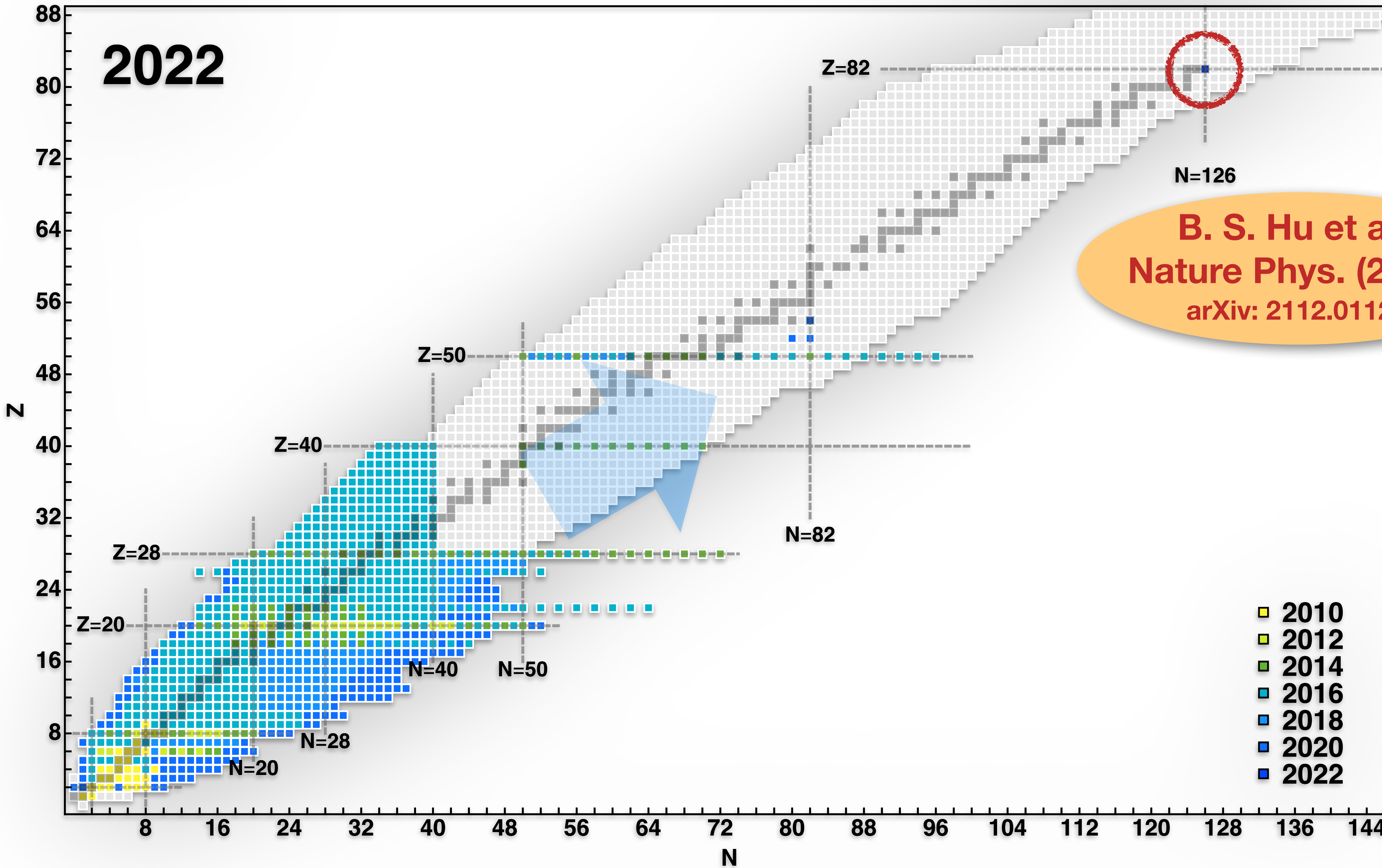
Progress in *Ab Initio* Calculations

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



B. S. Hu et al., Nature Phys. (2022), arXiv: 2112.01125

(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)

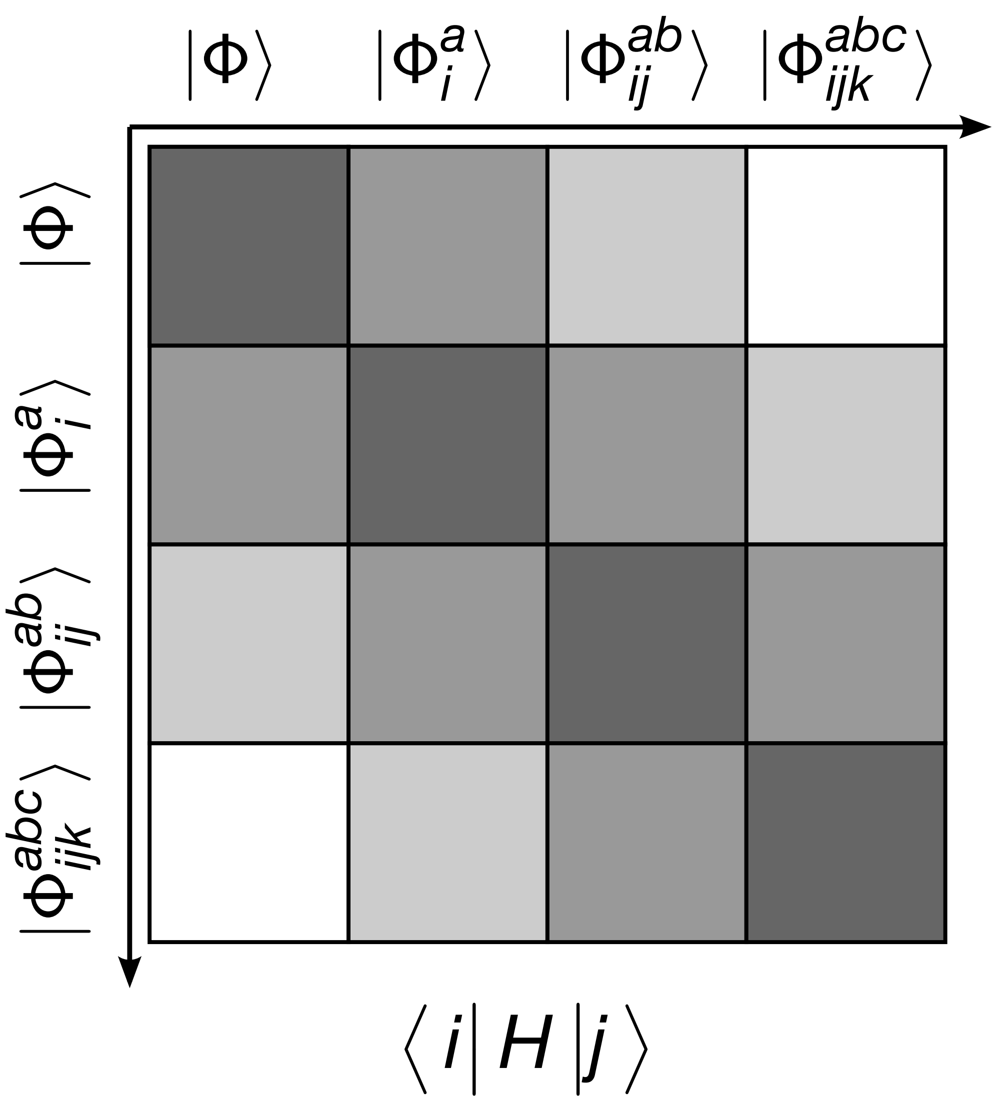
HH, S. K. Bogner, T. Morris, S. Binder, A. Calci, J. Langhammer, R. Roth, Phys. Rev. C **90**, 041302 (2014)

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

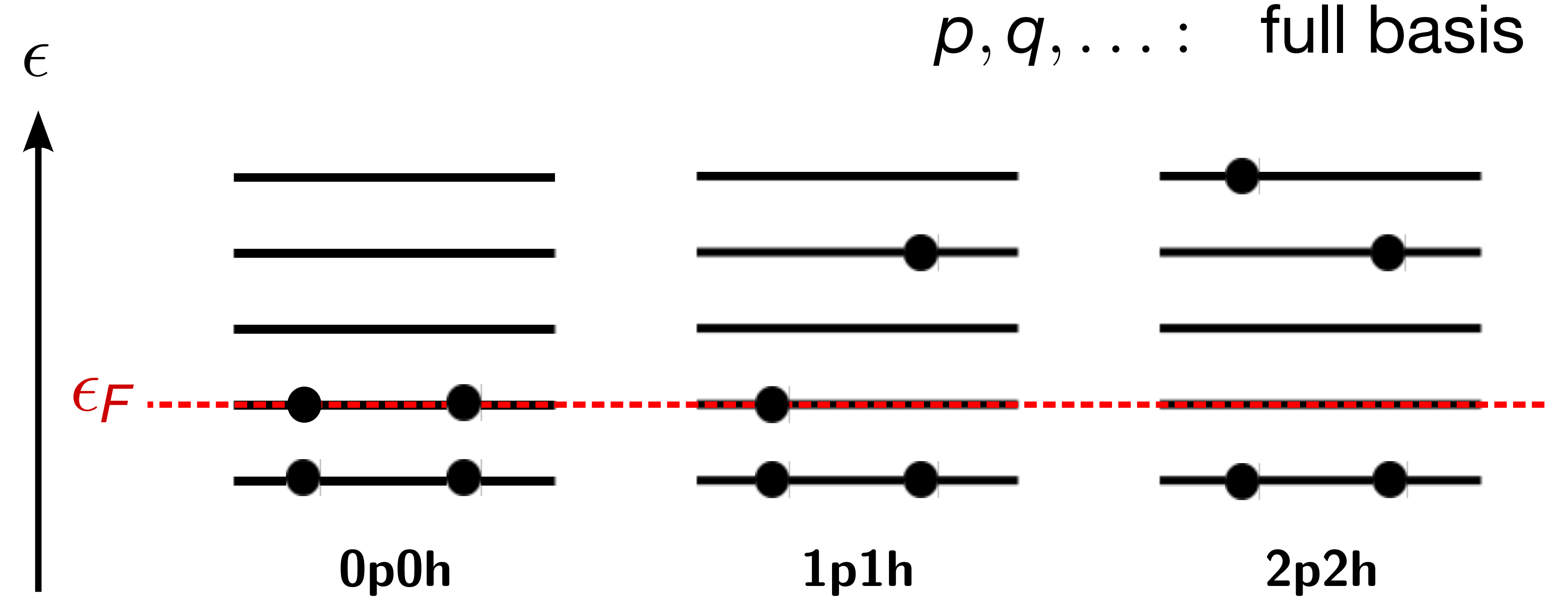
Transforming the Hamiltonian



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

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

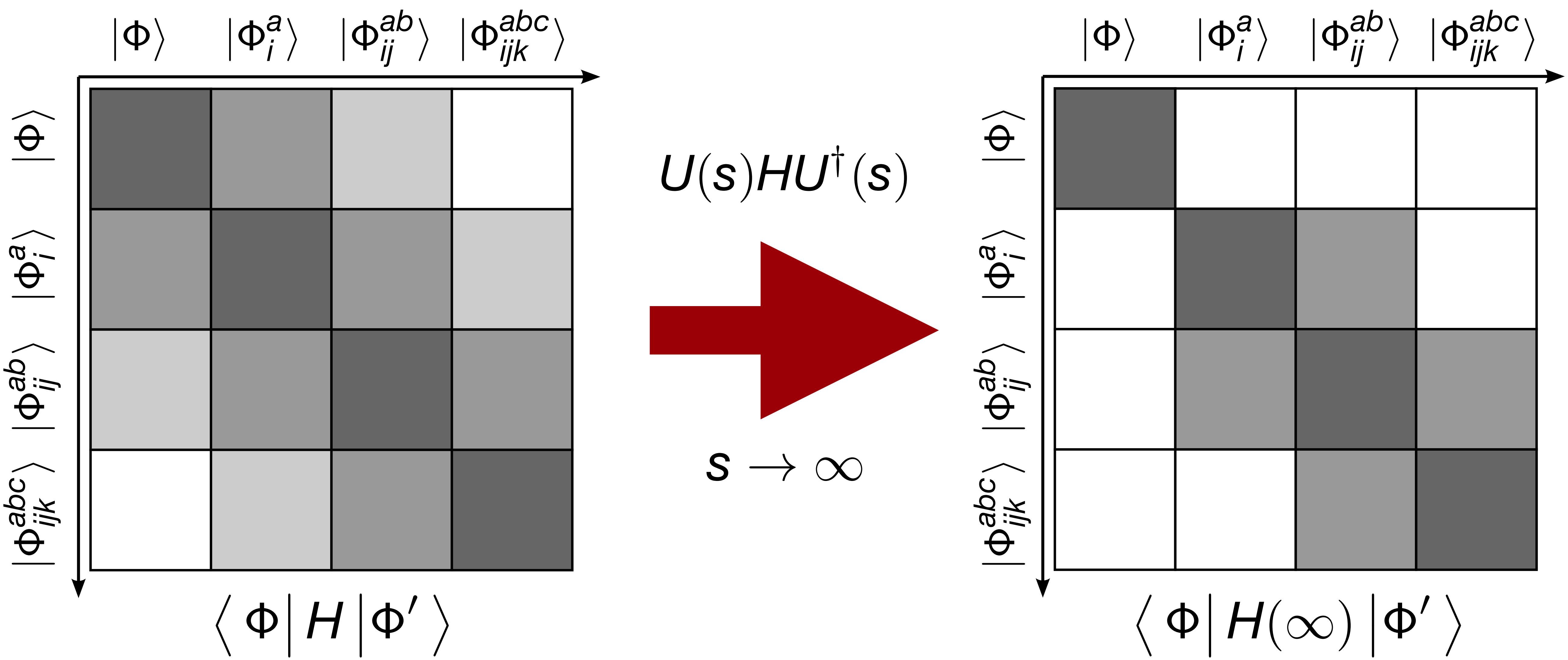
$p, q, \ldots :$ full basis



- reference state: **single Slater determinant**

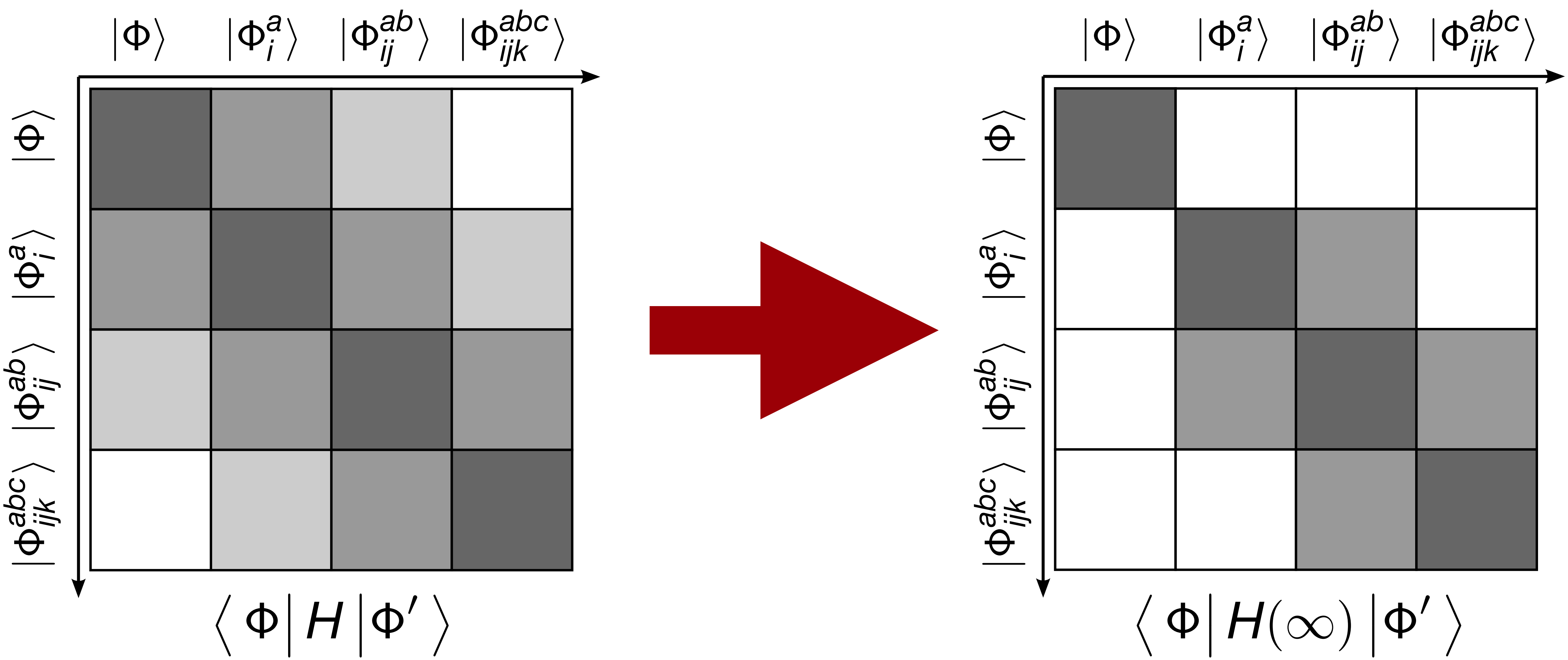
excitations relative to reference state: **normal-ordering**

Decoupling in A-Body Space



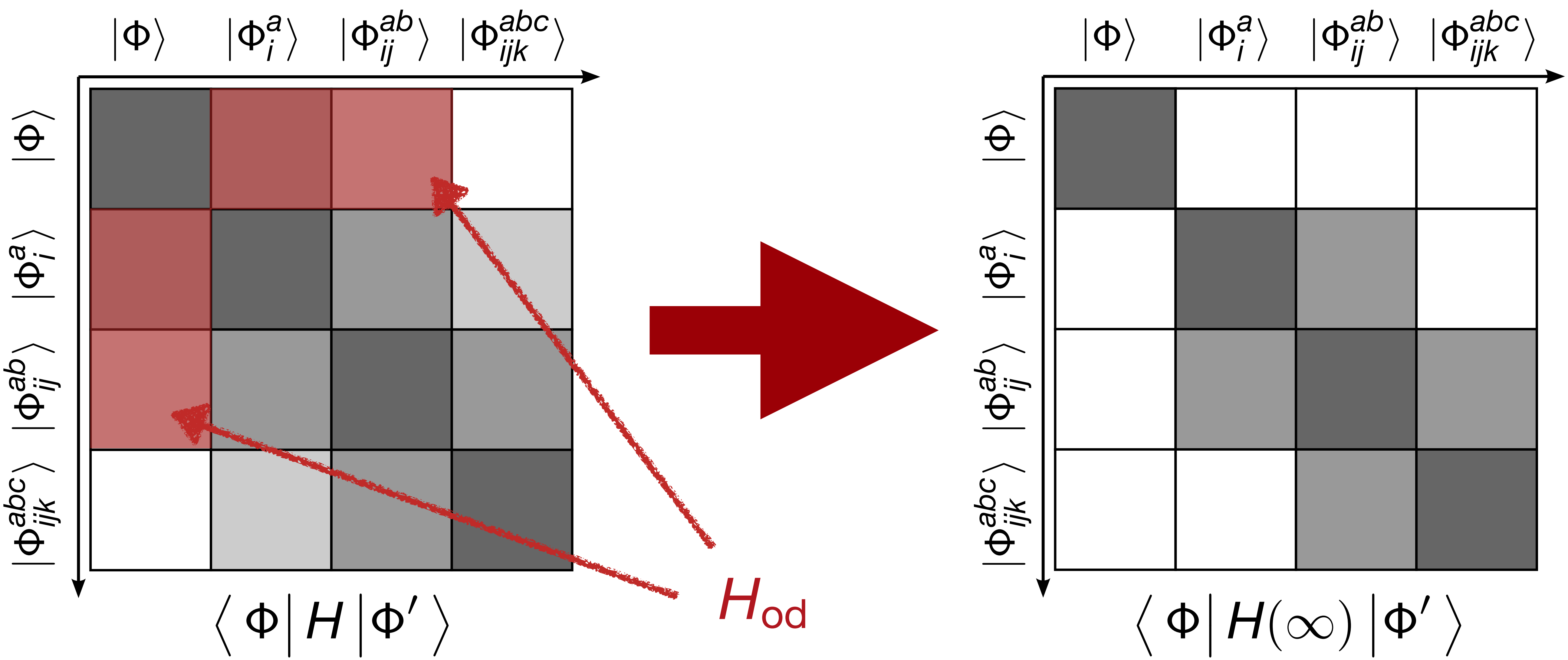
goal: decouple reference state $|\Phi\rangle$ from excitations

Flow Equation



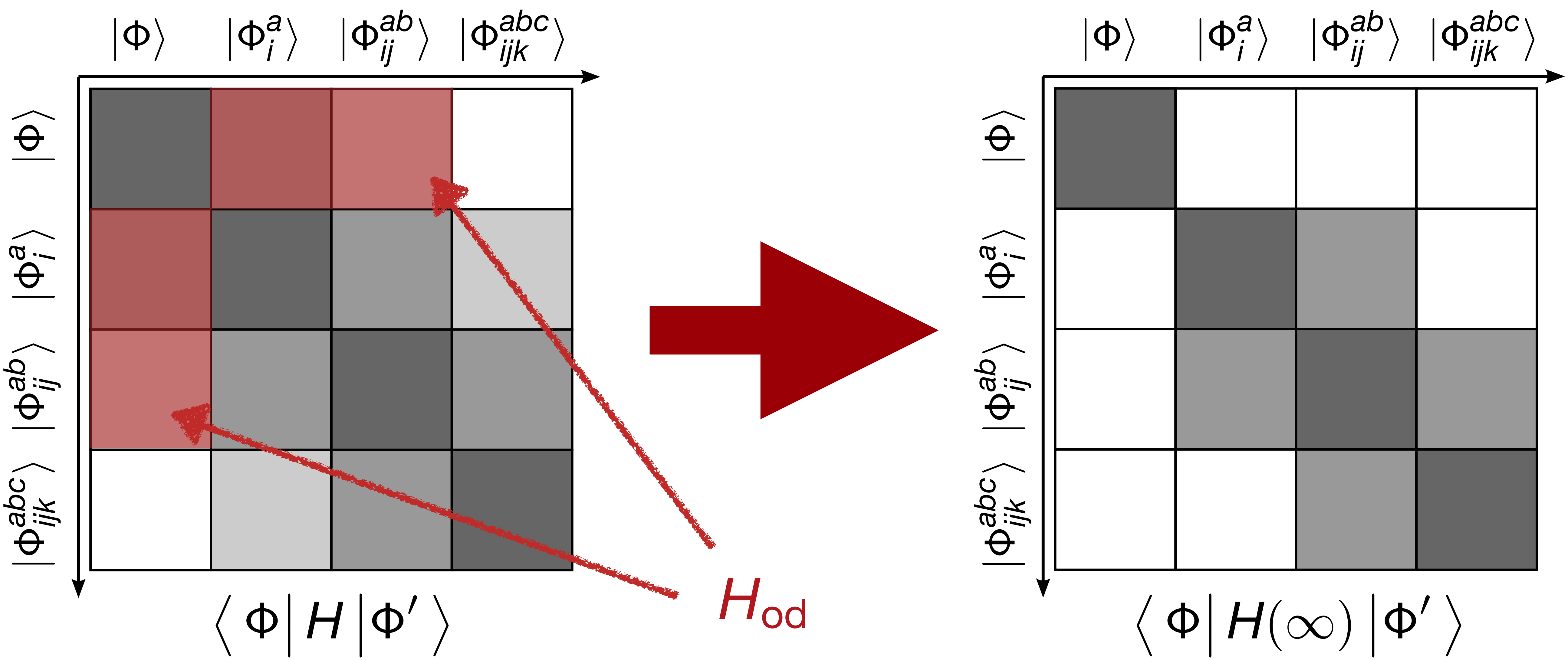
$$\frac{d}{ds}H(s) = \left[\eta(s), H(s)\right], \quad \text{e.g.,} \quad \eta(s) \equiv \left[H_d(s), H_{od}(s)\right]$$

Flow Equation



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

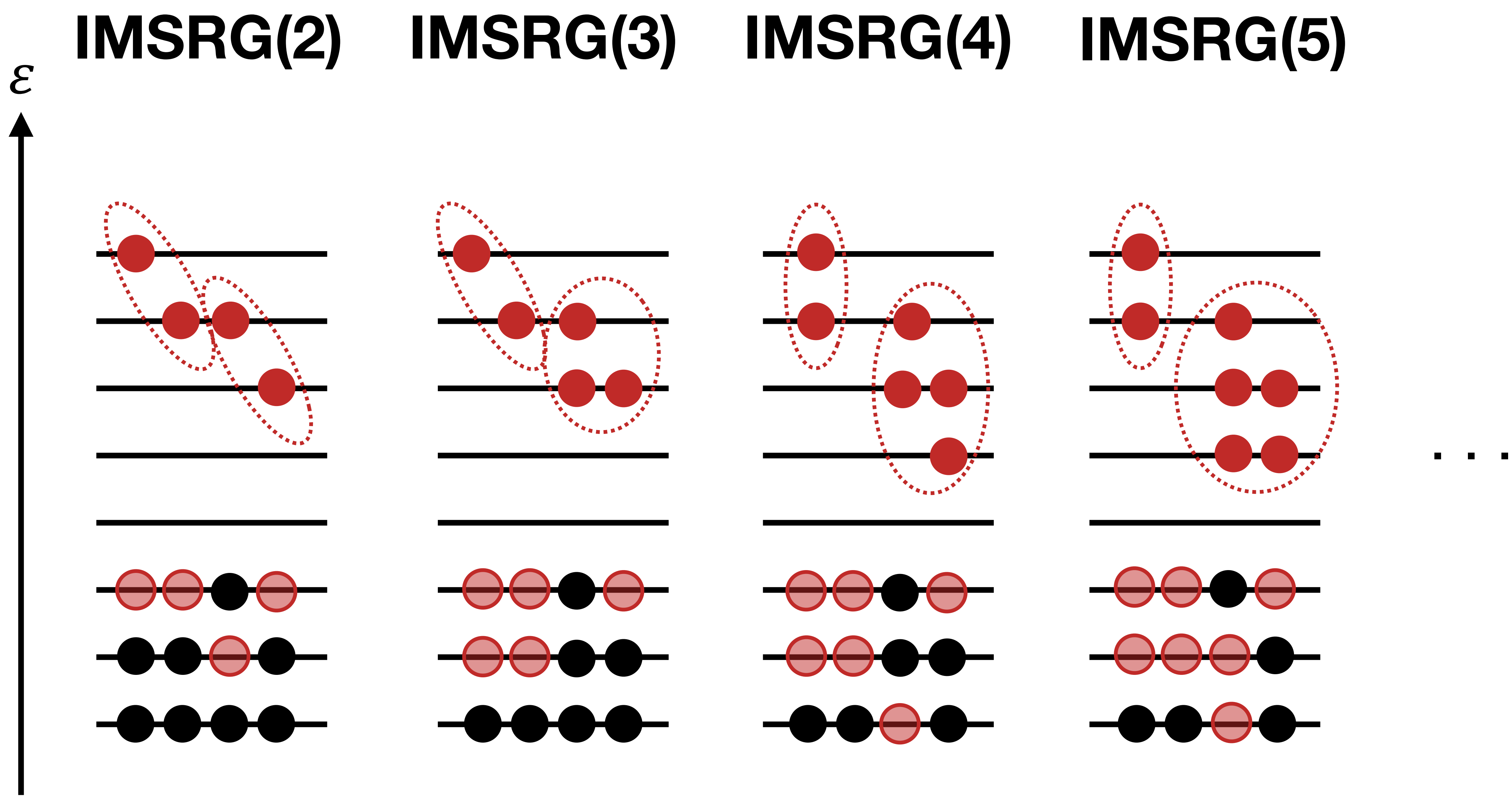
Flow Equation



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

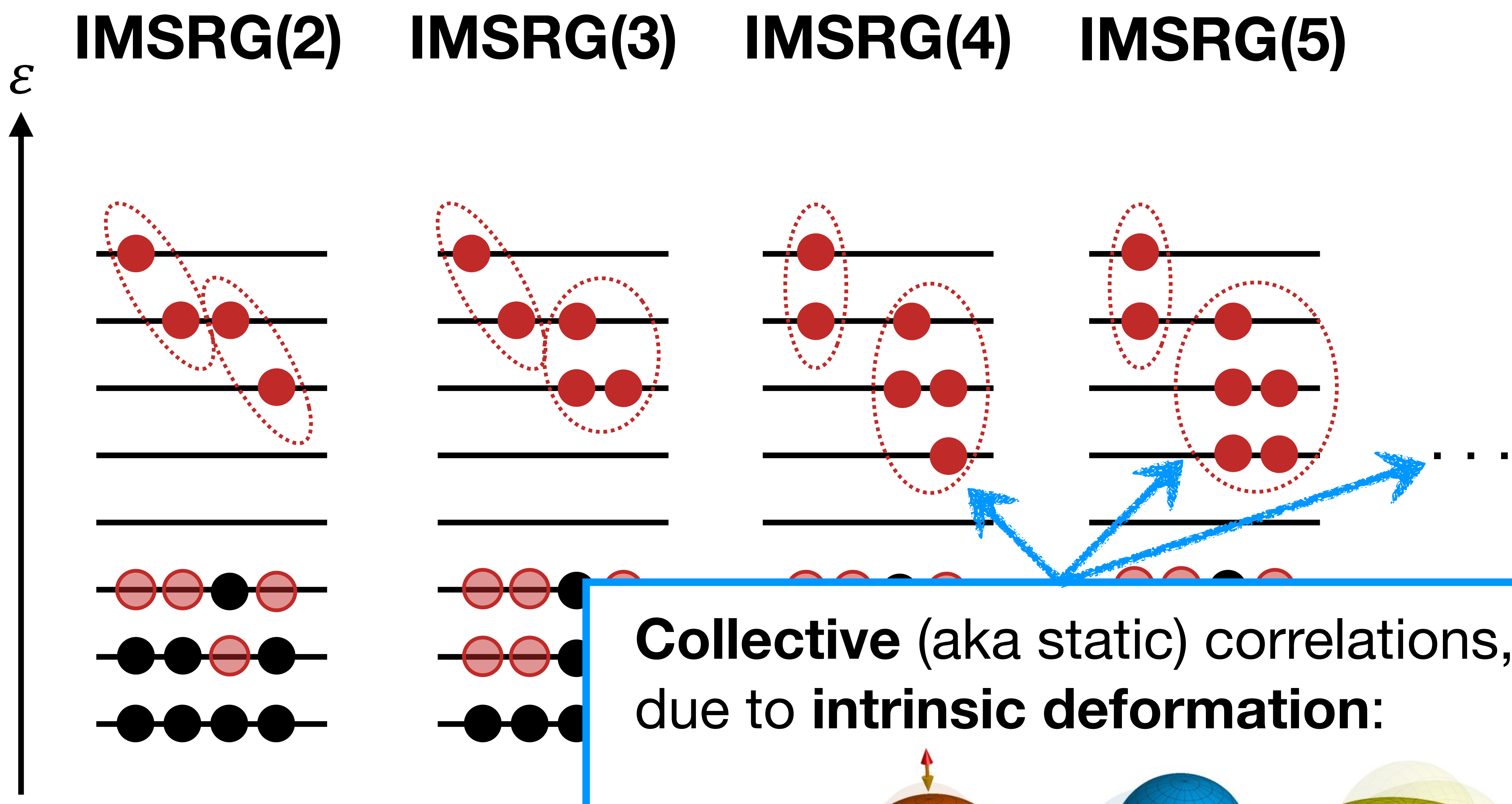
Operators
truncated at **two-body level** -
matrix is never constructed explicitly!

Correlated Reference States



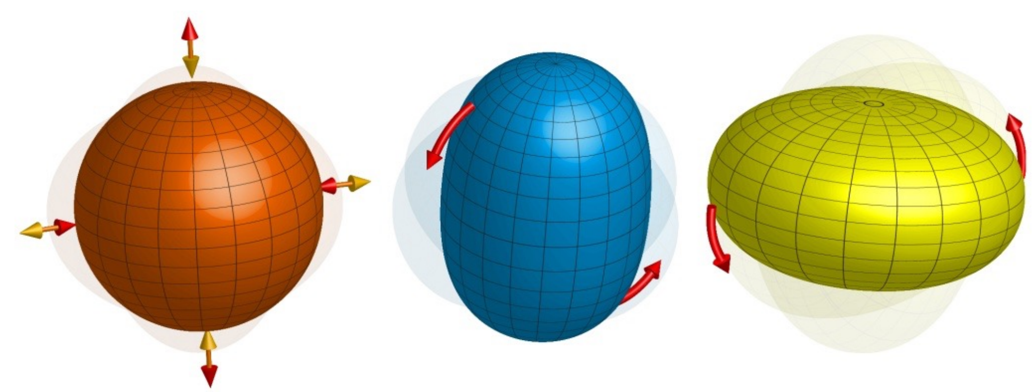
“standard” IMSRG: build correlations on top of Slater determinant (=**independent-particle state**)

Correlated Reference States

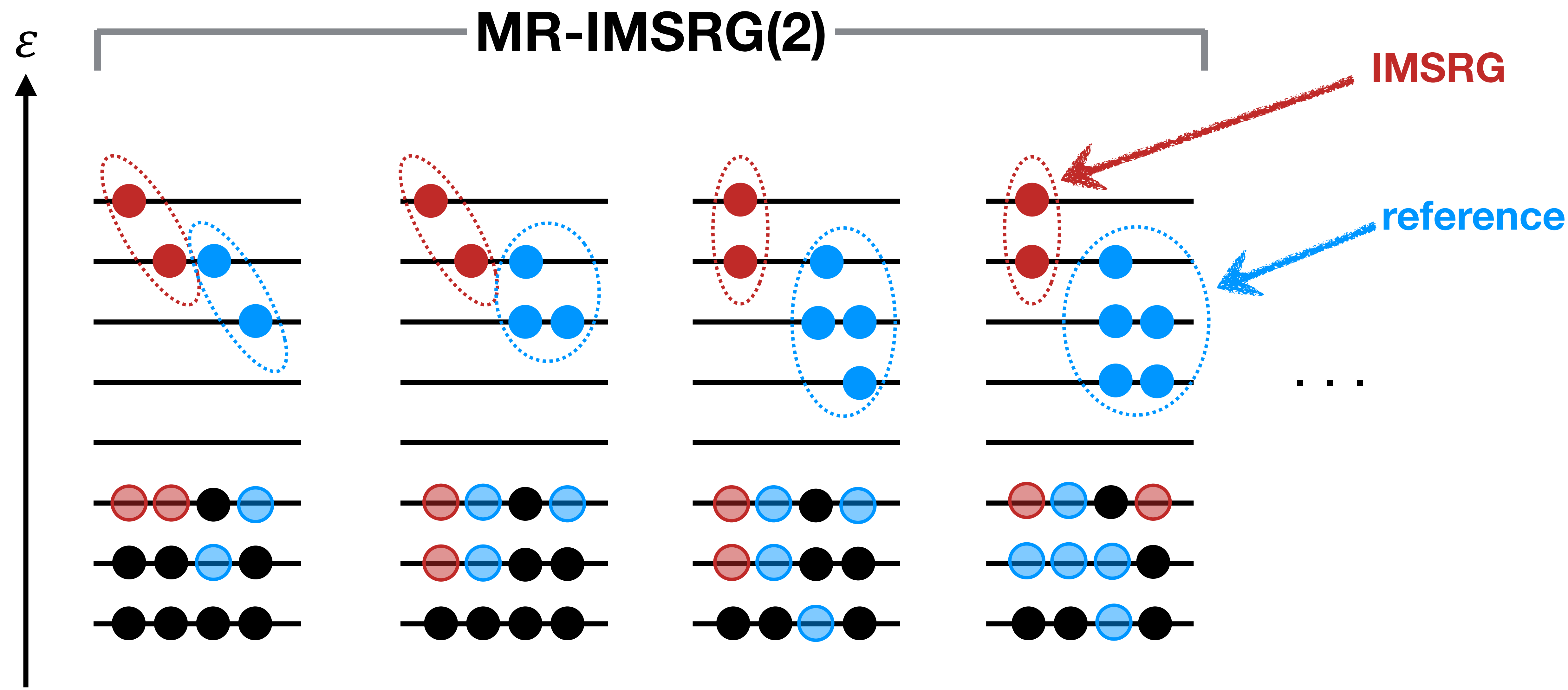


“standard” IMS
Slater determinan

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

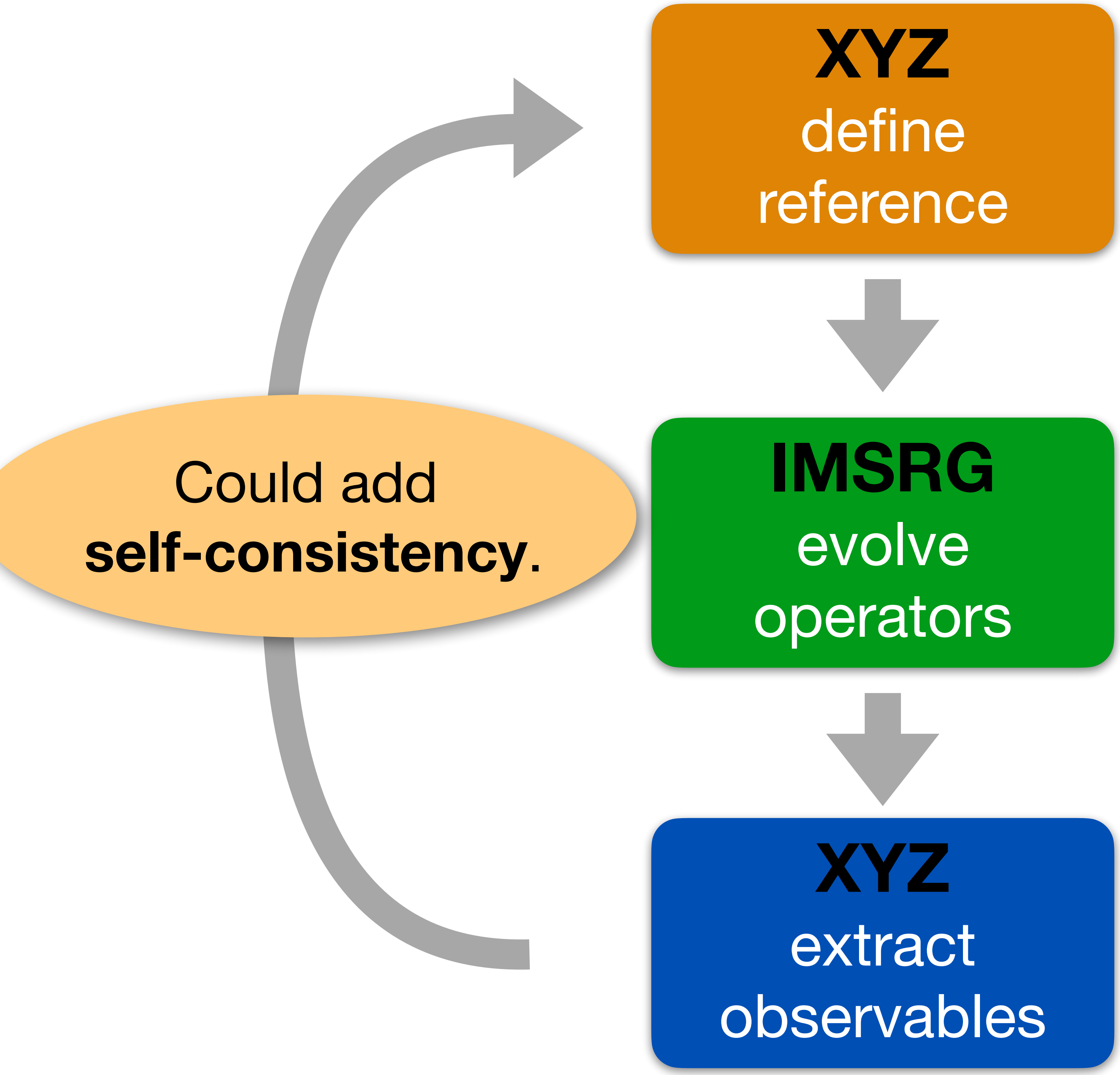


Correlated Reference States



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

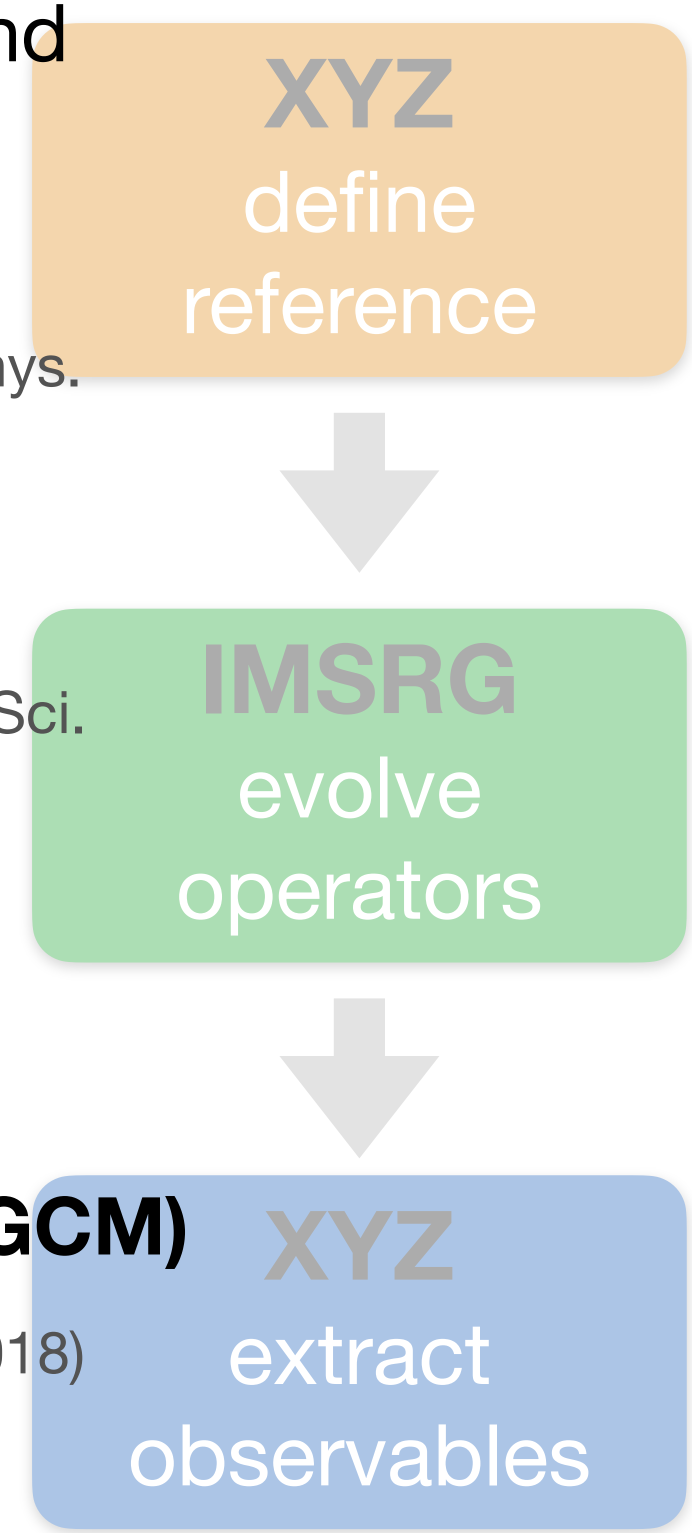
IMSRG-Improved Methods



* 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)



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)

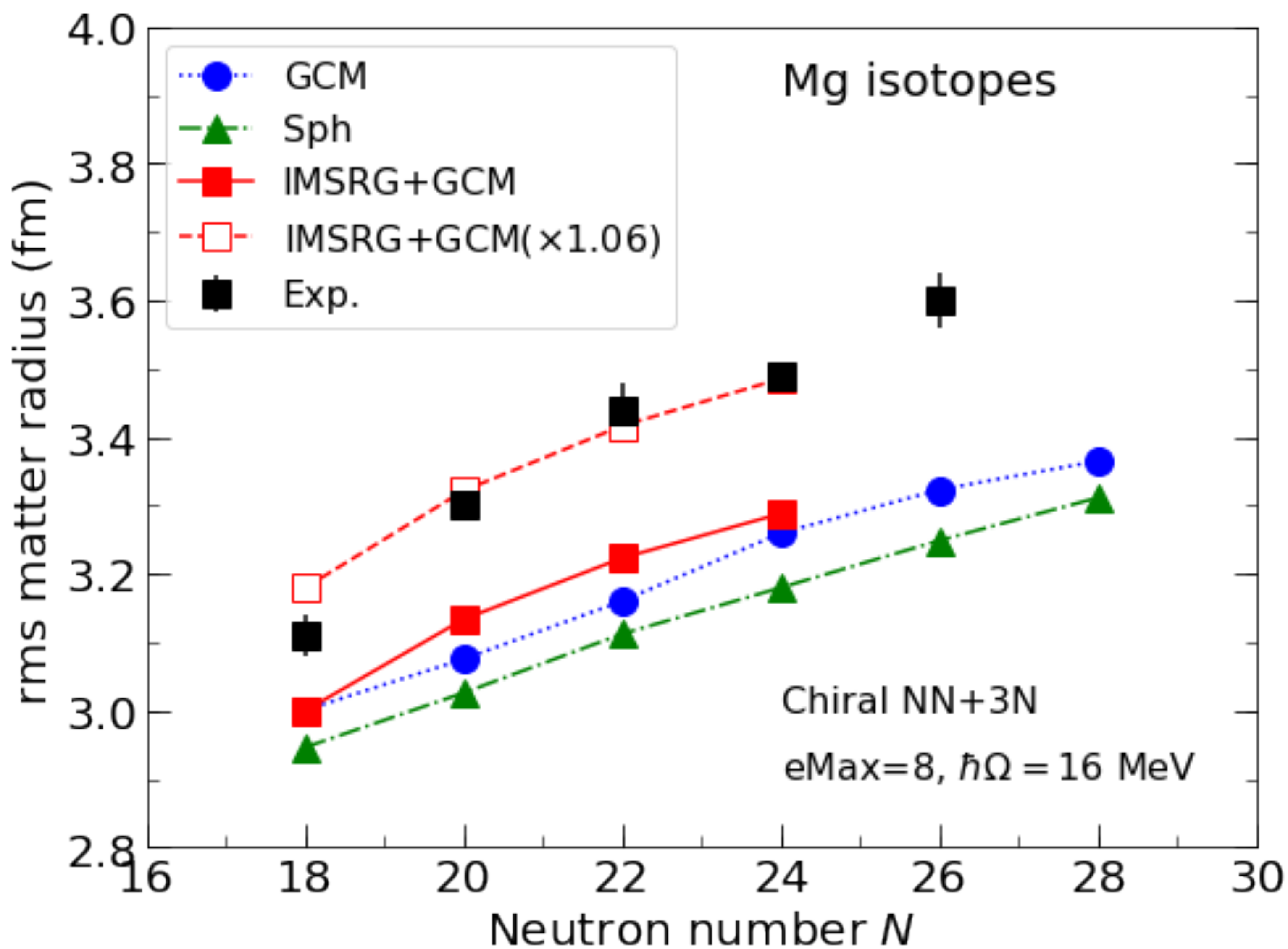
J. M. Yao, B. Bally, J. Engel, R. Wirth, T. R. Rodriguez, HH, PRL **124**, 232501 (2020)

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

HH, J. M. Yao, T. D. Morris, N. M. Parzuchowski, S. K. Bogner and J. Engel, J. Phys. Conf. Ser. 1041, 012007 (2018)

Magnesium Isotopes

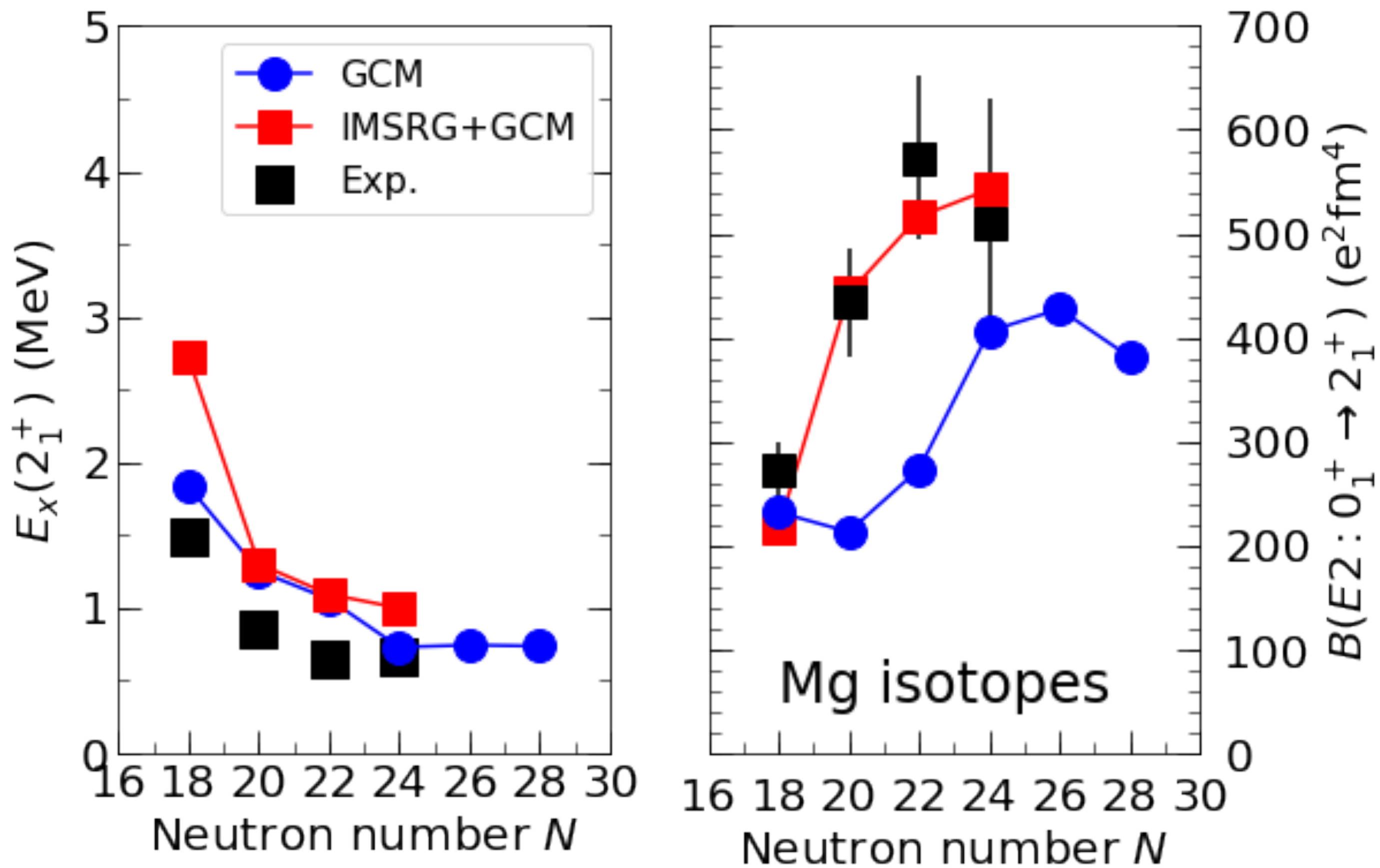
J. M. Yao, HH, in preparation



- note **improvement of rms radius trend** from IM-GCM
- global shifts (and/or rotation around "pivot") often associated with cutoff dependence of interactions

Magnesium Isotopes

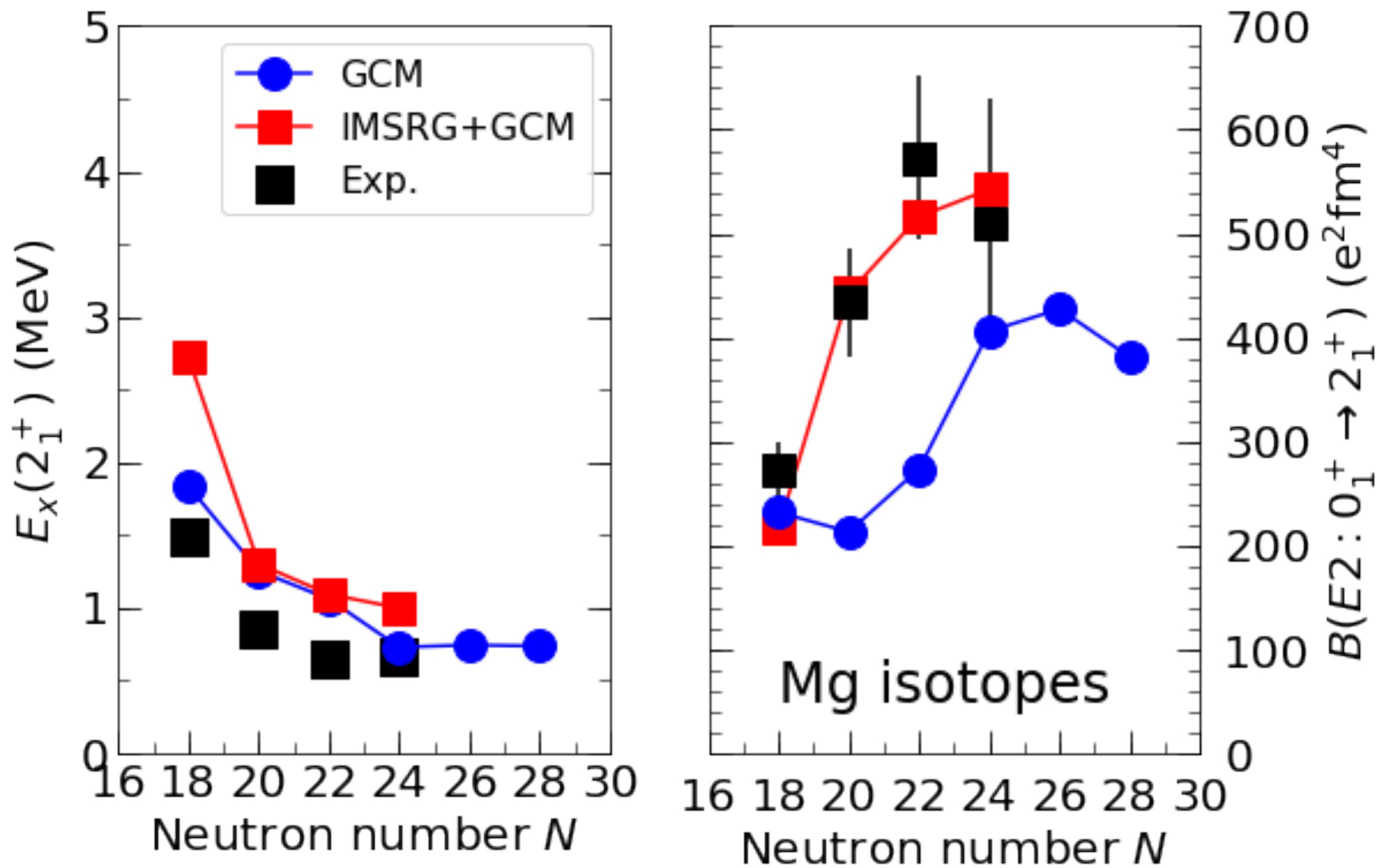
J. M. Yao, HH, in preparation



- 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

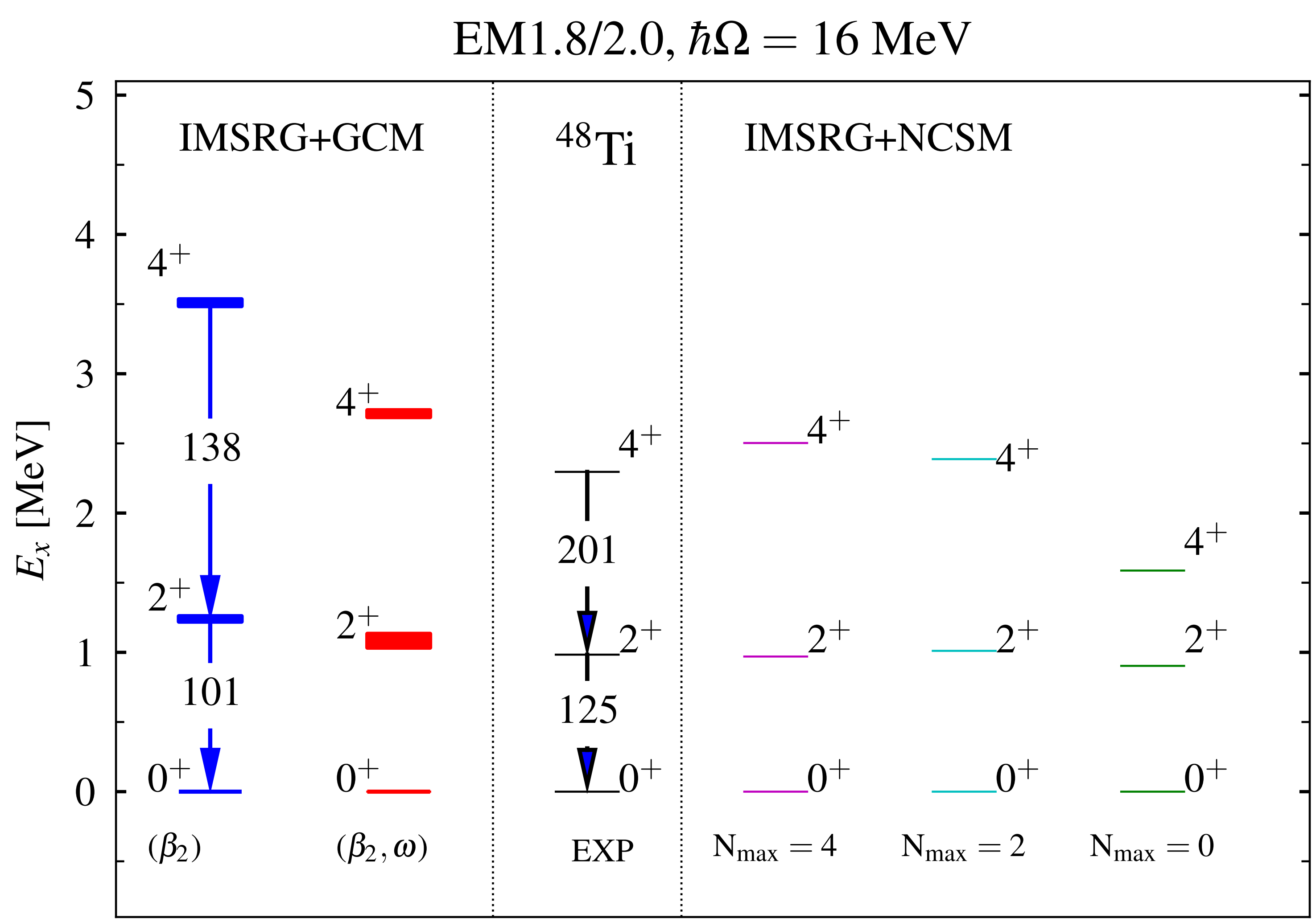


$$O = O^{(1)} \underset{s\to\infty}{\to} O(s) = O^{(1)}(s) + \underbrace{O^{(2)}(s) + \ldots}_{\text{induced contributions}}$$

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

IM-GCM: $0\nu\beta\beta$ Decay of ^{48}Ca

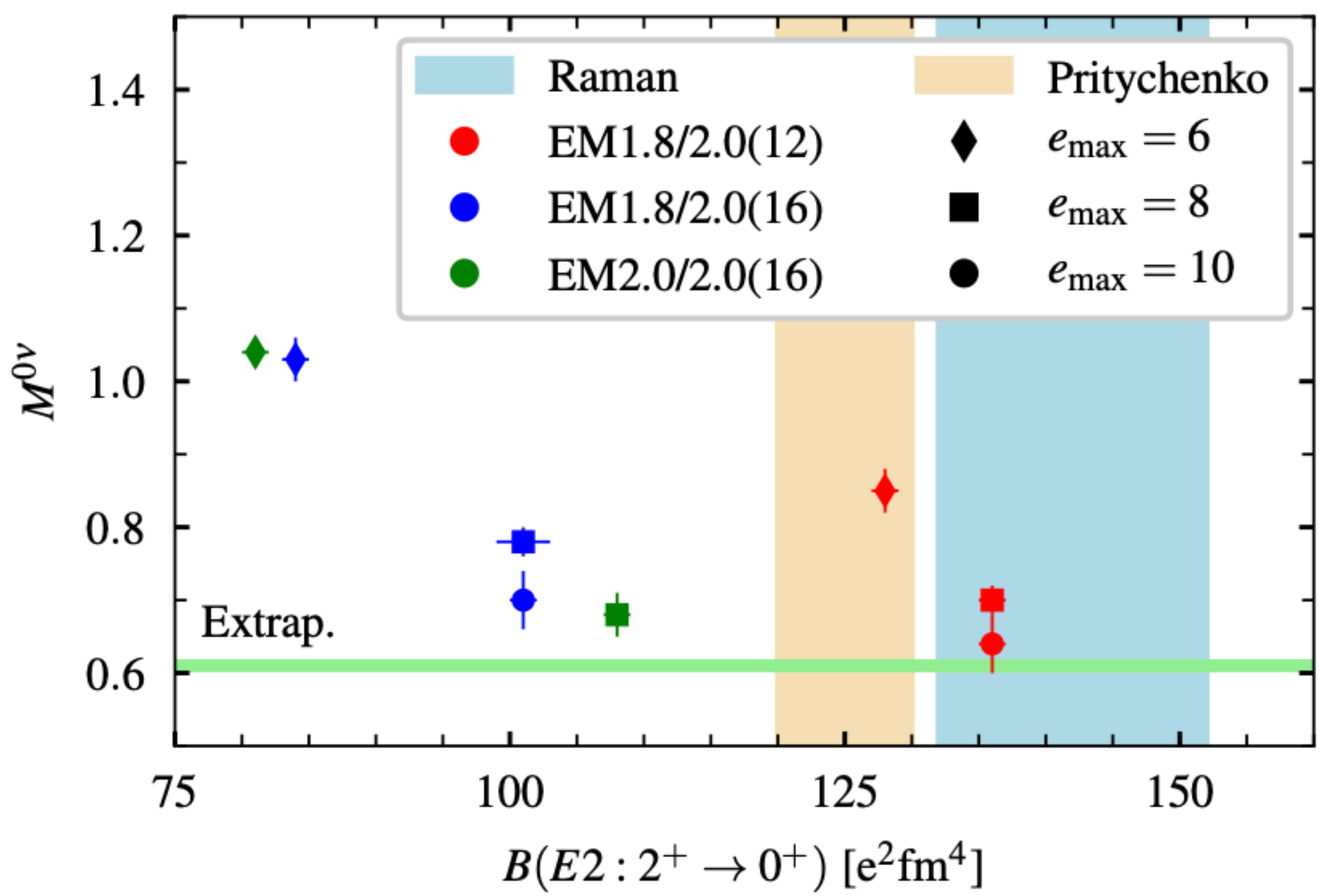
*J. M. Yao et al., PRL **124**, 232501 (2020); HH, Front. Phys. **8**, 379 (2020)*



- richer GCM state through **cranking**
- consistency between IM-GCM and IM-NCSM

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

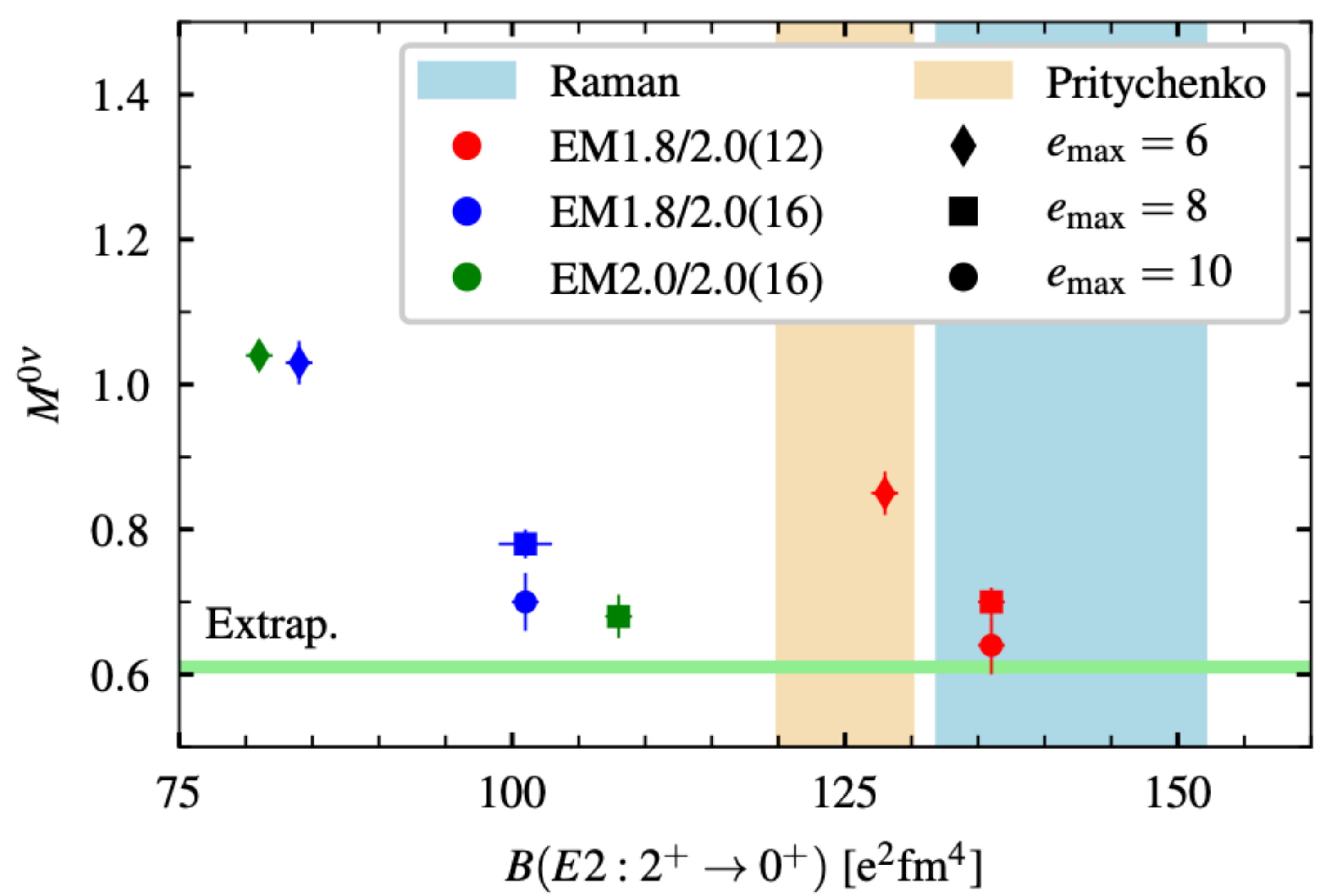
*J. M. Yao et al., PRL **124**, 232501 (2020); PRC **103**, 014315 (2021)*



- NME from different methods **consistent** for consistent interactions & transition operators
  (A. Belley et al., PRL 126, 042502, S. Novario et al., PRL 126, 182502)
- interpretation and features differ from empirical approaches (e.g., only **weak correlation** between NME and B(E2) value)

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

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



- NME from different methods **consistent** for consistent interactions & transition operators

  (A. Belley et al., PRL 126, 042502, S. Novario e

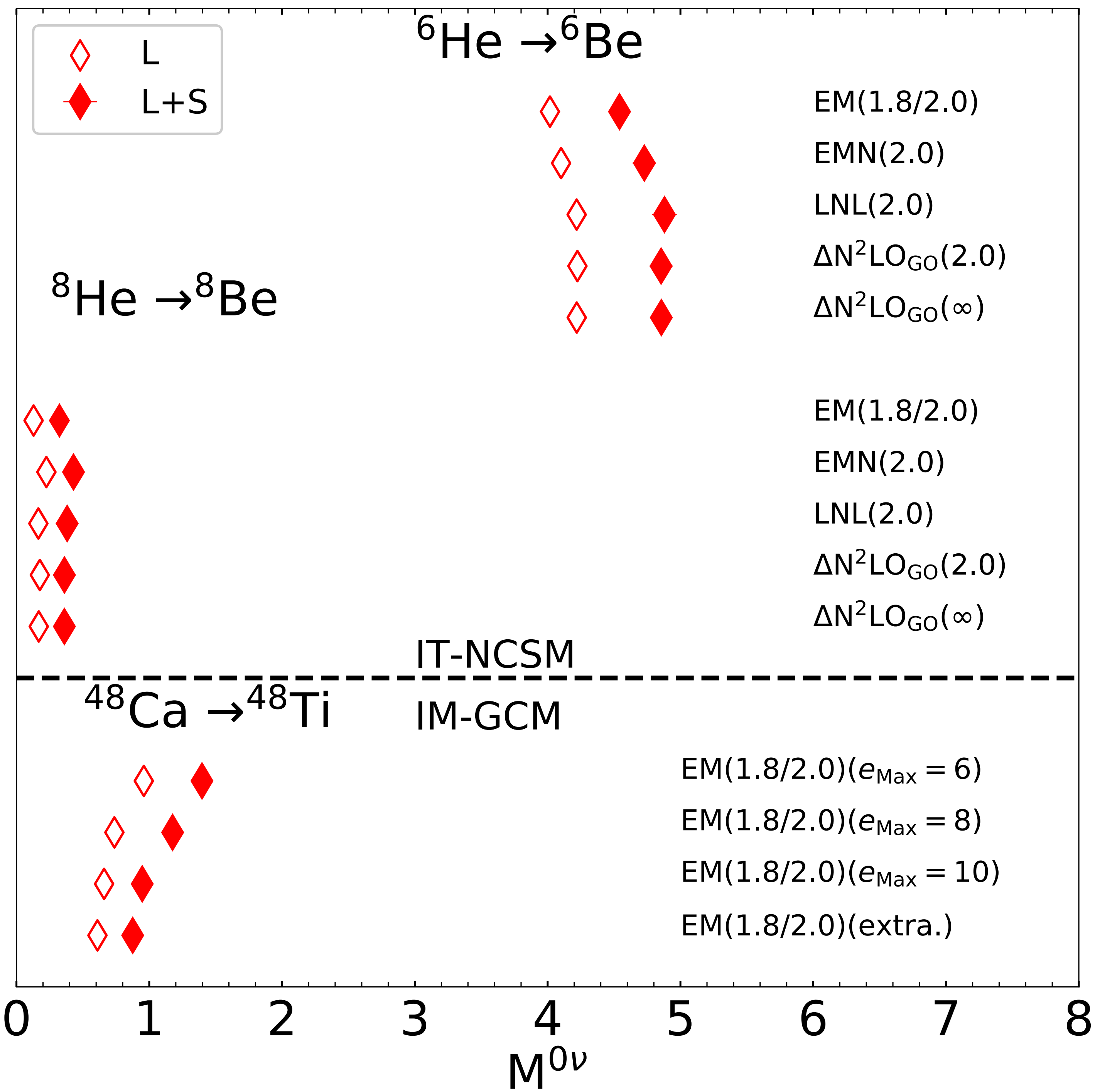
- interpretation and features differ from e

  only **weak correlation** between NME and

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

Counterterm in $0\nu\beta\beta$ Operator

R. Wirth, J. M. Yao, H. Hergert, PRL **127**, 242502 (2021)

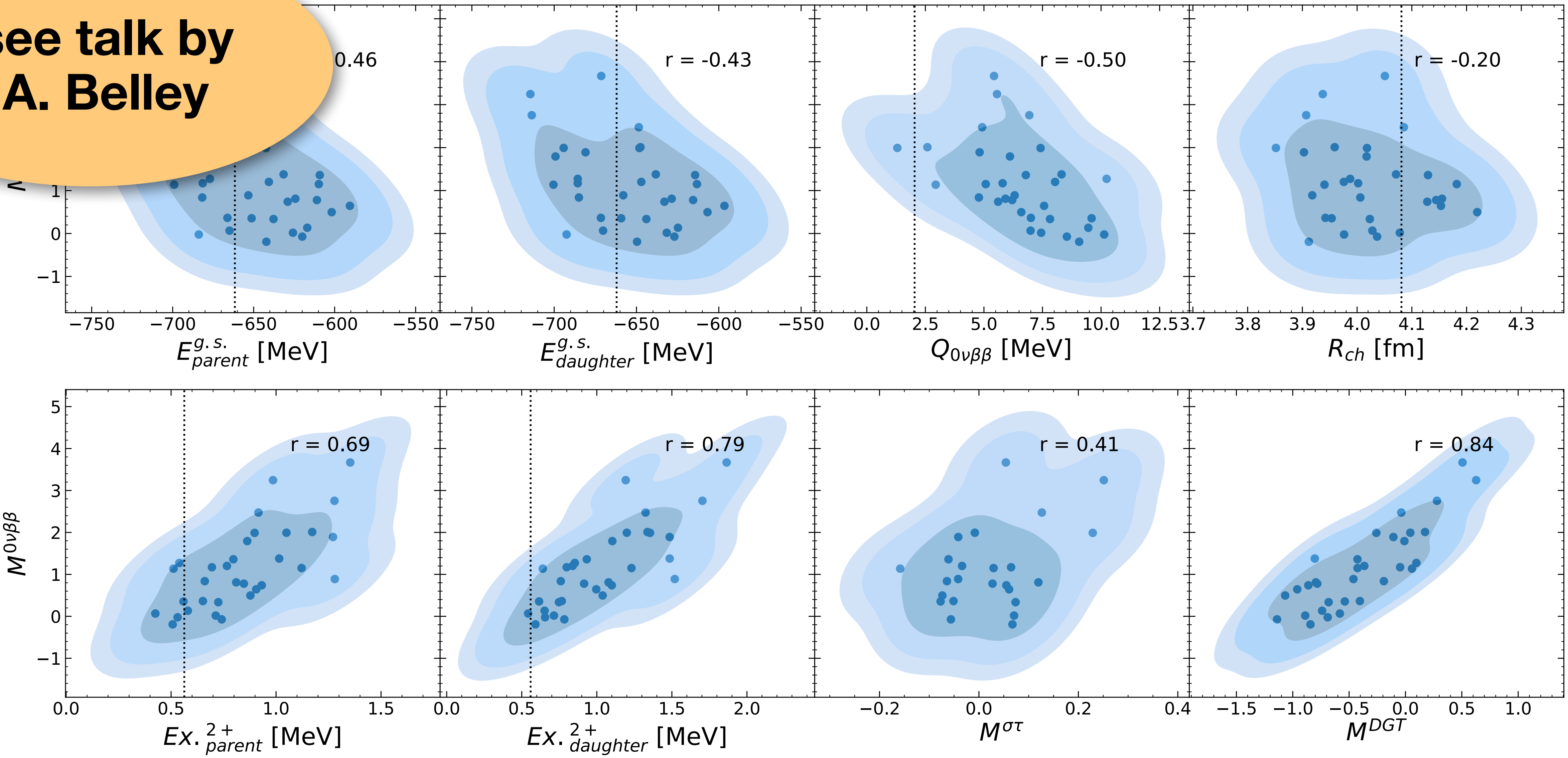


- Cirigliano et al.: RG invariance of the DBD transition operator requires **contact term**
- Counter term yields **robust enhancement**
  - varied EFT orders, RG scales, interactions
- **Next:**
  - more interactions
  - inclusion of currents
  - LEC sensitivity / UQ

Correlations revisited

A. Belley et al., arXiv:2210.05809 [nucl-th]; also see J. M. Yao et al., PRC 106, 014315

see talk by A. Belley



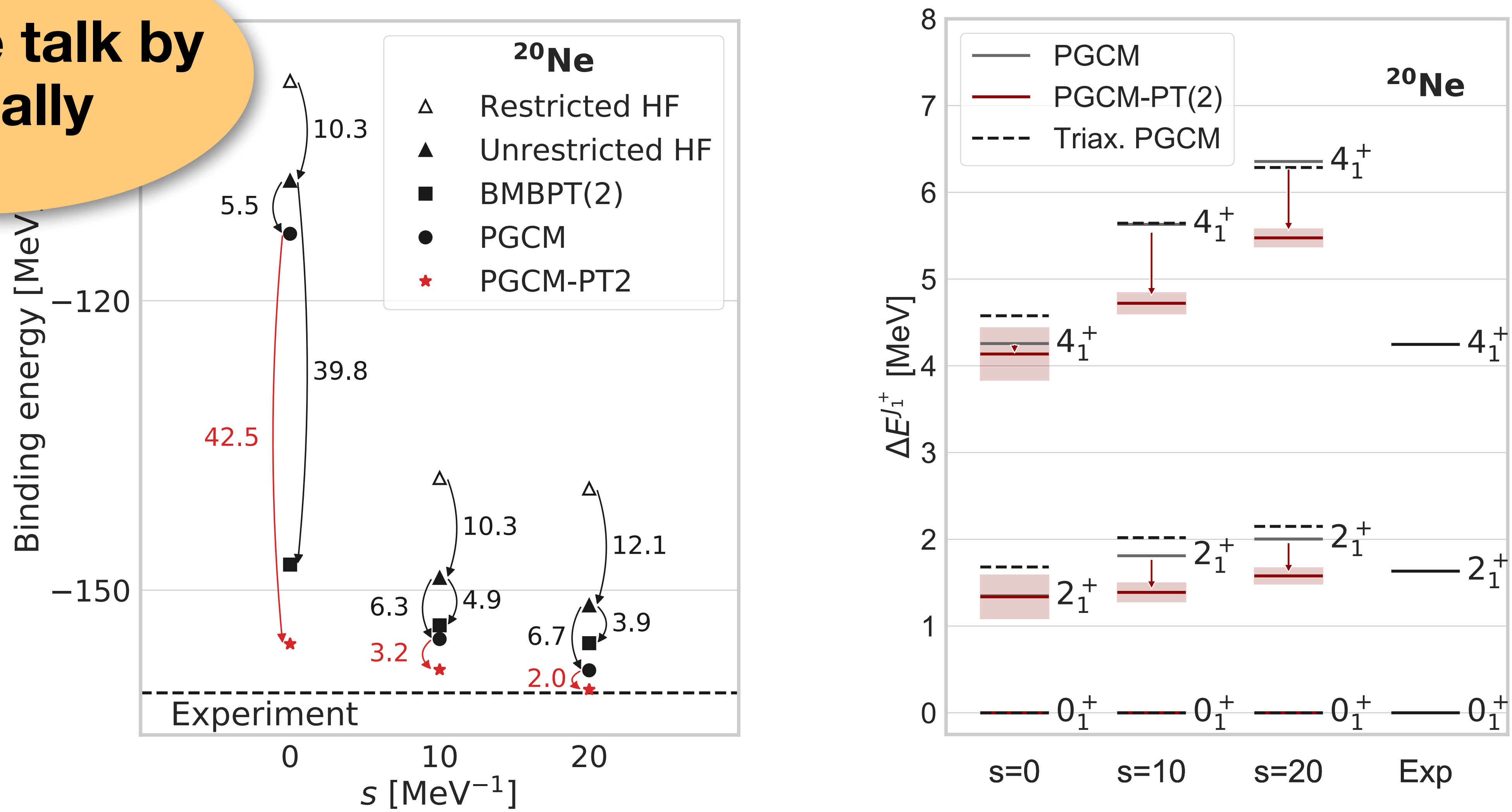
^{76}Ge, VS-IMSRG, 34 non-implausible Δ-full N2LO interactions
(cf. B.S. Hu et al., Nature Phys.)

- possible correlation with **Double Gamow Teller** transition, **2^{+} energies** (but the latter only in ^{76}Ge)

Perturbative Enhancement of IM-GCM

also see talk by B. Bally

*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

Looking Ahead

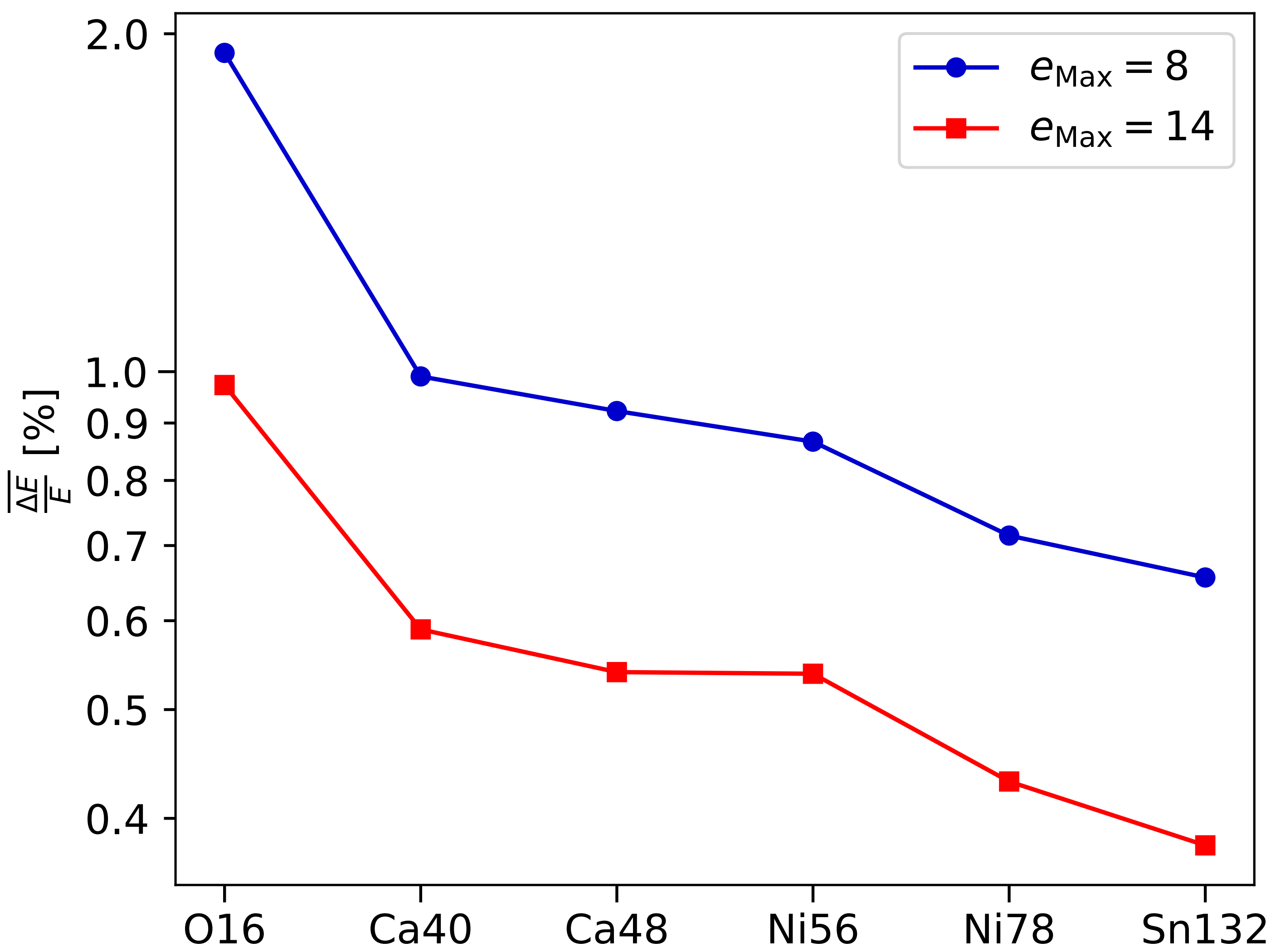
(Some) Physics Goals

- **Neutrinoless Double Beta Decay** matrix elements for ^{76}Ge and other candidates
  - use VS-IMSRG for heavy lifting in parameter sensitivity analysis & UQ because IM-GCM is too costly
  - **accelerate IMSRG & IM-GCM** (GPUs, factorization, …)
- increased precision for **beta decays** & **Schiff moments**
  - IM-GCM for odd nuclei
  - tackle nuclei for which large multi-shell valence-spaces make VS-IMSRG difficult or prohibitive
- **Uncertainty Quantification / Sensitivity Analysis**
  - need cheap **surrogate models (emulators)**

Compression with Random Projections

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

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

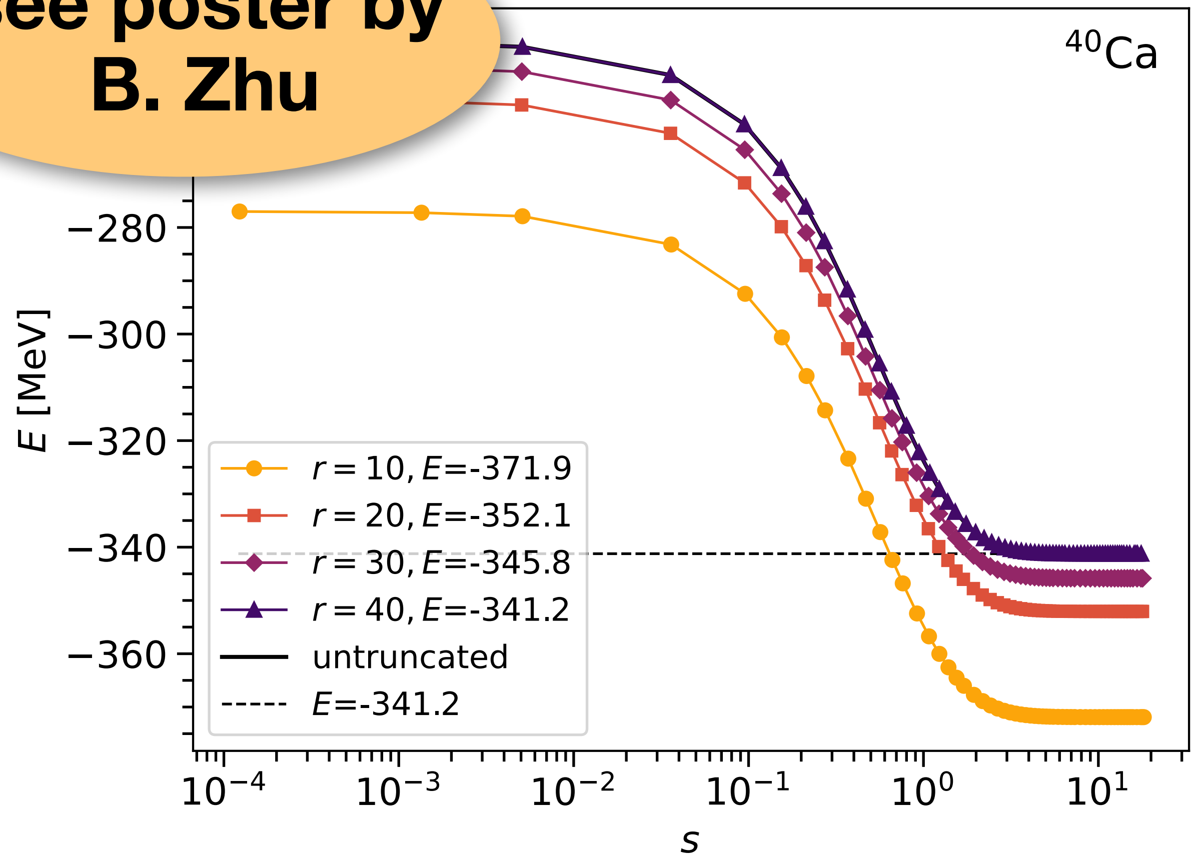


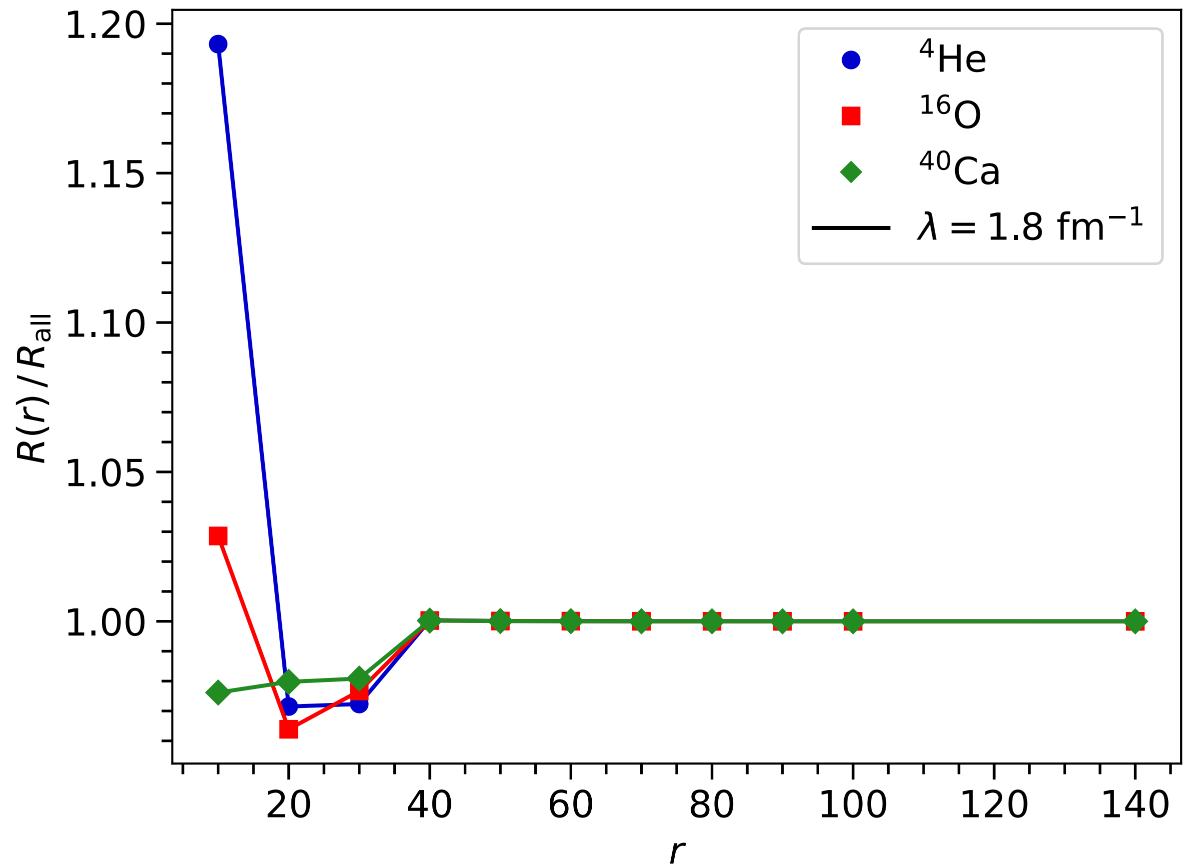
- tensorial (= modewise) **Johnson-Lindenstrauss embeddings**
- **purely based on features of (sparse) big data sets** - integrate with physics-based ideas?
- suitable for **streaming** transforms: compress on the fly while reading from disk

Leveraging Low-Rank Structures

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

see poster by B. Zhu



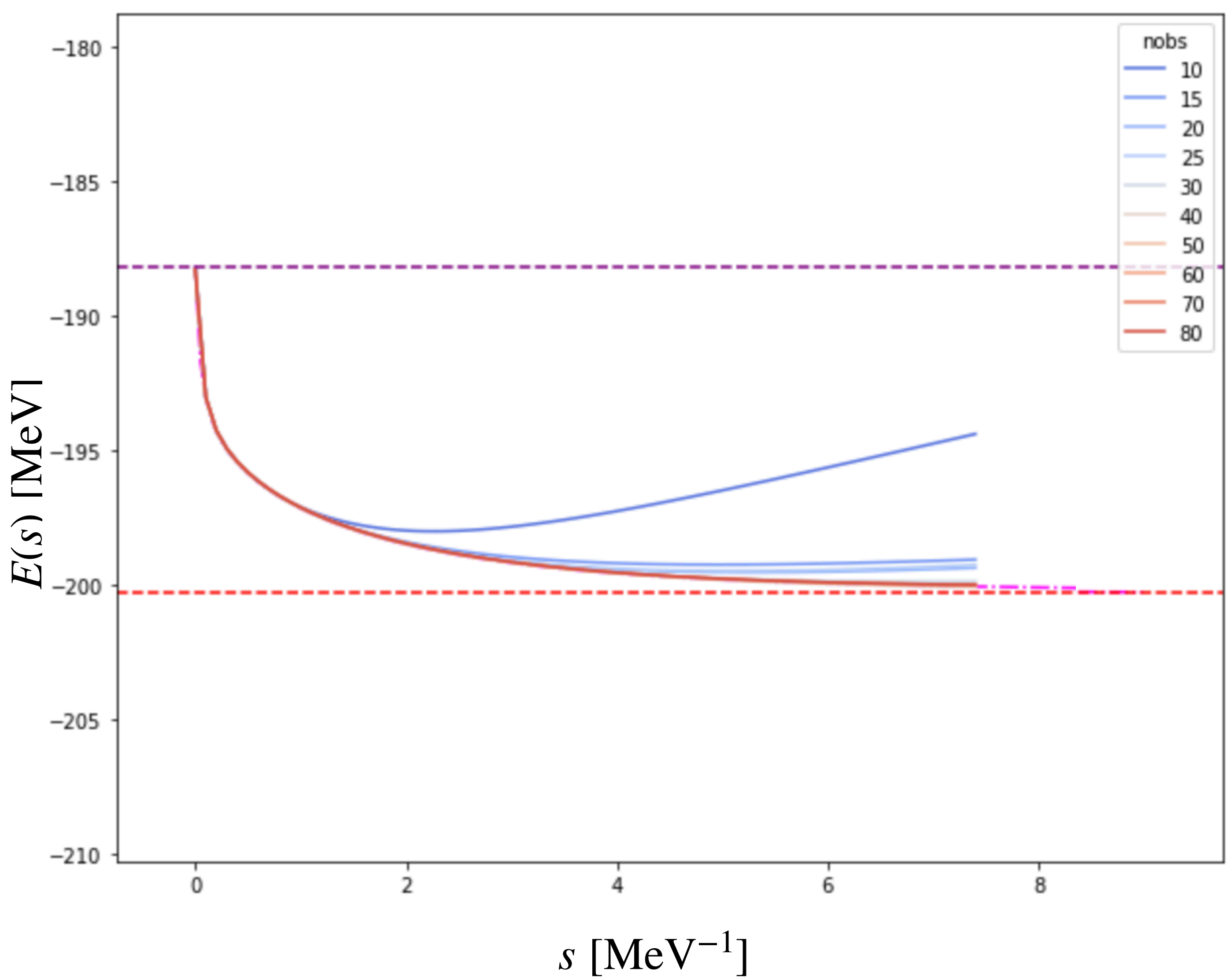


- **principal component analysis** of chiral interactions
  - free-space SRG effort and storage **reduced by several orders of magnitude** (but not a major bottleneck anyway)
  - **no adverse affect** on other (studied) observables
- **next: 3N & leverage factorization** in many-body calculation

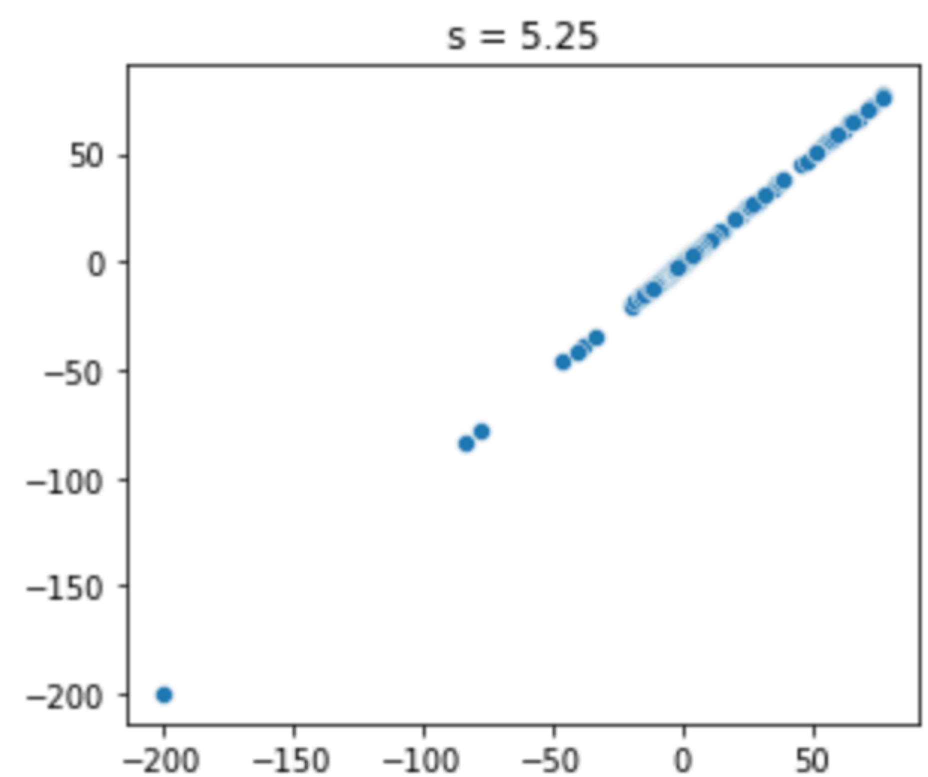
Emulating IMSRG Flows

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

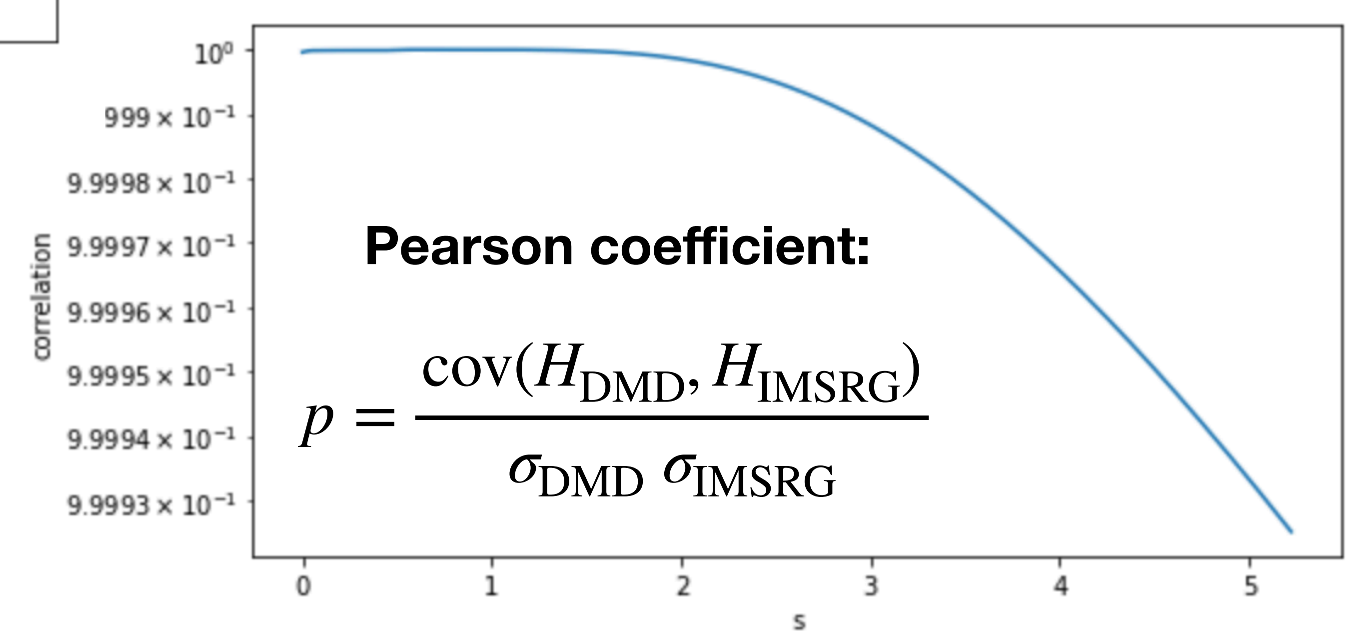
EM(500) N³LO, $\lambda = 2.0\,\mathrm{fm}^{-1}$



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



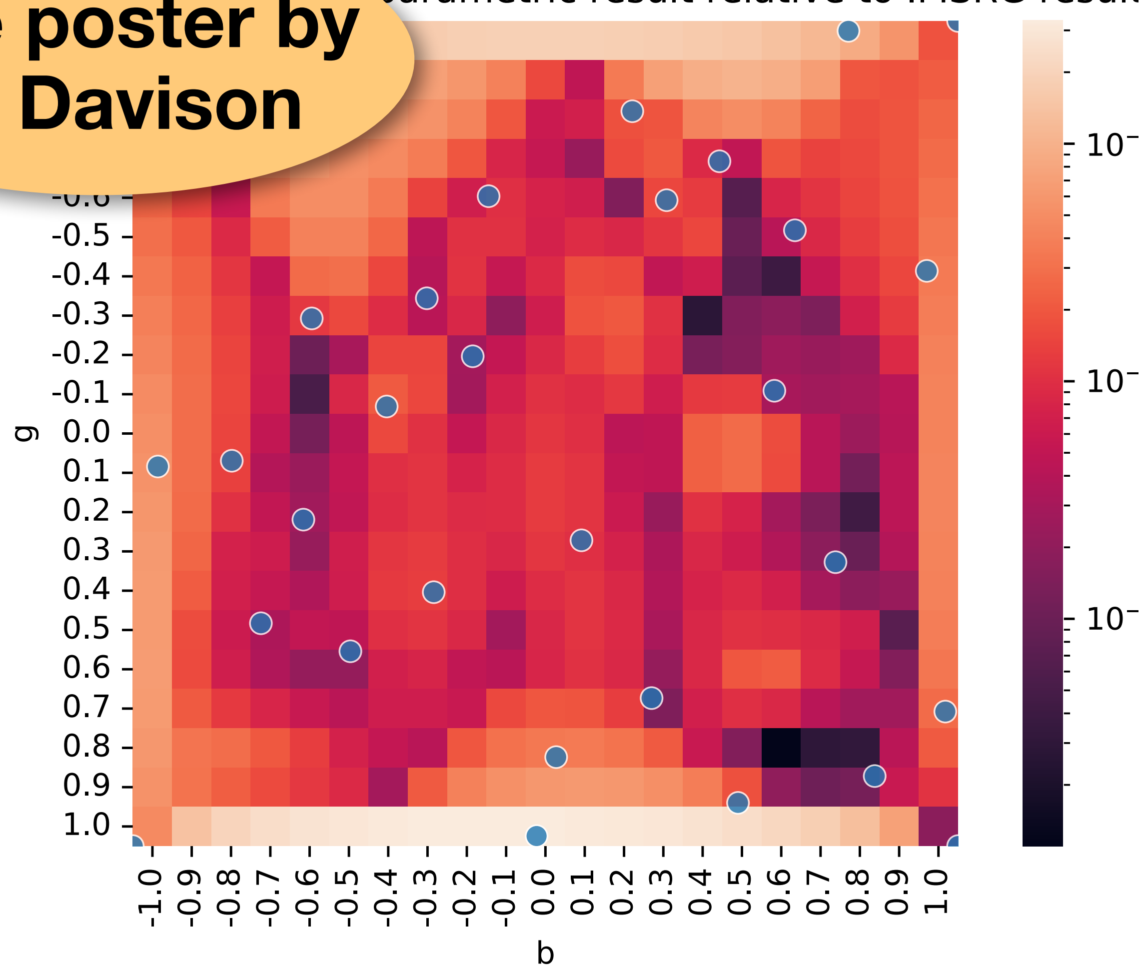
Dynamic Mode Decomposition **emulator** "learns" **all flowing operator coefficients** from snapshots!

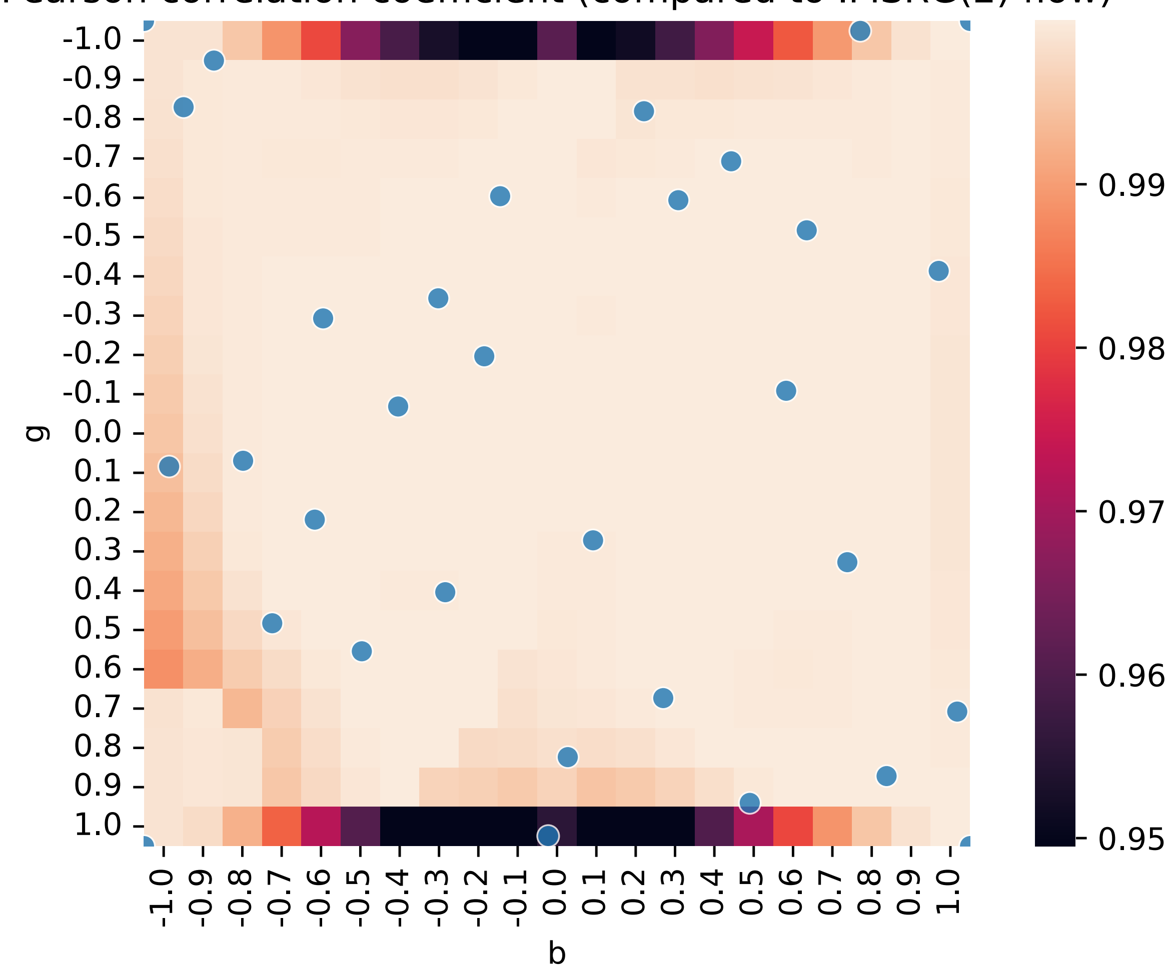


Parametric DMD

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

see poster by J. Davison





- pairing plus particle-hole model - 3 parameters + flow
- “naive” framework built for chiral LECs, but needs more optimization (more model reduction before DMD, etc.)
  - (still) ambitious by trying to predict full operators, could focus on observables (zero-body part of evolving operators) only

Summary

- developing **new capabilities:**
  - **transitions** (for structure, fundamental symmetry searches, …)
  - **(complex) deformations**
  - **clustering** (bridge to dynamics /reactions…)
- improve **precision**:
  - full or approximate **next-order truncations:** IMSRG(3) (see poster by M. Heinz)
  - alternative (?): improve **operator bases**
- tackling **computational cost & scalability (crucial for UQ):**
  - identify (and leverage) low-rank structures - **model order reduction**

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University of Notre Dame

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P. Arthuis, K. Hebeler, M. Heinz, R. Roth, T. Mongelli, T. Miyagi, A. Schwenk, A. Tichai
TU Darmstadt

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CMSE, Michigan State University

K. Fossez
Florida State University

A. Belley, J. D. Holt, P. Navrátil
TRIUMF

G. Hagen, G. Jansen, J. G. Lietz, T. D. Morris, T. Papenbrock
UT Knoxville & Oak Ridge National Laboratory

B. Bally, T. Duguet, M. Frosini, V. Somà
CEA Saclay, France

R. J. Furnstahl
The Ohio State University

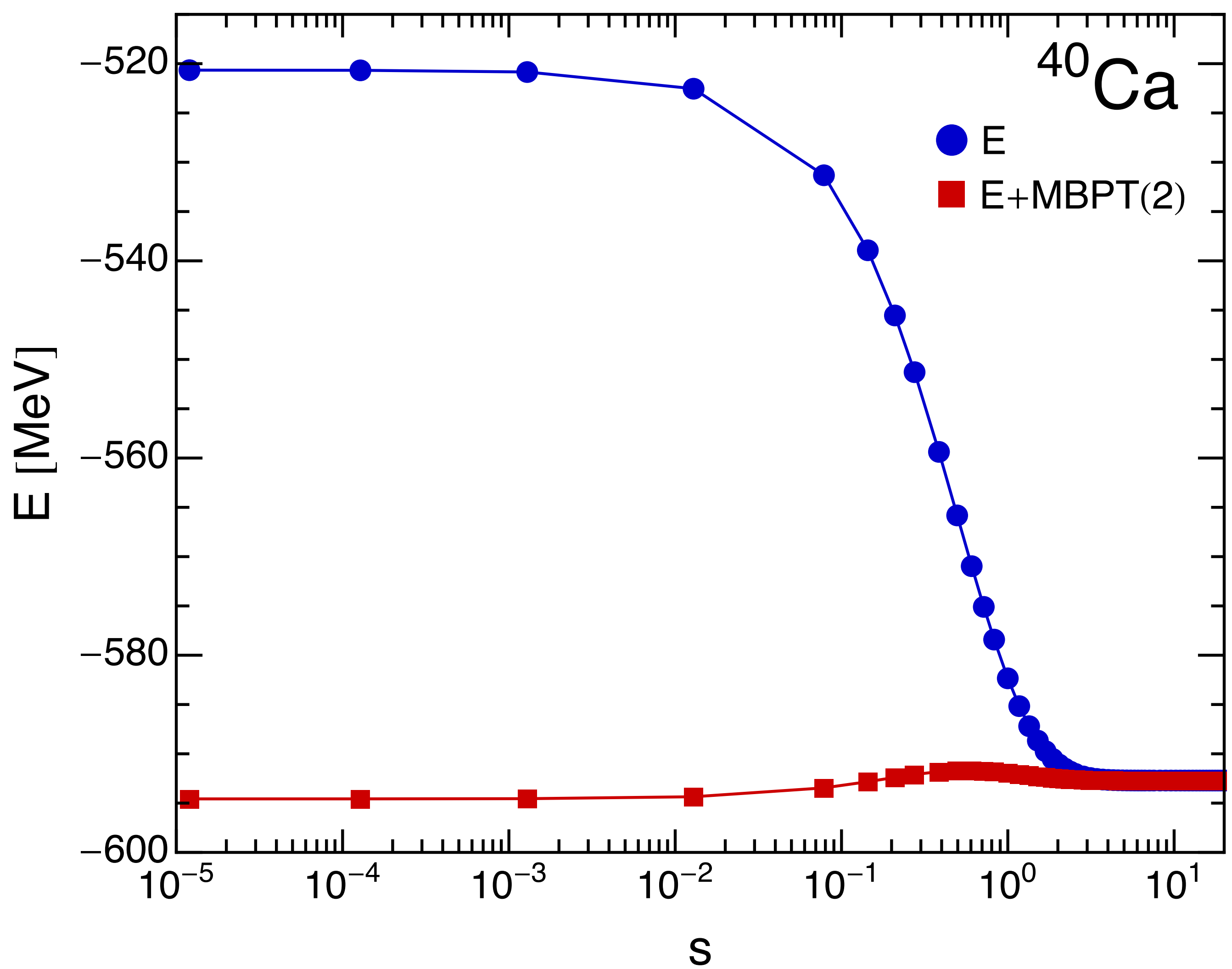
Grants: US Dept. of Energy, Office of Science, Office of Nuclear Physics **DE-SC0017887, DE-SC0023516,** as well as **DE-SC0018083, DE-SC0023175** (SciDAC NUCLEI Collaboration)

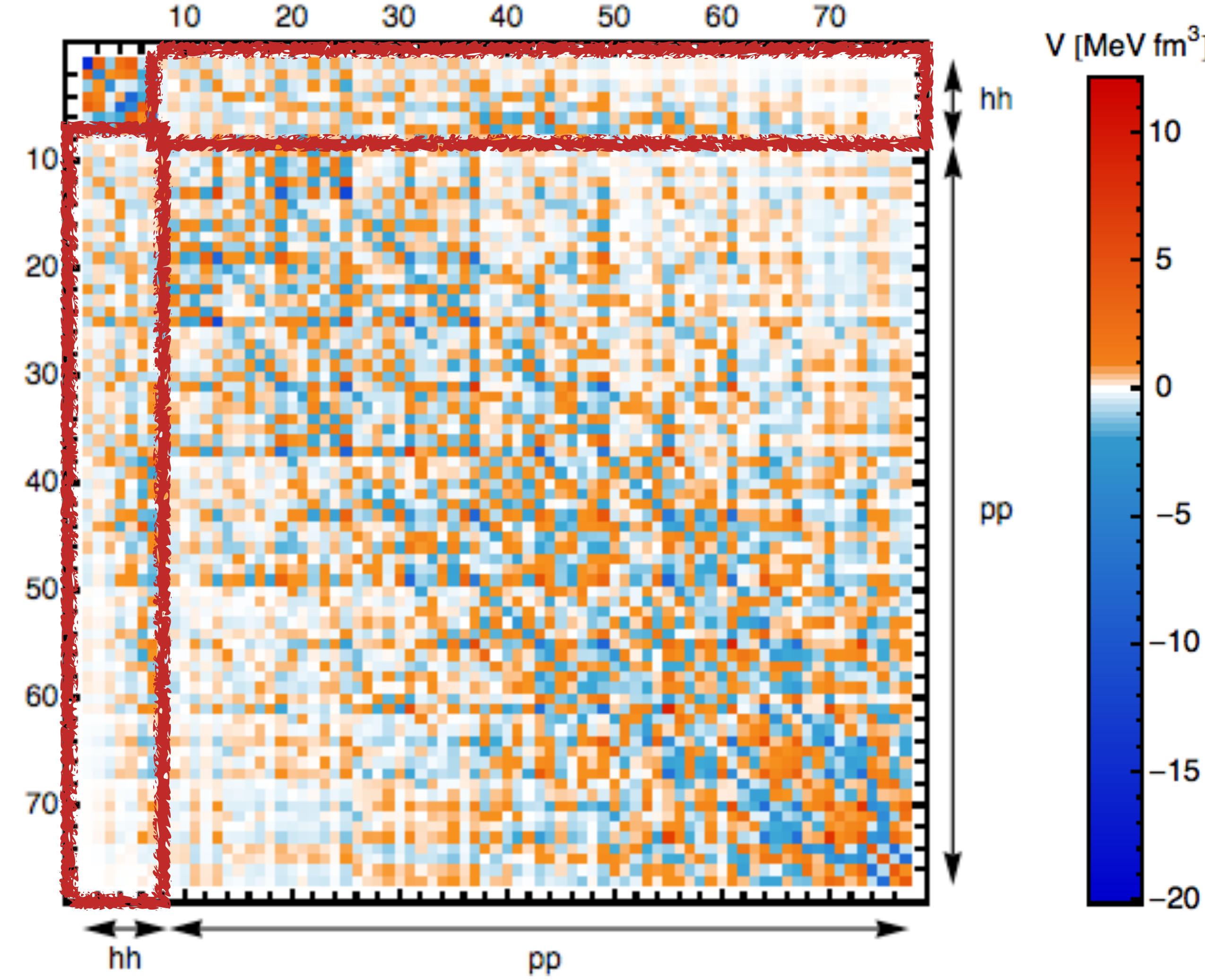
Postdoctoral Position @ FRIB

- **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, bit will continue until position is filled
- **Please encourage suitable candidates to apply!**

Supplements

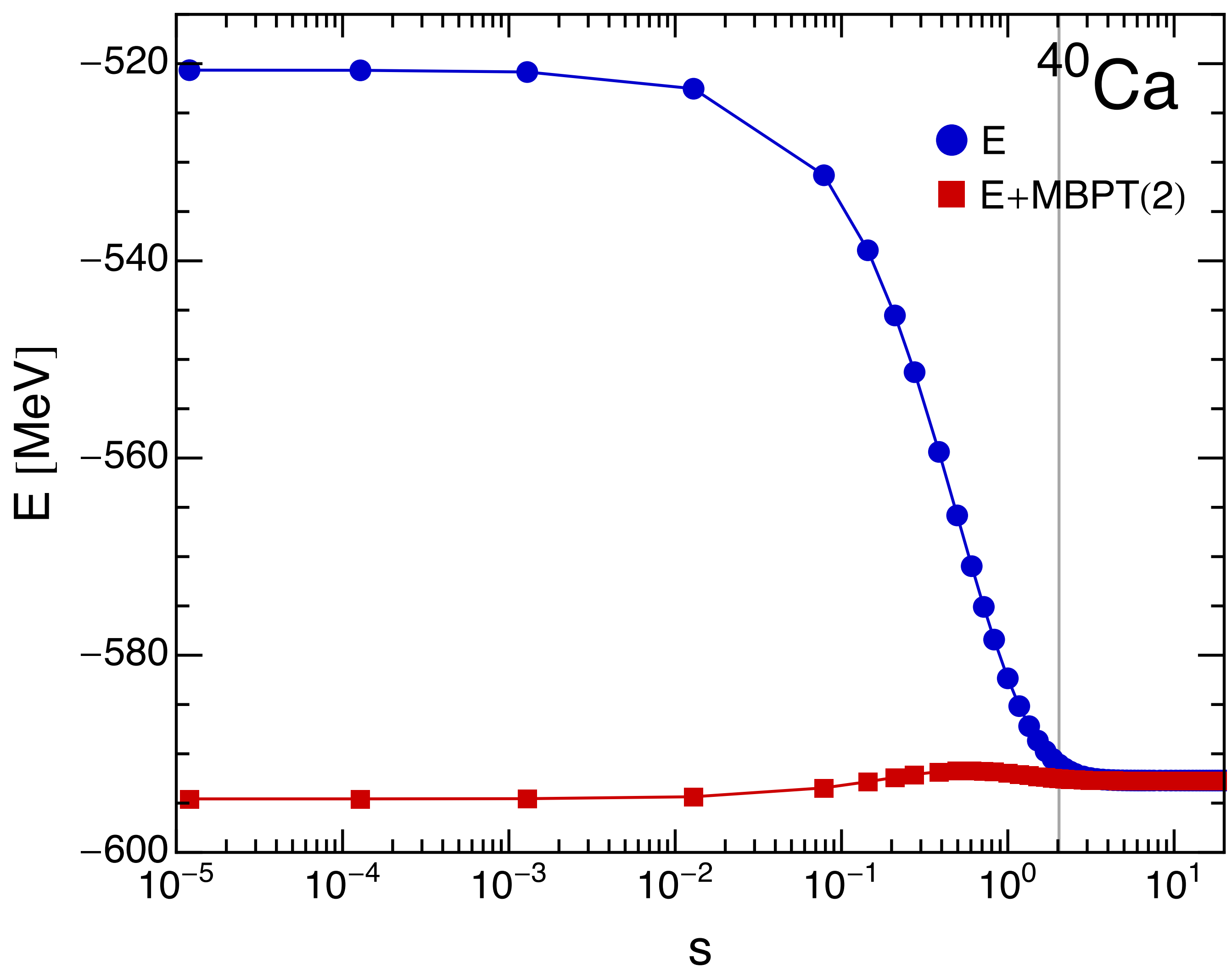
Decoupling

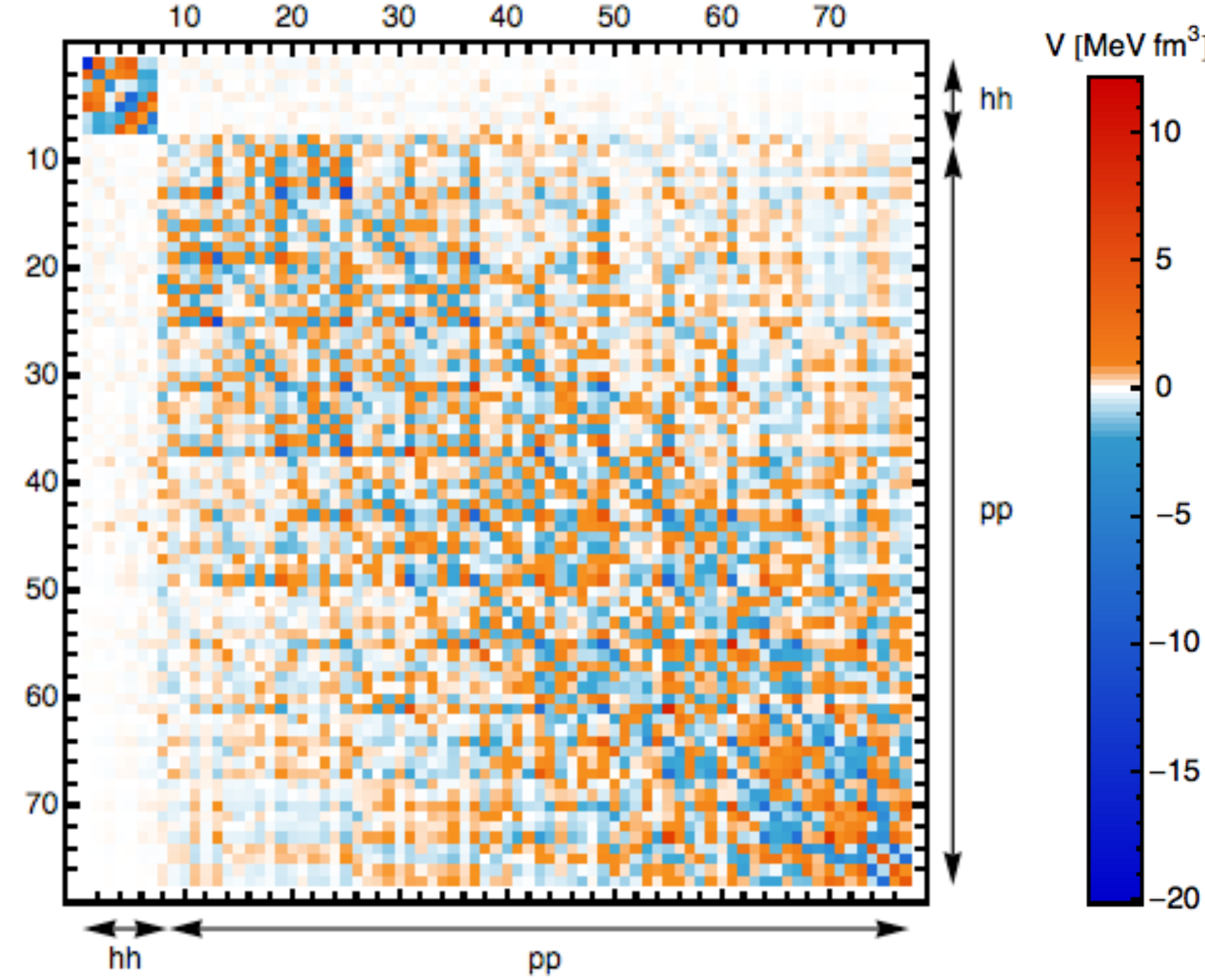




N3LO, $\lambda = 2.0\ \mathrm{fm}^{-1}, e_{\mathrm{Max}} = 8$

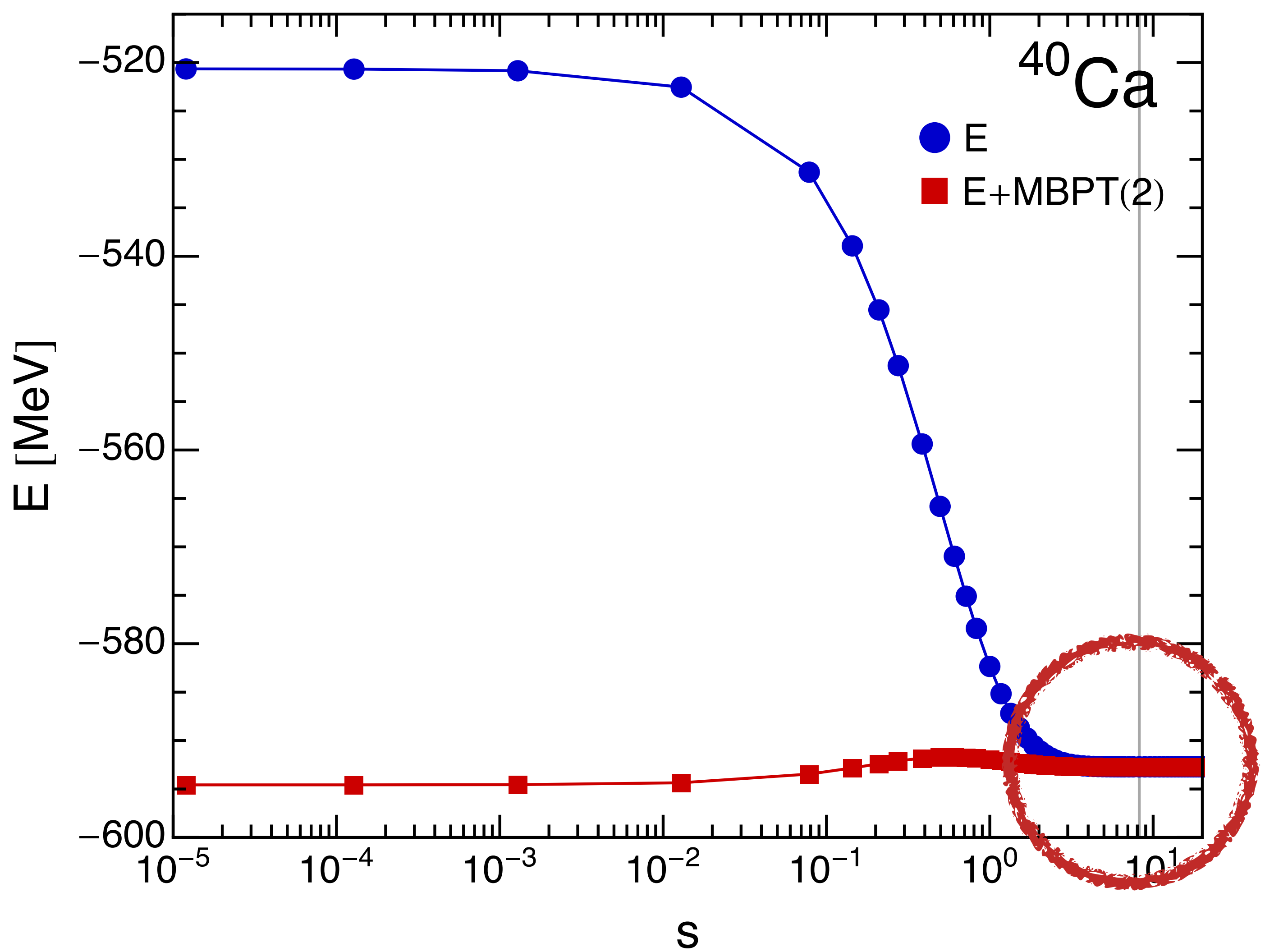
Decoupling

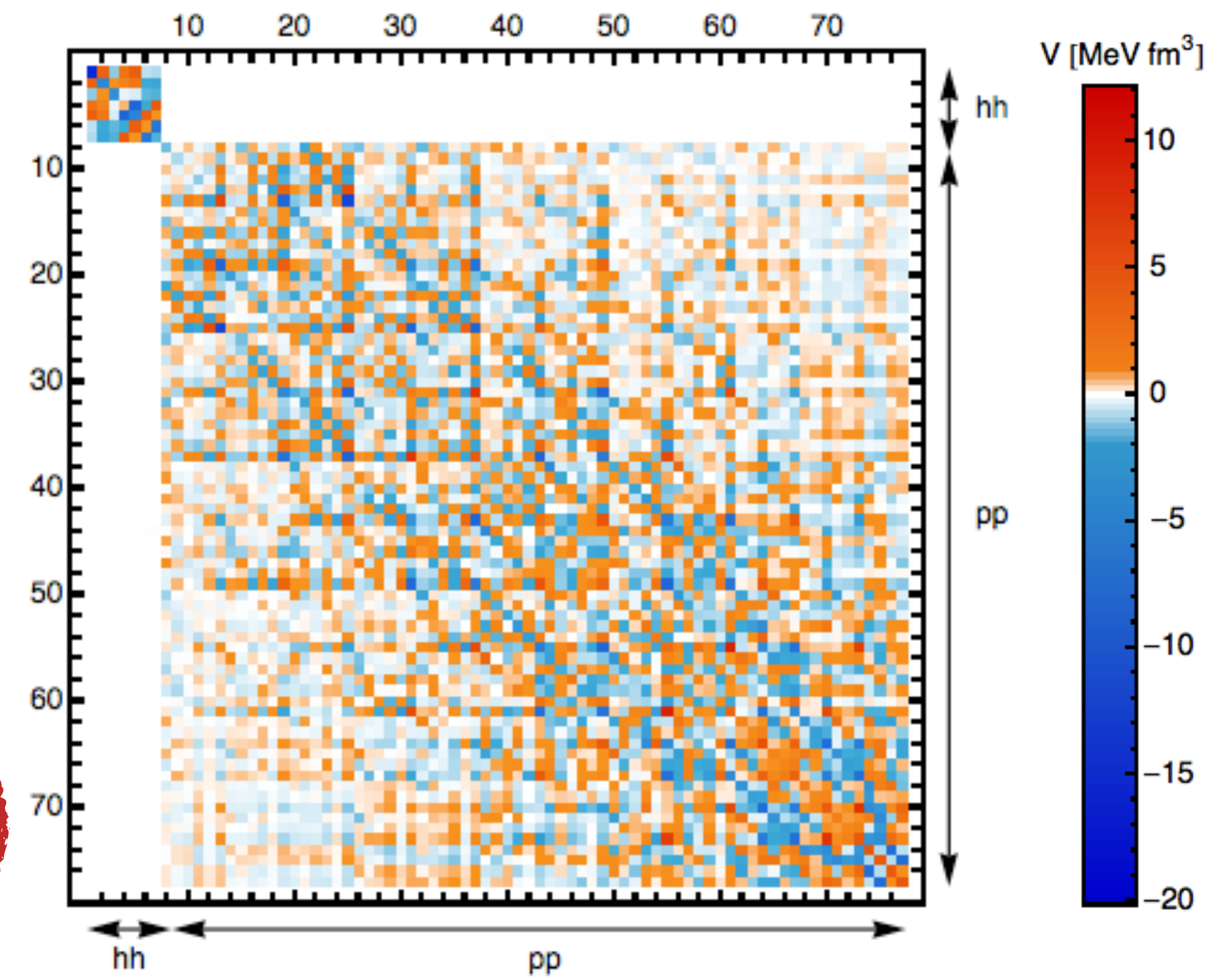




N3LO, $\lambda = 2.0\ \mathrm{fm}^{-1}, e_{\mathrm{Max}} = 8$

Decoupling



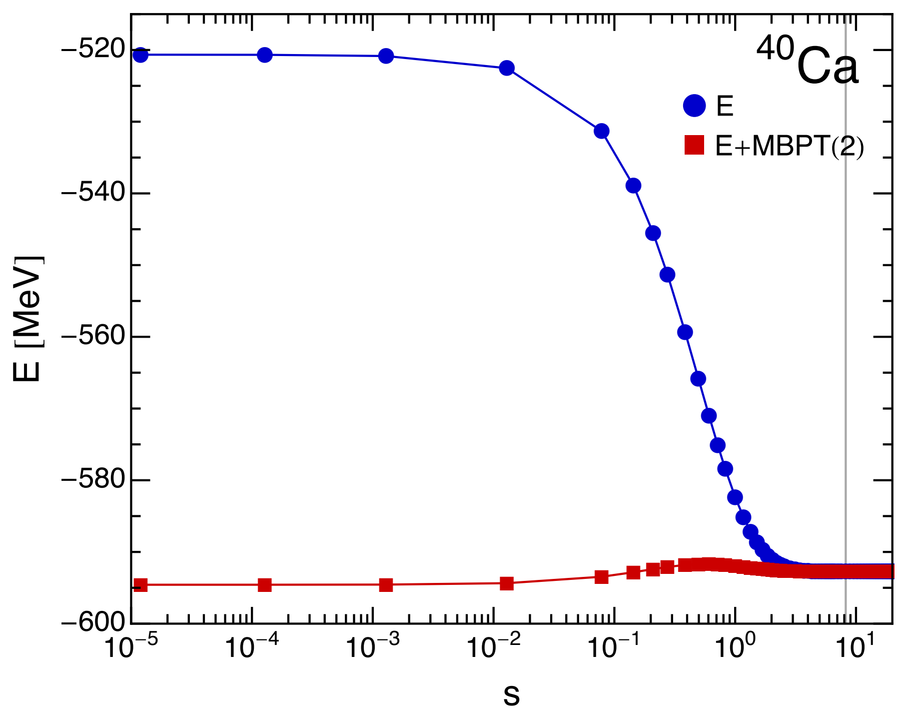


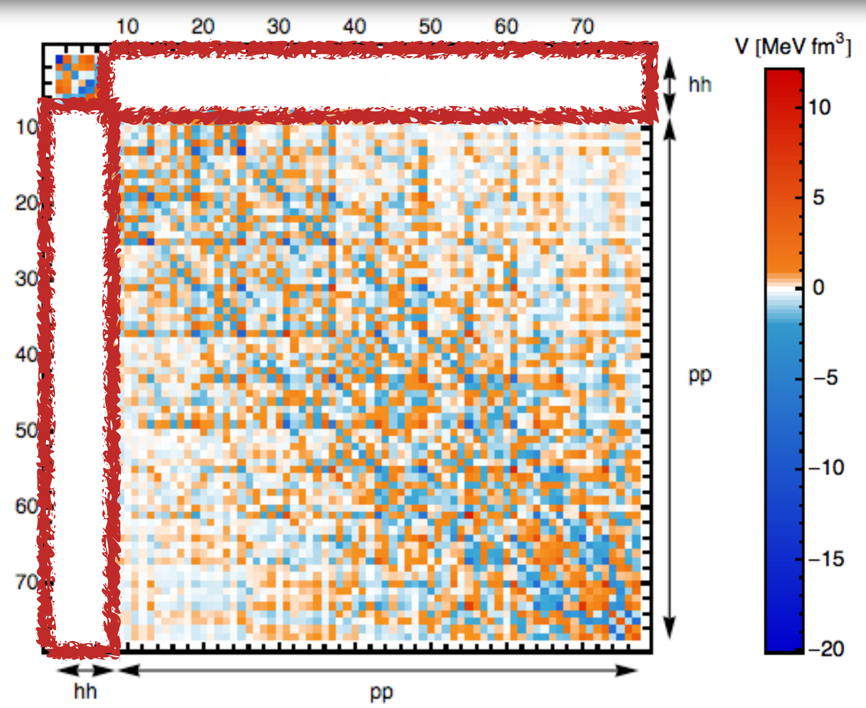
N3LO, $\lambda = 2.0\ \text{fm}^{-1}, e_{\text{Max}} = 8$

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**

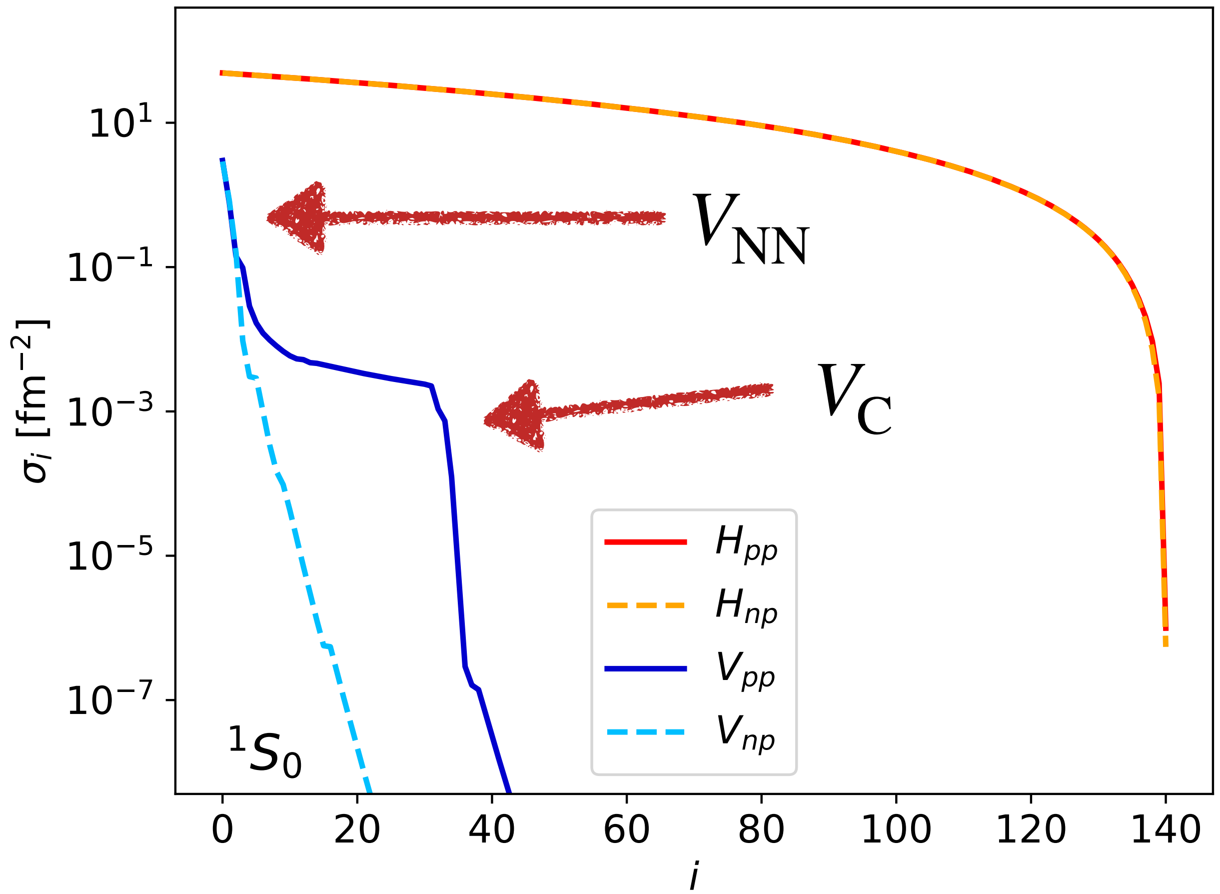
$$U(s)HU^{\dagger}(s)U(s)\left|\Psi_n\right\rangle = E_n U(s)\left|\Psi_n\right\rangle$$

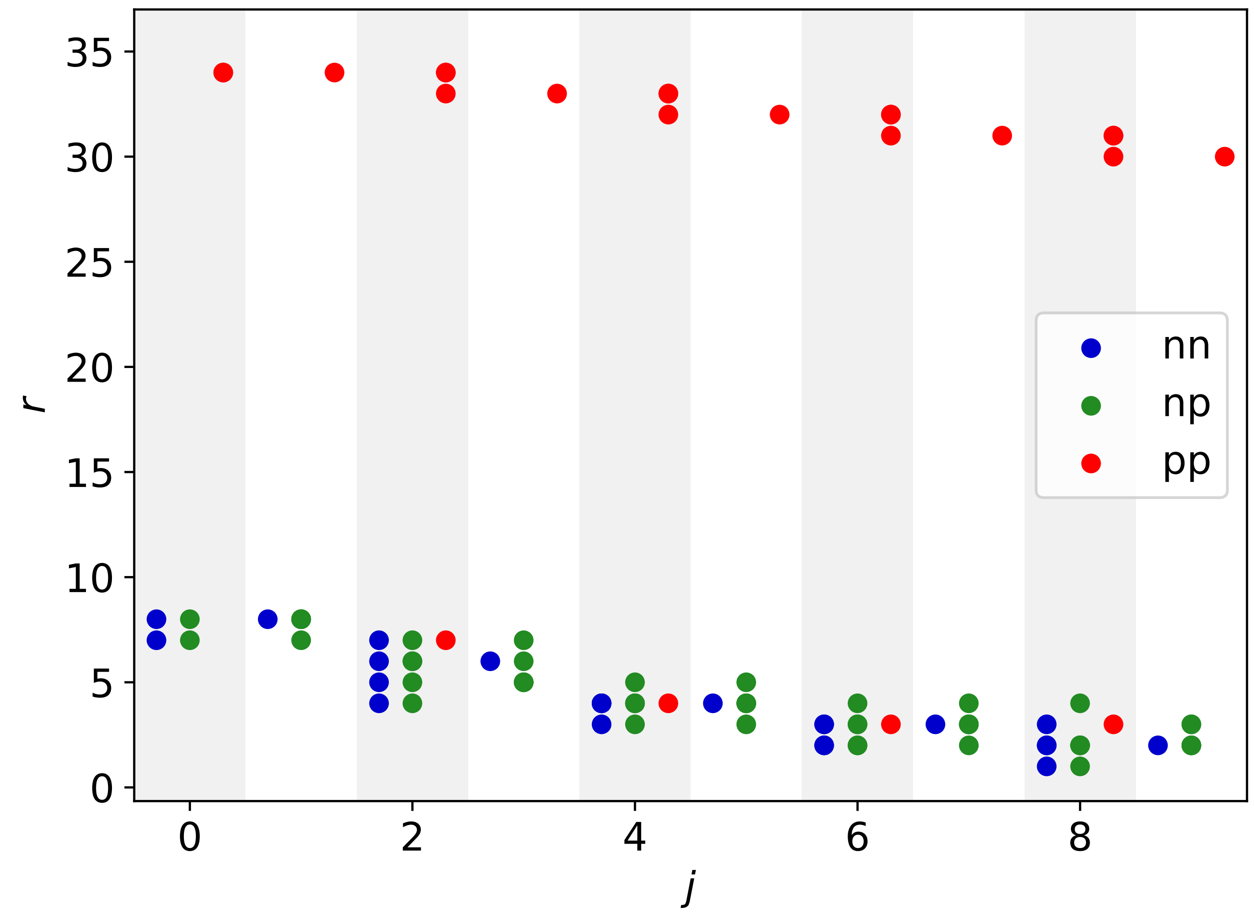
- reference state is ansatz for transformed, **less correlated** eigenstate:

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

Factorized Interactions

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

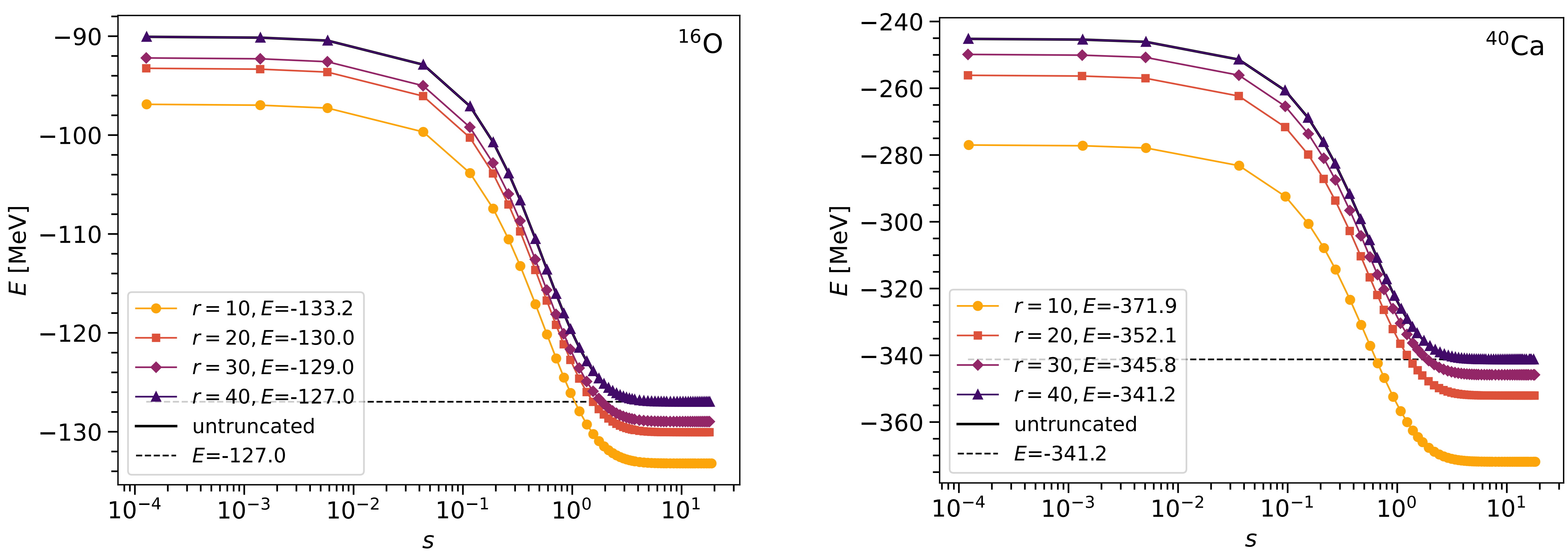




- O(10) operators, O(100) particles, but O(10^8-10^{12}) flow equations, basis dimension… there must be **redundancy**
- **NN interaction:** 5-10 SVD components (**short range**)
- **Coulomb interaction:** less well-behaved, but ~25-30 components sufficient (**long range, no explicit scale**)

Factorized Interactions

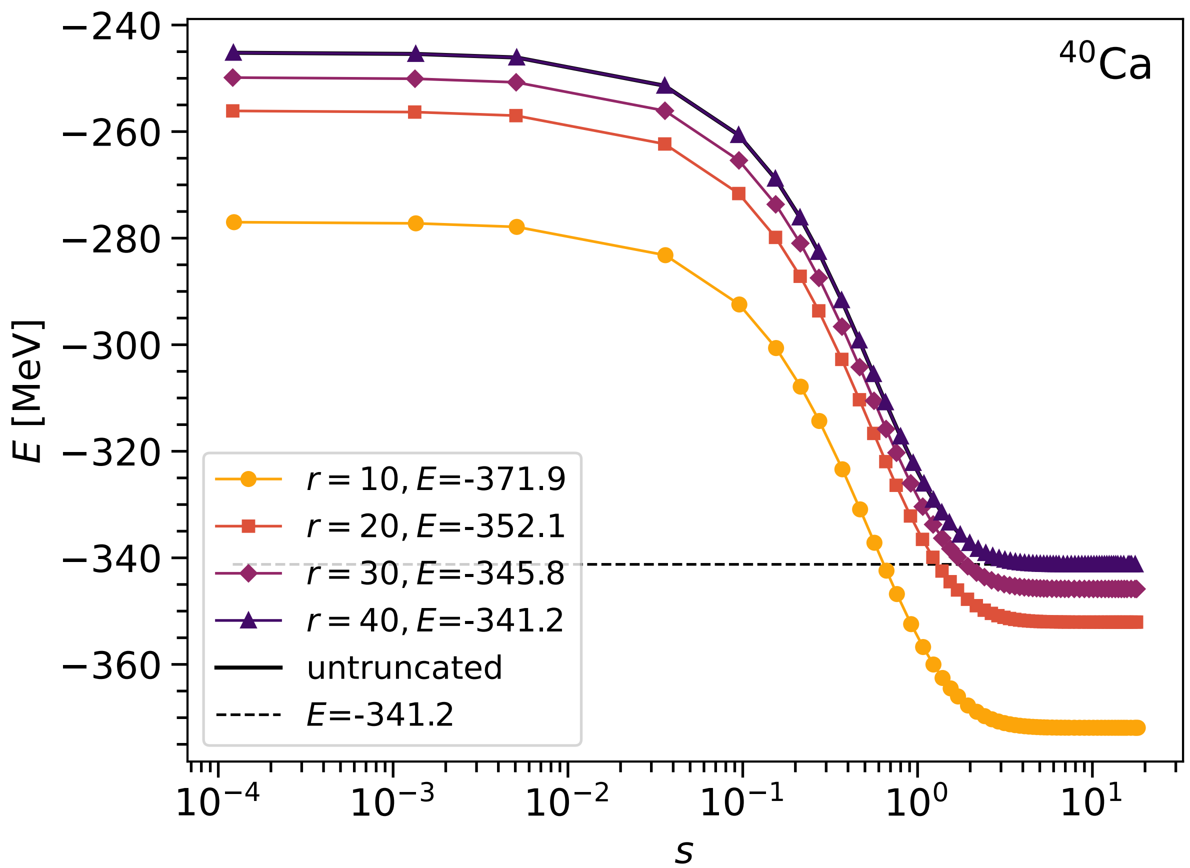
*B. Zhu, R. Wirth, HH, PRC **104**, 044002 (2021)*

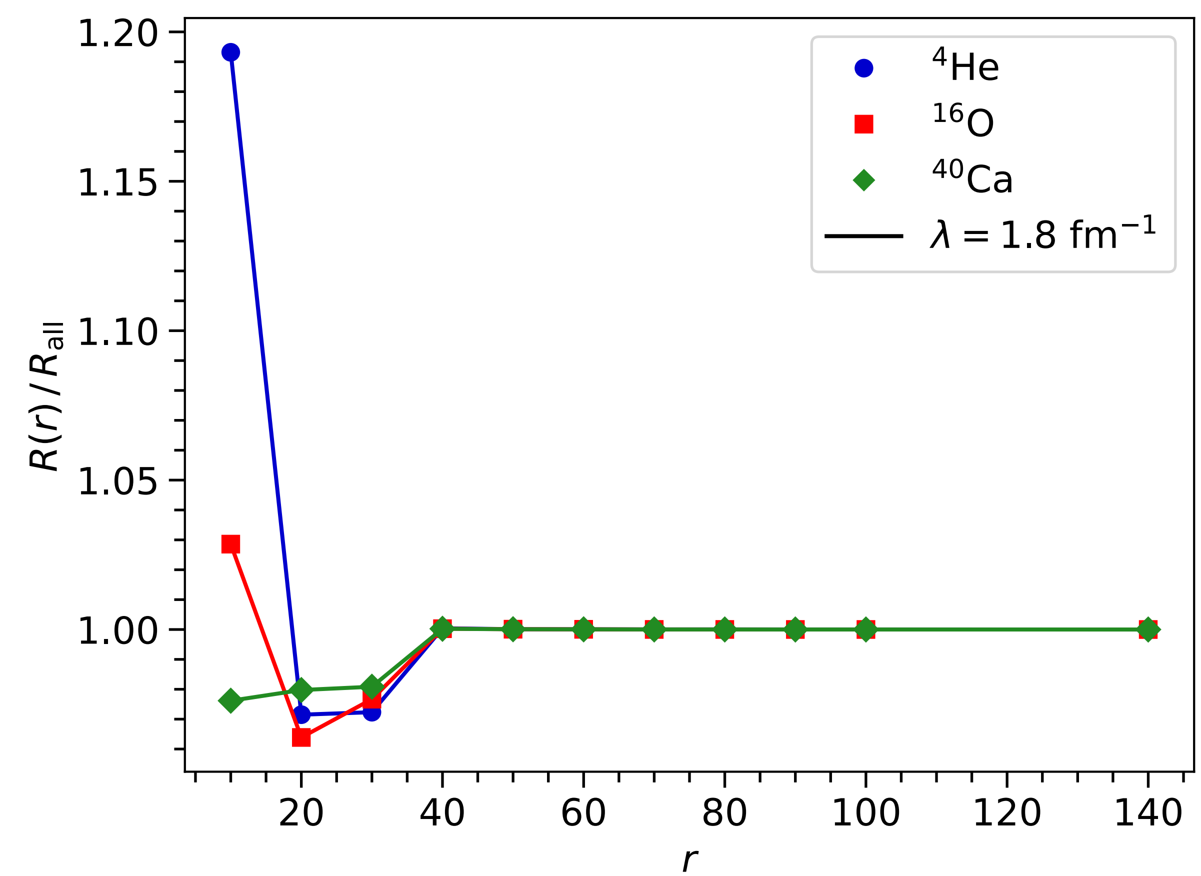


- NN interaction: free-space SRG evolution in component form (**IMSRG not yet**)
  - (3N interaction added to produce realistic binding / radii)
- free-space SRG effort and storage **reduced by several orders of magnitude**

Factorized Interactions

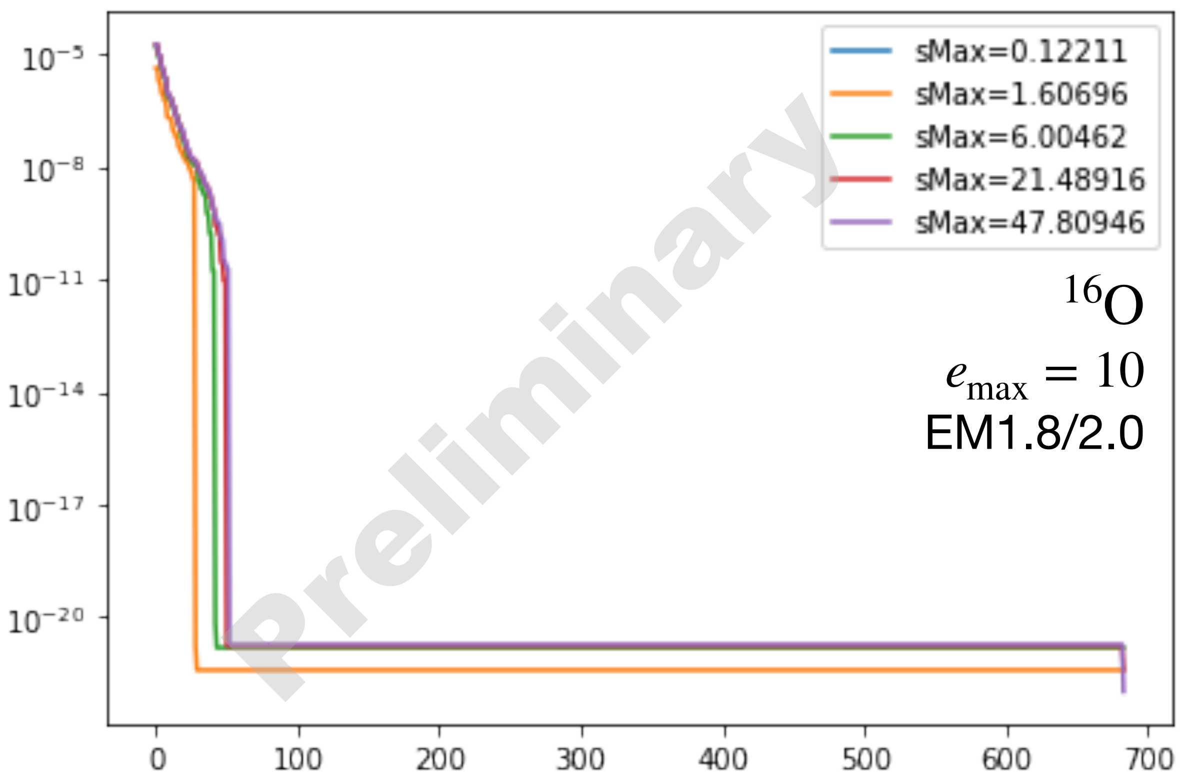
*B. Zhu, R. Wirth, HH, PRC **104**, 044002 (2021)*

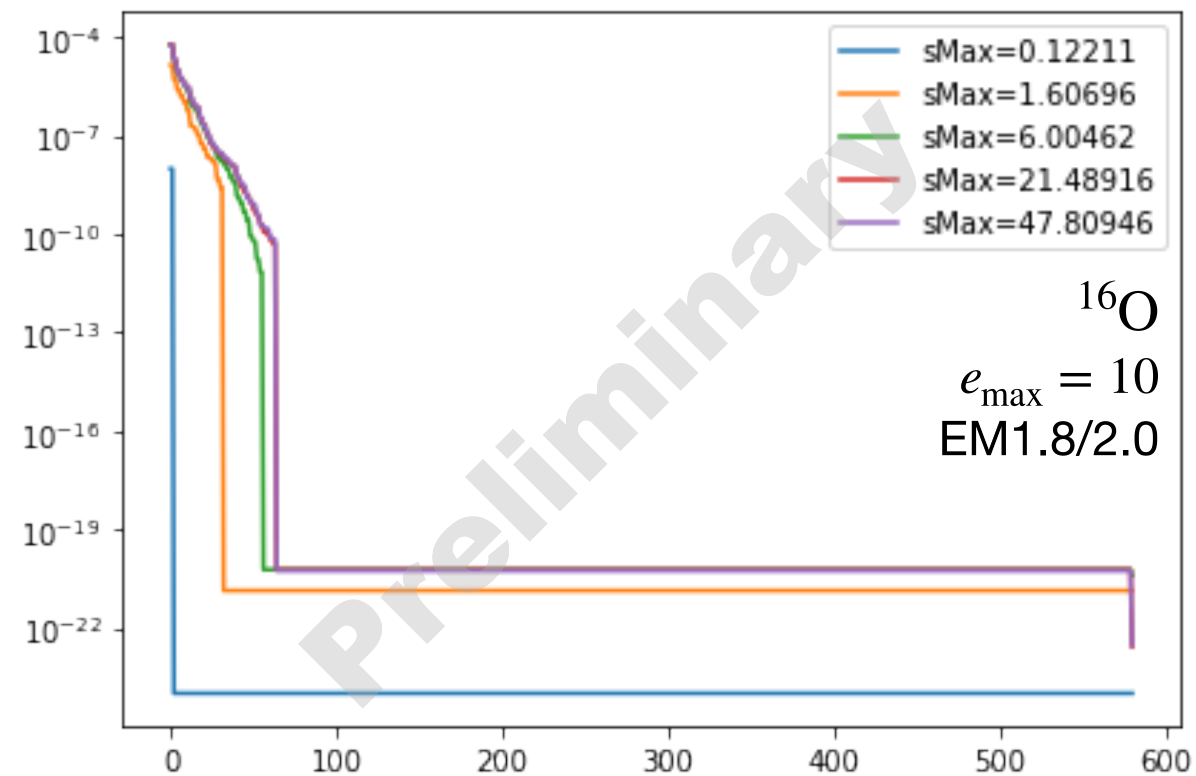




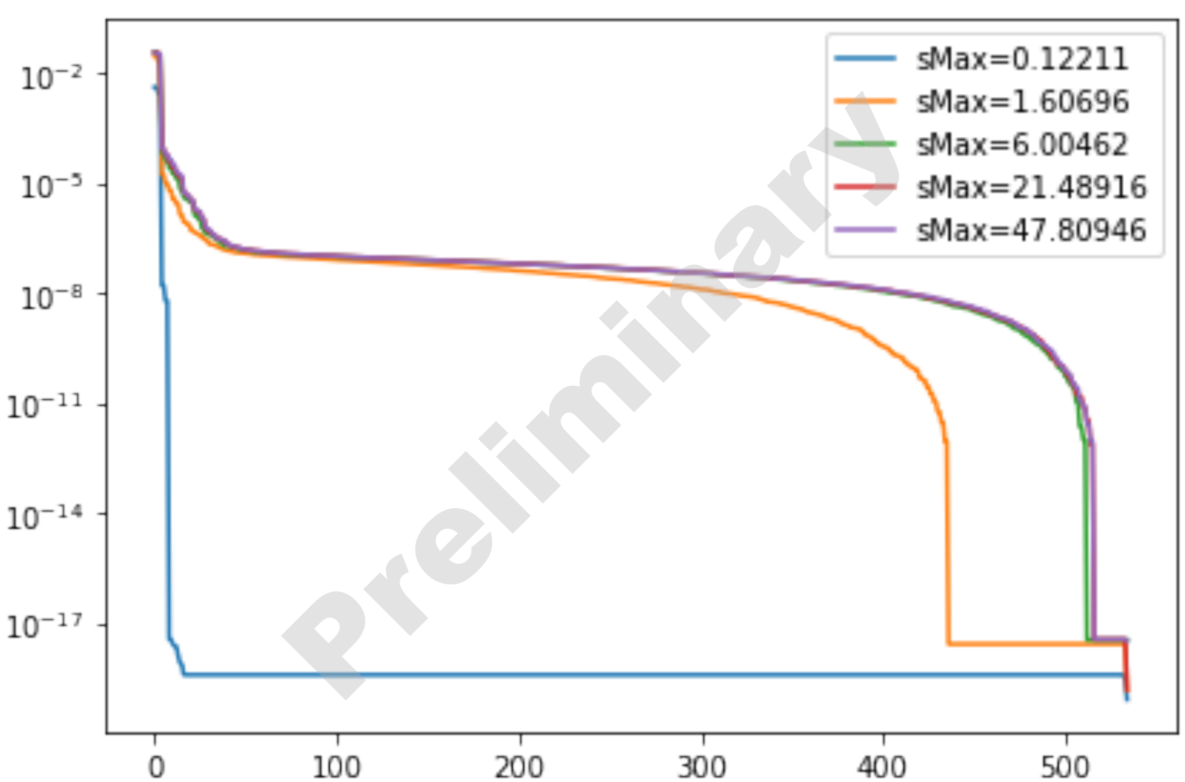
- implementing factorized SRG flow has **no adverse affect** on other observables / expectation values

SVD for Many-Body Calculation





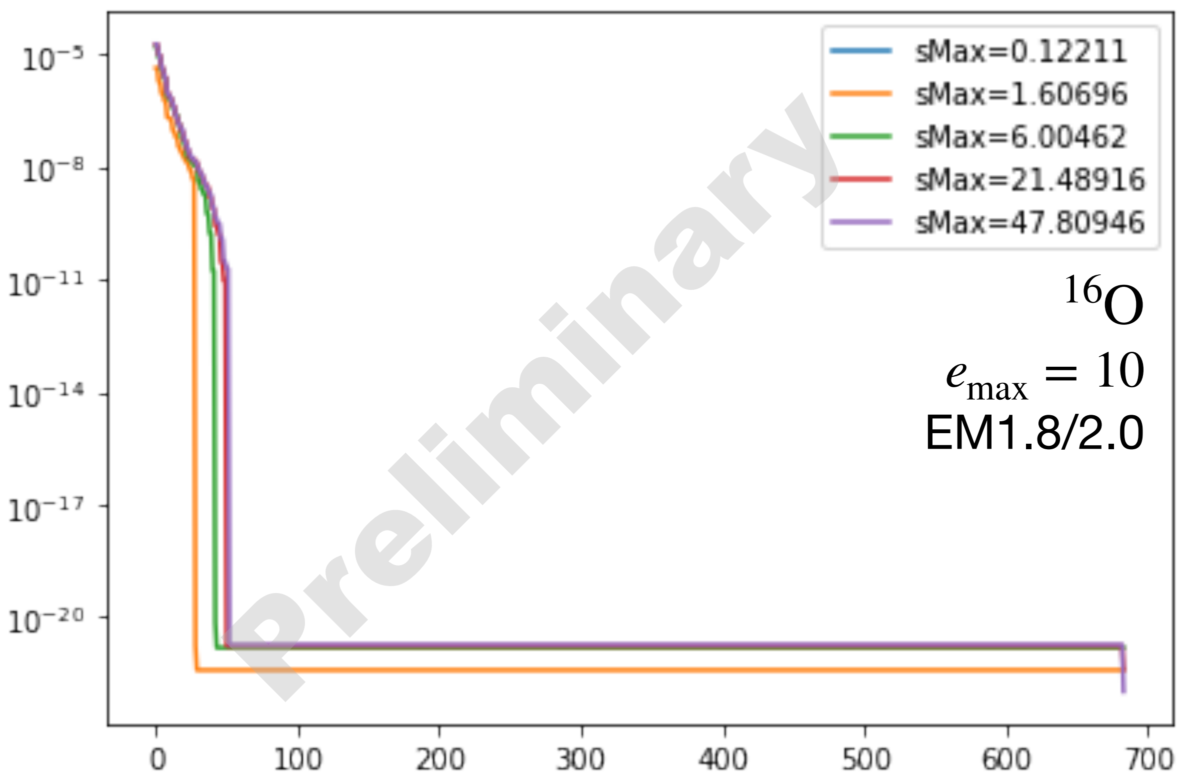
^{16}O, $e_{\rm max} = 10$, EM1.8/2.0

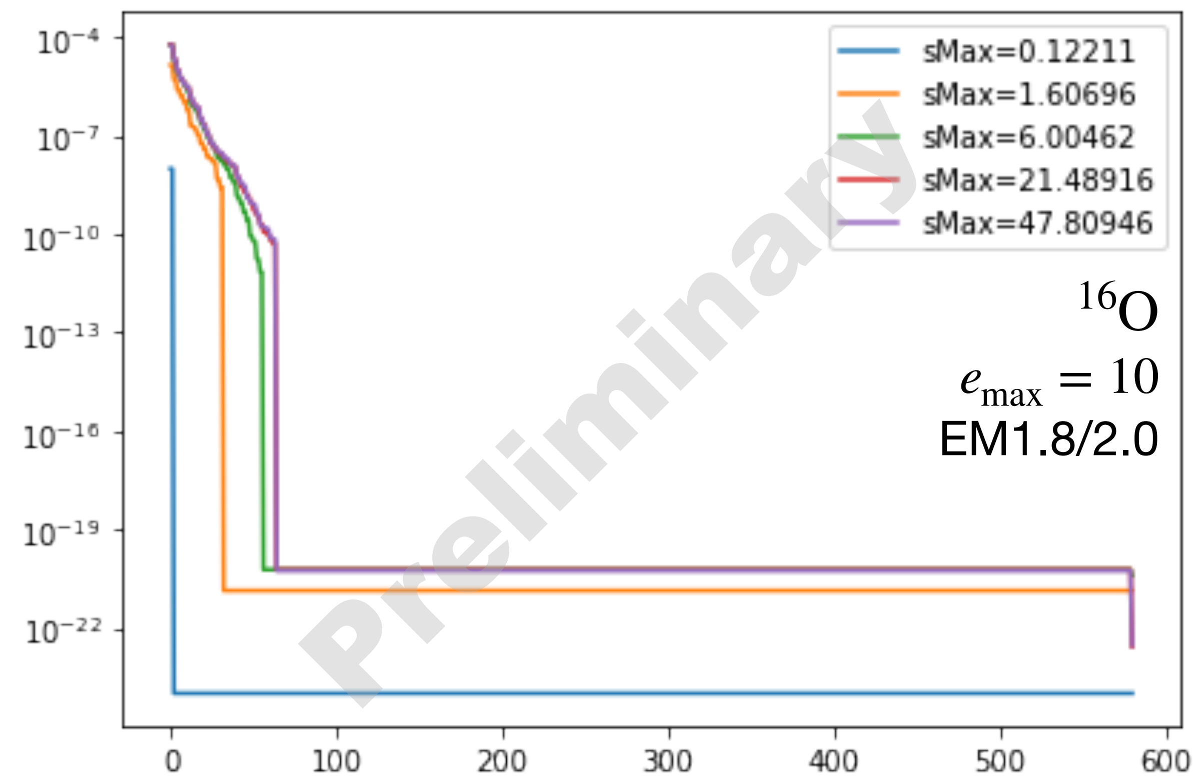


- **Magnus-IMSRG:**

$$U(s) = e^{\Omega(s)}$$

SVD for Many-Body Calculation





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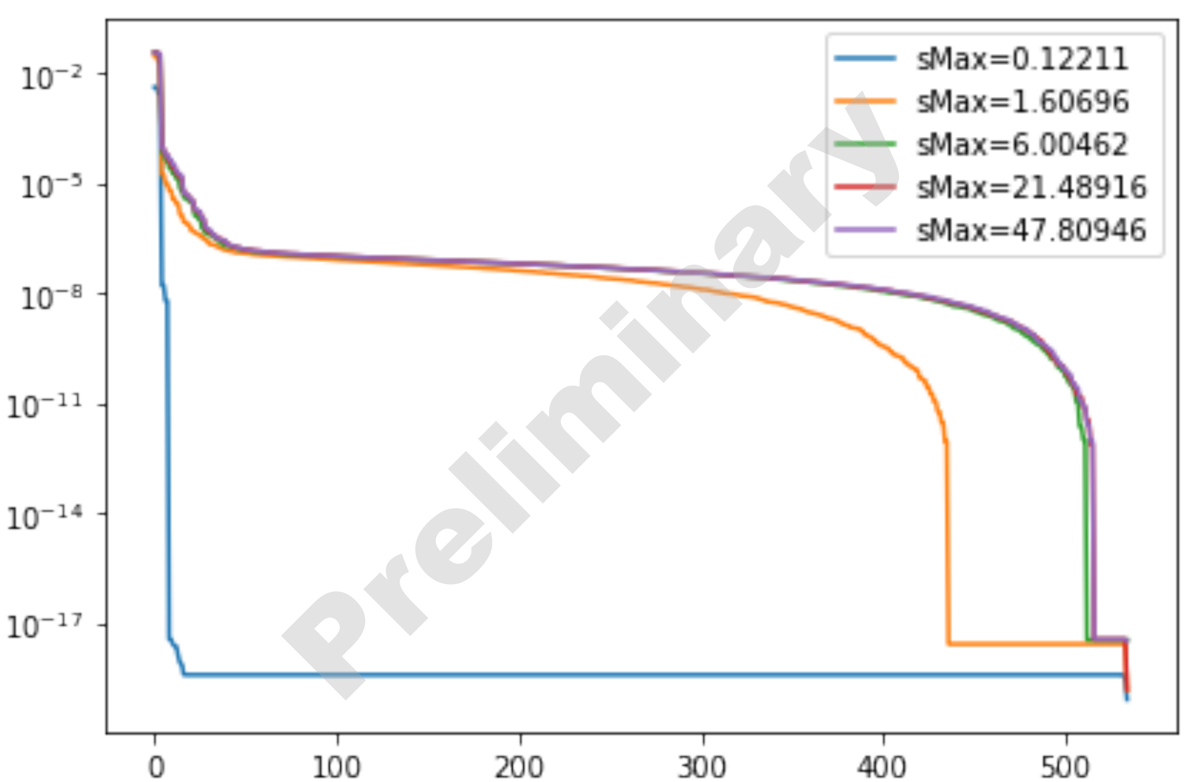

- **Magnus-IMSRG:**

$$U(s) = e^{\Omega(s)}$$

- SVD reveals that $\Omega(s)$ **has a low rank**