Advances in *ab initio* computations of atomic nuclei

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TECHNISCHE UNIVERSITÄT DARMSTADT

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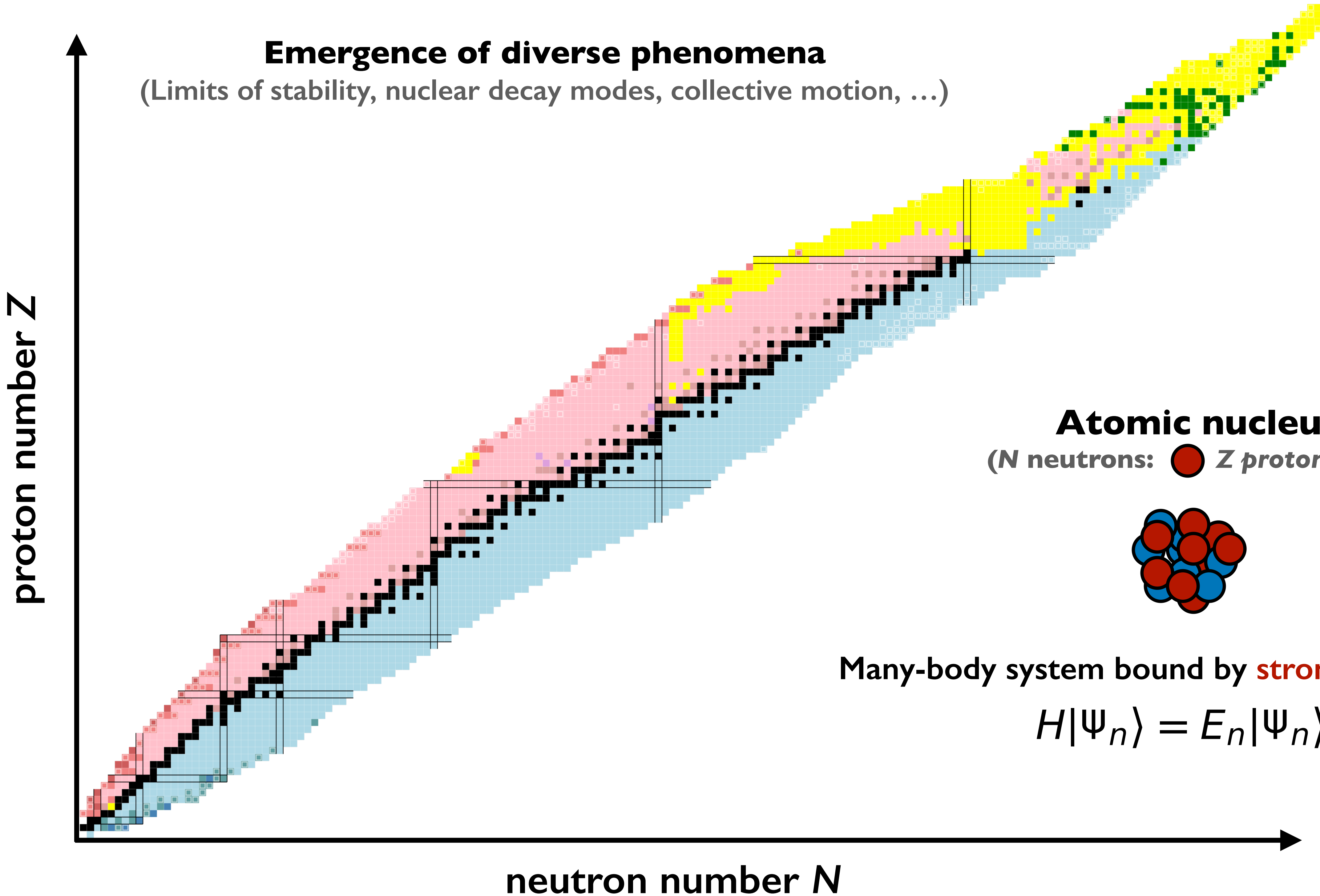
The nuclear landscape

Emergence of diverse phenomena

(Limits of stability, nuclear decay modes, collective motion, …)



Atomic nucleus

(*N* neutrons: *Z* protons:)

Many-body system bound by strong interaction!

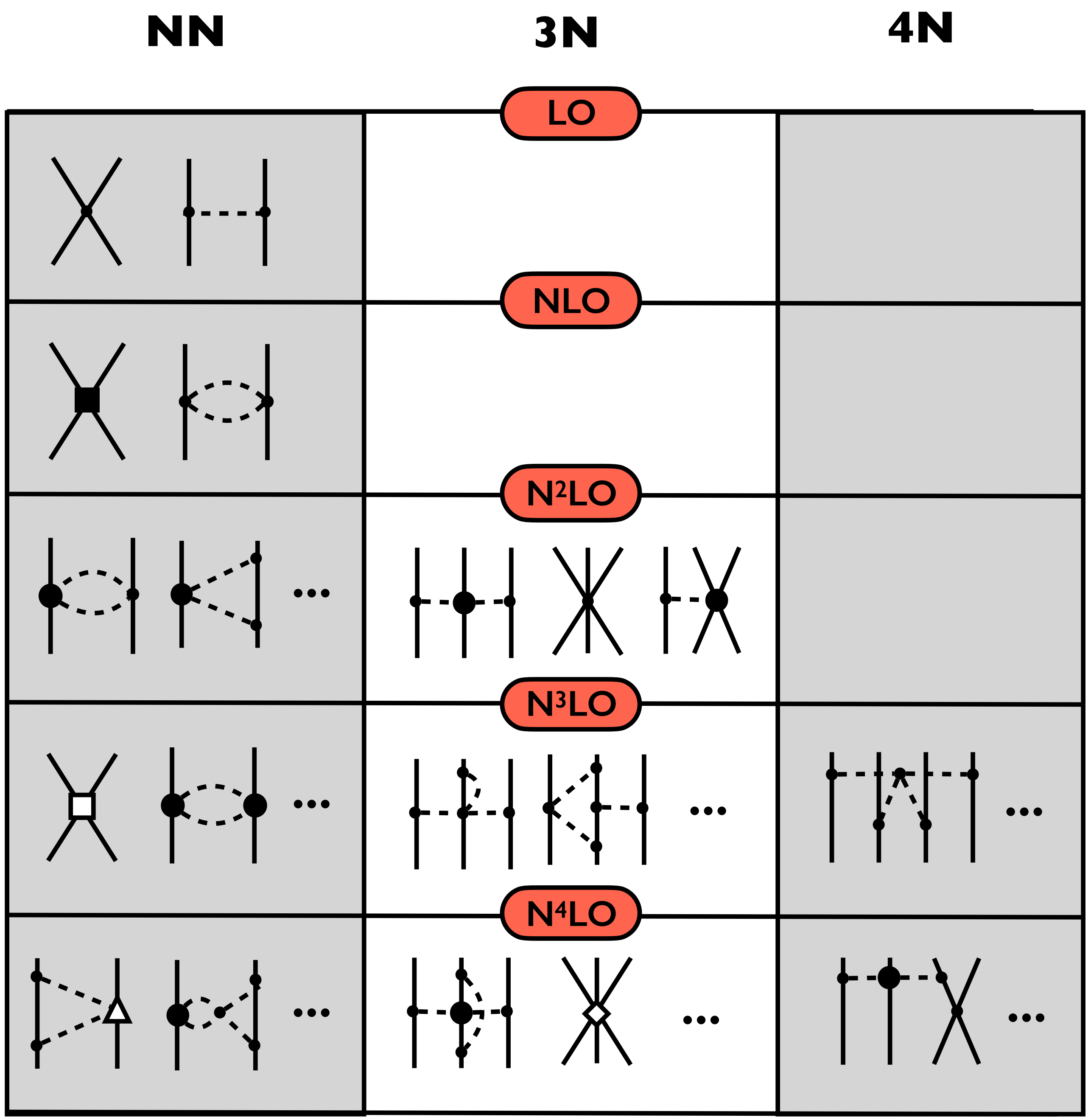
$$H|\Psi_n\rangle = E_n|\Psi_n\rangle$$

Chiral effective field theory

- Low-energy effective field theory with nucleons/pions as degrees of freedom
- Expansion parameter from separation of scales at low-energies

$$\frac{Q}{\Lambda_b} \approx \frac{1}{3}$$

- High-energy physics captured by few low-energy constants (LECs)
- Power counting predicts emergence (!) of higher-body operators



Many-body techniques

- **Goal: solution of Schrödinger equation**

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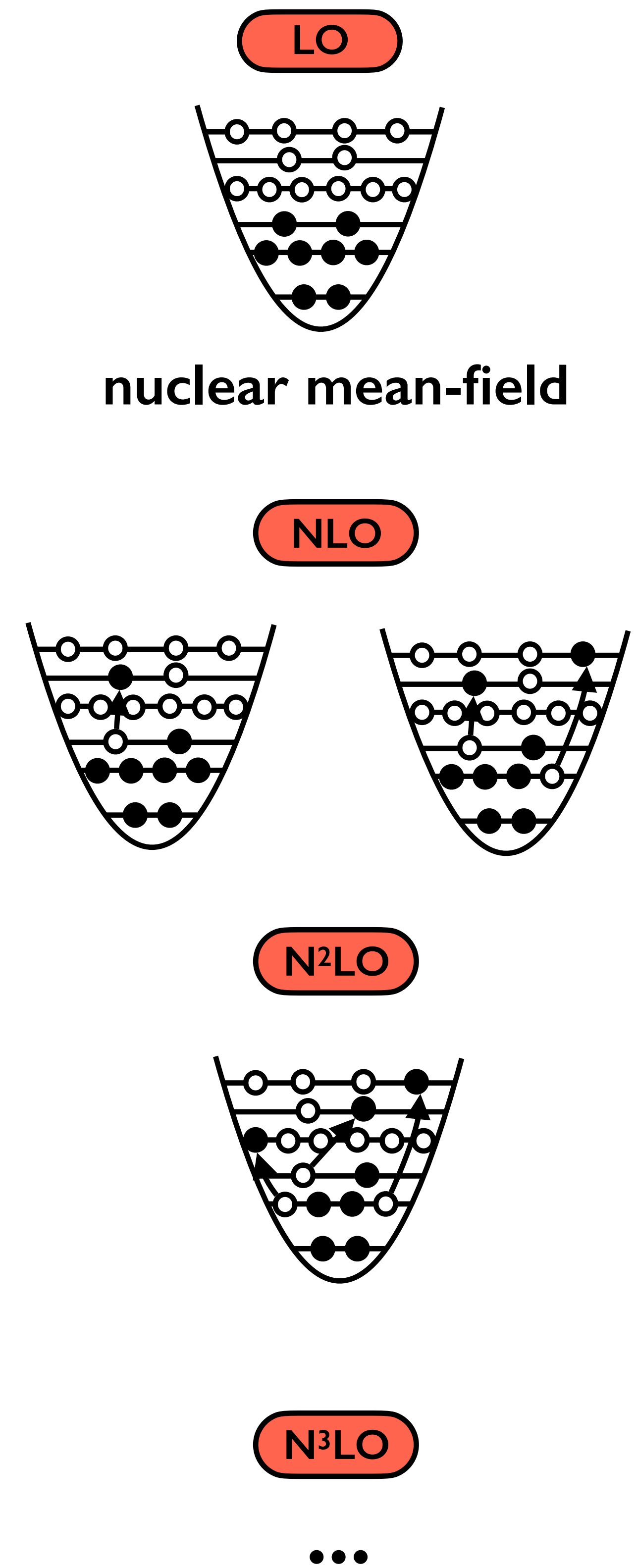
- **Idea: write exact many-body solution relative to an *A*-body reference state (leading order)**

$$|\Psi_{\text{exact}}\rangle = \hat{W}\,|\Phi\rangle$$

- **Leading order must qualitatively capture the dominant correlations of the system!**



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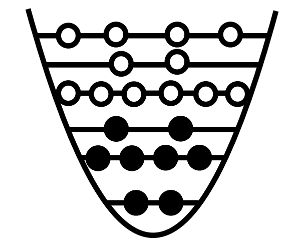
- **The unknown wave operator encapsulates all the complexity of the system**

$$W = W^{[0B]} + W^{[1B]} + W^{[2B]} + W^{[3B]} + \dots$$

work-horse / high-precision

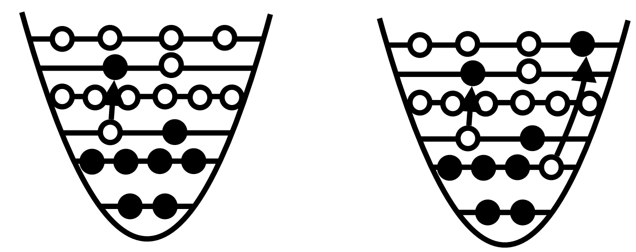
LO



$W^{[0B]}$

nuclear mean-field

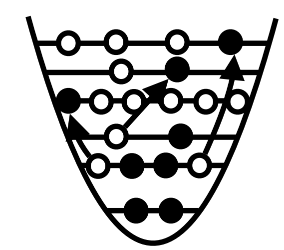
NLO



$W^{[1B]}$

$W^{[2B]}$

N²LO



$W^{[3B]}$

N³LO

...

$W^{[\geq 4B]}$

Quantification of uncertainties

- *Ab initio* theory allows for rigorous quantification of theory uncertainties

- Interaction uncertainties estimated from order-by-order calculations

$$\Delta X^{(k)} = Q \cdot \max\{|X^{(k)} - X^{(k-1)}|, \Delta X^{(k-1)}\}$$

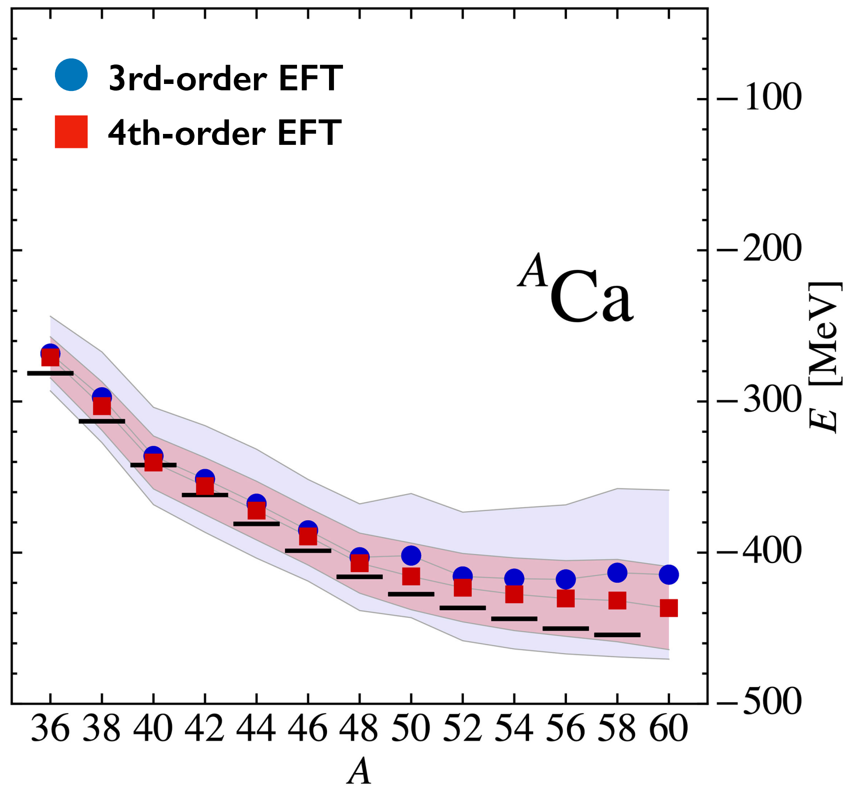
- Many-body uncertainties still based on empirical *ad-hoc* models

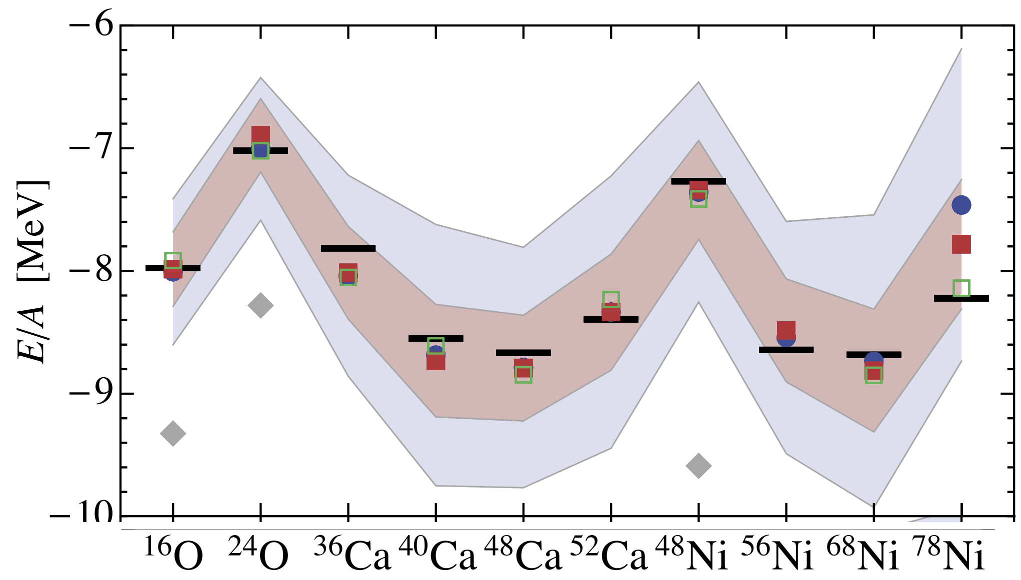
2-3% of ground-state energy

- Similar studies of theory uncertainties in nuclear-matter simulations

Drischler *et al.*, PRL (2020)
Keller *et al.*, PRL (2023)

Tichai *et al.*, Frontiers in Physics (2020)





Hüther *et al.*, PLB (2020)

Towards heavy nuclei

- *Ab initio* simulations are extended significantly beyond *A=100*
- Exotic drip line nuclei from first-principles frameworks available
- Pioneering *ab initio* calculations of doubly magic ^{208}Pb nucleus

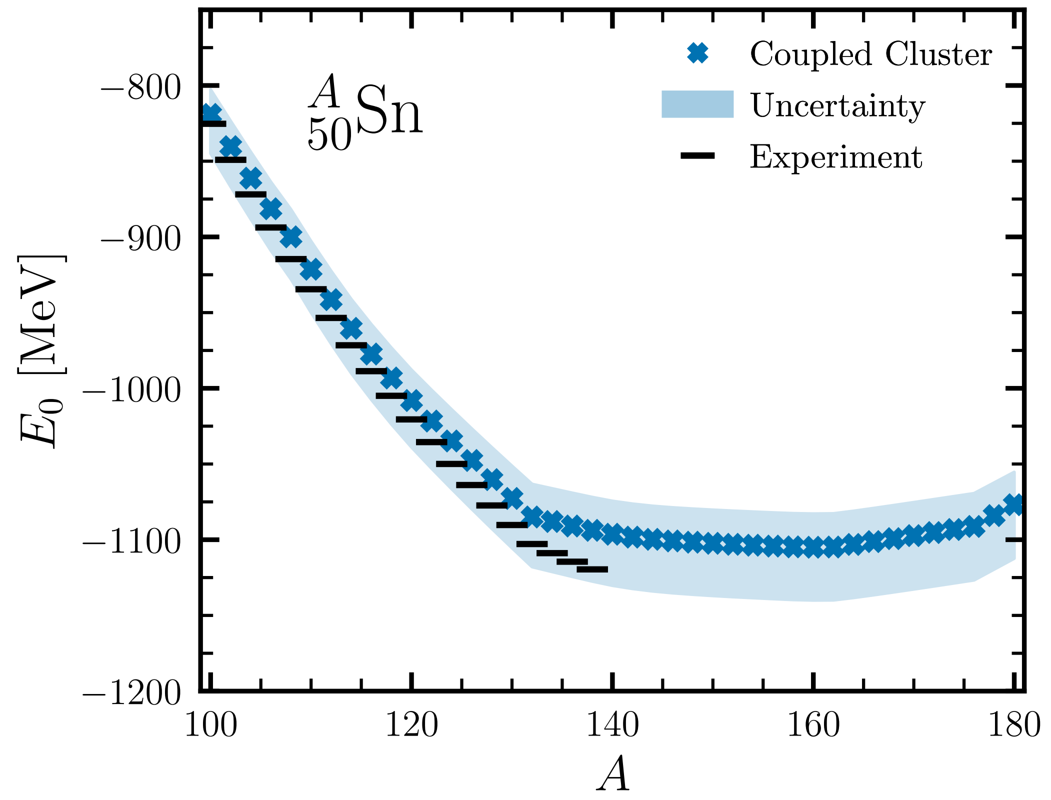
  → neutron-skin thickness

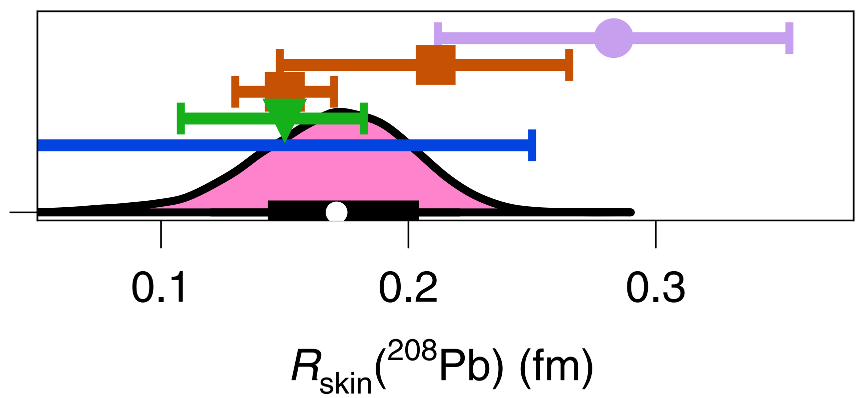
- Recent high-precision simulations in $^{170\text{-}176}$Yb for new physics searches

Door *et al.*, arXiv:2403.07792

***Ab initio* complements density functional theory!**

Tichai *et al.*, Phys. Lett. B (2024)

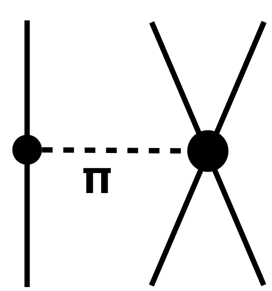




Hu *et al.*, Nat. Phys. (2022)

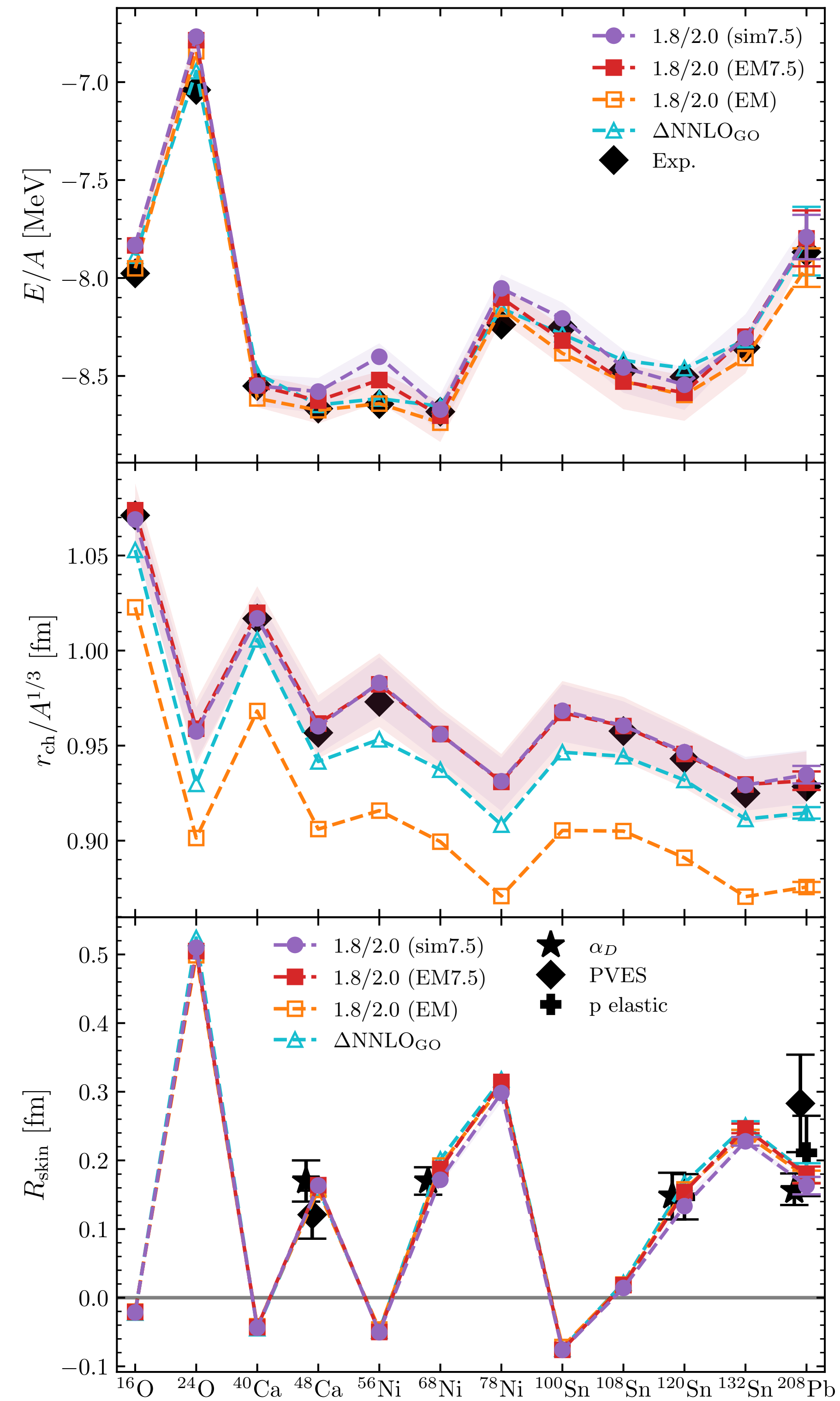
New interactions!

- **Chiral interaction give decent reproduction of ground-state energies**
- **Common problem: nuclear charge radii are underestimated in medium-mass nuclei**
- **Approach: re-fit c_D interaction to reproduce charge radius of ^{16}O**



one-pion exchange topology

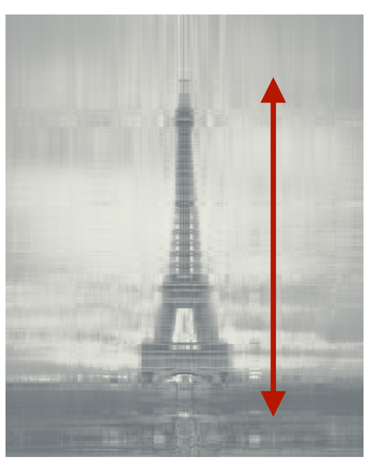
- **Great reproduction of experimental data from medium-light to heavy systems**



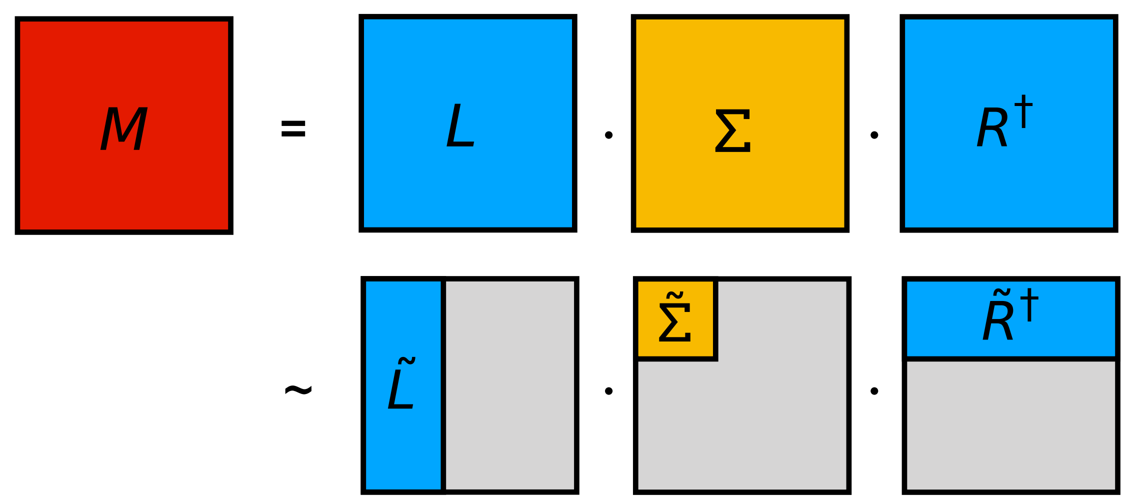
Arthuis *et al.*, arXiv:2401.06675

Concepts of data compression

Removal of 97% of information!



Singular value decomposition (SVD)

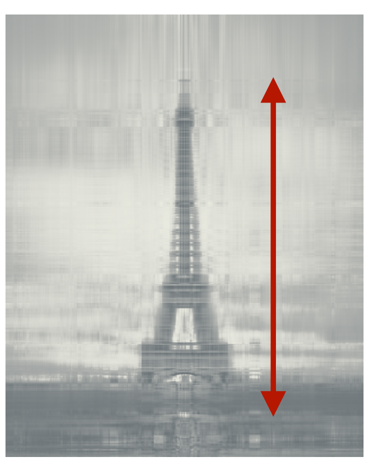


Low-rank approximation

Concepts of data compression

One can still tell the size of the Eiffel tower (observable) from a blurred picture (input data)!

Removal of 97% of information!



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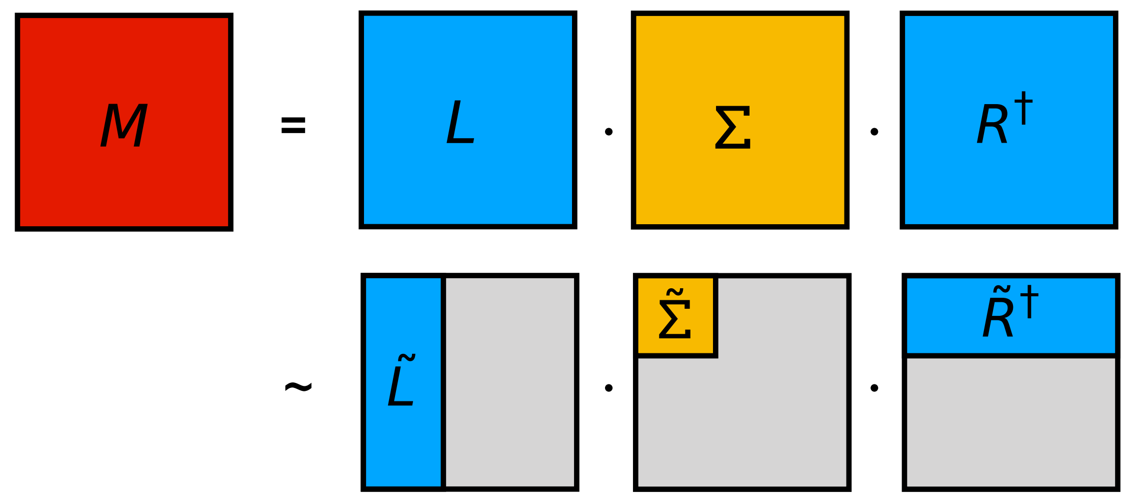
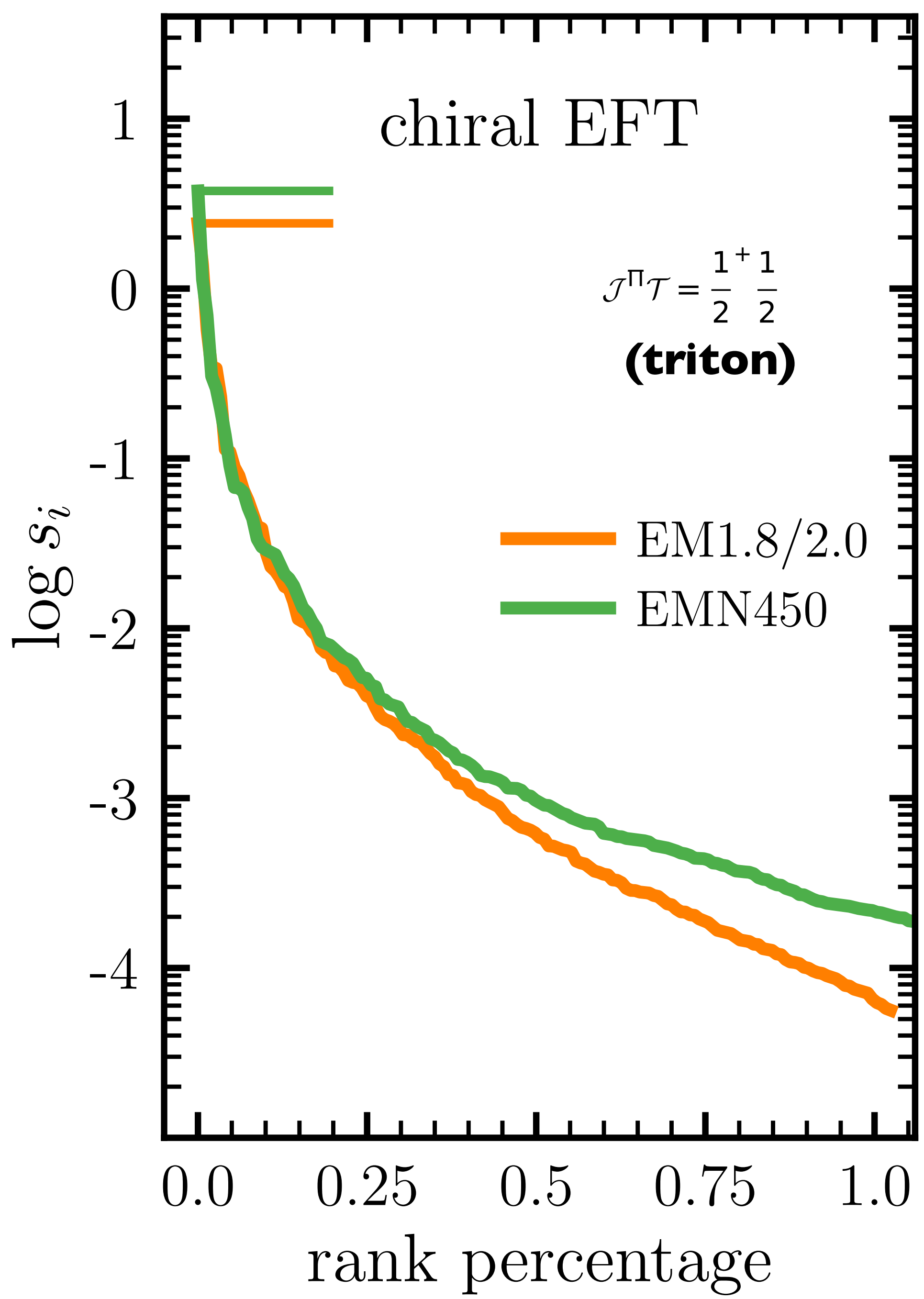


Low-rank approximation

Low-rank interactions from chiral EFT

Singular spectrum of three-body interaction



Tichai *et al.*, arXiv:2307.15572

- Application to partial-wave-decomposed three-body matrix elements

$$\langle pq, \alpha | V_{3N} | p'q', \alpha' \rangle$$

- Very few SVD components needed

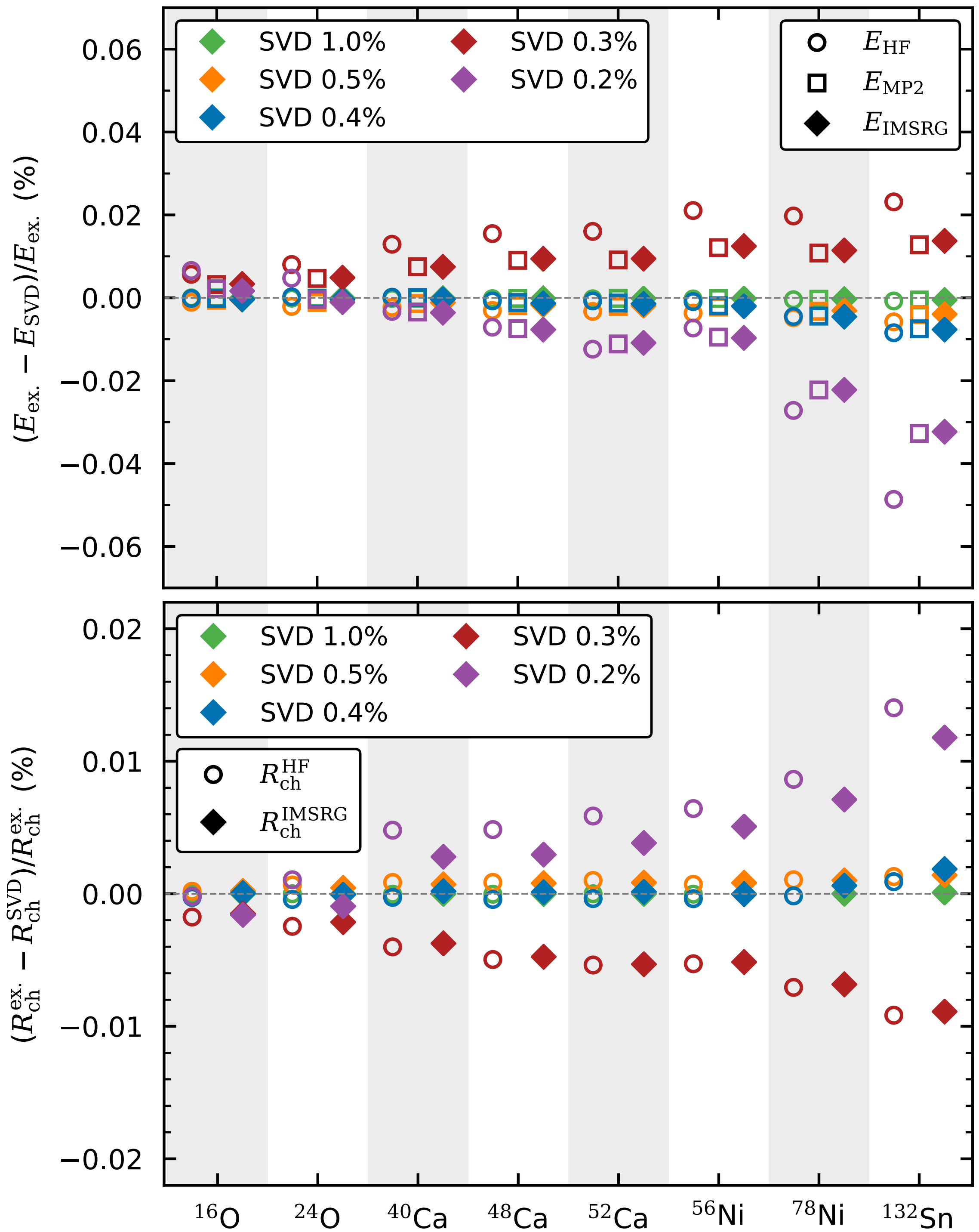
~100 out of 15.000

- Scalability: novel randomized SVD algorithm implemented

Singular spectrum reveals pronounced low-rank character!

Medium-mass nuclei

Ground-state observables for closed-shell nuclei



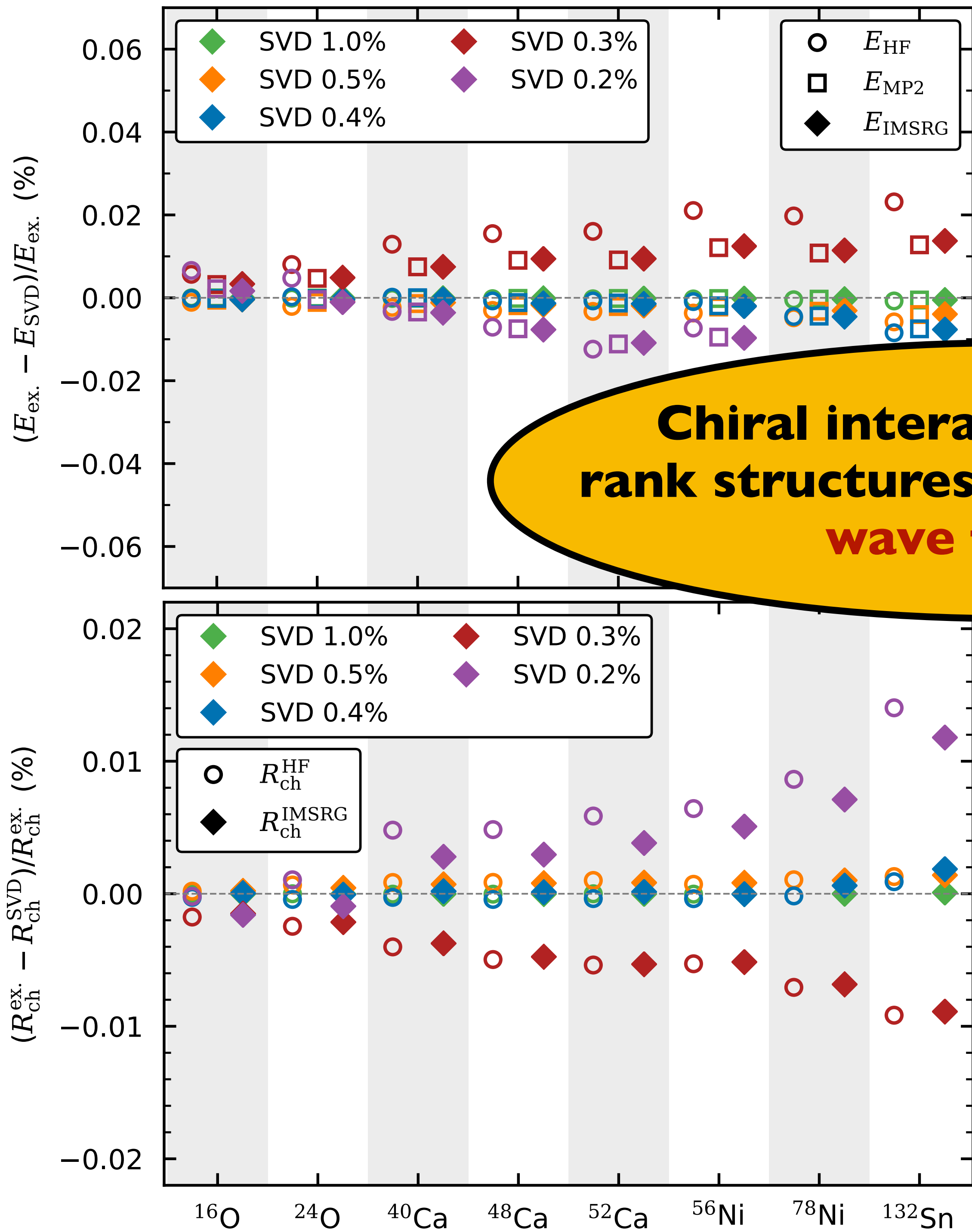
Tichai *et al.*, arXiv:2307.15572

- **Matrix elements from transformation of low-rank 3N interactions**
- **Low error on observables from different many-body schemes**
- **Slight increase of decomposition error with mass number**
- **1% of singular values yield less than keV errors on ground-state energy**

Many-body systems
99% of singular values can be discarded at zero loss in accuracy!

Medium-mass nuclei

Ground-state observables for closed-shell nuclei



Tichai *et al.*, arXiv:2307.15572

Chiral interaction have low-rank structures … what about the wave function?

- Matrix elements from transformation of low-rank 3N interactions
- Low error on observables from different many-body schemes
- …se of decomposition …ass number
- 1% of singular values yield less than keV errors on ground-state energy

Many-body systems
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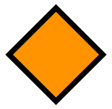
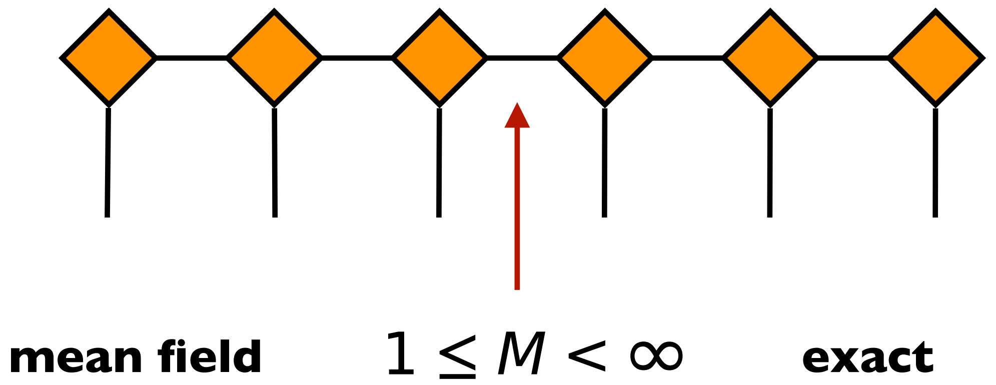
Nuclear tensor networks

- Factorized ansatz of the many-body function: matrix-product state (MPS)

- Novel many-body solver will solve for the factors themselves ()



Nuclear tensor networks

- Factorized ansatz of the many-body function: matrix-product state (MPS)

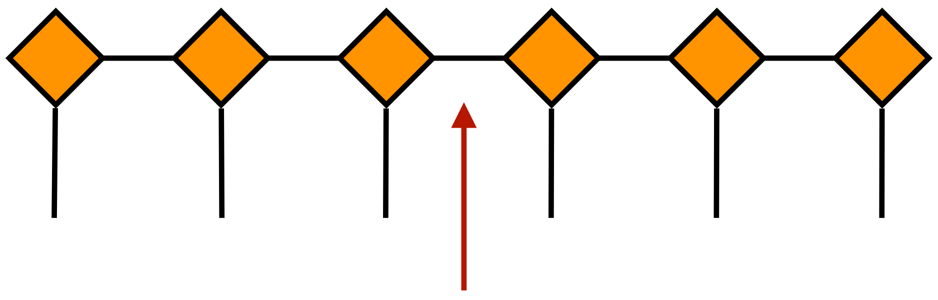
- Novel many-body solver will solve for the factors themselves (◆)

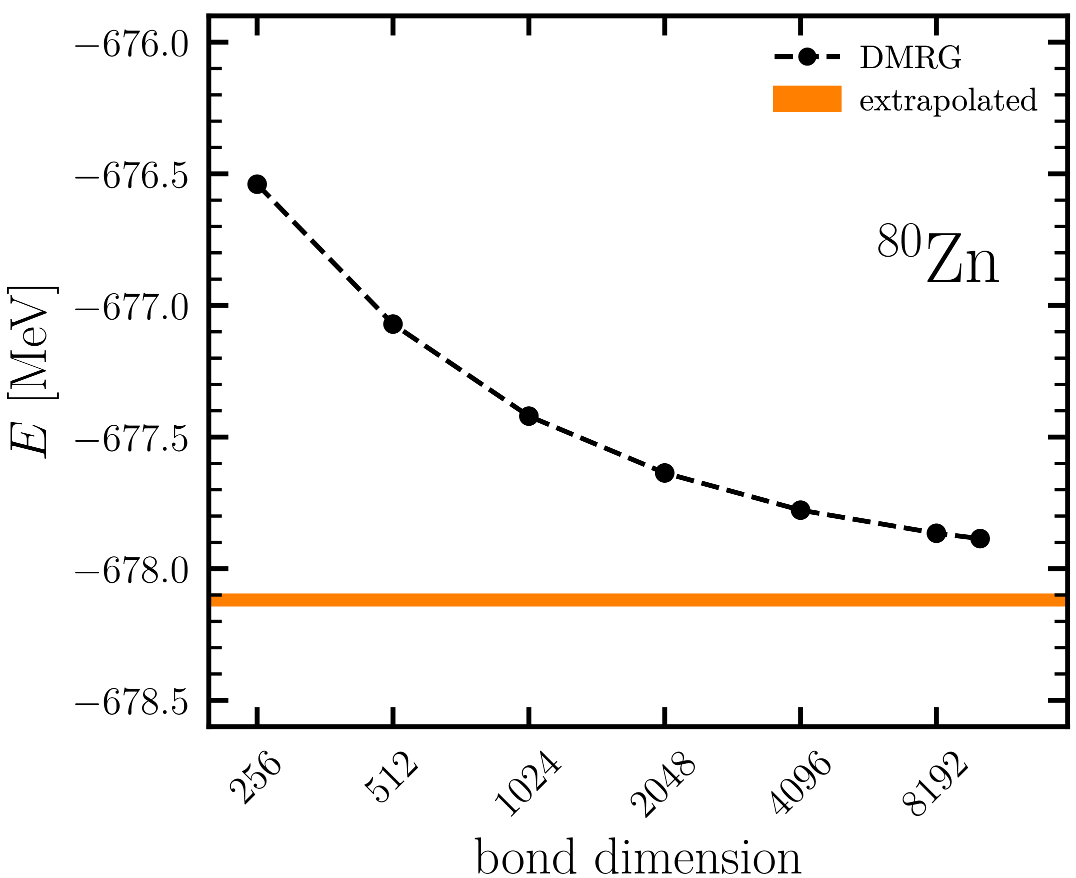
- Density matrix renormalization group: variational optimization of MPS

  White, PRL (1992)
  Schollwöck, Annals of Physics (2011)

- Systematically improvable by increasing the bond dimension (M)

- Method of choice for low-dimensional problems in condensed matter



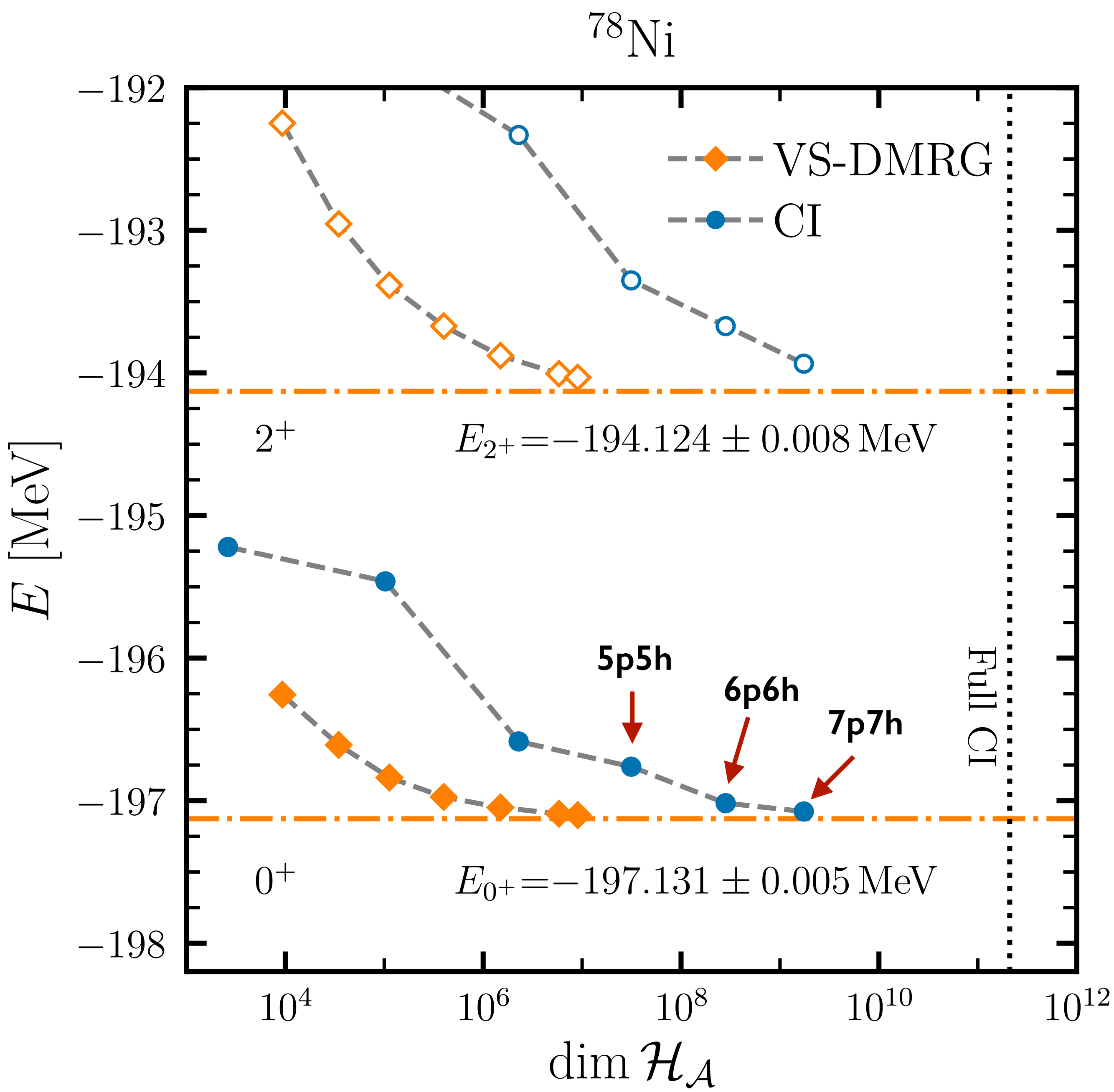


Tichai *et al.*, PLB (2024)

^{78}Ni: Why DMRG?

Taniuchi *et al.*, Nature (2019)

DMRG/CI energies vs. effective dimension of H_A



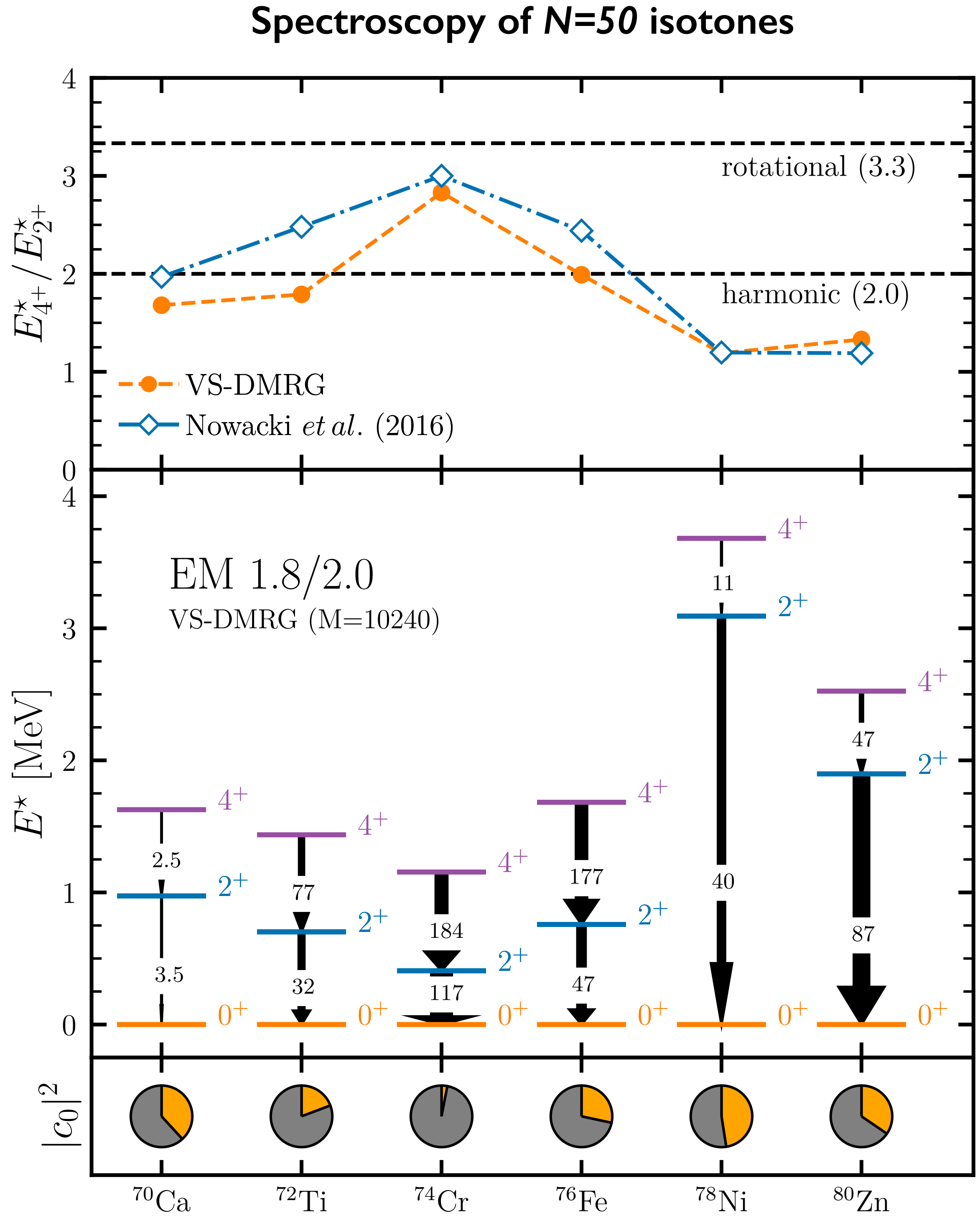
Tichai *et al.*, PLB (2023)

- **DMRG: economic representation of the many-body wave function**

Smaller Hilbert spaces!

- **Slow convergence of the 2^+ excited state in CI calculations**
- **Robust convergence of DMRG energies at large bond dimension**
- **DMRG outscales diagonalization**

Transitional nuclei at *N*=50



Tichai *et al.*, PLB (2024)

- **Onset of nuclear deformation**

$$E^{\star}_{\mathrm{rot}} \sim J(J+1)$$

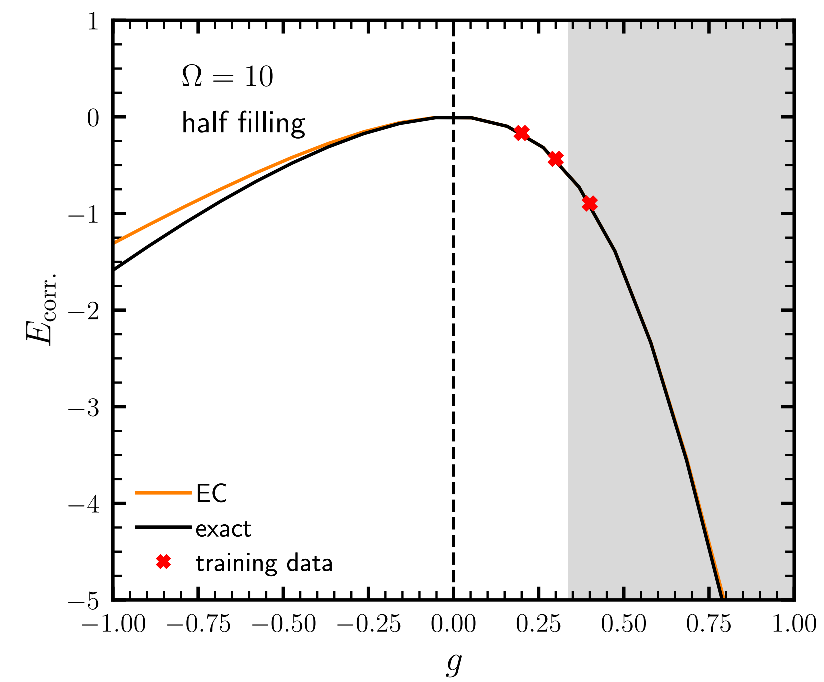
- **Rapid transition between single-particle-like and collective excitations**
- **Qualitative agreement with previous shell-model calculations**

  Nowacki *et al.*, PRL (2016)

- **Spectroscopy: DMRG extended to EM transitions strengths**
- **<u>Challenge</u>: description of excited rotational band in ^{78}Ni**

Emulators

Companys, Tichai *et al.*, PRC (2024)



- **Challenge**: **repeated solution** of many-body problem millions of times (~20 LECs)

$$H_{\mathrm{EFT}} = \sum_i c_i V_i$$

- **Idea**: train a surrogate model to **mimic the true many-body solution**

snapshots basis: $\{|\Psi_{\mathrm{training}}\rangle\}$

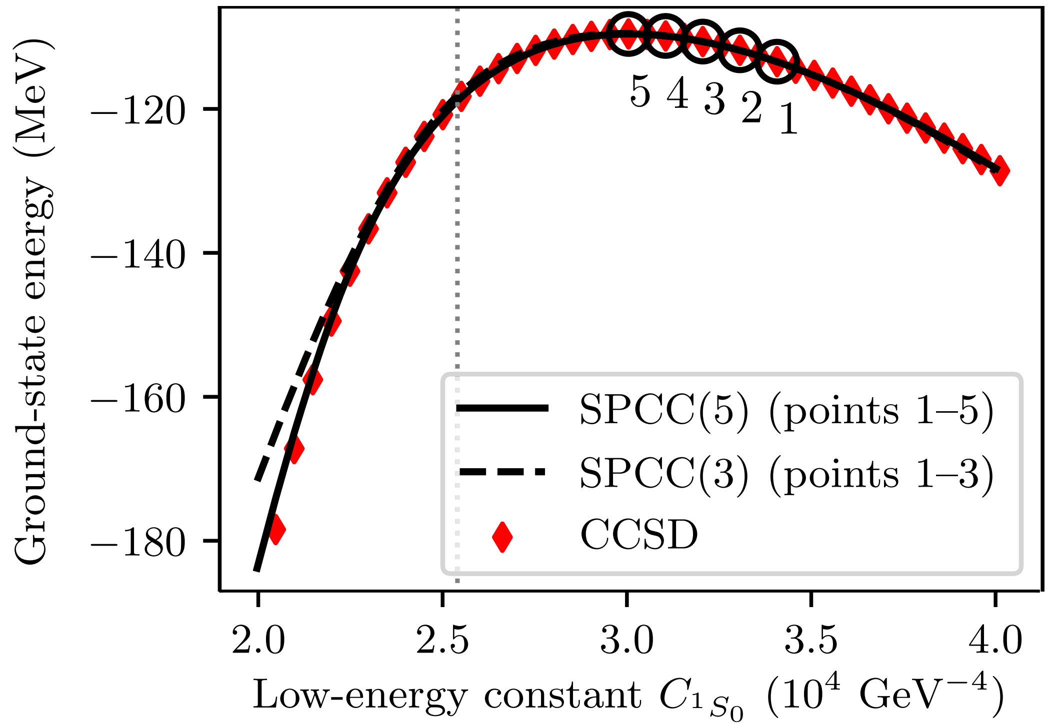
- **Eigenvector continuation**: re-expand solution in basis of training vectors

Frame *et al.*, PRL (2018)

$$H_{ij} = \langle \Psi(c_i) | H(c_\circ) | \Psi(c_j) \rangle$$

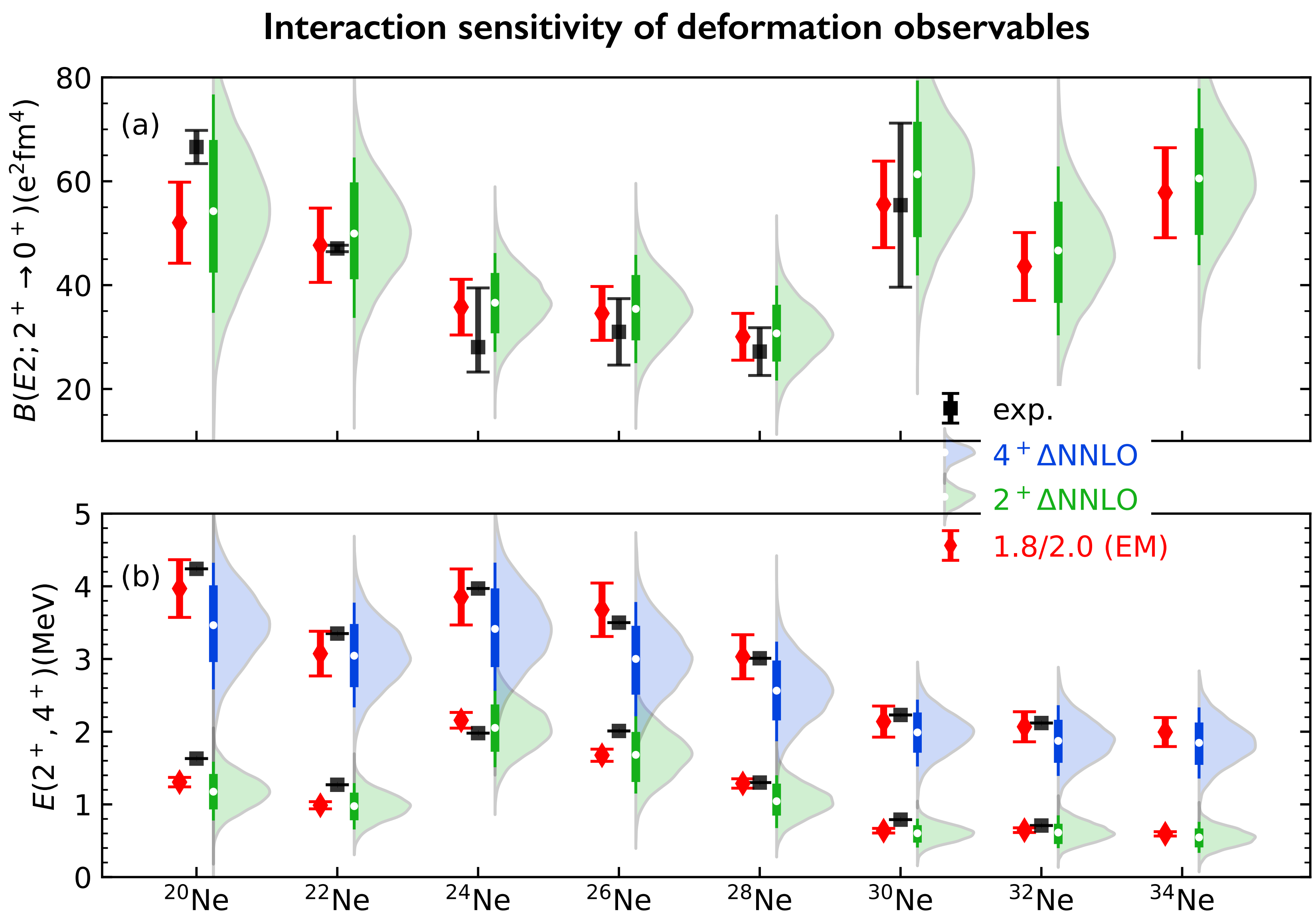
$$H\vec{x} = \lambda N \vec{x}$$

small-scale generalized eigenvalue problem



Ekström, Hagen, PRL (2019)

Global sensitivity analysis



Sun *et al.*, arXiv:240400058

Interaction uncertainties sampled from many-body emulator

Conclusions

Nuclear interactions from chiral effective field theory

- Systematically improvable from power counting
- Access to interaction uncertainties
- Extensive exploration of LEC values

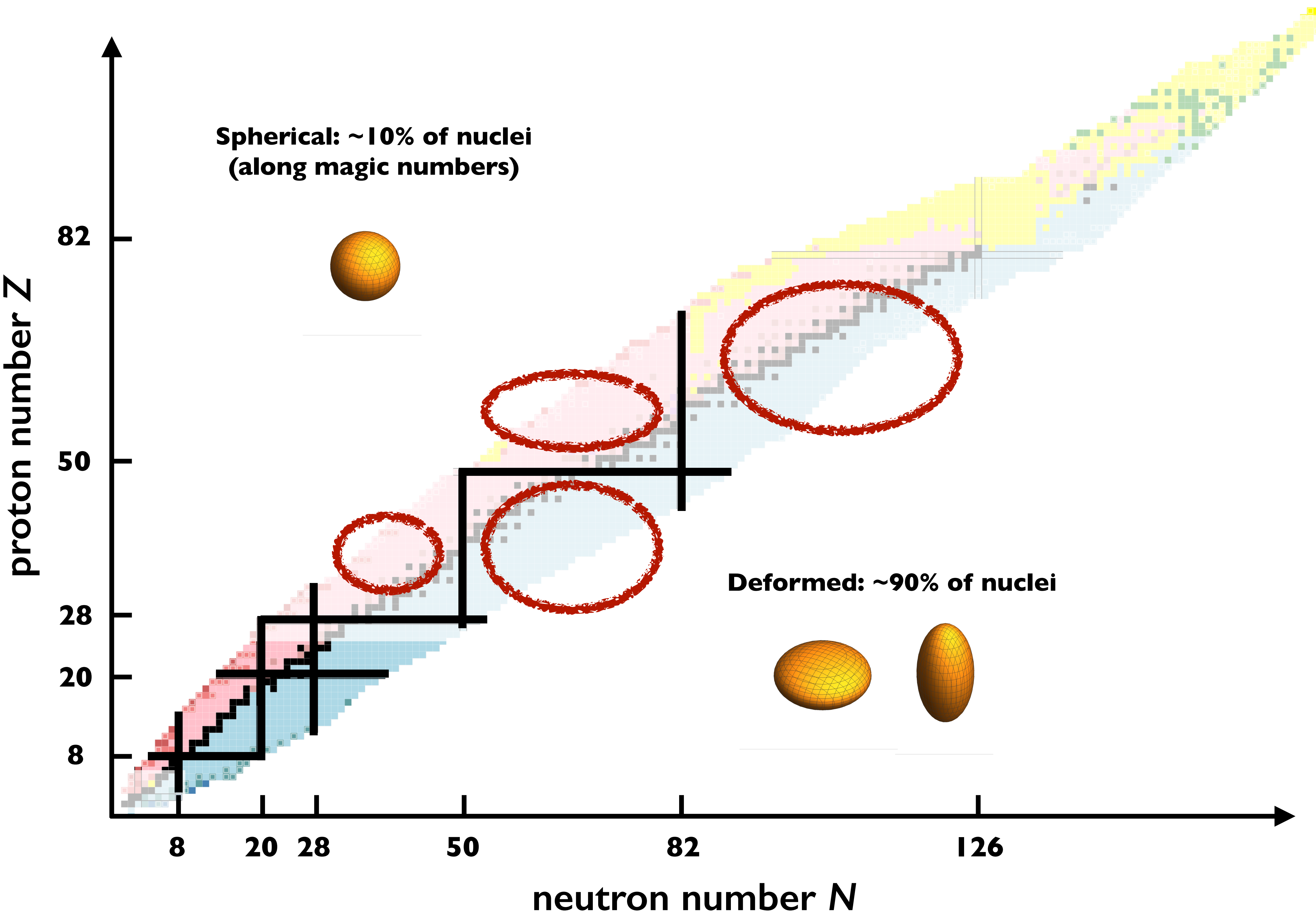
Next steps: exploring new interactions in atomic nuclei

Many-body theory from basis expansion methods

- Accurate predictions for heavy-mass regime
- Novel tensor-network approaches for strong correlations
- Design of many-body emulators for interaction surveys

Next steps: global account for nuclear deformation

Nuclear deformation: a grand challenge



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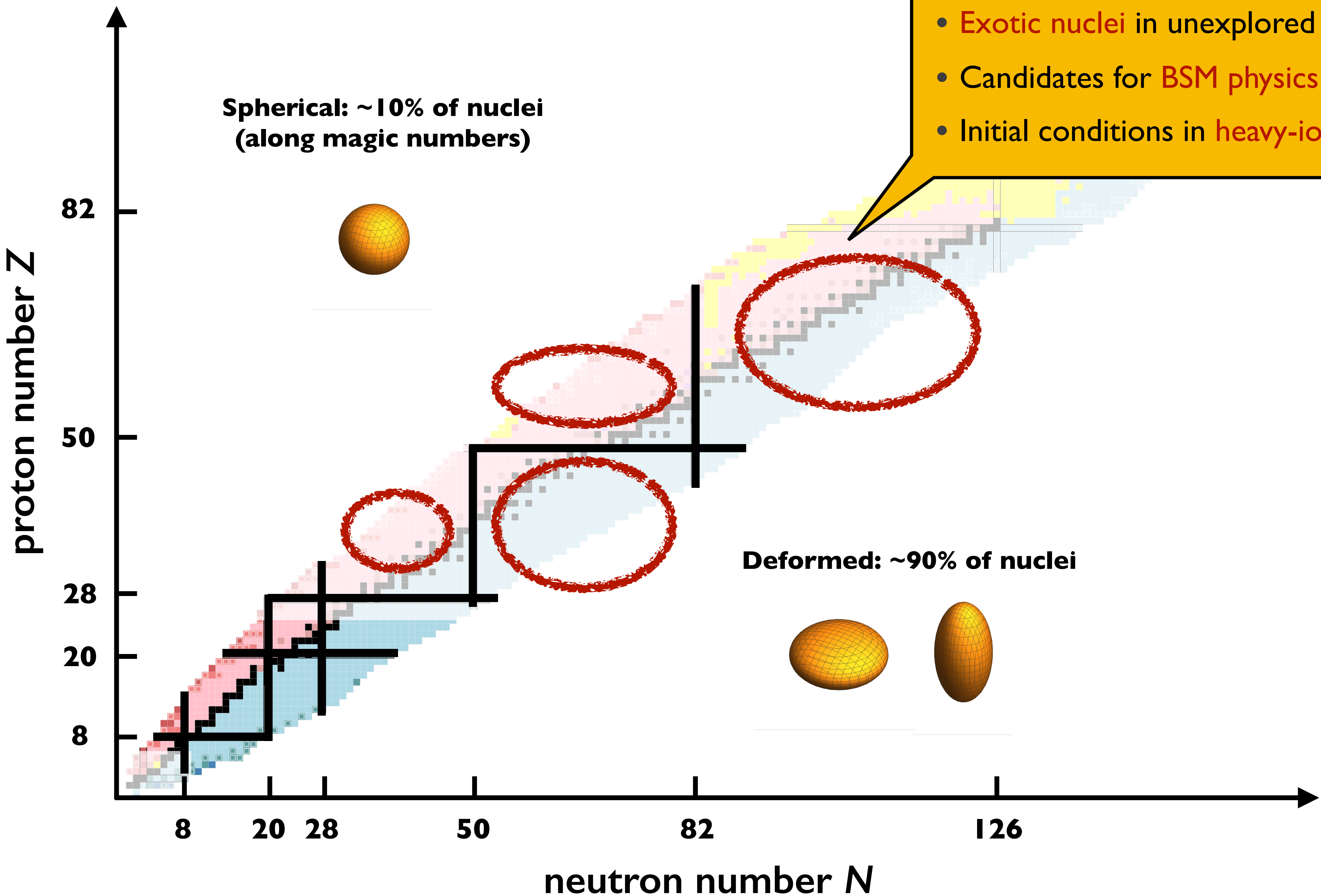

Science opportunities

- Exotic nuclei in unexplored territory
- Candidates for BSM physics searches
- Initial conditions in heavy-ion collisions