Towards a More Effective Nuclear Many-Body Problem

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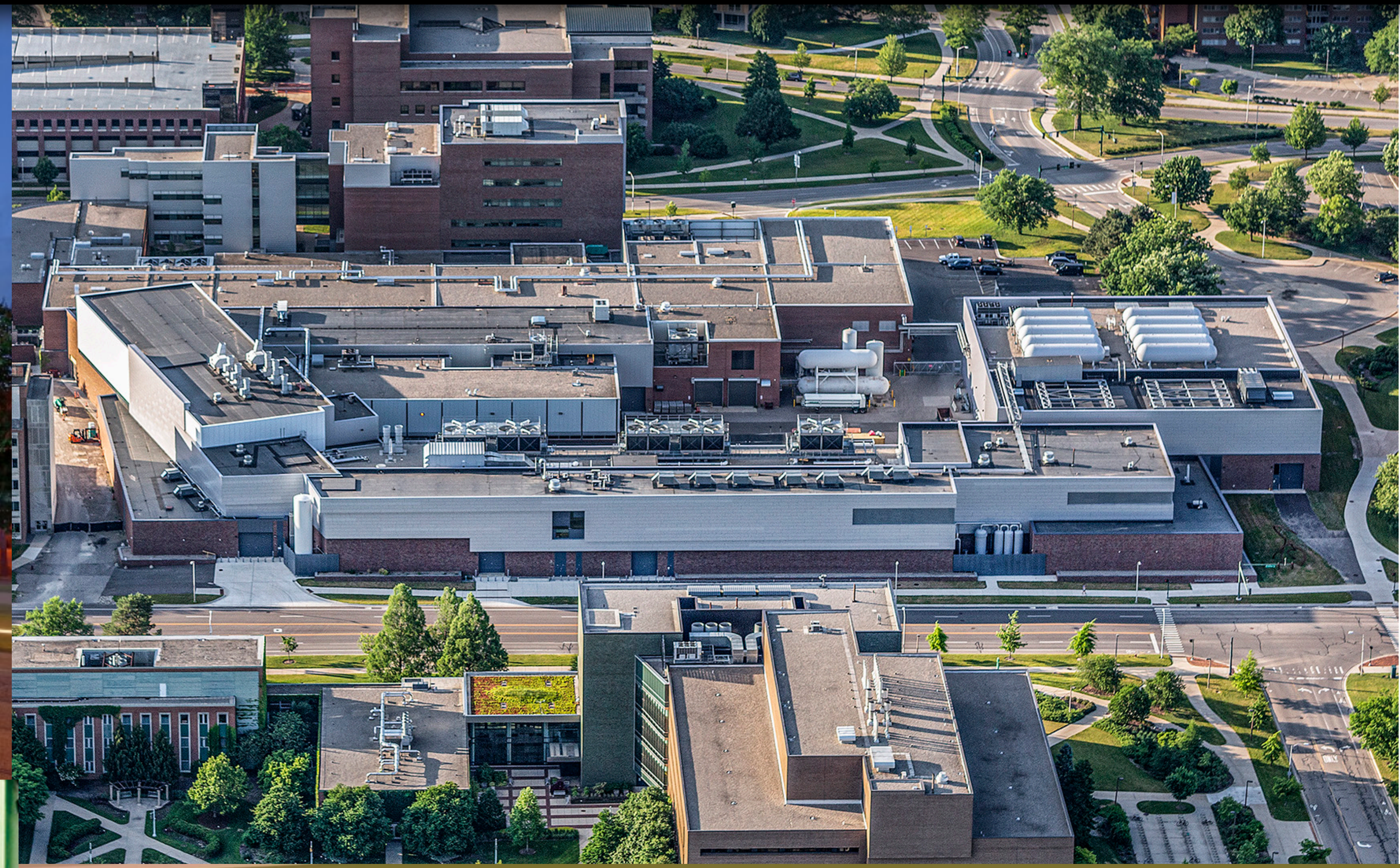
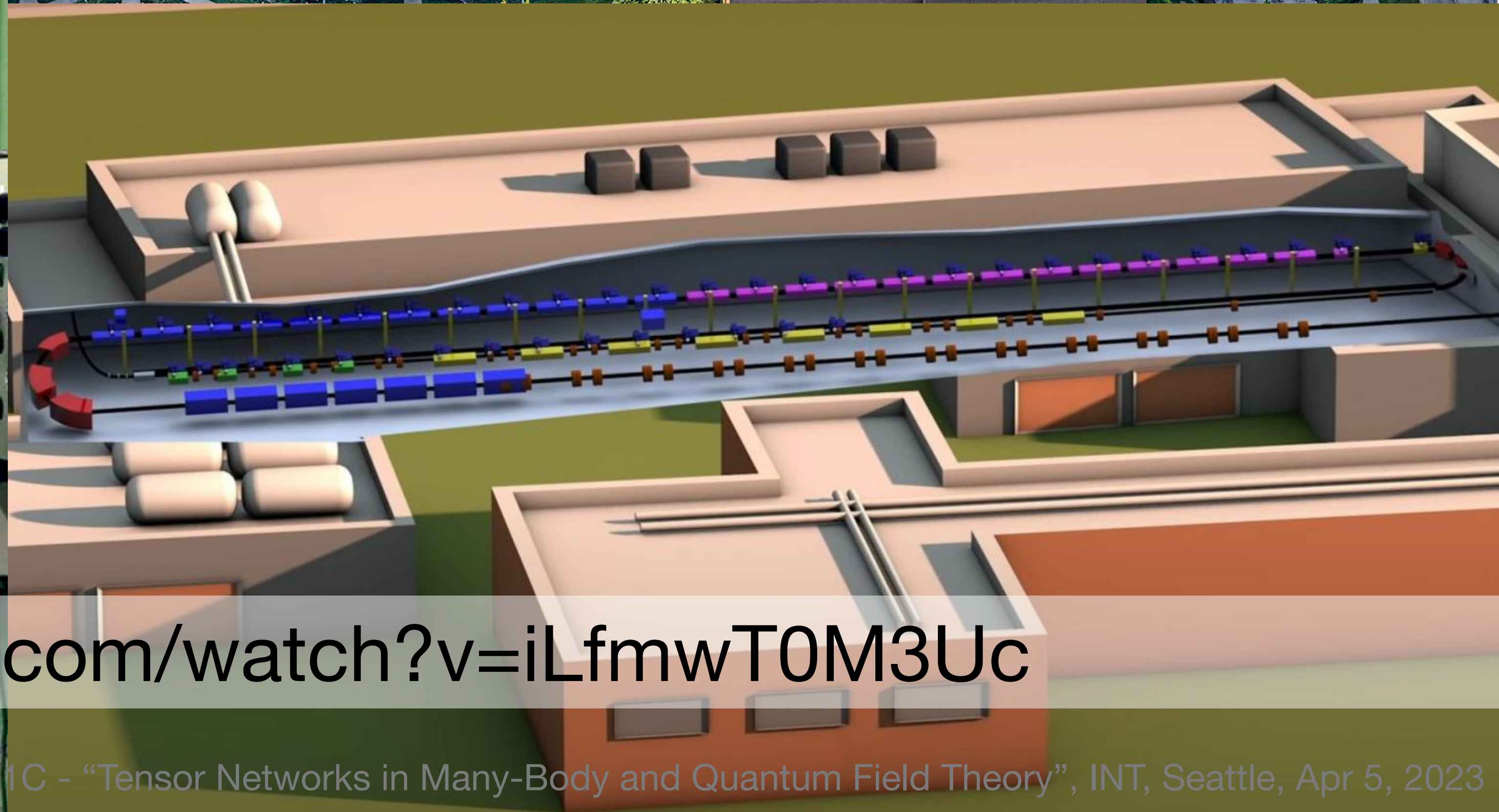
FRIB Has Commenced Operation





virtual tour: https://www.youtube.com/watch?v=iLfmwT0M3Uc

FRIB Has Commenced Operation

FRIB

PHYSICAL REVIEW LETTERS **129,** 212501 (2022)

Editors' Suggestion | Featured in Physics

Crossing $N = 28$ Toward the Neutron Drip Line: First Measurement of Half-Lives at FRIB

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New half-lives for exotic isotopes approaching the neutron drip-line in the vicinity of $N \sim 28$ for $Z =$ 12–15 were measured at the Facility for Rare Isotope Beams (FRIB) with the FRIB decay station initiator. The first experimental results are compared to the latest quasiparticle random phase approximation and shell-model calculations. Overall, the measured half-lives are consistent with the available theoretical descriptions and suggest a well-developed region of deformation below ^{48}Ca in the $N = 28$ isotones. The erosion of the $Z = 14$ subshell closure in Si is experimentally confirmed at $N = 28$, and a reduction in the ^{38}Mg half-life is observed as compared with its isotopic neighbors, which does not seem to be predicted well based on the decay energy and deformation trends. This highlights the need for both additional data in this very exotic region, and for more advanced theoretical efforts.

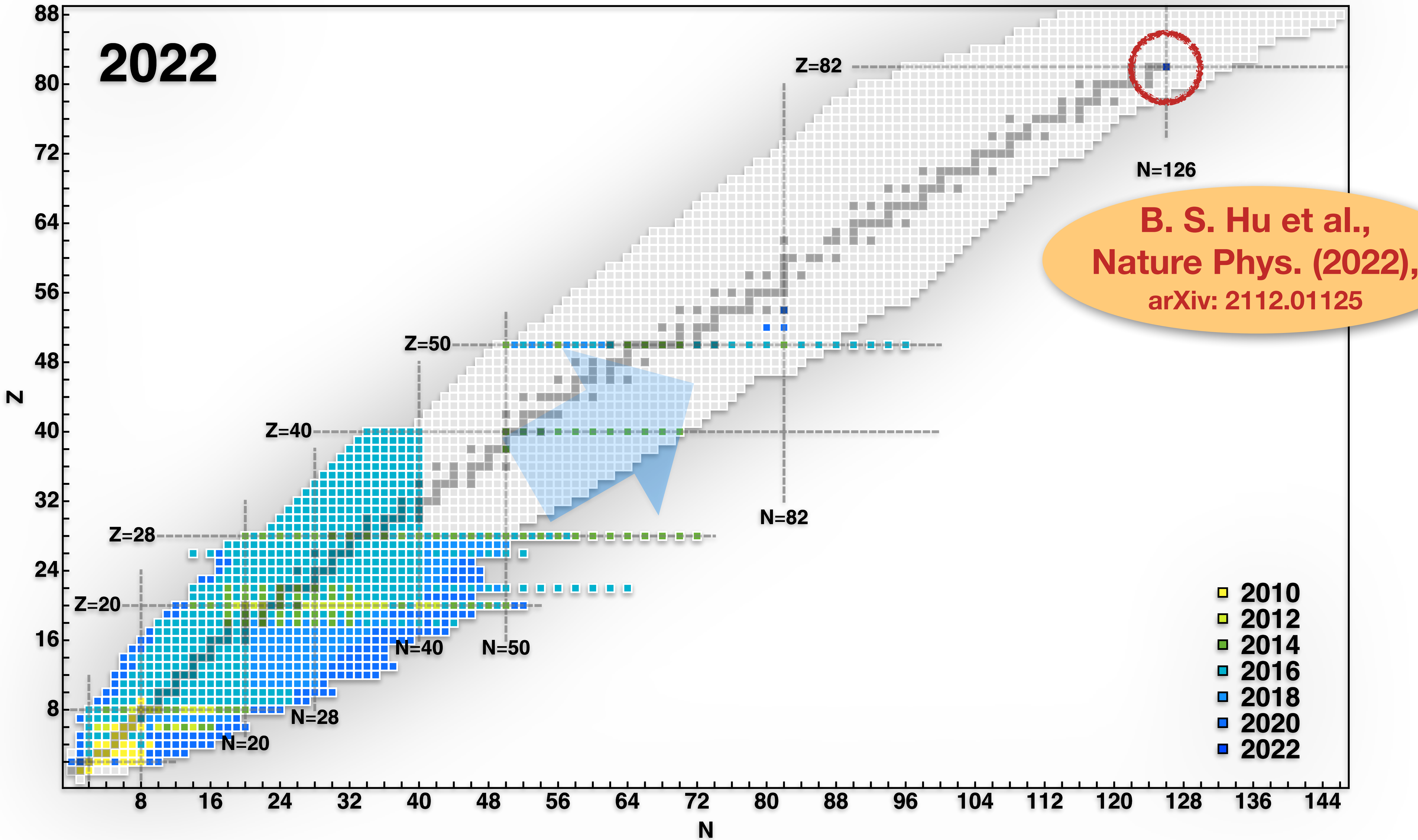
DOI: 10.1103/PhysRevLett.129.212501

Need for Precision Nuclear Structure

- understanding **nuclear forces** (i.e., low-energy QCD), **emergent phenomena** (clustering, halos, …)
- **nuclear & neutron matter equation of state**
  - crucial for supernovae and neutron star mergers
- **nucleosynthesis**
  - explaining processes and resulting abundances
- searches for **physics beyond the Standard Model**
  - **nuclei** and **radioactive molecules** offer alternatives to ever larger colliders
  - neutrinoless double beta decay, CKM unitarity Tests, electric dipole moments, …

Progress in *Ab Initio* Calculations

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



The Roadmap

Chiral EFT

↓

RG
(similarity trafos)

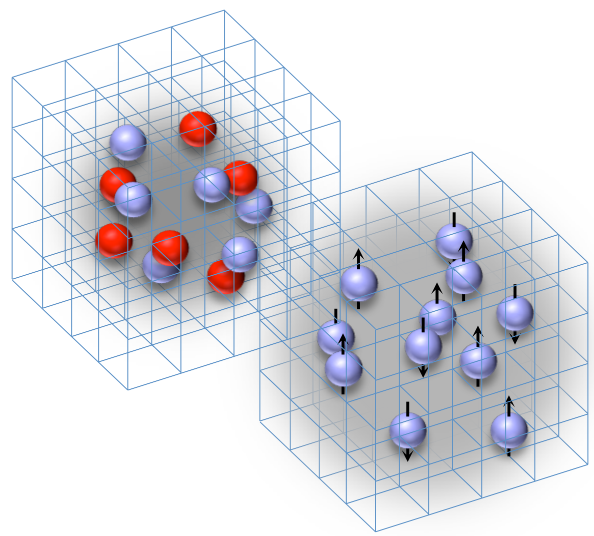
↓

many-body method

- **Interactions (& Operators) from Chiral EFT**
  - symmetries of low-energy QCD
  - power counting
- **(Similarity) Renormalization Group**
  - systematically dial resolution scales (cutoffs) of theory
  - trade-off: enhanced convergence & accuracy of many-body methods vs. omitted induced 4N, …, AN forces
- ***Ab Initio* Many-Body Methods**
  - systematically improvable towards exact solution

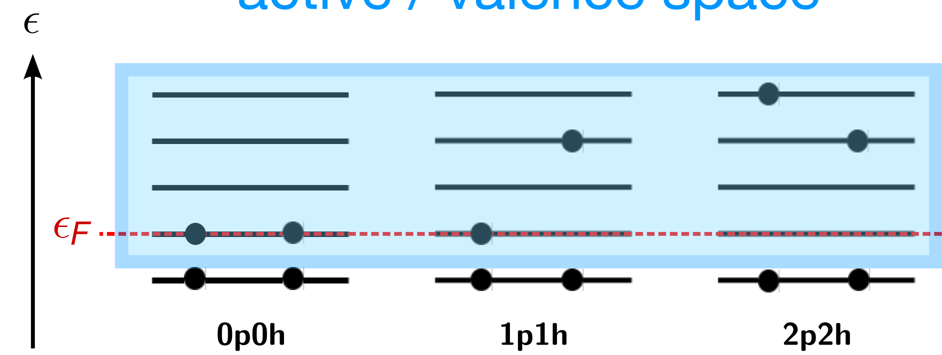
Paradigms

- **Coordinate Space**
  - Quantum Monte Carlo
  - Lattice EFT

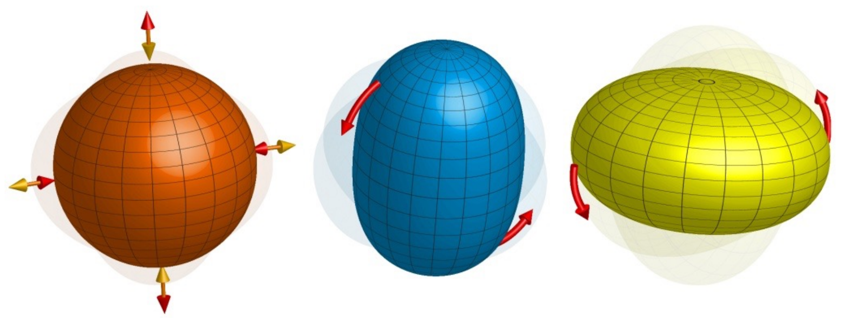


- **Configuration Space: Particle-Hole Expansions**
  - Many-Body Perturbation Theory (MBPT)
  - (No-Core) Configuration Interaction (aka Shell Model, (NC)SM)
  - Coupled Cluster (CC)
  - In-Medium Similarity Renormalization Group (IMSRG)

active / valence space

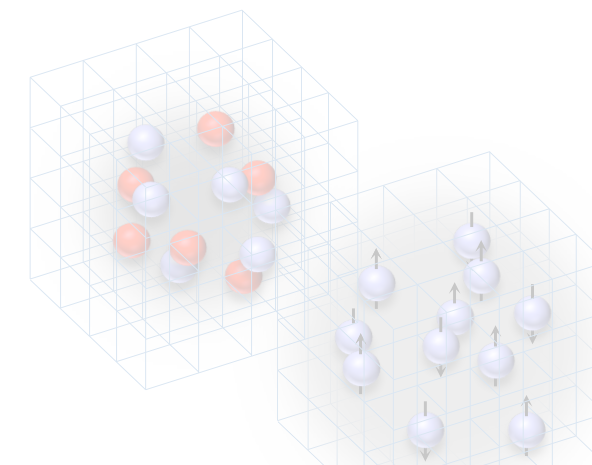


- **Configuration Space / Coordinate Space: Geometric Expansions**
  - deformed HF(B) + projection
  - projected Generator Coordinate Method (PGCM)
  - symmetry-adapted NCSM



Paradigms

- **Coordinate Space**
  - Quantum Monte Carlo
  - Lattice EFT



- **Configuration Space: Particle-Hole Expansions**

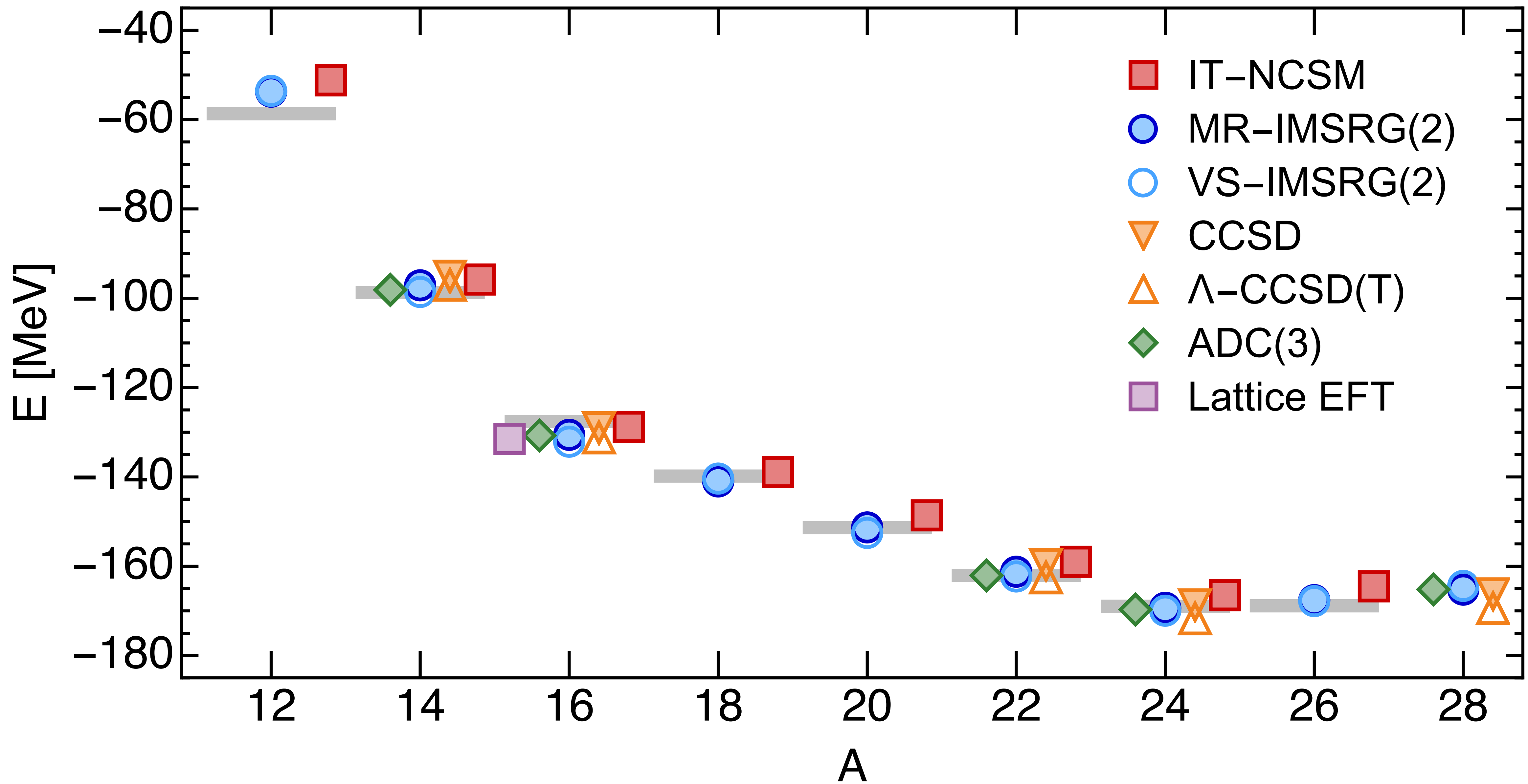
Recent(-ish) Reviews:
HH, Front. Phys. **8**, 379 (2020)
S. Gandolfi, D. Lonardoni, A. Lovato and M. Piarulli, Front. Phys. **8**, 117 (2020)
D. Lee, Front. Phys. **8**, 174 (2020)
V. Somà, Front. Phys. **8**, 340 (2020)

also see
“What is *ab initio* in nuclear theory?”, A. Ekström, C. Forssén, G. Hagen, G. R. Jansen, W. Jiang, T. Papenbrock, arXiv:2212.11064

  - deformed HF(B) + projection
  - projected Generator Coordinate Method (PGCM)
  - symmetry-adapted NCSM

Consistency: Oxygen Isotopes

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



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

Part I:

Renormalization

S. R. Stroberg, HH, S. K. Bogner and J. D. Holt, Ann. Rev. Nucl. Part. Sci 69, 307 (2019)

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)

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

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 $H(s) = U(s)HU^{\dagger}(s)$:

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

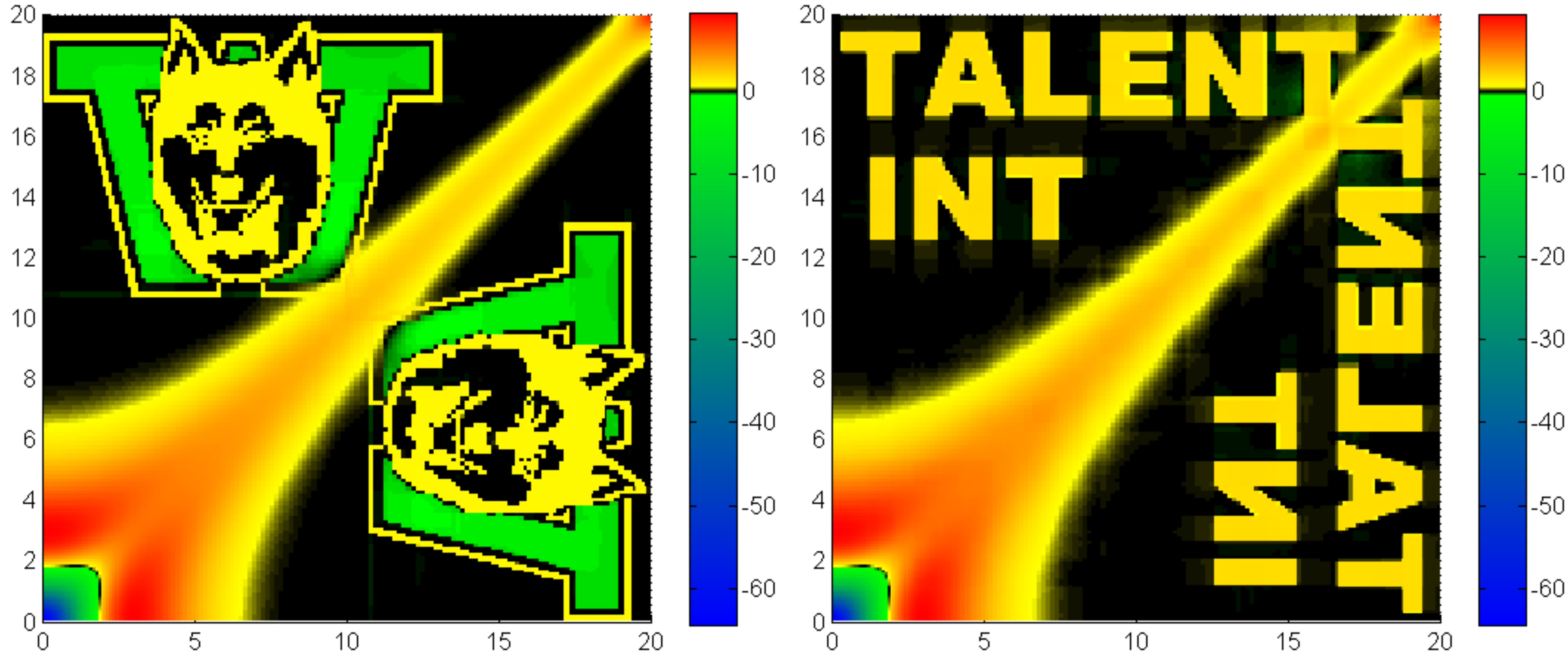
- choose $\eta(s)$ to achieve desired behavior, e.g.,

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

to suppress (suitably defined) off-diagonal Hamiltonian

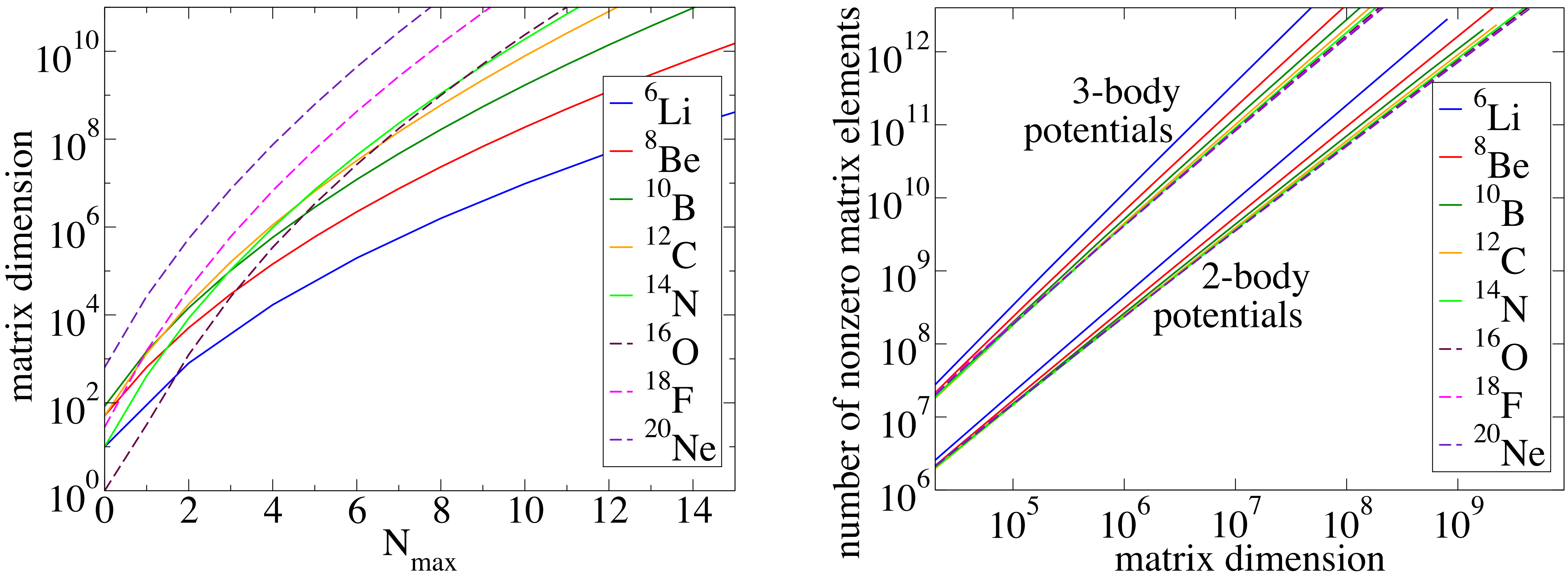
- consistent evolution for all observables of interest

Tailoring the Hamiltonian



SRG Evolution of an NN Interaction
with the Husky and TALENT Generators
[B. D. Carlsson, TALENT summer school at INT, 2013]

Dimensions for Exact Diagonalization



from: C. Yang, H. M. Aktulga, P. Maris, E. Ng, J. Vary, Proceedings of NTSE-2013

- basis-size "explosion": **exponential growth**
- **importance truncation** etc. cannot fully compensate this growth as A increases

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:

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

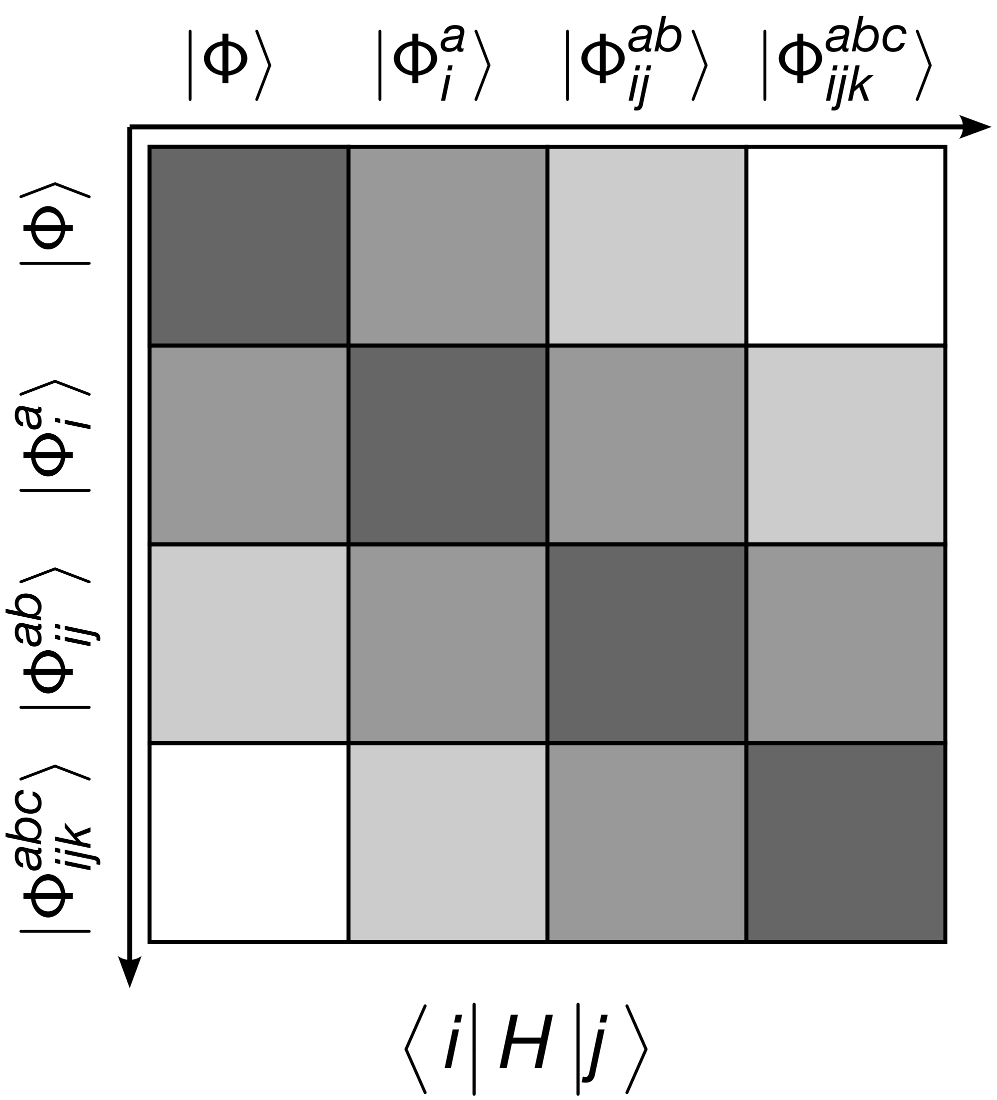
- **flow equations** for the coefficient (**coupling constants**):

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

- "obvious" choice for many-body problems:

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

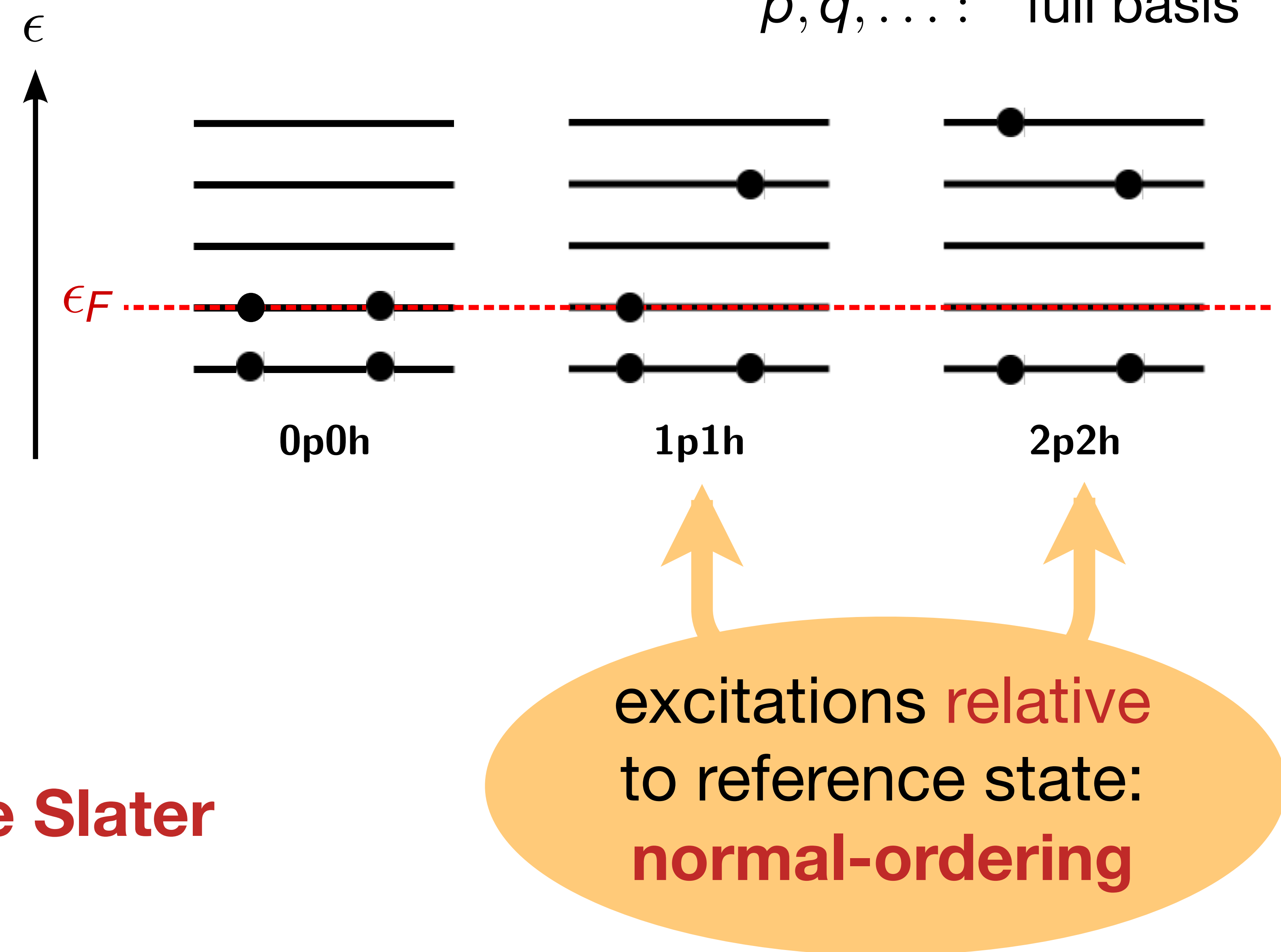
Transforming the Hamiltonian



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

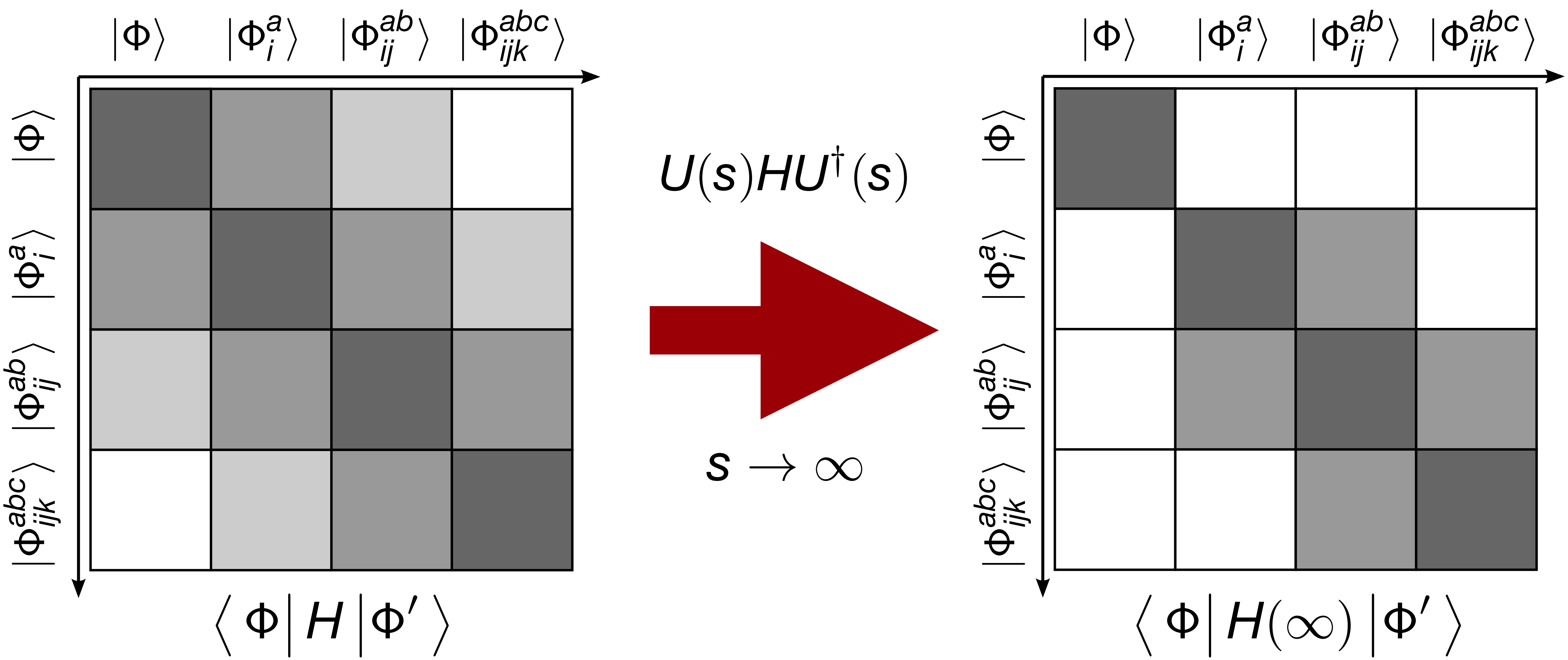
$i, j, \ldots : \quad \epsilon \leq \epsilon_F$

$p, q, \ldots :$ full basis



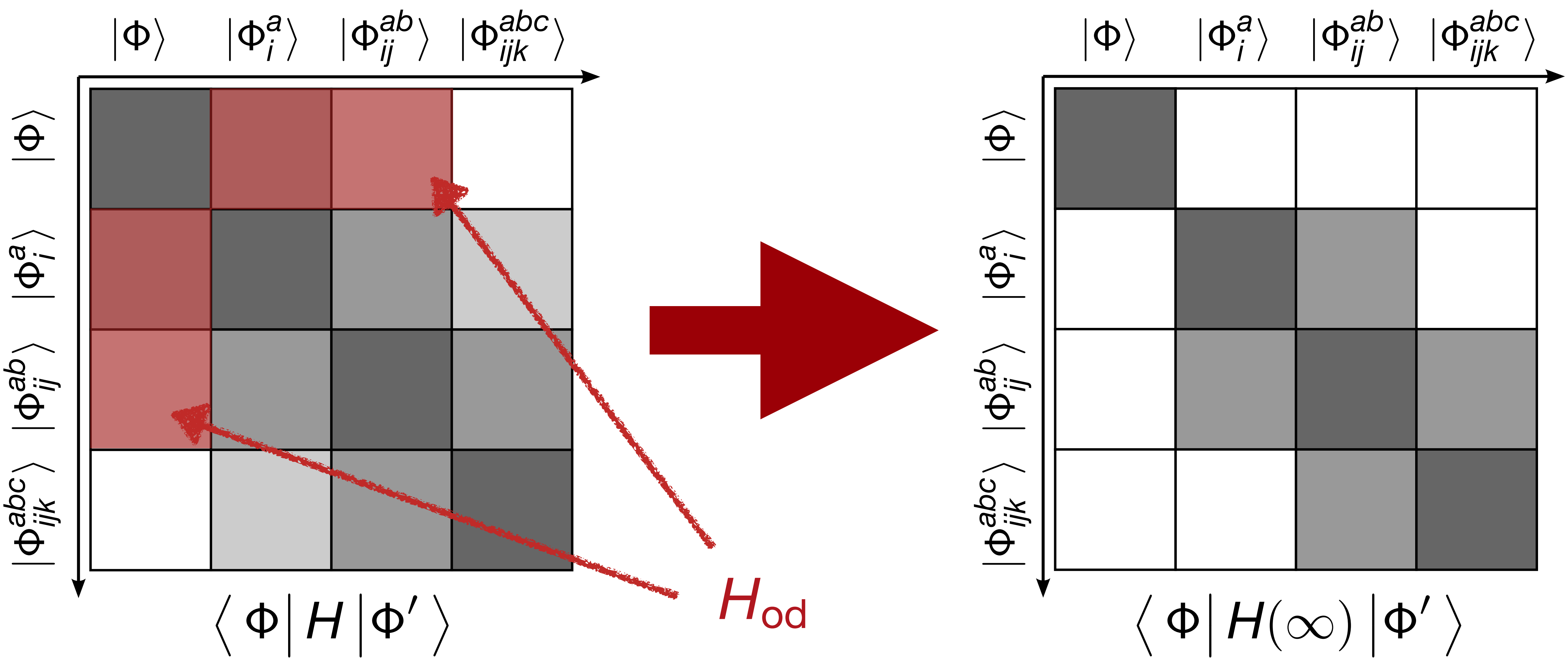
- reference state: **single Slater determinant**

Decoupling in A-Body Space



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

Flow Equation



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

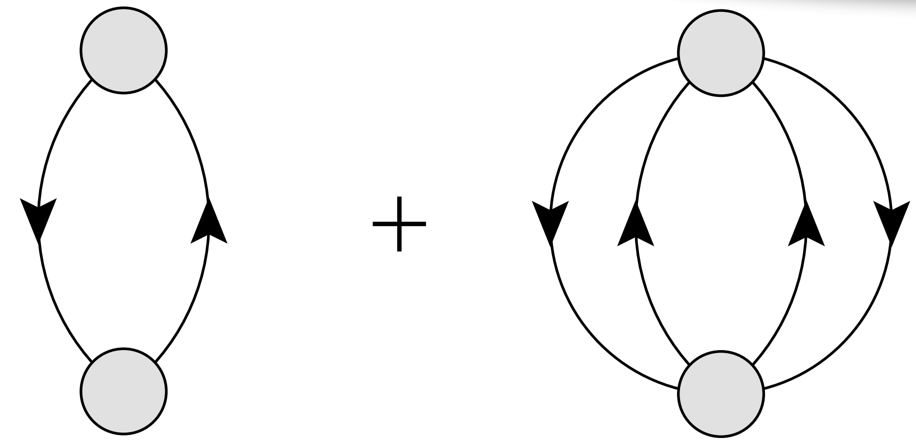
Operators
truncated at **two-body level** -
matrix is never constructed explicitly!

Standard IMSRG(2) Flow Equations

0-body Flow

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

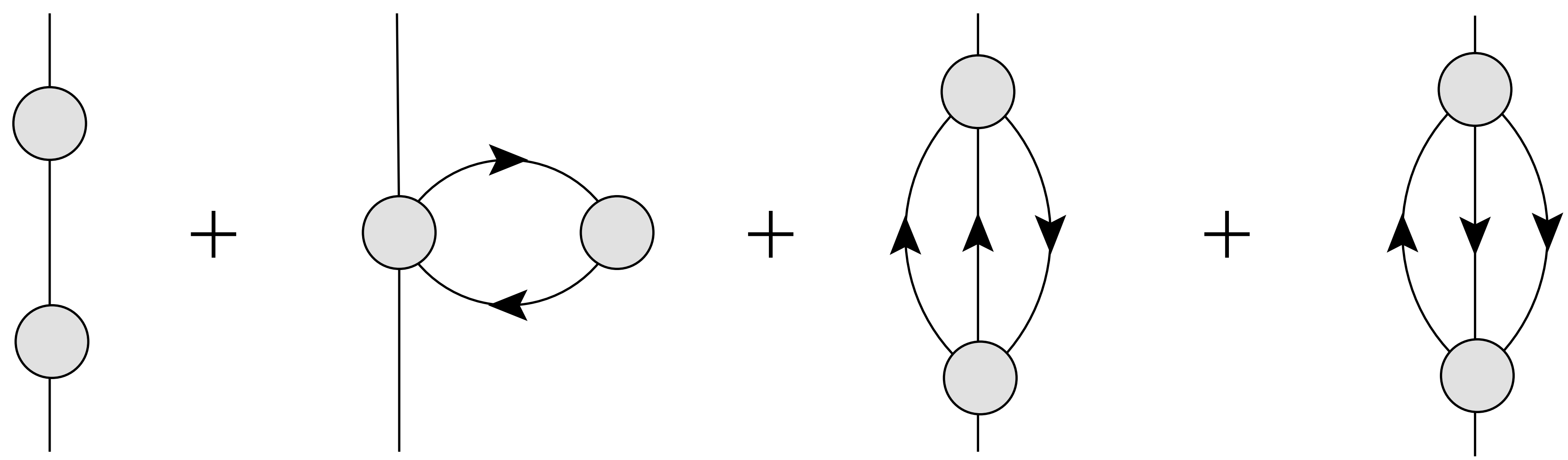
$$\frac{dE}{ds} =$$



1-body Flow

coefficients (couplings) of H(s)

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

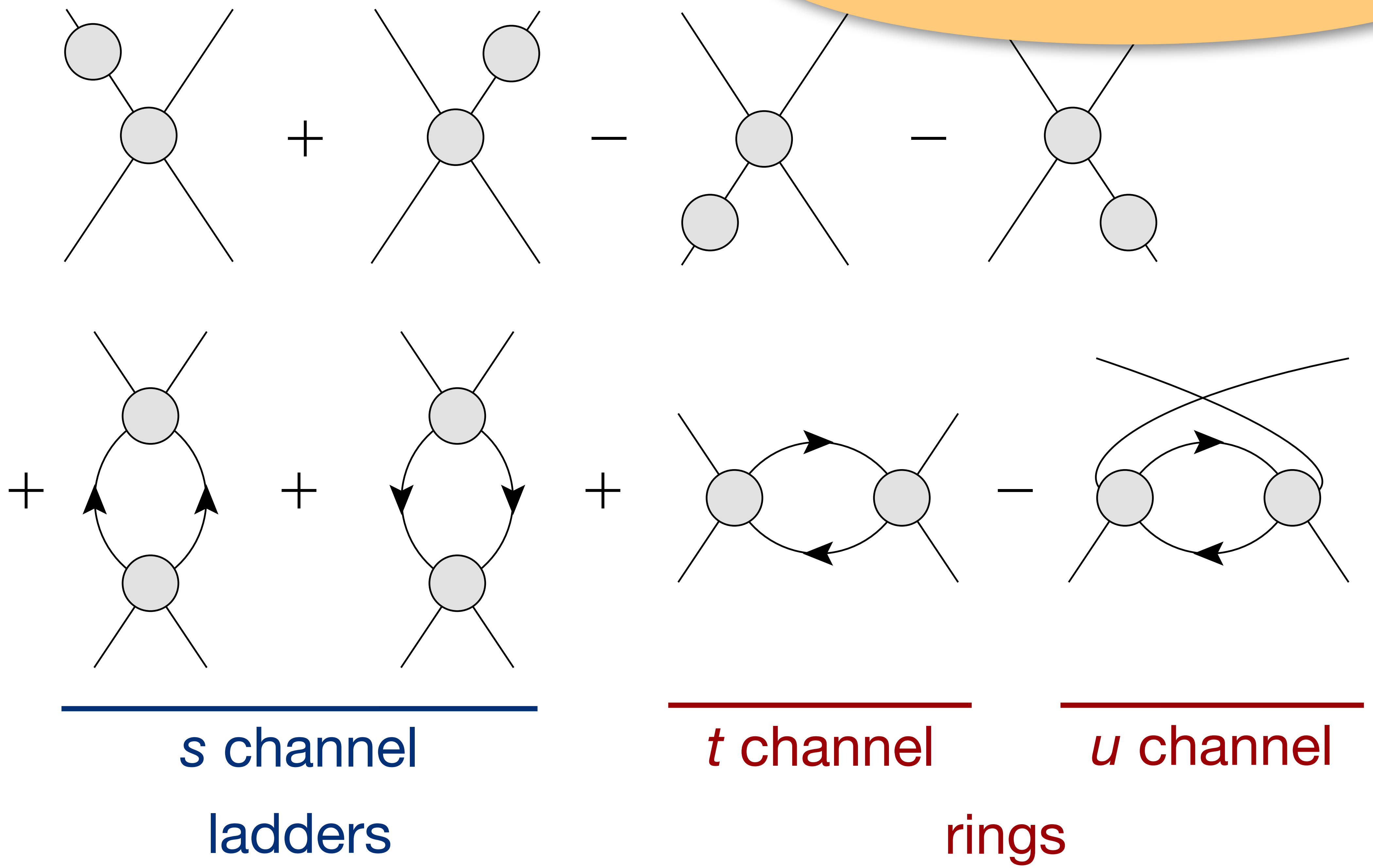


Standard IMSRG(2) Flow Equations

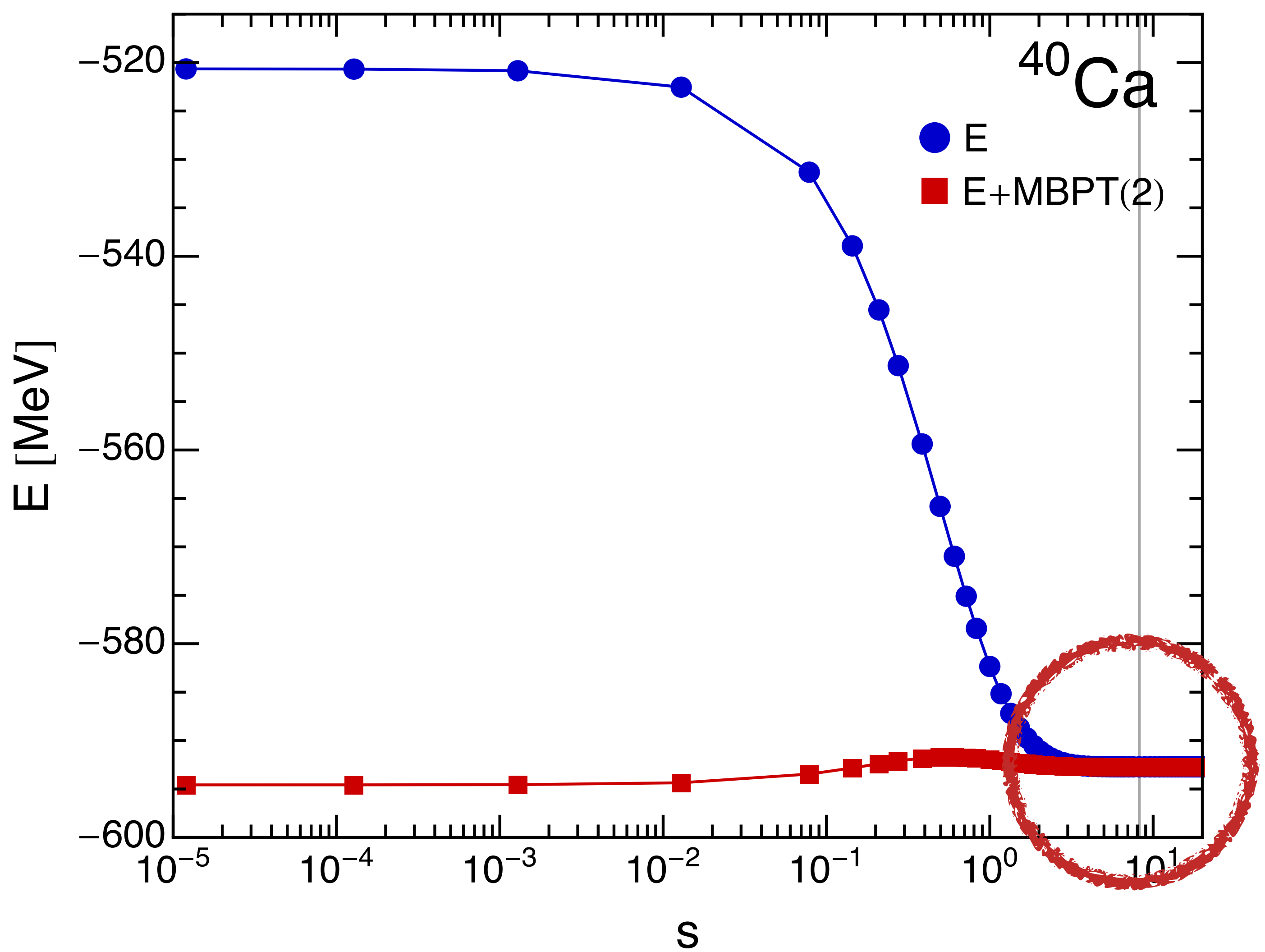
2-body Flow

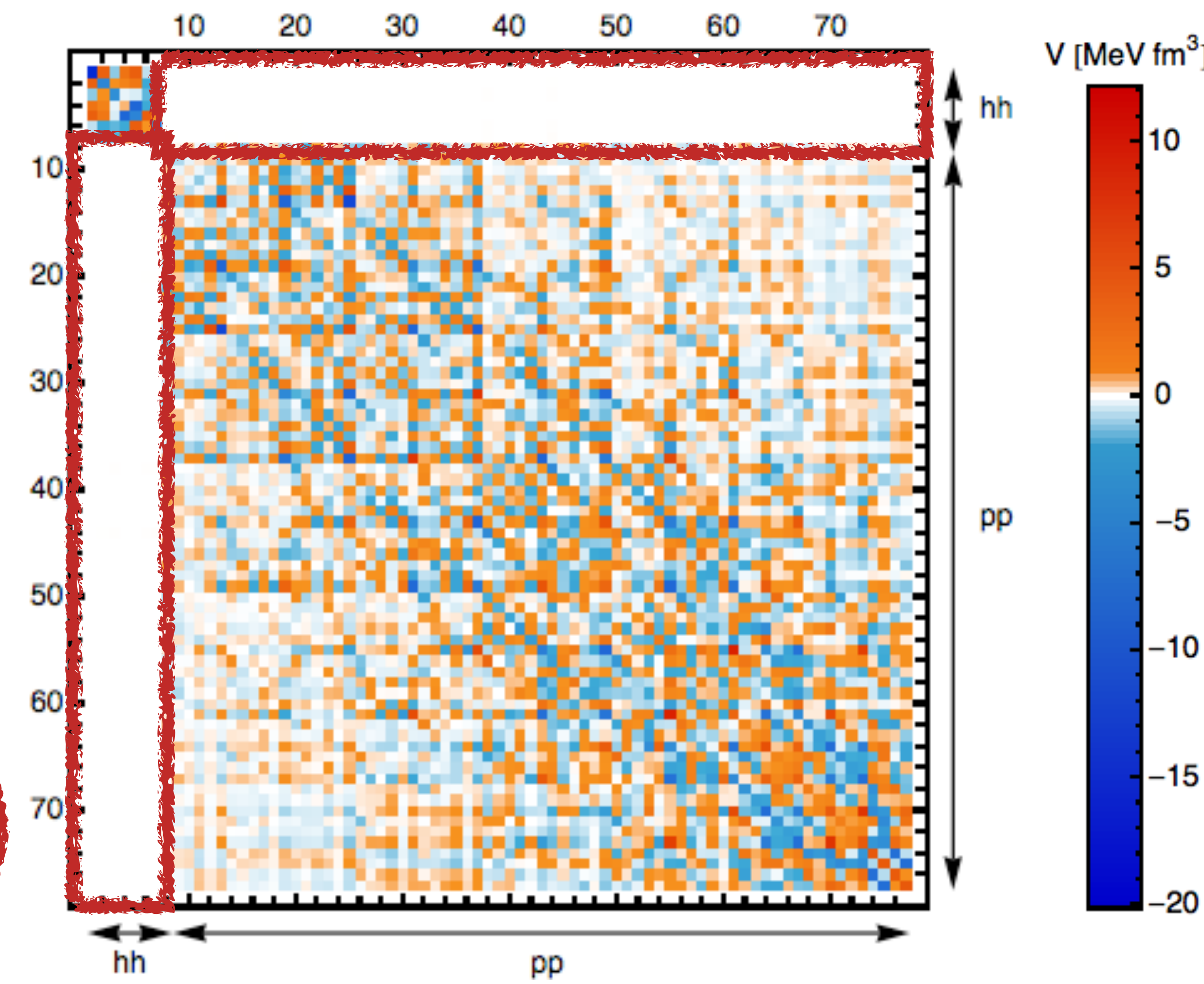
O(N⁶) scaling
(before particle/hole distinction)

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



Decoupling



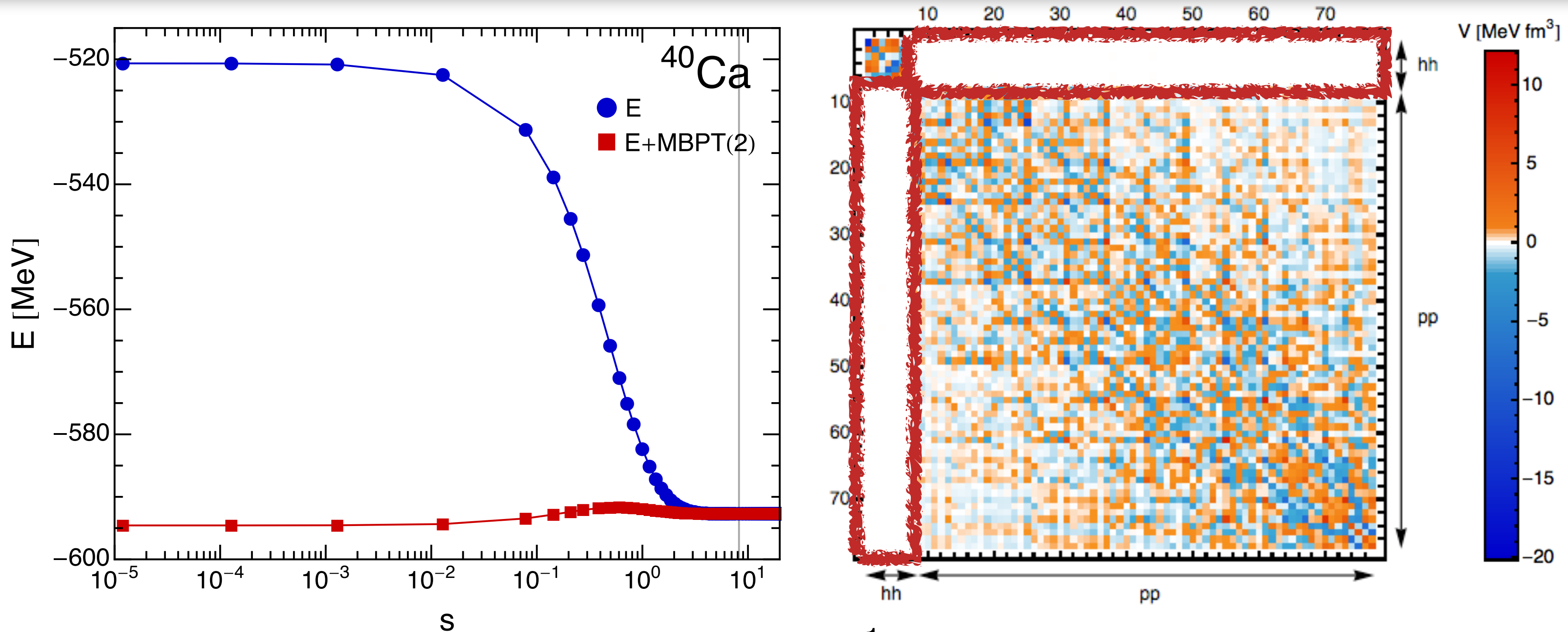


N3LO, $\lambda = 2.0\ \mathrm{fm}^{-1}, e_{\mathrm{Max}} = 8$

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

off-diagonal couplings are rapidly driven to zero

Decoupling



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

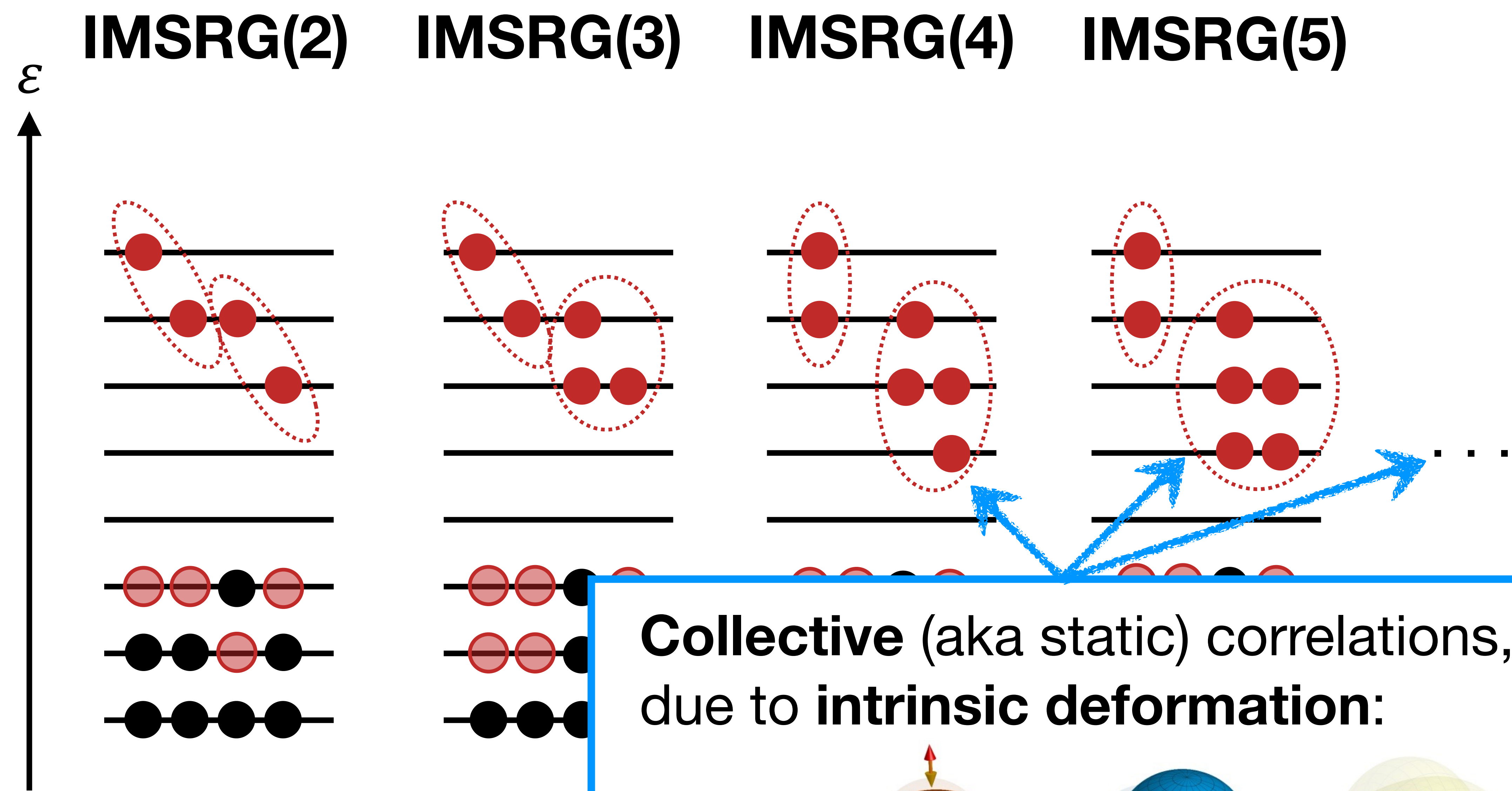
- absorb correlations into **RG-improved Hamiltonian**

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

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

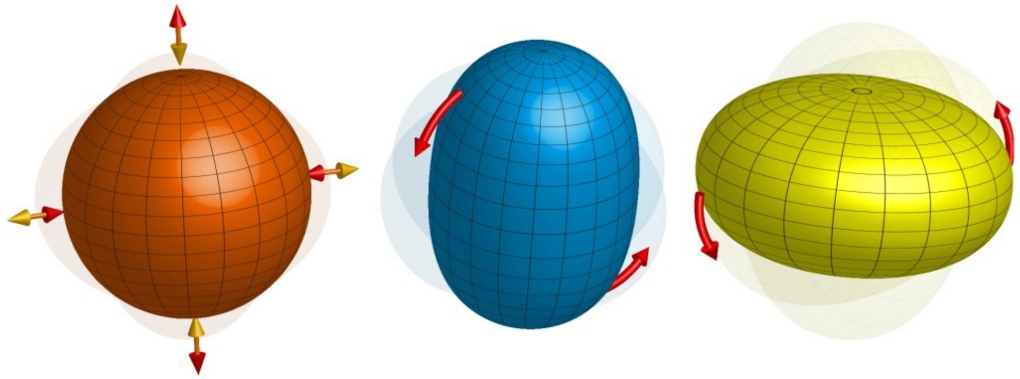
$$U(s)\left|\Psi_n\right\rangle \overset{!}{=} \left|\Phi\right\rangle$$

Correlated Reference States

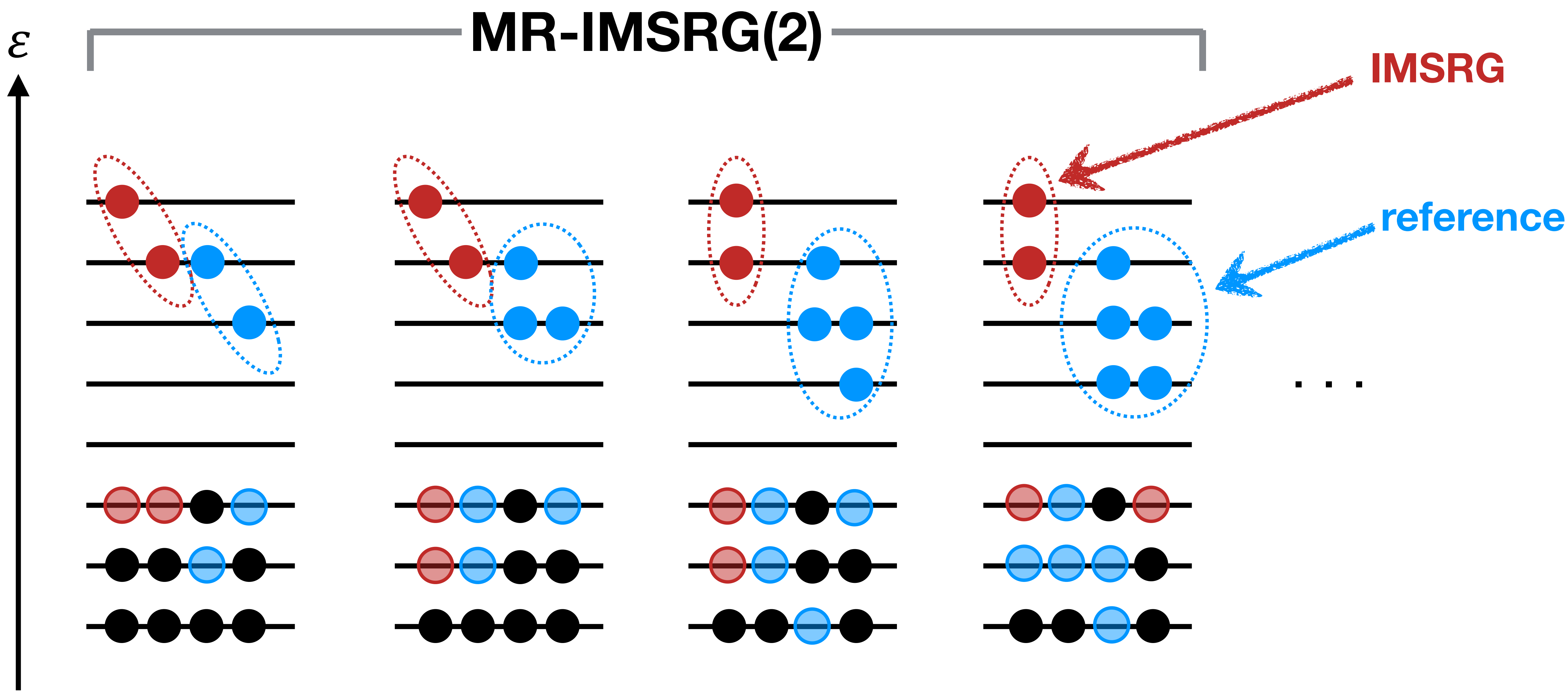


"standard" IMS
Slater determinar

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

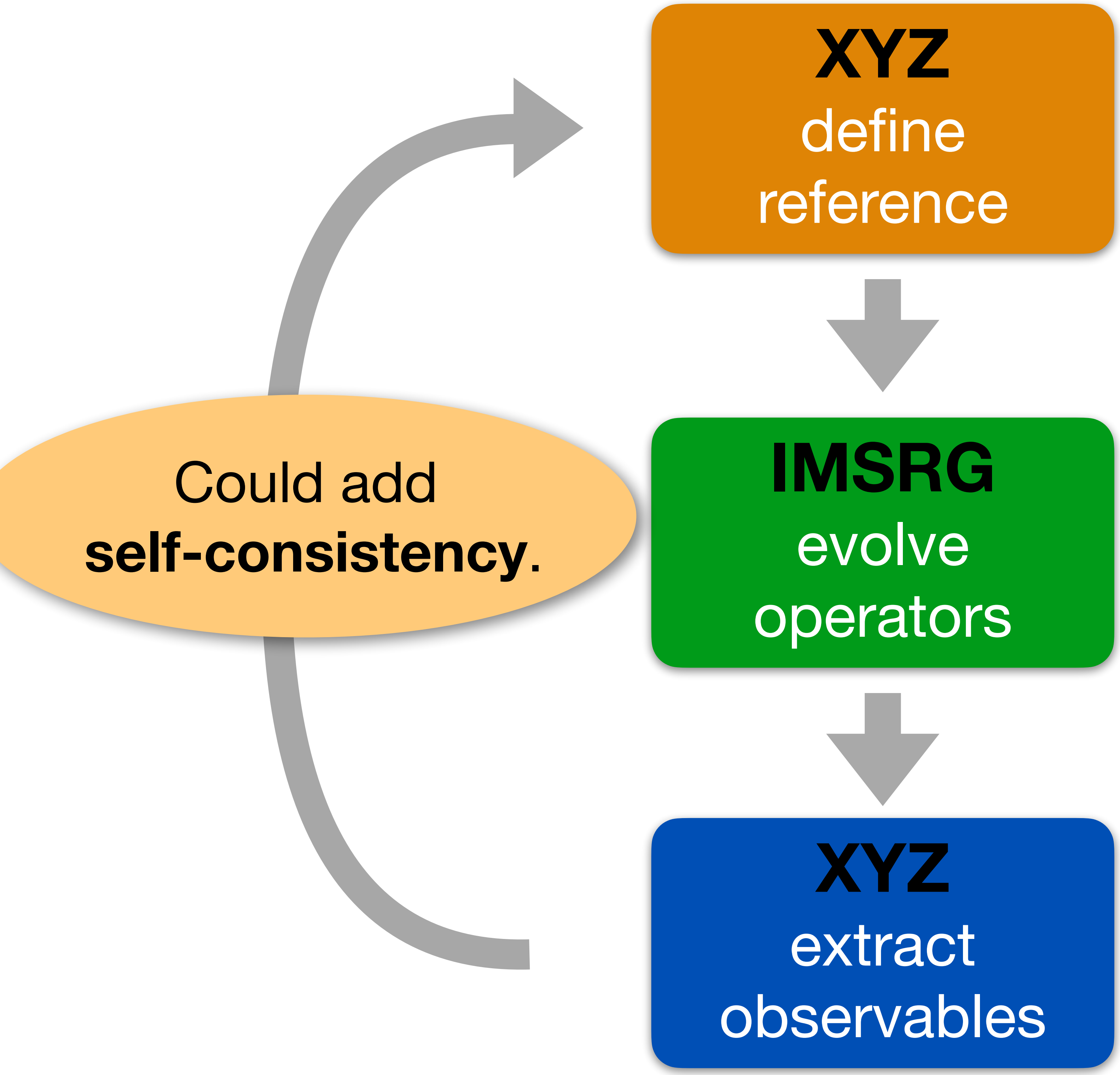


Correlated Reference States



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

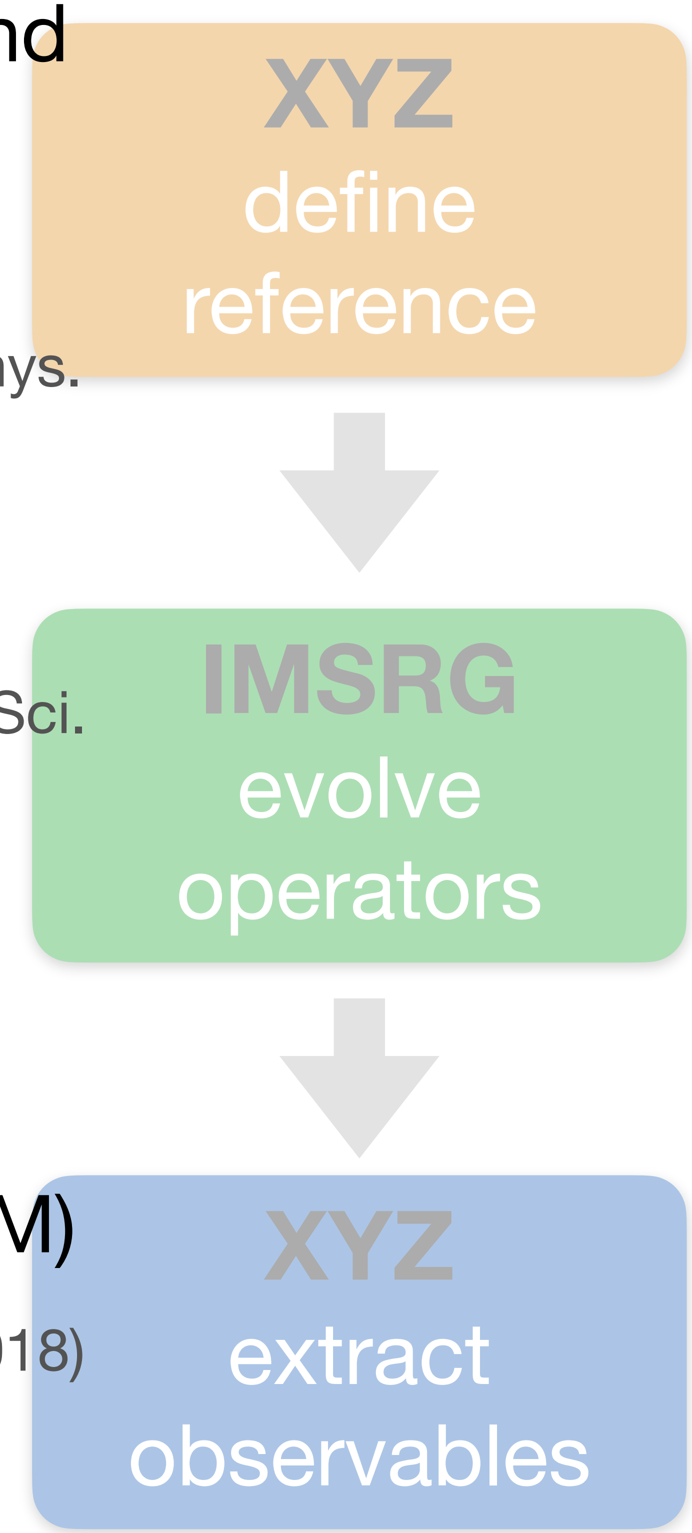
IMSRG-Improved Methods



* mean field or **explicitly correlated**

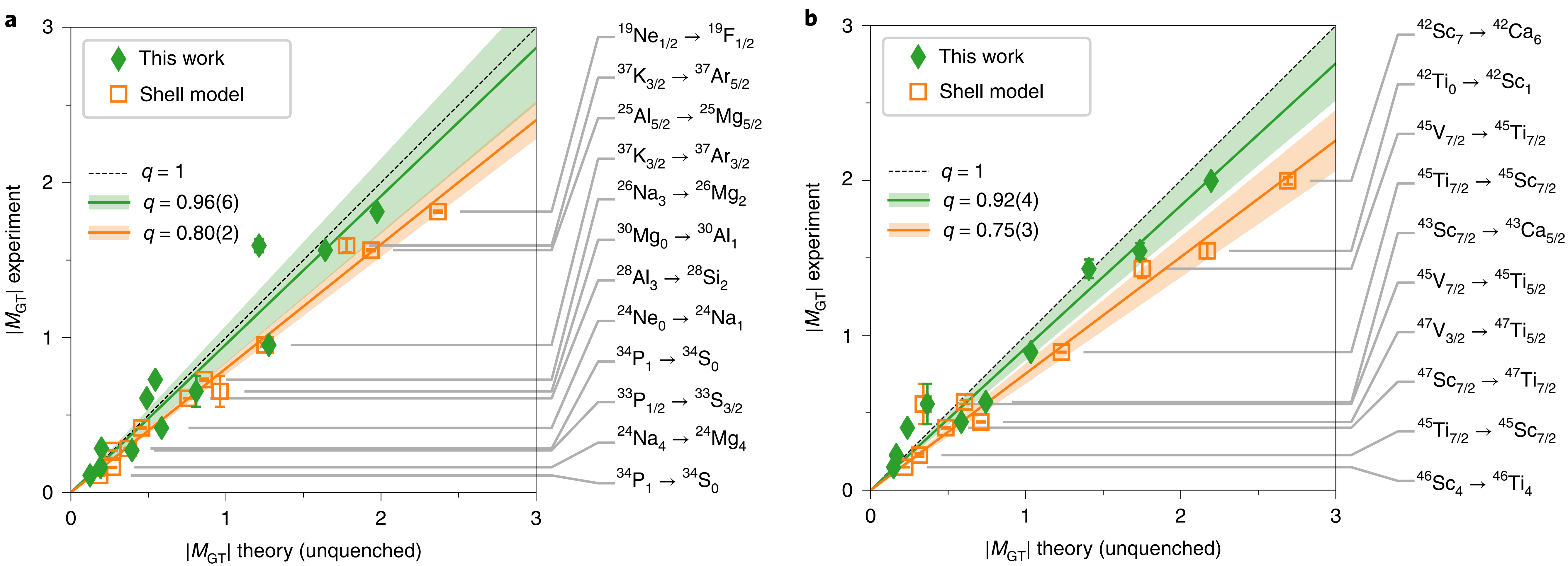
IMSRG-Improved Methods

- 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)



Application: Quenching of Gamow-Teller Decays

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



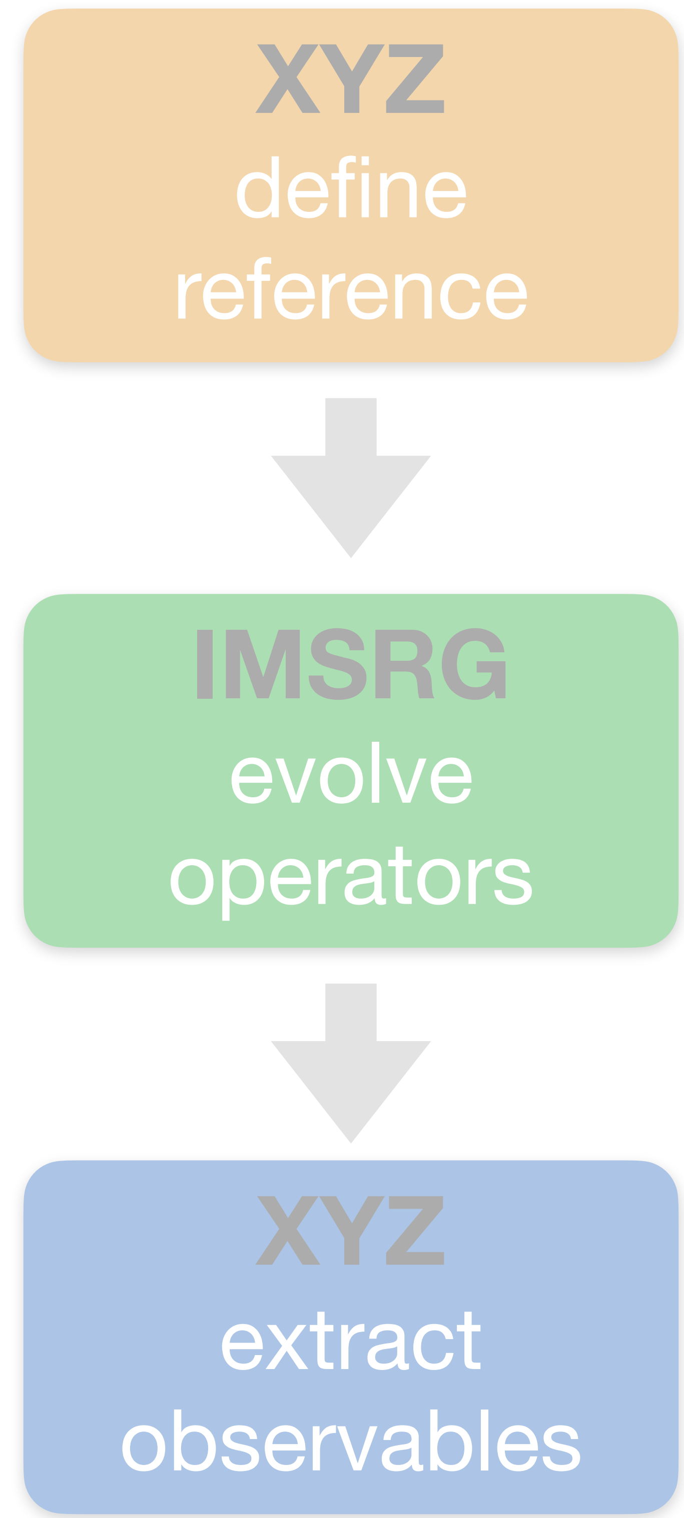
- **empirical Shell model** calculations require **quenching factors** of the weak axial-vector couling g_A
- **VS-IMSRG** explains this through consistent **renormalization** of transition operator, incl. **two-body currents**

Part II:

Entanglement

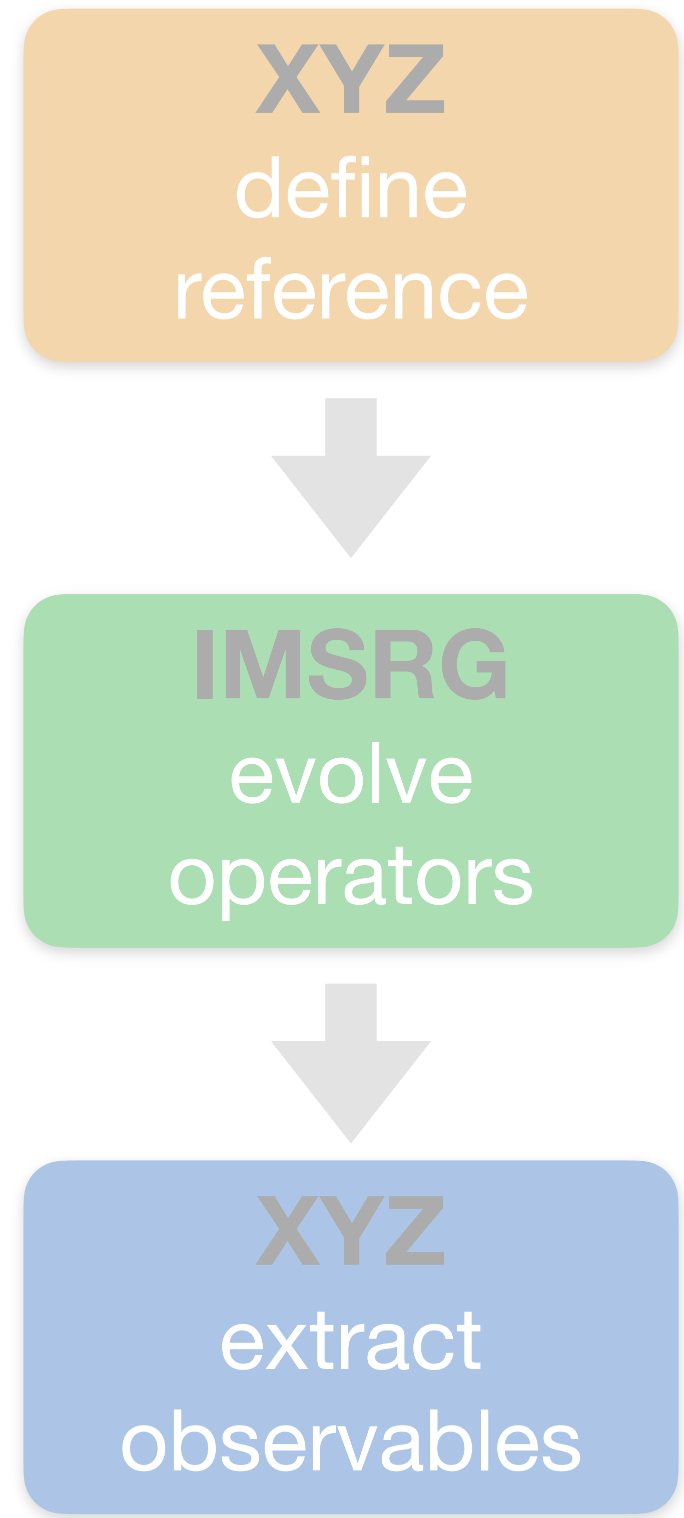
IMSRG Hybrid Approaches

- **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 ?**

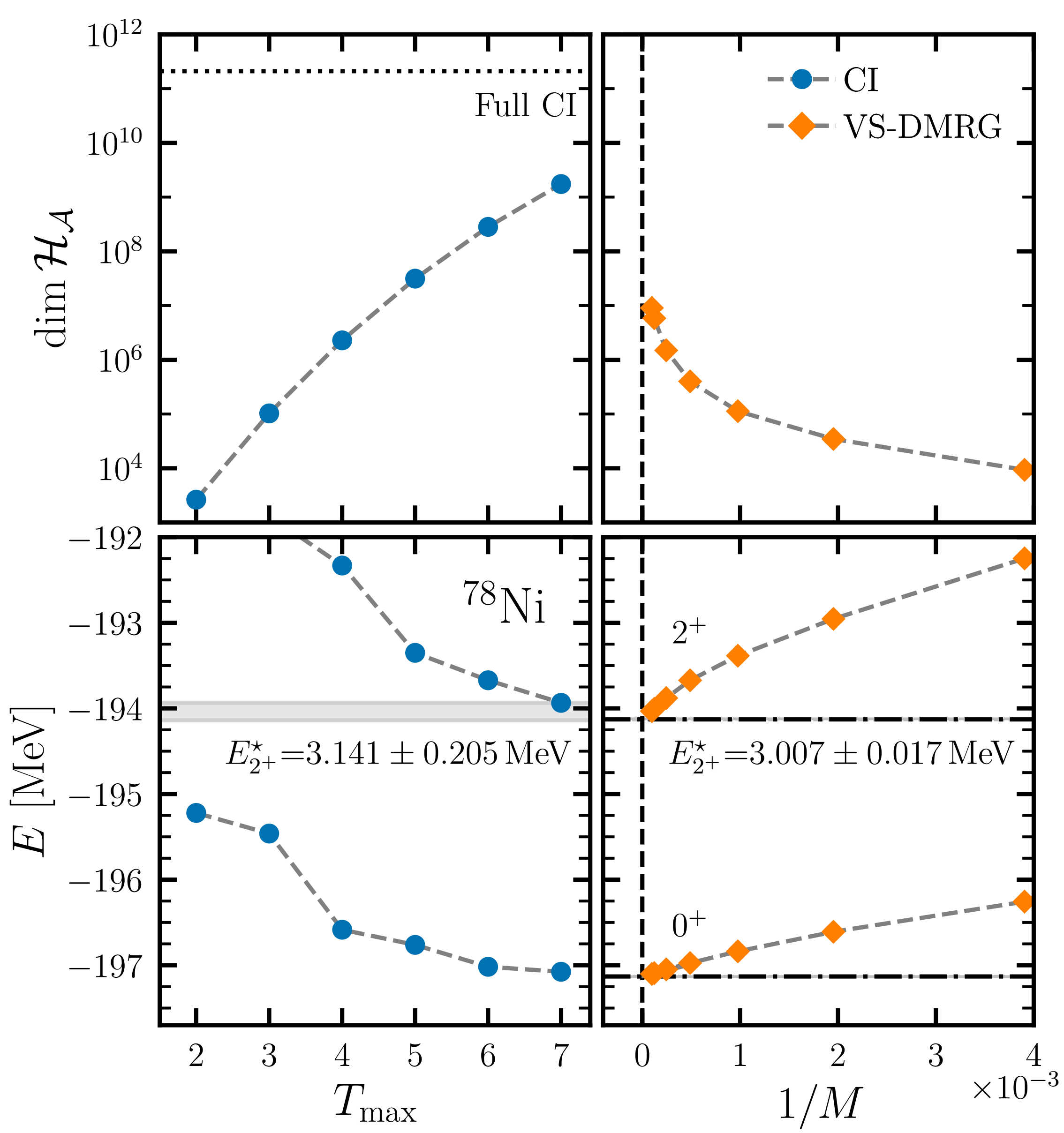


DMRG in Nuclear Physics

- **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**
  - **slow convergence** an issue beyond mass A=8-10

VS-IMSRG + DMRG

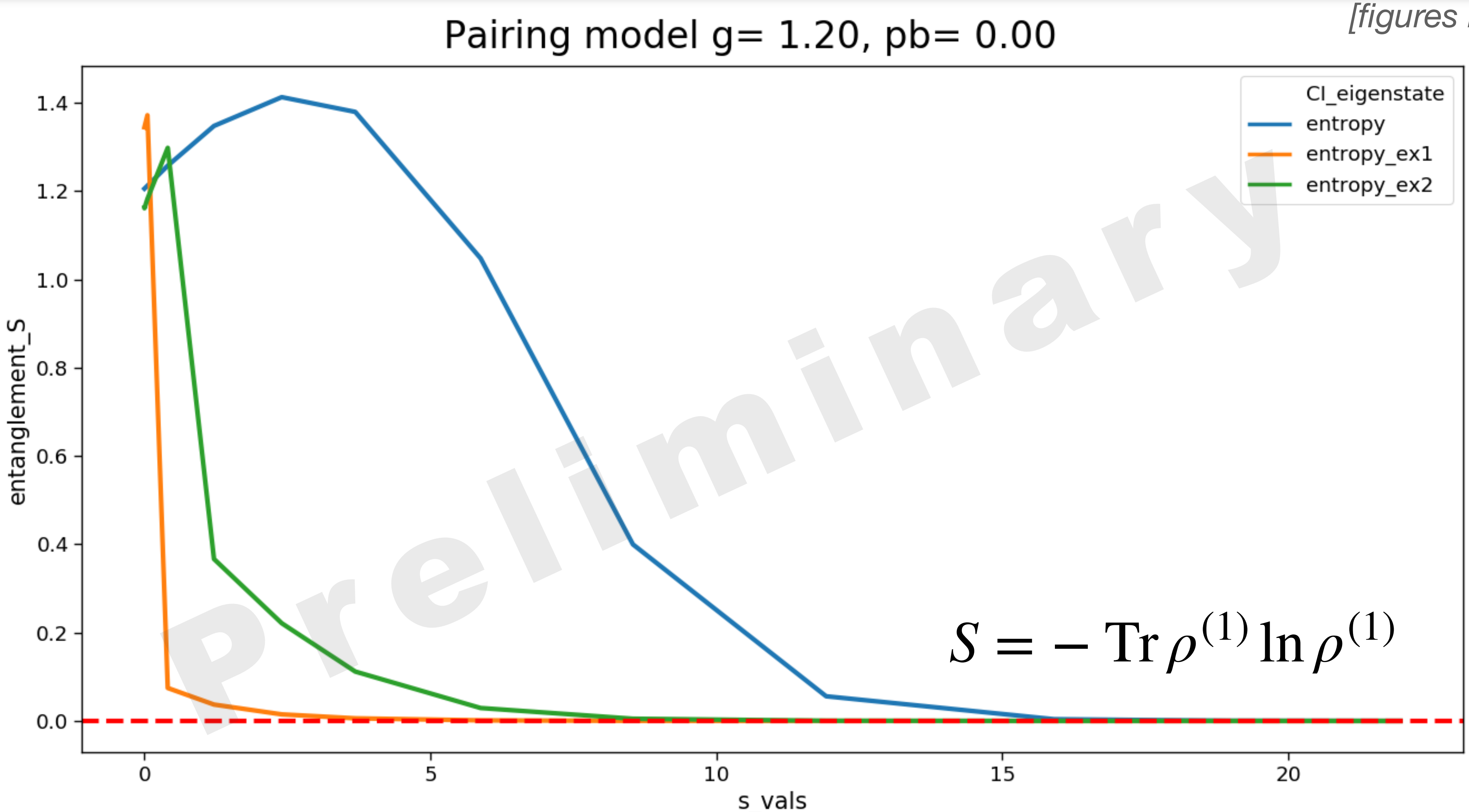
A. Tichai et al., arXiv:2207.01438



- no-core CI or DMRG with **unevolved** Hamiltonian **unfeasible** for medium-mass nuclei (Hilbert space/ bond dimension)
- **effective valence-space Hamiltonians** from IMSRG
- next: **no-core IM-DMRG** to better understand IMSRG as a disentangler
  [with K. Fossez (FSU), …]
    - naively: should enable smaller bond dimensions

IMSRG as a Disentangler

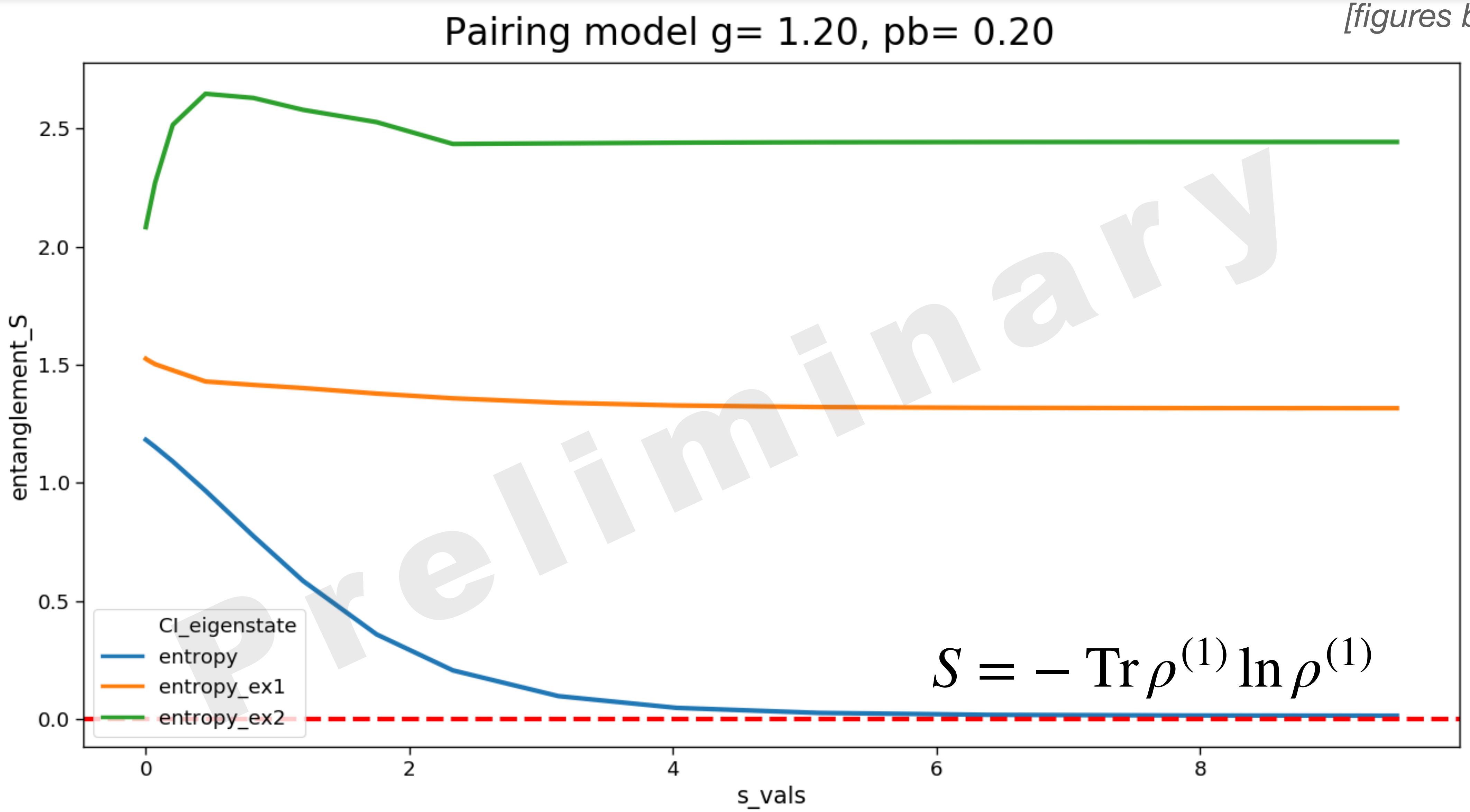
[figures by J. Davison]



- 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

- **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, Ann. Phys. 433, 168581]
- (IM)SRG transformations as **disentanglers** in tensor networks? Benefits compared to variational approaches?
- **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], **. . .**
- **And probably many more… I'm happy to discuss!**

Part III:

Model-Order Reduction

Control Problem Growth

- “obvious” operator basis for many-body problems:

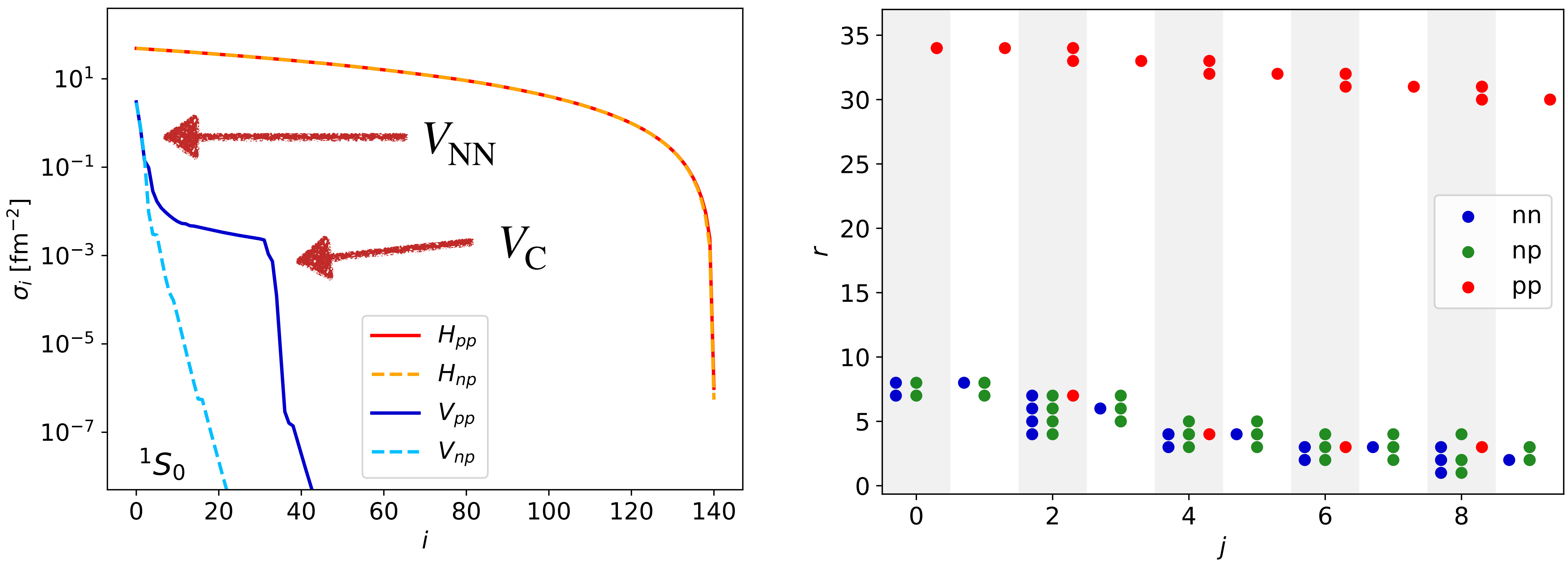
$$\{O_{pq}\,,\,O_{pqrs}\,,\,O_{pqrstu}\,,\,\ldots\} \equiv \{a^{\dagger}_{p}a_{q}\,,\,a^{\dagger}_{p}a^{\dagger}_{q}a_{s}a_{r}\,,\,a^{\dagger}_{p}a^{\dagger}_{q}a^{\dagger}_{r}a_{u}a_{t}a_{s}\,,\,\ldots\}$$

- 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**

Factorized Interactions

B. Zhu, R. Wirth, HH, PRC **104**, 044002 (2021)



- O(10) operators, O(100) particles, but O(10^8-10^{12}) flow equations, basis dimension… there must be **redundancy**
- **NN interaction:** 5-10 SVD components (**short range**)
- **Coulomb interaction:** less well-behaved, but ~25-30 components sufficient (**long range, no explicit scale**)

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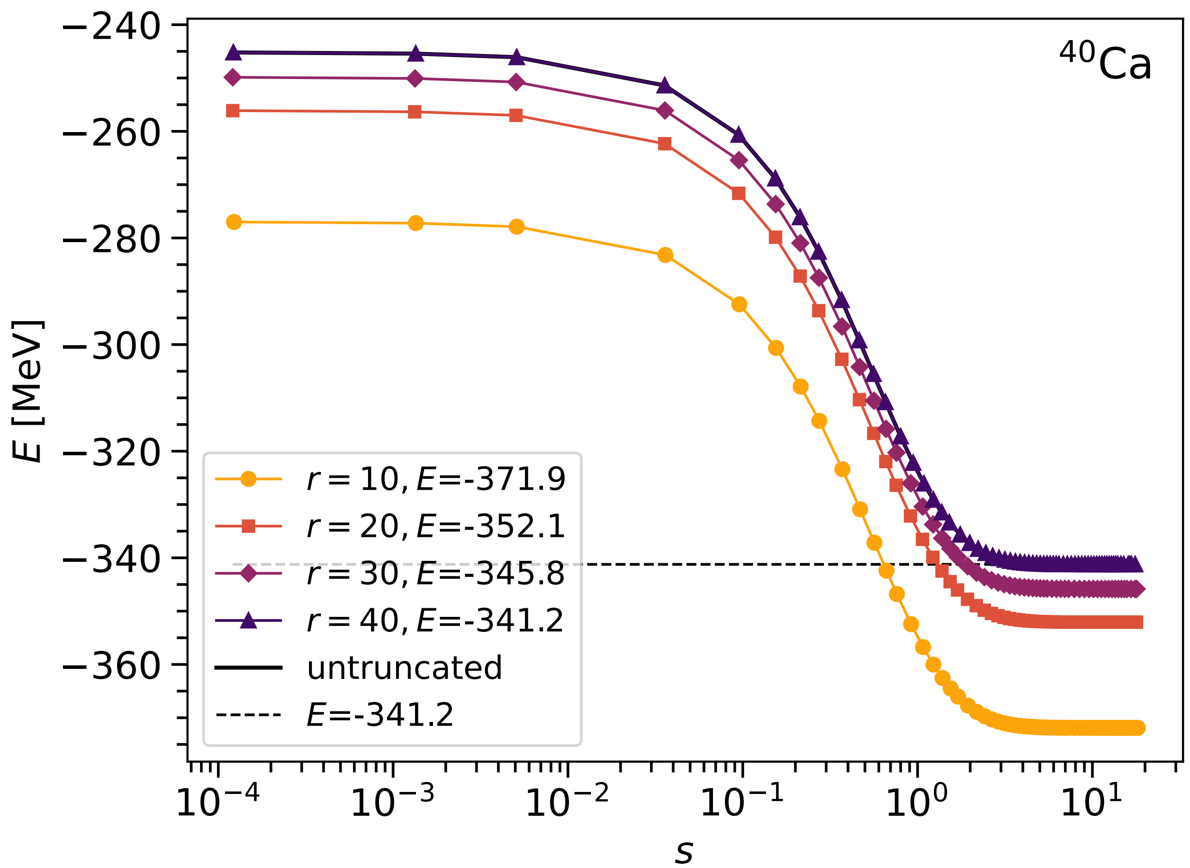
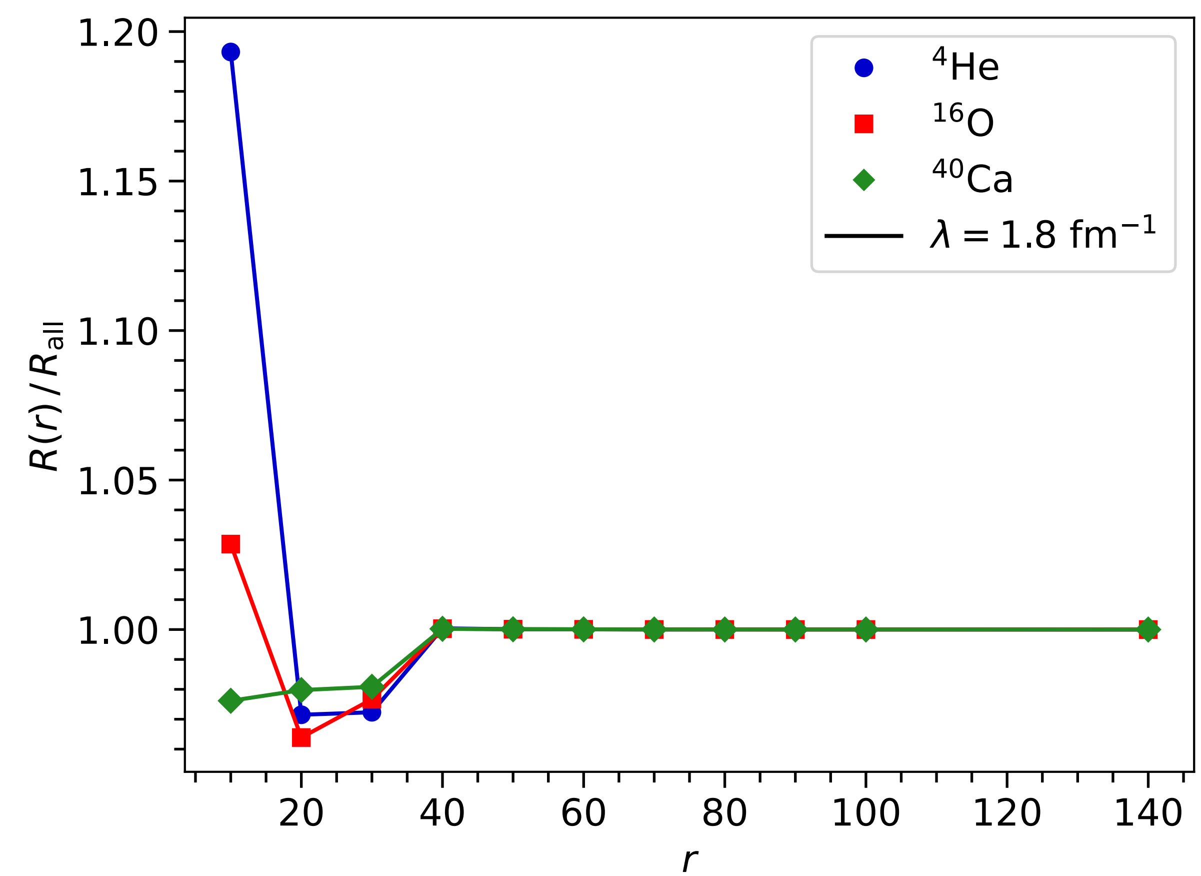
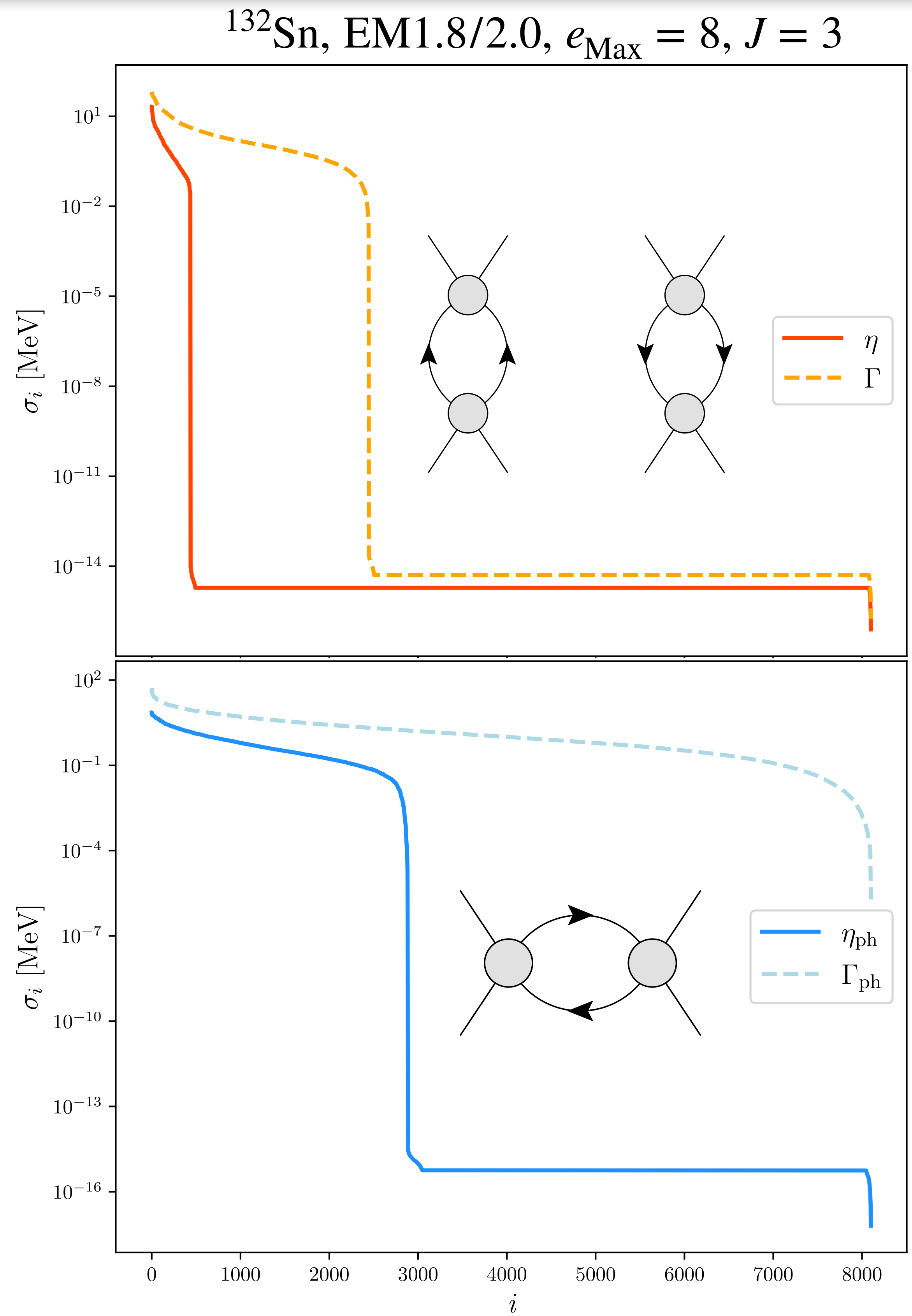




- implementing factorized SRG flow has **no adverse affect** on other observables / expectation values
- **But:** rank is **inflated** when we transform to single-particle coordinates (lab frame) - can **tensor representations** help?

Low-Rank Structures in Flow Equations

- η, H_{od} coefficient tensors can have inherent reduced rank based on definition
- SVD rank depends on **type of representation**: particle-particle/ladder vs. particle-hole/ring
- **problem:** need both representations in 2B flow equation - either ladder or ring terms prevent reduction
- **next:** tensor decompositions, but symmetries might cause issues (?)



Dynamic Mode Decomposition

S. L. Brunton et al., arXiv:2102.12086
Kutz et al., "Dynamic Mode Decomposition" (SIAM, 2016), https://www.dmdbook.com

- create snapshot matrices of discretized dynamic system

$$\mathbf{X} = \begin{pmatrix} \mathbf{h}_0 & \cdots \mathbf{h}_{n-1} \end{pmatrix}, \qquad \mathbf{X}' = \begin{pmatrix} \mathbf{h}_1 & \cdots \mathbf{h}_n \end{pmatrix}$$

- express evolution with the help of the **Koopman operator** $\mathbf{K}$

$$\mathbf{h}_{i+1} = \mathbf{K}\mathbf{h}_i \qquad \rightarrow \qquad \mathbf{X}' = \mathbf{K}\mathbf{X}$$

- take the Moore-Penrose pseudo-inverse $\mathbf{X}^+$ to compute an (approximate) matrix representation of $\mathbf{K}$:

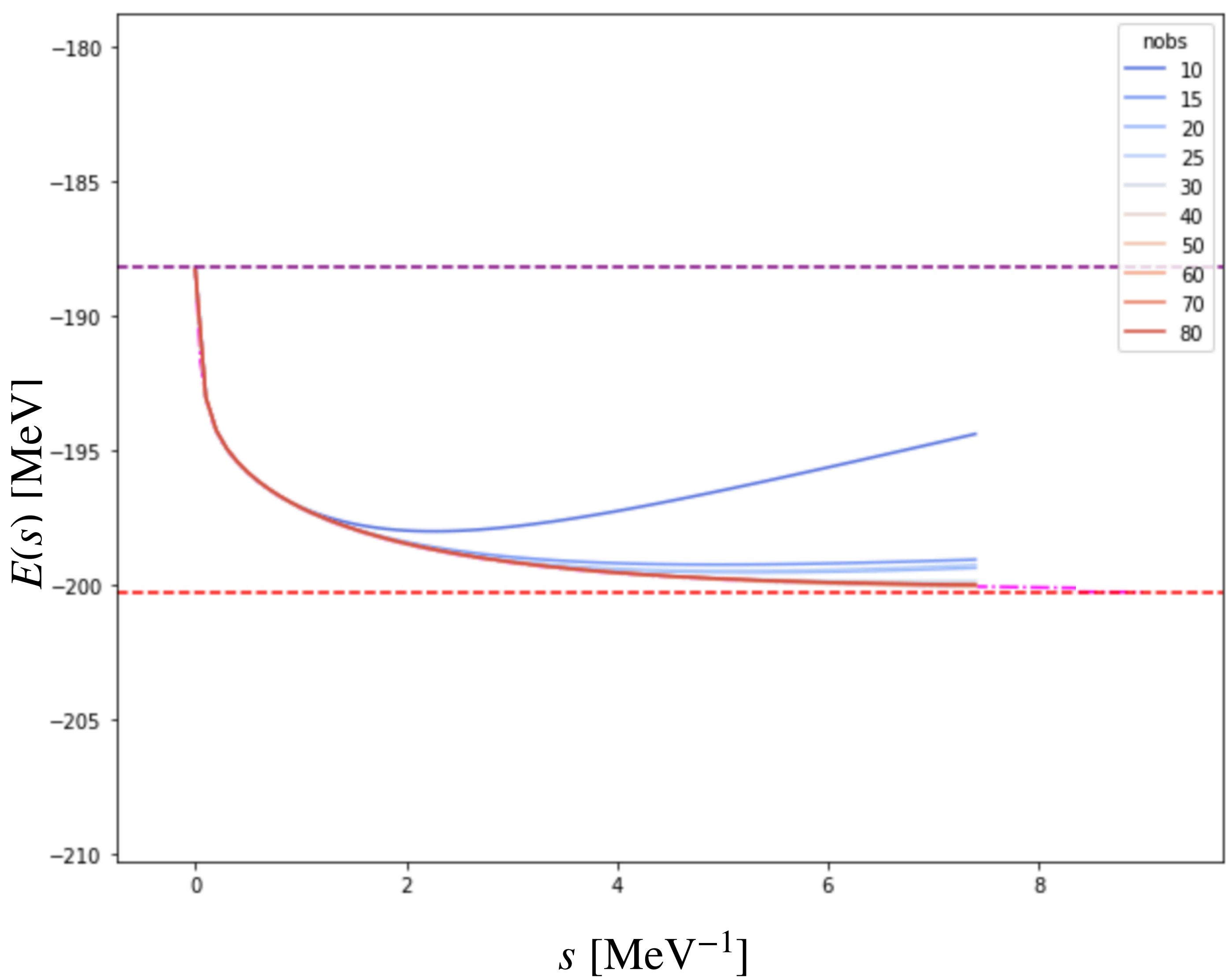
$$\mathbf{K} = \mathbf{X}'\mathbf{X}^+$$

- solve **eigenvalue problem** for Koopman operator to construct **reduced basis** of **dynamic modes**

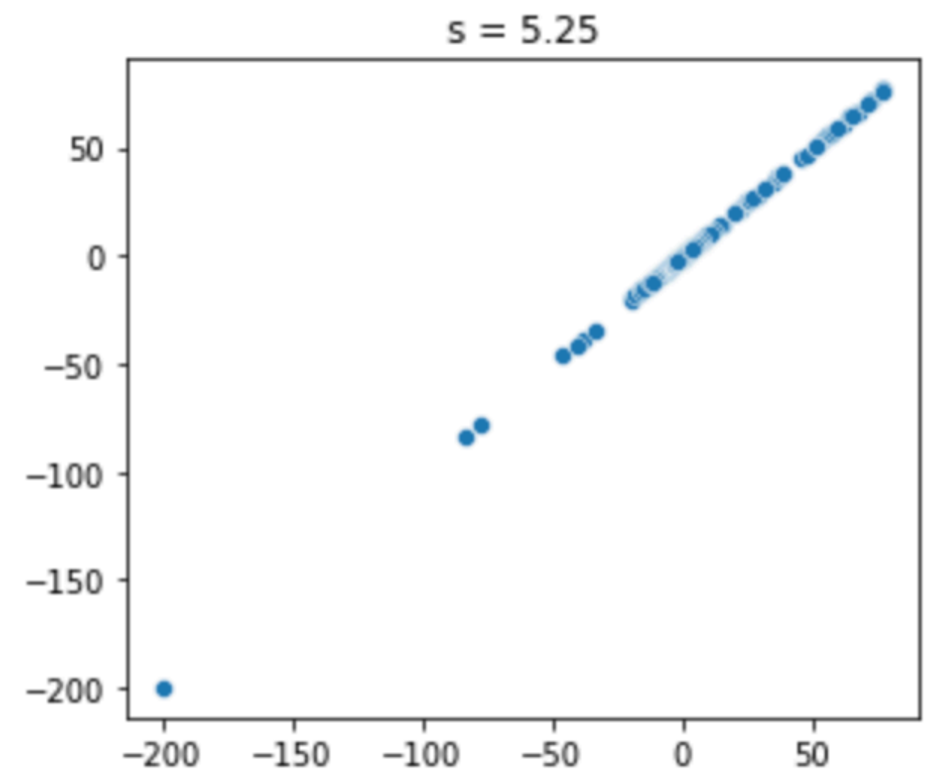
Application: Emulating IMSRG Flows

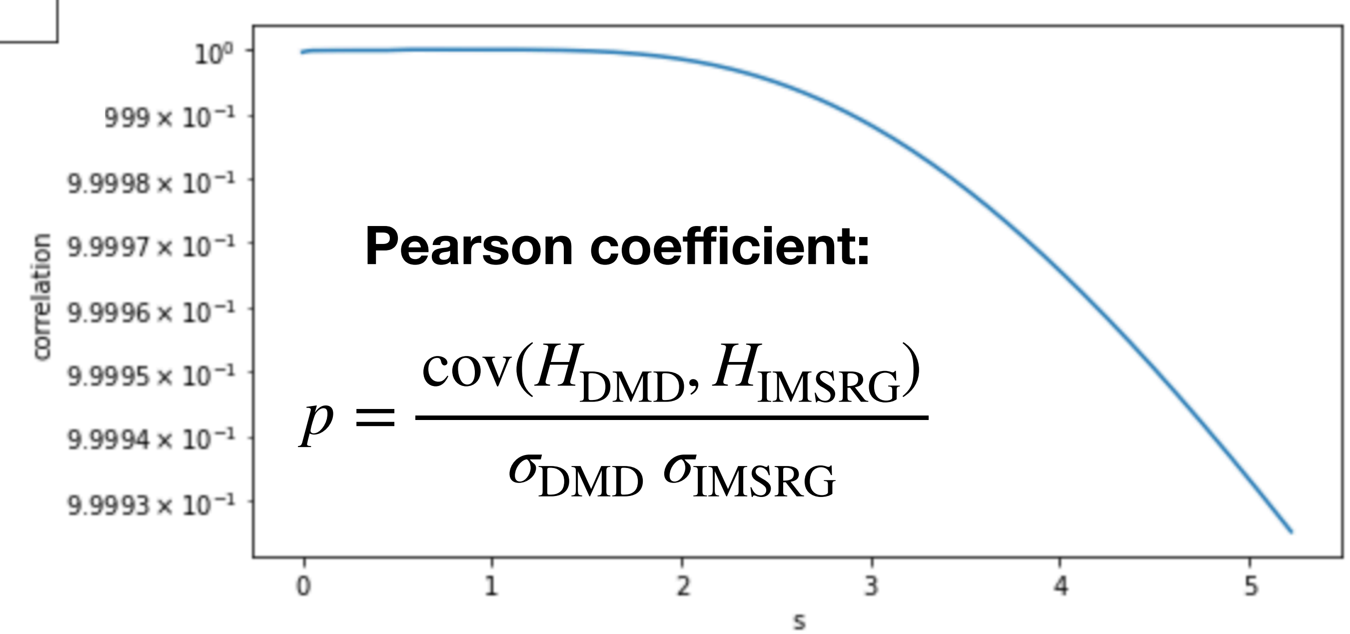
J. Davison, J. Crawford, *S. Bogner, HH, in preparation*

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



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





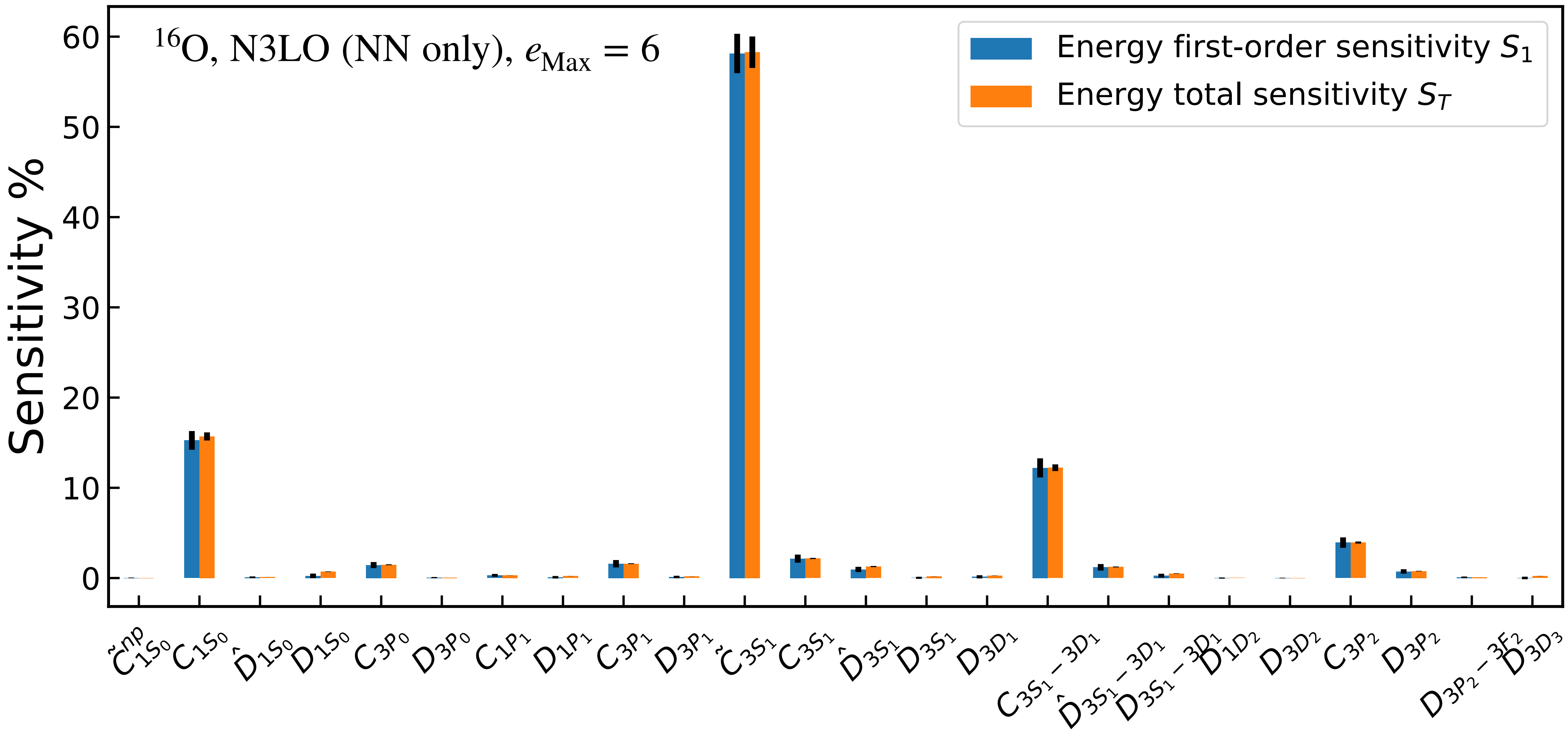
Pearson coefficient:

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

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

Application: Sensitivity Analysis & UQ

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



- reduction to **dominant DMD modes** allows sensitivity studies & uncertainty quantification (**while still generating full H(s)**)
- showing 200k+ Monte Carlo samples in LEC parameter space: **4-5 order of magnitude computing time reduction**

Epilogue

Summary

- Nuclear many-body theory plays a crucial role in answering a variety of fundamental questions
  - need **predictive *ab initio* theory** with systematic uncertainties & convergence to exact result
  - expand capabilities: spectra, radii, transitions, **clustering,** bridge to **dynamics /reactions**…
  - **scalable** methods: from day-to-day data analysis to leadership calculations
- **(How) Can we unlock more efficiency?**
  - apply quantum information theory (**entanglement**)
  - DMRG, tensor networks, … (**improve scaling**)

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NUCLEI Nuclear Computational Low-Energy Initiative

Postdoctoral Position @ FRIB

- **focus:** extensions of IMSRG Framework and applications (incl. fundamental symmetries)
- broad portfolio of nuclear theory research @ FRIB, great opportunities for collaboration
- 2 years (+ possible renewal)
- Contact me: hergert@frib.msu.edu …
- … or apply directly at https://careers.msu.edu/en-us/job/513047/research-associatefixed-term
- **review of applications has started, but will continue until position is filled**
- **Please encourage suitable candidates to apply!**

Supplements

Sources of Uncertainty

Chiral EFT

- selection of degrees of freedom
- regulators
- truncation
- low-energy constant (**LEC**) uncertainties

RG
(similarity trafos)

- selection of operator basis / model space
- truncation

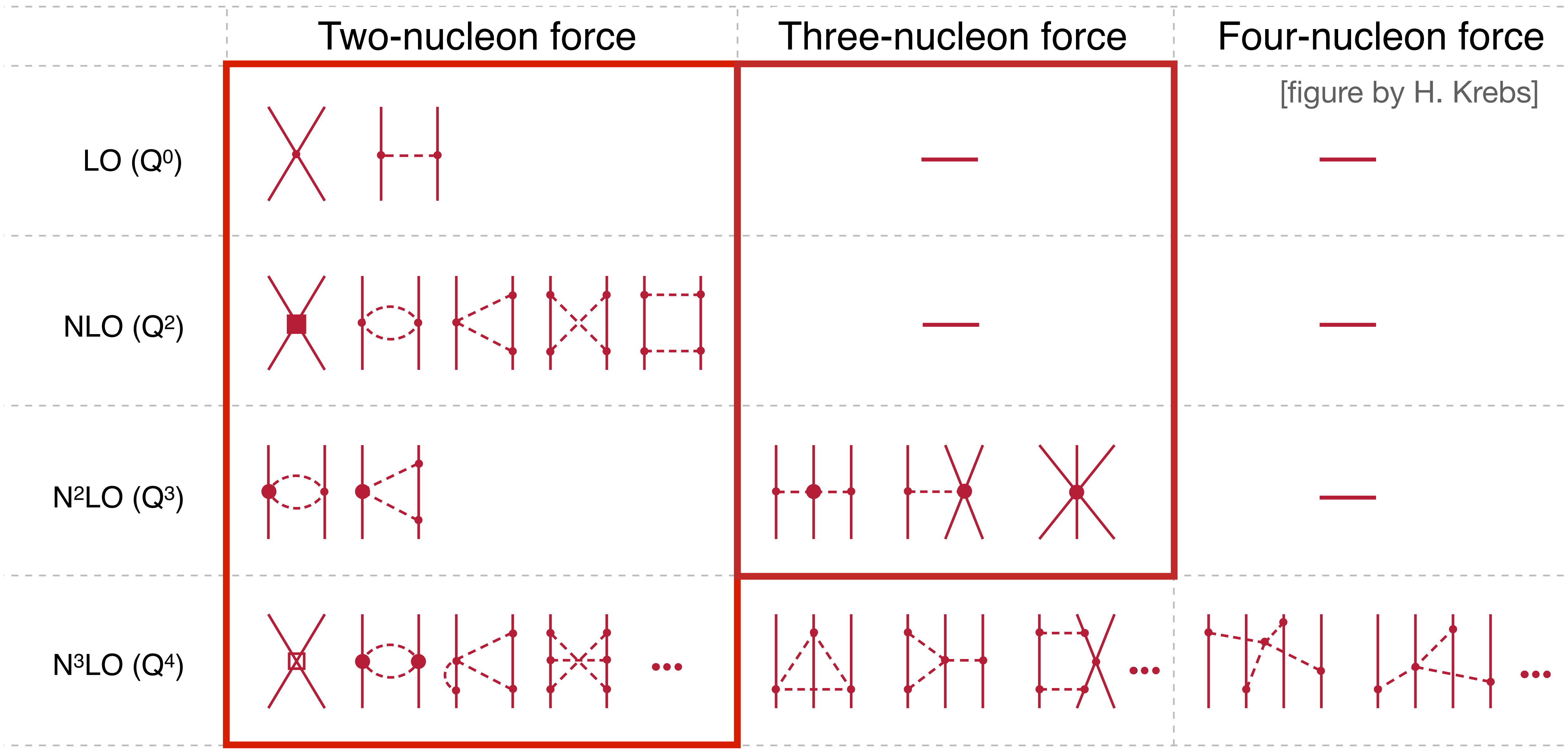
many-body method

- symmetry restrictions
- model-space & many-body truncation(s)
- continuum

Nuclear Interactions from Chiral Effective Field Theory

Recent(-ish) Reviews:
E. Epelbaum, H. Krebs and P. Reinert, Front. Phys. **8**, 98 (2002)
M. Piarulli and I. Tews, Front. Phys. **7**, 245 (2020)
R. Machleidt and F. Sammarruca, Phys. Scripta **91**, 083007 (2016)

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!**)

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 $H(s) = U(s)HU^{\dagger}(s)$:

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

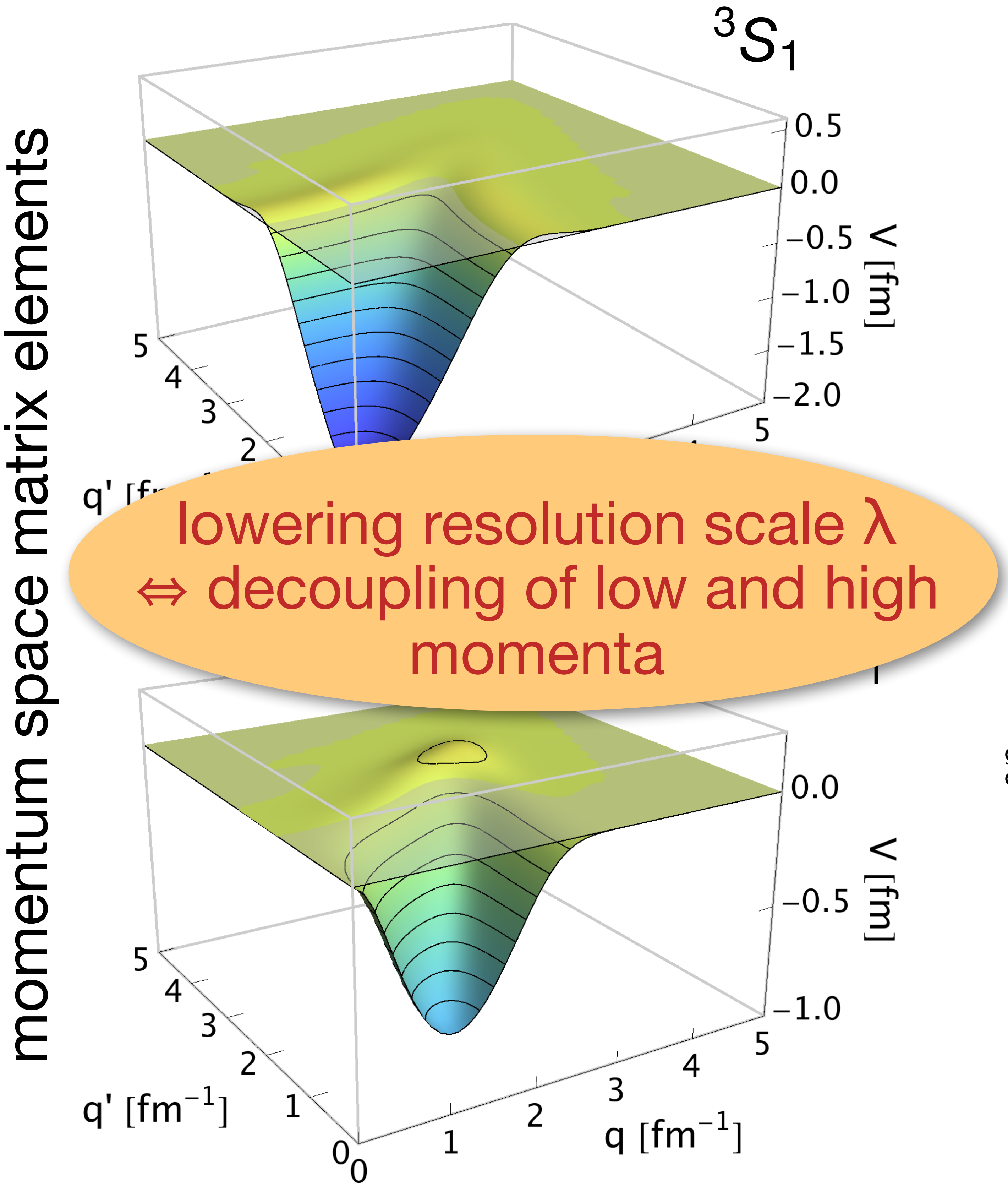
- choose $\eta(s)$ to achieve desired behavior, e.g.,

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

to suppress (suitably defined) off-diagonal Hamiltonian

- consistent evolution for all observables of interest

SRG in Two-Body Space

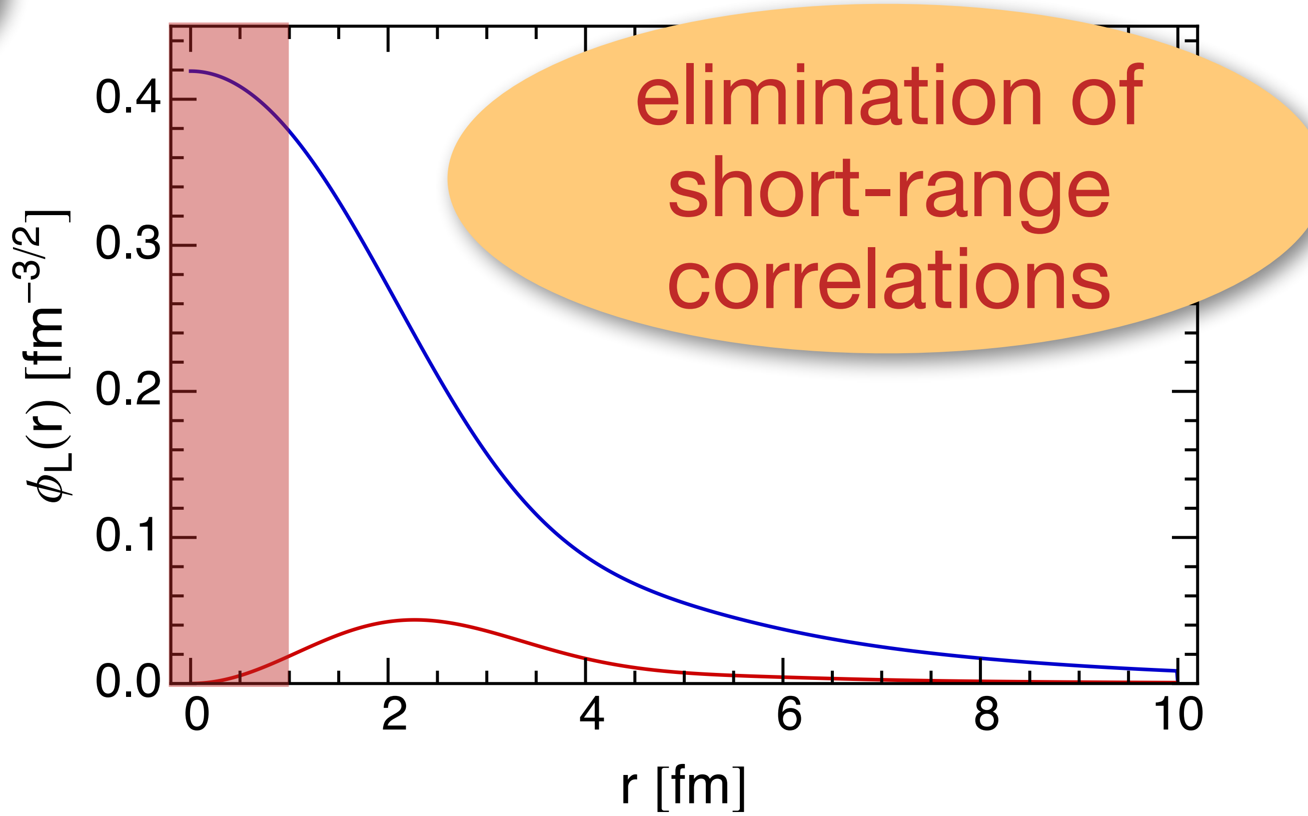


$\lambda = 1.8\ \text{fm}^{-1}$

$$\eta(\lambda) = 2\mu\left[T_{\rm rel}, H(\lambda)\right]$$

$$\lambda = s^{-1/4}$$

deuteron wave function



Induced Interactions

- SRG is a unitary transformation in A-body space
- up to A-body interactions are induced during the flow:

$$\frac{dH}{d\lambda} = [[\sum a^\dagger a, \sum \underbrace{a^\dagger a^\dagger a a}_{\text{2-body}}], \sum \underbrace{a^\dagger a^\dagger a a}_{\text{2-body}}] = \ldots + \sum \underbrace{a^\dagger a^\dagger a^\dagger a a a}_{\text{3-body}} + \ldots$$

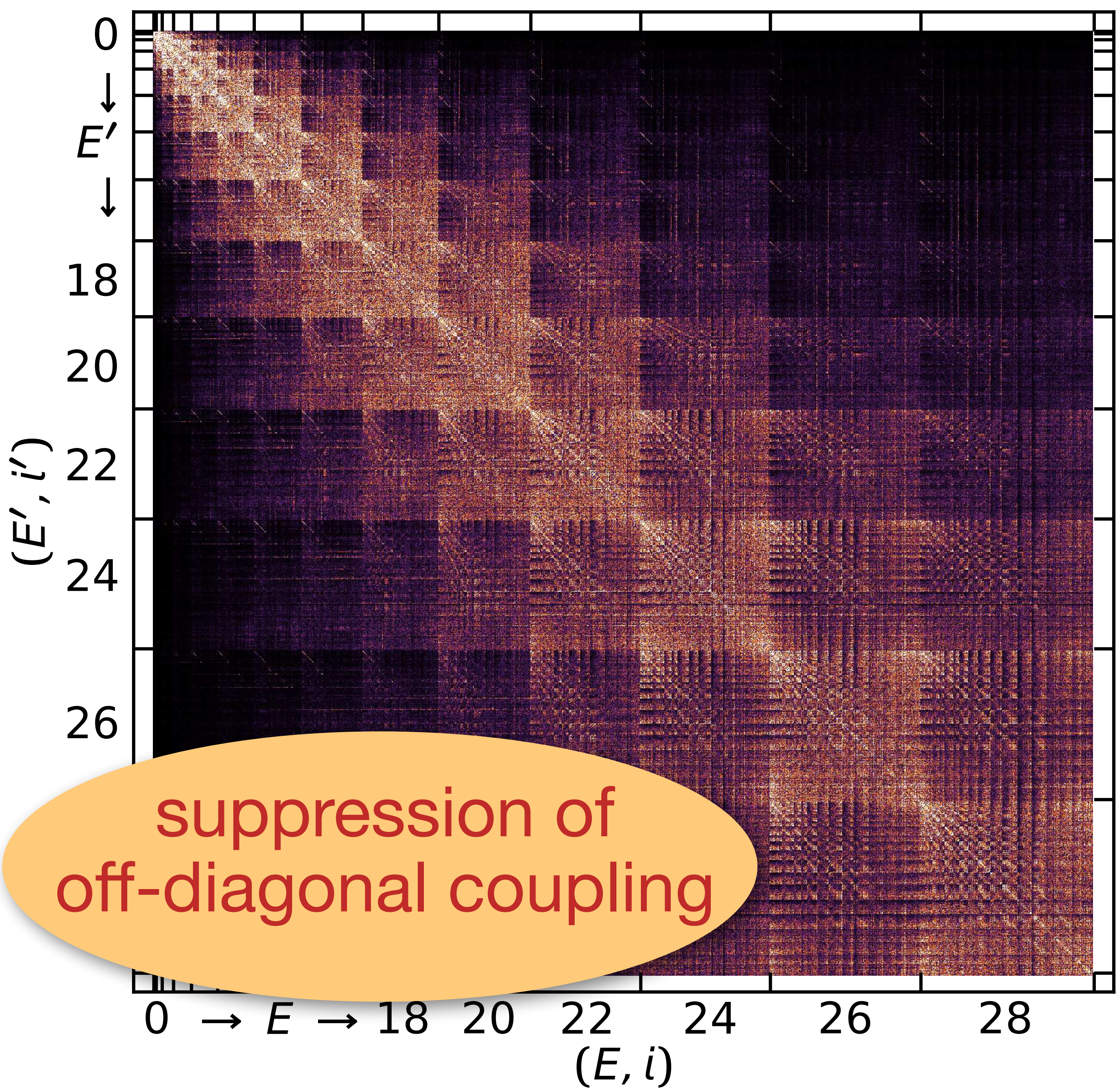
- state-of-the-art: evolve in three-body space, truncate induced four- and higher many-body forces
(Jurgenson, Furnstahl, Navratil, PRL 103, 082501; Hebeler, PRC 85, 021002; Wendt, PRC 87, 061001)
- λ-dependence of eigenvalues is a diagnostic for size of omitted induced interactions

SRG in Three-Body Space

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

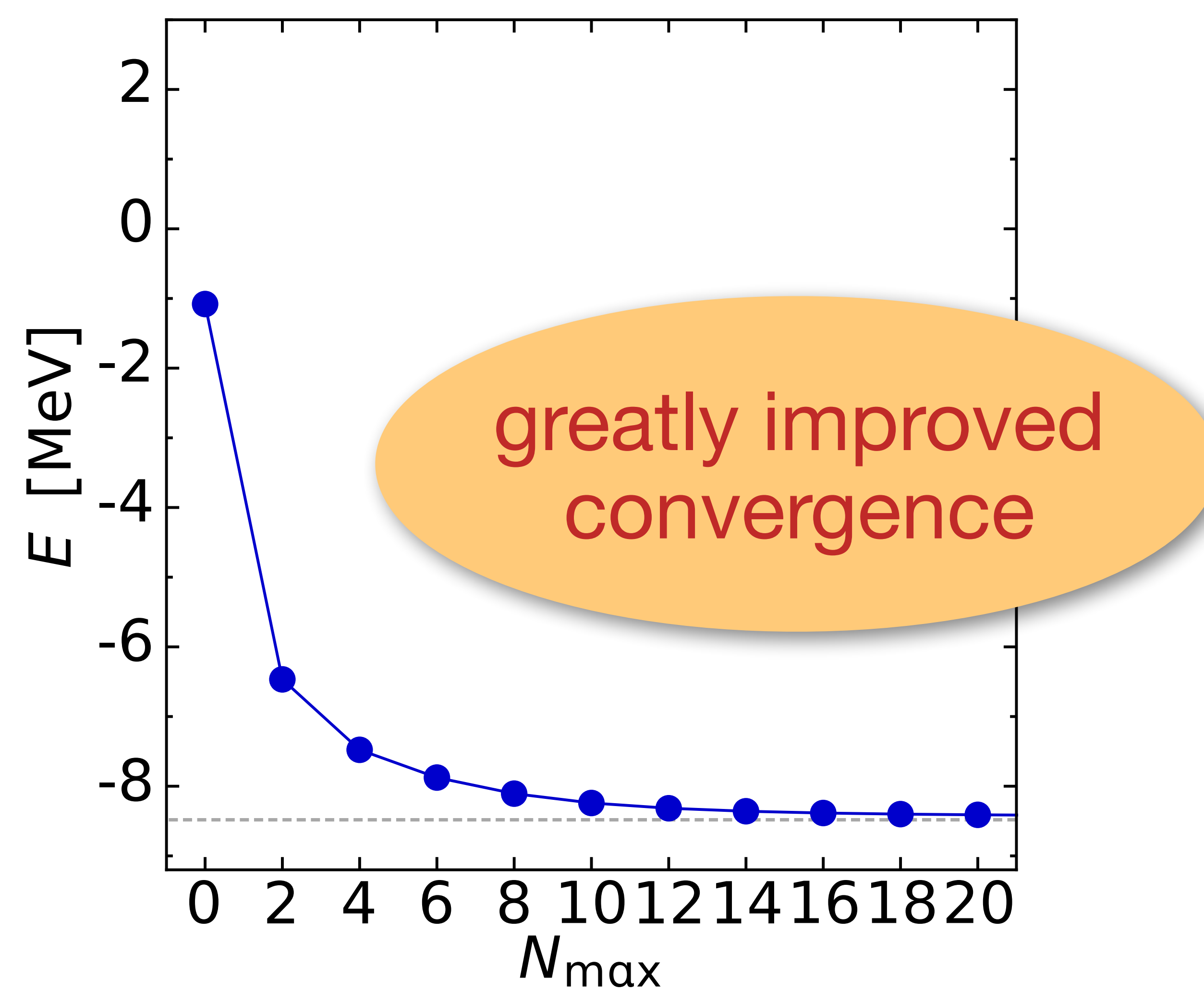
3B Jacobi-HO Matrix Elements

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



λ = 1.33 fm^{-1}

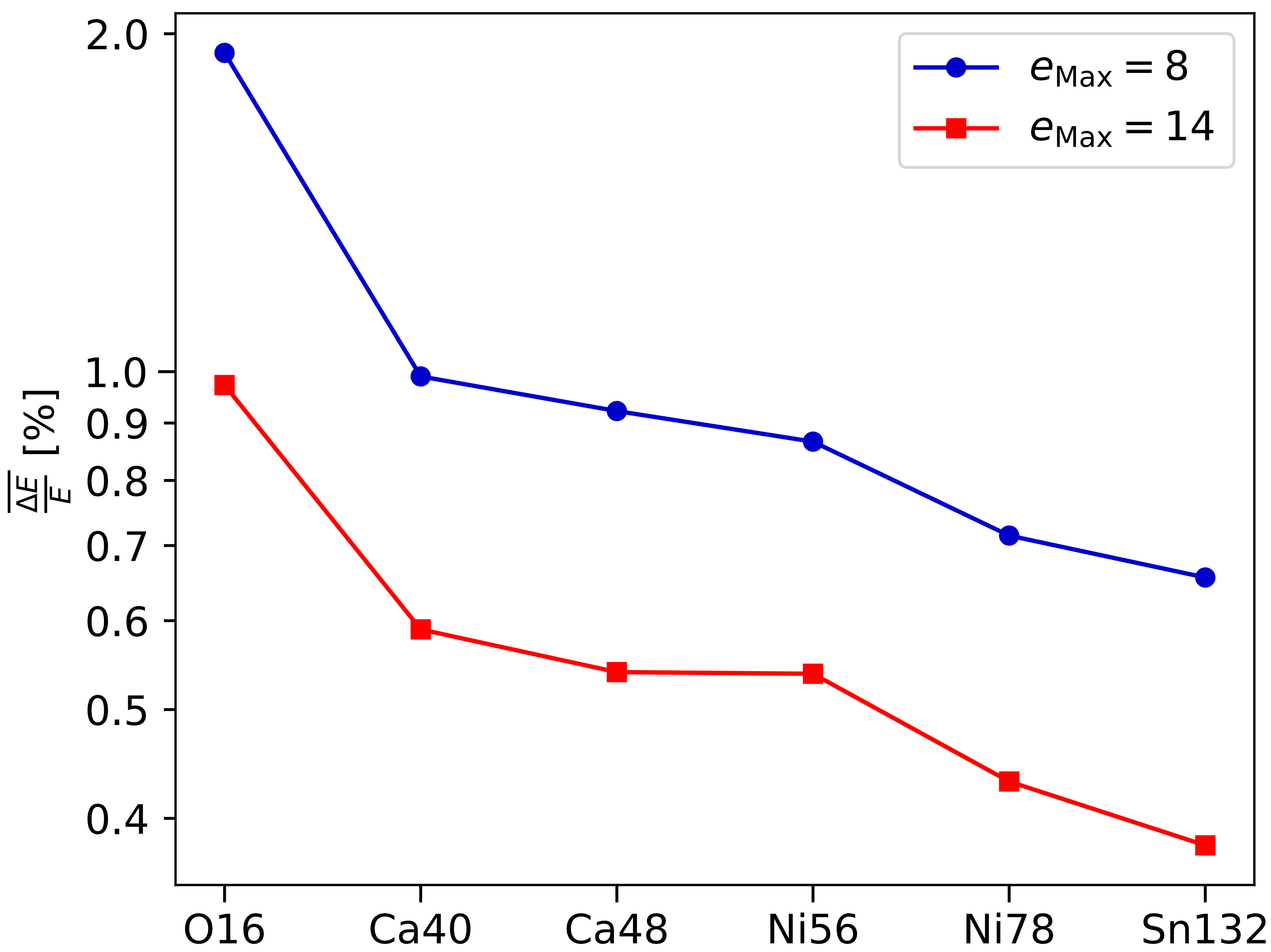
^{3}H ground-state (NCSM)



Compression with Random Projections

A. Zare, R. Wirth, C. Haselby, HH, M. Iwen, arXiv:2211.01315

EM1.8/2.0 NN+3N, MBPT(2); $c_{\text{tot}} < 10^{-3}$



- tensorial (= modewise) **Johnson-Lindenstrauss embeddings**
- **purely based on features of (sparse) big data sets** - integrate with physics-based ideas?
- suitable for **streaming** transforms: compress on the fly while reading from disk

Koopman Operator Theory

- **nonlinear** dynamical system:
  - $\mathbf{x} \in X \subseteq \mathbb{R}^n, \quad \mathbf{F}^t : X \to X, \qquad \mathbf{x}(t) = \mathbf{F}^t(\mathbf{x}(0))$
  - flow map $\mathbf{F}^t$ propagates $\mathbf{x}(0)$ forward in time
- define a set $\mathcal{G}(X)$ of **observables or measurement functions** $g : X \to \mathbb{C}$
- define the semi-group of **Koopman operators** by
  - $K^t : \mathcal{G}(X) \to \mathcal{G}(X), \qquad K^t g(\mathbf{x}) = g(F^t(\mathbf{x}))$
  - K^t is **linear** if $\mathcal{G}(X)$ is a **linear** function space, e.g., $L^2(\mathbb{R})$
- Describe **nonlinear dynamics** through a generally **infinite-dimensional linear operator** that acts on **measurements**!

Koopman Operators & IMSRG

- IMSRG flow is a **nonlinear** “dynamical” system **Review:** S. L. Brunton et al., arXiv:2102.12086
- Hamiltonian in (NO2B) operator algebra:

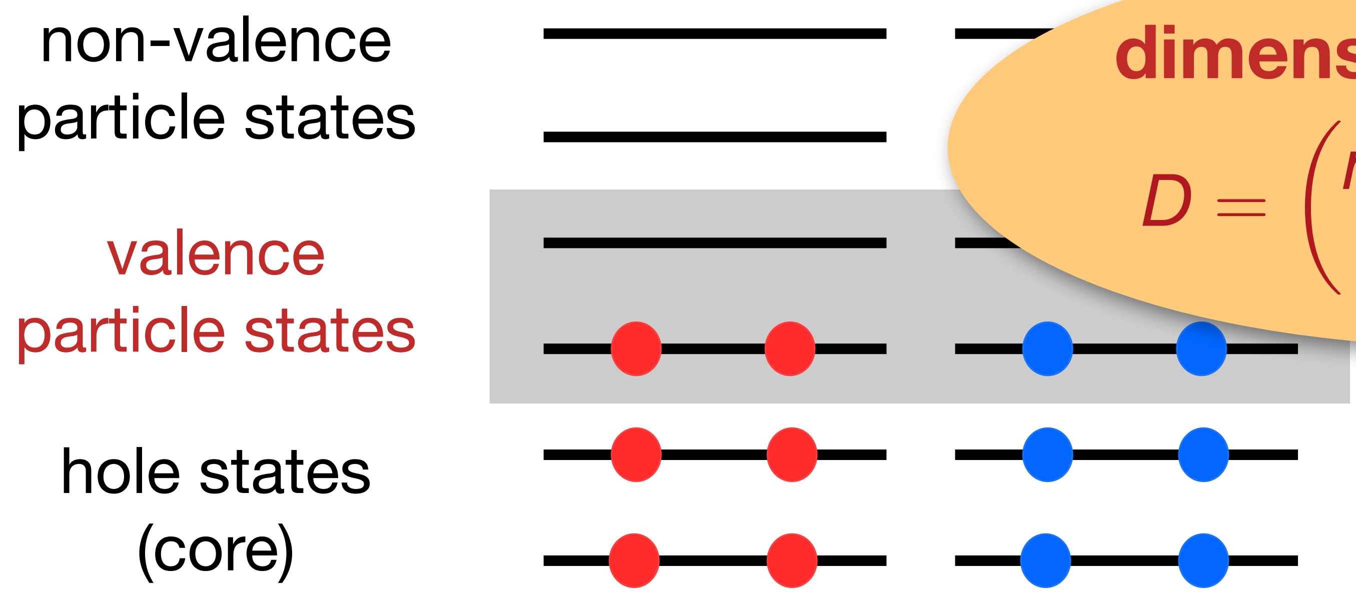
$$H \equiv E_0 + \sum_{pq} f_{pq} : a_p^\dagger a_q : + \frac{1}{4} \sum_{pqrs} \Gamma_{pqrs} : a_p^\dagger a_q^\dagger a_s a_r :$$

- define $\mathbf{h} \equiv \begin{pmatrix} E_0 & \cdots & f_{pq} & \cdots & \Gamma_{pqrs} & \cdots \end{pmatrix}^T$ …
- … and write the evolution in **Koopman operator form:**

$$K^{\bar{s}}\mathbf{h} = \begin{pmatrix} (U_{\bar{s}} H U_{\bar{s}}^\dagger)_0 & \cdots & (U_{\bar{s}} H U_{\bar{s}}^\dagger)_{pq} & \cdots & (U_{\bar{s}} H U_{\bar{s}}^\dagger)_{pqrs} & \cdots \end{pmatrix}^T$$

- **What have we gained compared to other approaches? We can construct Koopman operators from “observations”!**

Core and Valence Spaces



dimension reduced to

$$D = \binom{n_v^{(p)}}{Z_v} \times \binom{n_v^{(n)}}{N_v}$$

- introduce an **inert core:** restrict states to the form

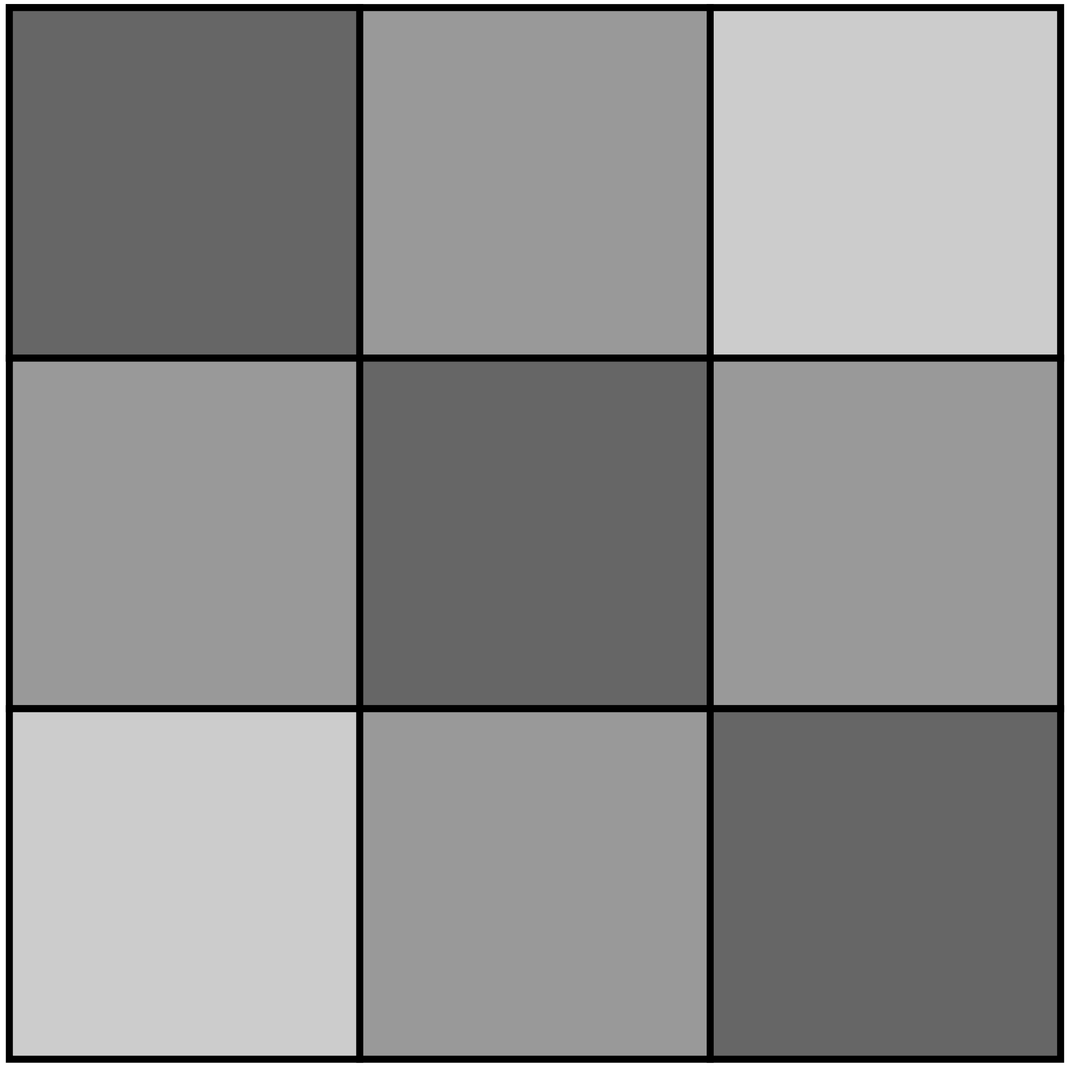
$$\left|\Psi_i\right\rangle = \left|\overline{\Psi}_i\right\rangle \otimes \left|\text{core}\right\rangle$$

- basis states:

$$\left|\Phi_{v_1,\dots,v_{A_v}}\right\rangle = a^\dagger_{v_1}\dots a^\dagger_{v_{A_v}}\left|\text{core}\right\rangle$$

- wave functions for $A_v < A$ ($A_v \ll A$) particles (**core implicit**)

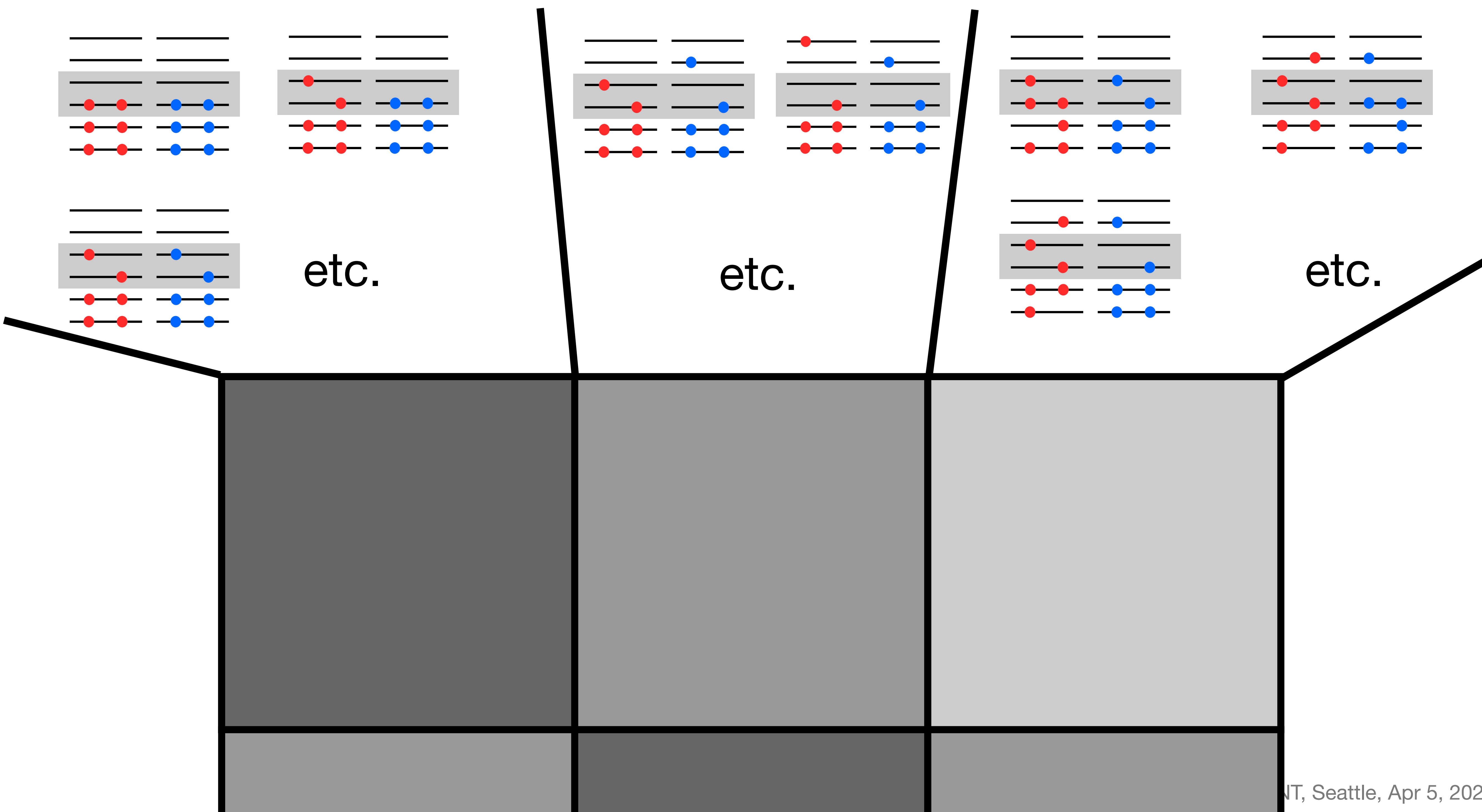
Effective Hamiltonian



Effective Hamiltonian

P **space**
(included configurations)

Q **space**
(excluded configurations)



Effective Hamiltonian