In-Medium Similarity Renormalization Group Methods for Deformed Nuclei

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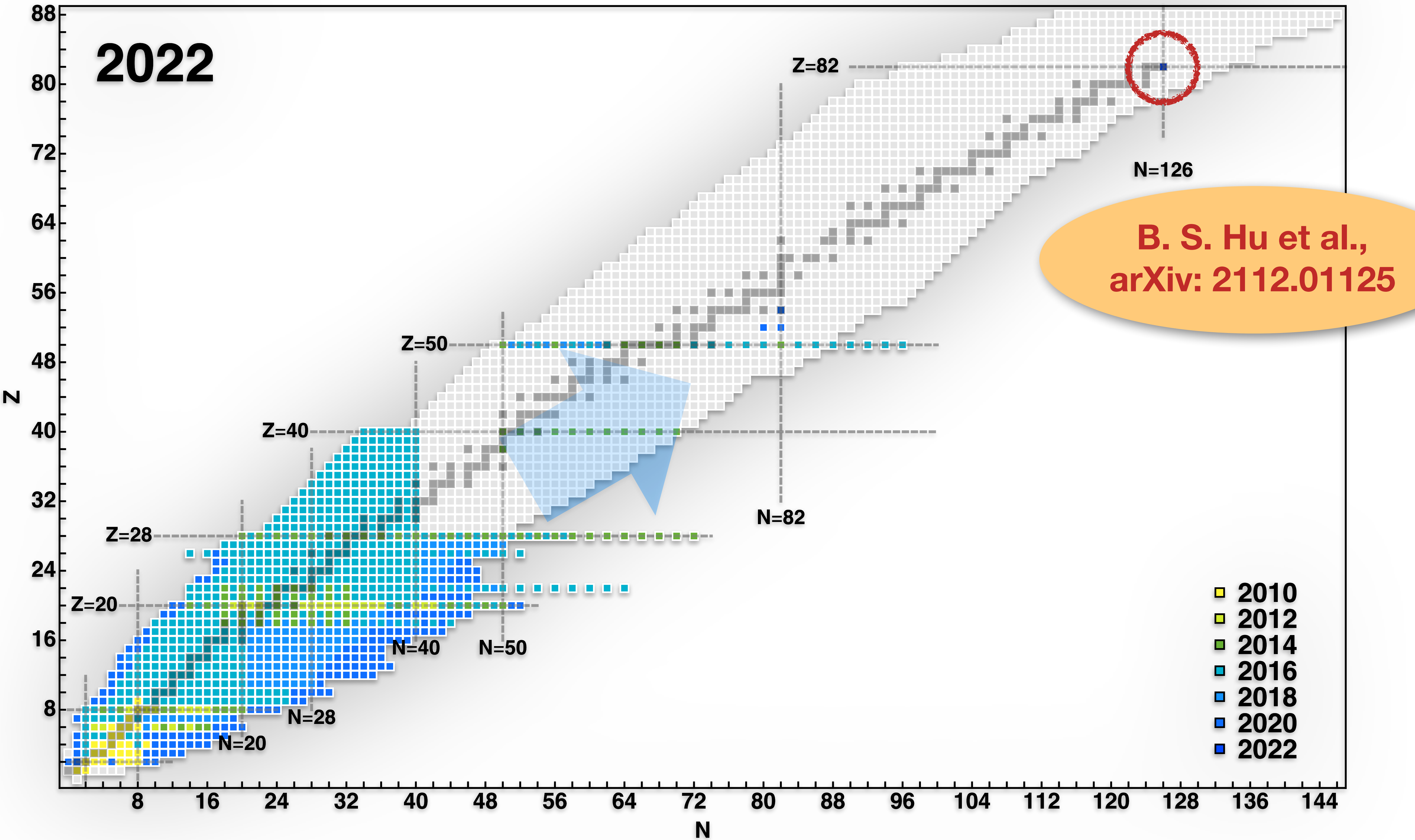
Progress in *Ab Initio* Calculations

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



(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)

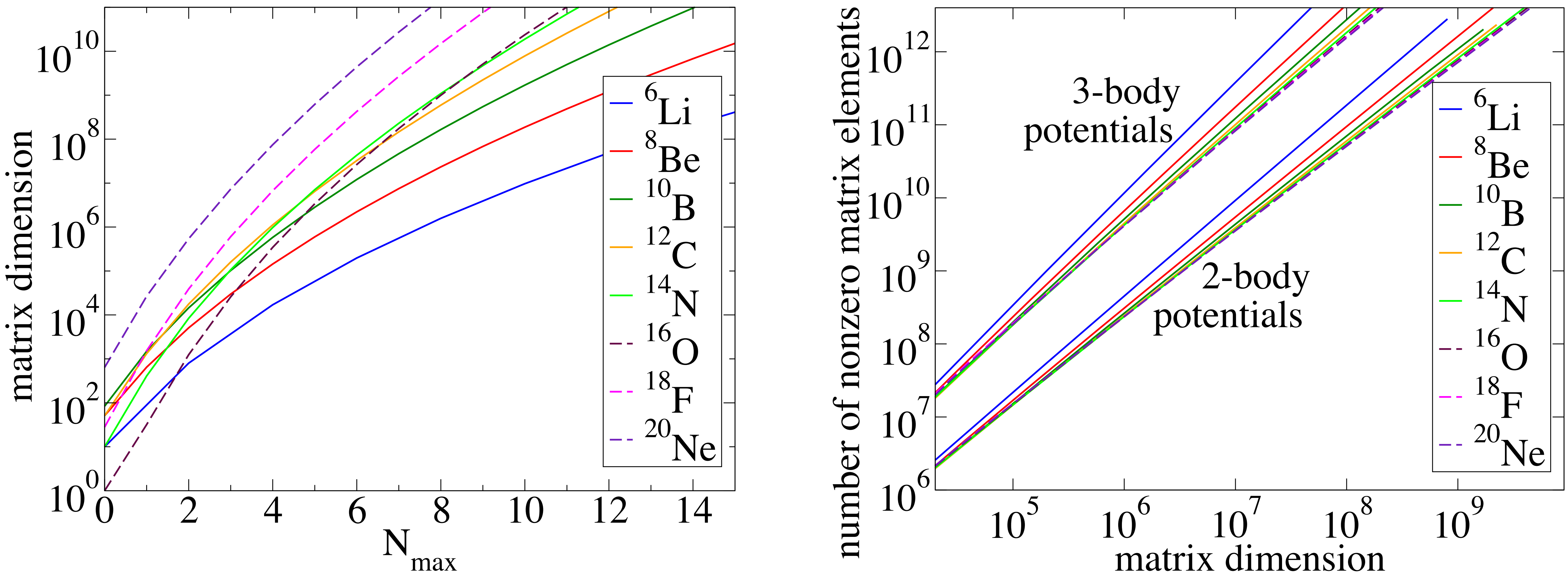
HH, S. K. Bogner, T. Morris, S. Binder, A. Calci, J. Langhammer, R. Roth, Phys. Rev. C **90**, 041302 (2014)

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

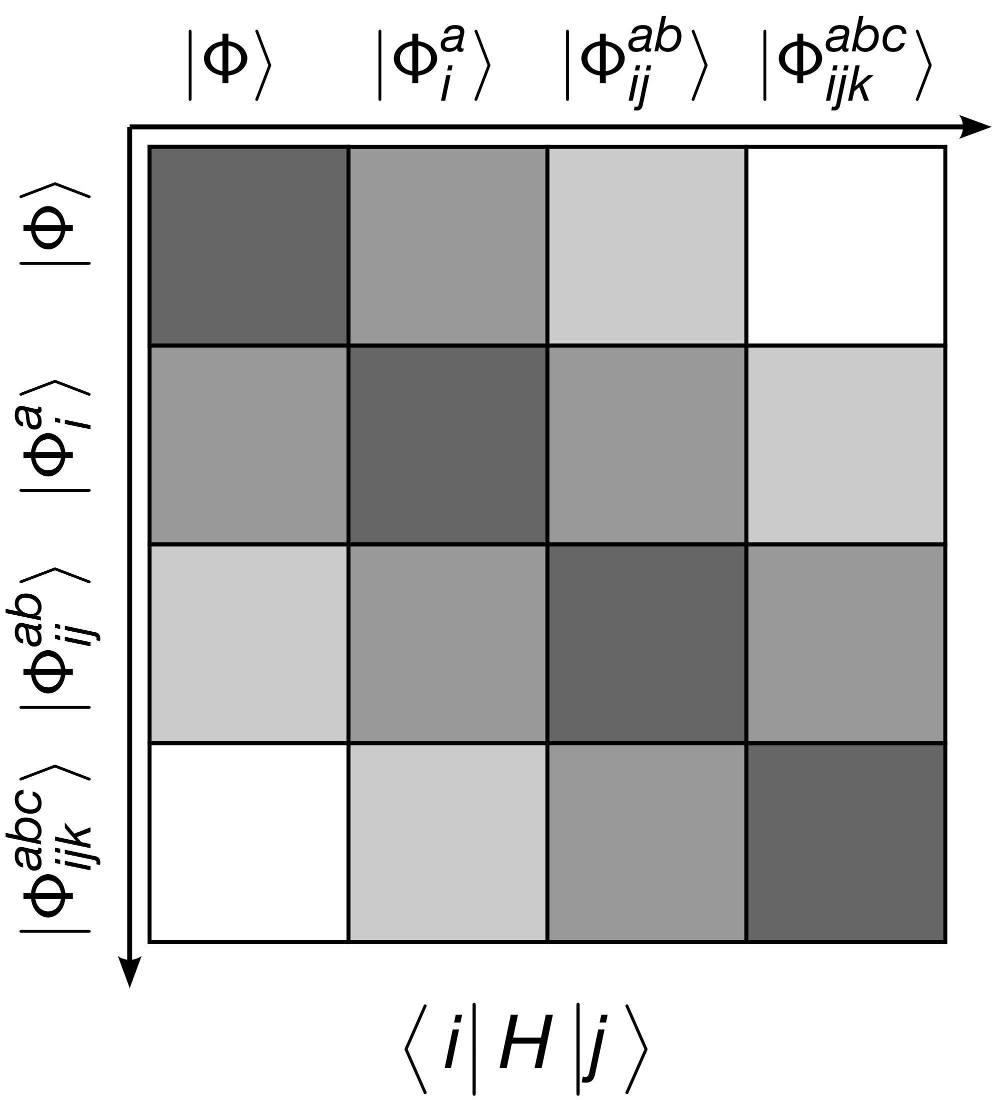
Large-Scale Diagonalization



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

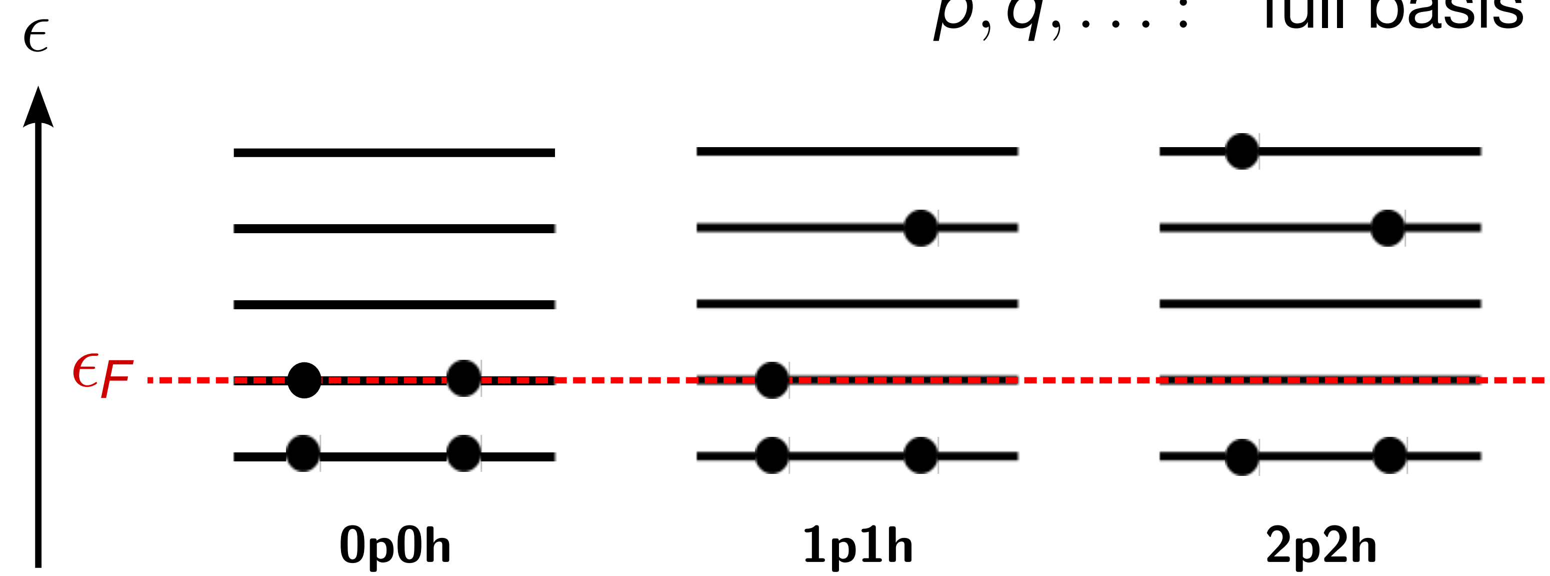
Transforming the Hamiltonian



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

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

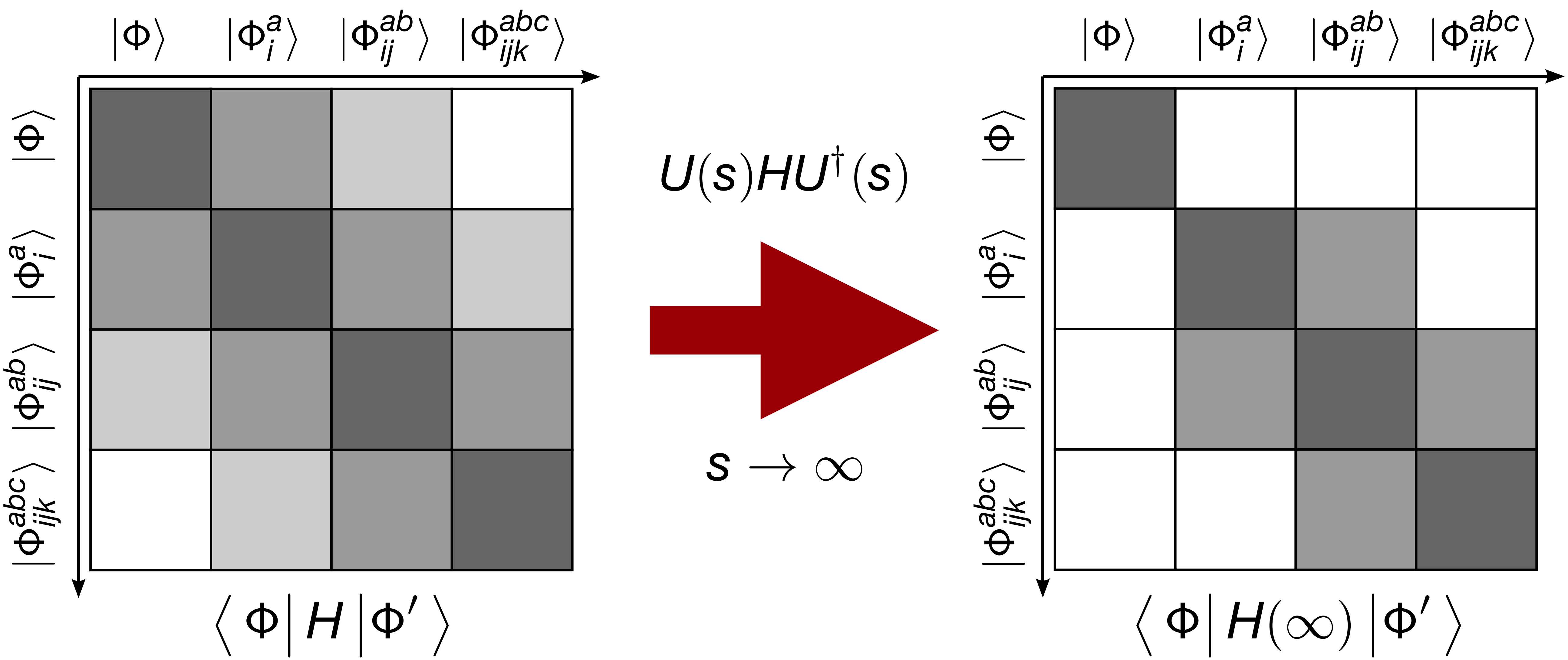
$p, q, \ldots :\quad$ full basis



- reference state: **single Slater determinant**

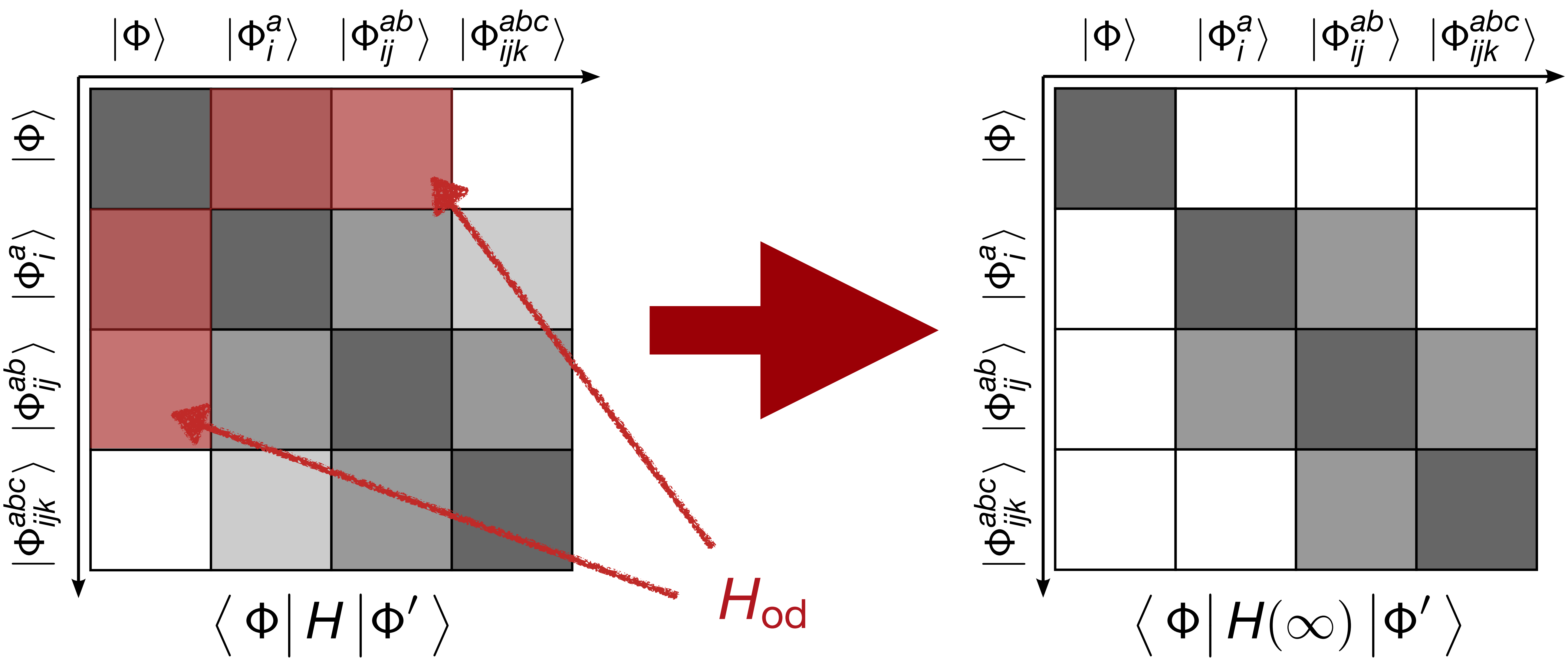
excitations relative to reference state: **normal-ordering**

Decoupling in A-Body Space



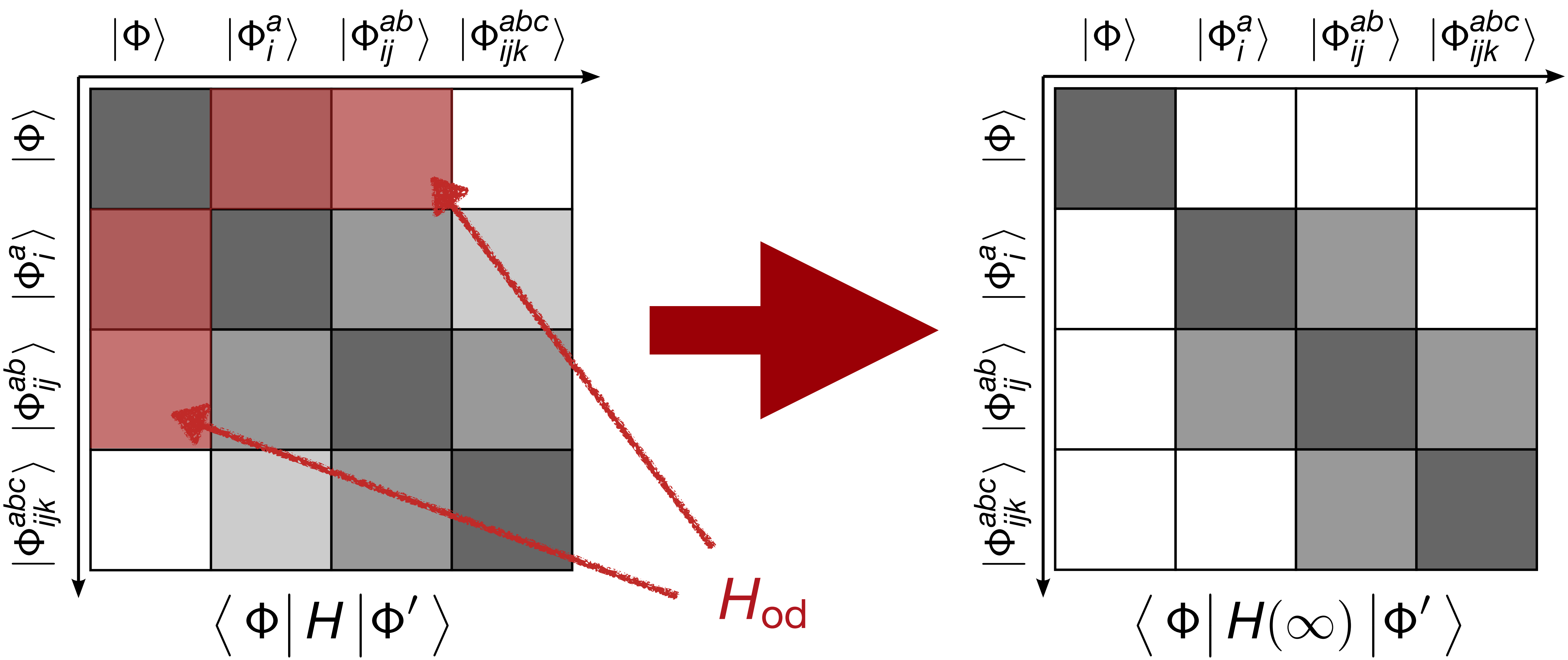
goal: decouple reference state $|\Phi\rangle$ from excitations

Flow Equation



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

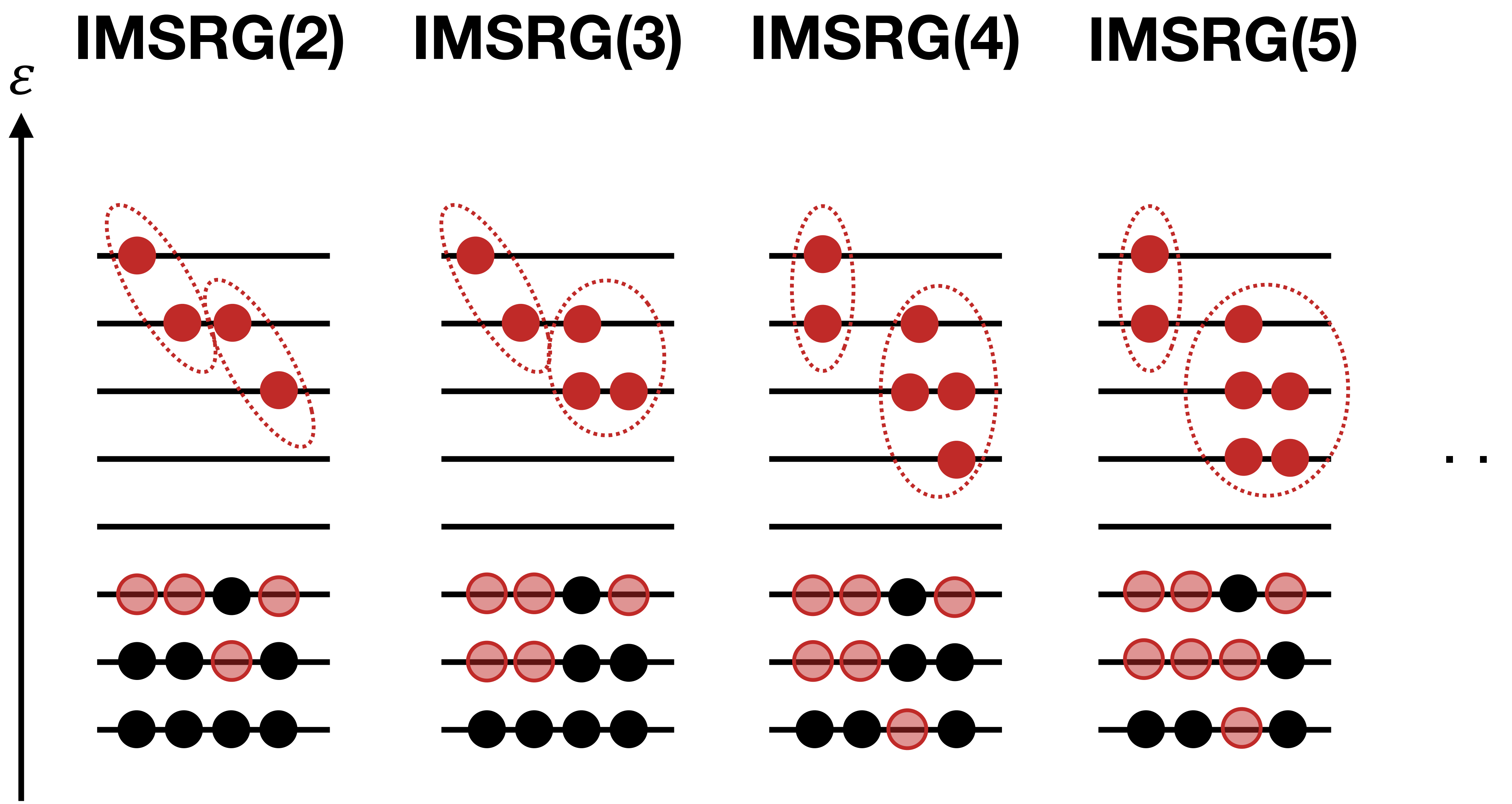
Flow Equation



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

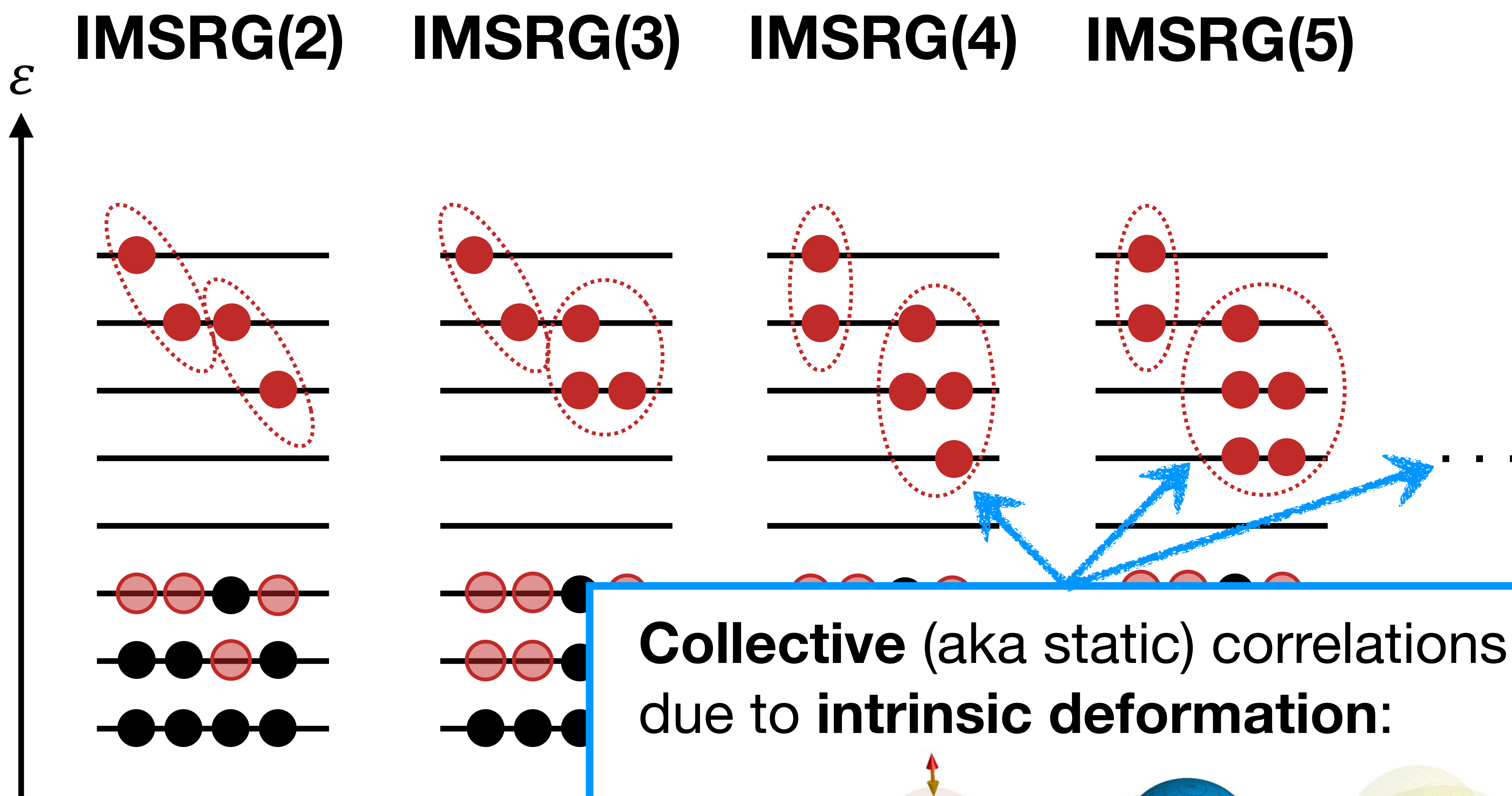
Operators
truncated at **two-body level** -
matrix is never constructed explicitly!

Correlated Reference States



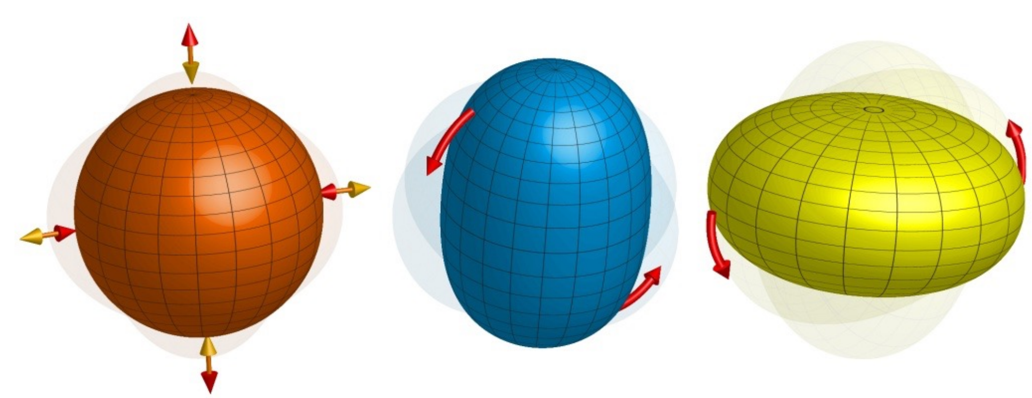
“standard” IMSRG: build correlations on top of Slater determinant (=**independent-particle state**)

Correlated Reference States

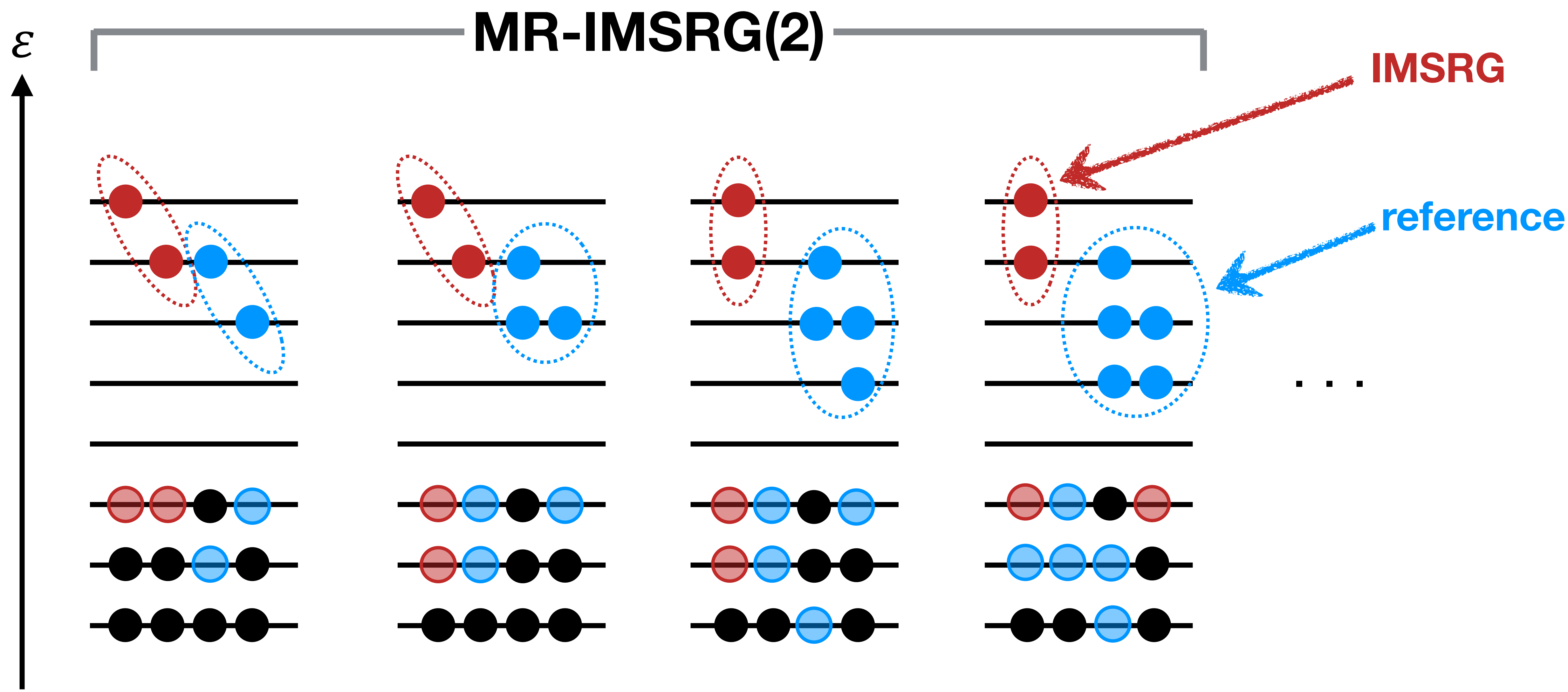


“standard” IMS
Slater determinan

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

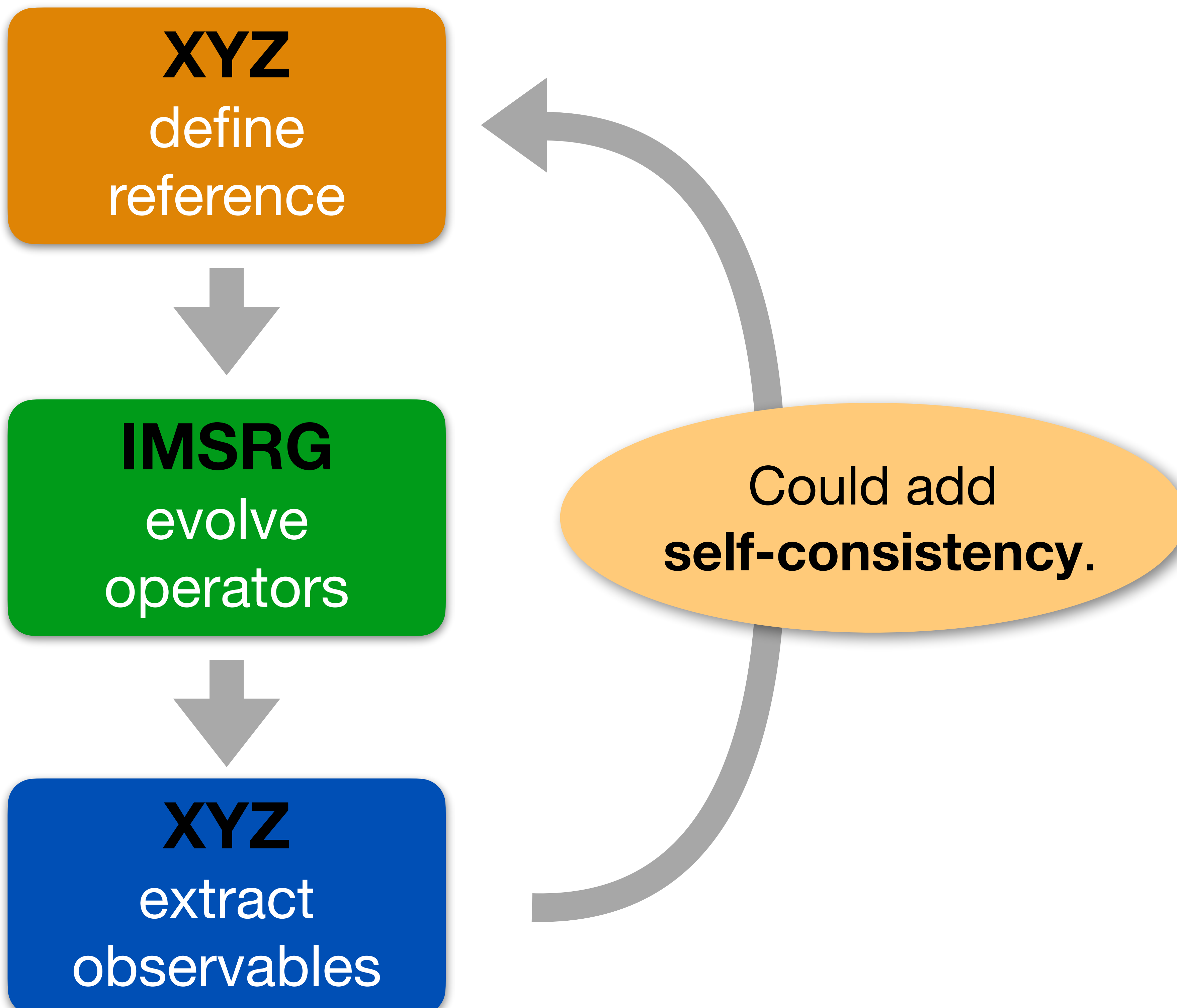


Correlated Reference States



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

IMSRG-Improved Methods



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)

XYZ
define
reference

IMSRG
evolve
operators

XYZ
extract
observables

Merging IMSRG and CI: Valence-Space IMSRG

Review:

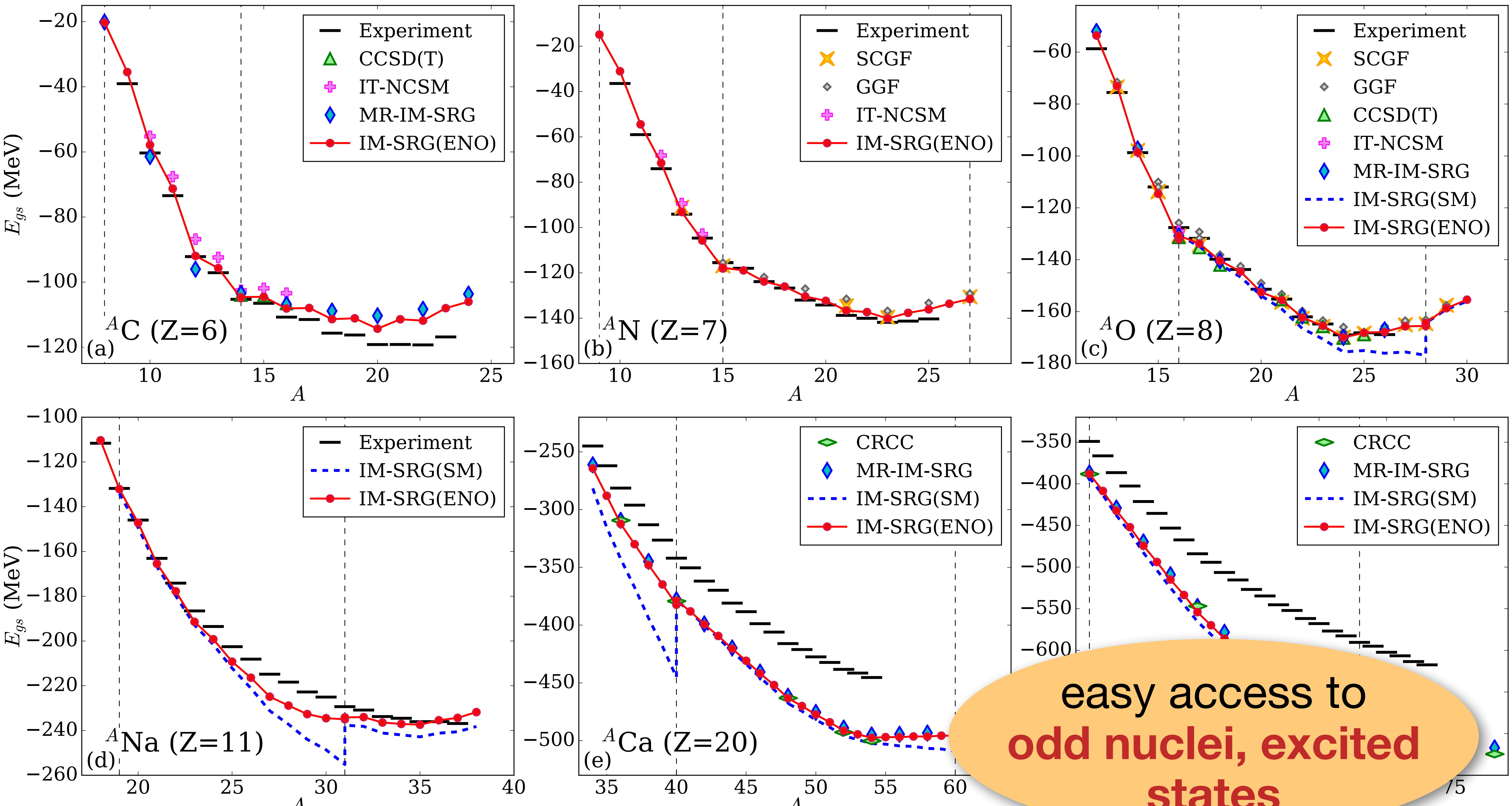
S. R. Stroberg, HH, S. K. Bogner, and J. D. Holt, Ann. Rev. Part. Nucl. Sci. **69**, 165 (2019)

Full CI:

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

Ground-State Energies

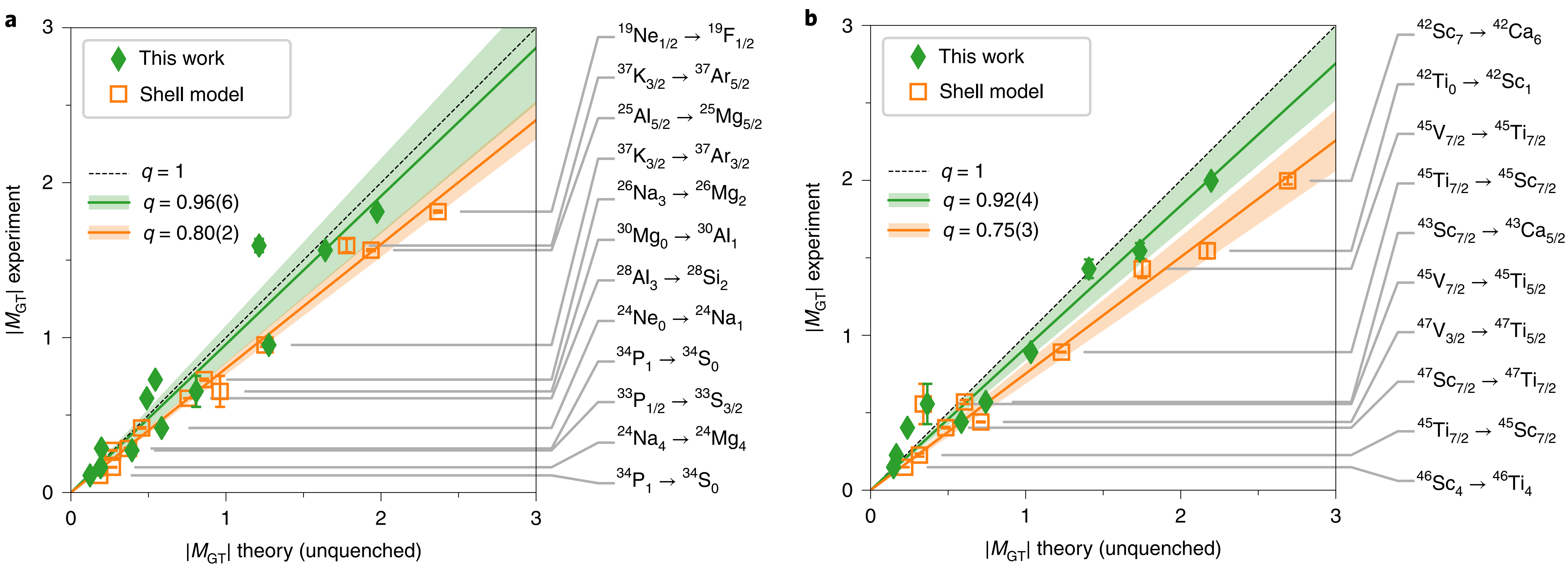
S. R. Stroberg, A. Calci, HH, J. D. Holt, S. K.Bogner, R. Roth, A. Schwenk, PRL **118**, 032502 (2017)
S. R. Stroberg, HH, S. K. Bogner, J. D. Holt, Ann. Rev. Part. Nucl. Sci. **69**, 307 (2019)



easy access to
odd nuclei, excited states

Quenching of Gamow-Teller Decays

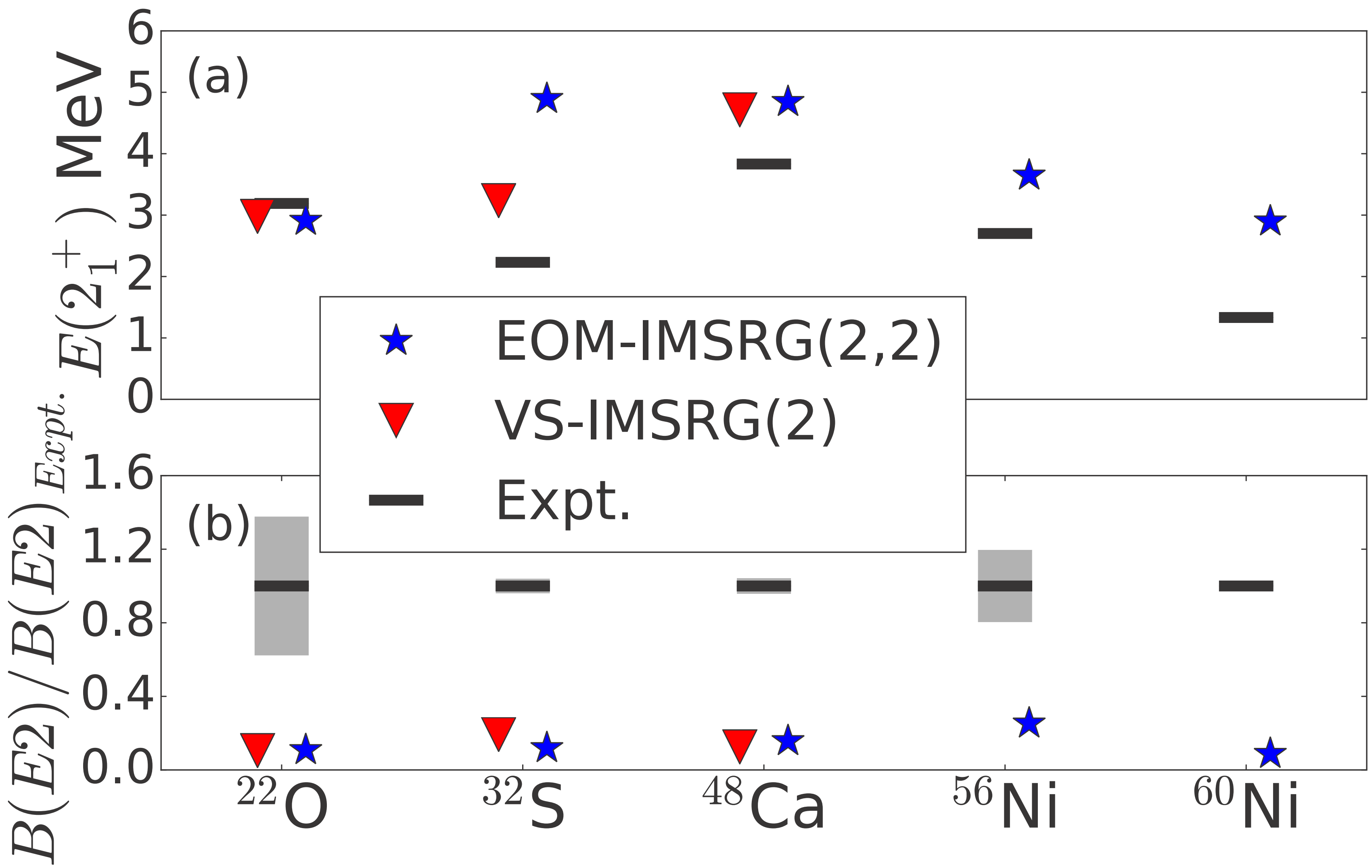
P. Gysbers et al., Nature Physics ***15****, 428 (2019)*



- **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

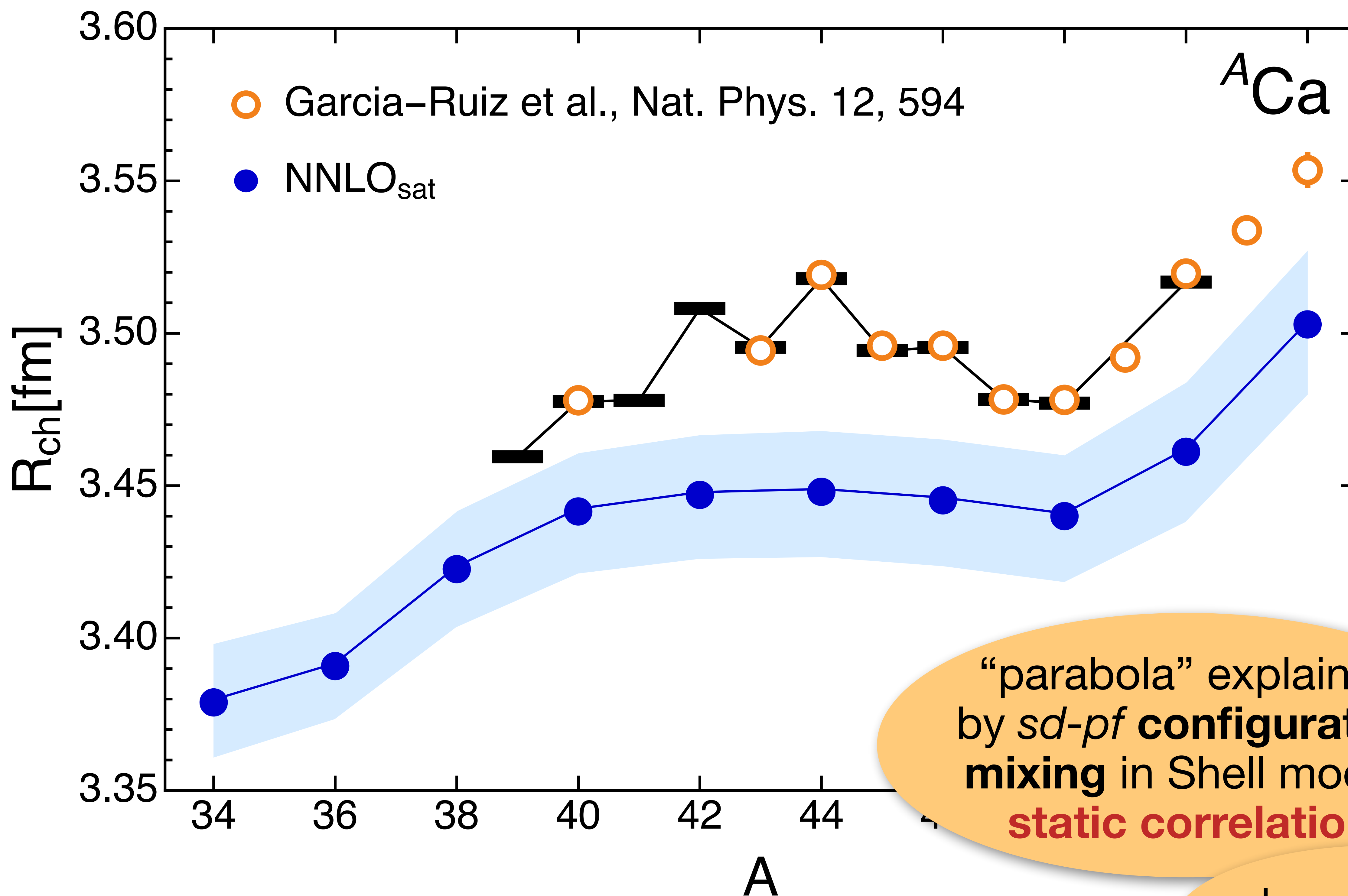
*N. M. Parzuchowski, S. R. Stroberg et al., PRC **96**, 034324*
*S. R. Stroberg, HH, S. K. Bogner, J. D. Holt, Ann. Rev. Part. Nucl. Sci. **69**, 307 (2019)*
*S. R. Stroberg et al. PRC **105**, 034333 (2022*



- **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**

also cf. talk by K. Minamisono

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)

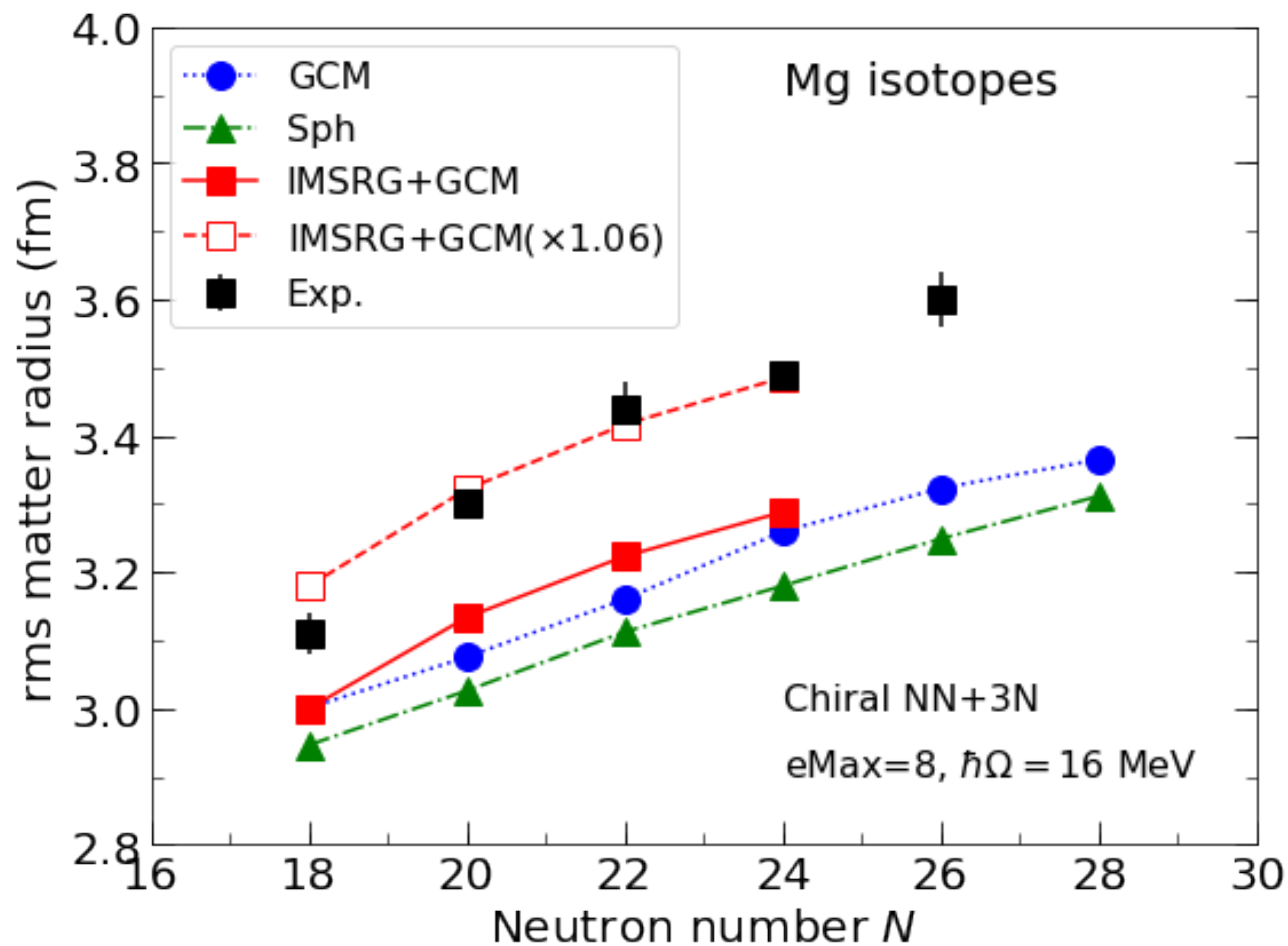
J. M. Yao, B. Bally, J. Engel, R. Wirth, T. R. Rodriguez, HH, PRL **124**, 232501 (2020)

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

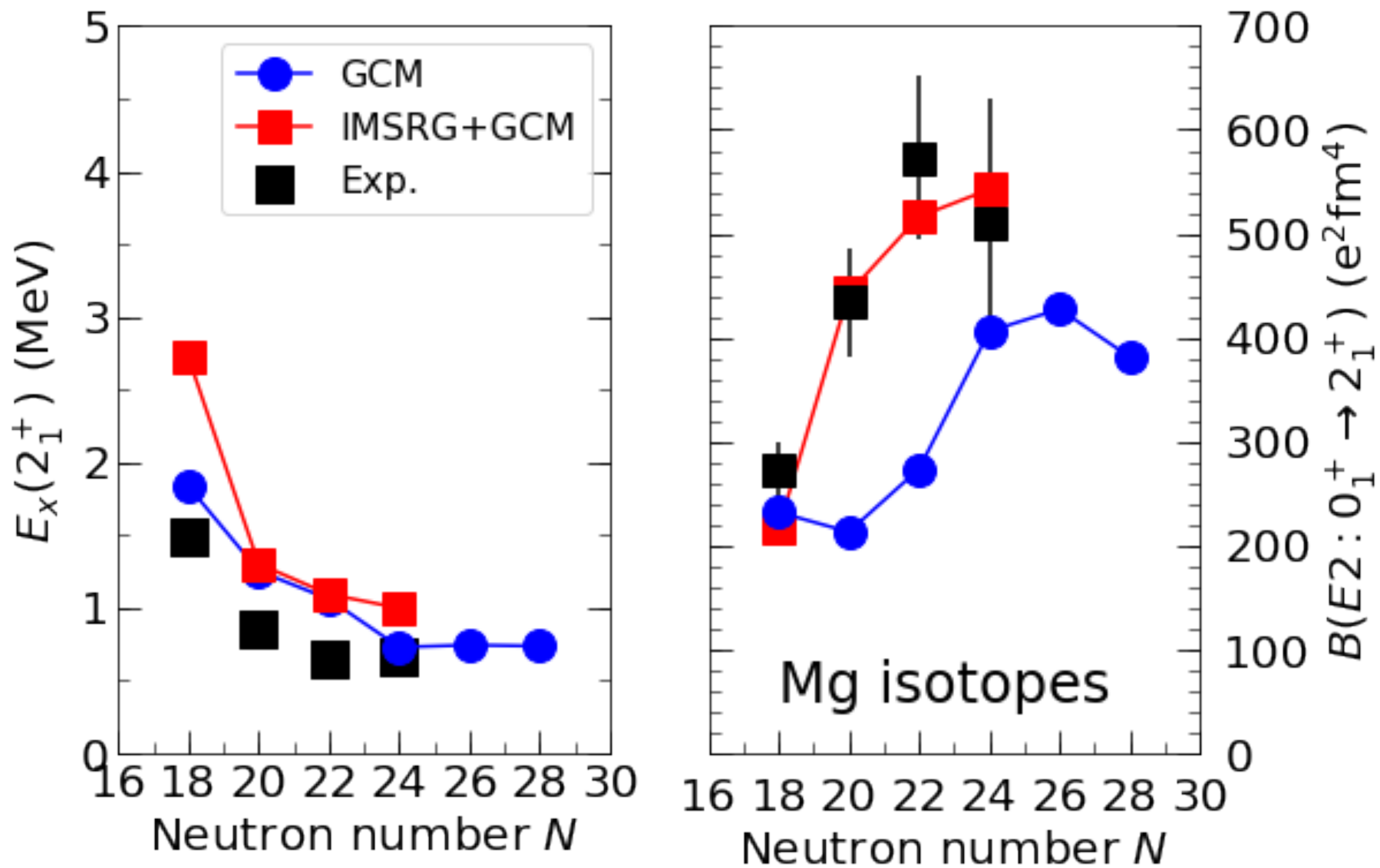


- note **improvement of rms radius trend** from IM-GCM
- global shifts (and/or rotation around "pivot") often associated with cutoff dependence of interactions

cf. talk by K. Flanagan

Magnesium Isotopes

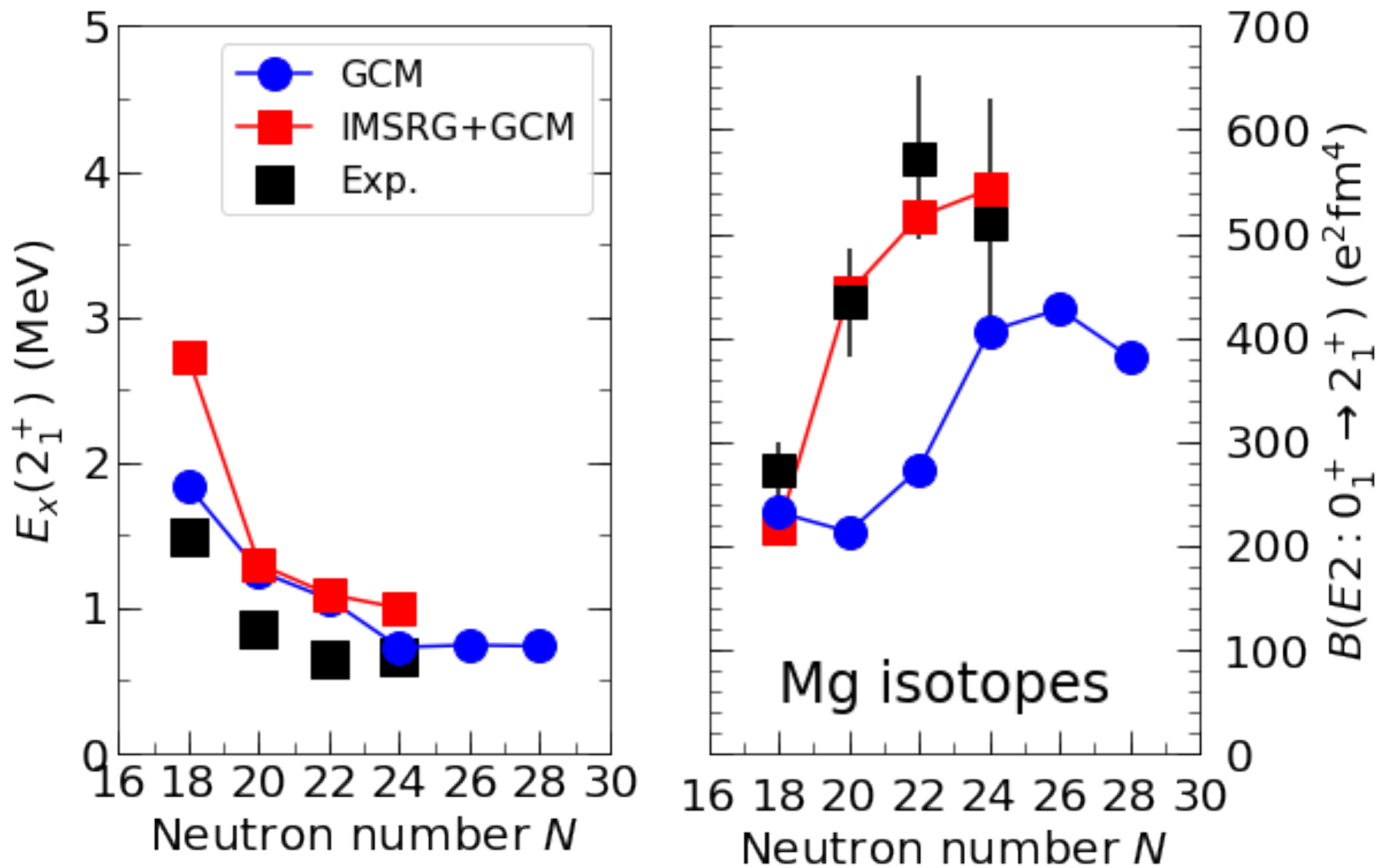
J. M. Yao, HH, in preparation



- 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

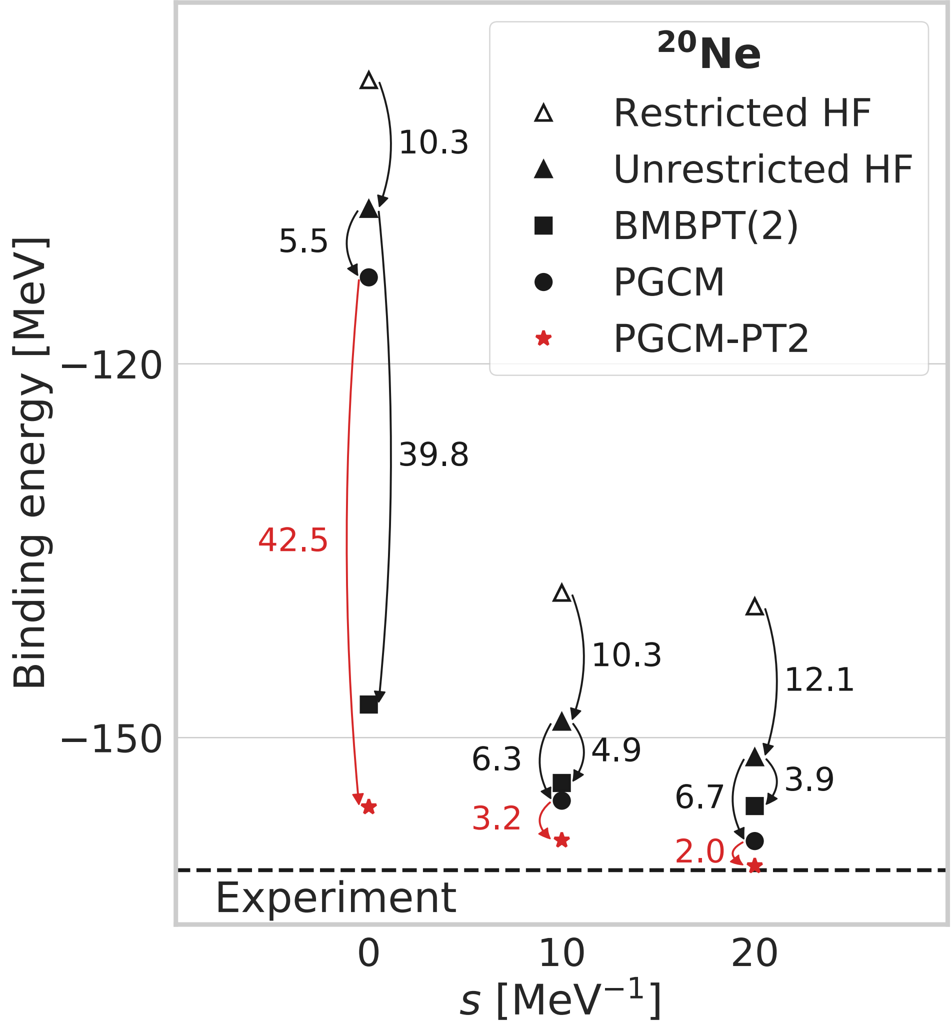


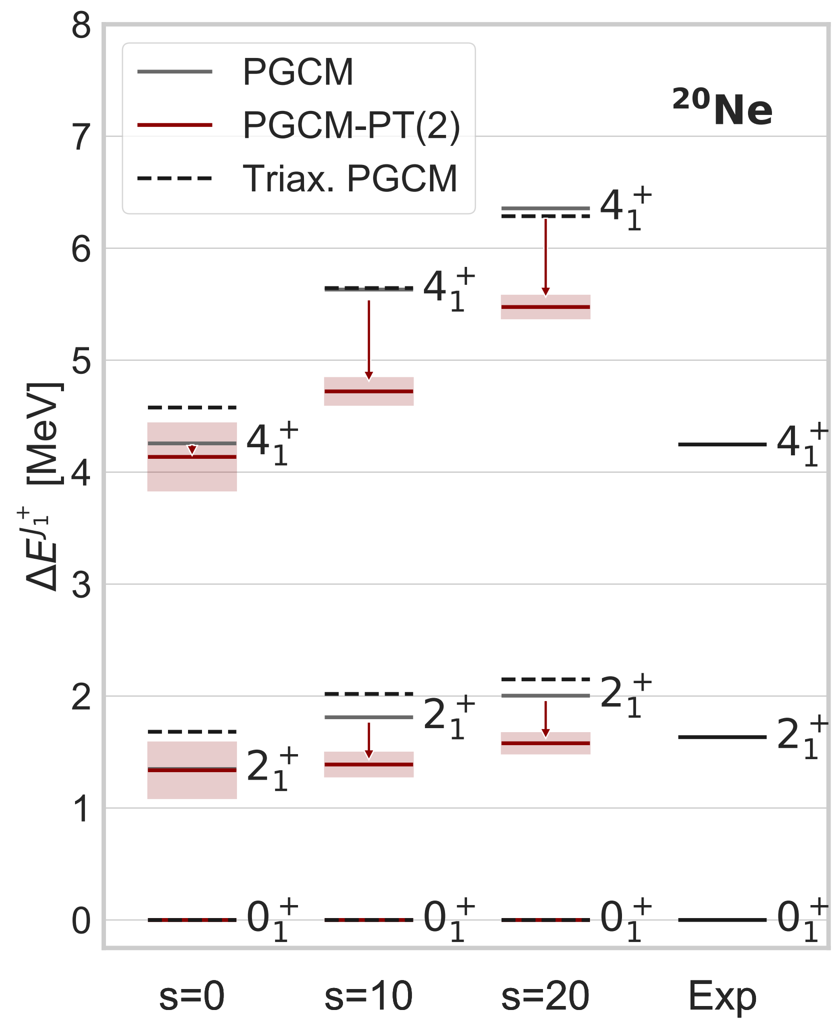
$$O = O^{(1)} \underset{s\to\infty}{\to} O(s) = O^{(1)}(s) + \underbrace{O^{(2)}(s) + \ldots}_{\text{induced contributions}}$$

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

Perturbative Enhancement of IM-GCM

M. Frosini et al., arXiv:2110.15737, arXiv:2111.00757, arXiv:2111.01461

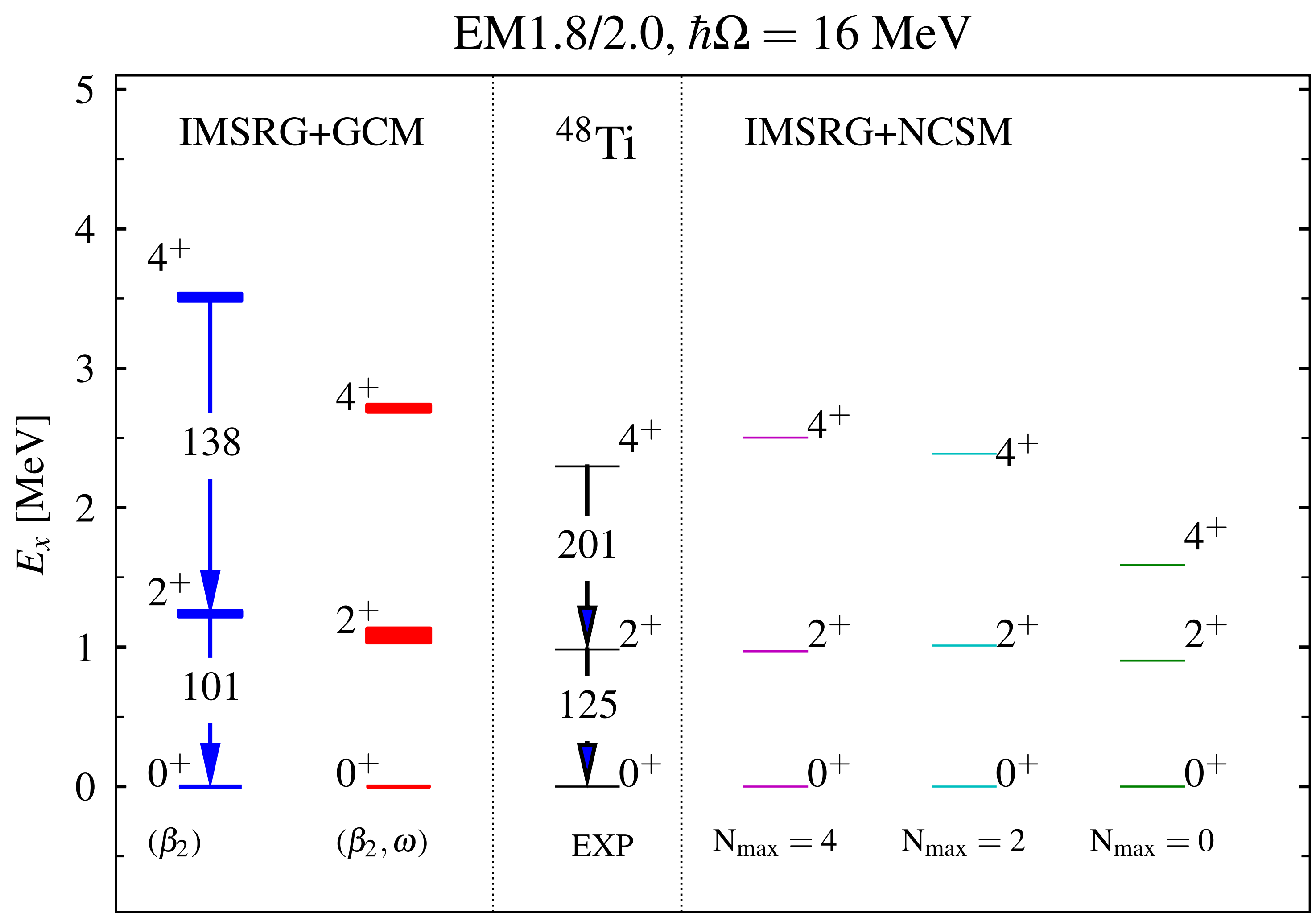




- s-dependence is a **built-in diagnostic tool** for IM-GCM **(not available in phenomenological GCM)**
  - if operator and wave function offer sufficient degrees of freedom, evolution of observables is unitary
- need **richer references and/or IMSRG(3)** for certain observables

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

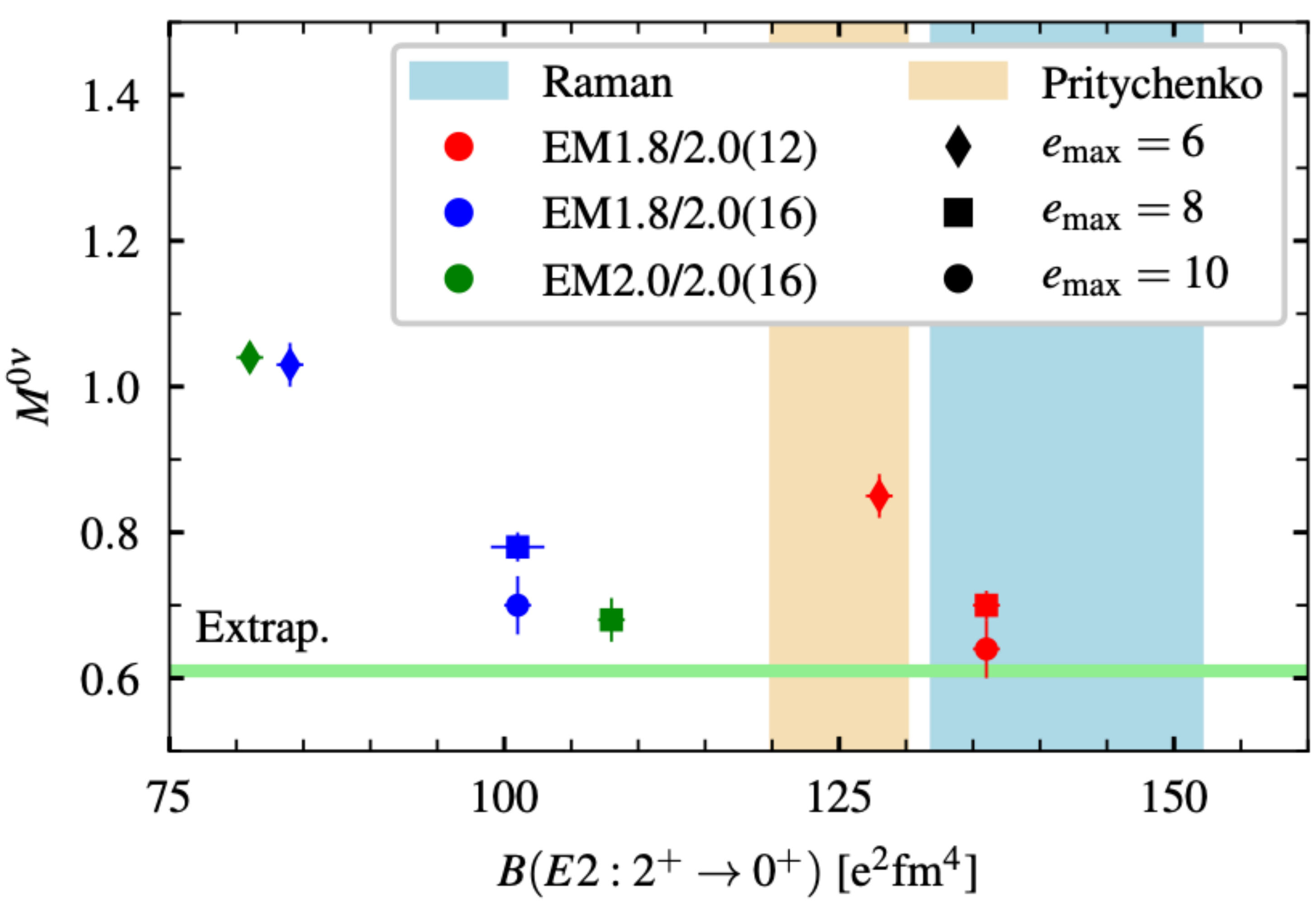
*J. M. Yao et al., PRL **124**, 232501 (2020); HH, Front. Phys. **8**, 379 (2020)*



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

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

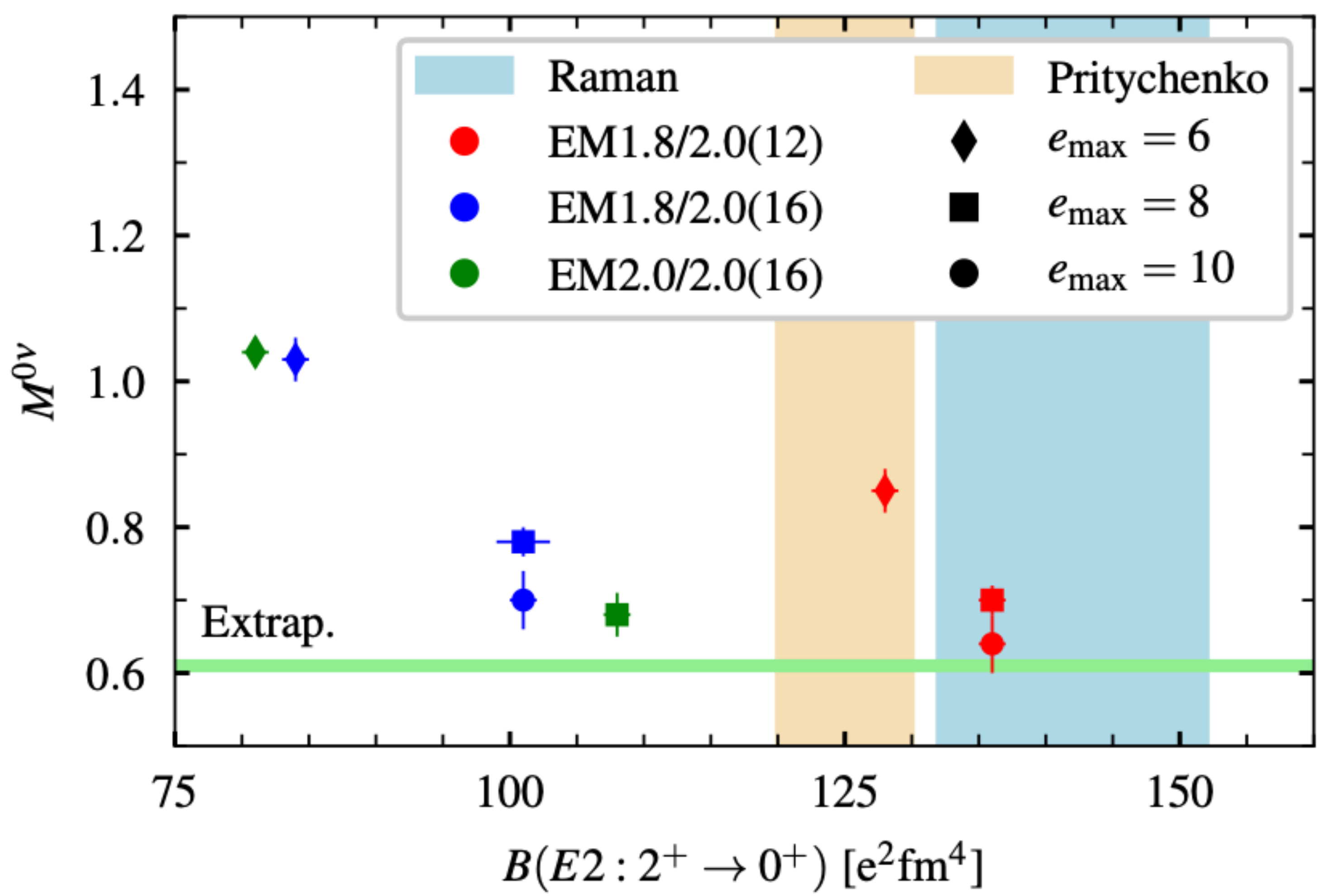
*J. M. Yao et al., PRL **124**, 232501 (2020); PRC **103**, 014315 (2021)*



- NME from different methods **consistent** for consistent interactions & transition operators
  (A. Belley et al., PRL 126, 042502, S. Novario 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

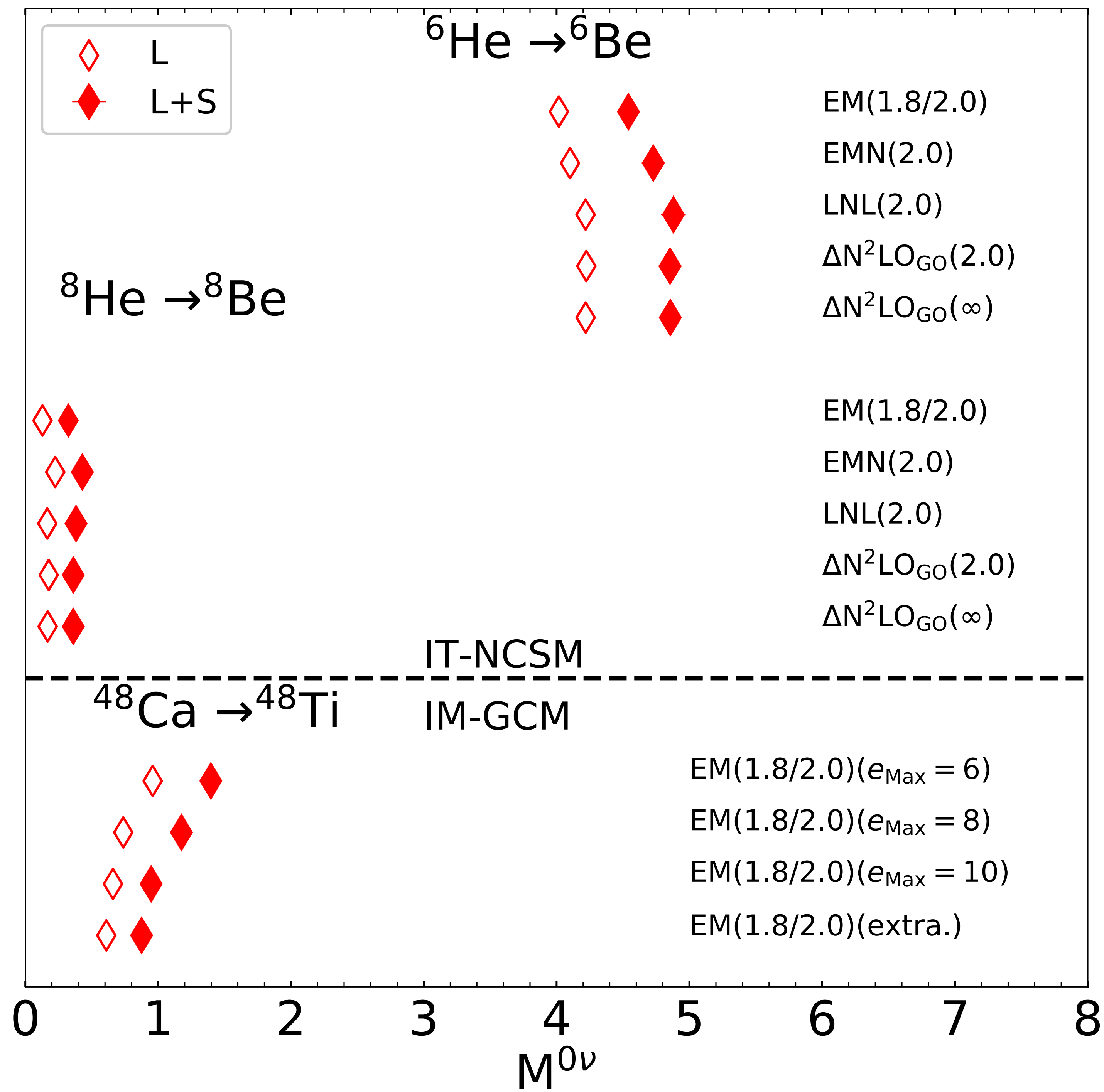
- interpretation and features differ from e

  only **weak correlation** between NME anc

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

Challenges

- inclusion of **IMSRG(3) correlations:**
    - assessment of many-body truncation errors & cutoff dependence effects
    - leverage tensor factorization / hidden low-rank structures?
- 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**… stay tuned)
- enhancement of computational performance & scalability

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 IMSRG: from day-to-day data analysis to leadership calculations

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NUCLEI
Nuclear Computational Low-Energy Initiative