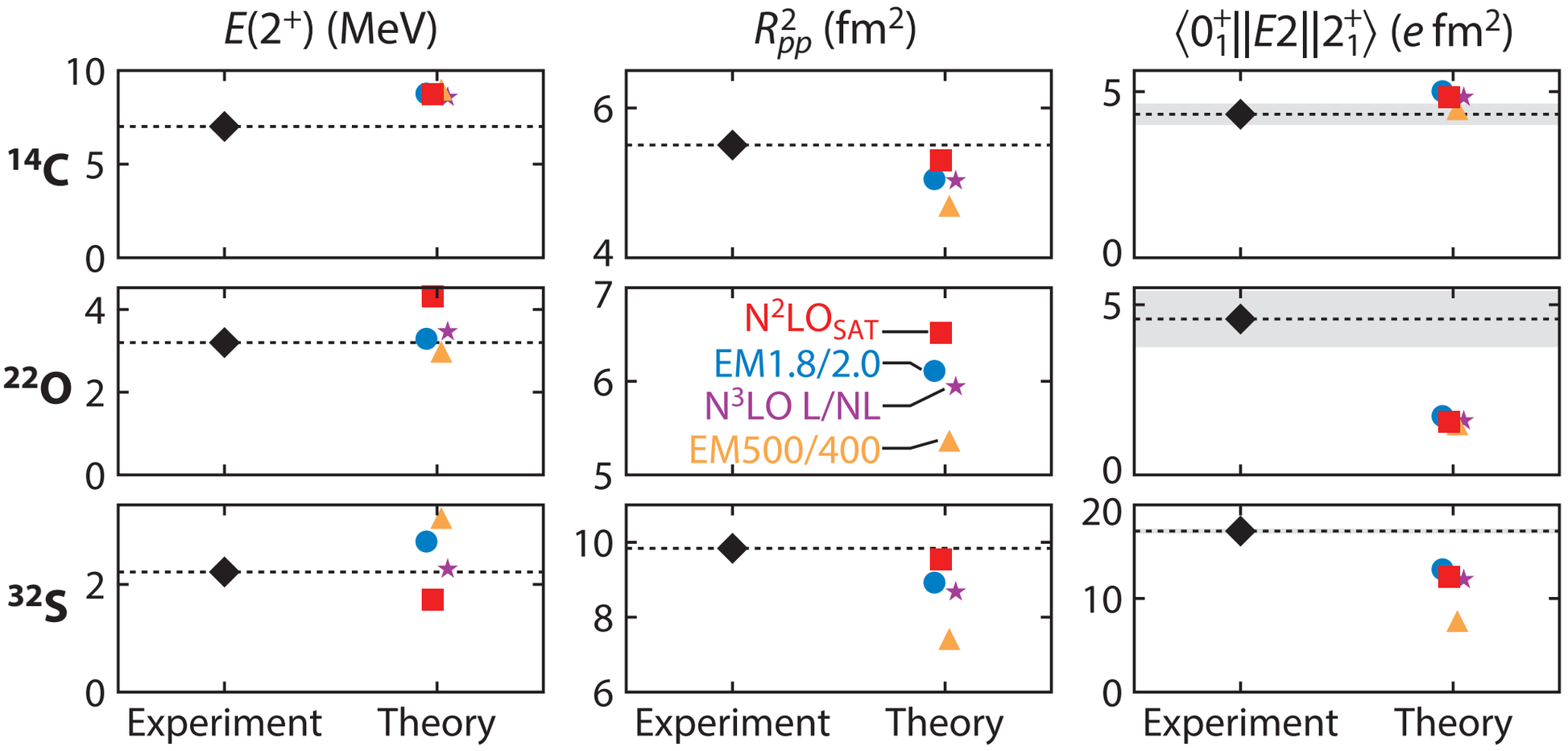


- **differential observables** like ΔR_{ch} are insensitive to variations of interaction cutoffs / resolution scale

cf. talk by W. Nazarewicz

Transitions

S. R. Stroberg, HH, S. K. Bogner, J. D. Holt, Ann. Rev. Part. Nucl. Sci. ***69****, 307 (2019)*
N. M. Parzuchowski, S. R. Stroberg et al., PRC ***96****, 034324 (2017)*
S. R. Stroberg et al. PRC ***105****, 034333 (2022)*



- **B(E2)s too small:** missing collectivity due to intermediate 3p3h, … states that are truncated in IMSRG evolution (**static correlation**)

Capturing Collective Correlations: In-Medium Generator Coordinate Method

J. M. Yao, A. Belley, R. Wirth, T. Miyagi, C. G. Payne, S. R. Stroberg, HH, J. D. Holt, PRC **103**, 014315 (2021)

J. M. Yao, B. Bally, J. Engel, R. Wirth, T. R. Rodriguez, HH, PRL **124**, 232501 (2020)

J. M. Yao, J. Engel, L. J. Wang, C. F. Jiao, HH, PRC **98**, 054311 (2018)

In-Medium GCM

*J. M. Yao, et al., PRC **98**, 054311 (2018), PRL **124**, 232501 (2020), PRC **103**, 014315 (2021)*

GCM
define reference

- no-core (or valence space) GCM calculation to prepare reference state

IMSRG
evolve operators

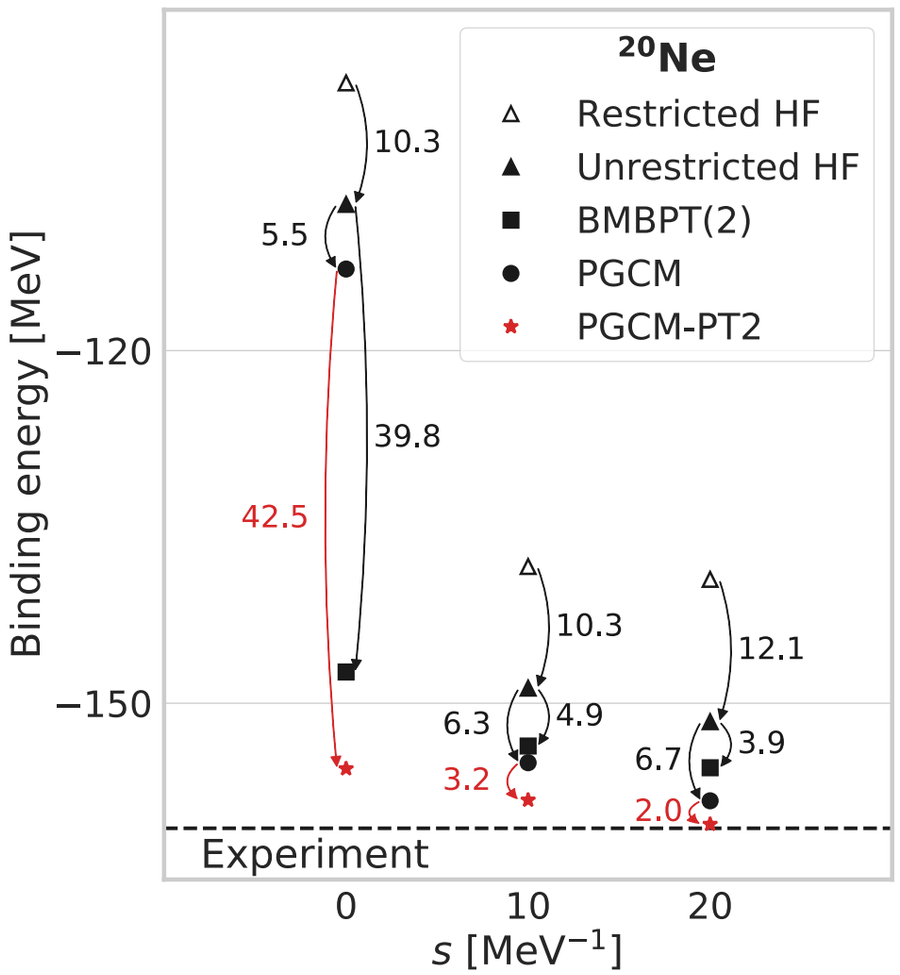
- evolve Hamiltonian and observables with MR-IMSRG
- decoupling in A-body space

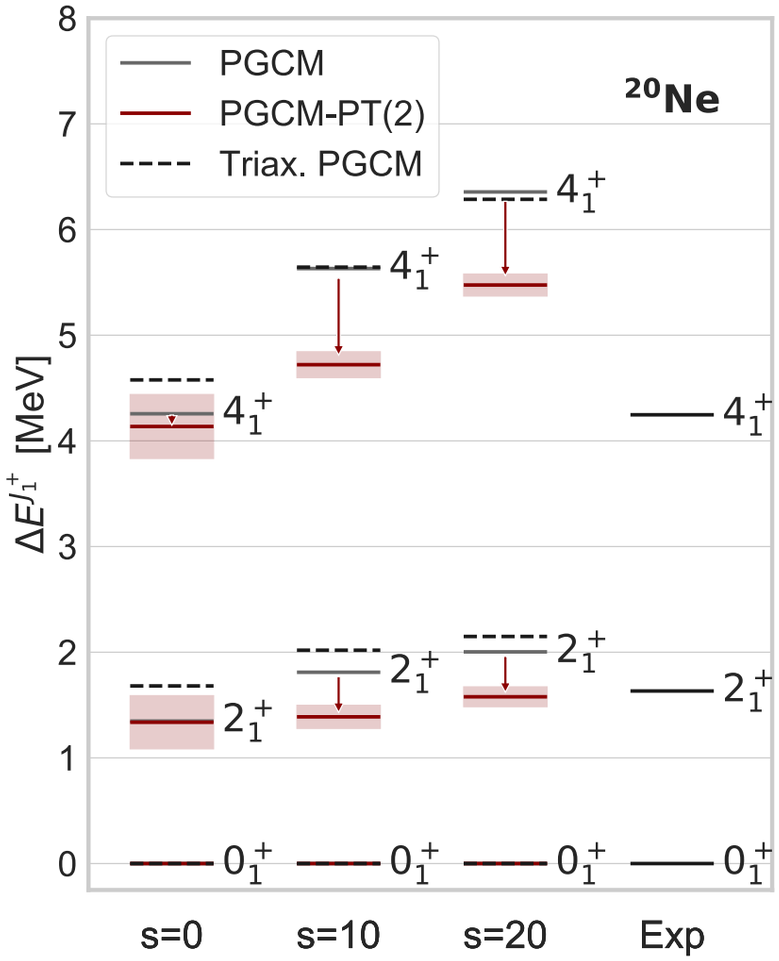
GCM
extract observables

- no-core GCM calculation using evolved Hamiltonian
- calculate GCM wave functions, observables

Perturbative Enhancement of IM-GCM

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

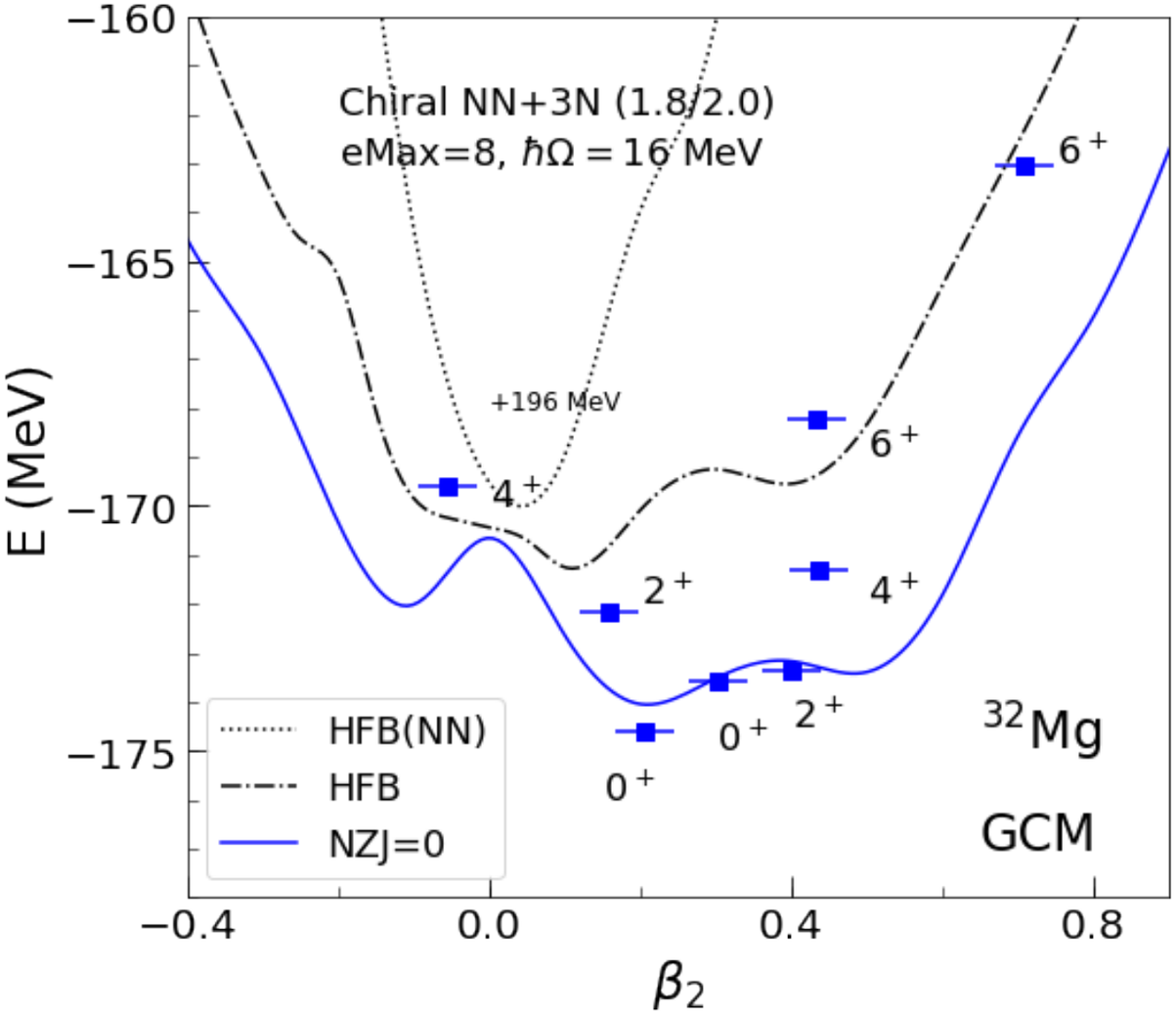


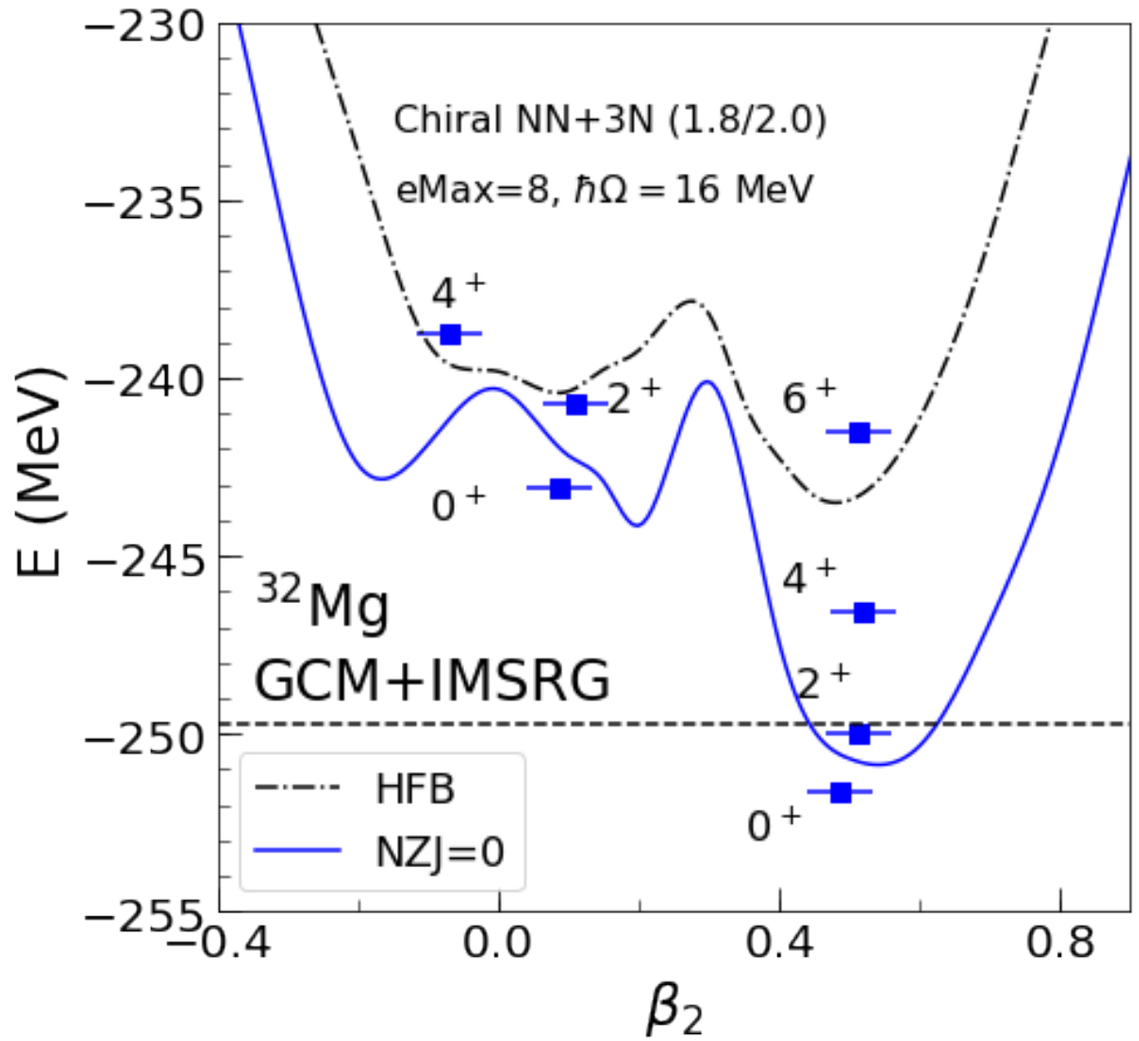


- s-dependence is a **built-in diagnostic tool** for IM-GCM **(not available in phenomenological GCM)**
  - if operator and wave function offer sufficient degrees of freedom, evolution of observables is unitary
- need **richer references and/or IMSRG(3)** for certain observables

Collectivity in ^{A}Mg: IM-GCM

J. M. Yao, HH, in preparation



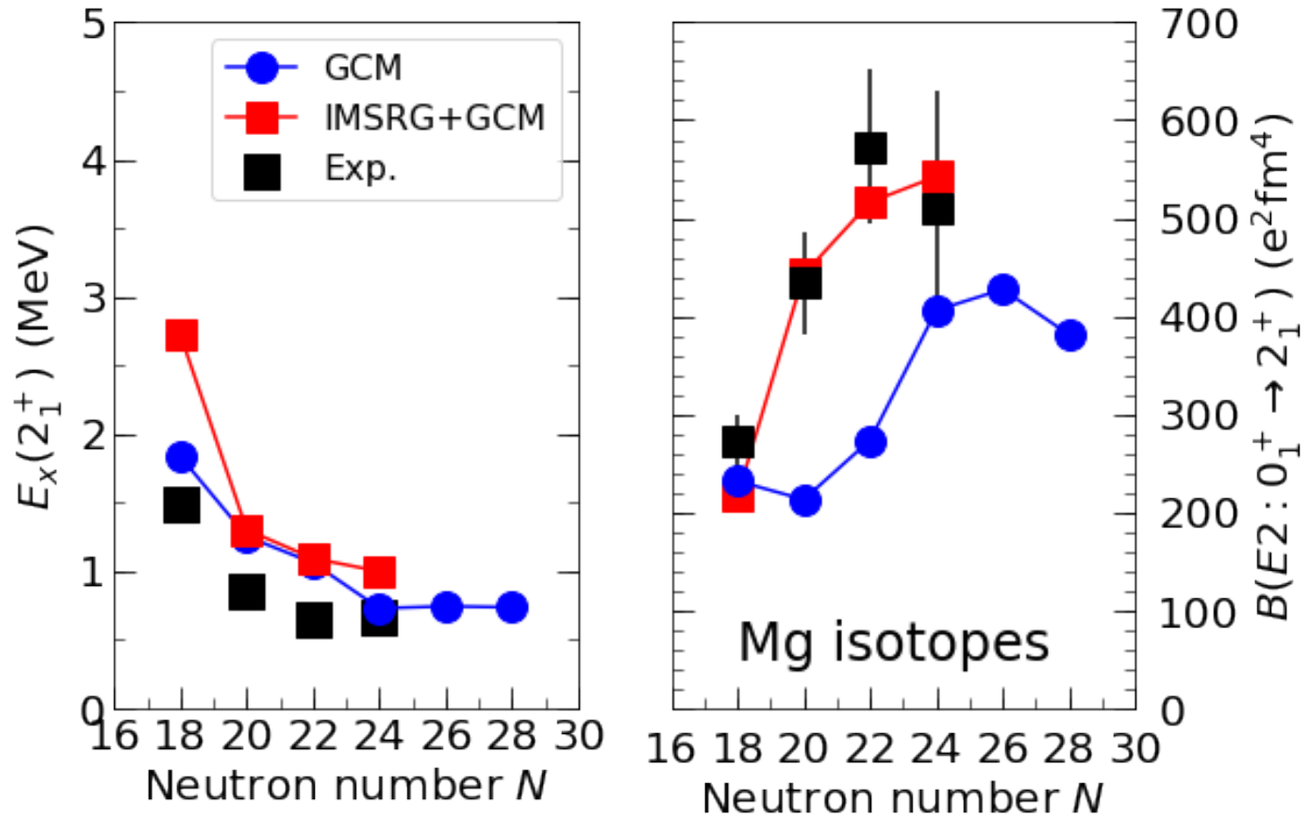


- Prolate configurations gain more energy than the weakly deformed one via IMSRG flow (**targeting states or groups/bands of states**)
- Dominant configuration is more concentrated at **large prolate deformation**, which **enhances the quadrupole collectivity** in ^{32}Mg.

Magnesium Isotopes

J. M. Yao, HH, in preparation

EM1.8/2.0

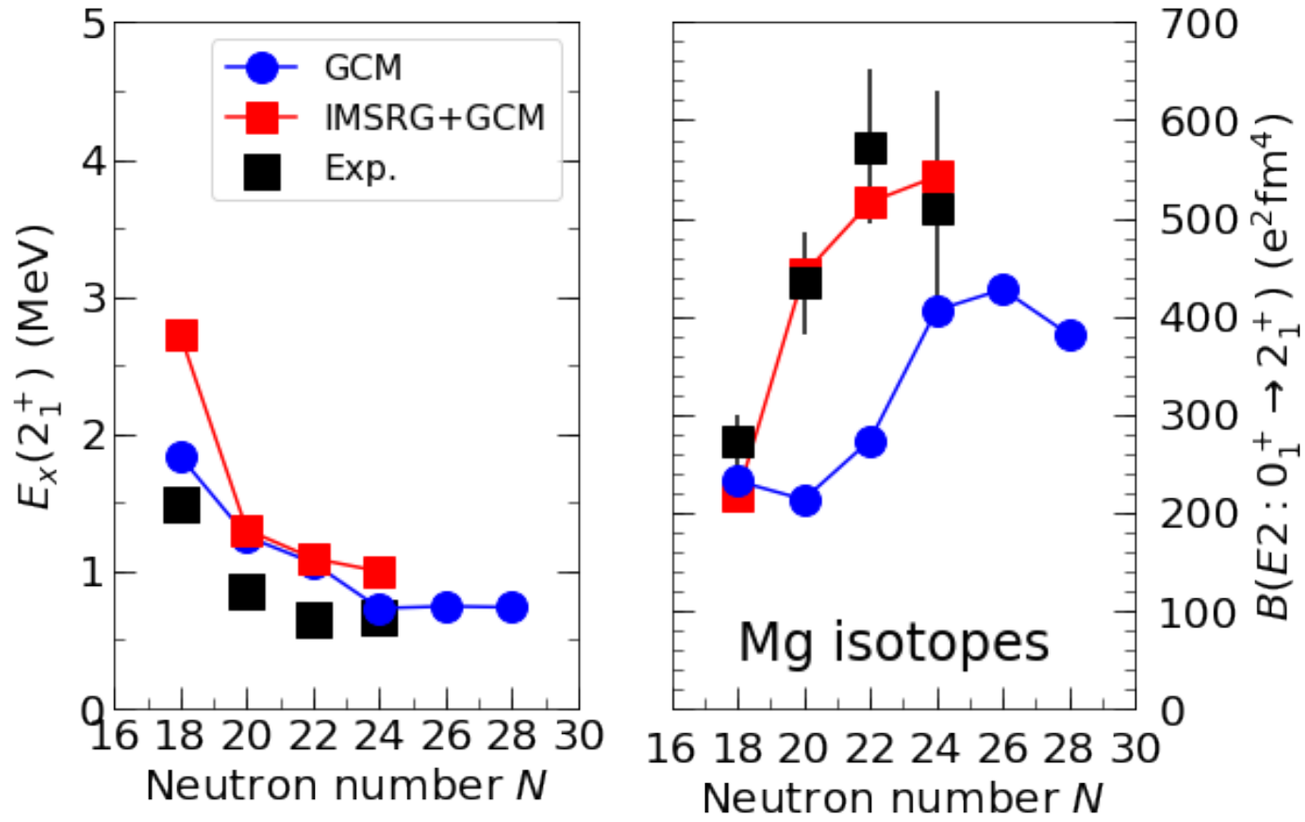


- much **improved B(E2)** values compared to standard GCM or VS-IMSRG calculations: IM-GCM captures **dynamical and static correlations**!

Magnesium Isotopes

J. M. Yao, HH, in preparation

EM1.8/2.0

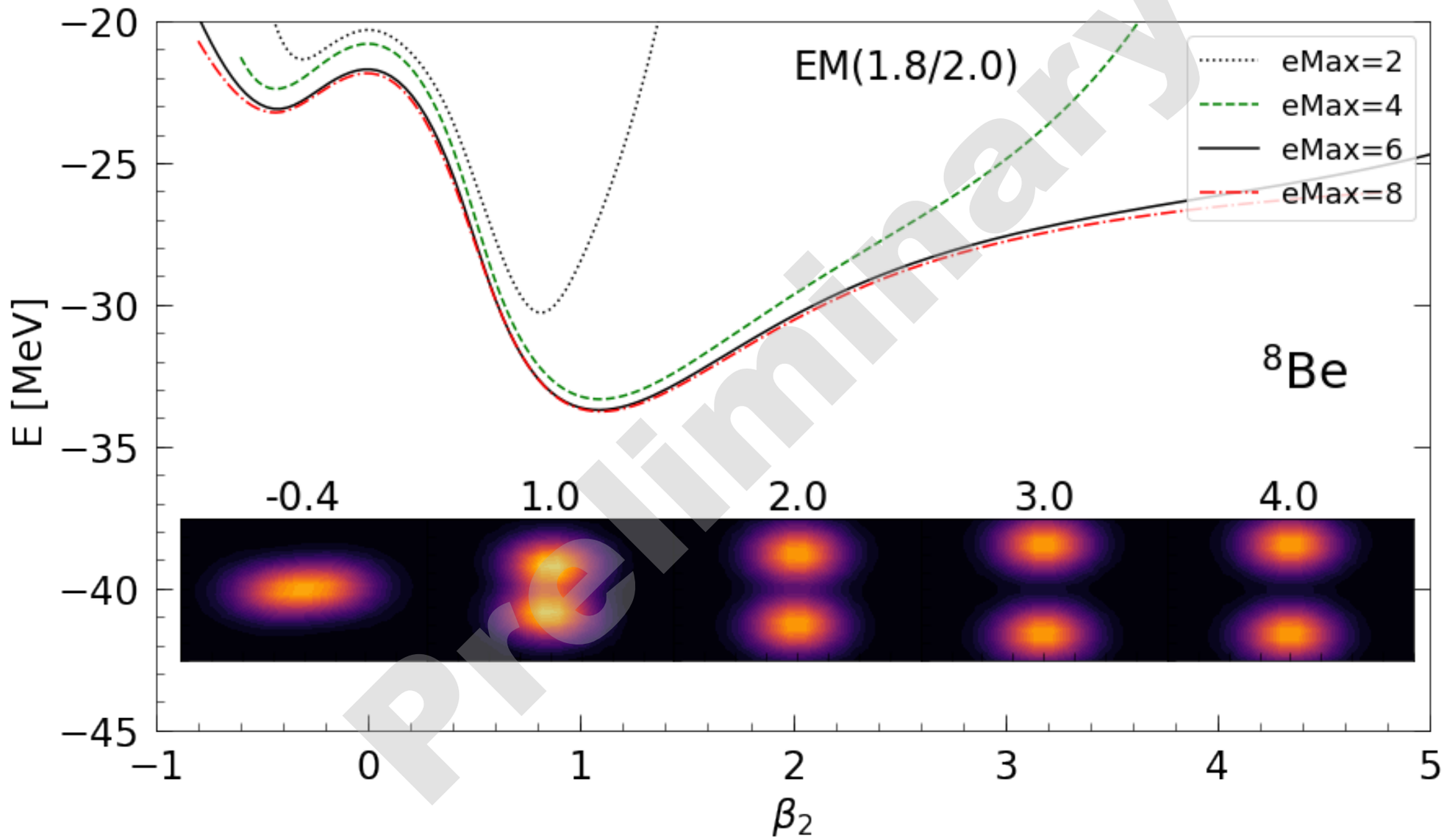


$$O = O^{(1)} \quad \underset{s\to\infty}{\to} \quad O(s) = O^{(1)}(s) + \underbrace{O^{(2)}(s) + \ldots}_{\text{induced contributions}}$$

- **induced 2B quadrupole operator is small (~5%),** contrary to typical VS-IMSRG (~50%): GCM reference equips operator basis with better capability to capture collectivity

Cluster Structures: ^{8}Be

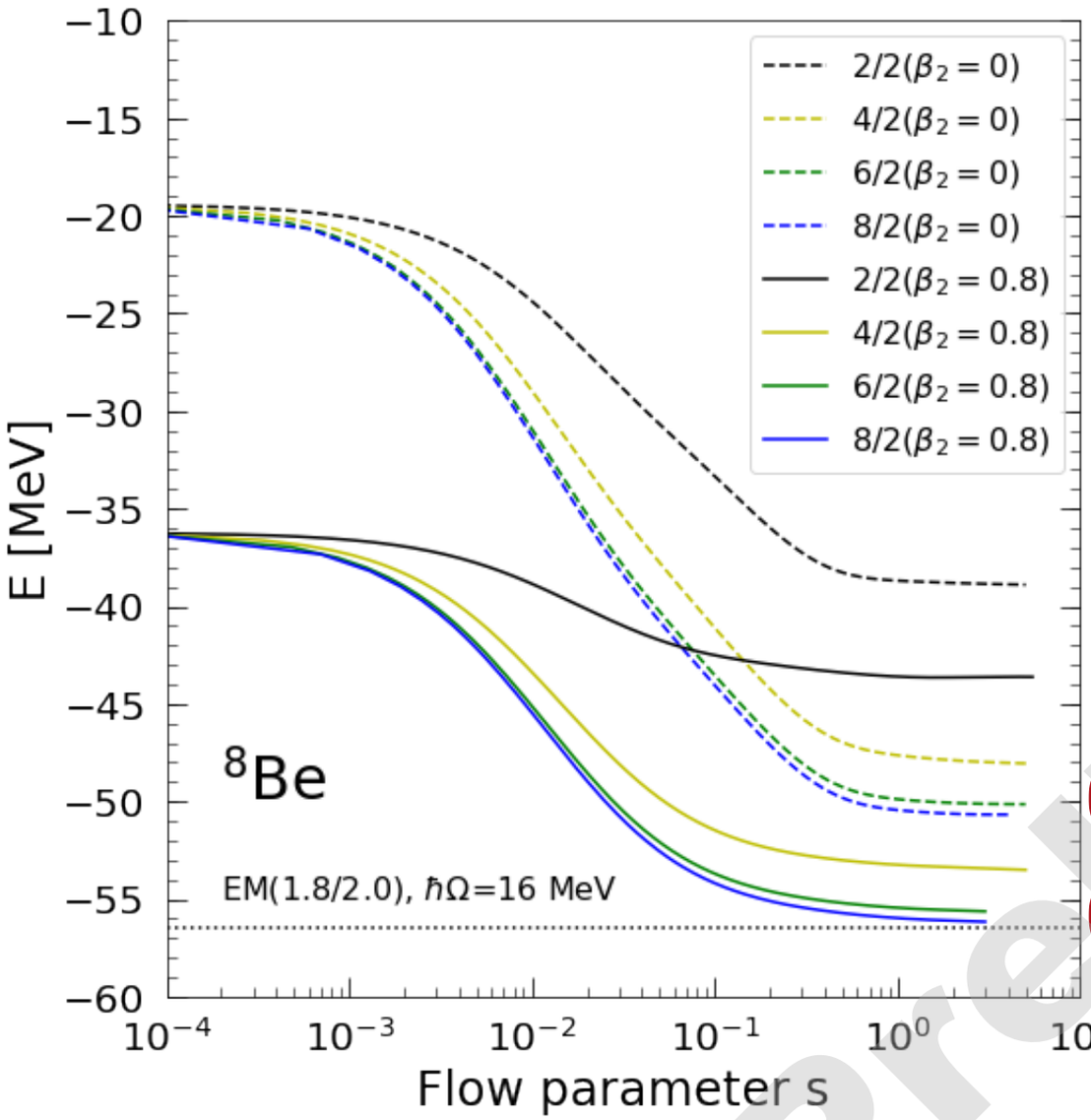
J. M. Yao, R. Wirth, HH, in progress

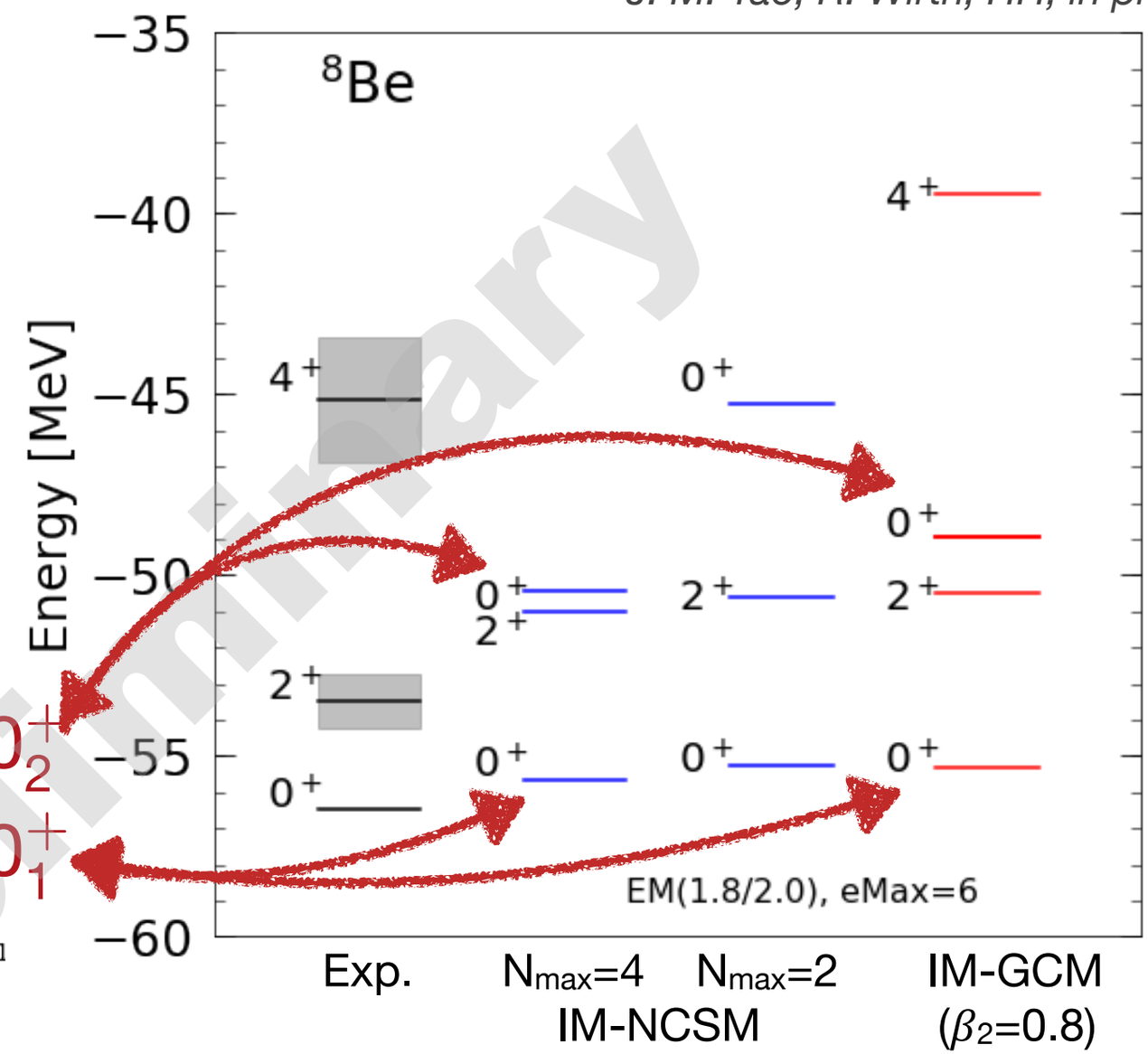


HFB potential energy surface

Cluster Structures: ^{8}Be

J. M. Yao, R. Wirth, HH, in progress





- **Prolate** and **spherical** references flow towards $\mathbf{0_1^+}$ and $\mathbf{0_2^+}$ states
  [cf. Sargsyan et al., PRL128, 202503; Caurier et al., PRC64, 051301(R)]
- **seems consistent with IM-NCSM**

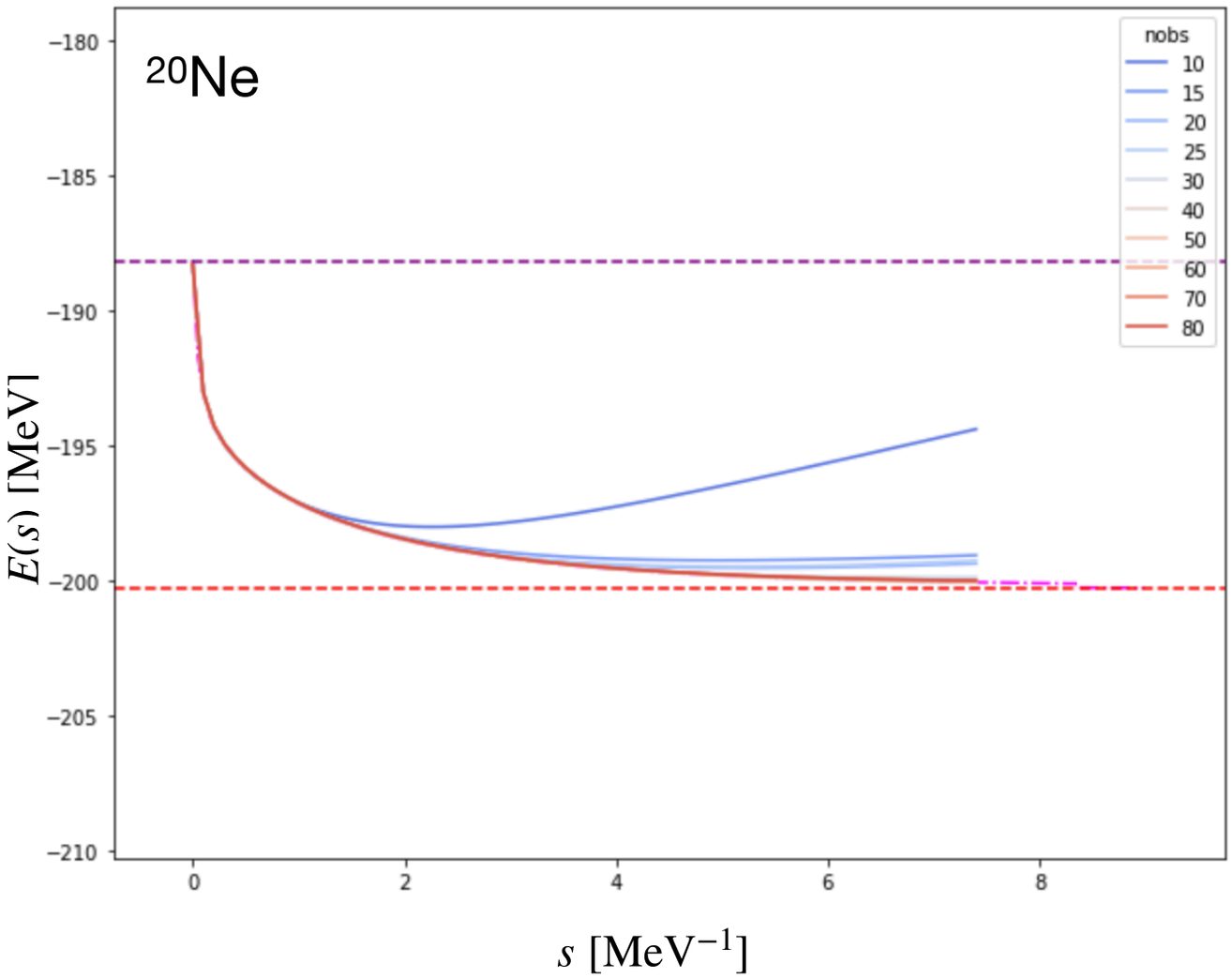
Looking Ahead

What Is Next?

- nuclear structure (and reaction) studies with **multiple complementary methods**: IM-GCM, VS-IMSRG, Coupled Cluster, (symmetry-adapted) NCSM(C)…
- **improved truncations:** IMSRG(3) and tailored operator bases
- **accelerate IMSRG & IM-GCM** (GPUs, factorization, Machine Learning, …)
  [A. M. Romero et al., PRC 104, 054317; X. Zhang et al., PRC 107, 024304]
- **Uncertainty Quantification / Sensitivity Analysis**
  - need cheap **surrogate models** (**emulators**)

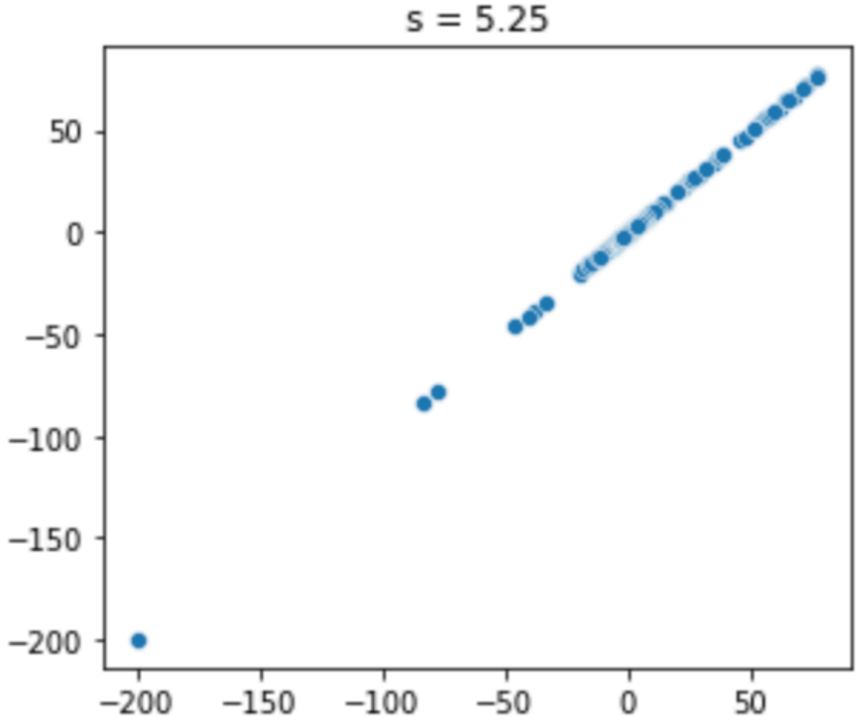
Emulating IMSRG Flows

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

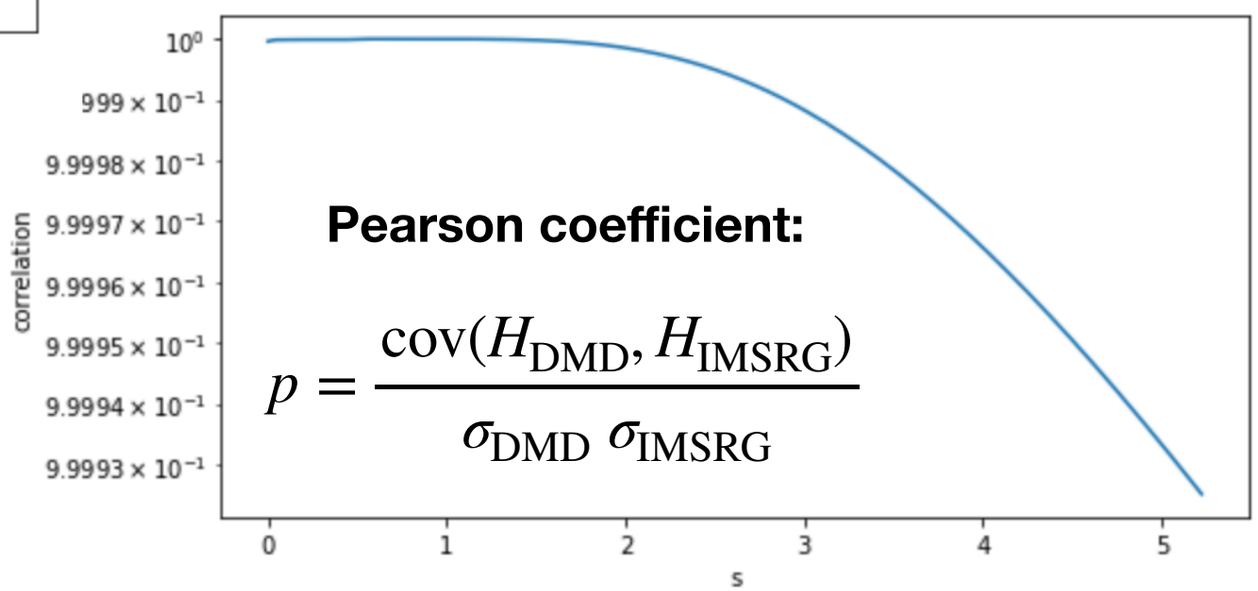


***J. Davison, J. Crawford**, S. Bogner, HH, in preparation*

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



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

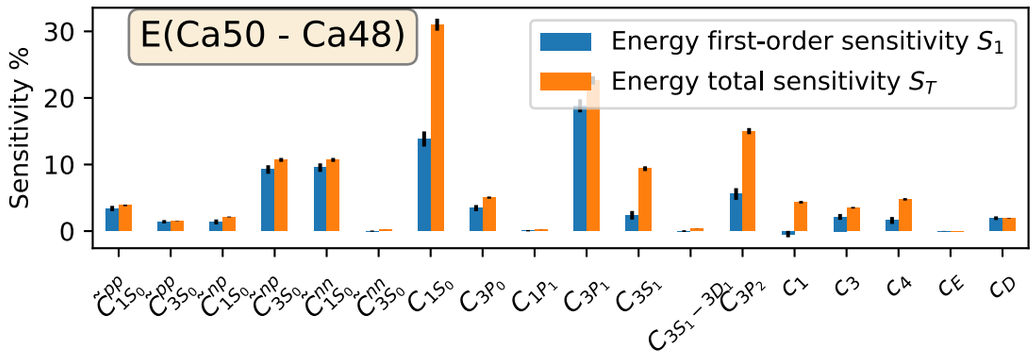


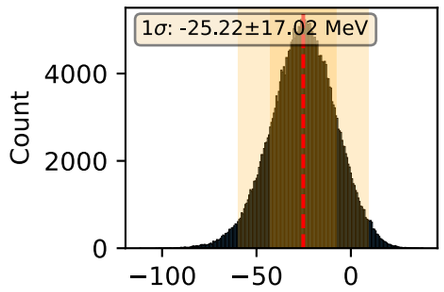
Pearson coefficient:

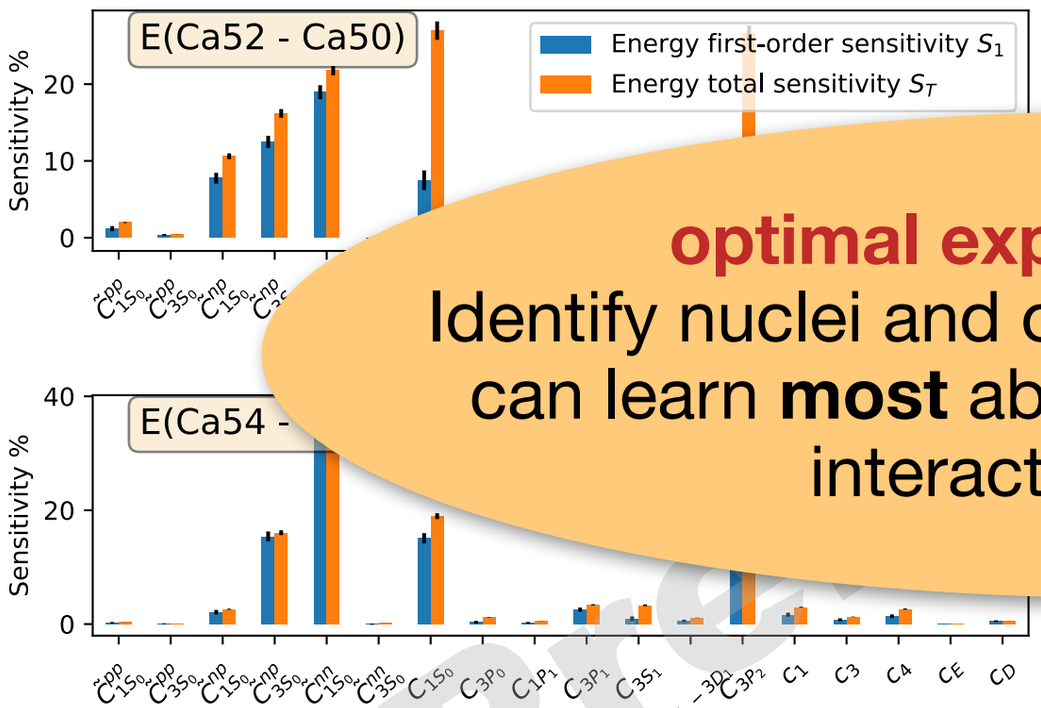
$$p = \frac{\mathrm{cov}(H_{\mathrm{DMD}}, H_{\mathrm{IMSRG}})}{\sigma_{\mathrm{DMD}}\,\sigma_{\mathrm{IMSRG}}}$$

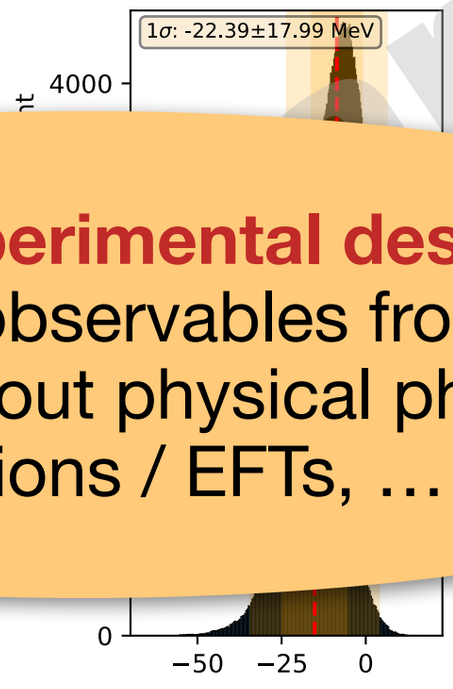
Parametric DMD

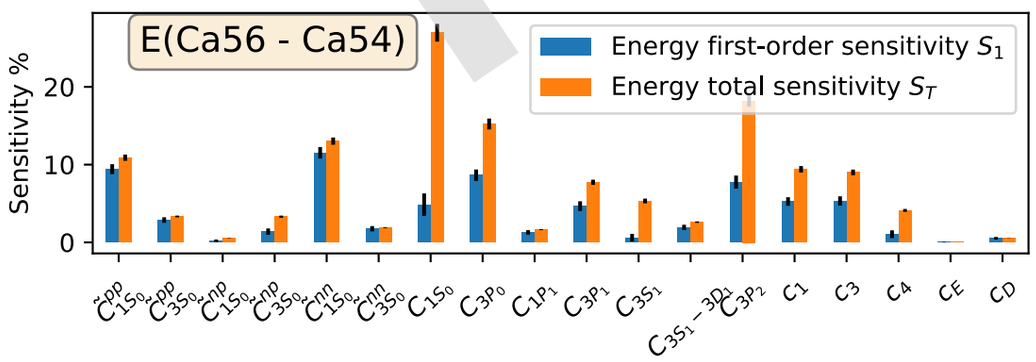
***J. Davison, J. Crawford**, S. Bogner, HH, in preparation*

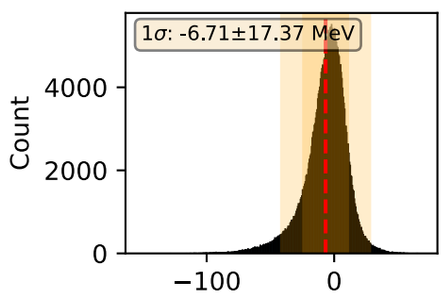












optimal experimental design:
Identify nuclei and observables from which we can learn **most** about physical phenomena, interactions / EFTs, …

- Δ-full, NNLO NN+3N
- $e_{max} = 12$, $E_{3max} = 14$
- 0+ es
- **4-5 order of magnitude reduction in computational effort**

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R. J. Furnstahl
The Ohio State University

and many more…

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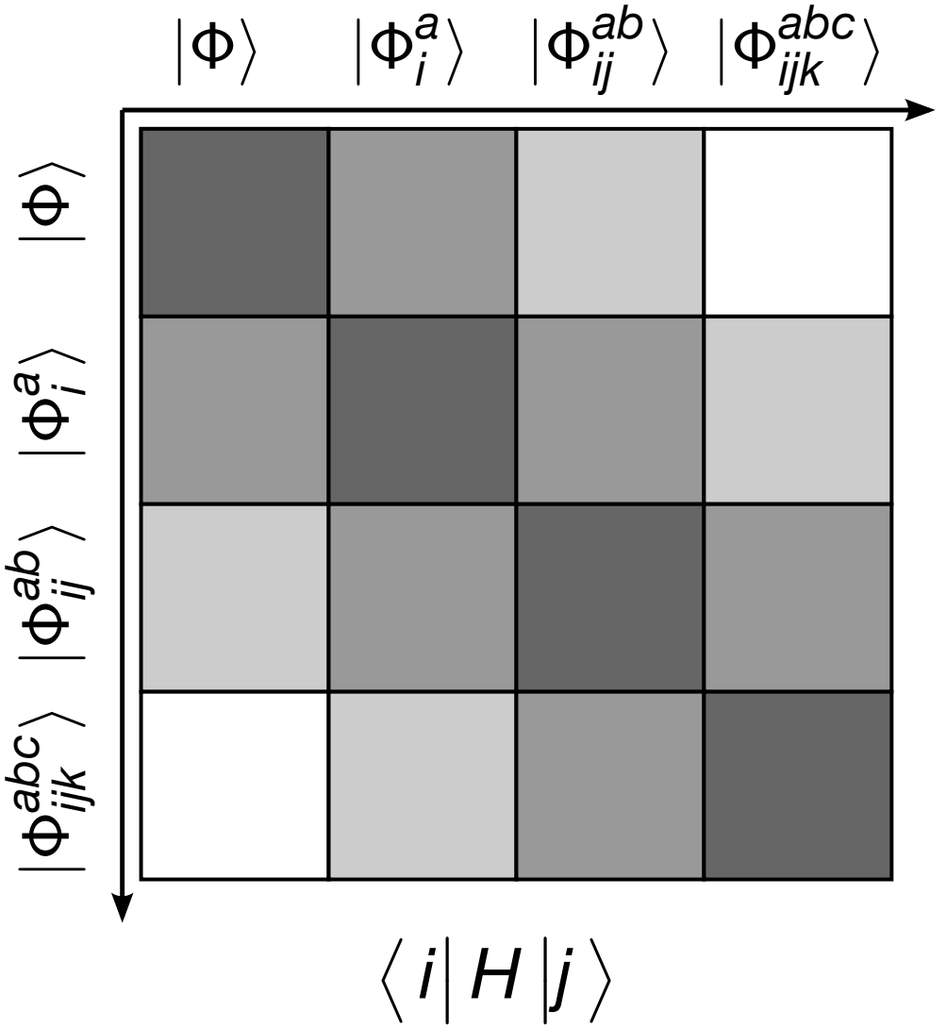
Supplements

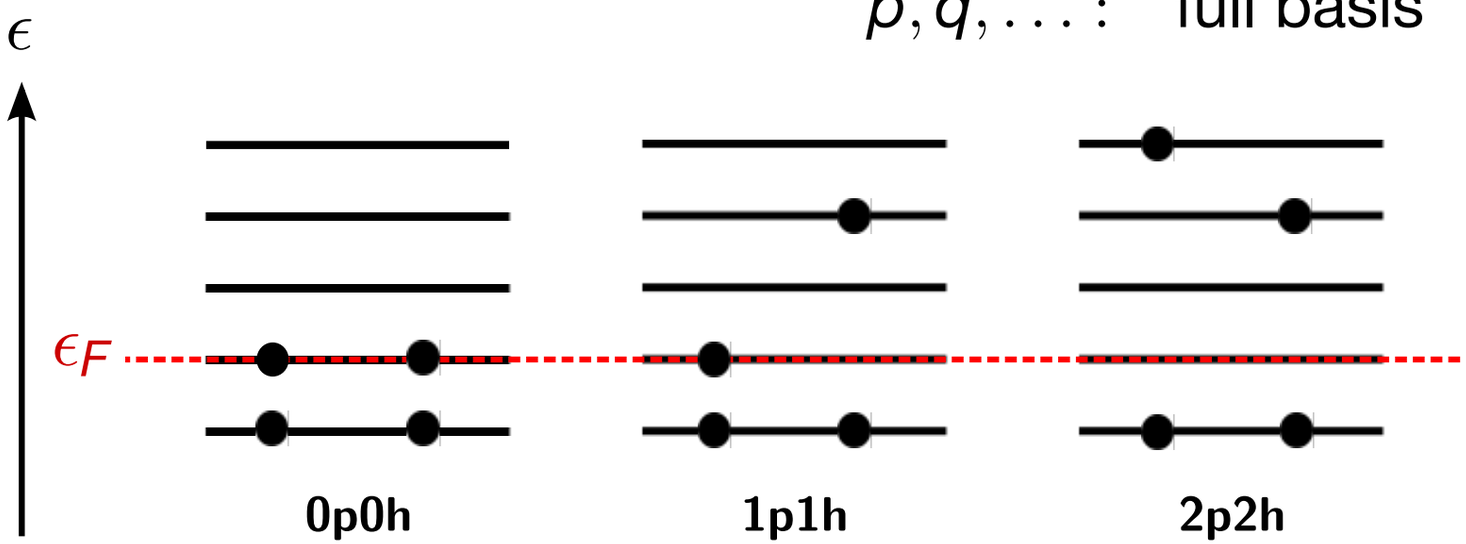
Transforming the Hamiltonian



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

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

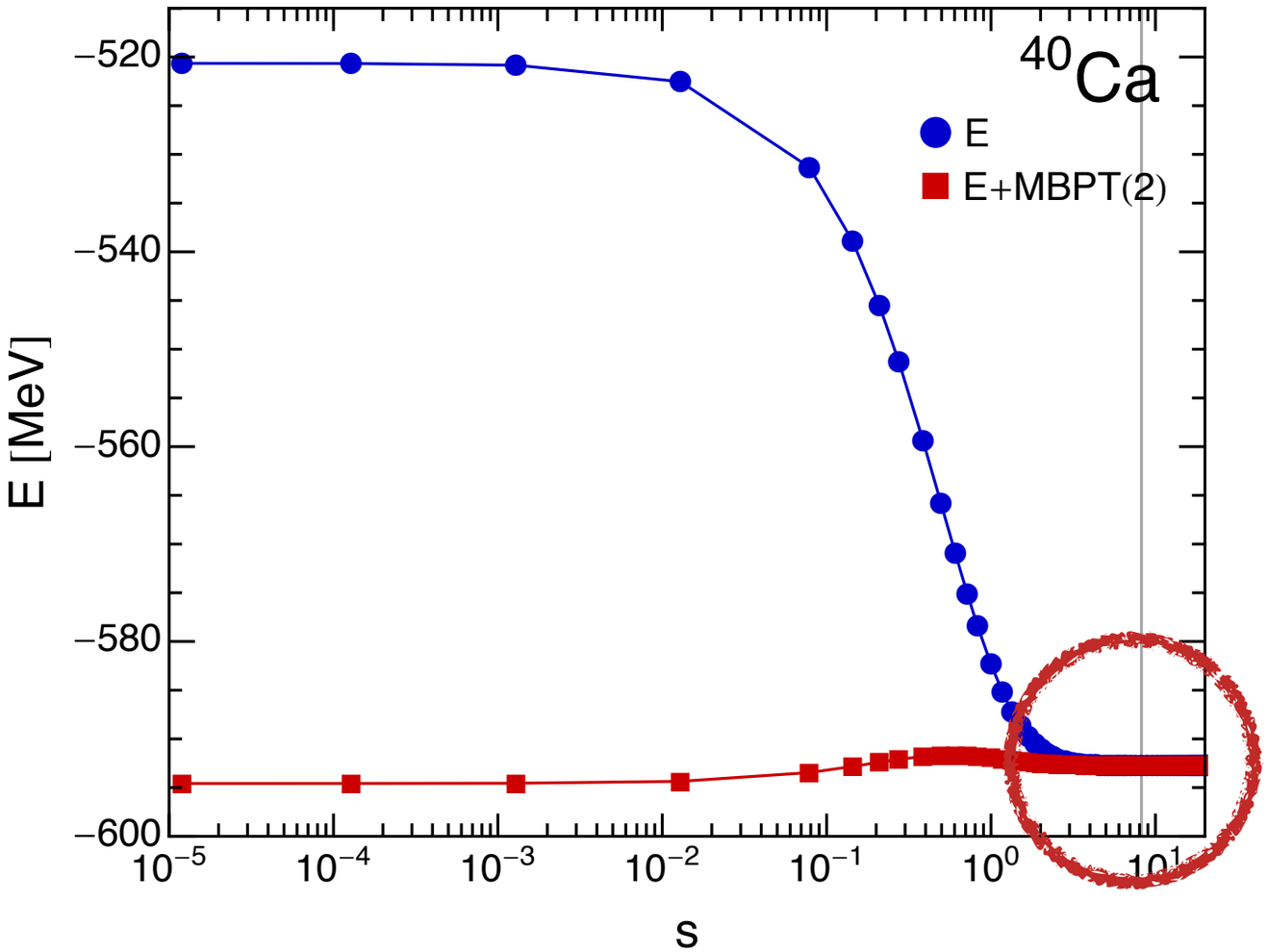
$p, q, \ldots$: full basis

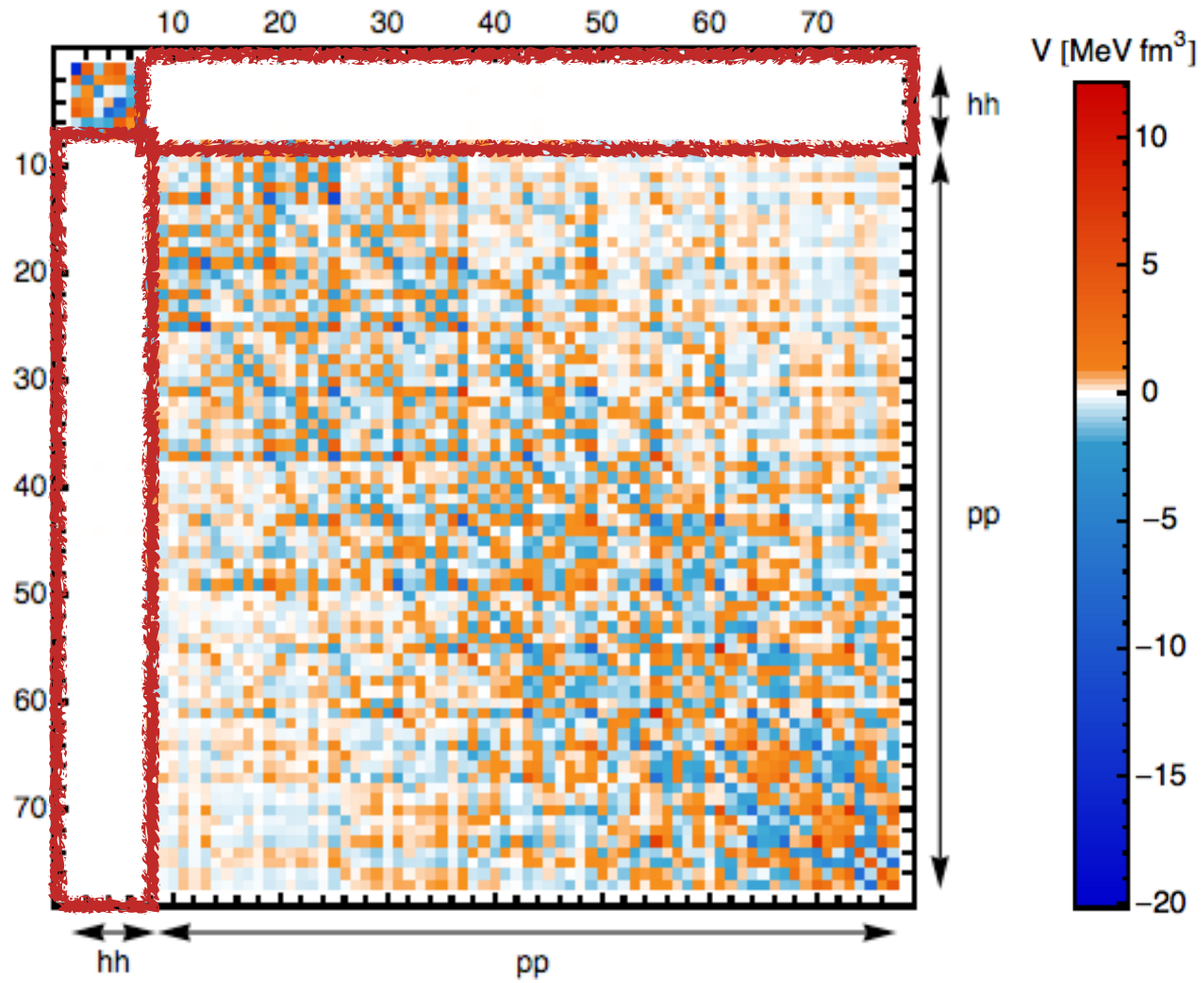


excitations relative to reference state: **normal-ordering**

- reference state: **single Slater determinant**

Decoupling



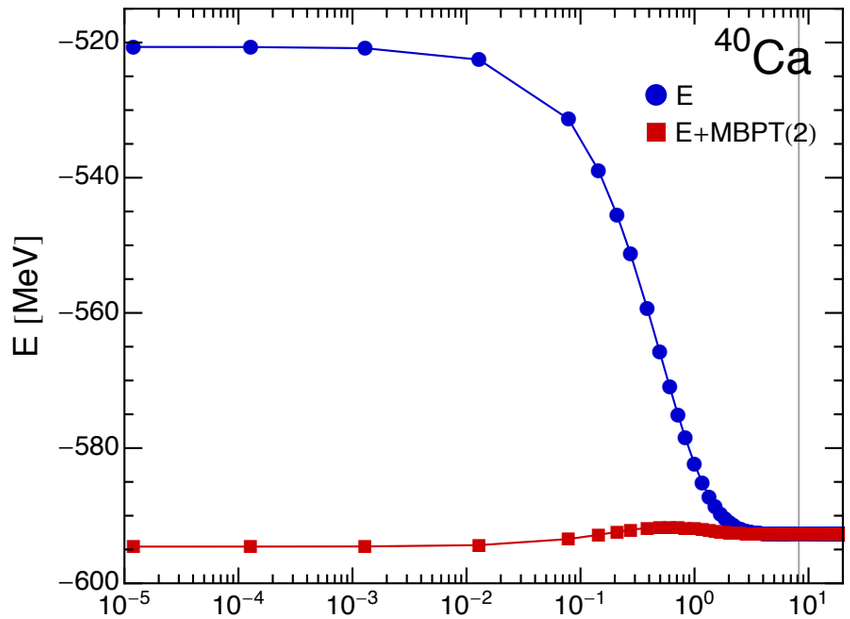


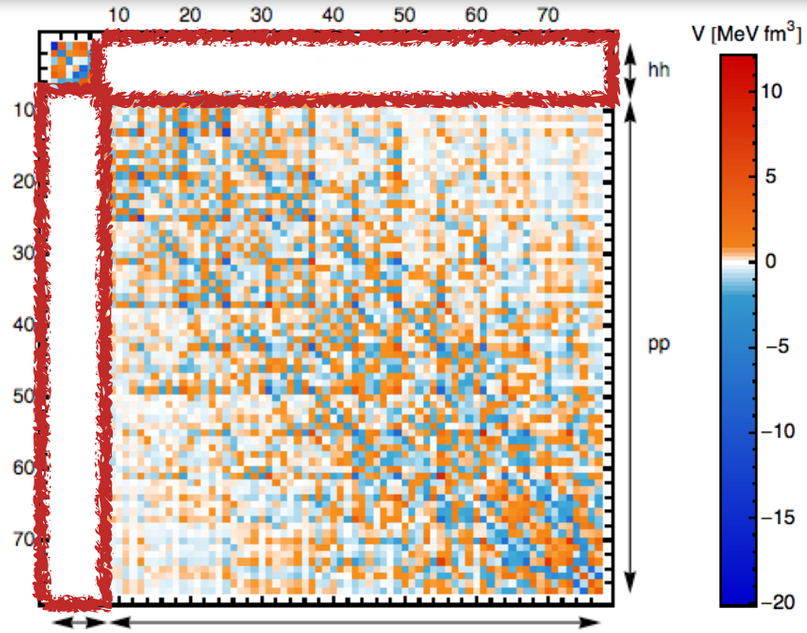
N3LO, $\lambda = 2.0$ fm^{-1}, $e_{\text{Max}} = 8$

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

off-diagonal couplings are rapidly driven to zero

Decoupling





- 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:

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