Innovative many-body methods for nuclear structure

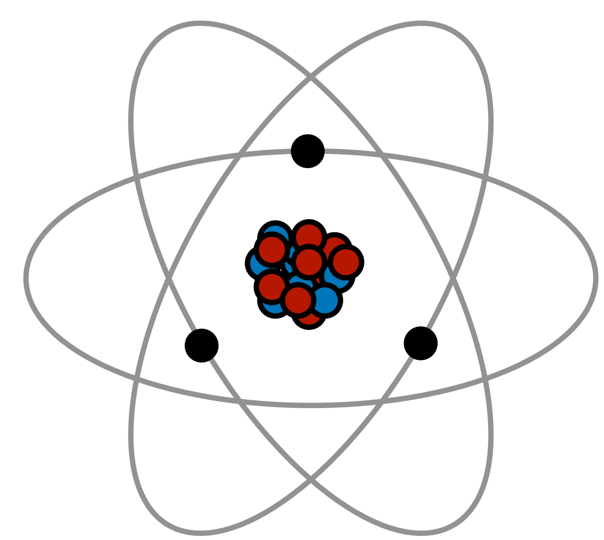
KHuK Annual Meeting

Physikzentrum Bad Honnef

December 9th, 2022

Alexander Tichai

Technische Universität Darmstadt

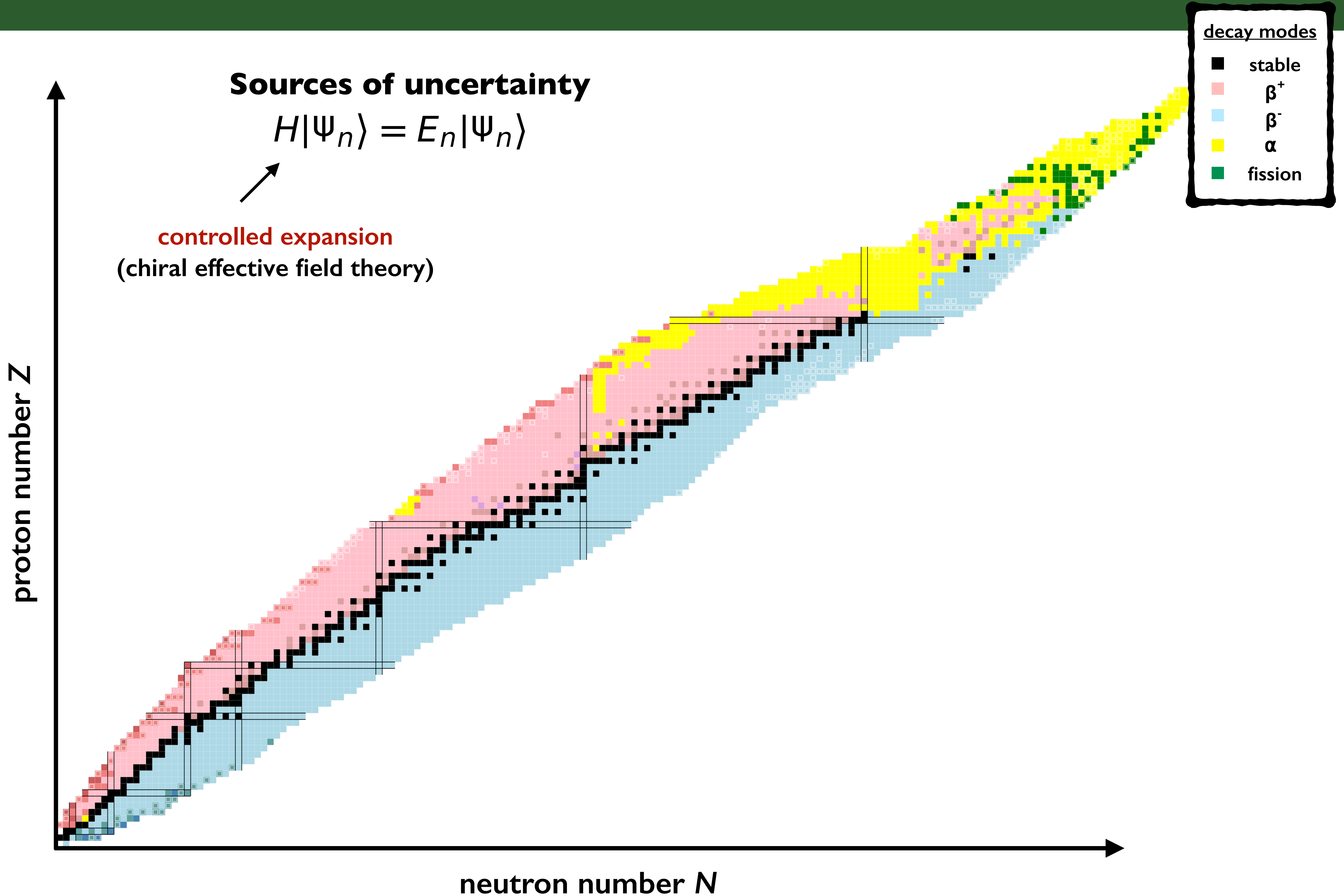


Ab initio nuclear structure

Sources of uncertainty

$$H|\Psi_n\rangle = E_n|\Psi_n\rangle$$

controlled expansion
(chiral effective field theory)



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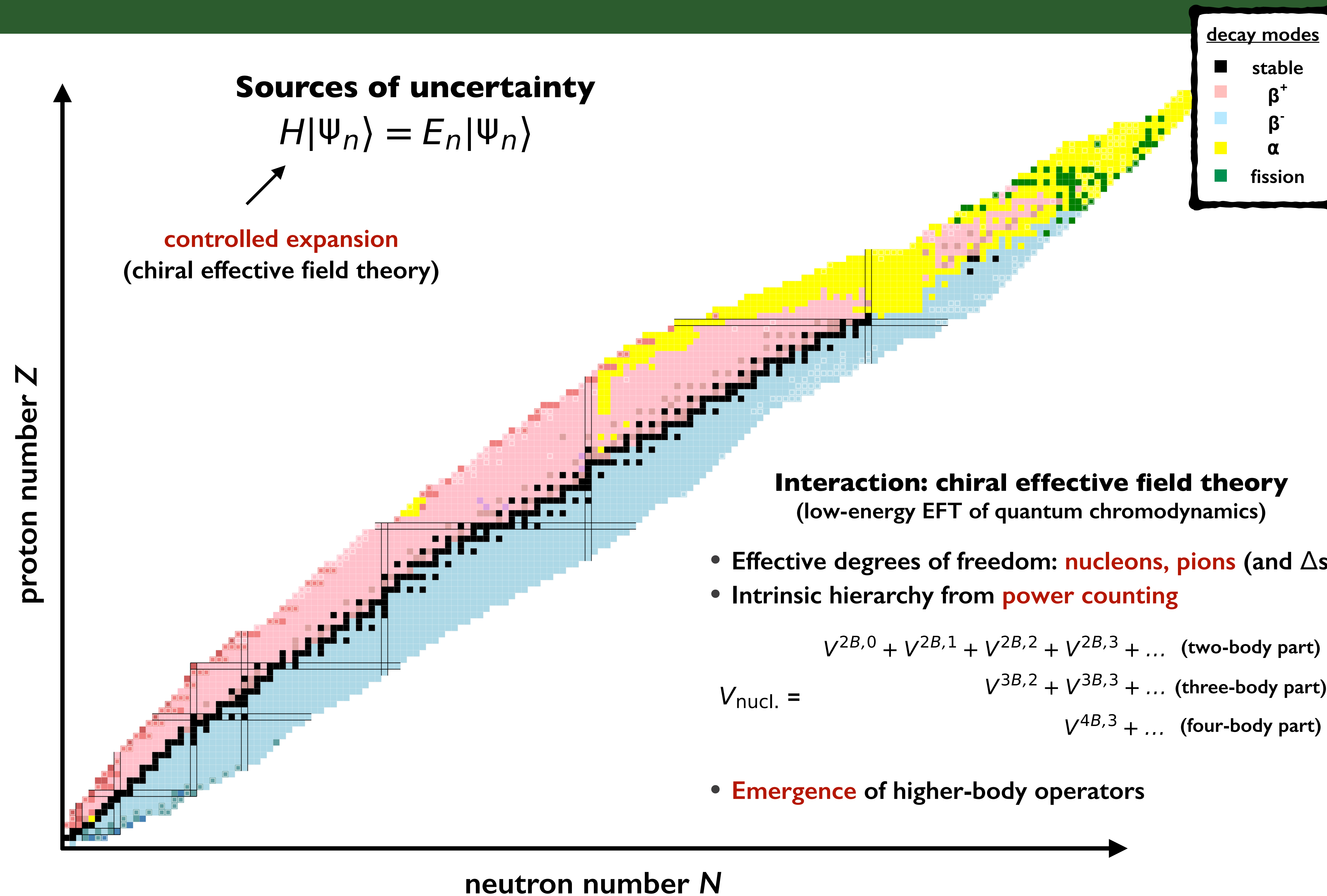

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Interaction: chiral effective field theory
(low-energy EFT of quantum chromodynamics)

- Effective degrees of freedom: nucleons, pions (and Δs)
- Intrinsic hierarchy from power counting

$$V_{\text{nucl.}} = \begin{array}{rl} V^{2B,0} + V^{2B,1} + V^{2B,2} + V^{2B,3} + \ldots & \text{(two-body part)} \\ V^{3B,2} + V^{3B,3} + \ldots & \text{(three-body part)} \\ V^{4B,3} + \ldots & \text{(four-body part)} \end{array}$$

- Emergence of higher-body operators

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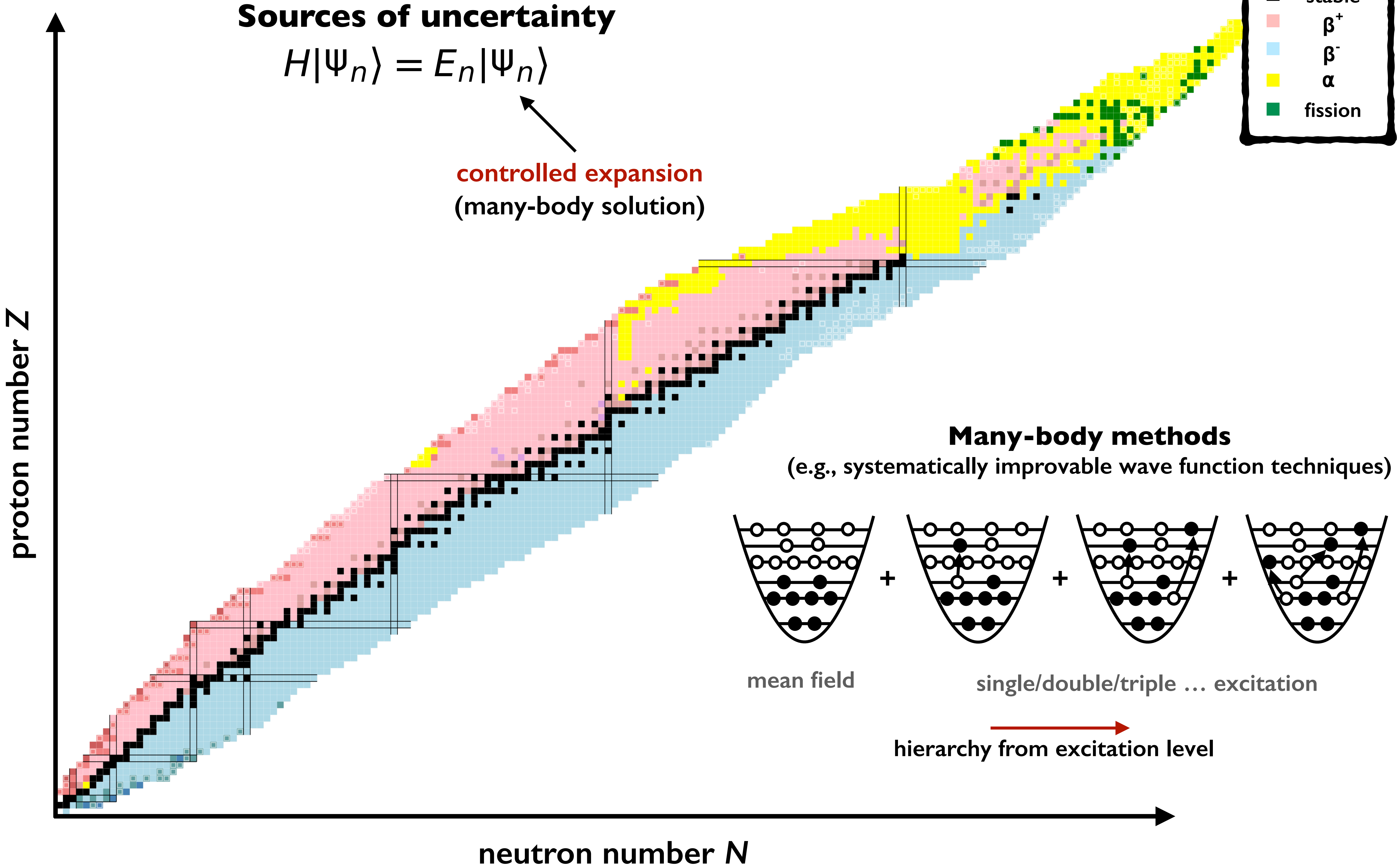
(many-body solution)



Many-body methods
(e.g., systematically improvable wave function techniques)

hierarchy from excitation level

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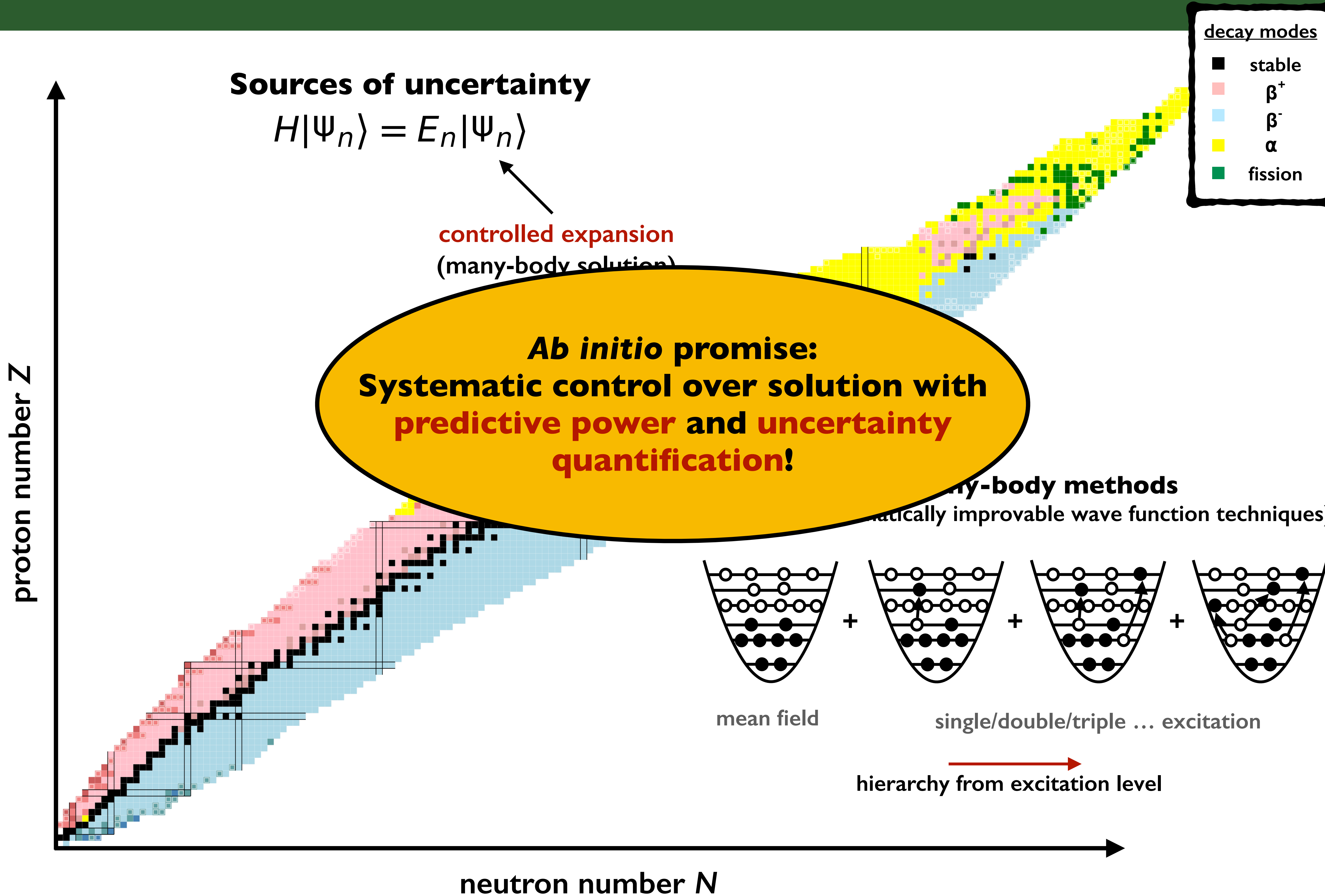


***Ab initio* promise:**

Systematic control over solution with predictive power and uncertainty quantification!

…y-body methods

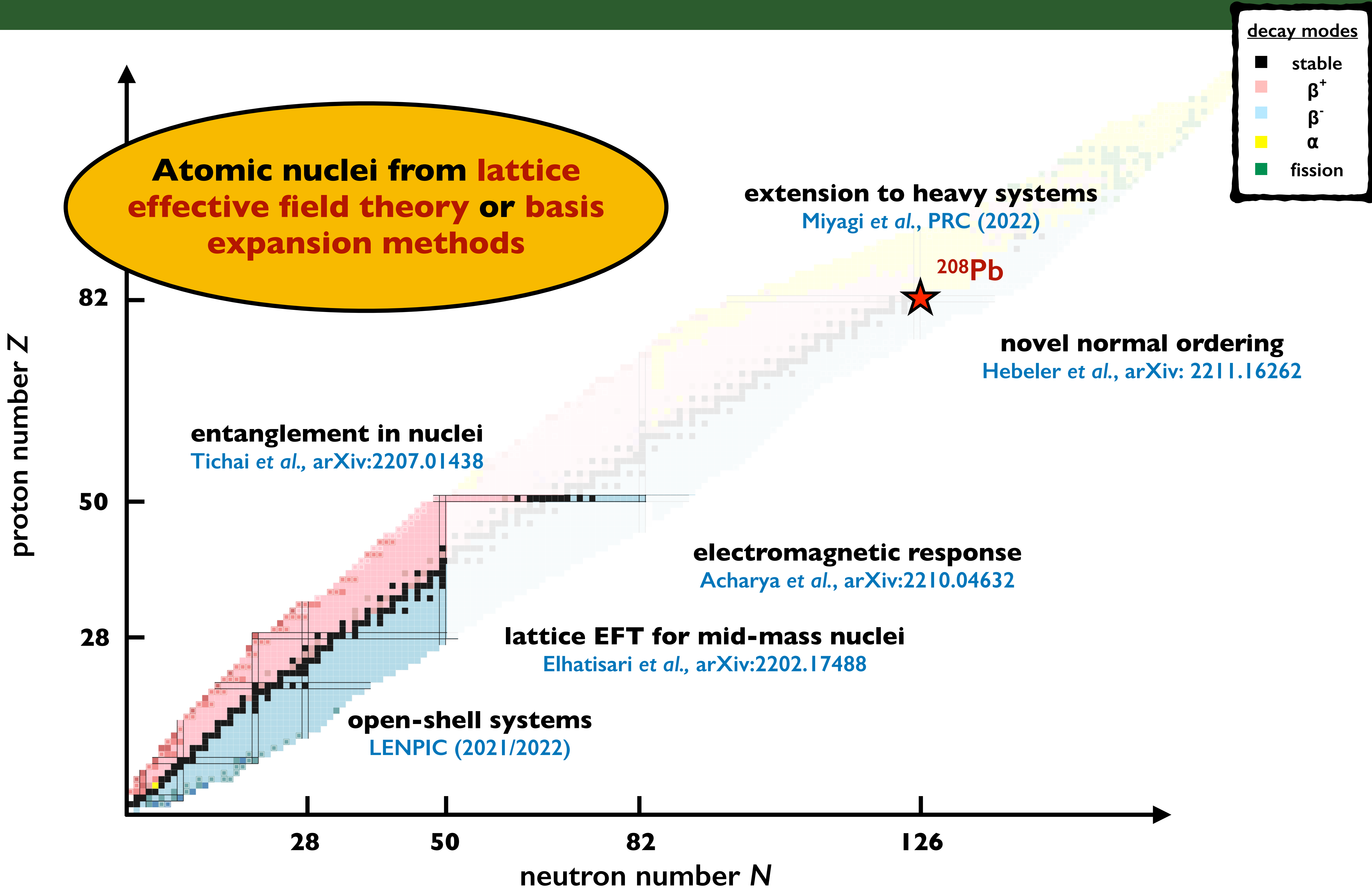
(…atically improvable wave function techniques)

mean field

single/double/triple … excitation

hierarchy from excitation level

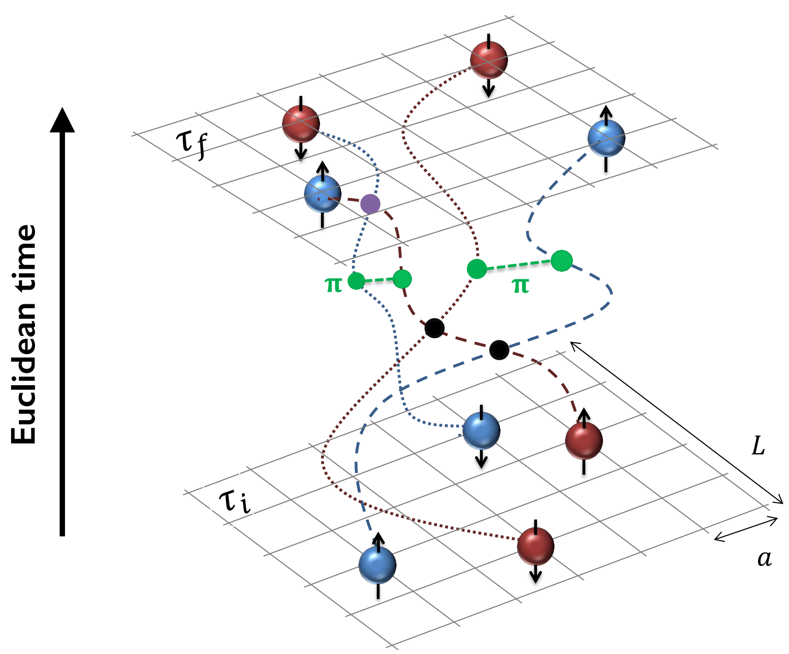
Recent highlights from 2021/22



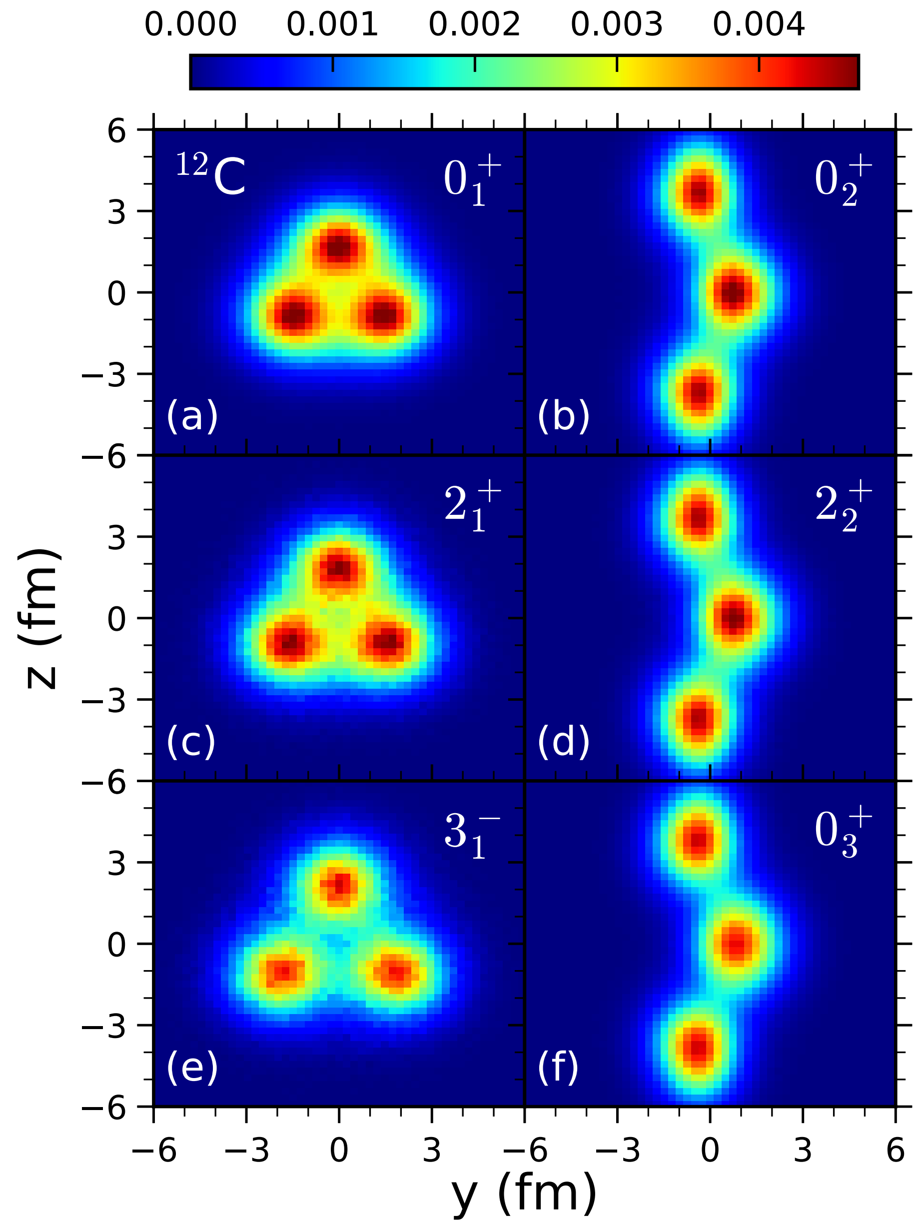
Nuclear lattice EFT

Lähde, Meißner, Lee, Shen, Elhatisari, Epelbaum, Krebs, …

- Nuclear dynamics on space-time lattice



Geometry of ^{12}C states



Shen *et al.*, arXiv:2202.13596

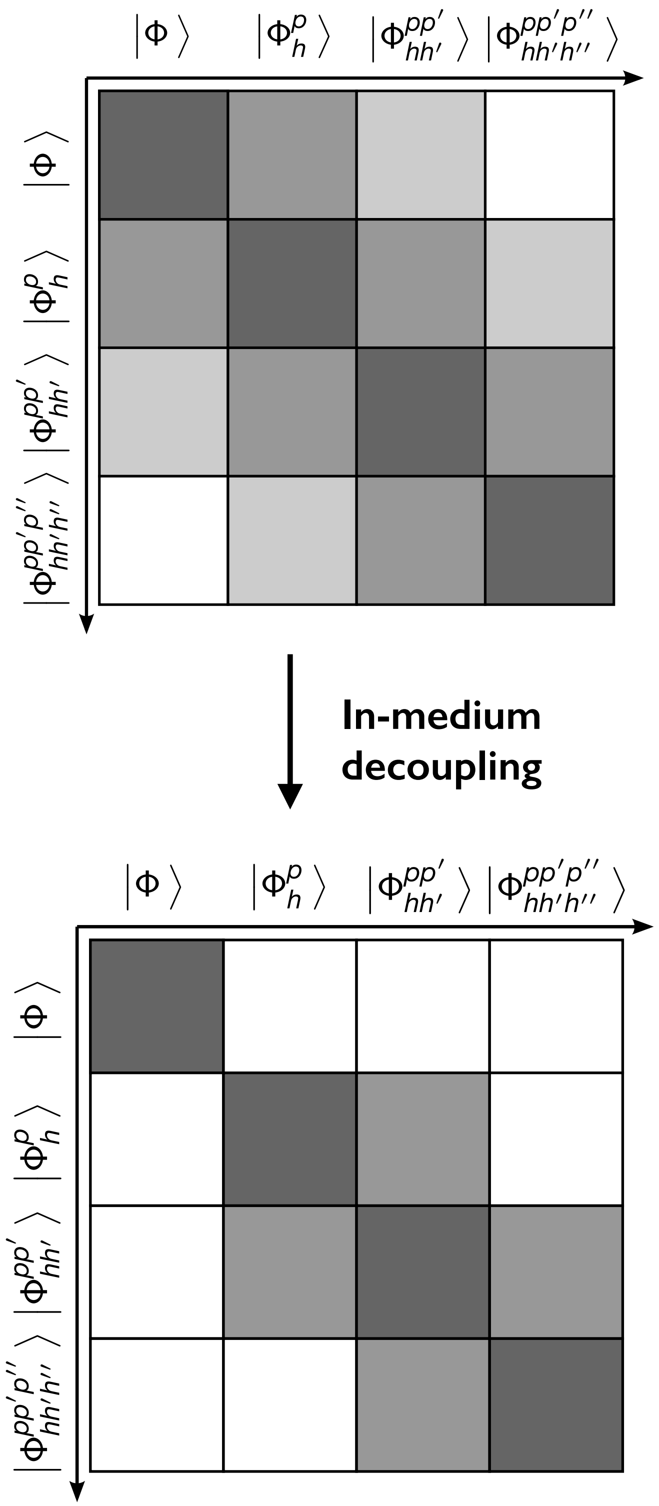
- Sampling via Quantum Monte Carlo techniques
- Emergence of clustering phenomena

Very complicated in basis-expansion methods!

- Recent extension to mid-mass systems (A < 40)

Elhatisari *et al.*, arXiv:2202.17488

In-medium similarity renormalization group



Hergert *et al.*, Phys. Rep. (2016)

- **Input: nuclear Hamiltonian in second quantization**

$$H_{\text{nucl.}} = T + V_{2N} + V_{3N} + \dots$$

- **Goal: decoupling of elementary ph-excitations**

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

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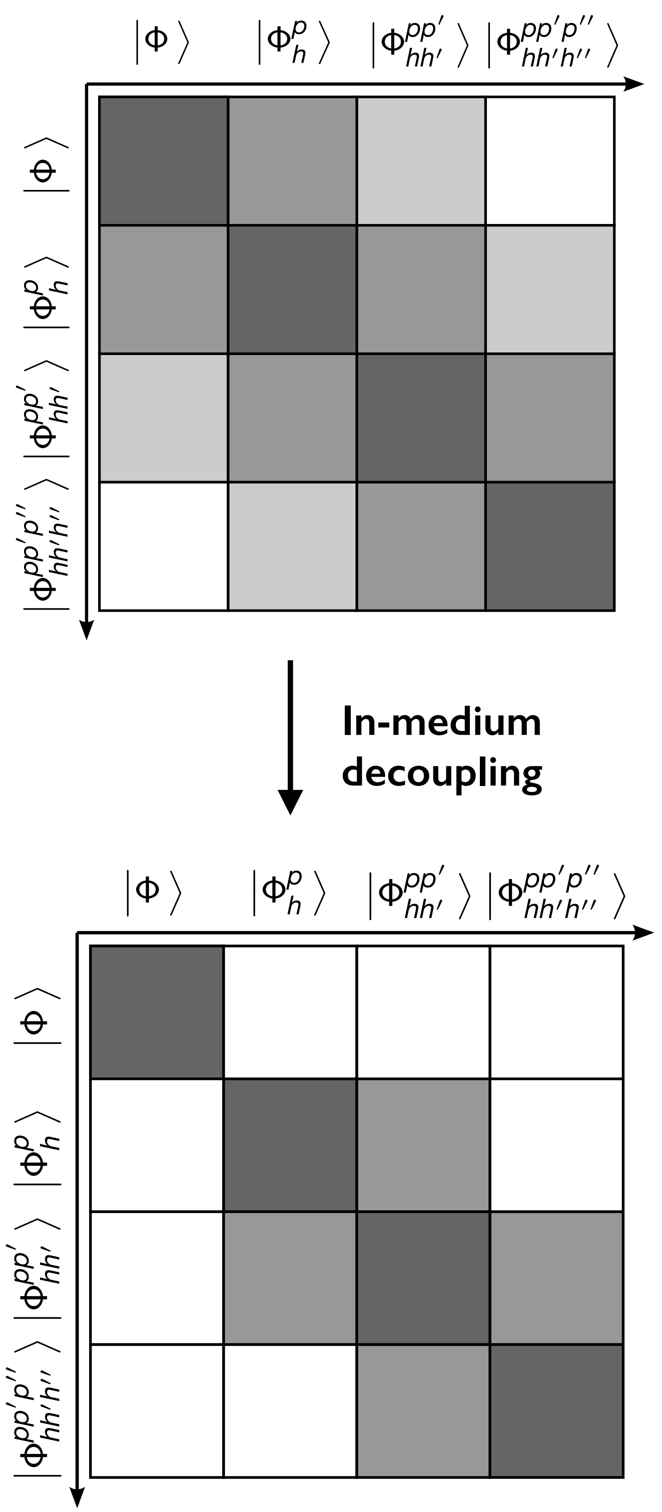

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Keep operators to *k*-body level:
IMSRG(*k*)

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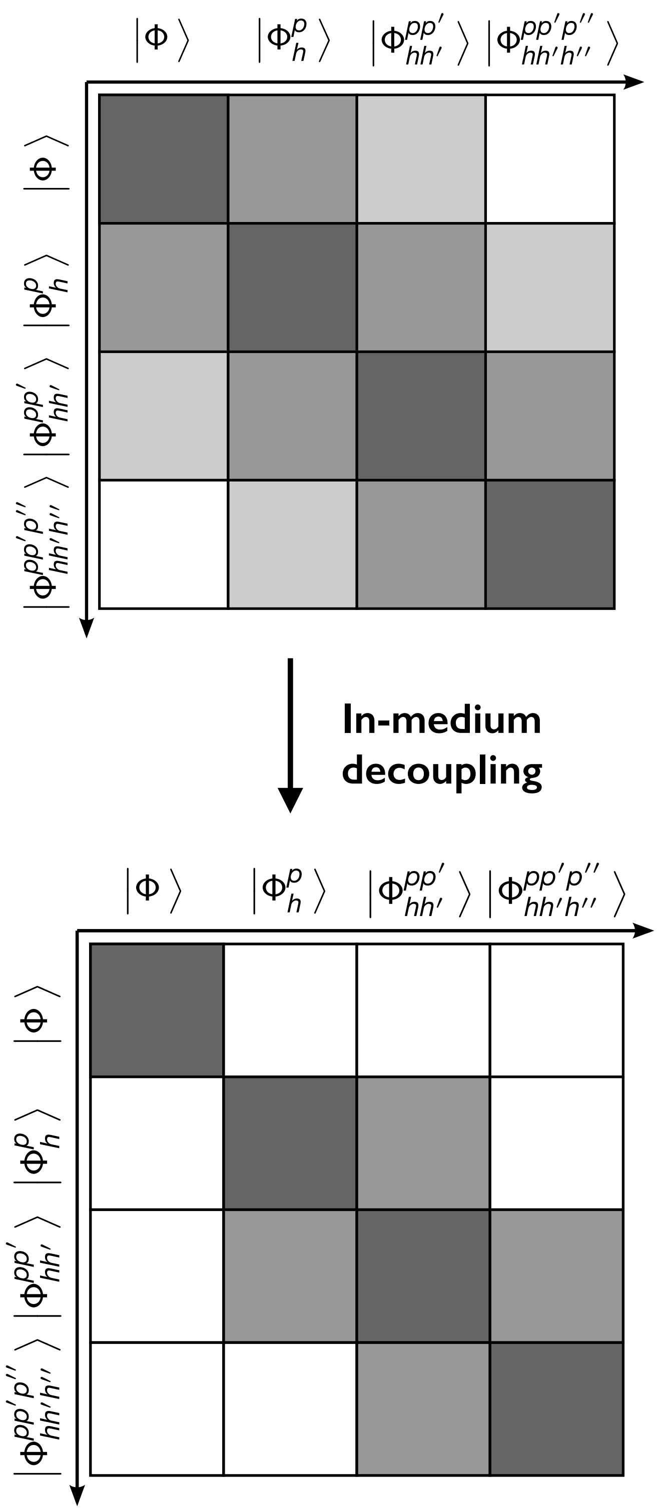

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- **Ground-state energy from flowing Hamiltonian**

$$\lim_{s\to\infty} \langle\Phi|H(s)|\Phi\rangle = E_0$$

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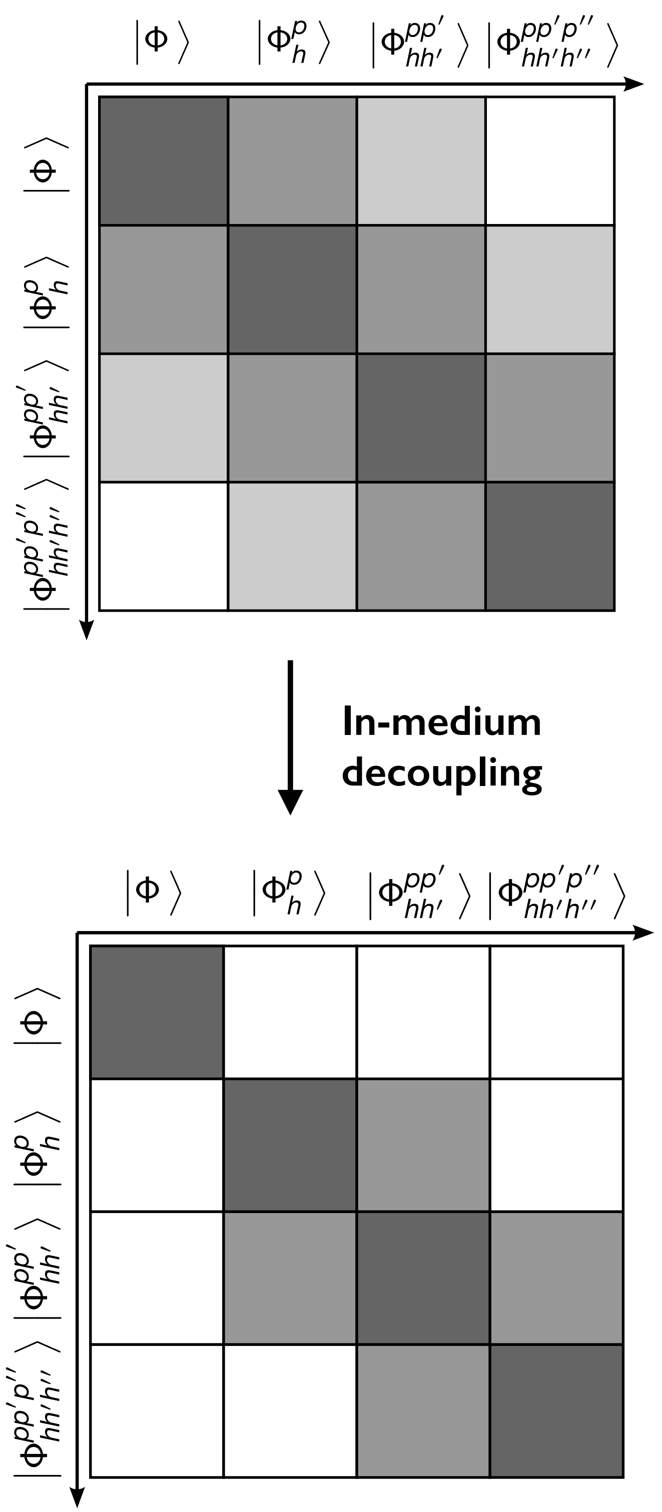

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- **Versatility: generate input for other approaches**

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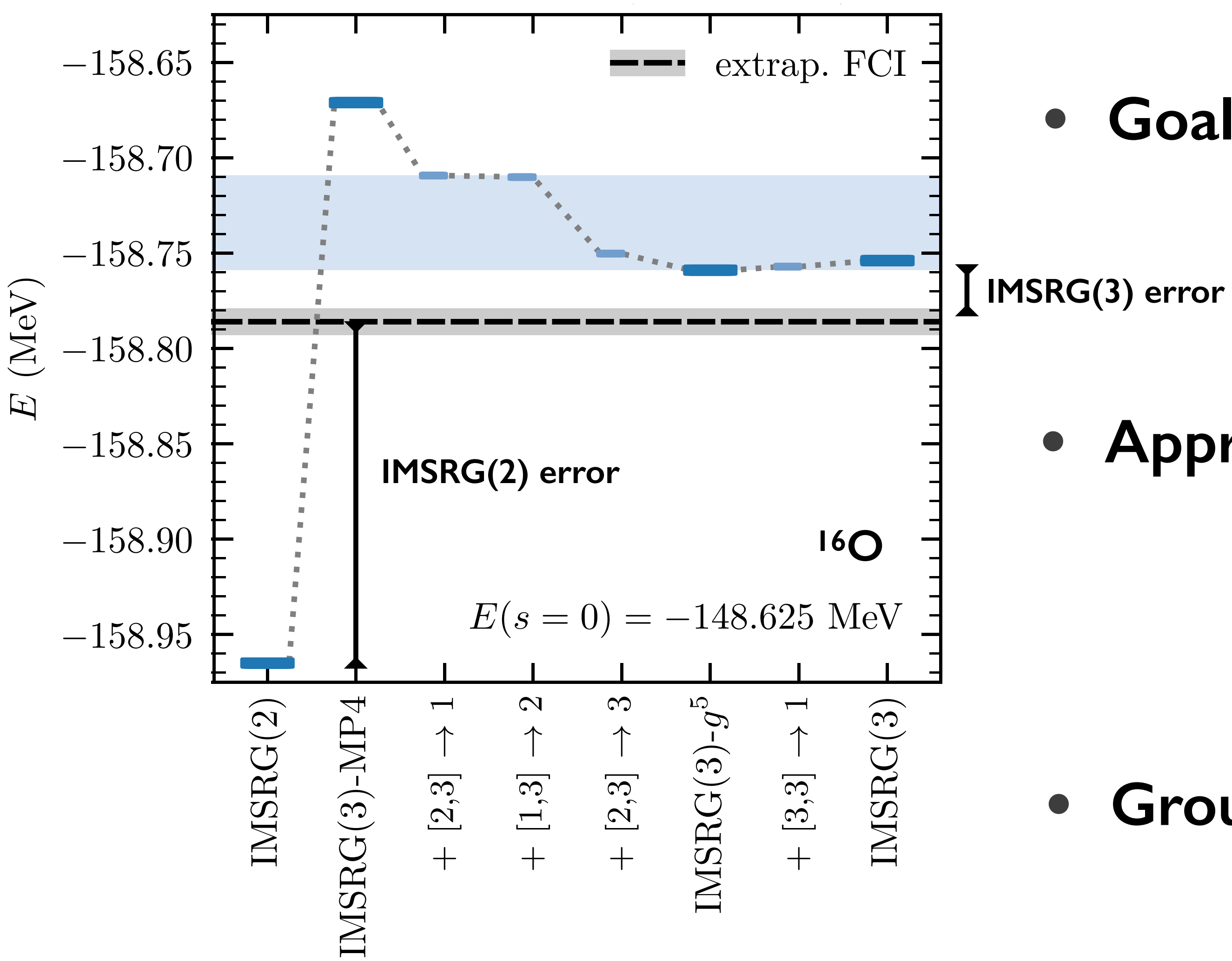
Systematic relaxation of many-body truncation



Heinz, Hebeler, Hoppe, Schwenk, Tichai
PRC (2021)

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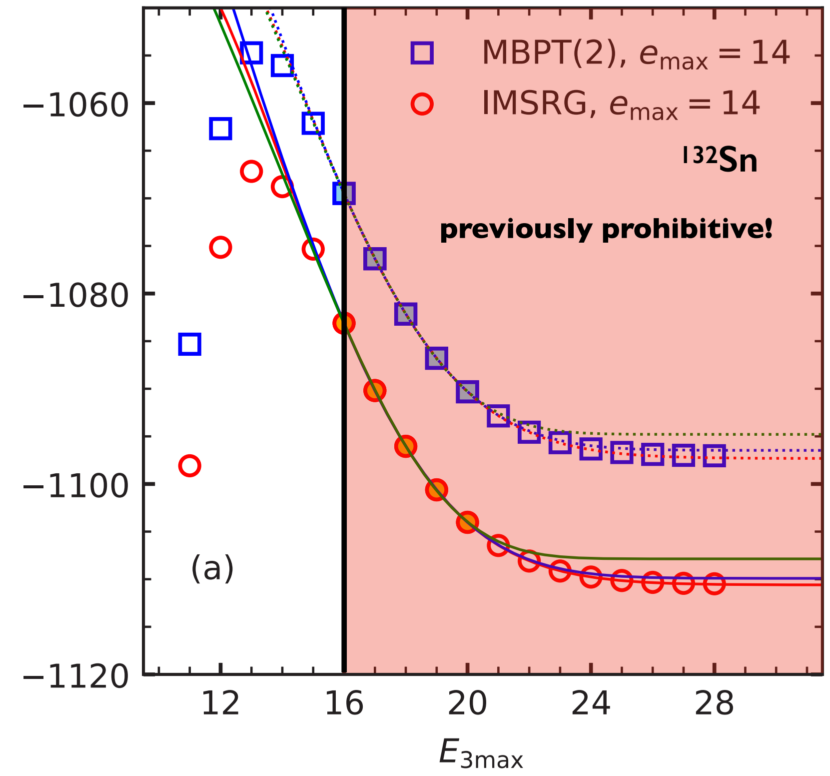
Towards heavy nuclei

Miyagi *et al.*, PRC (2022)



- **Normal ordering:** effective 2-body operator

$$v_{pqrs} = \sum_{tu} w_{pqtrsu} \rho_{tu}$$

- **Convergence gauged from 3B-truncation**

$$e_1 + e_2 + e_3 \leq E_{3max}$$

- ***Ab initio* frameworks can for the first time provide a controlled description of ^{208}Pb**

Hu *et al.*, Nature Physics (2022)

Neutron skin ⟷ EOS parameters

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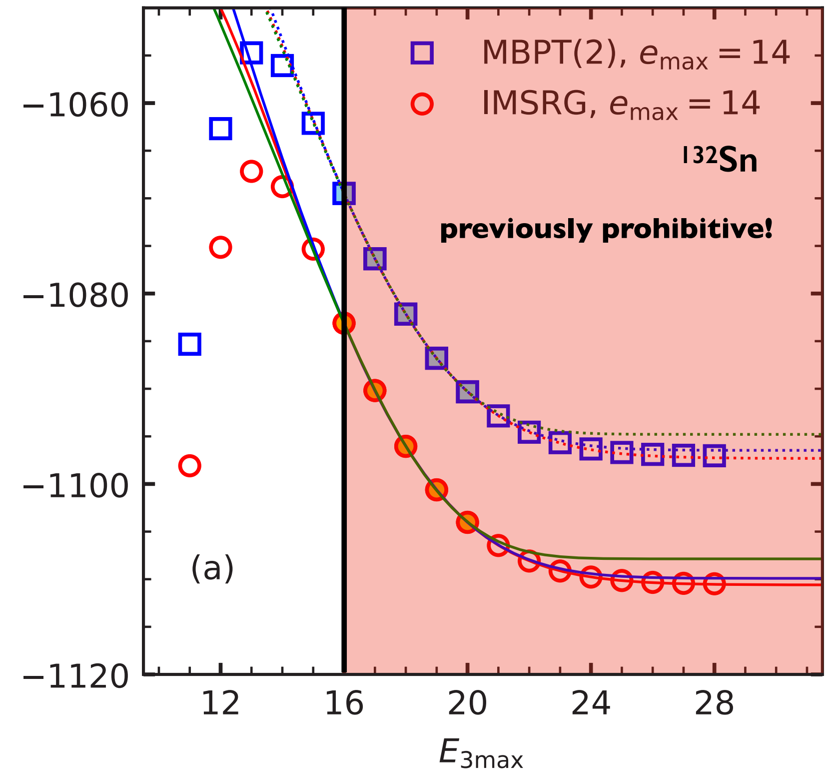

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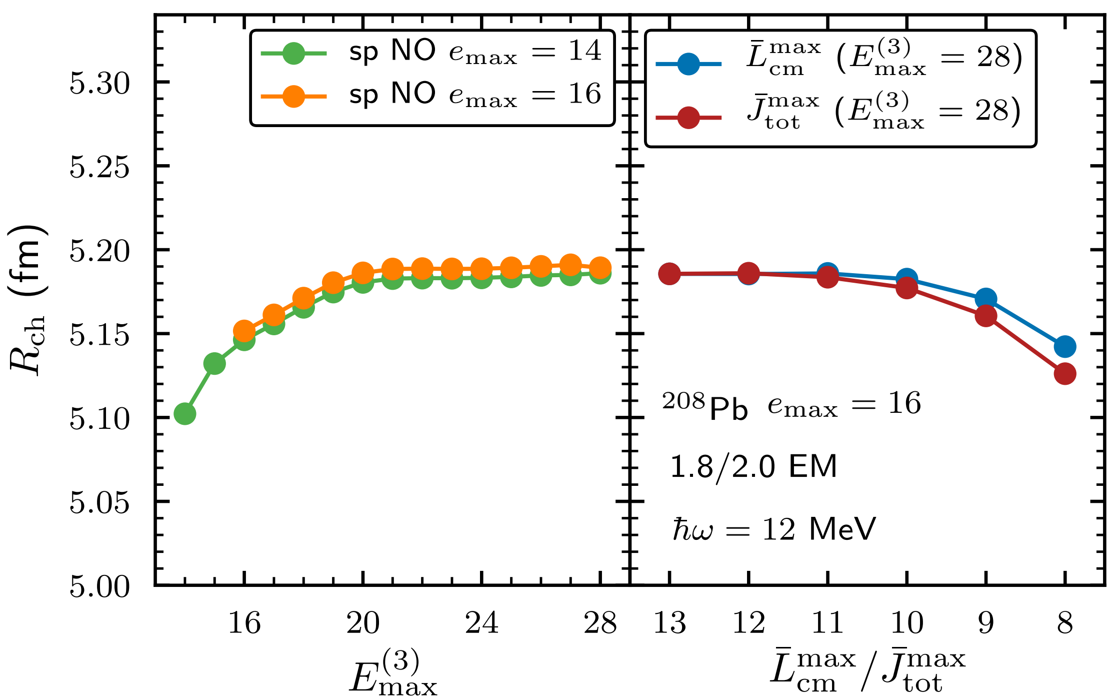


- Recent work fully **circumvents the storage of 3B matrix elements** in bound-state basis

Hebeler, Durant, Heinz, Hoppe, Schwenk, Simonis, Tichai
arXiv: 2211.16262

In-medium no-core shell model

Gebrerufael, Vobig, Roth, Mongelli, Hergert, …

- Hybrid approach based on multi-reference extension of IMSRG flow equation

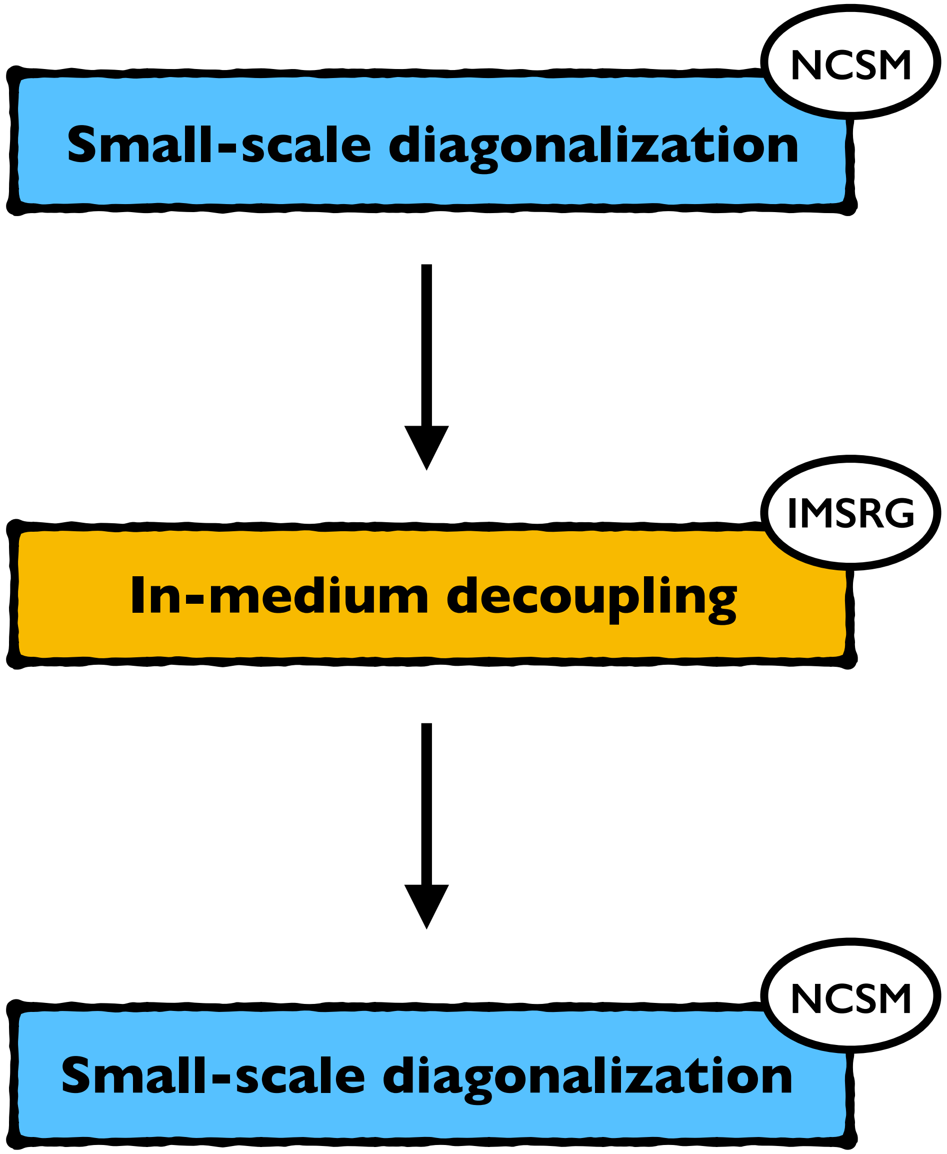
Merge IMSRG and no-core shell model (NCSM)

- Initial diagonalization captures static correlations in the reference state

… no mean-field reference state!

- Final diagonalization gives immediate access to various many-body observables

- No-core character limits available mass range to medium-light nuclei (A < 30)



IM-NCSM: open-shell nuclei

- IM-NCSM calculations for ground-state observables in oxygen chain

- Many-body uncertainties from reference state variations and comparison to NCSM

Energies: ~ 2 MeV

Radii: ~ 0.05 fm

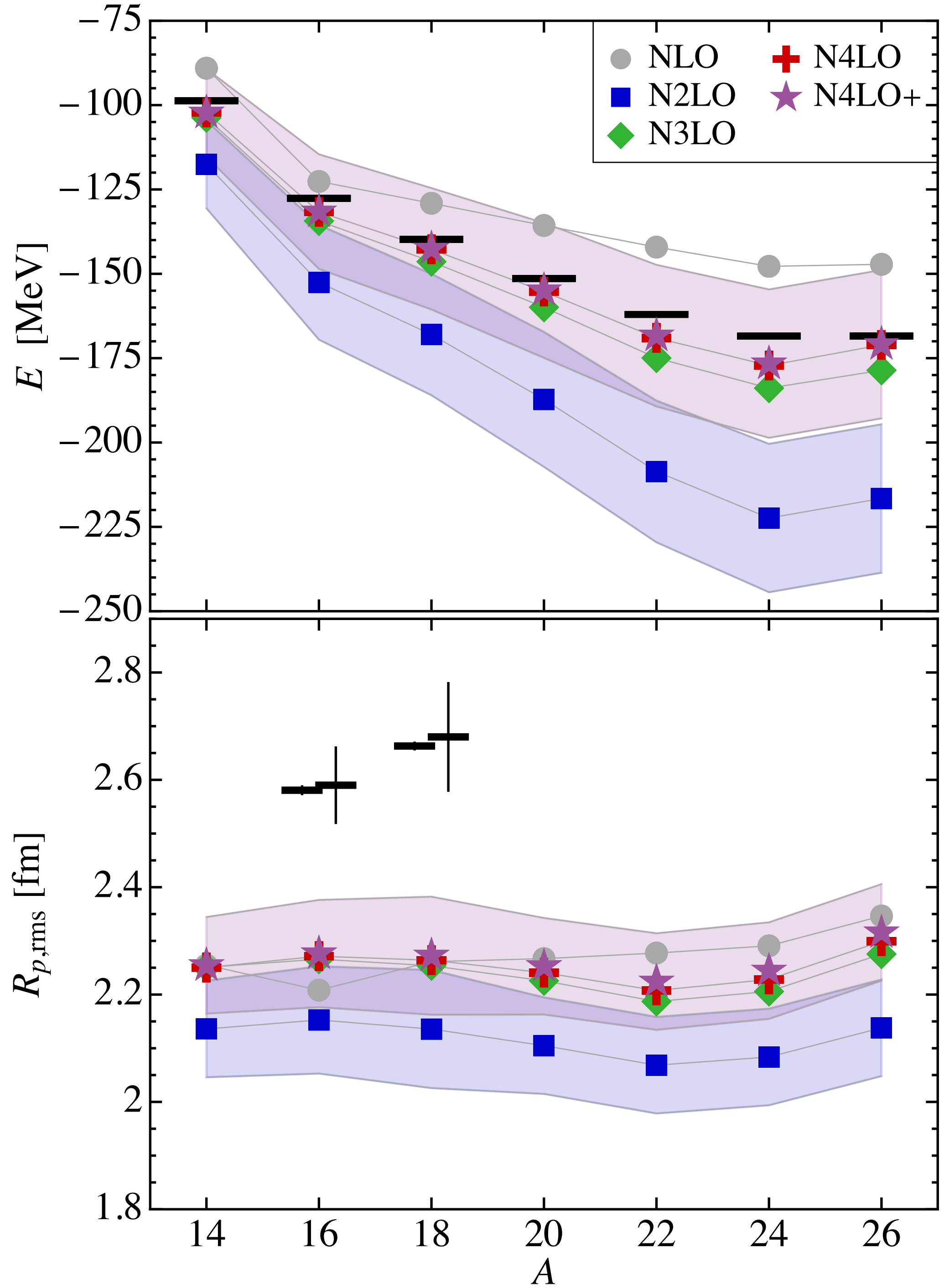
- Interaction uncertainties from systematic variation of chiral order of Hamiltonian

- Construction of total error bands from Bayesian analysis using Gaussian processes

extension to deformed Ne/Mg isotopes ongoing

Mongelli, PhD thesis (2022)

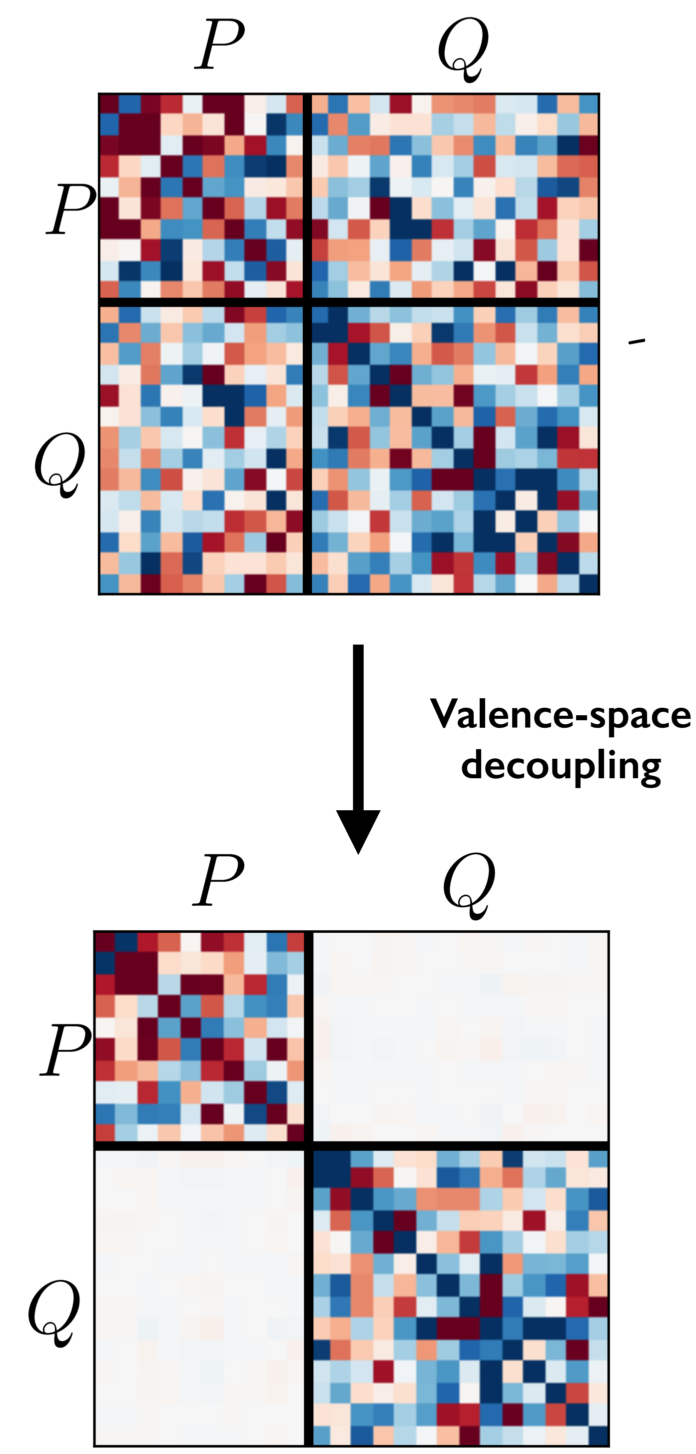
Energies/radii for oxygen isotopes



LENPIC collaboration, arXiv:2206.13303

Ab initio shell-model interactions

- Modify decoupling to target valence space
- Construction of *ab-initio* inspired valence-space interactions based on chiral EFT



Stroberg *et al.*, Ann. Rev. Nucl. Part. Sci (2019)

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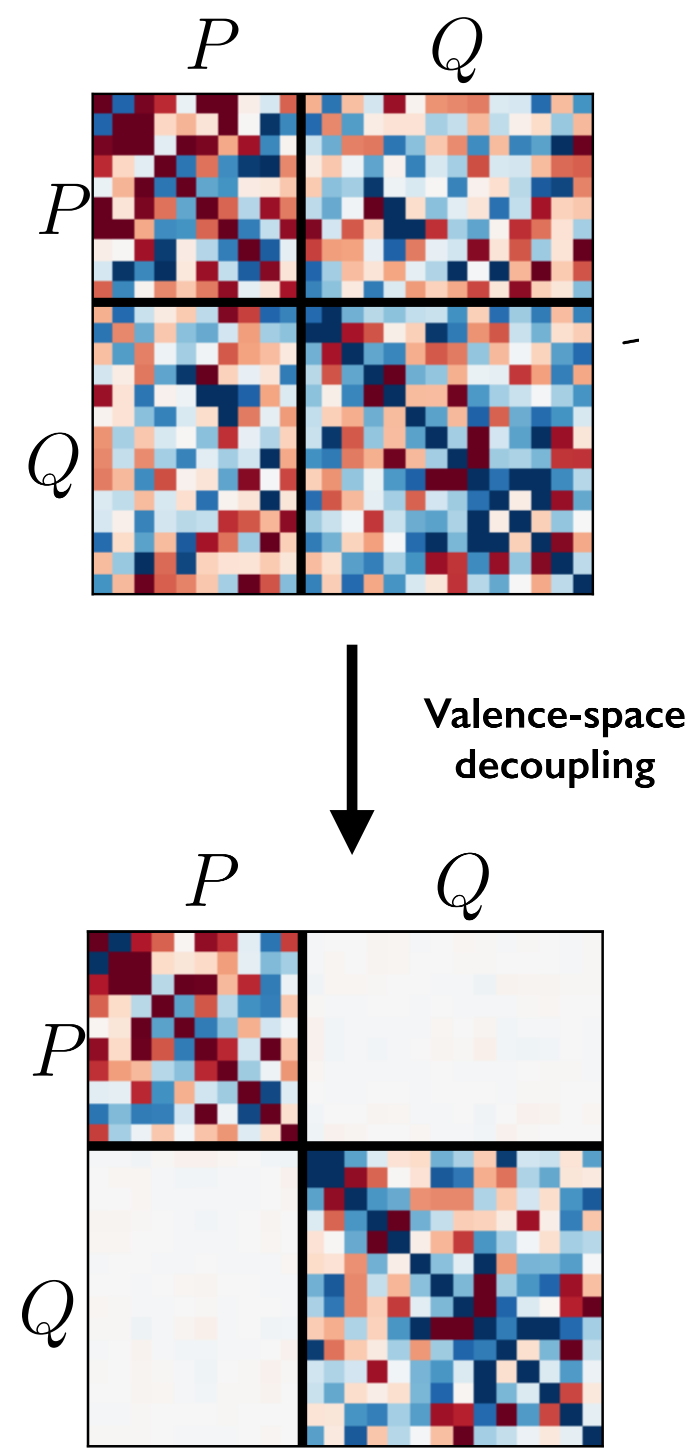
- Non-perturbative resummation of ph-correlations into active-space Hamiltonian
- Final computational step requires large-space shell-model diagonalization



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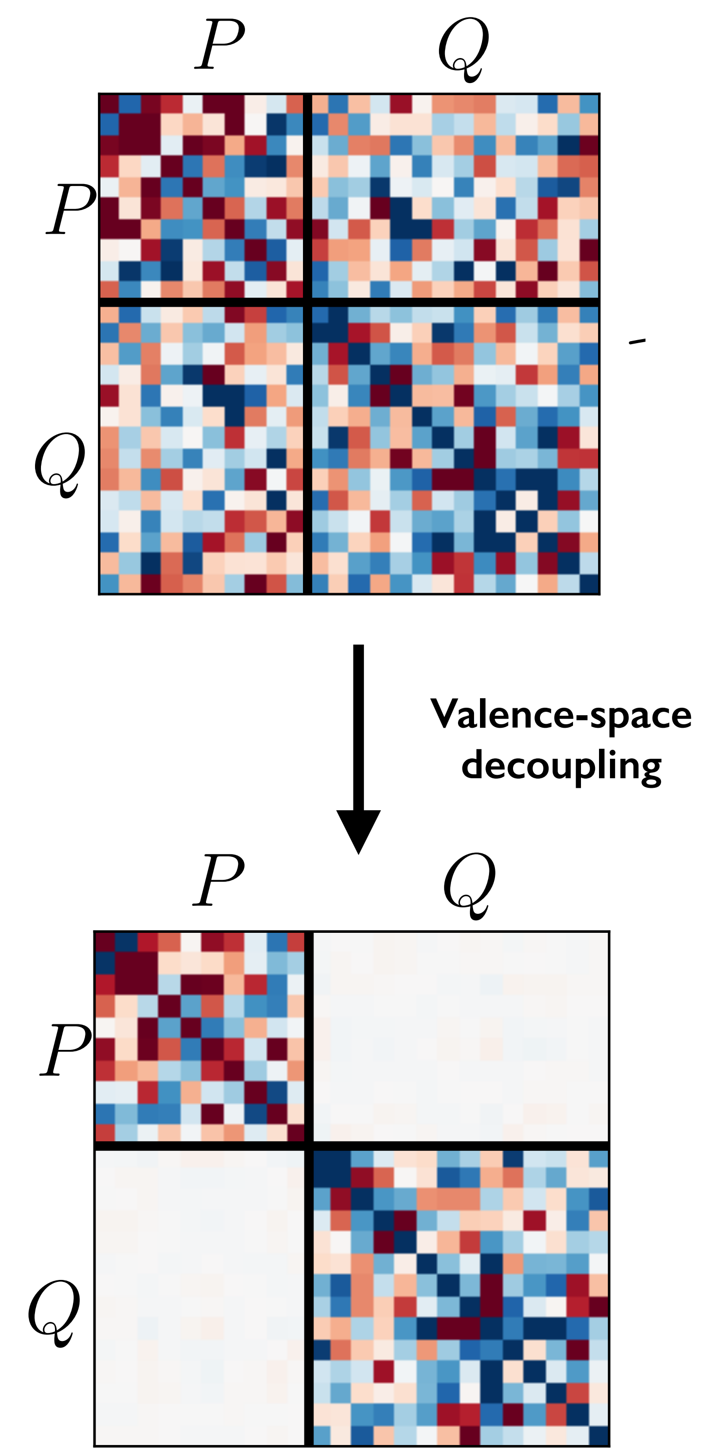
- Versatility: access to diverse set of observables from shell-model codes



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Ab initio shell-model interactions

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correlations into act

Challenge:
Computational cost of diagonalization

- Final computational step requires large-space shell-model diagonalization

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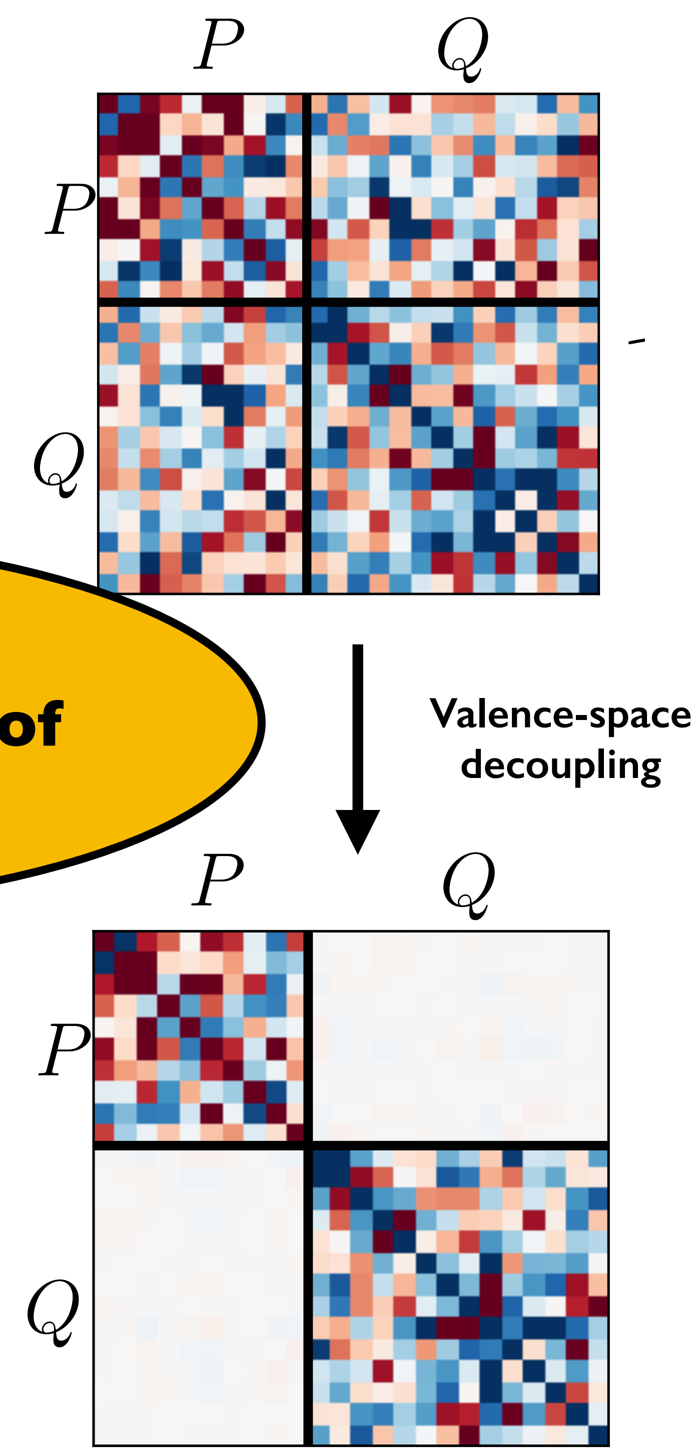

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The (nuclear) density matrix renormalization

Papenbrock, Pittel, Dukelsky, Poves, Legeza, Fossez, …

- **Configuration interaction:** inefficient representation of many-body state

$$|\Psi\rangle = \sum_{p_1 \dots p_N} \Psi_{p_1 \dots p_N} |p_1 \cdots p_N\rangle$$

complexity 2^N
(*occupied/unoccupied for N orbitals*)

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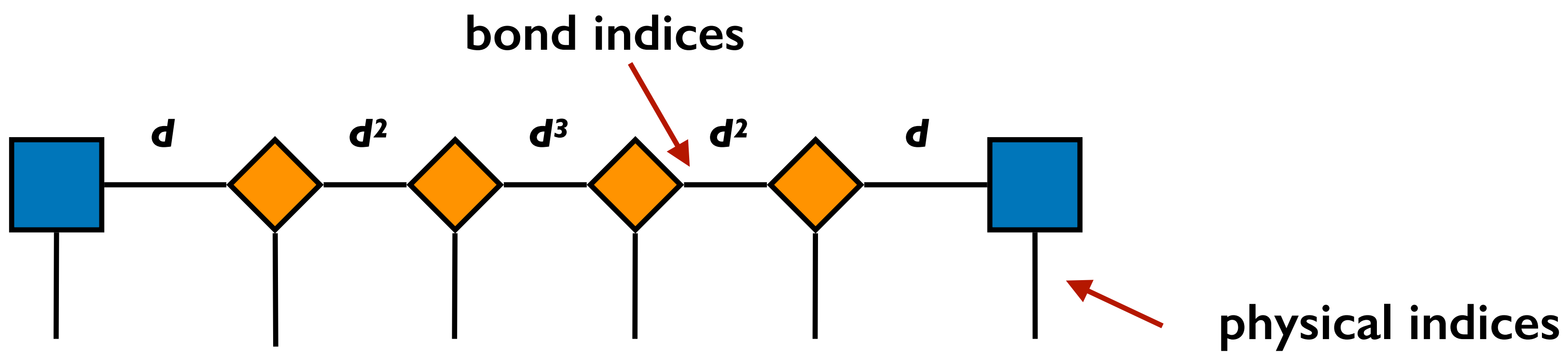
- Factorization of CI wave function using **matrix product state** (MPS) ansatz



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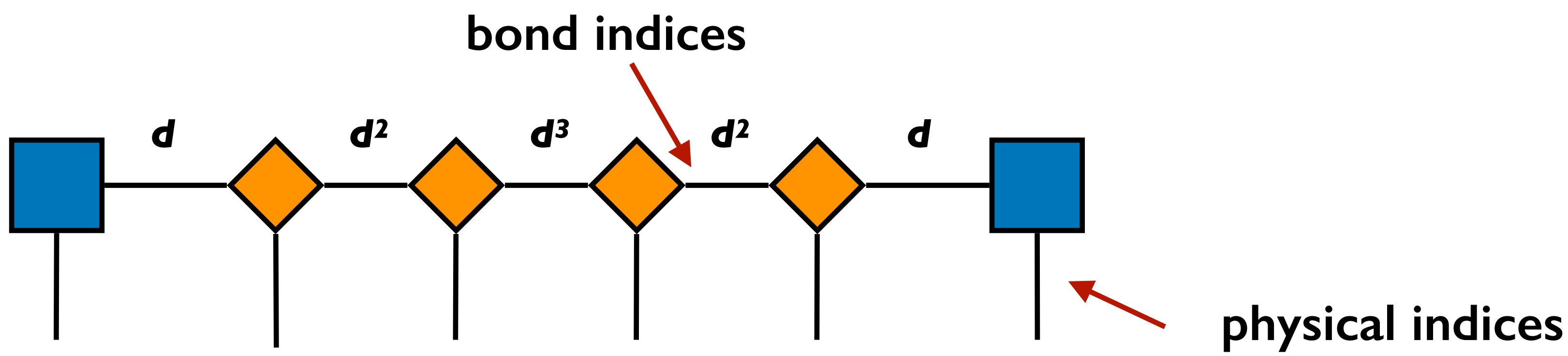

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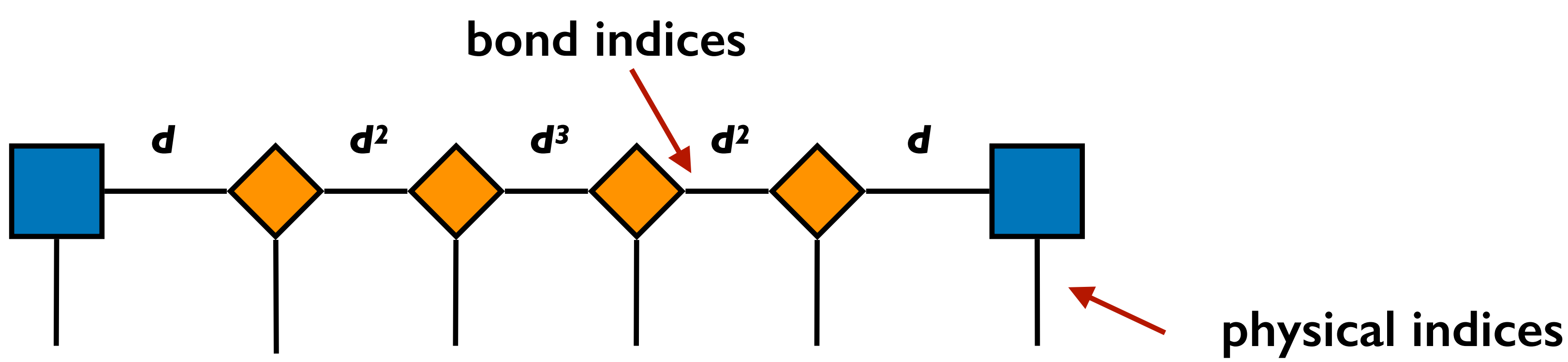

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- DMRG provides a variational procedure for the calculation of expectation values

White, PRL (1992/93)
Schollwöck, Ann. Phys. (2011)

$$E = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

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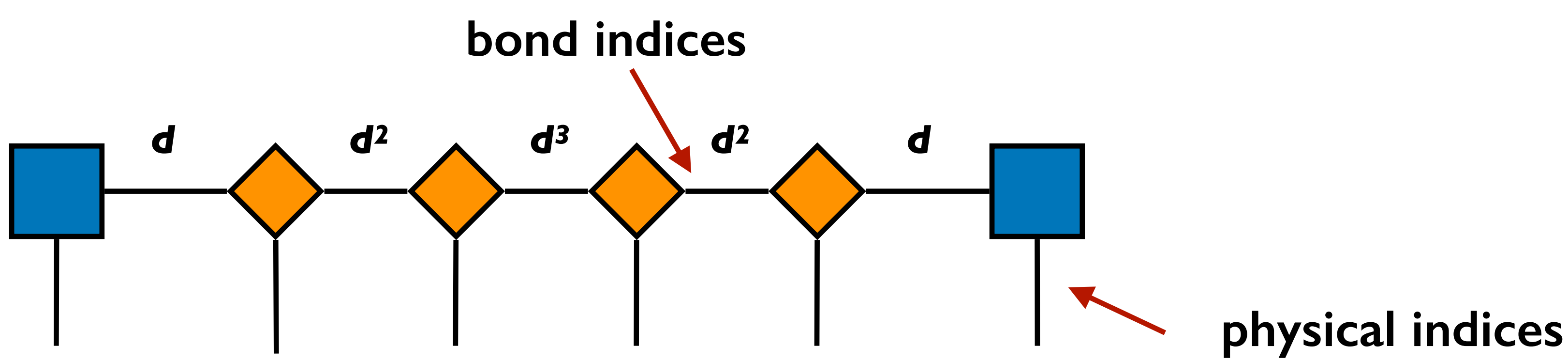

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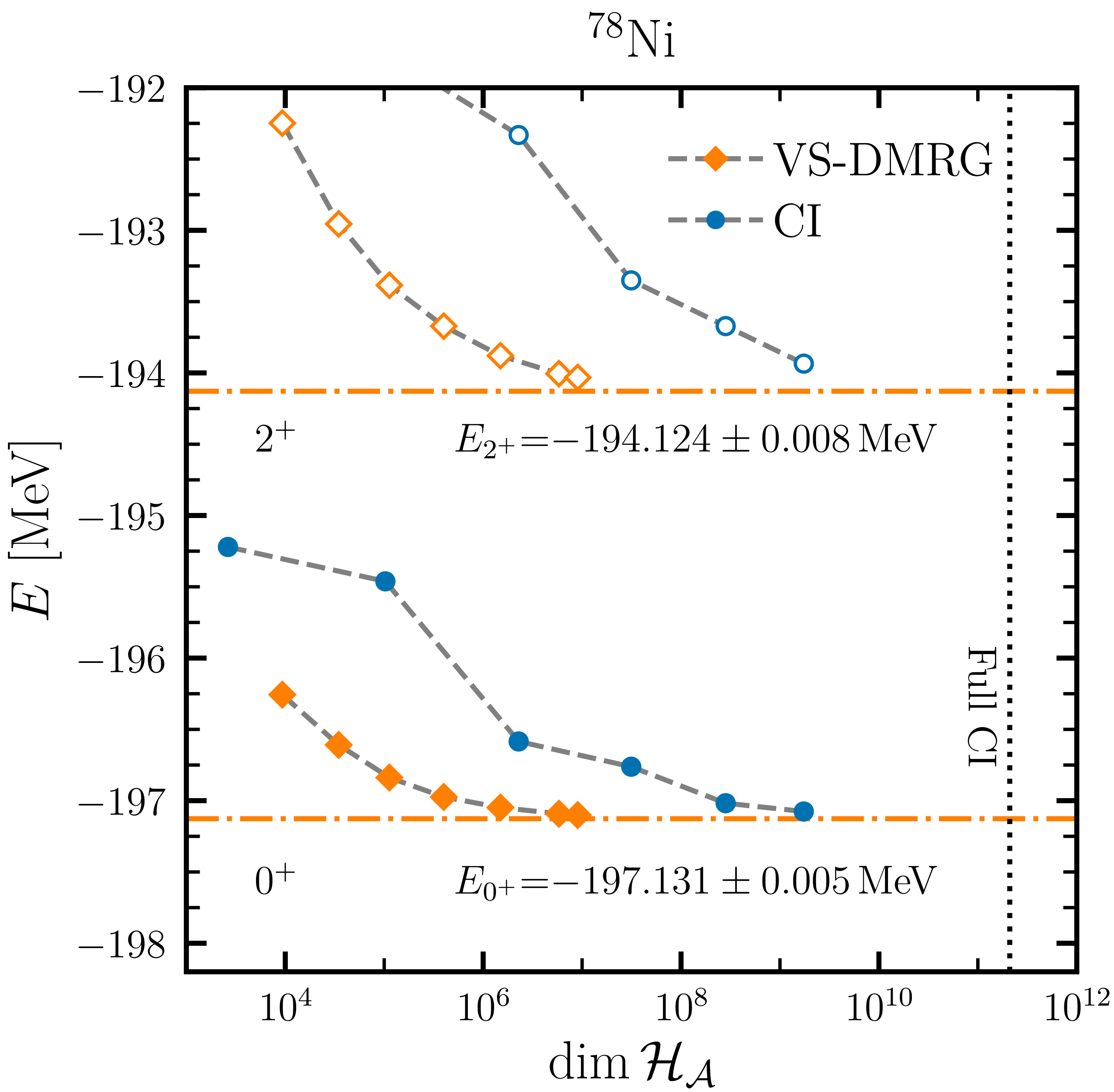
- Repeat calculations for different values of M and perform extrapolation

^{78}Ni: DMRG versus CI

DMRG/CI energies vs. effective dimension of H_A



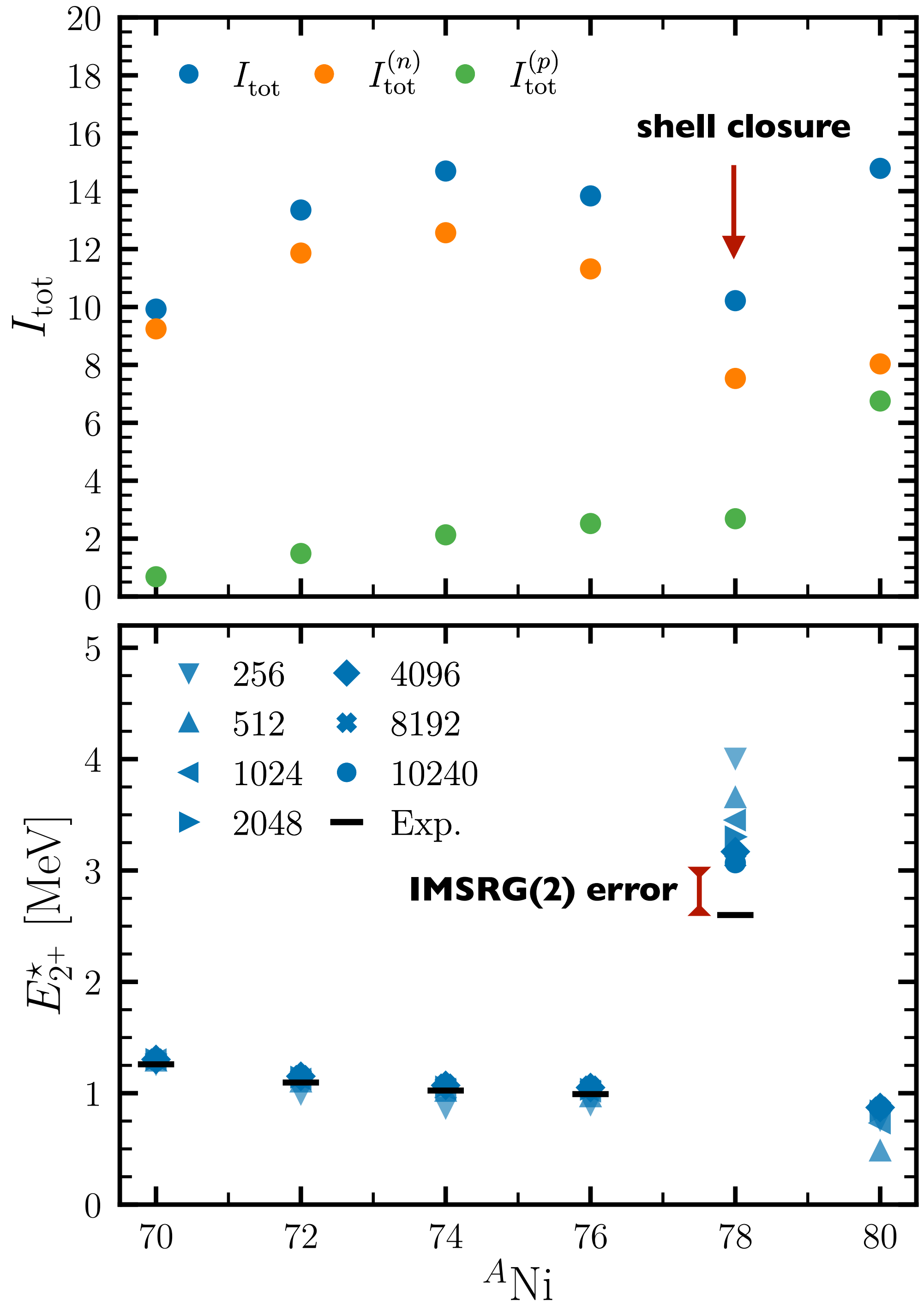
Tichai, Knecht, Kruppa, Legeza, Moca, Schwenk, Werner, Zarand
arXiv:2207.01438

- **DMRG: economic representation of the many-body wave function**
- **Very slow convergence of the 2$^+$ excited state in CI calculations**
- **Robust convergence of DMRG energies at large bond dimension**
- **DMRG does extend CI capacities**

Experimental input for neutron-rich nuclei needed!

Entanglement and shell structure

Total entropy in even-mass nickel isotopes



Tichai *et al.*, arXiv:2207.01438

experiment: Taniuchi *et al.*, Nature (2019)

- Extract entanglement entropy from one-body density of nuclear ground state

see alse Robin *et al.*, PRC (2021)

$$S_{\rm tot} = \sum_i \log(n_i)\,\log(1-n_i)$$

- Characterization of many-body systems

Closed-shell system: weak correlations

Open-shell system: strong correlations

- Pronounced kink at ^{78}Ni hints at neutron shell closure (~ dominated by HF)

Entropy is a good proxy for shell closures!

More observables!

Acharya, Sobczyk, Bacca, Bonaiti, Miorelli, Hagen, …

- Calculation of electromagnetic observables from first principles in medium-mass systems

Merge coupled cluster (CC) theory with integral transformations

- Dipole polarizability from weighted sum rules

$$\alpha_D = 2\alpha \int d\omega \frac{R_D(\omega)}{\omega}$$

- Strong sensitivity to higher-body correlations

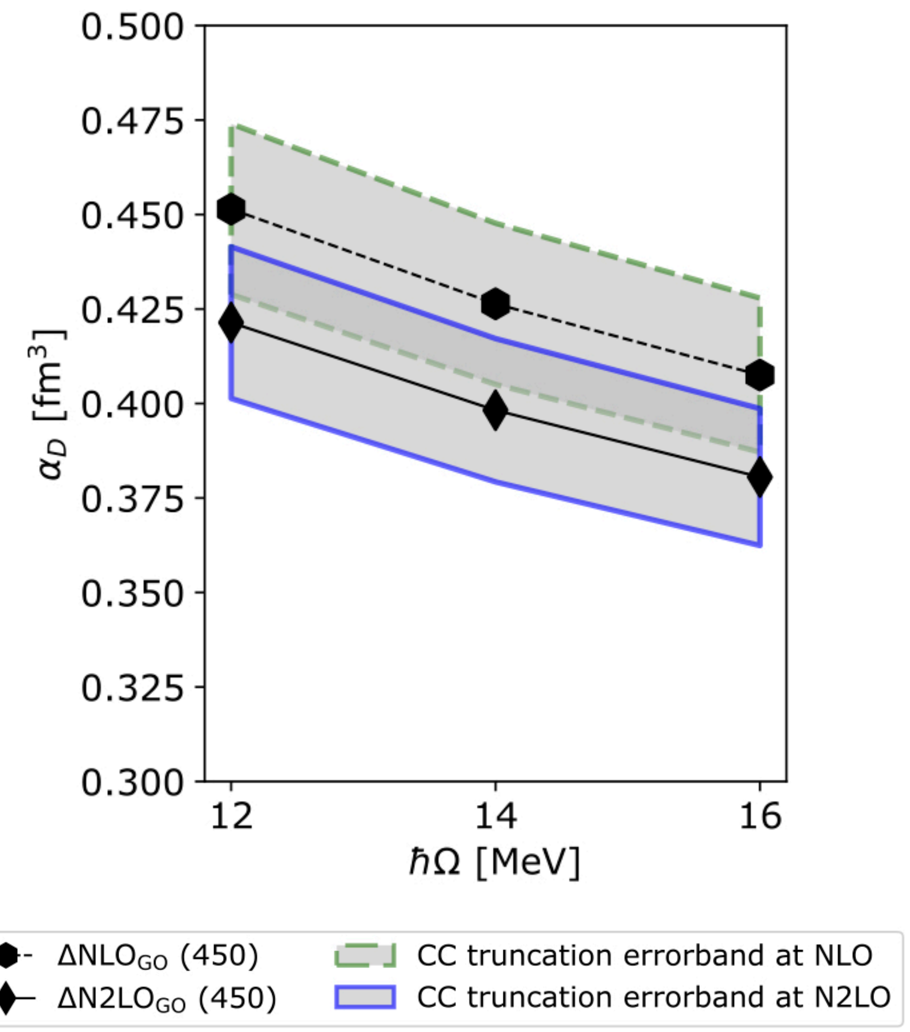
~4% from 3p3h contributions
(interaction dependent!)

- Future extensions to deformed nuclei

Axially deformed coupled cluster!

Novario, Hagen, Papenbrock, Duguet, Tichai, … PRC (2021/22)

Dipole polarizability in ^{8}He



Acharya *et al.*, arXiv:2210.04632
Bonaiti *et al.*, PRC (2022)

Conclusion and outlook

Progress in *ab initio* nuclear structure at various fronts

- Heavier: controlled expansions beyond *A=100*
- Exotic: extensions to open-shell nuclei

Long-term goals: nuclear deformation/collectivity from first principles

Further advances not covered today

- Nuclear-matter calculations at finite *T* and arbitrary proton fraction (Keller, Hebeler, Schwenk, …)
- Design of many-body emulators and machine-learning tools (Companys-Franzke, Tichai, Hebeler, Knöll, Roth, Schwenk, …)
- All interaction developments!
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