From Low-Energy QCD to Nuclear Structure

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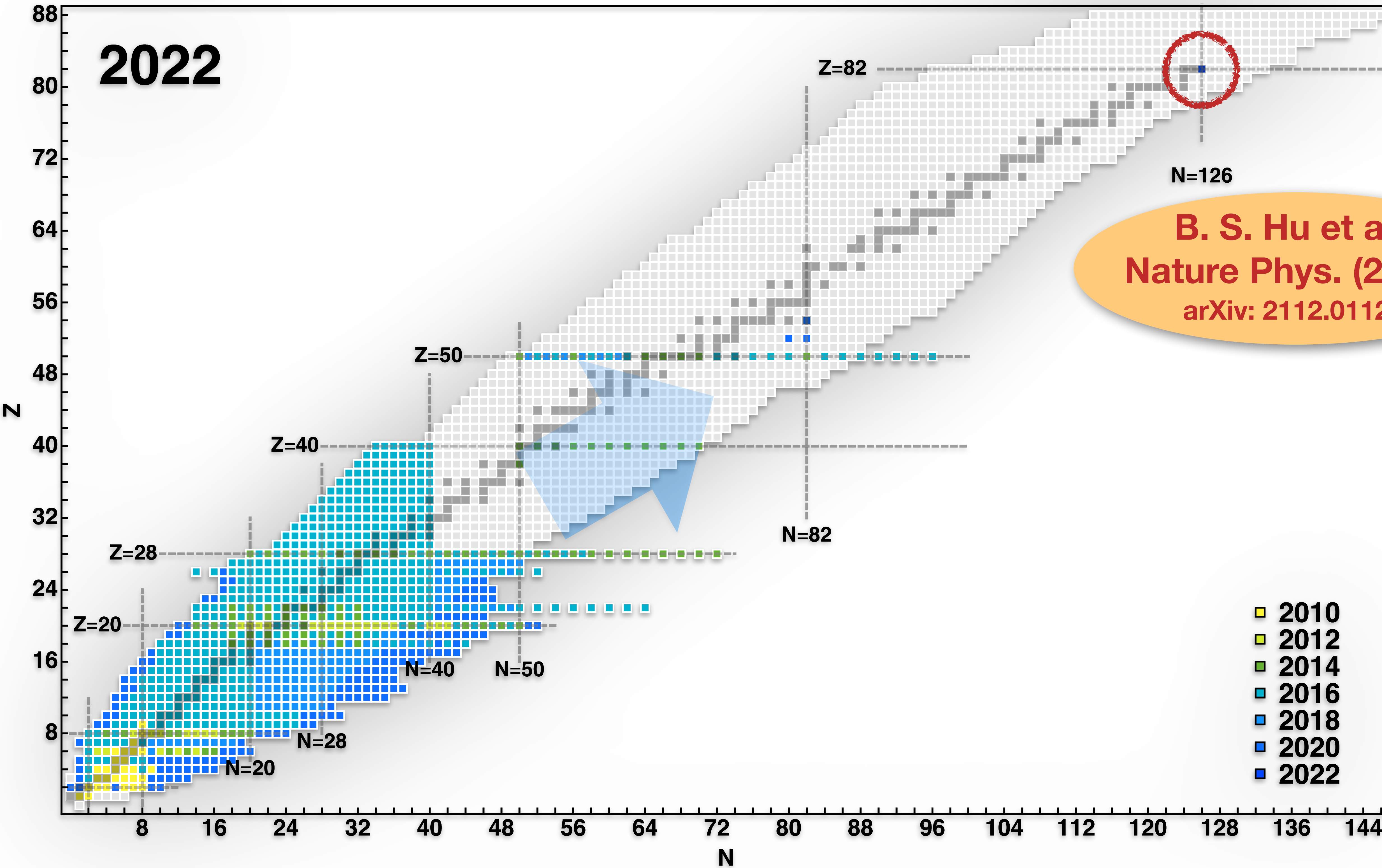
Progress in *Ab Initio* Calculations

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



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

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

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

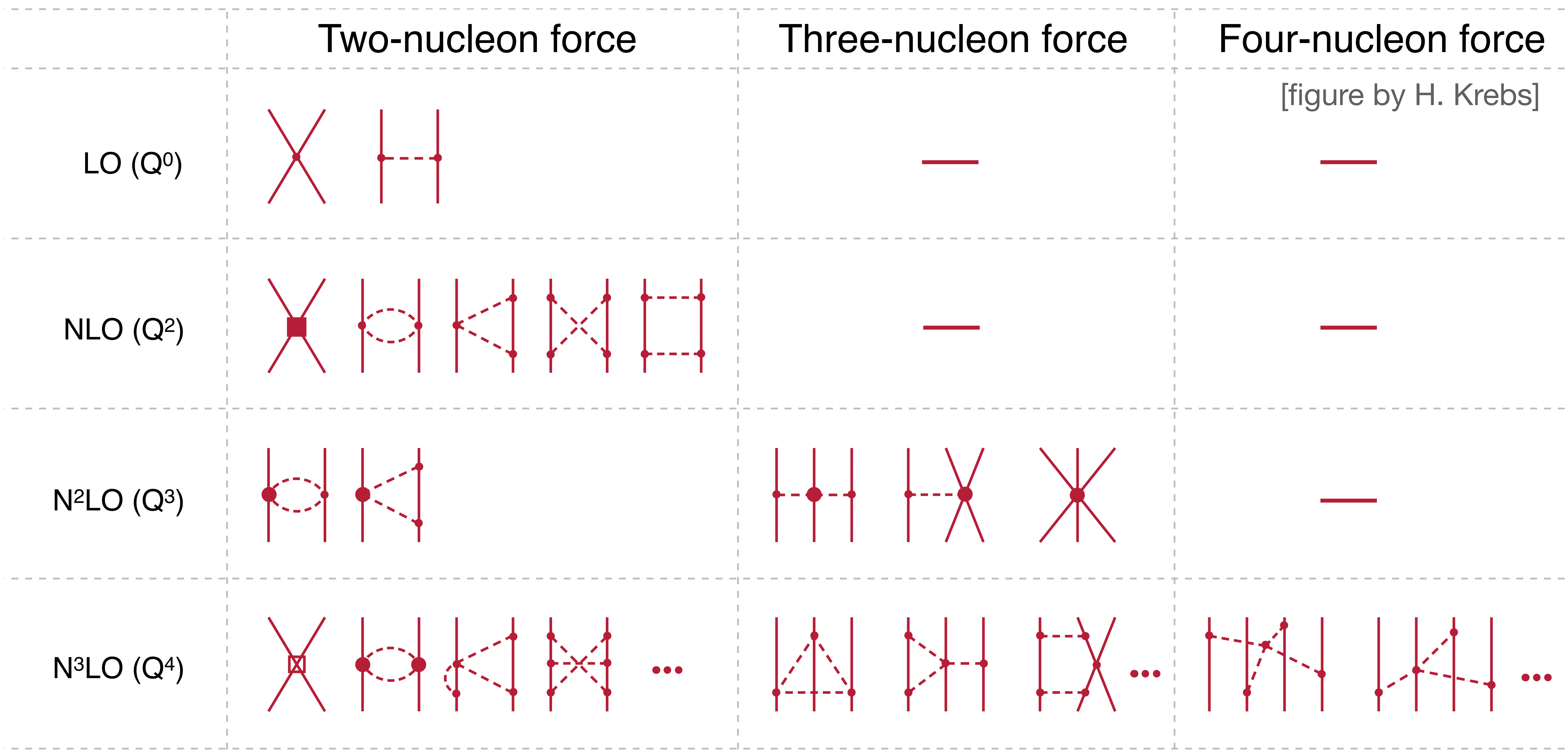
- symmetry restrictions
- model-space & many-body truncation(s)
- continuum

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 (e.g. **electroweak transitions**)

Current Interactions

PHYSICAL REVIEW C 91, 051301(R) (2015)

Accurate nuclear radii and binding energies from a chiral interaction

A. Ekström,[1,2] G. R. Jansen,[2,1] K. A. Wendt,[1,2] G. Hagen,[2,1] T. Papenbrock,[1,2] B. D. Carlsson,[3] C. Forssén,[3,1,2] M. Hjorth-Jensen,[4,5] P. Navrátil,[6] and W. Nazarewicz[4,2,7]
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[6]TRIUMF, 4004 Wesbrook Mall, Vancouver, British Columbia, V6T 2A3 Canada
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(Received 5 December 2014; revised manuscript received 10 April 2015; published 1 May 2015)

With the goal of developing predictive *ab initio* capability for light and medium-mass nuclei, two-nucleon and three-nucleon forces from chiral effective field theory are optimized simultaneously to low-energy nucleon-nucleon scattering data, as well as binding energies and radii of few-nucleon systems and selected isotopes of carbon and oxygen. Coupled-cluster calculations based on this interaction, named NNLO$_{sat}$, yield accurate binding energies and radii of nuclei up to ^{40}Ca, and are consistent with the empirical saturation point of symmetric nuclear matter. In addition, the low-lying collective $J^\pi = 3^-$ states in ^{16}O and ^{40}Ca are described accurately, while spectra for selected p- and sd-shell nuclei are in reasonable agreement with experiment.

DOI: 10.1103/PhysRevC.91.051301 PACS number(s): 21.30.−x, 21.10.−k, 21.45.−v, 21.60.De

PHYSICAL REVIEW LETTERS 120, 052503 (2018)

Light-Nuclei Spectra from Chiral Dynamics

M. Piarulli,[1] A. Baroni,[2] L. Girlanda,[3,4] A. Kievsky,[5] A. Lovato,[1,6] Ewing Lusk,[7] L. E. Marcucci,[5,8] Steven C. Pieper,[1] R. Schiavilla,[2,9] M. Viviani,[5] and R. B. Wiringa[1]
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(Received 31 July 2017; published 1 February 2018)

In recent years local chiral interactions have been derived and implemented in quantum Monte Carlo methods in order to test to what extent the chiral effective field theory framework impacts our knowledge of few- and many-body systems. In this Letter, we present Green's function Monte Carlo calculations of light nuclei based on the family of local two-body interactions presented by our group in a previous paper in conjunction with chiral three-body interactions fitted to bound- and scattering-state observables in the three-nucleon sector. These interactions include Δ intermediate states in their two-pion-exchange components. We obtain predictions for the energy levels and level ordering of nuclei in the mass range $A = 4$–12, accurate to $\leq 2\%$ of the binding energy, in very satisfactory agreement with experimental data.

DOI: 10.1103/PhysRevLett.120.052503

PHYSICAL REVIEW LETTERS 120, 122502 (2018)

Properties of Nuclei up to $A = 16$ using Local Chiral Interactions

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(Received 26 September 2017; revised manuscript received 29 January 2018; published 22 March 2018)

We report accurate quantum Monte Carlo calculations of nuclei up to $A = 16$ based on local chiral two- and three-nucleon interactions up to next-to-next-to-leading order. We examine the theoretical uncertainties associated with the chiral expansion and the cutoff in the theory, as well as the associated operator choices in the three-nucleon interactions. While in light nuclei the cutoff variation and systematic uncertainties are rather small, in ^{16}O these can be significant for large coordinate-space cutoffs. Overall, we show that chiral interactions constructed to reproduce properties of very light systems and nucleon-nucleon scattering give an excellent description of binding energies, charge radii, and form factors for all these nuclei, including open-shell systems in $A = 6$ and 12.

Eur. Phys. J. A (2018) 54: 86
DOI 10.1140/epja/i2018-12516-4
THE EUROPEAN PHYSICAL JOURN
Regular Article – Theoretical Physics

Semilocal momentum-space regularized chiral two-nucleon potentials up to fifth order

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Published online: 28 May 2018

Communicated by T. Duguet

Abstract. We introduce new semilocal two-nucleon potentials up to fifth order in the chiral expansion. We employ a simple regularization approach for the pion exchange contributions which i) maintains the long-range part of the interaction, ii) is implemented in momentum space and iii) can be straightforwardly applied to regularize many-body forces and current operators. We discuss in detail the two-nucleon contact interactions at fourth order and demonstrate that three terms out of fifteen used in previous calculations can be eliminated via suitably chosen unitary transformations. The removal of the redundant contact terms results in a drastic simplification of the fits to scattering data and leads to interactions which are much softer (*i.e.*, more perturbative) than our recent semilocal coordinate-space regularized potentials. Using the pion-nucleon low-energy constants from matching pion-nucleon Roy-Steiner equations to chiral perturbation theory, we perform a comprehensive analysis of nucleon-nucleon scattering and the deuteron properties up to fifth chiral order and study the impact of the leading F-wave two-nucleon contact interactions which appear at sixth order. The resulting chiral potentials at fifth order lead to an outstanding description of the proton-proton and neutron-proton scattering data from the self-consistent Granada-2013 database below the pion production threshold, which is significantly better than for any other chiral potential. For the first time, the chiral potentials match in precision and even outperform the available high-precision phenomenological potentials, while the number of adjustable parameters is, at the same time, reduced by about ∼ 40%. Last but not least, we perform a detailed error analysis and, in particular, quantify for the first time the statistical uncertainties of the fourth- and the considered sixth-order contact interactions.

PHYSICAL REVIEW C 100, 024318 (2019)

Probing chiral interactions up to next-to-next-to-next-to-leading order in medium-mass nuclei

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(Received 29 April 2019; published 12 August 2019)

We study ground-state energies and charge radii of closed-shell medium-mass nuclei based on novel chiral nucleon-nucleon (*NN*) and three-nucleon (3*N*) interactions, with a focus on exploring the connections between finite nuclei and nuclear matter. To this end, we perform in-medium similarity renormalization group (IM-SRG) calculations based on chiral interactions at next-to-leading order (NLO), N^{2}LO, and N^{3}LO, where the 3*N* interactions at N^{2}LO and N^{3}LO are fit to the empirical saturation point of nuclear matter and to the triton binding energy. Our results for energies and radii at N^{2}LO and N^{3}LO overlap within uncertainties, and the cutoff variation of the interactions is within the EFT uncertainty band. We find underbound ground-state energies, as expected from the comparison to the empirical saturation point. The radii are systematically too large, but the agreement with experiment is better. We further explore variations of the 3*N* couplings to test their sensitivity in nuclei. While nuclear matter at saturation density is quite sensitive to the 3*N* couplings, we find a considerably weaker dependence in medium-mass nuclei. In addition, we explore a consistent momentum-space SRG evolution of these *NN* and 3*N* interactions, exhibiting improved many-body convergence. For the SRG-evolved interactions, the sensitivity to the 3*N* couplings is found to be stronger in medium-mass nuclei.

DOI: 10.1103/PhysRevC.100.024318

PHYSICAL REVIEW C 101, 014318 (2020)

Novel chiral Hamiltonian and observables in light and medium-mass nuclei

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(Received 23 July 2019; revised manuscript received 6 November 2019; published 22 January 2020)

Background: Recent advances in nuclear structure theory have led to the availability of several complementary *ab initio* many-body techniques applicable to light and medium-mass nuclei as well as nuclear matter. After successful benchmarks of different approaches, the focus is moving to the development of improved models of nuclear Hamiltonians, currently representing the largest source of uncertainty in *ab initio* calculations of nuclear systems. In particular, none of the existing two- plus three-body interactions is capable of satisfactorily reproducing all the observables of interest in medium-mass nuclei.
Purpose: A novel parametrization of a Hamiltonian based on chiral effective field theory is introduced. Specifically, three-nucleon operators at next-to-next-to-leading order are combined with an existing (and successful) two-body interaction containing terms up to next-to-next-to-next-to-leading order. The resulting potential is labeled $NN + 3N$(lnl). The objective of the present work is to investigate the performance of this new Hamiltonian across light and medium-mass nuclei.

PHYSICAL REVIEW C 102, 054301 (2020)

Accurate bulk properties of nuclei from $A = 2$ to ∞ from potentials with Δ isobars

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(Received 2 July 2020; revised 26 August 2020; accepted 16 October 2020; published 2 November 2020)

We optimize Δ-full nuclear interactions from chiral effective field theory. The low-energy constants of the contact potentials are constrained by two-body scattering phase shifts, and by properties of bound state of $A = 2$ to 4 nucleon systems and nuclear matter. The pion-nucleon couplings are taken from a Roy-Steiner analysis. The resulting interactions yield accurate binding energies and radii for a range of nuclei from $A = 16$ to $A = 132$, and provide accurate equations of state for nuclear matter and realistic symmetry energies. Selected excited states are also in agreement with data.

DOI: 10.1103/PhysRevC.102.054301

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Family of chiral two- plus three-nucleon interactions for accurate nuclear structure studies

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ABSTRACT
We present a family of nucleon-nucleon (NN) plus three-nucleon (3N) interactions up to N^{3}LO in the chiral expansion that provides an accurate *ab initio* description of ground-state energies and charge radii up to the medium-mass regime with quantified theory uncertainties. Starting from the NN interactions proposed by Entem, Machleidt and Nosyk, we construct 3N interactions with consistent chiral order, non-local regulator, and cutoff value and explore the dependence of nuclear observables over a range of mass numbers on the 3N low-energy constants. By fixing these constants using the ^{3}H and ^{16}O ground-state energies, we obtain interactions that robustly reproduce experimental energies and radii for a large range from p-shell nuclei to the nickel isotopic chain and resolve many of the deficiencies of previous interactions. Based on the order-by-order convergence and the cutoff dependence of nuclear observables, we assess the uncertainties due the interaction, which yield a significant contribution to the total theory uncertainty.

Current Interactions

FRIB

- **NN and 3N forces at through order** N3LO, some NN forces available at even higher orders
  [cf. Epelbaum et al., Front. Phys. 8, 98 (2020) and references therein]
  - local, semilocal, nonlocal **regulators**
  - with and without **virtual Δ isobars**

also see talk by M. Piarulli

- need to account f… **ween LECs as well as observables**
  [see, e.g., Reinert et al., EPJA 54, 86; Wesolowski et. al, PRC 104, 064001 and refs. therein]

- **tensions revealed in LEC fits:** e.g., optimal 3NF LECs for medium-mass nuclei vs. nuclear matter
  [cf. Hoppe et al., PRC 100, 024318; Hüther et al., PLB 808, 135651, …]

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)

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

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

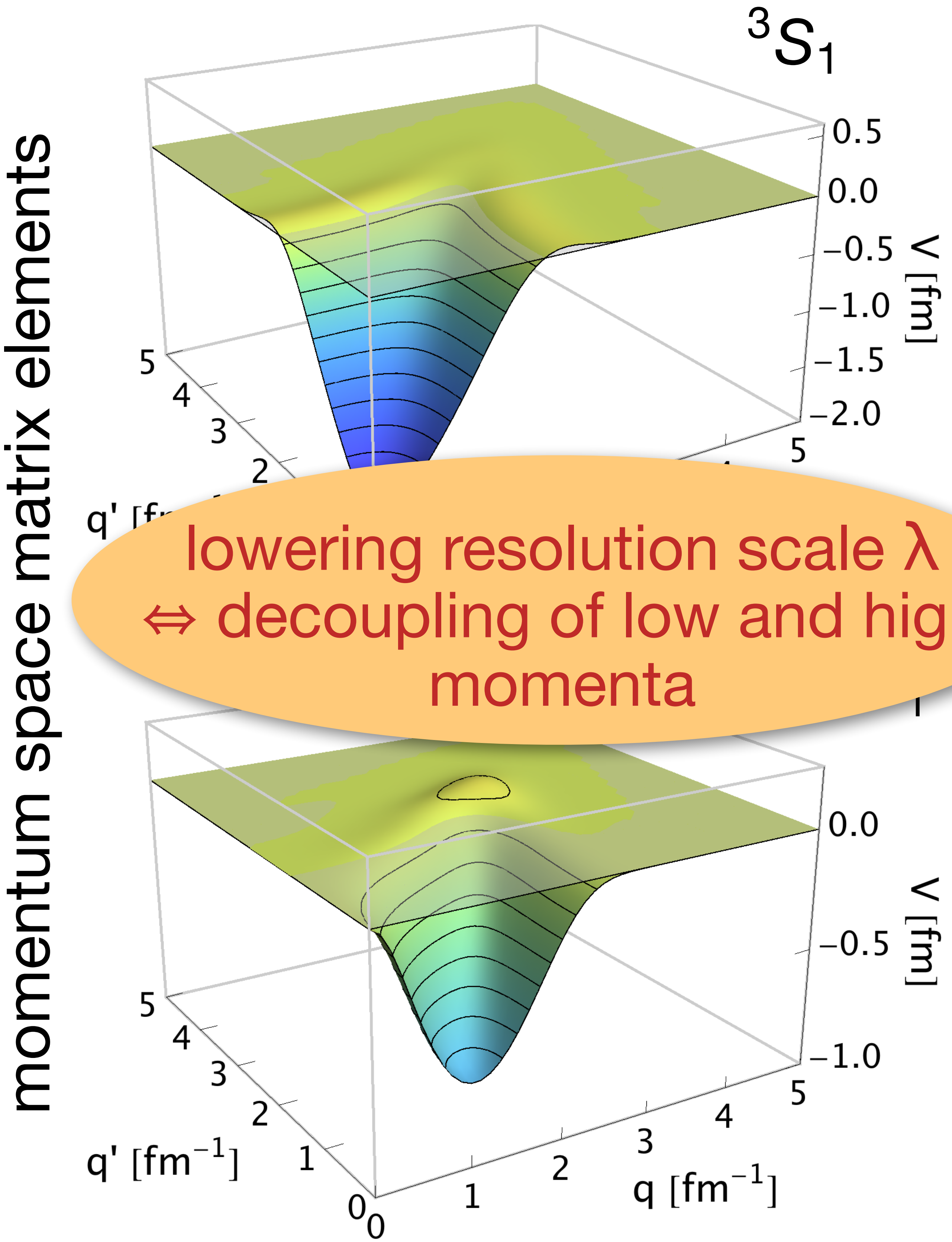
- choose $\eta(s)$ to achieve desired behavior, e.g.,

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

  to suppress (suitably defined) off-diagonal Hamiltonian

- consistent evolution for all observables of interest

SRG in Two-Body Space



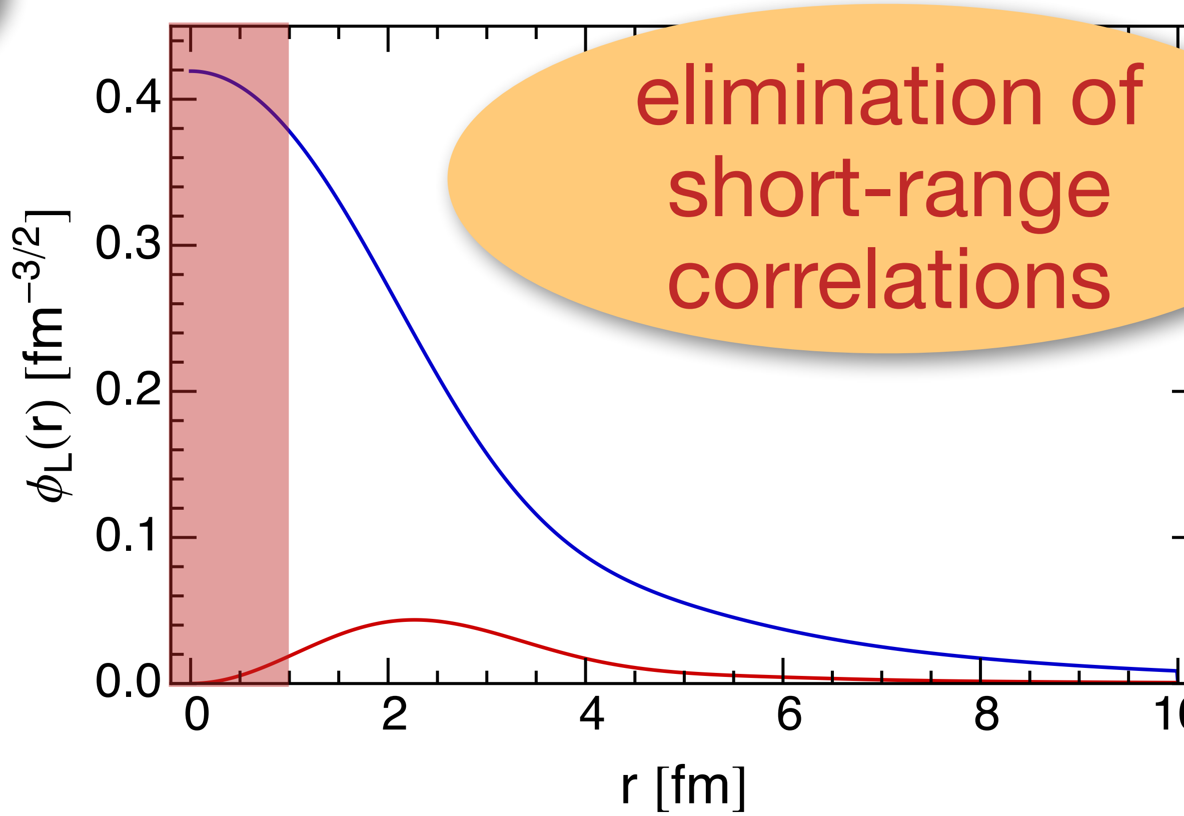
lowering resolution scale λ
⇔ decoupling of low and high momenta

λ = 1.8 fm^{-1}

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

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

deuteron wave function



elimination of short-range correlations

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

Ab Initio Many-Body Methods

Recent(-ish) Reviews:

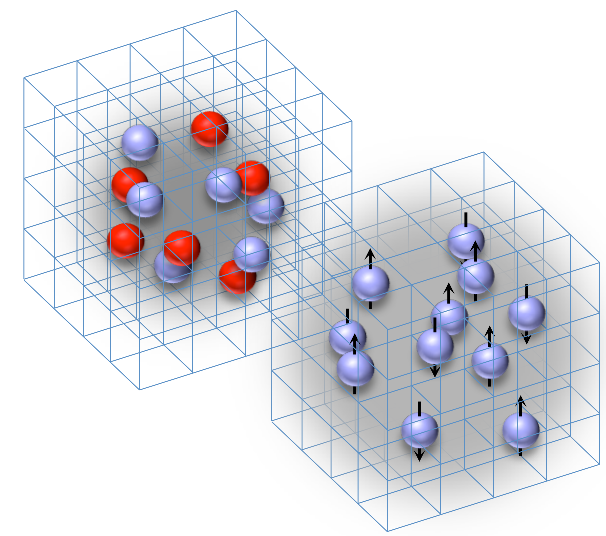
HH, Front. Phys. **8**, 379 (2020)
S. Gandolfi, D. Lonardoni, A. Lovato and M. Piarulli, Front. Phys. **8**, 117 (2020)
D. Lee, Front. Phys. **8**, 174 (2020)
V. Somà, Front. Phys. **8**, 340 (2020)

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

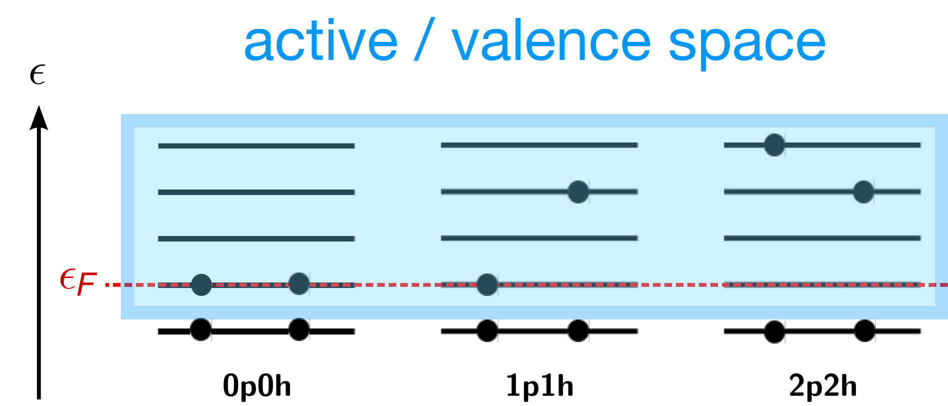
Paradigms

- **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)

talks by T. Papenbrock & G. Hagen

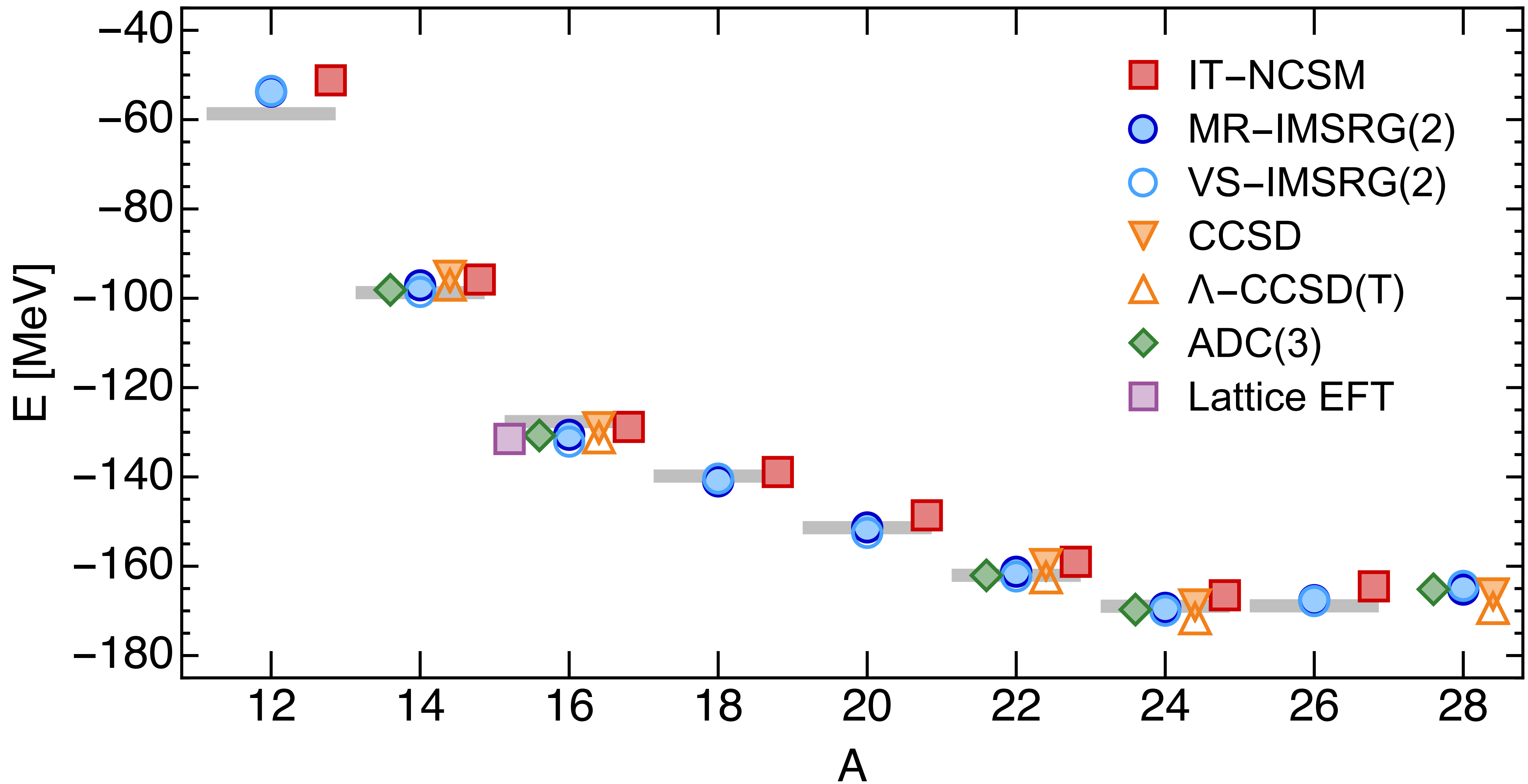


- **Configuration Space / Coordinate Space: Geometric Expansions**
  - deformed HF(B) + projection
  - projected Generator Coordinate Method (PGCM)
  - symmetry-adapted NCSM

also see talk by J.-P. Ebran

Consistency: Oxygen Isotopes

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



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

(Multi-Reference) In-Medium Similarity Renormalization Group

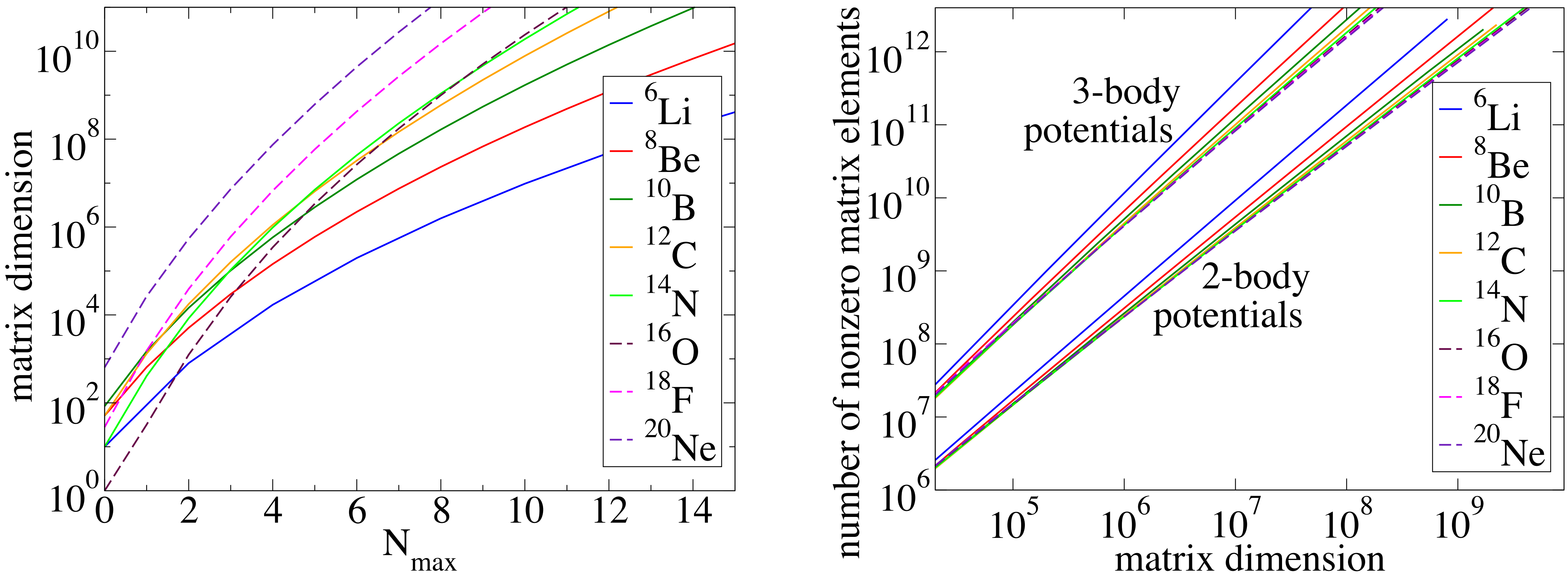
HH, Phys. Scripta, Phys. Scripta 92, 023002 (2017)

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)

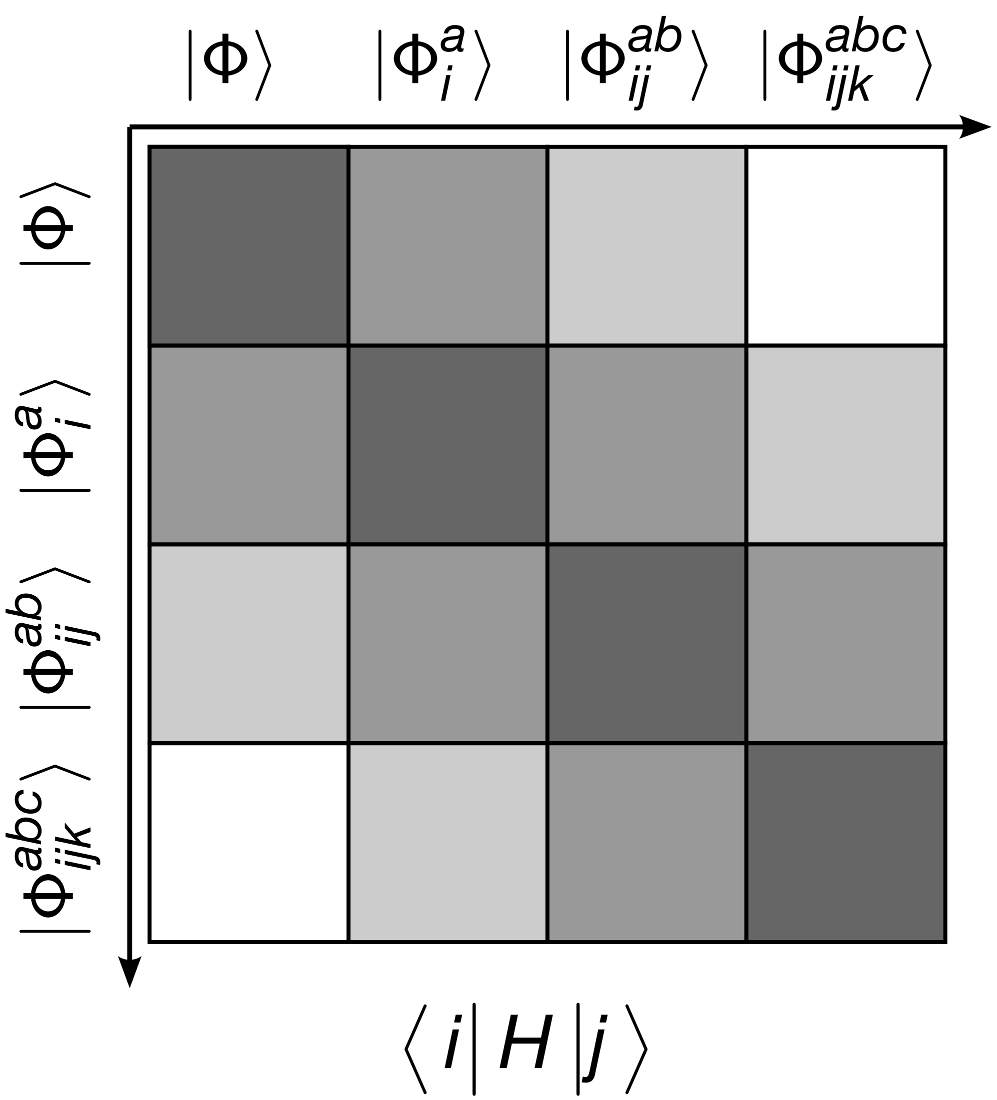
Large-Scale Diagonalization



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

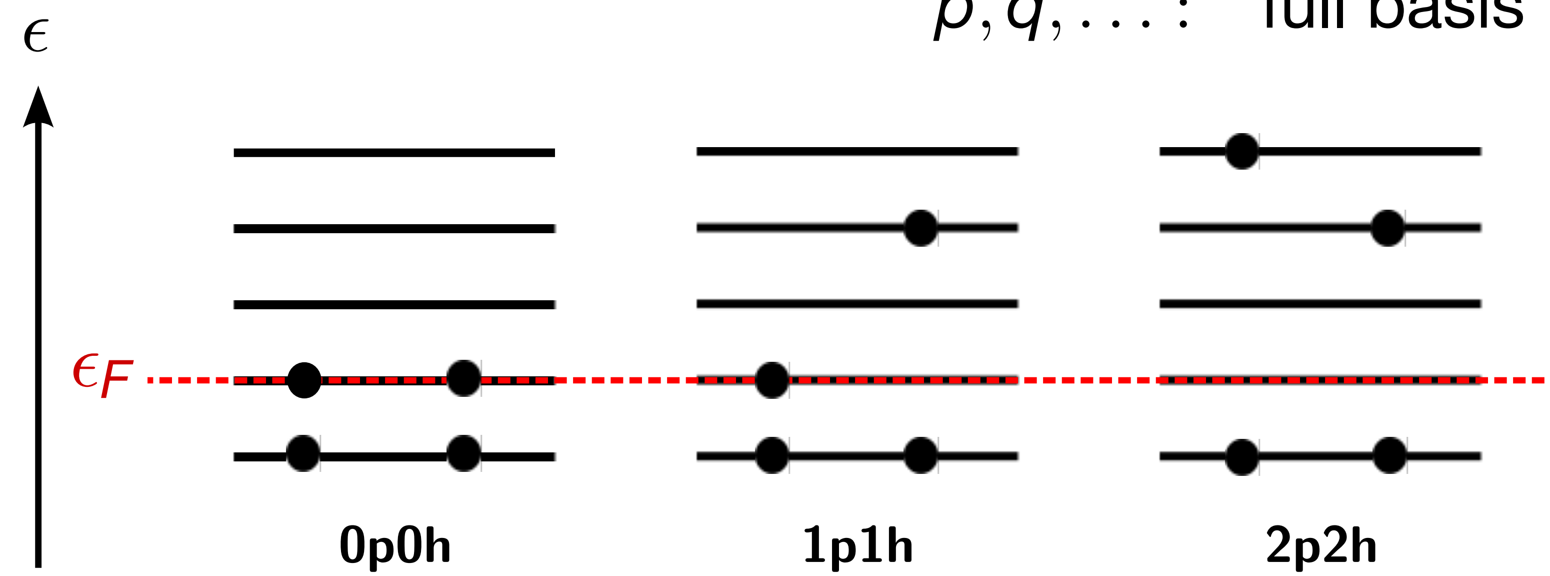
Transforming the Hamiltonian



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

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

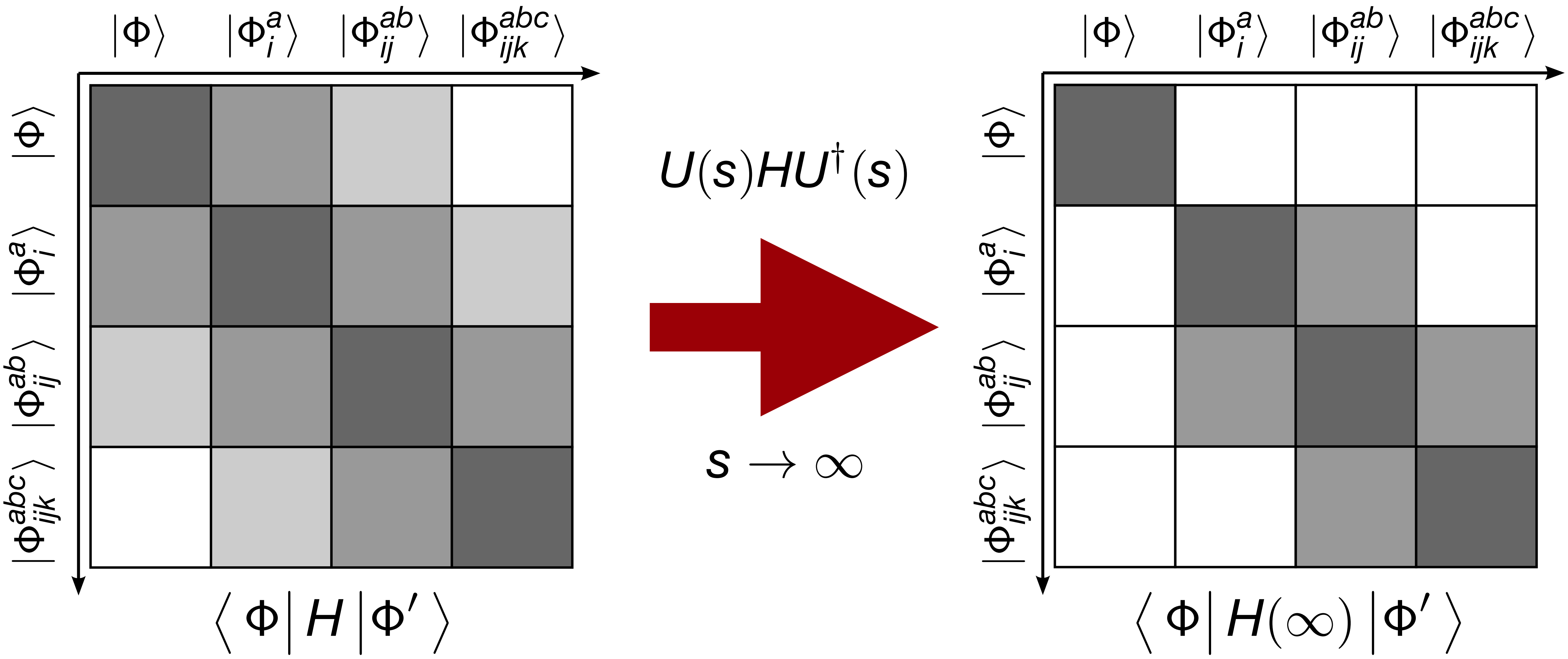
$p, q, \ldots :\quad$ full basis



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

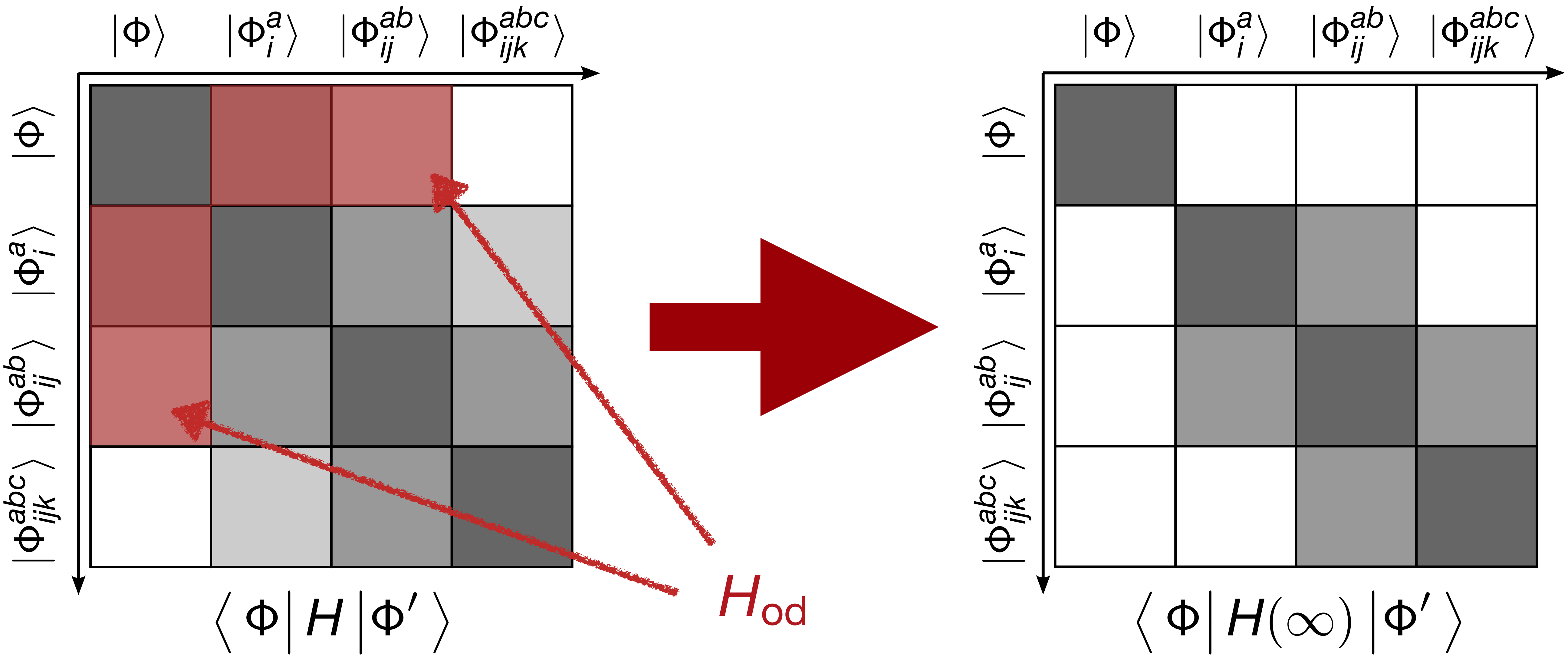
- reference state: **single Slater determinant**

Decoupling in A-Body Space



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

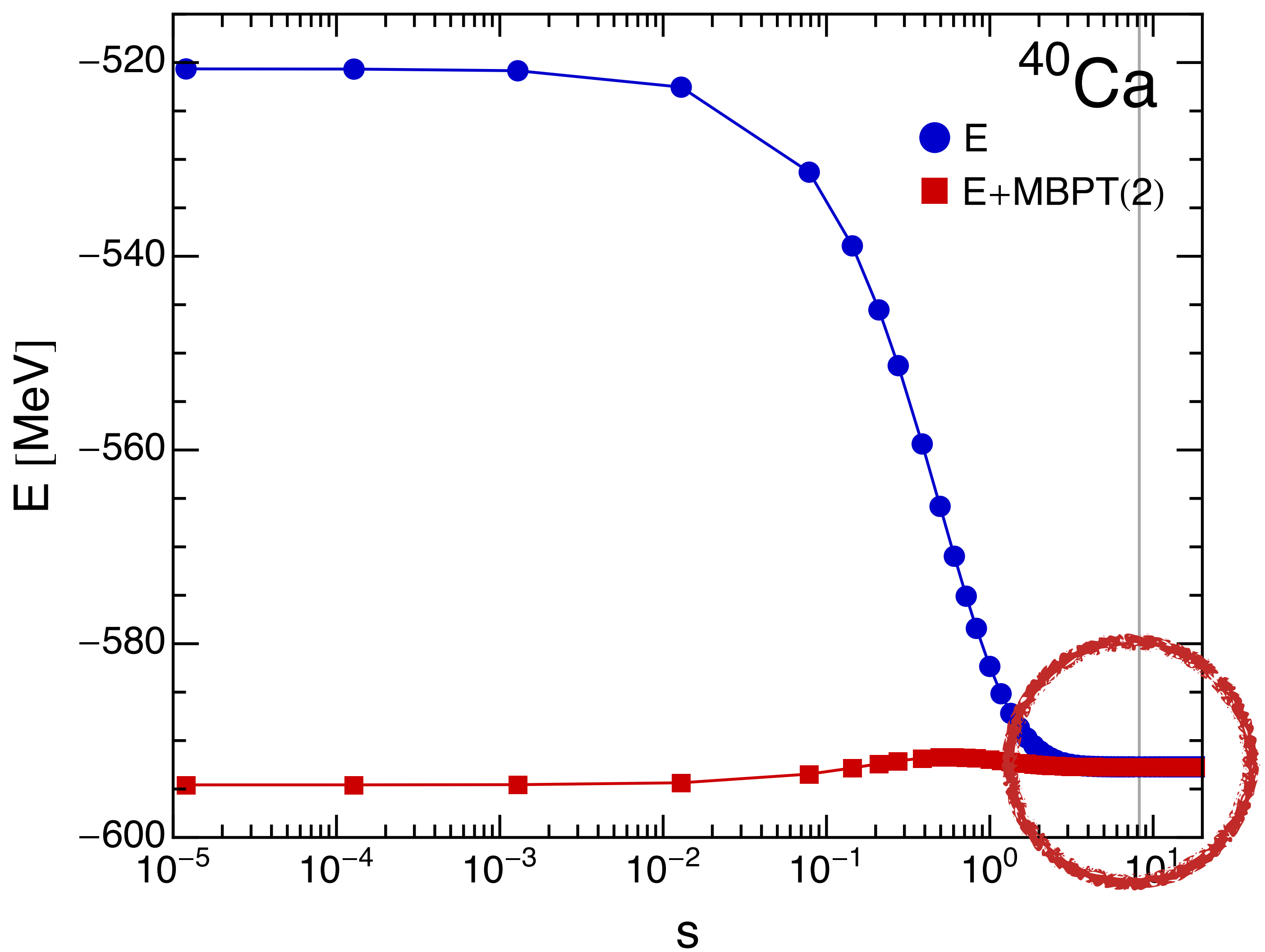
Flow Equation

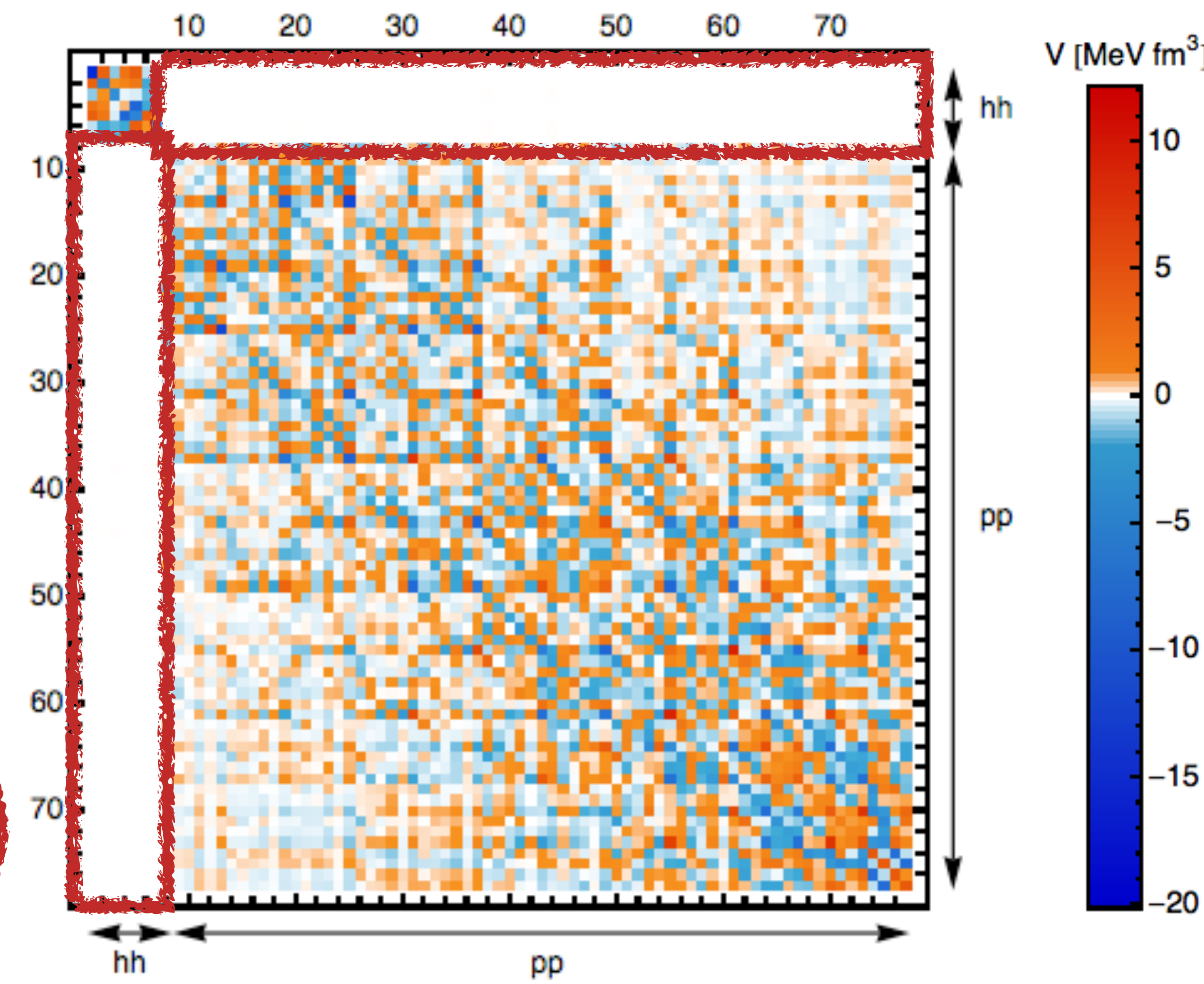


$$\frac{d}{ds} H(s) = [\eta(s), H(s)],$$

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

Decoupling



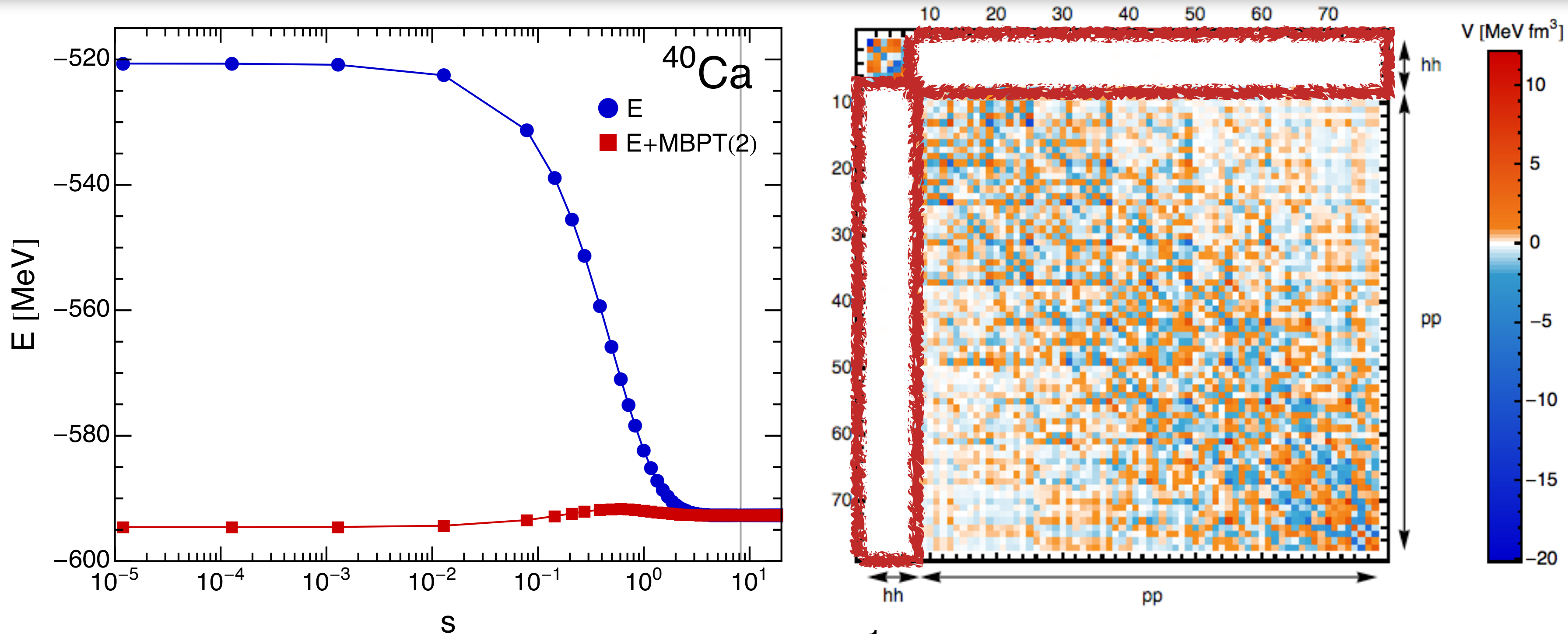


N3LO, $\lambda = 2.0\ \mathrm{fm}^{-1}, e_{\mathrm{Max}} = 8$

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

off-diagonal couplings are rapidly driven to zero

Decoupling



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

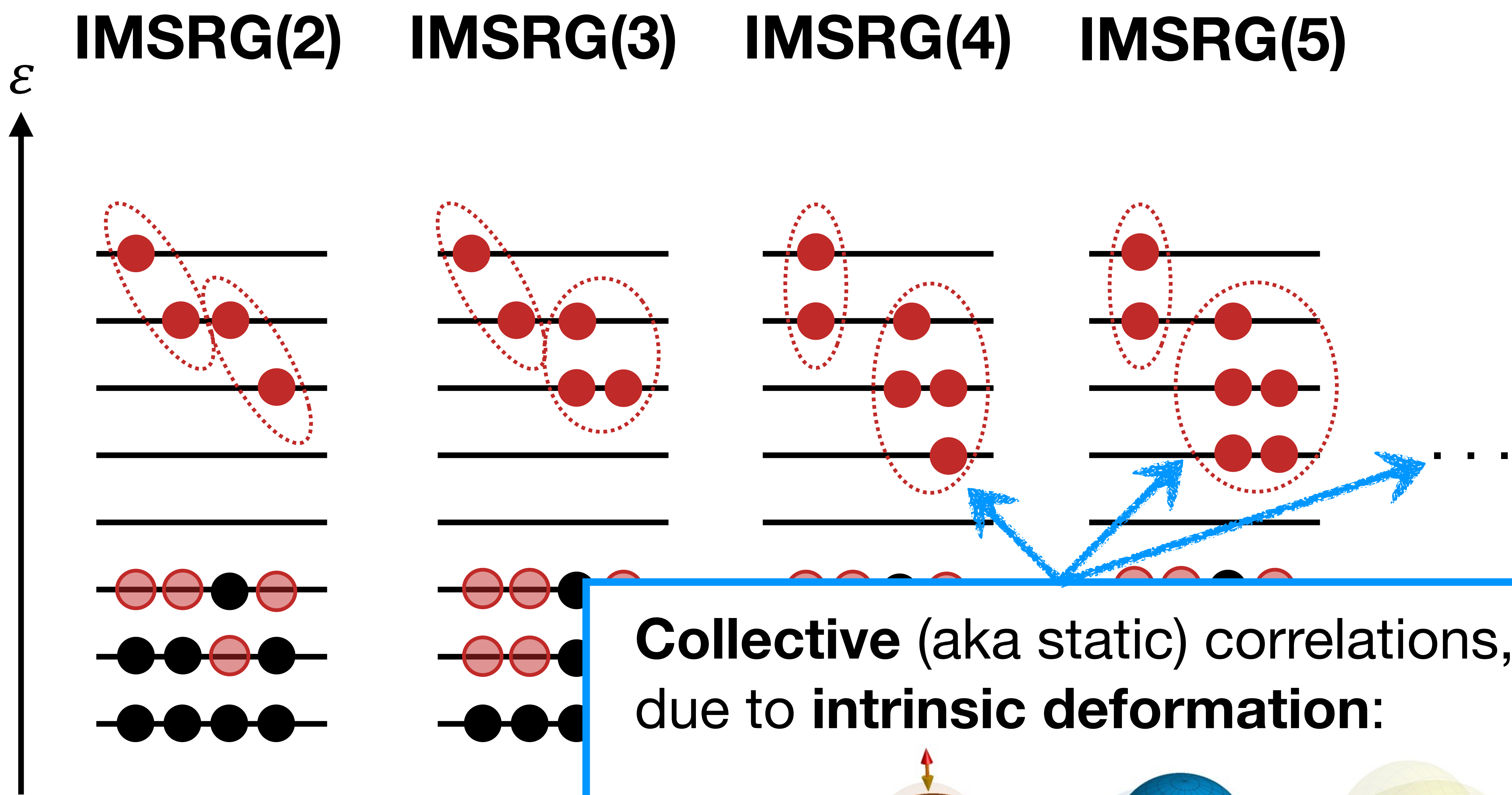
- absorb correlations into **RG-improved Hamiltonian**

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

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

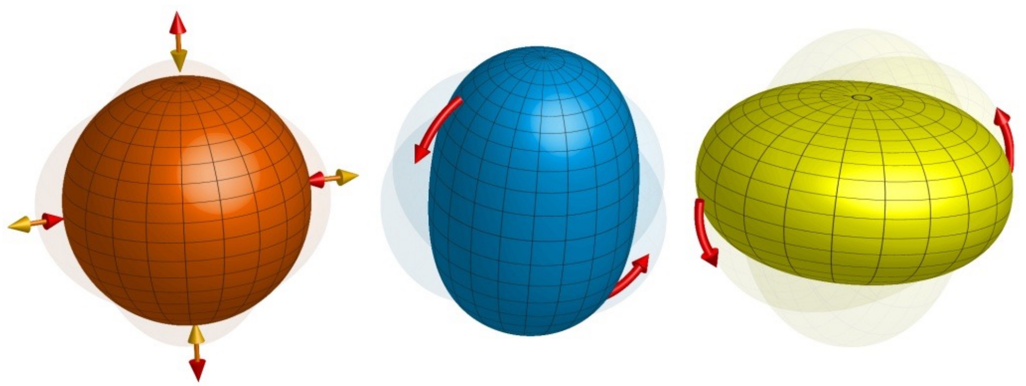
$$U(s) \left|\Psi_n\right\rangle \stackrel{!}{=} \left|\Phi\right\rangle$$

Correlated Reference States

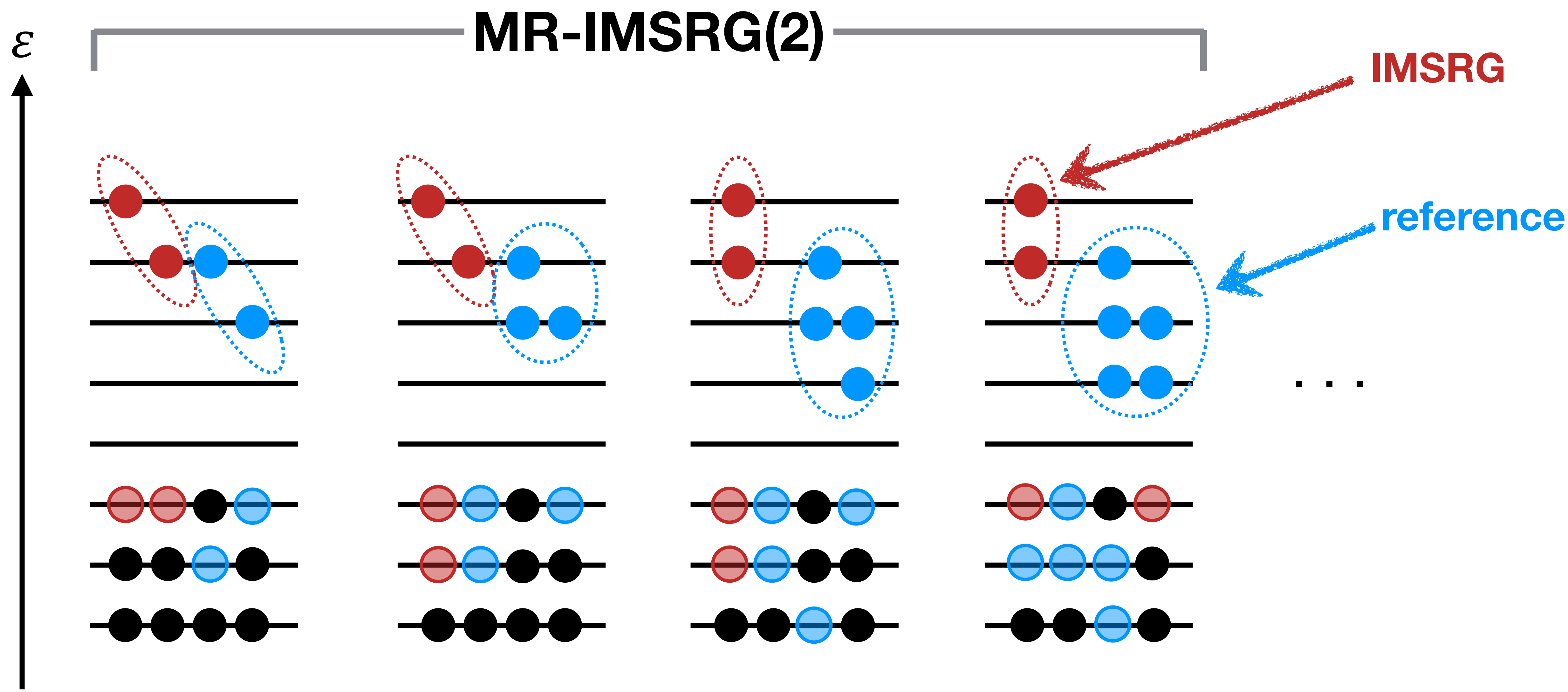


"standard" IMS
Slater determinar

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

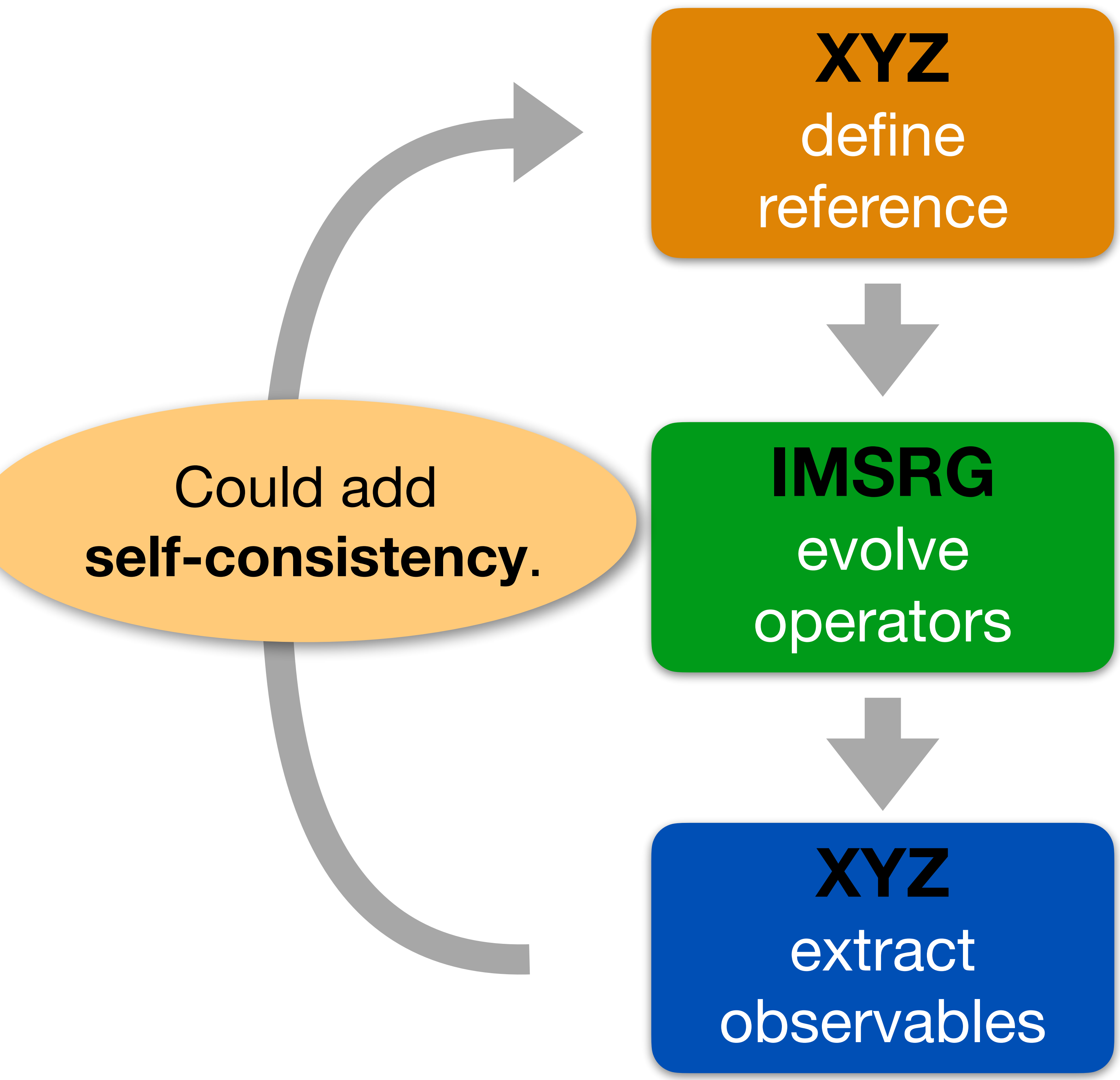


Correlated Reference States



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

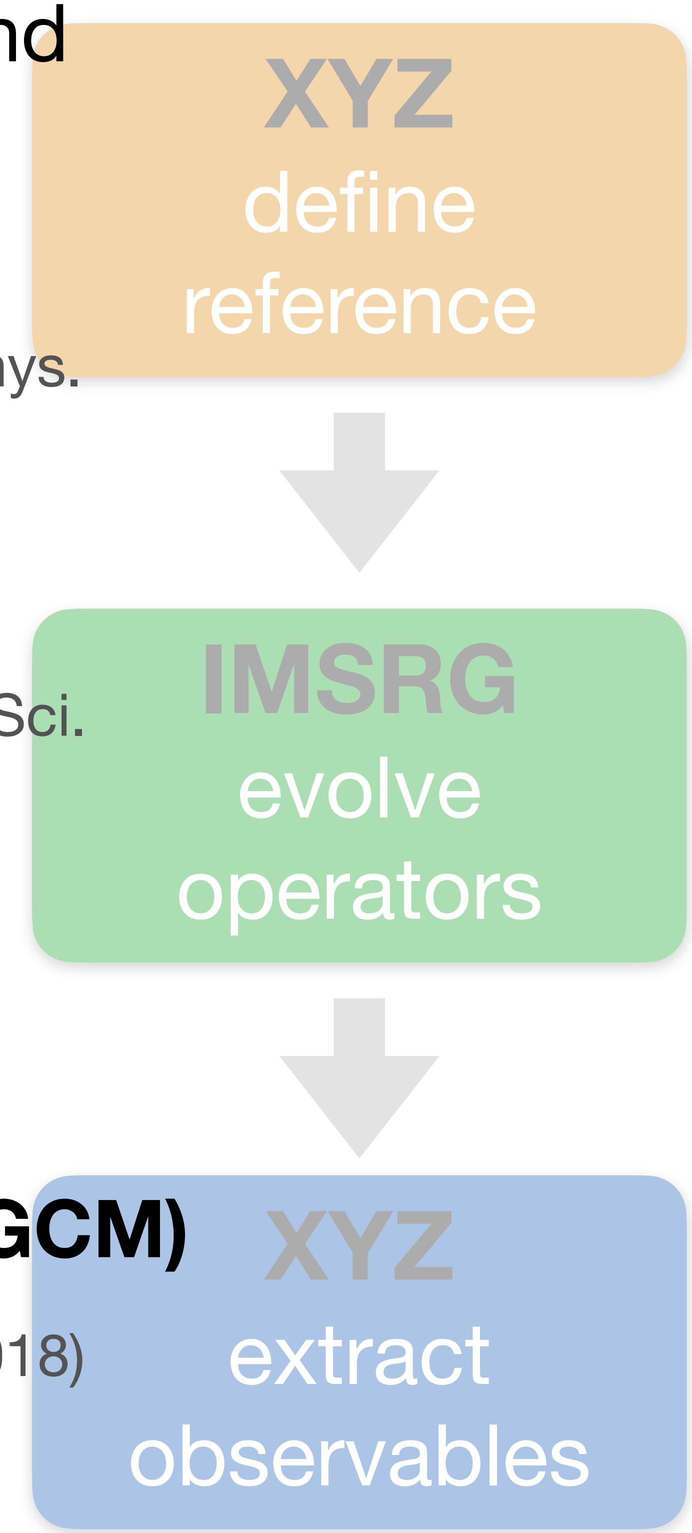
IMSRG-Improved Methods



* 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)



Merging IMSRG and CI: Valence-Space IMSRG

Review:

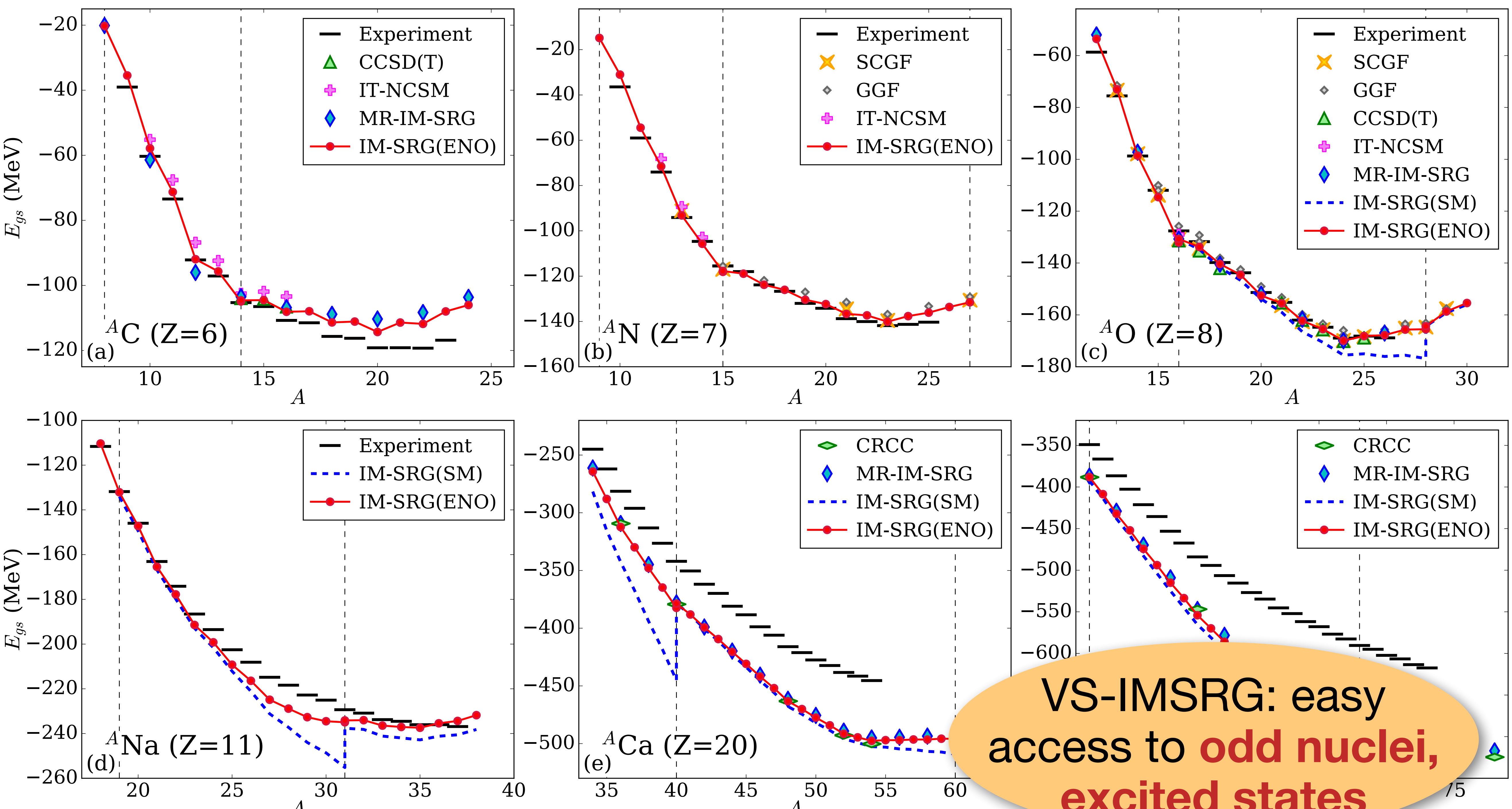
S. R. Stroberg, HH, S. K. Bogner, and J. D. Holt, Ann. Rev. Part. Nucl. Sci. **69**, 165 (2019)

Full CI:

E. Gebrerufael, K. Vobig, HH, and R. Roth, Phys. Rev. Lett. **118**, 152503 (2017)

Ground-State Energies

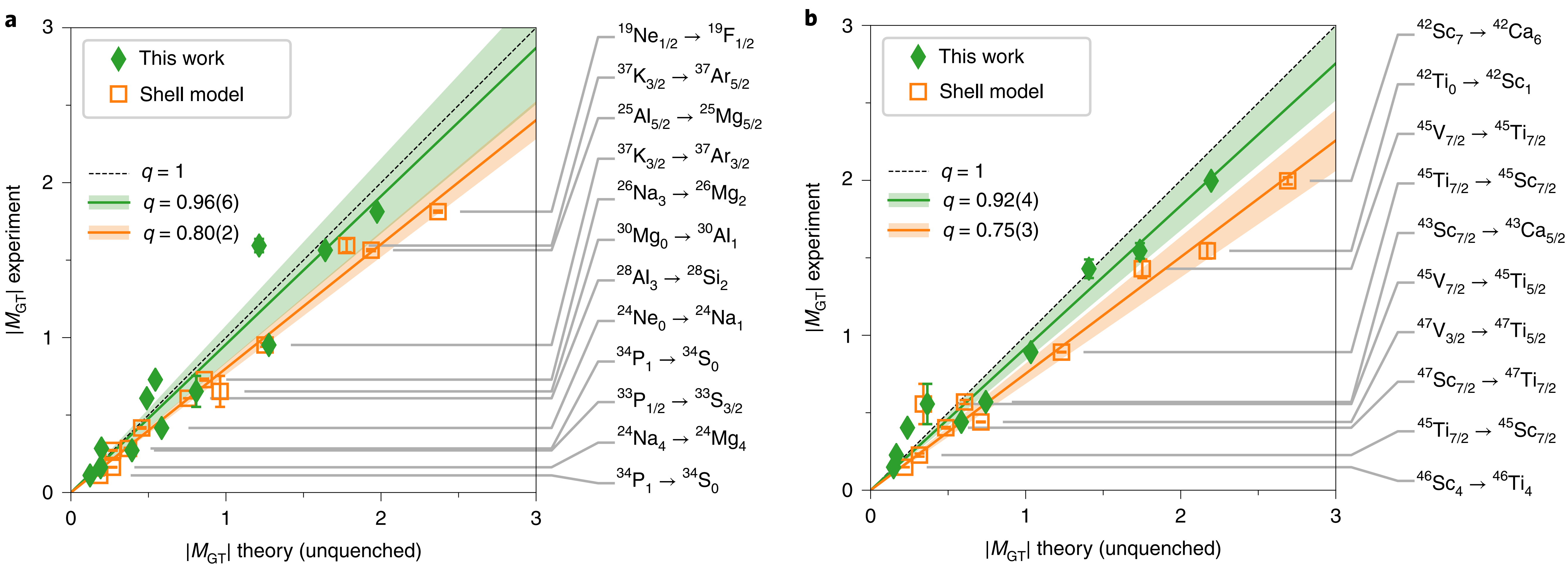
*S. R. Stroberg, A. Calci, HH, J. D. Holt, S. K.Bogner, R. Roth, A. Schwenk, PRL **118**, 032502 (2017)*
*S. R. Stroberg, HH, S. K. Bogner, J. D. Holt, Ann. Rev. Part. Nucl. Sci. **69**, 307 (2019)*



VS-IMSRG: easy access to **odd nuclei, excited states**

Quenching of Gamow-Teller Decays

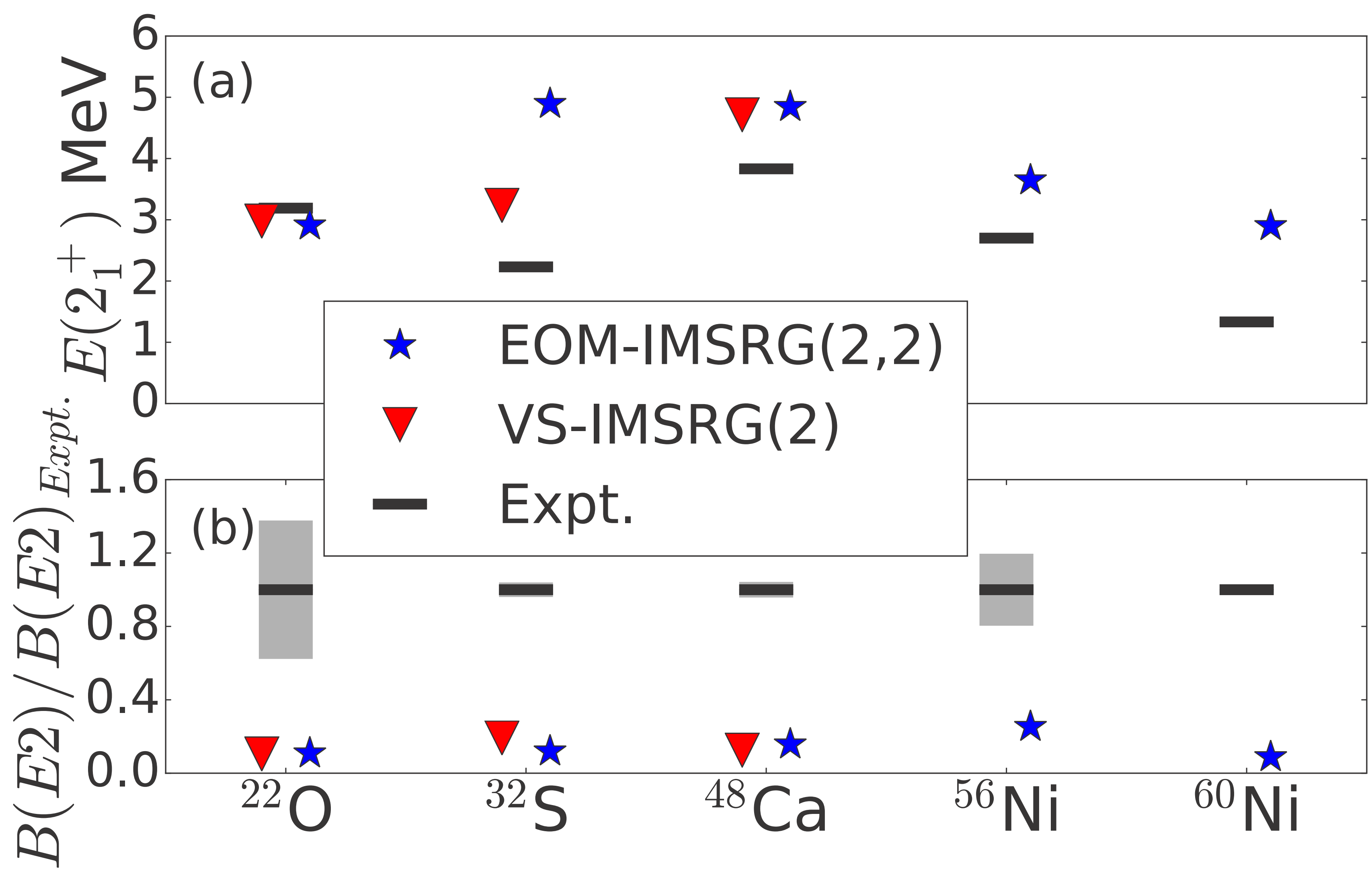
P. Gysbers et al., Nature Physics **15**, 428 (2019)



- **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**

Transitions

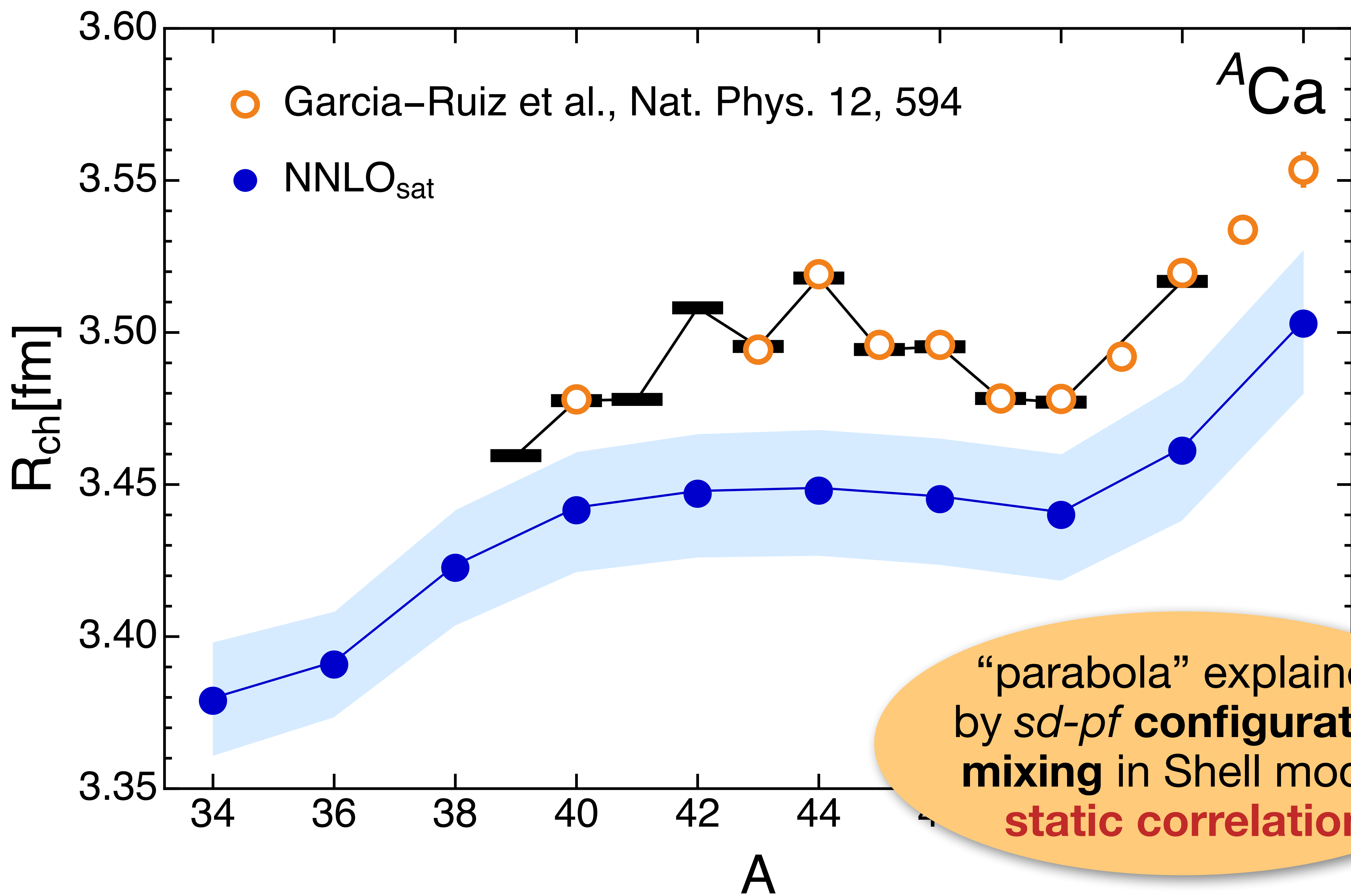
*N. M. Parzuchowski, S. R. Stroberg et al., PRC **96**, 034324*
*S. R. Stroberg, HH, S. K. Bogner, J. D. Holt, Ann. Rev. Part. Nucl. Sci. **69**, 307 (2019)*
*S. R. Stroberg et al. PRC **105**, 034333 (2022*



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

Calcium Isotopes

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



"parabola" explained by *sd-pf* **configuration mixing** in Shell model: **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)

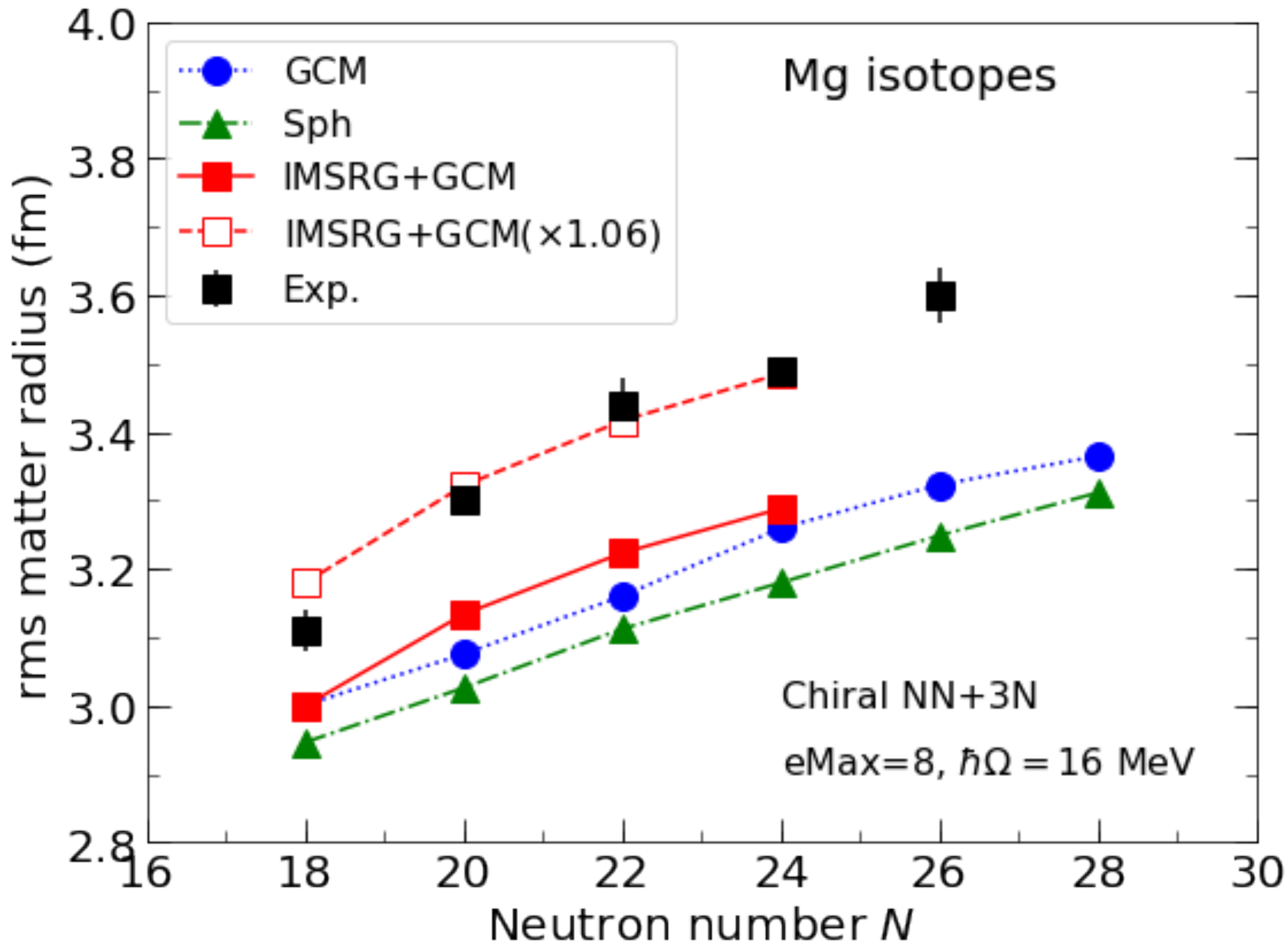
J. M. Yao, B. Bally, J. Engel, R. Wirth, T. R. Rodriguez, HH, PRL **124**, 232501 (2020)

J. M. Yao, J. Engel, L. J. Wang, C. F. Jiao, 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

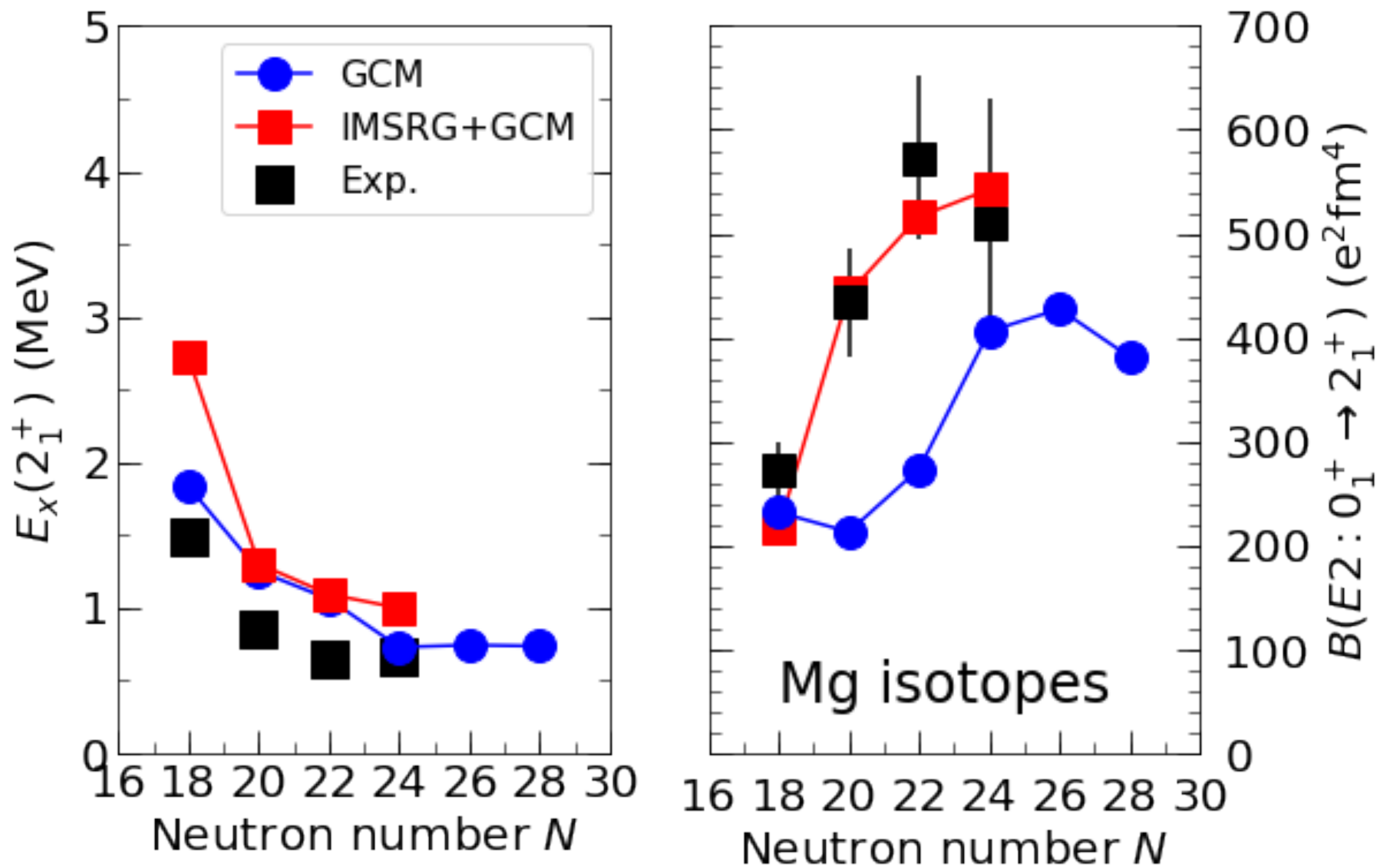
J. M. Yao, HH, in preparation



- 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

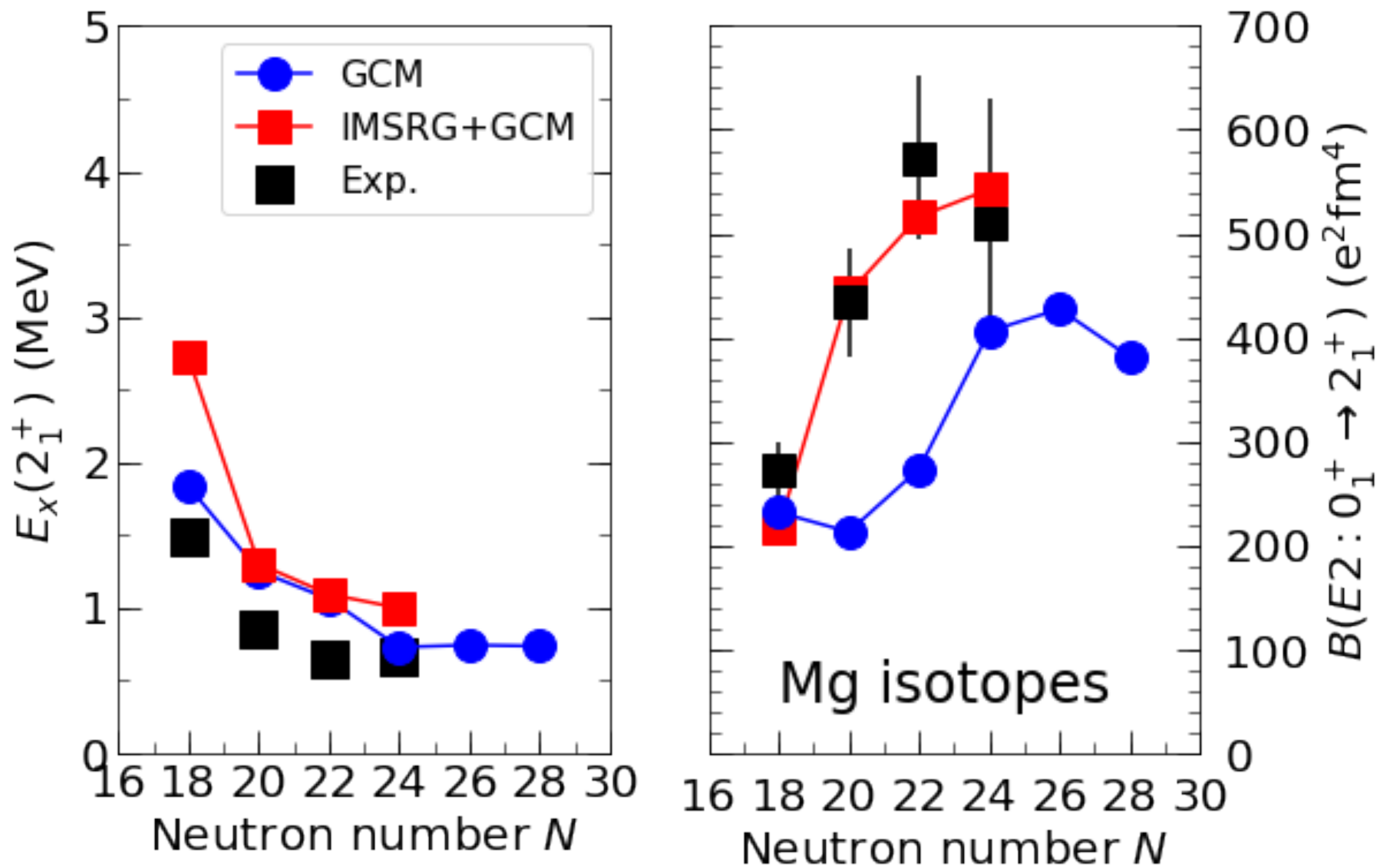
J. M. Yao, HH, in preparation



- 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

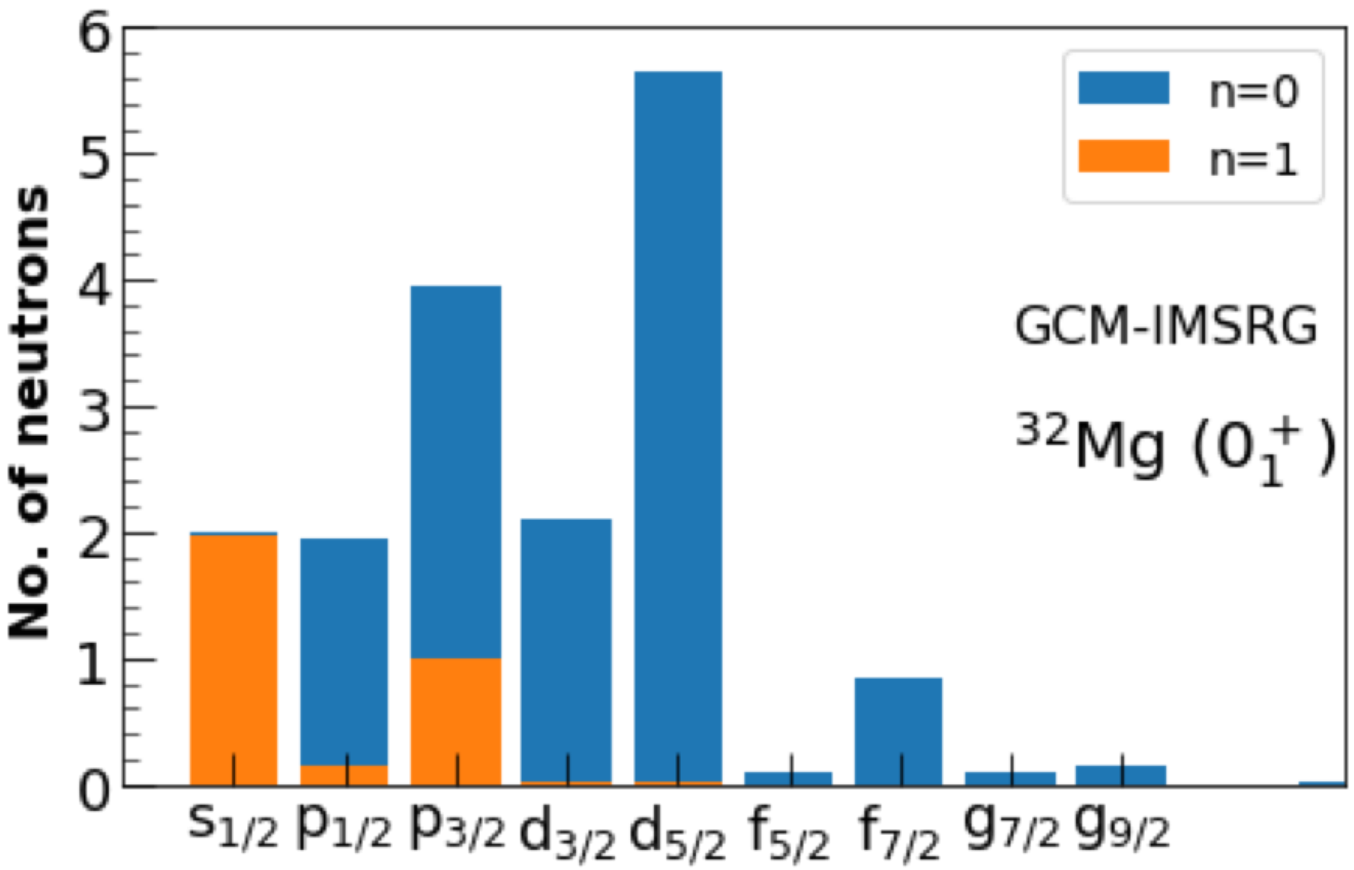


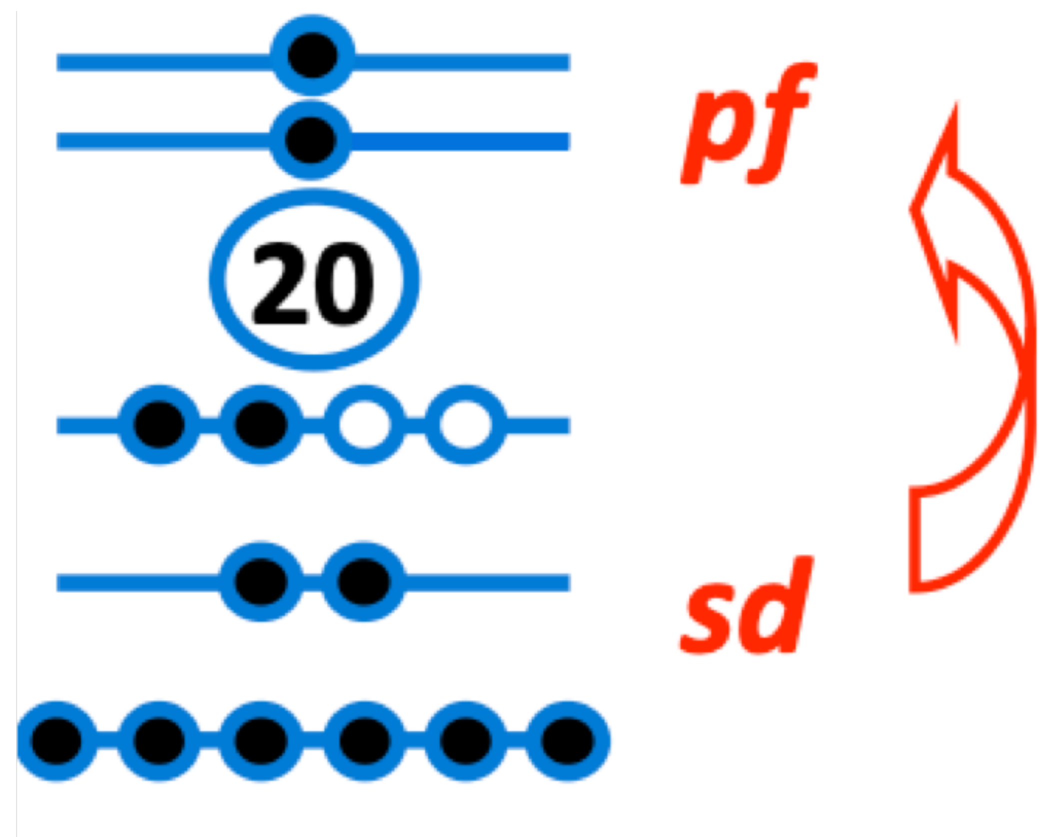
$$O = O^{(1)} \underset{s\to\infty}{\rightarrow} O(s) = O^{(1)}(s) + \underbrace{O^{(2)}(s) + \ldots}_{\text{induced contributions}}$$

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

Collectivity in Magnesium Isotopes

J. M. Yao, HH, in preparation





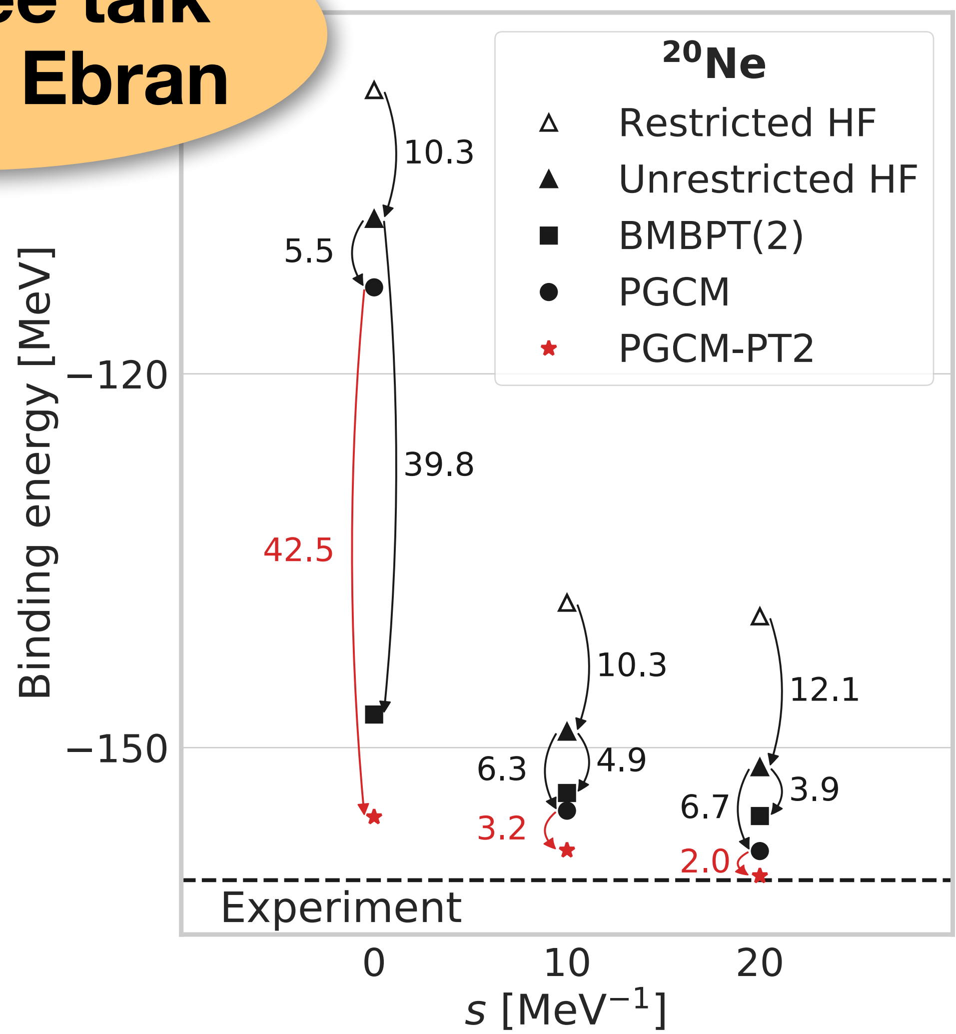
$$\nu(0d_{3/2})^{-2}(0f_{7/2})^1(1p_{3/2})^1$$

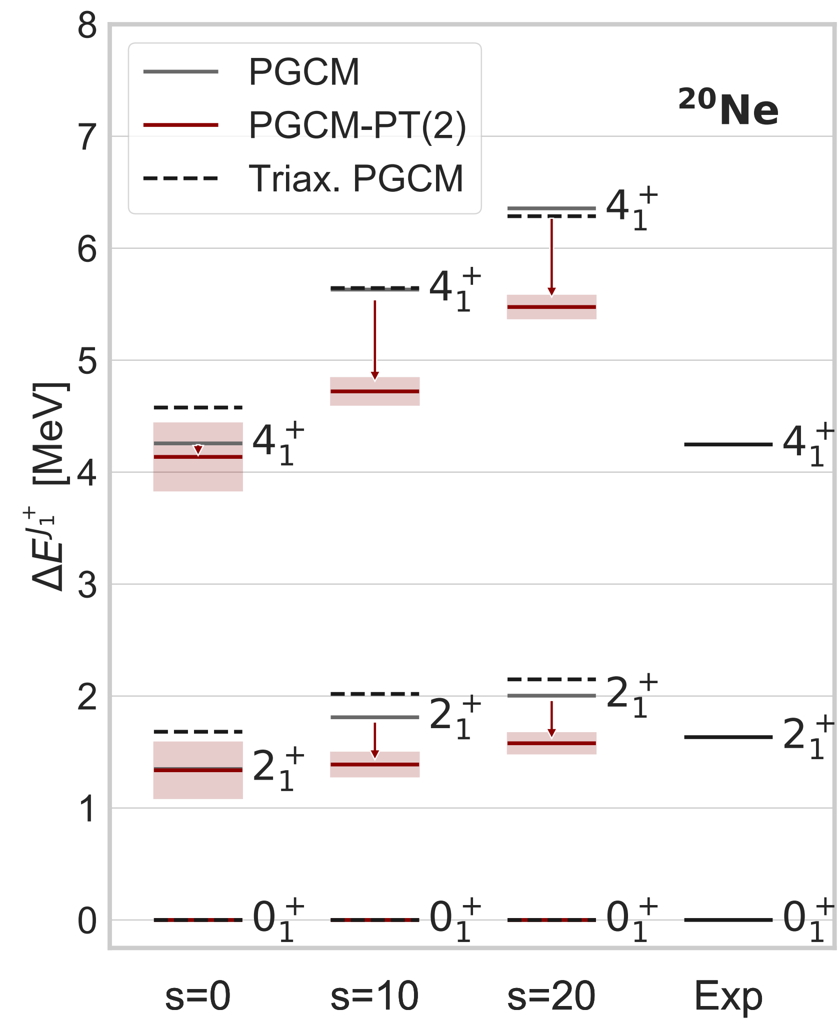
- **Caution:** occupation numbers are **not observables**, interpret with care (scale/scheme dependence)!
- For **low-resolution interactions**, the (no-core) IM-GCM and Shell Model interpretations of ^{32}Mg are **qualitatively** the same: two neutrons are excited from the sd- into the pf shell.

Perturbative Enhancement of IM-GCM

also see talk by J.-P. Ebran

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

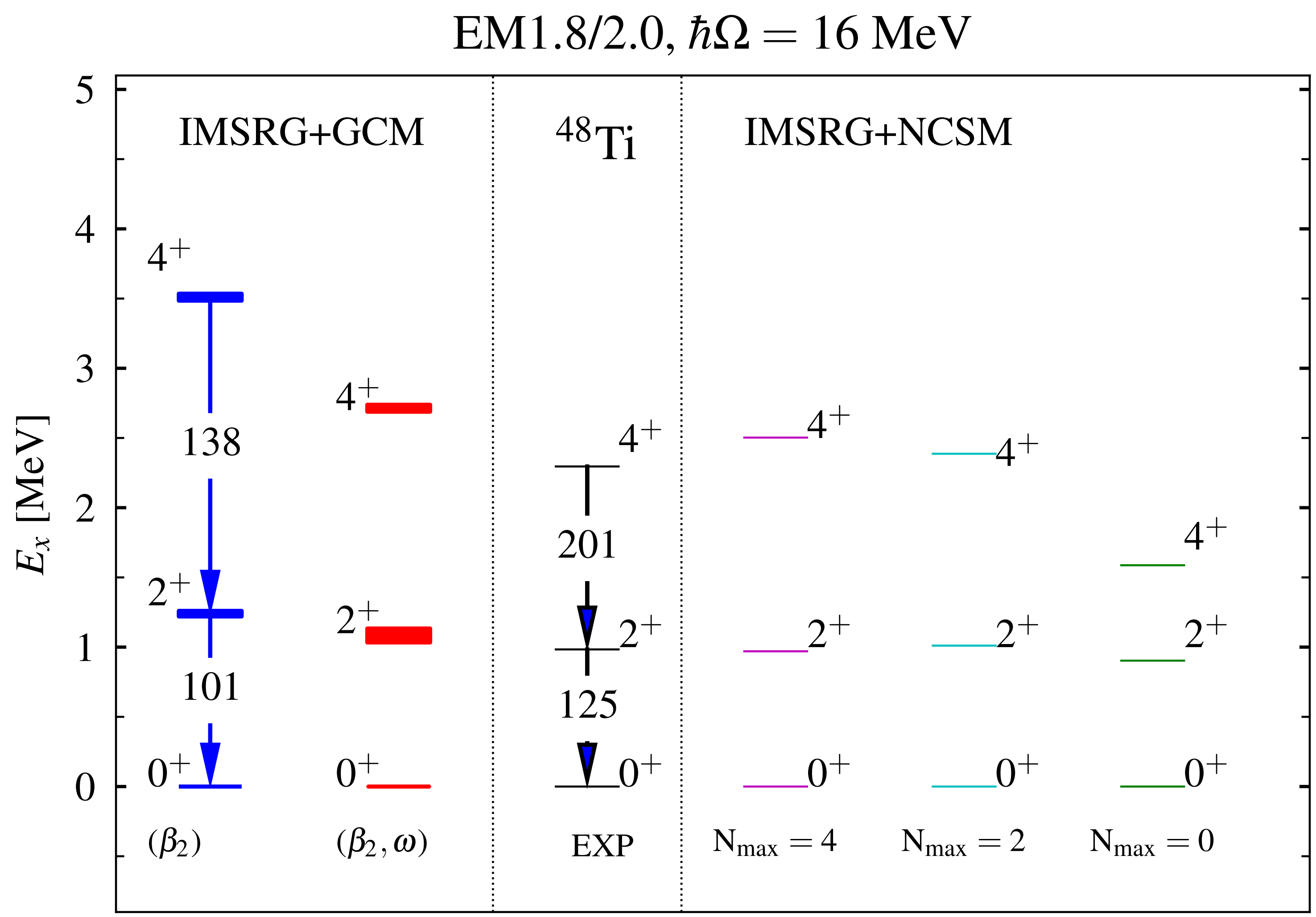




- s-dependence is a **built-in diagnostic tool** for IM-GCM **(not available in phenomenological GCM)**
  - if operator and wave function offer sufficient degrees of freedom, evolution of observables is unitary
- need **richer references and/or IMSRG(3)** for certain observables

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

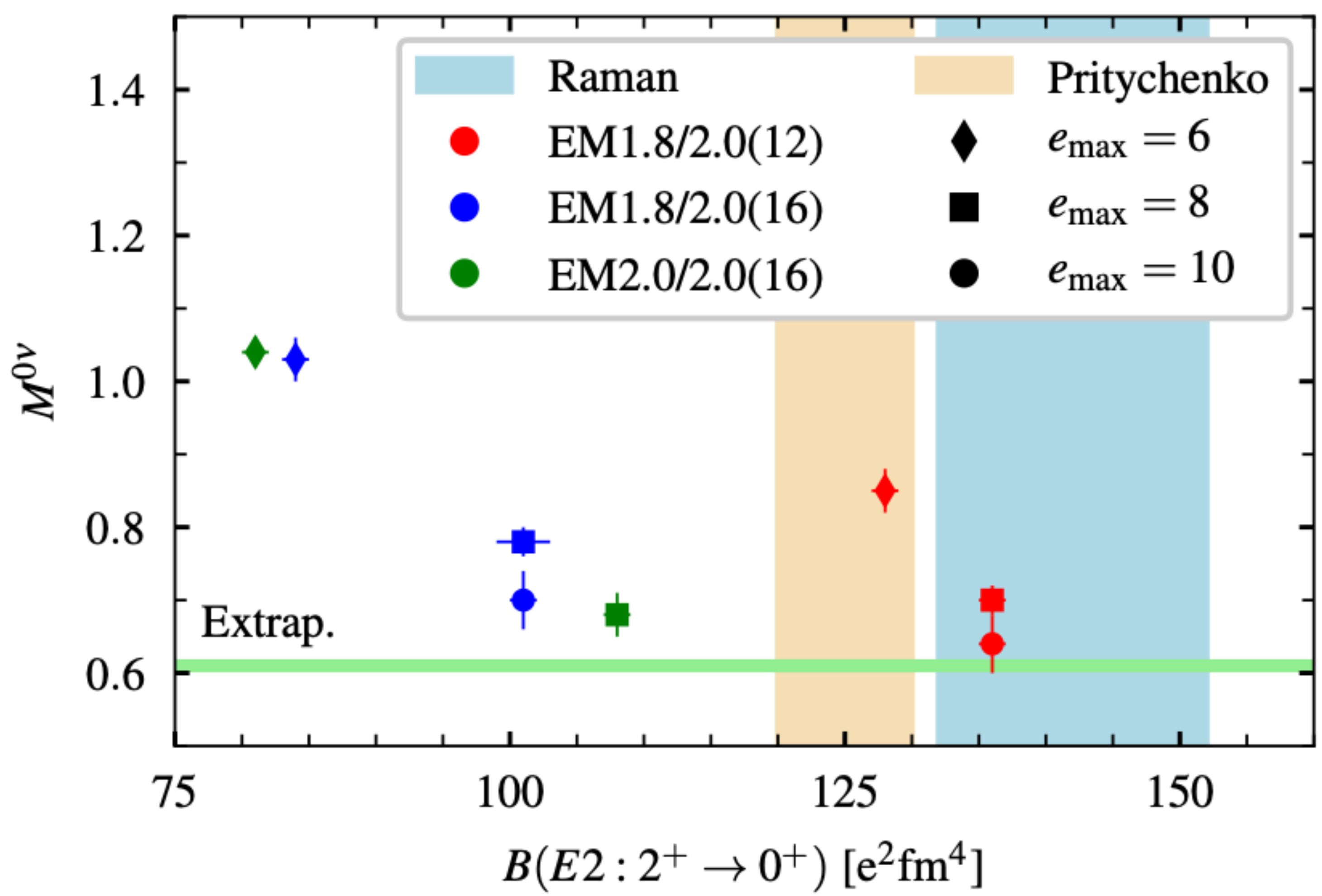
*J. M. Yao et al., PRL **124**, 232501 (2020); HH, Front. Phys. **8**, 379 (2020)*



- 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)

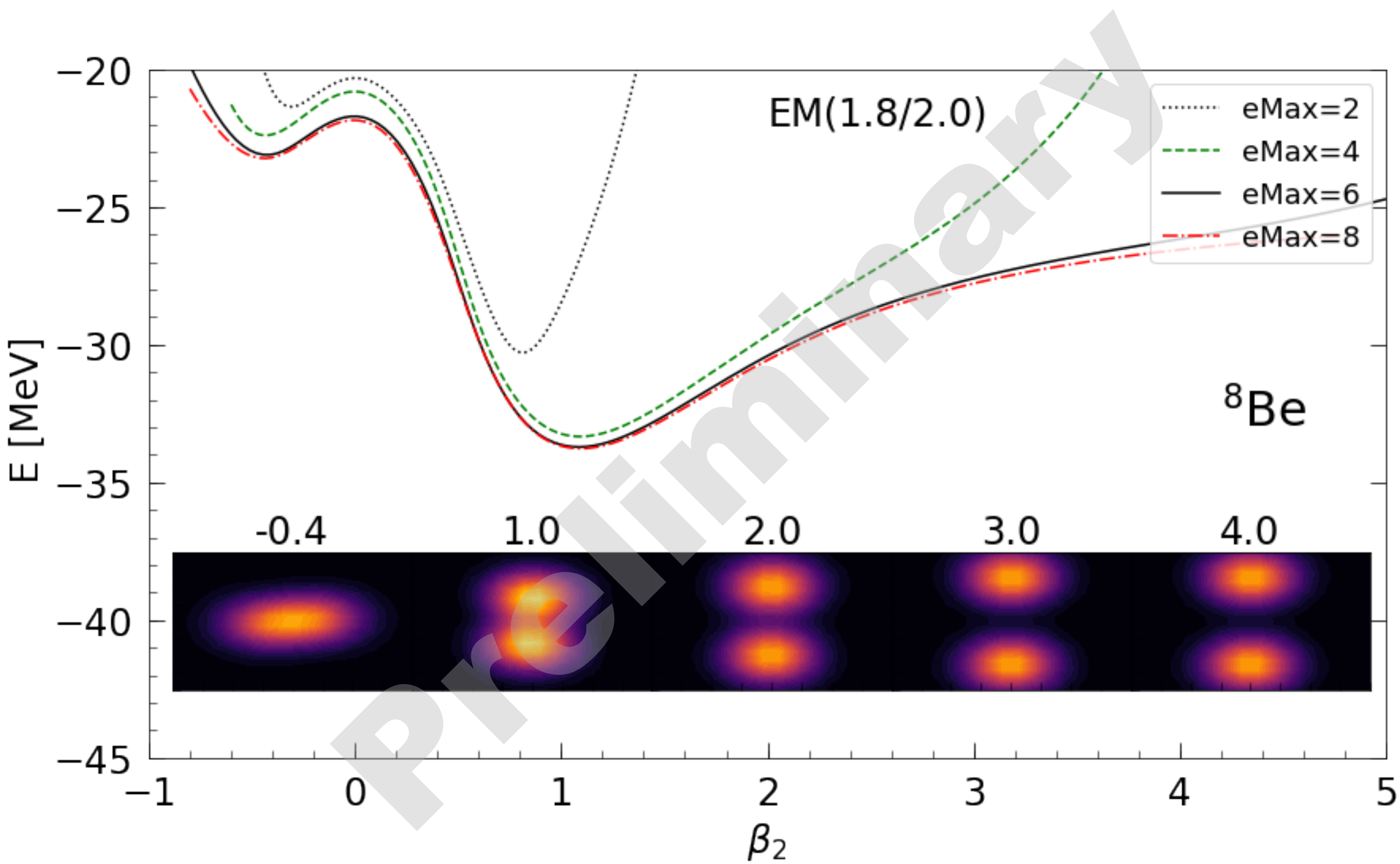


- NME from different methods **consistent** for consistent interactions & transition operators
  (A. Belley et al., PRL 126, 042502, S. Novario e
- interpretation and features differ from e
  only **weak correlation** between NME and

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

Cluster Structures: ^{8}Be

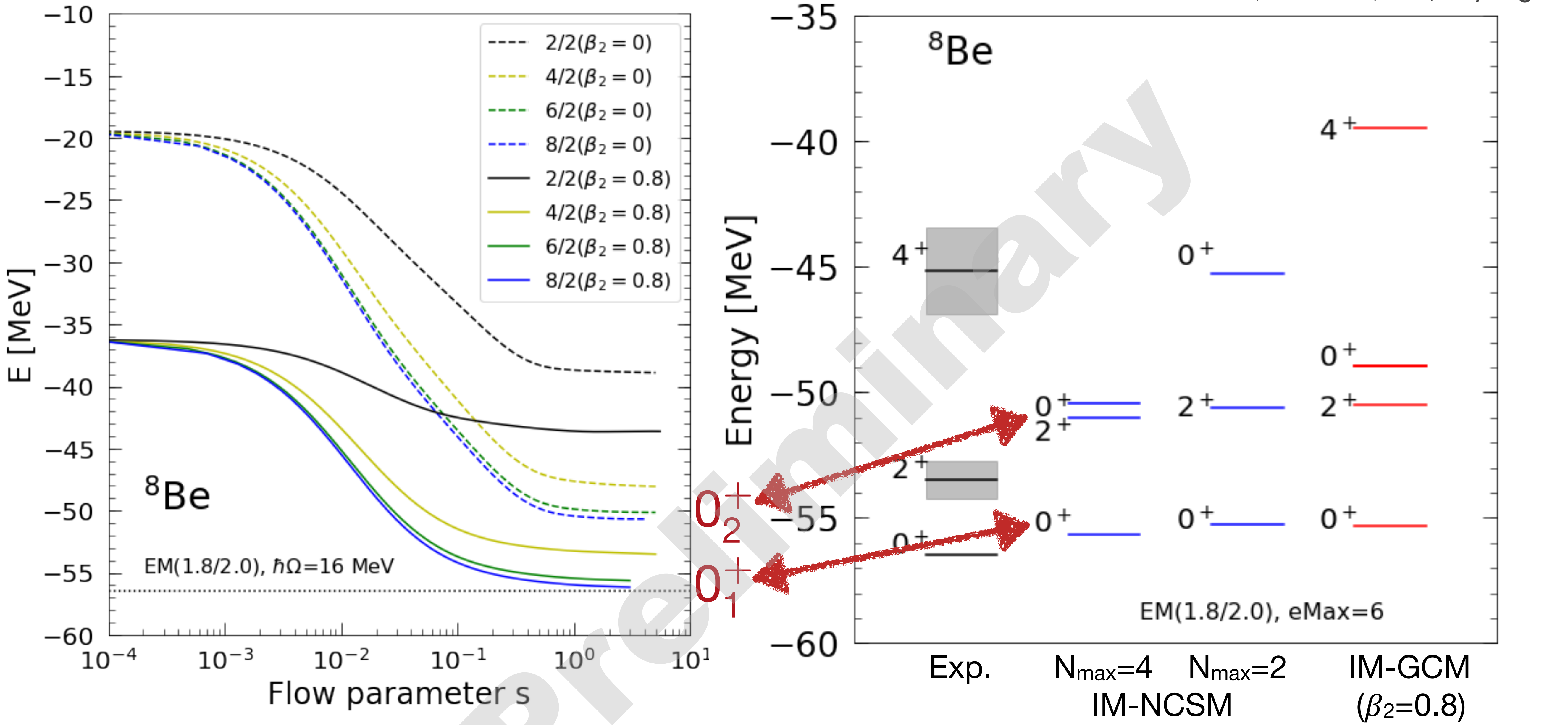
J. M. Yao, R. Wirth, HH, in progress



HFB potential energy surface

Cluster Structures: ^{8}Be

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



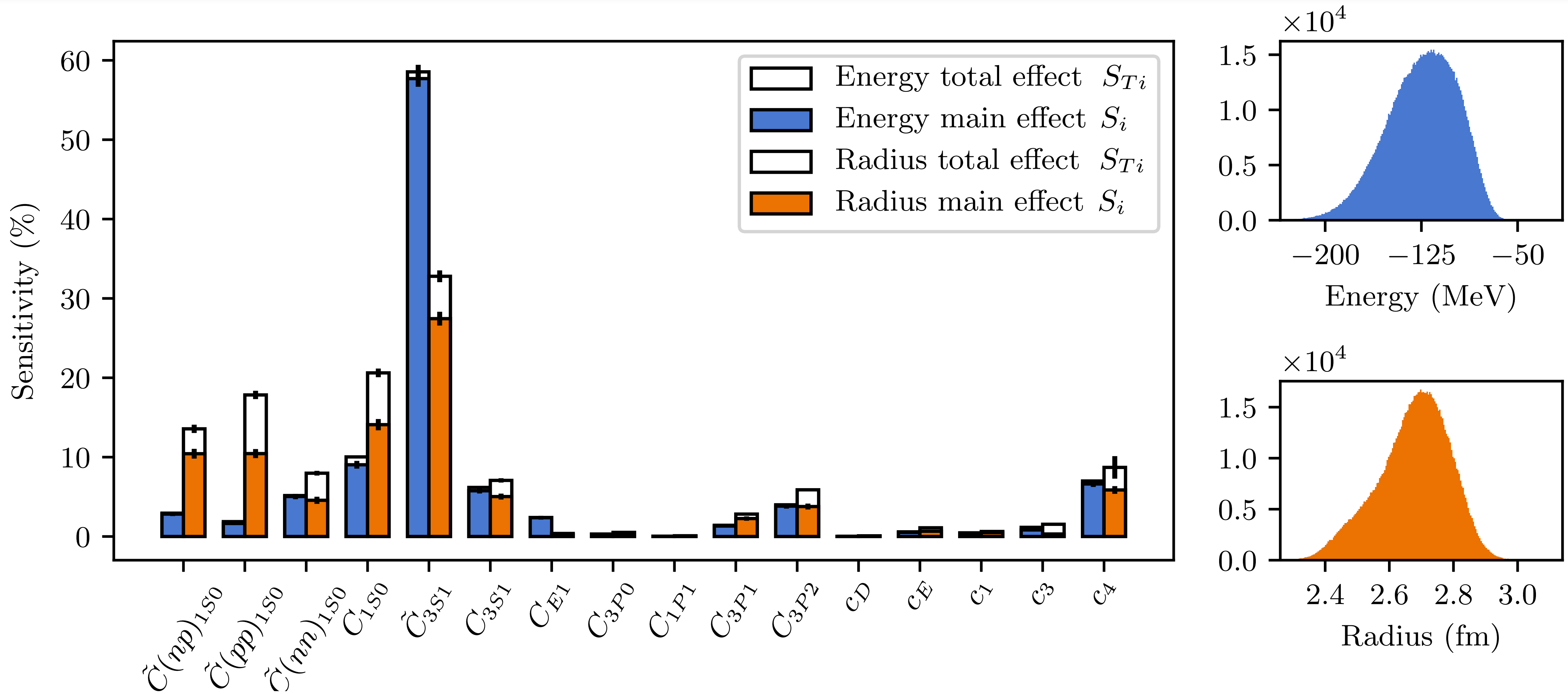
- Spherical and prolate references flow towards **different 0^+ states**.
- Consistent with IM-NCSM:
  - **prolate reference:** ground state and excited 2^+ state
  - **spherical reference:** first excited 0^+

Looking Ahead

Goals

- **precision** nuclear physics
  - structure of (exotic and stable) nuclei with **complex deformations**: shape coexistence, clustering, halos, …
  - inputs for fundamental symmetry programs: **neutrinoless double beta decay, EDMs / Schiff moments**, beta decay for unitarity tests…
- **explore opportunities with heavy ion collisions**
  - **caveat:** needs careful assessment of scale and scheme dependences
- **Uncertainty Quantification / Sensitivity Analysis**
  - identify strongly constraining nuclear observables (usually difficult to compute)
  - need surrogate models/emulators (**model reduction**)

Surrogate Models



Sensitivity of ^{16}O ground-state energy to variations of chiral LECs (through NNLO) [Ekström & Hagen, PRL 123, 252501]

Emulators from eigenvector continuation:
D. Frame et al., PRL **121**, 032501 (2017); S. König et al., PLB **810**, 135814 (2018); …

“Reviews” of model reduction for nuclear physicists:
E. Bonilla et al., PRC **106**, 054322 (2022); J. Melendez et al., JPG **49,** 102001 (2022)

The Horizon

- **predictive *ab initio* theory** with **systematic uncertainties** & convergence to exact result

- expanding capabilities: spectra, radii, transitions, **clustering,** bridge to **dynamics /reactions**…

- **scalable** techniques and codes: from day-to-day data analysis to leadership calculations

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NUCLEI
Nuclear Computational Low-Energy Initiative

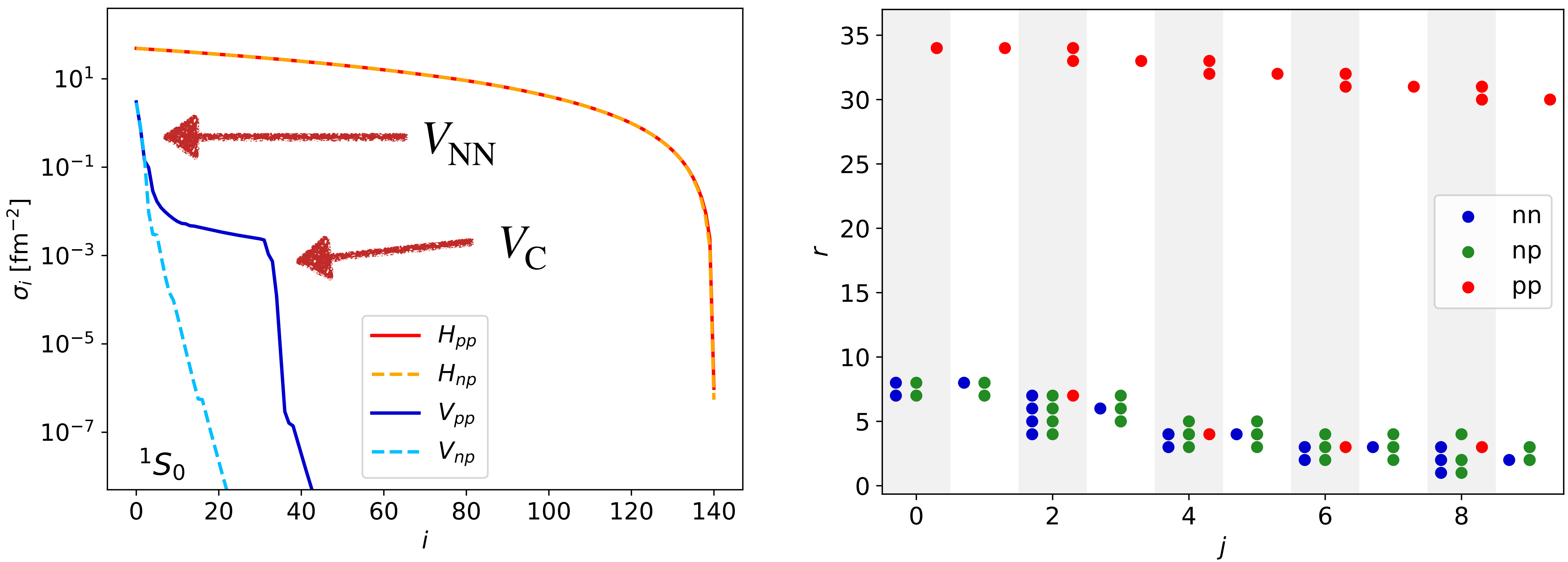
Postdoctoral Position @ FRIB

- **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 on Jan 30th, but will continue until position is filled**
- **Please encourage suitable candidates to apply!**

Supplements

Factorized Interactions

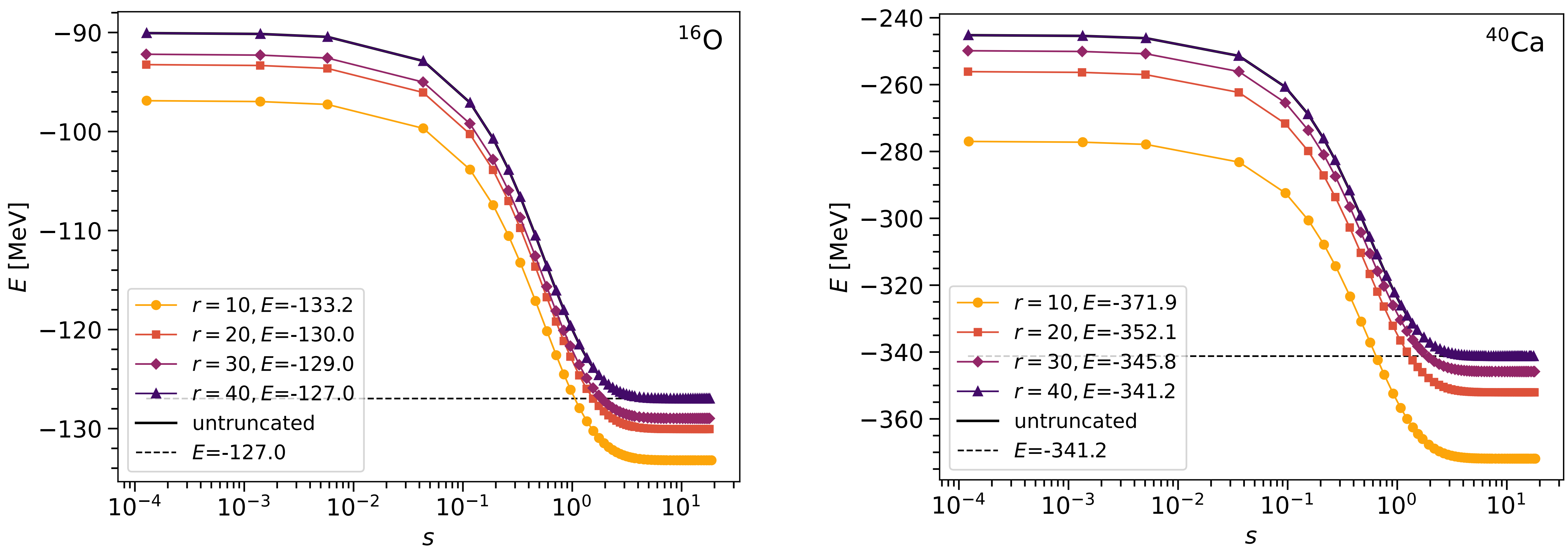
B. Zhu, R. Wirth, HH, PRC 104, 044002 (2021)



- 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

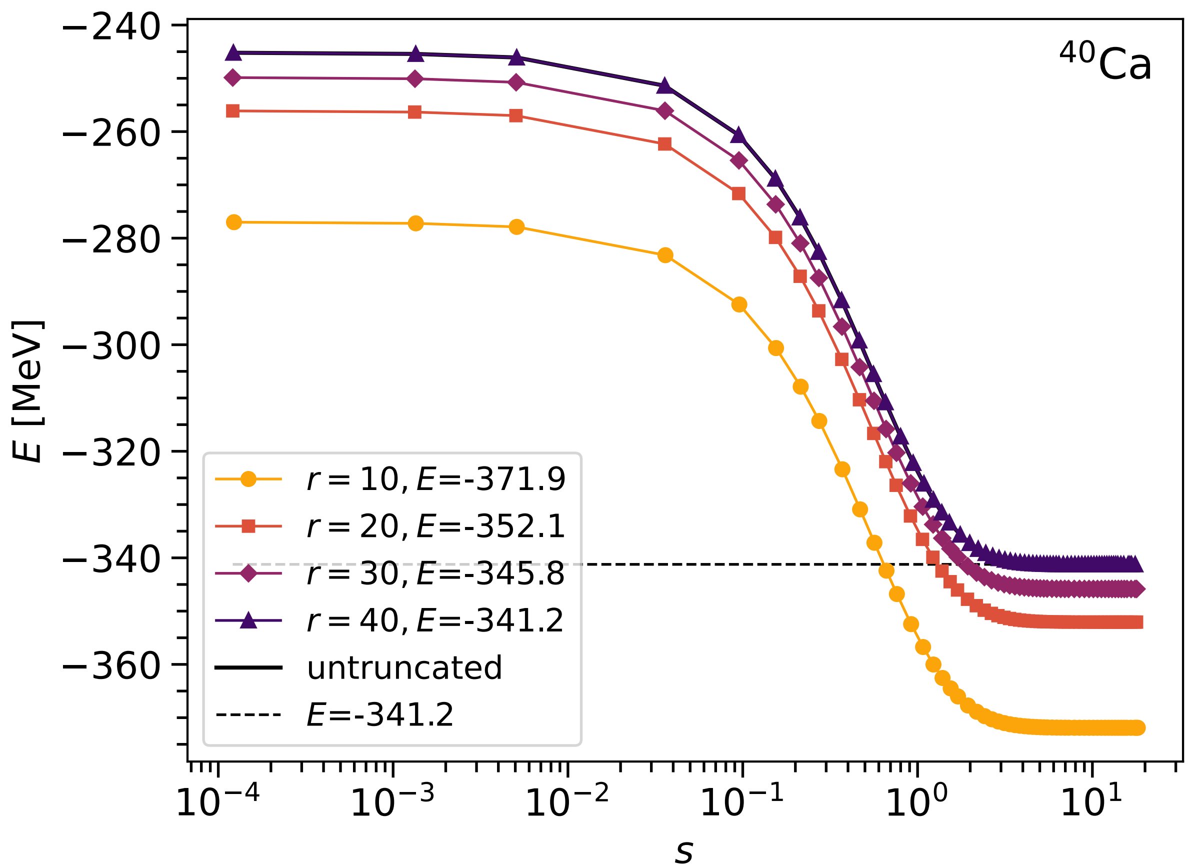
B. Zhu, R. Wirth, HH, PRC 104, 044002 (2021)

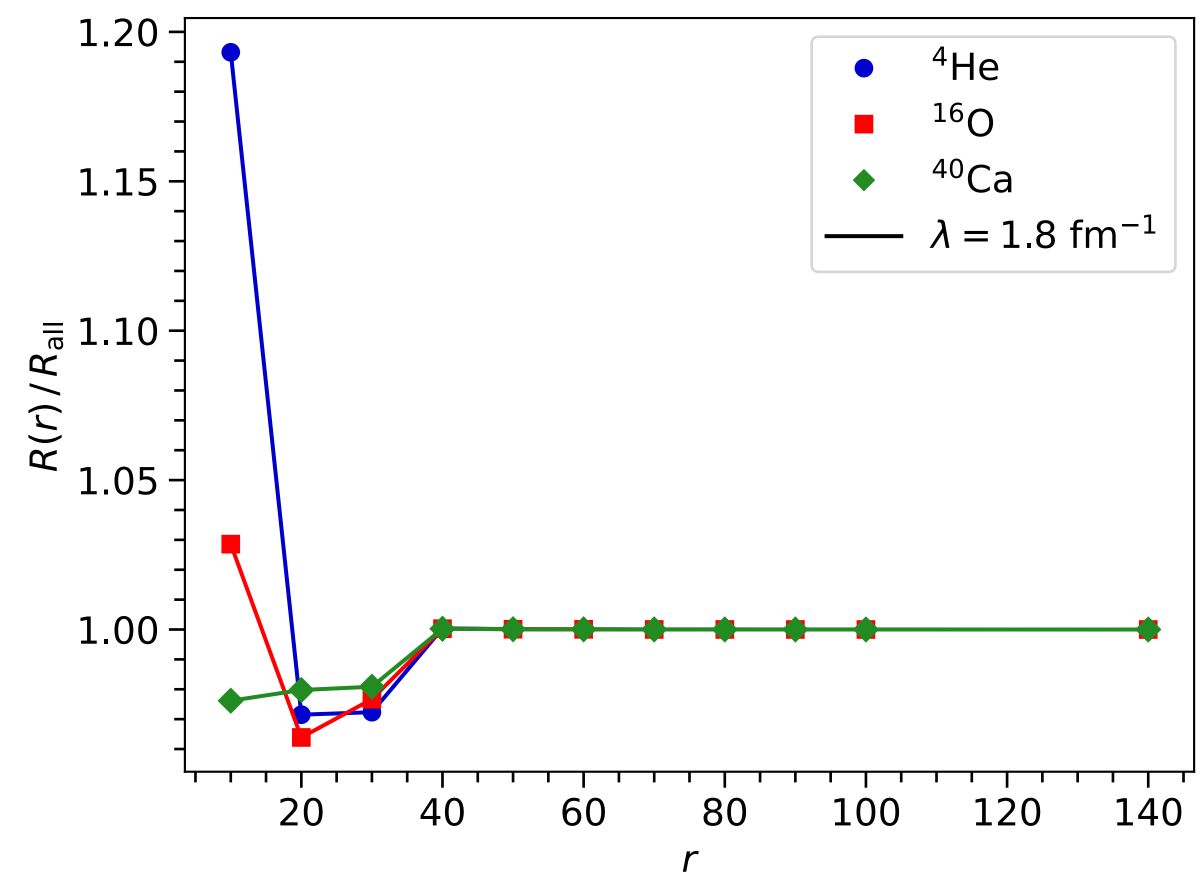


- NN interaction: free-space SRG evolution in component form (**IMSRG not yet**)
  - (3N interaction added to produce realistic binding / radii)
- free-space SRG effort and storage **reduced by several orders of magnitude**

Factorized Interactions

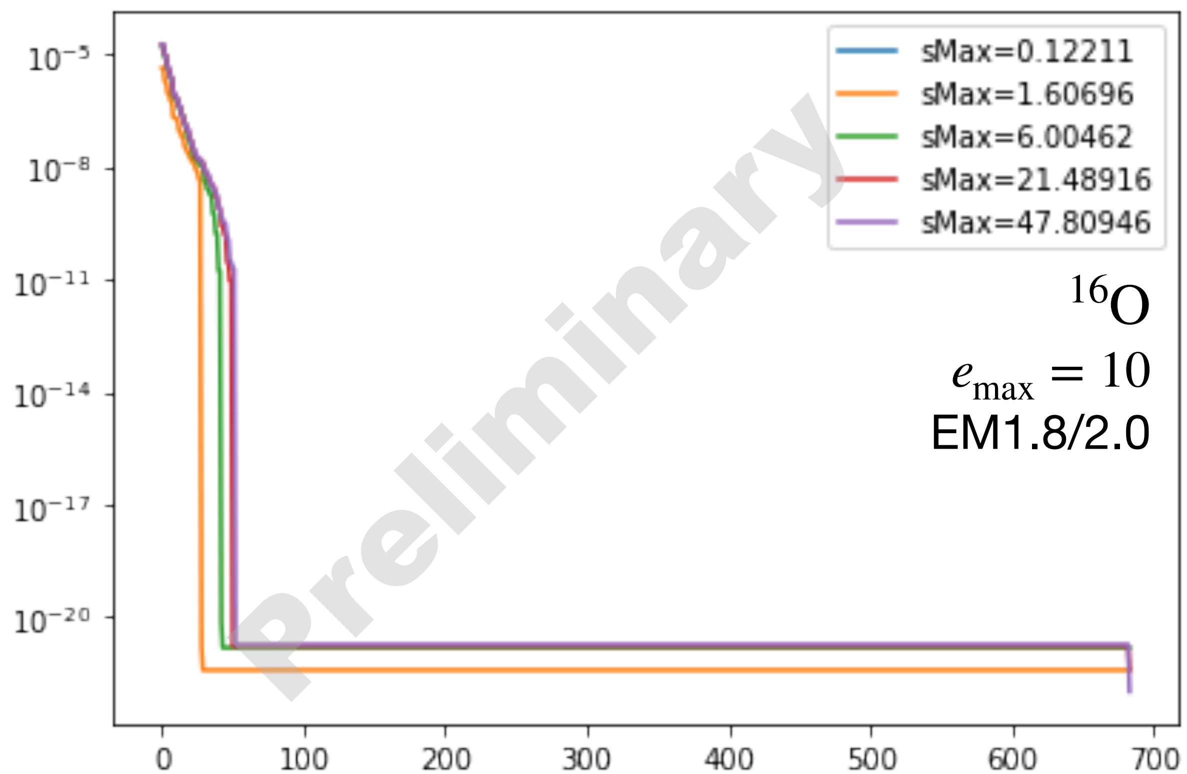
B. Zhu, R. Wirth, HH, PRC ***104****, 044002 (2021)*

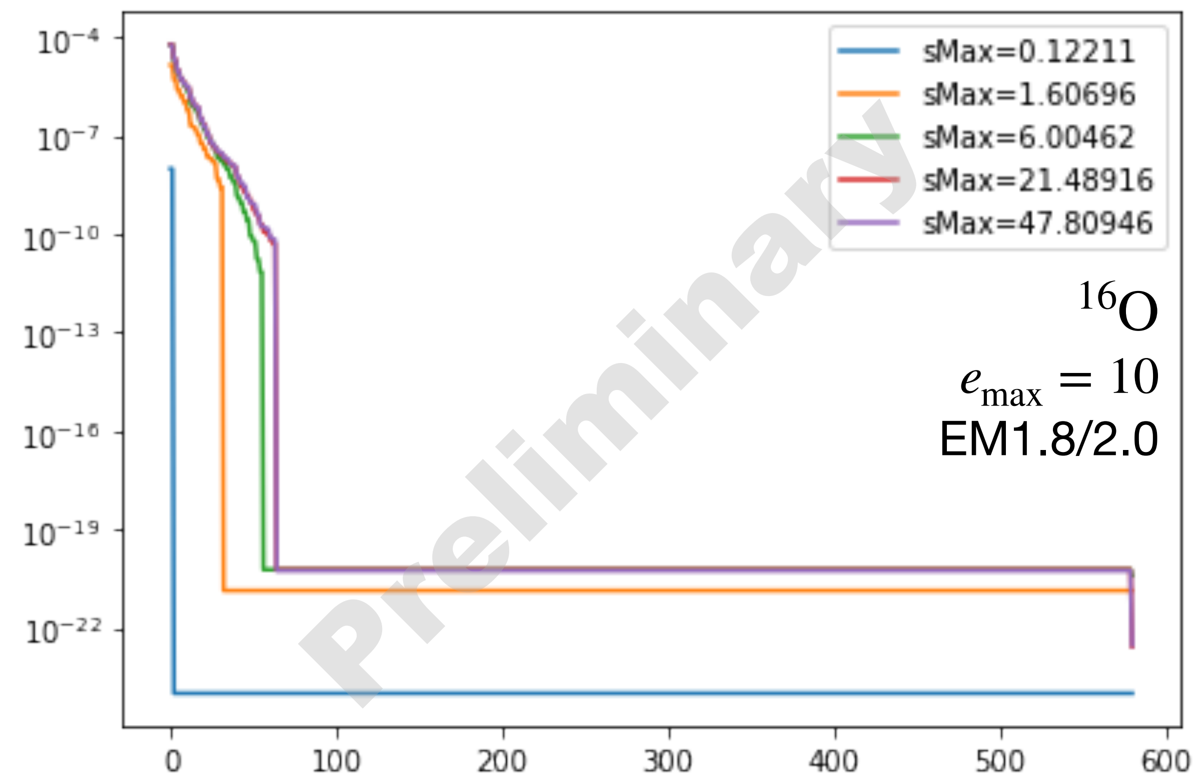




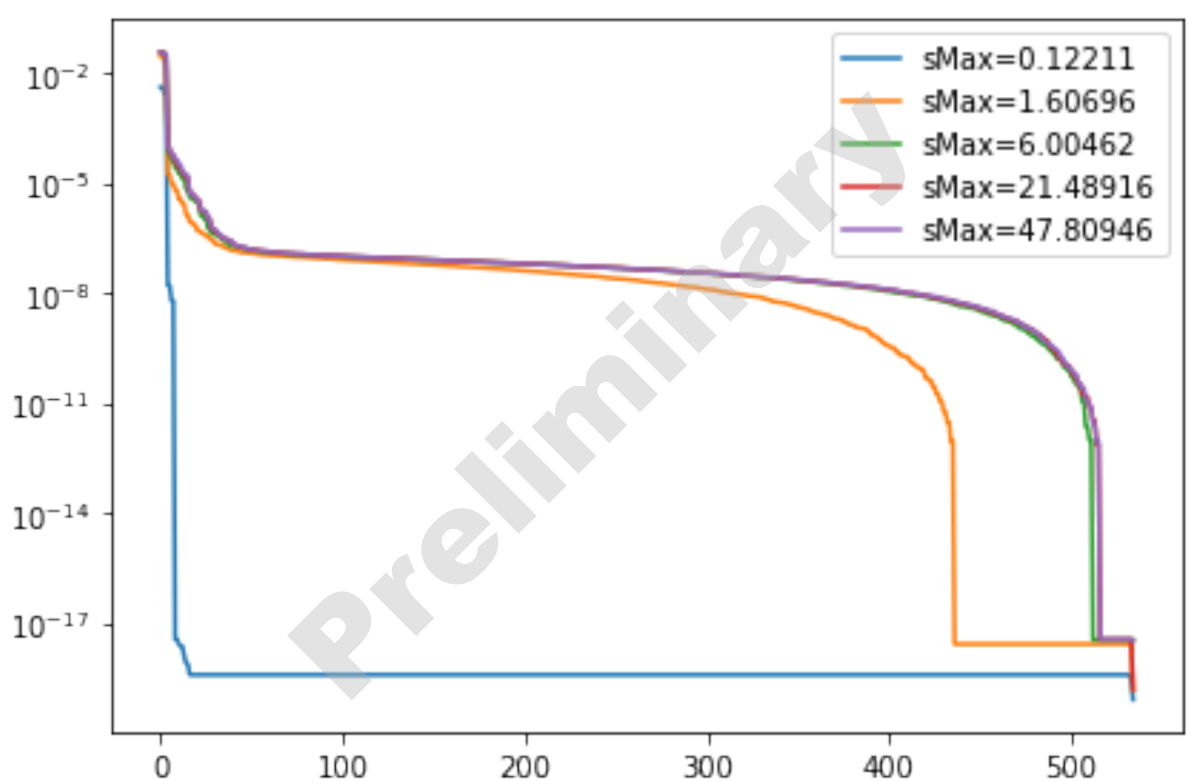
- implementing factorized SRG flow has **no adverse affect** on other observables / expectation values

SVD for Many-Body Calculation





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



- **Magnus-IMSRG:**

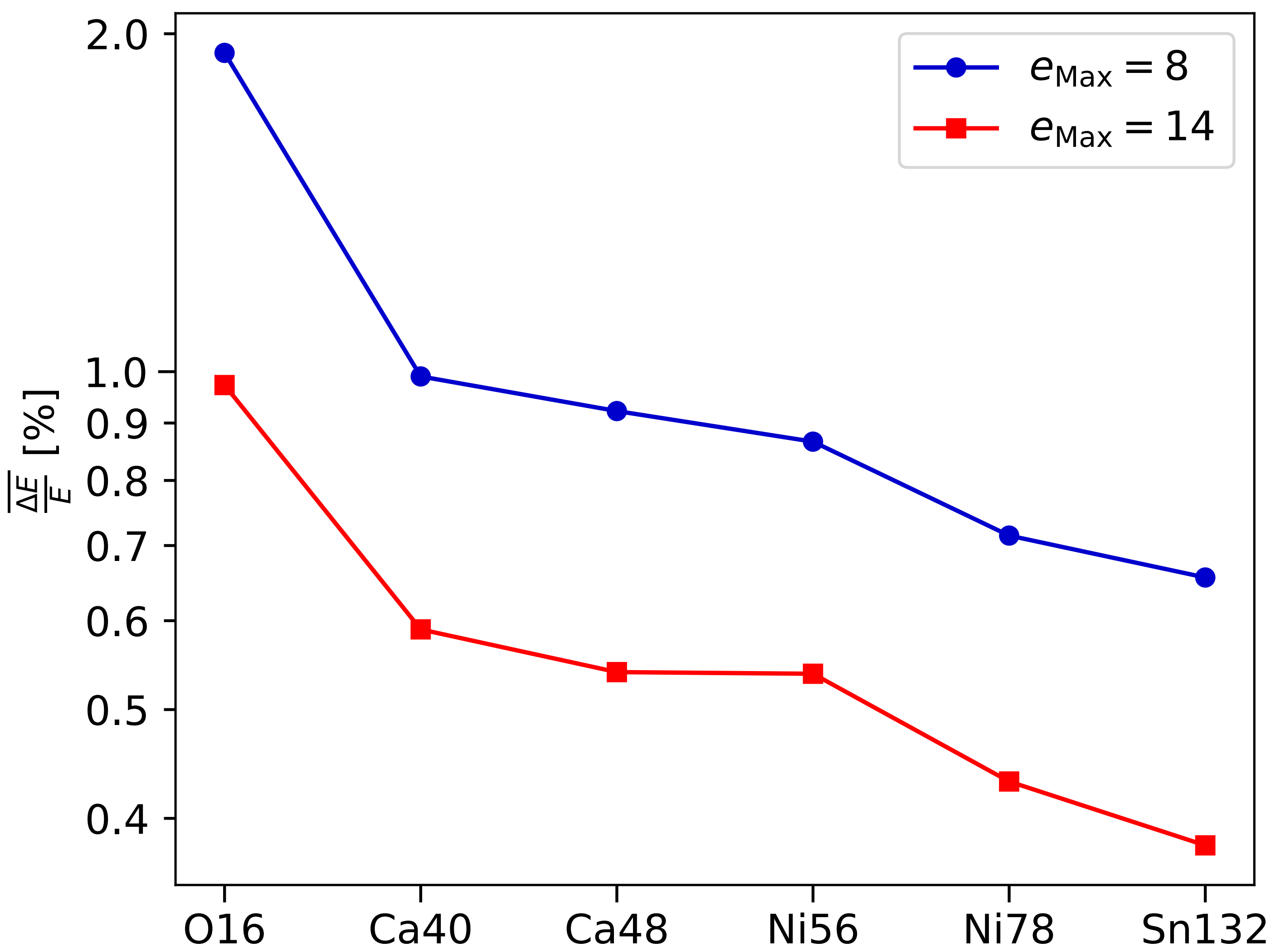
$$U(s) = e^{\Omega(s)}$$

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

Compression with Random Projections

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

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

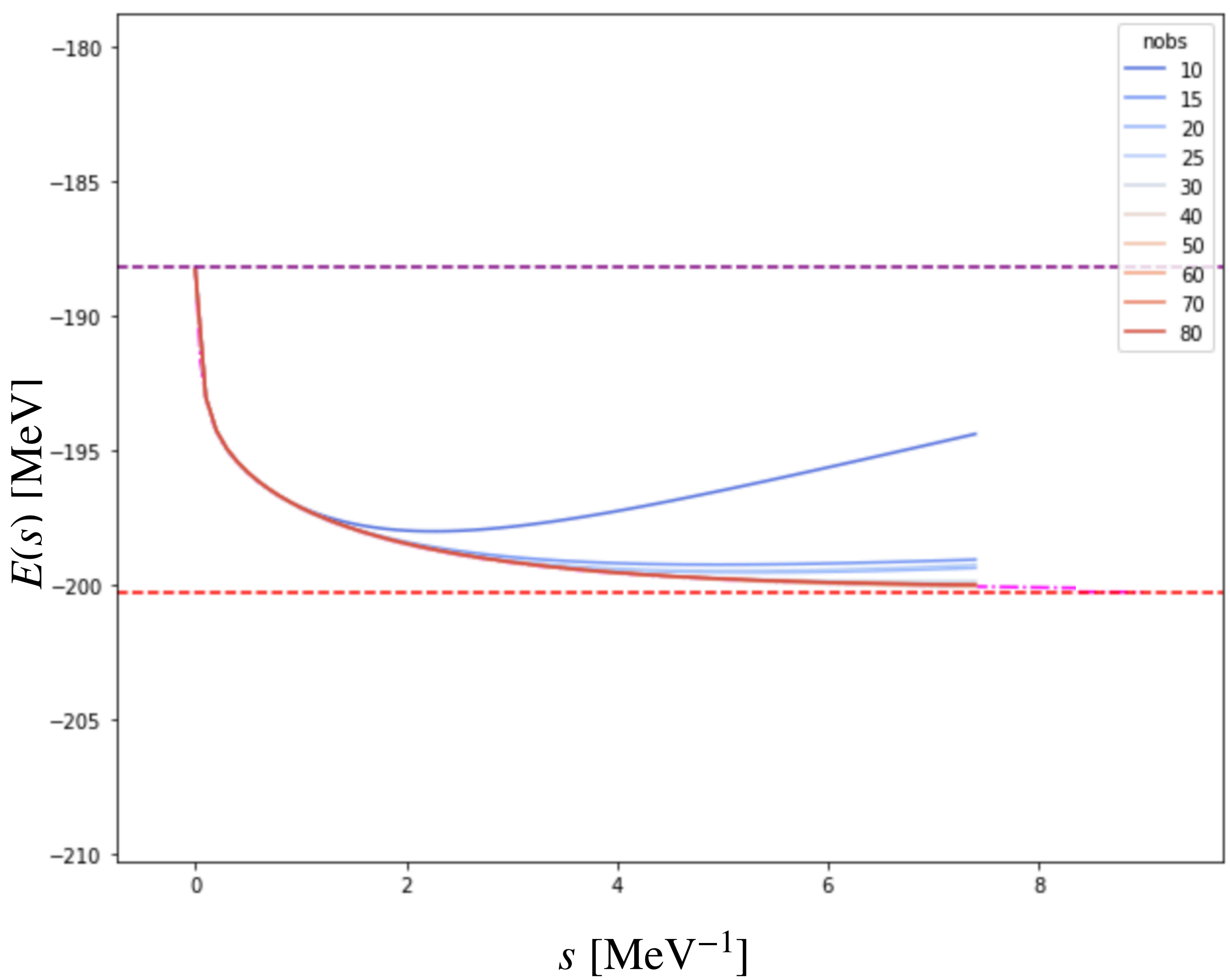


- tensorial (= modewise) **Johnson-Lindenstrauss embeddings**
- **purely based on features of (sparse) big data sets** - integrate with physics-based ideas?
- suitable for **streaming** transforms: compress on the fly while reading from disk

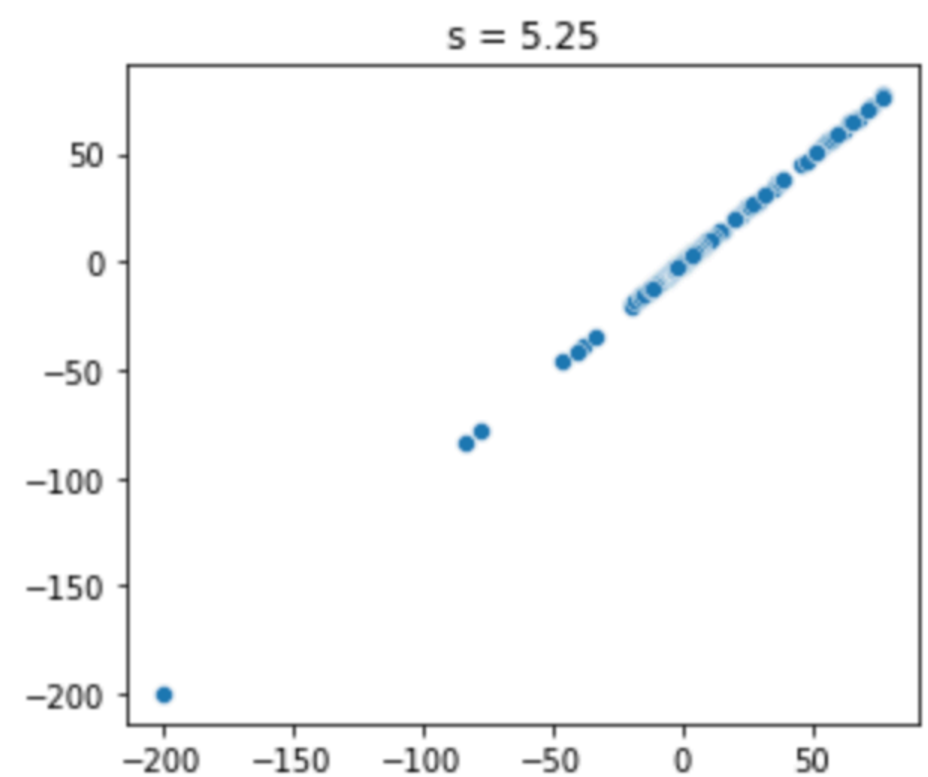
Emulating IMSRG Flows

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

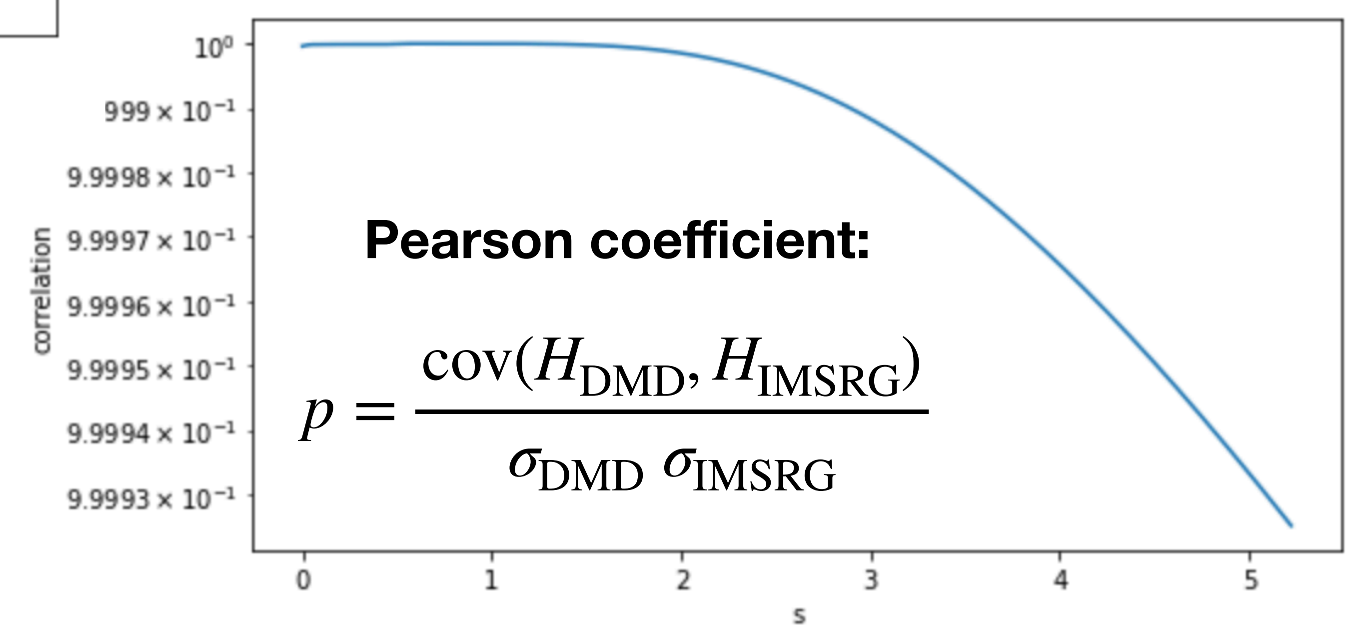
EM(500) N³LO, $\lambda = 2.0\,\mathrm{fm}^{-1}$



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



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

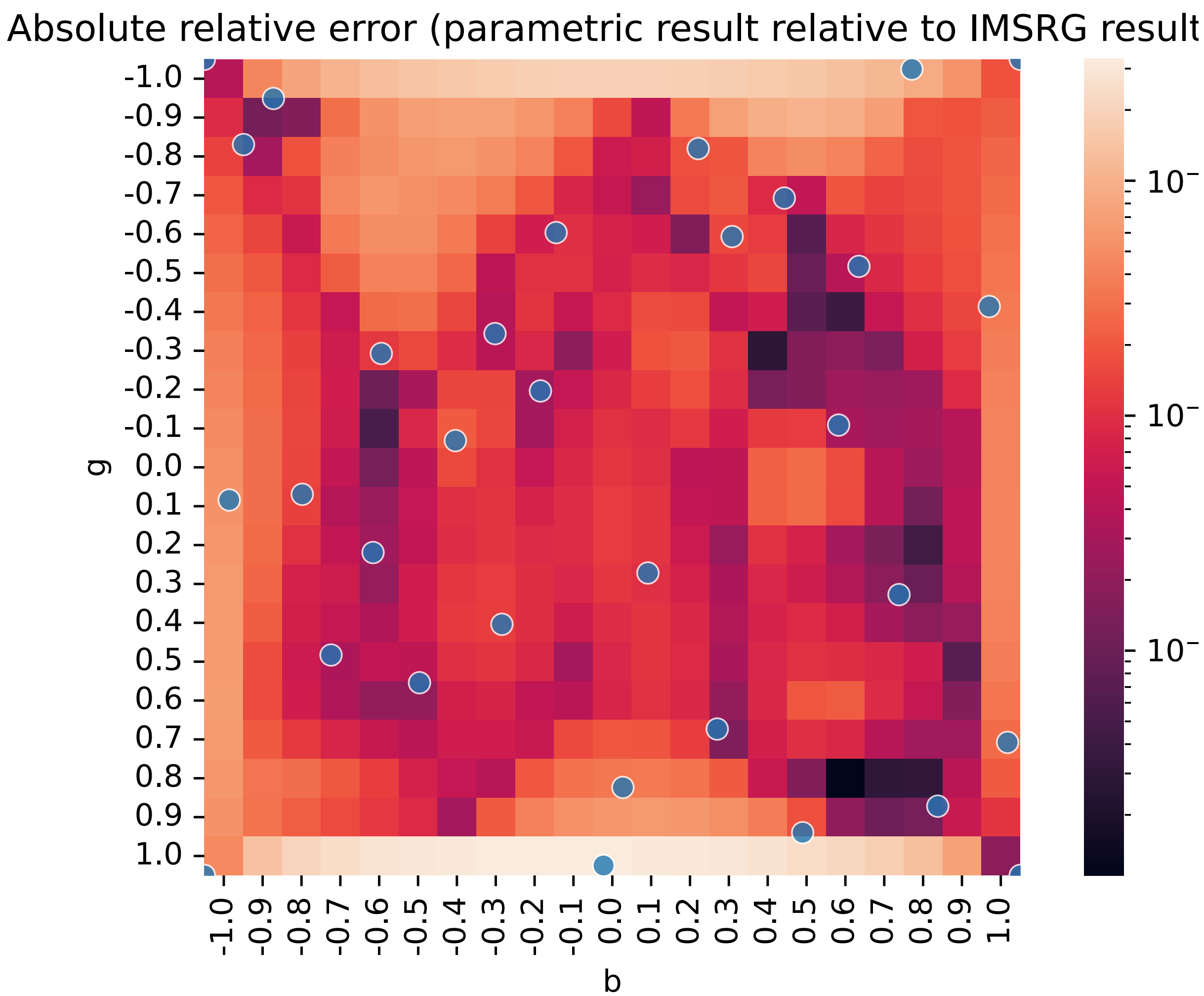


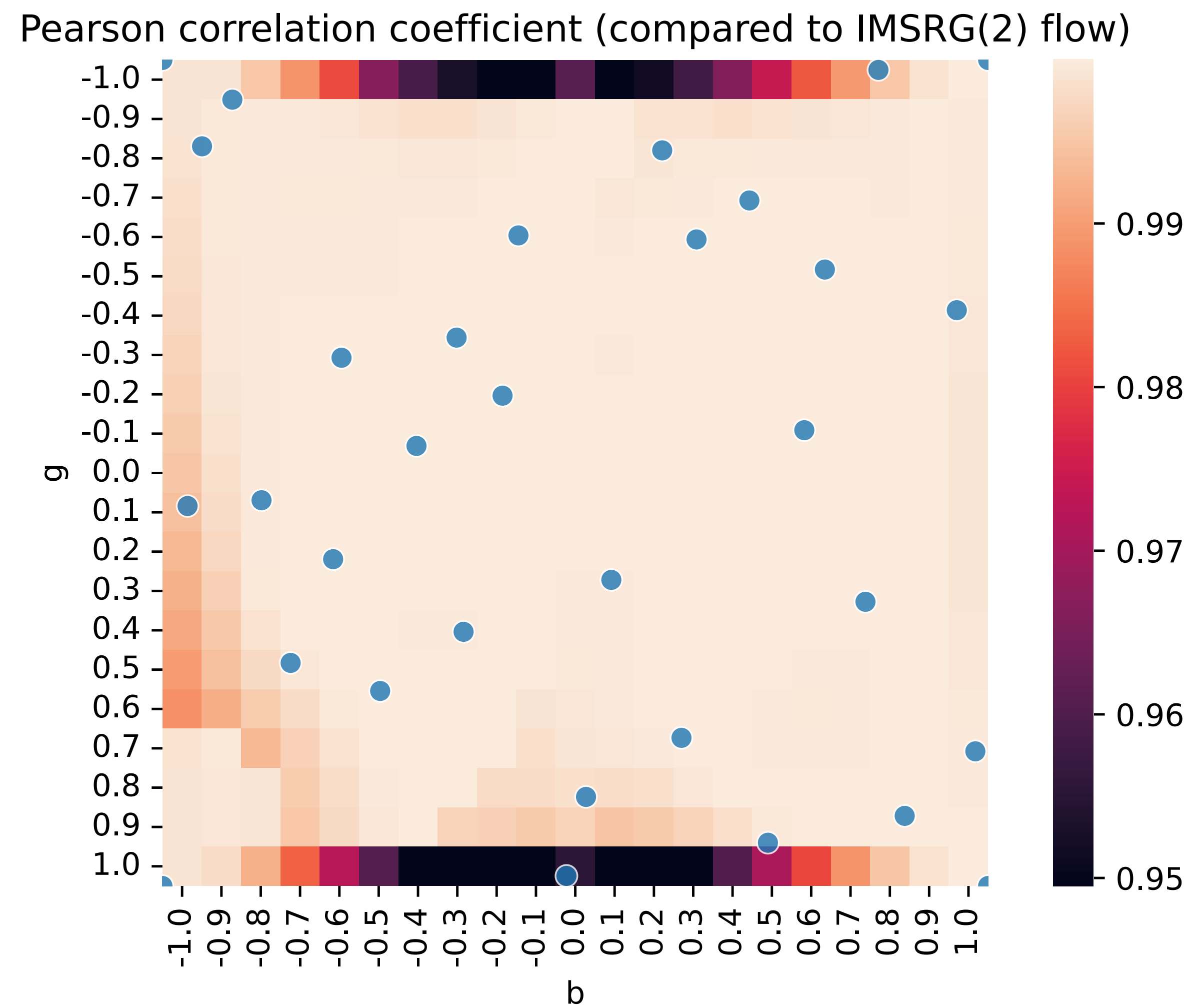
Pearson coefficient:

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

Parametric DMD

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





- 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