A Status Update on *Ab Initio* Calculations in Nuclear Physics

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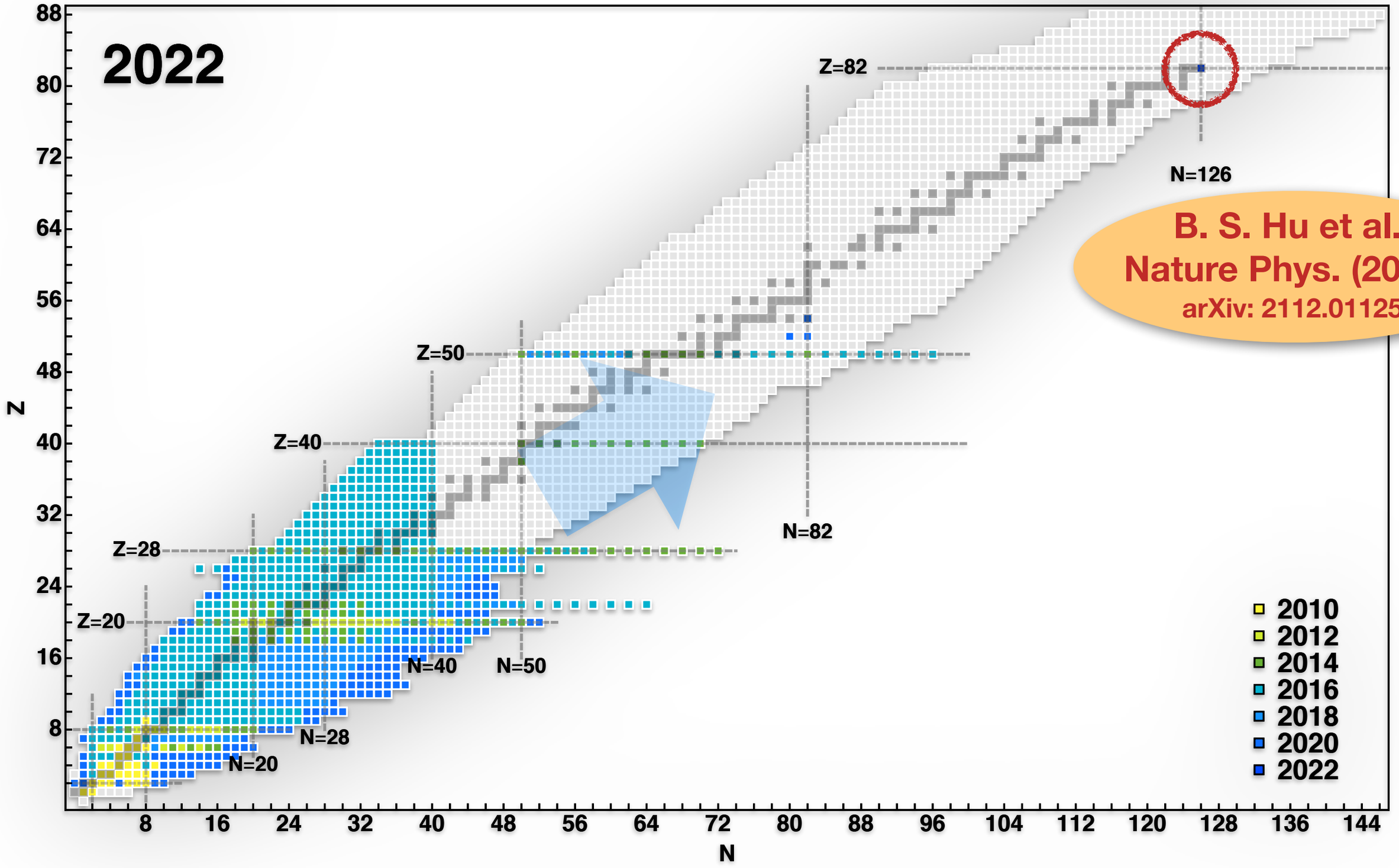
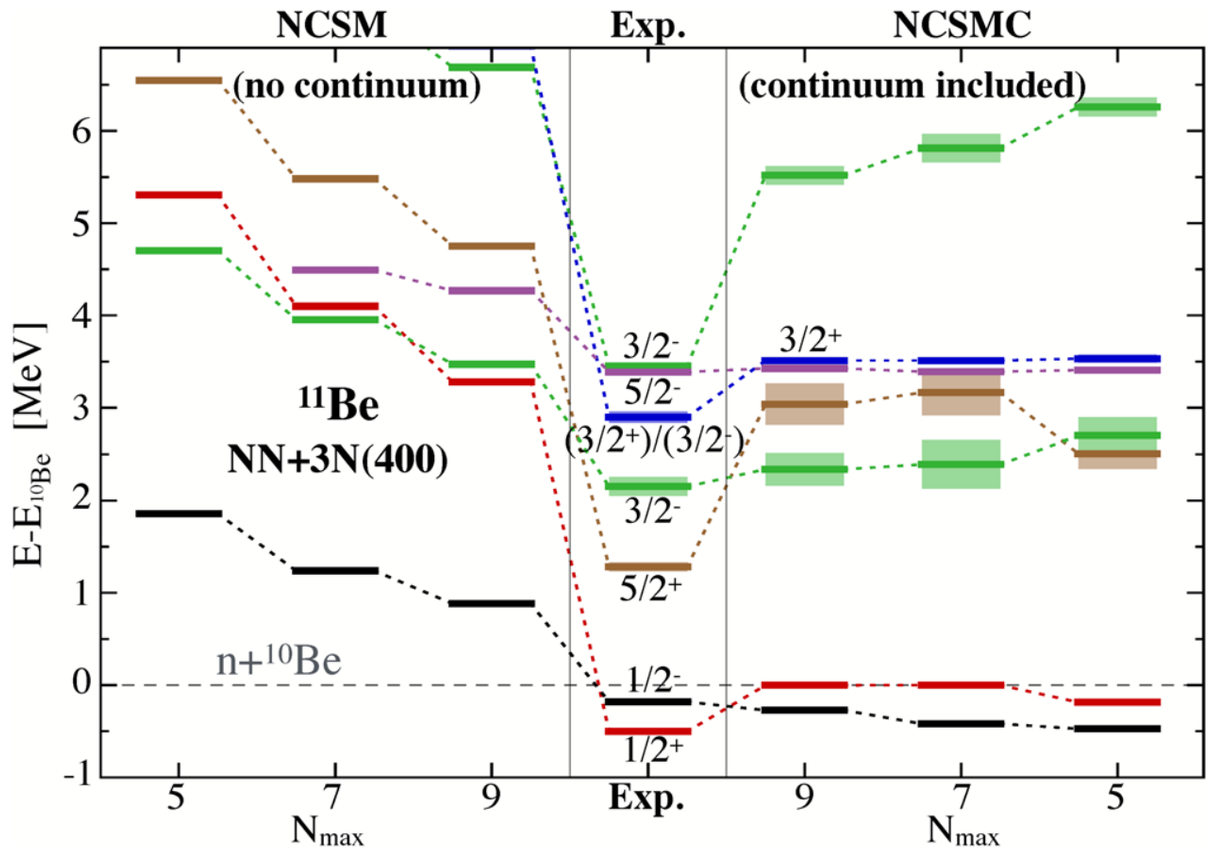
Progress in *Ab Initio* Calculations

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



Progress in *Ab Initio* Calculations

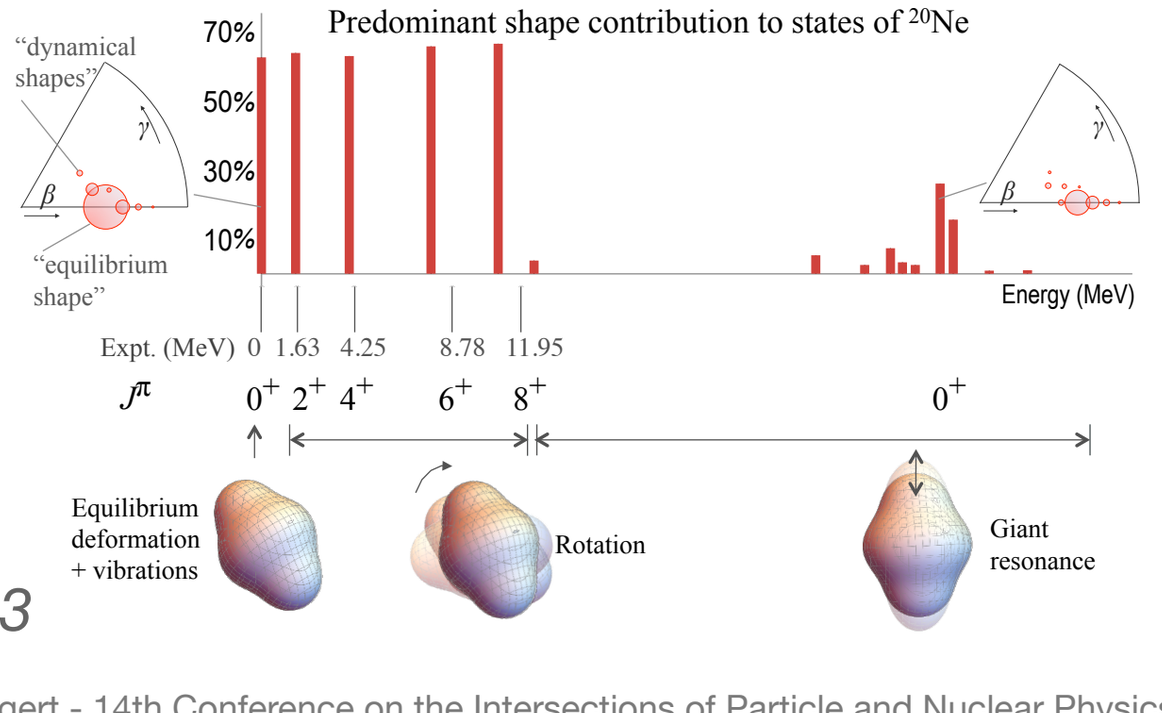


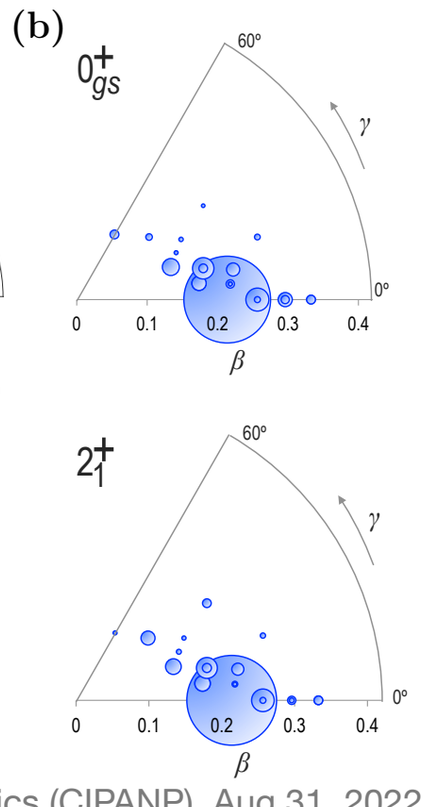
No-Core Shell Model with Continuum

*Calci et al., PRL **117**, 242501*
*Hupin et al., Nature Comm. **10**, 351*
*Hebborn et al., PRL **124**, 042503*

Symmetry-Adapted NCSM

*Dytrych et al., PRL **124**, 042501*
*Burkey et al., PRL **128**, 202502*
*Sargsyan et al., PRL **128**, 202503*

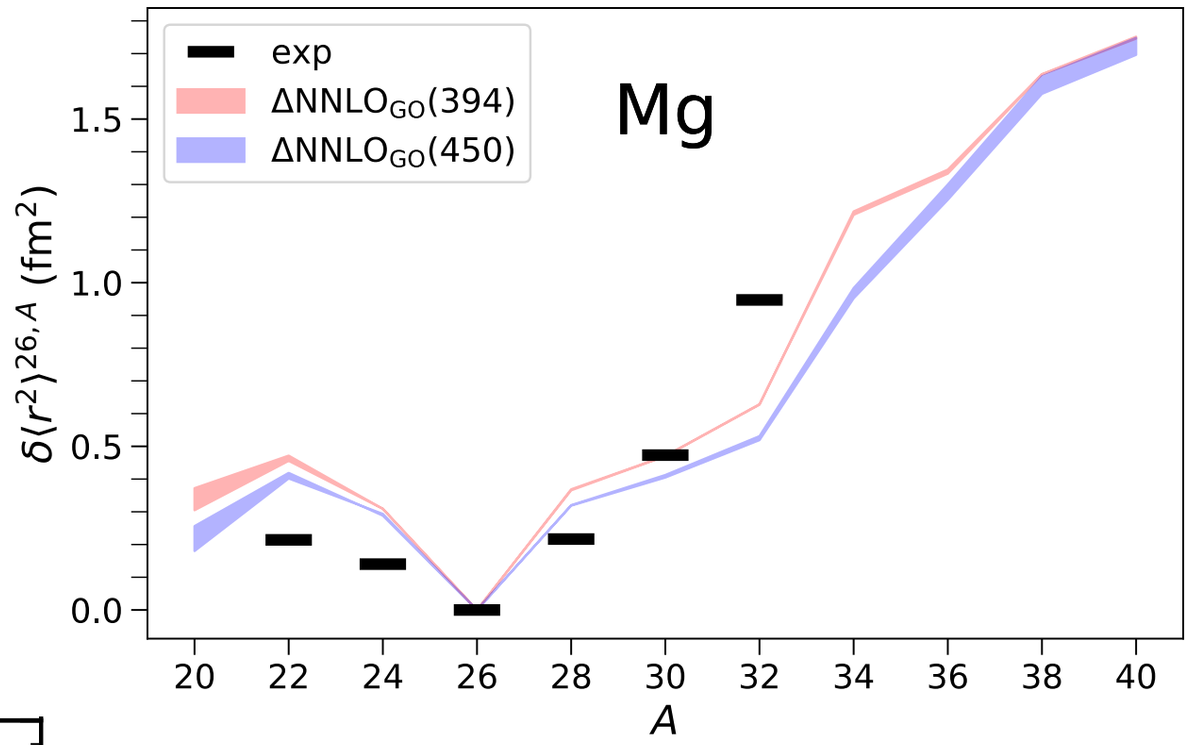


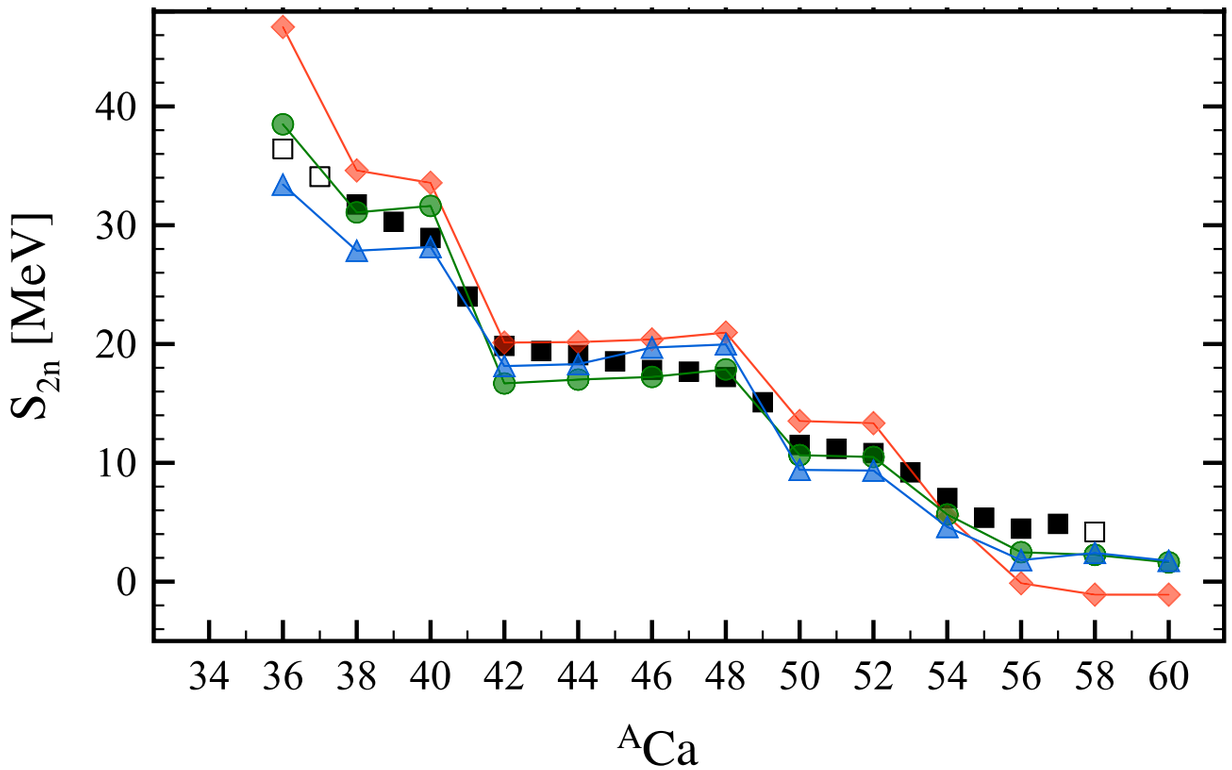


Progress in *Ab Initio* Calculations

Coupled Cluster
(with deformation)

*Novario et al., PRC **102**, 051303*
*Bonaiti et al., PRC **105**, 034313*
*Hagen et al., PRC **105**, 064311*

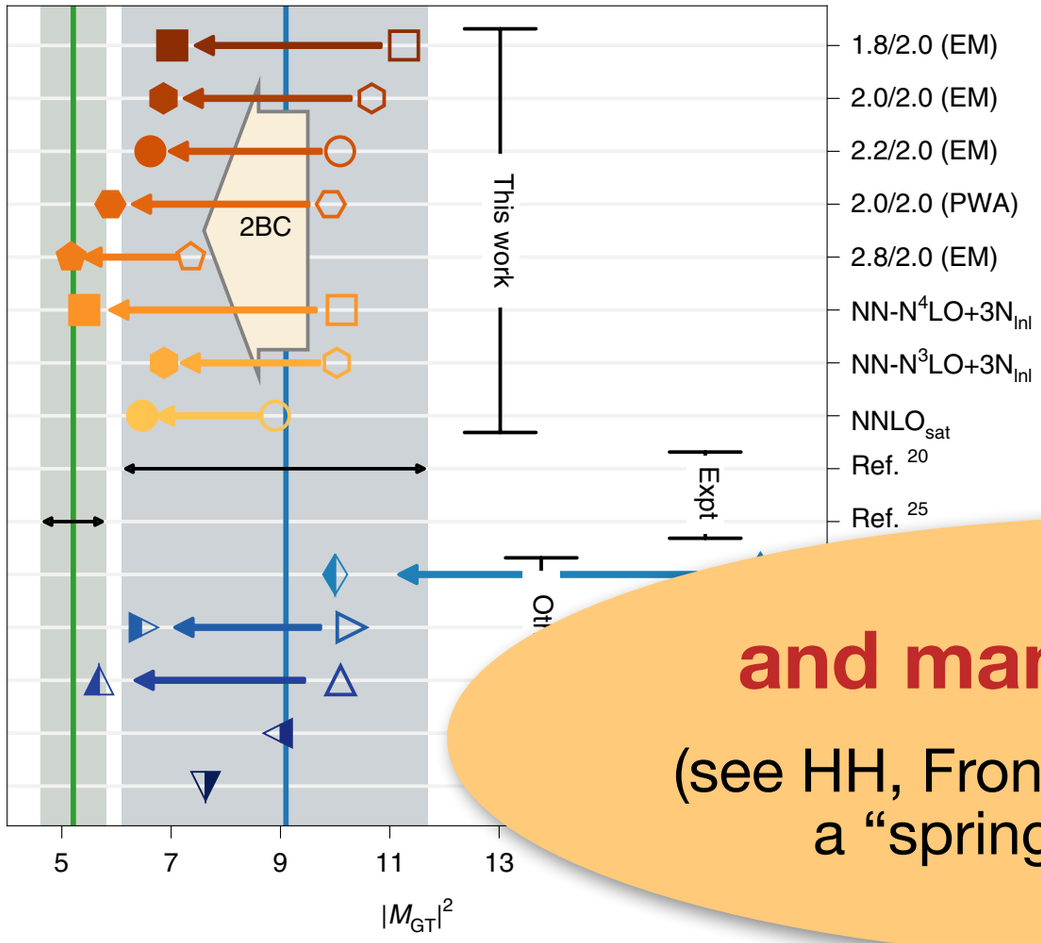




Gor'kov Greens Functions

*Somà et al., PRC **101**, 014318*

Progress in *Ab Initio* Calculations



NCSM, CC & Valence-Space In-Medium Similarity RG

Gysbers et al., Nature Phys. ***15****, 428*

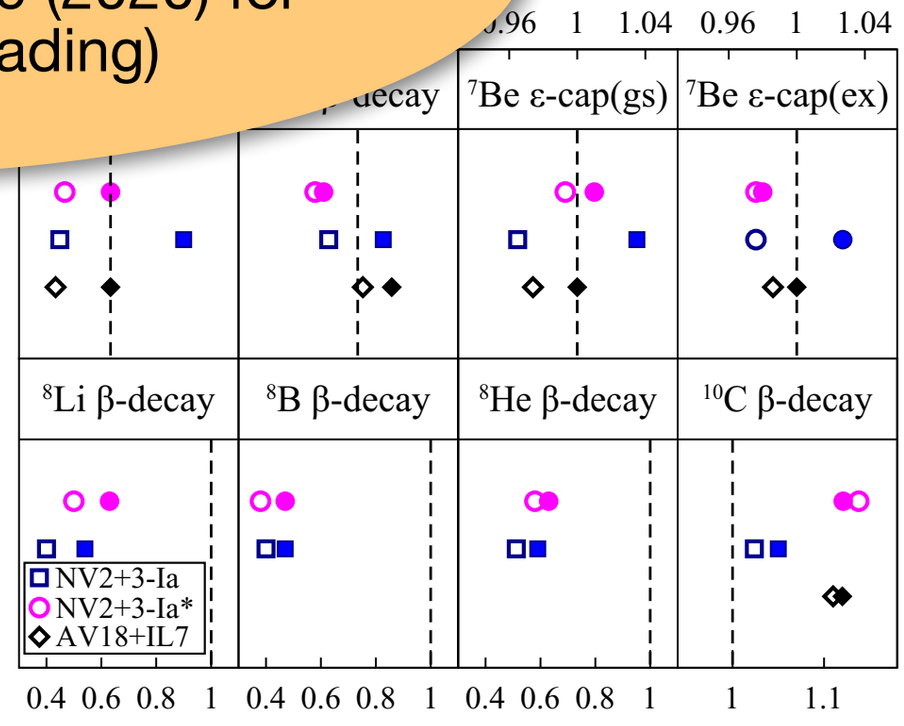
and many, many more…

(see HH, Front. Phys. 8, 379 (2020) for a “springboard" for reading)

cf. talk by S. Gandolfi

Green’s Function Monte Carlo

King et al., PRC ***102****, 025501*
King et al., arXiv: 2207.11179



(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)

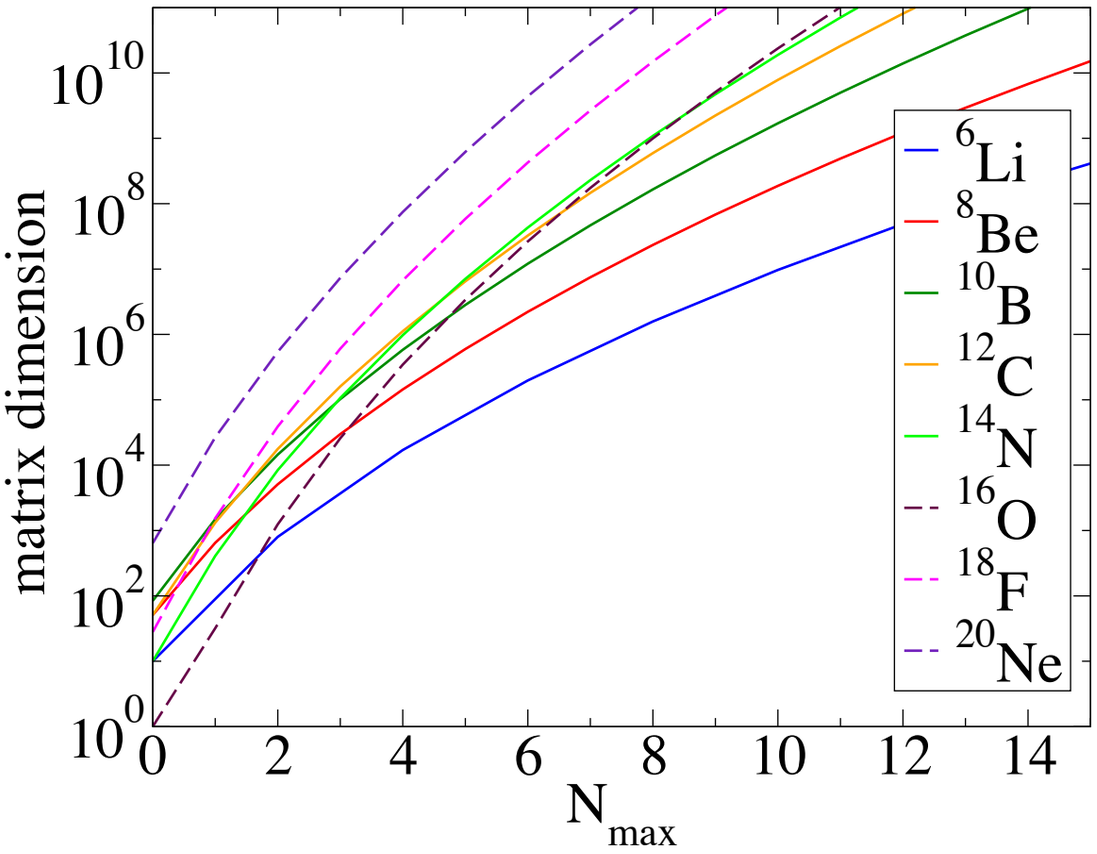
HH, S. K. Bogner, T. Morris, S. Binder, A. Calci, J. Langhammer, R. Roth, Phys. Rev. C **90**, 041302 (2014)

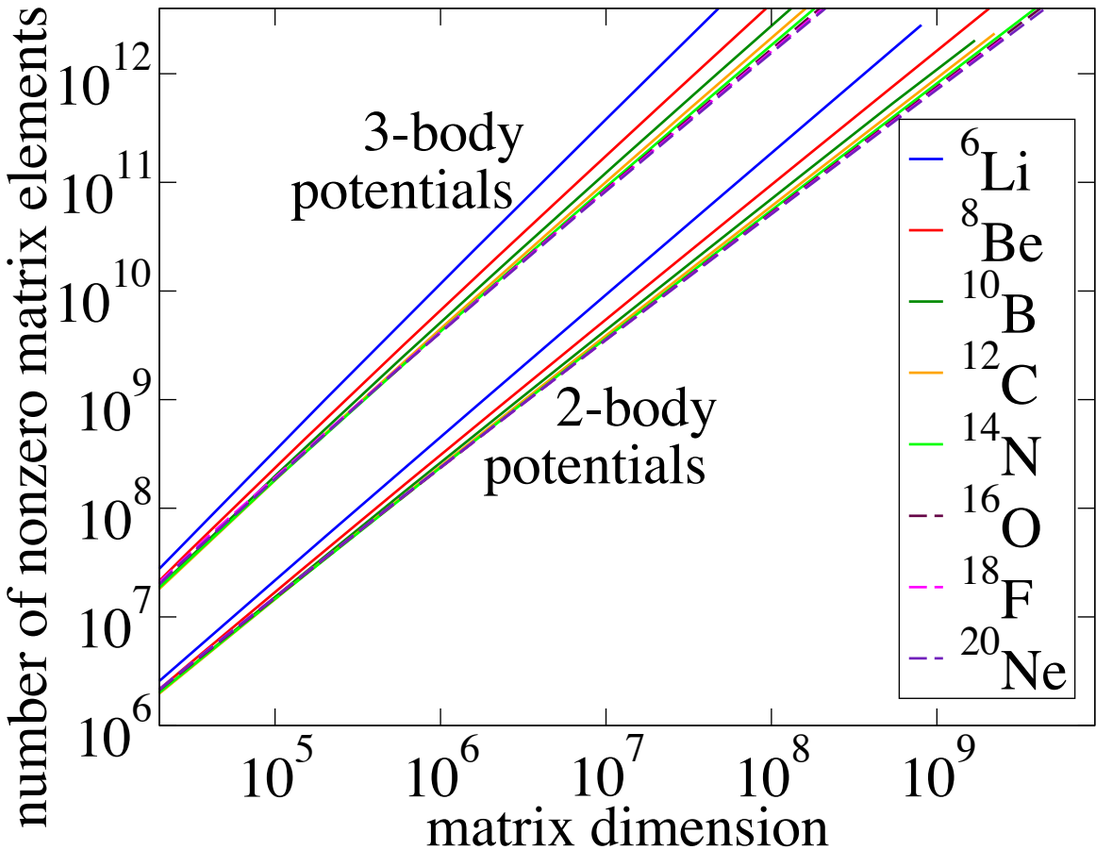
HH, S. Binder, A. Calci, J. Langhammer, and R. Roth, Phys. Rev. Lett **110**, 242501 (2013)

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

Large-Scale Diagonalization

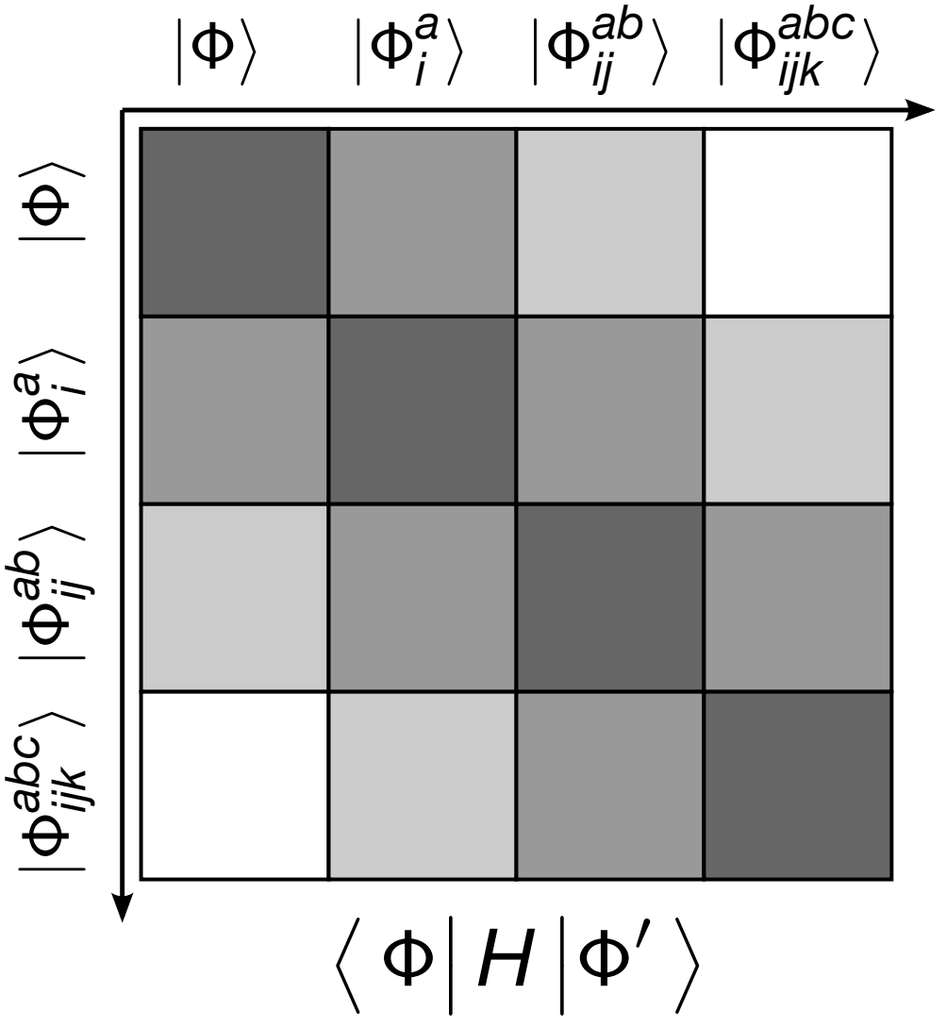




from: C. Yang, H. M. Aktulga, P. Maris, E. Ng, J. Vary, Proceedings of NTSE-2013

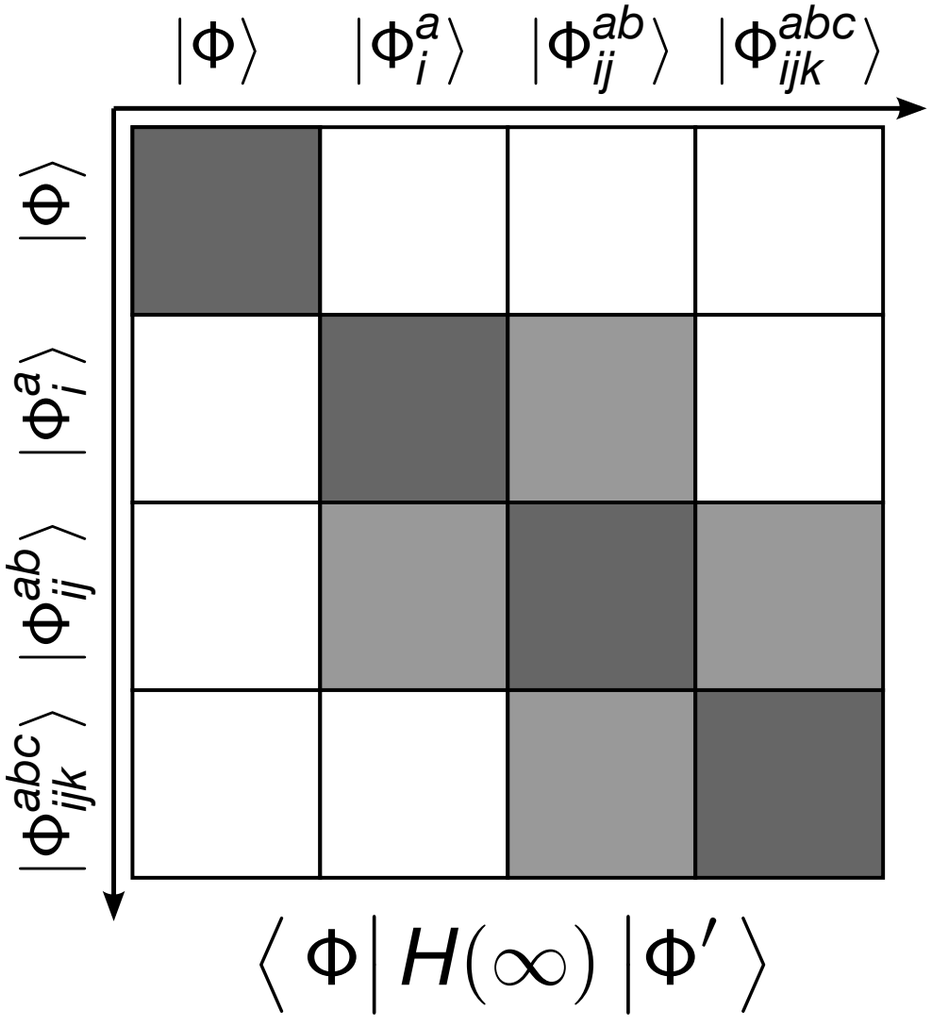
- basis-size “explosion”: **exponential growth**
- **importance truncation** etc. cannot fully compensate this growth as A increases

Decoupling in A-Body Space



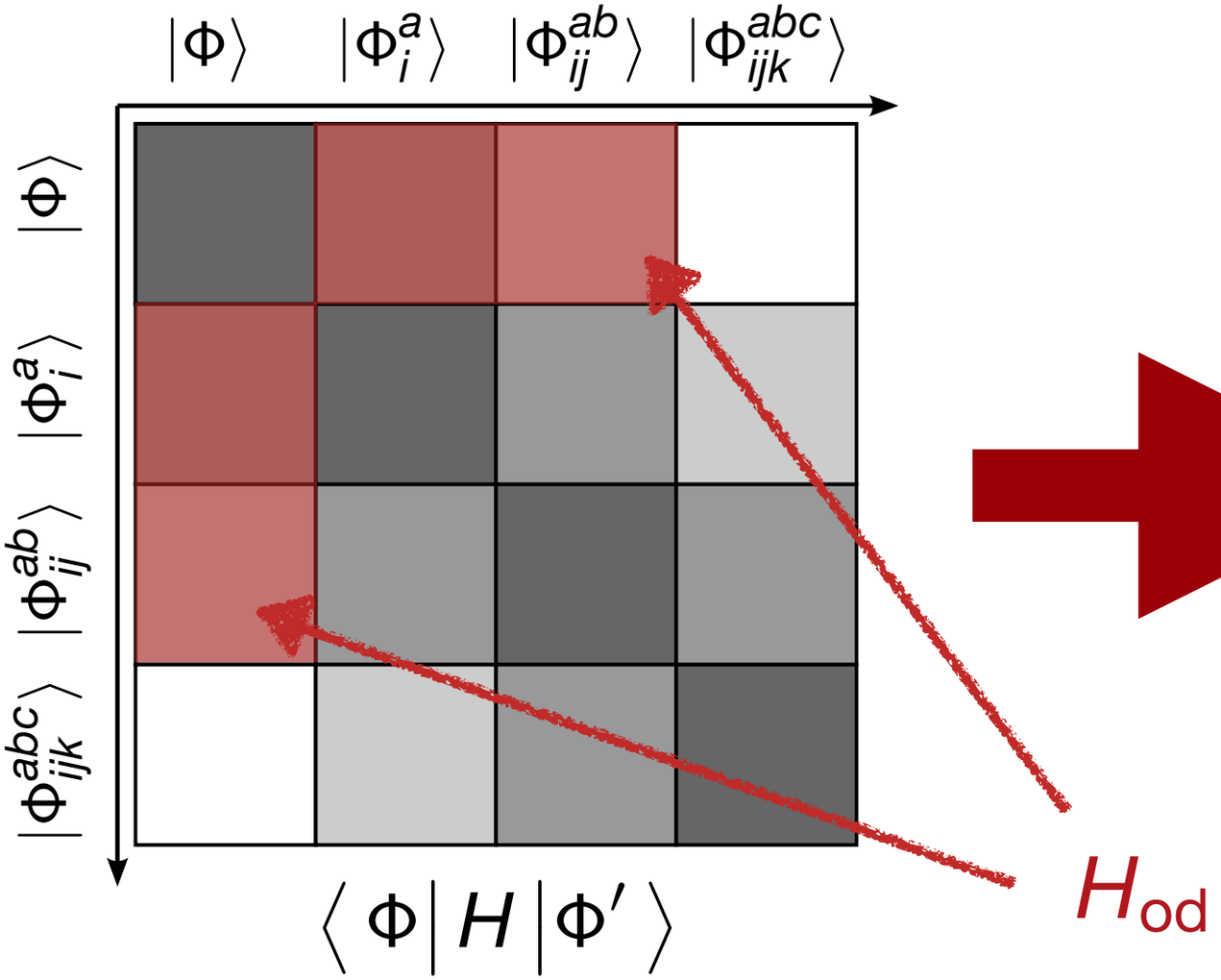
$U(s)HU^\dagger(s)$

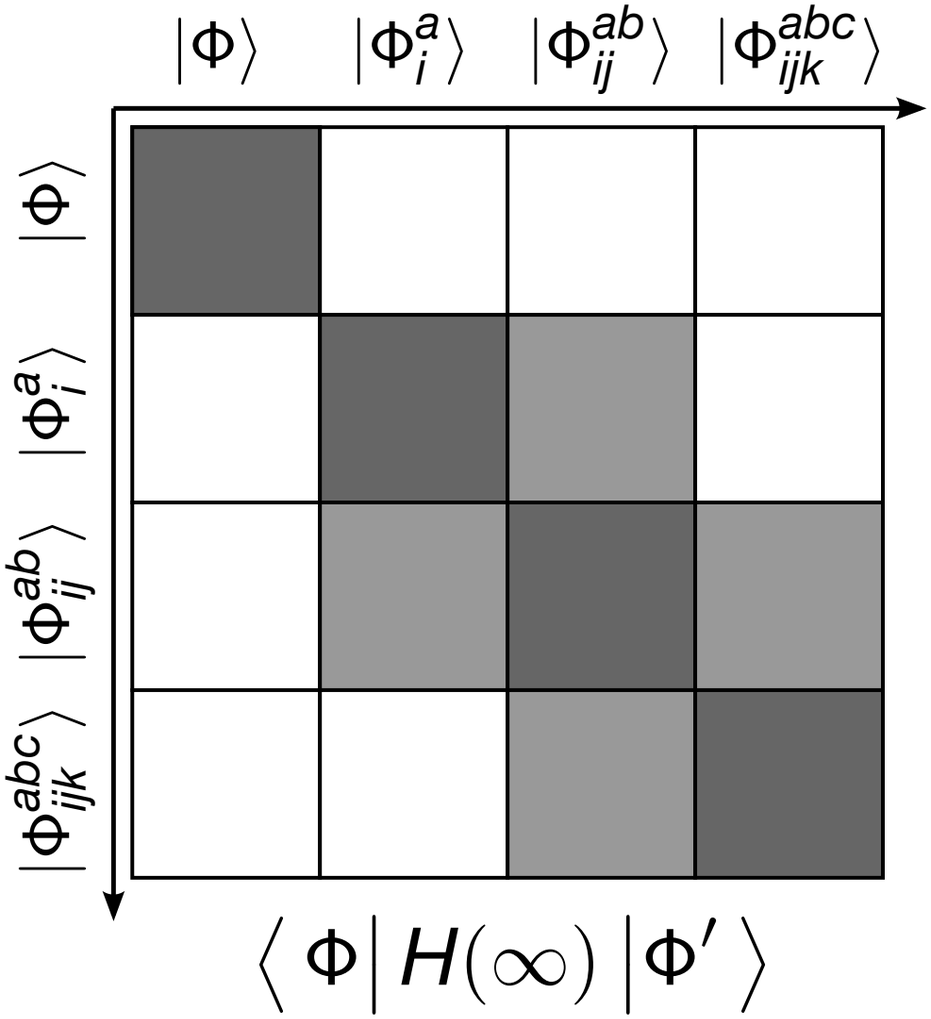
$s \to \infty$



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

Flow Equation

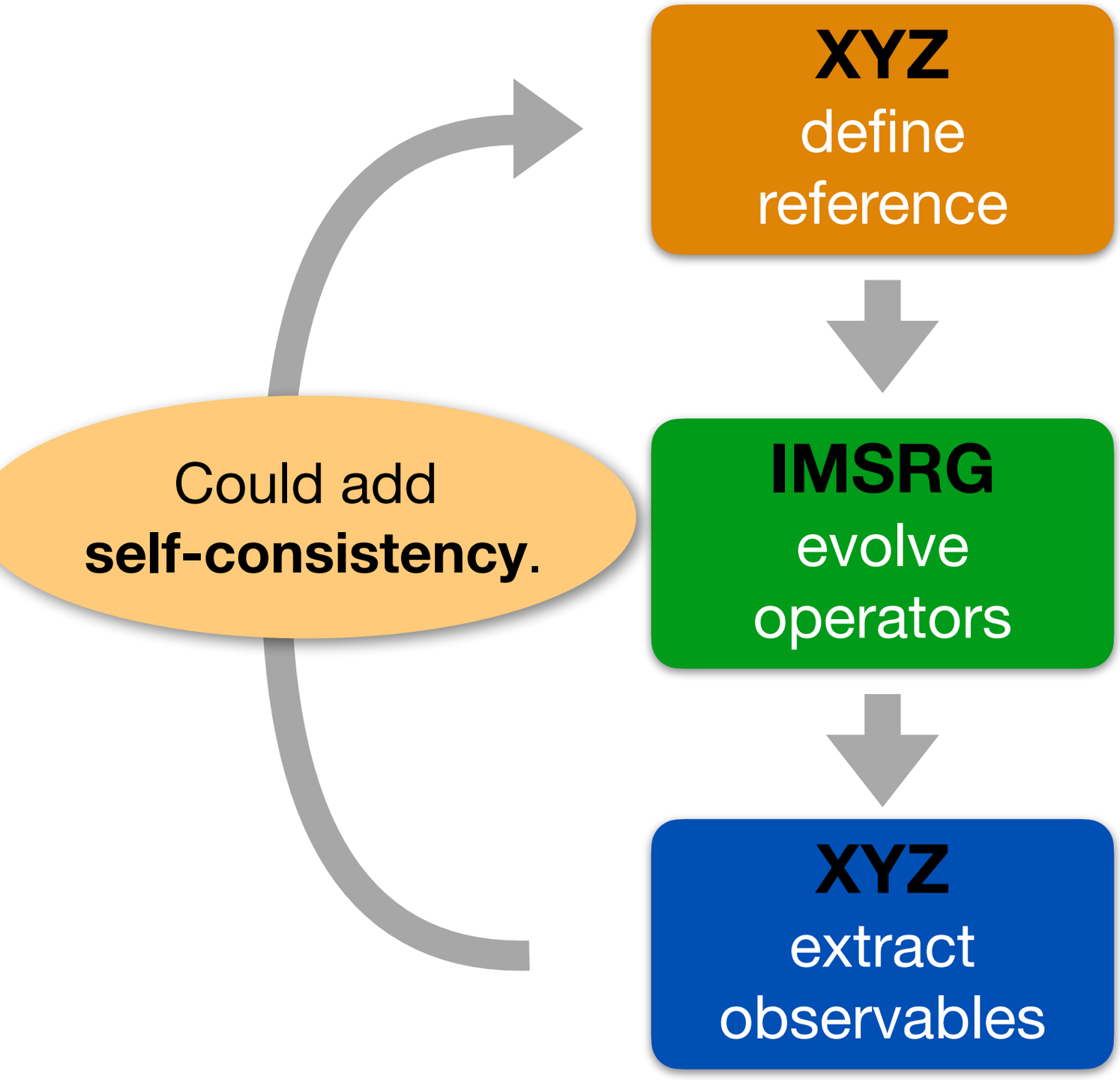




$$\frac{d}{ds}H(s) = \left[\eta(s), H(s)\right],$$

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

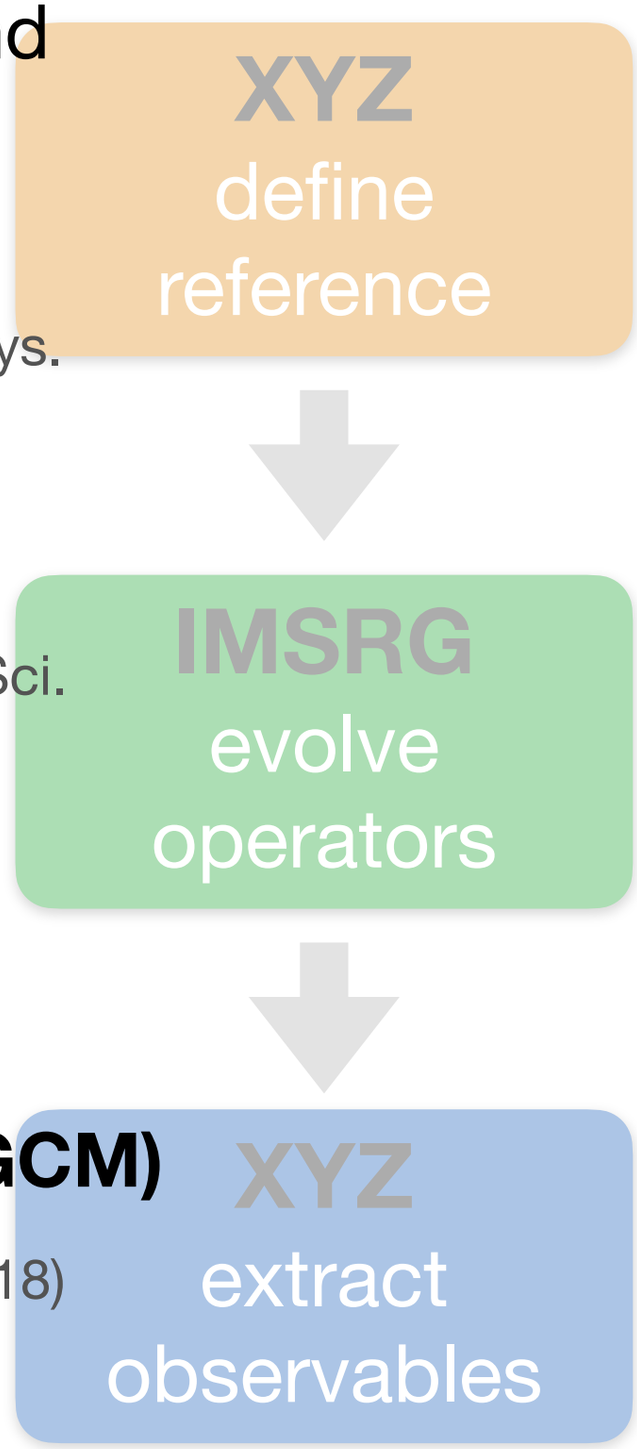
IMSRG-Improved Methods



* 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:

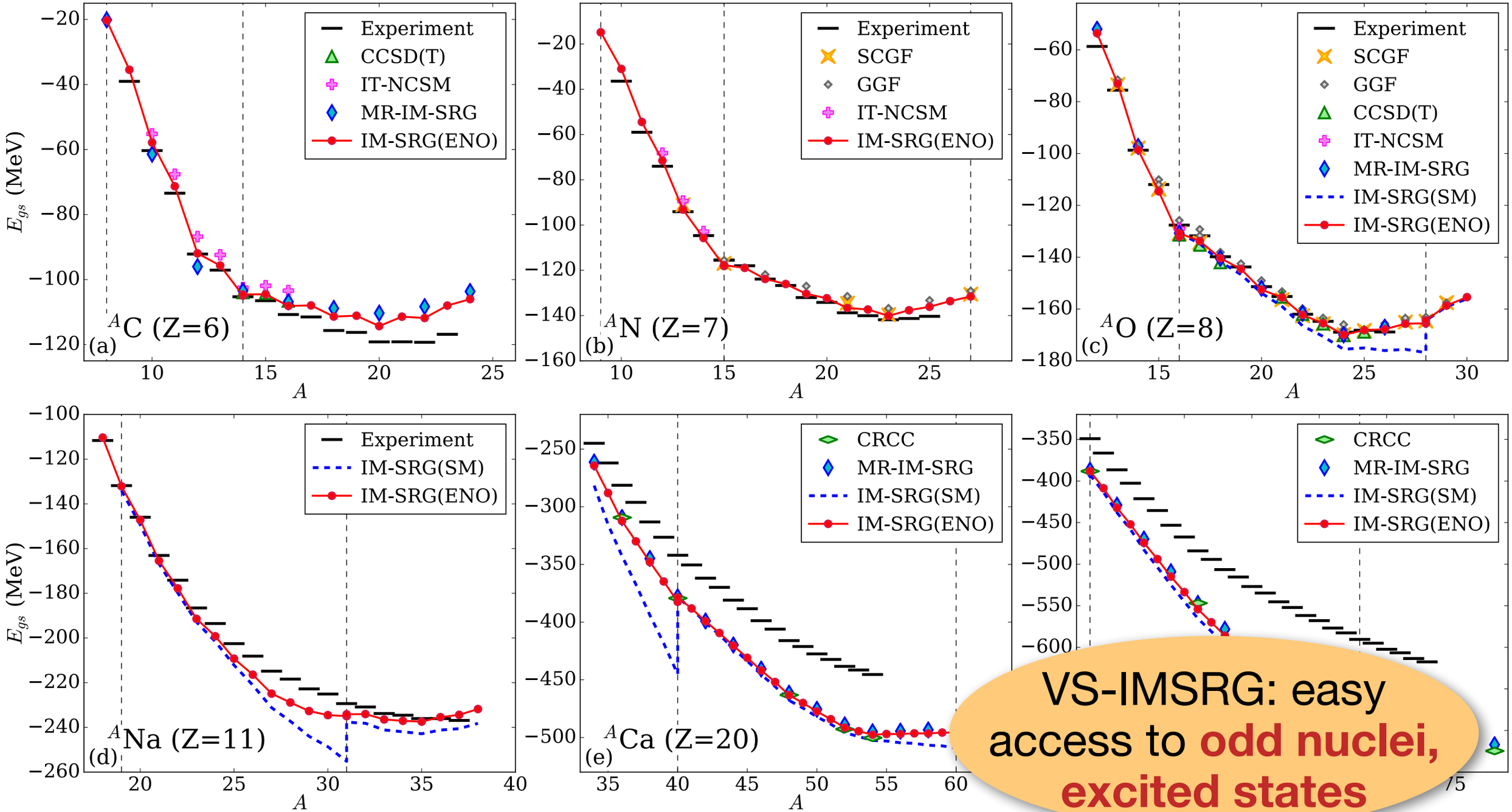
S. R. Stroberg, HH, S. K. Bogner, and J. D. Holt, Ann. Rev. Part. Nucl. Sci. **69**, 165 (2019)

Full CI:

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

Ground-State Energies

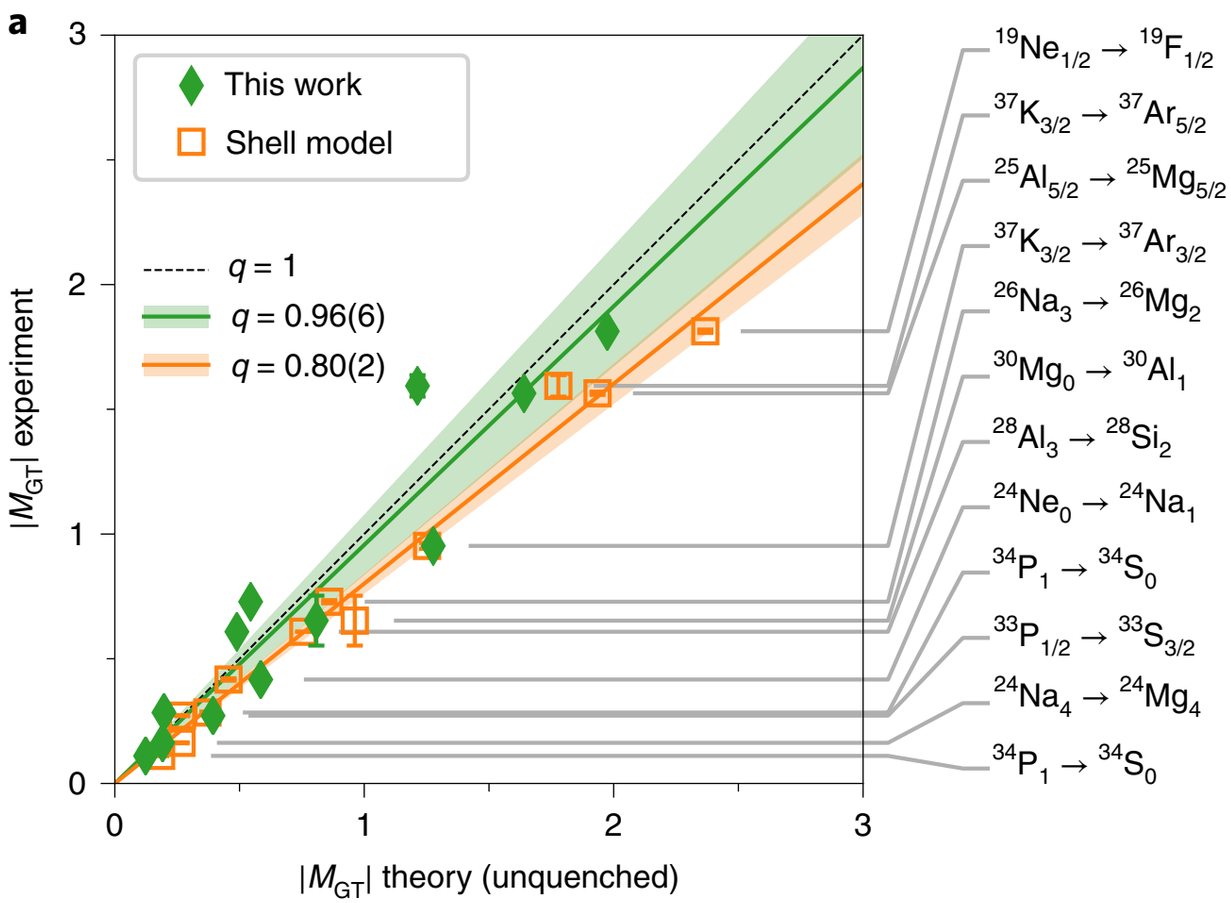
*S. R. Stroberg, A. Calci, HH, J. D. Holt, S. K.Bogner, R. Roth, A. Schwenk, PRL **118**, 032502 (2017)*
*S. R. Stroberg, HH, S. K. Bogner, J. D. Holt, Ann. Rev. Part. Nucl. Sci. **69**, 307 (2019)*

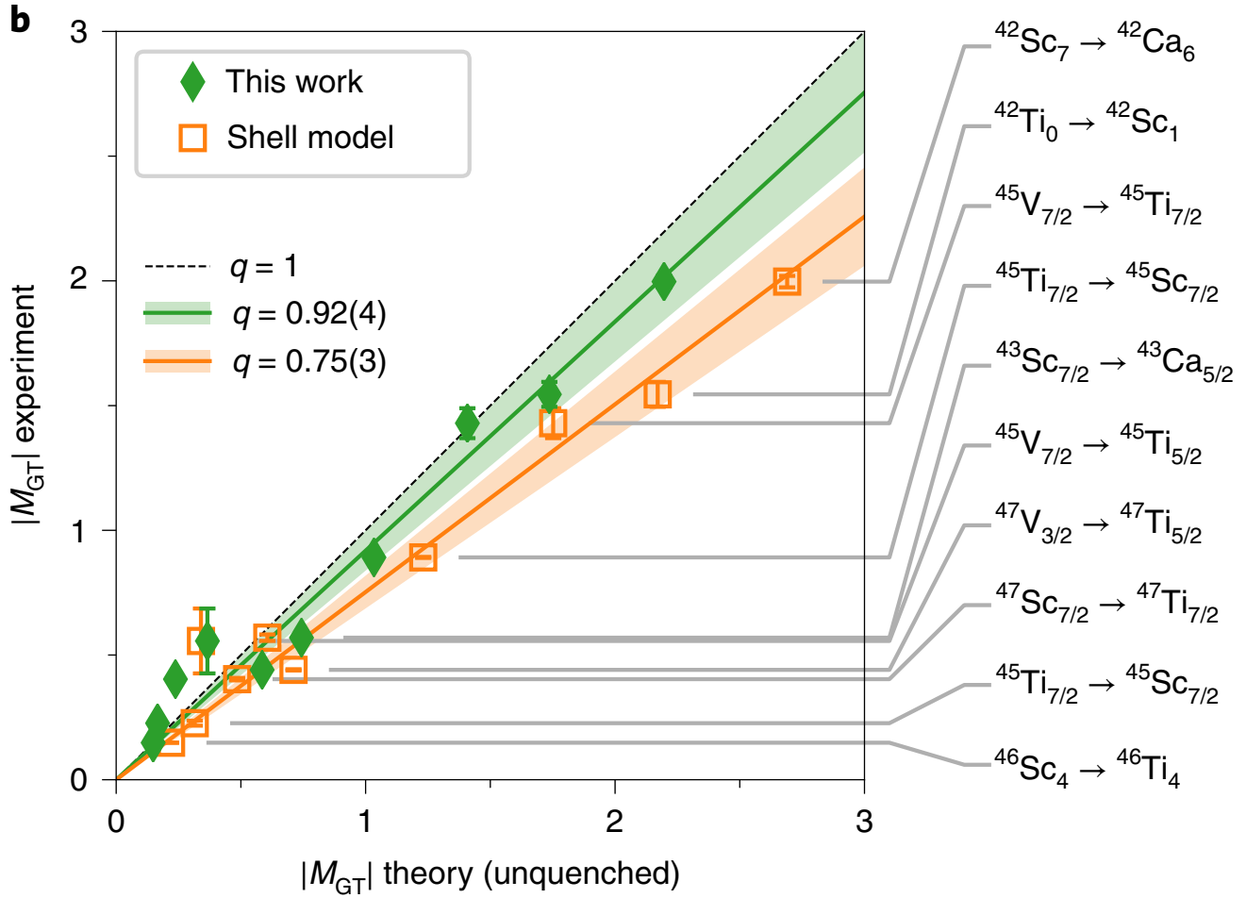


VS-IMSRG: easy access to odd nuclei, excited states

Quenching of Gamow-Teller Decays

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

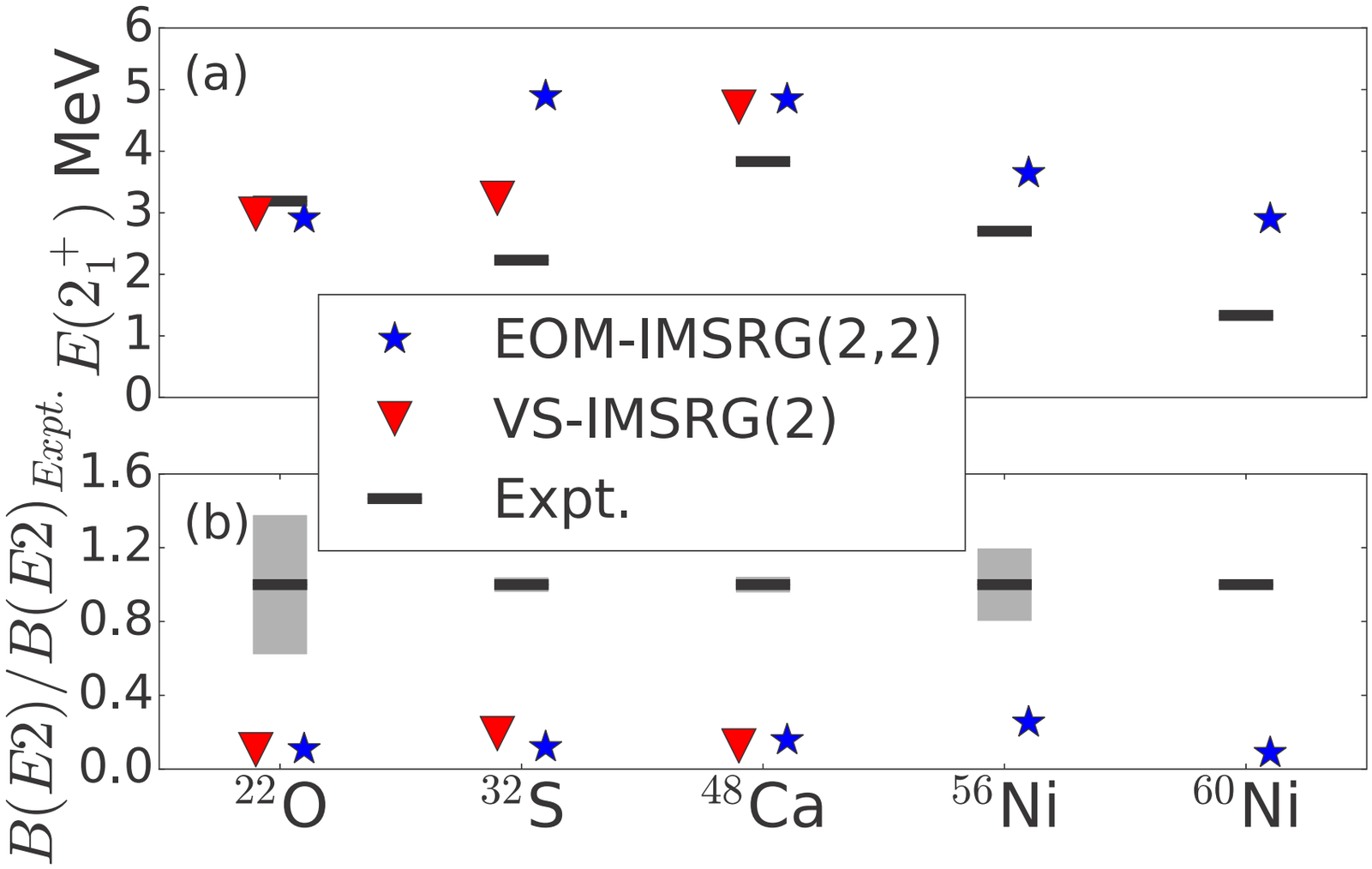




- **empirical Shell model** calculations require **quenching factors** of the weak axial-vector couling g_A
- **VS-IMSRG** explains this through consistent **renormalization** of transition operator, incl. **two-body currents**

Transitions

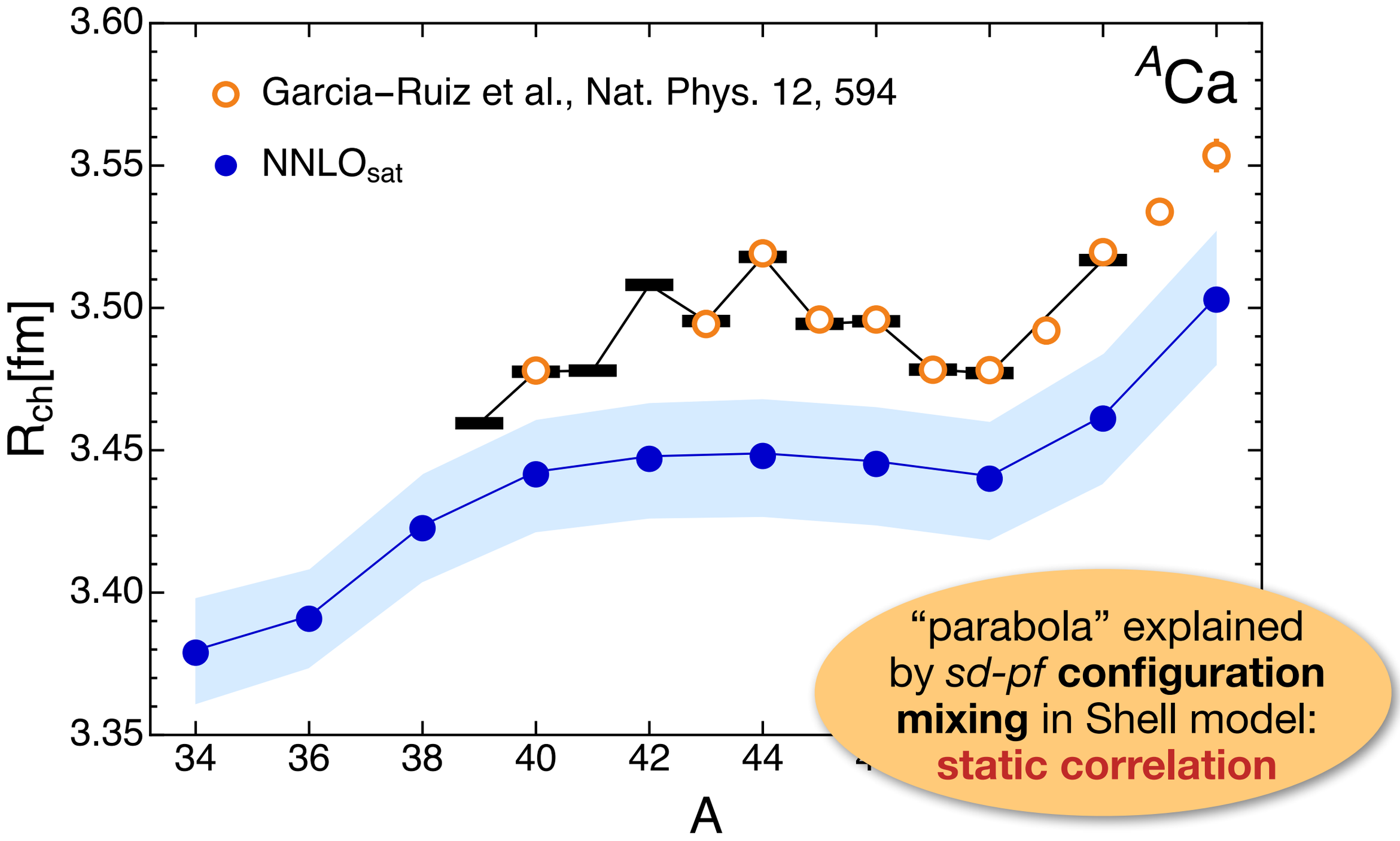
*N. M. Parzuchowski, S. R. Stroberg et al., PRC **96**, 034324*
*S. R. Stroberg, HH, S. K. Bogner, J. D. Holt, Ann. Rev. Part. Nucl. Sci. **69**, 307 (2019)*
*S. R. Stroberg et al. PRC **105**, 034333 (2022*



- **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)*



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)

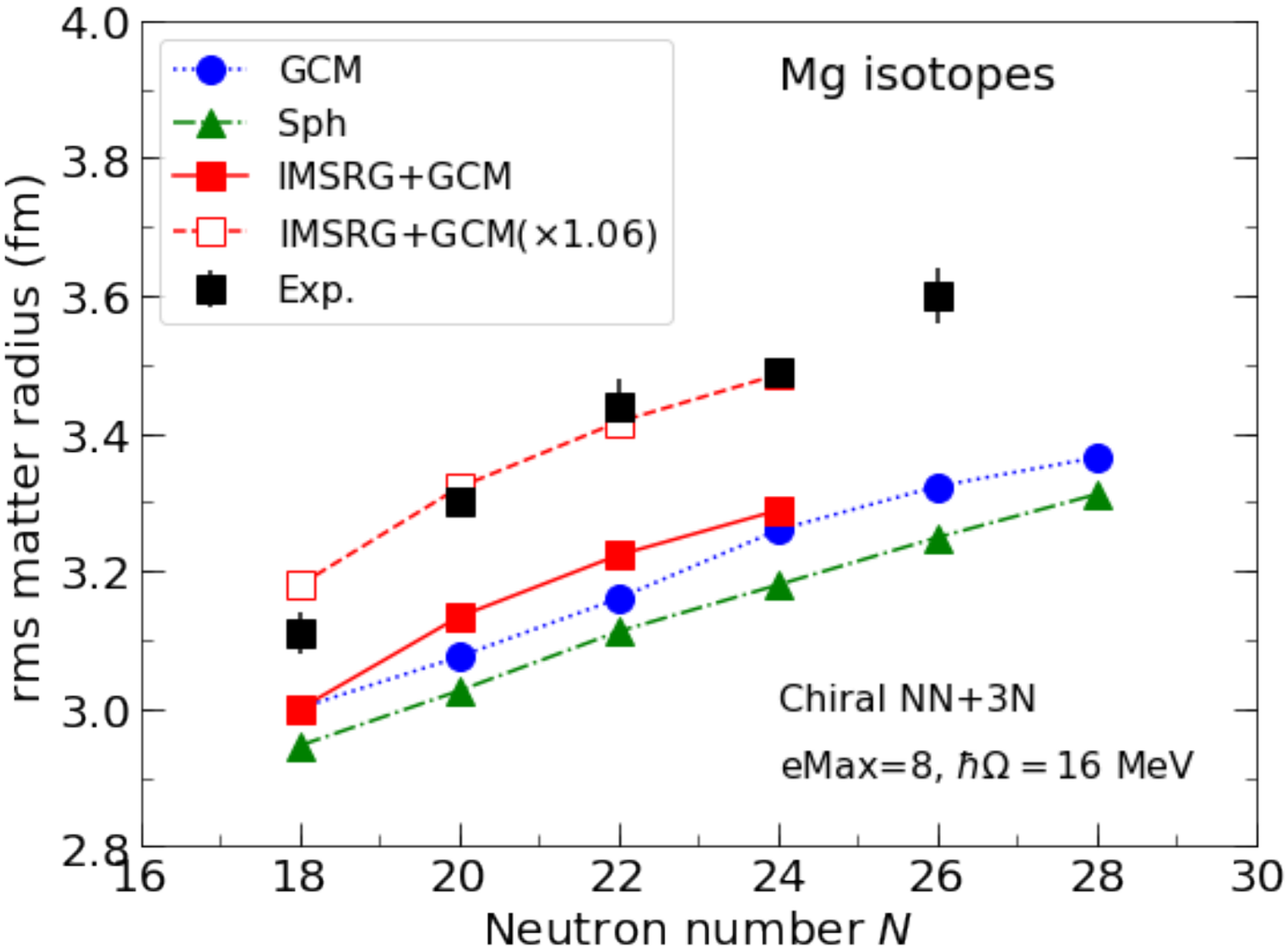
J. M. Yao, B. Bally, J. Engel, R. Wirth, T. R. Rodriguez, HH, PRL **124**, 232501 (2020)

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

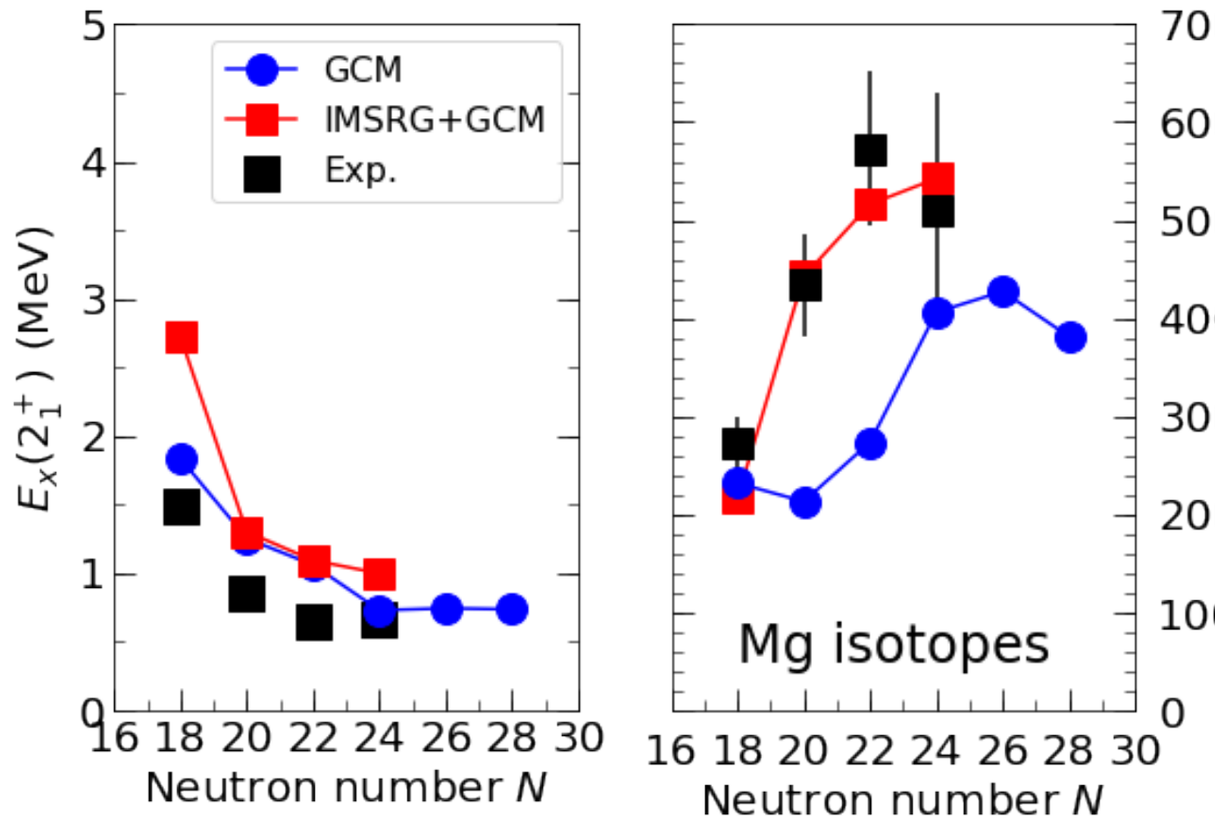
J. M. Yao, HH, in preparation



- 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

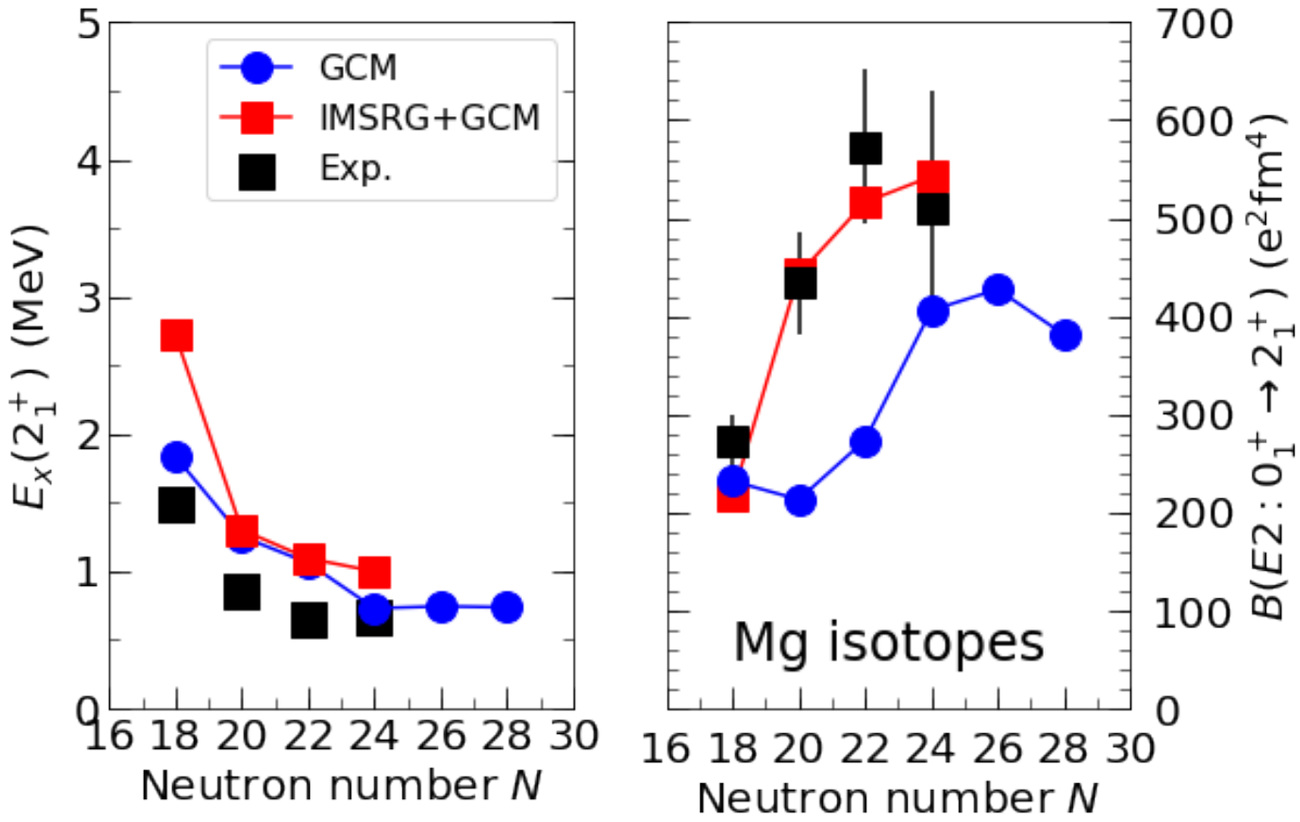
J. M. Yao, HH, in preparation



- 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

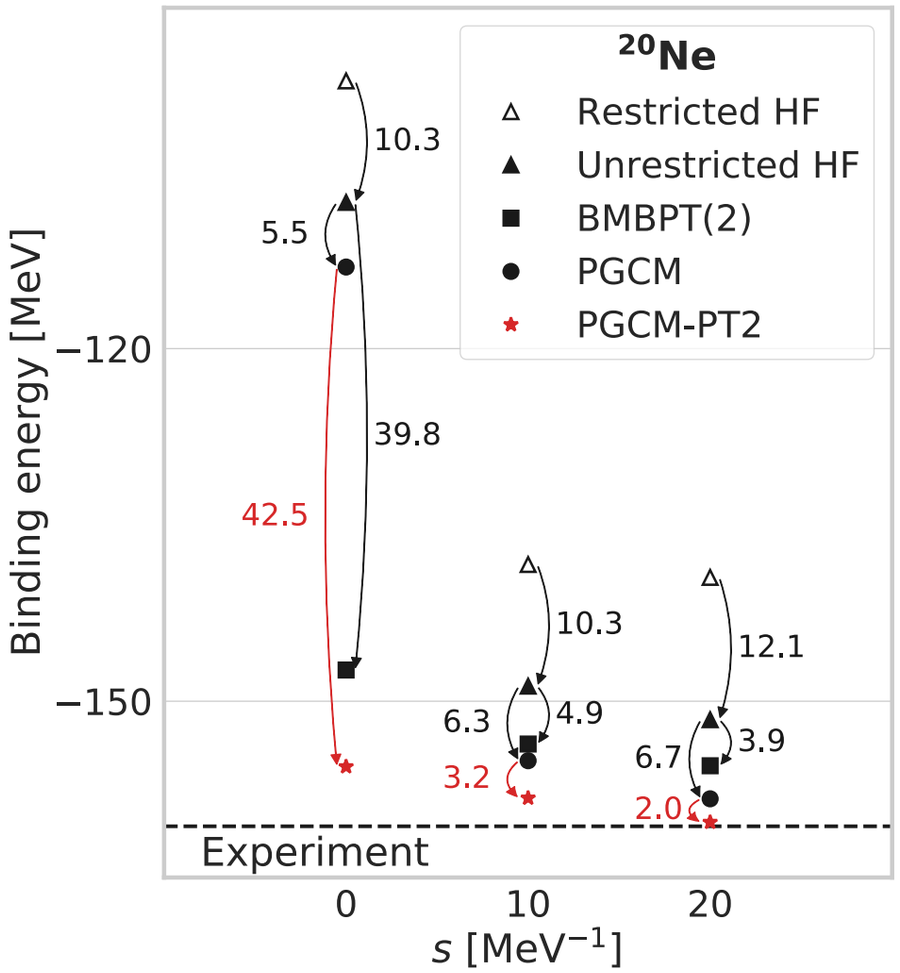


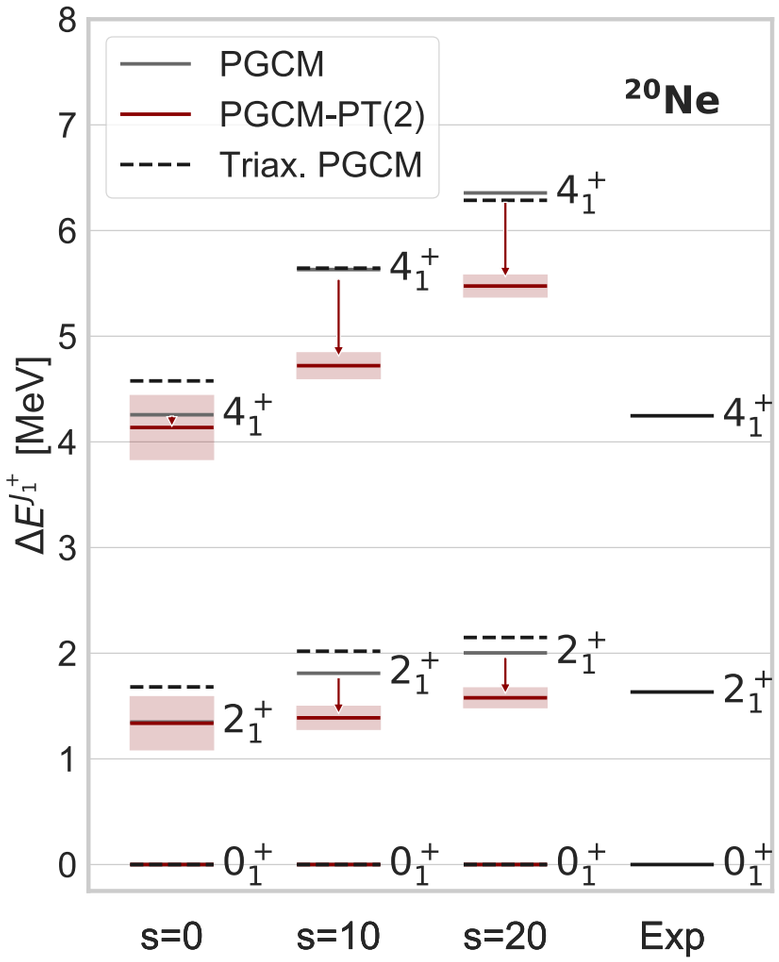
$$O = O^{(1)} \quad \underset{s\to\infty}{\to} \quad O(s) = O^{(1)}(s) + \underbrace{O^{(2)}(s) + \ldots}_{\textbf{induced contributions}}$$

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

Perturbative Enhancement of IM-GCM

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

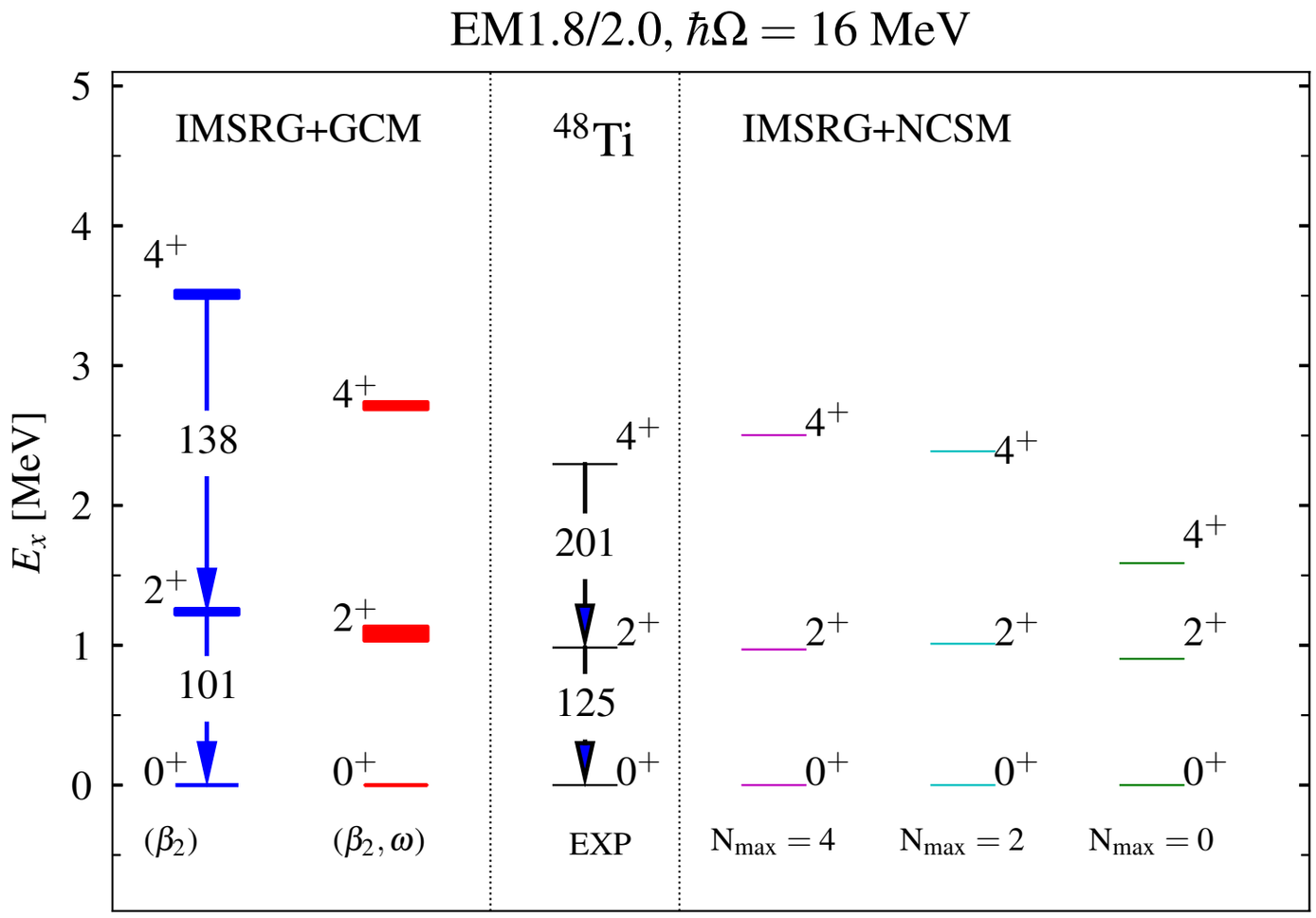




- s-dependence is a **built-in diagnostic tool** for IM-GCM **(not available in phenomenological GCM)**
  - if operator and wave function offer sufficient degrees of freedom, evolution of observables is unitary
- need **richer references and/or IMSRG(3)** for certain observables

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

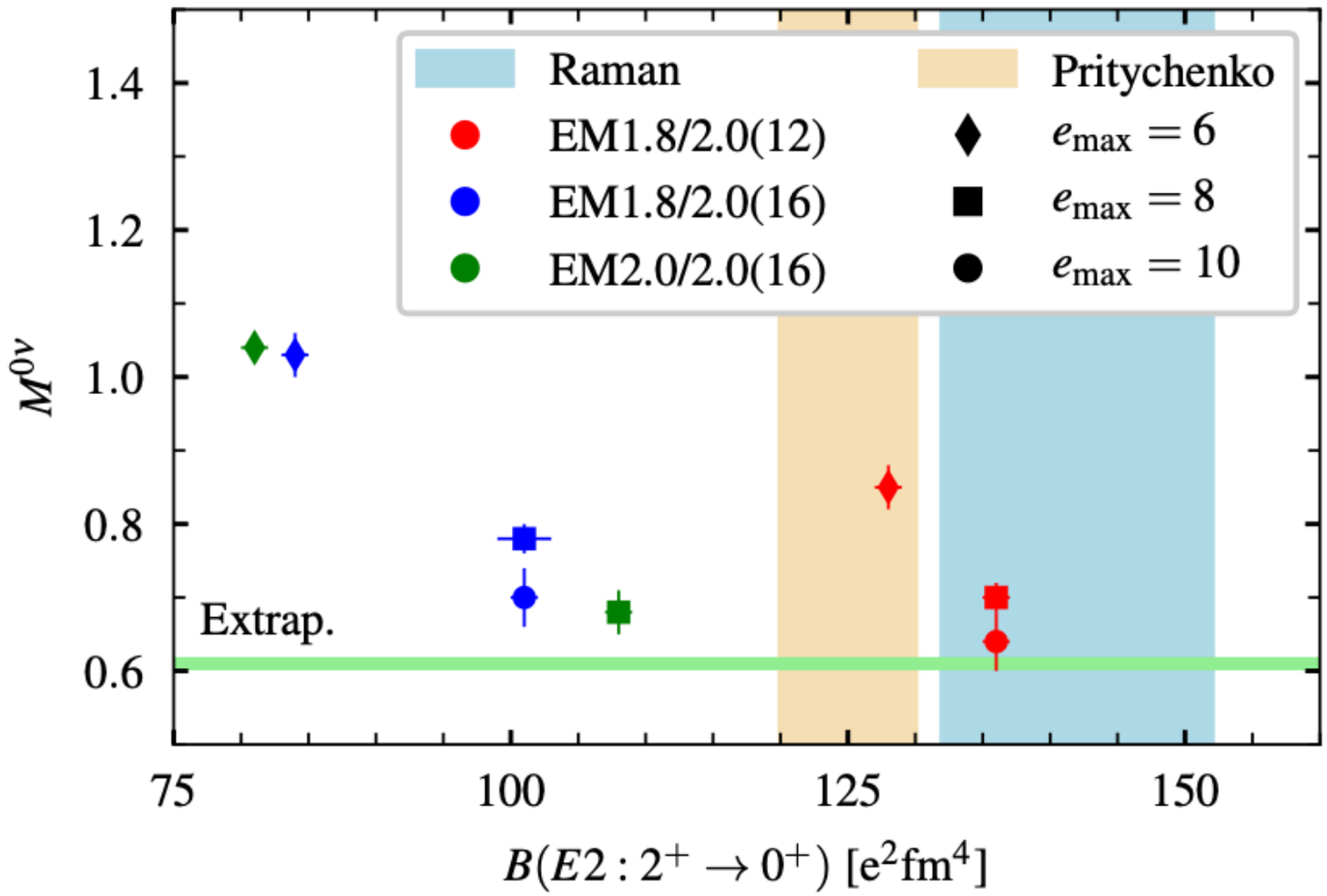
*J. M. Yao et al., PRL **124**, 232501 (2020); HH, Front. Phys. **8**, 379 (2020)*



- 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)*

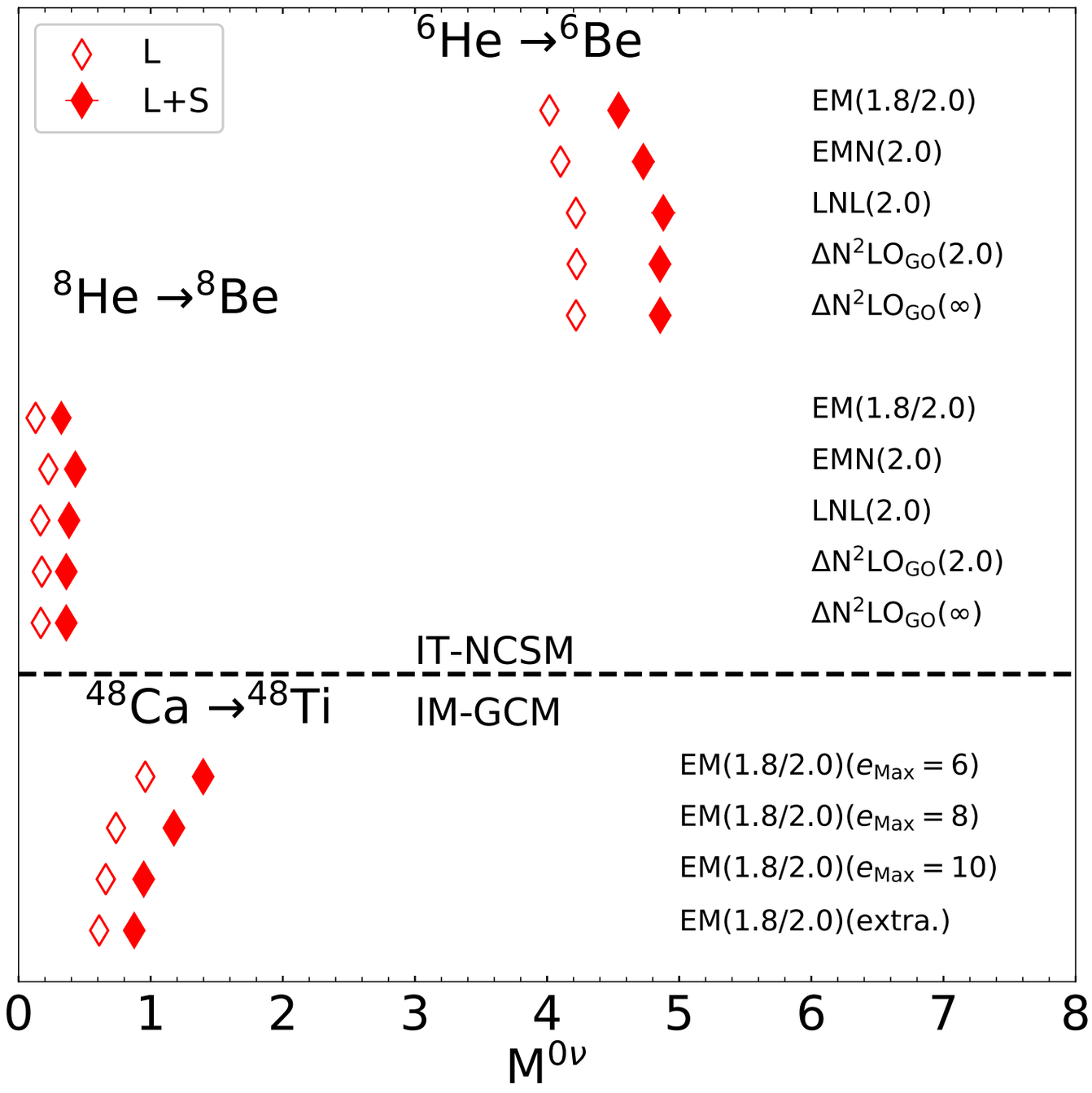


- NME from different methods **consistent** for consistent interactions & transition operators
  (A. Belley et al., PRL 126, 042502, S. Novario e
- interpretation and features differ from e
  only **weak correlation** between NME and

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

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

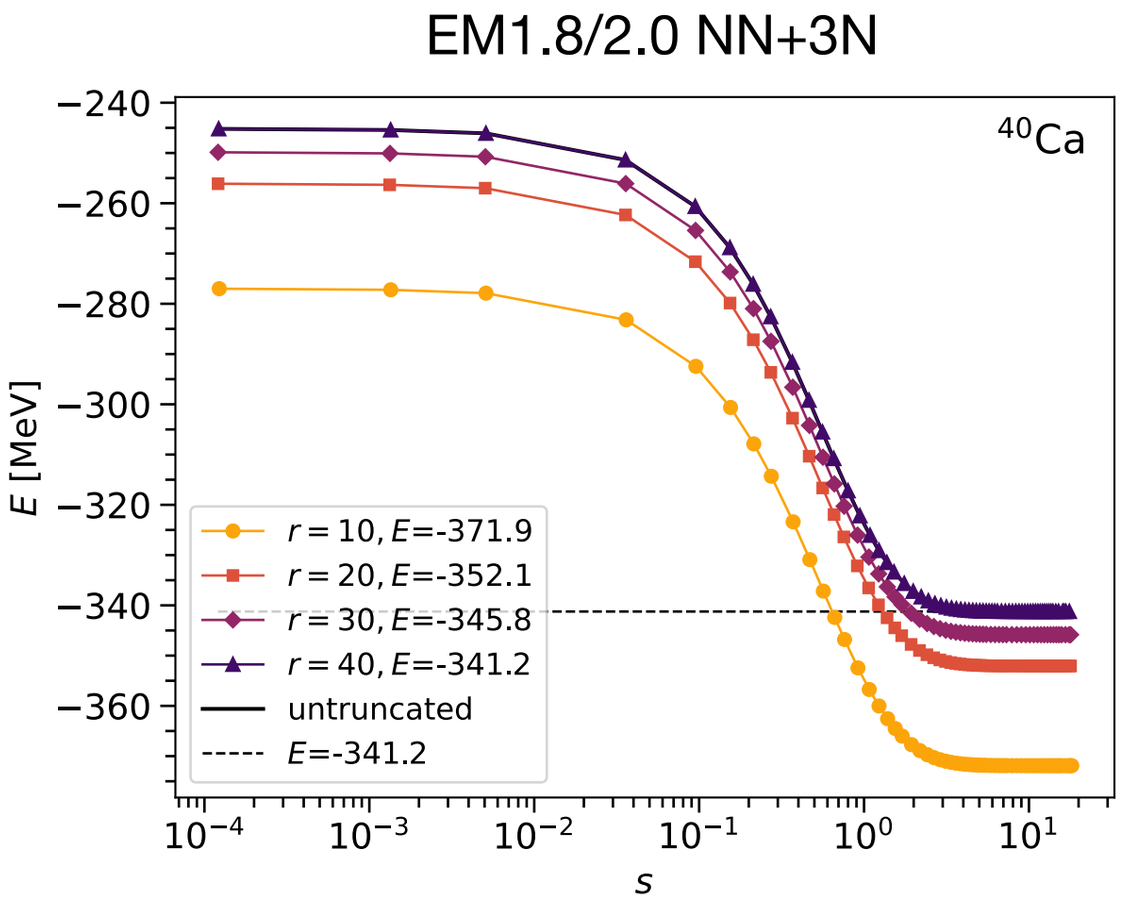
Looking Ahead

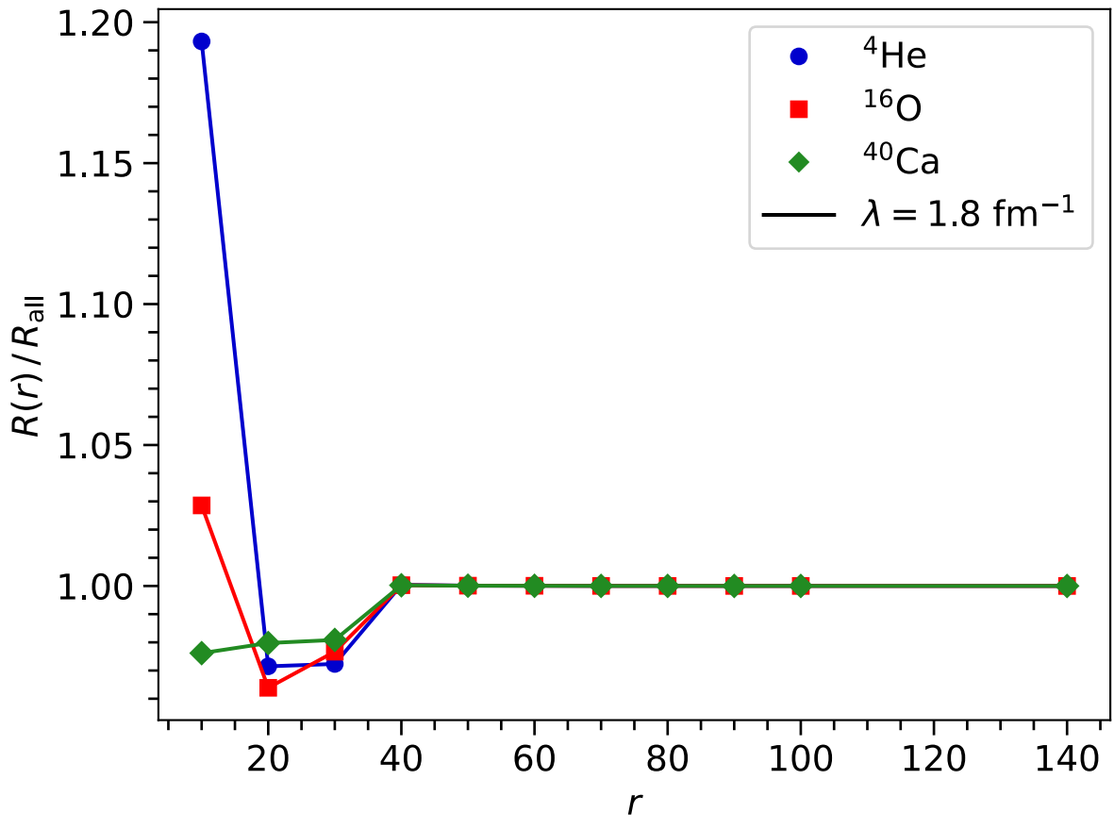
(Some) Physics Goals

- **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**)

Leveraging Low-Rank Structures

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

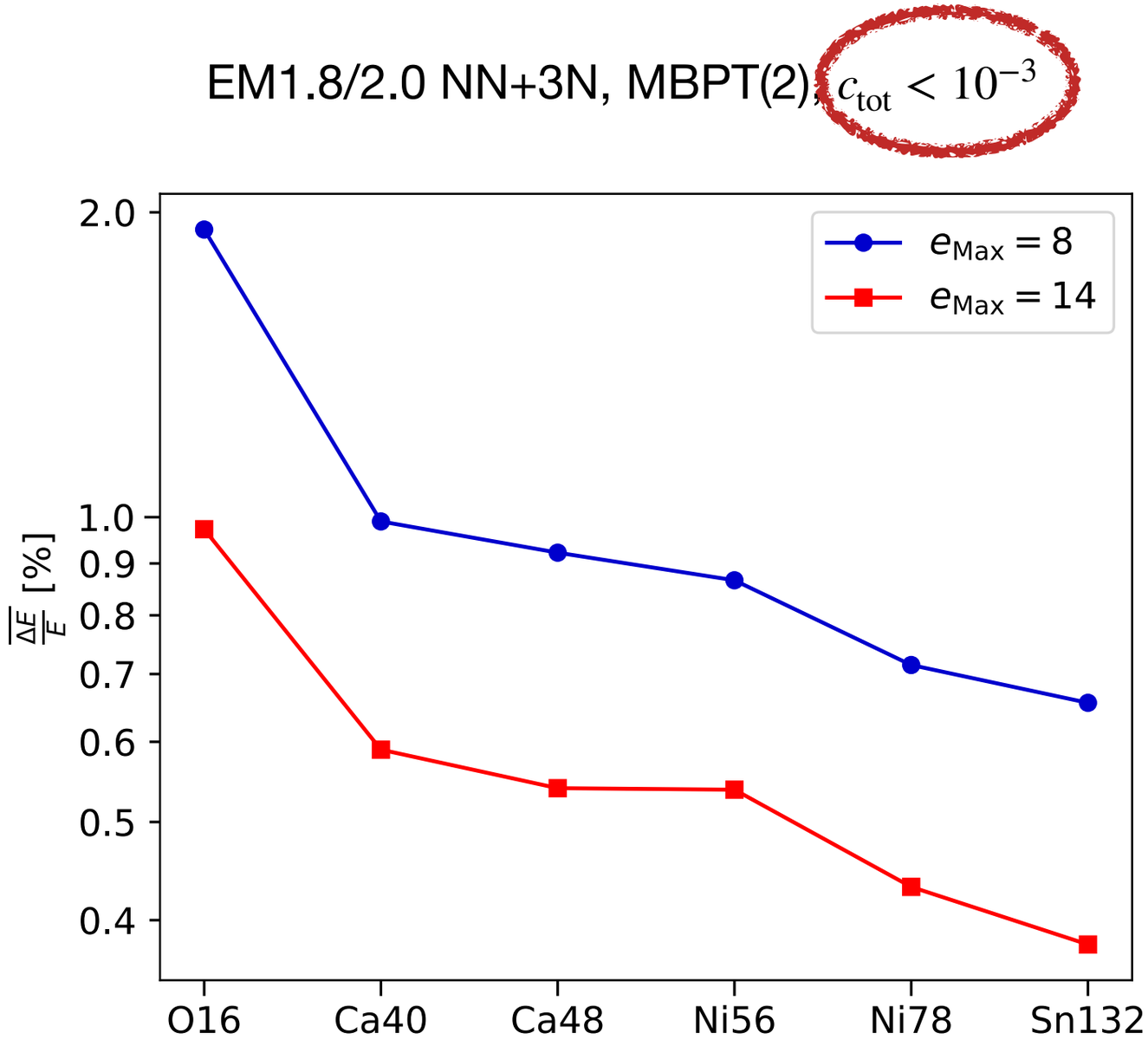




- **principal component analysis** of chiral interactions
  - free-space SRG effort and storage **reduced by several orders of magnitude** (but not a major bottleneck anyway)
  - **no adverse affect** on other (studied) observables
- **next: 3N & leverage factorization** in many-body calculation

Compression with Random Projections

***A. Zare, R. Wirth**, C. Haselby, HH, M. Iwen, in preparation*

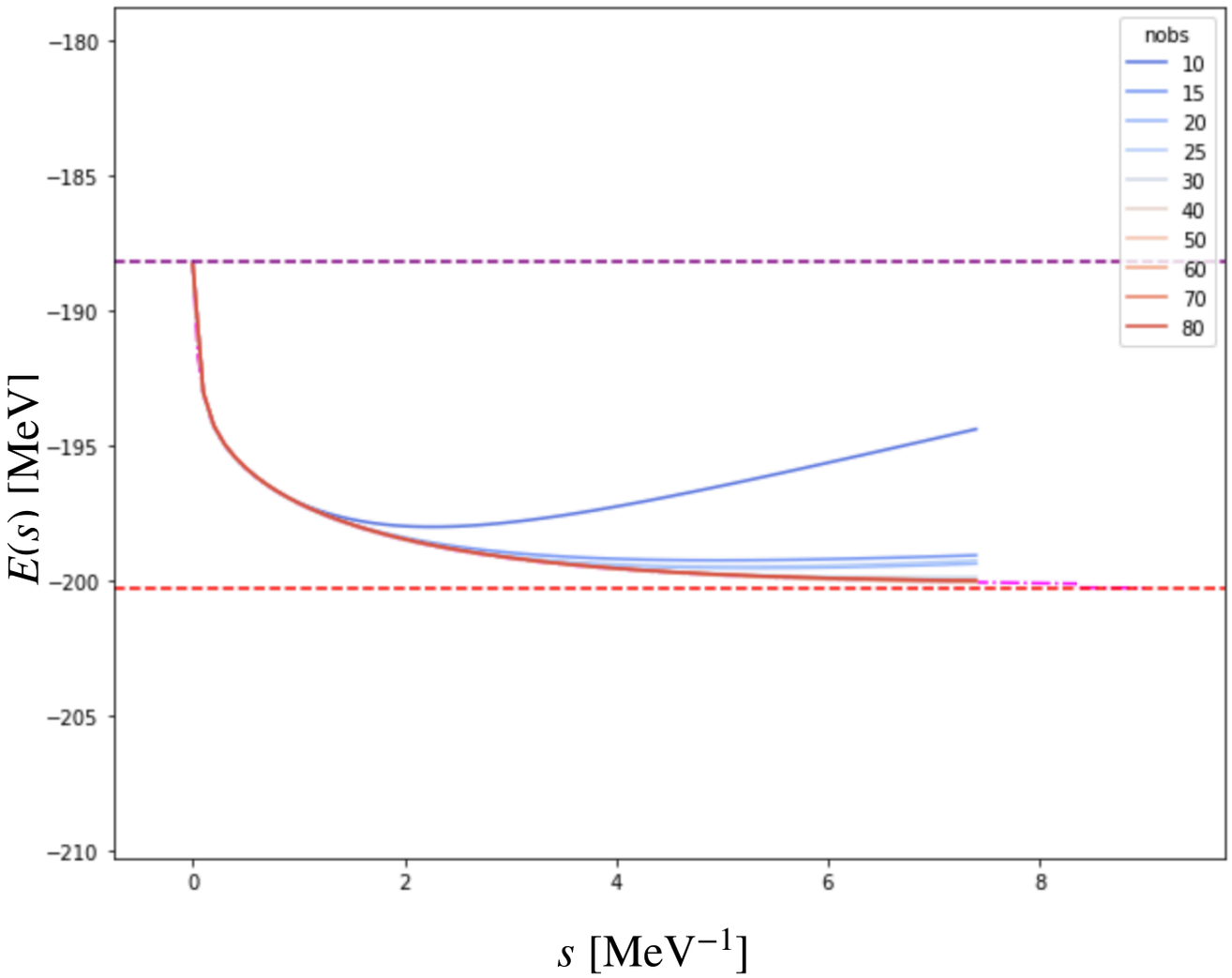


- tensorial (= modewise) **Johnson-Lindenstrauss embeddings**
- **purely based on features of (sparse) big data sets** - integrate with physics-based ideas?
- suitable for **streaming** transforms: compress on the fly while reading from disk

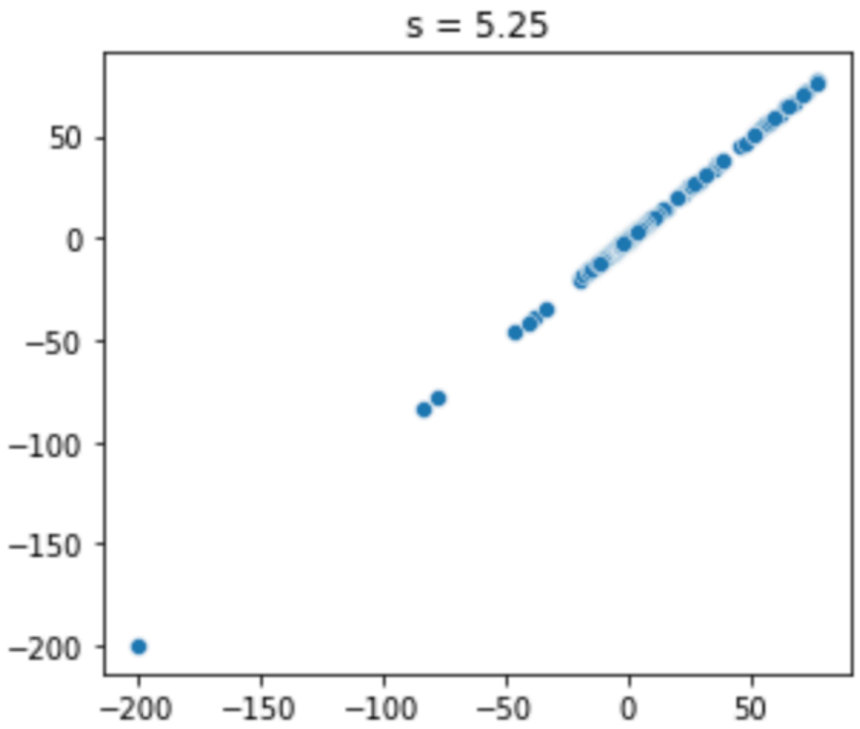
Emulating IMSRG Flows

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

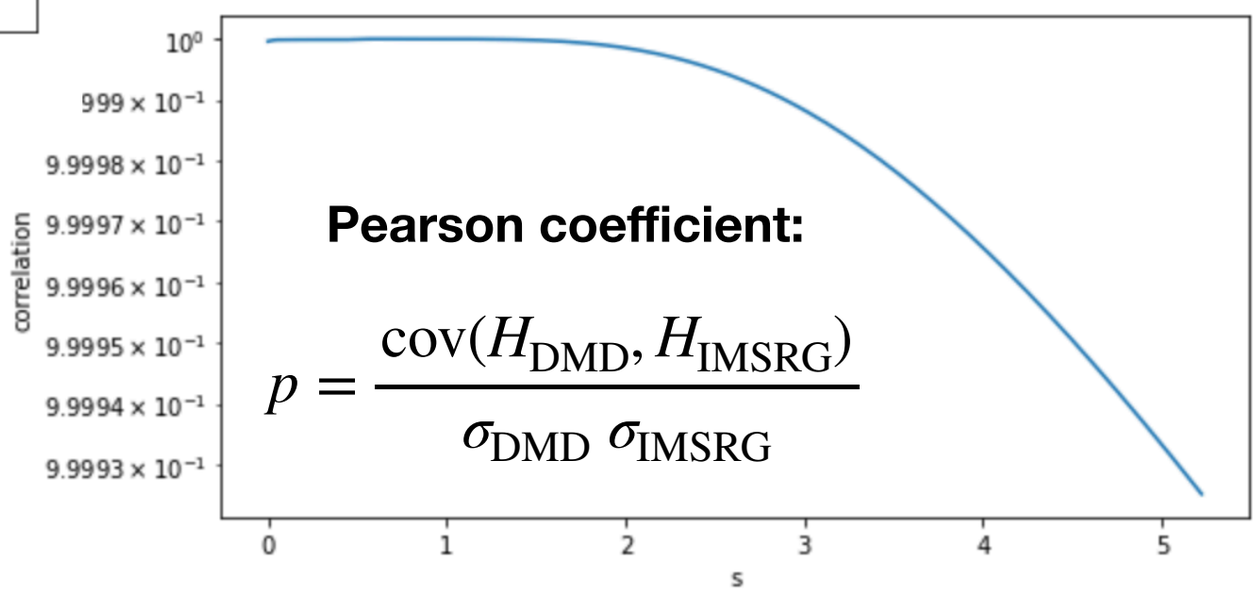
EM(500) N³LO, $\lambda = 2.0\,\mathrm{fm}^{-1}$



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



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



Pearson coefficient:

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

The Horizon

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

- developing new 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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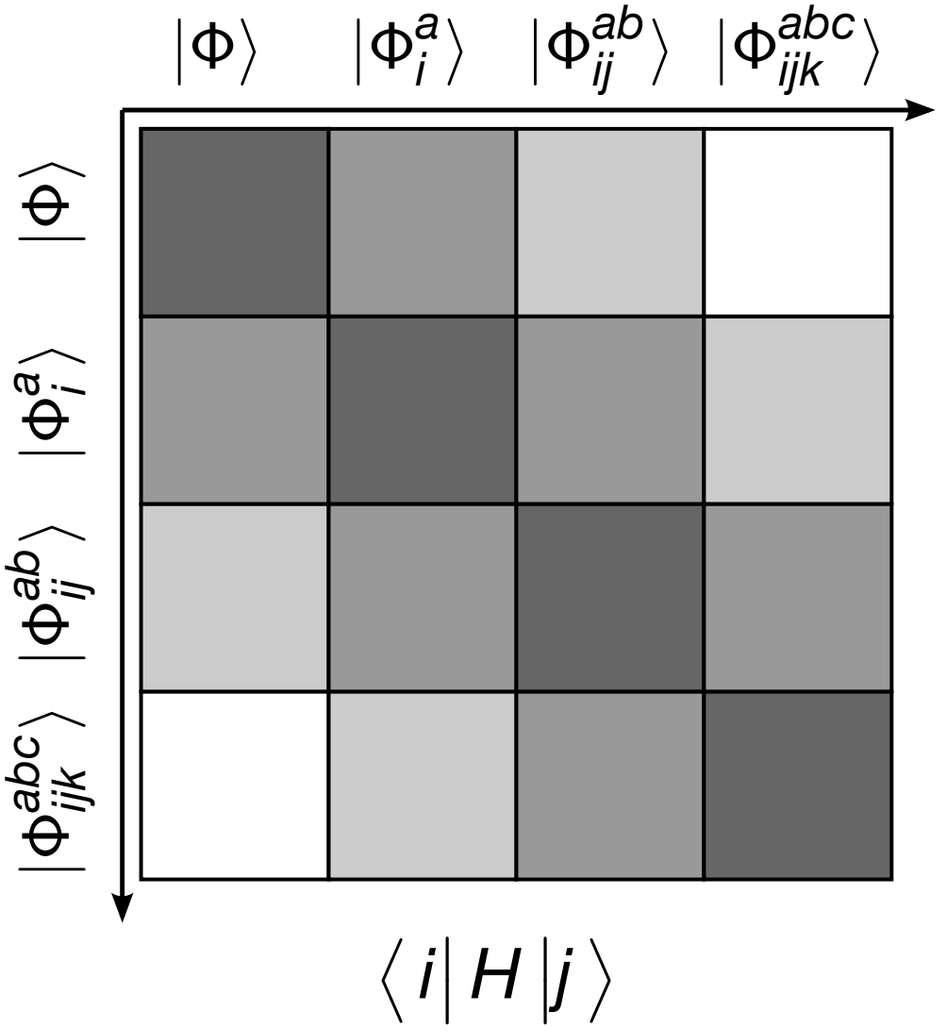
Supplements

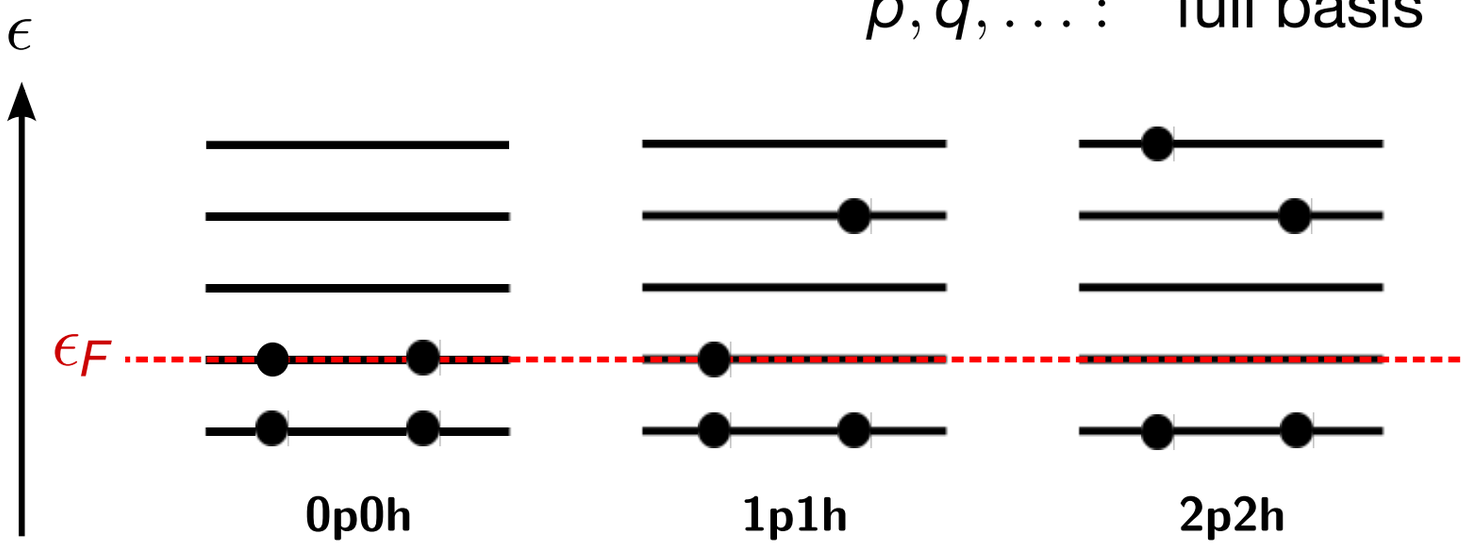
Transforming the Hamiltonian



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

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

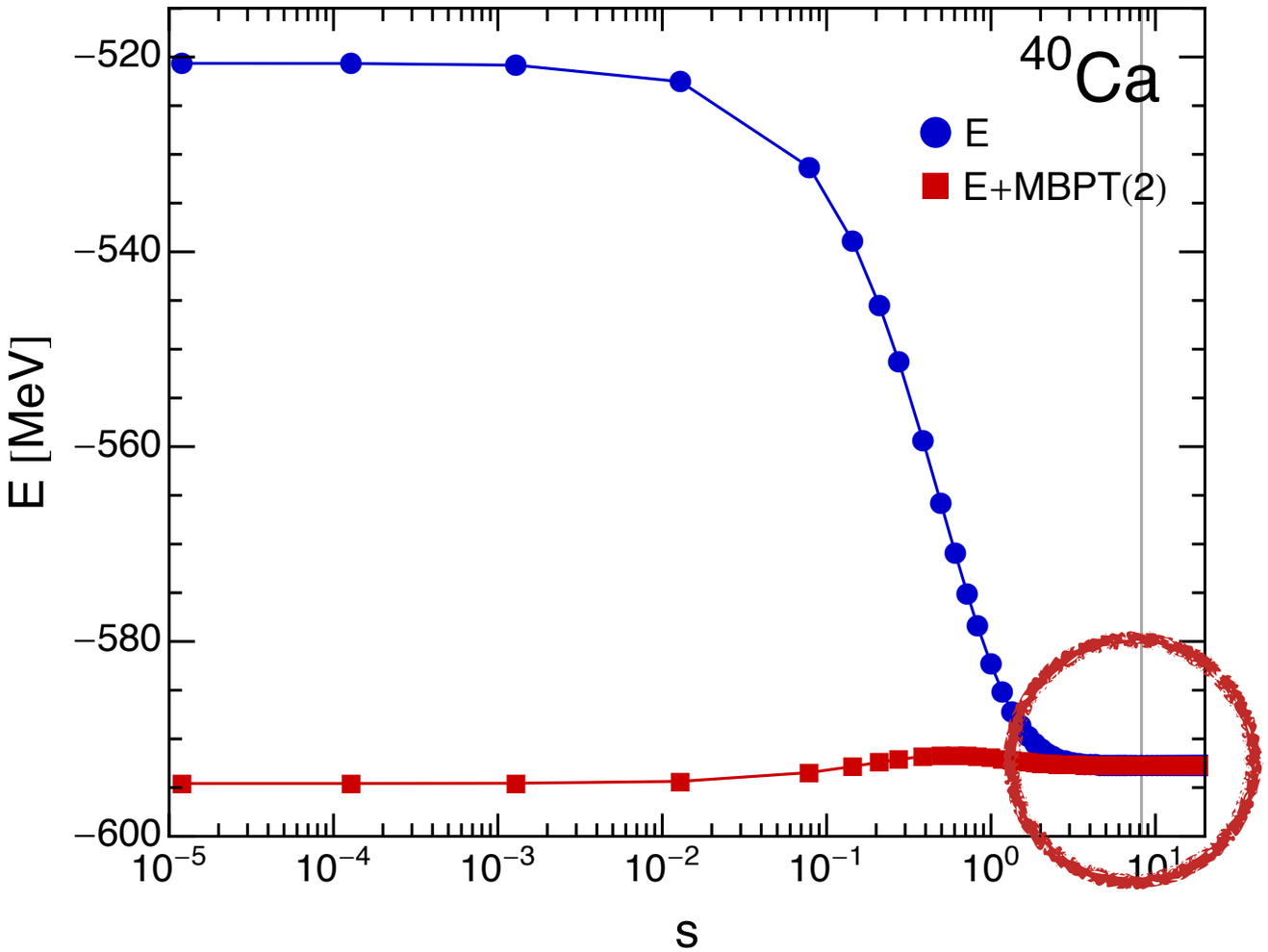
$p, q, \ldots$: full basis

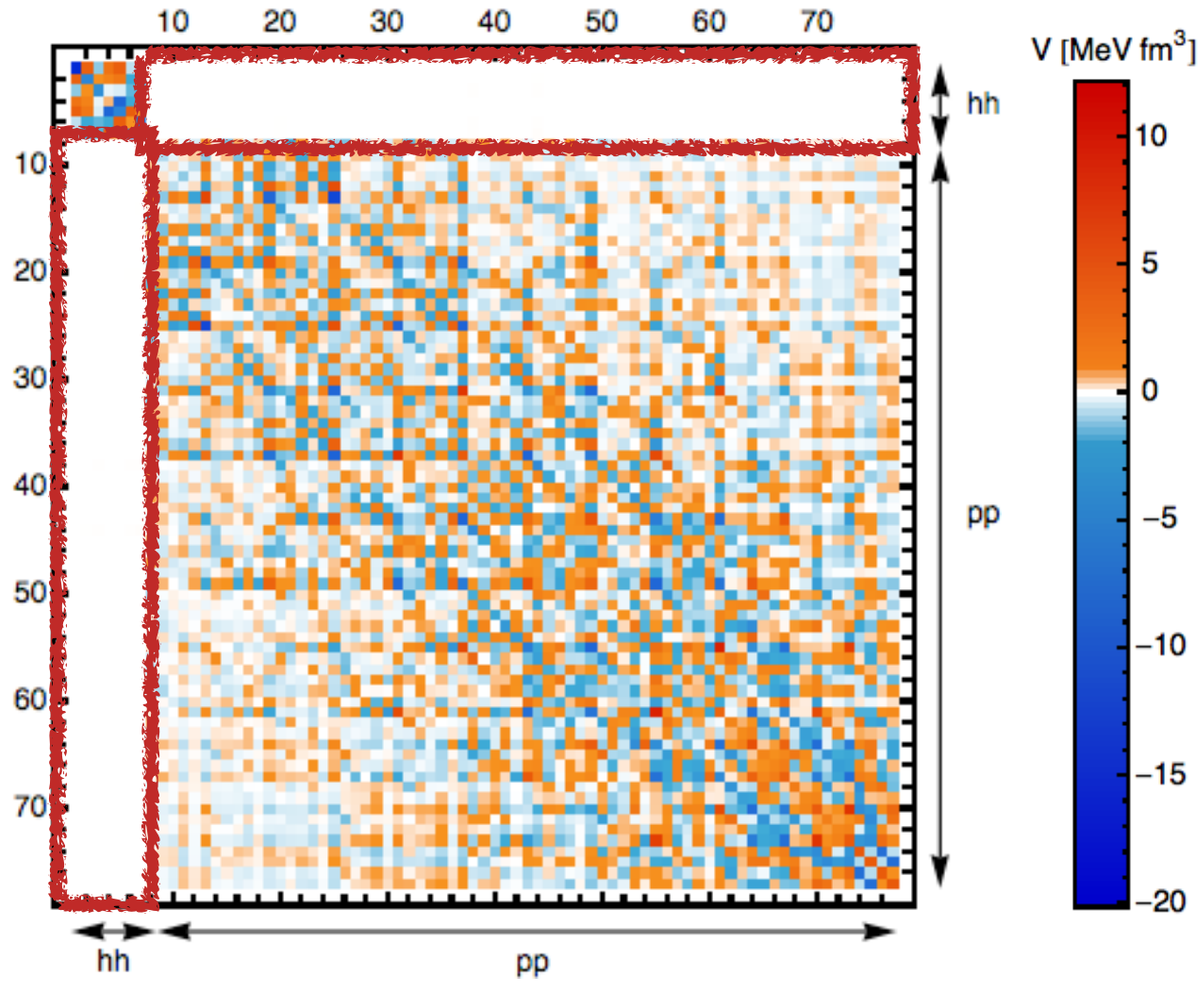


excitations relative to reference state: **normal-ordering**

- reference state: **single Slater determinant**

Decoupling



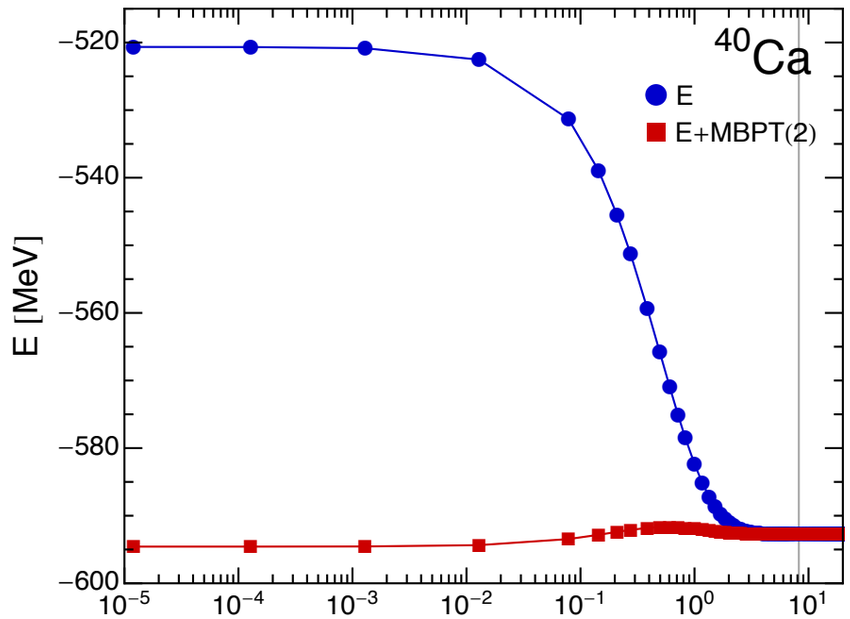


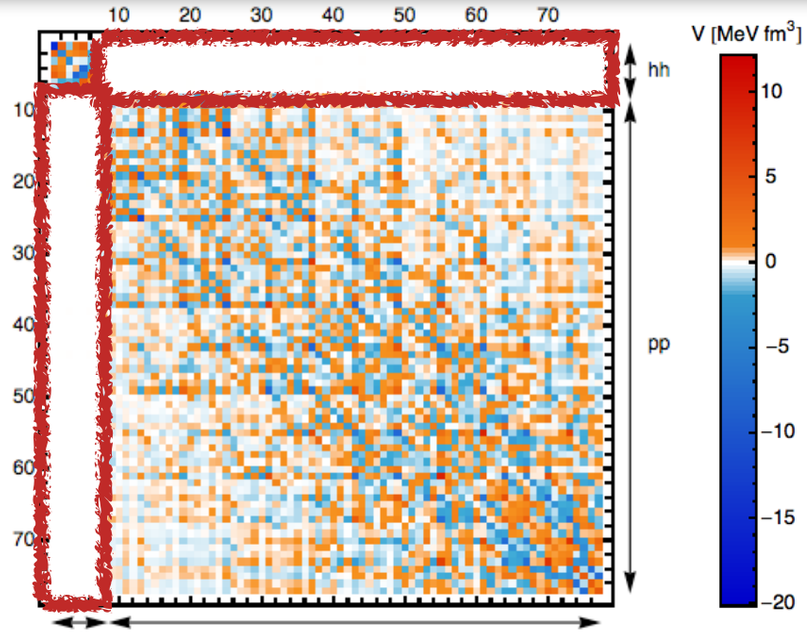
N3LO, $\lambda = 2.0$ fm^{-1}, $e_{\text{Max}} = 8$

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

off-diagonal couplings are rapidly driven to zero

Decoupling





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

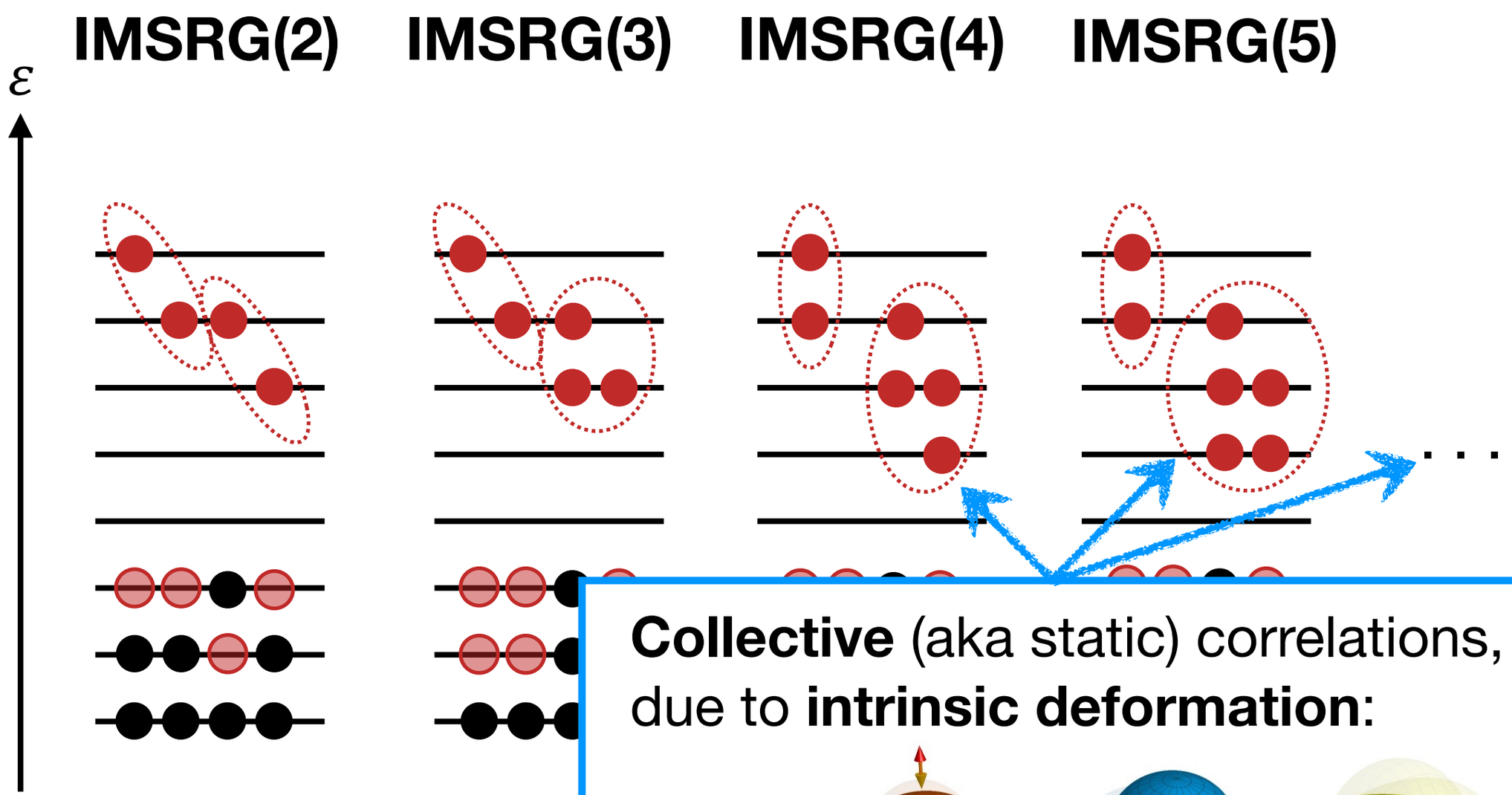
- absorb correlations into **RG-improved Hamiltonian**

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

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

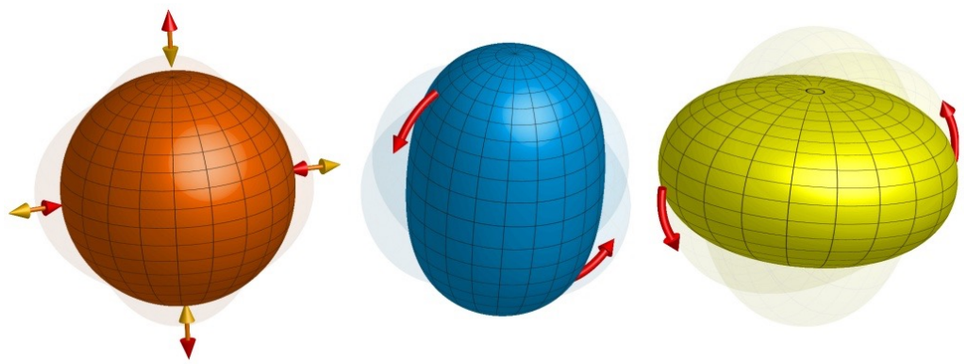
$$U(s)\left|\Psi_n\right\rangle \stackrel{!}{=} \left|\Phi\right\rangle$$

Correlated Reference States

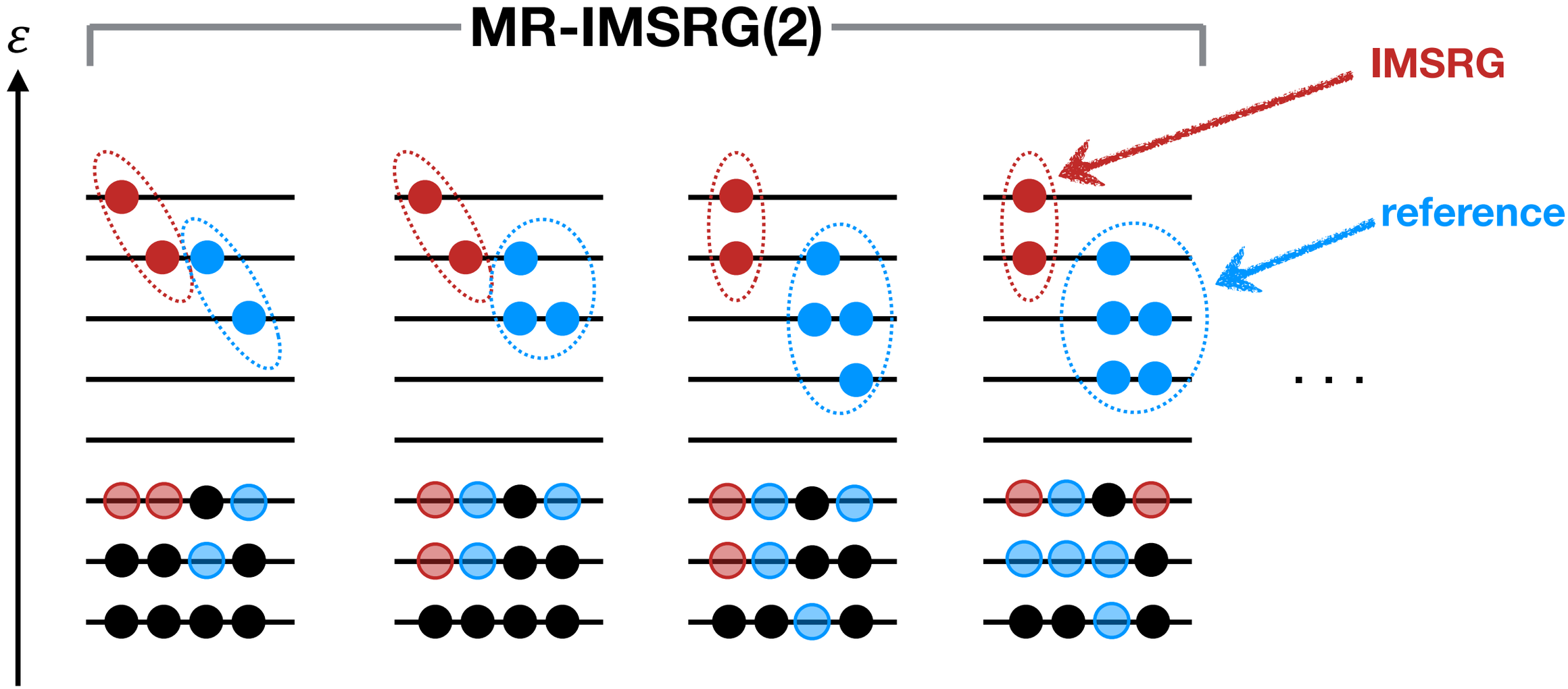


“standard” IMS
Slater determinar

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

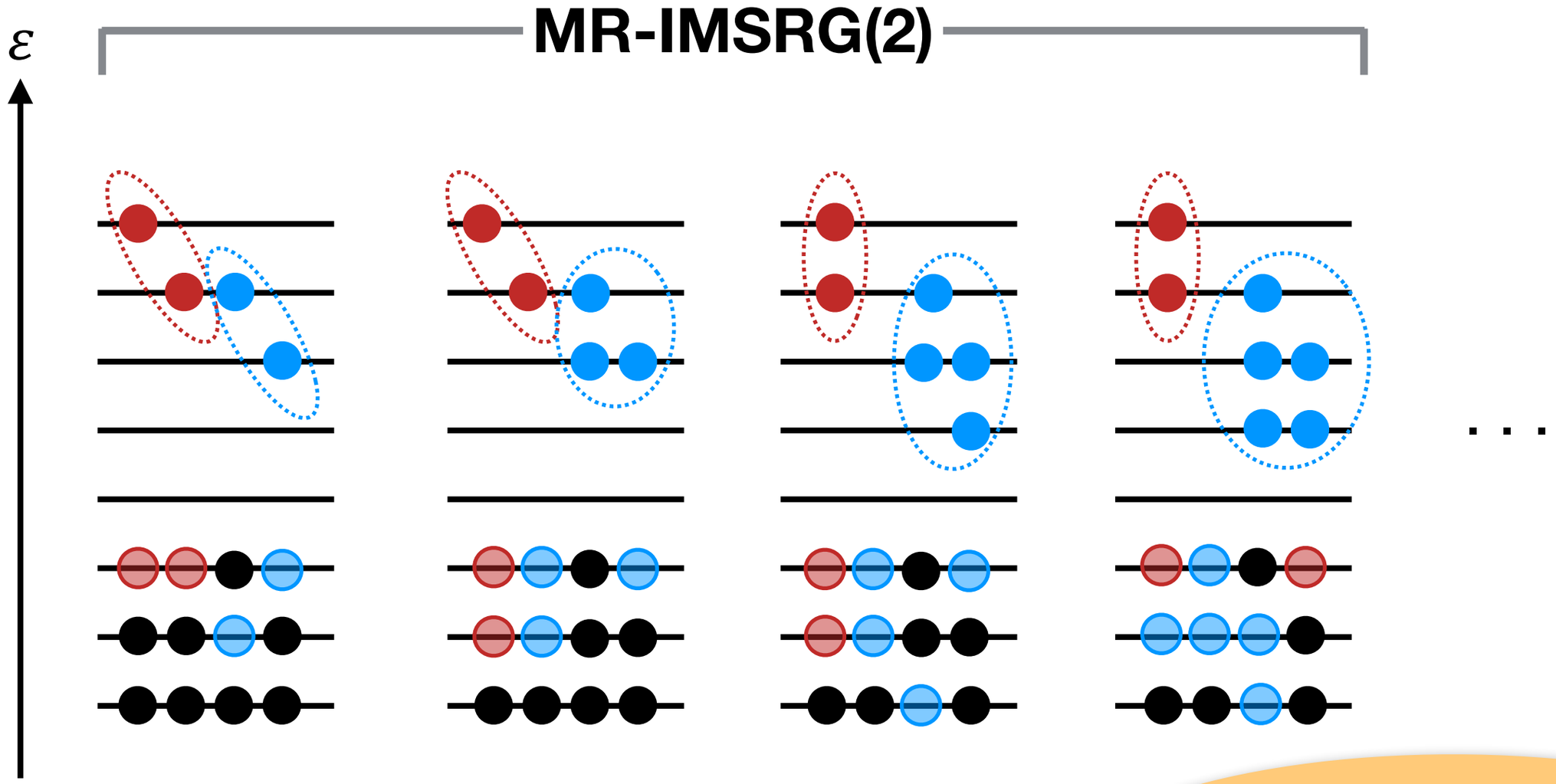


Correlated Reference States



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

Correlated Reference States

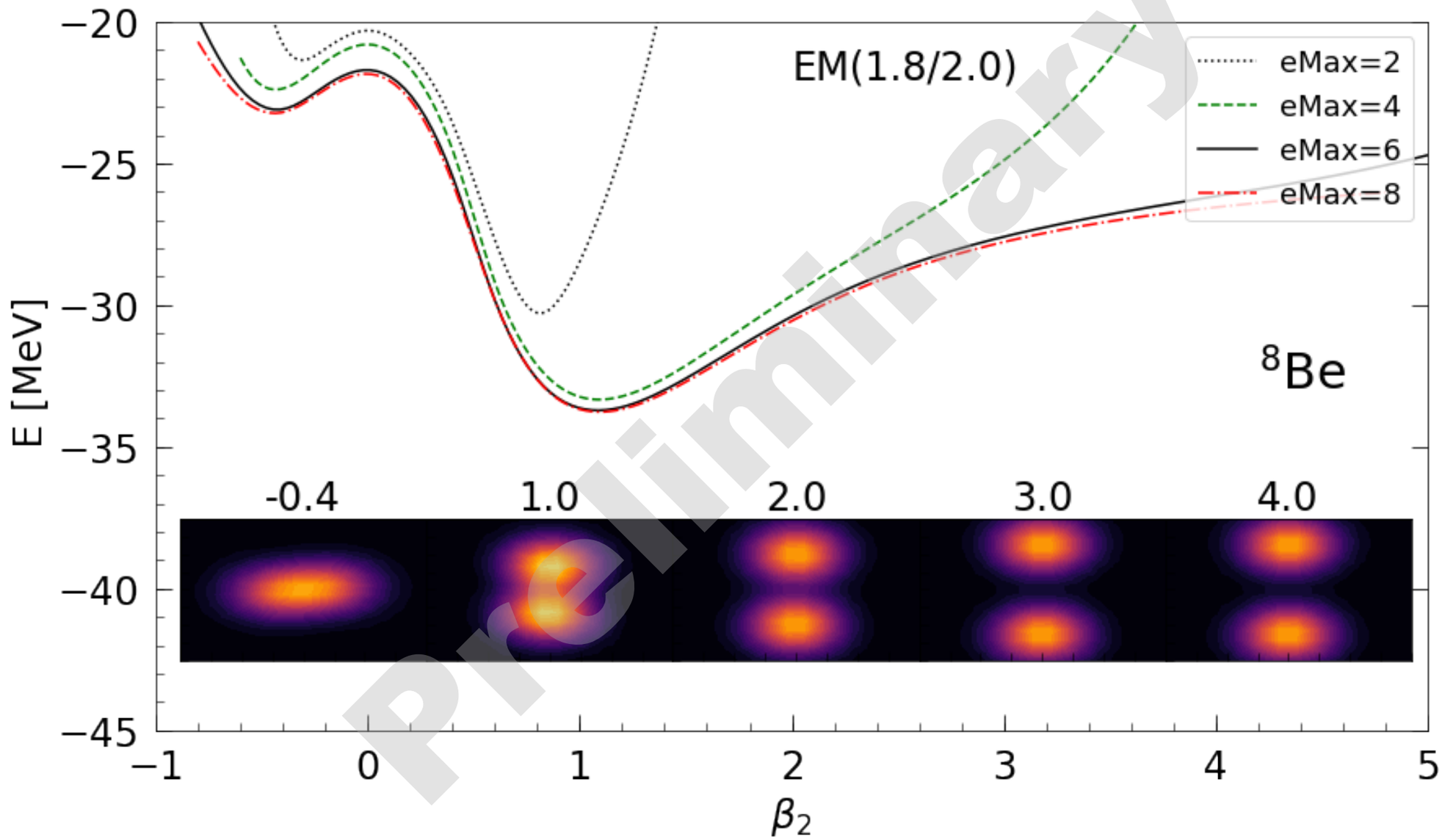


MR-IMSRG: build correlations
already correlated state (e.g., fro
describes static correlation

use generalized normal ordering with 2B,... densities

Cluster Structures: ^{8}Be

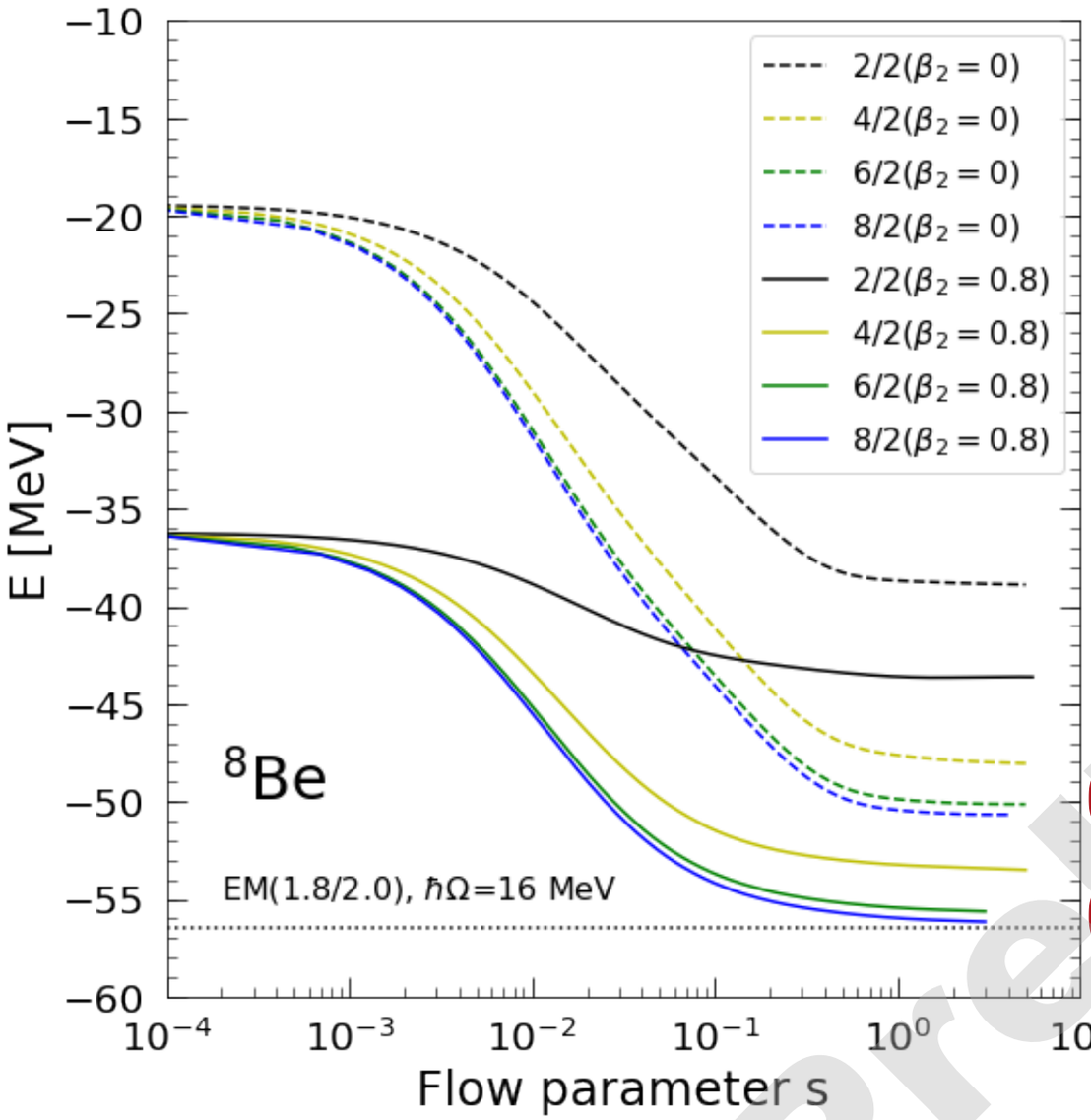
J. M. Yao, R. Wirth, HH, in progress

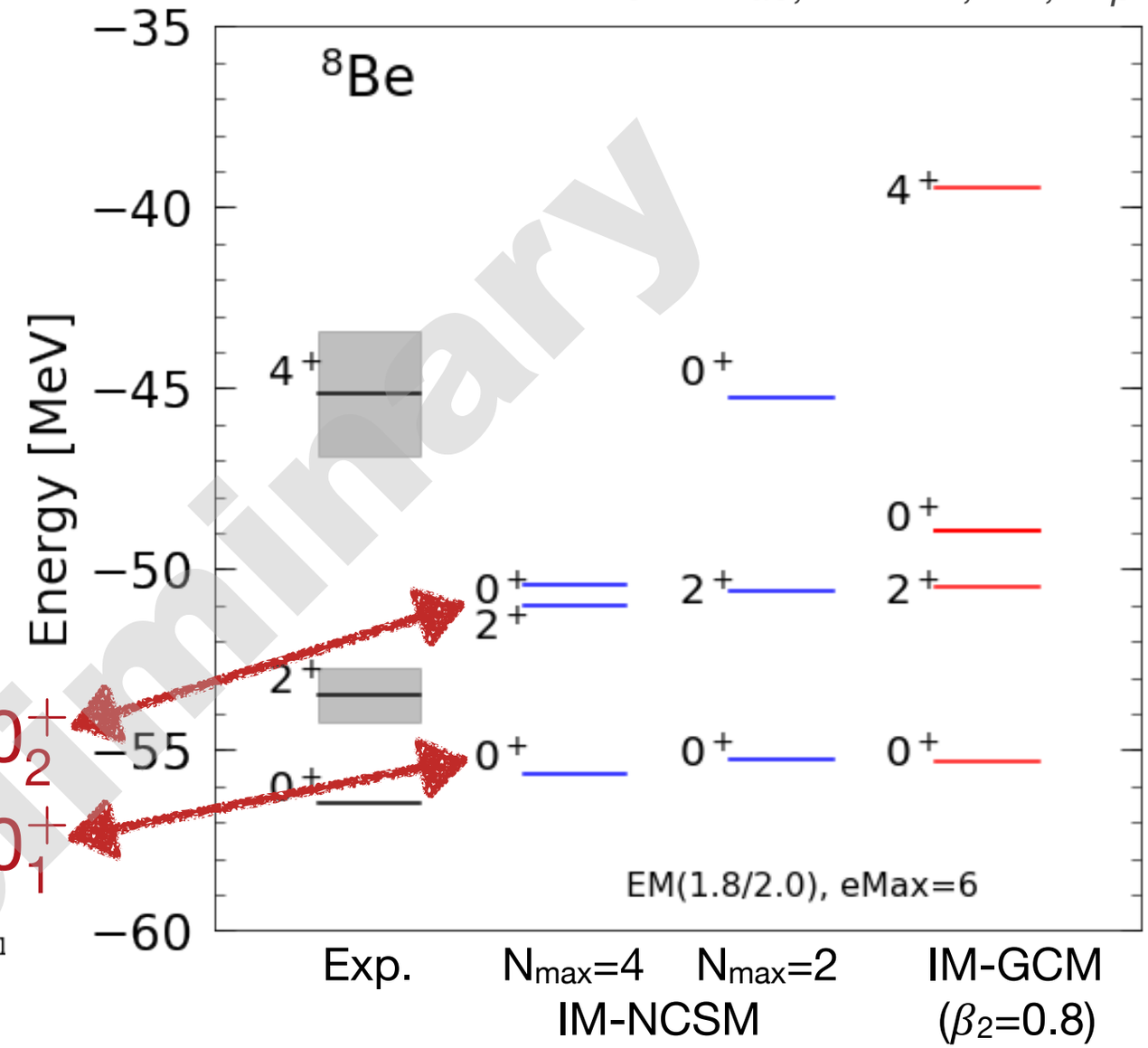


HFB potential energy surface

Cluster Structures: ^{8}Be

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

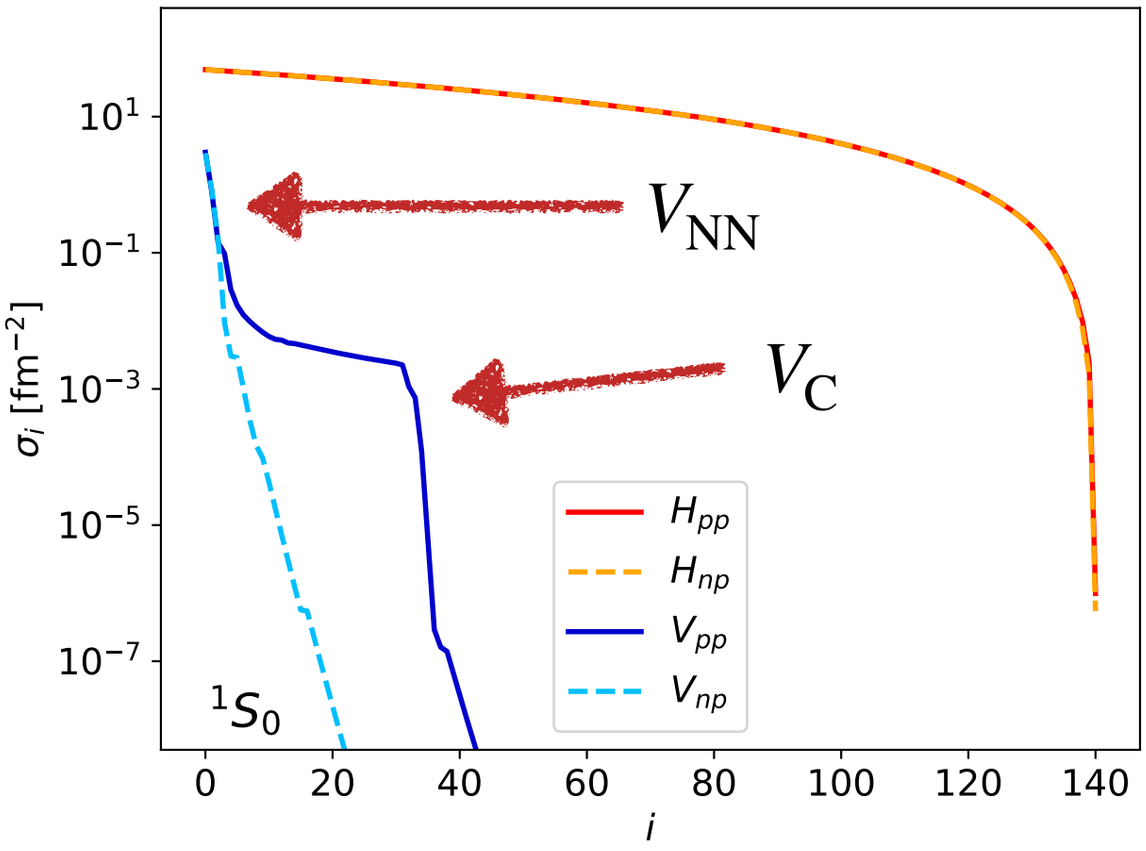


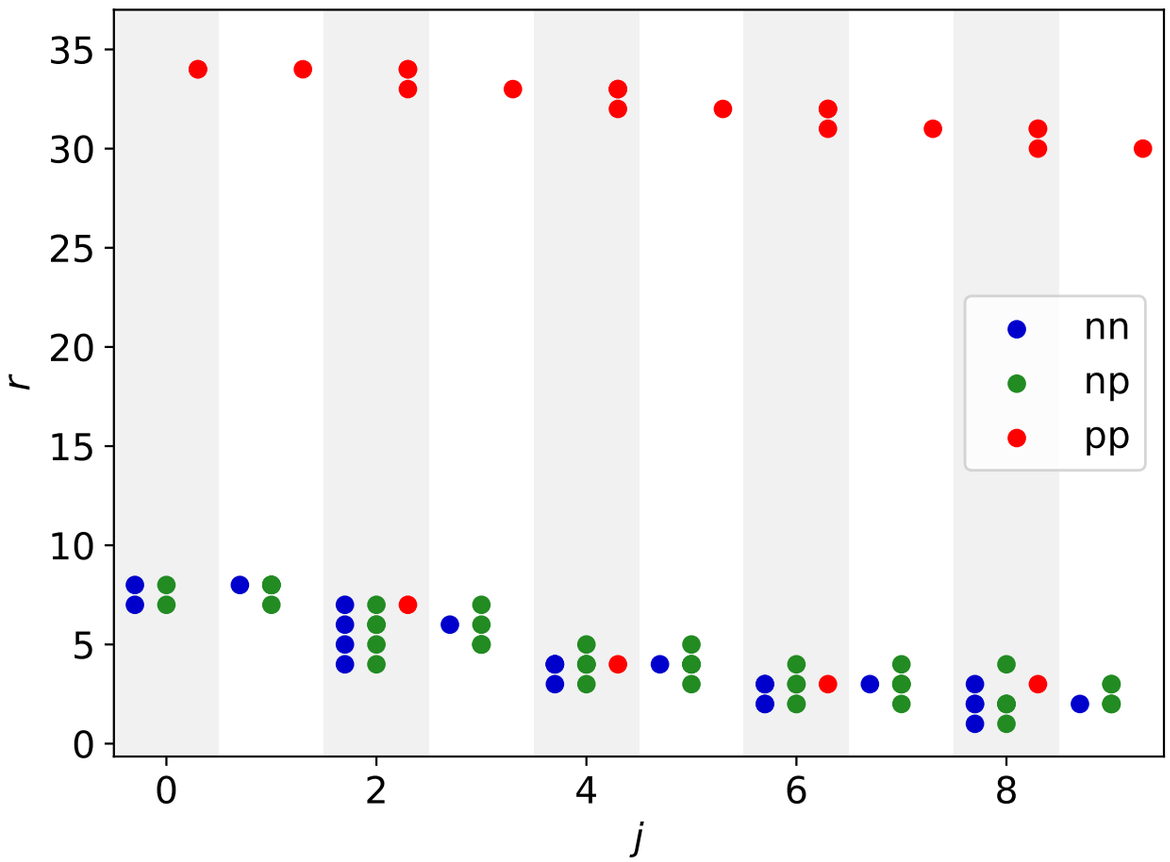


- Spherical and prolate references flow towards **different 0⁺ states**.
- Consistent with IM-NCSM:
  - **prolate reference:** ground state and excited 2⁺ state
  - **spherical reference:** first excited 0⁺

Factorized Interactions

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

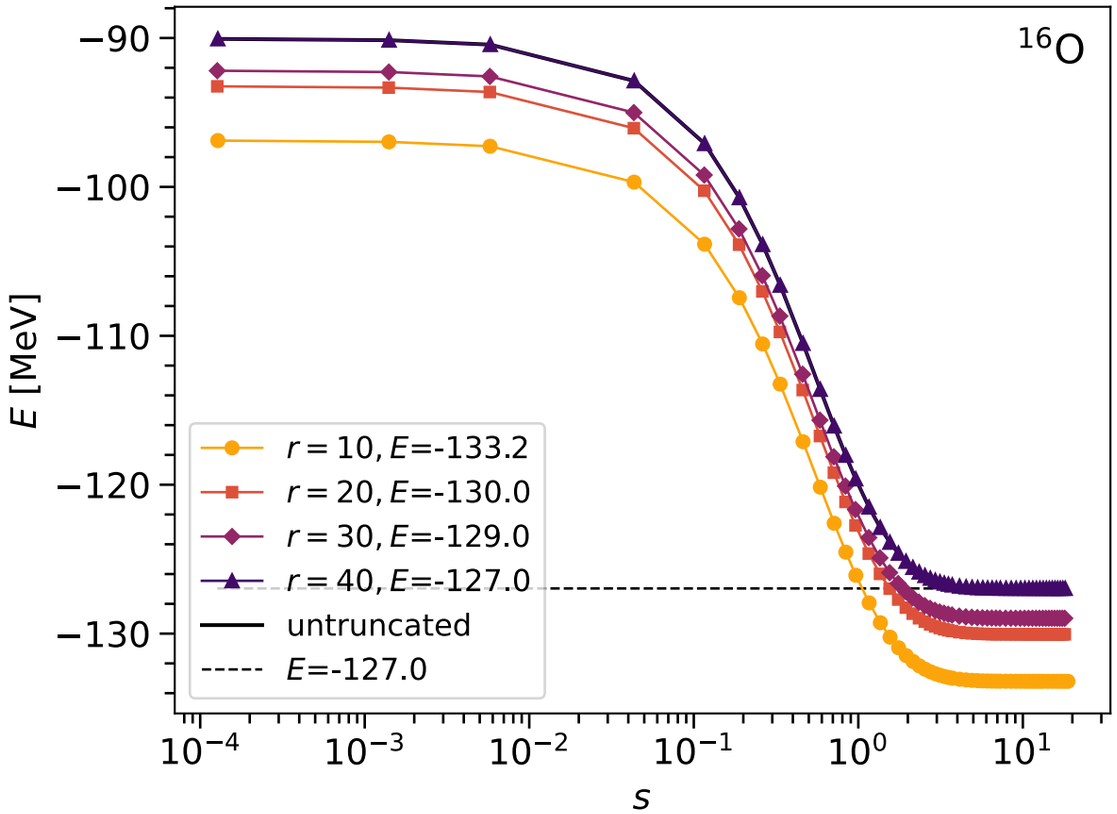


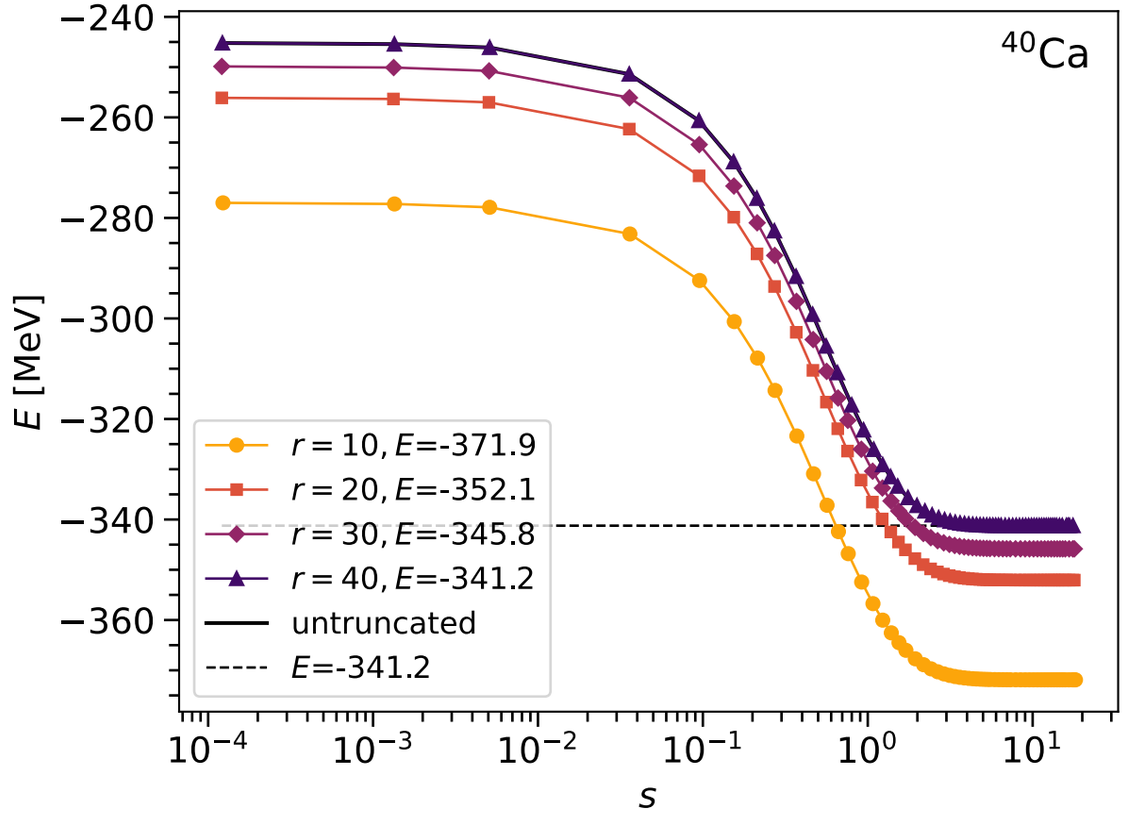


- O(10) operators, O(100) particles, but O(10^8-10^{12}) flow equations, basis dimension… there must be **redundancy**
- **NN interaction:** 5-10 SVD components (**short range**)
- **Coulomb interaction:** less well-behaved, but ~25-30 components sufficient (**long range, no explicit scale**)

Factorized Interactions

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

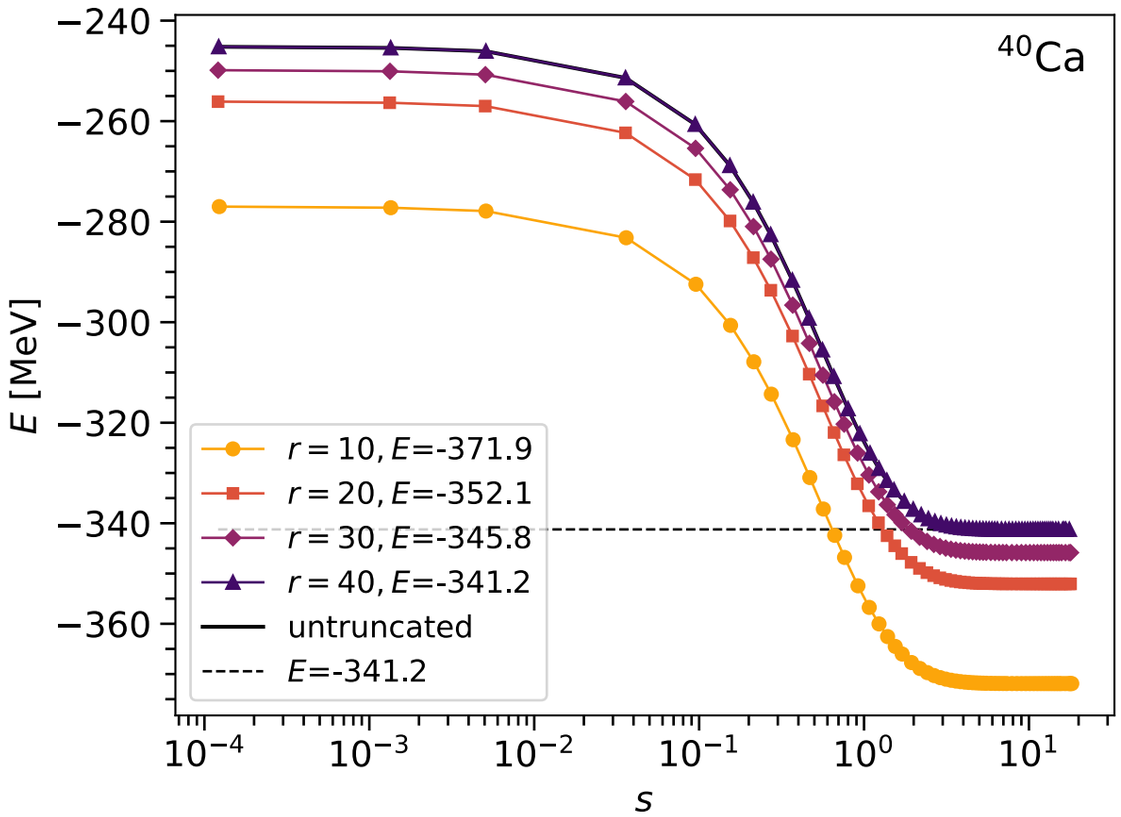


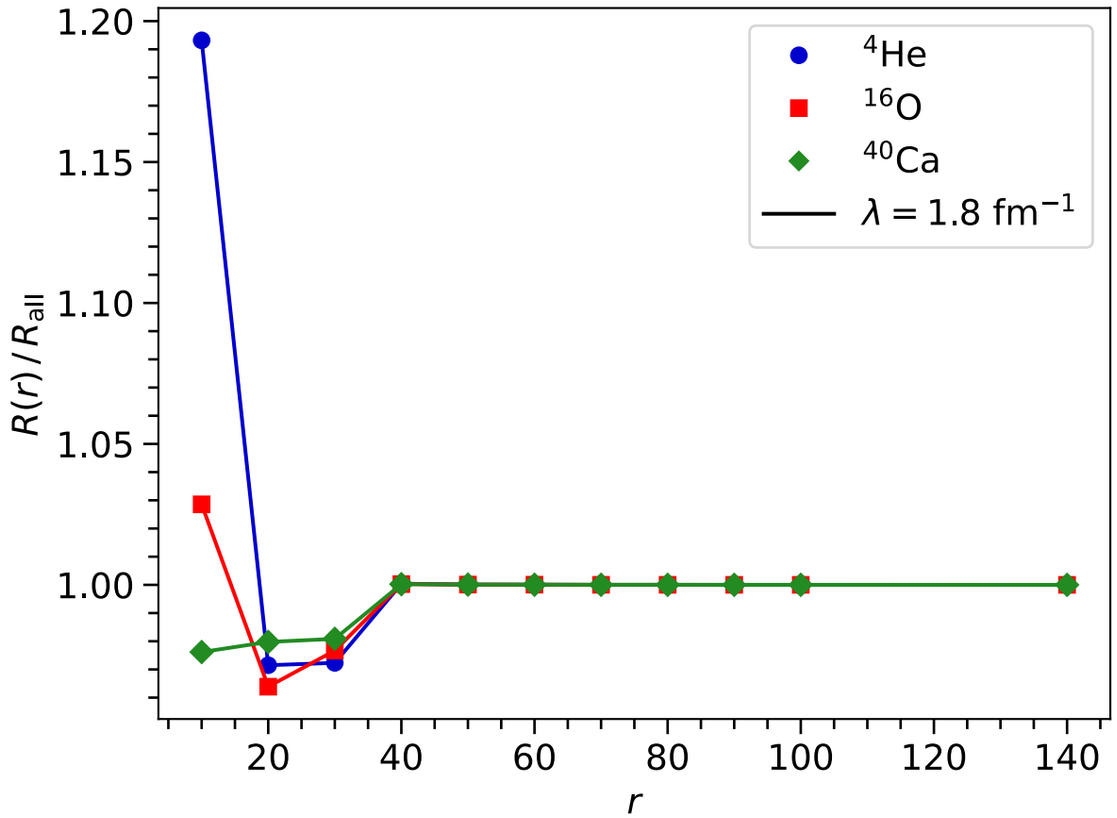


- NN interaction: free-space SRG evolution in component form (**IMSRG not yet**)
  - (3N interaction added to produce realistic binding / radii)
- free-space SRG effort and storage **reduced by several orders of magnitude**

Factorized Interactions

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





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