Recent Developments in *Ab Initio* Nuclear Many-Body Theory

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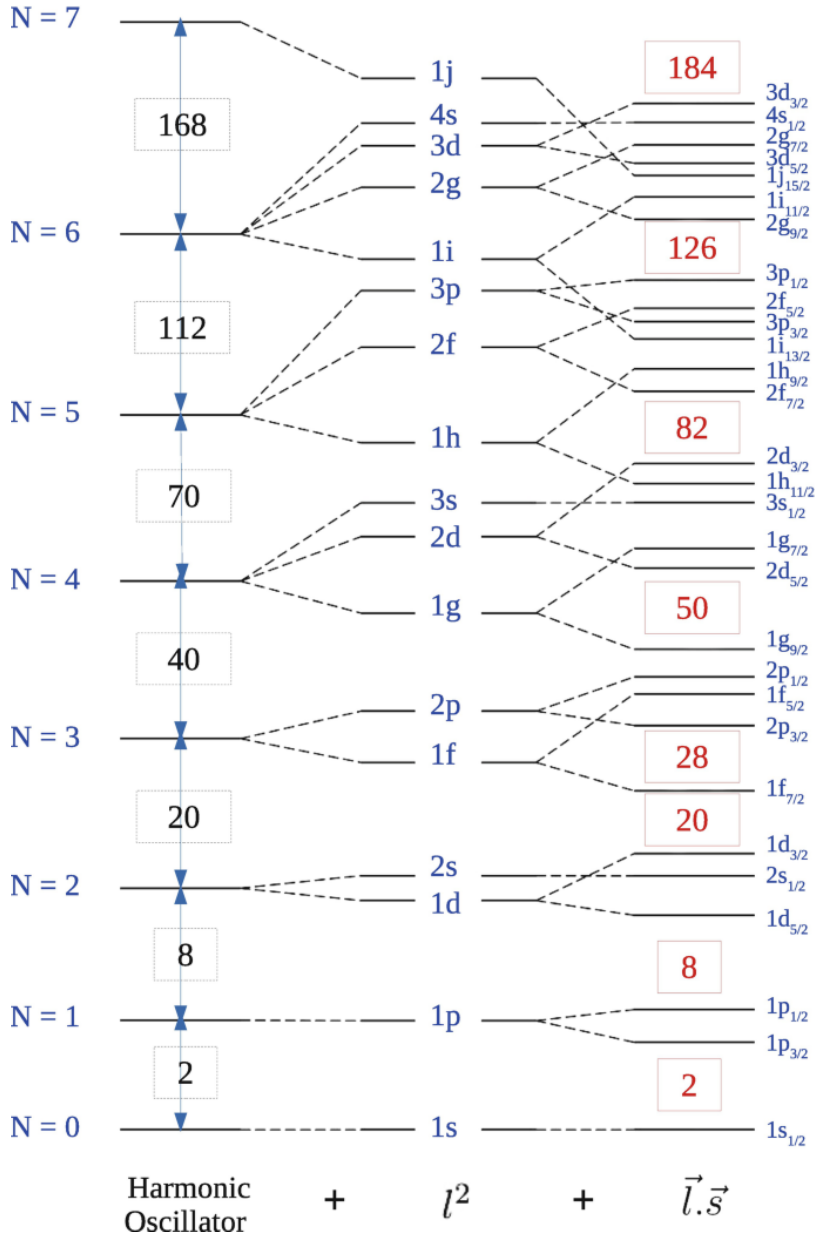
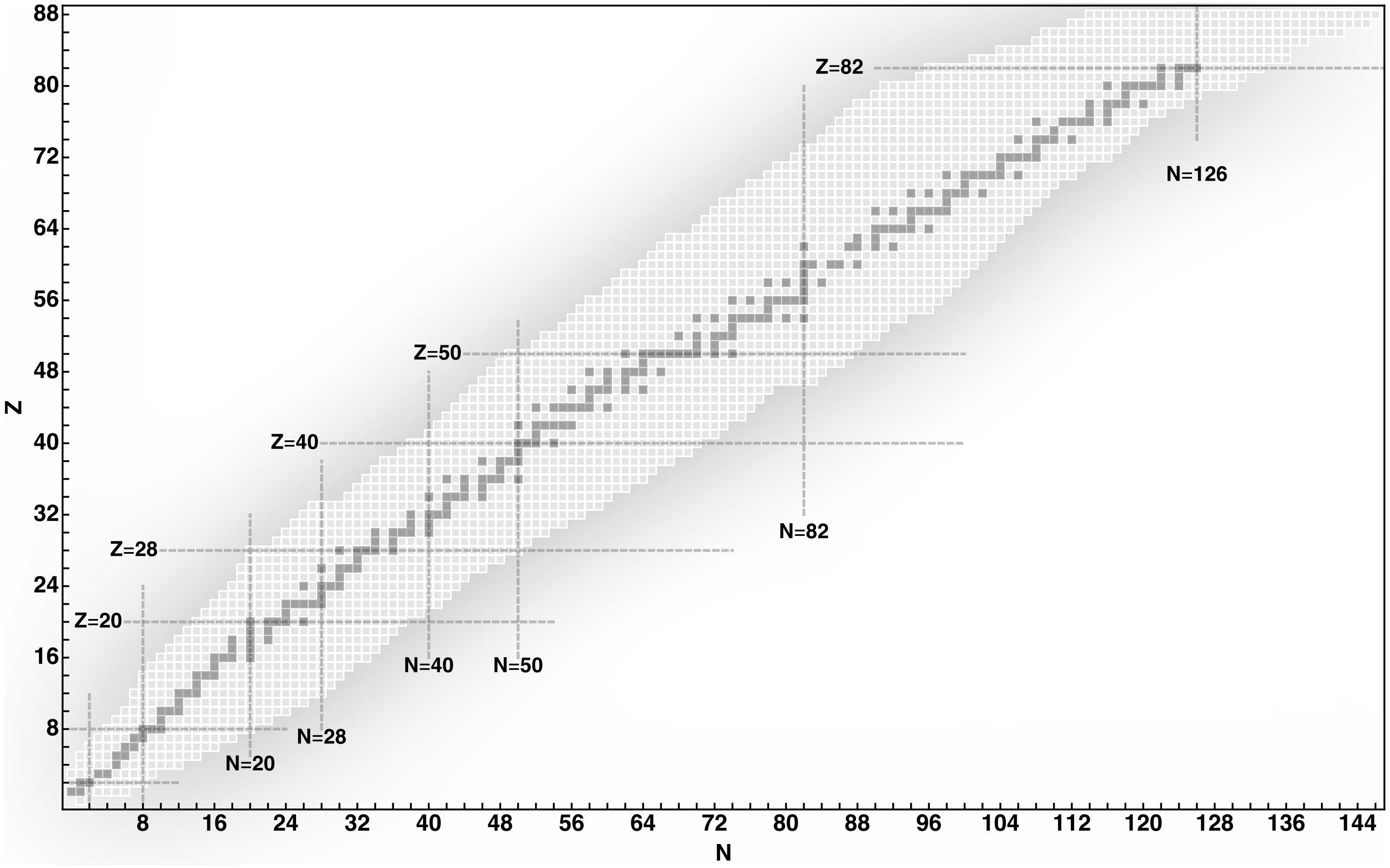
Where Do We Want to Go (Today)?

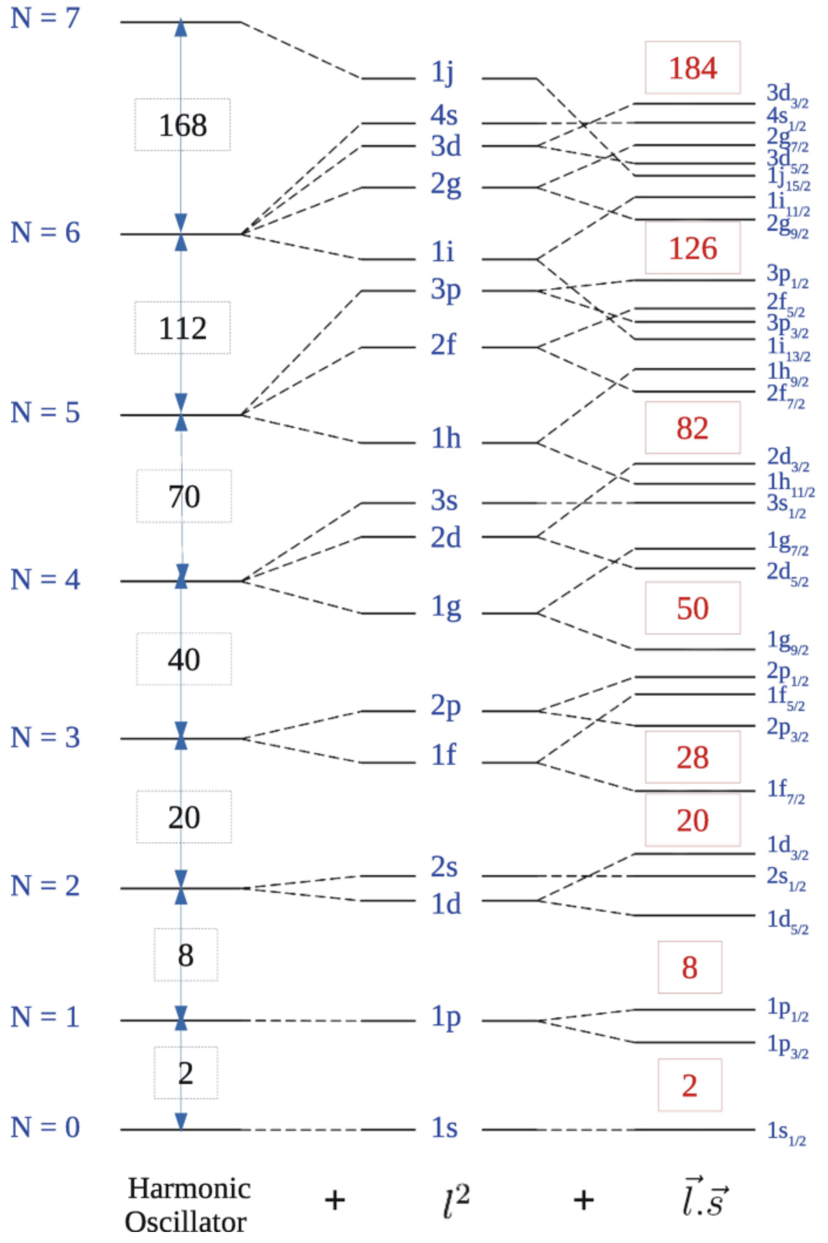
How Does Nuclear Structure Evolve?

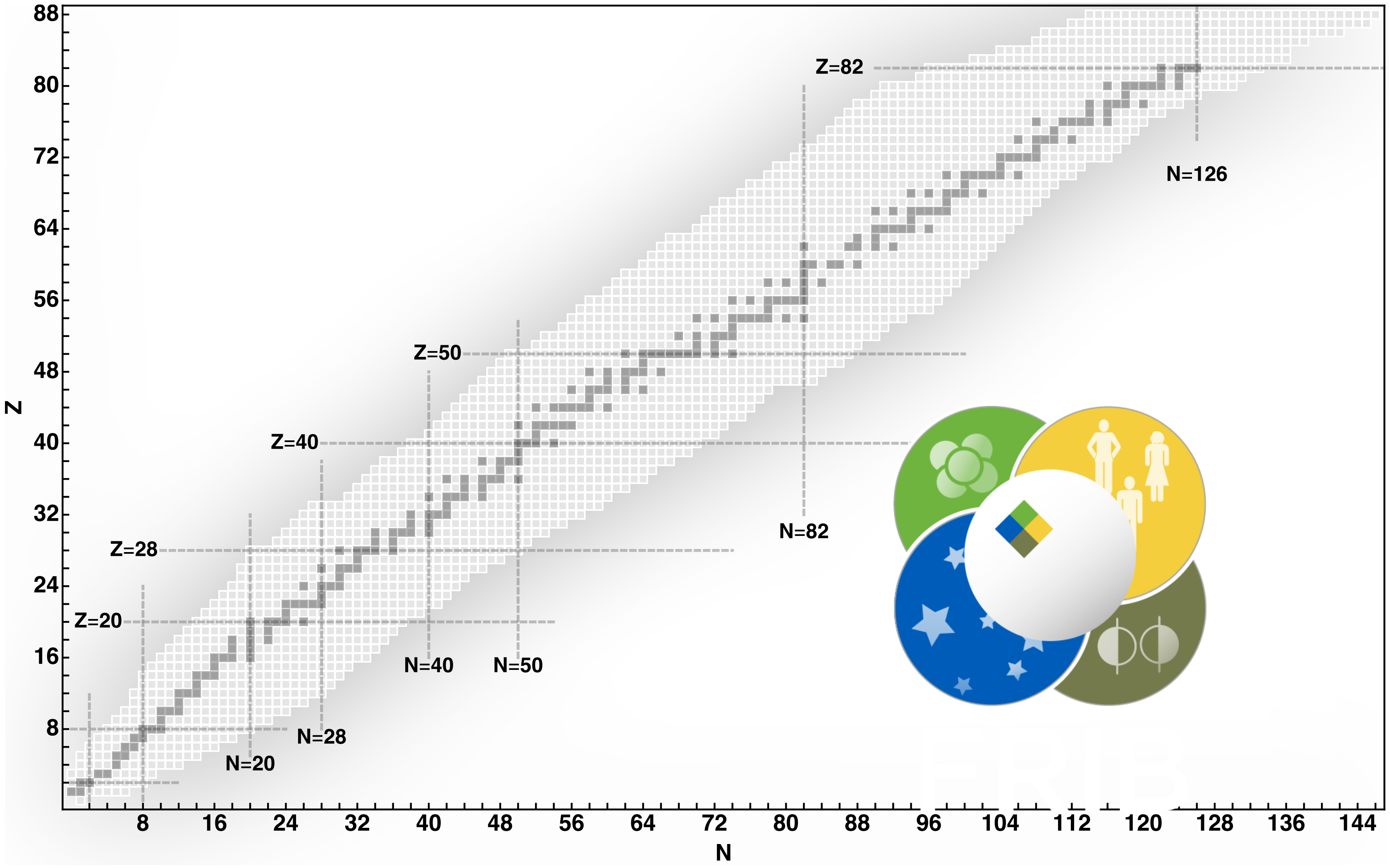




- Evolution of **(intrinsic) shapes** along isotopic chains
- New phenomena: **neutron skins, halos**, …
- Emergence of **new magic numbers** (and absence of old ones)

How Does Nuclear Structure Evolve?





- Evolution of **(intrinsic) shapes** along isotopic chains
- New phenomena: **neutron skins, halos**, …
- Emergence of **new magic numbers** (and absence of old ones)

What Are the Limits of Nuclear Existence?

PRL **100,** 152502 (2008) PHYSICAL REVIEW LETTERS week ending 18 APRIL 2008

Determination of the $N = 16$ Shell Closure at the Oxygen Drip Line

C. R. Hoffman,^{1,*} T. Baumann,^{2} D. Bazin,^{2} J. Brown,^{3} G. Christian,^{2,4} P. A. DeYoung,^{5} J. E. Finck,^{6} N. Frank,^{2,4,†}
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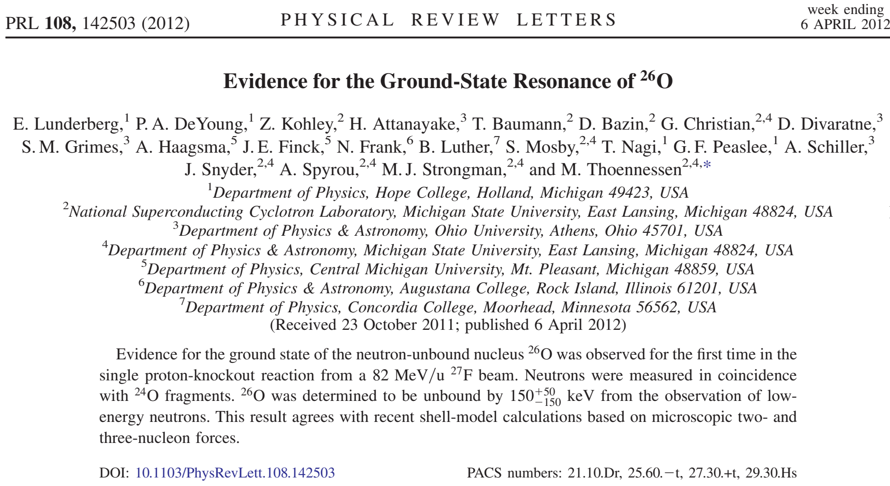
(Received 22 December 2007; published 17 April 2008)

The neutron unbound ground state of ^{25}O ($Z = 8$, $N = 17$) was observed for the first time in a proton knockout reaction from a ^{26}F beam. A single resonance was found in the invariant mass spectrum corresponding to a neutron decay energy of 770^{+20}_{-10} keV with a total width of 172(30) keV. The $N = 16$ shell gap was established to be 4.86(13) MeV by the energy difference between the $\nu 1s_{1/2}$ and $\nu 0d_{3/2}$ orbitals. The neutron separation energies for ^{25}O agree with the calculations of the universal *sd* shell model interaction. This interaction incorrectly predicts an ^{26}O ground state that is bound to two-neutron decay by 1 MeV, leading to a discrepancy between the theoretical calculations and experiment as to the particle stability of ^{26}O. The observed decay width was found to be on the order of a factor of 2 larger than the calculated single-particle width using a Woods-Saxon potential.

DOI: 10.1103/PhysRevLett.100.152502 PACS numbers: 21.10.Pc, 25.60.−t, 27.30.+t, 29.30.Hs



PRL **108,** 142503 (2012) PHYSICAL REVIEW LETTERS week ending 6 APRIL 2012

Evidence for the Ground-State Resonance of ^{26}O

E. Lunderberg,^{1} P. A. DeYoung,^{1} Z. Kohley,^{2} H. Attanayake,^{3} T. Baumann,^{2} D. Bazin,^{2} G. Christian,^{2,4} D. Divaratne,^{3}
S. M. Grimes,^{3} A. Haagsma,^{5} J. E. Finck,^{5} N. Frank,^{6} B. Luther,^{7} S. Mosby,^{2,4} T. Nagi,^{1} G. F. Peaslee,^{1} A. Schiller,^{3}
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(Received 23 October 2011; published 6 April 2012)

Evidence for the ground state of the neutron-unbound nucleus ^{26}O was observed for the first time in the single proton-knockout reaction from a 82 MeV/u ^{27}F beam. Neutrons were measured in coincidence with ^{24}O fragments. ^{26}O was determined to be unbound by 150^{+50}_{-150} keV from the observation of low-energy neutrons. This result agrees with recent shell-model calculations based on microscopic two- and three-nucleon forces.

DOI: 10.1103/PhysRevLett.108.142503 PACS numbers: 21.10.Dr, 25.60.−t, 27.30.+t, 29.30.Hs

PHYSICAL REVIEW C **88**, 034313 (2013)

Beyond the neutron drip line: The unbound oxygen isotopes ^{25}O and ^{26}O

C. Caesar,^{1,2} J. Simonis,^{1,3} T. Adachi,^{4} Y. Aksyutina,^{2,3} J. Alcantara,^{5} S. Altstadt,^{6} H. Alvarez-Pol,^{5} N. Ashwood,^{7}
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R. Gernhäuser,^{22} P. Golubev,^{8} D. Gonzalez Diaz,^{1} J. Hagdahl,^{23} T. Heftrich,^{6} M. Heil,^{2} M. Heine,^{1} A. Heinz,^{23} A. Henriques,^{21}
M. Holl,^{1} J. D. Holt,^{24,25} G. Ickert,^{2} A. Ignatov,^{1} B. Jakobsson,^{8} H. T. Johansson,^{23} B. Jonson,^{23} N. Kalantar-Nayestanaki,^{4}
R. Kanungo,^{18} A. Kelic-Heil,^{2} R. Knöbel,^{2} T. Kröll,^{1} R. Krücken,^{22,†} J. Kurcewicz,^{2} M. Labiche,^{26} C. Langer,^{6} T. Le Bleis,^{22}
R. Lemmon,^{26} O. Lepyoshkina,^{22} S. Lindberg,^{23} J. Machado,^{21} J. Marganiec,^{3} V. Maroussov,^{27} J. Menéndez,^{1,3} M. Mostazo,^{5}
A. Movsesyan,^{1} A. Najafi,^{4} T. Nilsson,^{23} C. Nociforo,^{2} V. Panin,^{1} A. Perea,^{11} S. Pietri,^{2} R. Plag,^{6} A. Prochazka,^{2}
A. Rahaman,^{15} G. Rastrepina,^{2} R. Reifarth,^{6} G. Ribeiro,^{11} M. V. Ricciardi,^{2} C. Rigollet,^{4} K. Riisager,^{20} M. Röder,^{28,9}
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V. Volkov,^{1} A. Wagner,^{9} F. Wamers,^{1} H. Weick,^{2} M. Weigand,^{6} C. Wheldon,^{7} G. Wilson,^{32} C. Wimmer,^{6} J. S. Winfield,^{2}
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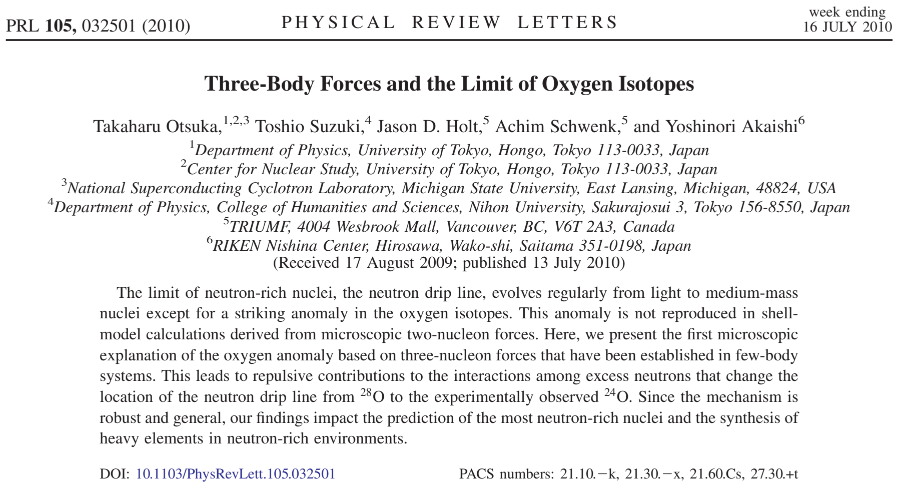
(Received 2 September 2012; revised manuscript received 13 August 2013; published 16 September 2013)

The very neutron-rich oxygen isotopes ^{25}O and ^{26}O are investigated experimentally and theoretically. The unbound states are populated in an experiment performed at the R3B-LAND setup at GSI via proton-knockout reactions from ^{26}F and ^{27}F at relativistic energies around 442 and 414 MeV/nucleon, respectively. From the kinematically complete measurement of the decay into ^{24}O plus one or two neutrons, the ^{25}O ground-state energy and width are determined, and upper limits for the ^{26}O ground-state energy and lifetime are extracted. In addition, the results provide indications for an excited state in ^{26}O at around 4 MeV. The experimental findings are compared to theoretical shell-model calculations based on chiral two- and three-nucleon ($3N$) forces, including for the first time residual $3N$ forces, which are shown to be amplified as valence neutrons are added.

DOI: 10.1103/PhysRevC.88.034313 PACS number(s): 21.10.−k, 25.60.−t, 27.30.+t, 29.30.Hs



PRL **105,** 032501 (2010) PHYSICAL REVIEW LETTERS week ending 16 JULY 2010

Three-Body Forces and the Limit of Oxygen Isotopes

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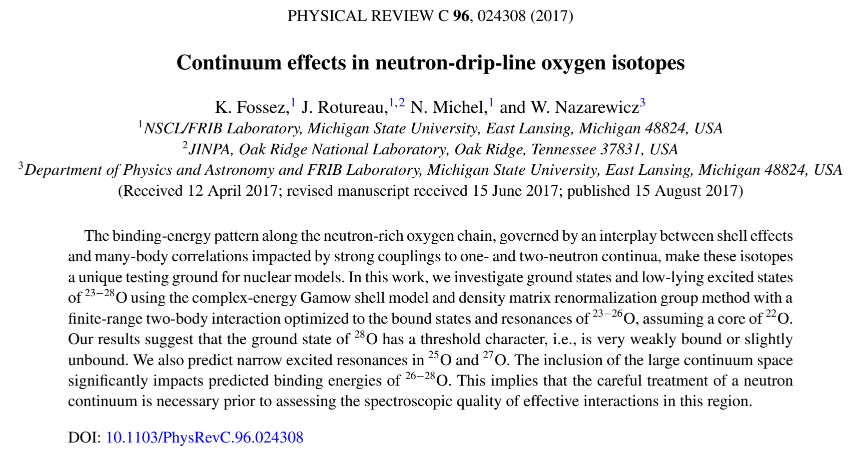
(Received 17 August 2009; published 13 July 2010)

The limit of neutron-rich nuclei, the neutron drip line, evolves regularly from light to medium-mass nuclei except for a striking anomaly in the oxygen isotopes. This anomaly is not reproduced in shell-model calculations derived from microscopic two-nucleon forces. Here, we present the first microscopic explanation of the oxygen anomaly based on three-nucleon forces that have been established in few-body systems. This leads to repulsive contributions to the interactions among excess neutrons that change the location of the neutron drip line from ^{28}O to the experimentally observed ^{24}O. Since the mechanism is robust and general, our findings impact the prediction of the most neutron-rich nuclei and the synthesis of heavy elements in neutron-rich environments.

DOI: 10.1103/PhysRevLett.105.032501 PACS numbers: 21.10.−k, 21.30.−x, 21.60.Cs, 27.30.+t



PHYSICAL REVIEW C **96**, 024308 (2017)

Continuum effects in neutron-drip-line oxygen isotopes

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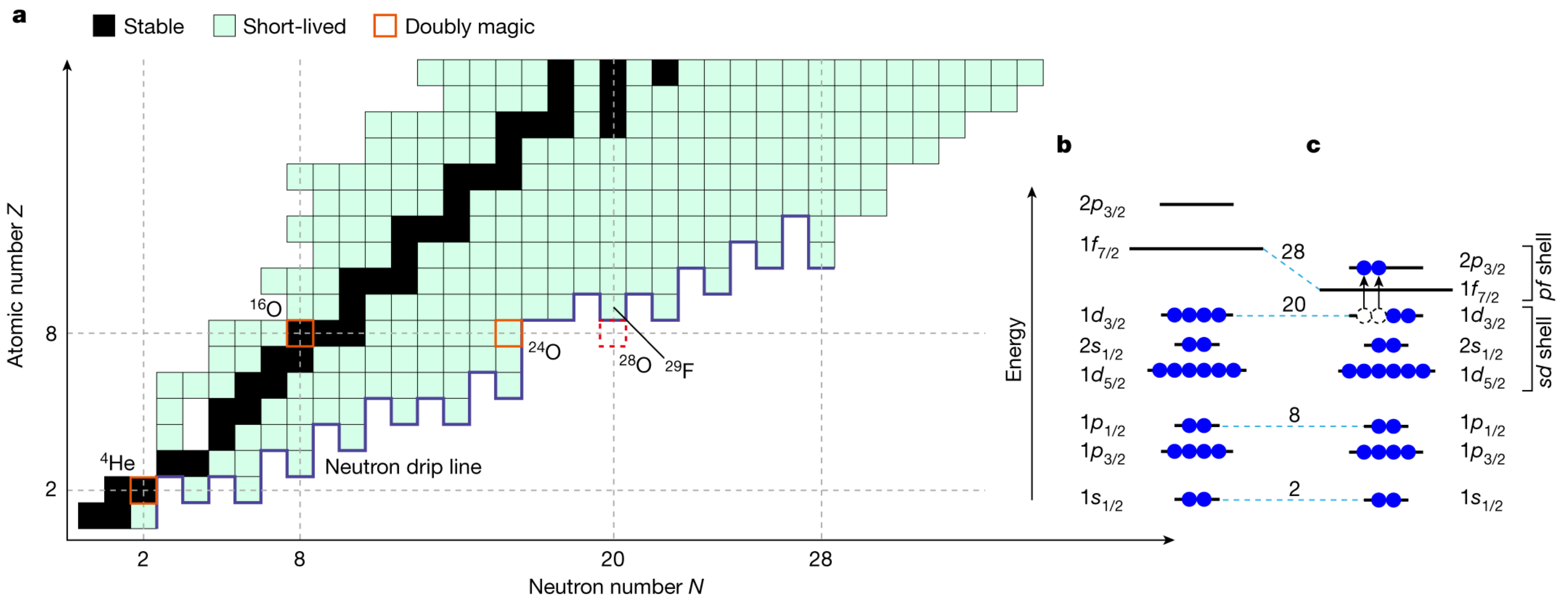
(Received 12 April 2017; revised manuscript received 15 June 2017; published 15 August 2017)

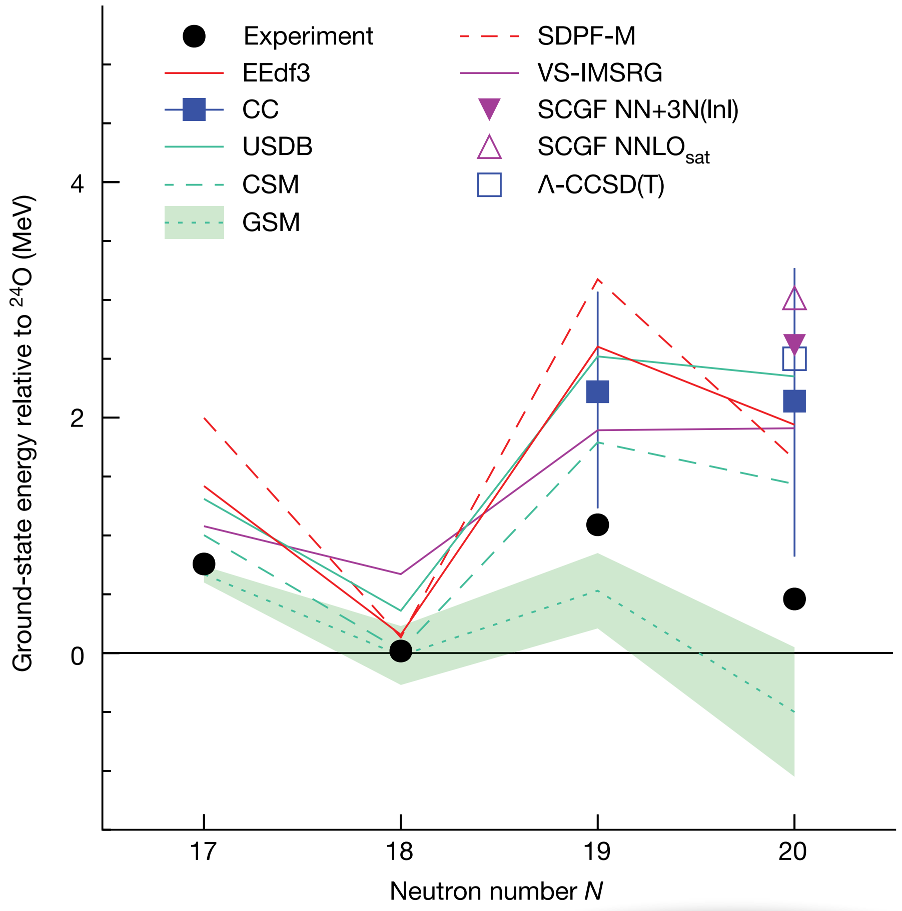
The binding-energy pattern along the neutron-rich oxygen chain, governed by an interplay between shell effects and many-body correlations impacted by strong couplings to one- and two-neutron continua, make these isotopes a unique testing ground for nuclear models. In this work, we investigate ground states and low-lying excited states of $^{23-28}$O using the complex-energy Gamow shell model and density matrix renormalization group method with a finite-range two-body interaction optimized to the bound states and resonances of $^{23-26}$O, assuming a core of ^{22}O. Our results suggest that the ground state of ^{28}O has a threshold character, i.e., is very weakly bound or slightly unbound. We also predict narrow excited resonances in ^{25}O and ^{27}O. The inclusion of the large continuum space significantly impacts predicted binding energies of $^{26-28}$O. This implies that the careful treatment of a neutron continuum is necessary prior to assessing the spectroscopic quality of effective interactions in this region.

DOI: 10.1103/PhysRevC.96.024308

e.g., emergence of **new N=16 magic number** and location of **the neutron drip line in oxygen** isotopes

What Are the Limits of Nuclear Existence?



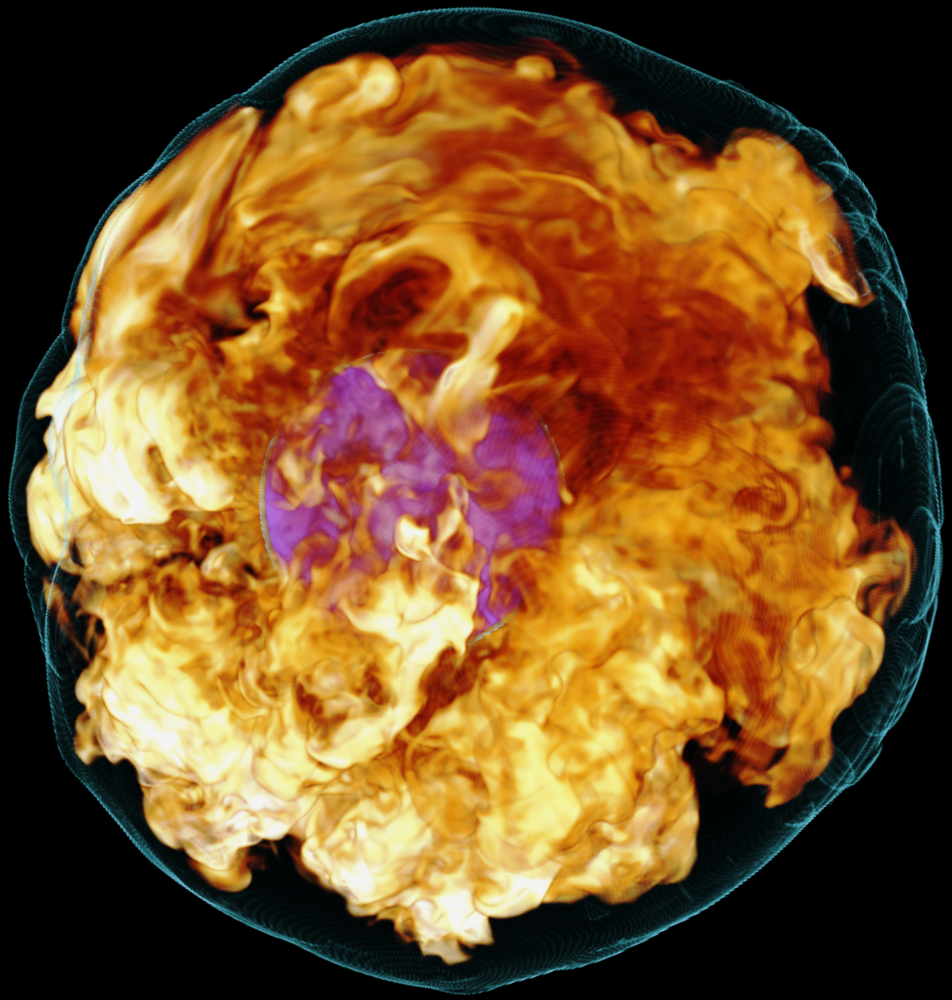


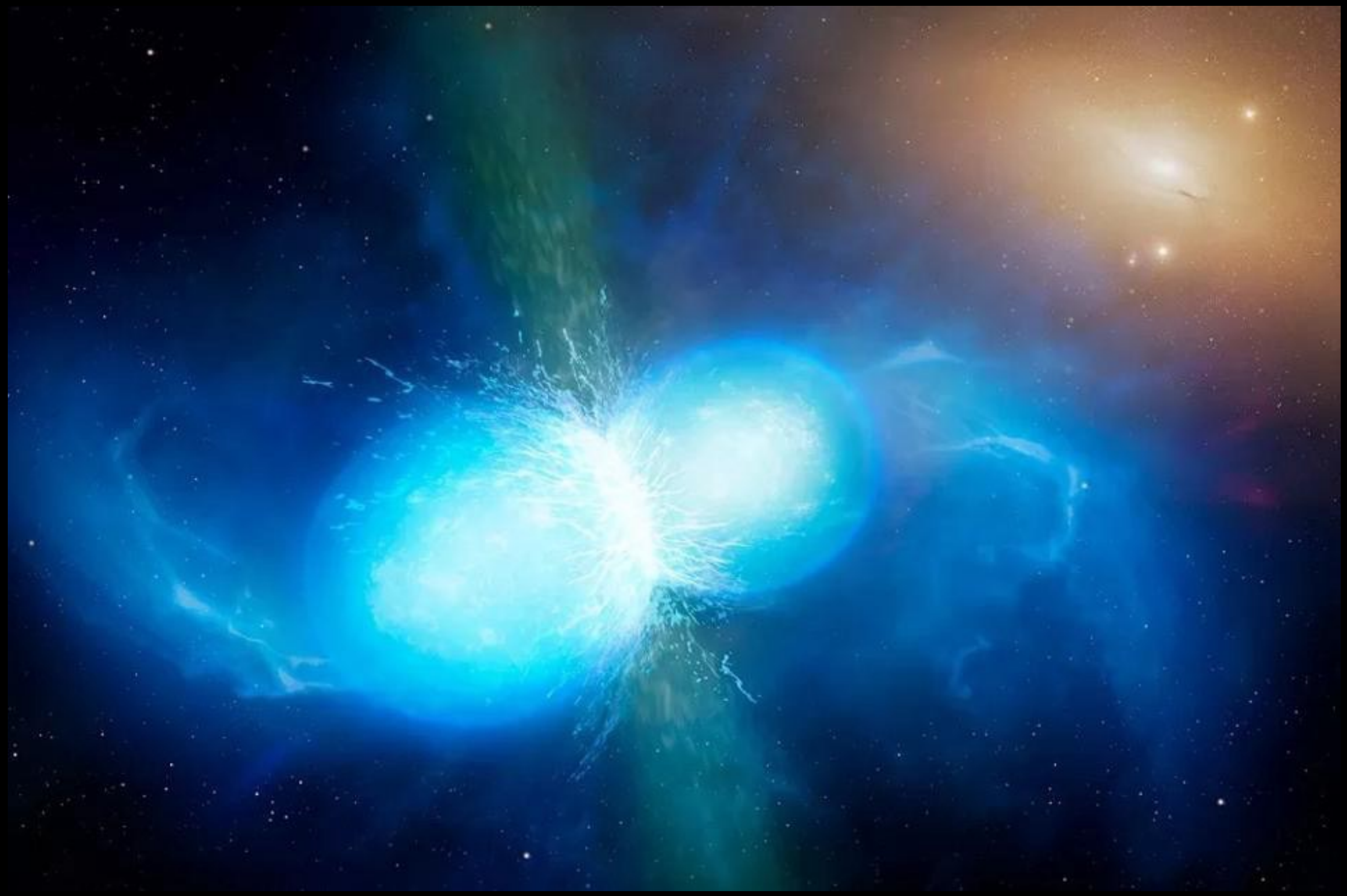
Y. Kondo et al., Nature **620**, 965 (2023)

cf. talk by A. Obertelli

- ^{28}O found to be a **resonance**
- spread of theory predictions: phenomenology, ab initio **with different interactions**, methods with and without **continuum**, potential **deformation** effects, …

How Were the Elements Made?





Core-Collapse Supernovae **Neutron-Star Mergers**

Multi-physics problem that requires microscopic inputs

- **Equation of state (EOS)** of strongly interacting matter
  - including **supra-nuclear** densities (exotic matter)
- **Neutrino interactions**

Physics Beyond the Standard Model

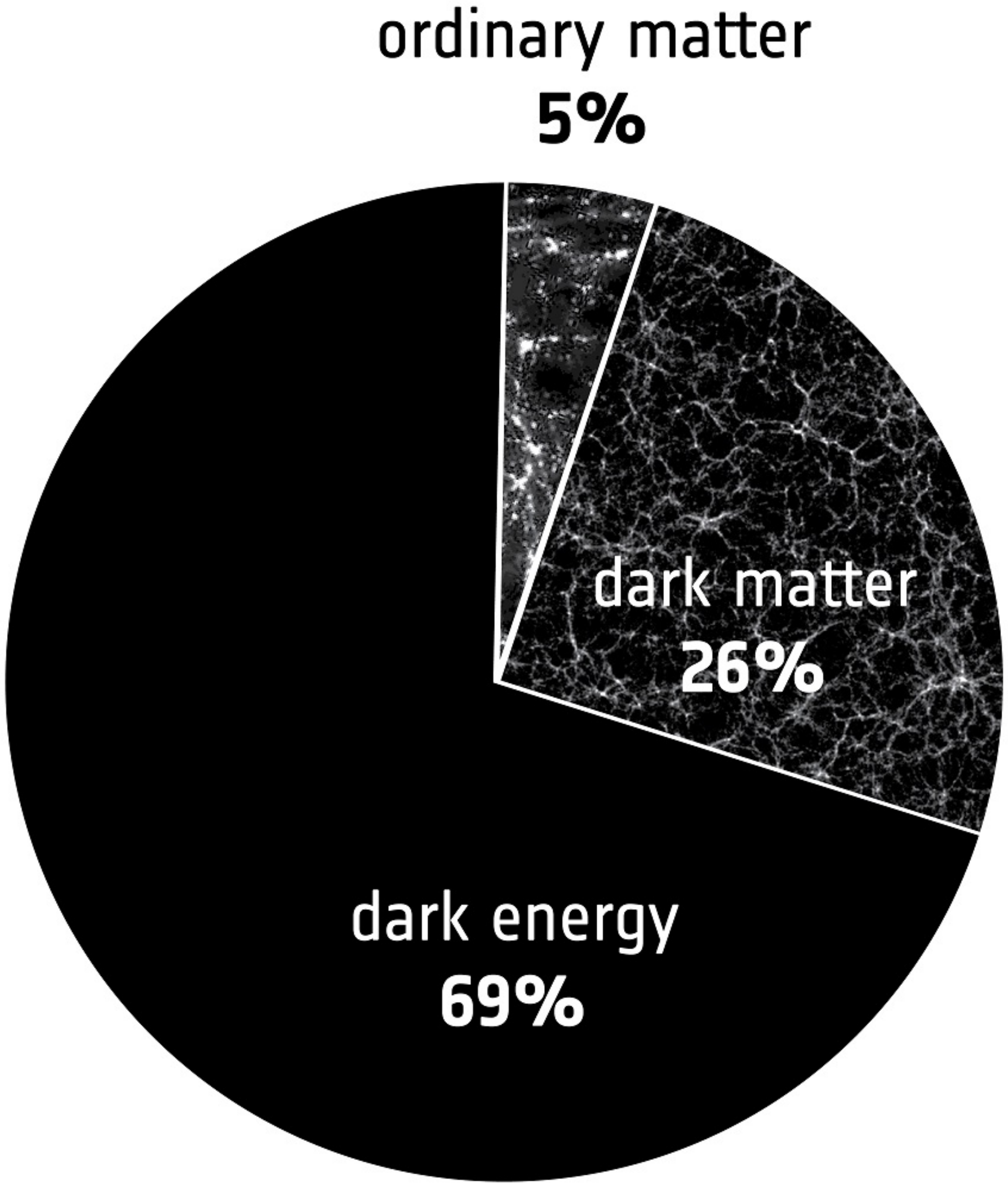
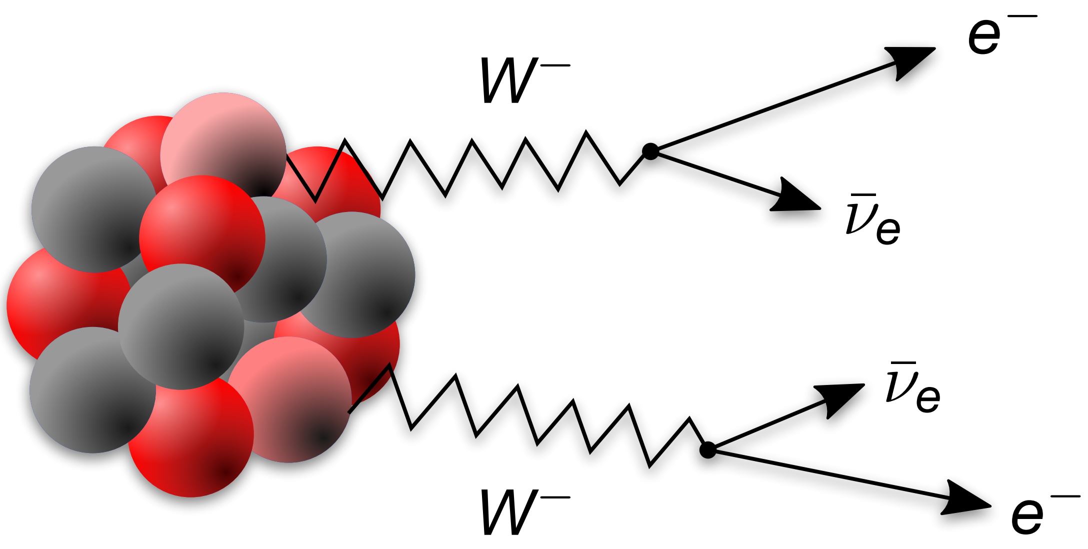


image credit: ESA
https://sci.esa.int/web/euclid/-/42267-science
[EUCLID expected to launch on July 1, 2023]

- Standard Model does **not contain** **dark matter or dark energy**
- SM neutrinos are massless, but **neutrino flavor oscillations** that require mass have been **confirmed experimentally**
- SM does not explain observed **matter-antimatter asymmetry** (**insufficient CP symmetry violation**)

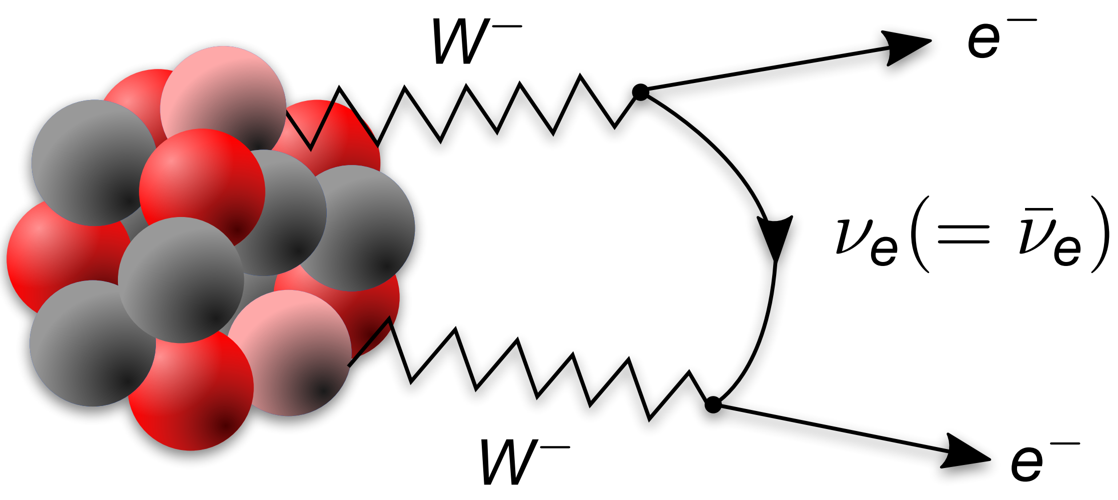
Physics Beyond the Standard Model

“Standard” Double Beta Decay



- neutrinos are **Dirac** particles
- Standard Model valid

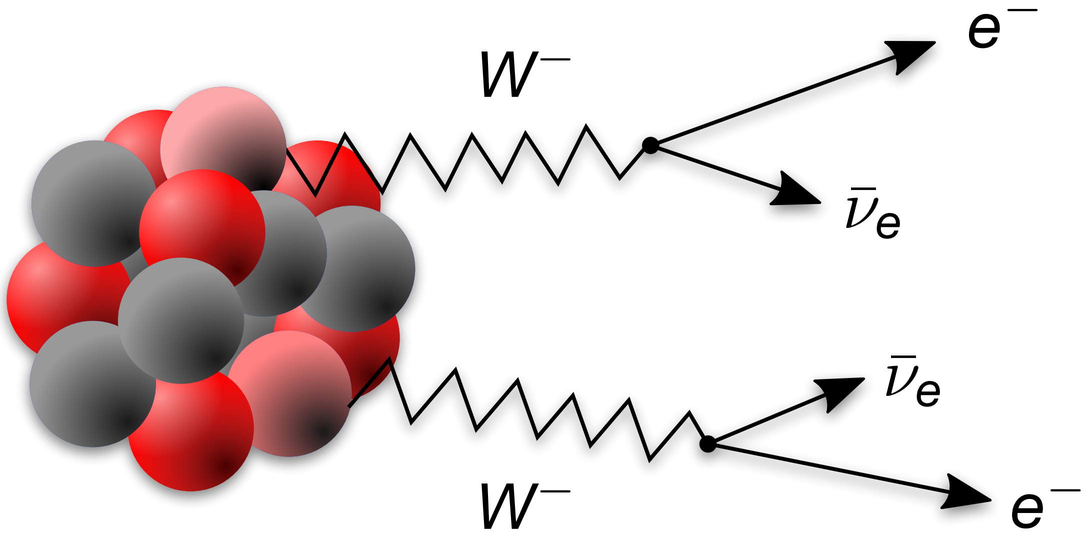
Neutrinoless Double Beta Decay



- neutrinos are **Majorana** particles
- beyond Standard Model: **new physics**

Physics Beyond the Standard Model

“Standard” Double Beta Decay



- neutrinos are **Dirac** particles
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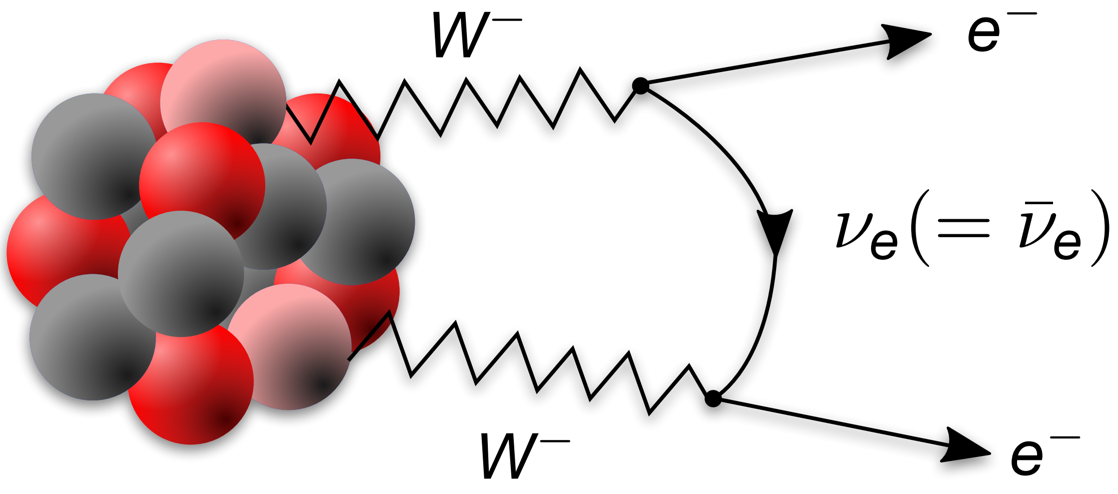
Neutrinoless Double Beta Decay



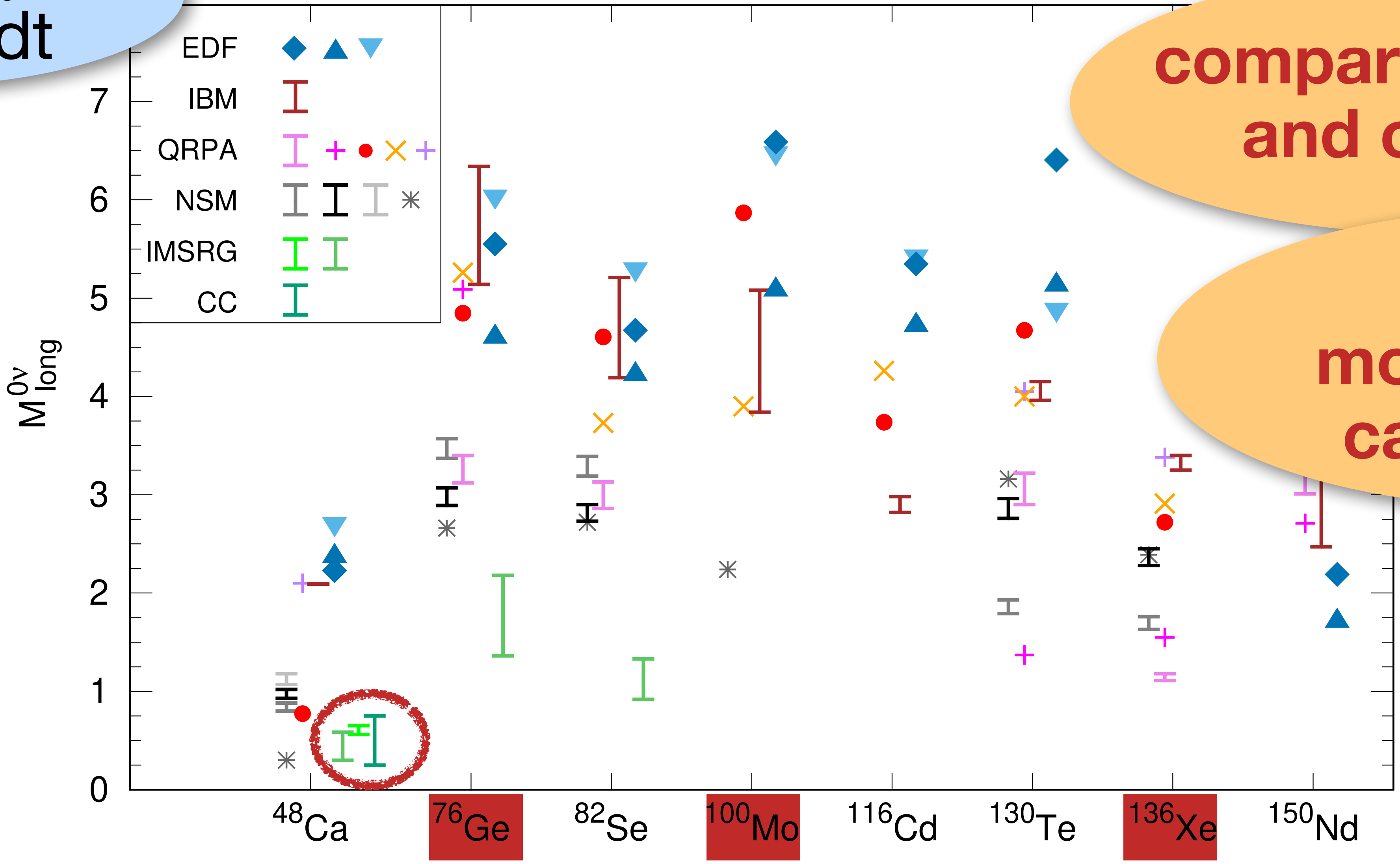
- neutrinos are **Majorana** particles

yields **absolute neutrino mass scale** if we can compute **nuclear matrix elements** accurately

Nuclear Matrix Elements

M. Agostini et al., RMP **95**, 025002 (2023)

cf. talk by B. Schmidt



comparing apples and oranges

need more *ab initio* calculations

- inputs tailored to specific methods: phenomenological EDFs, Shell Model interactions, …
- quenched g_A, “renormalization” of operators, etc.

CP Violation and EDMs

- need **BSM CP violation** to explain **matter-antimatter asymmetry -** e.g., CP-violating πNN vertex in (chiral) EFT
- induces neutron EDM and nuclear EDMs via a (P)T-violating interaction V_{PT}
- Probed by **screened dipole** (=**Schiff**) **moment**

$$\langle S_z\rangle = \sum_k \frac{\langle 0|S_z|k\rangle\langle k|V_{PT}|0\rangle}{E_0 - E_k} + \mathrm{c.c.}$$

- enhanced by **large deformation** and **small energy denominator** - e.g., parity doublet of $\frac{1}{2}^+$ ground state and $\frac{1}{2}^-$ excited state in ^{225}Ra

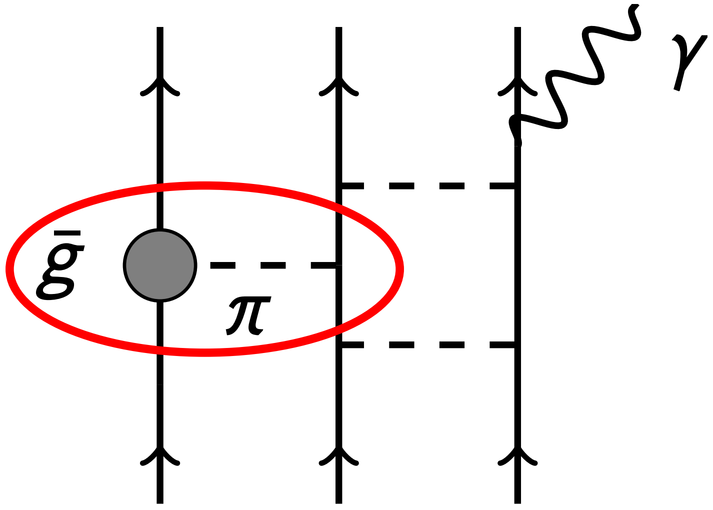


image credit: J. Engel

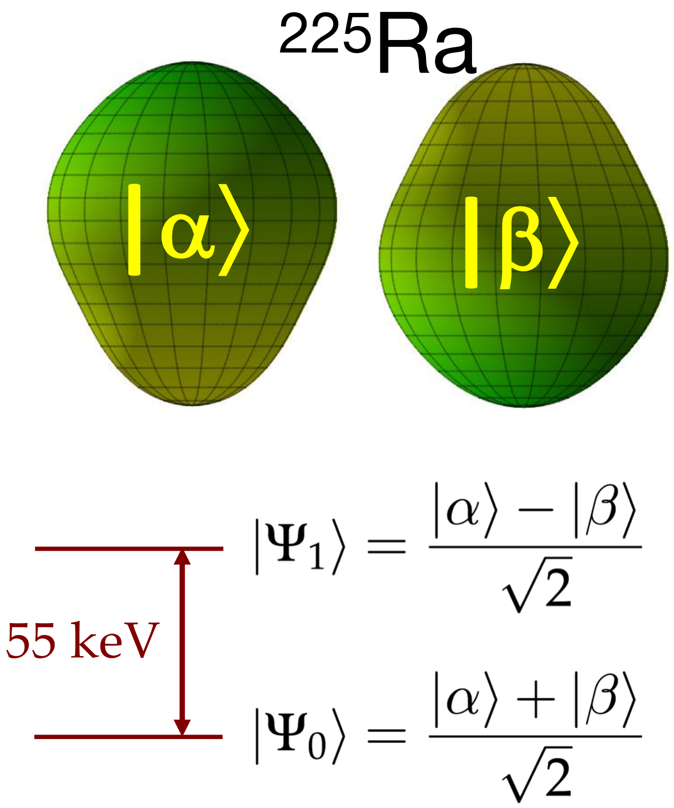


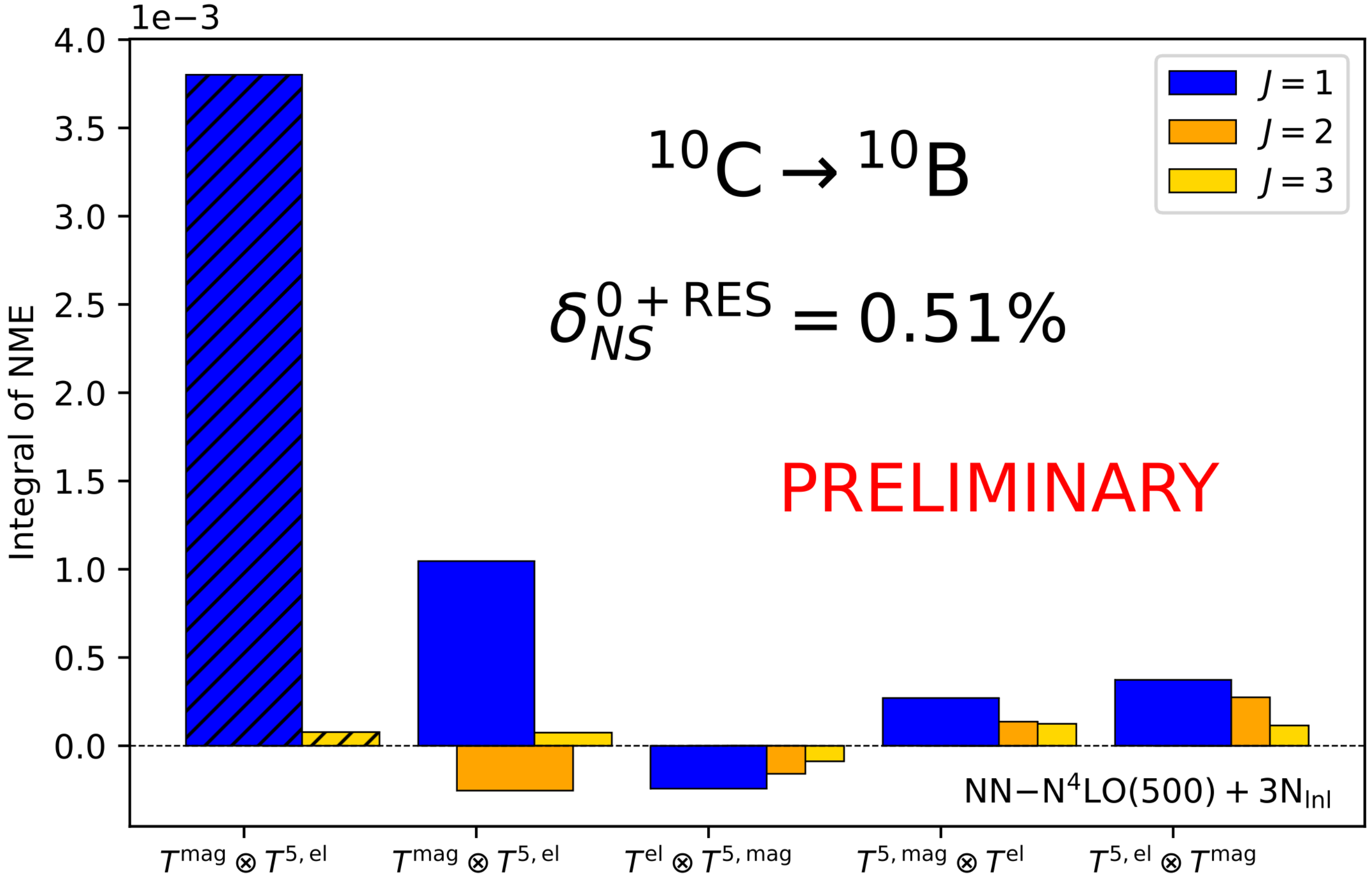
image credit: J. Singh

CKM Unitarity and Beta Decays

- new insights from ***ab initio* analysis of radiative corrections** to (super allowed) beta decays

- e.g., **No-Core Shell Model with Continuum** calculations of δ_{NS}, δ_C in ^{10}C

- Towner & Hardy used $\delta_{NS} = -0.40\,\%$



Gennari, Navratil, in progress

cf. talk by
P. Plattner

NTNP Topical Collaboration

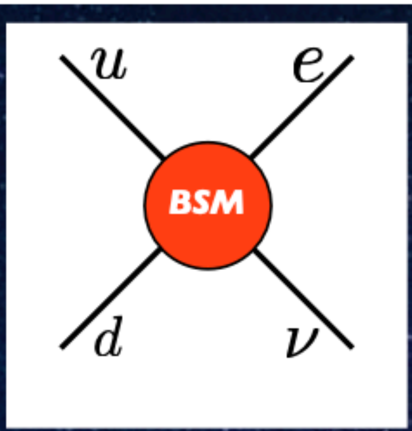
Nuclear Theory for New Physics
co-chairs: *Vincenzo Cirigliano & Saori Pastore*

DEI Coordinator: *Maria Piarulli*

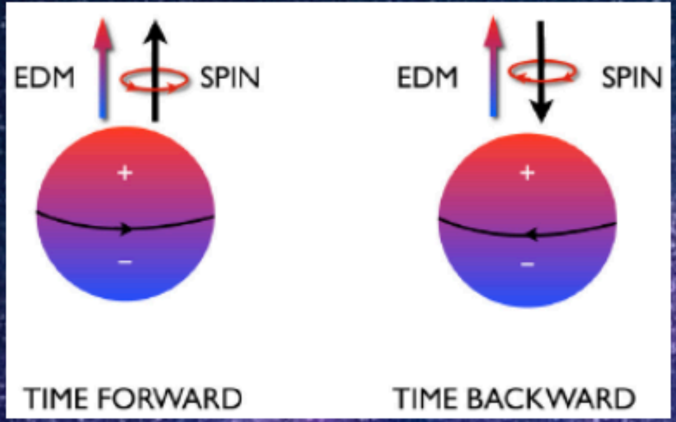
Lattice QCD
Coordinator:
Andre' Walker-Loud

EFT / phenomenology
Coordinator:
Emanuele Mereghetti

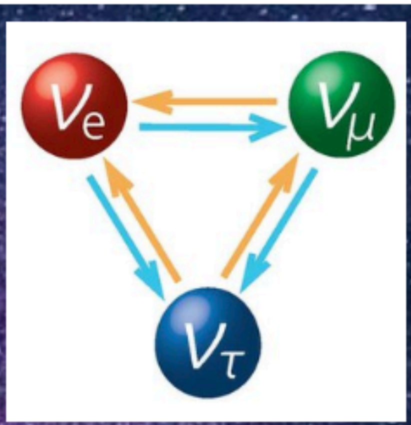
Nuclear Structure
Coordinator:
Heiko Hergert



β decays and new particles



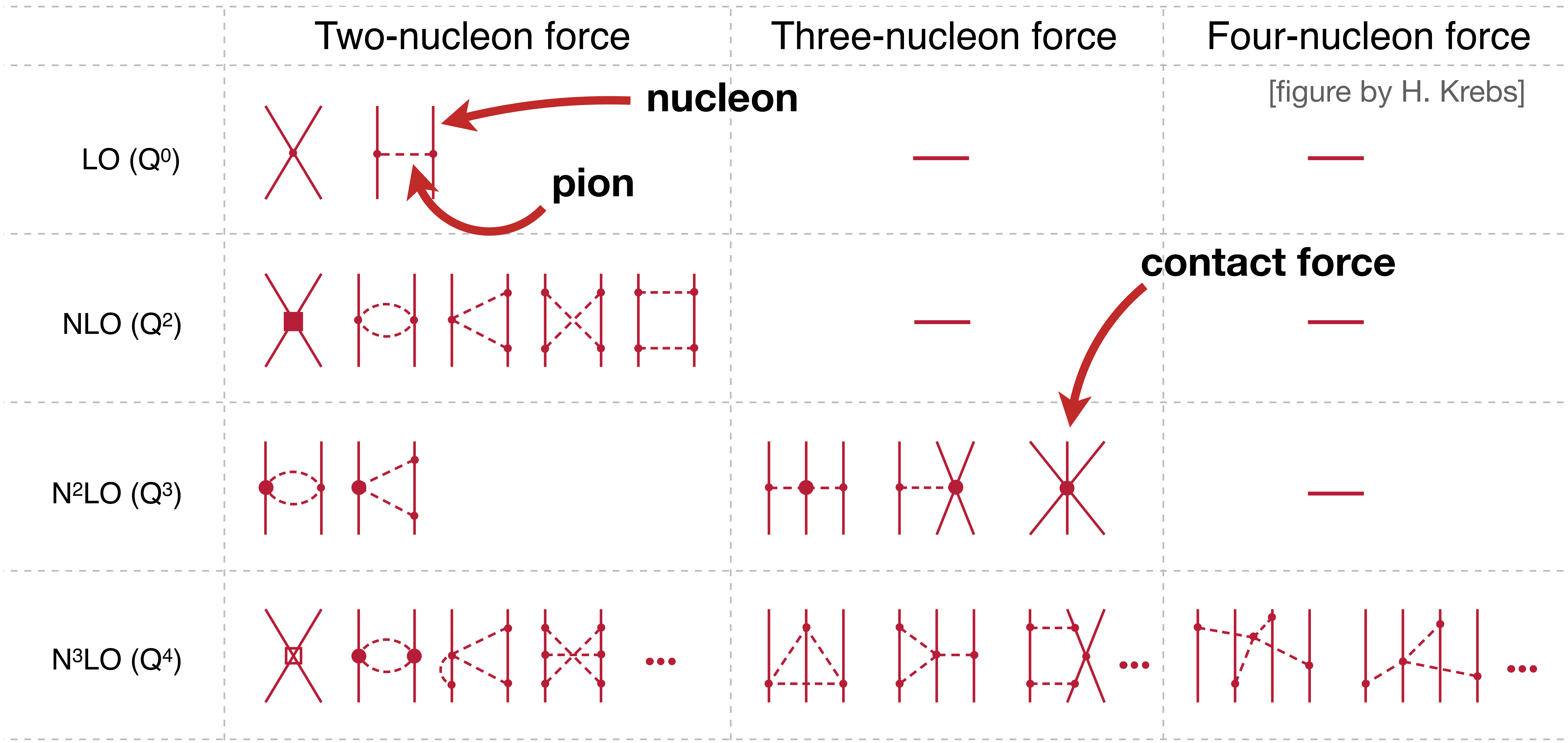
T & CP violation and the Origin of Matter



Neutrino properties & CP violation

Where Do We Start?

Chiral Effective Field Theory



- 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 & transition operators

Renormalization

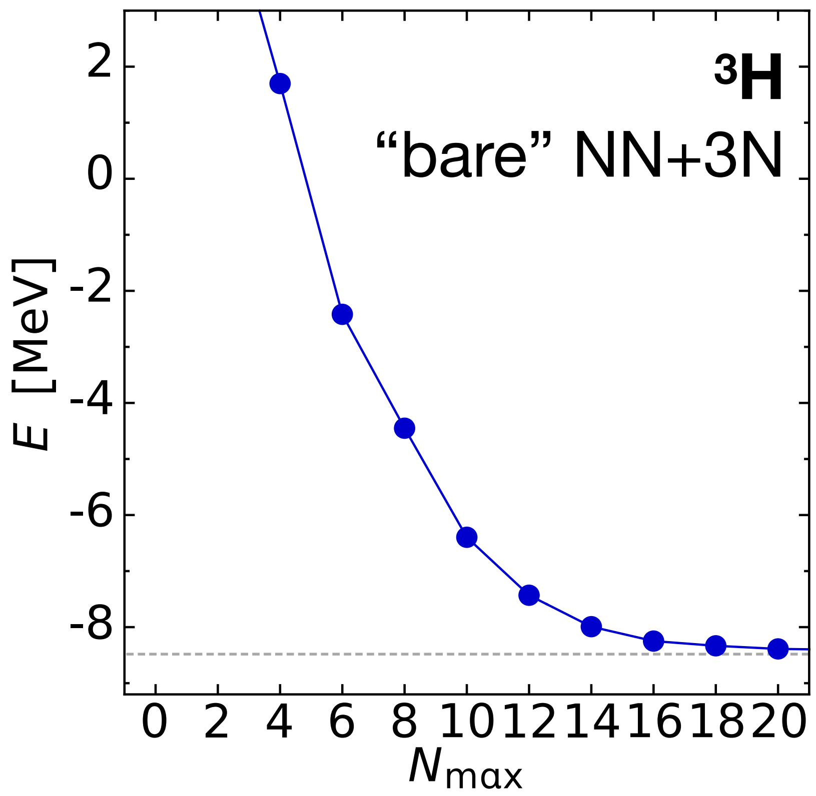
- tune **resolution scale** of a **theory** in **systematic fashion** with **Renormalization Group** methods

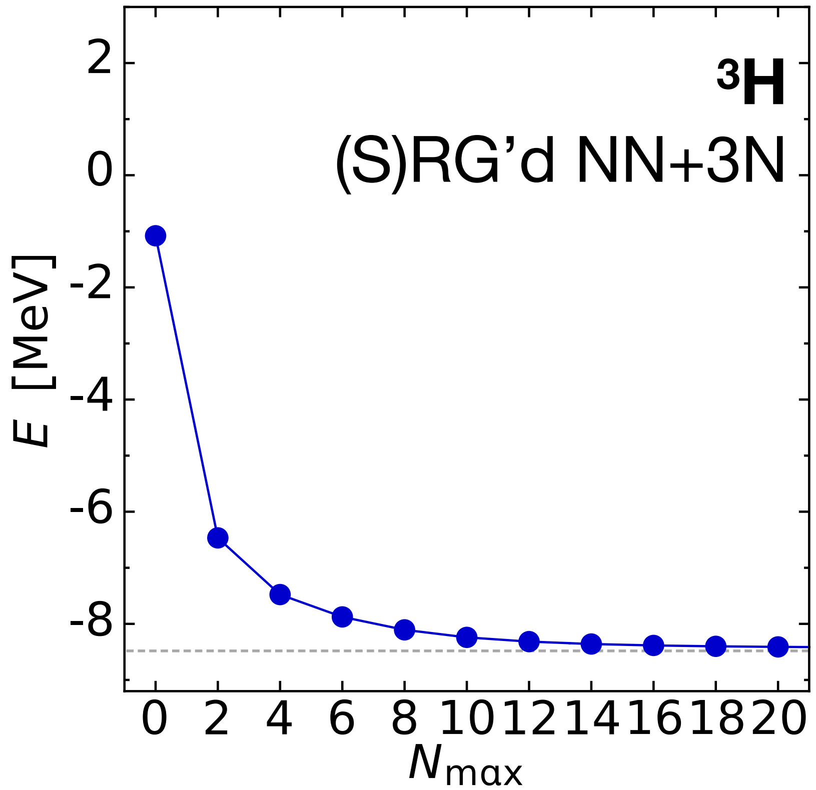
- **conserve relevant information** in low-resolution theory

- renormalization reduces effort by **orders of magnitude**, allows our methods to **reach heavier nuclei**

  - **example:** ^{3}H ground-state energy from exact diagonalization

- **must be applied consistently to all observables**

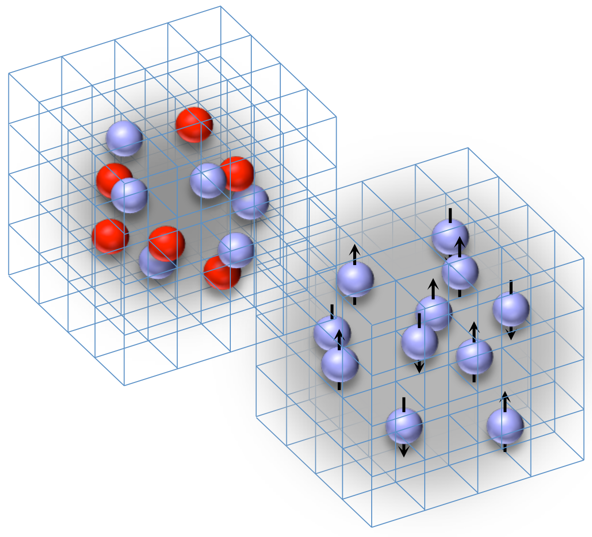




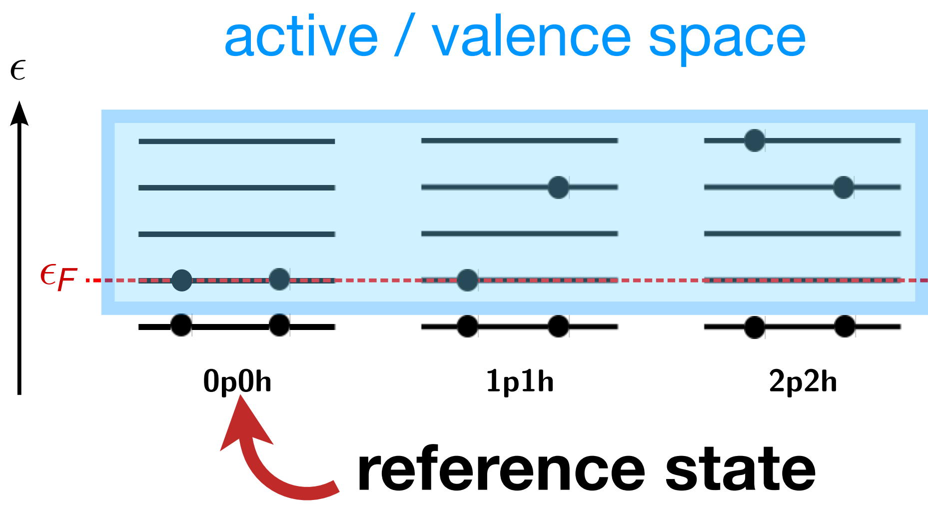
Many Roads Lead to Rome

Paradigms

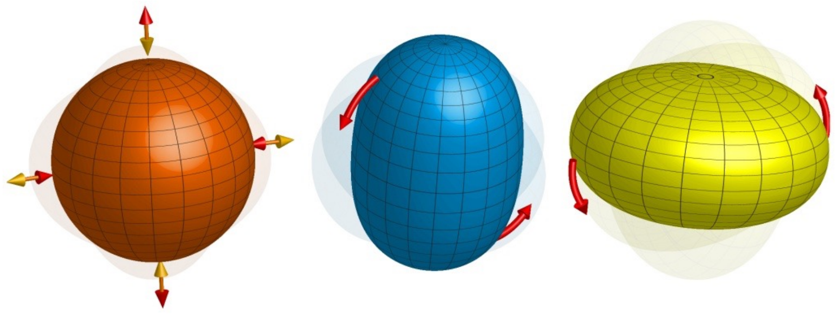
- **Coordinate Space**
  - Quantum Monte Carlo
  - Lattice EFT



- **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)

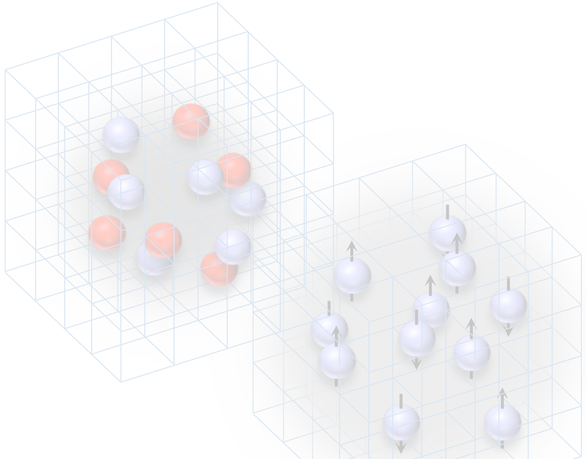


- **Configuration Space / Coordinate Space: Geometric Expansions**
  - deformed HF(B) + projection
  - projected Generator Coordinate Method (PGCM)
  - symmetry-adapted NCSM



Paradigms

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

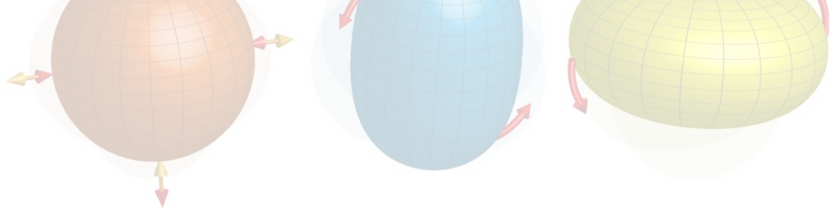


- **Configuration Space: Particle-Hole Expansions**

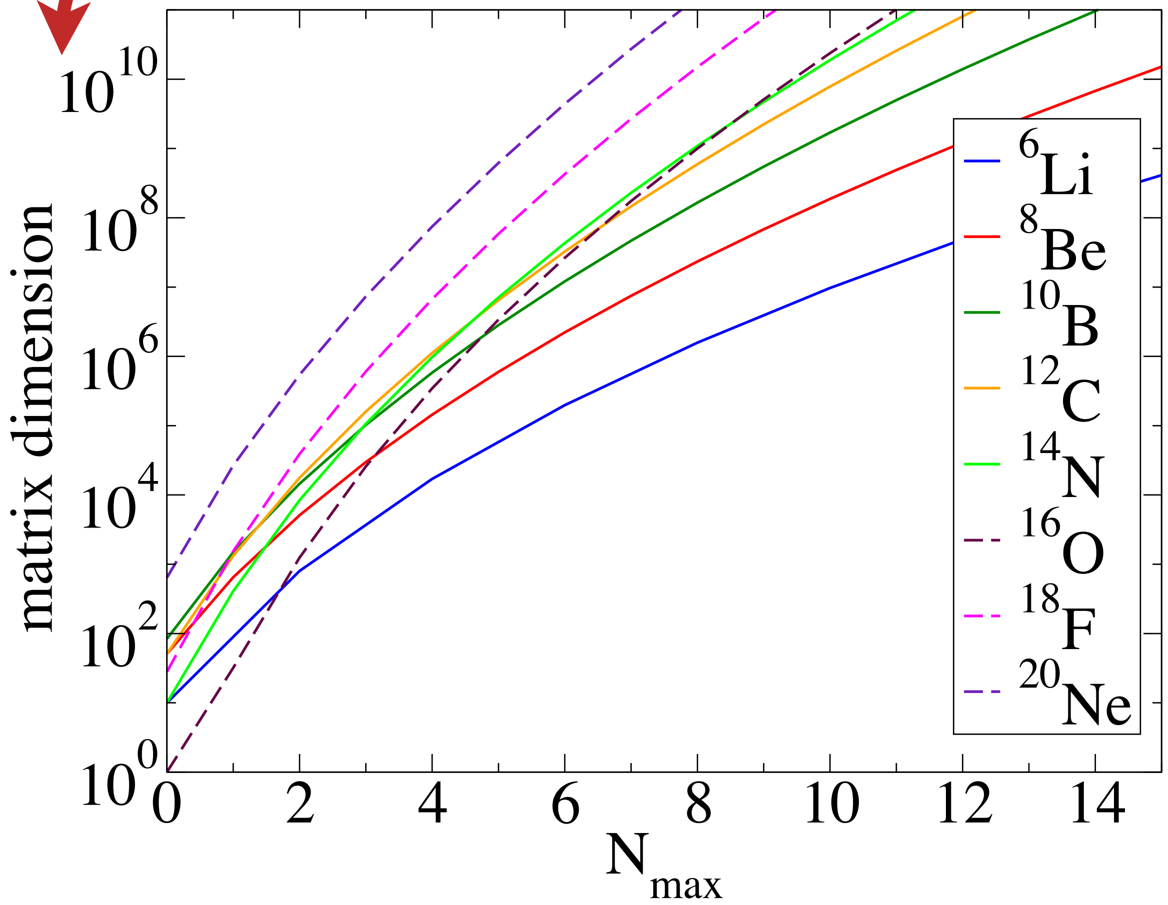
Recent(-ish) Reviews:
HH, Front. Phys. **8**, 379 (2020)
S. Gandolfi, D. Lonardoni, A. Lovato and M. Piarulli, Front. Phys. **8**, 117 (2020)
D. Lee, Front. Phys. **8**, 174 (2020)
V. Somà, Front. Phys. **8**, 340 (2020)

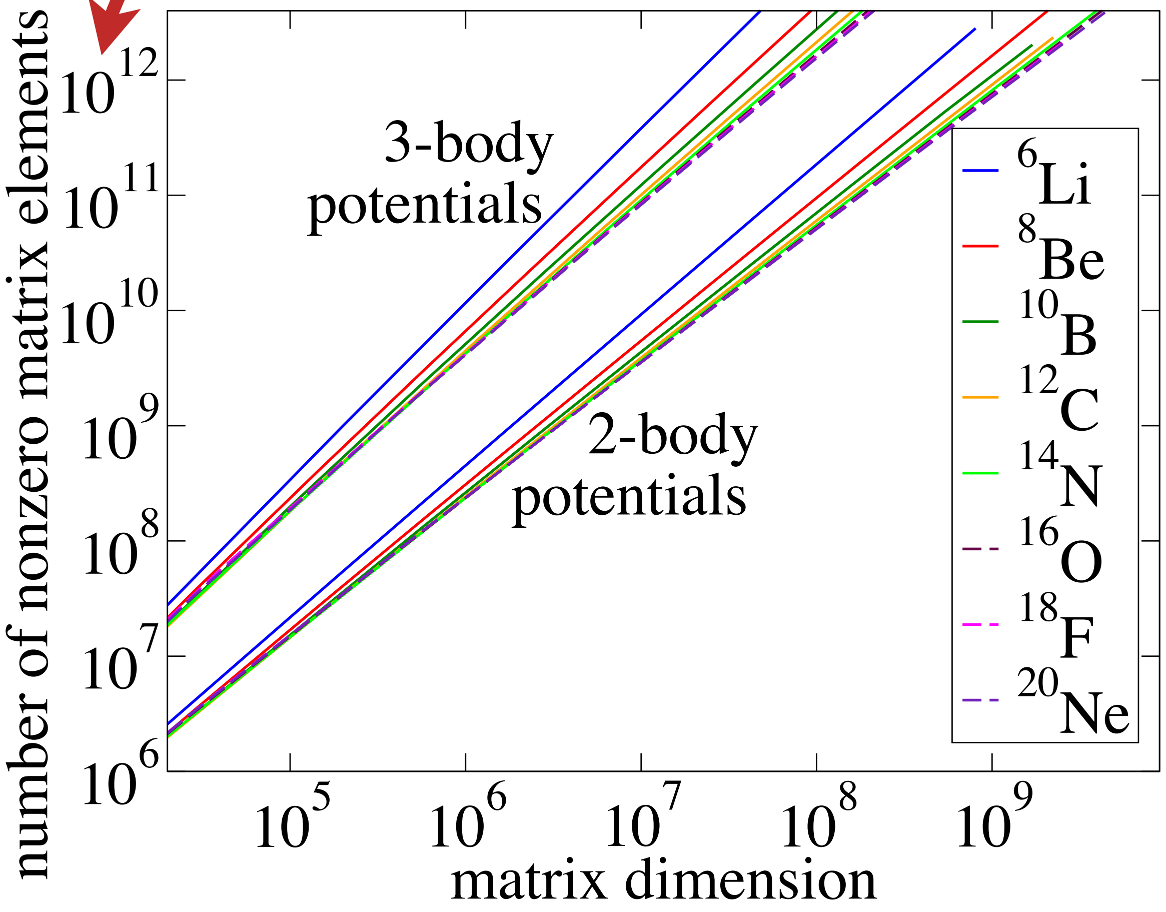
also see
“What is *ab initio* in nuclear theory?”, A. Ekström, C. Forssén, G. Hagen, G. R. Jansen, W. Jiang, T. Papenbrock, arXiv:2212.11064

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



Basis Size “Explosion”

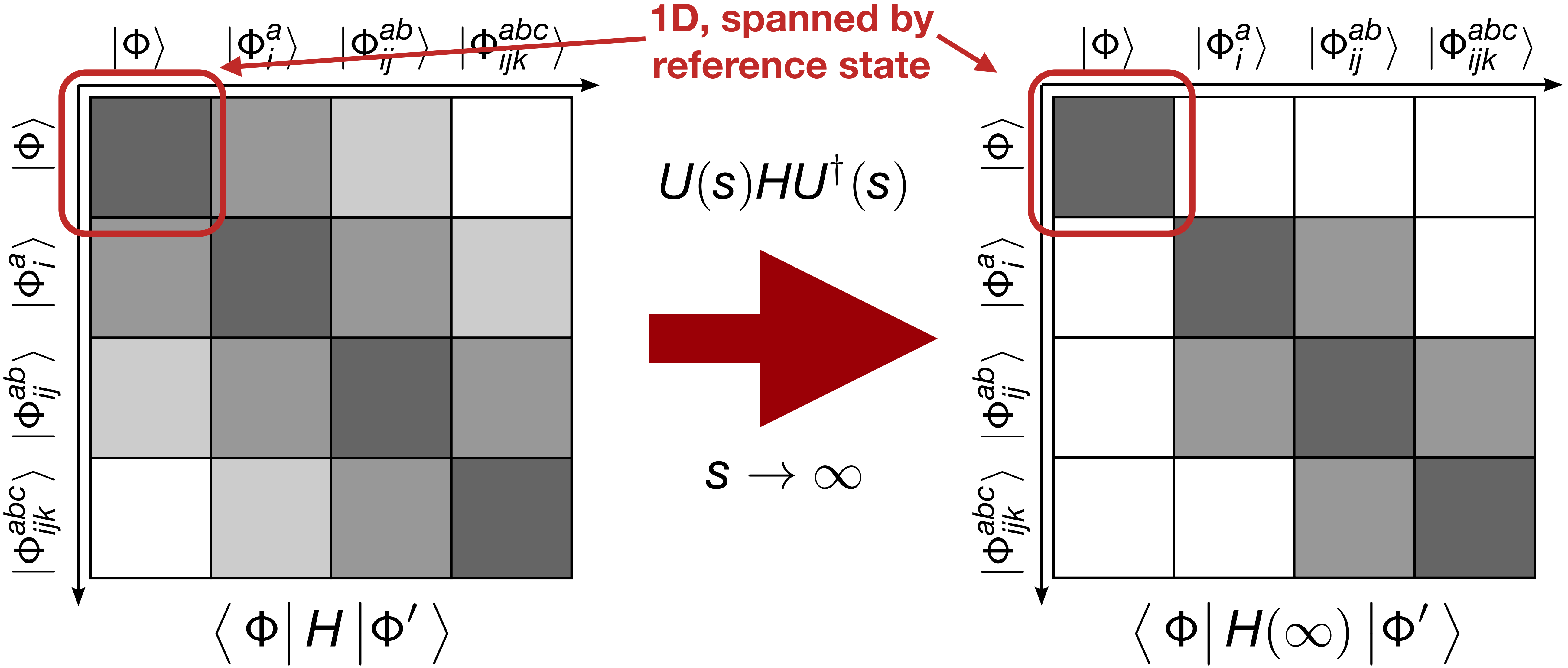

75 GB per vector


7.5 TB

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

- **constructing and storing full *H* matrix is impossible**
- exploit **matrix sparseness**, but problem is still **hard**

Decoupling in A-Body Space



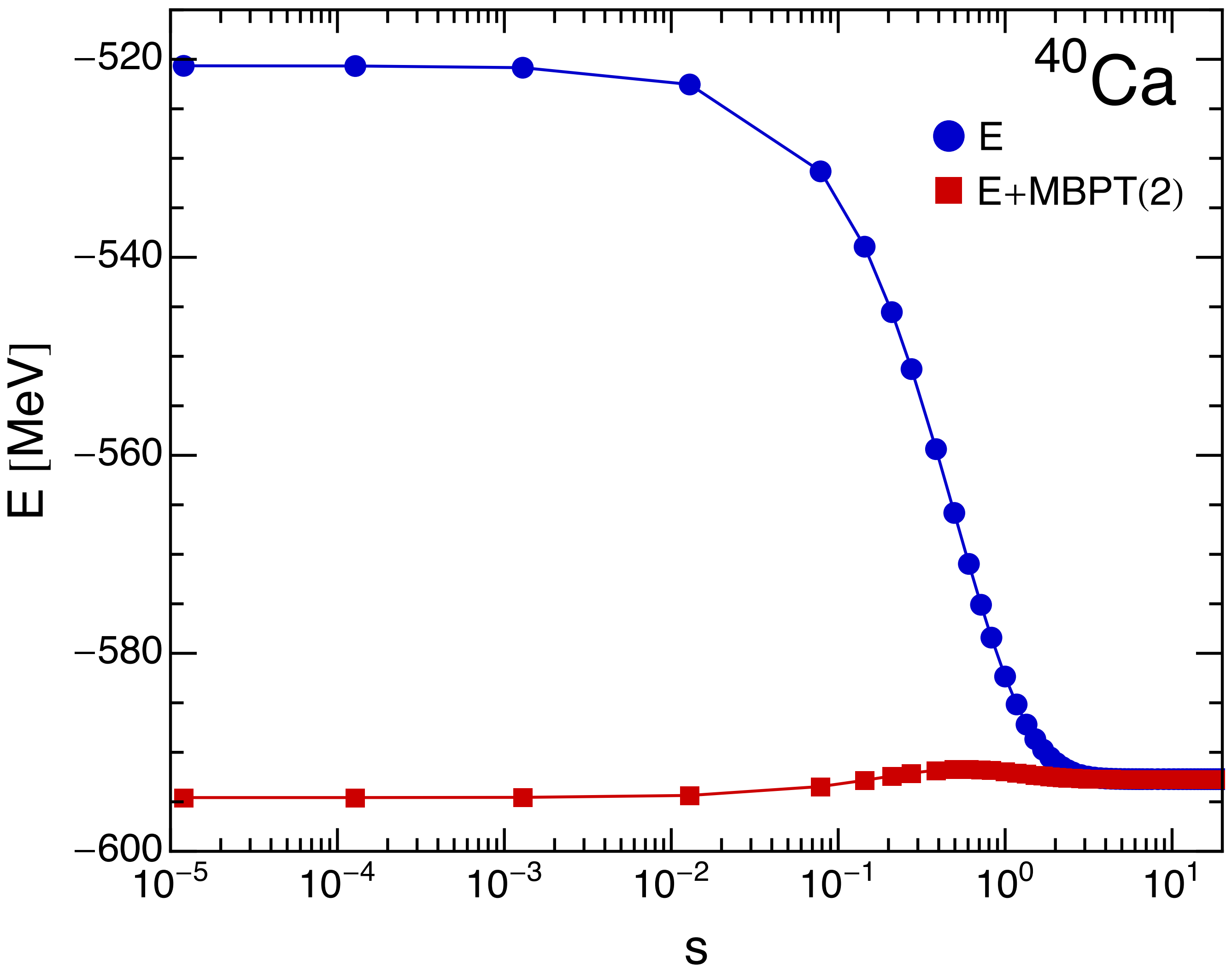
1D, spanned by reference state

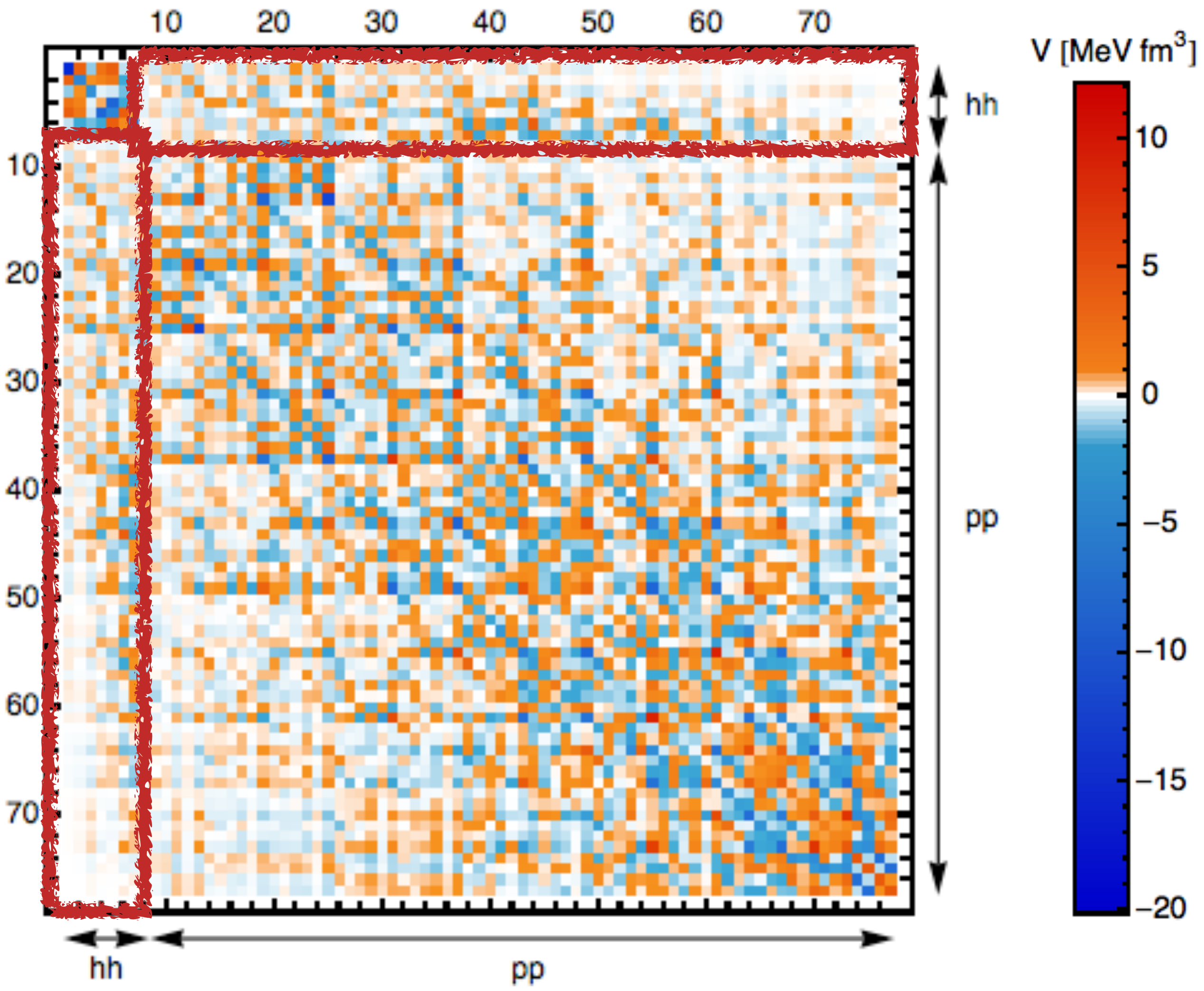
$$U(s)HU^\dagger(s)$$

$$s \to \infty$$

- **identify** the parts of the **operator *H*** which **couple reference state to excitations**
- **eliminate** them with SRG (or other similarity transformations)
- **efficient: polynomial scaling,** no need to construct matrix !

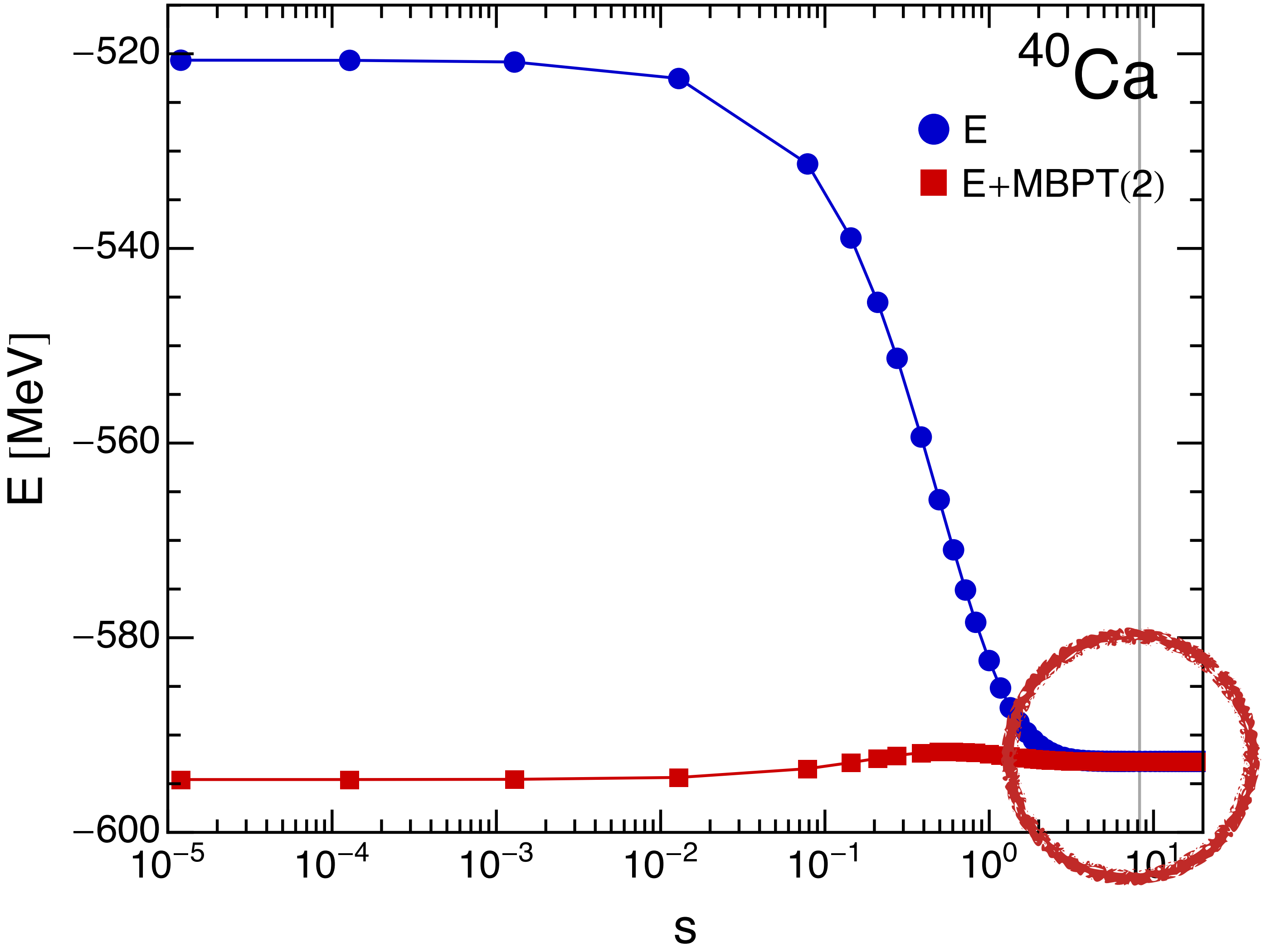
Decoupling

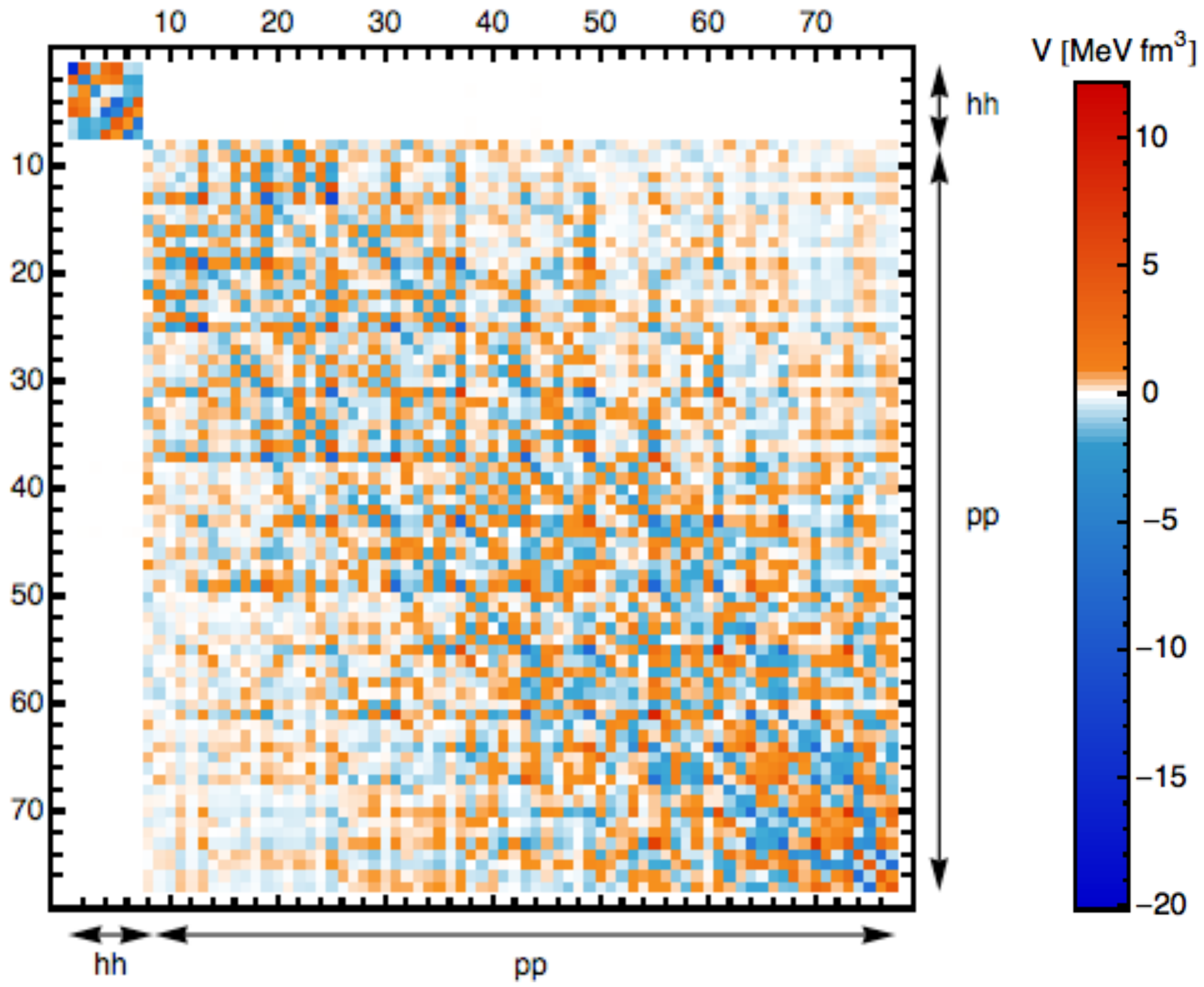




$$\text{N3LO}, \lambda = 2.0\ \text{fm}^{-1}, e_{\text{Max}} = 8$$

Decoupling



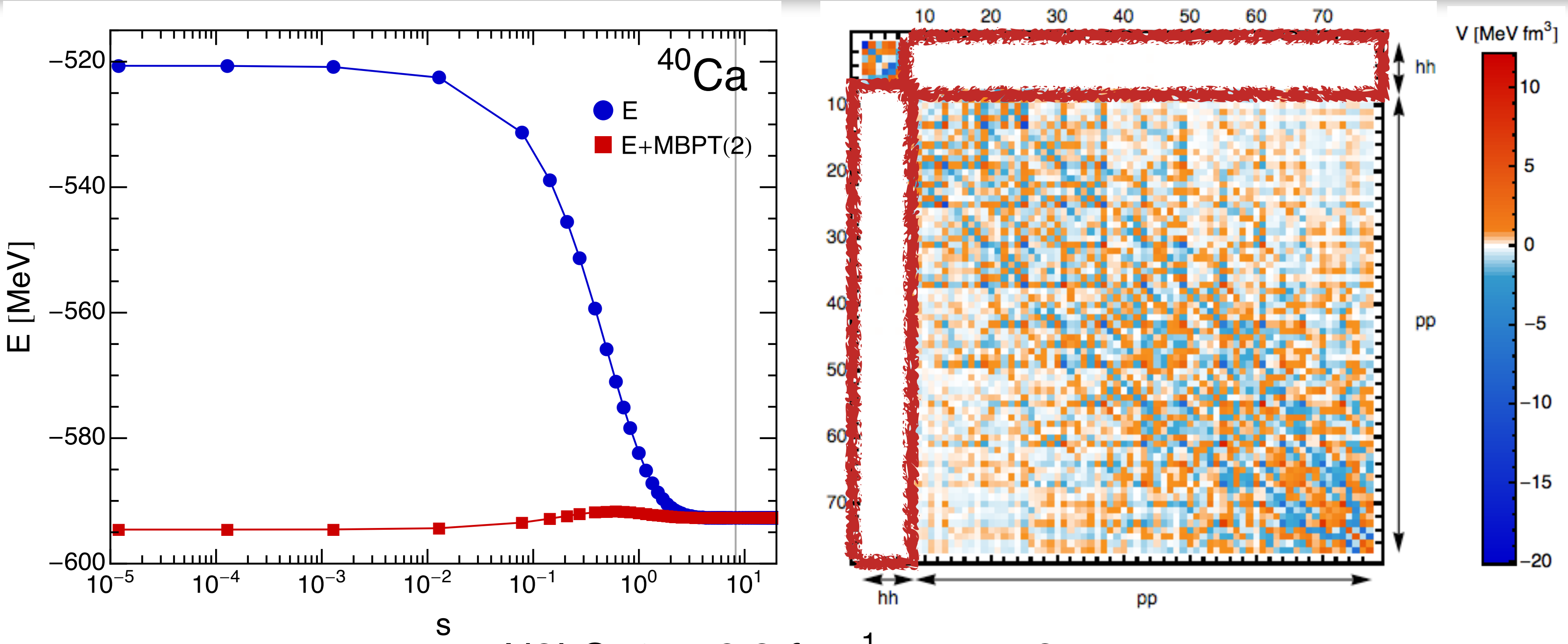


N3LO, $\lambda = 2.0\ \mathrm{fm}^{-1}, e_{\mathrm{Max}} = 8$

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

off-diagonal couplings are rapidly driven to zero

Decoupling



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

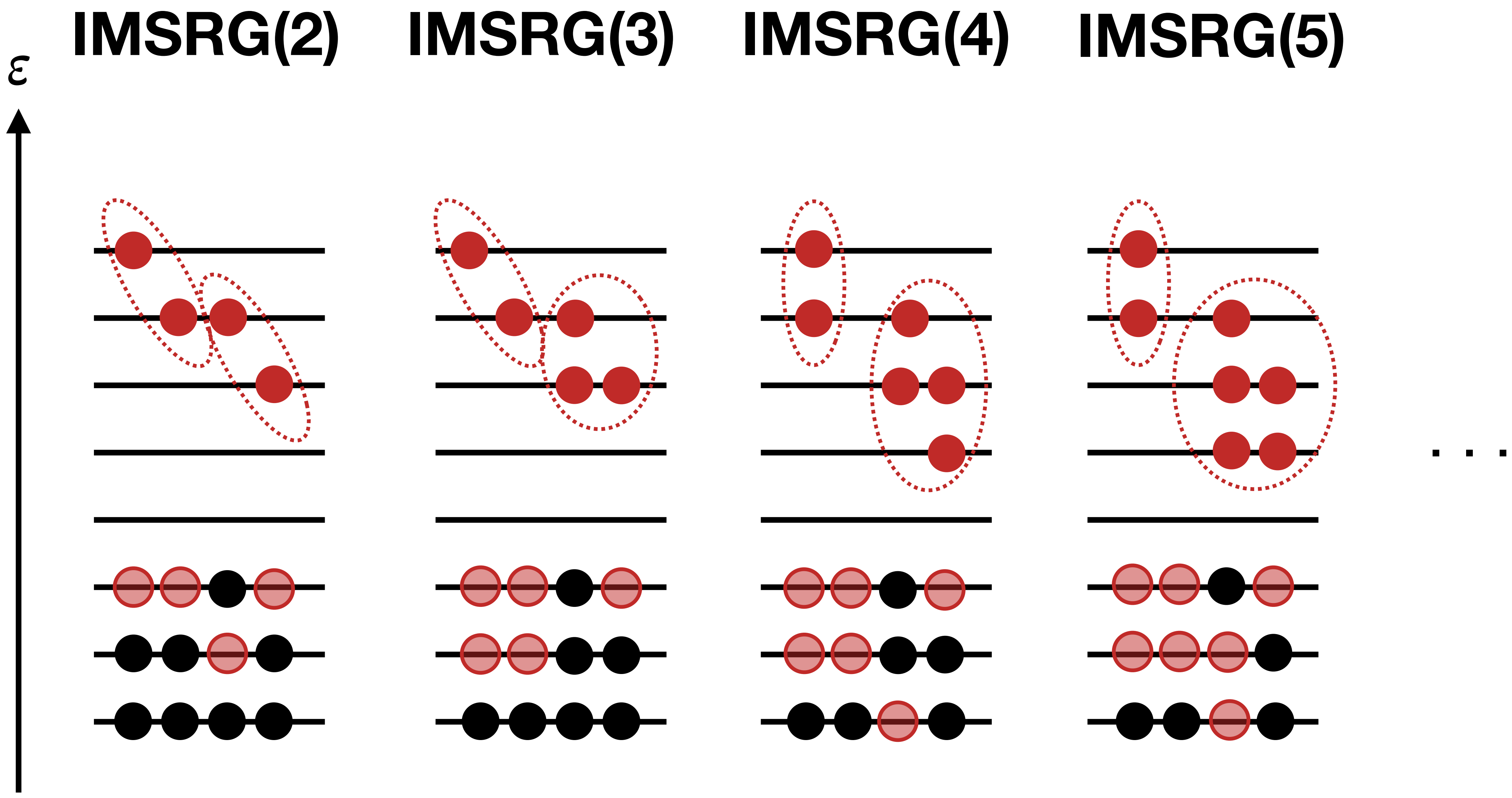
- absorb correlations into **RG-improved Hamiltonian**

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

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

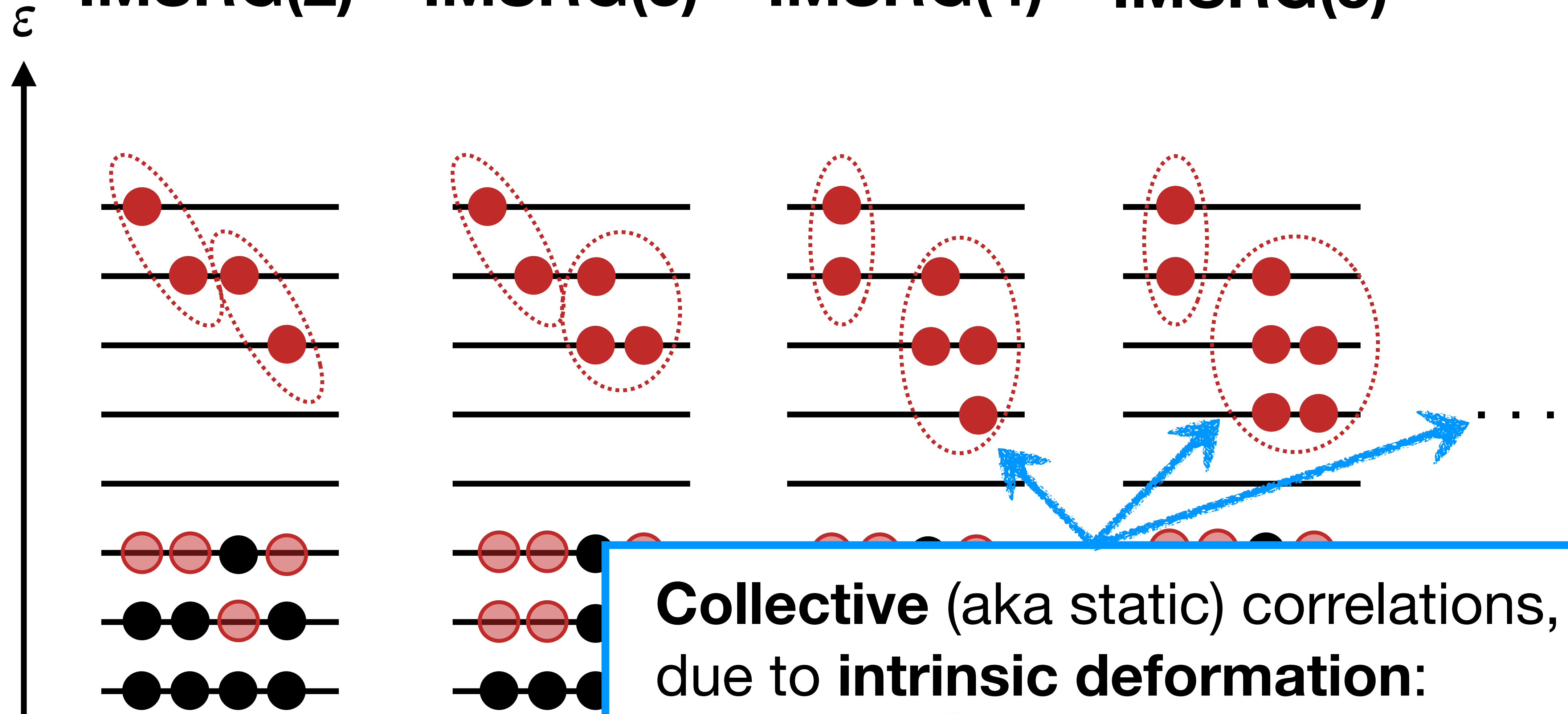
$$U(s)\left|\Psi_n\right\rangle \overset{!}{=} \left|\Phi\right\rangle$$

Correlated Reference States



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

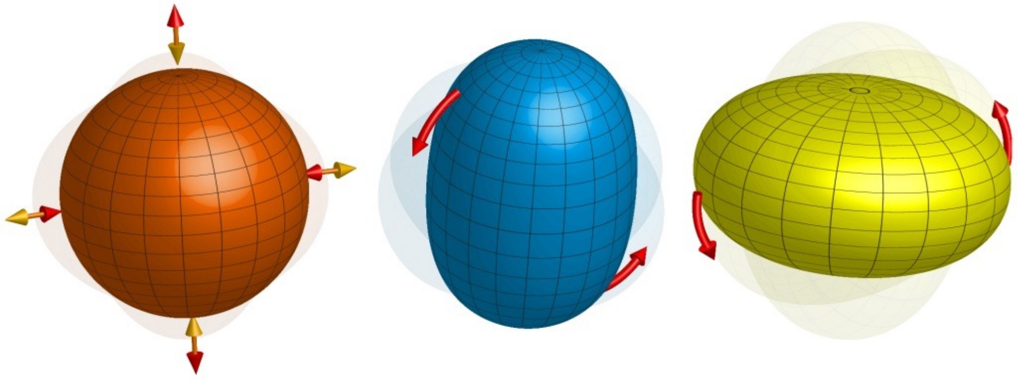
Correlated Reference States



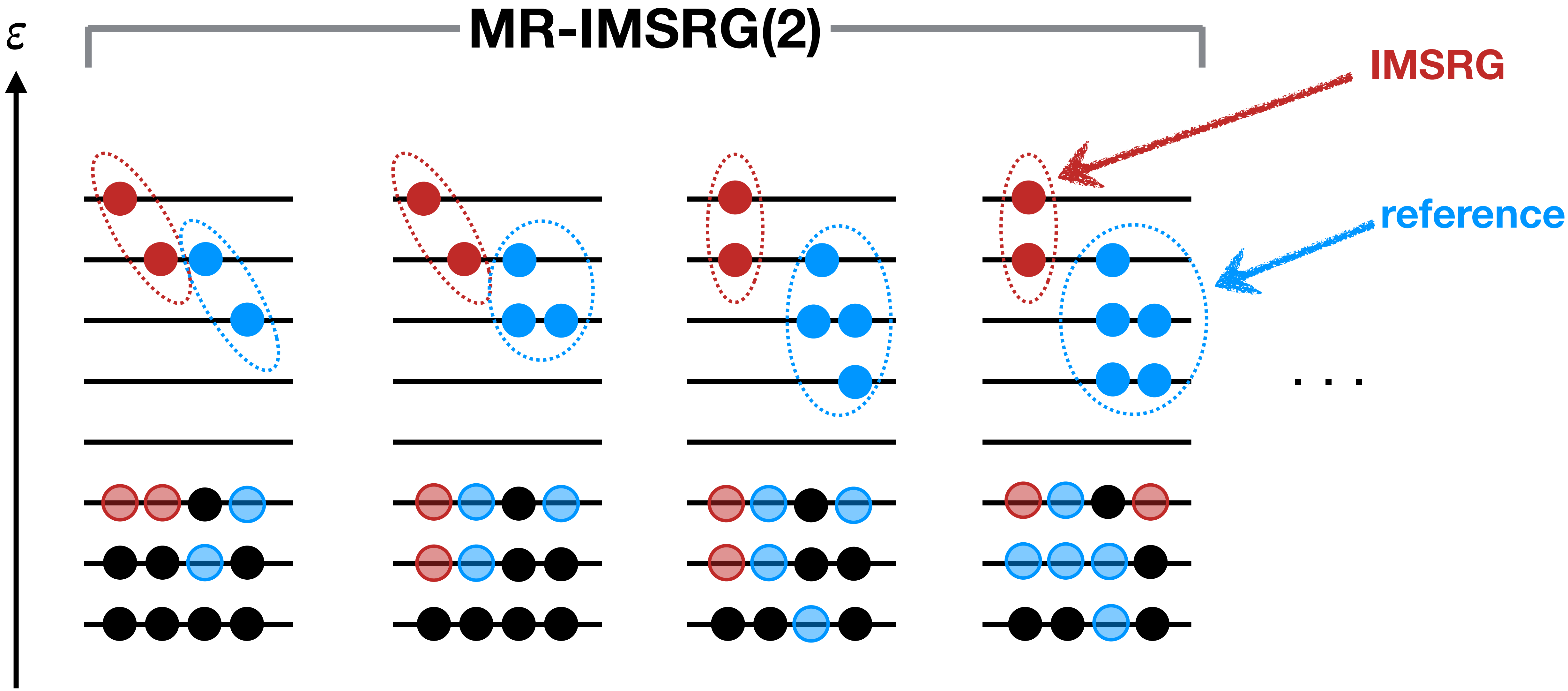
IMSRG(2) **IMSRG(3)** **IMSRG(4)** **IMSRG(5)**

“standard” IMS
Slater determinan

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

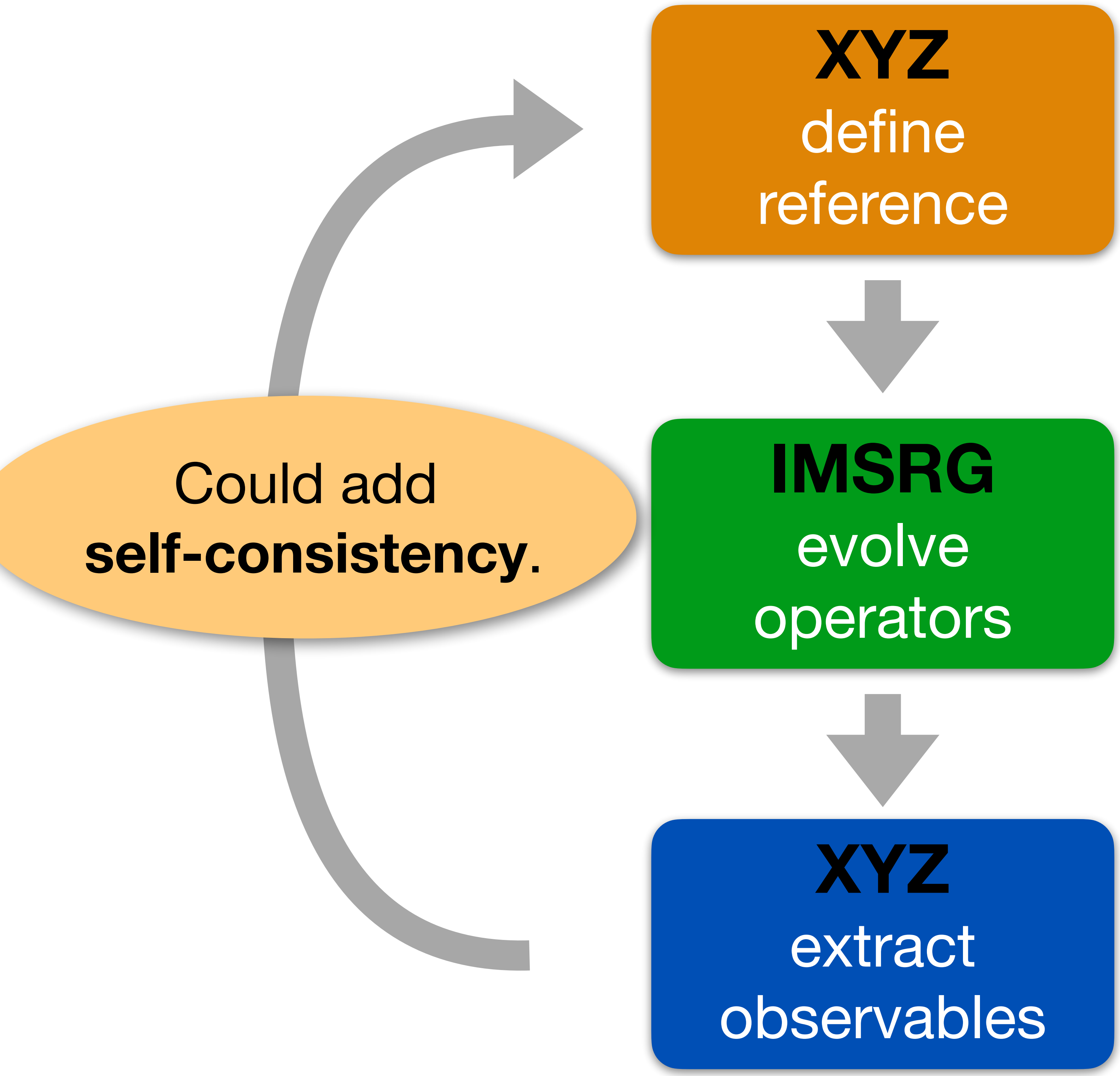


Correlated Reference States



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

IMSRG-Improved Methods



XYZ
define
reference

IMSRG
evolve
operators

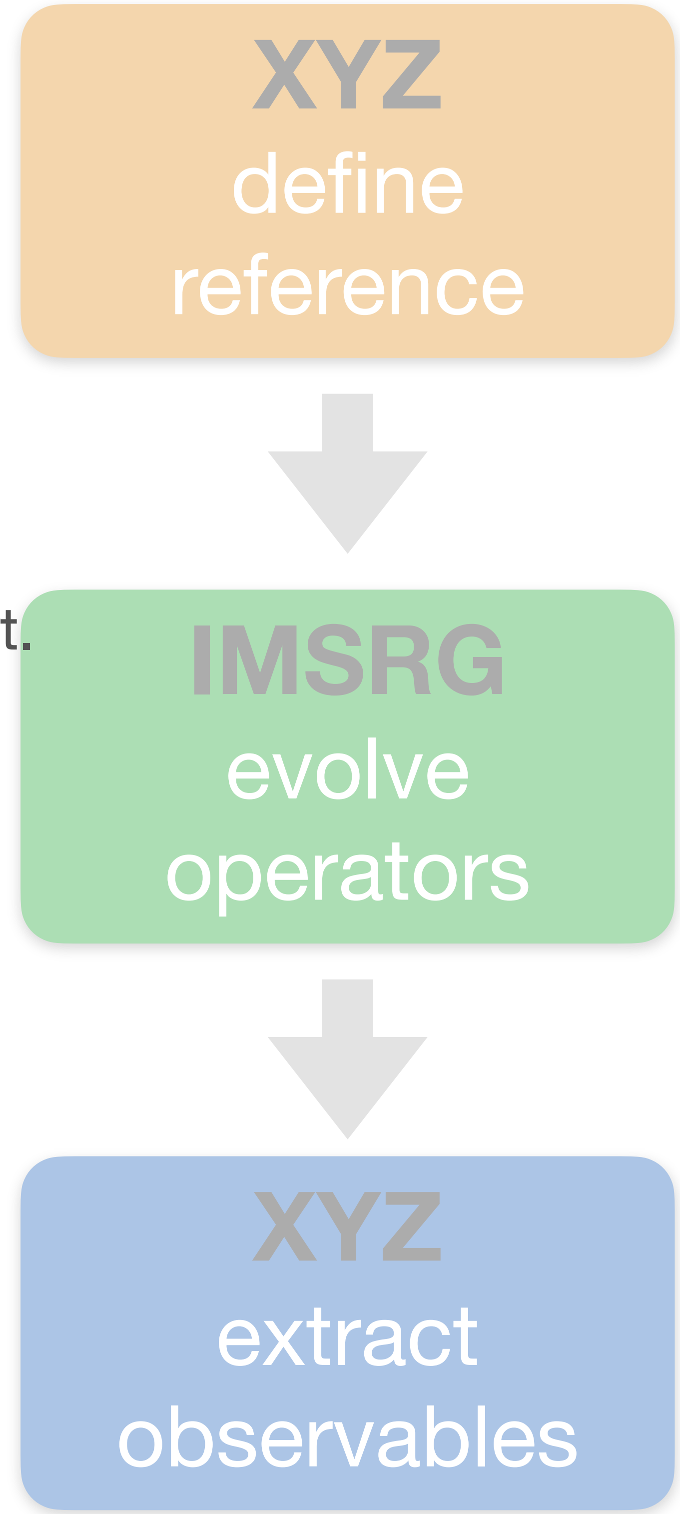
XYZ
extract
observables

Could add
self-consistency.

* 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)



XYZ
define reference

IMSRG
evolve operators

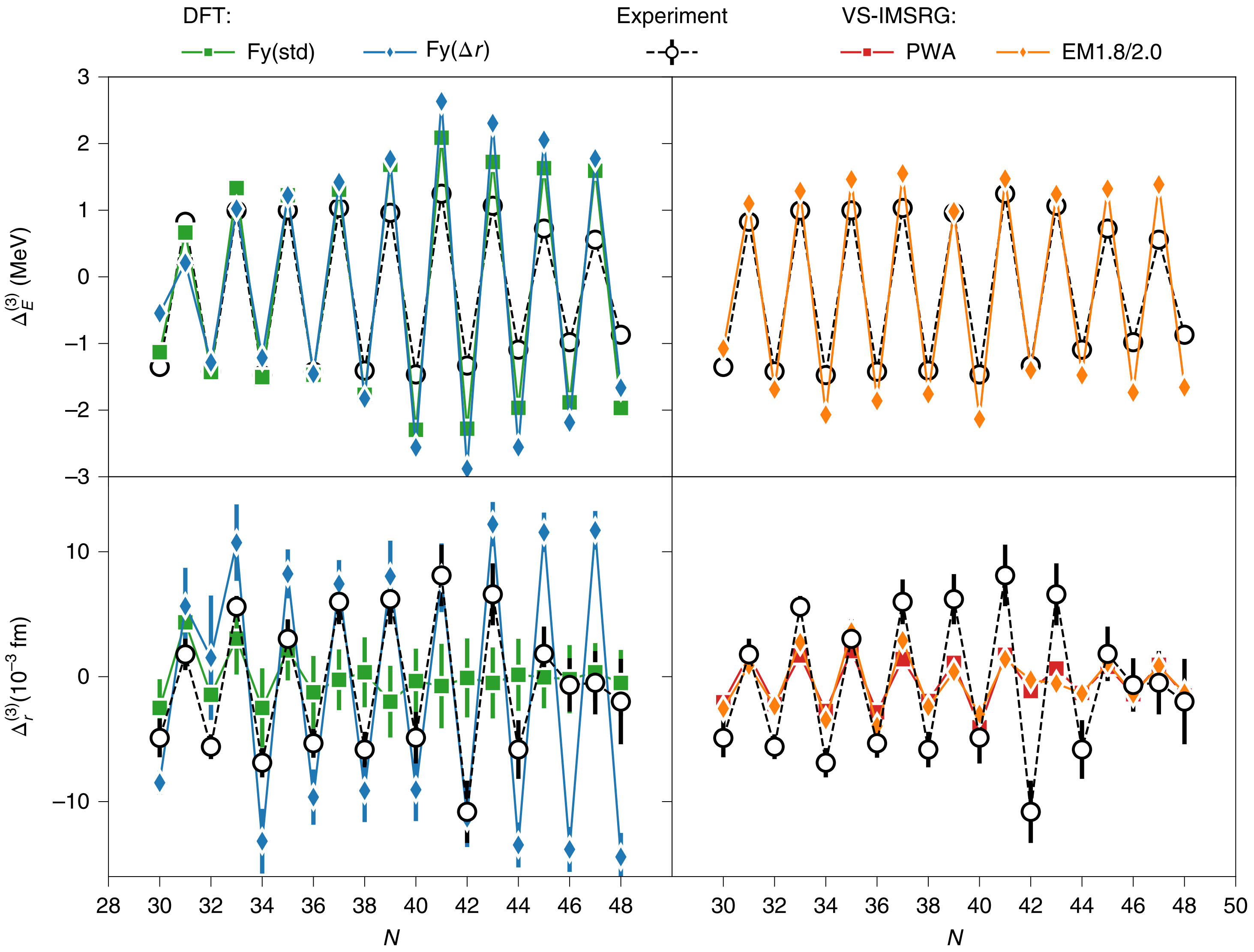
XYZ
extract observables

Are We There Yet?

Uncertainty

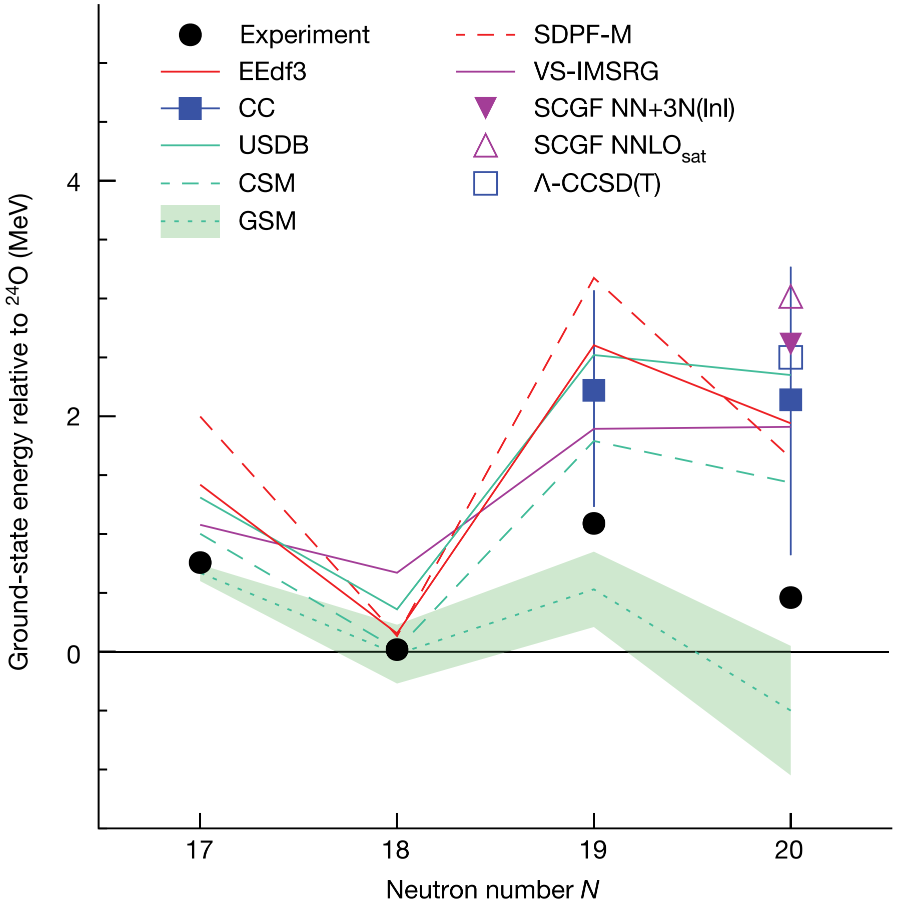
chromium isotopes

R. de Groote et al., Nat. Phys. ***16****, 620 (2020)*



oxygen isotopes

Y. Kondo et al., Nature ***620****, 965 (2023)*



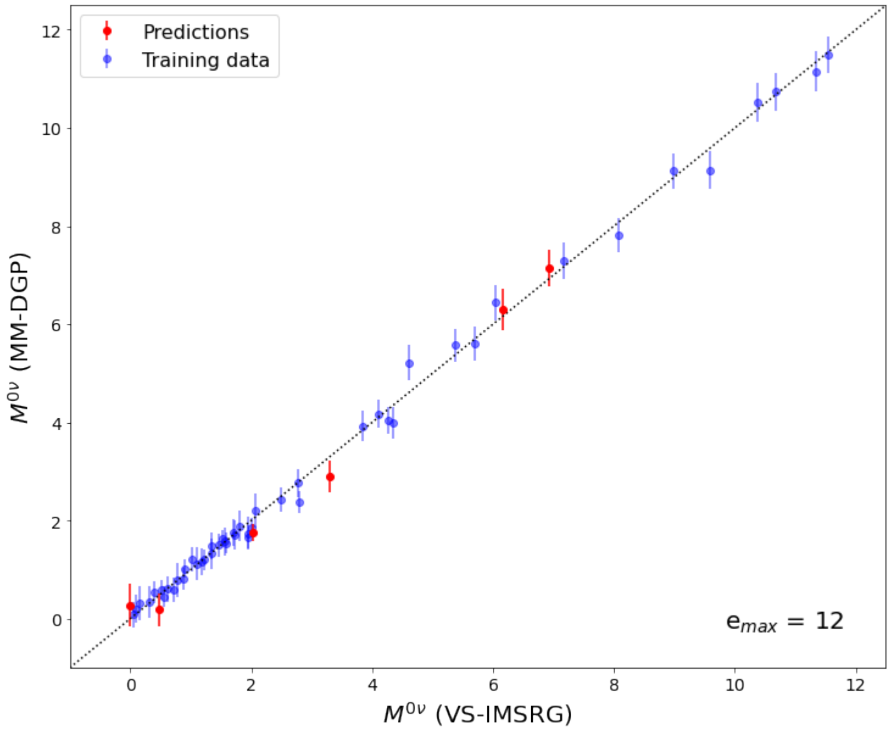
Are these results good, bad, or just ok? Is there genuine tension between theory and experiment? **How can we know?**

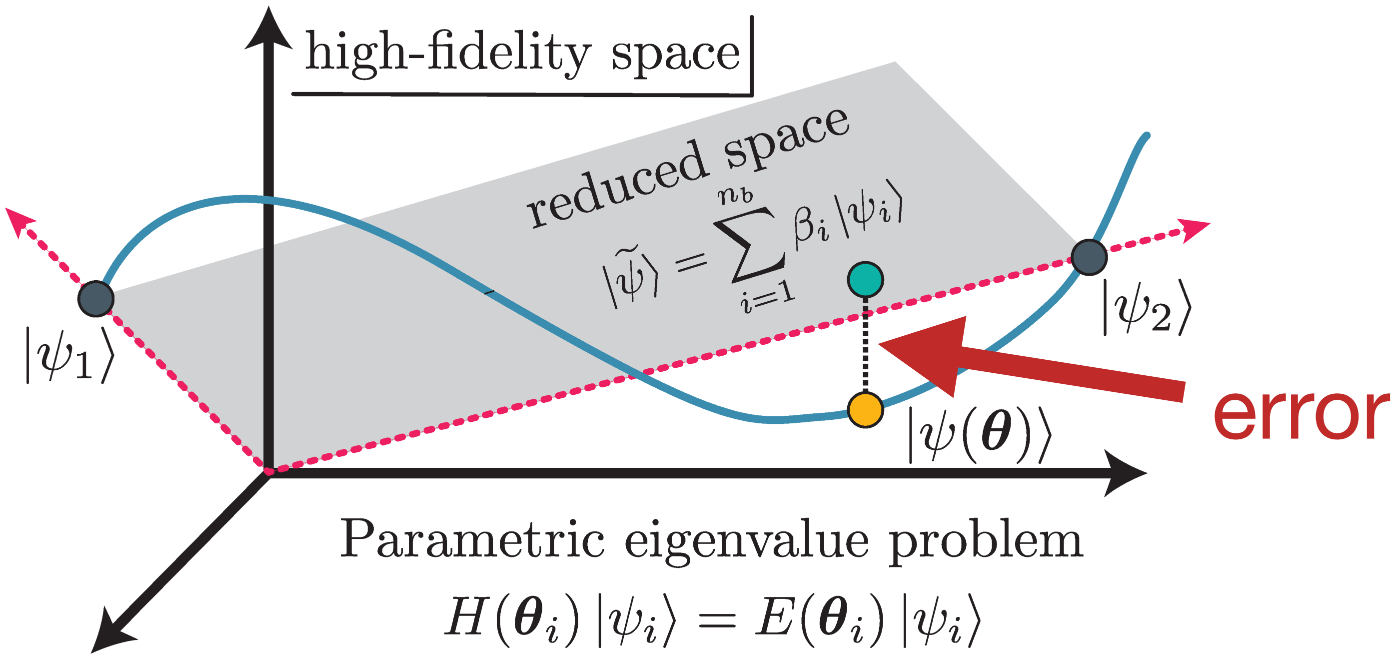
Modern Uncertainty Quantification

- treat **model parameters** as **probability distributions** rather than just numbers
    - condition, calibrate, and validate with data
- **predictions for observables** become **probability distributions** as well
    - allows characterization of likelihood, standard deviations (=error bars), correlations, parameter sensitivity, …
- **challenge:** need **lots** of **expensive** many-body calculations
- **solution:** construct **emulators** for costly simulations - can reduce computational effort by **many orders of magnitude** (but still need **training data**)

Emulators

J. Melendez et al., JPG 49, 102001 (2022), C. Drischler et al., Front. Phys. 10, 1092931 (2023)
E. Bonilla et al., PRC 106, 054322 (2022), P. Giuliani et al., Front. Phys. 10, 1054524 (2023)
J. Pitcher, A. Belley et al., in preparation, A. Belley et al., arXiv:2308.15643 (v2)



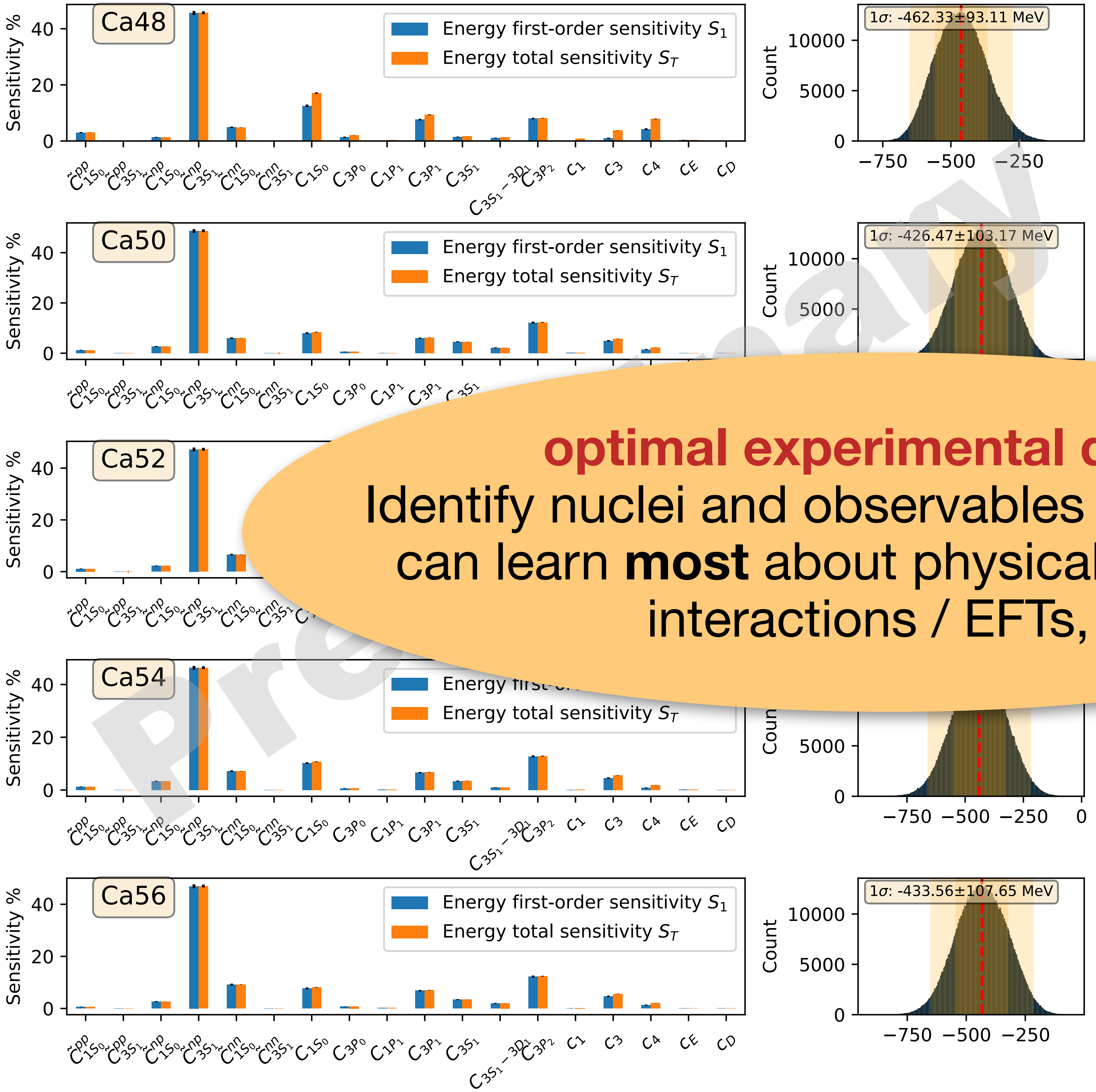


- Data driven (only expectation values)
- E.g. Multi-output, Multi-fidelity Deep Gaussian Processes (MM-DGP)

- Physics driven reduced-order models (ROMs)
- E.g., Galerkin projection for bound-state or scattering wave functions

Emulation for Operators (IMSRG)

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



optimal experimental design:

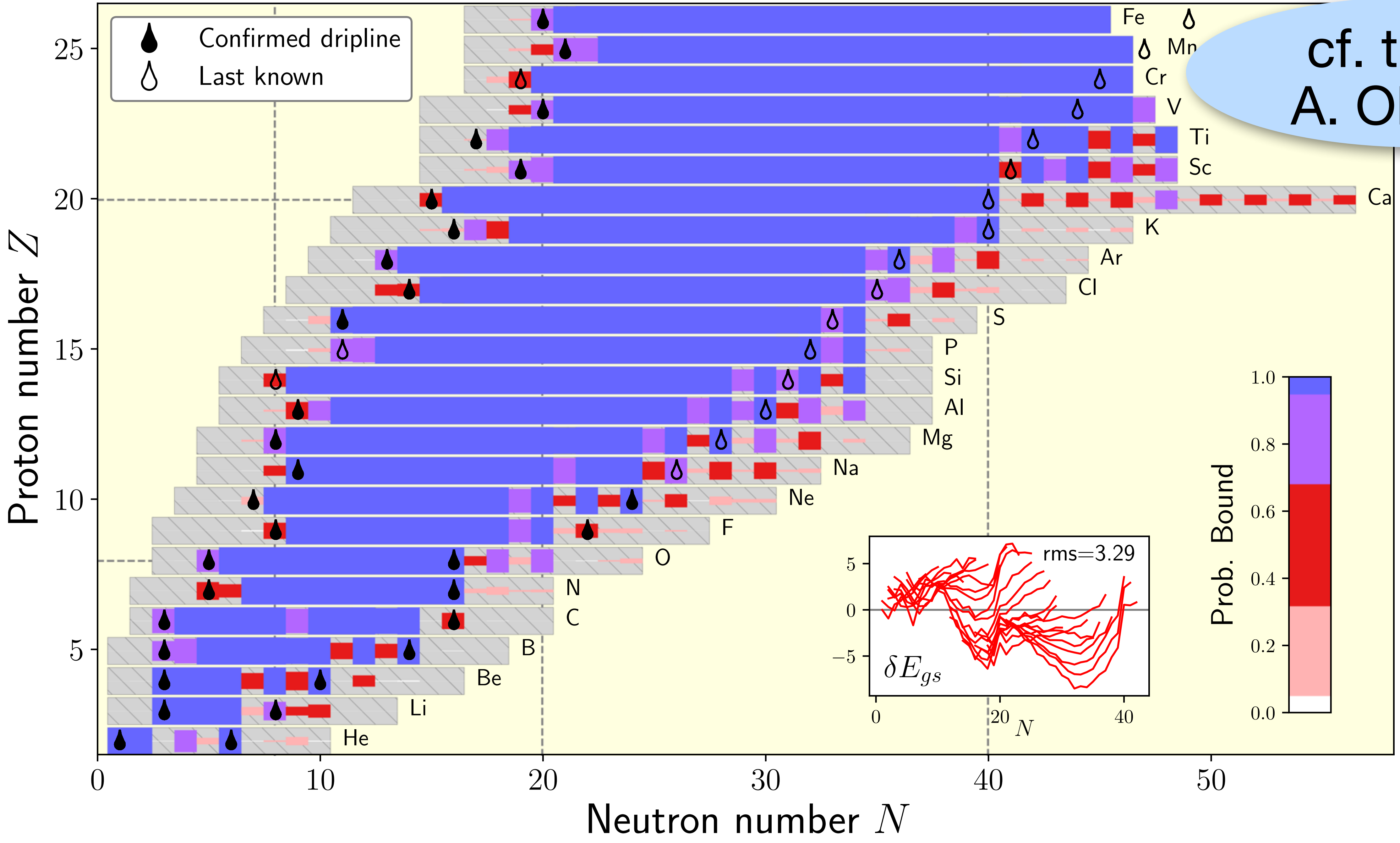
Identify nuclei and observables from which we can learn **most** about physical phenomena, interactions / EFTs, …

- non-invasive ROM emulator based on Dynamic Mode Decomposition
- …NLO$_{GO}$, NN+3N, $E_{3max} = 14$
- …samples
- **computational effort reduced by 5+ orders of magnitude**

No Matter Where You Go… There You Are

Towards *Ab Initio* Mass Tables

*S. R. Stroberg et al., PRL **126**, 022501 (2021)*

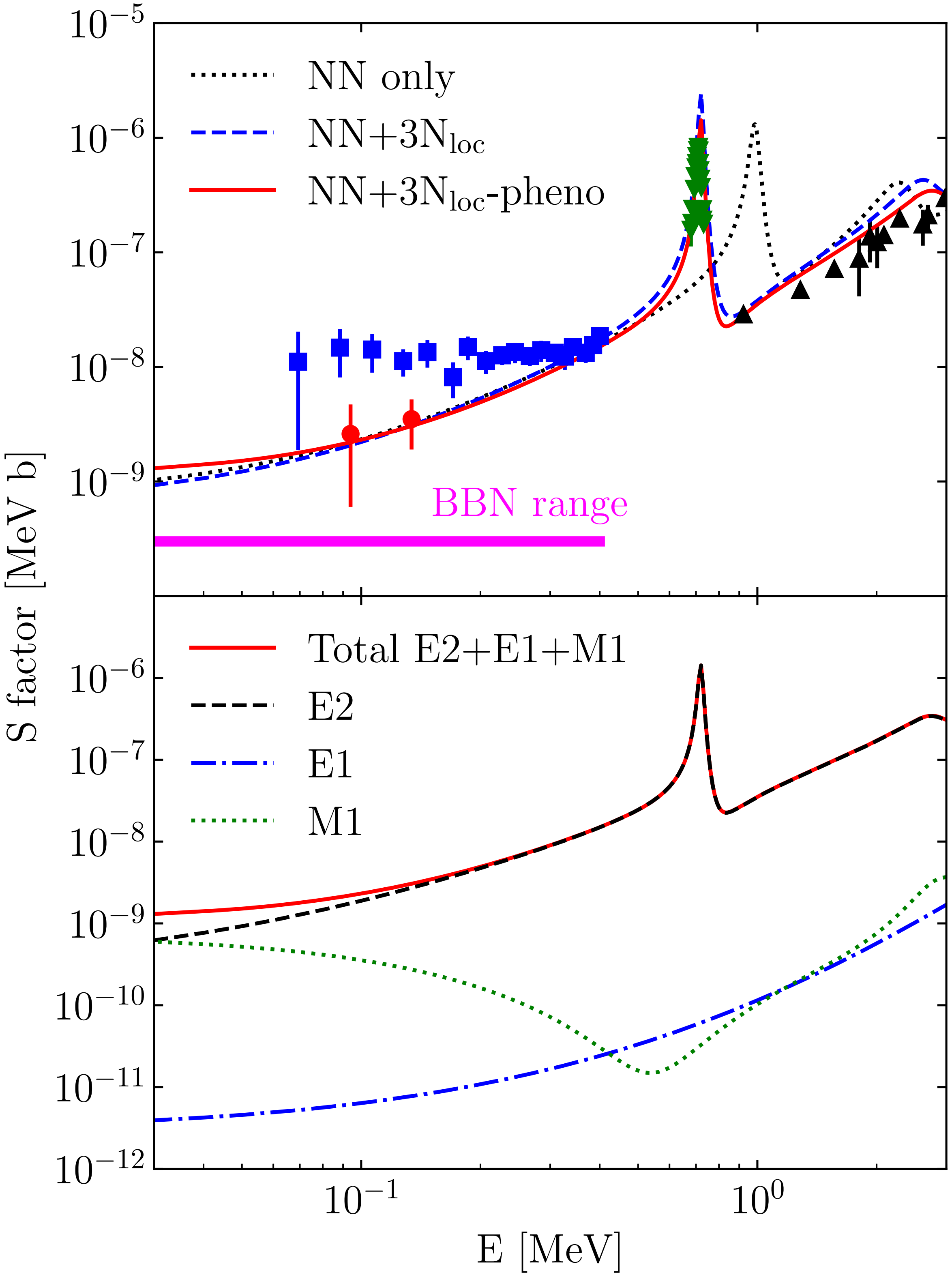


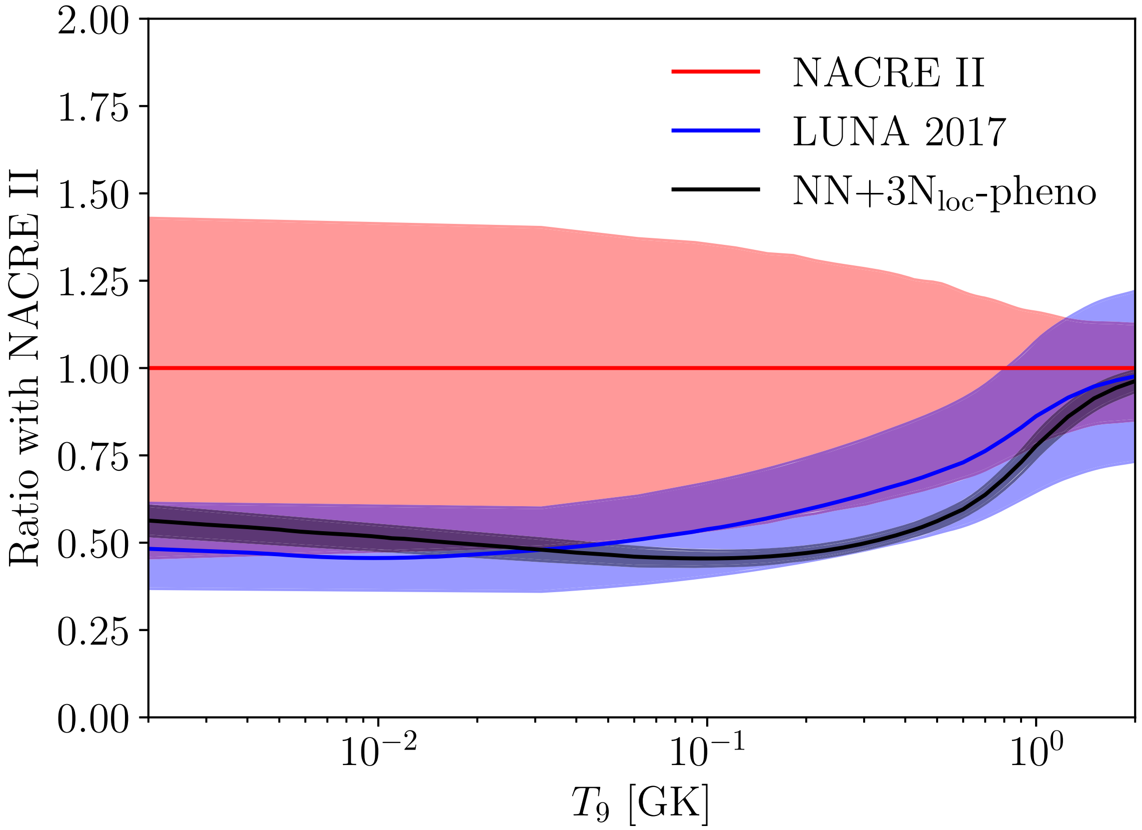
cf. talk by
A. Obertelli

Valence-Space IMSRG “mass table” based on a chiral NN+3N interaction (EM1.8/2.0)

^{4}He (d,γ) ^{6}Li Big Bang Radiative Capture

C. Hebborn et al., PRL **129**, 042503 (2021)



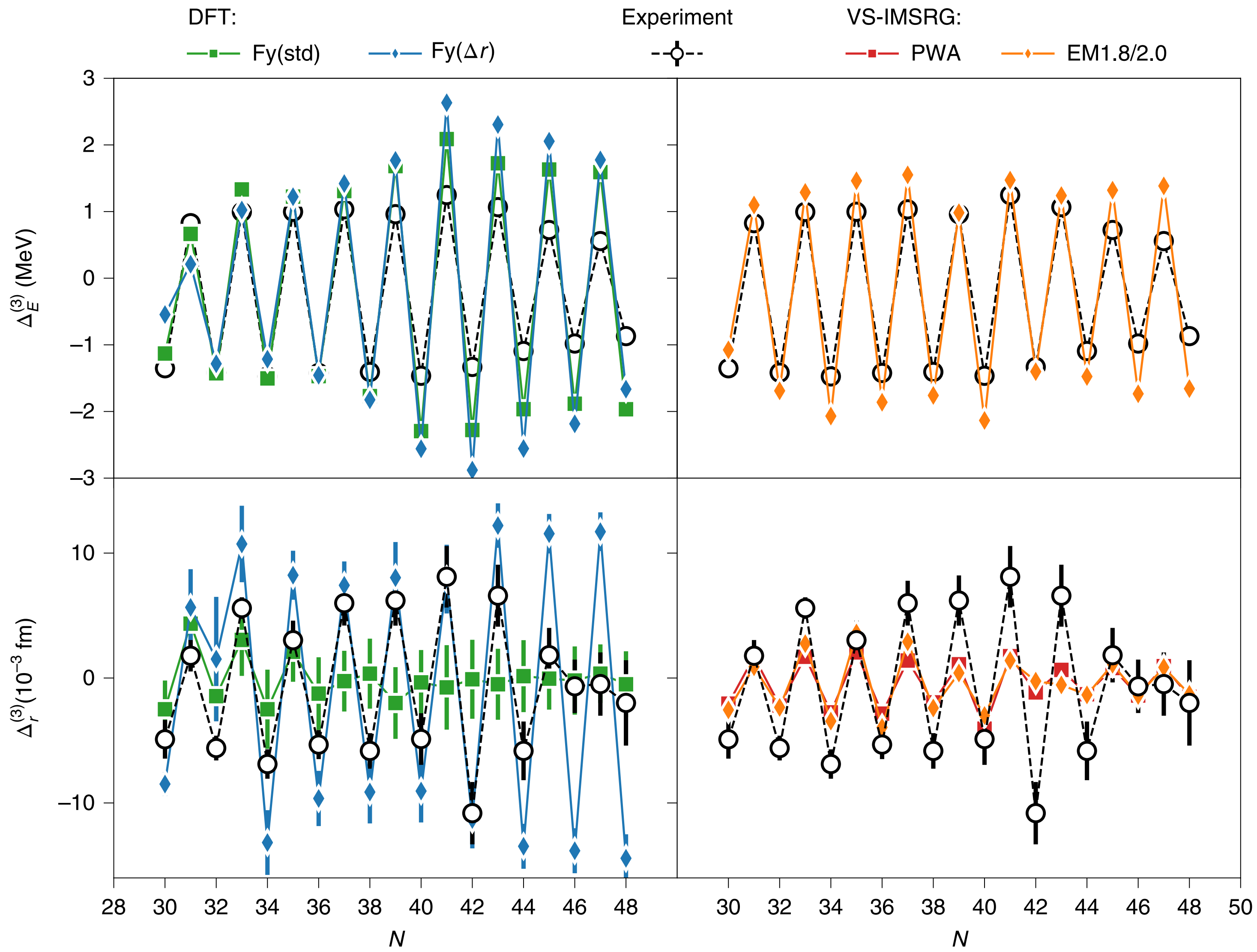


- BB nucleosynthesis models under-predict ^{6}Li abundance - one cause could be inaccurate **reaction rates**
- NCSMC computation based on chiral EFT interactions

Differential Radii and Trends

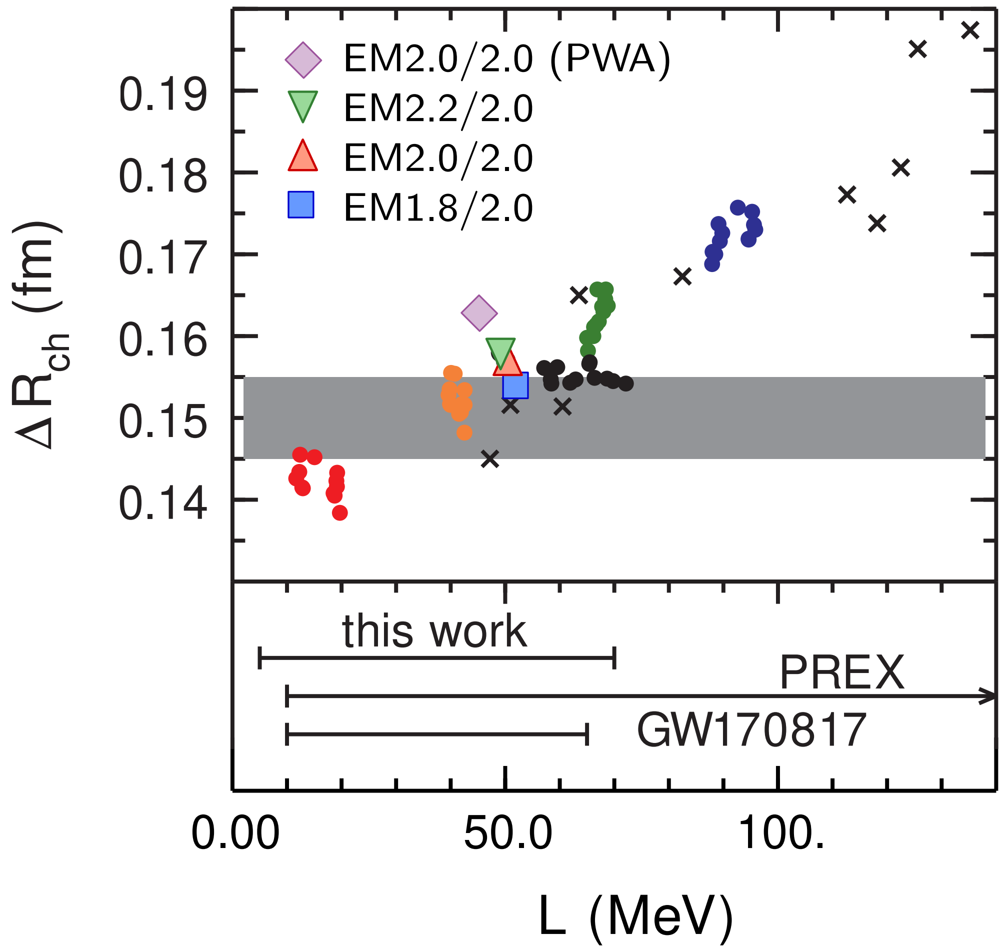
chromium isotopes

*R. de Groote et al., Nat. Phys. **16**, 620 (2020)*



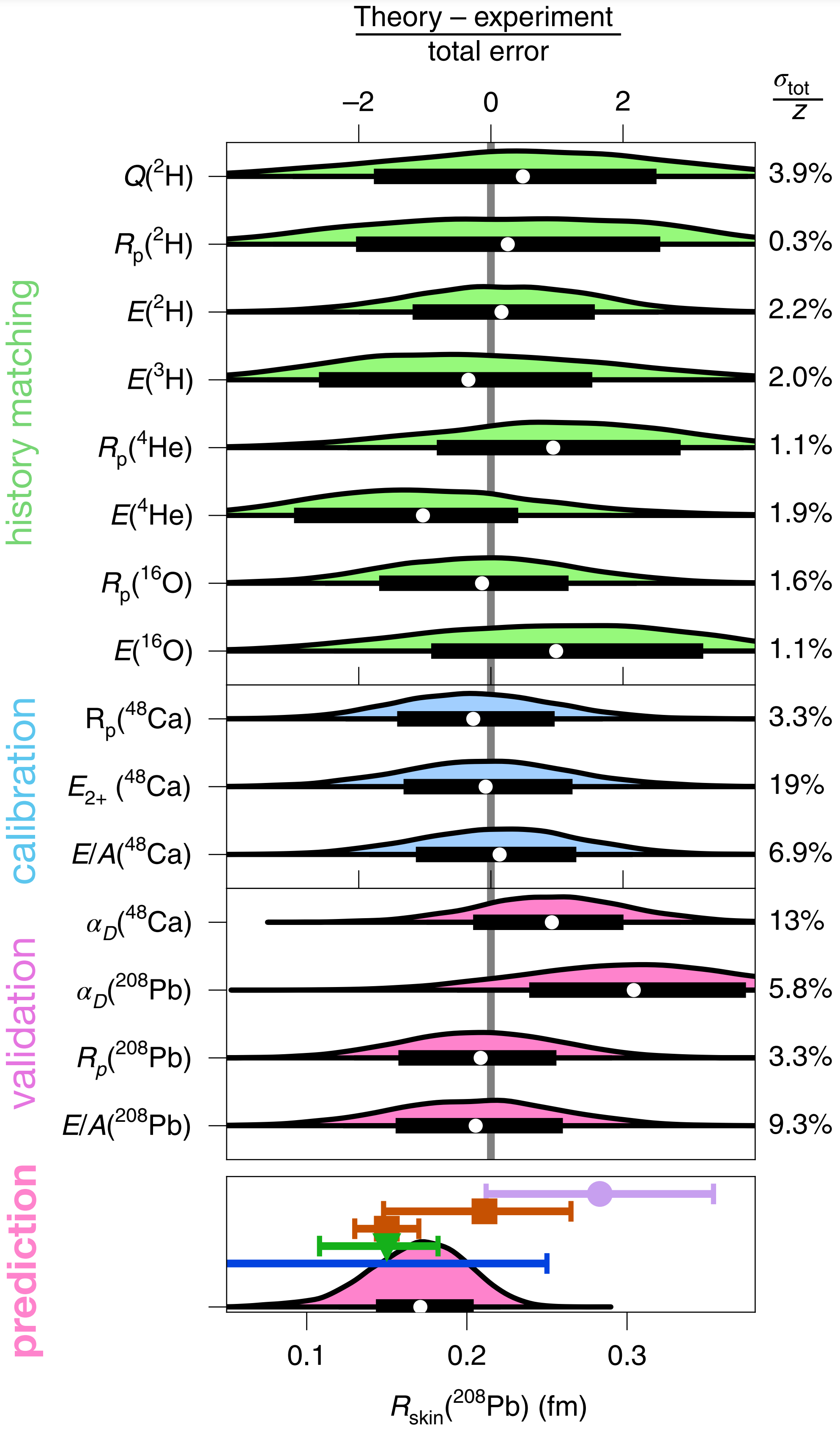
^{36}Ca - ^{36}S

*B. A. Brown et al., PRR **2**, 022305(R) (2020)*

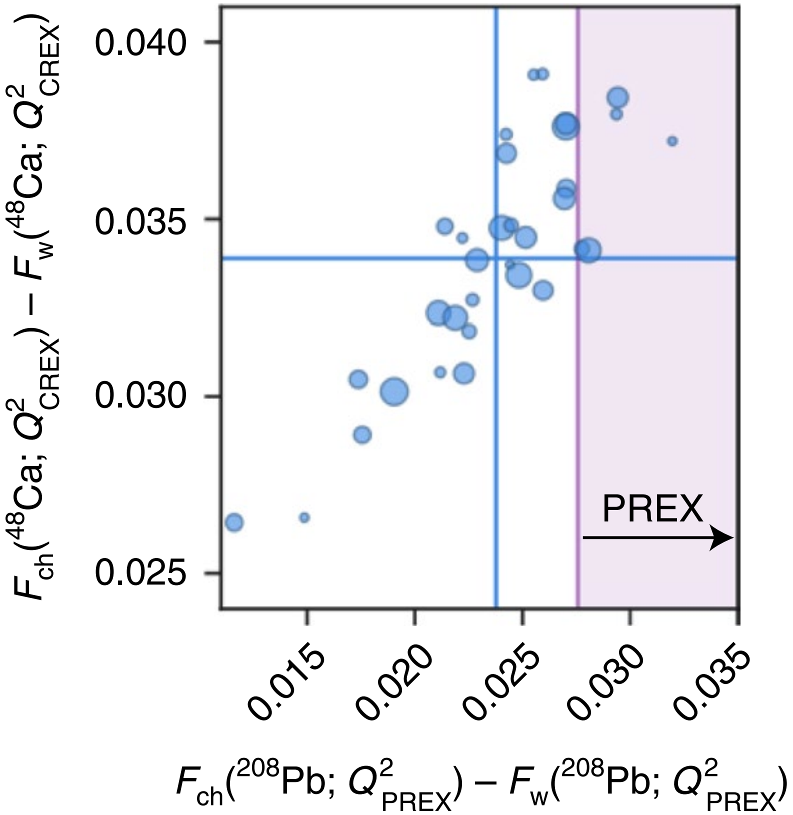


differential observables like the staggering of energies ($\Delta_E^{(3)}$) and radii ($\Delta_r^{(3)}$) or the charge radius difference of mirror nuclei, ΔR_{ch}, are **insensitive** to variations of interaction cutoffs / resolution scale

Neutron Skin in ^{208}Pb



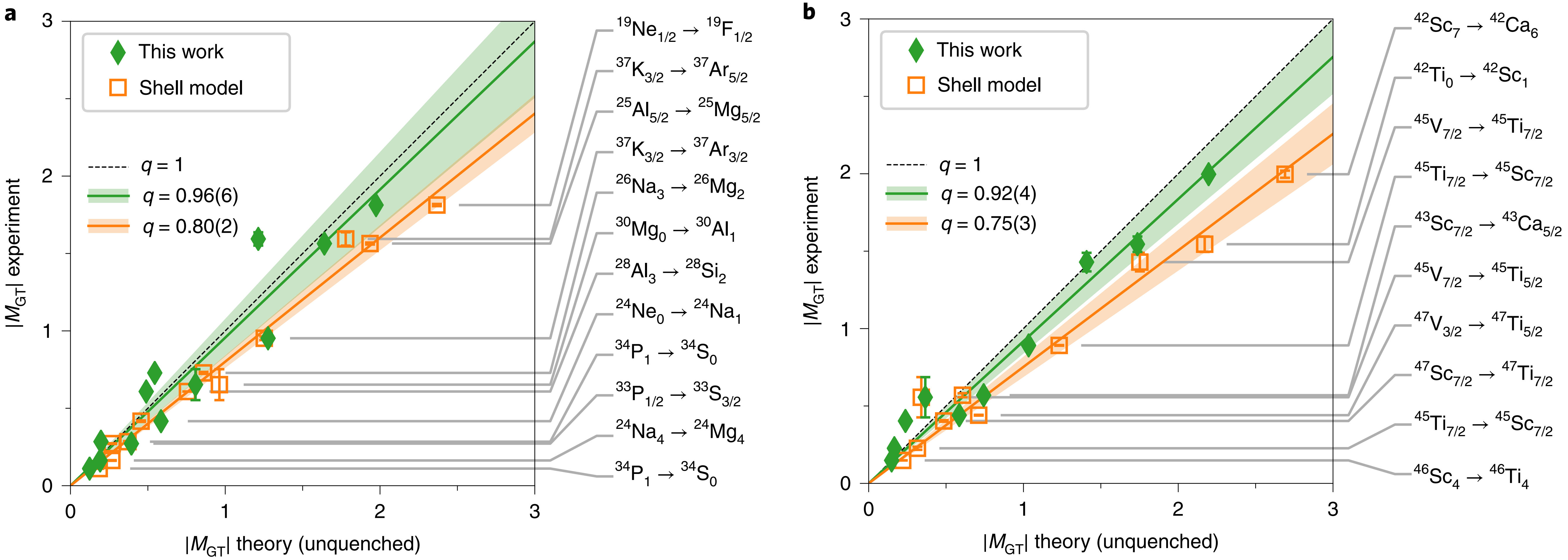
B. S. Hu et al., Nat. Phys. **18**, 1196 (2022)



- ^{208}Pb is **heaviest nucleus** for which converged *ab initio* calculations have been achieved (VS-IMSRG, CC)
- chiral forces favor **thin neutron skin,** in **mild tension** with recent experimental result from PREX

Quenching of Gamow-Teller Decays

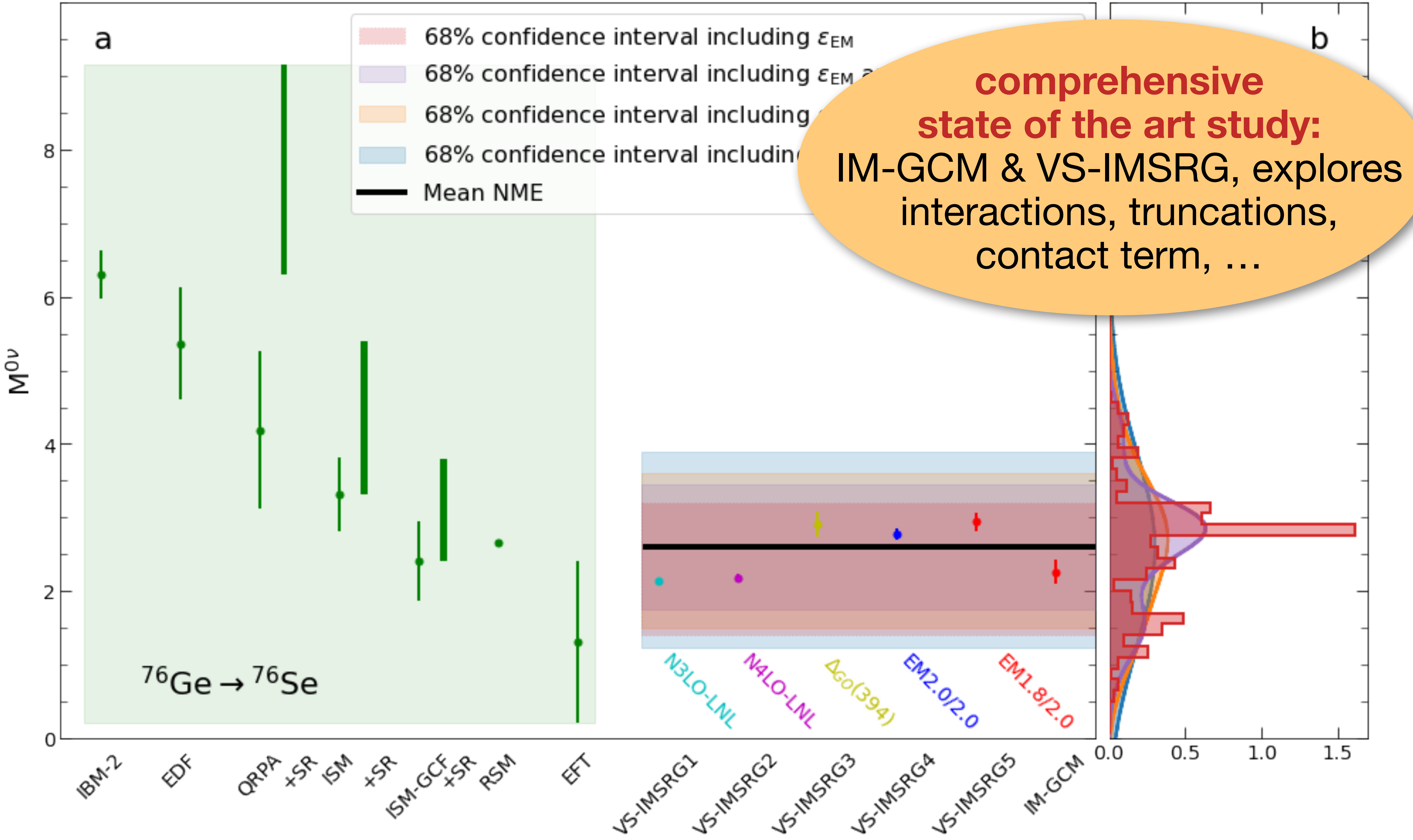
P. Gysbers et al., Nature Physics ***15****, 428 (2019)*



- **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**

^{76}Ge

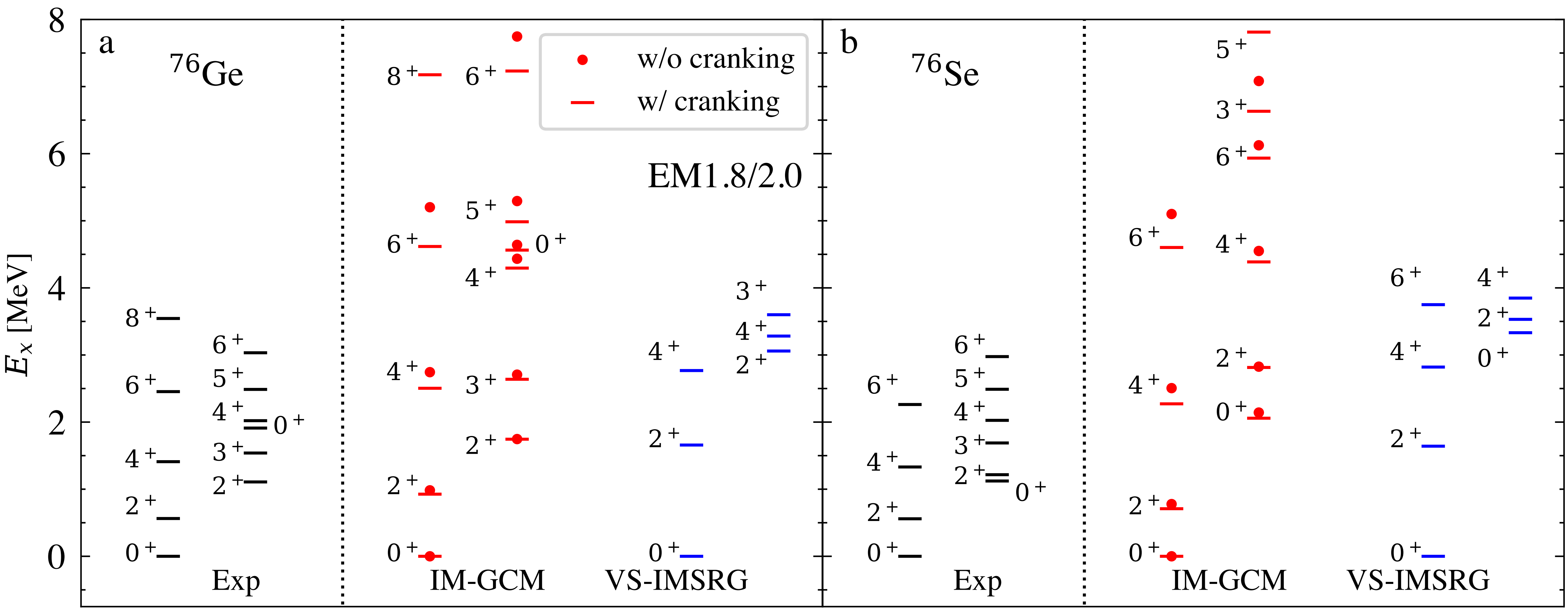
*A. Belley et al., arXiv:2308.15643 (**v2**)*



comprehensive state of the art study:
IM-GCM & VS-IMSRG, explores interactions, truncations, contact term, …

^{76}Ge / ^{76}Se Structure

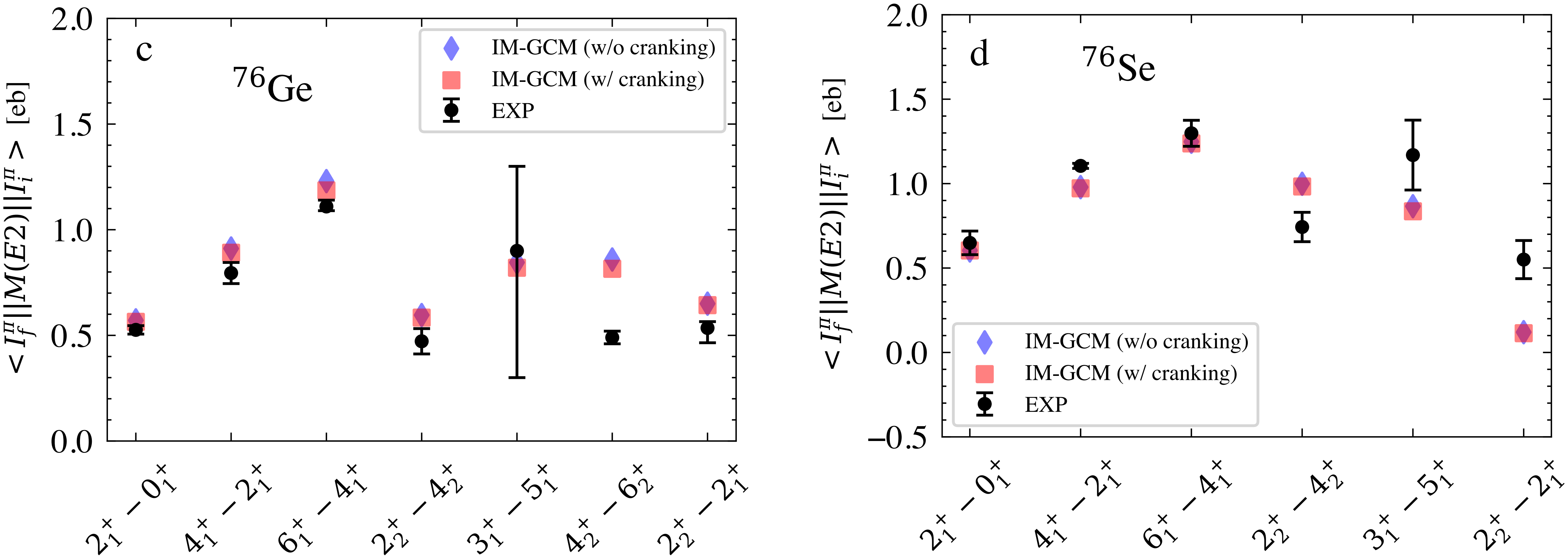
*A. Belley et al., arXiv:2308.15643 (**v2**)*



EM1.8/2.0 NN+3N interaction, $\hbar\omega = 12\,\mathrm{MeV}, e_{max} = 10$

^{76}Ge / ^{76}Se Structure

*A. Belley et al., arXiv:2308.15643 (**v2**)*



EM1.8/2.0 NN+3N interaction, $\hbar\omega = 12\,\text{MeV}, e_{max} = 10$

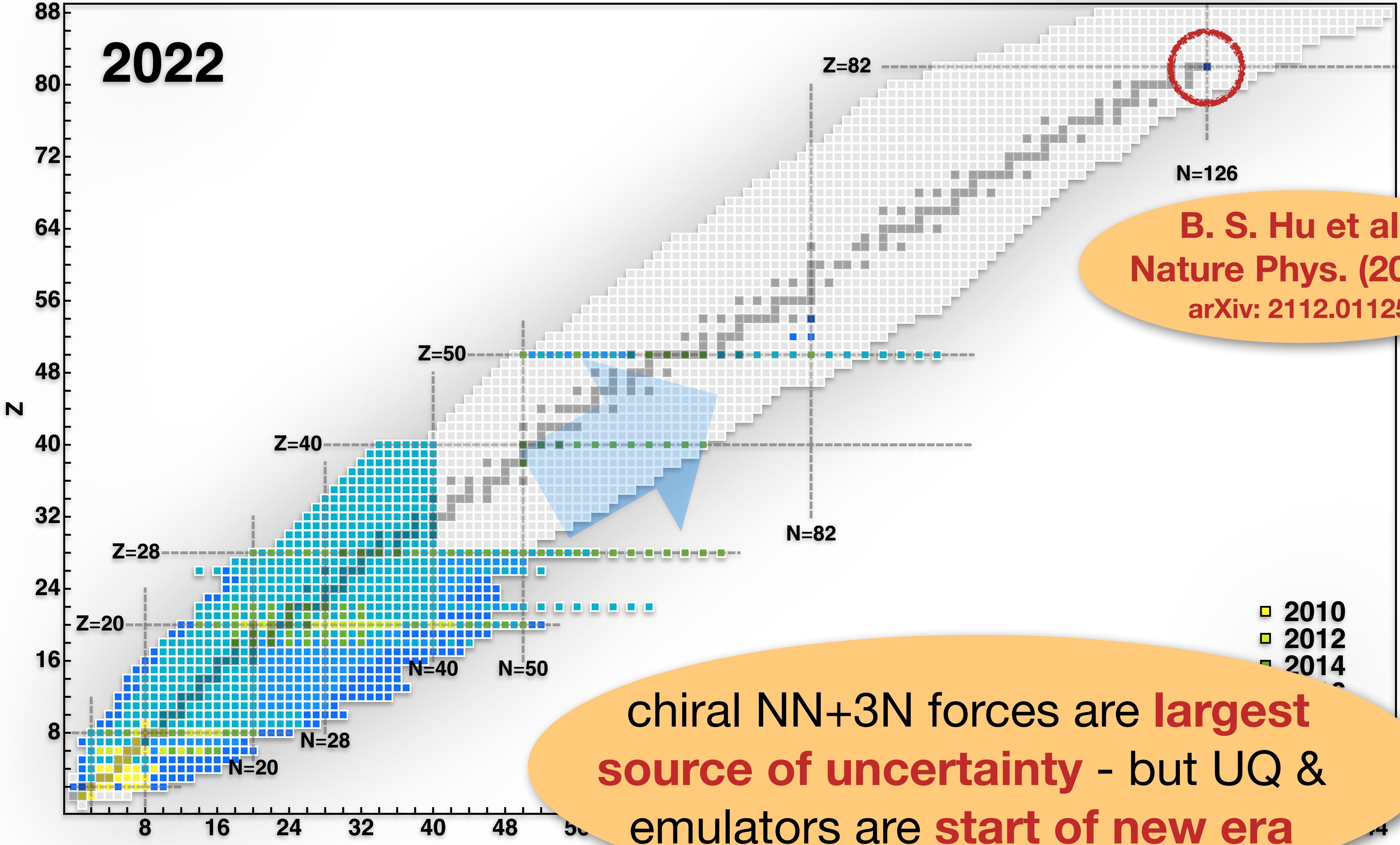
Where Do We Go From Here?

Conclusions & Outlook

- ***ab initio*** **approach** is key for a **predictive theory** of nuclear structure and reactions
    - rooted in QCD (**proper symmetries**)
    - **systematically improvable interactions and operators** (through Chiral EFT)
    - **systematically improvable many-body methods**
    - **quantified uncertainties** (theoretical error bars)
- **renormalization group** methods are a **powerful tool** for nuclear theory
- always growing capabilities, many **exiting applications** ahead

Progress in *Ab Initio* Calculations

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

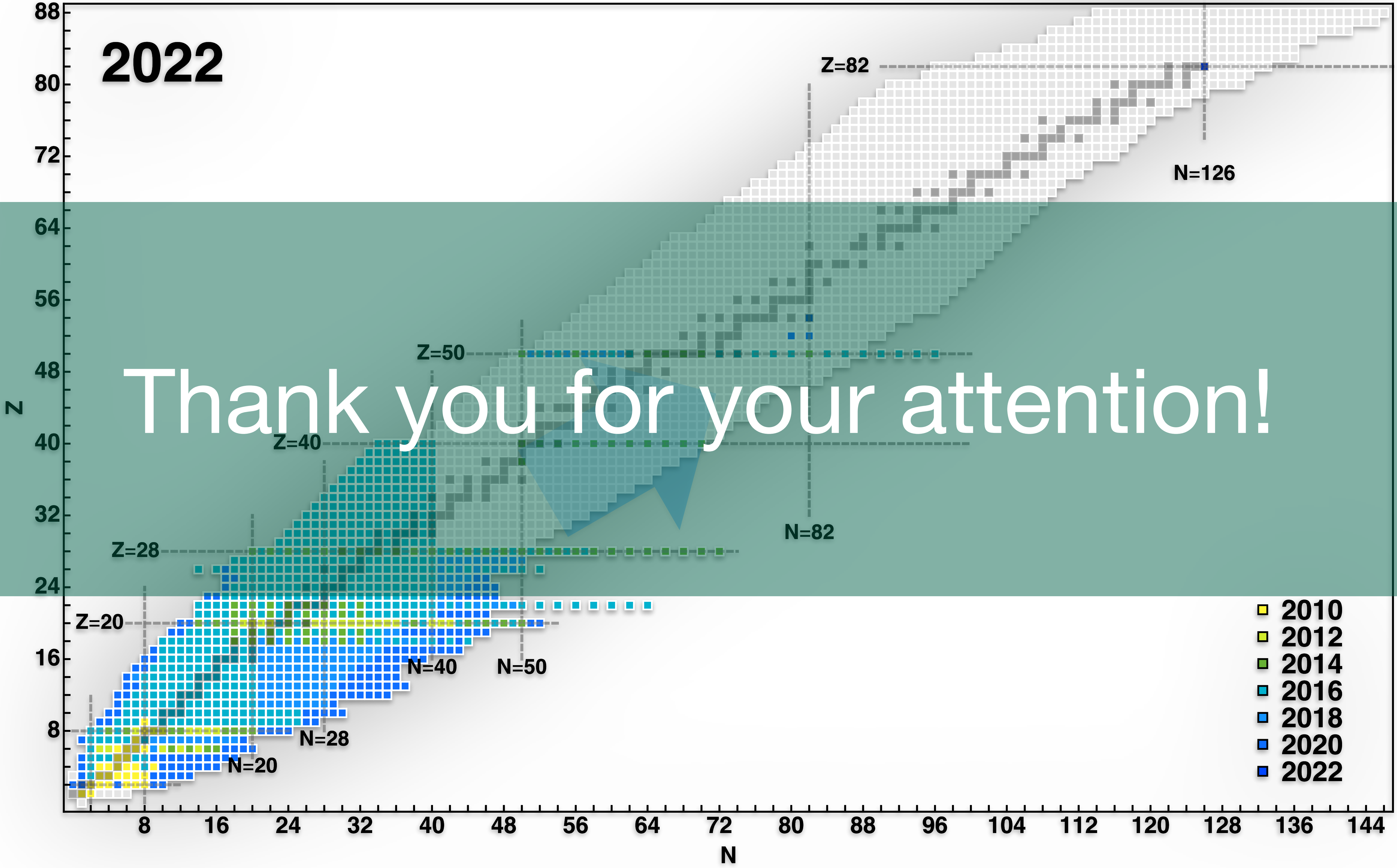


B. S. Hu et al., Nature Phys. (2022), arXiv: 2112.01125

chiral NN+3N forces are **largest source of uncertainty** - but UQ & emulators are **start of new era**

Progress in *Ab Initio* Calculations

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



Thank you for your attention!

FRIB

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Universidad Complutense de Madrid, Spain

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Florida State University

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UT Knoxville & Oak Ridge National Laboratory

R. J. Furnstahl
The Ohio State University

and everyone I forgot to list...

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NUCLEI
Nuclear Computational Low-Energy Initiative

NERSC

ICER

Supplements

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.,

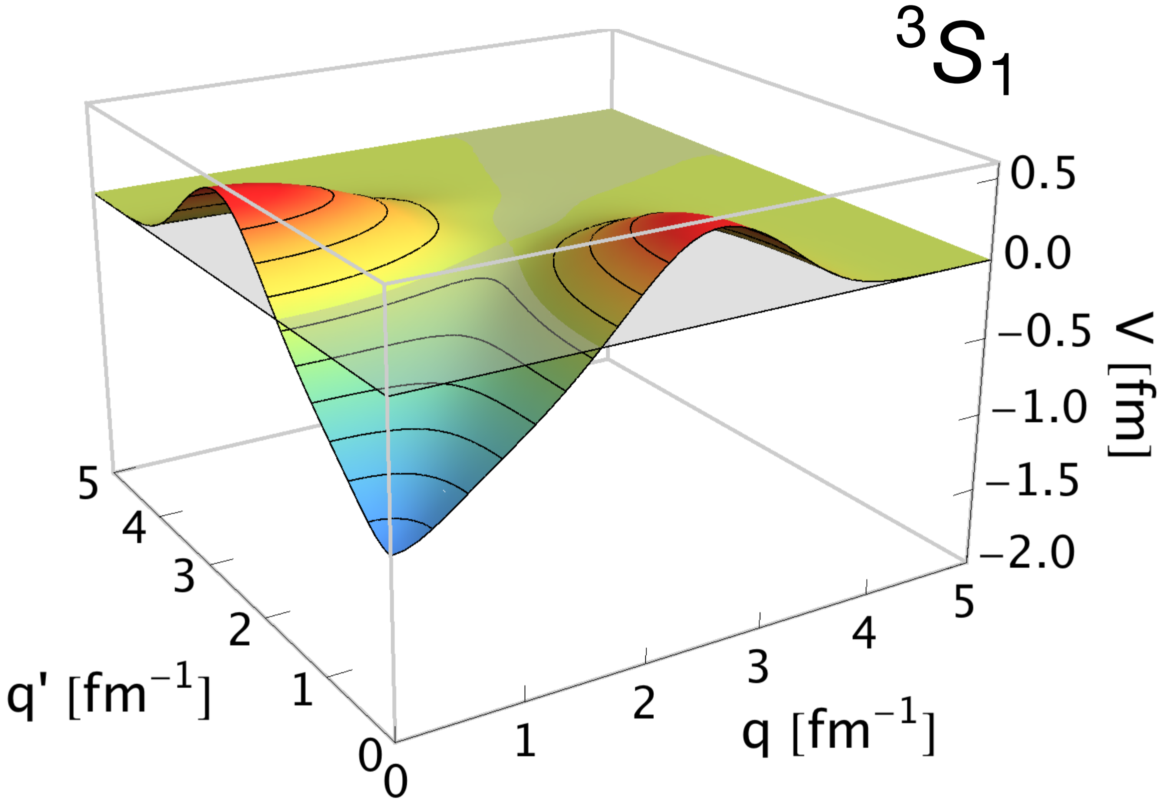
$$\eta(s) = \left[H_d(s), H_{od}(s)\right]$$

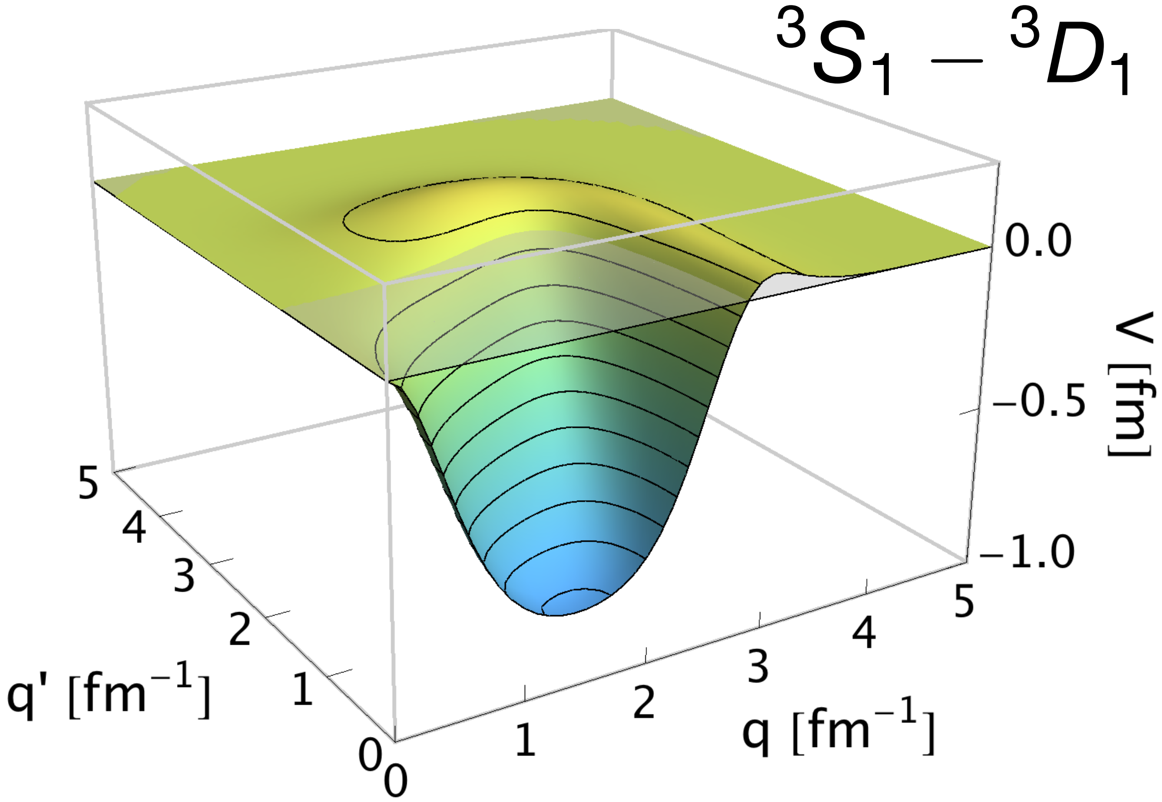
to suppress (suitably defined) off-diagonal Hamiltonian

- consistent evolution for all observables of interest

SRG in Two-Body Space

momentum space matrix elements


$^3S_1$


$^3S_1 - {}^3D_1$

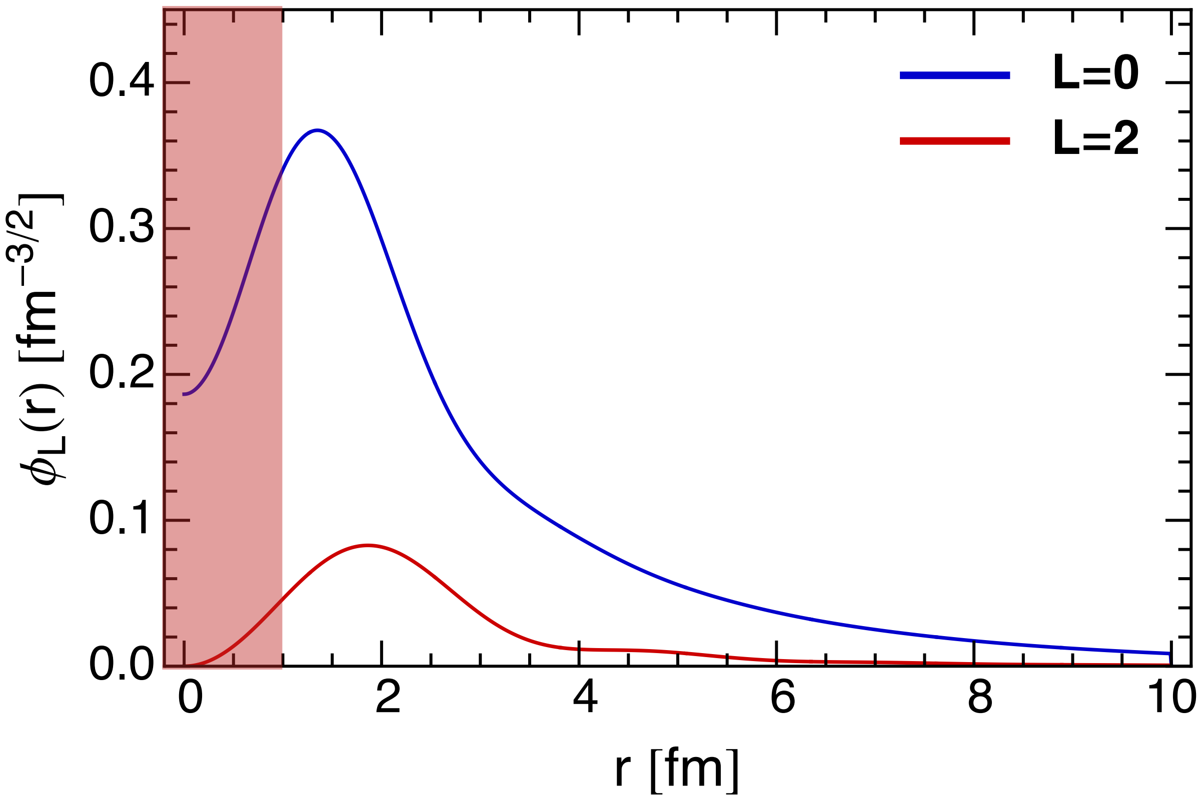
chiral NN

Entem & Machleidt, N3LO

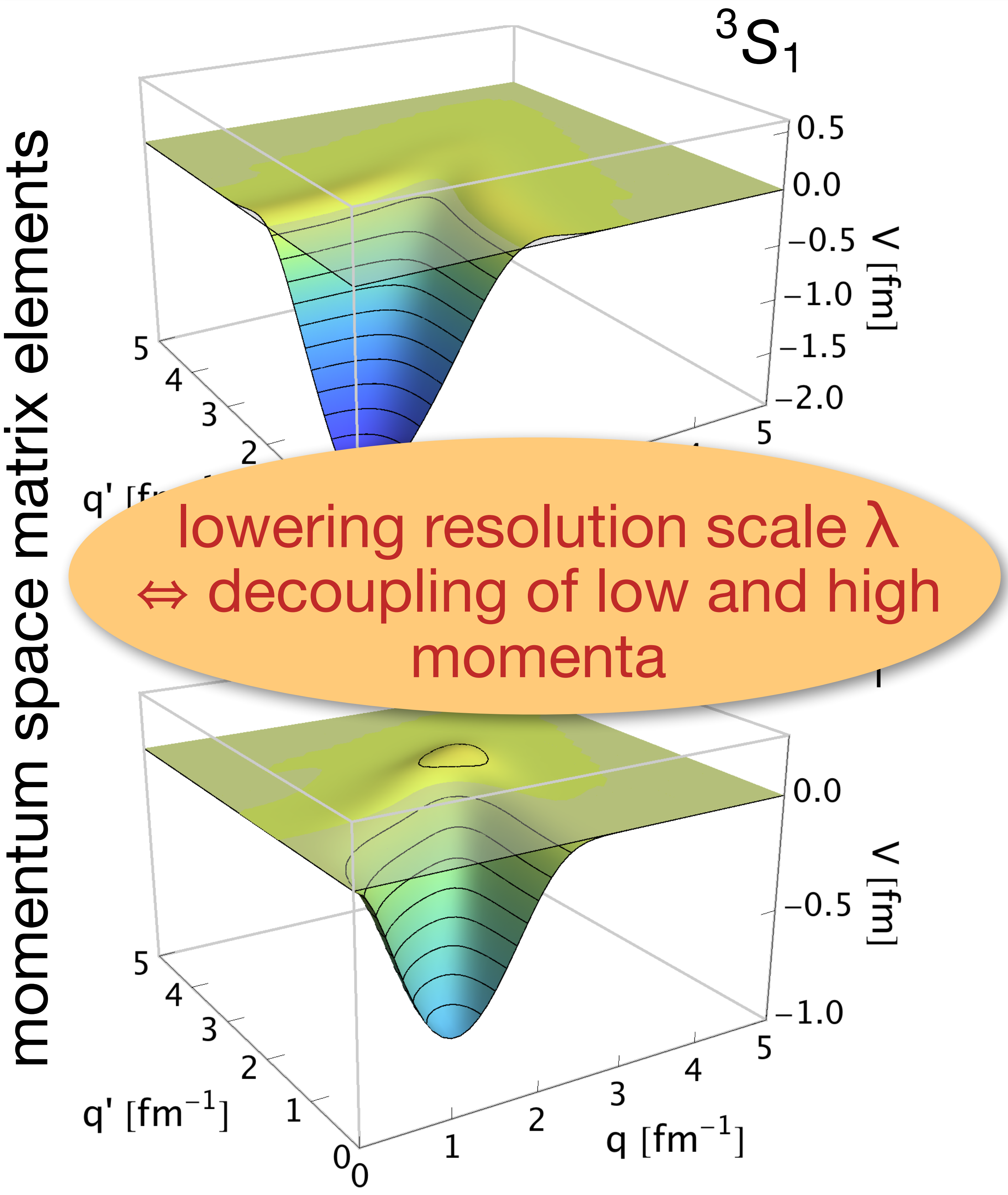
$$\eta(\lambda) = 2\mu\left[T_{\mathrm{rel}}, H(\lambda)\right]$$

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

deuteron wave function



SRG in Two-Body Space



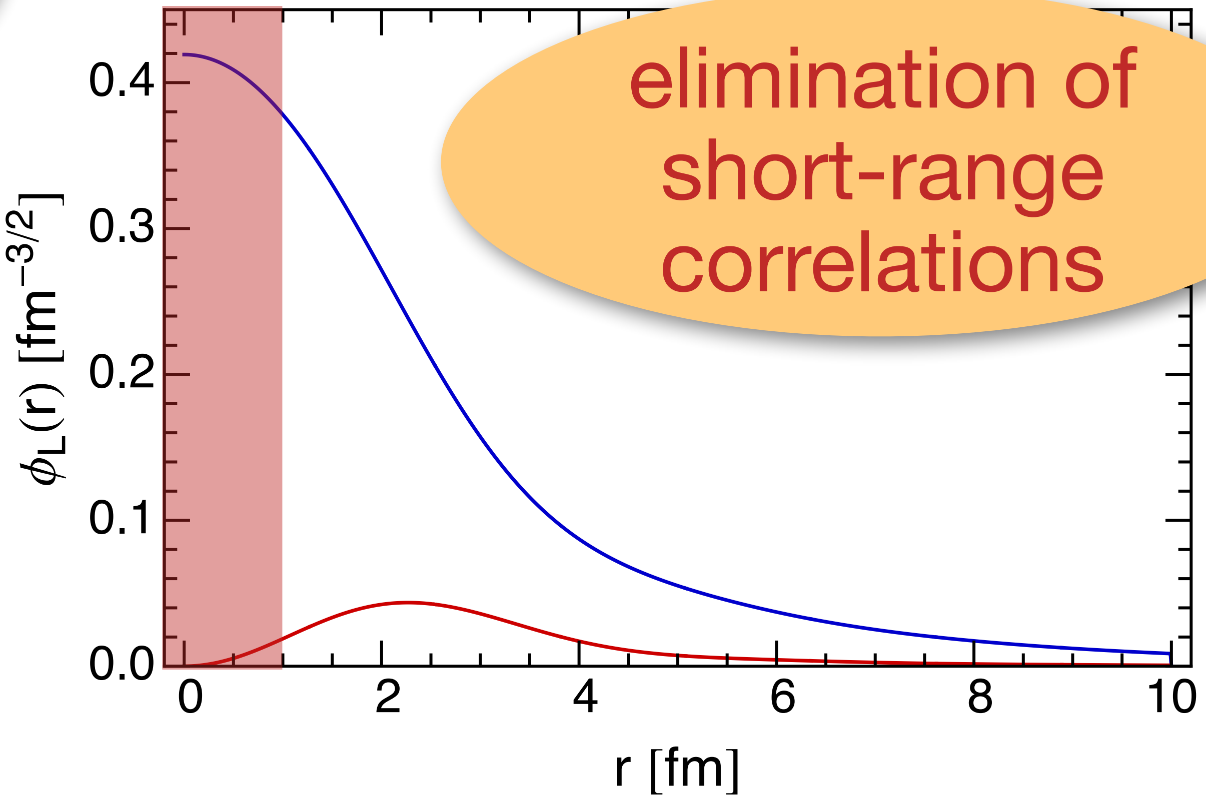
lowering resolution scale λ
⇔ decoupling of low and high momenta

λ = 1.8 fm^{-1}

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

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

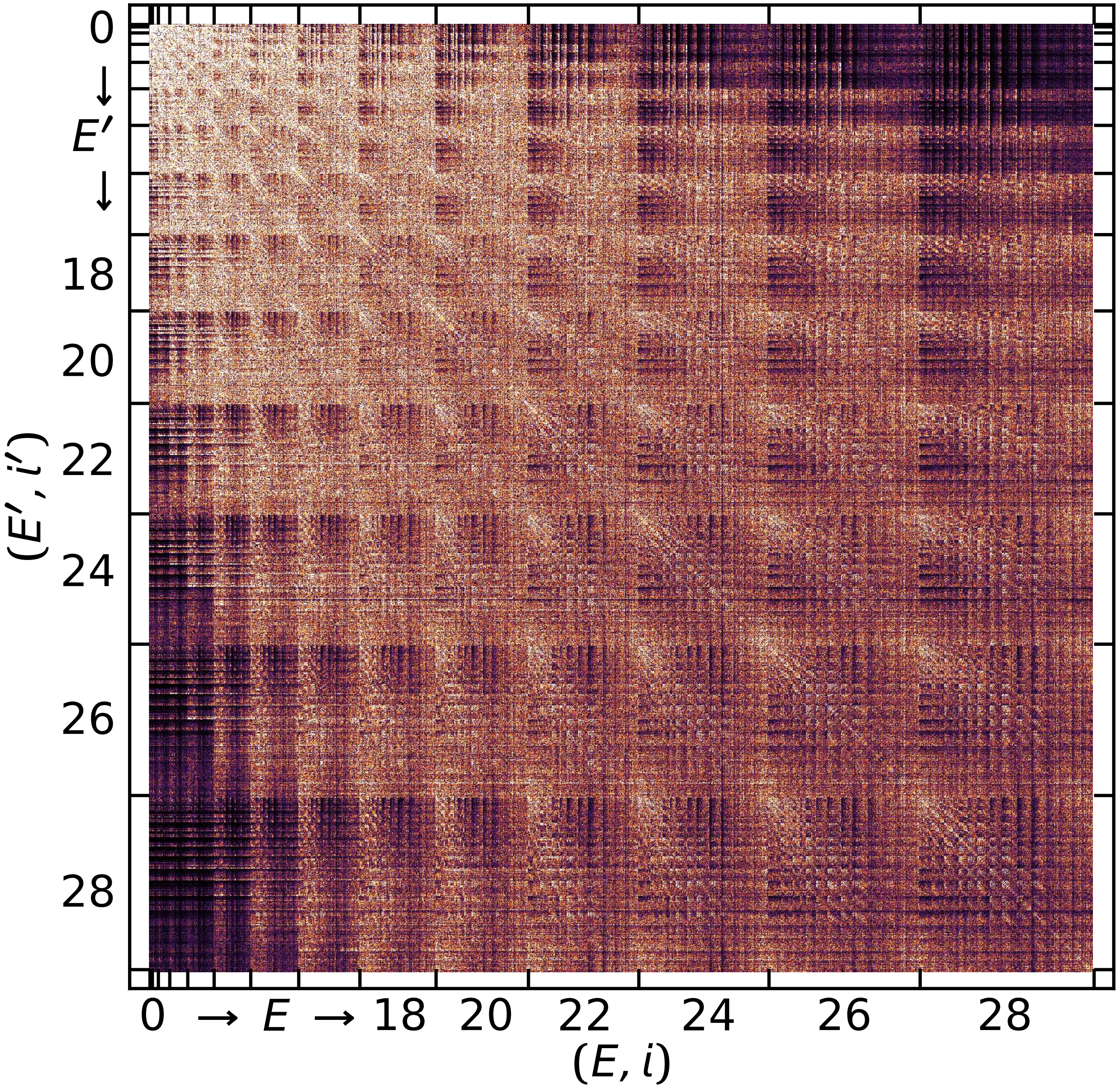
deuteron wave function



elimination of short-range correlations

SRG in Three-Body Space

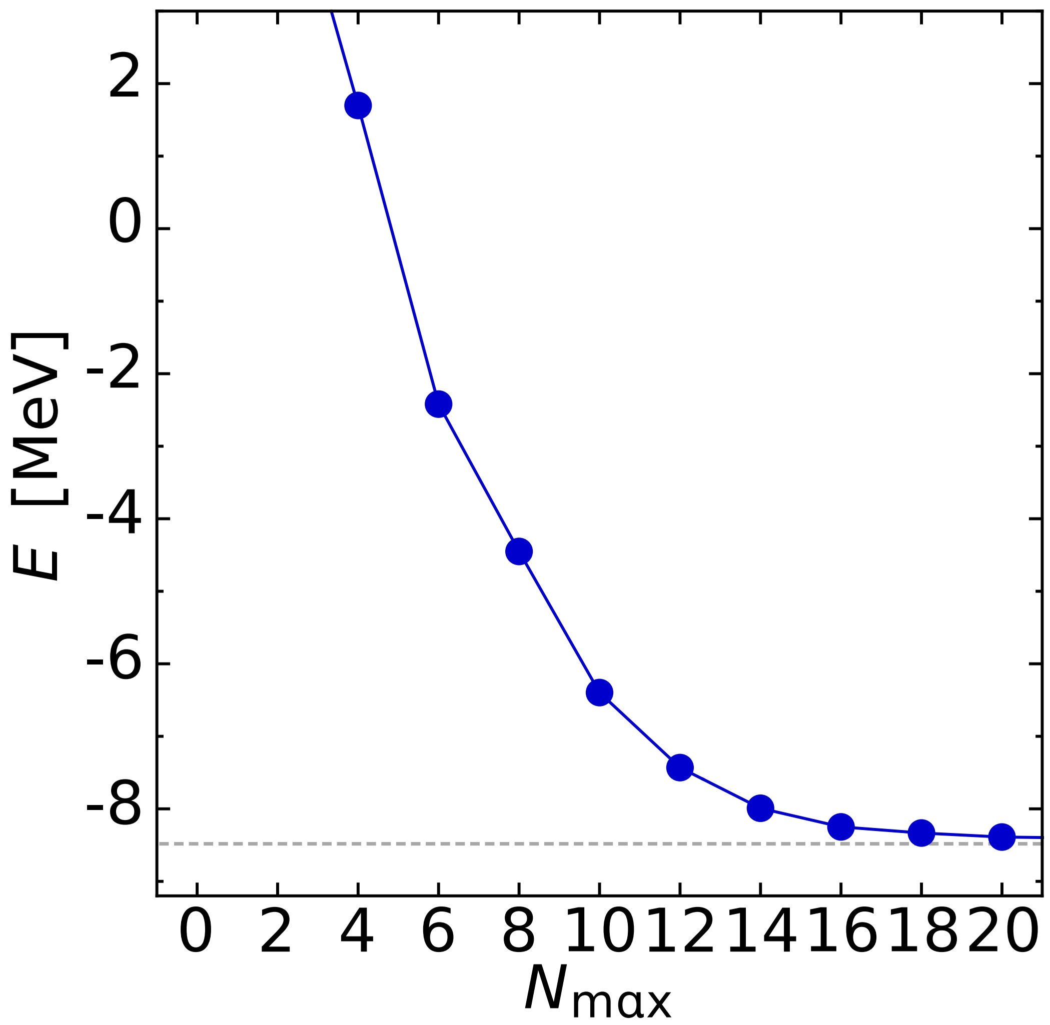
$J^\pi = \frac{1}{2}^+, T = \frac{1}{2}, \hbar\Omega = 28$ MeV



chiral NN + 3N

N^{3}LO + N^{2}LO (³H fit)

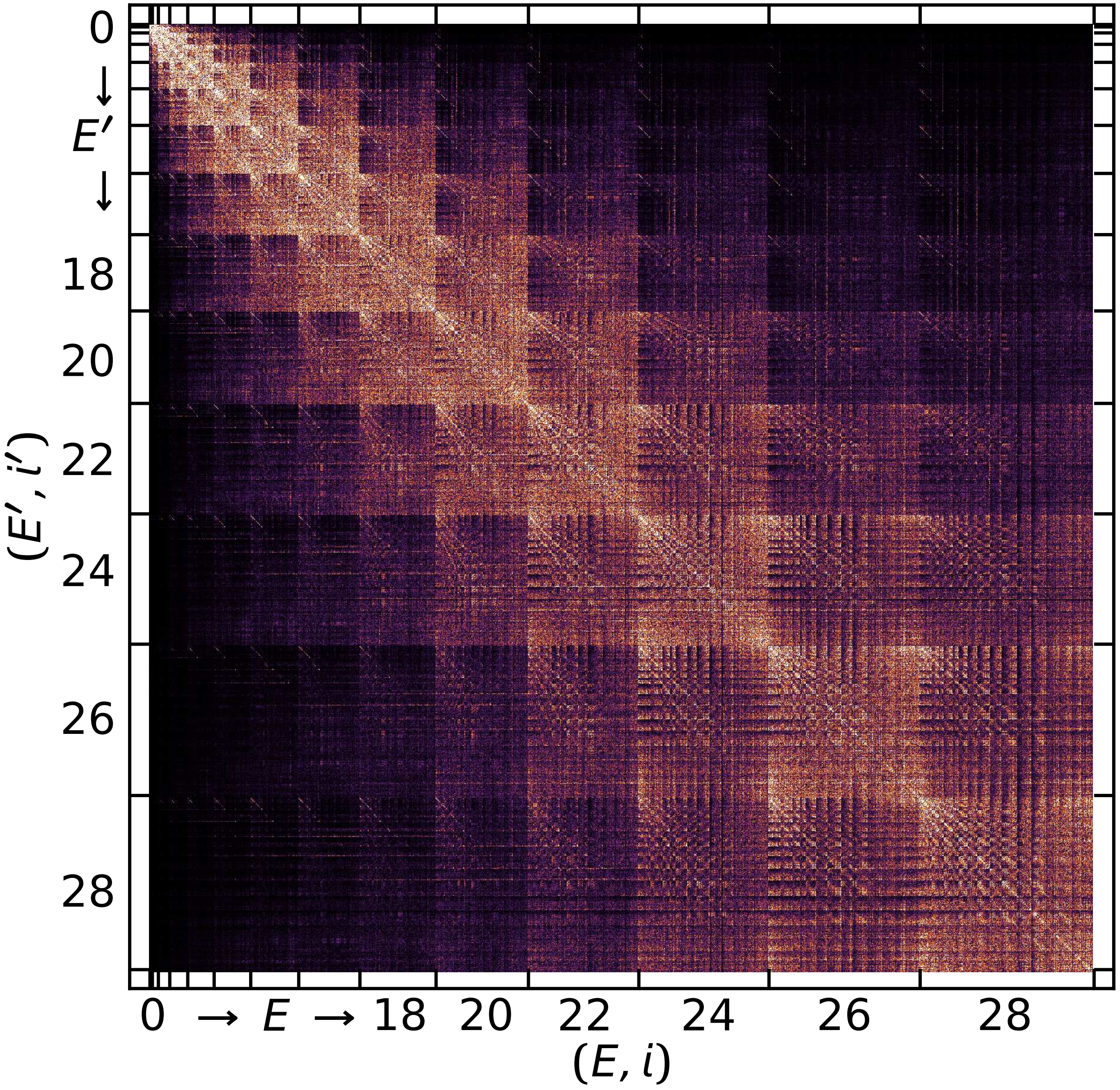
^{3}H ground-state (NCSM)



[figures courtesy of A. Calci and R. Roth]

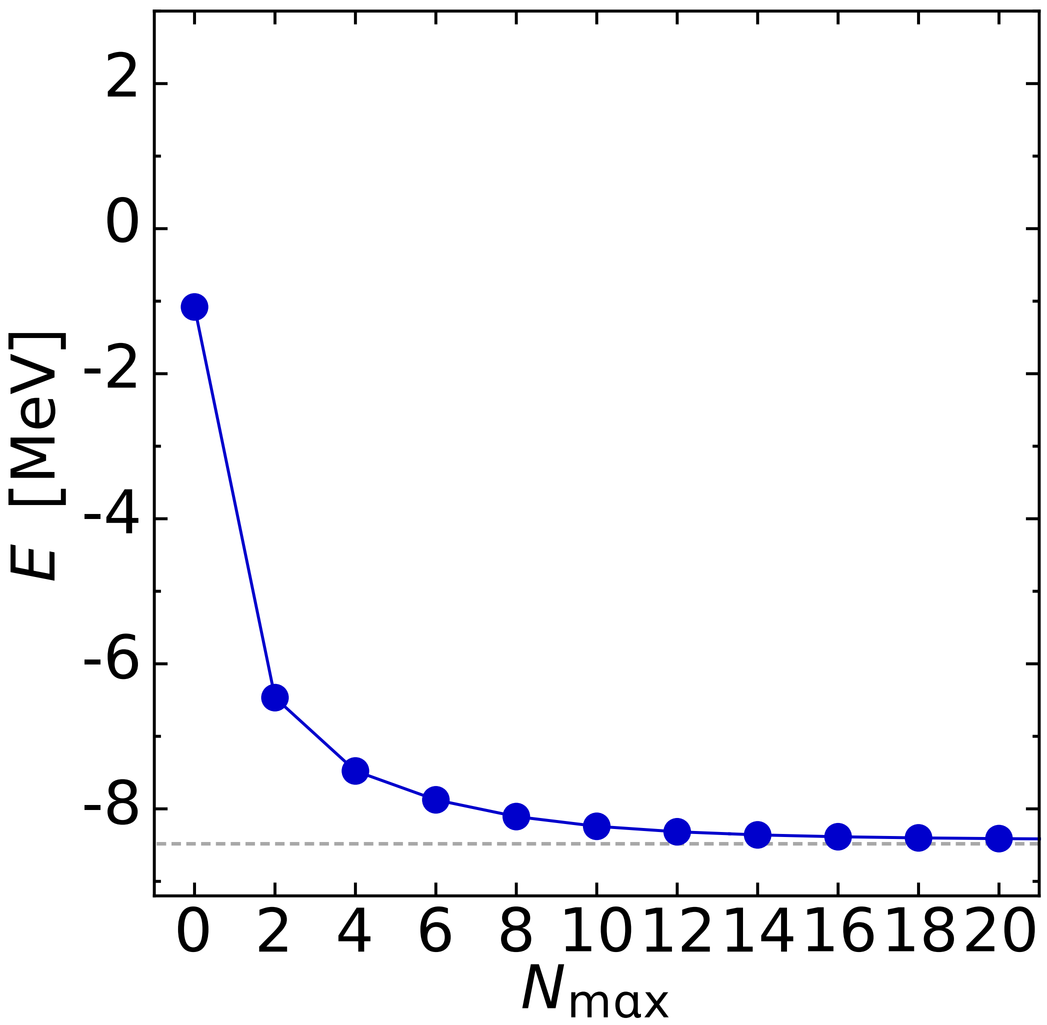
SRG in Three-Body Space

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



$\lambda = 1.33 \text{ fm}^{-1}$

^{3}H ground-state (NCSM)



[figures courtesy of A. Calci and R. Roth]

Operator Bases for the IMSRG

- choose a **basis of operators** to represent the flow (make an educated guess about physics):

$$H(s) = \sum_i c_i(s) O_i \,, \quad \eta(s) = \sum_i f_i(\{c(s)\}) O_i$$

- **close algebra by truncation,** if necessary:

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

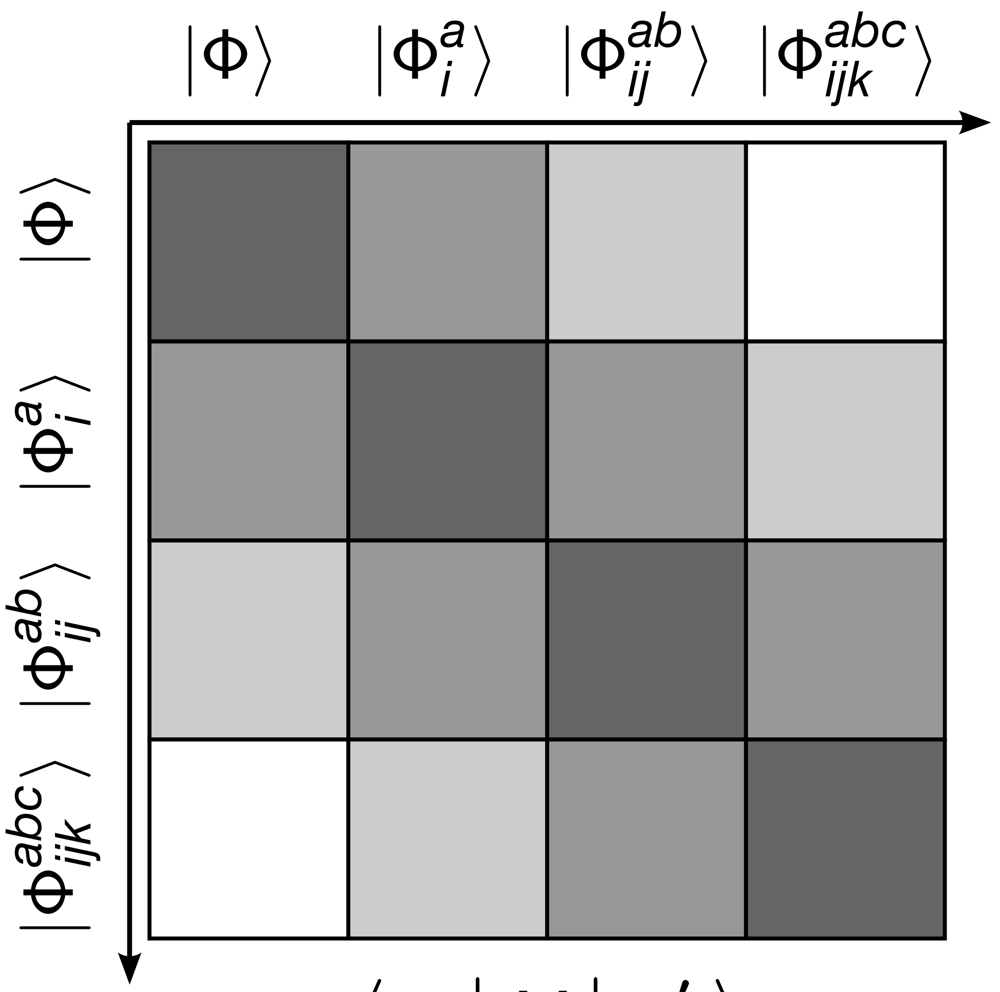
- **flow equations** for the coefficient (**coupling constants**):

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

- "obvious" choice for many-body problems:

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

Transforming the Hamiltonian

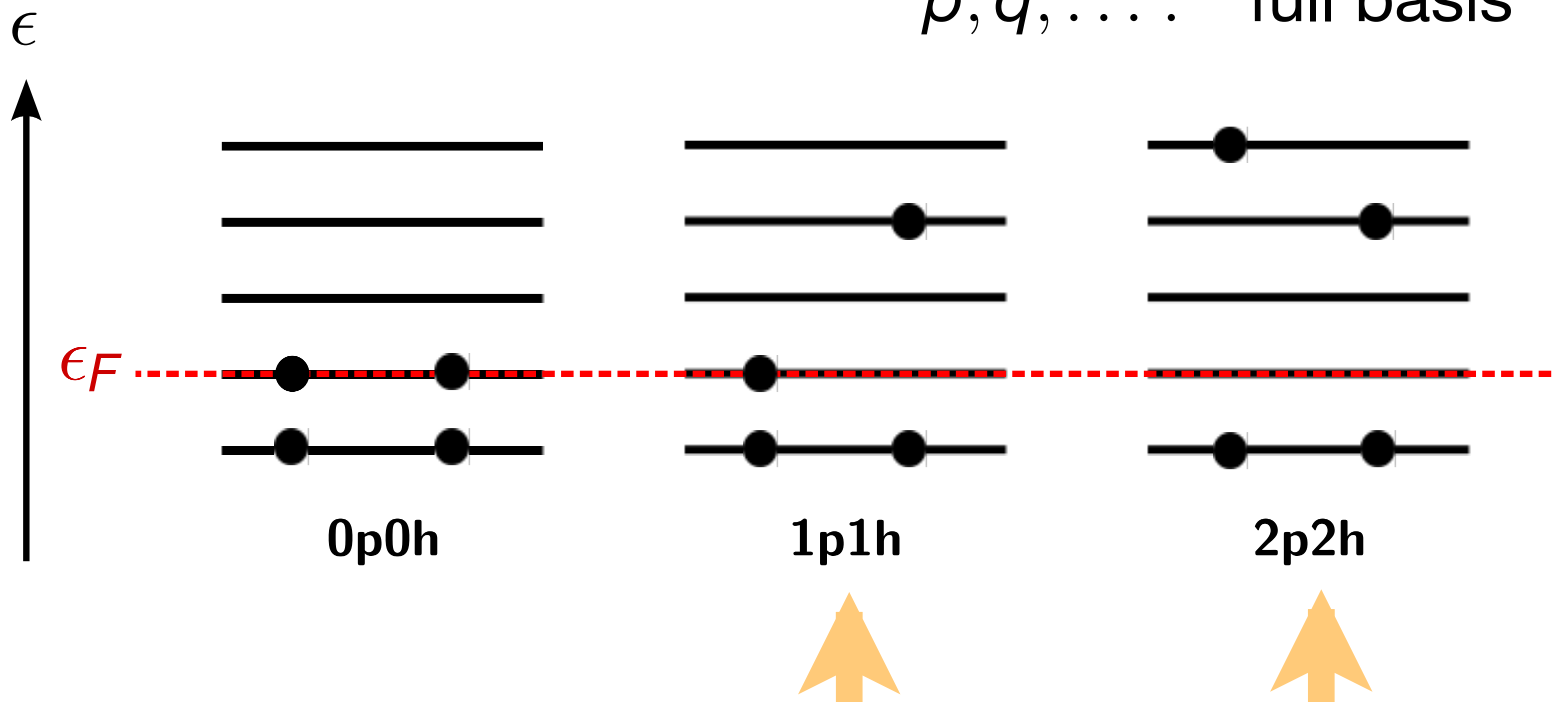


$$\left\langle \Phi \middle| H \middle| \Phi' \right\rangle$$

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

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

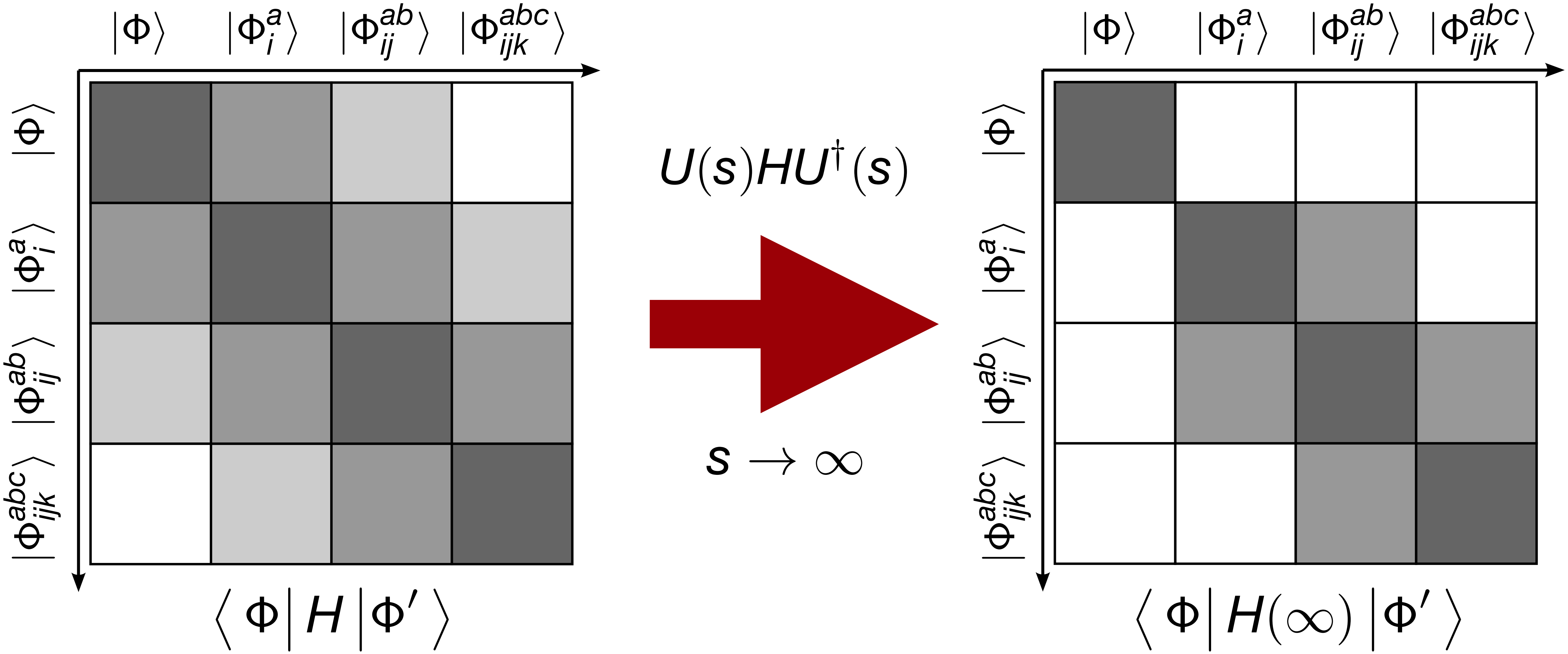
$p, q, \ldots :$ full basis



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

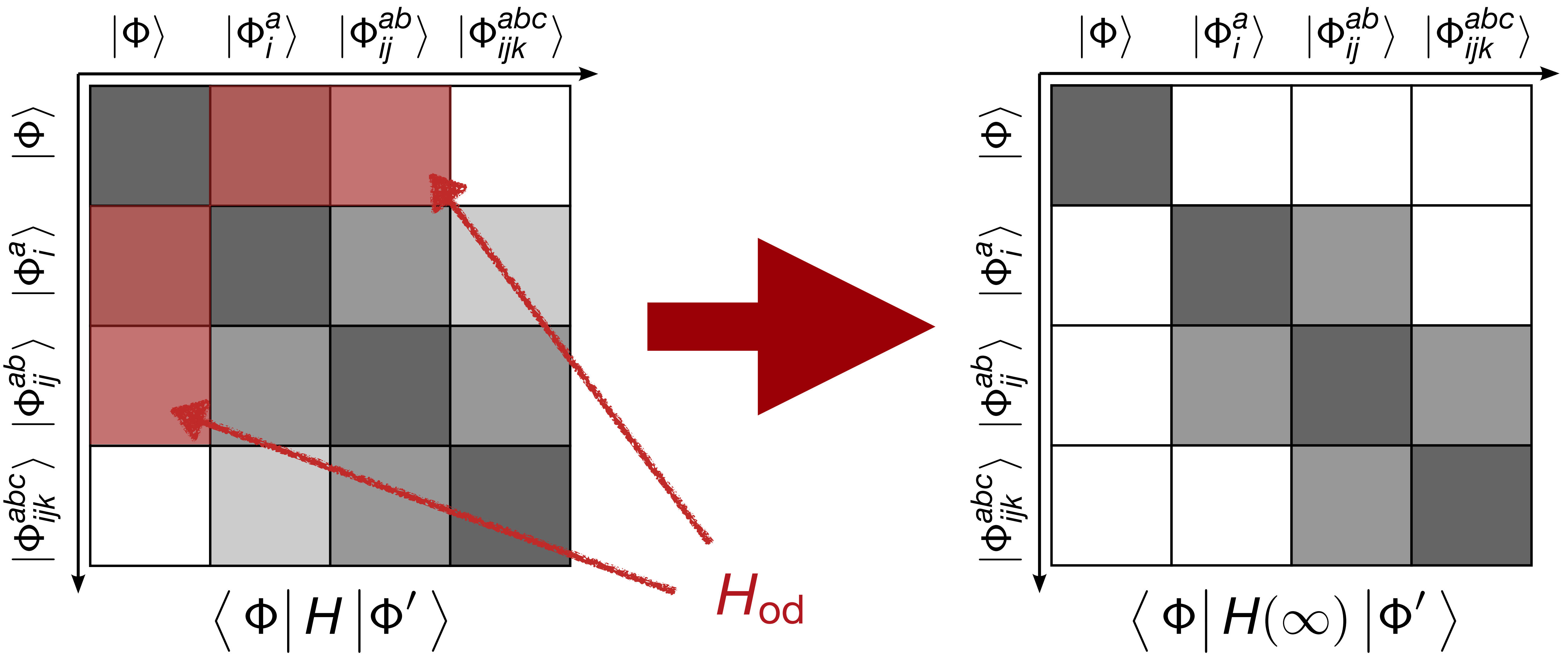
- reference state: **single Slater determinant**

Decoupling in A-Body Space



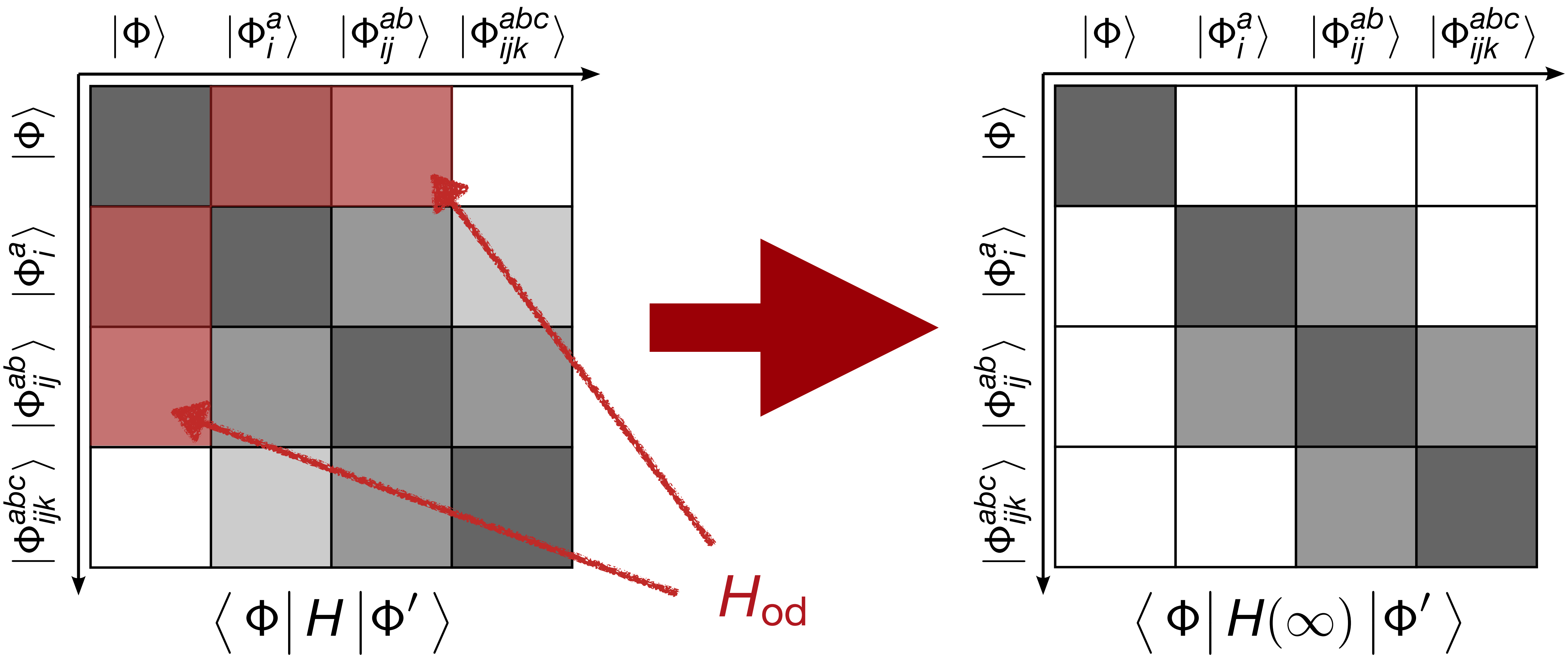
goal: decouple reference state $|\Phi\rangle$ from excitations

Flow Equation



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

Flow Equation



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

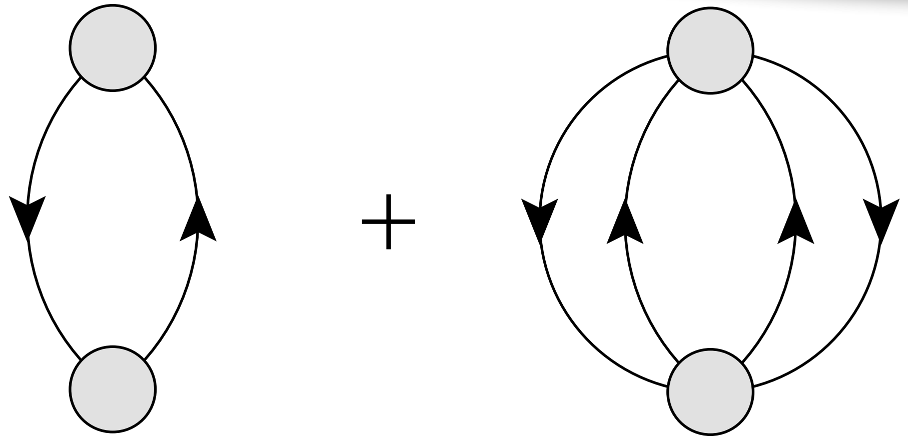
Operators
truncated at **two-body level** -
matrix is never constructed explicitly!

Standard IMSRG(2) Flow Equations

0-body Flow

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

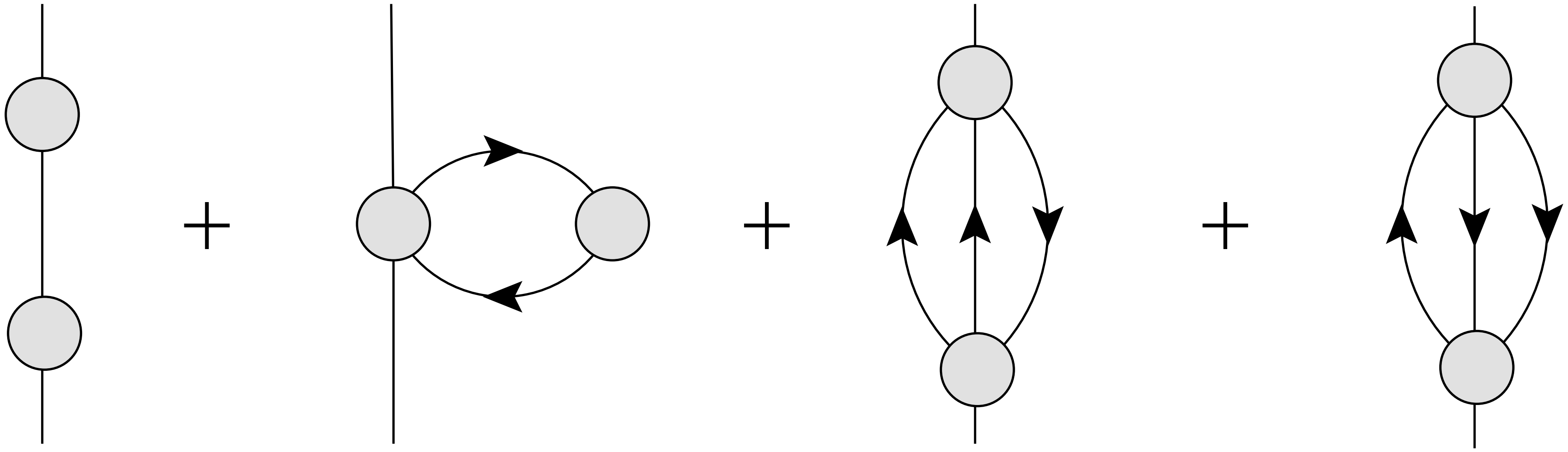
$$\frac{dE}{ds} =$$



coefficients (couplings) of H(s)

1-body Flow

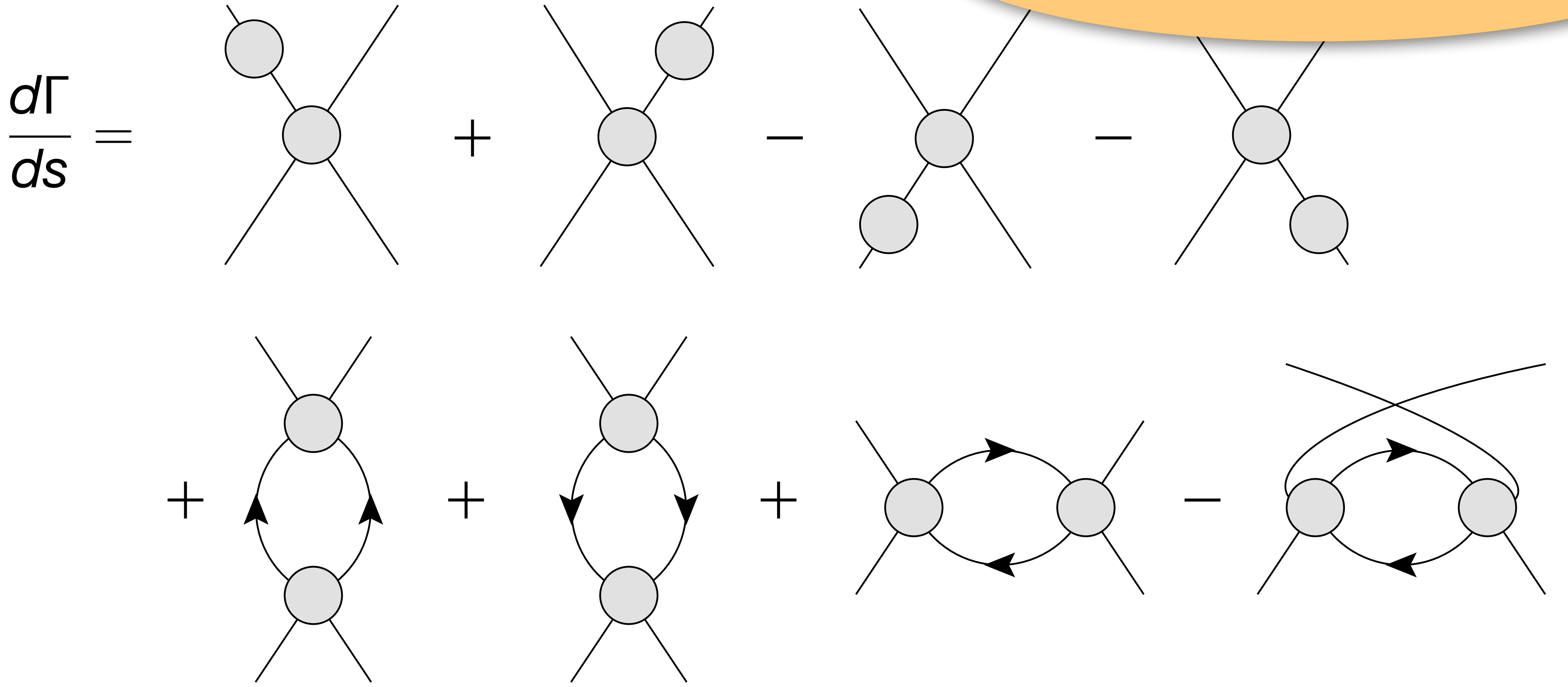
$$\frac{df}{ds} =$$



Standard IMSRG(2) Flow Equations

2-body Flow

O(N^6) scaling
(before particle/hole distinction)



s channel

ladders

t channel

u channel

rings

Coupled Cluster Method

- explicit ansatz for **similarity transformation**:

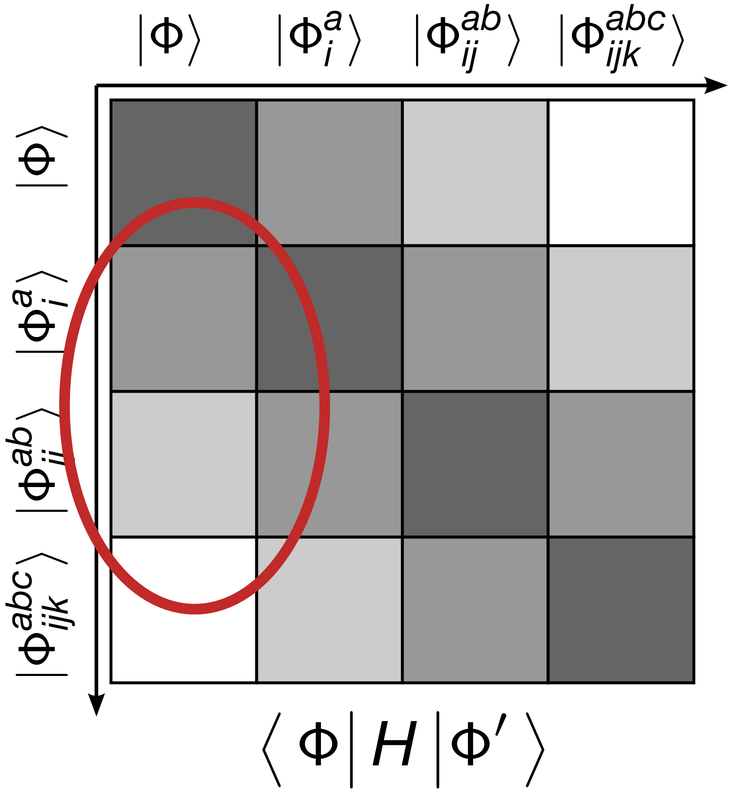
$$\bar{H} = e^{T} H e^{-T}, \qquad T = T^{[1]} + T^{[2]} + \dots$$

- **project** on 1p1h, 2p2h, ... spaces and demand that coupling terms vanish:

$$\langle \Phi_i^a | \bar{H} | \Phi \rangle = 0$$

$$\langle \Phi_{ij}^{ab} | \bar{H} | \Phi \rangle = 0$$

  - Note: effective Hamiltonian is **not Hermitian (symmetric)**!



- solve **non-linear algebraic equations** (e.g., conjugate gradient, quasi-Newton, ...)

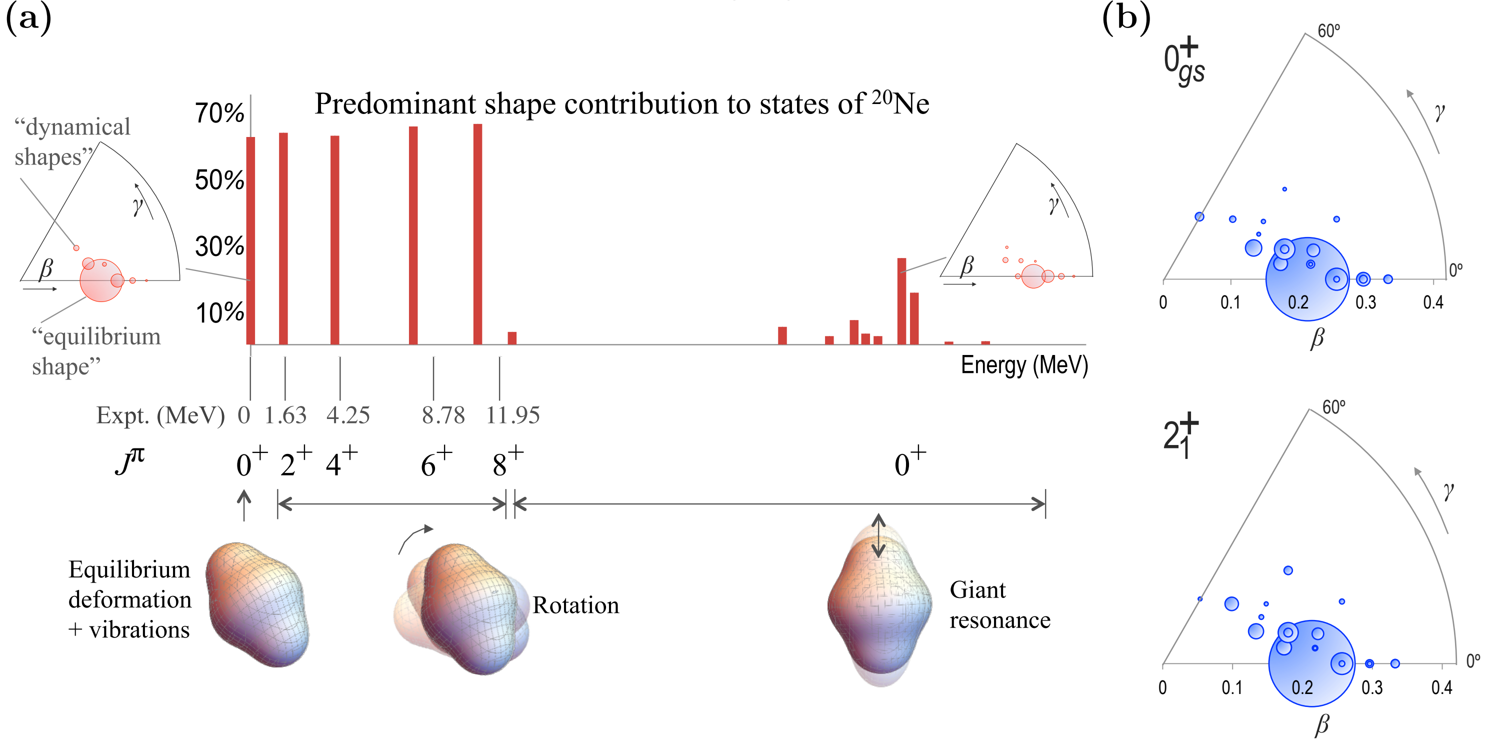
Symmetry-Adapted NCSM

- Demonstration of emergent **symplectic Sp(3,ℝ) symmetry** in nuclei

- Collective states in nuclei **dominated by few specific irreps**

- irreps allow **much smaller model spaces** than“brute force” particle-hole expansion

T. Dytrych et al., PRL ***124****, 042501 (2021)*



A. E. McCoy et al., PRL ***125****, 102505 (2021)*