Ab Initio Calculations for Deformed Nuclei with IMSRG Techniques

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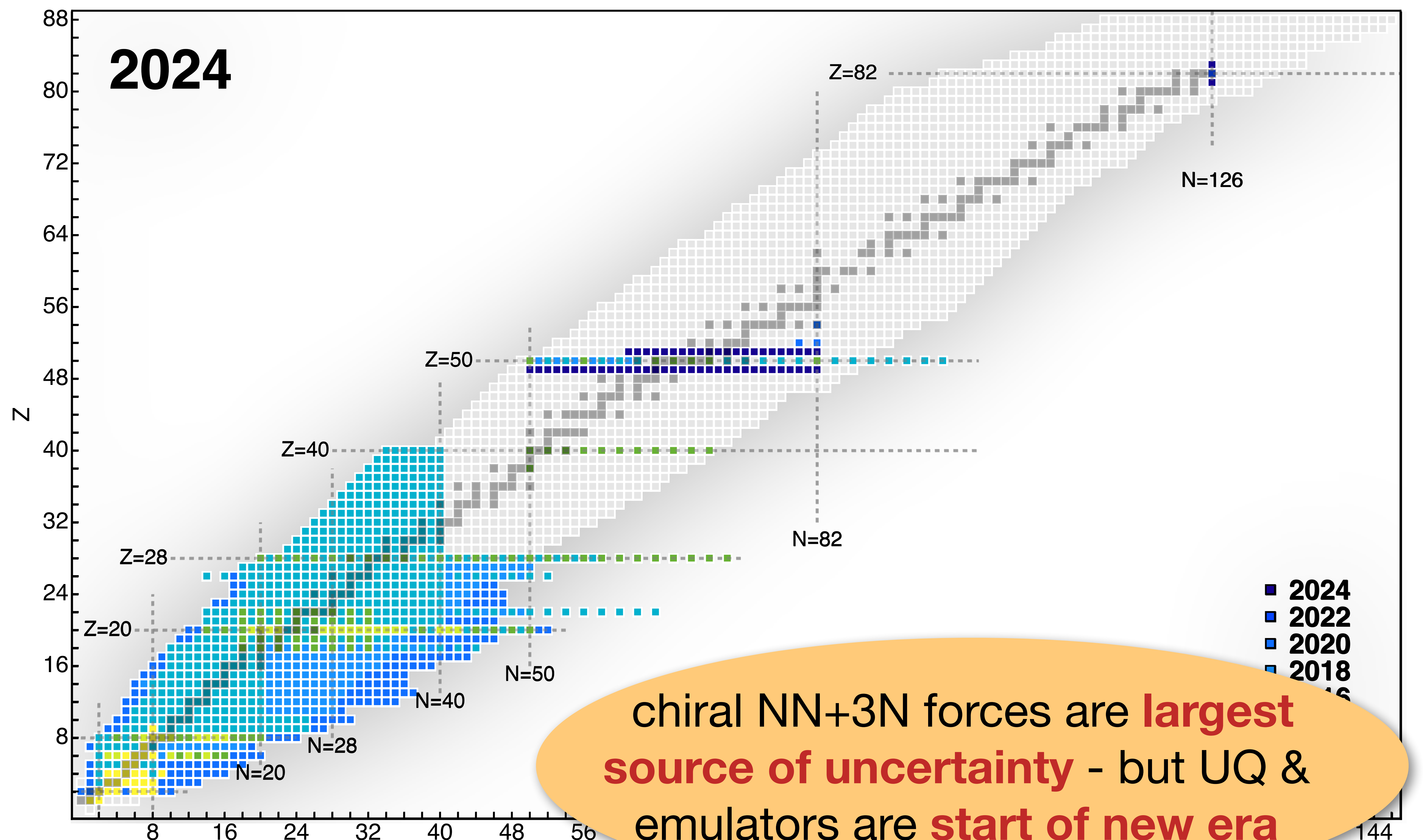
Progress in *Ab Initio* Calculations

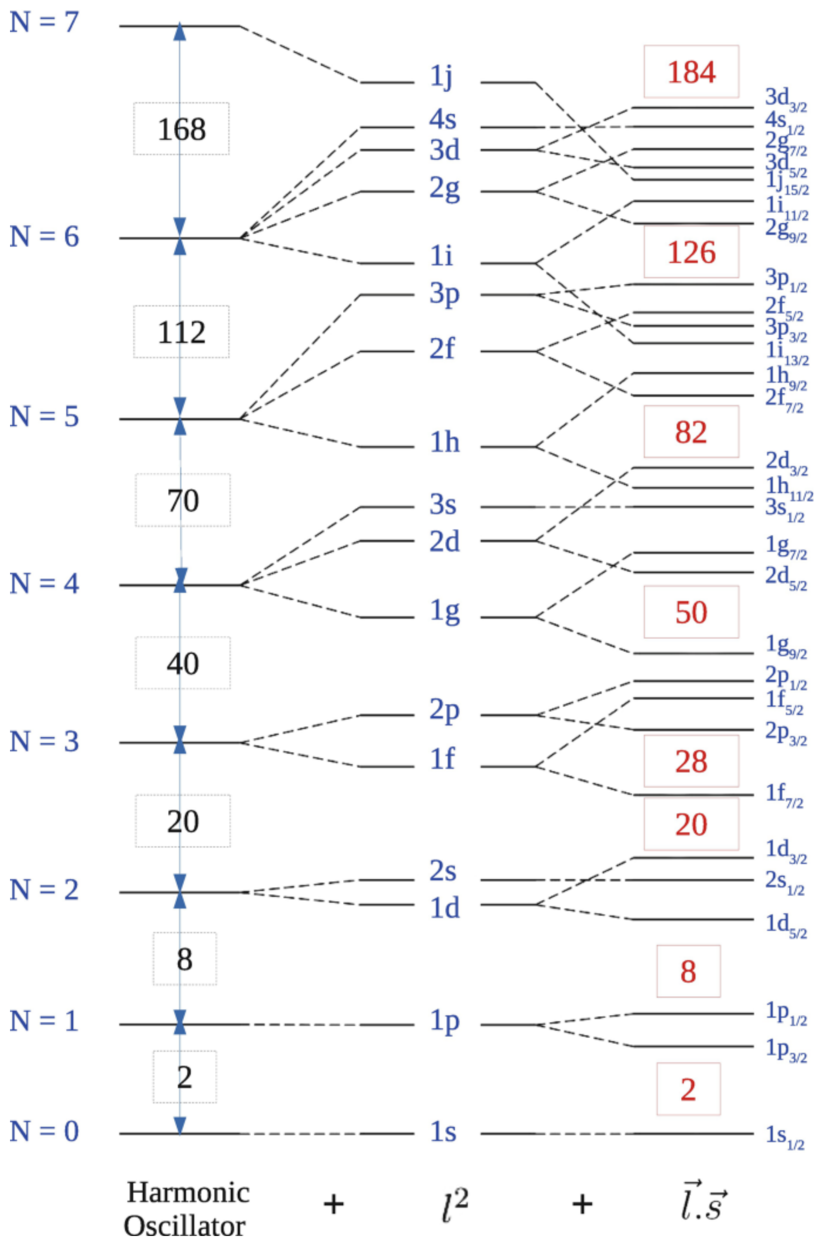
[cf. HH, Front. Phys. **8**, 379 (2020)]

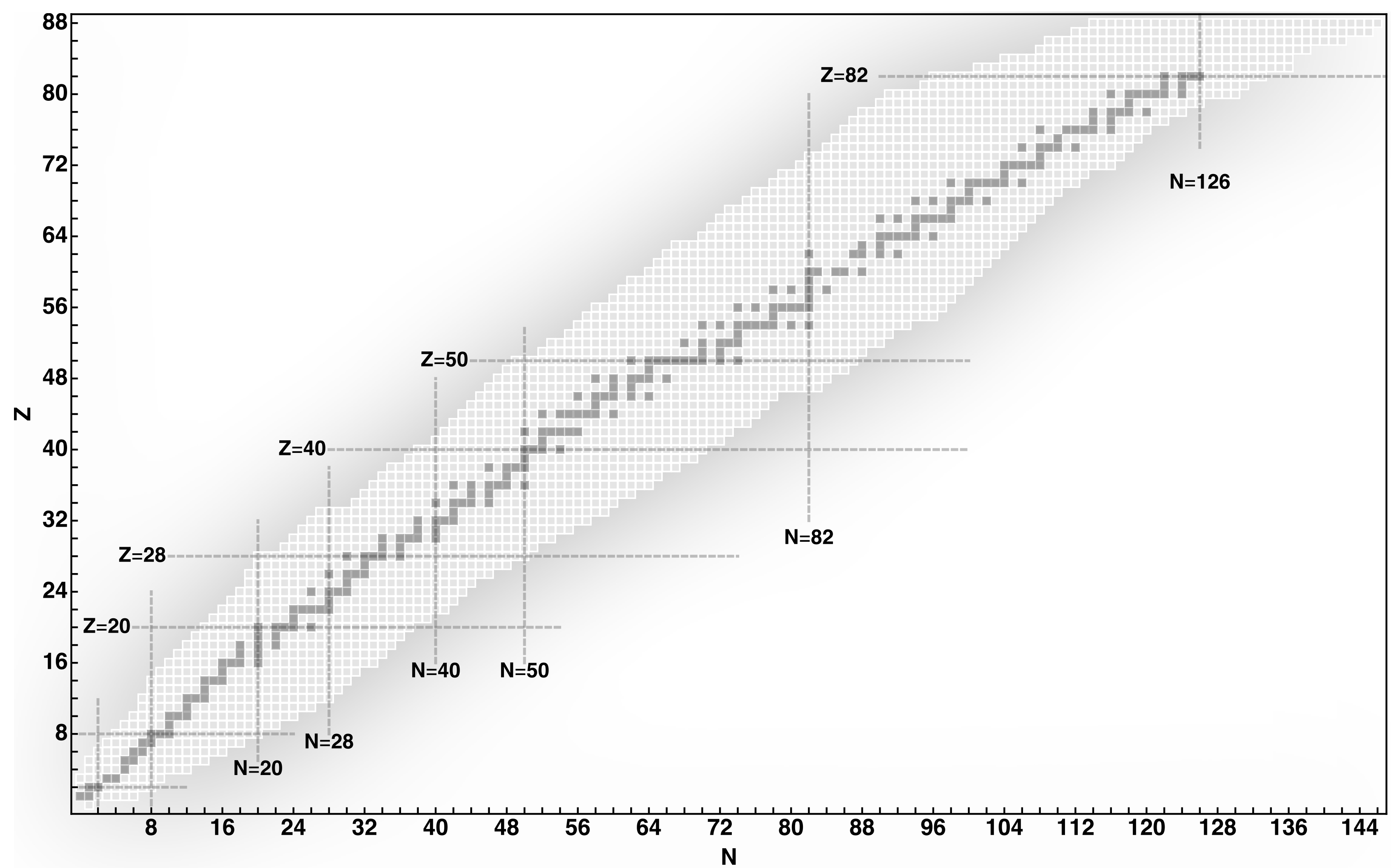


chiral NN+3N forces are **largest source of uncertainty** - but UQ & emulators are **start of new era**

Where Do We Want to Go (Today)?

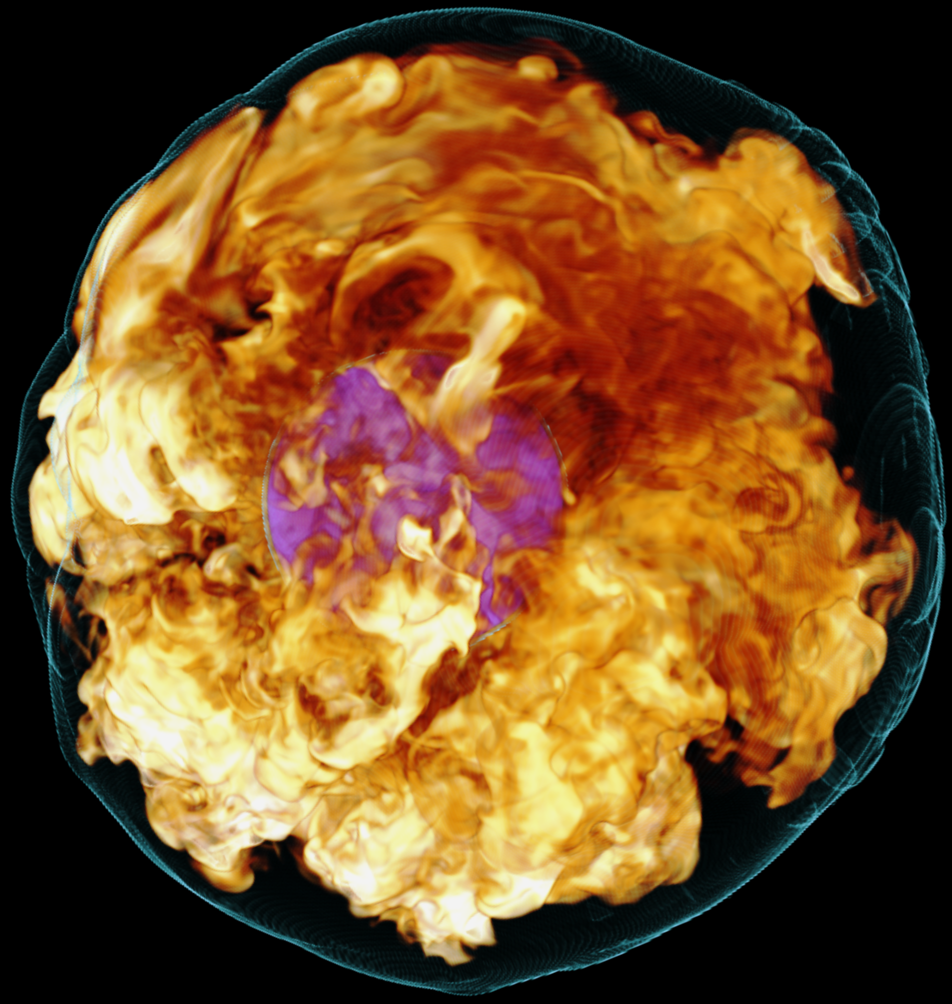
How Does Nuclear Structure Evolve?



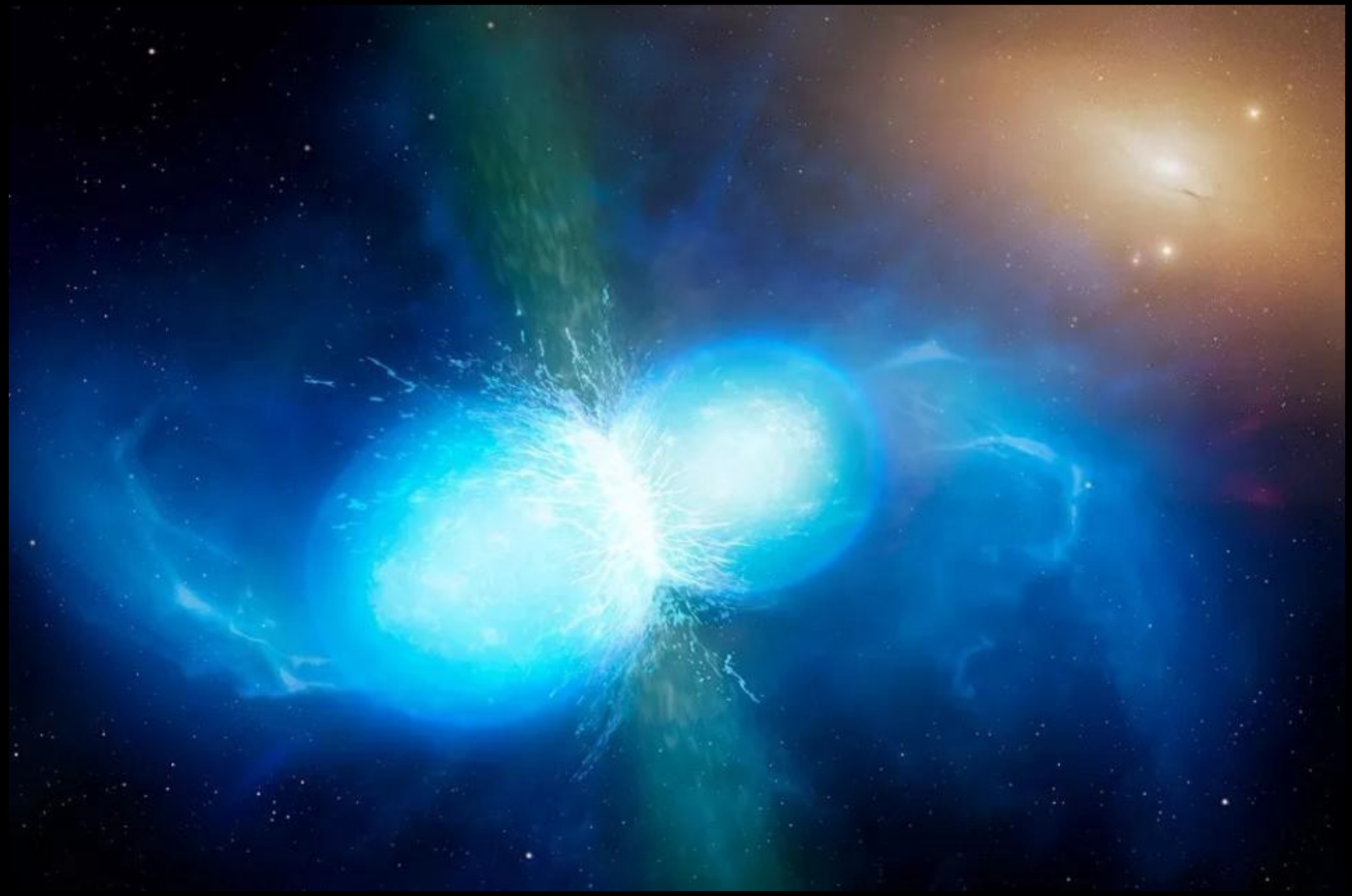


- Evolution of **(intrinsic) shapes** along isotopic chains
- New phenomena: **neutron skins, halos**, …
- Emergence of **new magic numbers** (and absence of old ones)

How Were the Elements Made?



Core-Collapse Supernovae



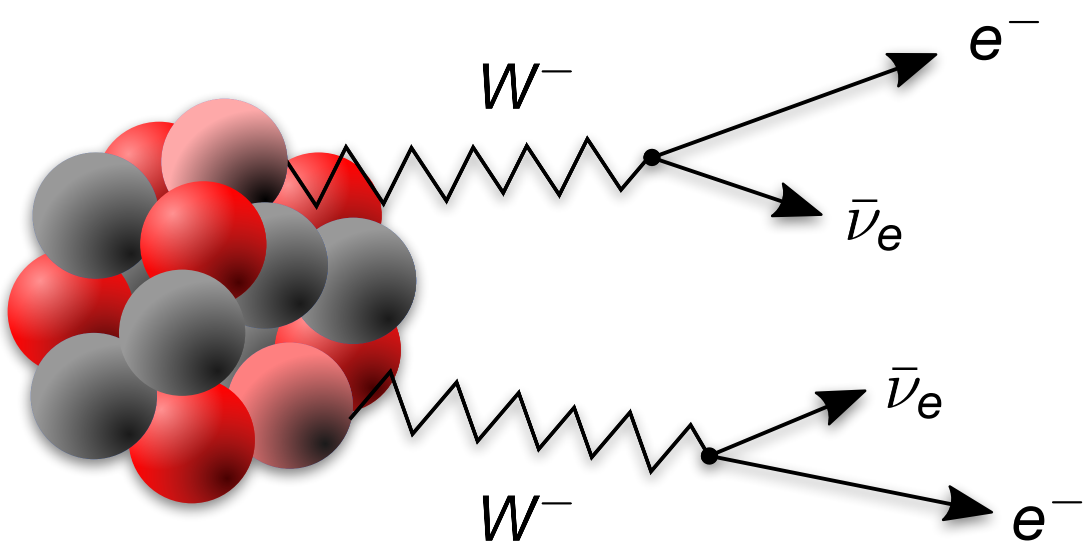
Neutron-Star Mergers

Multi-physics problem that requires microscopic inputs

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

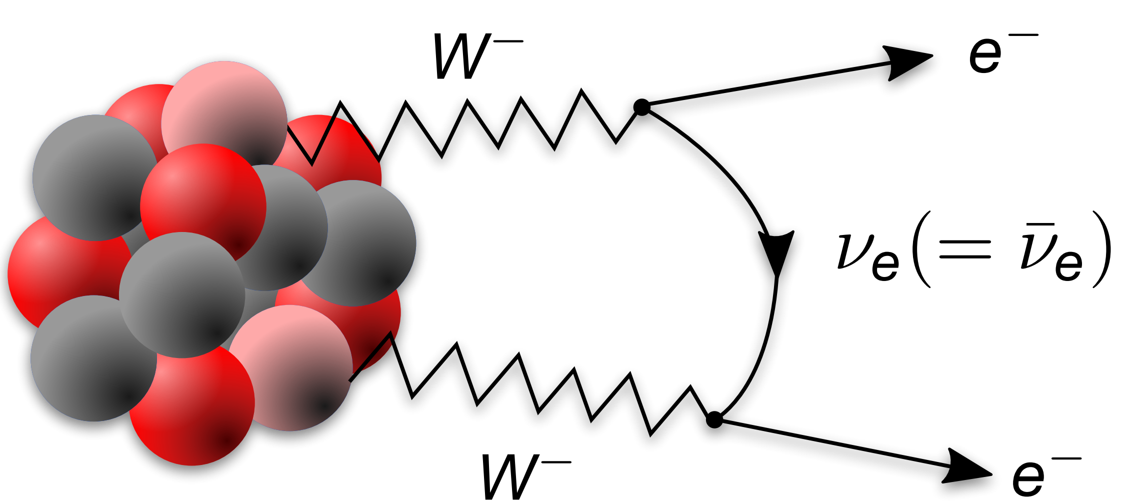
Physics Beyond the Standard Model

“Standard” Double Beta Decay



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

Neutrinoless Double Beta Decay

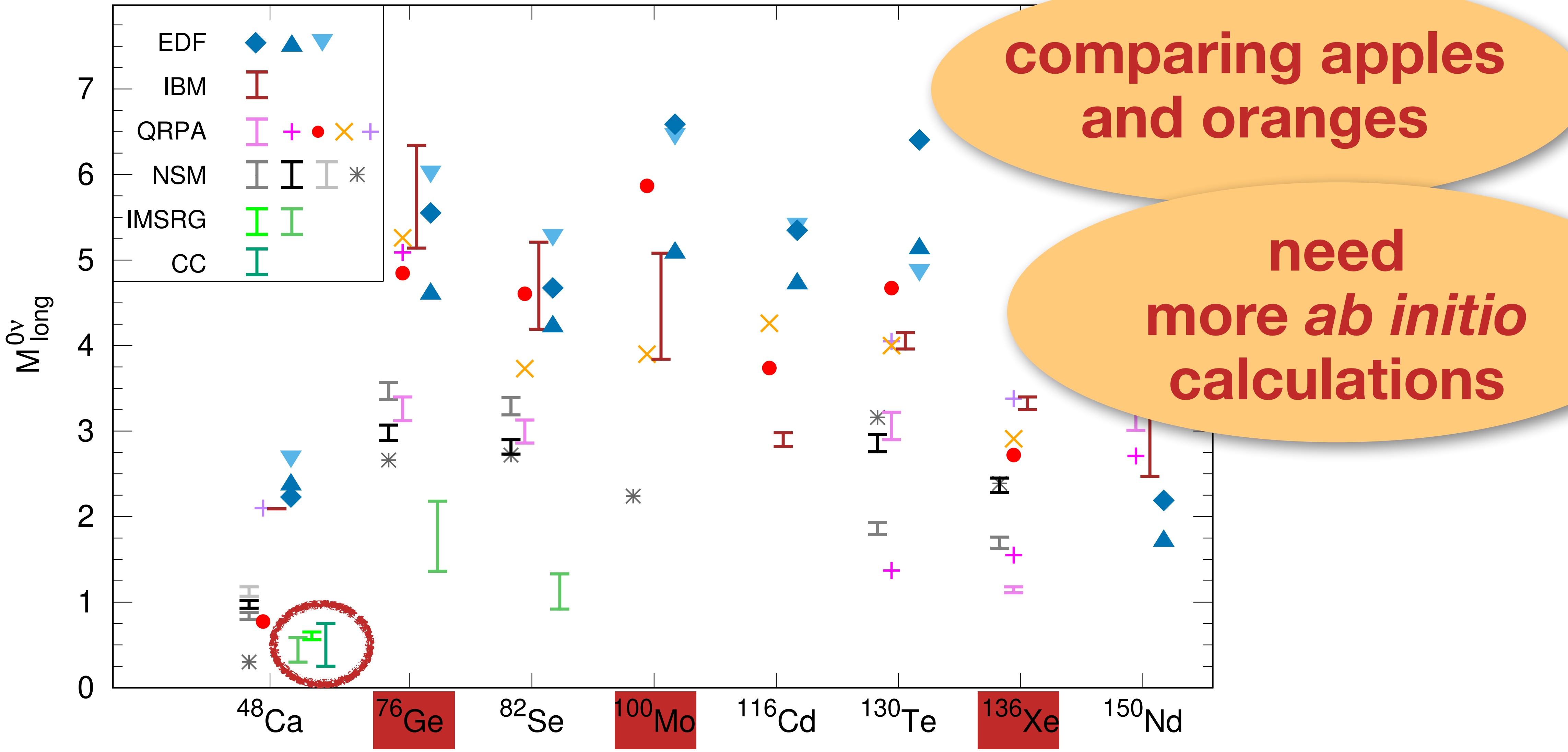


- neutrinos are **Majorana** particles

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

Nuclear Matrix Elements

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



- 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

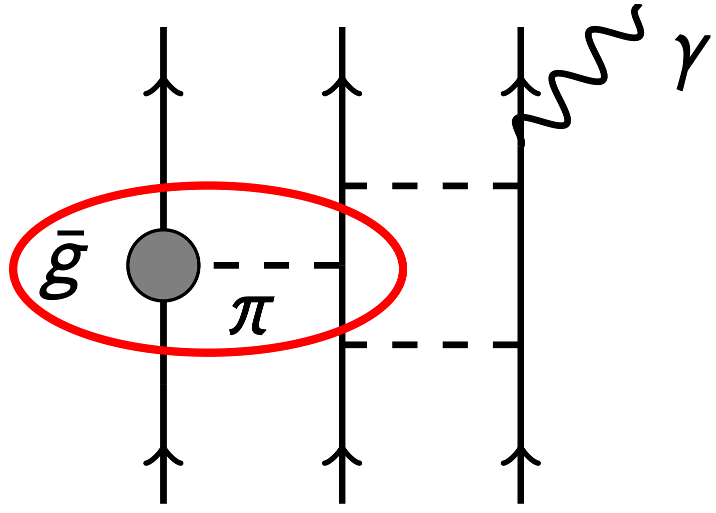
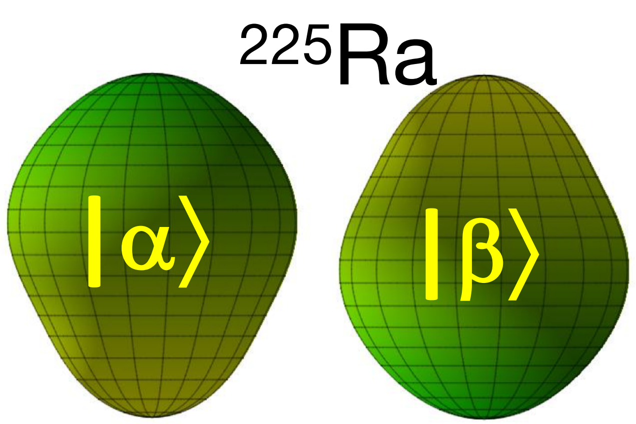


image credit: J. Engel

- 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

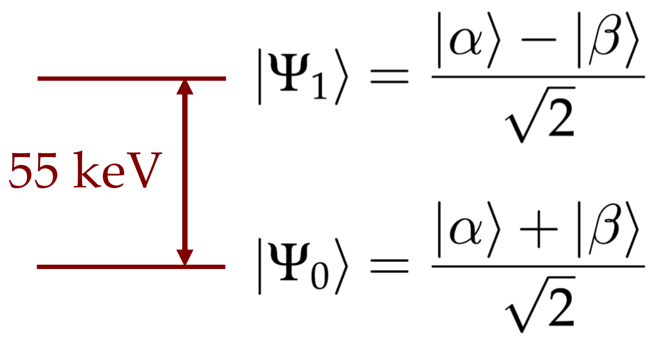
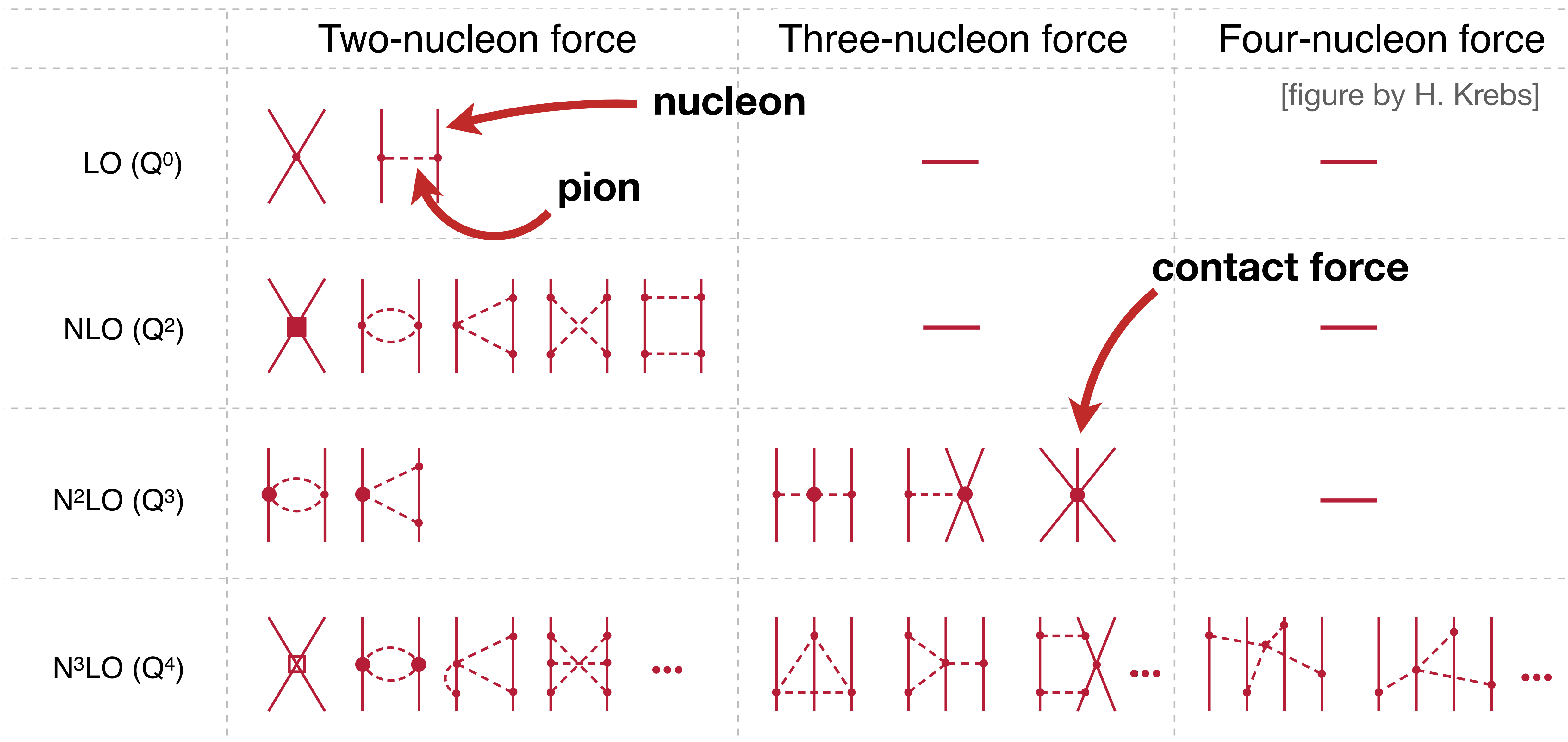


image credit: J. Singh

Where Do We Start?

Chiral Effective Field Theory

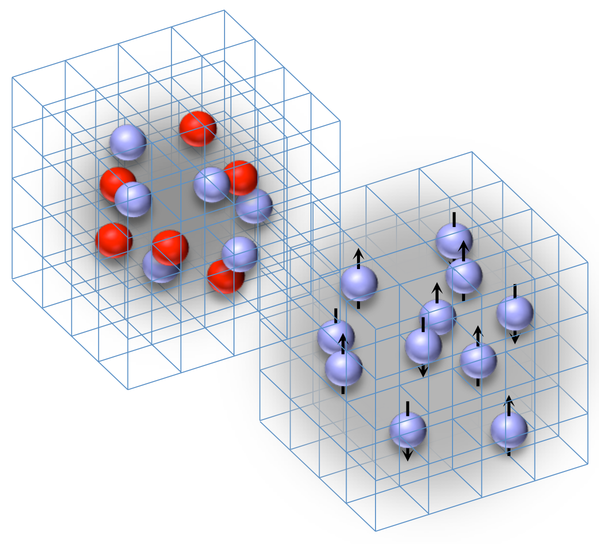


- organization in powers $(Q/\Lambda_\chi)^\nu$ allows systematic improvement
- low-energy constants fit to NN, 3N data (future: from Lattice QCD (?))
- consistent NN, 3N, ... interactions & transition operators

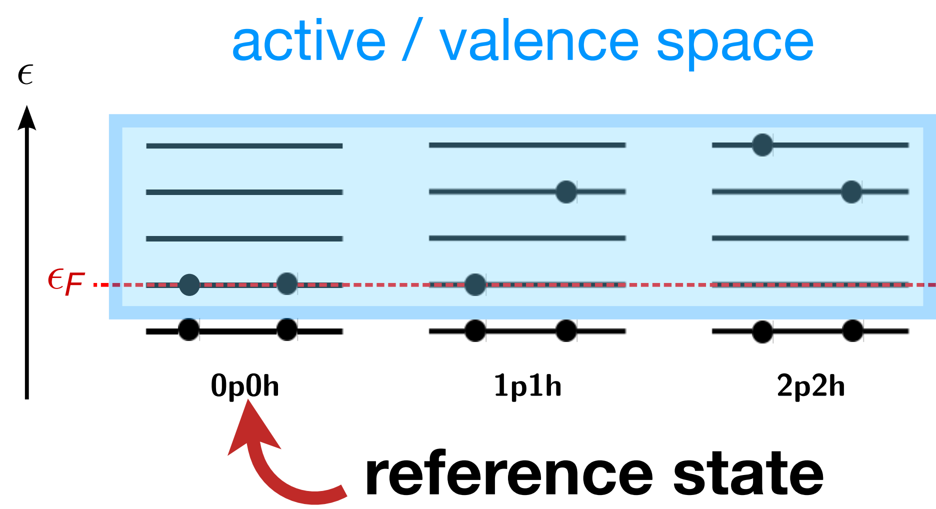
Many Roads Lead to Rome

Paradigms

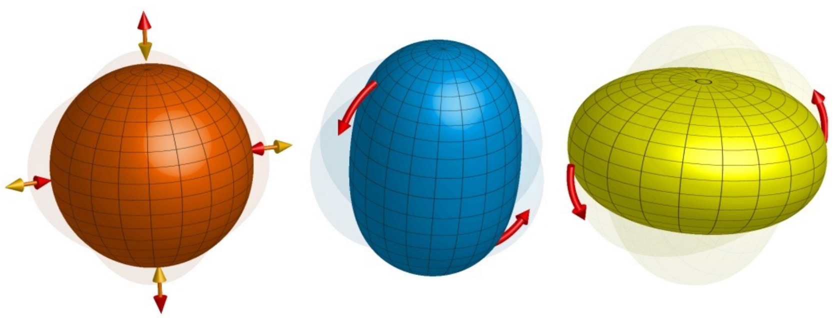
- **Coordinate Space**
  - Quantum Monte Carlo
  - Lattice EFT



- **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)

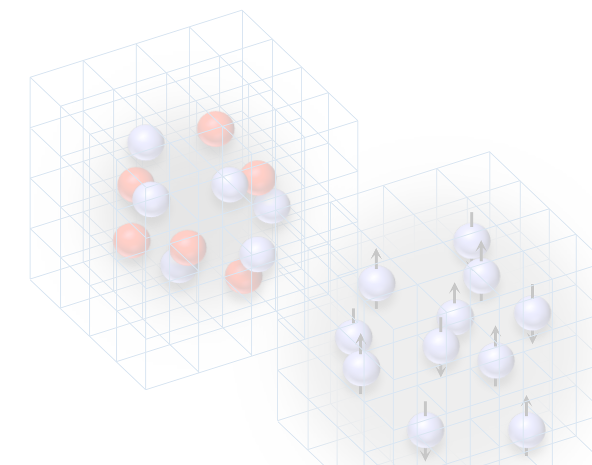


- **Configuration Space / Coordinate Space: Geometric Expansions**
  - deformed HF(B) + projection
  - projected Generator Coordinate Method (PGCM)
  - symmetry-adapted NCSM



Paradigms

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

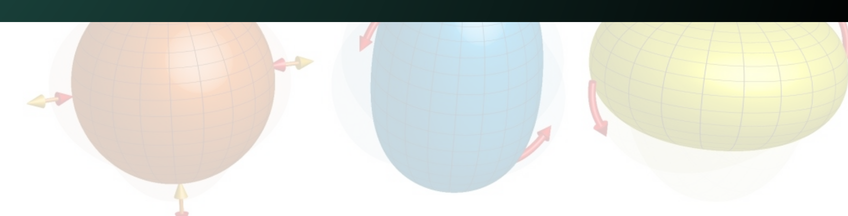


- **Configuration Space: Particle-Hole Expansions**

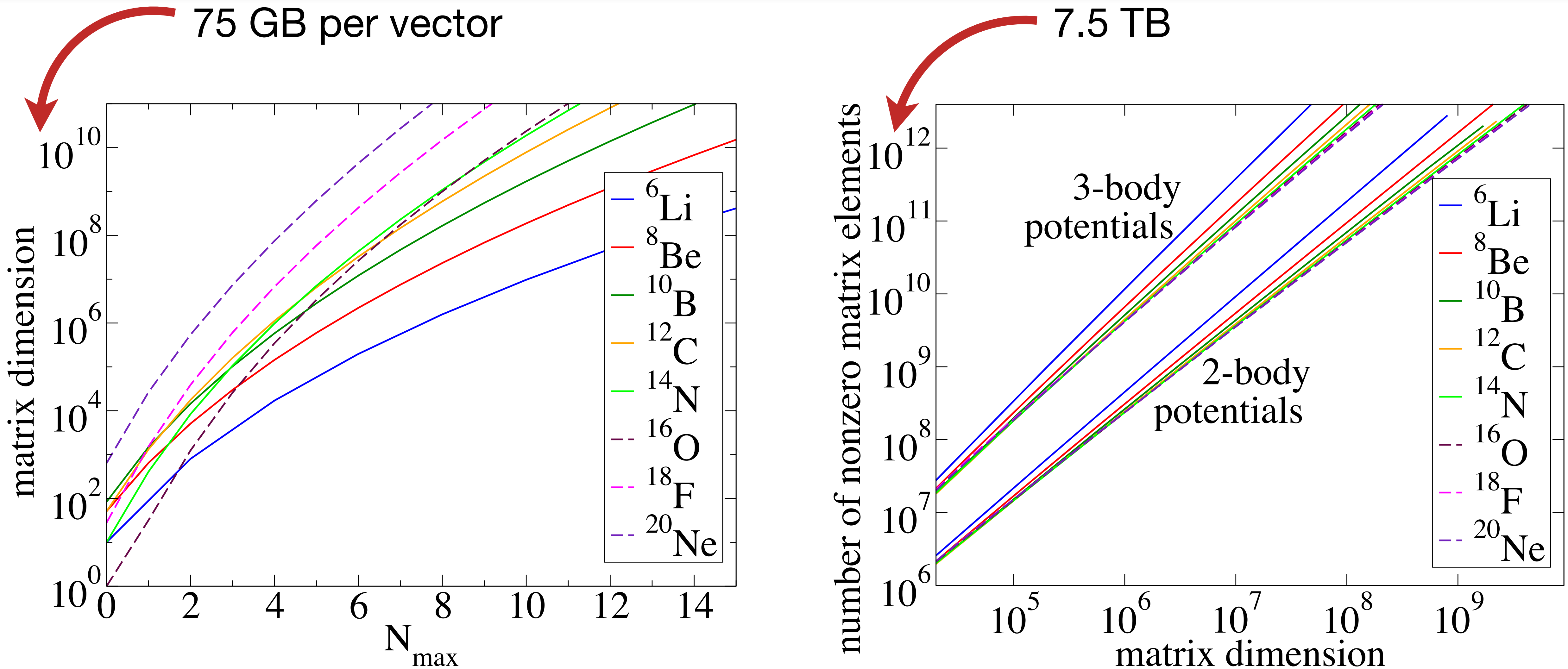
Recent(-ish) Reviews:
HH, Front. Phys. **8**, 379 (2020)
S. Gandolfi, D. Lonardoni, A. Lovato and M. Piarulli, Front. Phys. **8**, 117 (2020)
D. Lee, Front. Phys. **8**, 174 (2020)
V. Somà, Front. Phys. **8**, 340 (2020)

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



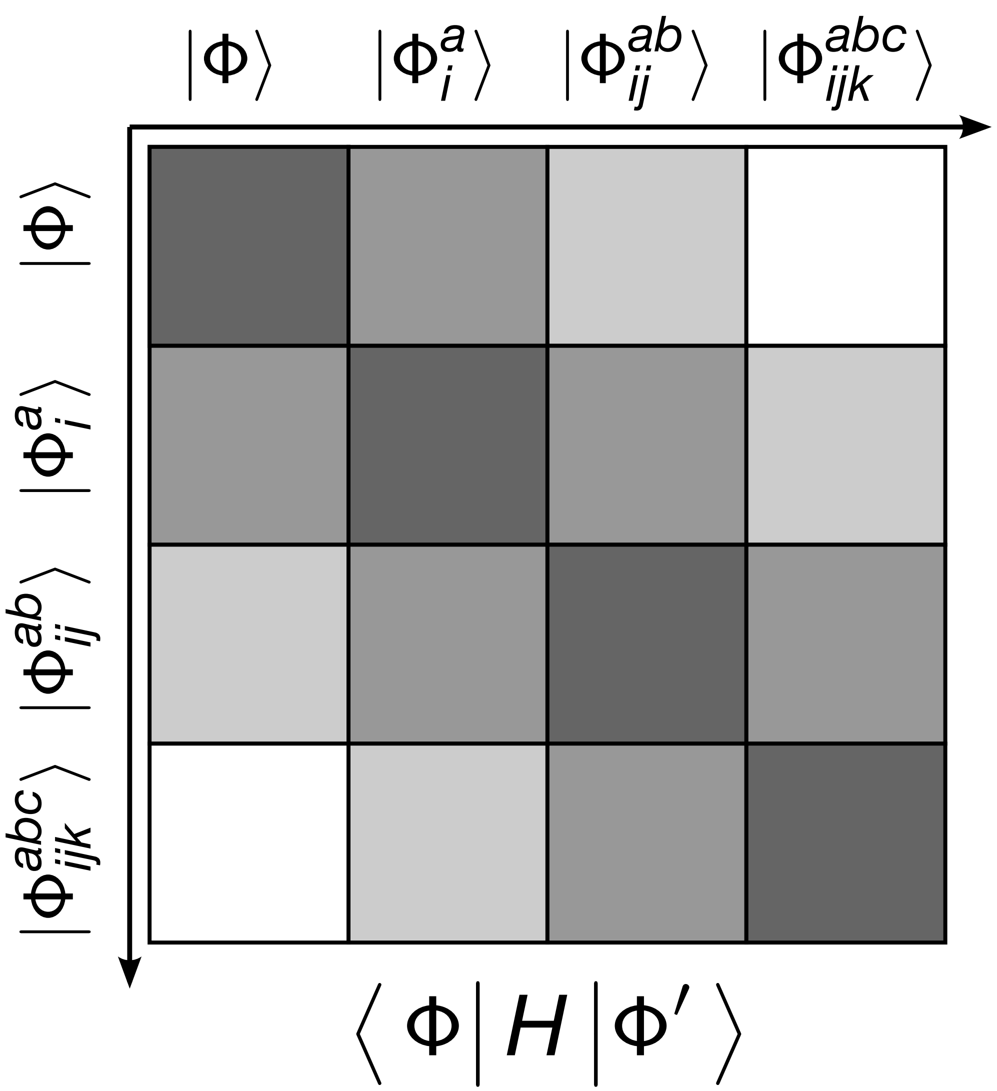
Basis Size “Explosion”



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**

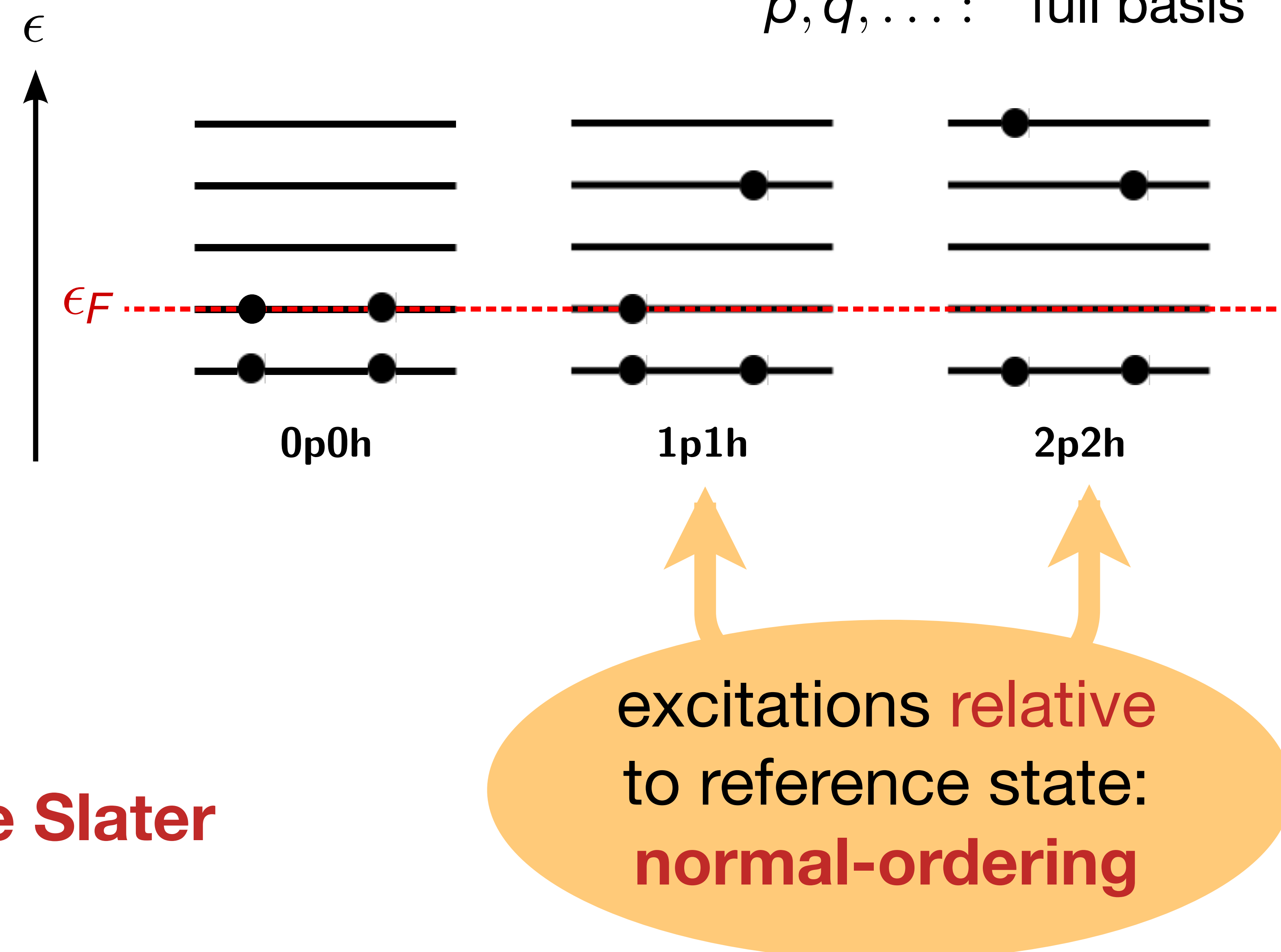
Transforming the Hamiltonian



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

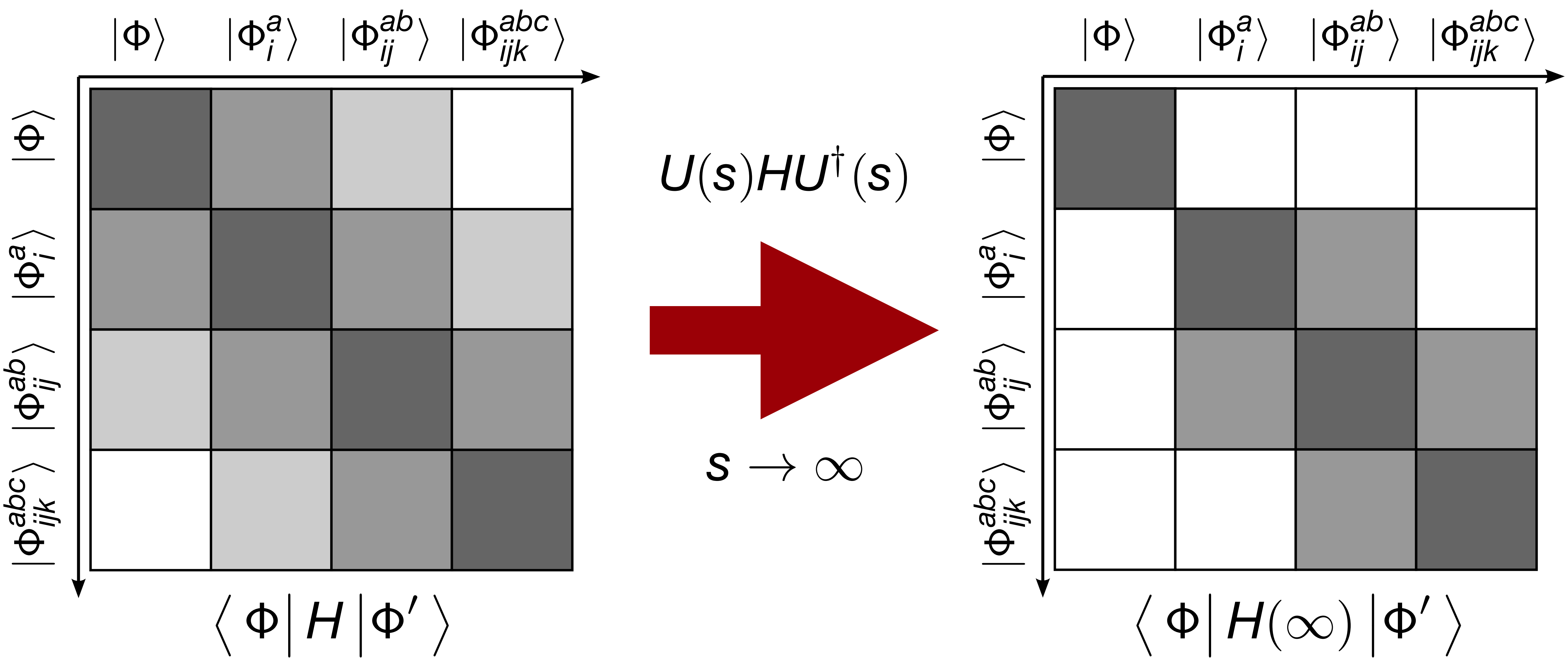
$i, j, \ldots :\quad \epsilon \leq \epsilon_F$

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



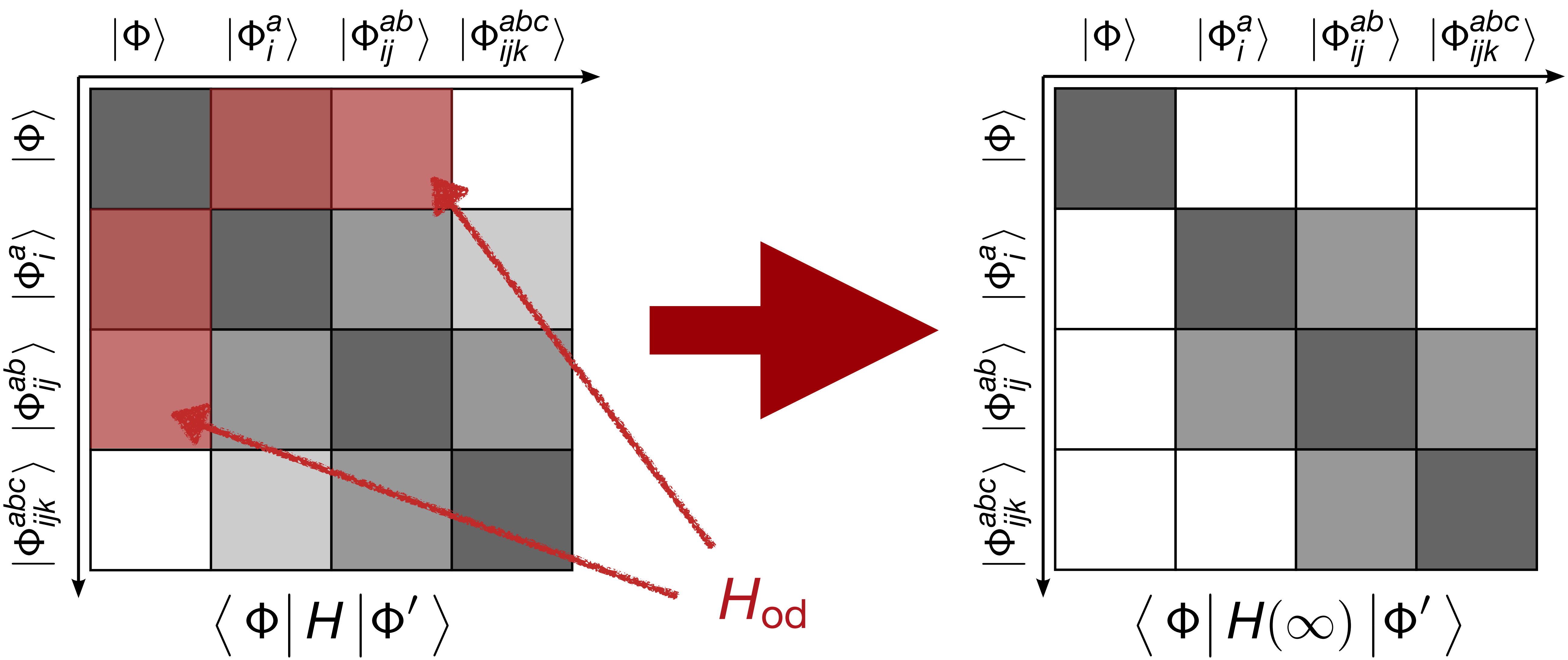
- reference state: **single Slater determinant**

Decoupling in A-Body Space



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

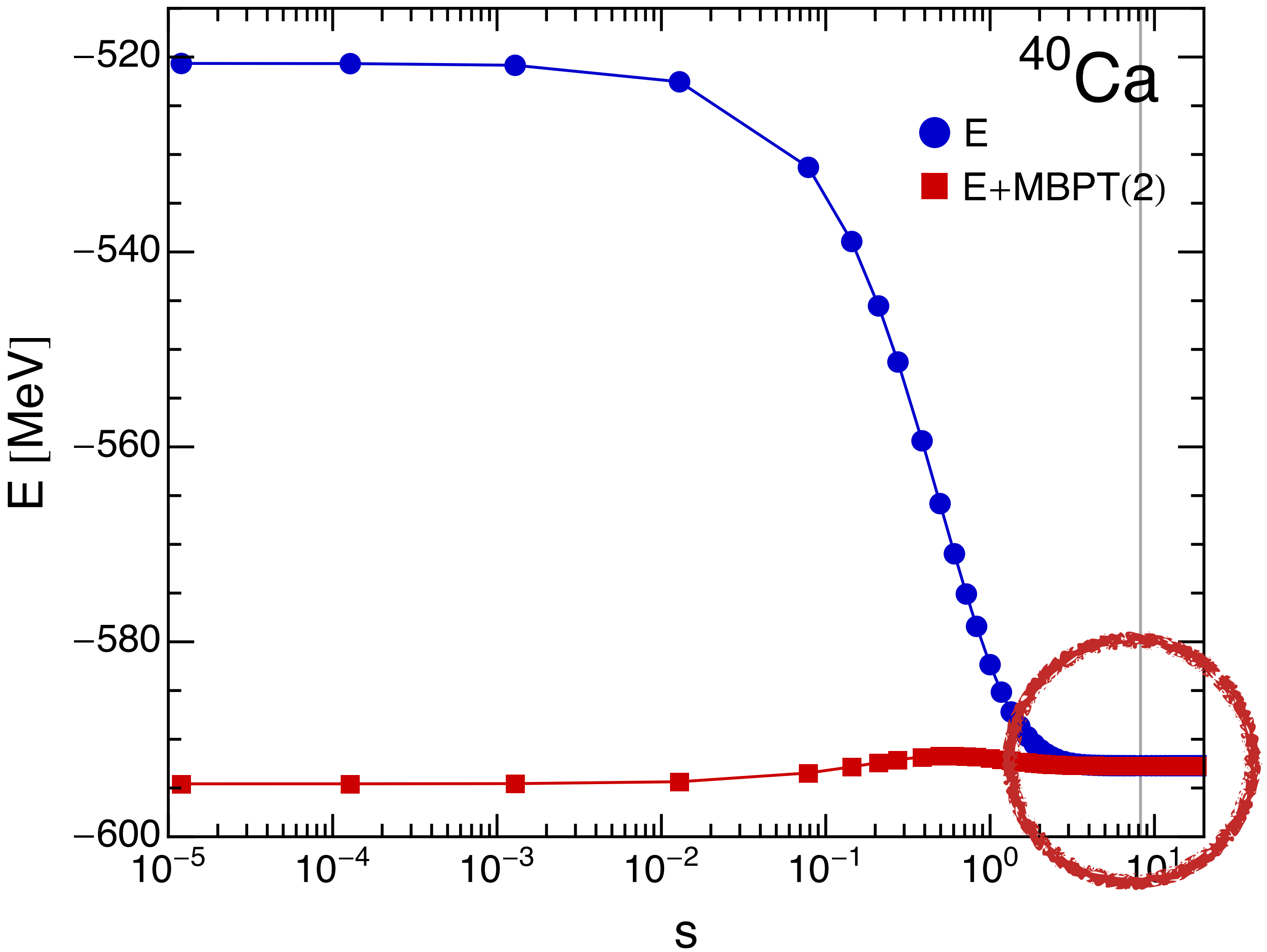
Flow Equation

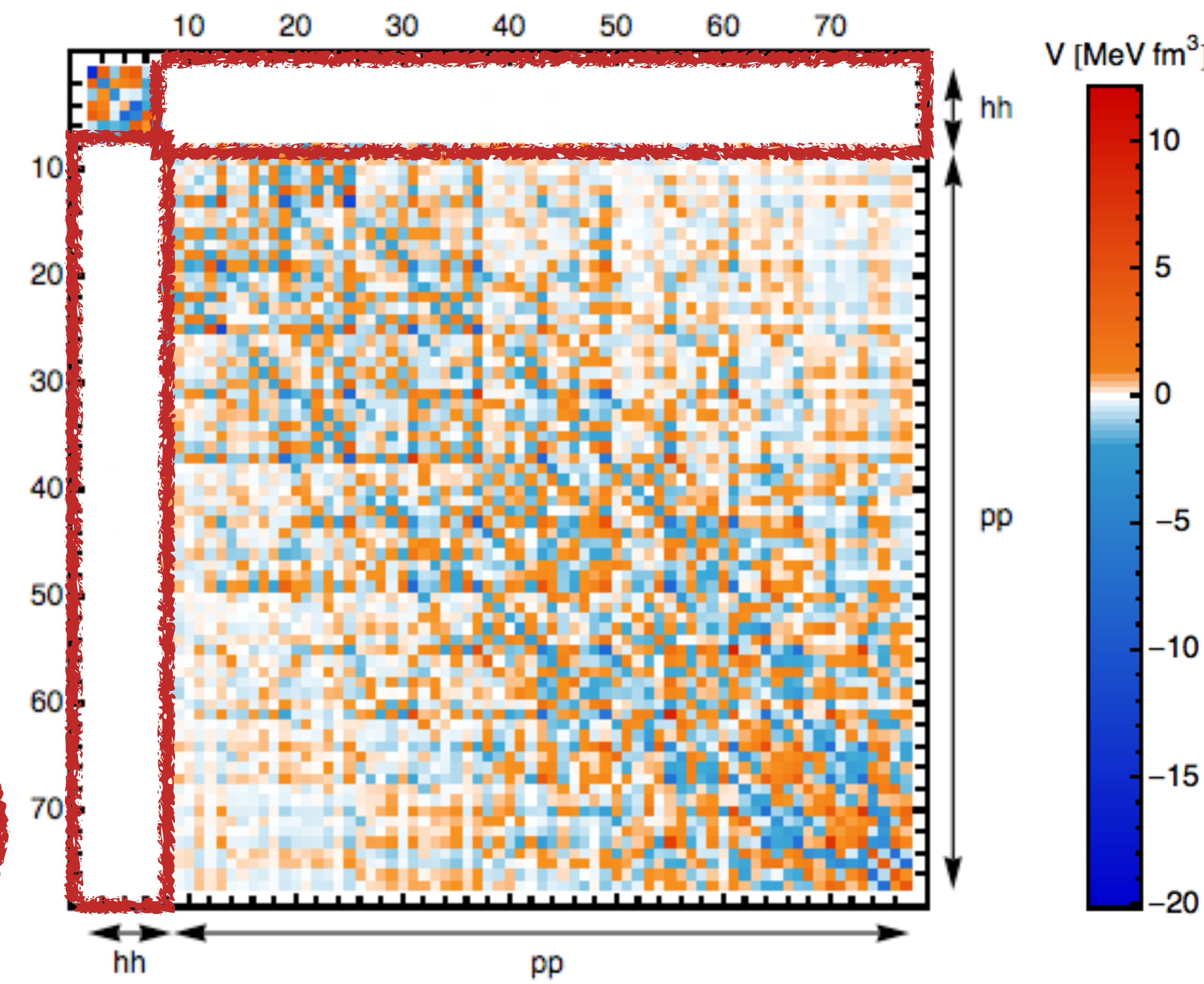


$$\frac{d}{ds}H(s) = \left[\eta(s), H(s)\right],$$

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

Decoupling



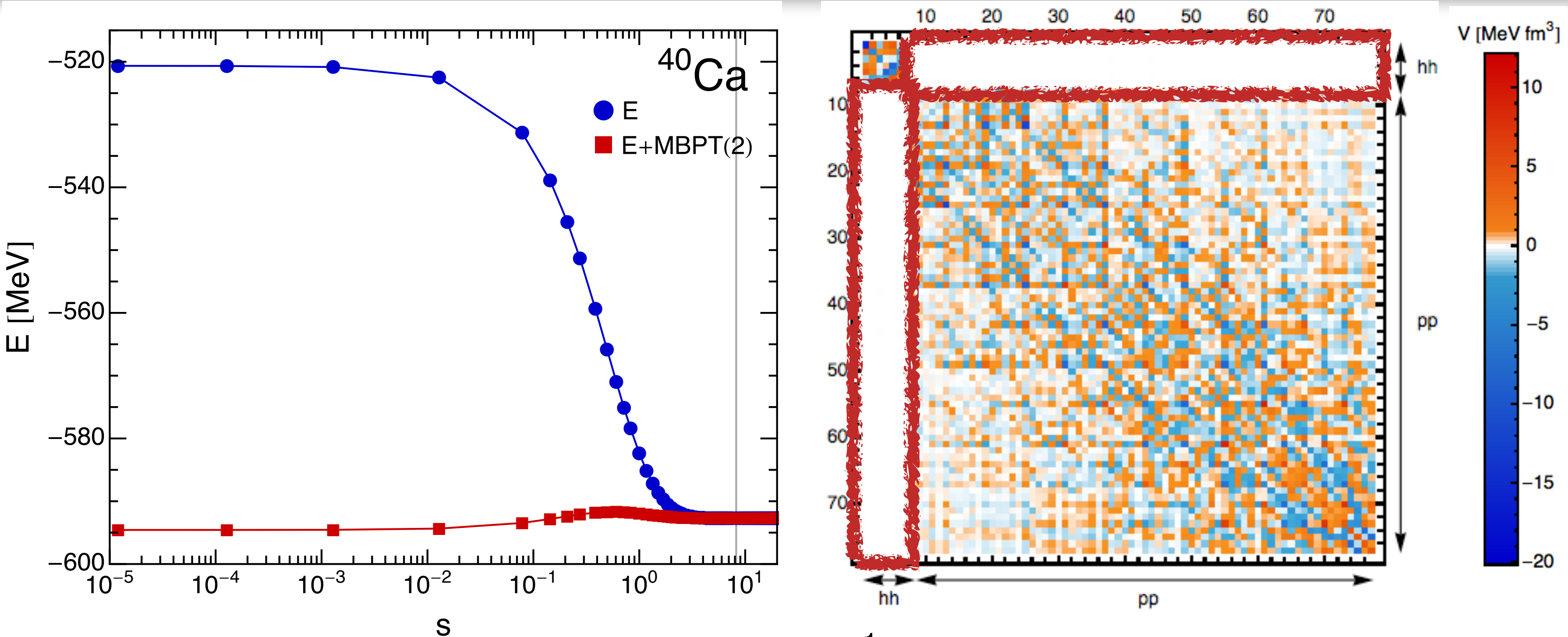


N3LO, $\lambda = 2.0\ \text{fm}^{-1}, e_{\text{Max}} = 8$

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

off-diagonal couplings are rapidly driven to zero

Decoupling



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

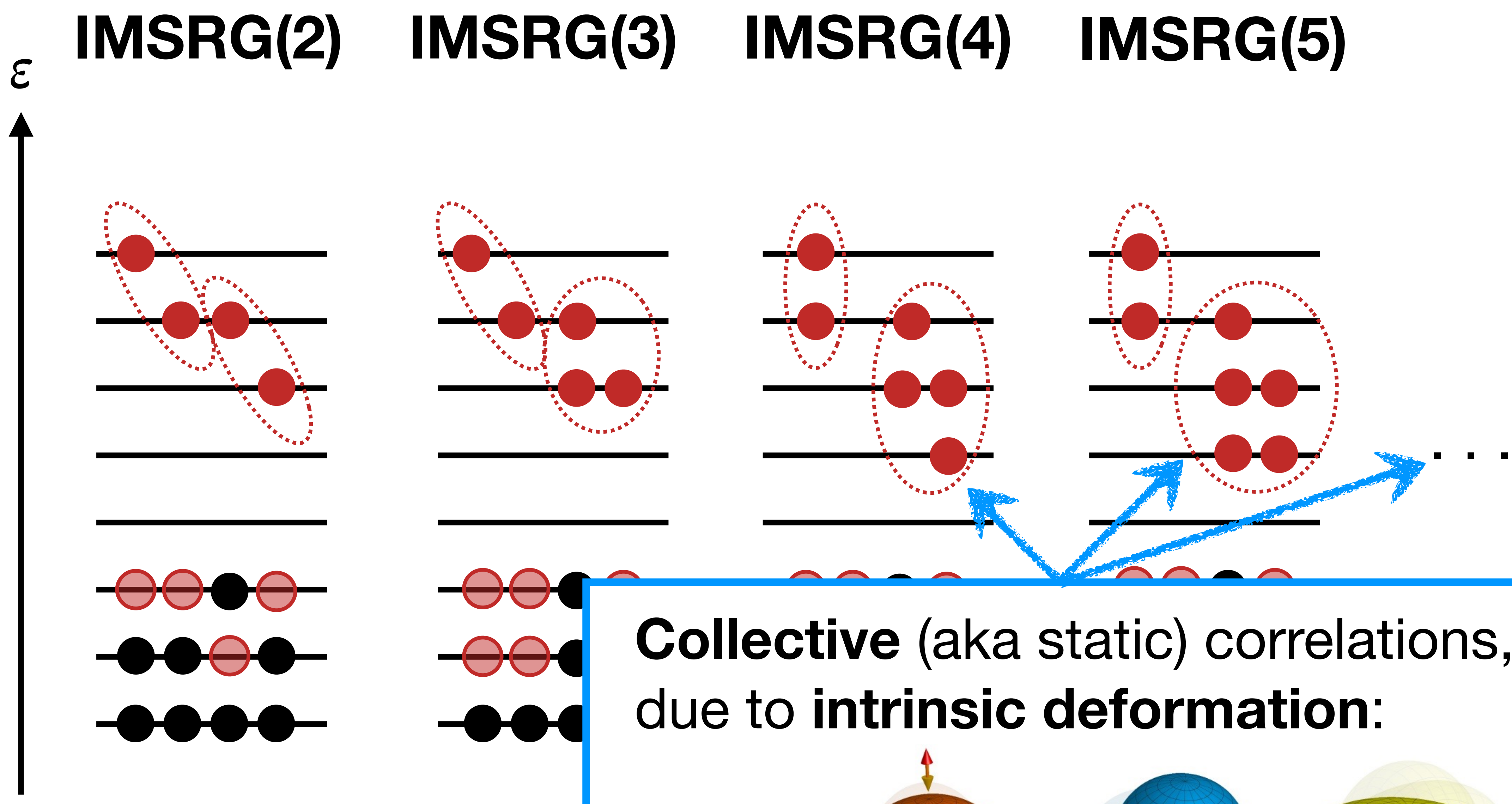
- absorb correlations into **RG-improved Hamiltonian**

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

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

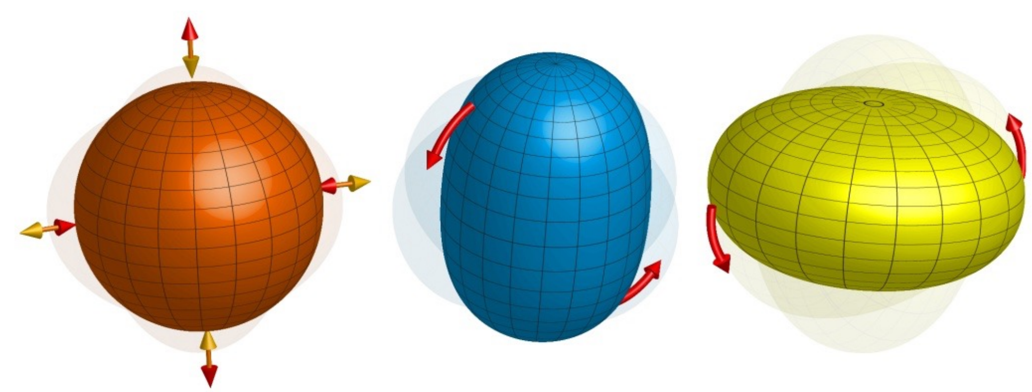
$$U(s) \left|\Psi_n\right\rangle \stackrel{!}{=} \left|\Phi\right\rangle$$

Correlated Reference States

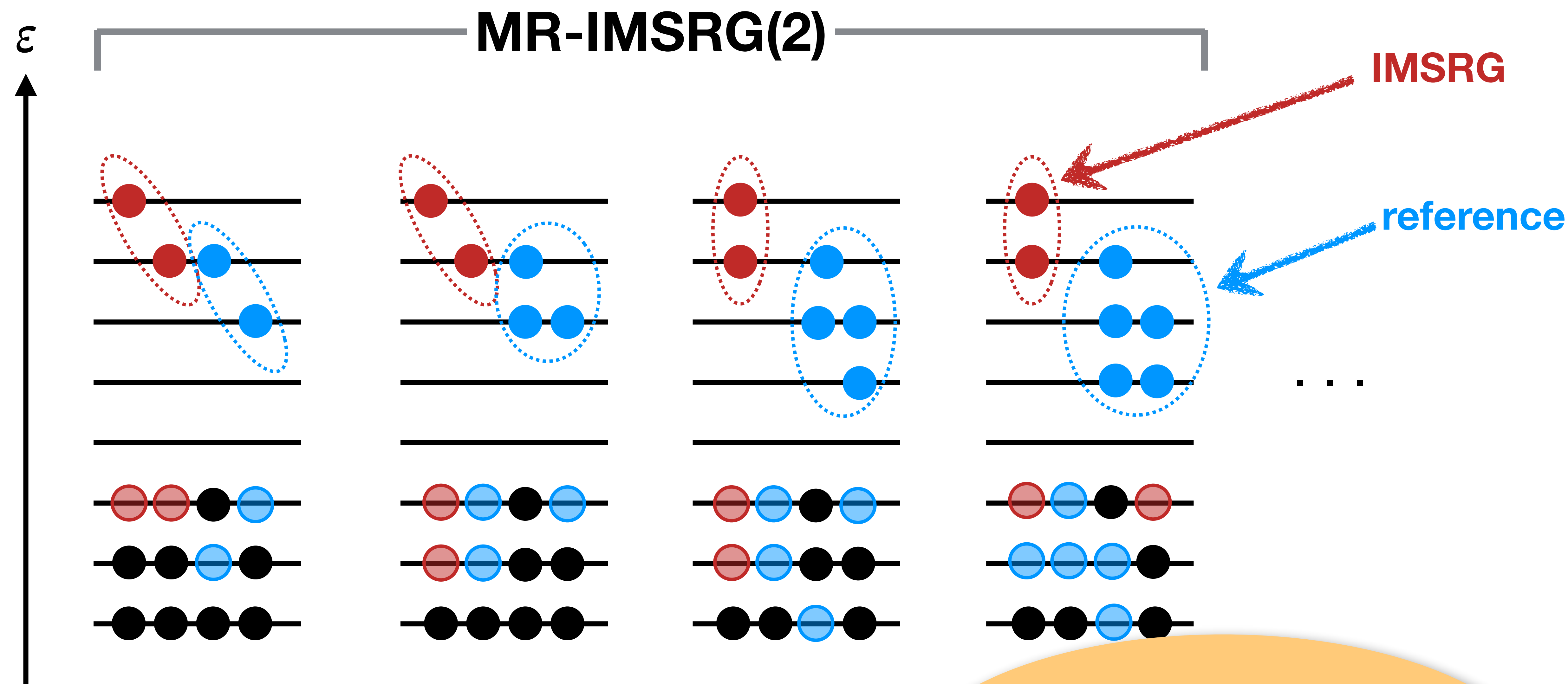


“standard” IMS
Slater determinan

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



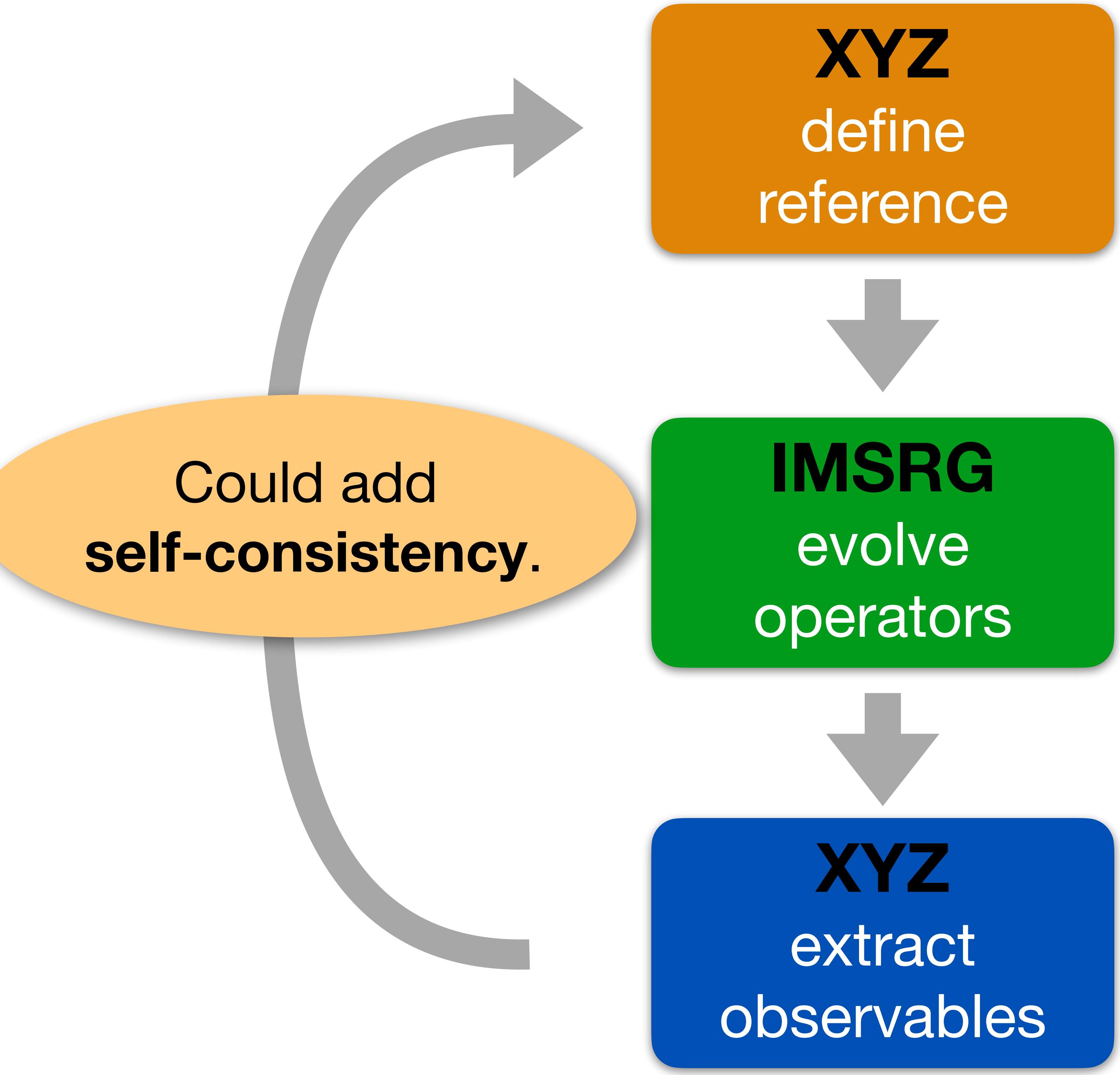
Correlated Reference States



MR-IMSRG: build correlation[s on top of]
already correlated state (e.g., fro[m ...])
describes static correlation

new contractions (two-body and higher densities), but **scaling remains unchanged**

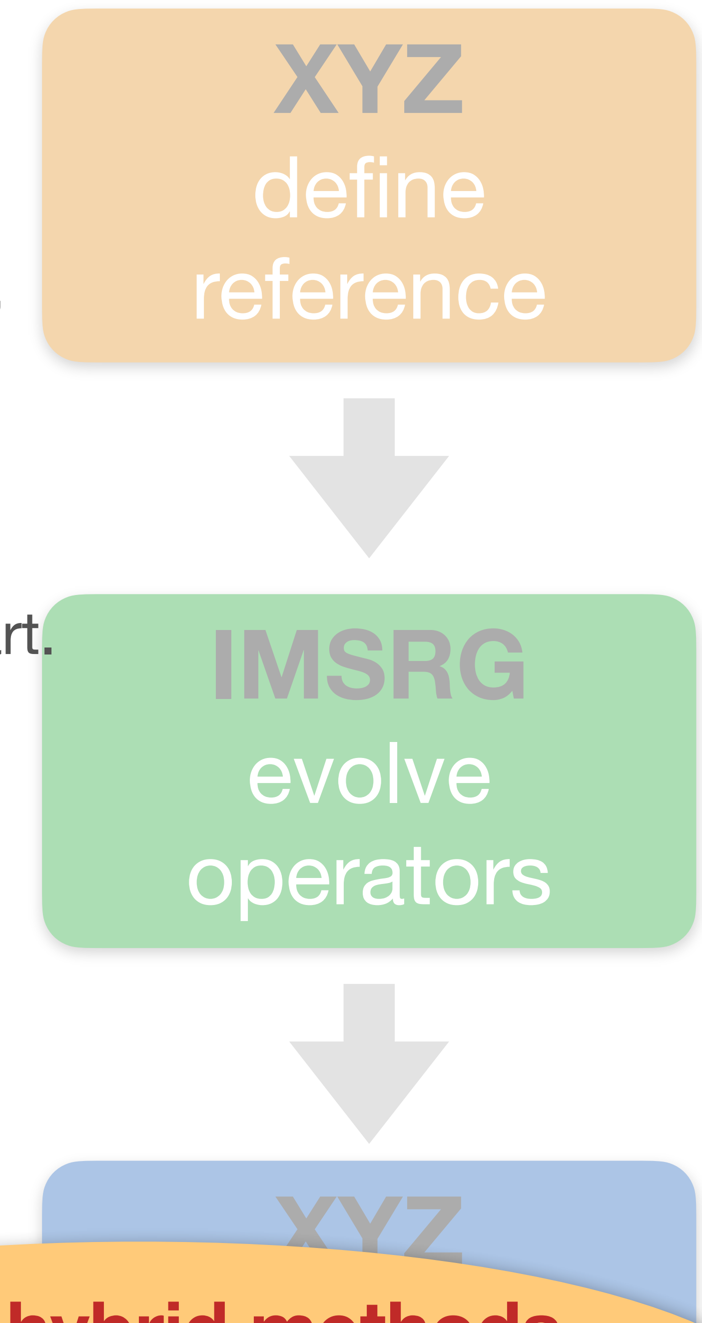
IMSRG-Improved Methods



* 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, H
    (2018)
  - J. M. Yao et al., PRL 124, 232501 (2020)



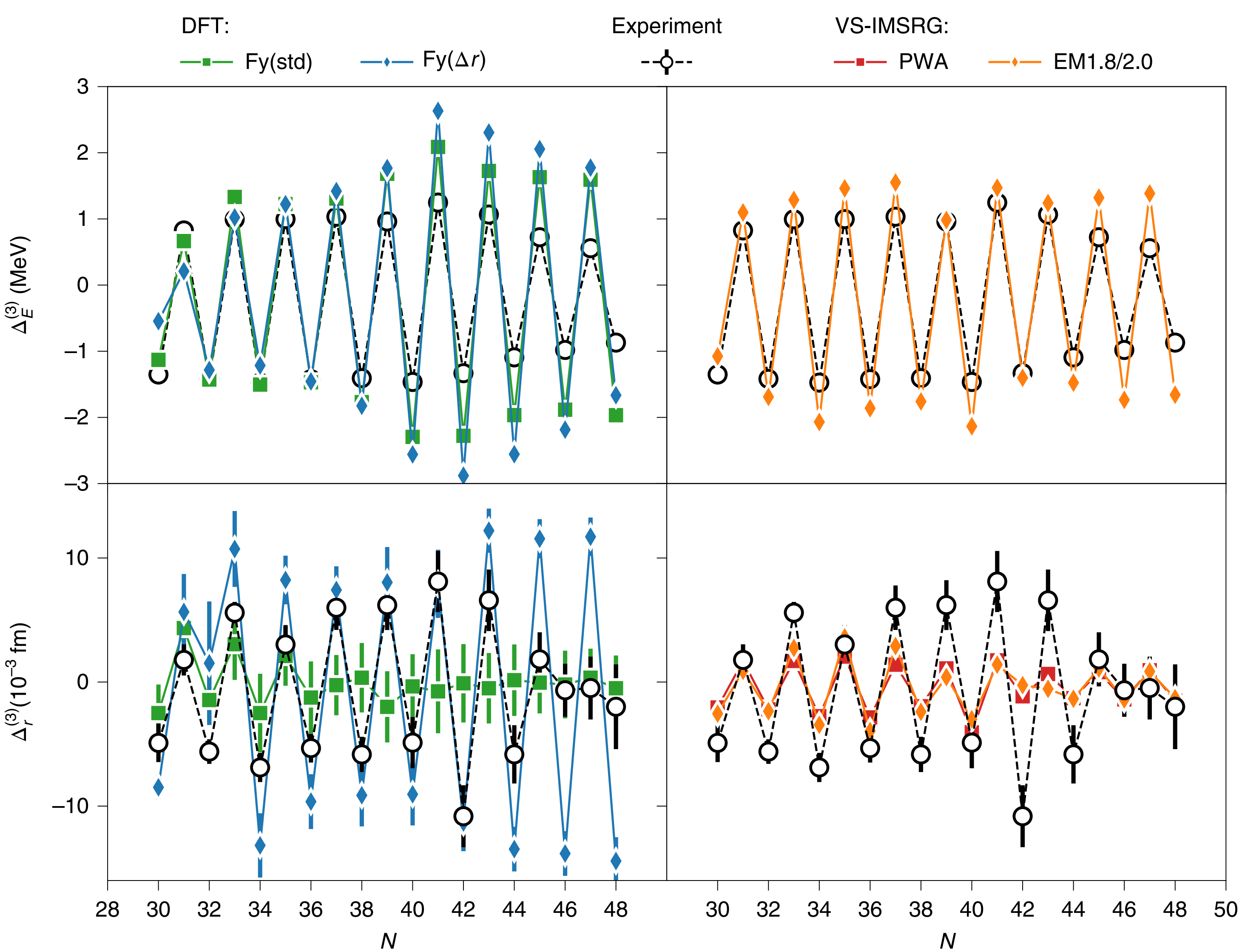
more hybrid methods in development (SA-NCSM, DMRG, …)

Are We There Yet?

Uncertainty

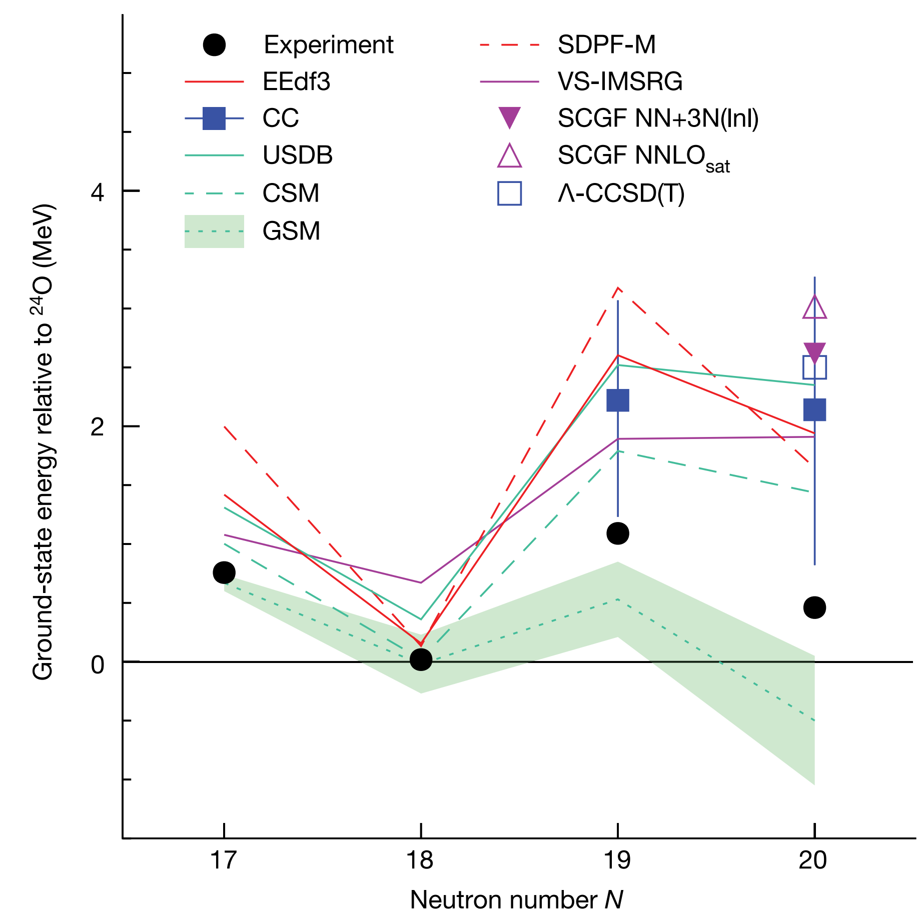
copper isotopes

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



oxygen isotopes

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



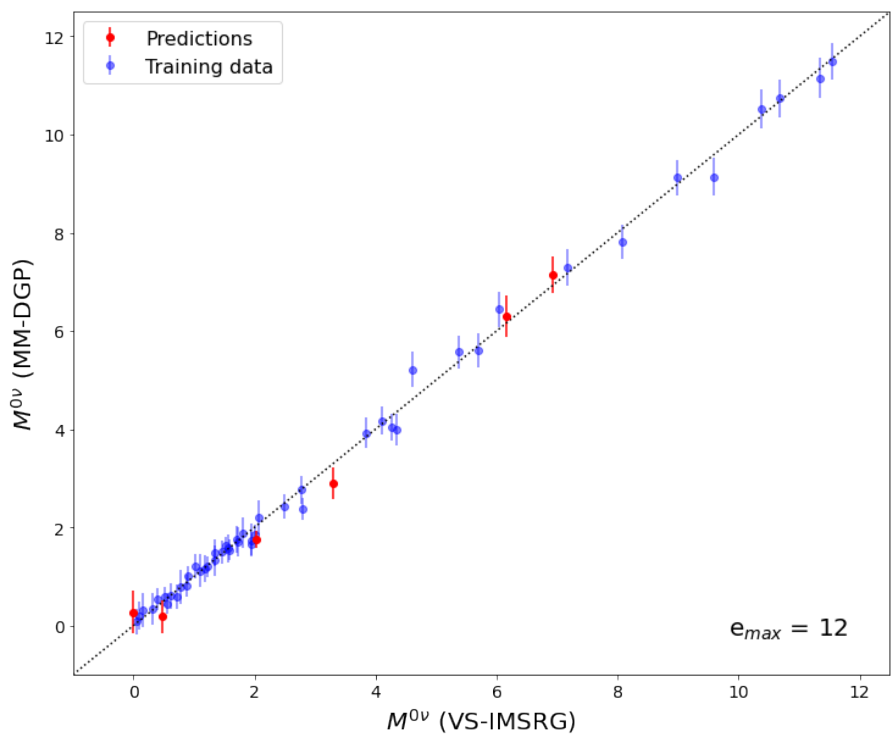
Are these results good, bad, or just ok? Is there genuine tension between theory and experiment? **How can we know?**

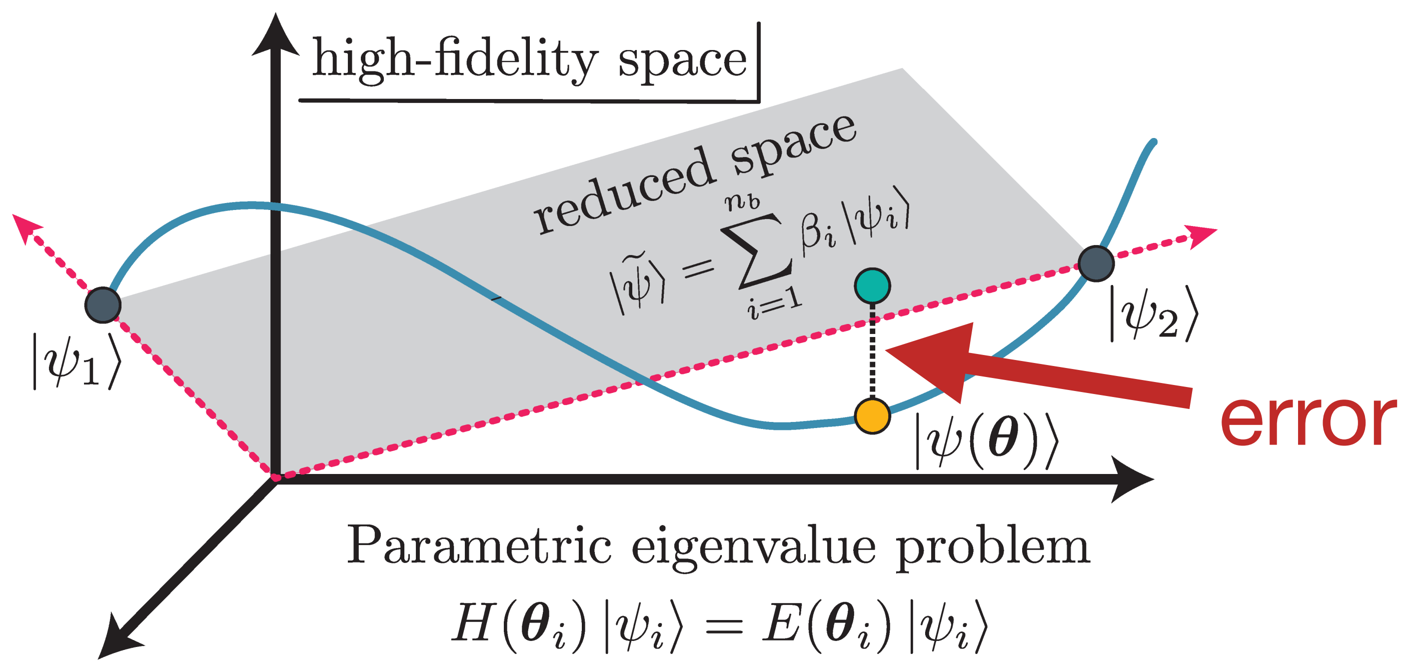
Modern Uncertainty Quantification

- 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)





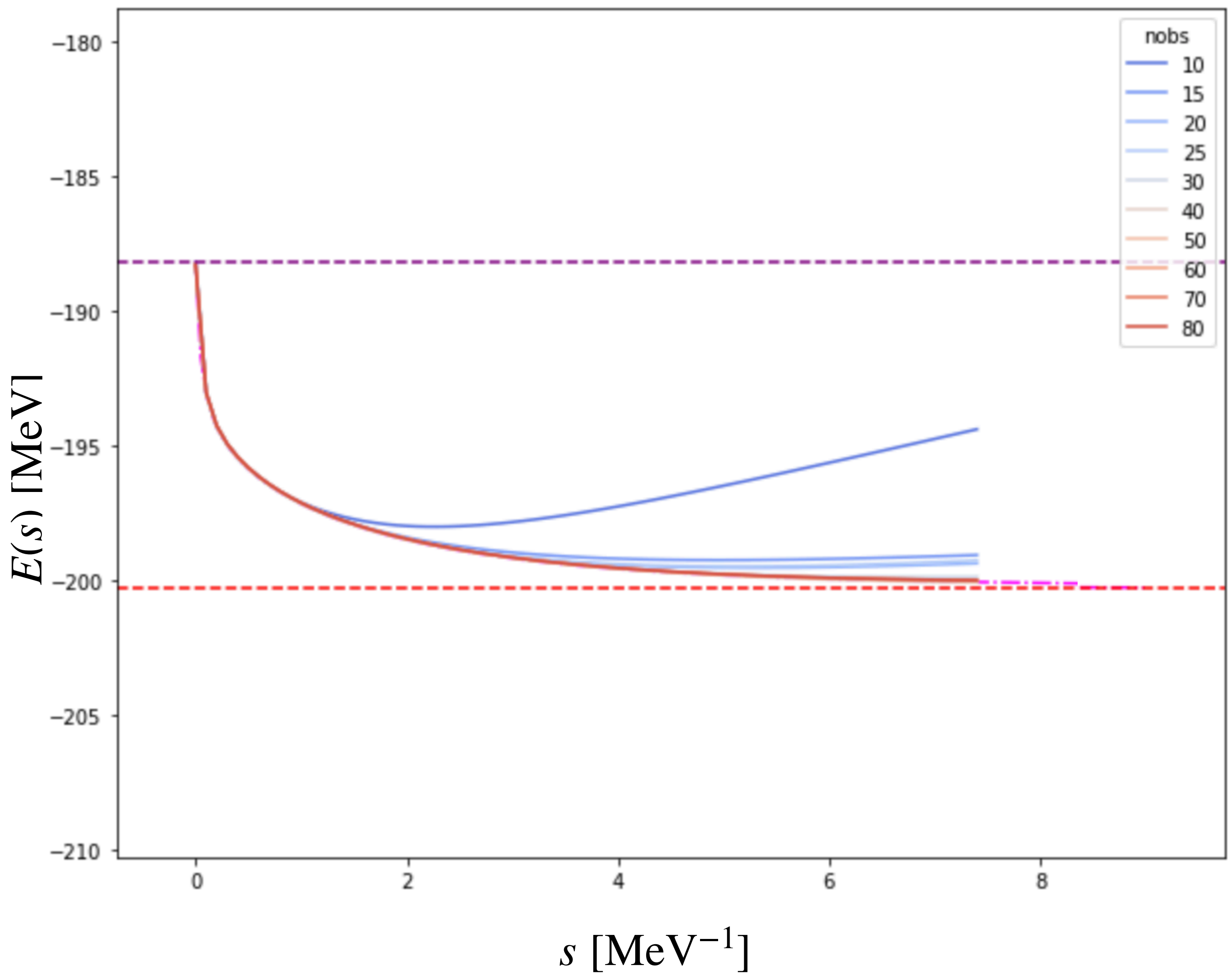
- **Data driven** (only expectation values)
- E.g. Multi-output, Multi-fidelity **Deep Gaussian Processes** (MM-DGP)

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

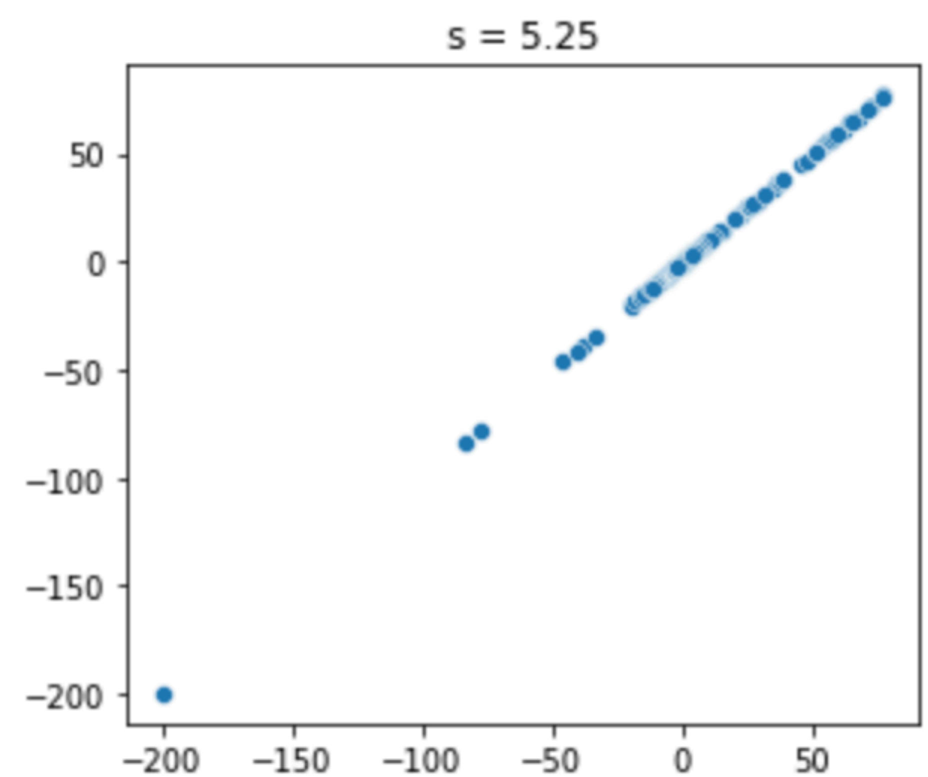
Emulating IMSRG Flows

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

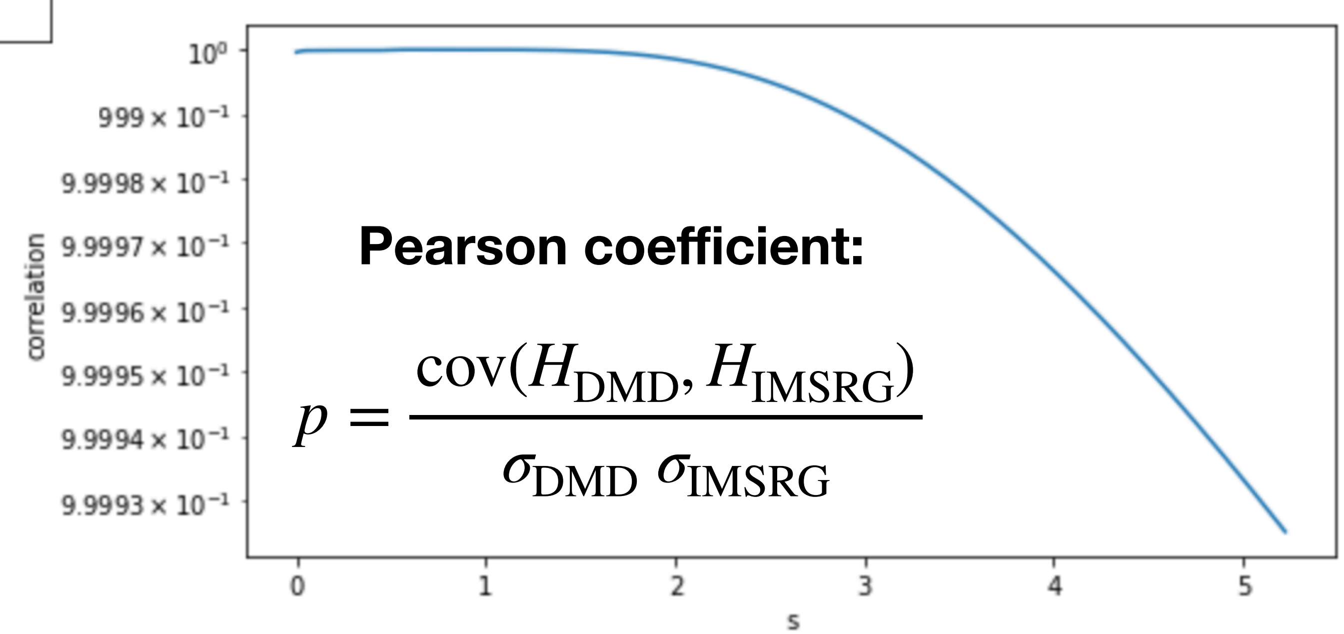
EM(500) N³LO, $\lambda = 2.0\,\mathrm{fm}^{-1}$



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



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

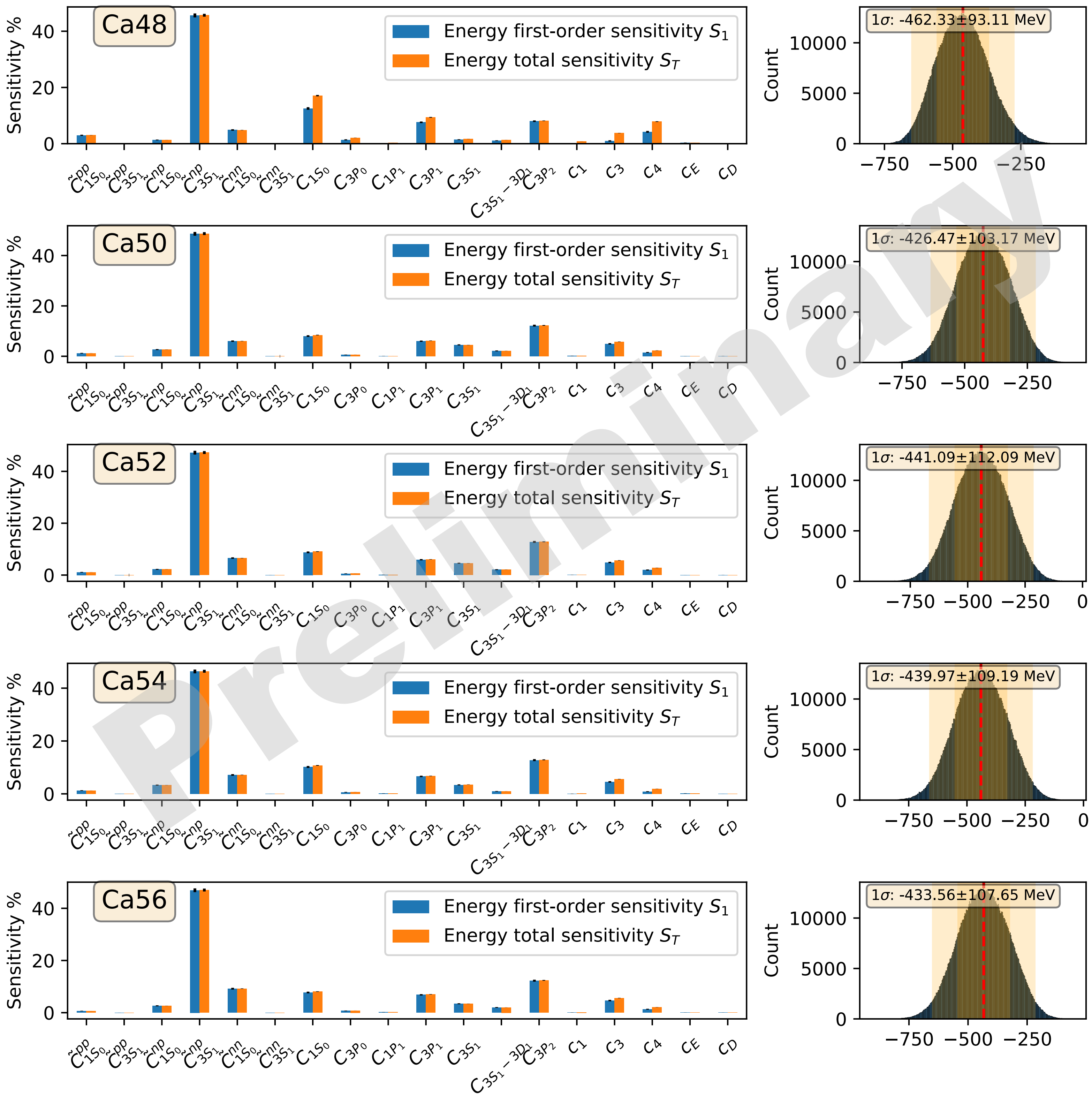


Pearson coefficient:

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

Emulation for Operators (IMSRG)

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

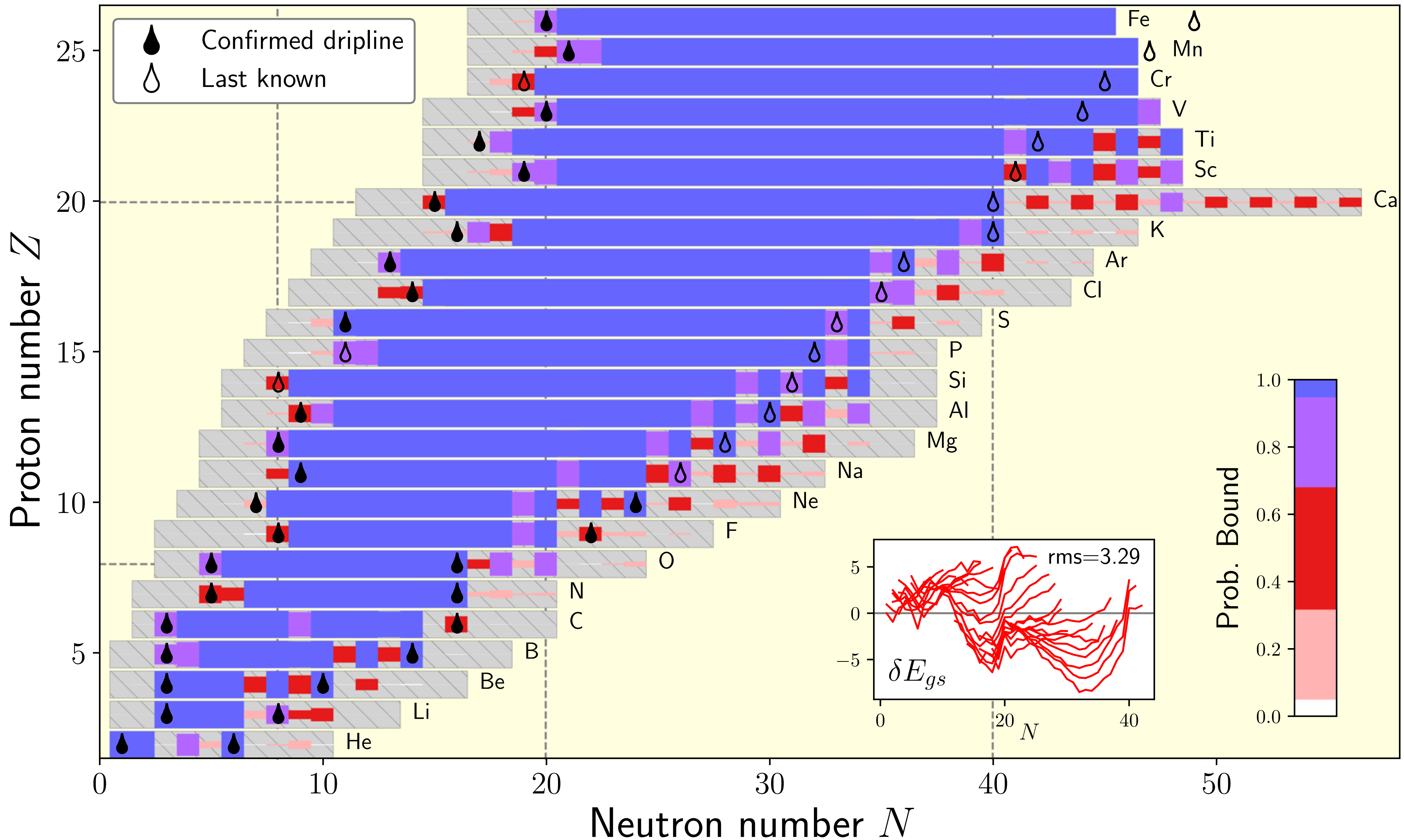


- non-invasive **ROM emulator** based on Dynamic Mode Decomposition
- ΔNNLOGO, NN+3N, $e_{max} = 12, E_{3max} = 14$
- O(10M) samples
- **computational effort reduced by 5+ orders of magnitude**

No Matter Where You Go… There You Are

Towards *Ab Initio* Mass Tables

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

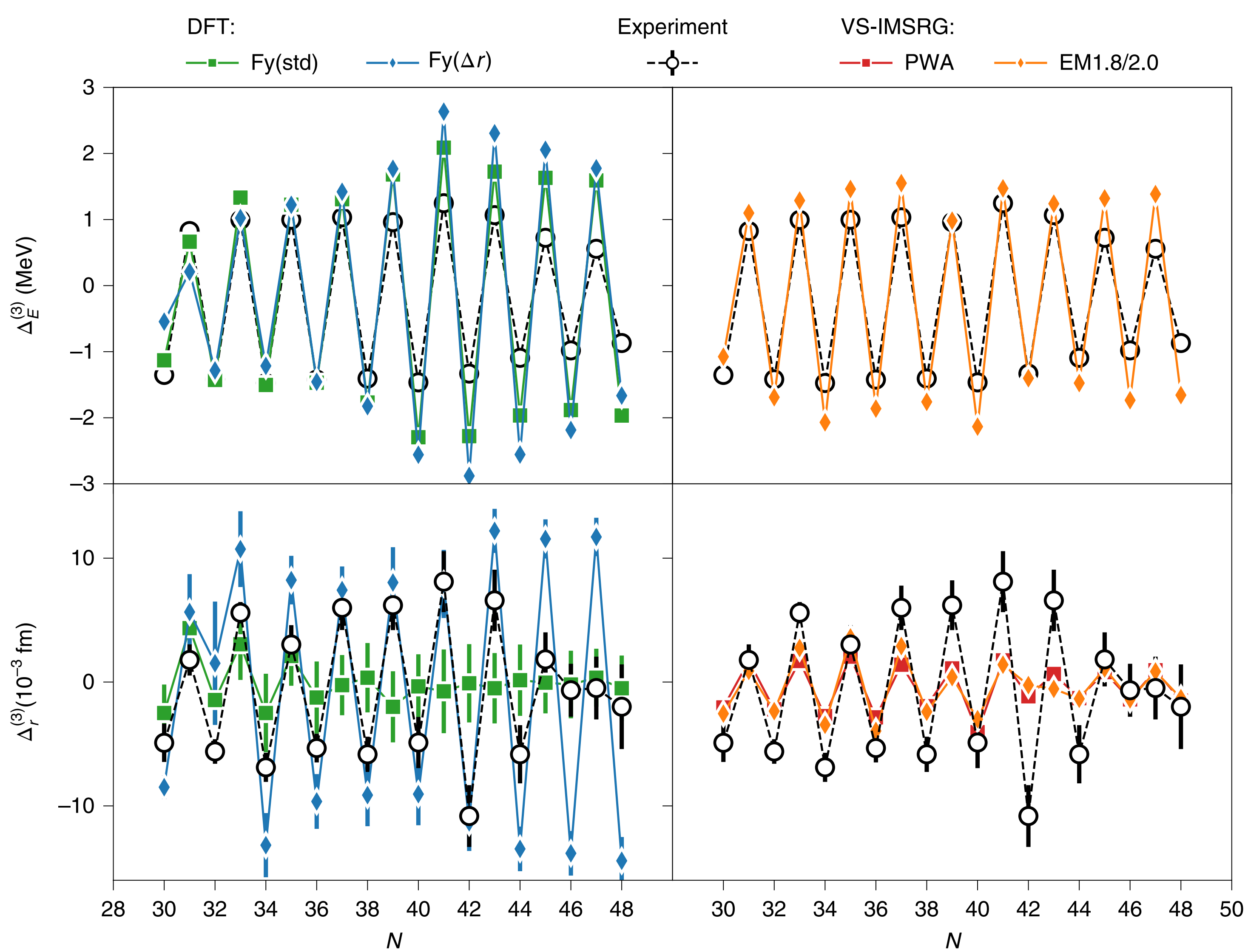


Valence-Space IMSRG "mass table" based on a chiral NN+3N interaction (EM1.8/2.0)

Differential Radii and Trends

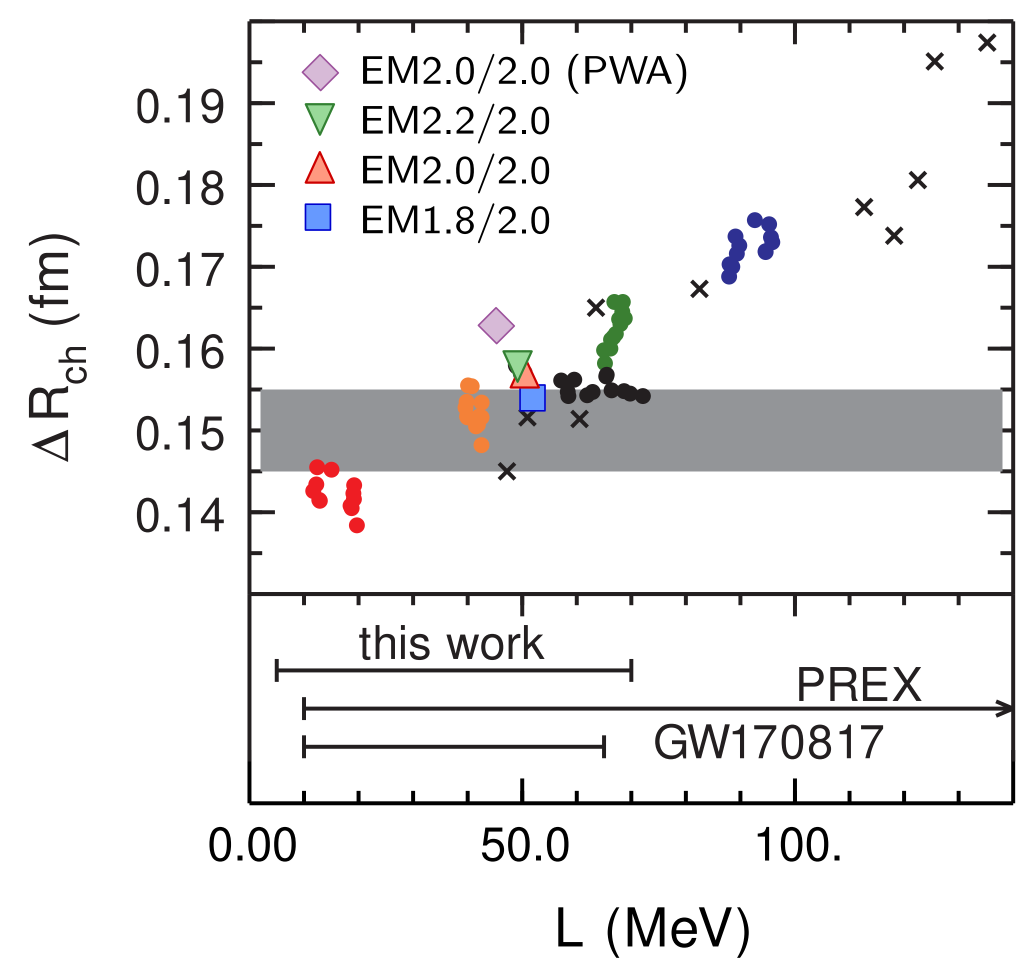
copper isotopes

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



^{36}Ca - ^{36}S

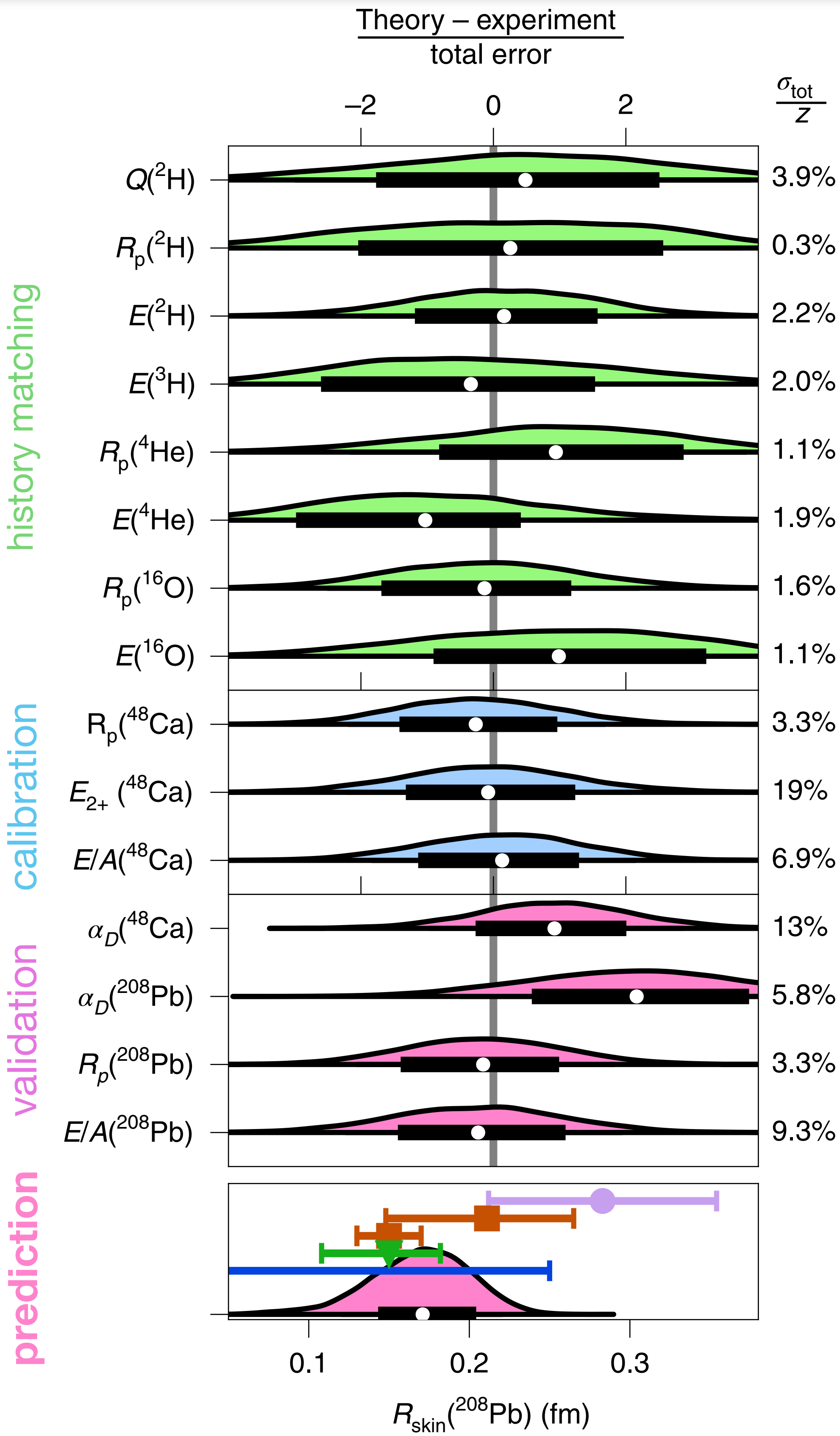
*B. A. Brown et al., PRR **2**, 022305(R) (2020)*

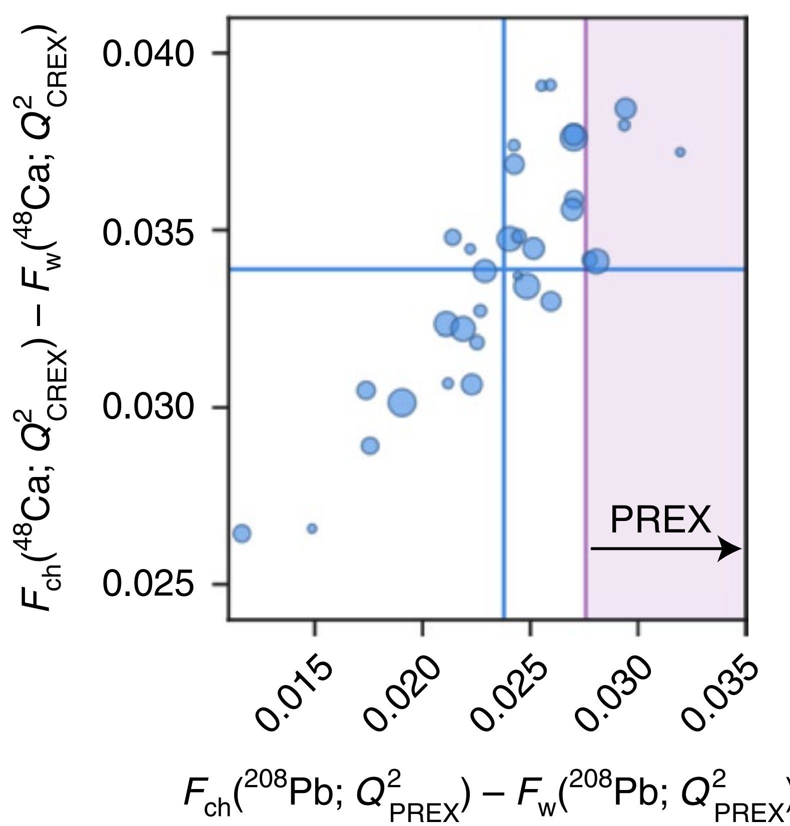


differential observables like the staggering of energies ($\Delta_E^{(3)}$) and radii ($\Delta_r^{(3)}$) or the charge radius difference of mirror nuclei, ΔR_{ch}, are **insensitive** to variations of interaction cutoffs / resolution scale

Neutron Skin in ^{208}Pb

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

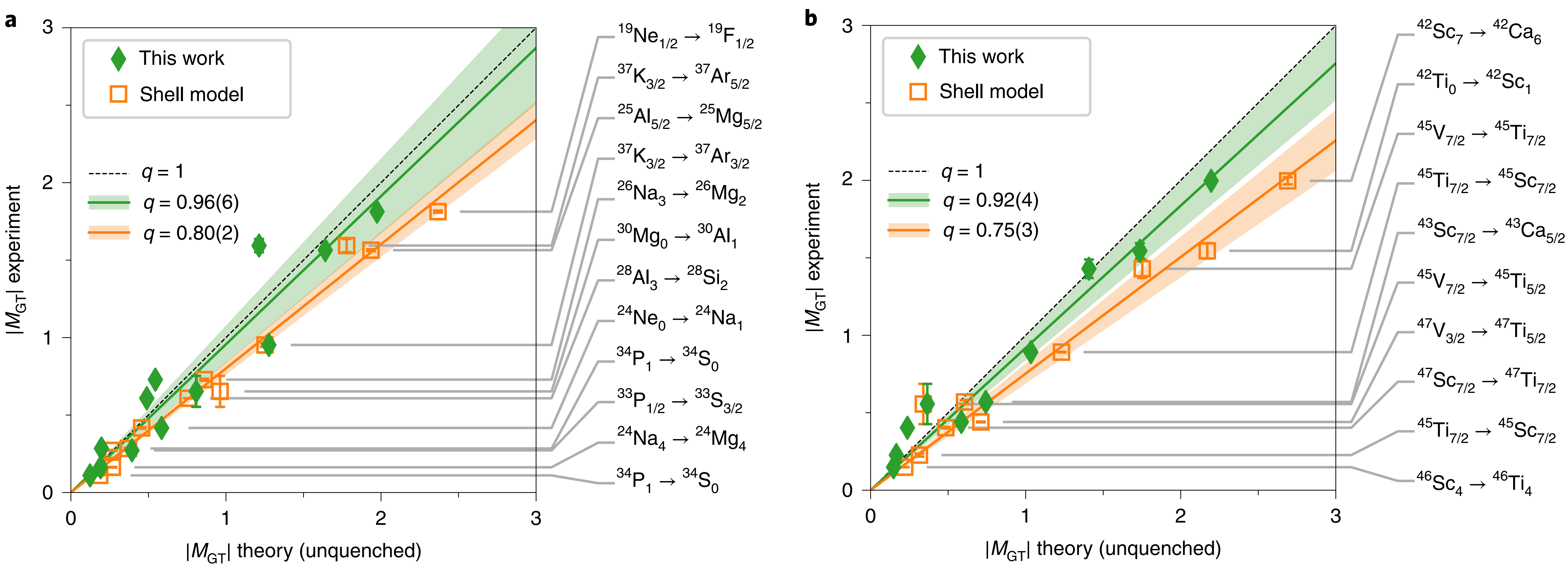




- ^{208}Pb is **heaviest nucleus** for which converged *ab initio* calculations have been achieved (VS-IMSRG, CC)
- chiral forces favor **thin neutron skin,** in **mild tension** with recent experimental result from PREX

Quenching of Gamow-Teller Decays

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

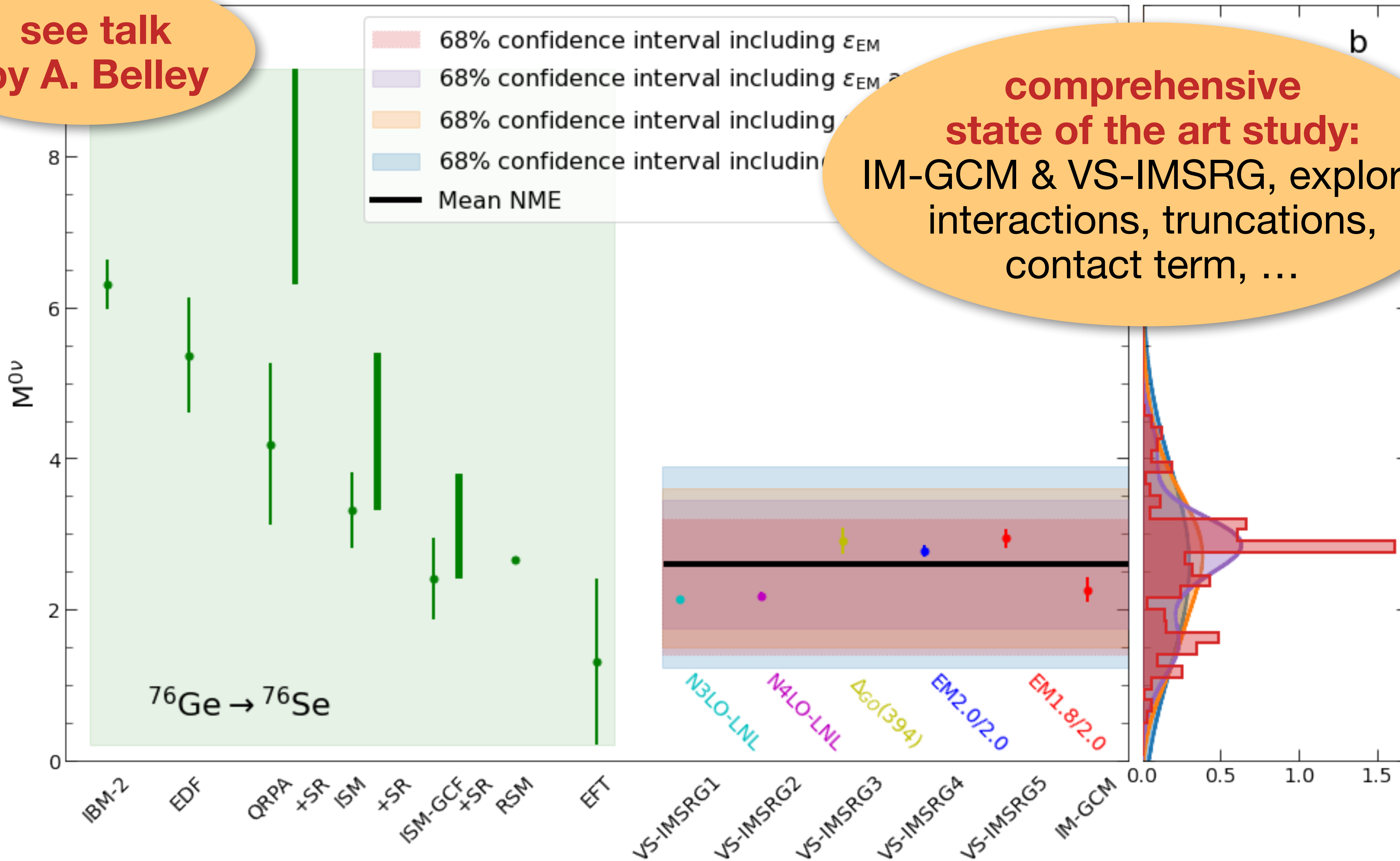


- **empirical Shell model** calculations require **quenching factors** of the weak axial-vector couling g_A
- **VS-IMSRG** explains this through consistent **renormalization** of transition operator, incl. **two-body currents**

^{76}Ge

A. Belley et al., to appear in PRL, arXiv:2308.15643 (**v2**)

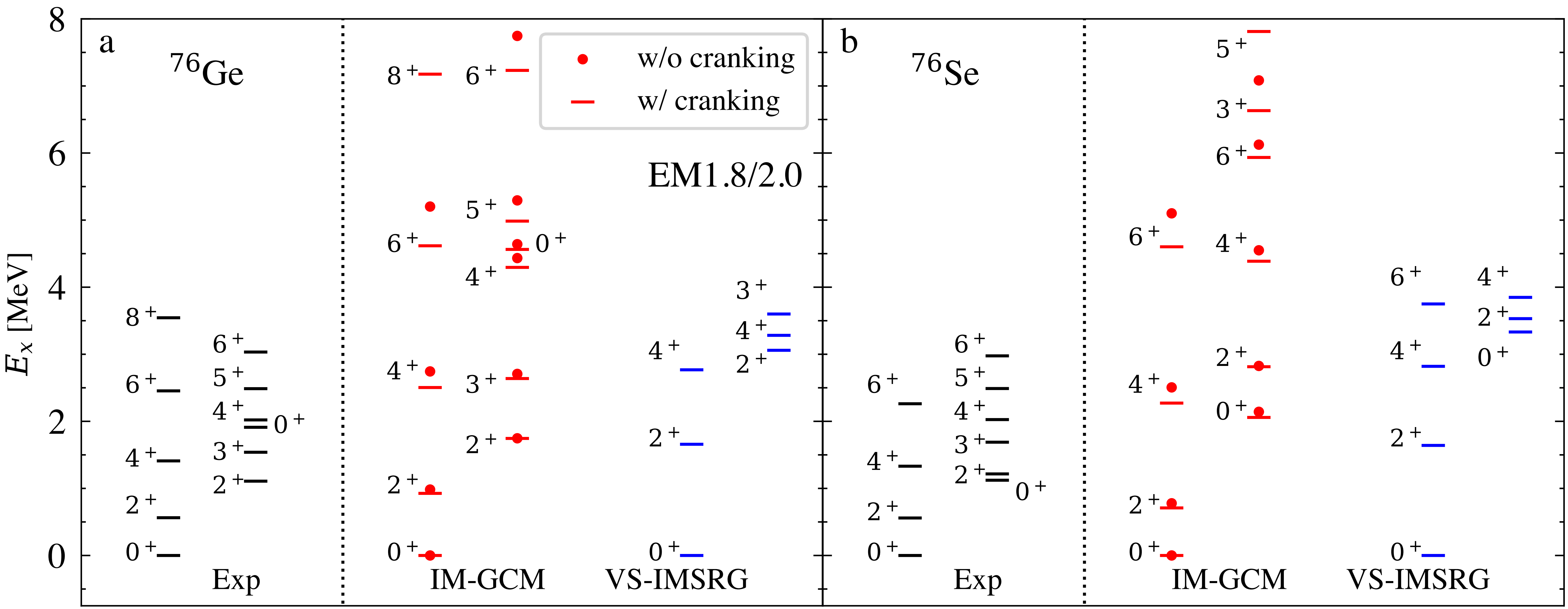
see talk by A. Belley



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

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

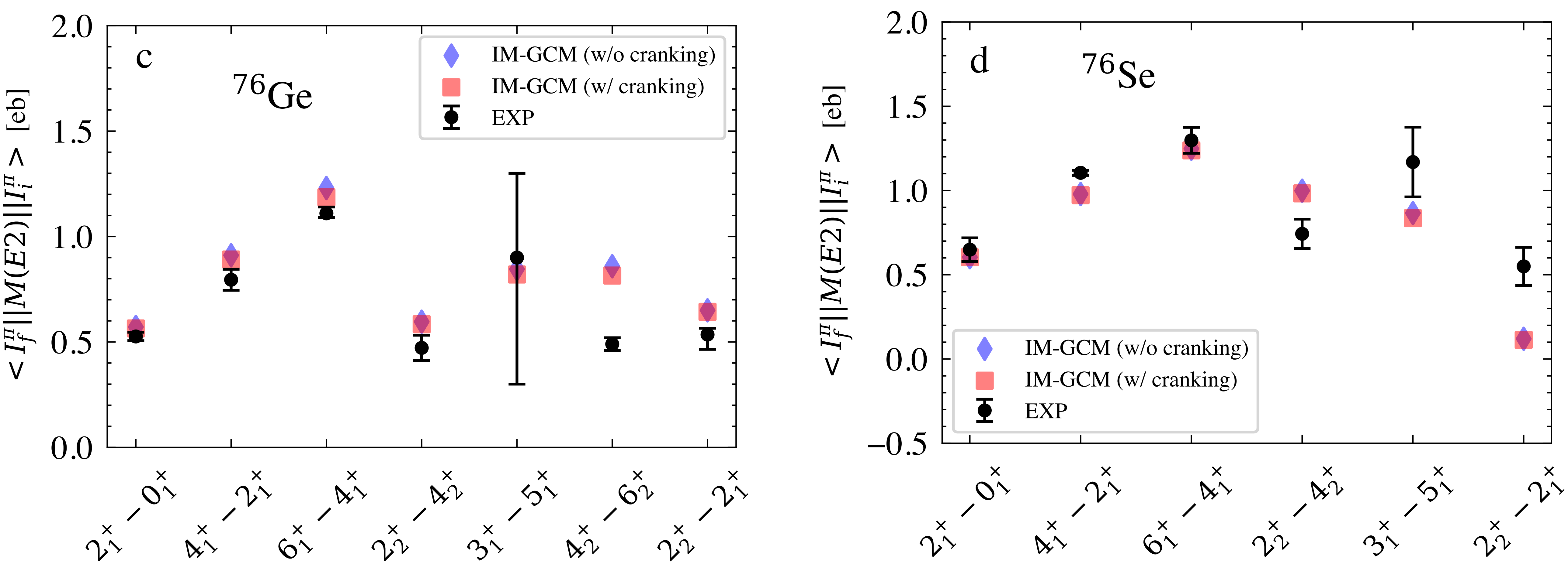
A. Belley et al., to appear in PRL, arXiv:2308.15643 (**v2**)



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

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

A. Belley et al., to appear in PRL, arXiv:2308.15643 (**v2**)

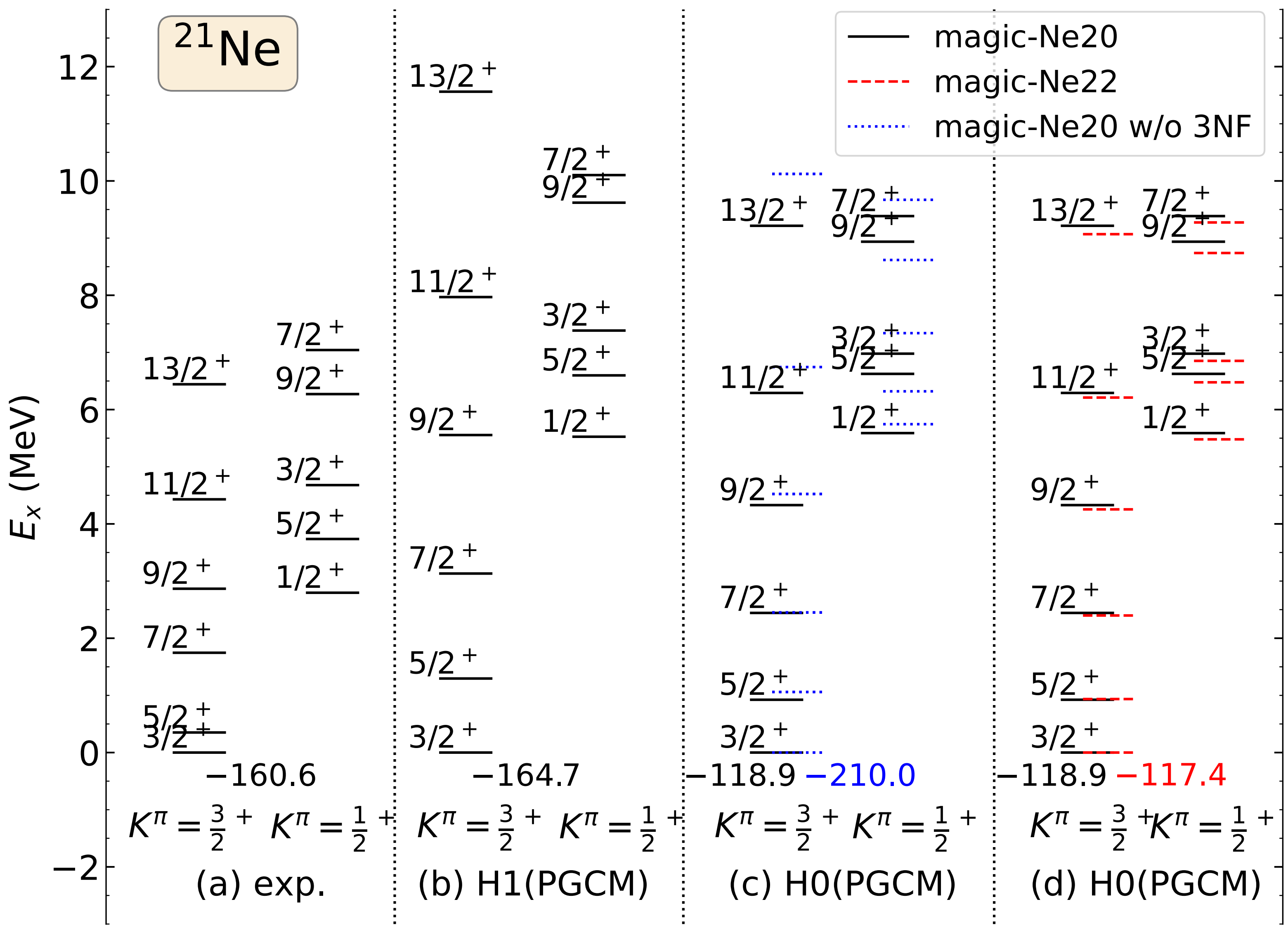


EM1.8/2.0 NN+3N interaction, $\hbar\omega = 12\,\mathrm{MeV}, e_{max} = 10$

caveat: EM1.8/2.0 gives radii that are a few percent too small

IM-GCM for Odd Nuclei

W. Lin, J. M. Yao, E. F. Zhou, HH, in preparation



- IMSRG evolution improves **absolute energies**
- working to understand how/why evolution increases **spread of spectrum**: reshaping of PES, tailoring to g.s.
- **weak sensitivity to choice of reference** (even neighbors, ensemble, …)

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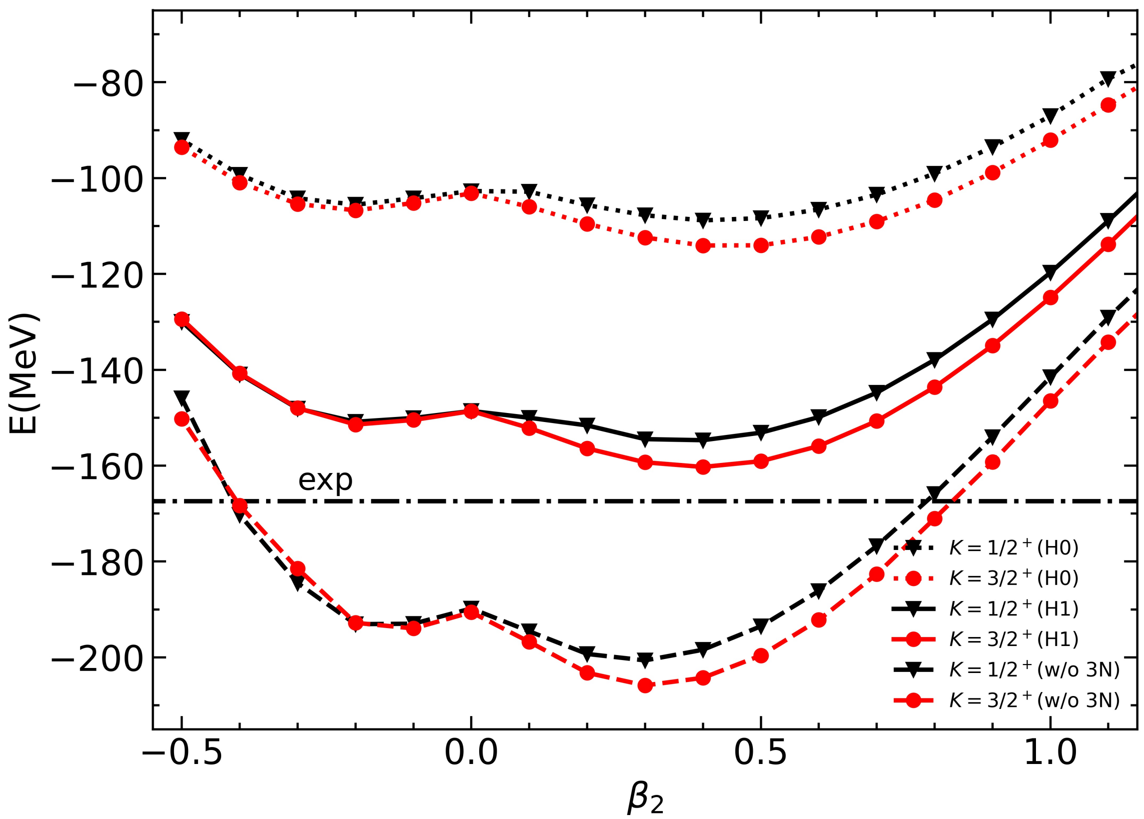

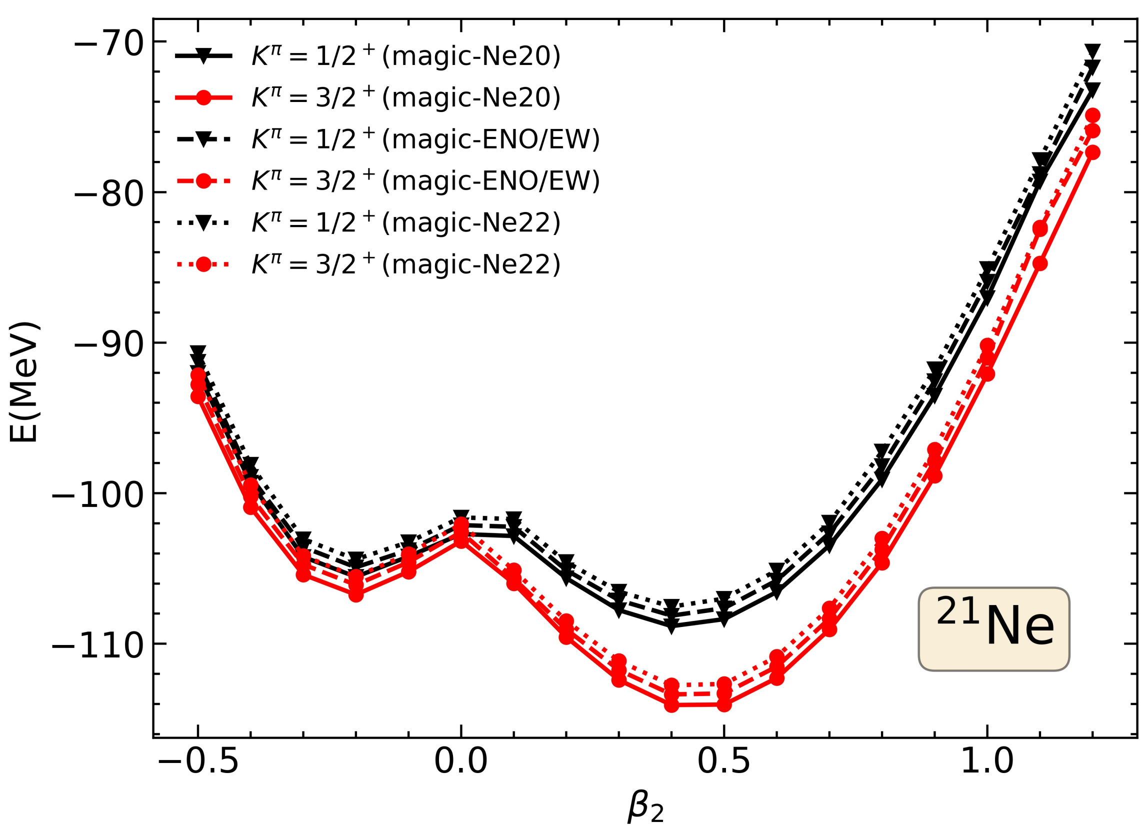

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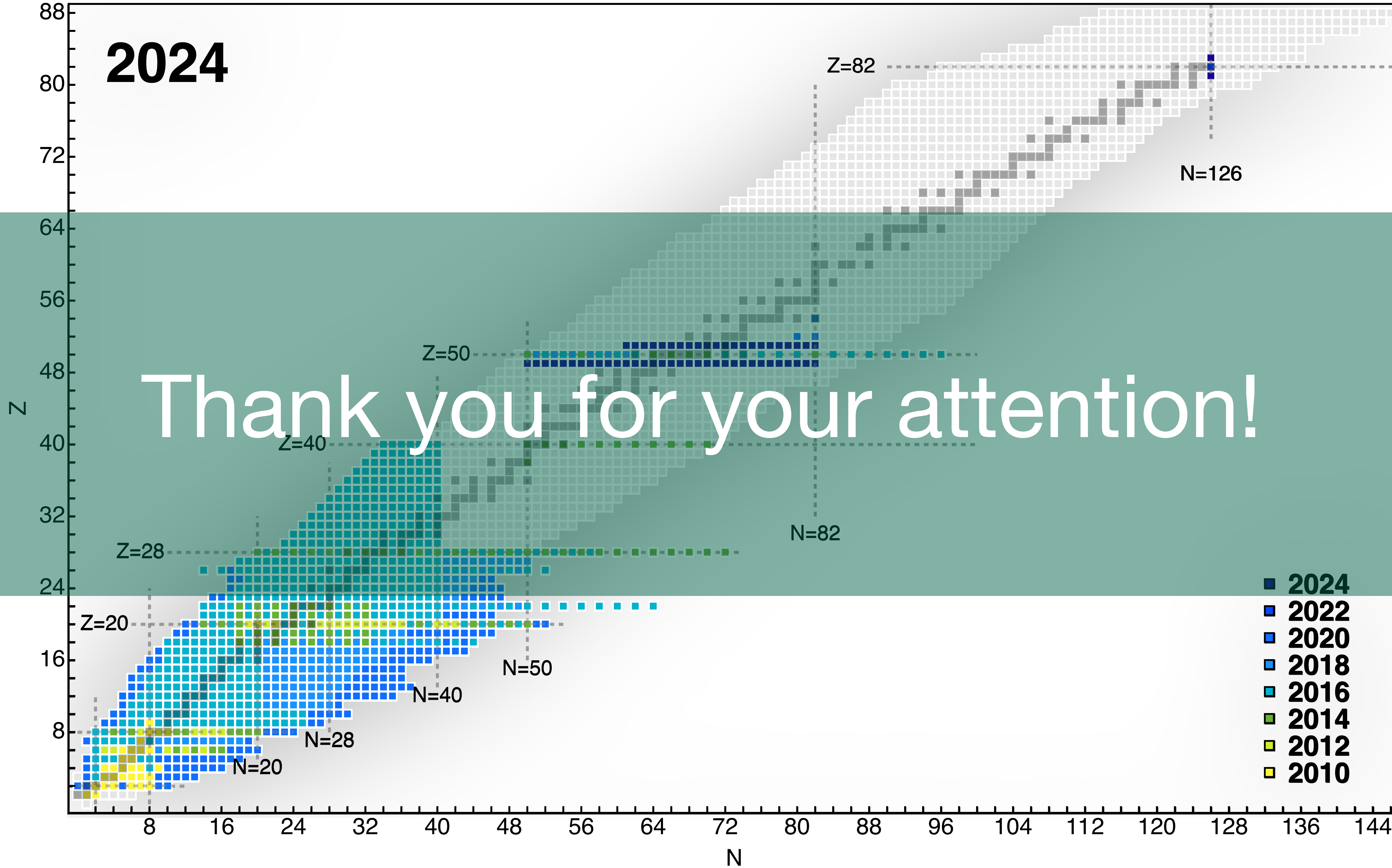
Where Do We Go From Here?

What Is Next?

- **improved truncations:** IMSRG(3), tailored operator bases
- **accelerate IMSRG & IM-GCM**
    - GPUs, factorization, Machine Learning, …
    - (random) **compression & tensor factorization**
- **uncertainty quantification / sensitivity analysis**
    - emulators for GCM (wave function / Galerkin methods)
    - **emulation workflow based on (IM)SRG ROMs ?**
- **applications**
    - incl. nuclear observables relevant for BSM physics (beta decays for CKM unitarity, Schiff moments, …)

Progress in *Ab Initio* Calculations

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



Thank you for your attention!

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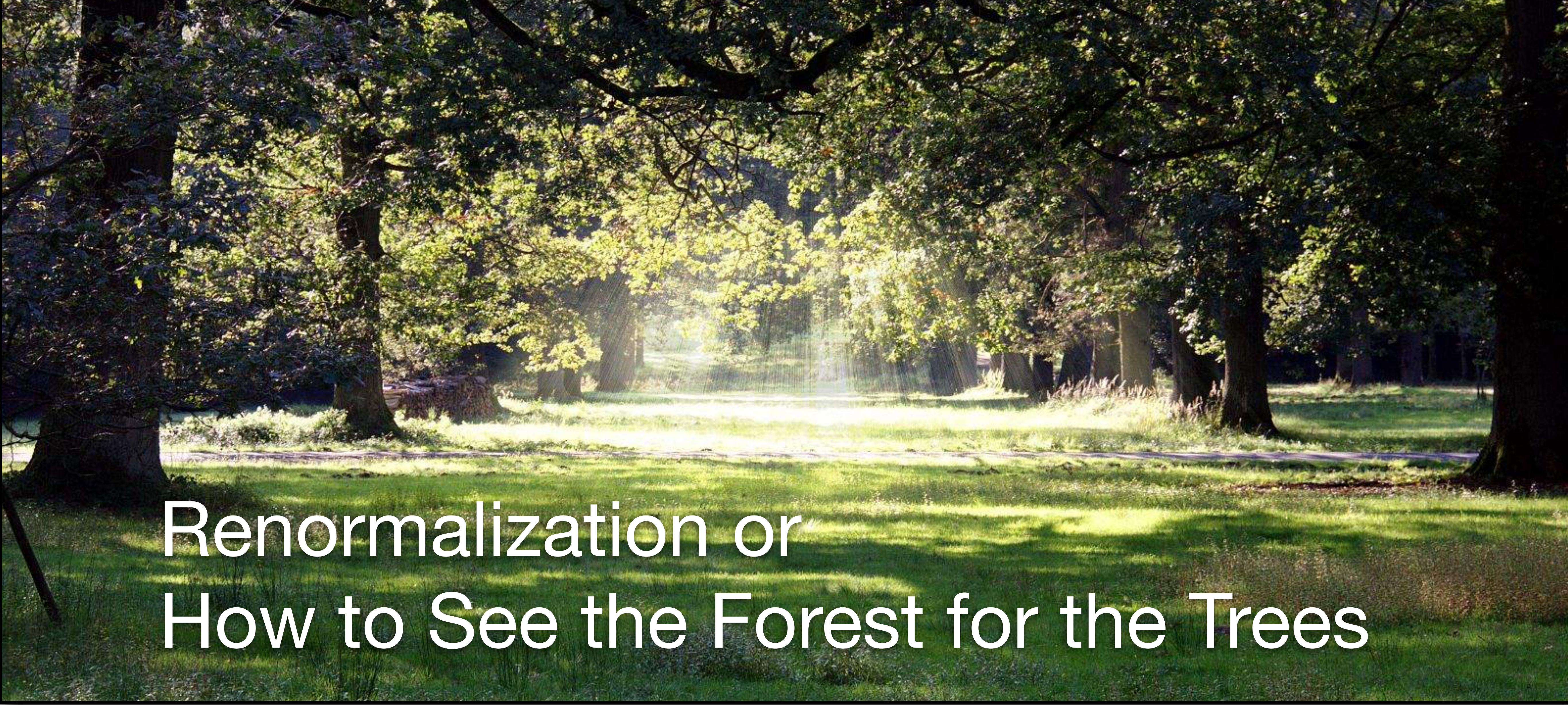
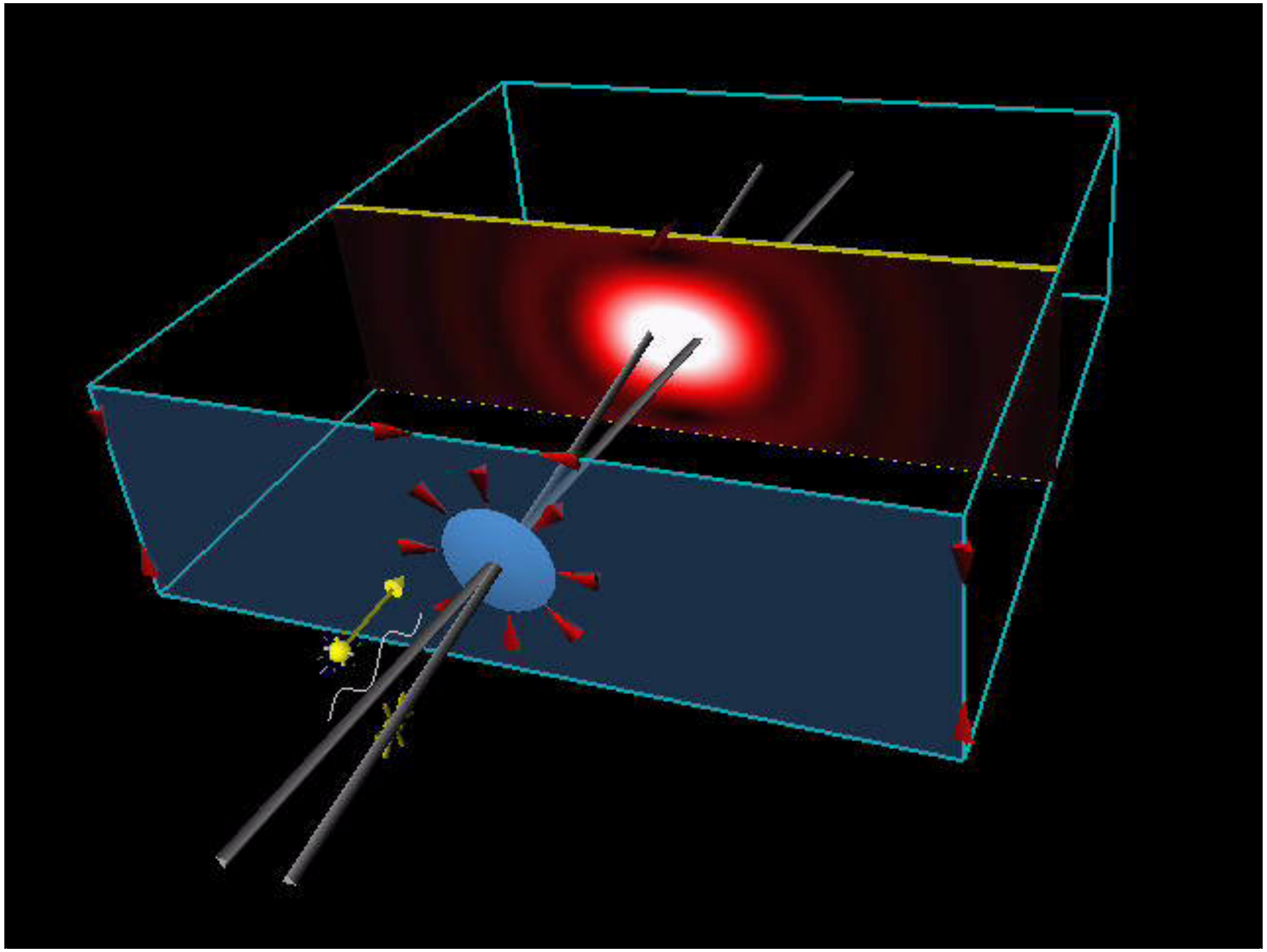
NUCLEI Nuclear Computational Low-Energy Initiative

Supplements


Renormalization or
How to See the Forest for the Trees

Resolution



We must use probes of **sufficiently short wavelength to resolve small structures**… **but do we need to**?

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

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

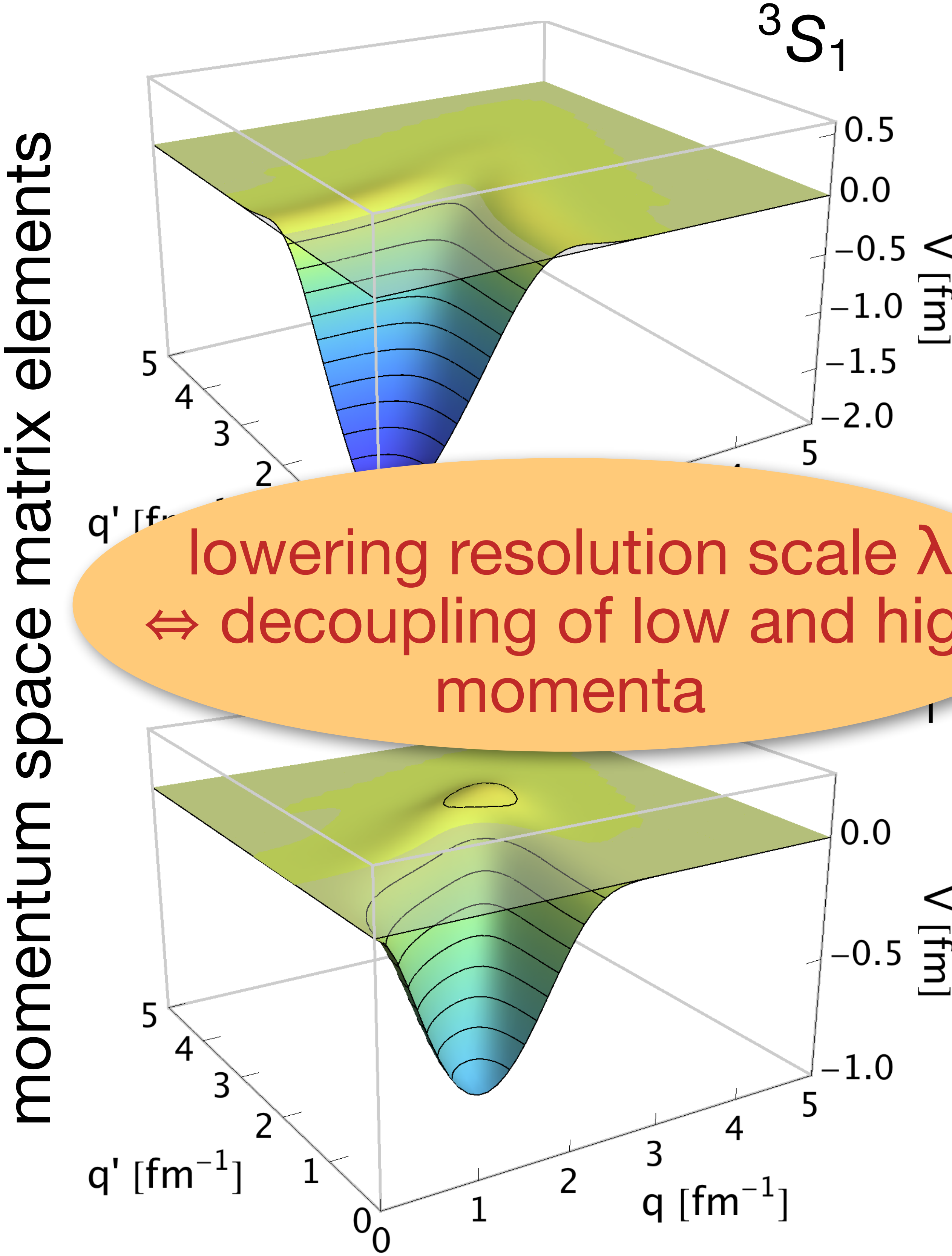
- choose $\eta(s)$ to achieve desired behavior, e.g.,

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

to suppress (suitably defined) off-diagonal Hamiltonian

- consistent evolution for all observables of interest

SRG in Two-Body Space



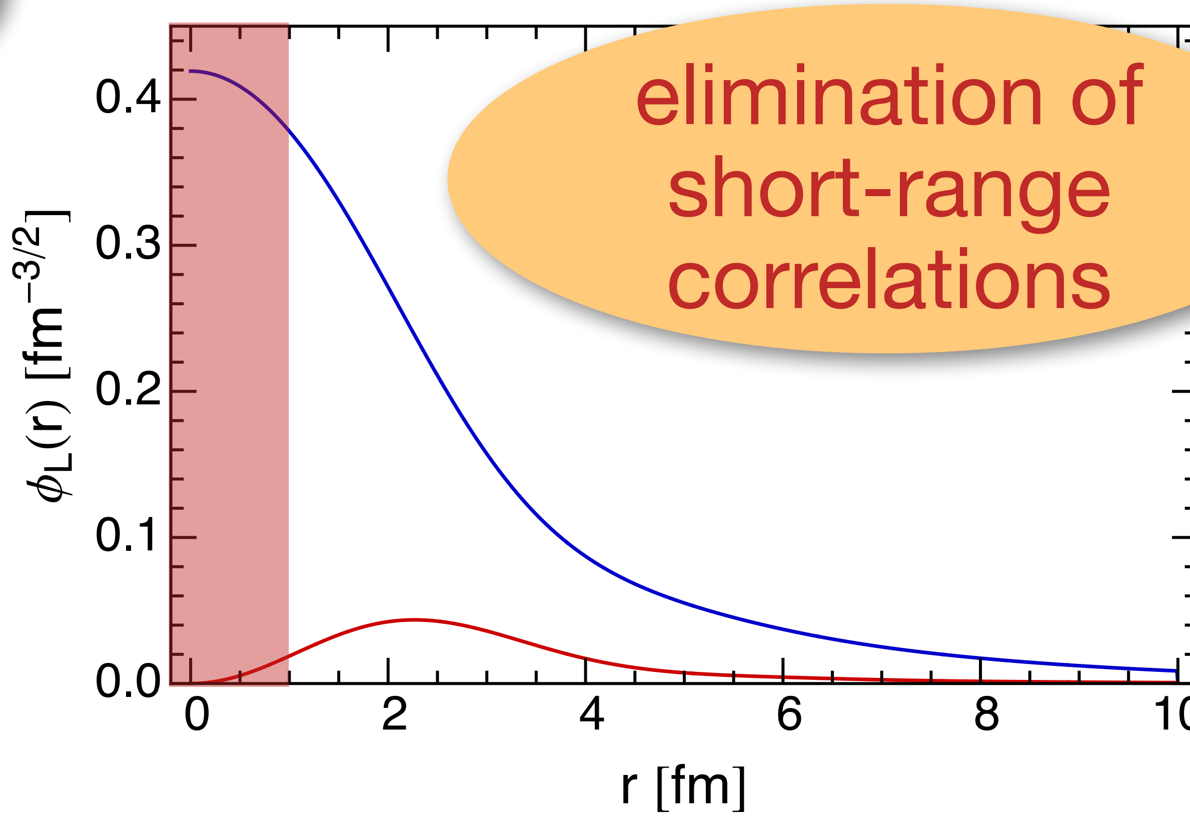
lowering resolution scale λ
⇔ decoupling of low and high momenta

$\lambda = 1.8\ \mathrm{fm}^{-1}$

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

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

deuteron wave function



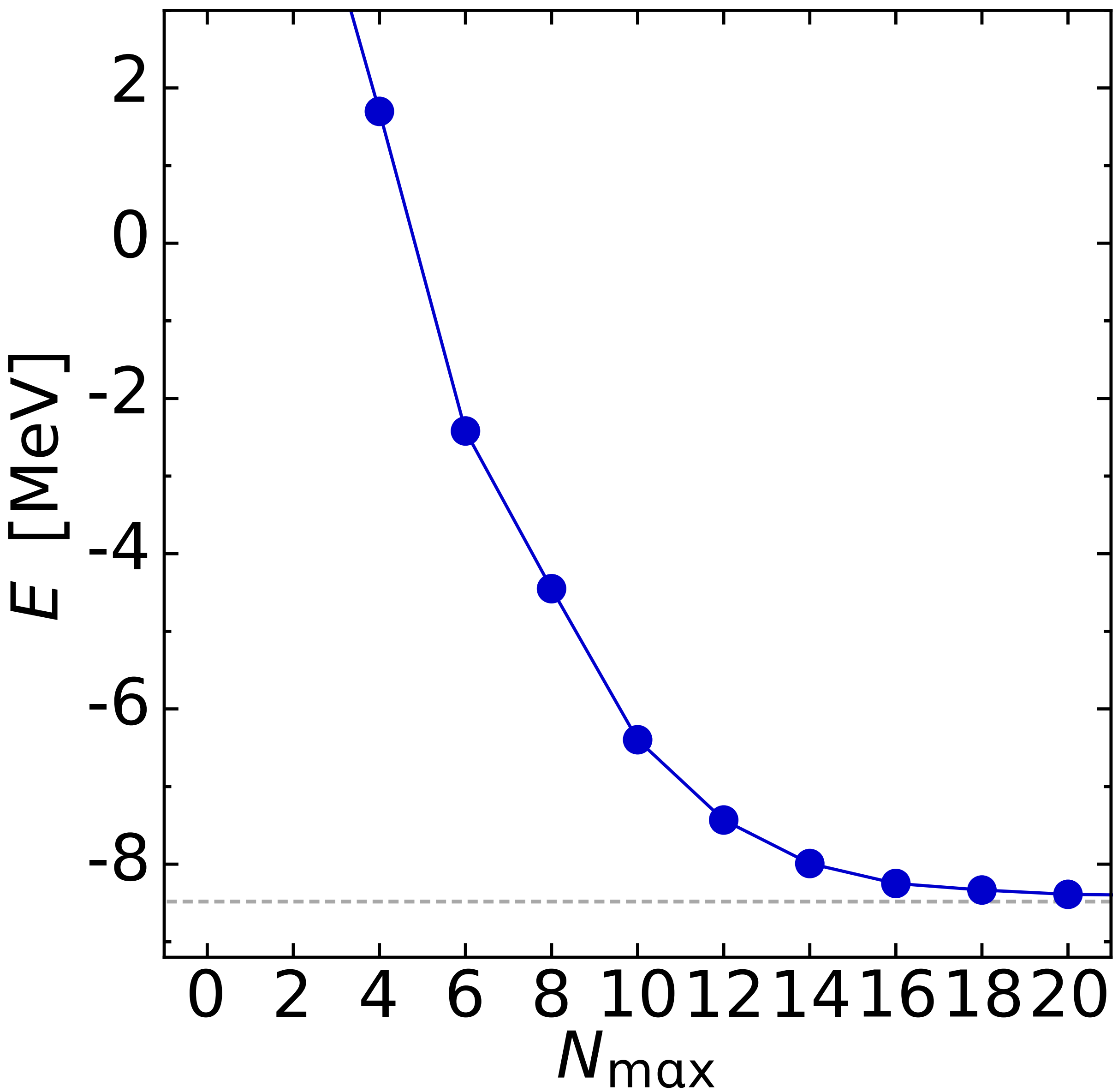
elimination of short-range correlations

Renormalization

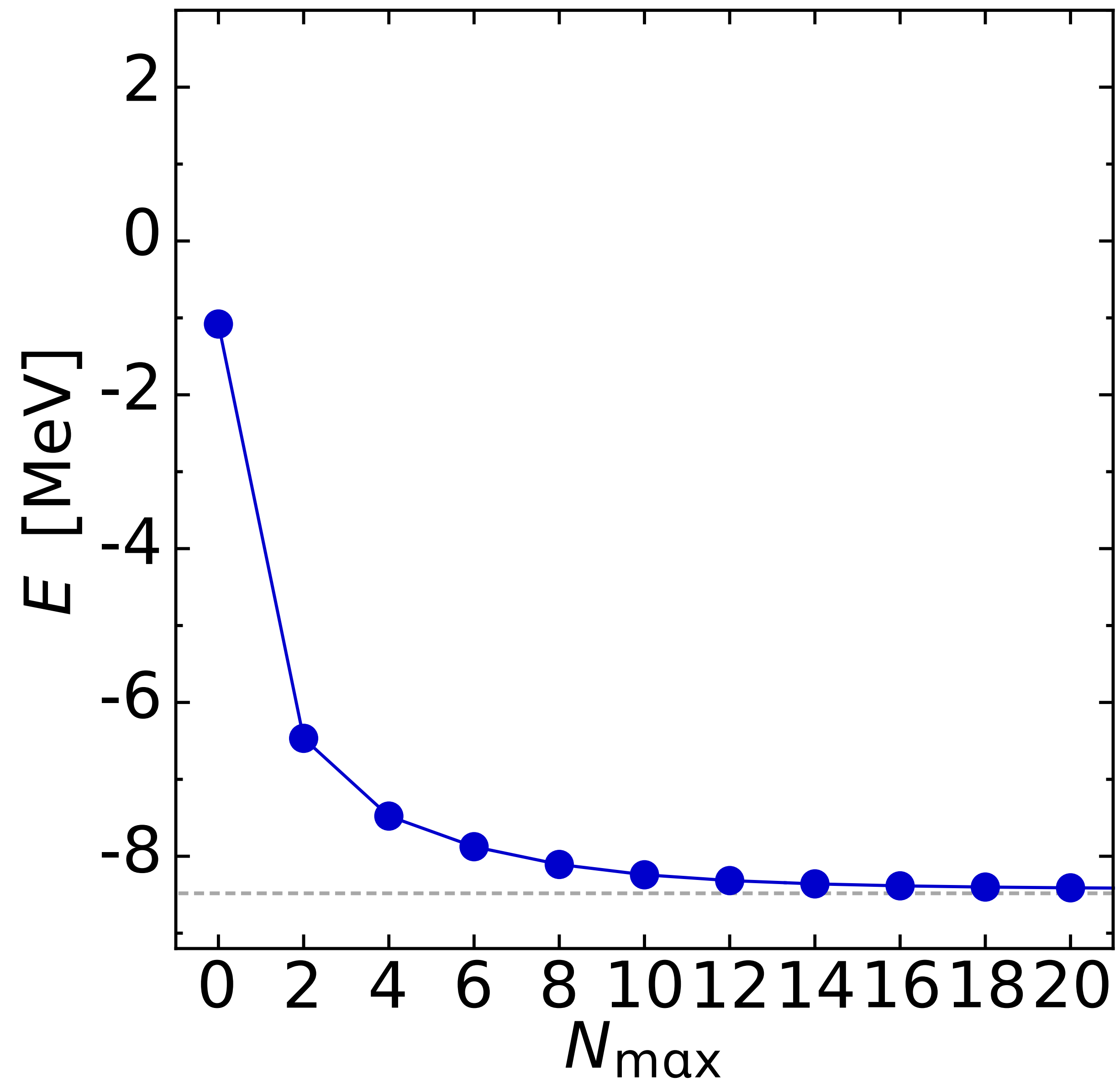
- tune **resolution scale** of a **theory** in **systematic fashion** with **Renormalization Group** methods
  - analogous to adjusting optics of a microscope / tuning energy of accelerator beam
- **conserve relevant information** in low-resolution theory
- **profit:** calculations of low-resolution observables become easier computationally (and maybe even analytically)

Benefits of SRG Evolution

without renormalization



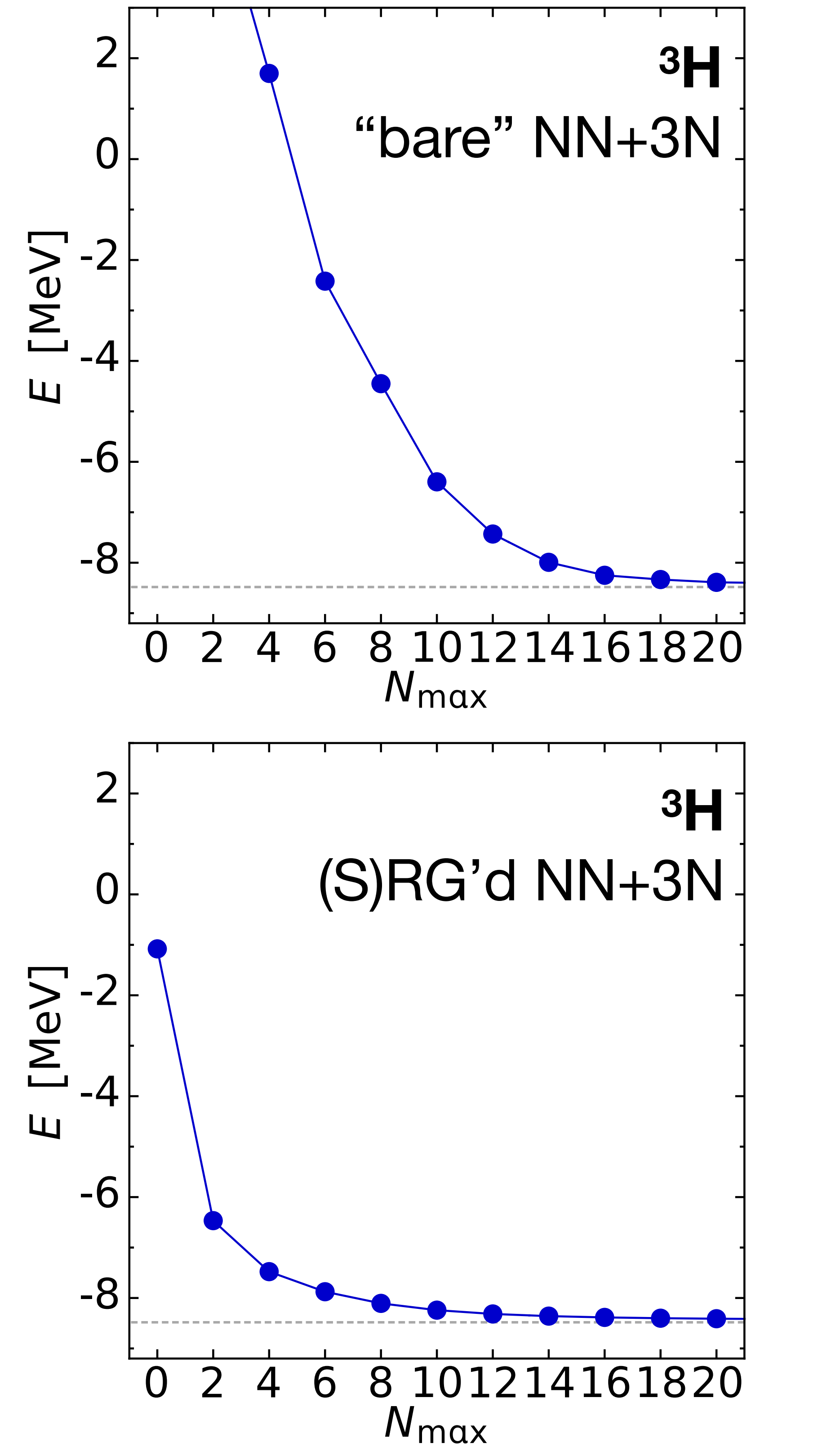
with renormalization



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

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**



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:

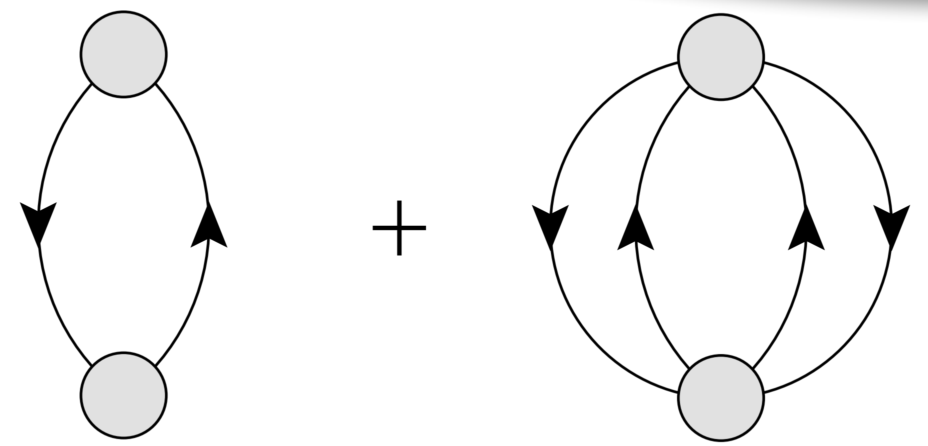
$$\{O_{pq}, O_{pqrs}, \ldots\} = \{a^\dagger_p a_q, a^\dagger_p a^\dagger_q a_s a_r, \ldots\}$$

Standard IMSRG(2) Flow Equations

0-body Flow

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

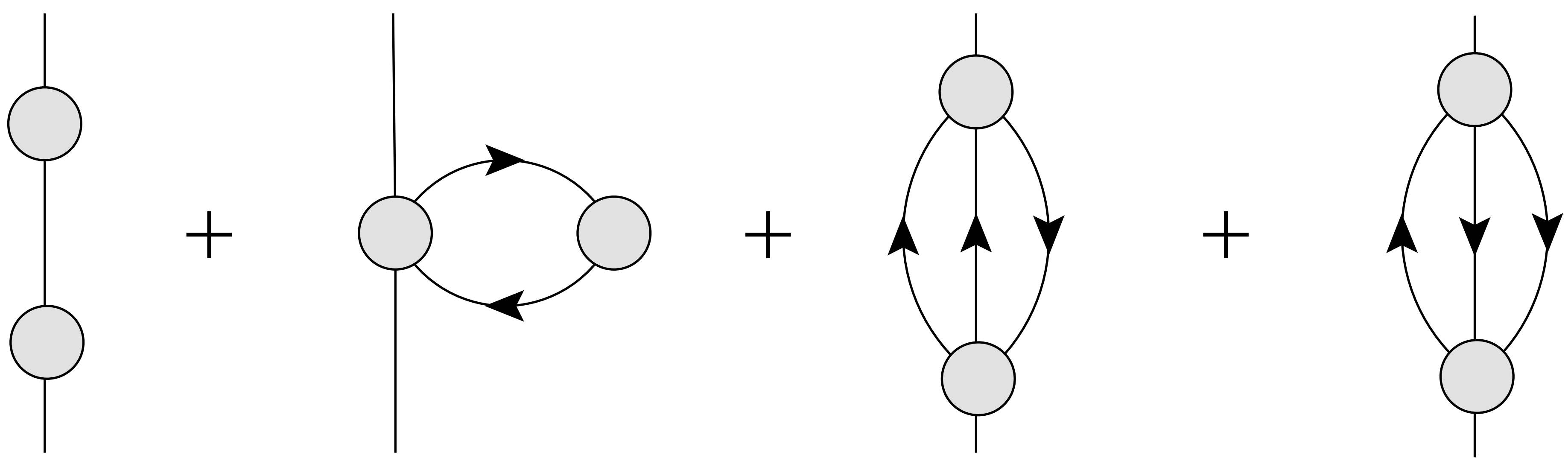
$$\frac{dE}{ds} =$$



coefficients (couplings) of H(s)

1-body Flow

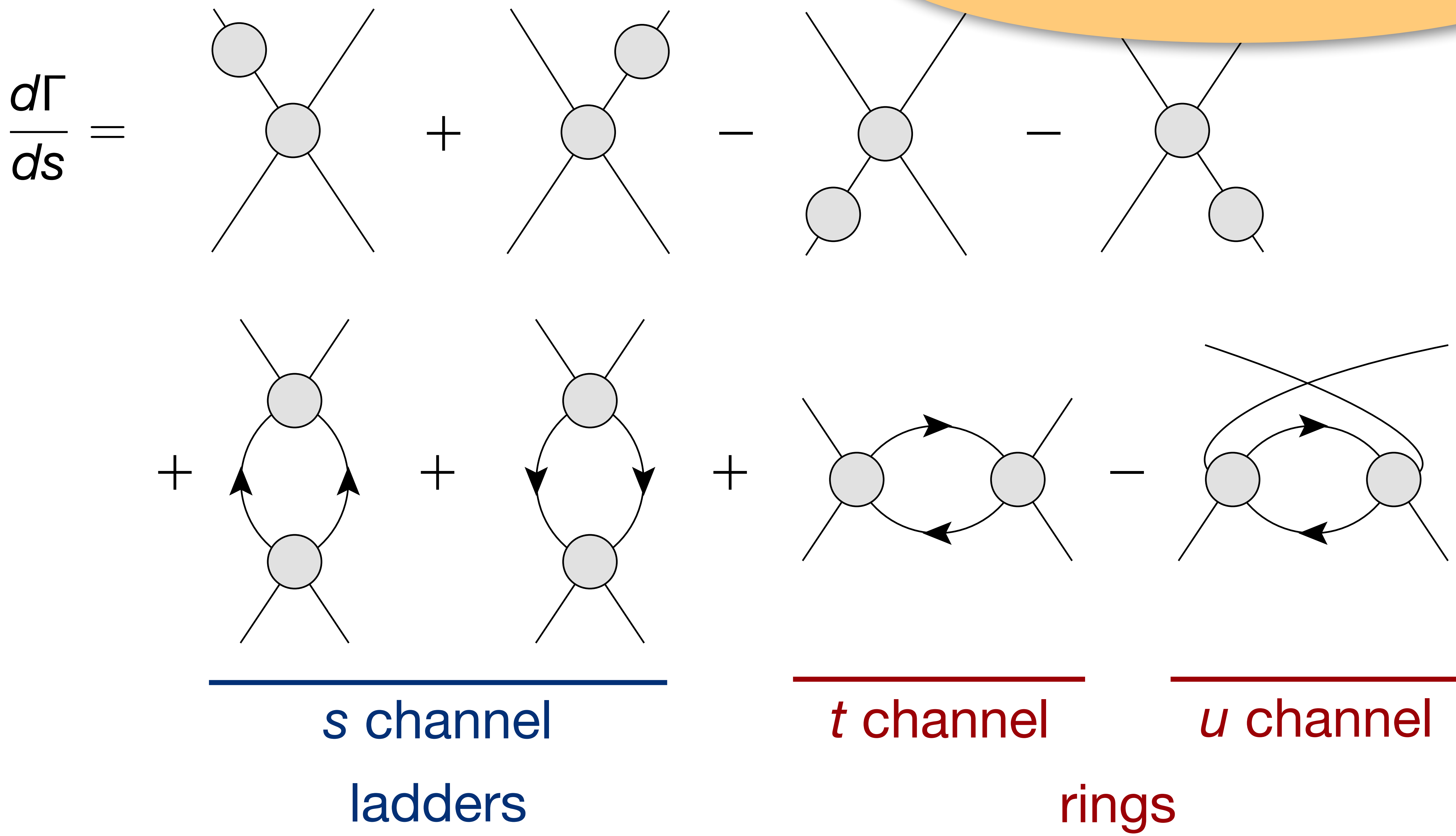
$$\frac{df}{ds} =$$



Standard IMSRG(2) Flow Equations

O(N⁶) scaling
(before particle/hole distinction)

2-body Flow



Coupled Cluster Method

- explicit ansatz for **similarity transformation**:

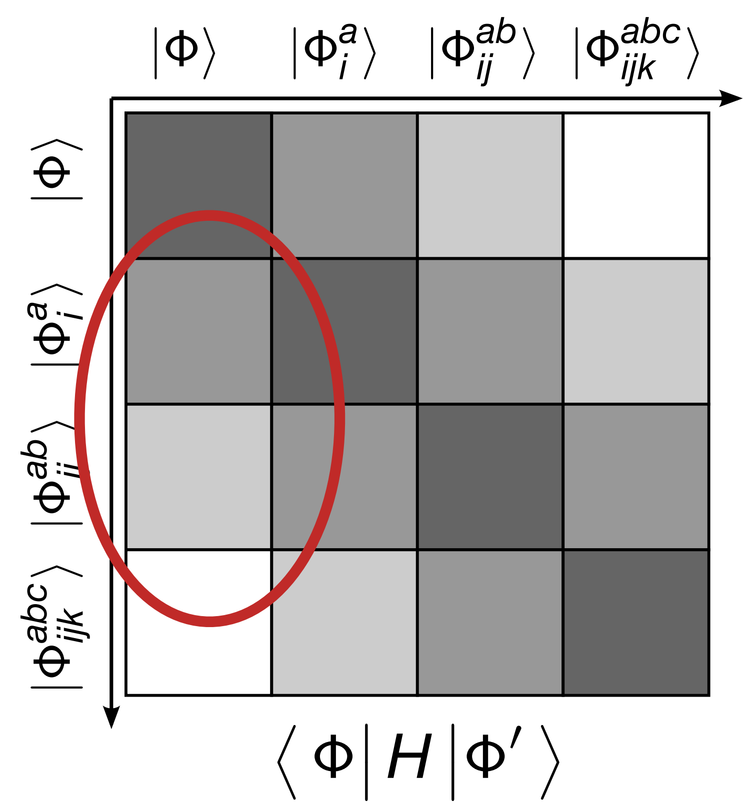
$$\bar{H} = e^{T} H e^{-T}, \qquad T = T^{[1]} + T^{[2]} + \ldots$$

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

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

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

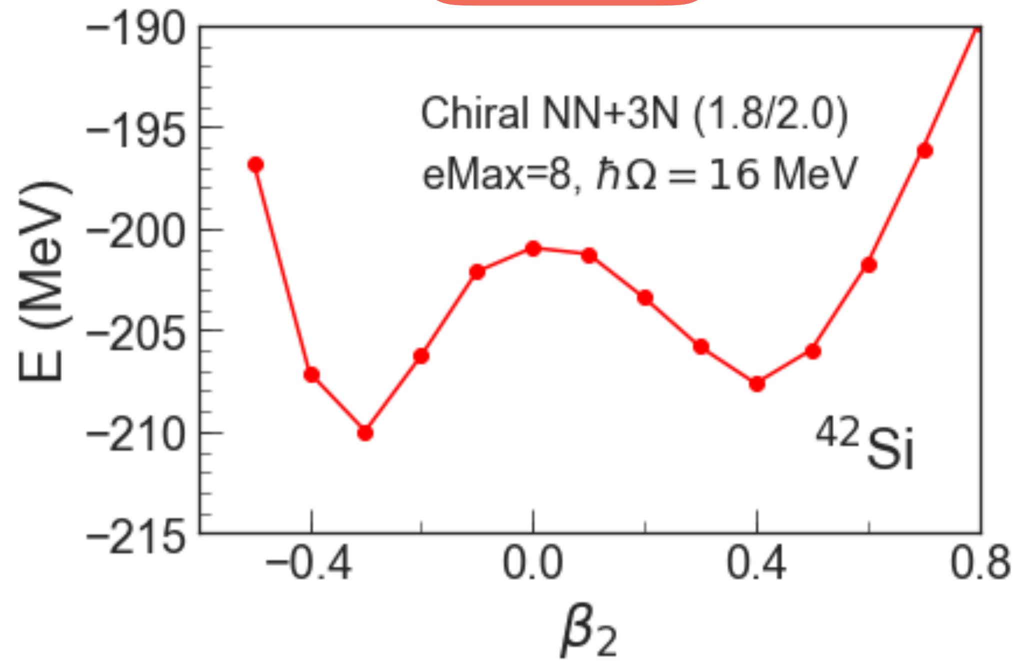
  - Note: effective Hamiltonian is **not Hermitian (symmetric)**!



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

Projected GCM

HFB
Generate reference state



$$\frac{\langle \mathrm{HFB}(\mathbf{q})|\hat{H}|\mathrm{HFB}(\mathbf{q})\rangle}{\langle \mathrm{HFB}(\mathbf{q})|\mathrm{HFB}(\mathbf{q})\rangle}$$

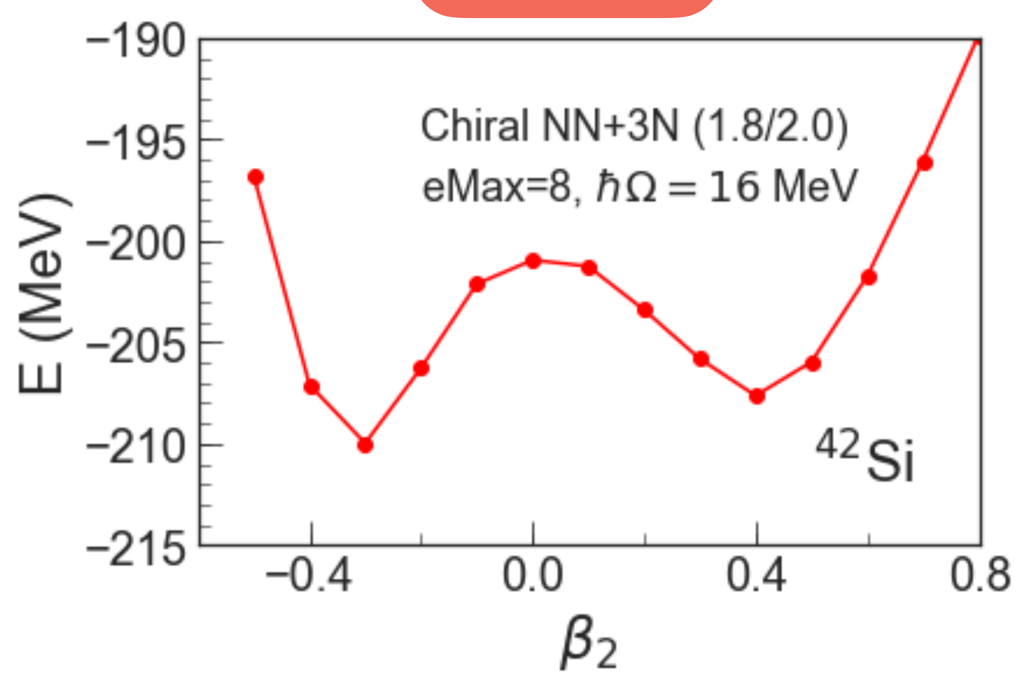
Potential Energy Surface

Take into account static correlations (pairing, deformation) via symmetry breaking.

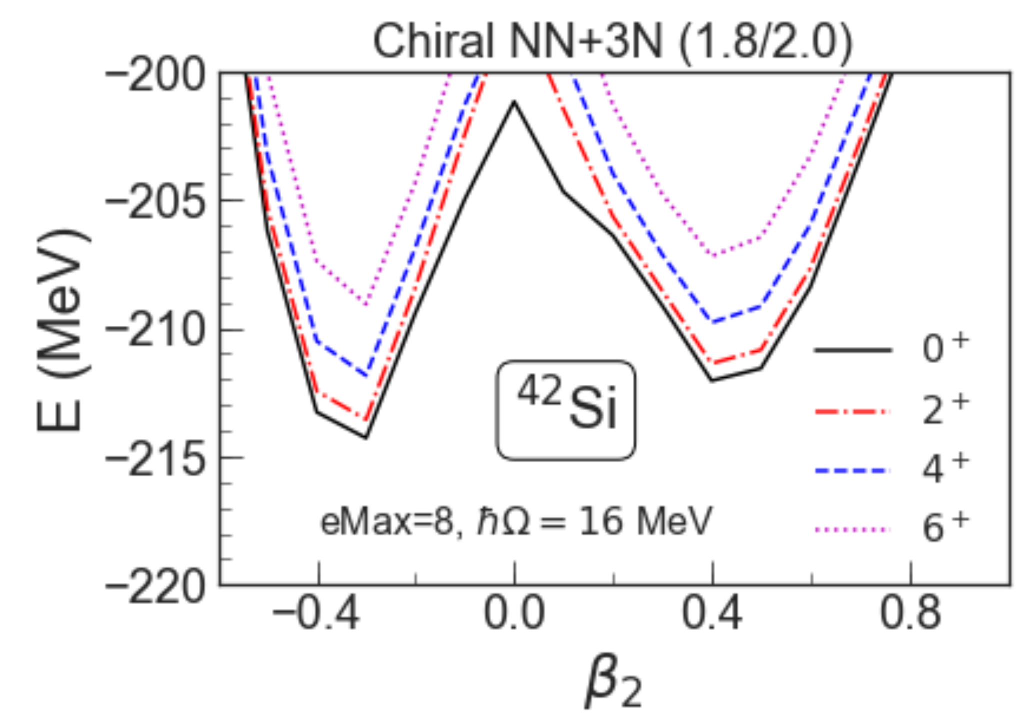
[slides by **J. M. Yao**]

Projected GCM

HFB
Generate reference state

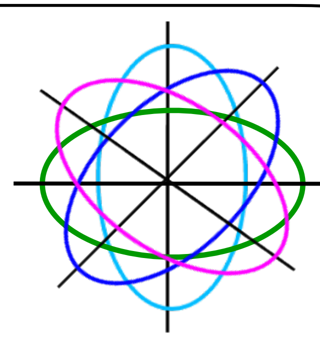


Projection
Compute different kernels



particle-number projector

$$\hat{P}_{N_0} = \frac{1}{2\pi}\int_0^{2\pi} d\phi_N \underbrace{e^{-i\phi_N N_0}}_{\text{weight}} \overbrace{e^{i\phi_N \hat{N}}}^{\text{rotation in gauge space}}$$



angular-momentum restoration operator

$$\hat{P}^J_{MK} = \frac{2J+1}{16\pi^2}\int_0^{4\pi} d\alpha \int_0^{\pi} d\beta\ \sin(\beta) \int_0^{2\pi} d\gamma\ \underbrace{\mathcal{D}^{*J}_{MK}(\alpha,\beta,\gamma)}_{\text{Wigner function}} \overbrace{\hat{R}(\alpha,\beta,\gamma)}^{\text{rotation in real space}}$$

$$|\Phi^{JNZ}(\mathbf{q})\rangle = \hat{P}^J_{MK}\hat{P}_{N_0}\hat{P}_{Z_0}|\mathbf{q}\rangle$$

$$\frac{\langle\Phi^{JNZ}(\mathbf{q})|\hat{H}|\Phi^{JNZ}(\mathbf{q})\rangle}{\langle\Phi^{JNZ}(\mathbf{q})|\Phi^{JNZ}(\mathbf{q})\rangle}$$

[slides by **J. M. Yao**]

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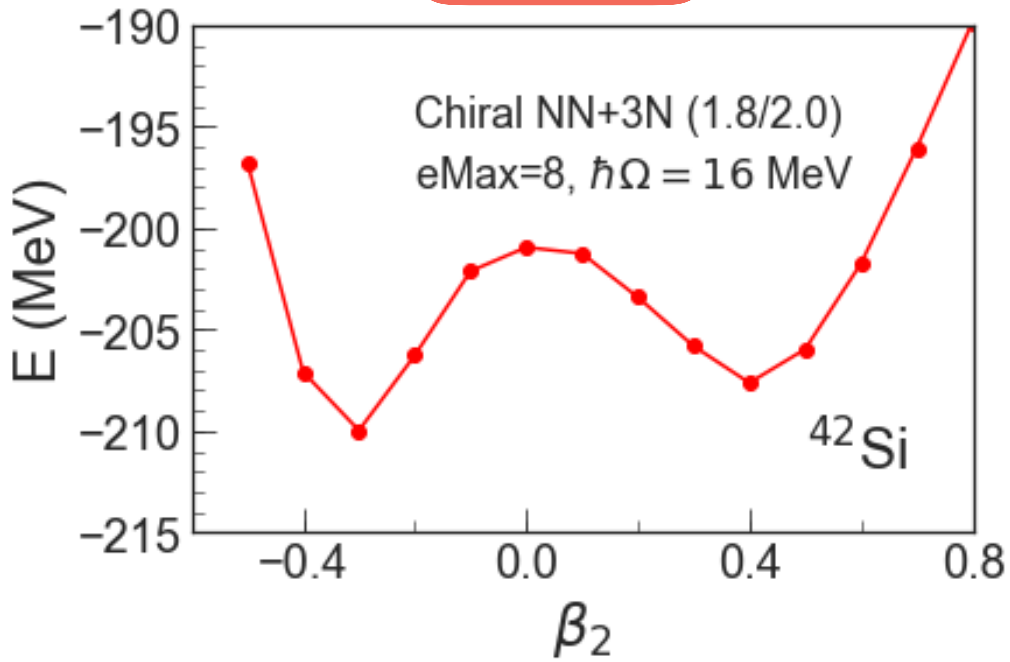
HFB
Generate reference state



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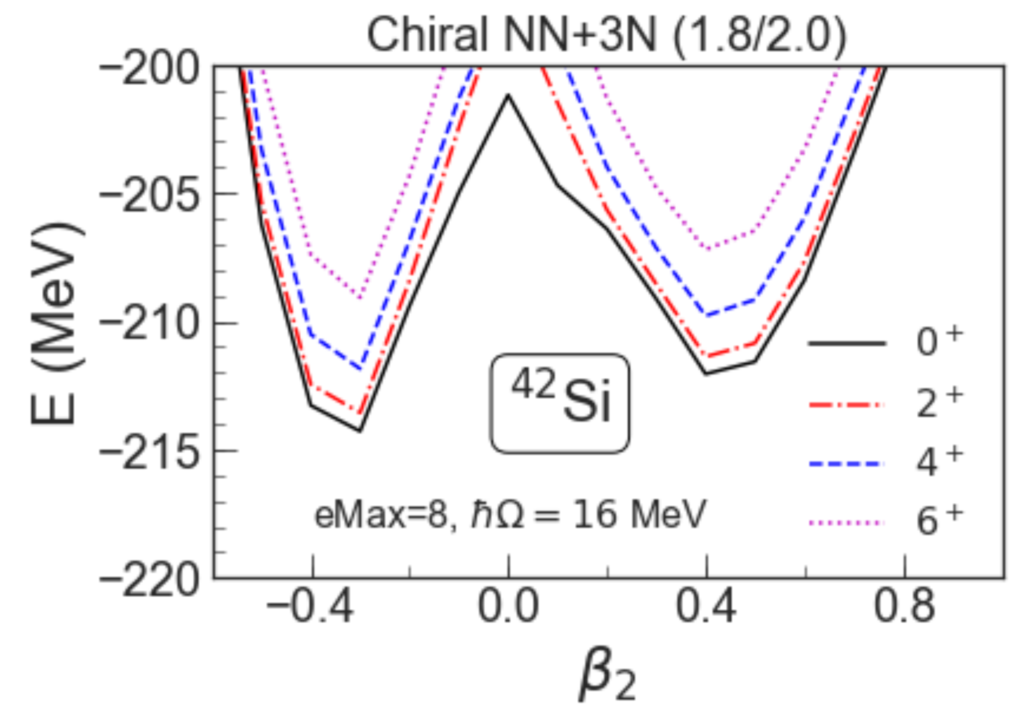
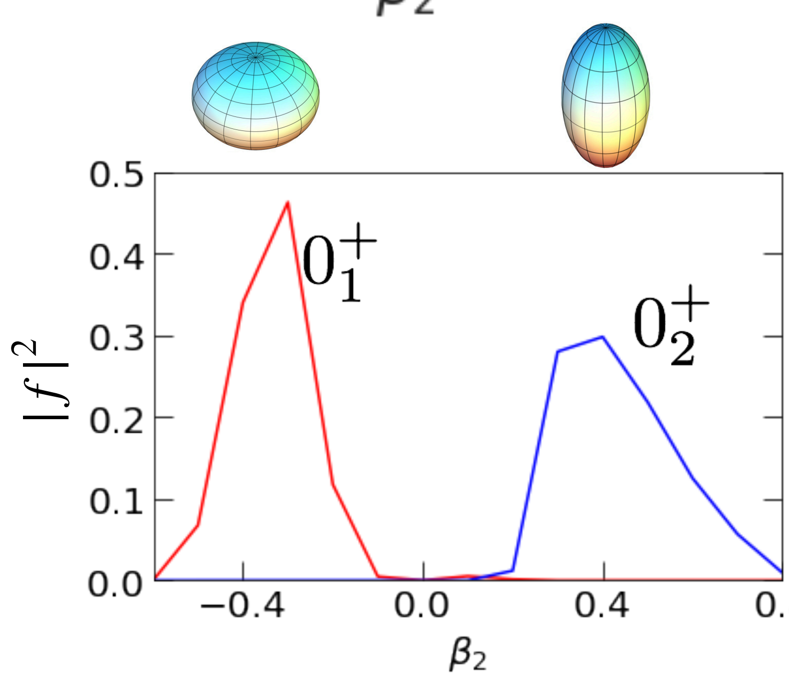


GCM
Solve Hill-Wheeler equation

$$|\Phi\rangle = \sum_{\mathbf{q}} f^J(\mathbf{q})|\Phi^{JNZ}(\mathbf{q})\rangle$$

$$\sum_{\mathbf{q}_b}\left[\mathscr{H}^J_{\mathbf{q}_a,\mathbf{q}_b} - E^J_\alpha \mathscr{N}^J_{\mathbf{q}_a,\mathbf{q}_b}\right] f^J_\alpha(\mathbf{q}_b) = 0$$



[slides by **J. M. Yao**]

Projected GCM

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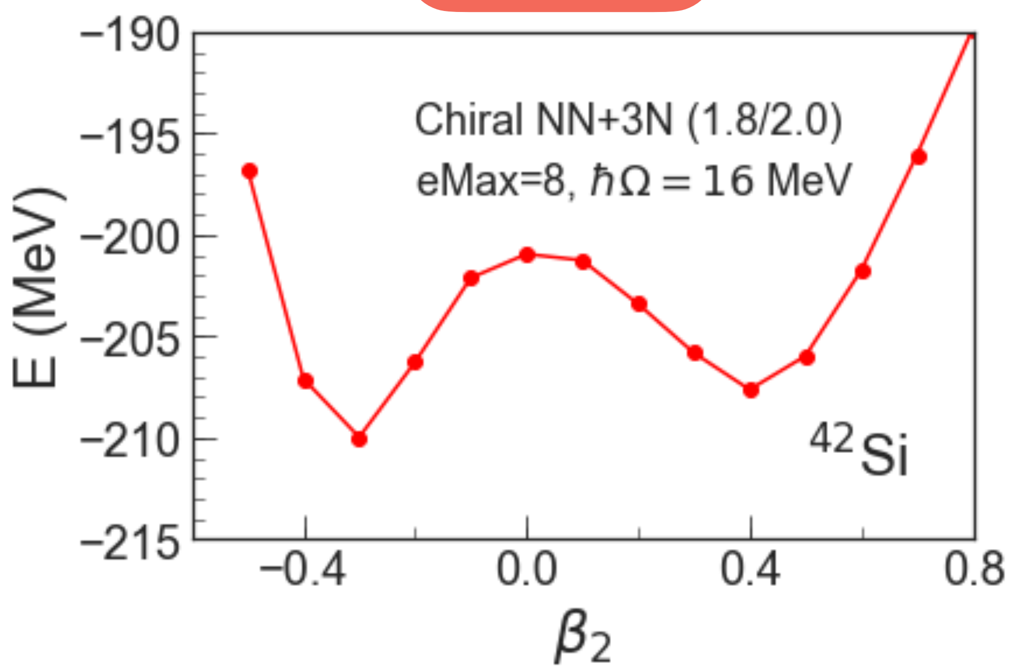

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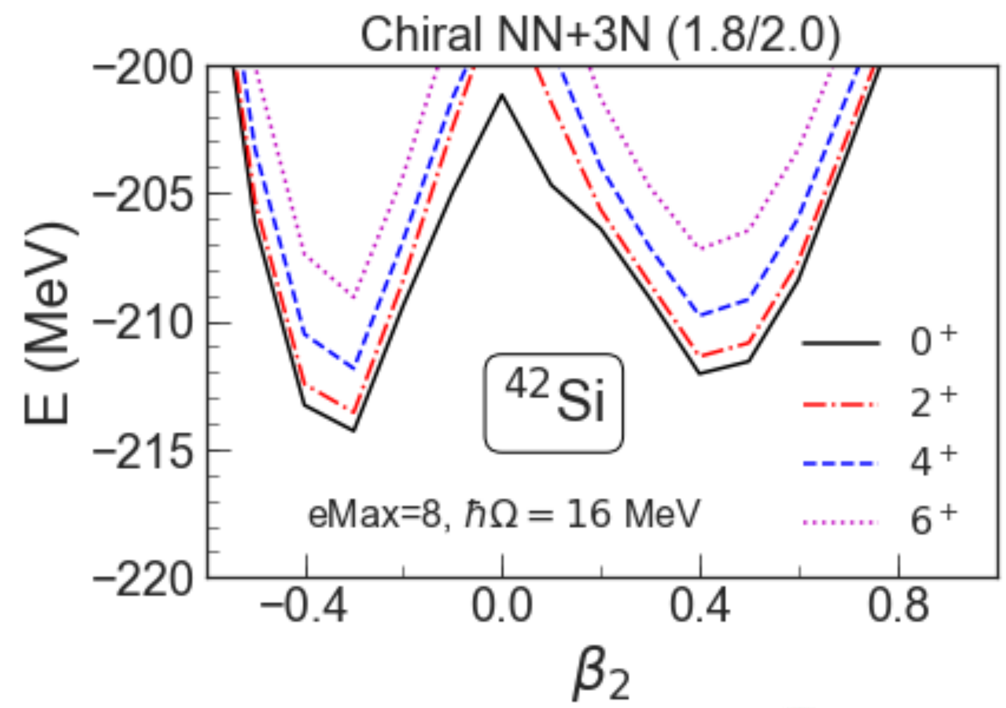
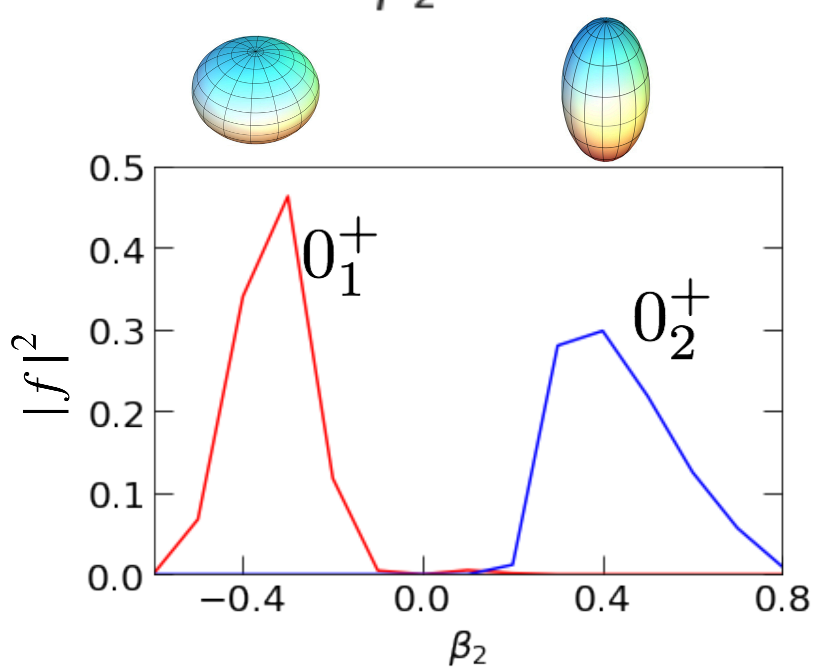
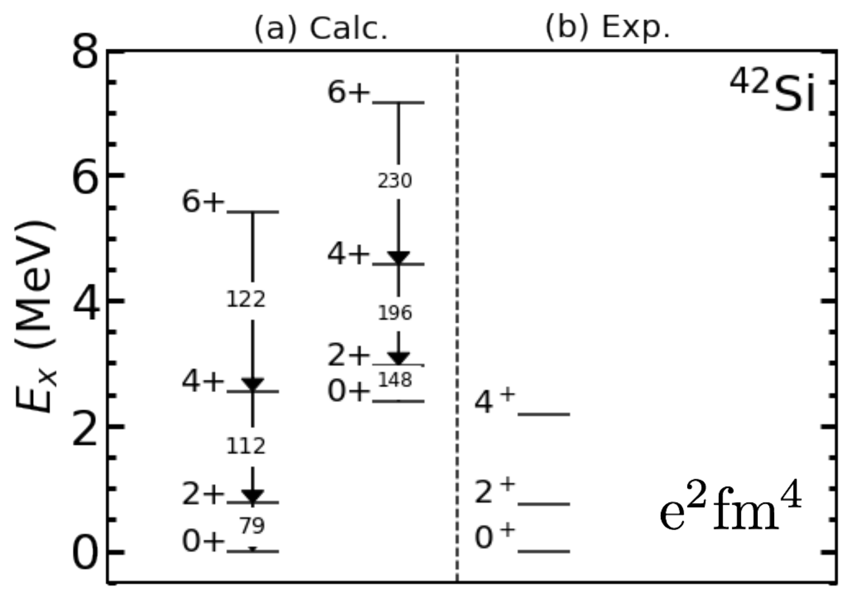


GCM
Solve Hill-Wheeler equation

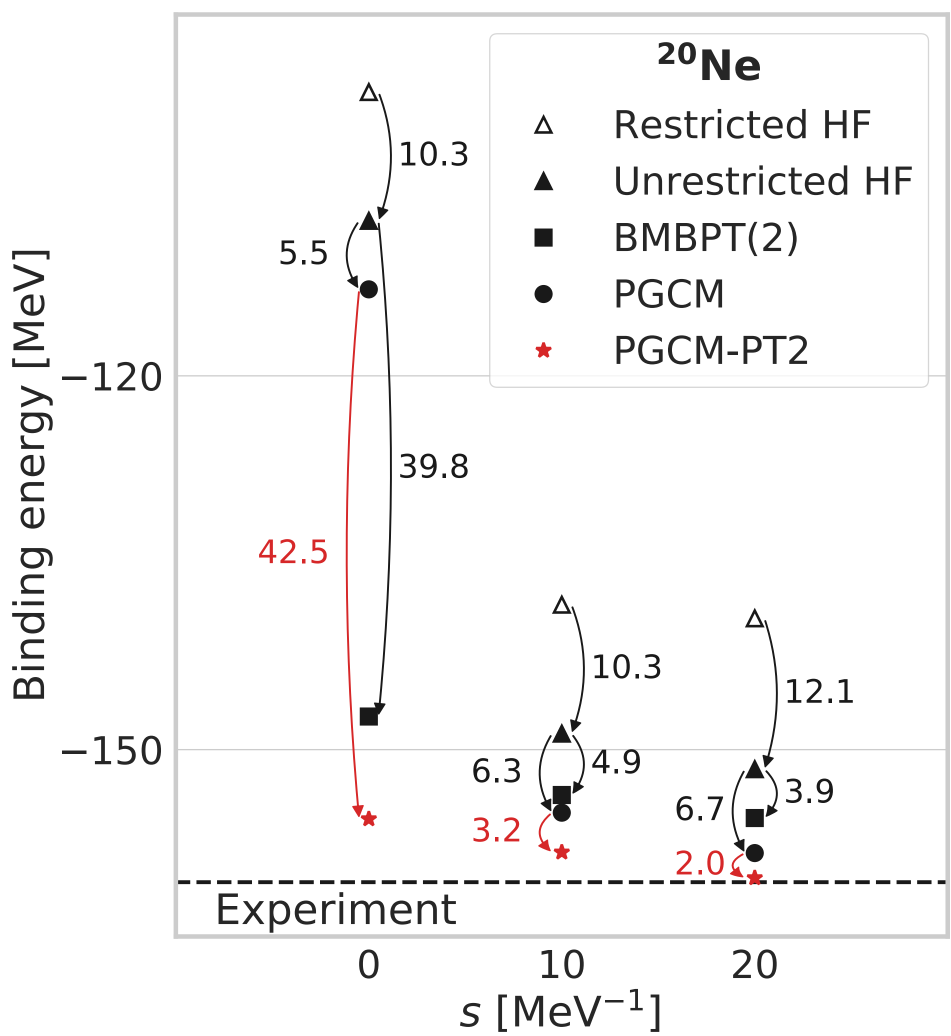


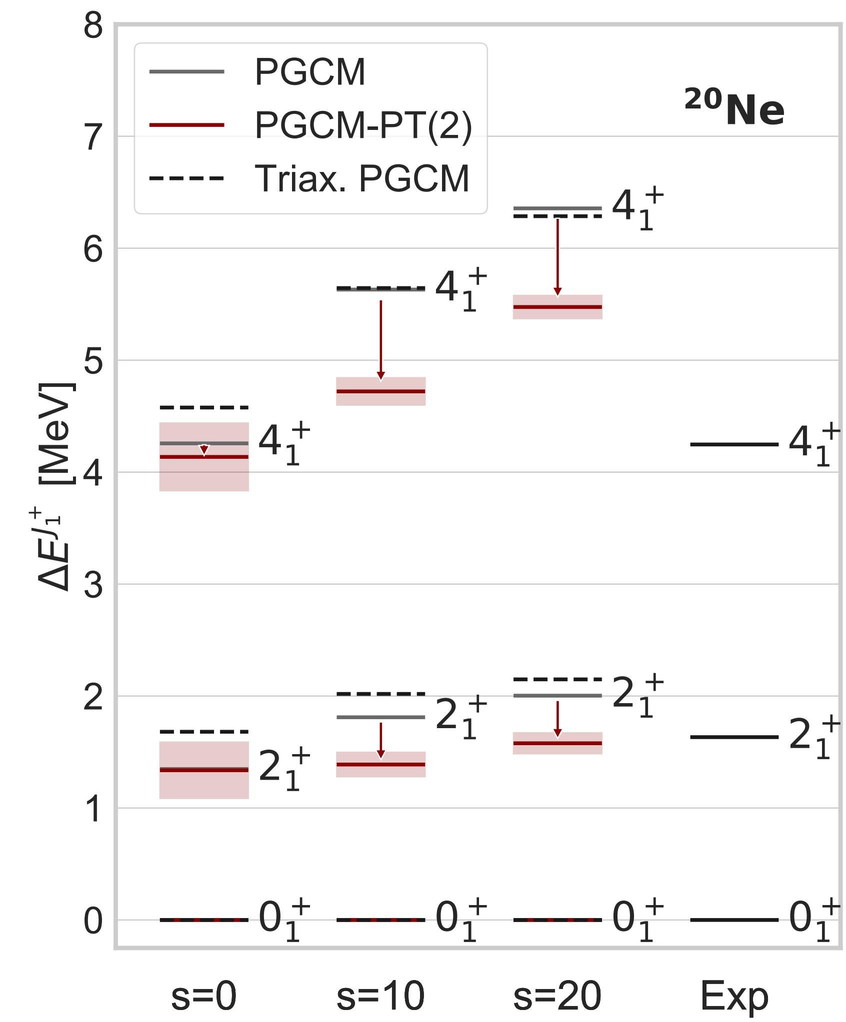


[slides by **J. M. Yao**]

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