In-Medium Similarity Renormalization Group Techniques in Nuclear Physics

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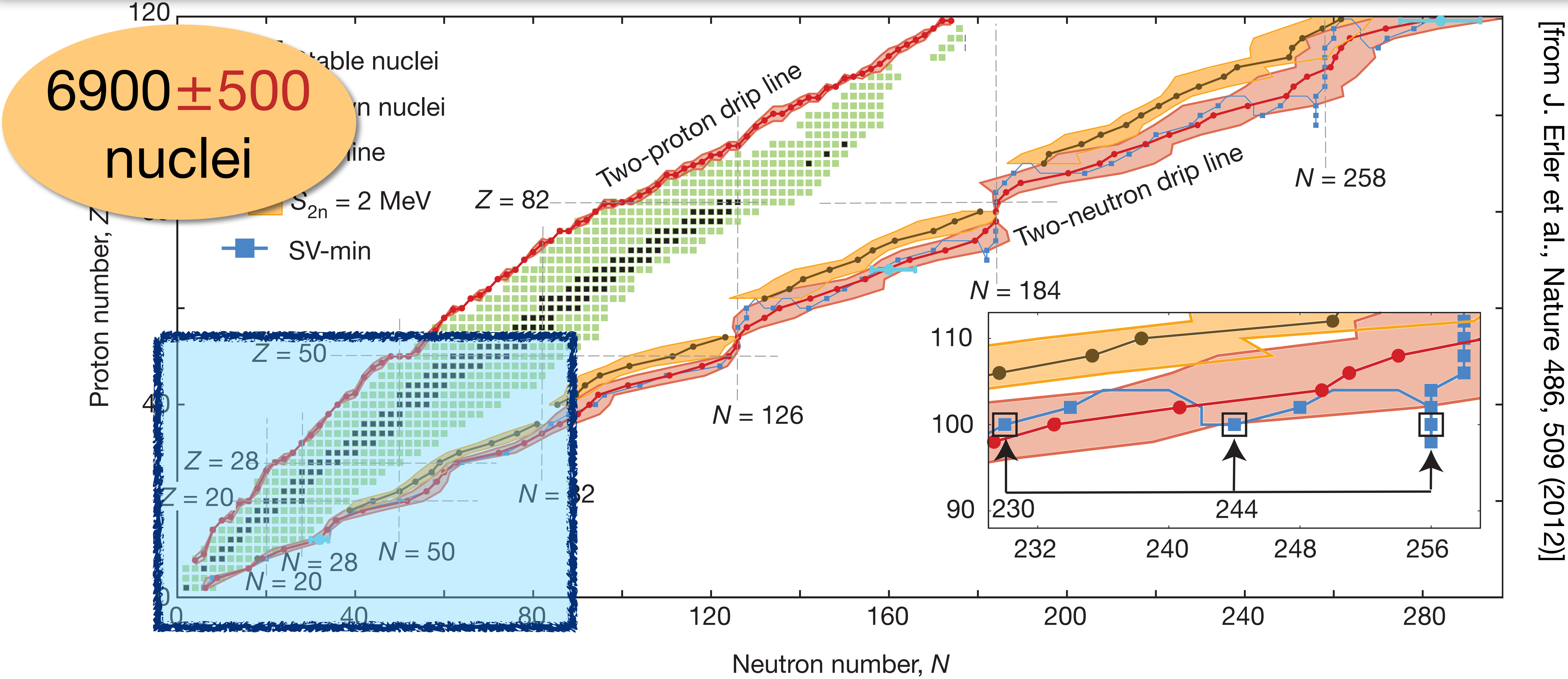
FRIB

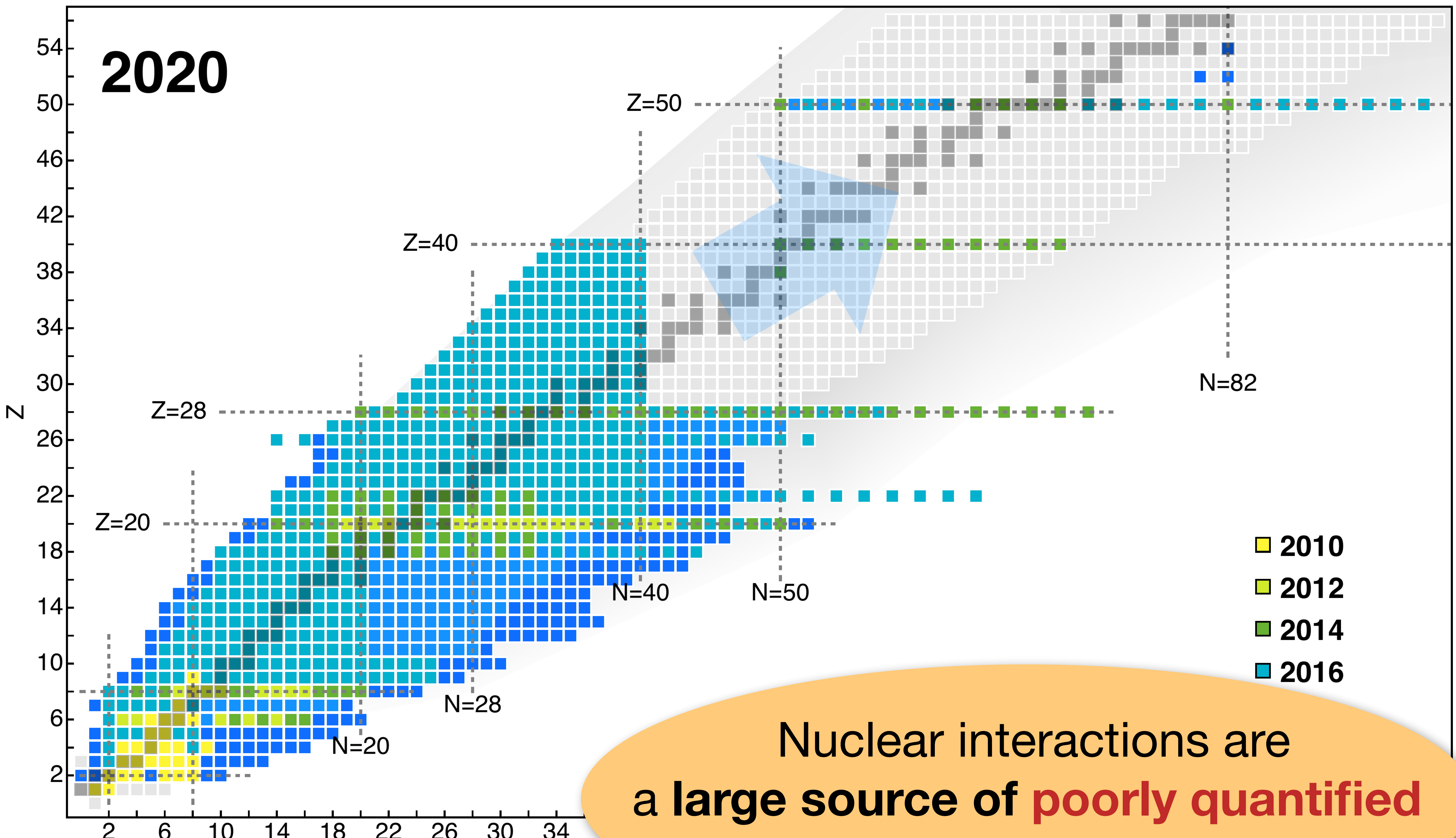
Key Directions for Nuclear Physics



- Limits of nuclear existence
- Evolution of nuclear structure towards the drip lines
- Nucleosynthesis in stellar (or cosmic) environments
- Tests of fundamental symmetries

Progress in *Ab Initio* Calculations

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

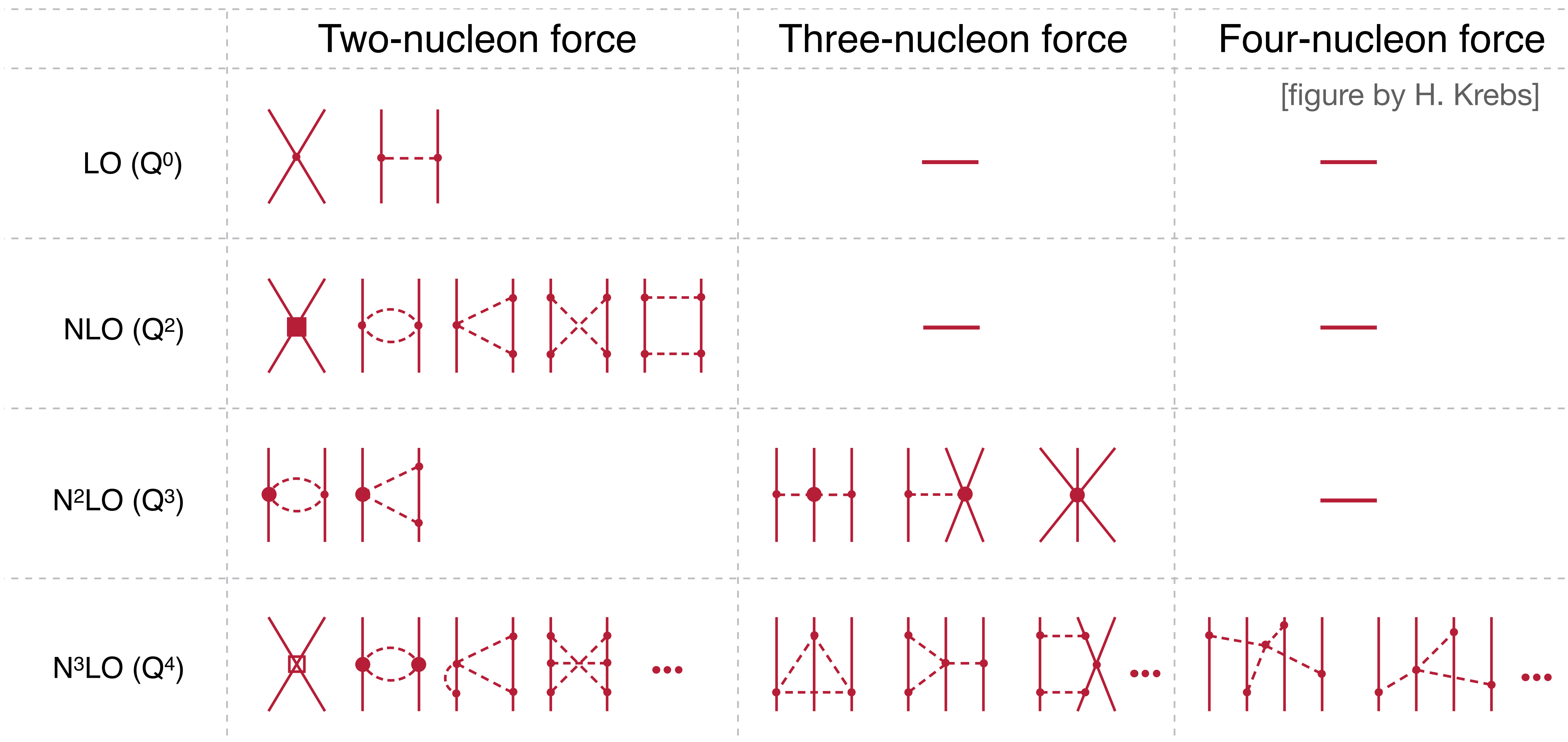


Nuclear interactions are
a **large source of poorly quantified uncertainty**

The Nuclear Many-Body Problem in a Nutshell

- **non-relativistic** many-body Schrödinger equation
  - this talk: **configuration space** methods
- nuclei are **compact, self-bound** objects
  - **rotational** symmetry
  - **translational (& boost) symmetry:** at least need decoupling of intrinsic and center-of-mass d.o.f.
- Hamiltonian: low-energy QCD
  - (approximate) **chiral symmetry**
  - **neutrons & protons** interact via **pion** exchange (and contact interactions)
  - **composite, effective** degrees of freedom: 3N, … forces

Interactions from Chiral EFT



- organization in powers $(Q/\Lambda_\chi)^\nu$ allows systematic improvement
- low-energy constants fit to NN, 3N data (future: from Lattice QCD (?))
- consistent NN, 3N, ... interactions & operators (**electroweak transitions!**)

The Similarity Renormalization Group

Review:
S. Bogner, R. Furnstahl, and A. Schwenk, Prog. Part. Nucl. Phys. **65**, 94 (2010)

E. Anderson, S. Bogner, R. Furnstahl, and R. Perry, Phys. Rev. C **82**, 054001 (2011)
E. Jurgenson, P. Navratil, and R. Furnstahl, Phys. Rev. C **83**, 034301 (2011)
R. Roth, S. Reinhardt, and H. H., Phys. Rev. C **77**, 064003 (2008)
H. H. and R. Roth, Phys. Rev. C **75**, 051001 (2007)

SRG in a Nutshell

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

Operator Bases for the RG Flow

- choose a **basis of operators** $\{O_i\}_{i\in\mathbb{N}}$ to represent the flow (make an educated guess about physics):

$$H(s) \equiv \sum_i h_i(s) O_i\,, \quad \eta(s) \equiv \sum_i \eta_i(s) O_i\,.$$

- **close algebra by truncating induced terms** (if necessary)

$$\left[O_i, O_k\right] = \sum c_{ikl} O_l + \ldots$$

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

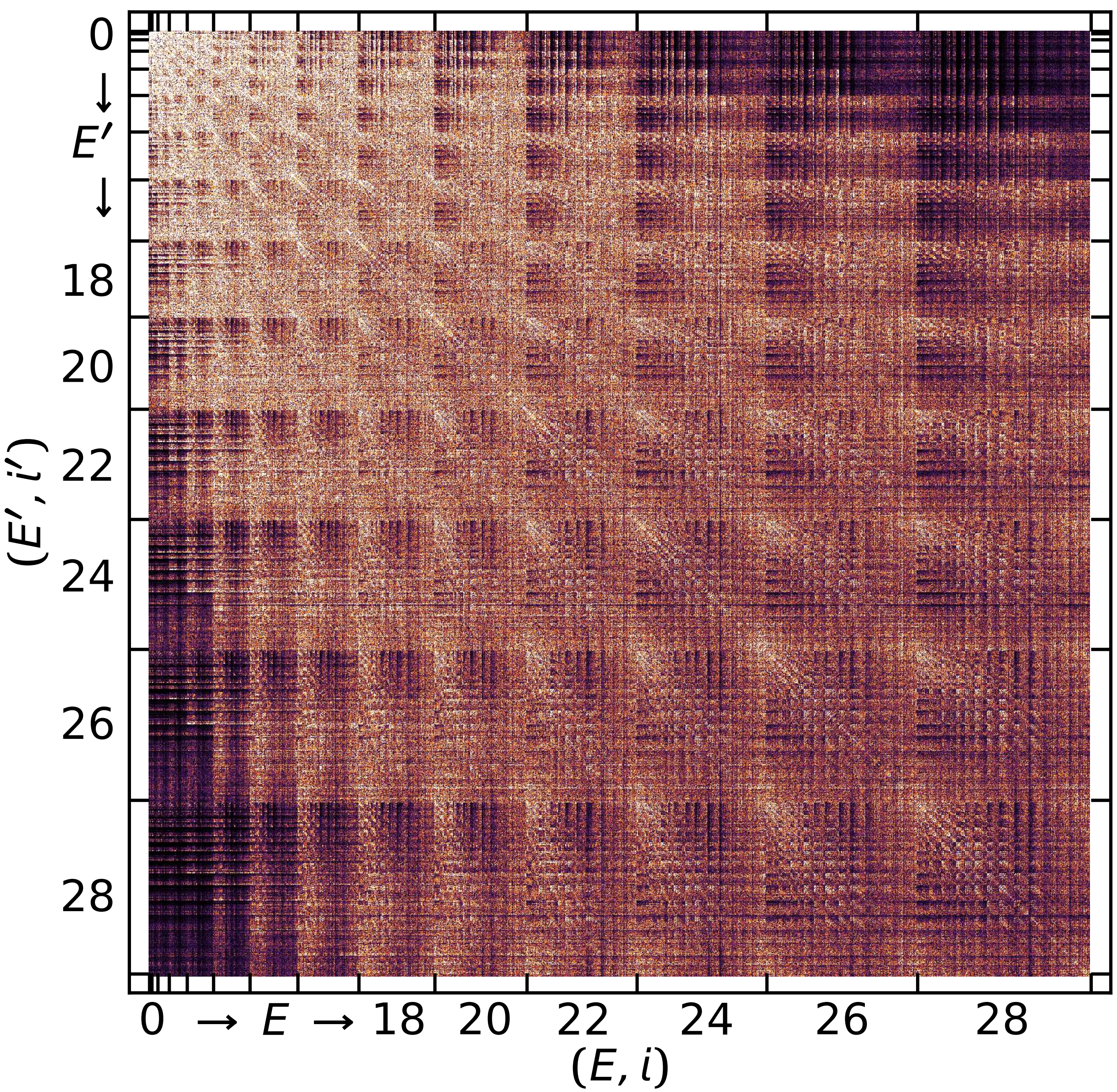
$$\frac{dh_i}{ds} = \sum_k f_{ik}(h,\eta)\, O_k$$

SRG in Three-Body Space

[figures by R. Roth, A. Calci, J. Langhammer]

3B Jacobi-HO Matrix Elements

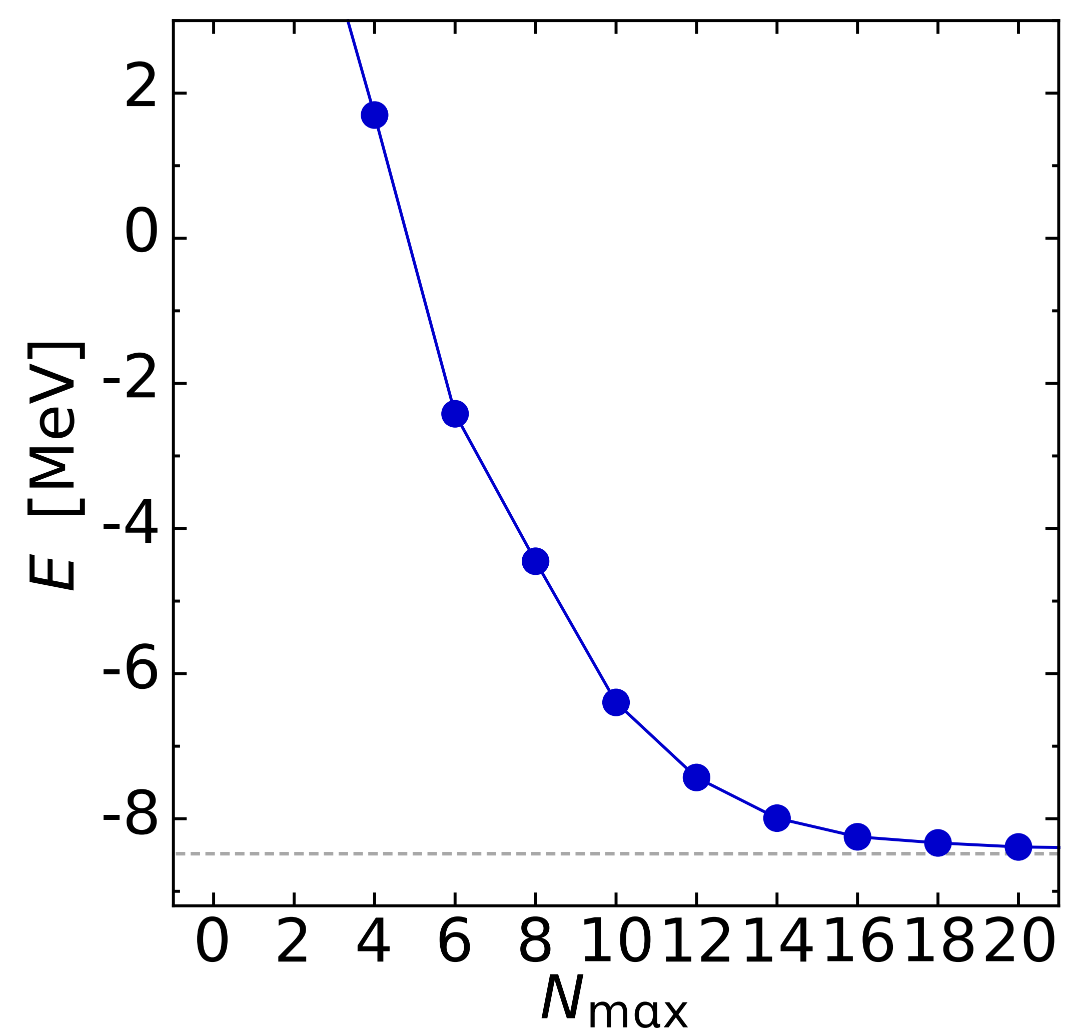
$J^\pi = \frac{1}{2}^+, T = \frac{1}{2}, \hbar\Omega = 28$ MeV



chiral NN + 3N

N³LO + N²LO (³H fit)

³H ground-state (NCSM)



SRG in Three-Body Space

[figures by R. Roth, A. Calci, J. Langhammer]

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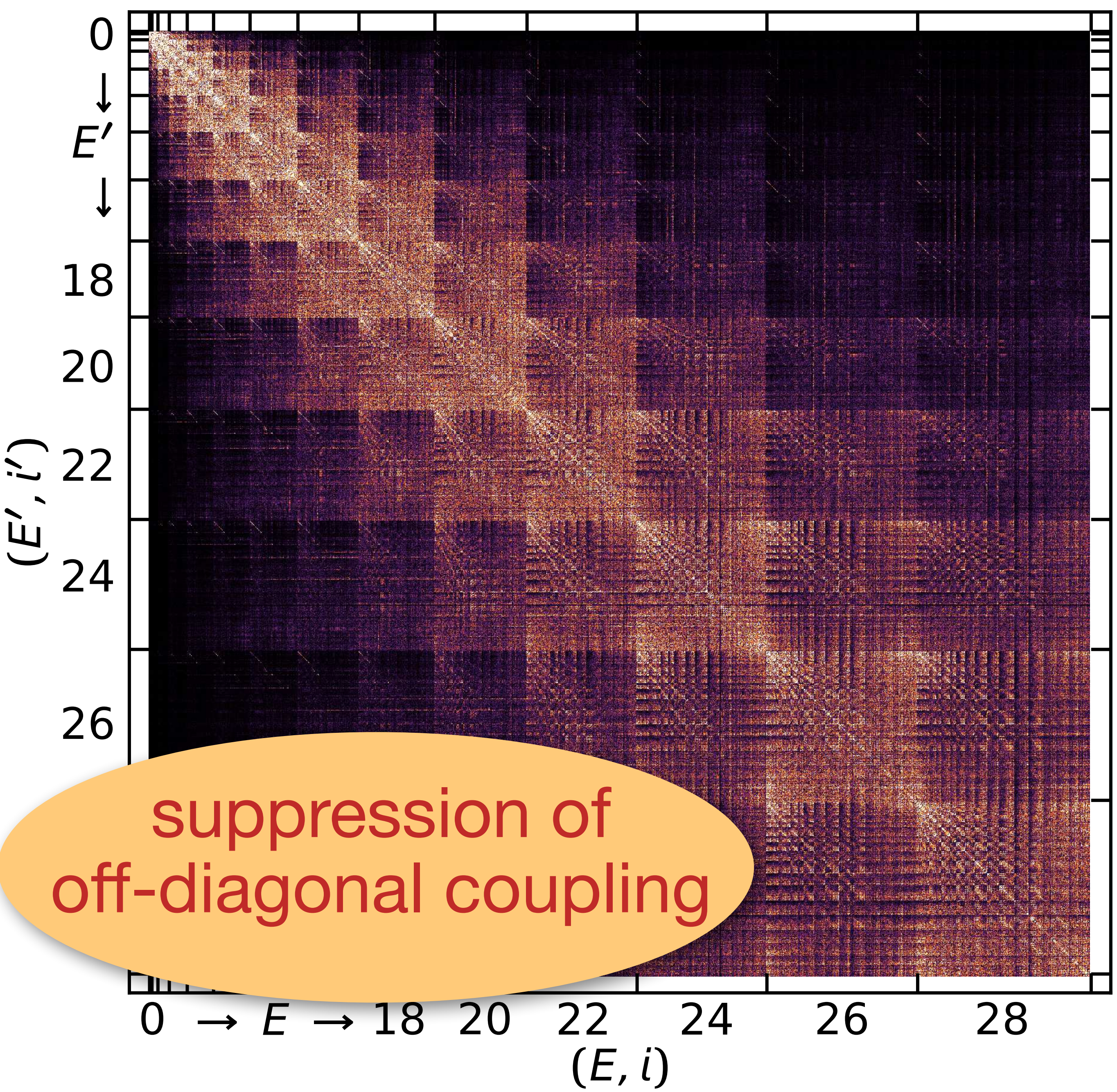
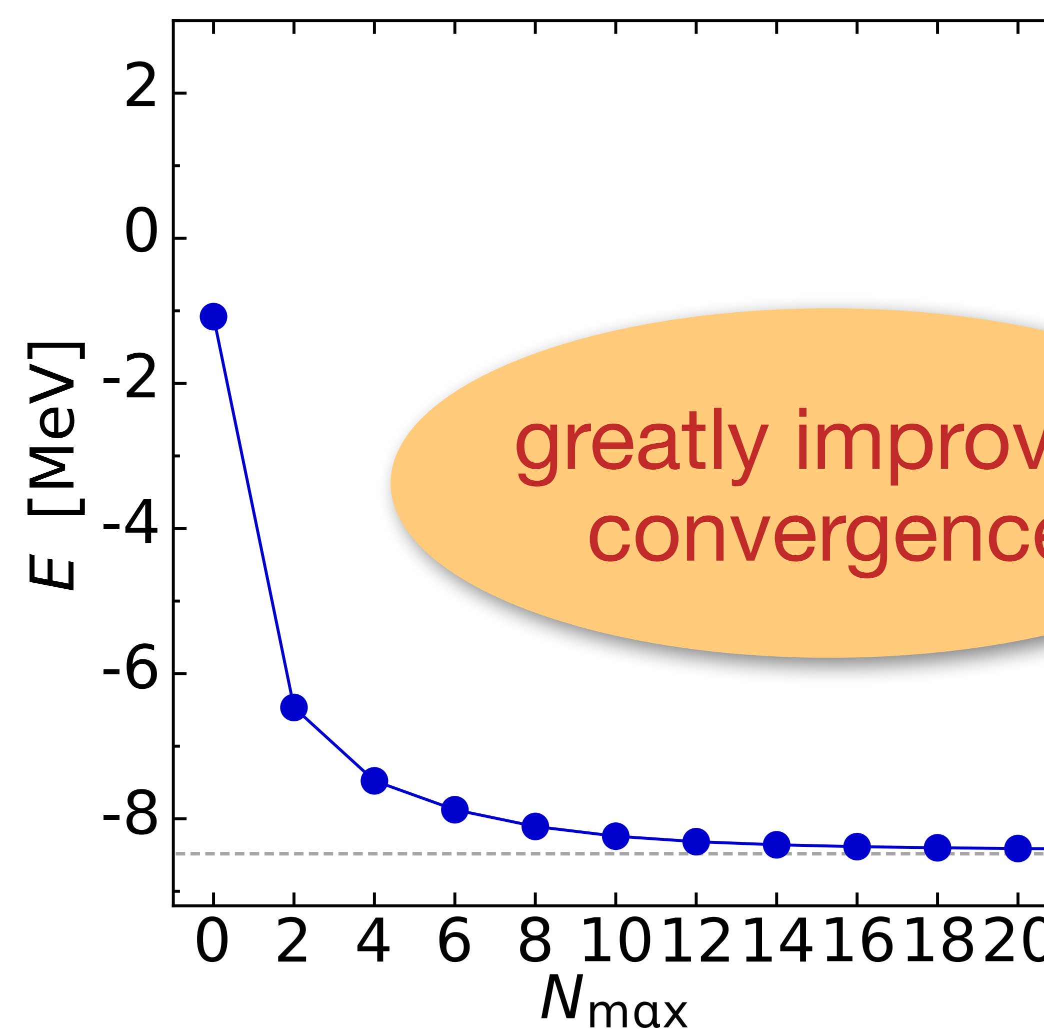


suppression of off-diagonal coupling

$\lambda = 1.33\ \text{fm}^{-1}$

^{3}H ground-state (NCSM)



greatly improved convergence

(Multi-Reference) In-Medium Similarity Renormalization Group

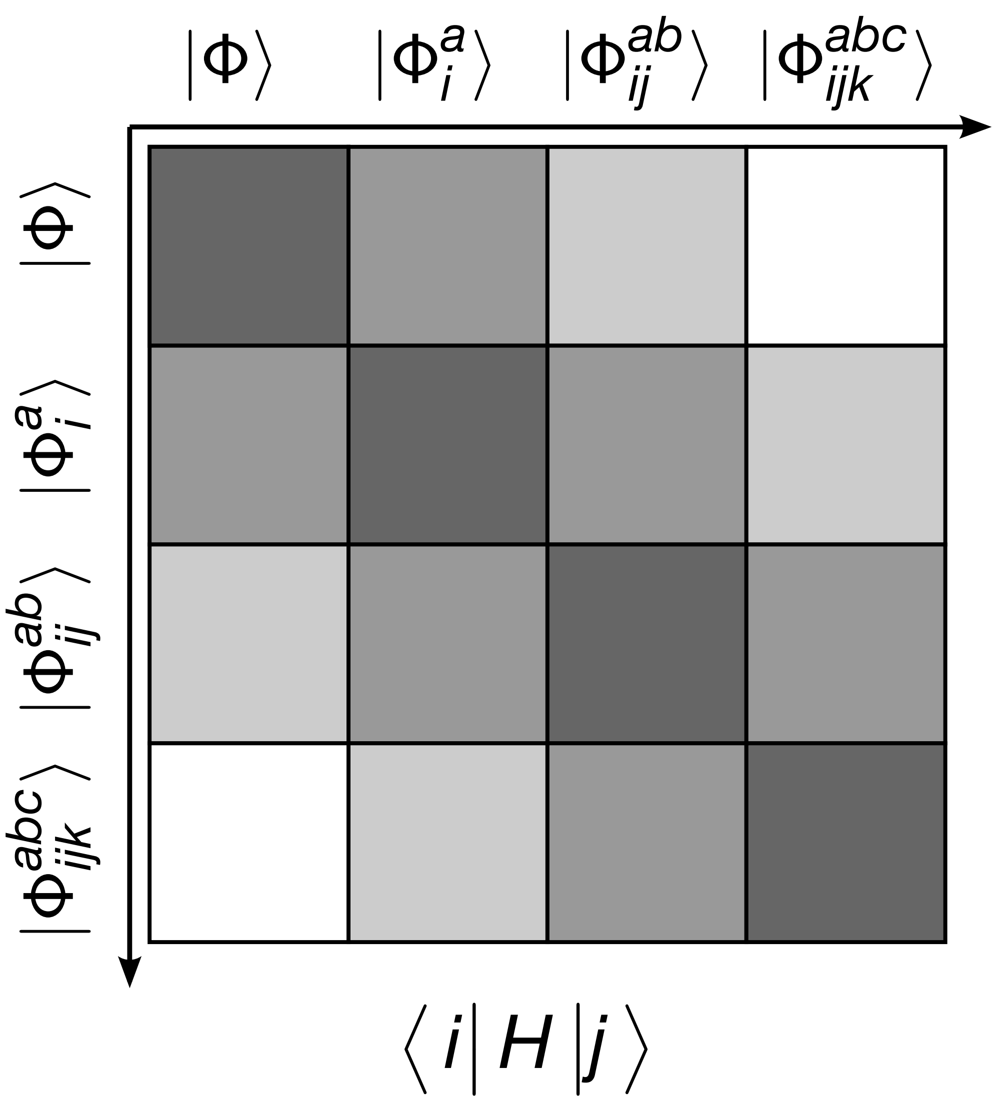
HH, Phys. Scripta, Phys. Scripta 92, 023002 (2017)

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

HH, S. 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)

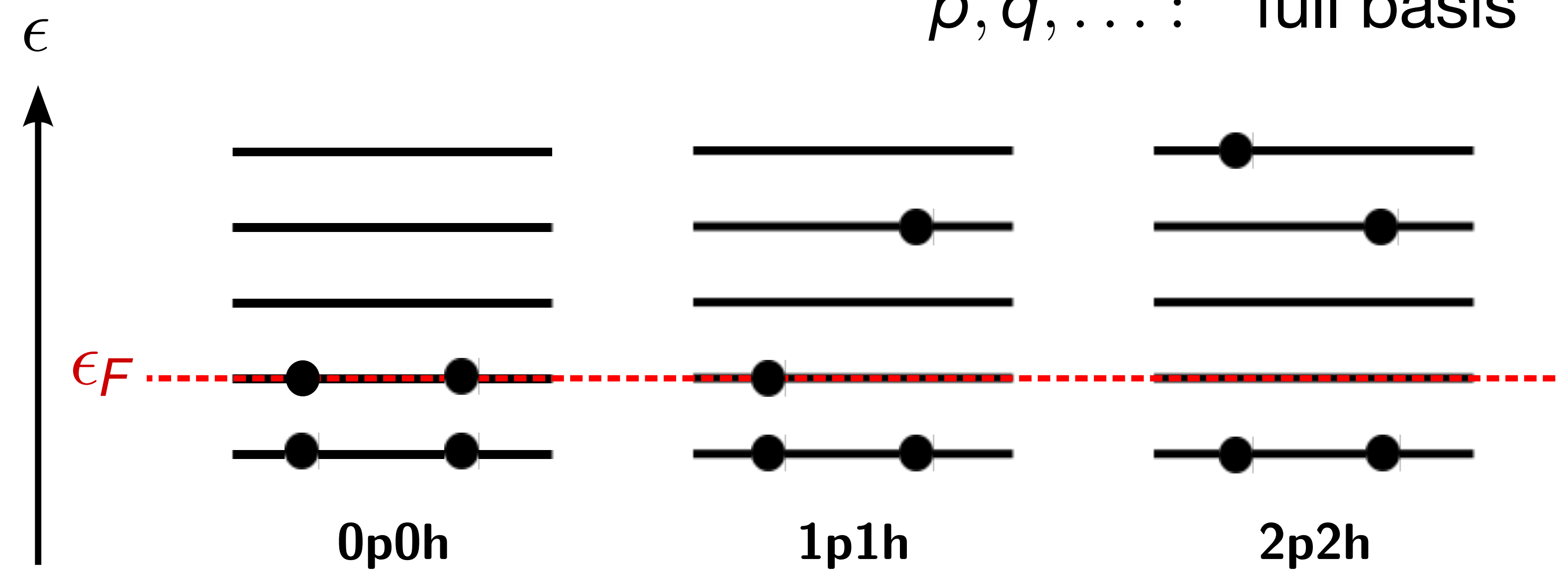
Transforming the Hamiltonian



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

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

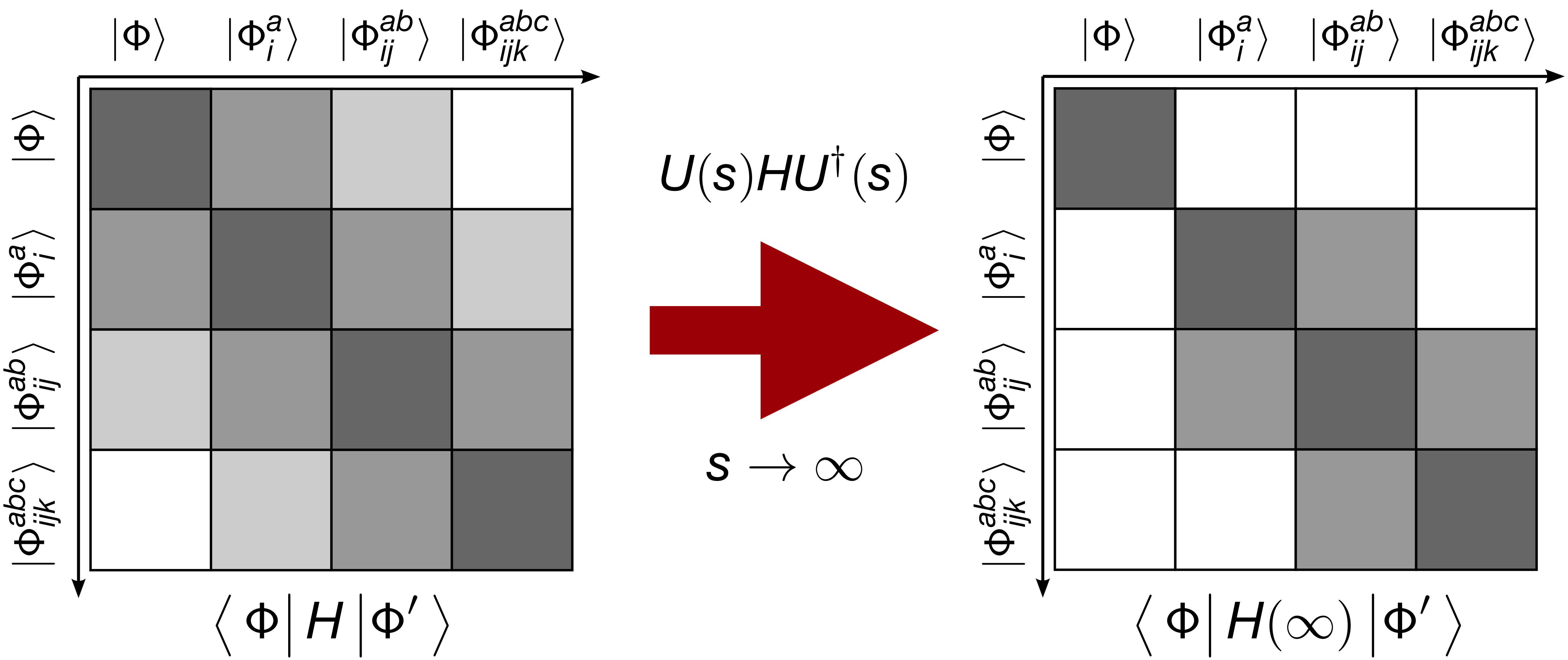
$p, q, \ldots :$ full basis



- reference state: **single Slater determinant**

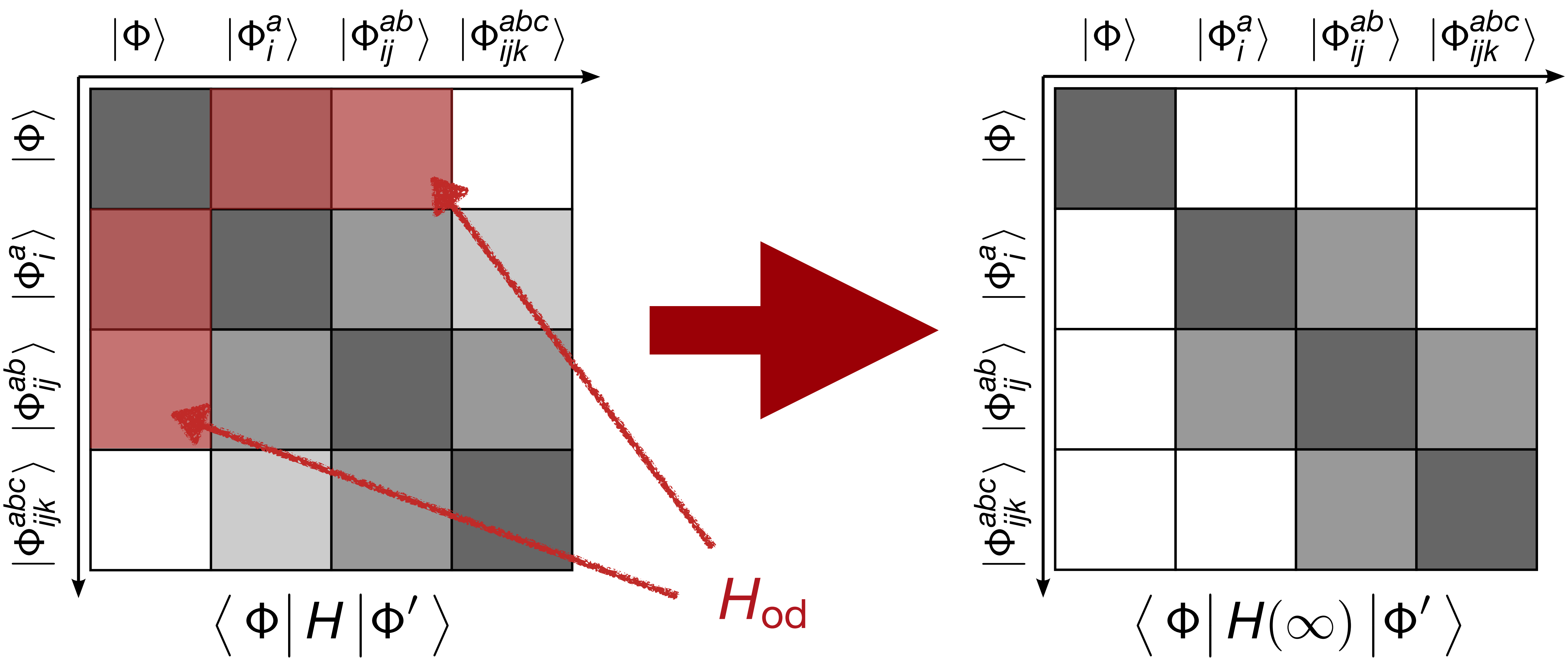
excitations relative to reference state: **normal-ordering**

Decoupling in A-Body Space



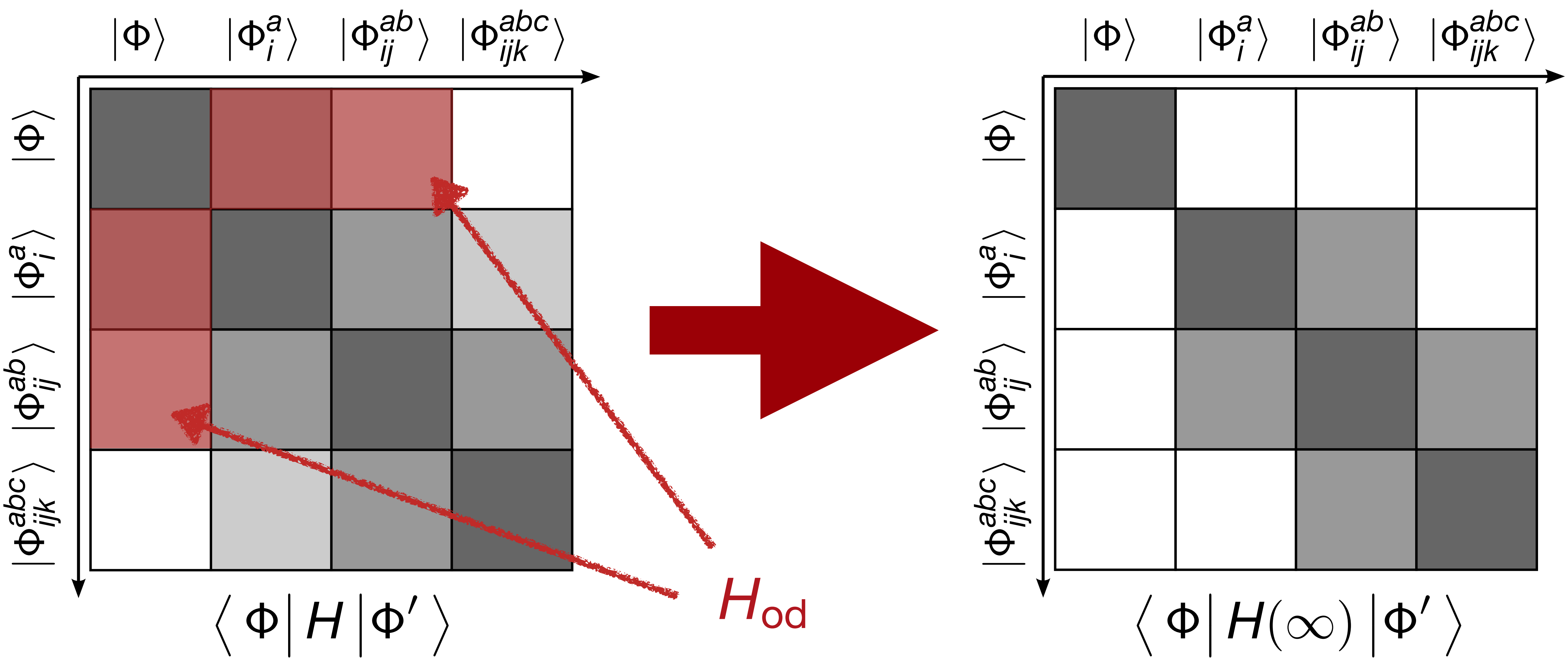
goal: decouple reference state $|\Phi\rangle$ from excitations

Flow Equation



$$\frac{d}{ds}H(s) = \left[\eta(s), H(s)\right], \quad \text{e.g.,} \quad \eta(s) \equiv \left[H_d(s), H_{od}(s)\right]$$

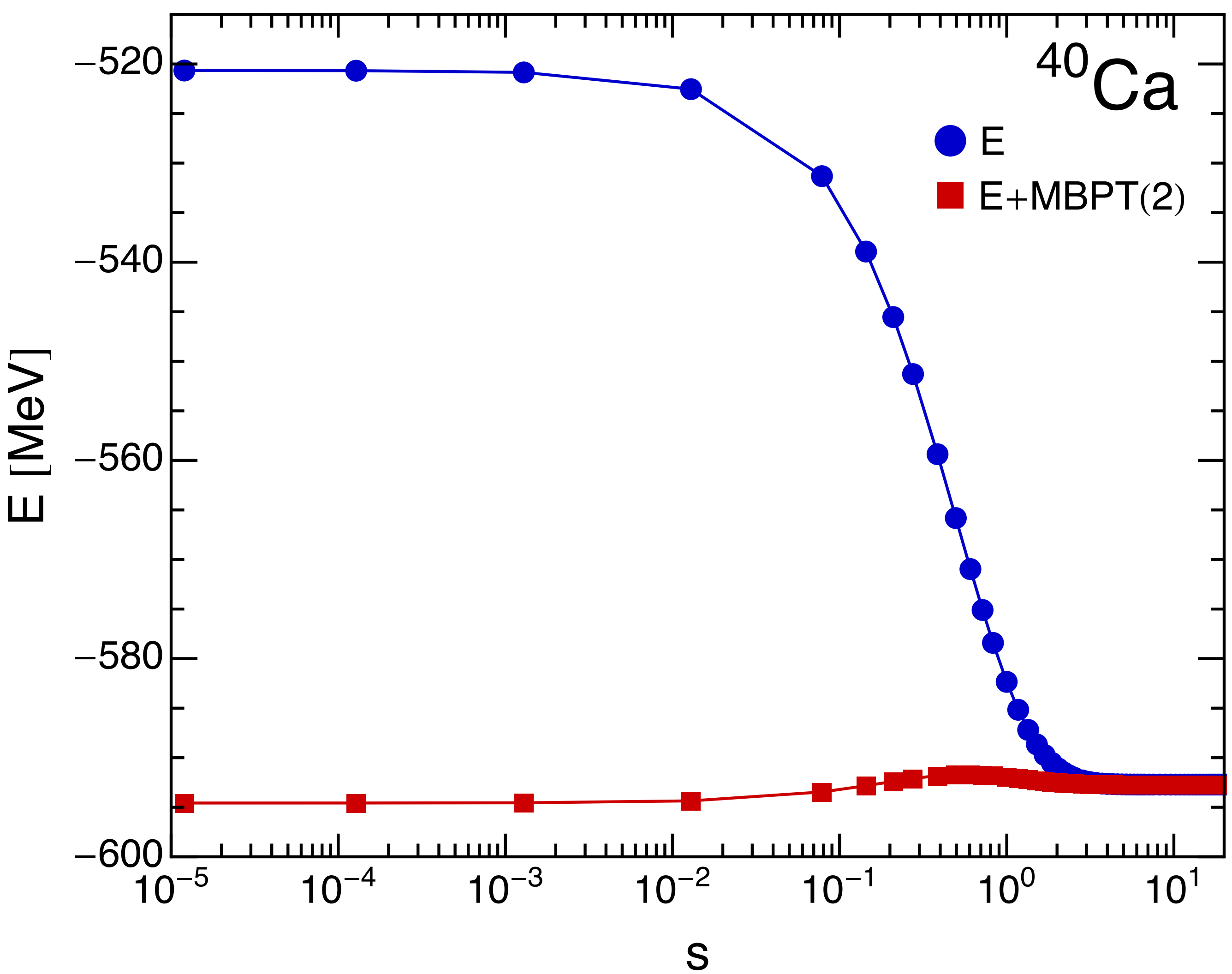
Flow Equation

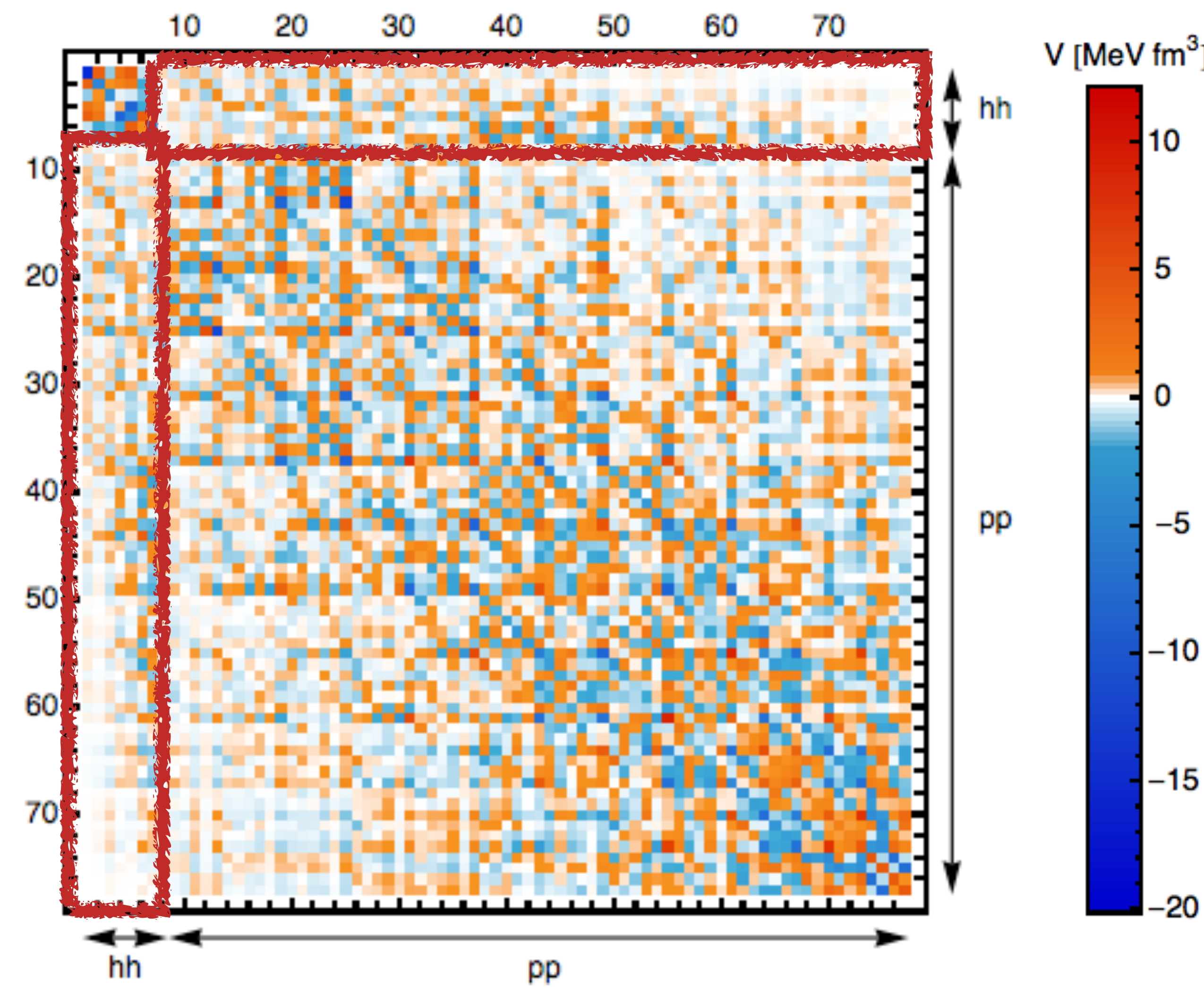


$$\frac{d}{ds}H(s) = \left[\eta(s), H(s)\right]$$

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

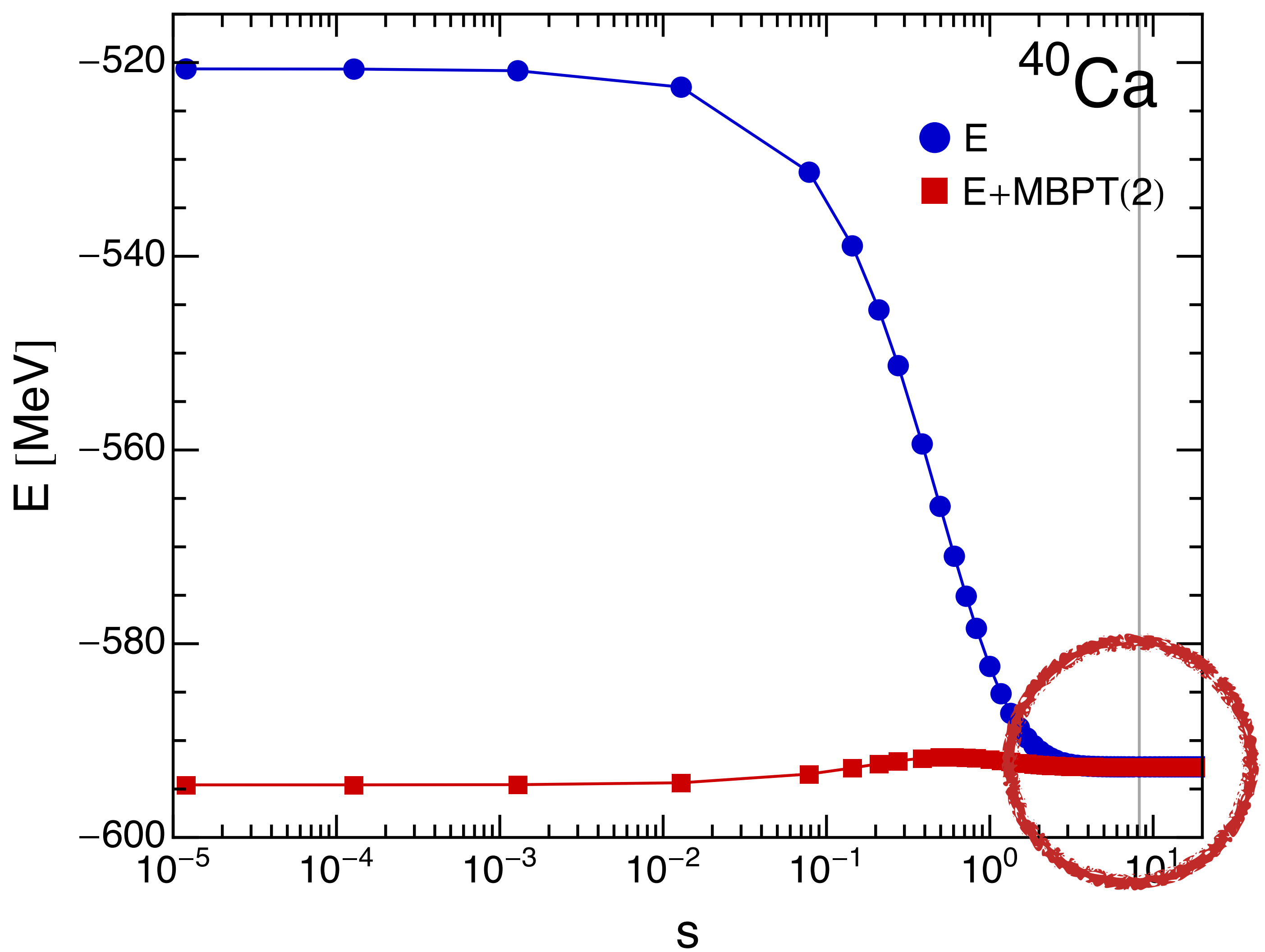
Decoupling

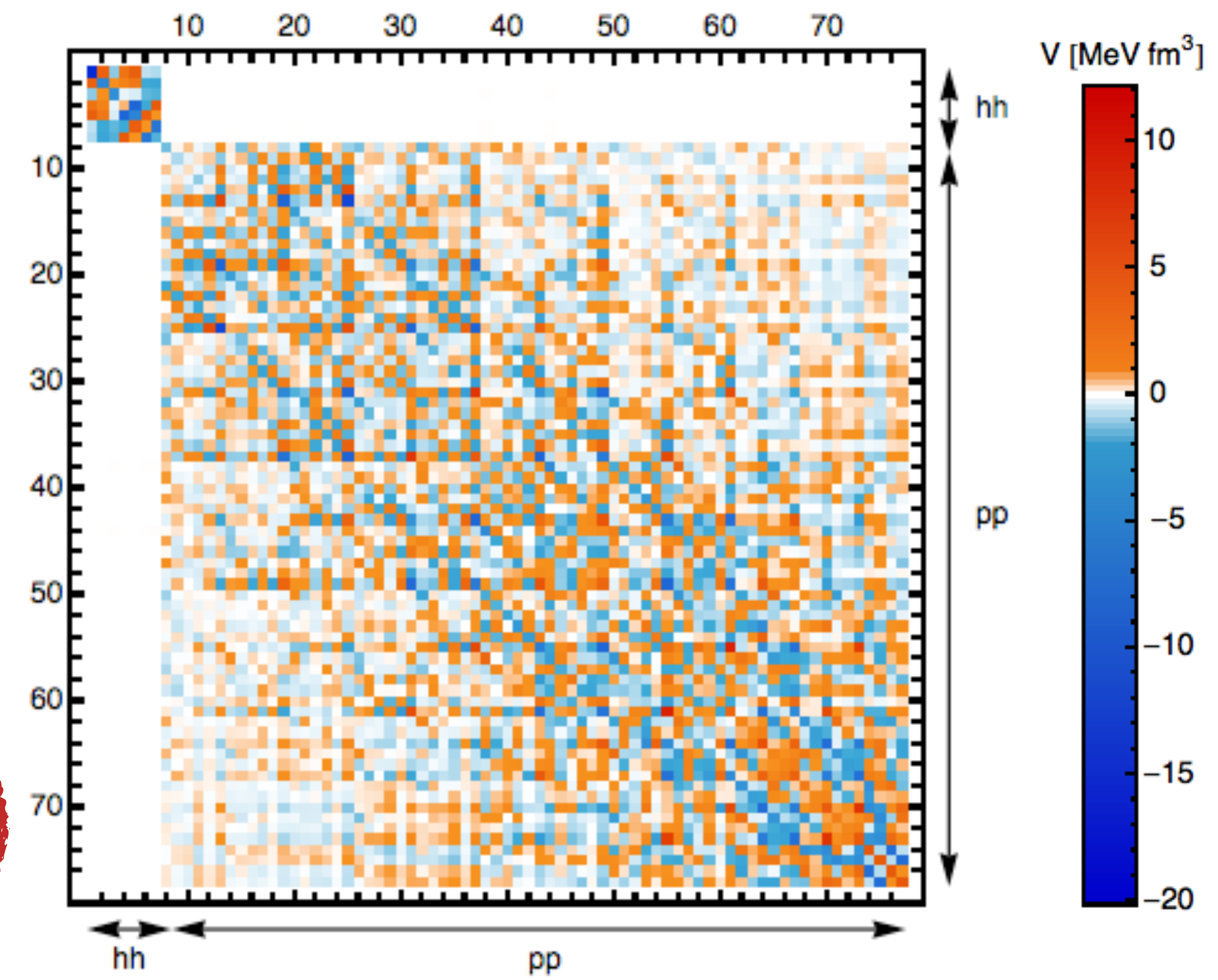




N3LO, $\lambda = 2.0\ \mathrm{fm}^{-1}, e_{\mathrm{Max}} = 8$

Decoupling



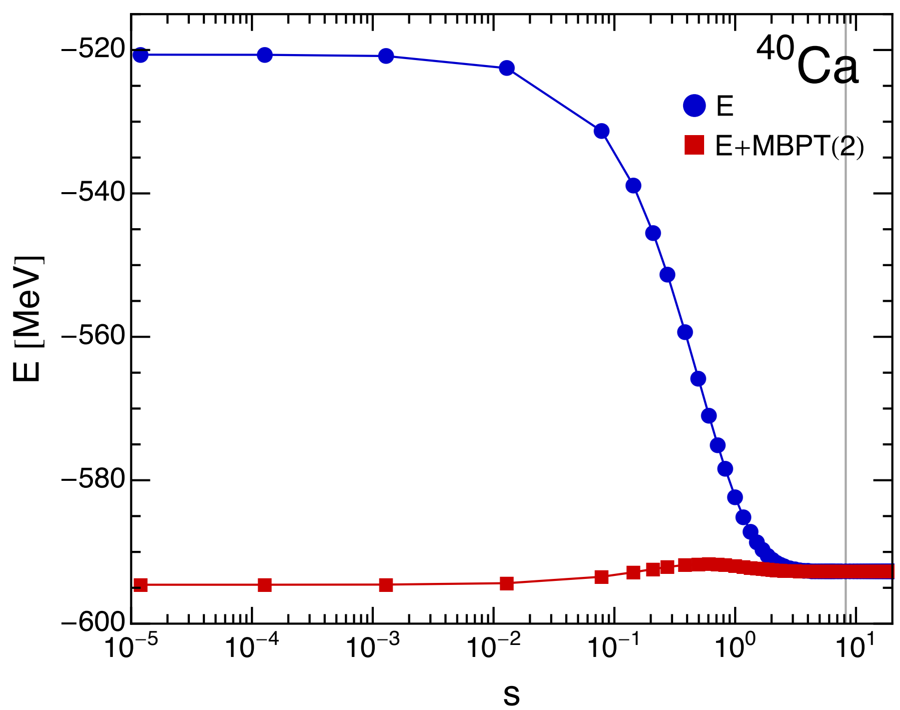


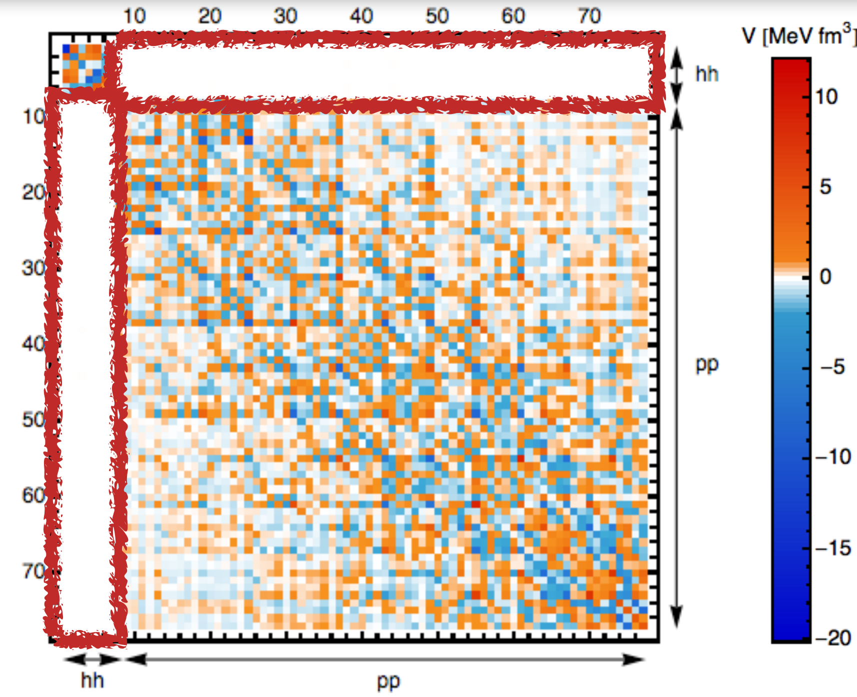
N3LO, $\lambda = 2.0\ \mathrm{fm}^{-1}, e_{\mathrm{Max}} = 8$

non-perturbative resummation of MBPT series (correlations)

off-diagonal couplings are rapidly driven to zero

Decoupling





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

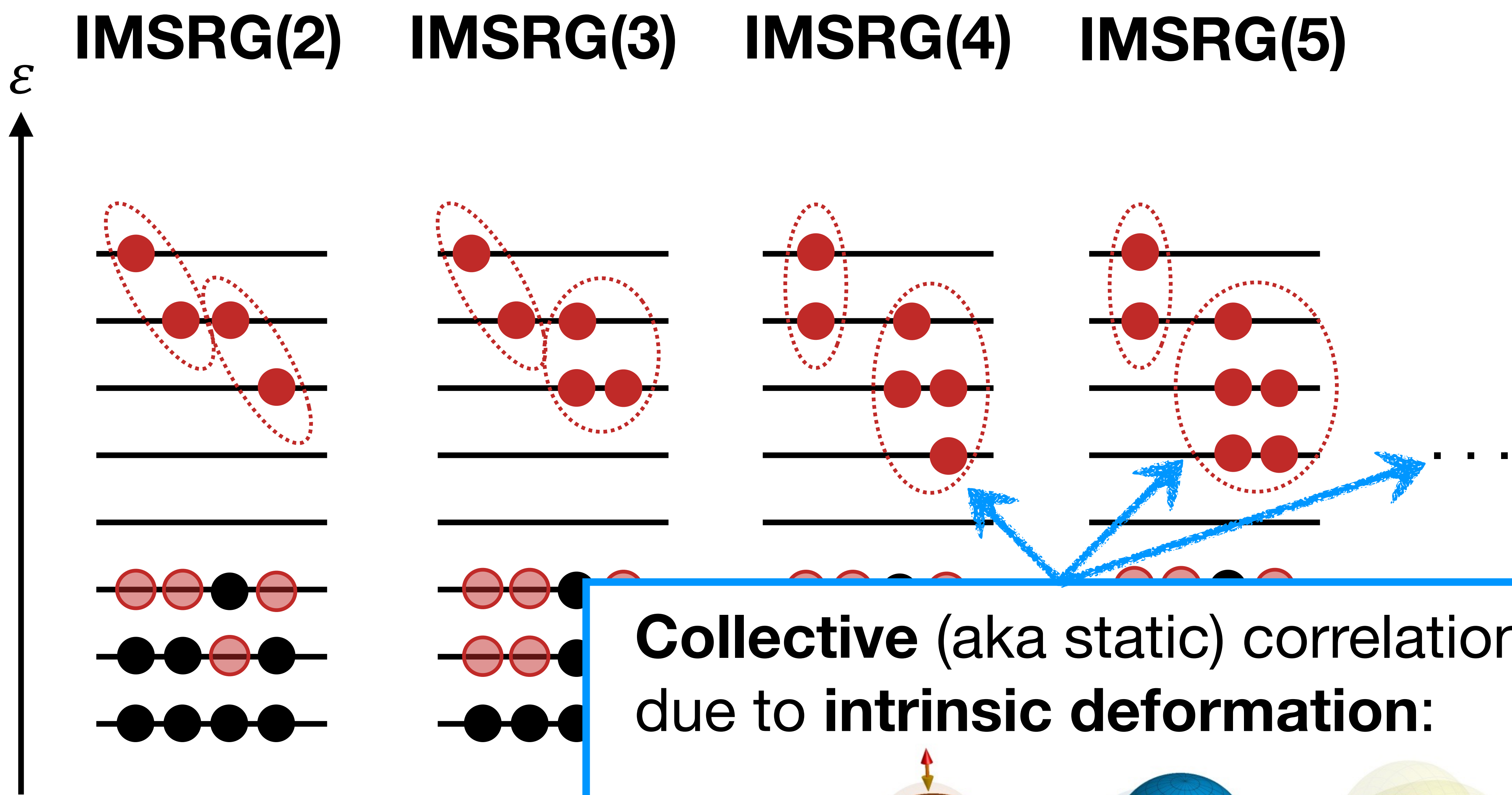
- absorb correlations into **RG-improved Hamiltonian**

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

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

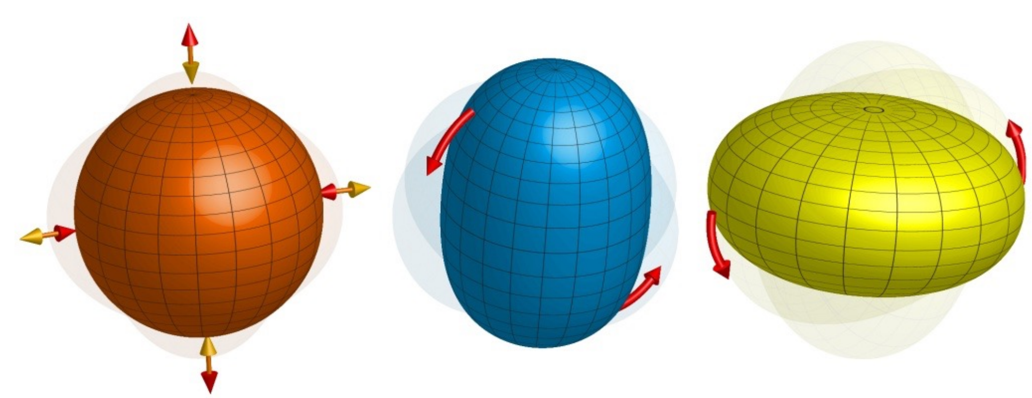
$$U(s)\left|\Psi_n\right\rangle \stackrel{!}{=} \left|\Phi\right\rangle$$

Correlated Reference States

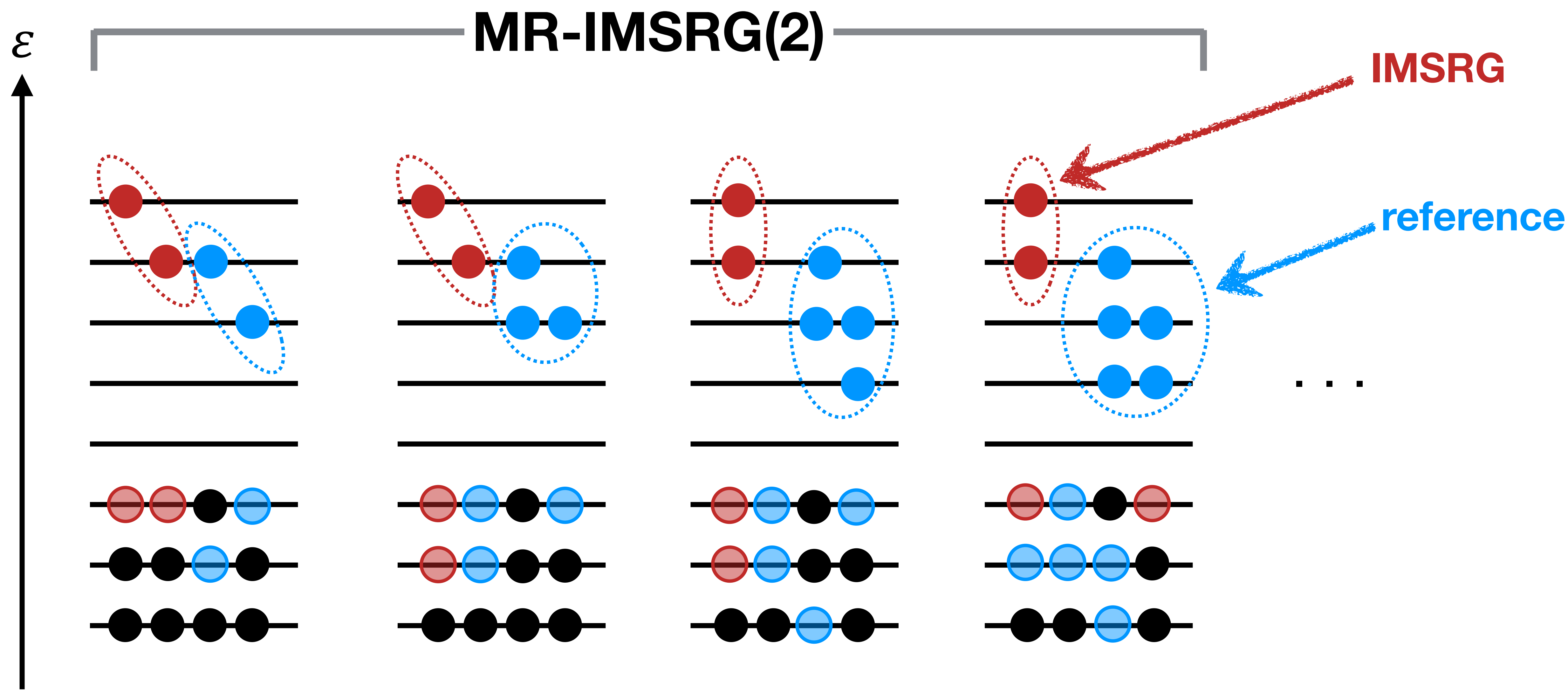


"standard" IMS
Slater determinar

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

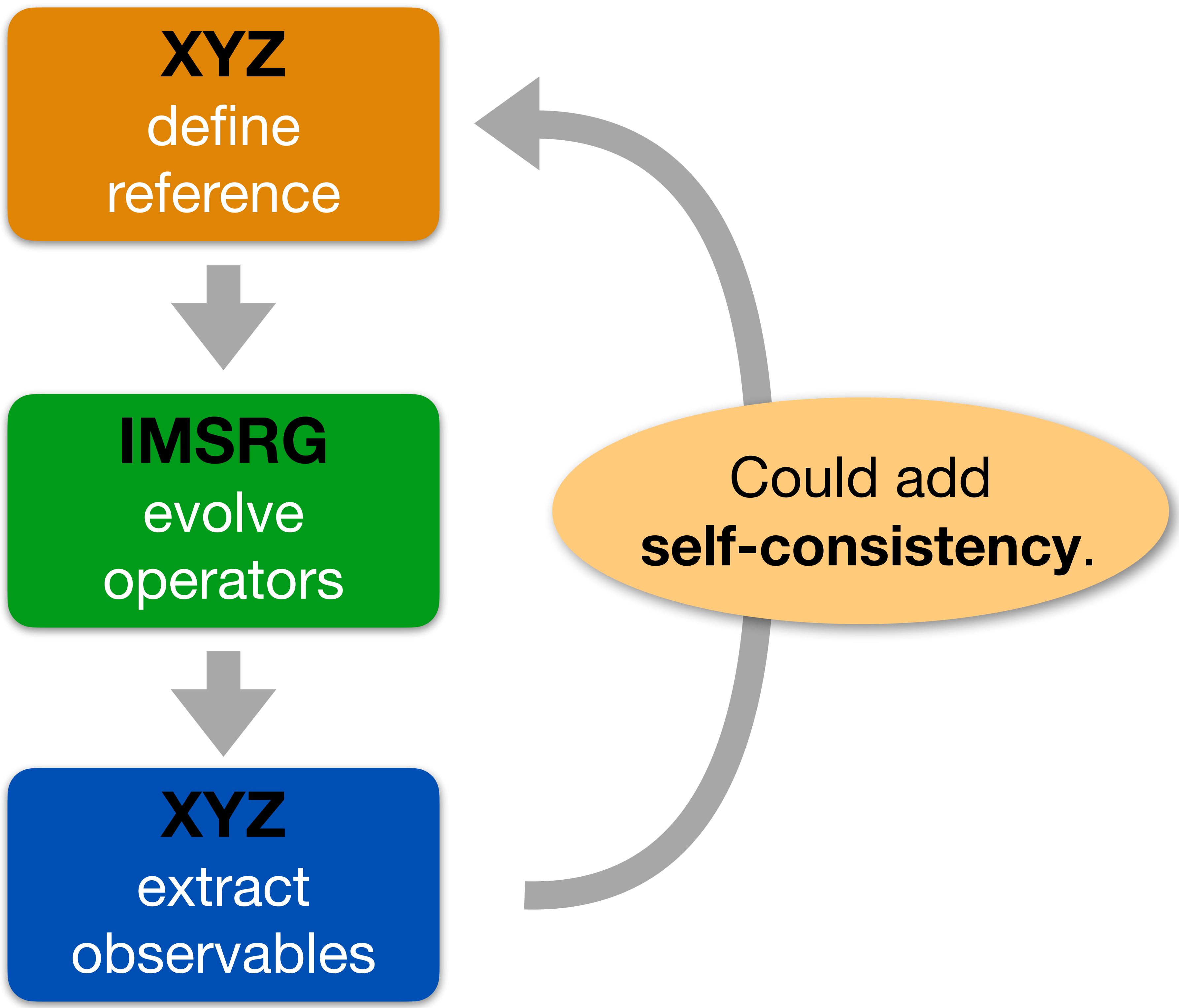


Correlated Reference States



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

IMSRG-Improved Methods



Selected Results

IMSRG-Improved HF and PHFB

HF / PHFB
define reference

- closed shell: HF Slater determinant
- open shell: number-projected HFB state

↓

IMSRG
evolve operators

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

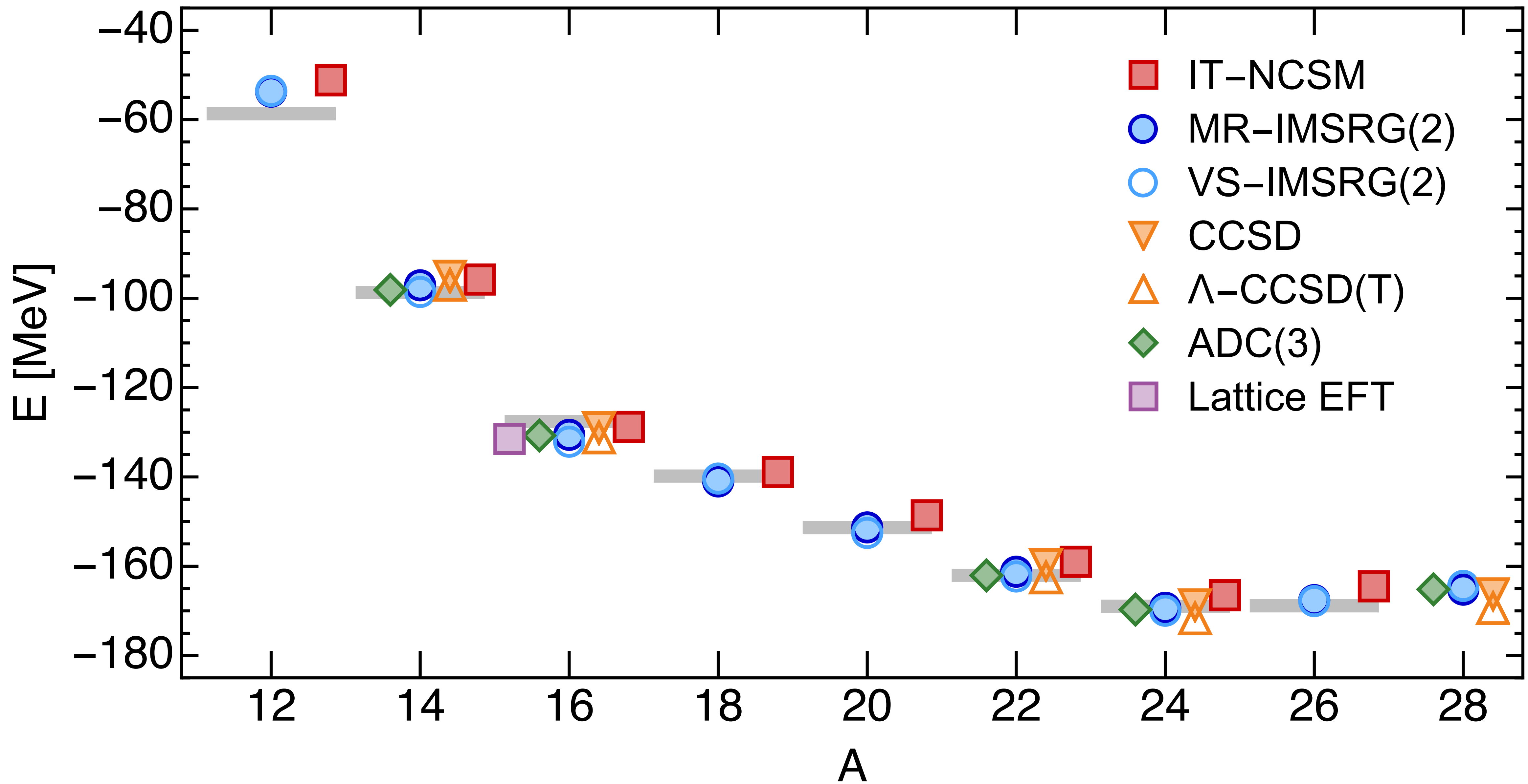
↓

HF / PHFB
extract observables

- calculation is trivial, energy can be directly read off the evolved Hamiltonian

Consistent Ground-State Energies

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



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

Valence-Space IMSRG

HF
define reference

- defines meaning of P (=valence) and Q(=core + non-valence excitation) spaces

IMSRG
evolve operators

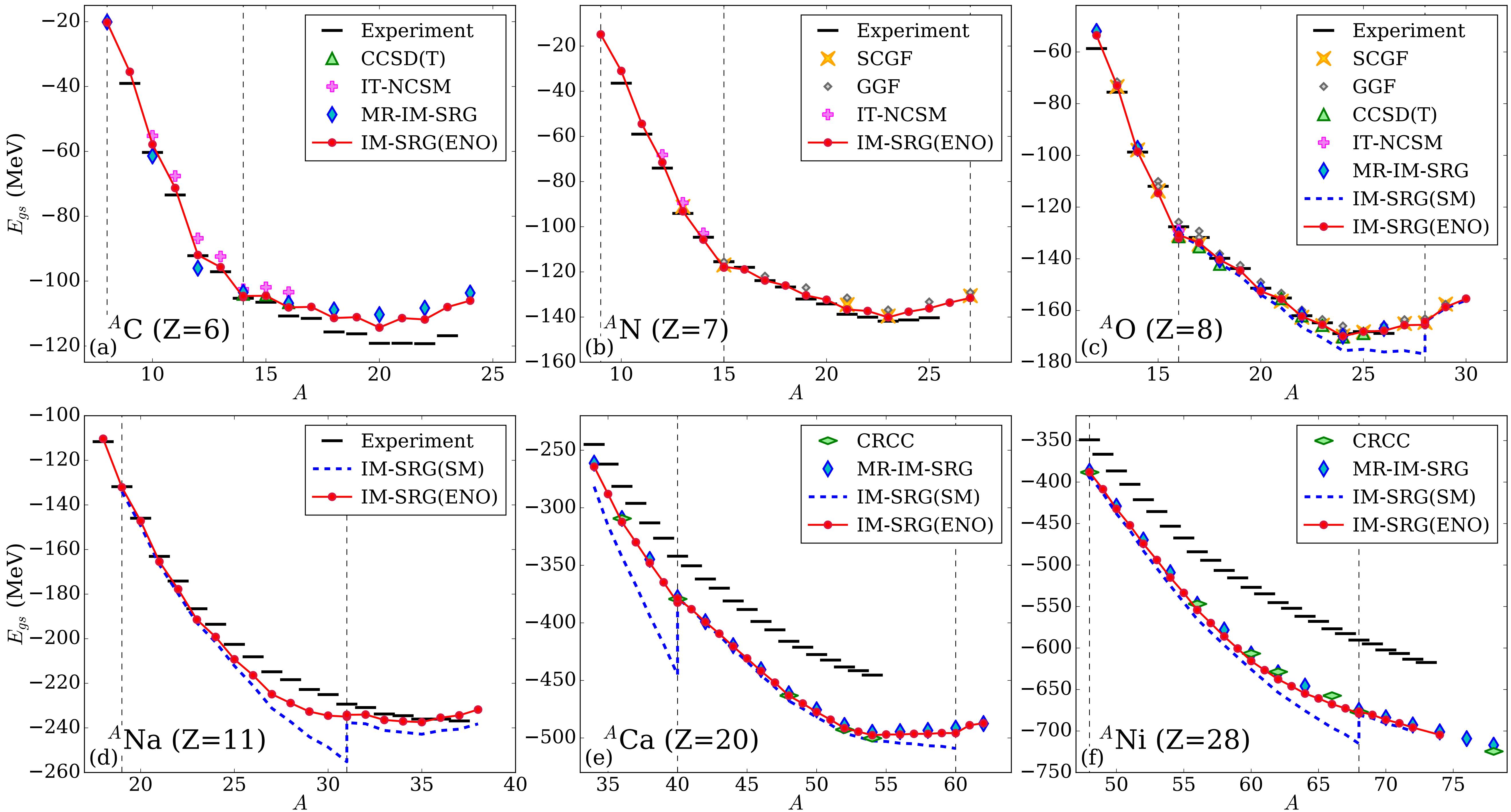
- evolve Hamiltonian and observables
- decouple P and Q spaces
- determines core part of w.f.

Valence CI
extract observables

- determines valence part of w.f.

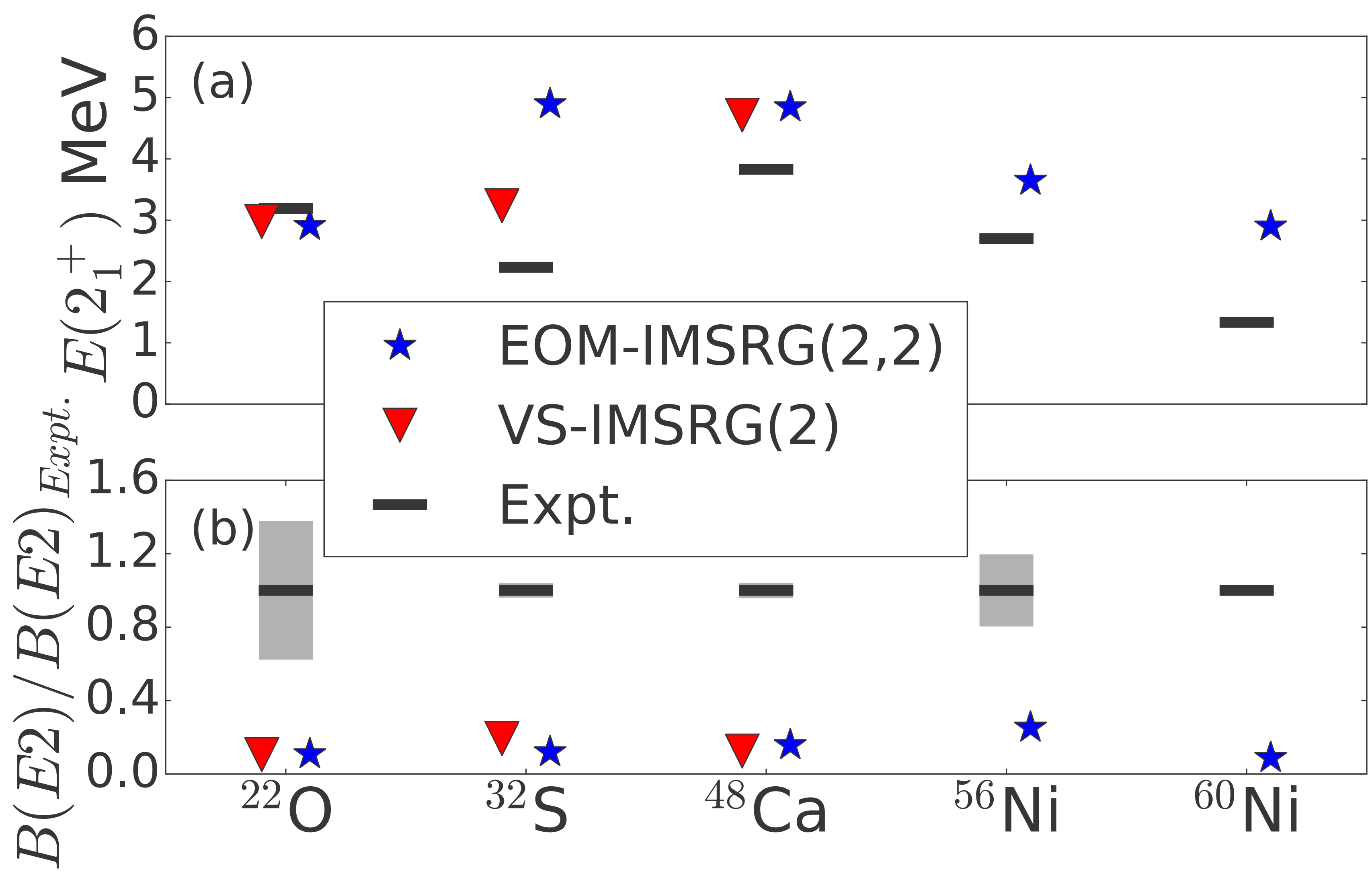
Consistent Ground-State Energies

*S. R. Stroberg, A. Calci, HH, J. D. Holt, S. K.Bogner, R. Roth, A. Schwenk, PRL **118**, 032502 (2017)*



Transitions

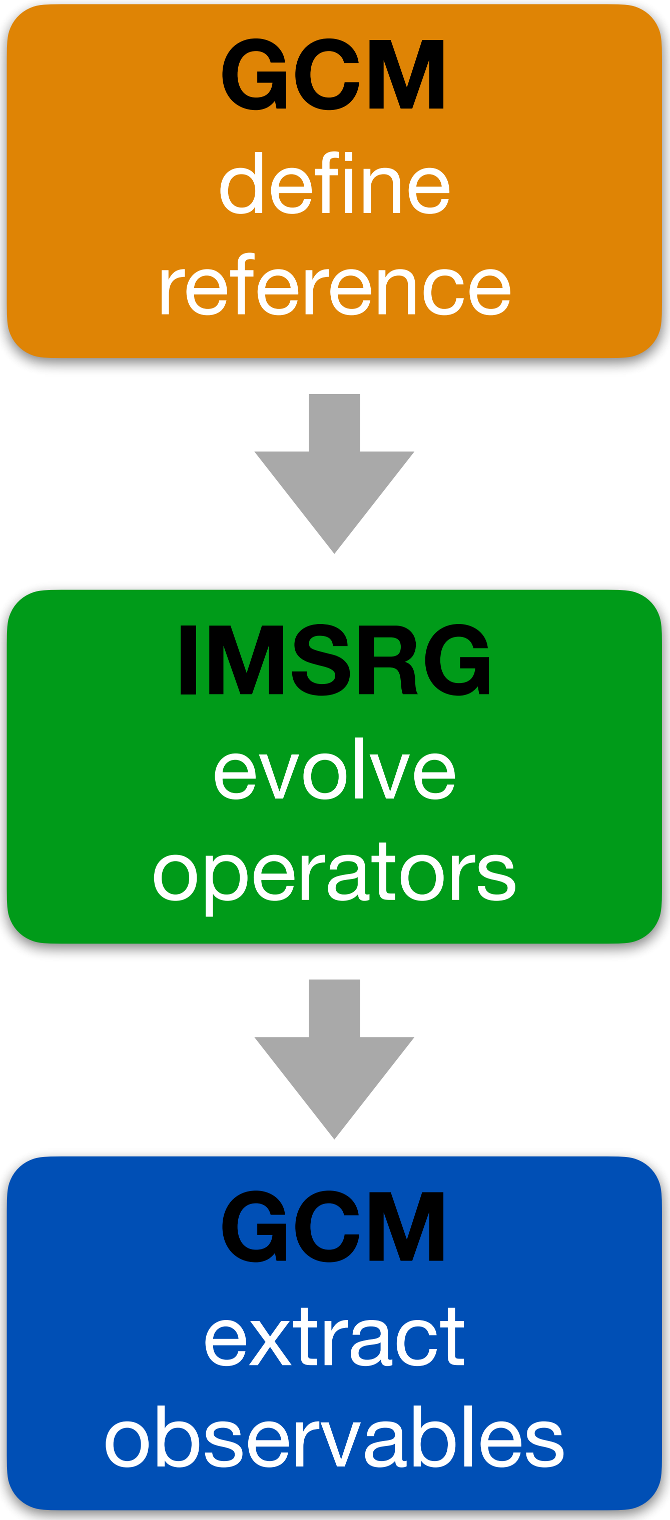
*N. M. Parzuchowski, S. R. Stroberg et al., PRC **96**, 034324*



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

In-Medium GCM

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



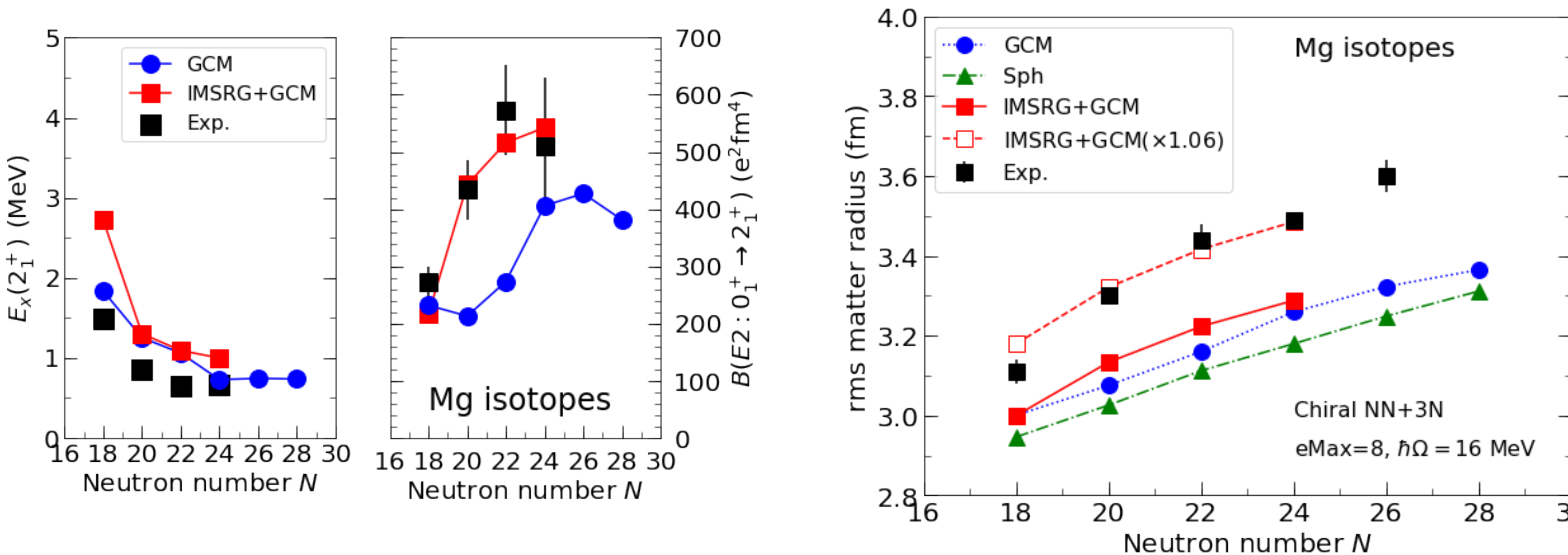
- no-core (or valence space) GCM calculation to prepare reference state

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

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

Collectivity in Magnesium Isotopes

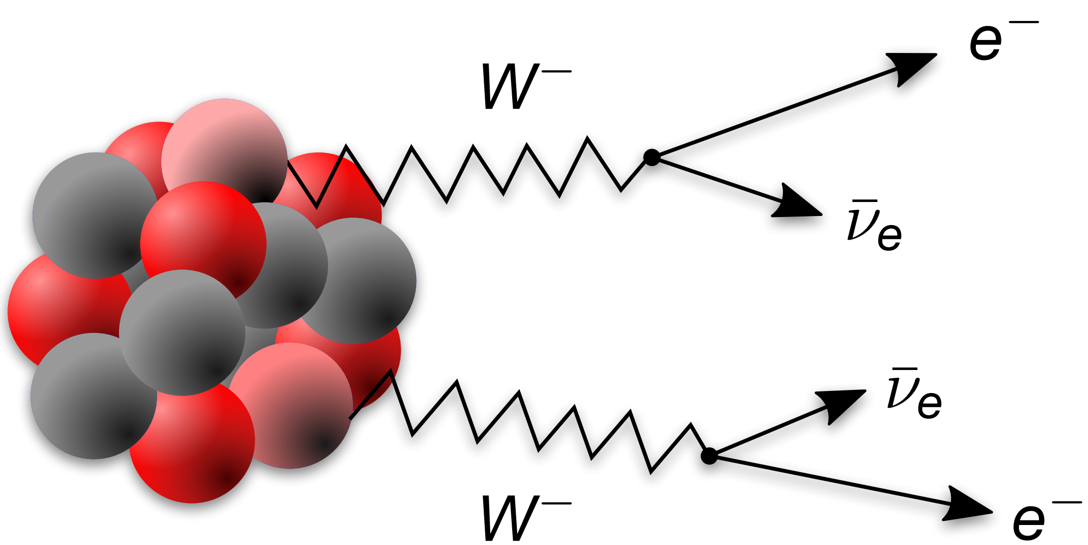
J. M. Yao, HH, in preparation



- **improved** B(E2) values compared to plain GCM or VS-IMSRG
  - **dynamical** **and** **static correlations included**
- **induced 2B quadrupole operator small in IM-GCM** but **dominant** in VS-IMSRG
  - GCM reference equips IMSRG operator basis with capability to capture collectivity

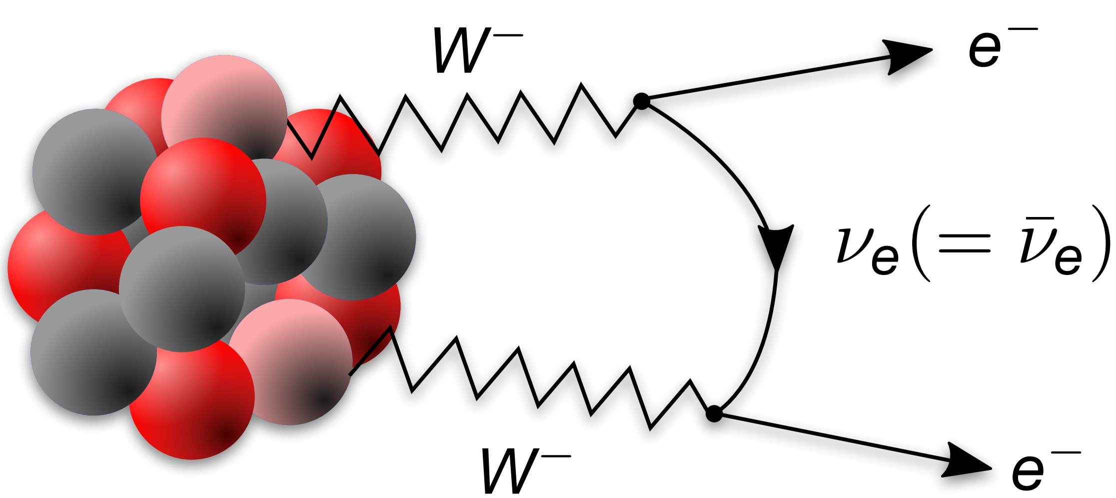
Testing Fundamental Symmetries

“Standard” Double Beta Decay



- neutrinos are **Dirac** particles
- Standard Model valid

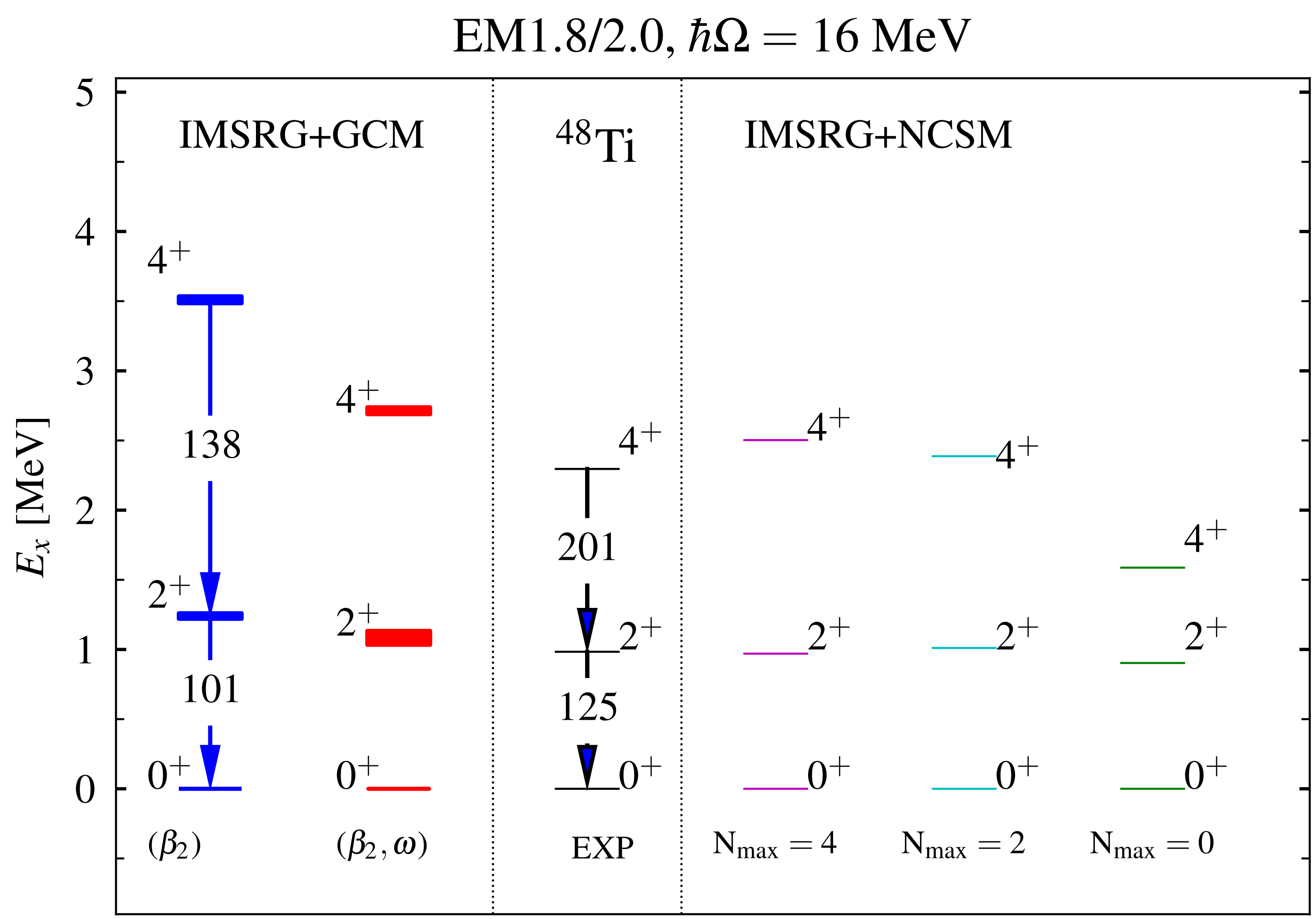
Neutrinoless Double Beta Decay



- neutrinos are **Majorana** particles
- beyond Standard Model: **new physics**

$0\nu\beta\beta$ Decay of ^{48}Ca

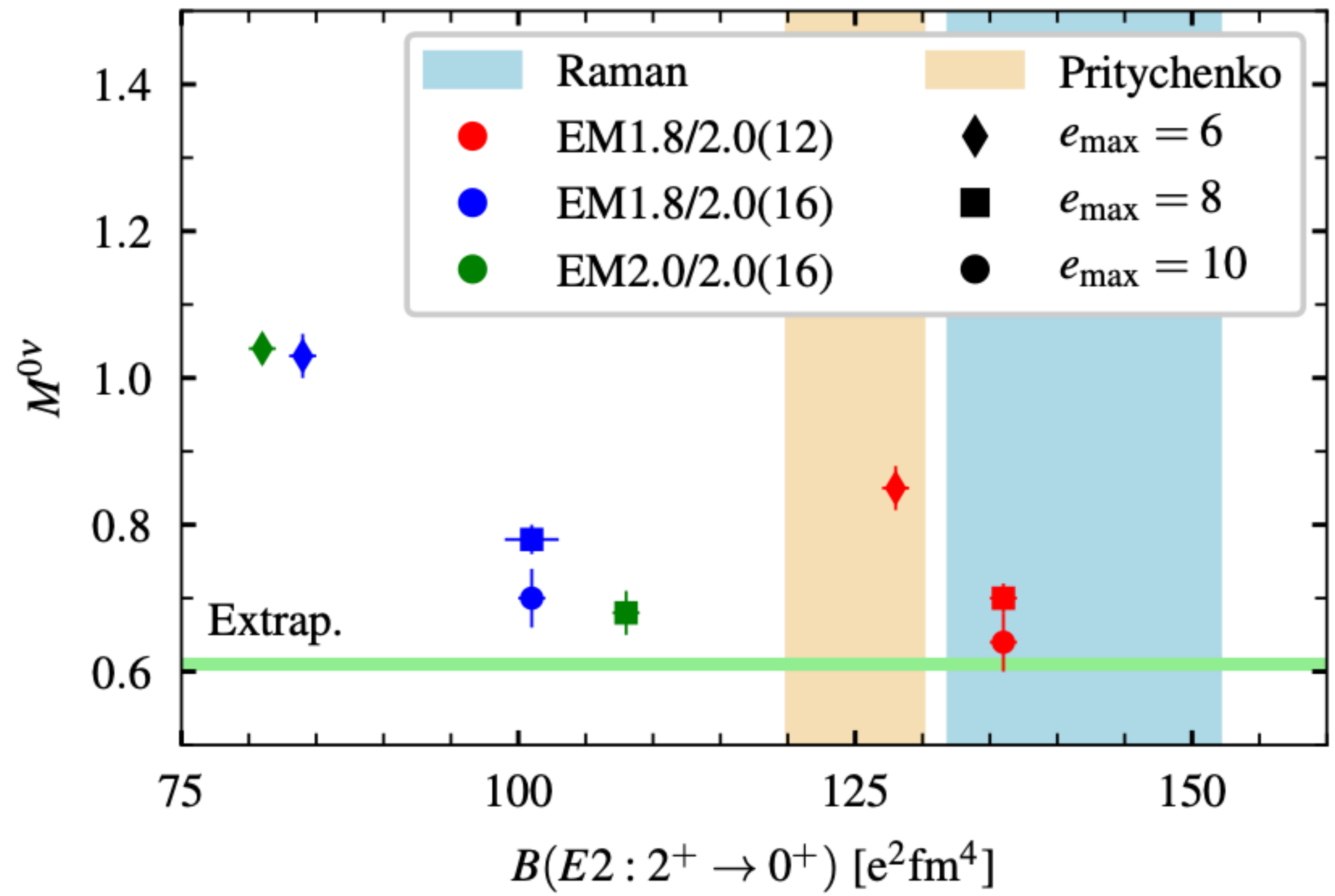
*J. M. Yao et al., PRL **124**, 232501 (2020); PRC **103**, 014315 (2021)*



- **consistency** between IM-GCM and IM-NCSM
- nuclear matrix element **insensitive to spread of spectrum**
  - “lore” based on phenomenological interactions may be misleading (scale/scheme dependence)

$0\nu\beta\beta$ Decay of ^{48}Ca

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



- NME **consistent** with **VS-IMSRG and CC** results (A. Belley et al., PRL 126, 042502, S. Novario et al
- only **weak correlation** with B(E2)
- ^{76}Ge and heavier candidates in progress

not the full story yet: improve IMSRG truncations, additional GCM correlations, include currents, …

Interfaces with Tensor Networks

Control Problem Growth

- "obvious" operator basis for many-body problems:

$$\{O_{pq}\,,\, O_{pqrs}\,,\, O_{pqrstu}\,,\, \ldots\} \equiv \{a^\dagger_p a_q\,,\, a^\dagger_p a^\dagger_q a_s a_r\,,\, a^\dagger_p a^\dagger_q a^\dagger_r a_u a_t a_s\,,\, \ldots\}$$

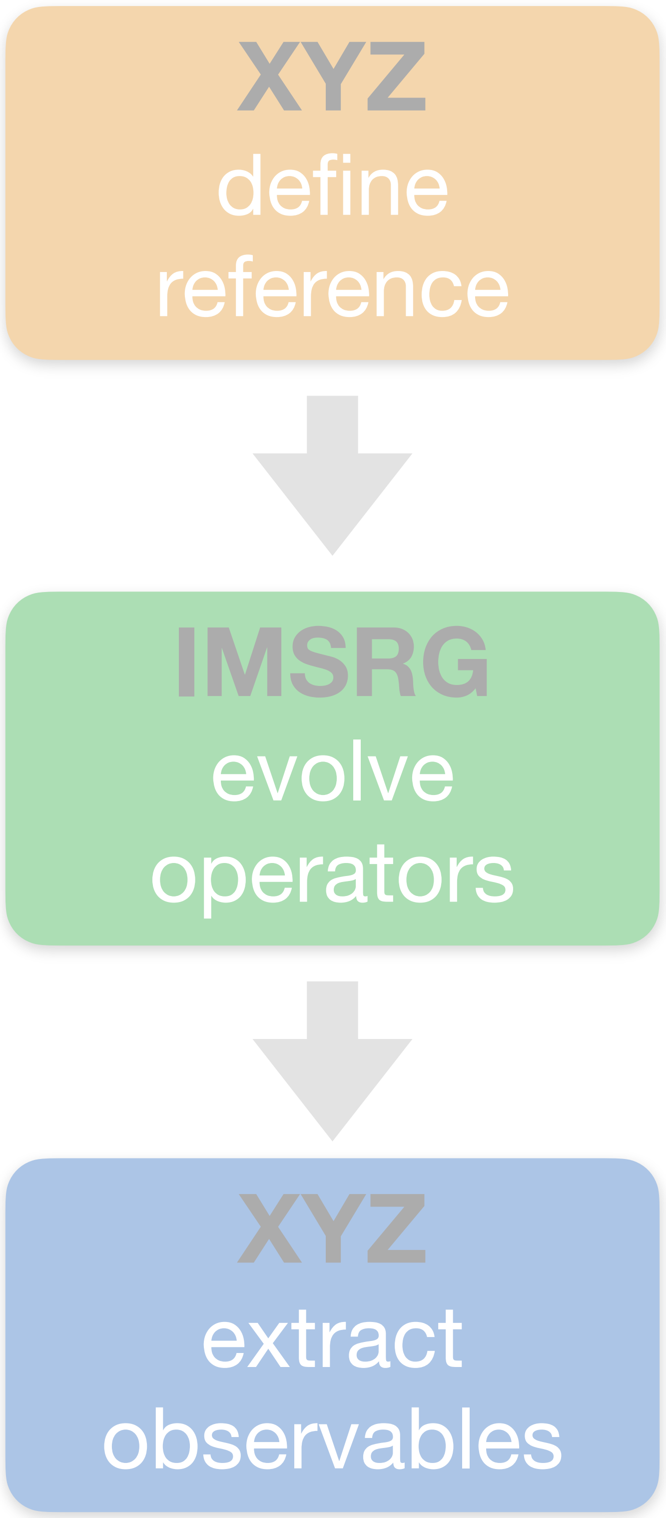
- state of the art: $O(10^8)$ operators & coupling coefficients, **next-level: $O(10^{12})$** or even more
- normal ordering "informs" the operator basis of physics, but doesn't change its size
- **in contrast:** O(10) interaction **operators** (even with 3N), O(100) particles - there must be **lots of redundancy**

➡ **principal component analysis & tensor factorization**

see talk by **A. Tichai**

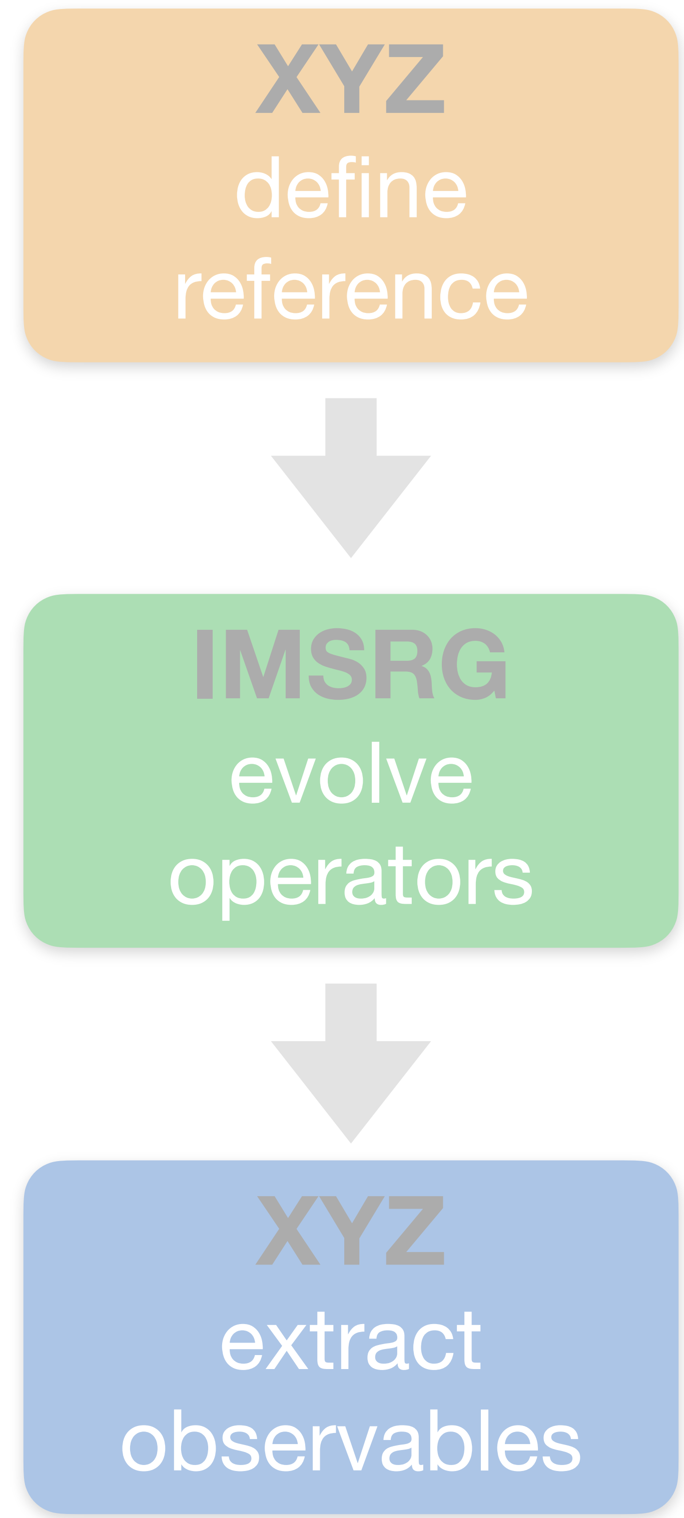
IMSRG Hybrid Approaches

- **VS-IMSRG**
  [review: S. R. Stroberg, HH, S. K. Bogner, J. D. Holt, Ann. Rev. Nucl. Part. Sci **69**, 307 (2019)]
- **IM-NCSM**
  [E. Gebrerufael, K. Vobig, HH, R. Roth, PRL **118**, 152503; with R. Roth, T. Mongolia, R. Wirth…]
  - **unbiased**
  - active-space CI / FCI: **exponential scaling**
- **IM-GCM**
  - requires **very few states (O(10)-O(100))**
  - **biased** selection of configurations and generator coordinates



Density Matrix Renormalization Group

- How about **IM-DMRG** (or IMSRG + other tensor network methods)?
    - aka **Canonical Transformation Theory + DMRG**
      [S. White, JCP **117**, 7472; Yanai et al. JCP **124**, 194106; JCP **127**, 104107; JCP **132**, 024105]
    - **Efficient and unbiased ?**

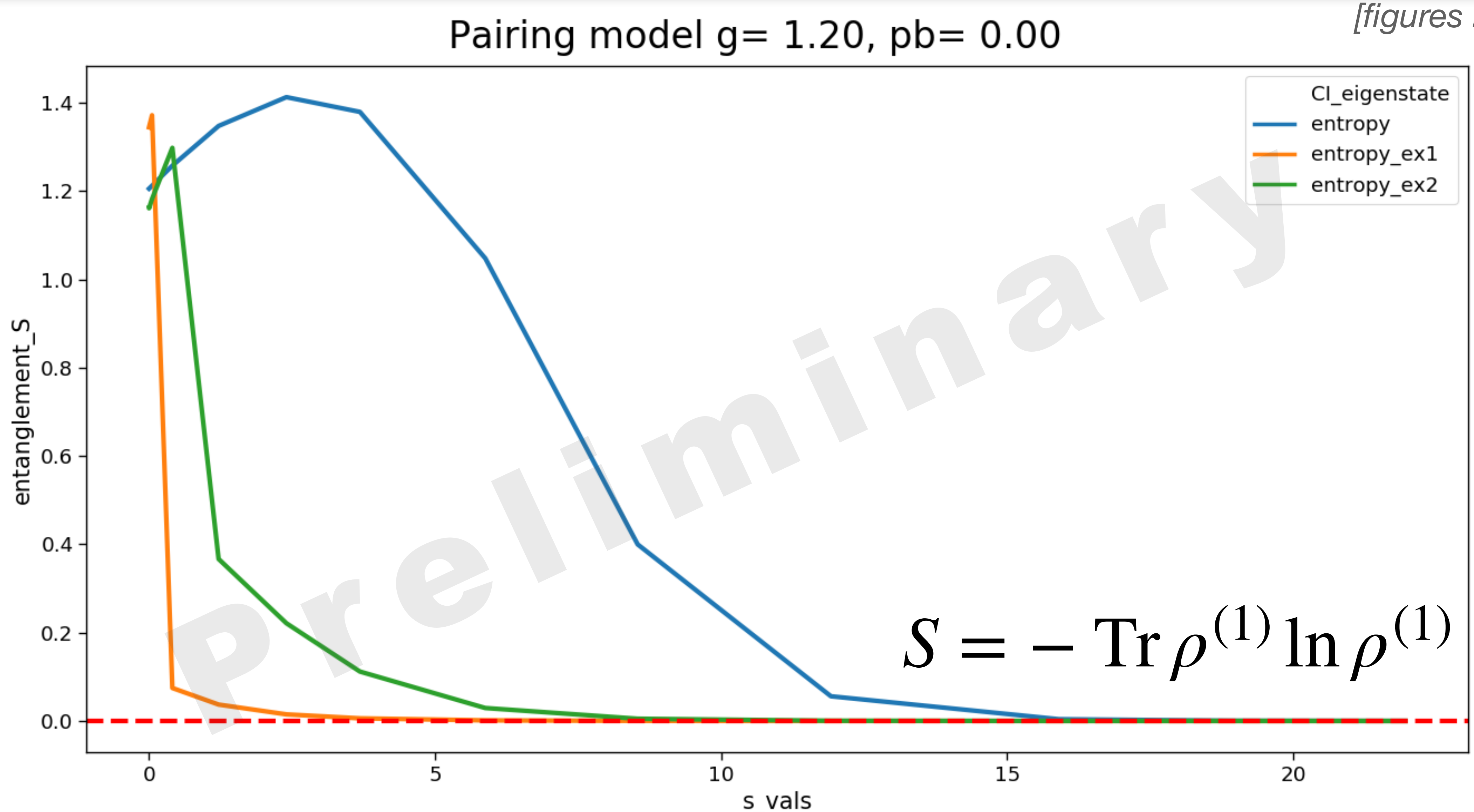


DMRG in Nuclear Physics

- **valence-space / active space DMRG**
  - based on **empirical** interactions (**= low-resolution**)
  - **issues:** mapping of orbitals to 1D chain, implementation of symmetries
    [Papenbrock & Dean, JPG 31, S1377 (2004); Thakur et al., PRC 78, 041303]
  - recent advances: better accounting for **entanglement**
    [Legeza et al., PRC 02, 051303; Kruppa et al., JPG 48, 025107]
  - inclusion of **continuum** possible via Gamow-DMRG
    [**J. Rotureau** et al., PRC 79, 014304; **K. Fossez** et al., PRC 98, 061302 and arXiv:2105.05287]
- ab initio **No-Core Gamow Shell Model / DMRG** based on RG-evolved **two-nucleon interactions** [J. Rotureau et al.]
  - **slow convergence** an issue beyond mass A=8-10

IMSRG as a Disentangler

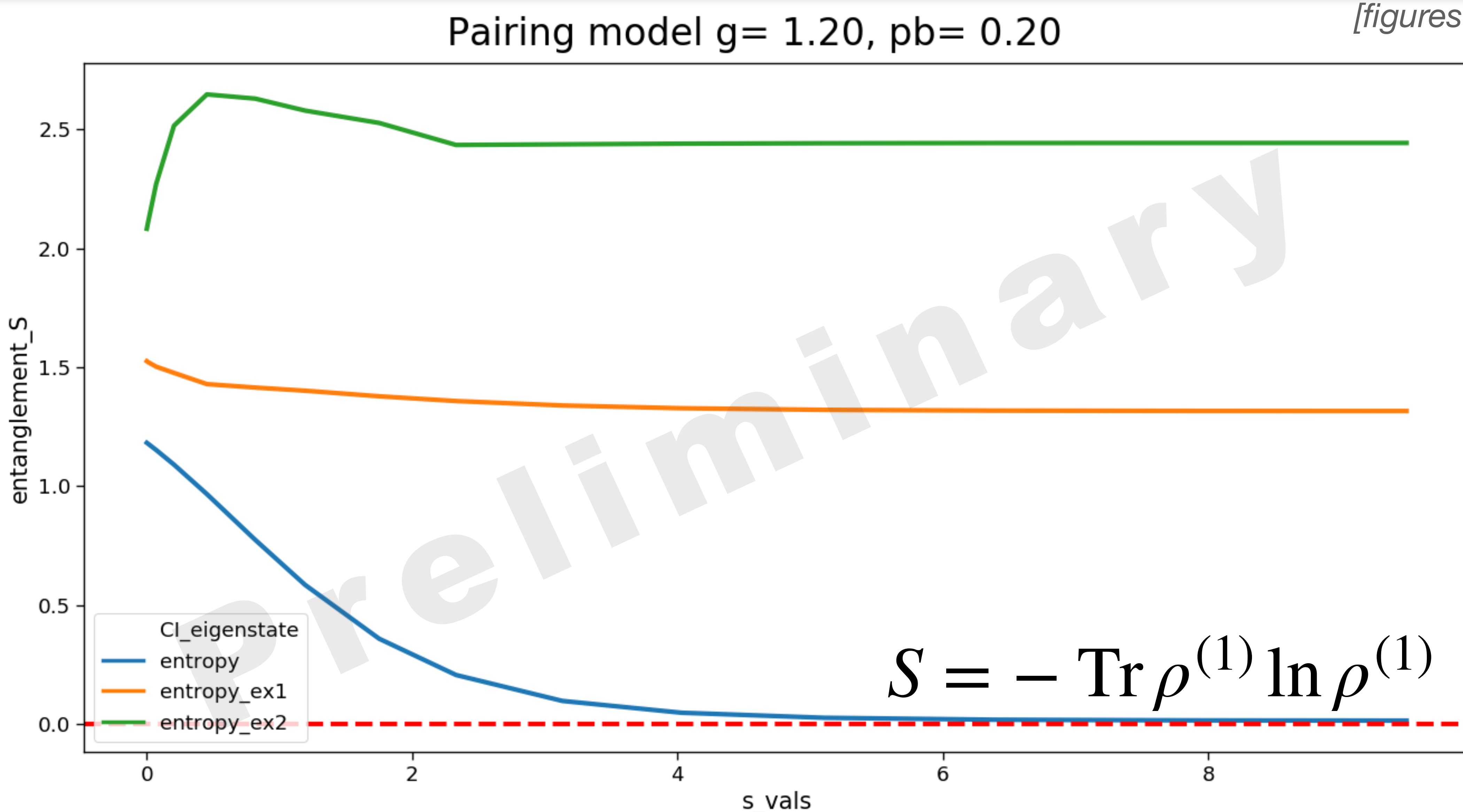
[figures by J. Davison]



- IMSRG maps **interacting ground state** to **reference state** (here, a Slater determinant)
- eigenstates with similar structure (fully paired) are mapped onto Slater determinants by the same transformation

IMSRG as a Disentangler

[figures by J. Davison]



- ground-state mapping still successful for more “complex” Hamiltonian (pairing plus pair-breaking)

Prospects & Opportunities

- **IM-DMRG** [with K. Fossez and J. Rotureau]
- **entanglement-based generators** for the IMSRG ?
  - need to translate entanglement from wave function property into operator property, e.g., **entangling power** [see, e.g., Zanardi et al., PRA **62**, 030301; Beane & Farrell, arXiv:2011.01278]
- derive **effective (no-core, active-space, schematic) Hamiltonians** using SRG and IMSRG flows
  - e.g., Coulomb: free-space SRG has little effect, but IMSRG decoupling of active space might

Prospects & Opportunities

- Could (IM)SRG transformations be used as **disentanglers** in tensor networks?
    - Computational cost benefits compared to variational optimization?
- **Tensor network structure** of the IMSRG transformation / wave function $|\Psi\rangle = U(s)|\Phi_{\text{ref}}\rangle$?
    - relation with tensor networks, e.g., (c)MERA [Haegemann et al., PRL **100**, 100402], ...
    - Unitary neural networks?
- **And probably many more… I'm happy to discuss!**

Acknowledgments

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R. J. Furnstahl
The Ohio State University

and many more…

NUCLEI Nuclear Computational Low-Energy Initiative

NERSC

ICER