Ab initio simulations of atomic nuclei

State-of-the-art and future challenges

Heavy Ion Coffee Seminar

February 4th, 2025

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TECHNISCHE UNIVERSITÄT DARMSTADT
ATHENE YOUNG INVESTIGATOR
European Research Council
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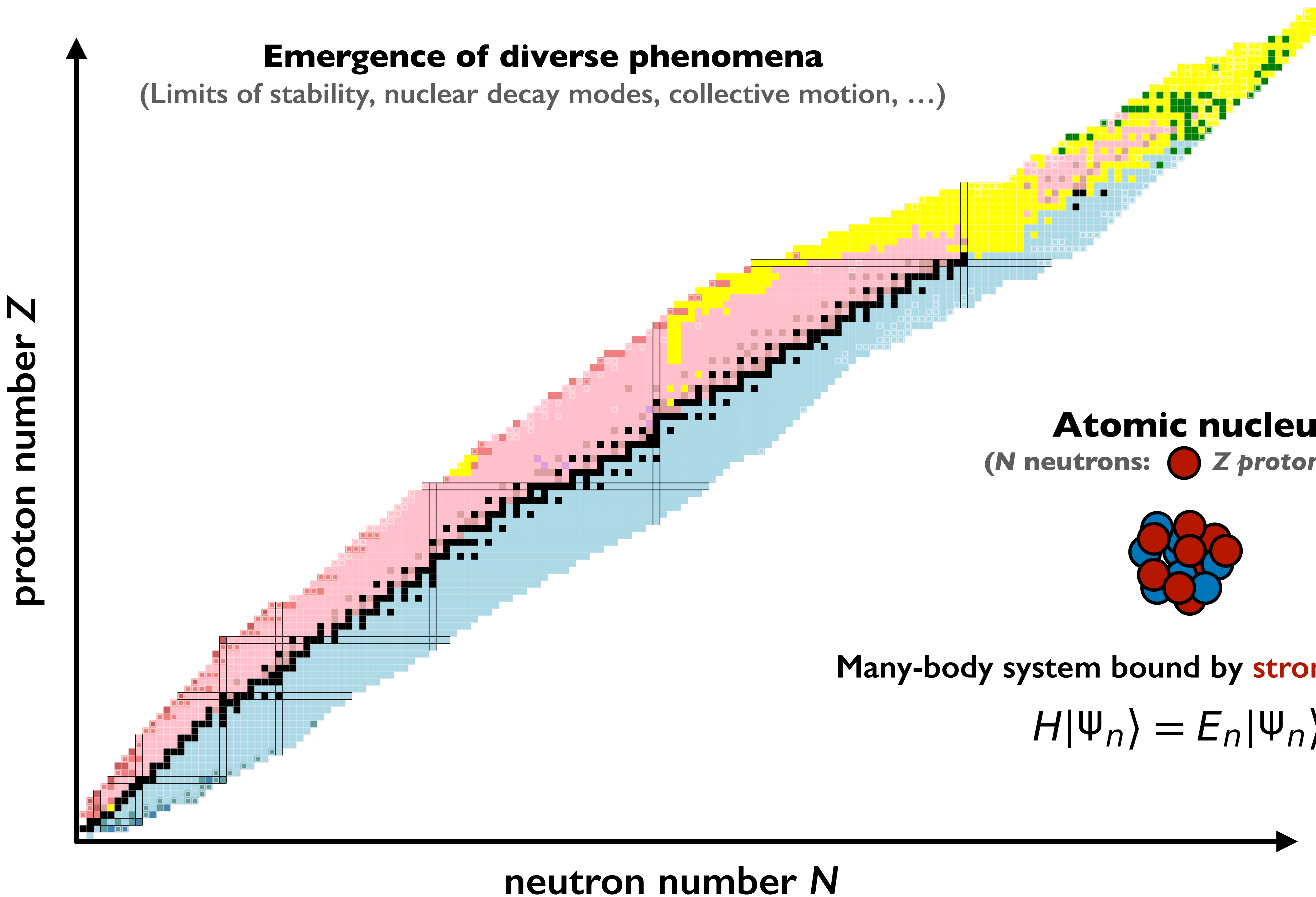
DeformedNuclei
SFB 1245

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!

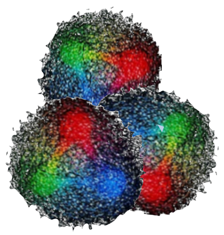
$$H|\Psi_n\rangle = E_n|\Psi_n\rangle$$

What is *ab initio* nuclear structure?

- Ideal scenario: solve for nuclear observables from QCD Lagrangian

- Practically requires (intractable) solution using lattice QCD techniques

Quantum chromodynamics



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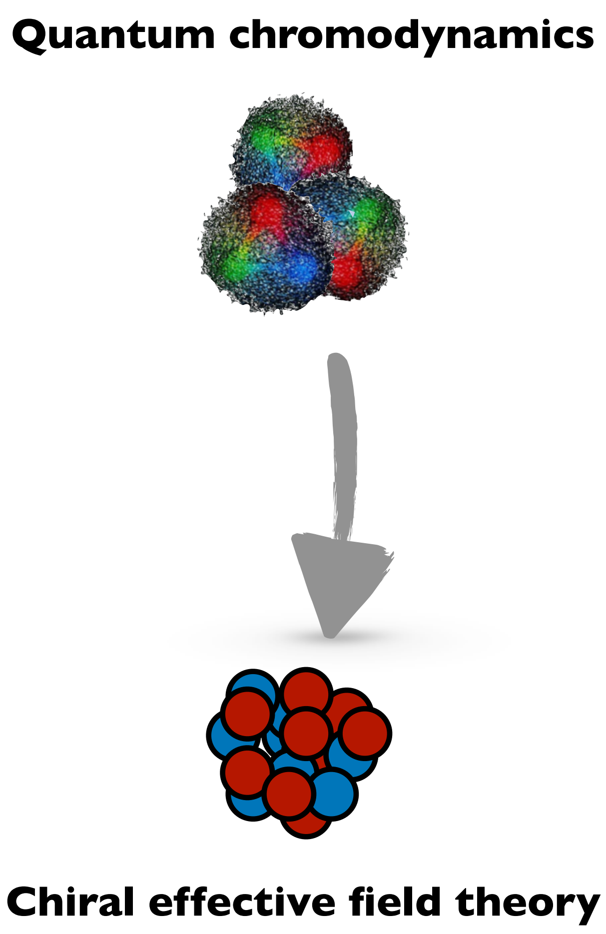
- Effective field-theory description

$$\mathcal{L}_{\mathrm{QCD}} \longrightarrow H_{\mathrm{EFT}}$$



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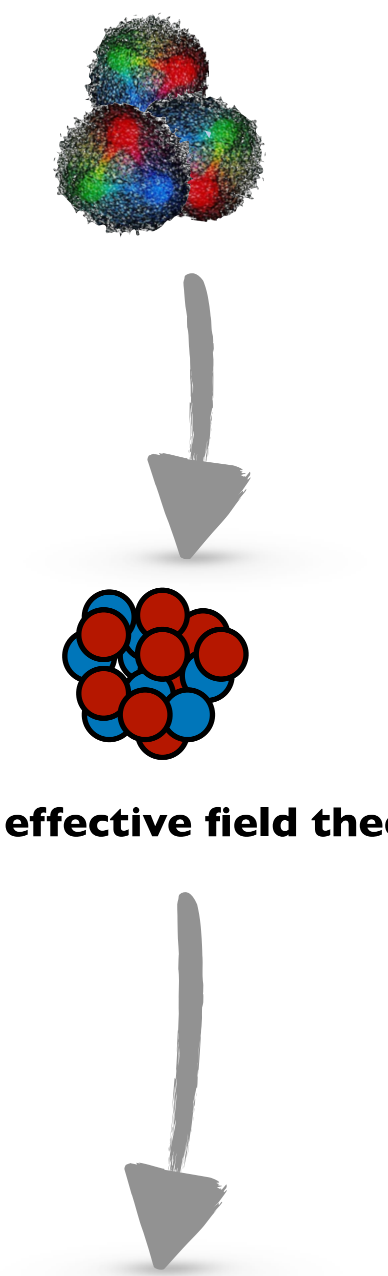
$$\mathcal{L}_{\text{QCD}} \longrightarrow H_{\text{EFT}}$$

- Solve many-body problem in a systematically improvable way

Quantum chromodynamics



Chiral effective field theory

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

Nuclear many-body problem

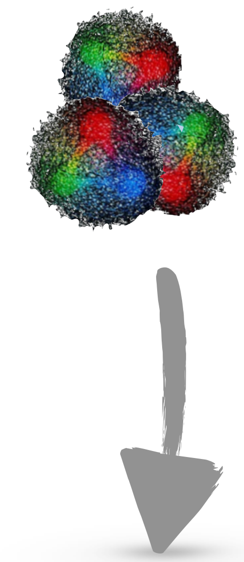
What is *ab initio* nuclear structure?

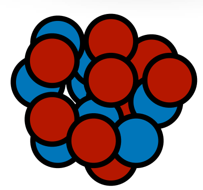
- Ideal scenario: solve for nuclear observables from **QCD Lagrangian**
- Practically requires (intractable) solution using **lattice QCD techniques**
- Effective field-theory description

$$\mathcal{L}_{\text{QCD}} \longrightarrow H_{\text{EFT}}$$

- Solve many-body problem in a **systematically improvable** way
- *Ab initio* promise: controlled uncertainties with **predictive power**

Quantum chromodynamics





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Nuclear many-body problem

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- Practically requ… solution using la…
- Effective field-th…

$\mathcal{L}_{\text{QCD}}$

- Solve many-body problem in a systematically improvable way
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Quantum chromodynamics

Chiral effective field theory

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

Nuclear many-body problem

Controlled expansions:

Accuracy → Complexity

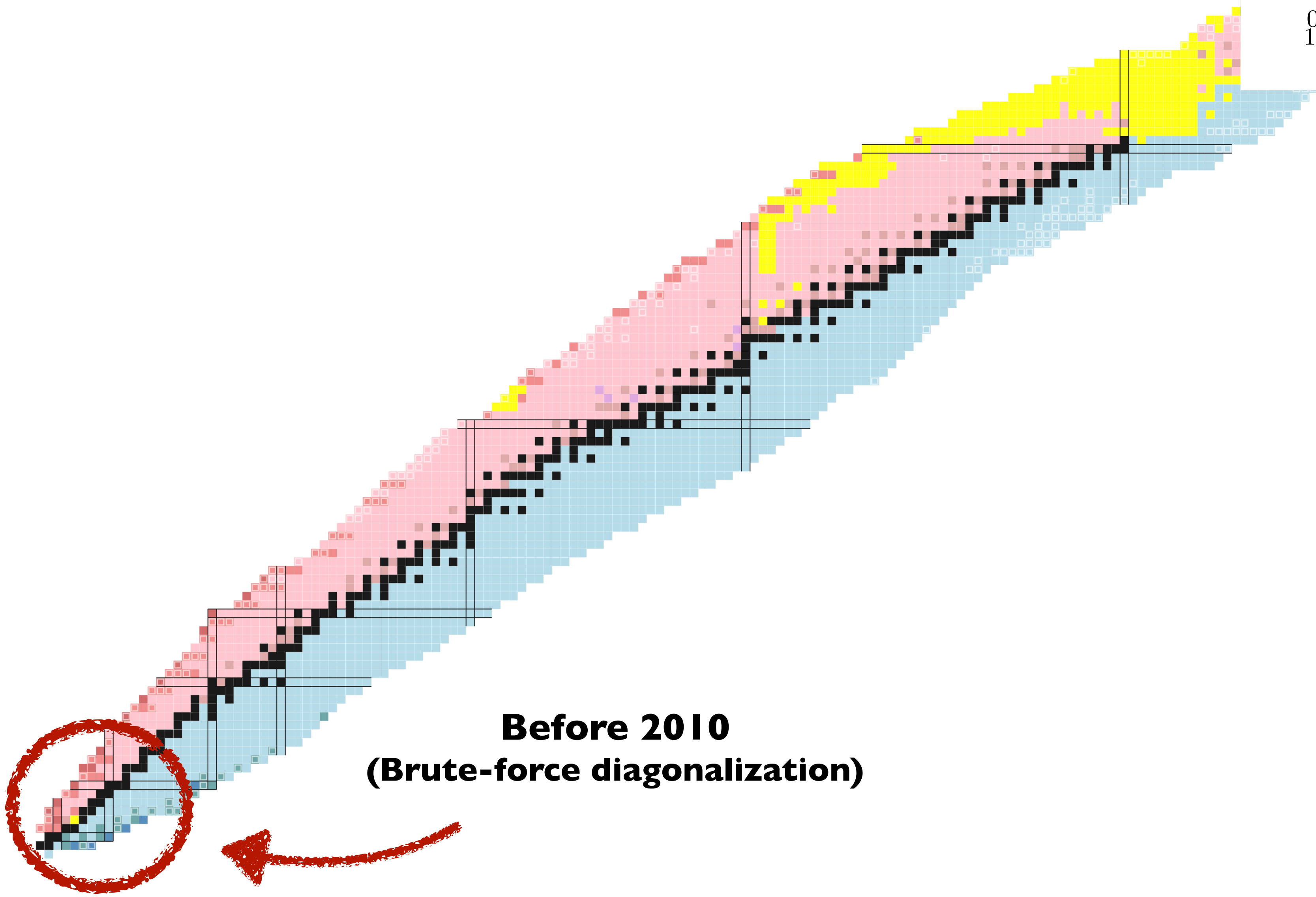
Complicated!

$$e^x = 1 + x + \frac{1}{2}x^2 + \frac{1}{6}x^3 + \mathcal{R}(x^4)$$

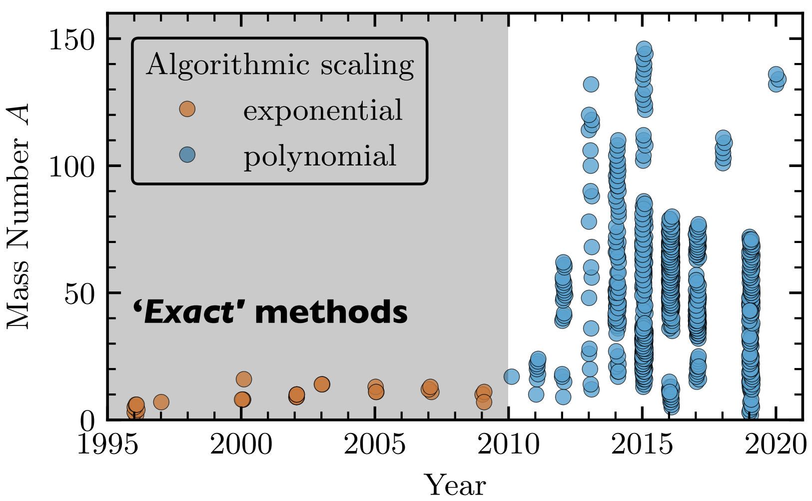
Simple!

Remainder term (uncertainty estimate!)

Evolution of *ab initio* nuclear structure



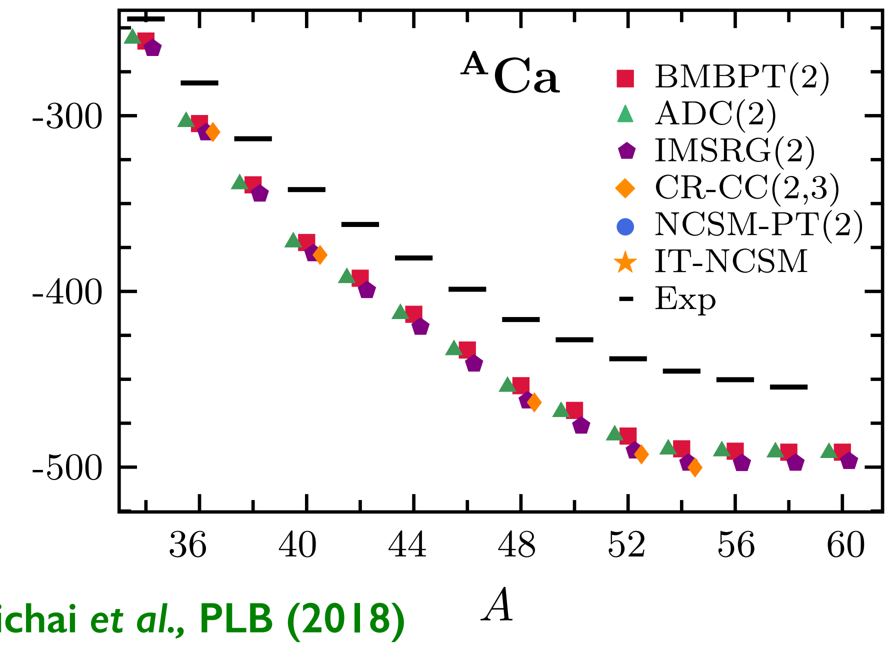
Explosion of *ab initio* simulations



Drischler, Bogner, Few-Body Systems (2021)

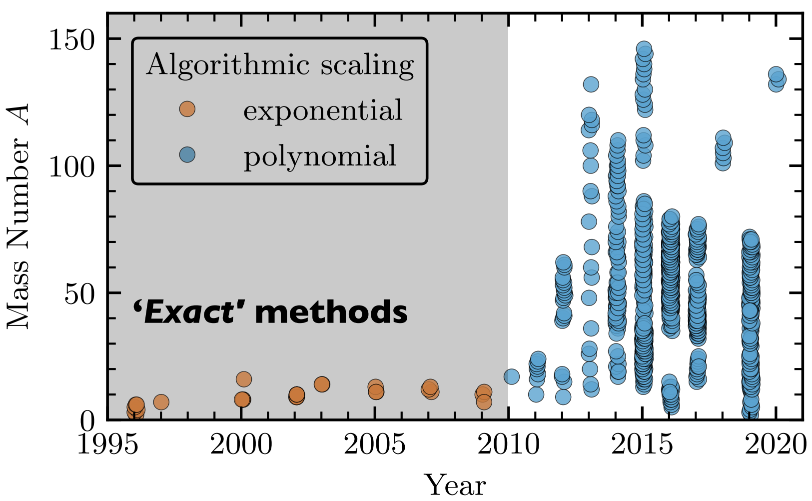
Evolution of *ab initio* nuclear structure

Consistency in many-body systems



Tichai *et al.*, PLB (2018)

Explosion of *ab initio* simulations



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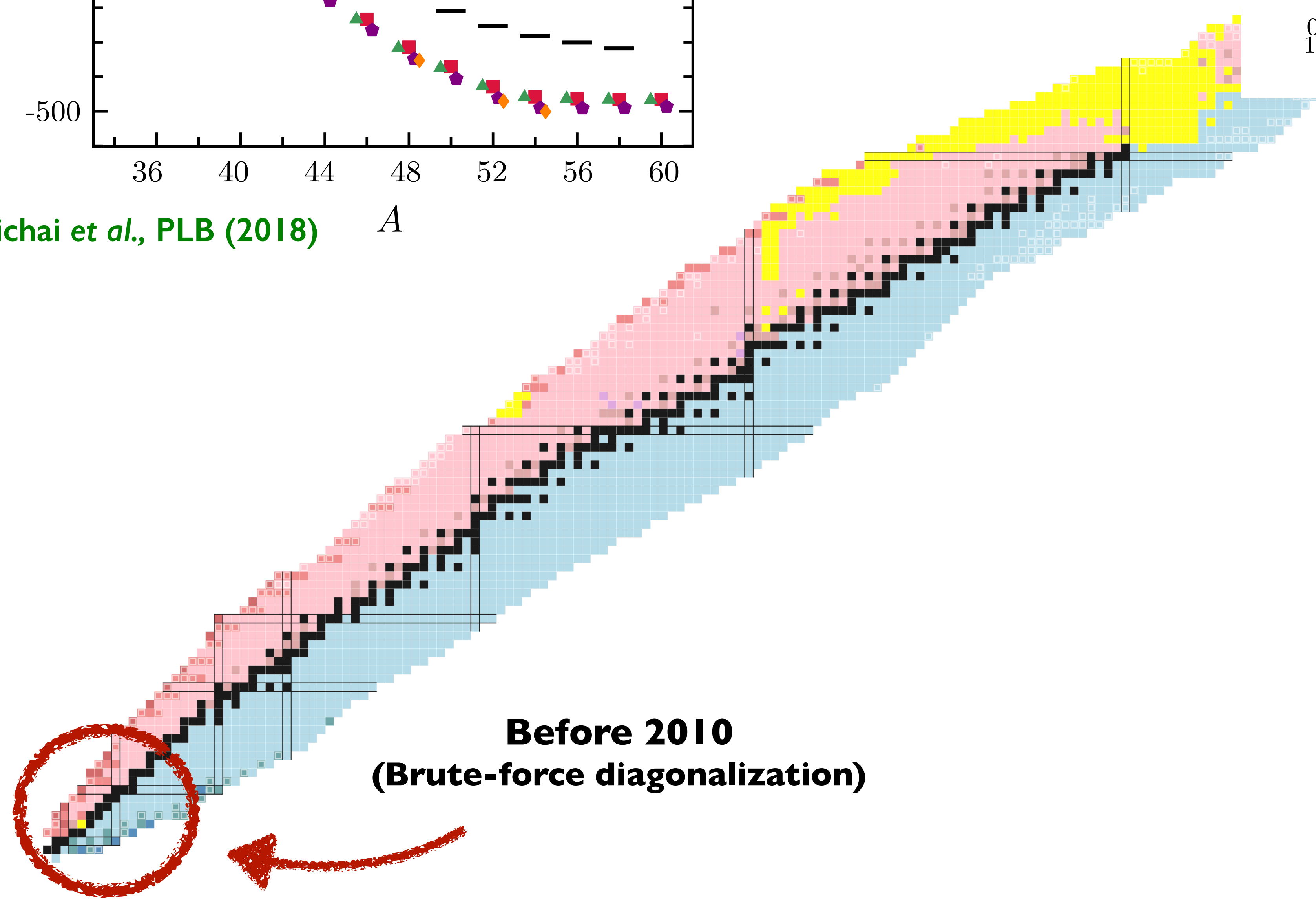

Before 2010
(Brute-force diagonalization)

Evolution of *ab initio* nuclear structure

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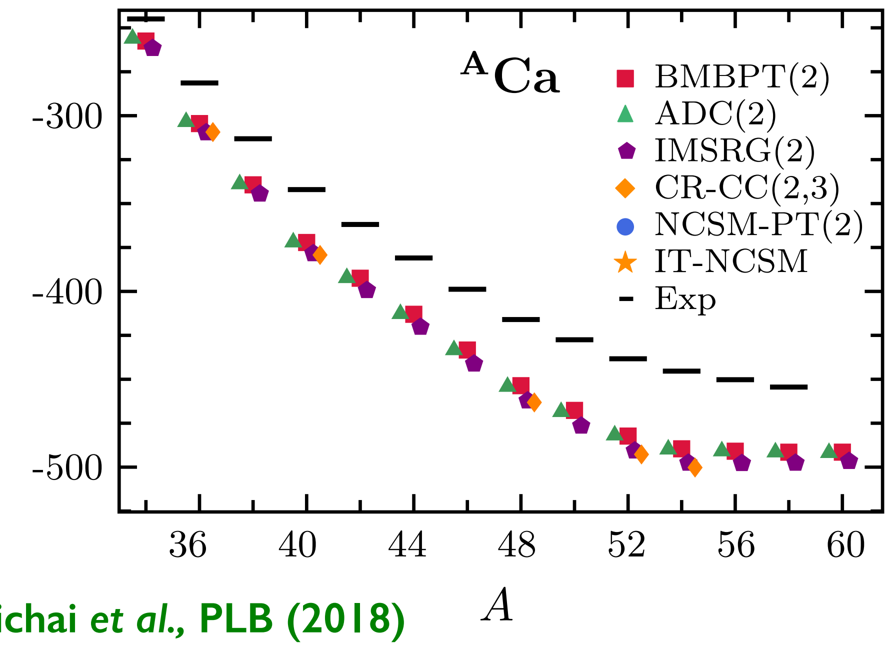

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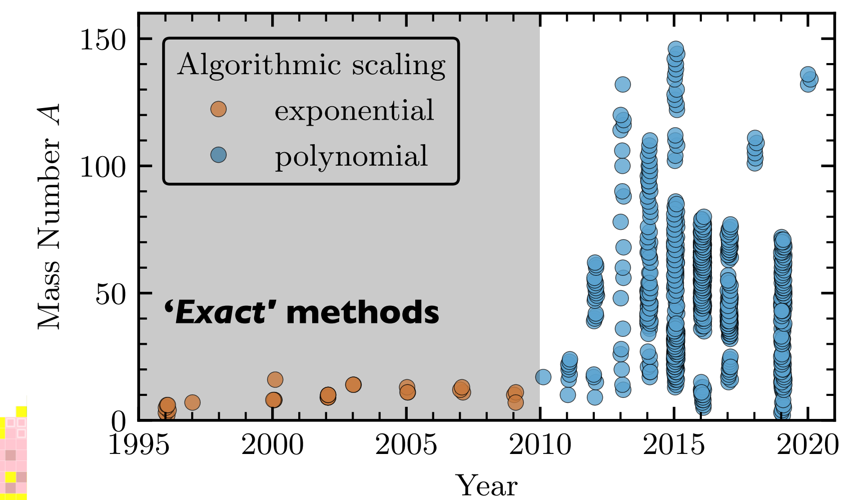

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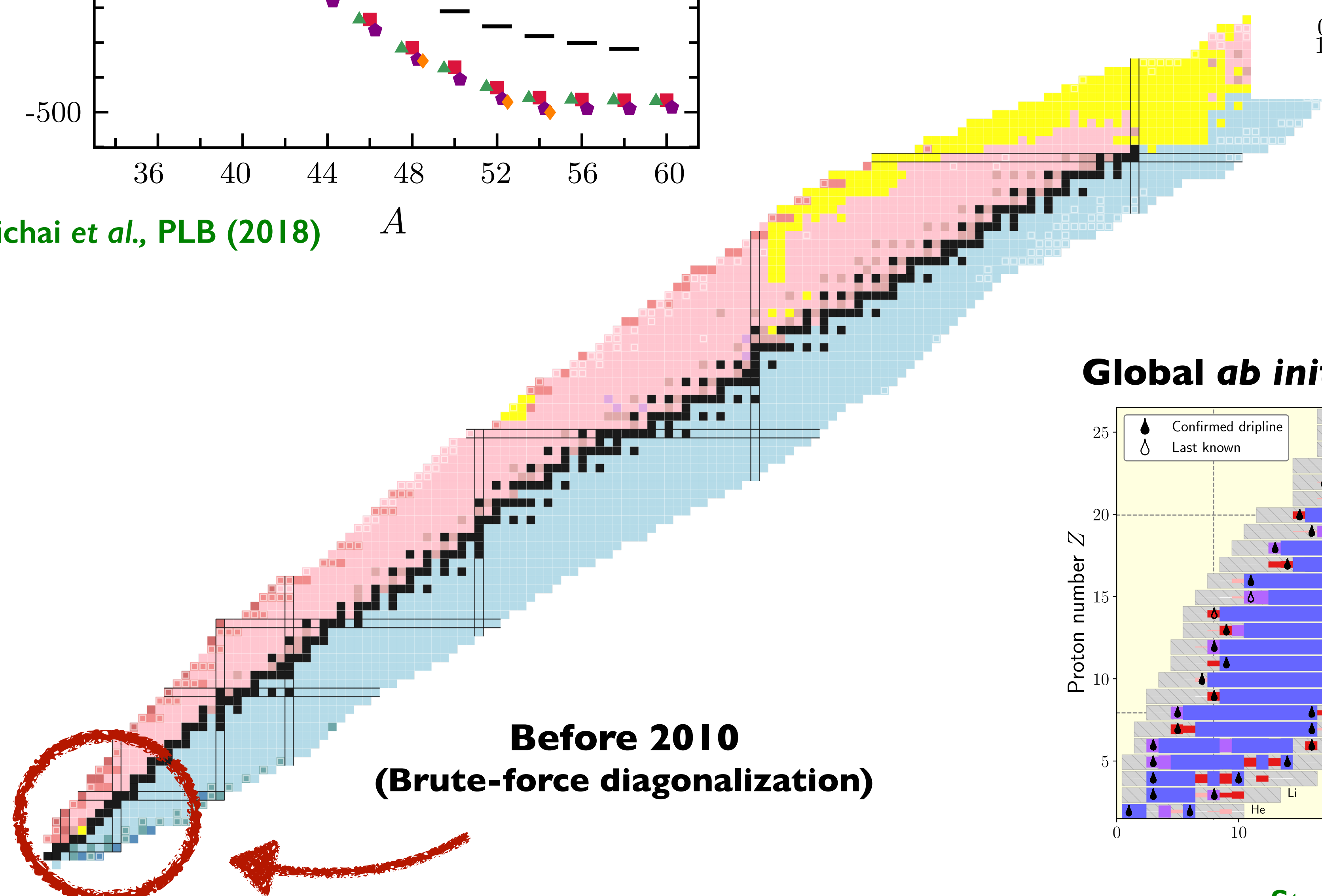
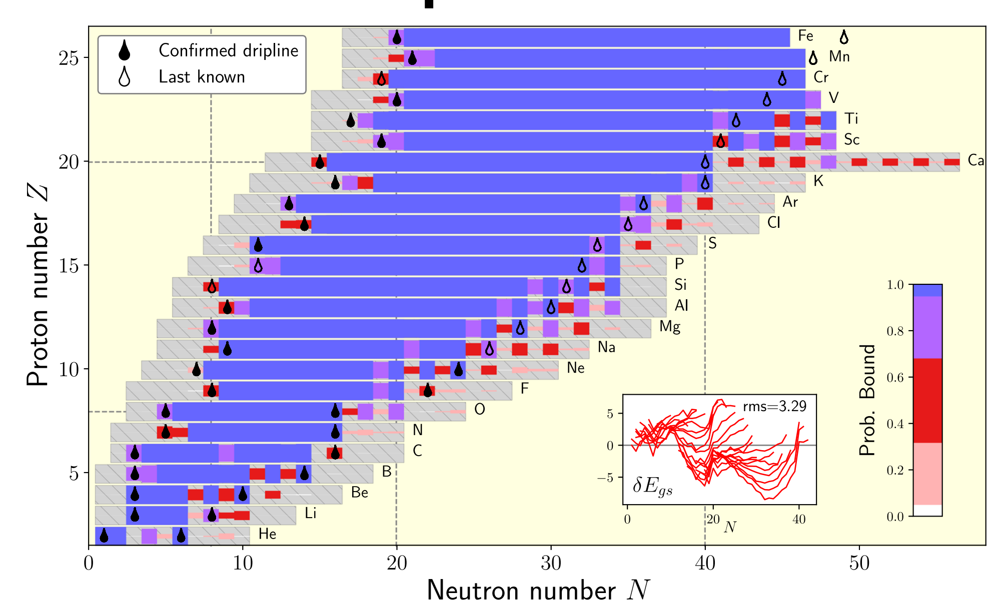


Global *ab initio* predictions of 700 nuclei

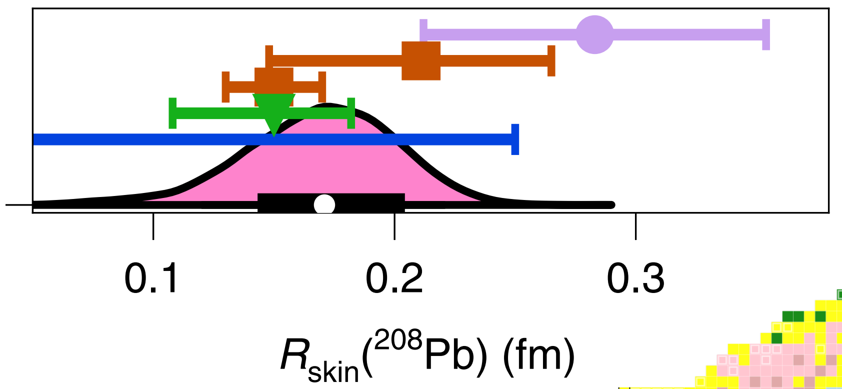


Stroberg *et al.*, PRL (2019)

Highlights in heavy nuclei!

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

Neutron skin in ^{208}Pb

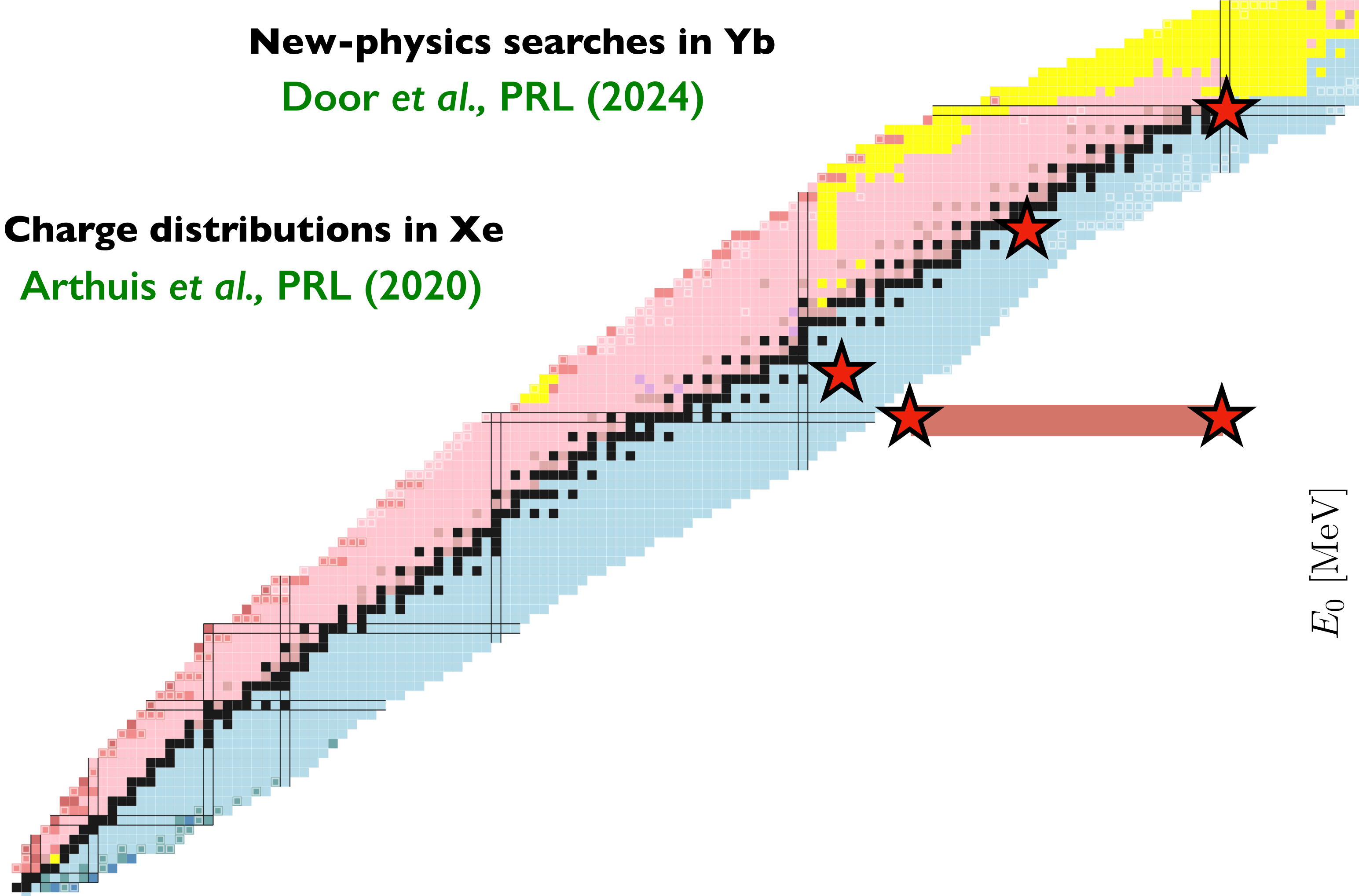


New-physics searches in Yb

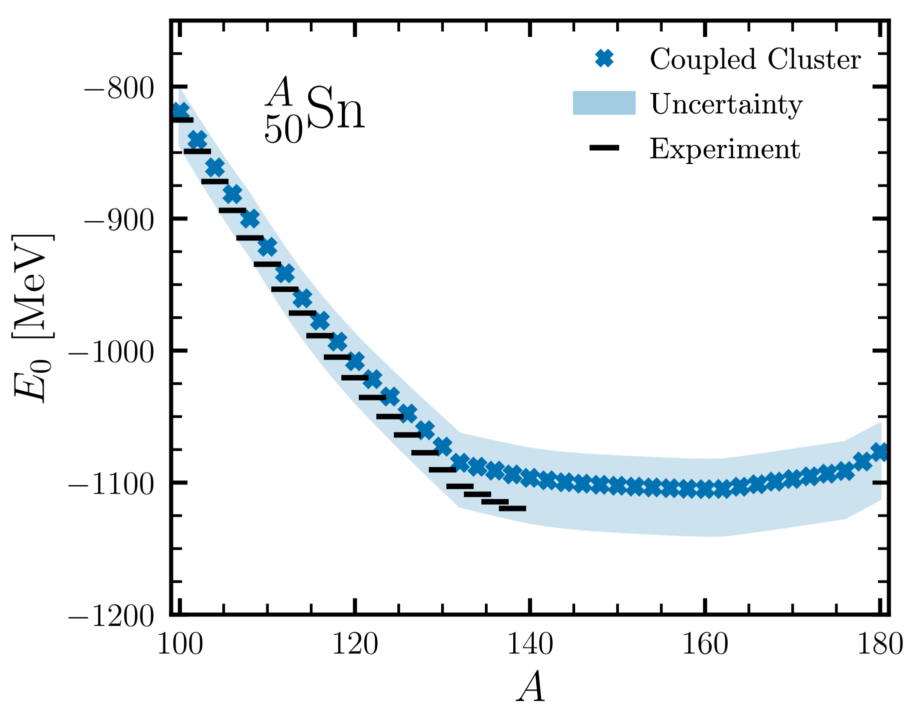
Door *et al.*, PRL (2024)

Charge distributions in Xe

Arthuis *et al.*, PRL (2020)



Neutron dripline in Sn



Tichai *et al.*, PLB (2024)

Chiral effective field theory

Weinberg, Epelbaum, Kaplan, van Kolck, Krebs, Machleidt, Meißner, Savage, …

- Low-energy effective field theory with nucleons/pions as degrees of freedom

- Expansion parameter from separation of scales at low-energies

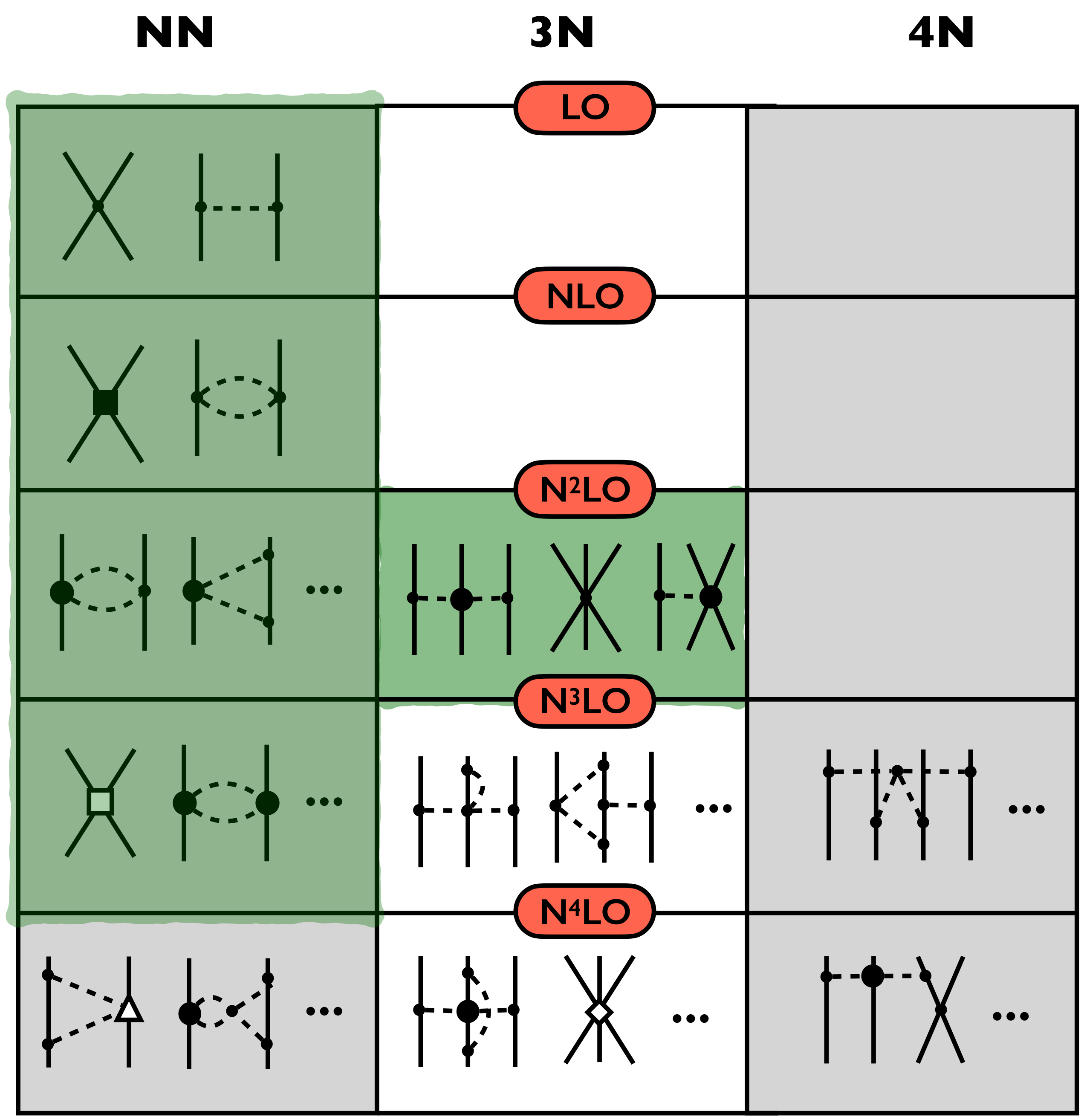
$$\frac{Q}{\Lambda_b} \approx \frac{1}{3}$$

(sets the scale of convergence)

- High-energy physics parametrised by few low-energy constants (LECs)

$$V_{\mathrm{EFT}} = V_0 + \sum_i c_i \cdot V_i$$

- Emergence (!) of higher-body operators



Many-body expansions

- **Goal: solution of Schrödinger equation**

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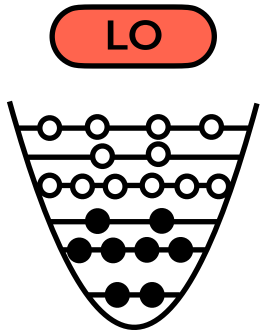
- **Idea: write exact many-body solution relative to an *A*-body reference state (leading order)**

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

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



nuclear mean-field
(e.g. Hartree-Fock)

$W^{[0B]}$

Many-body expansions

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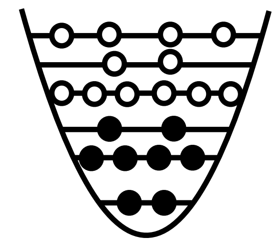
- **Leading order must qualitatively capture the dominant correlations of the system!**

- **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



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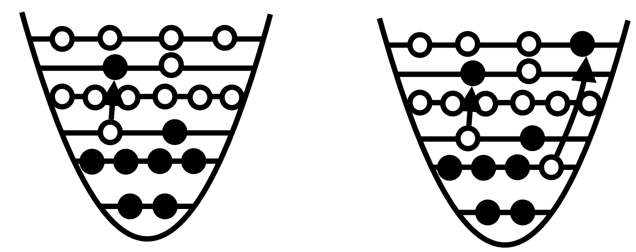
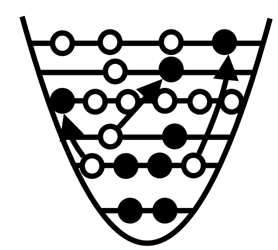
NLO



$W^{[1B]}$

$W^{[2B]}$

N²LO



$W^{[3B]}$

N³LO

...

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

Interaction uncertainties

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

- Interaction uncertainties estimated from order-by-order calculations

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

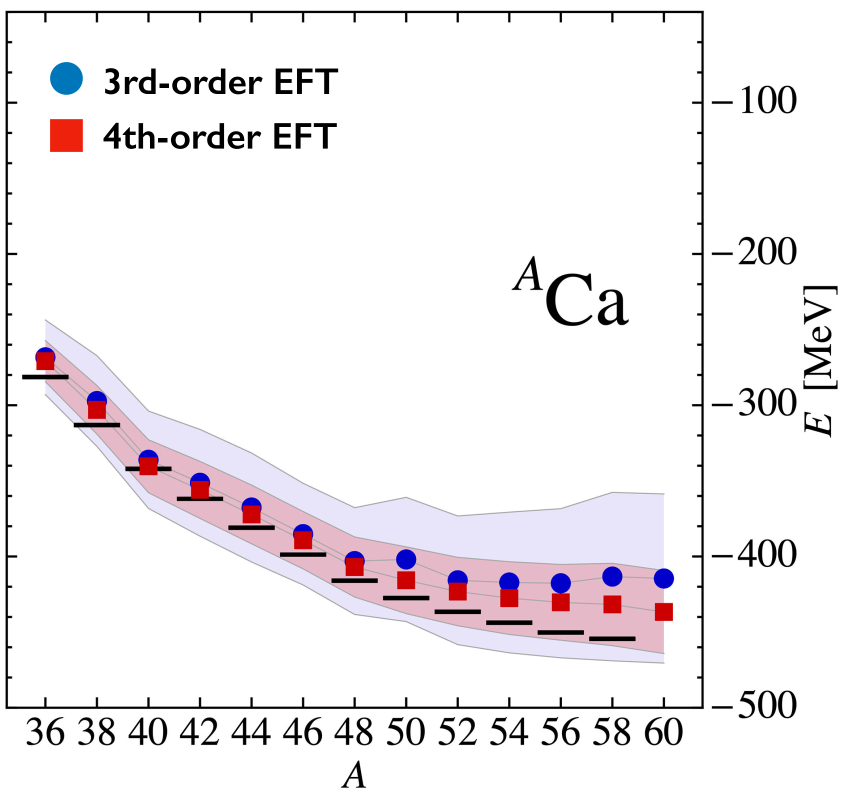
- Similar studies of theory uncertainties in nuclear-matter simulations

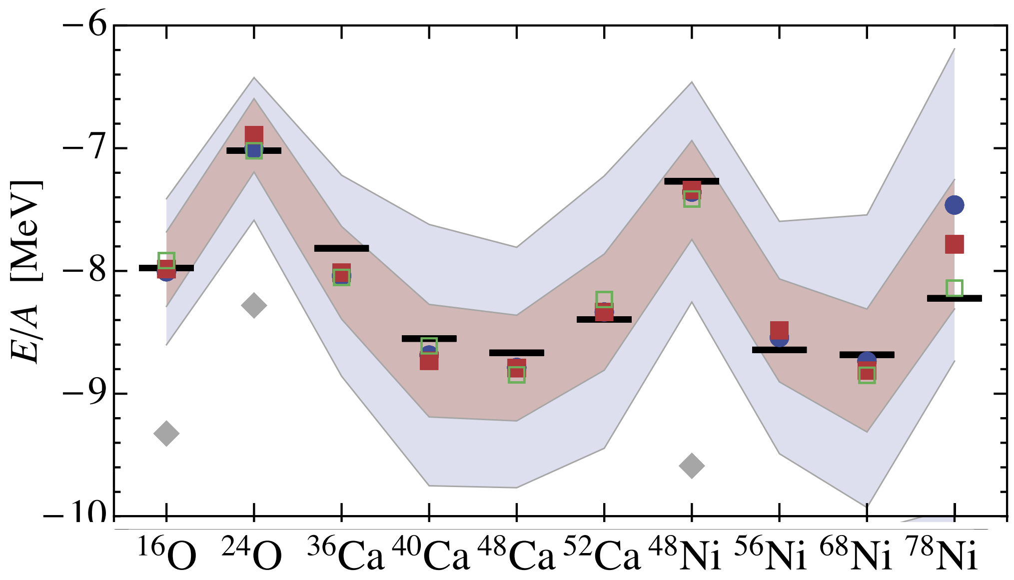
Drischler *et al.*, PRL (2020)
Keller *et al.*, PRL (2023)

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

2-3% of ground-state energy

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





Hüther *et al.*, PLB (2020)

Towards many-body uncertainties

- **Simple framework for ground states:** **many-body perturbation theory**

$$E_0 = E_{\text{ref}} + E^{(2)} + E^{(3)} + \ldots$$

- **Error model for truncated expansion**

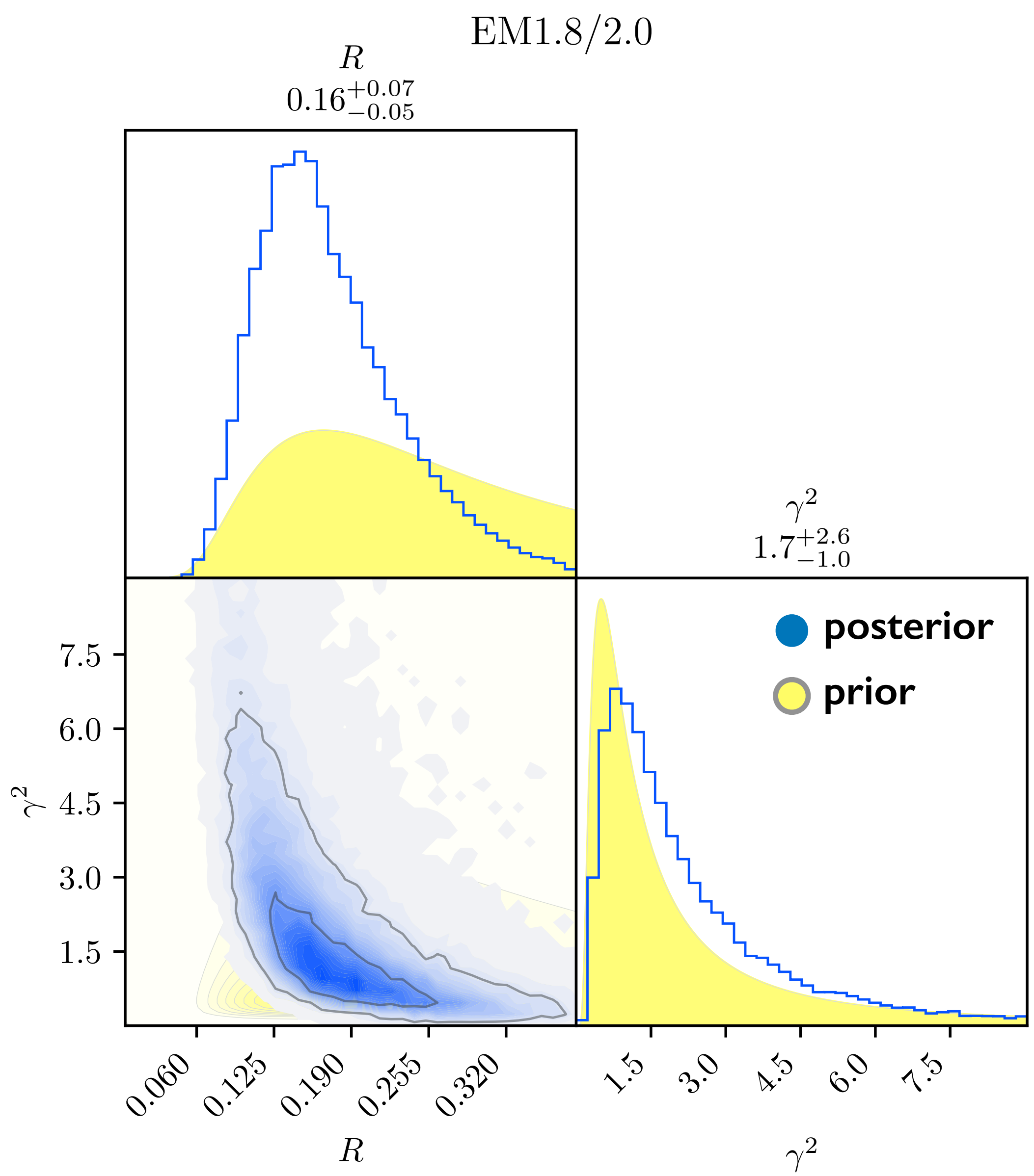
coefficient drawn from $N(0,\gamma^2)$

$$\delta E_0 = E_{\text{ref}} \sum_{i=k+1}^{\infty} \gamma_i R^i$$

reference scale (8 MeV/A)

suppression ratio (⟶ softness)

with I. Svensson, K. Hebeler, A. Schwenk



Probability distributions of parameters

Towards many-body uncertainties

with I. Svensson, K. Hebeler, A. Schwenk

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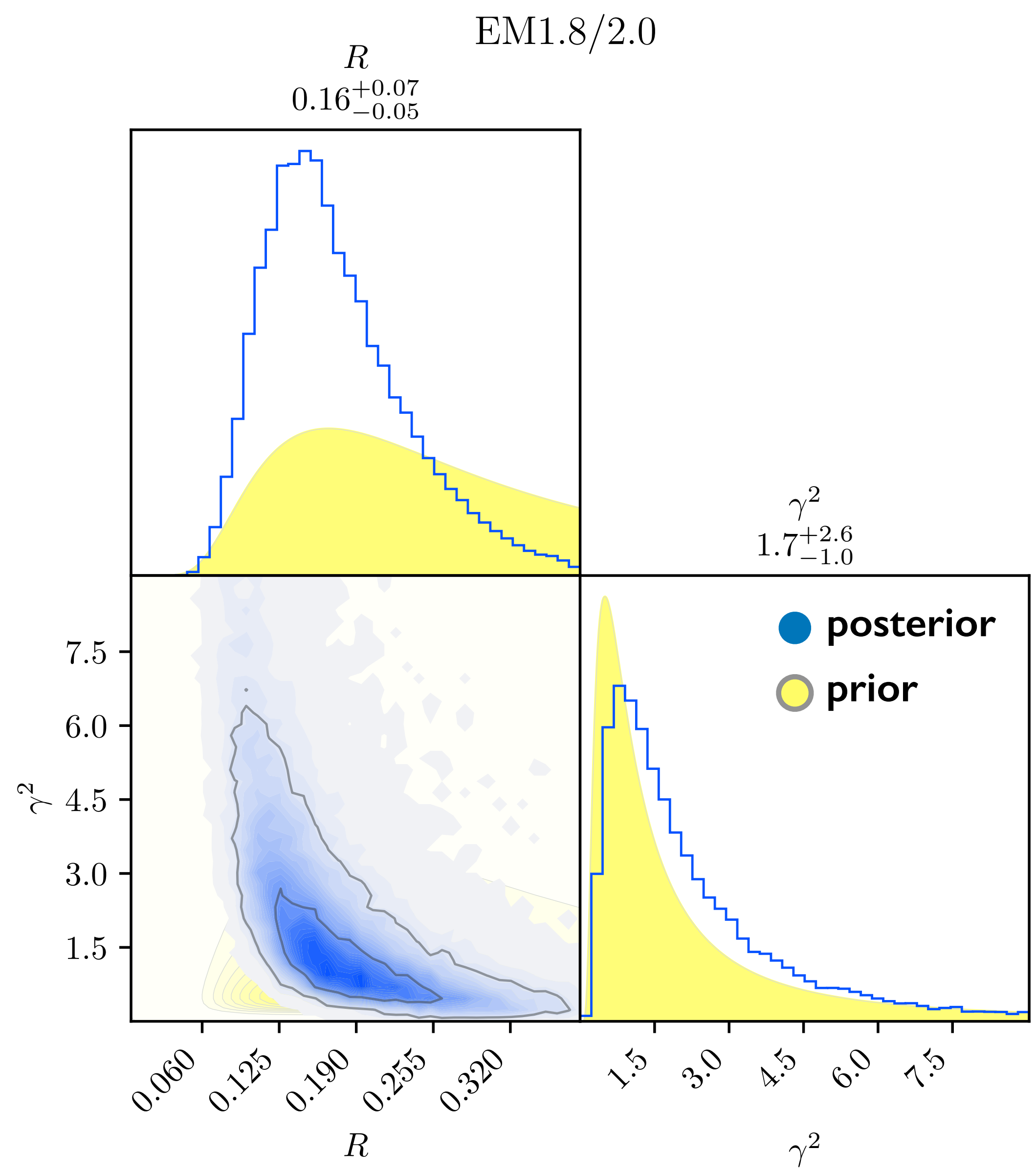
- **Learn coefficients of error model** from MBPT results for given interaction

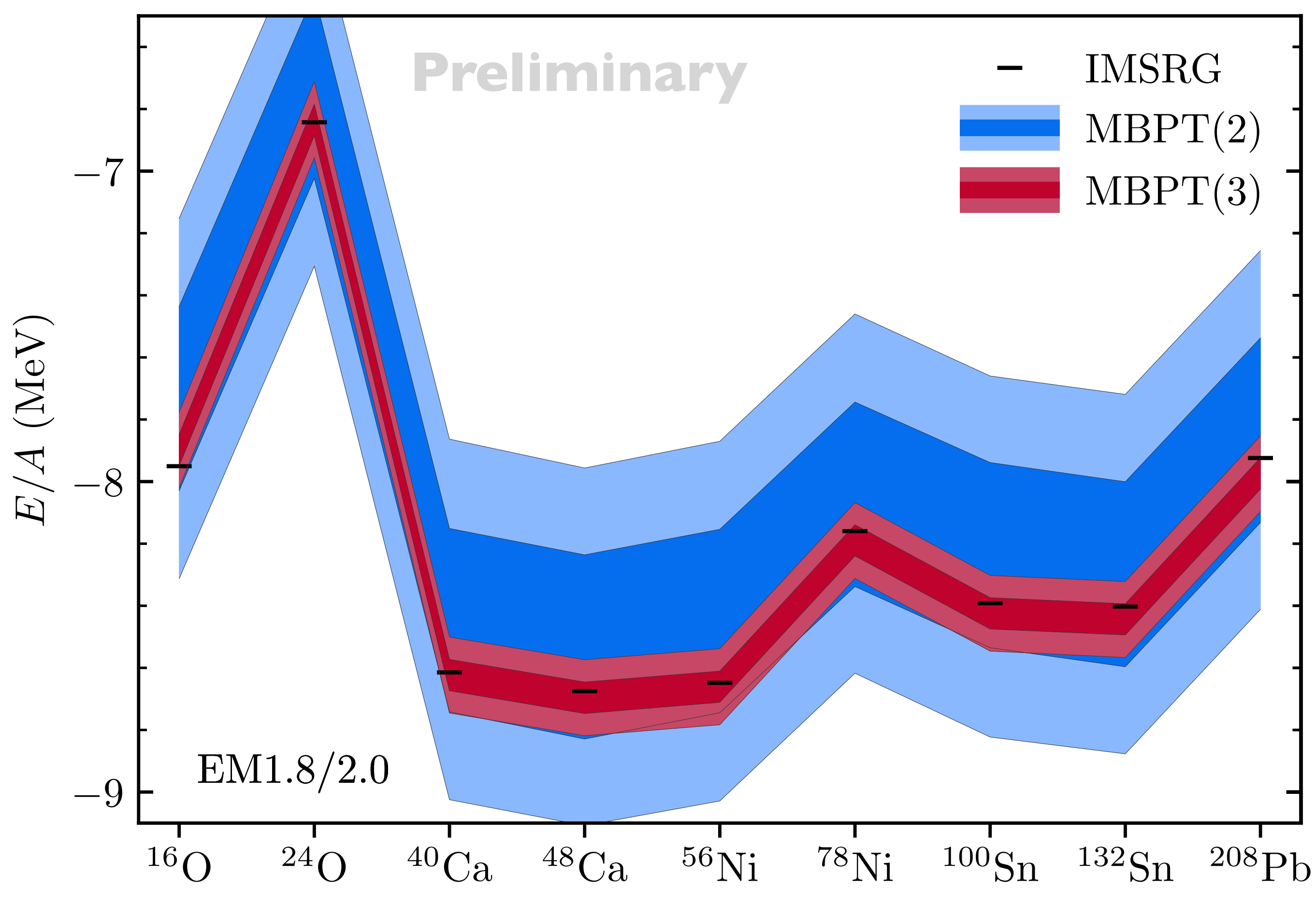
R < 1 indicates convergence!



Probability distributions of parameters

Medium-mass nuclei

1- and 2-*σ* error bands for closed-shell nuclei

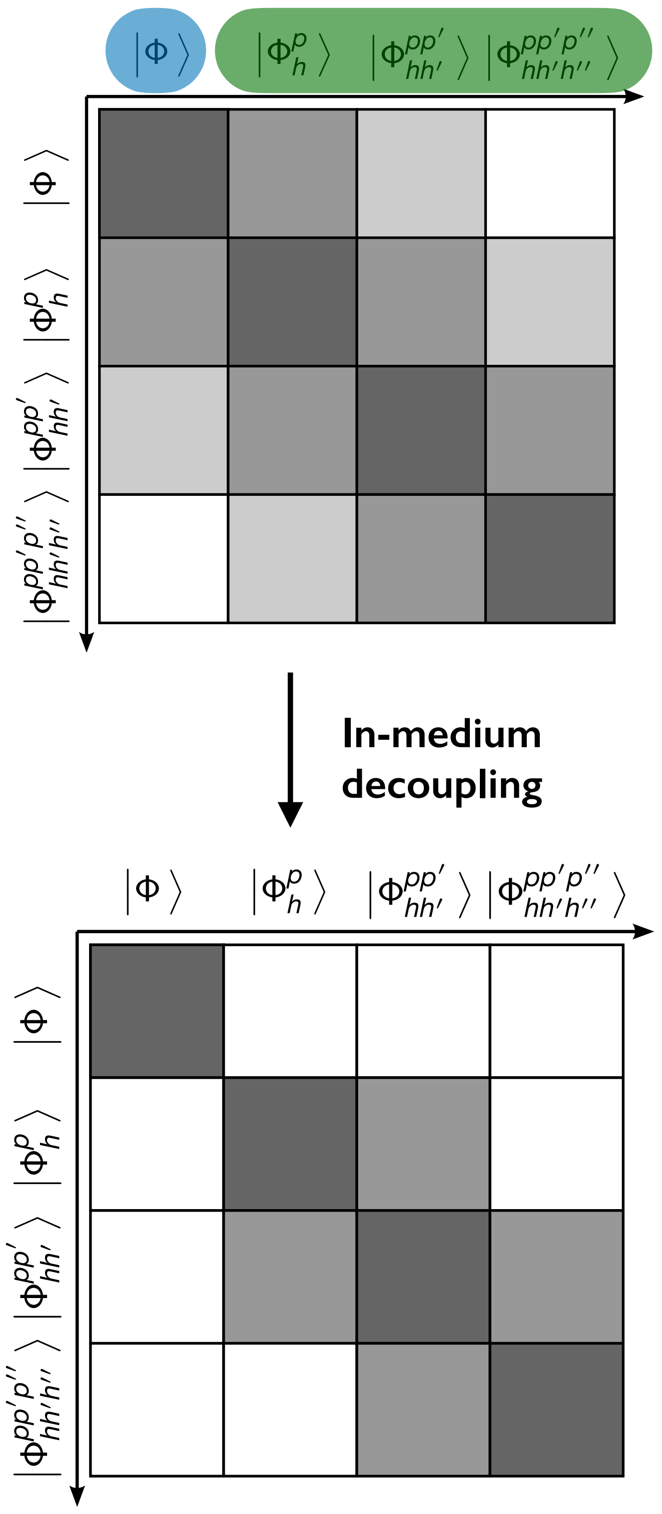


- **Large uncertainties for second-order MBPT calculations**
- **Significantly reduced uncertainty at third order for all nuclei**
- **'Interaction softness': strong suppression of higher-order terms**

Harder interactions: larger *R*

Replace *ad hoc* estimates with statistically sound predictions

In-medium similarity renormalization group



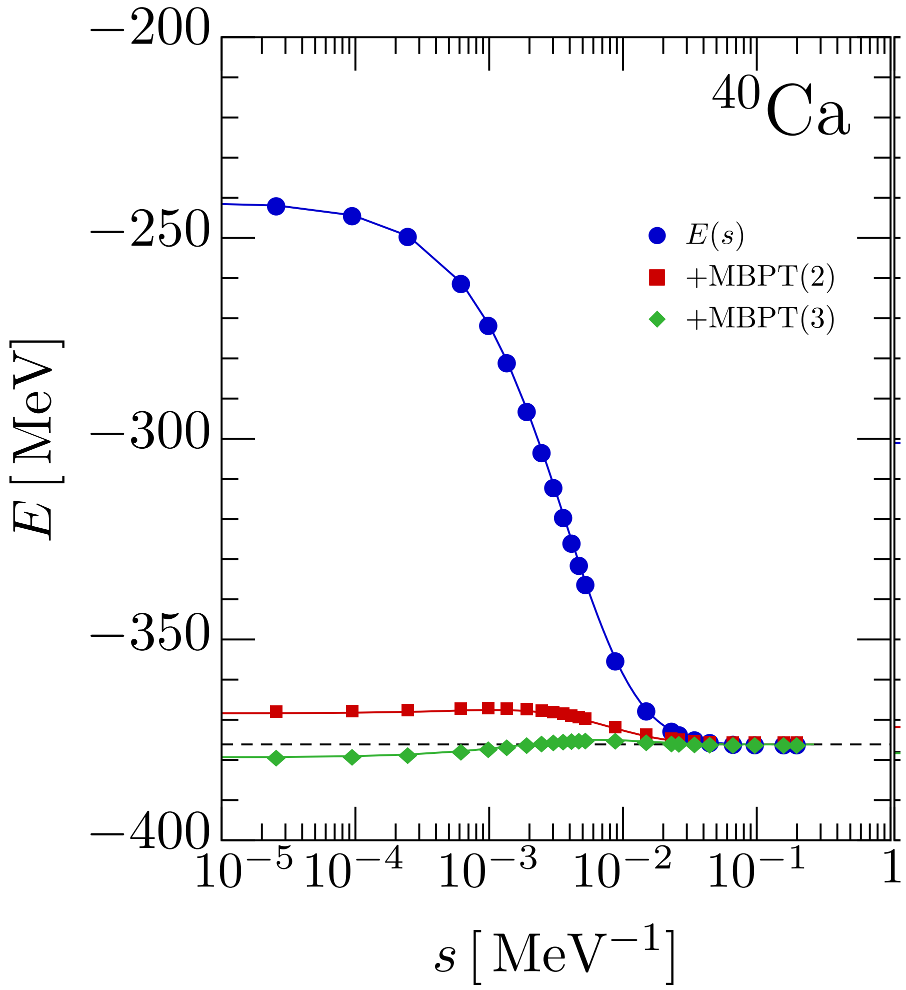
Hergert *et al.*, Phys. Rep. (2016)

- **Goal: decoupling of elementary particle-hole excitations from reference state**

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

$\uparrow$ *A*-body rotation

In-medium similarity renormalization group



- **Goal: decoupling of elementary particle-hole excitations from reference state**

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

A-body rotation

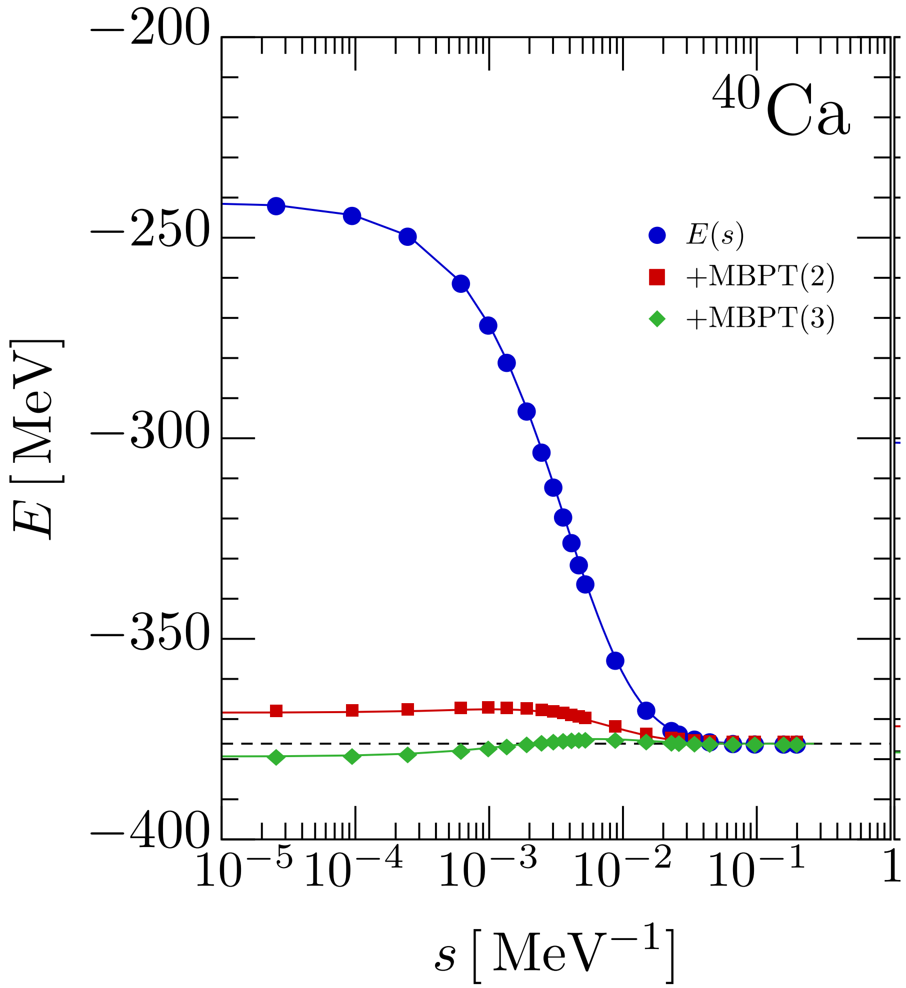
- **Basic formulation: ground-state energy from *H(s)***

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

- **Particle-hole correlations are absorbed into the renormalized Hamiltonian**

$$E^{(2)}, E^{(3)} \quad \longrightarrow \quad 0$$

In-medium similarity renormalization group



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A-body rotation (of H)

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- **Approximation: induced higher-body operators**

$$H(s=0) \quad \longrightarrow \quad H(s) \quad \neq \quad \tilde{H}(s)$$

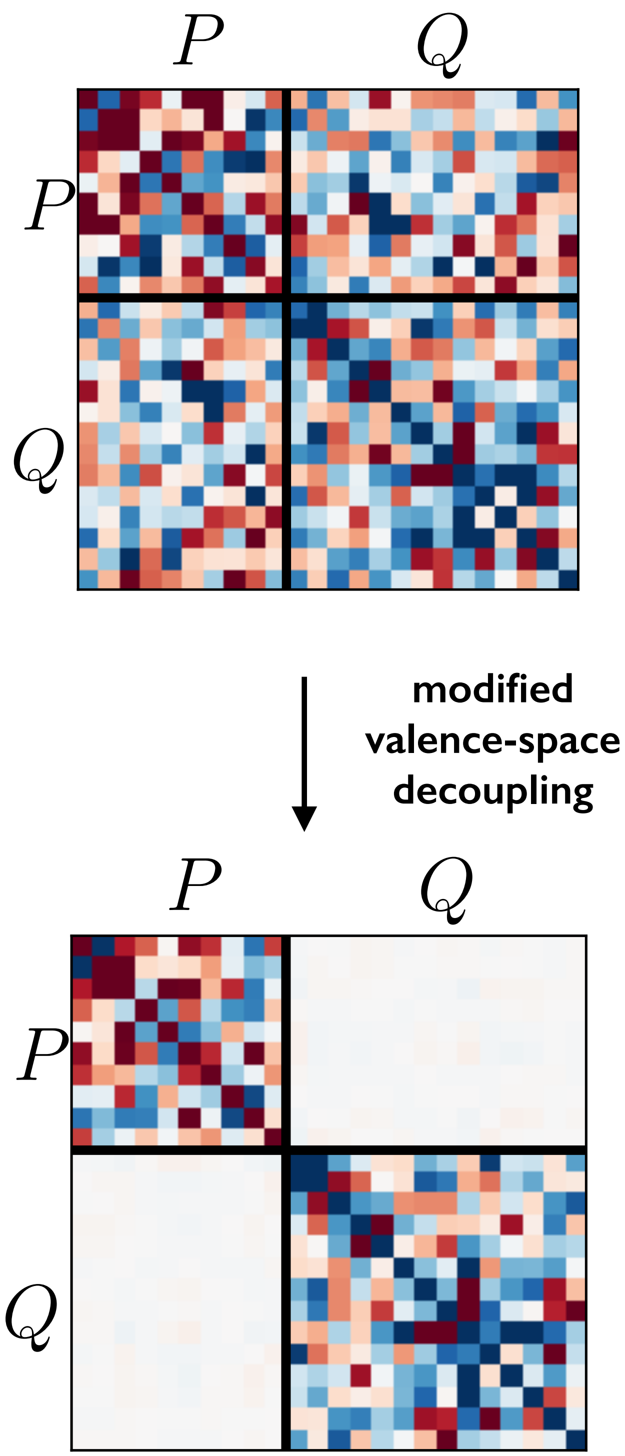
$H(s)$: *A*-body operator; $\tilde{H}(s)$: *two*-body operator

Valence-space formulation

- **Freezing of nucleons in an inert core**

$$\dim \mathcal{H}_A = \binom{\#\text{basis functions}}{A}$$

Valence-space formulation



- **Valence-space IMSRG: modified decoupling yields *ab initio* shell-model interactions**
- **Freezing of nucleons in an inert core**

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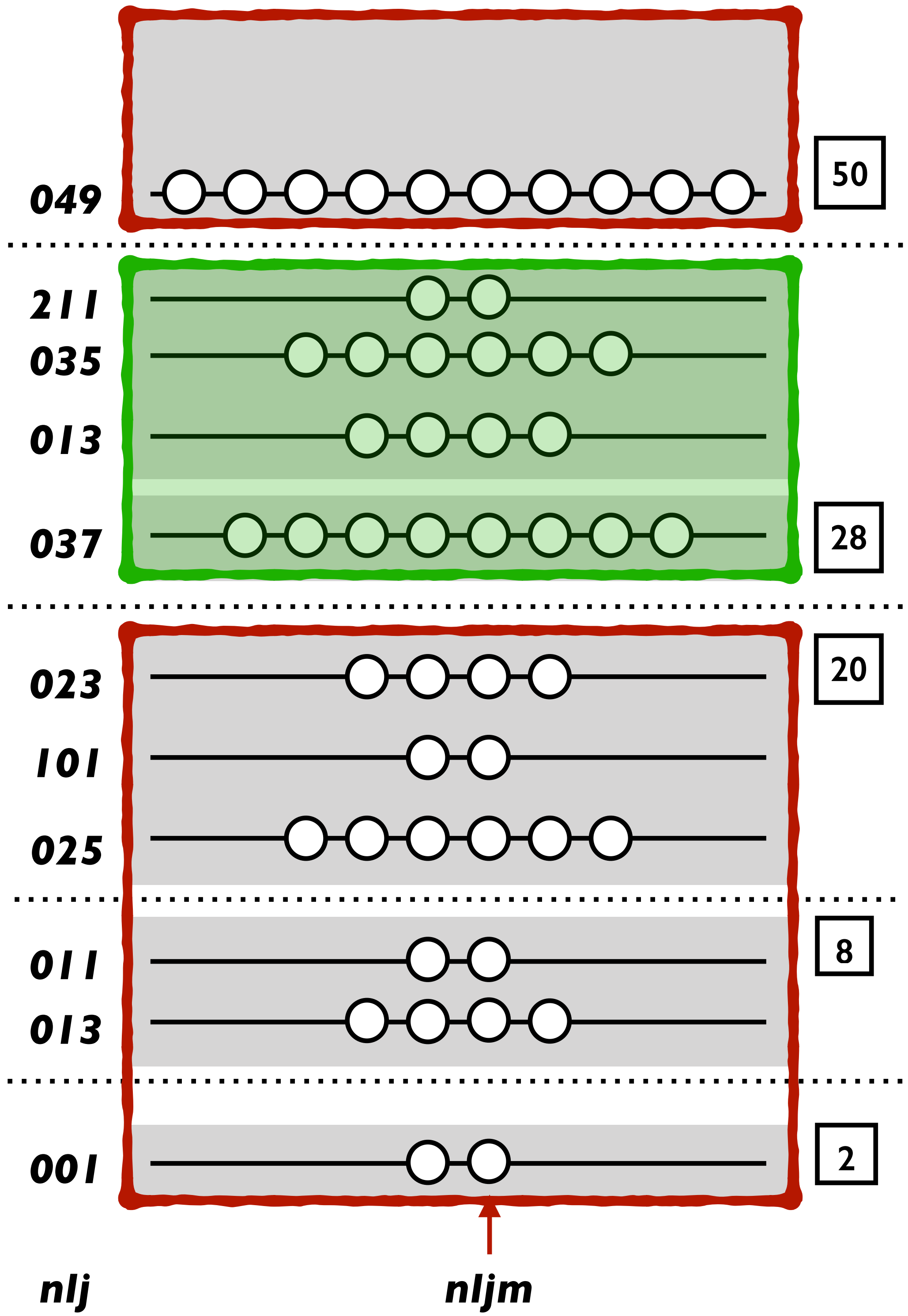
Stroberg *et al.*, Ann. Rev. Nucl. Part. Sci (2019)

Valence-space formulation



Bohr-Mottelson shell ordering

- Valence-space IMSRG: modified decoupling yields *ab initio* shell-model interactions
- Freezing of nucleons in an inert core

$$\dim \mathcal{H}_A = \binom{\#\text{basis functions}}{A}$$

- Solve large-scale eigenvalue problem within an active space of limited size
- Example: spectroscopy of ^{48}Ca with ^{40}Ca core and neutron *pf* orbits as active space (green)

No-core: 48 particles in 2000 states

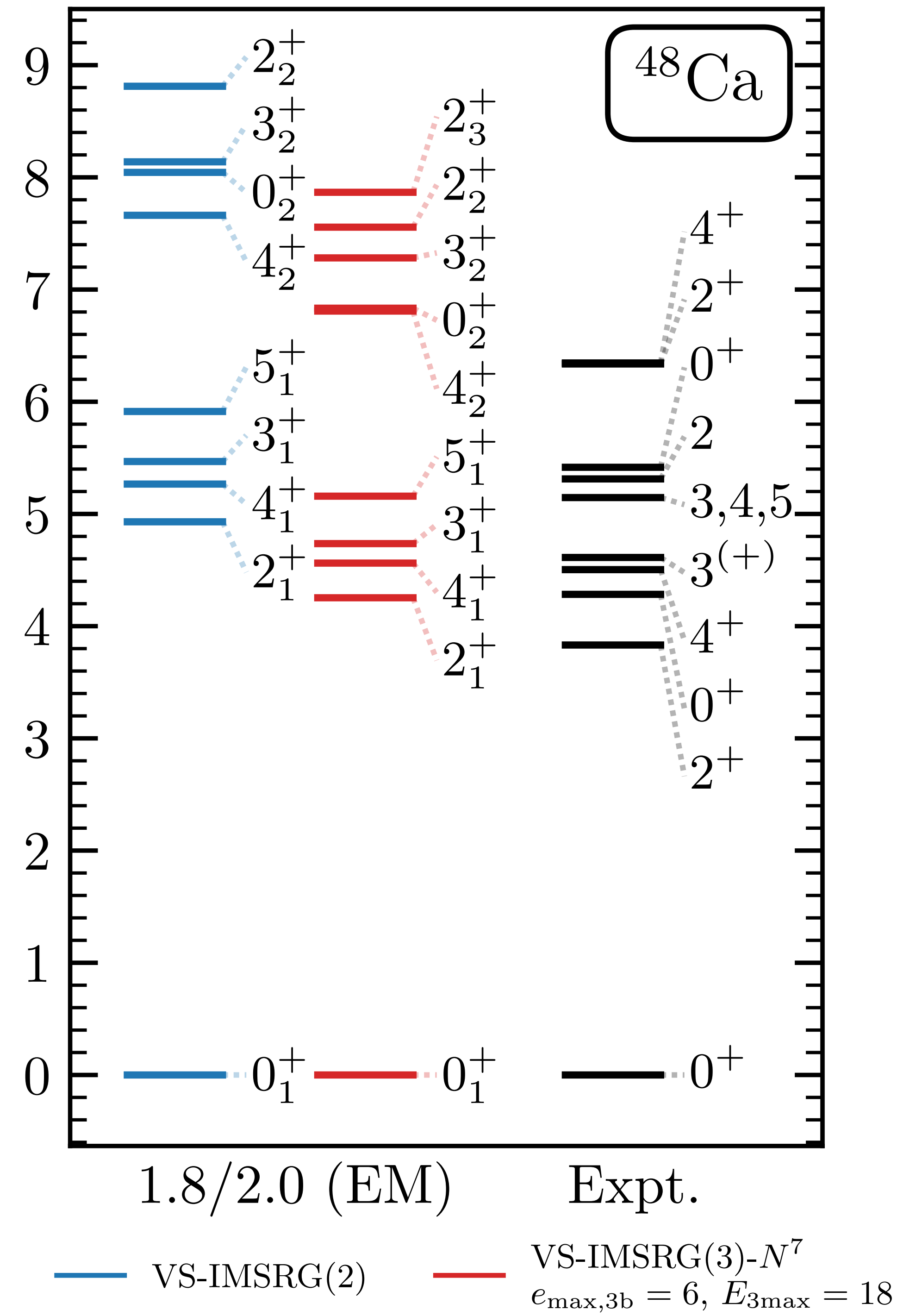
With core: 8 particles in 20 states

Precision simulations in calcium (Z=20)

Heinz, …, Tichai, arXiv:2411.16014

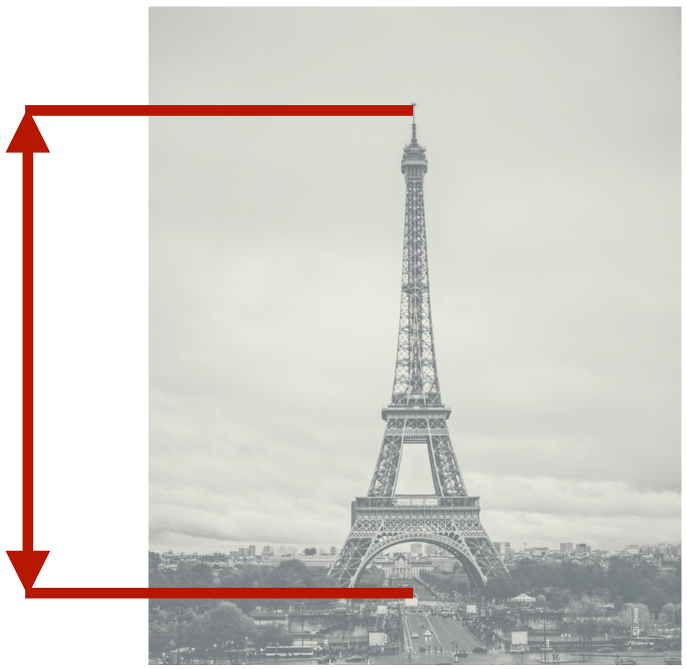
- Qualitative reproduction of experimental spectra in ^{48}Ca
- Inclusion of triples contributions from IMSRG(3) improve energies
- Shell closure at ^{48}Ca from large excitation energy of first 2^+ state
- Keep in mind: residual interaction uncertainty is not accounted for

But even the reduced active space can be too large!



Low-rank approximations

High-resolution picture



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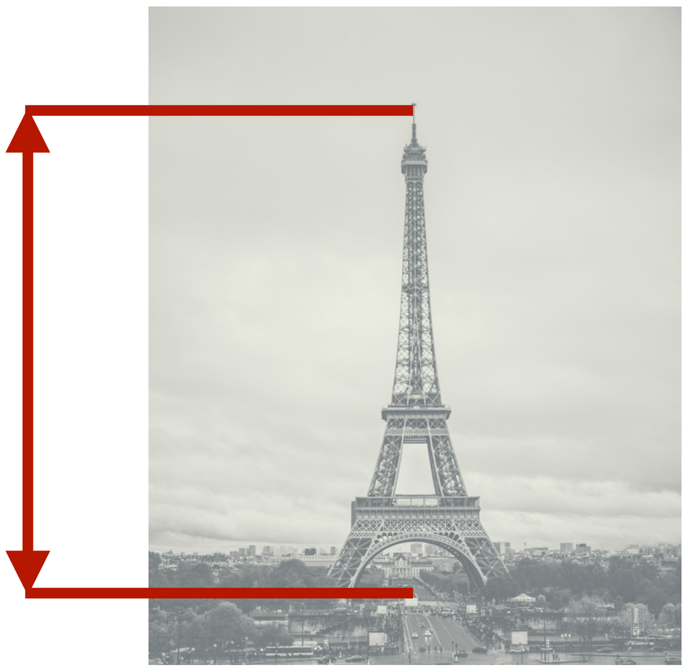


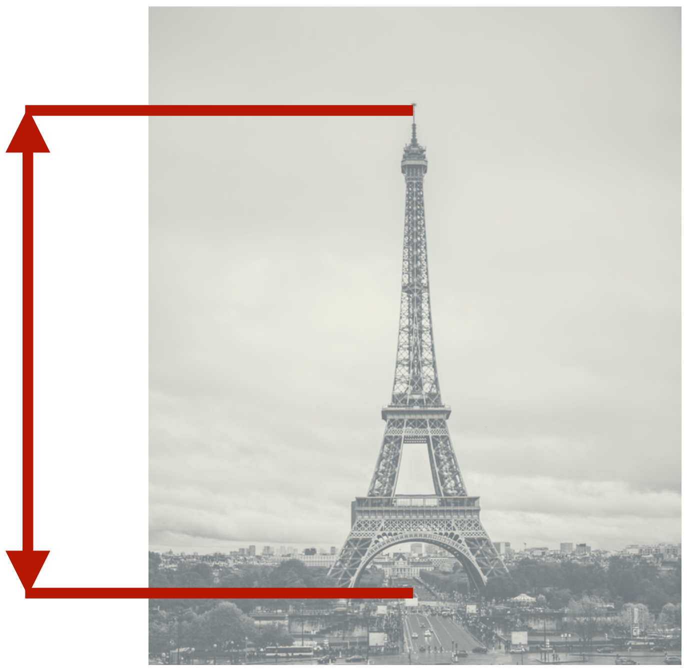
Removal of 97% of information!

('blurriness' induces uncertainty)

Low-resolution picture

Low-rank approximations

High-resolution picture



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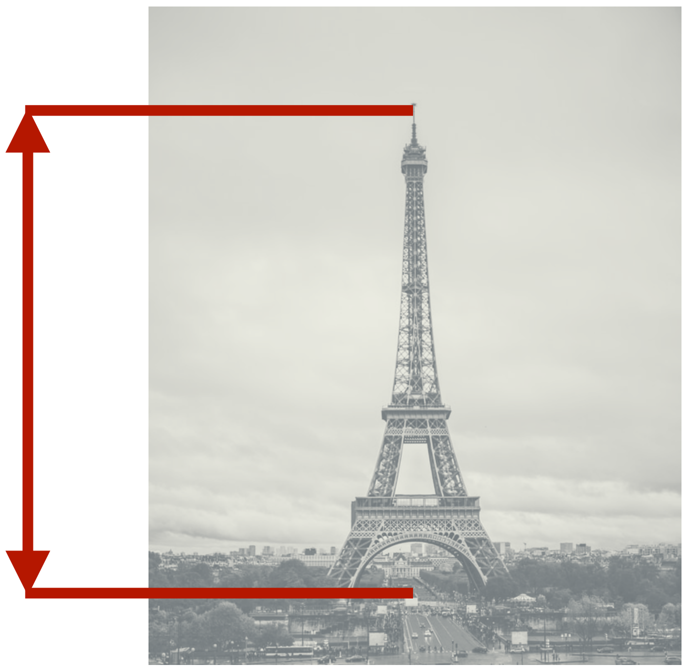
Low-resolution picture

Singular value decomposition (SVD)

$$M = L \cdot \Sigma \cdot R^\dagger$$

Low-rank approximations

High-resolution picture



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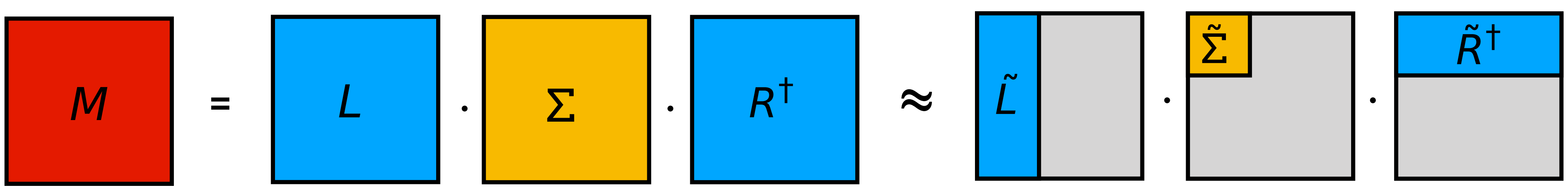

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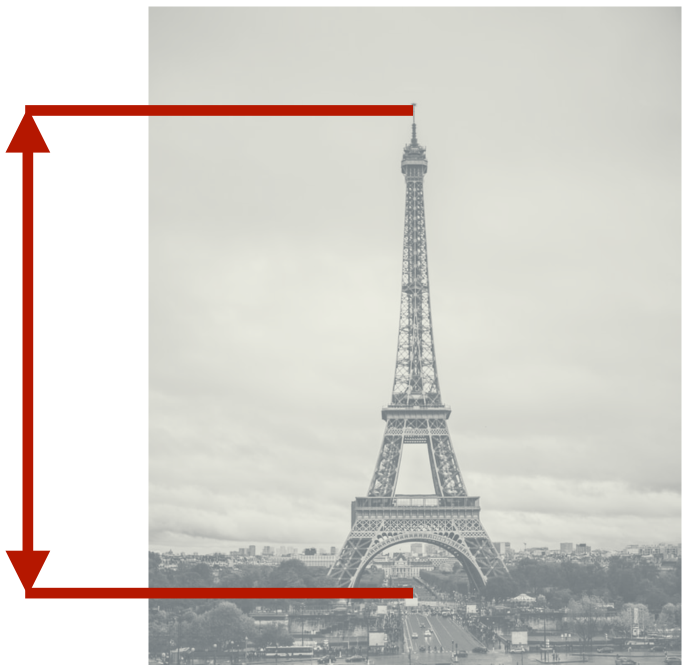

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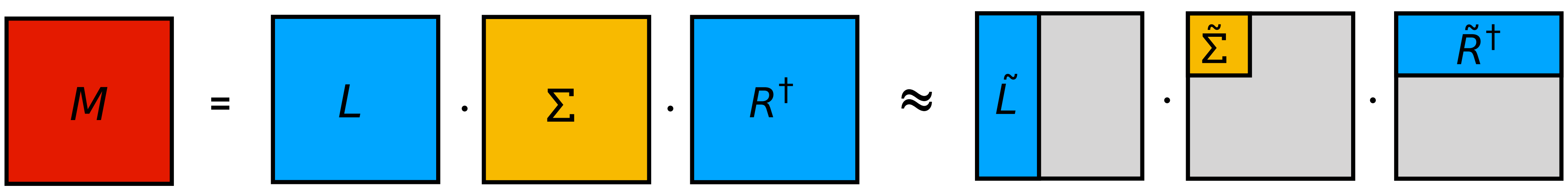
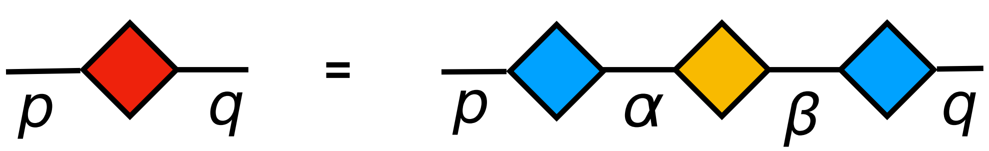


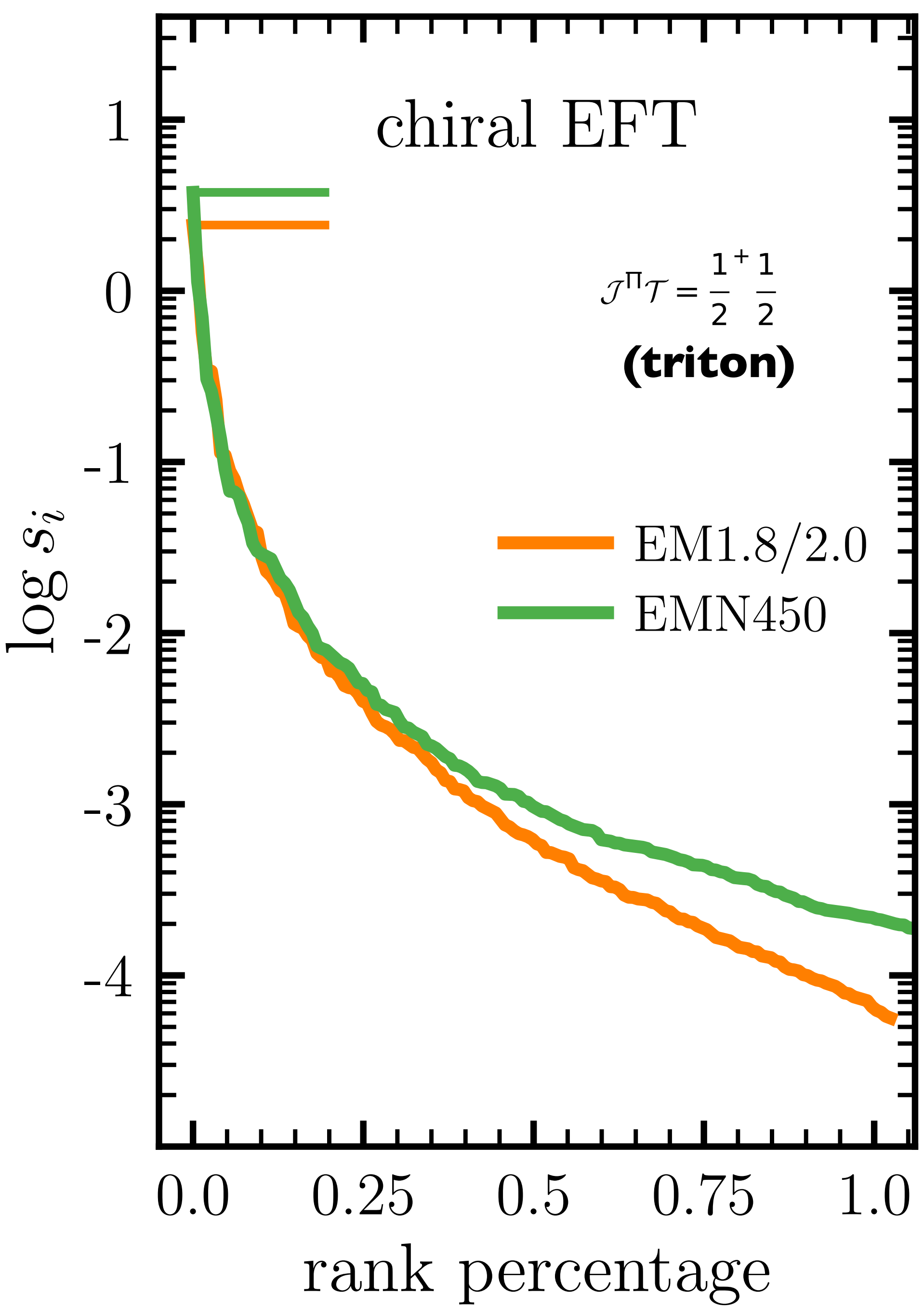
Tensor notation



$$M_{pq} = \sum_{\alpha\beta} L_{p\alpha} \Sigma_{\alpha\beta} R_{\beta q}$$

Low-rank interactions

Singular spectrum of three-body interaction



Tichai *et al.*, PRR (2024)

NN applications:
Tichai *et al.*, PRC (2019), EPJA(2019), PLB (2022), PRC(2023)
Zhu *et al.*, PRC (2022); Frosini *et al.* (2024)

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

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

- Very **few SVD components** needed

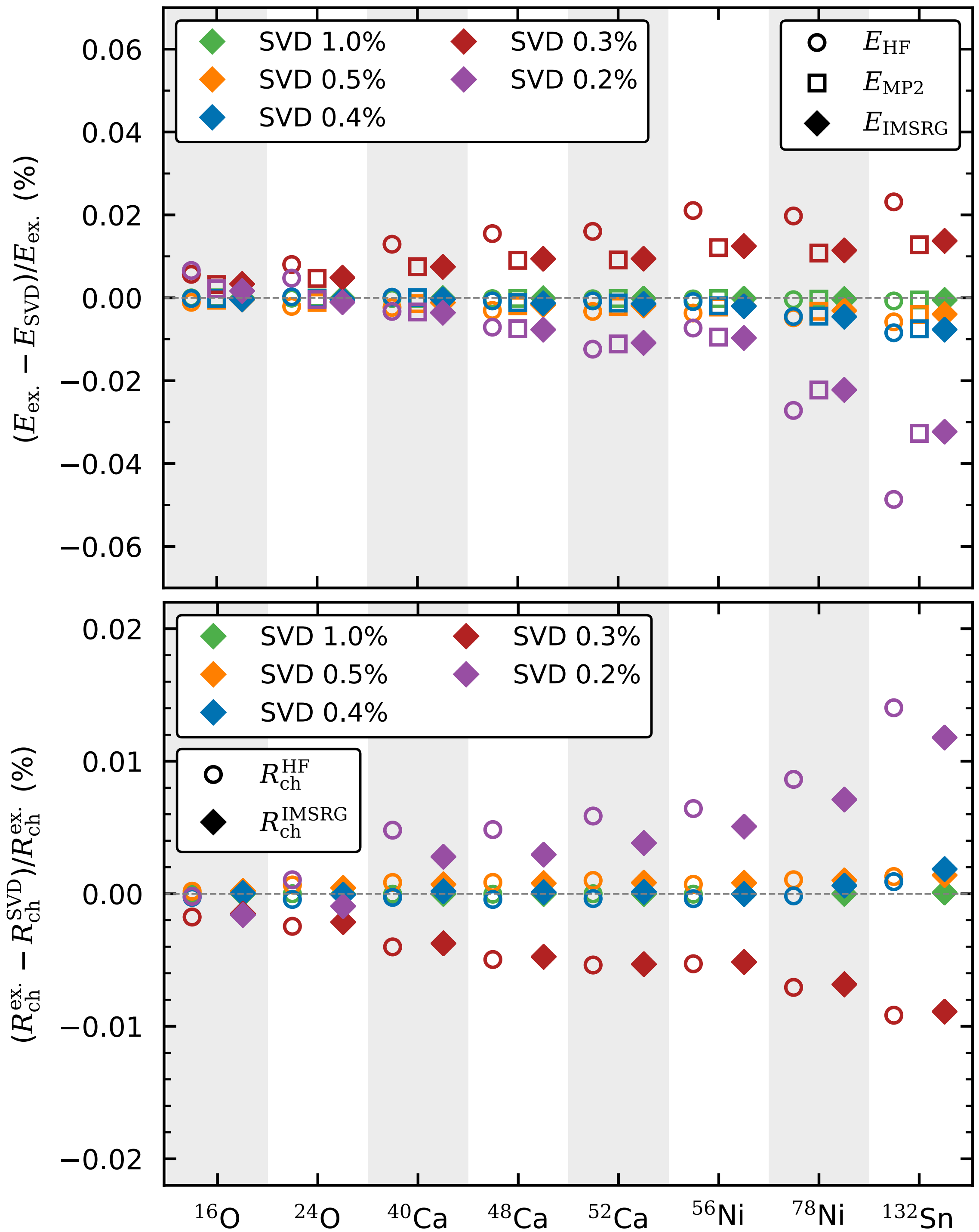
~100 out of 15.000

- Reminder: chiral EFT is built from **only ~20 parameters** (LECs)

Low-rank patterns:
Employed data representations is redundant.

Medium-mass nuclei

Ground-state observables for closed-shell nuclei

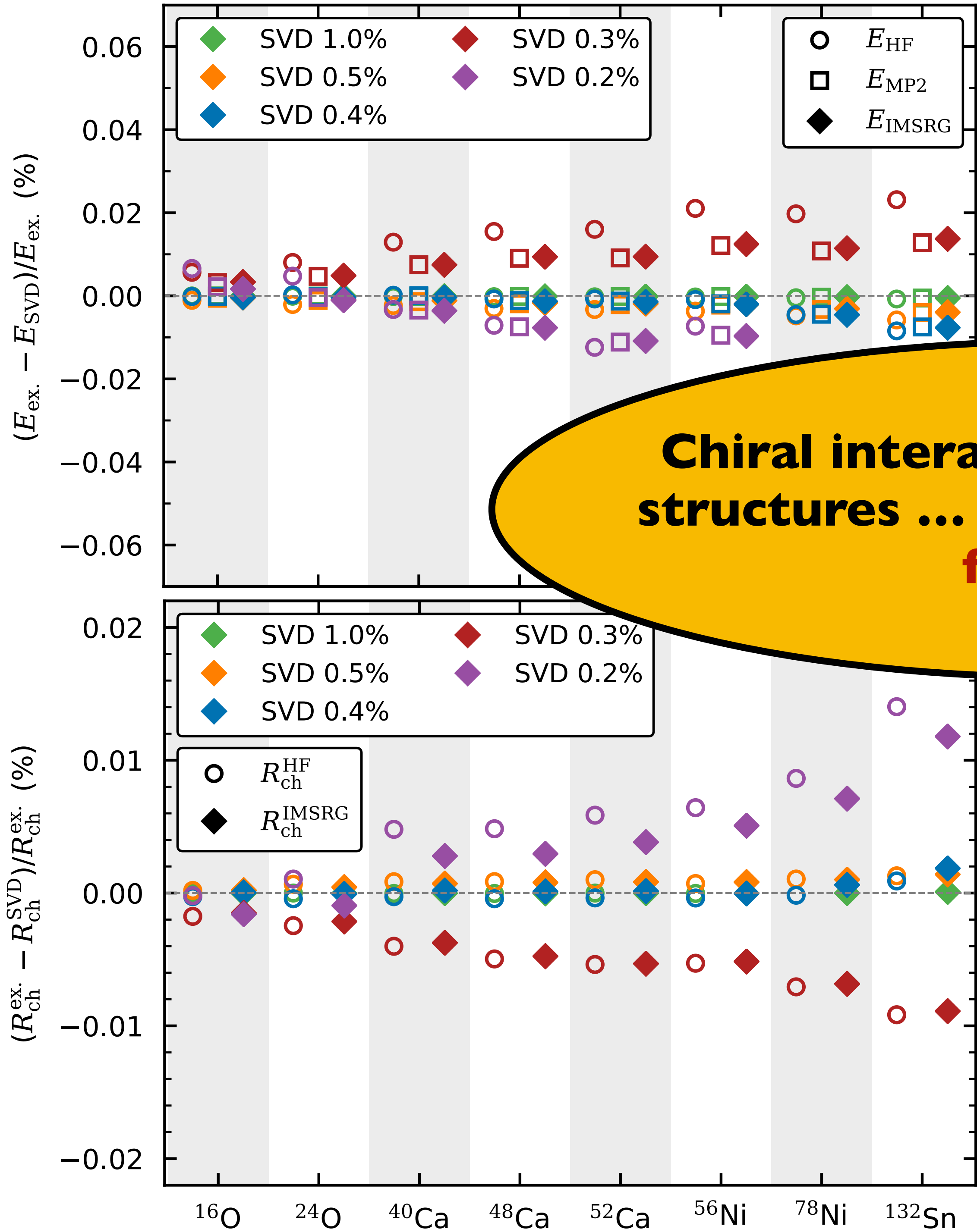


Tichai *et al.*, PRR (2025)

- 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!

Ground-state observables for closed-shell nuclei



Tichai *et al.*, PRR (2025)

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

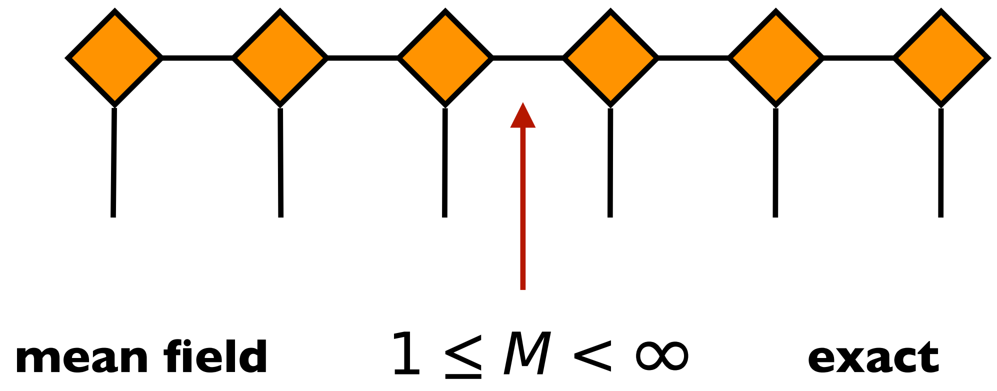
Chiral interaction have low-rank structures … what about the wave function?

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

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)

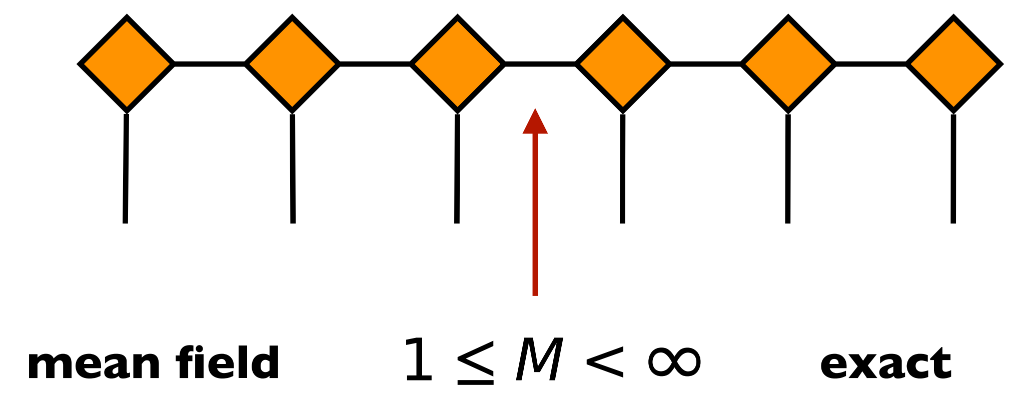


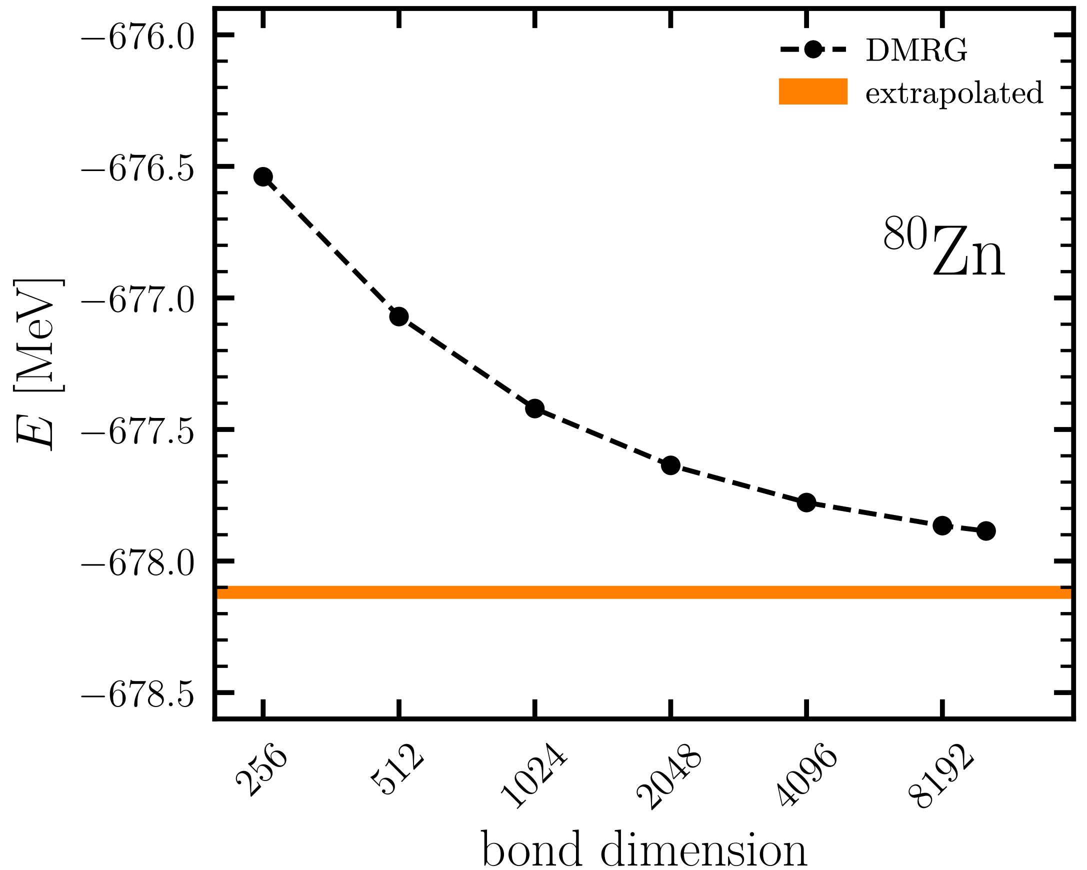
Nuclear tensor networks

- **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)

- **Systematically improvable by increasing the bond dimension *M***

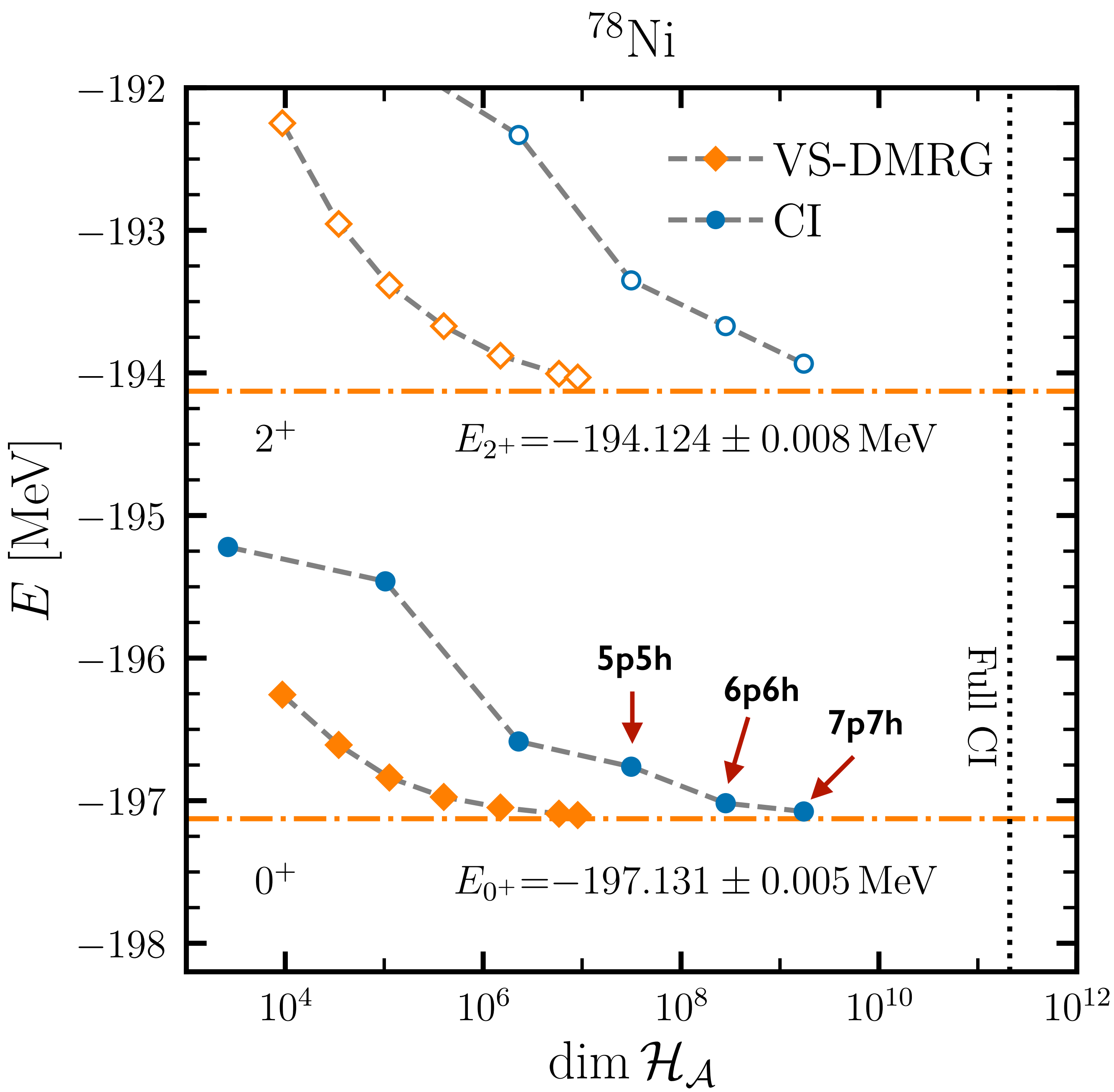




Tichai *et al.*, PLB (2024)

^{78}Ni: Why DMRG?

Energies vs. dimension of Hilbert space



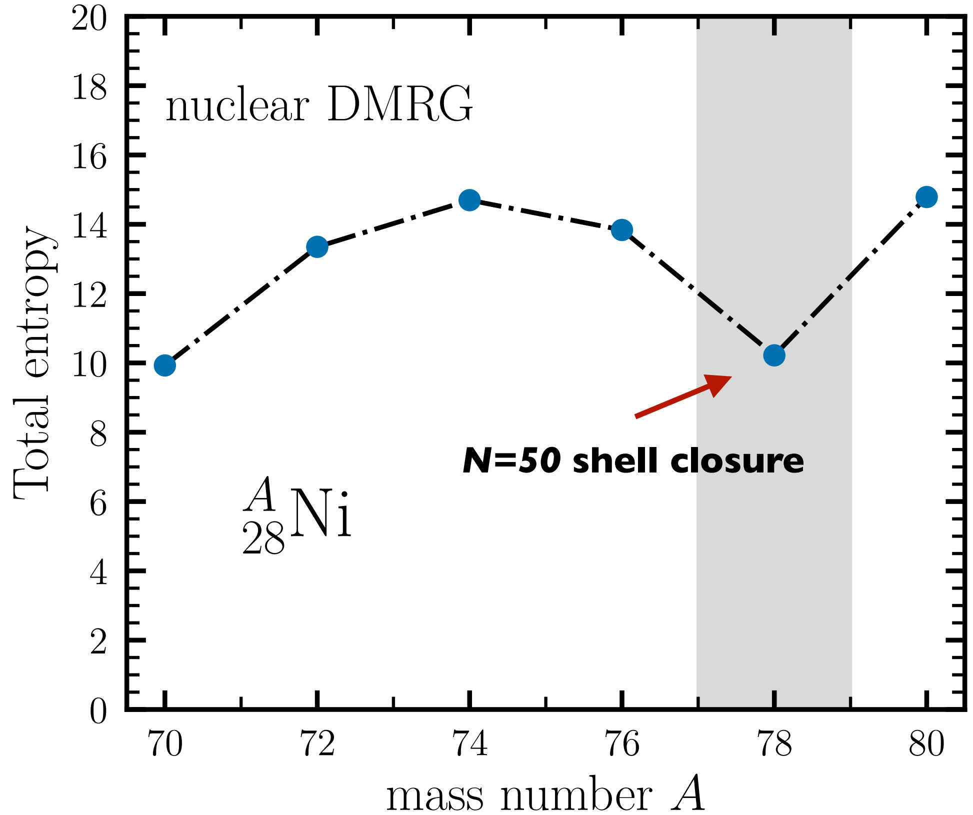
Tichai *et al.*, PLB (2023)

- **DMRG: economic representation of the many-body wave function**
- **Tensor networks select the important part of Hilbert space**
- **Robust convergence of DMRG energies at large bond dimension**
- **CI extrapolation: 2+ state exhibits linear convergence pattern**

Quantifying entanglement

Tichai *et al.*, PLB (2023)

see also Taniuchi *et al.*, Nature (2019)



- **Entanglement through information science**

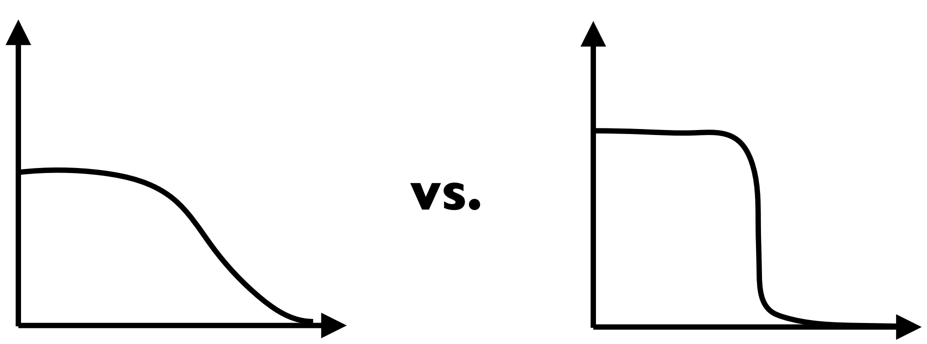
$$s_i = -[n_i \log n_i + \bar{n}_i \log \bar{n}_i]$$

n_i: occupation number

- **Total entropy quantifies entanglement**

$$I_{\text{tot}} = \sum_i s_i$$

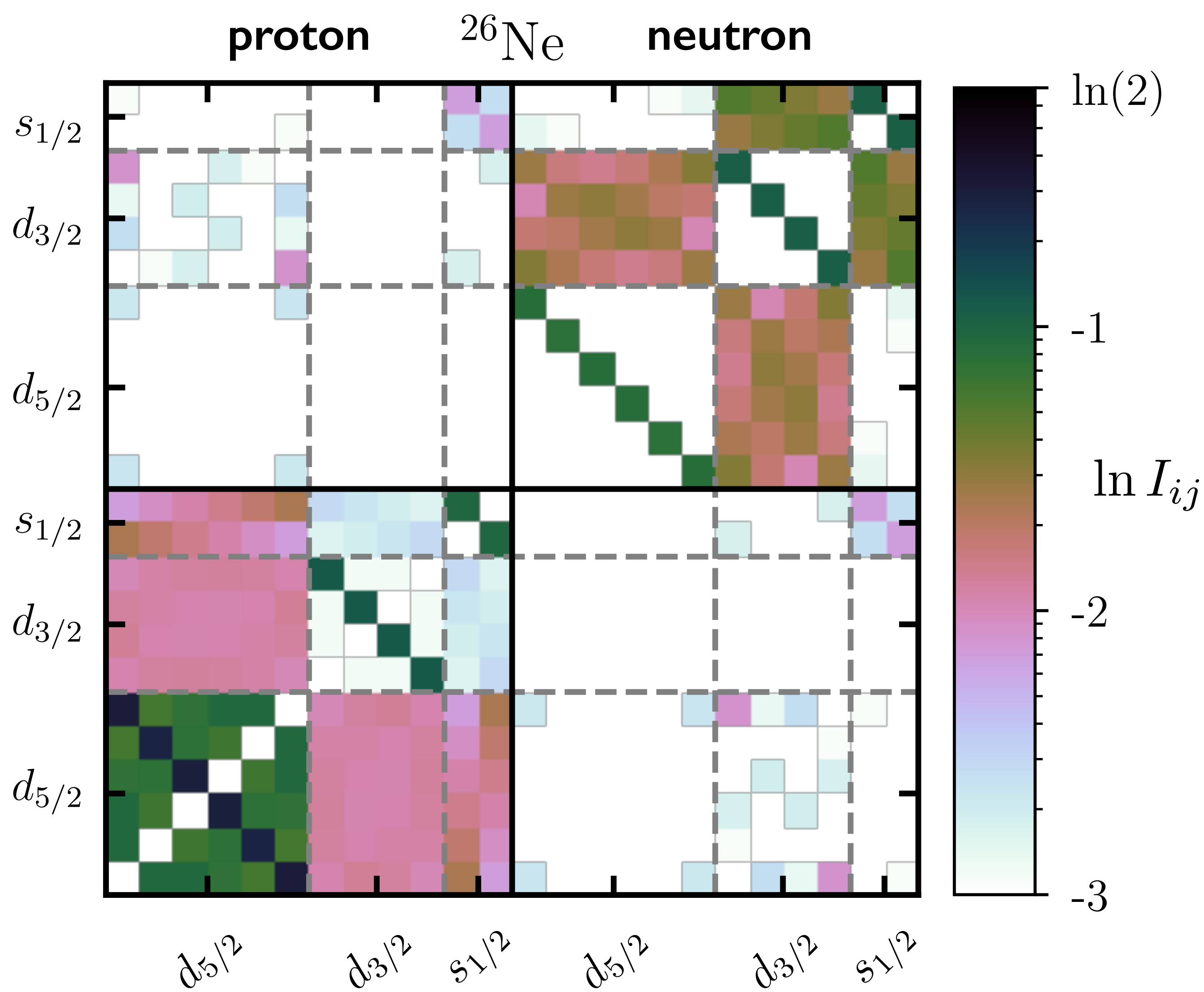
- **Kink at ^{78}Ni hints at neutron shell closure**



Different occupation profiles

Phenomenology through eyes of information theory

Many-body correlations



Tichai *et al.*, PLB (2023)

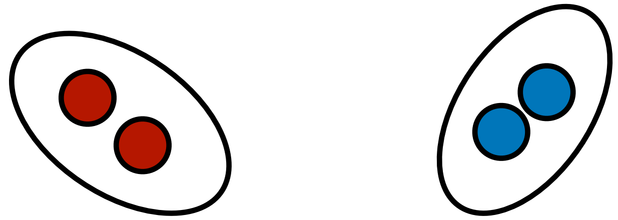
- Mutual information: pairwise correlations among orbitals

Two-body density matrix

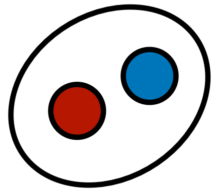
- Superfluidity: clear signals of BCS-type *n*-*n* and *p*-*p* correlations

Time-reversed pairs

$|nljmt\rangle \quad \longleftrightarrow \quad |nlj(-m)t\rangle$



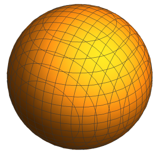
- Suppression of *n*-*p* correlations



Intermezzo: Nuclear deformation

- Closed-shell nuclei with N/Z = 8, 20, 28, 50,… have spherical shapes

Spherical



$\beta = 0$

Intermezzo: Nuclear deformation

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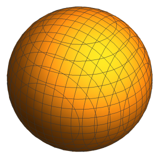
- Mass-independent deformation parameter

$$\beta \sim \frac{\langle Q_{20} \rangle}{R^2 A} \qquad \frac{r_x}{r_z} = 1 + \beta$$

(difference in semi axis of ellipsoid)

Spherical



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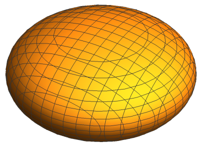
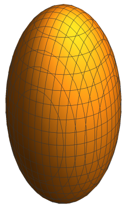
Axial deformation



$\beta < 0$



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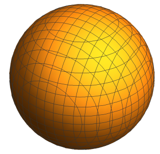
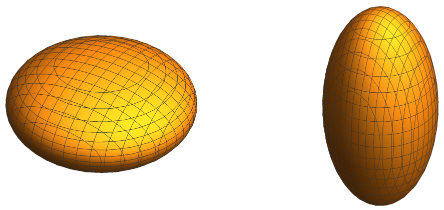
$$E_J \sim J(J+1)$$

Spherical

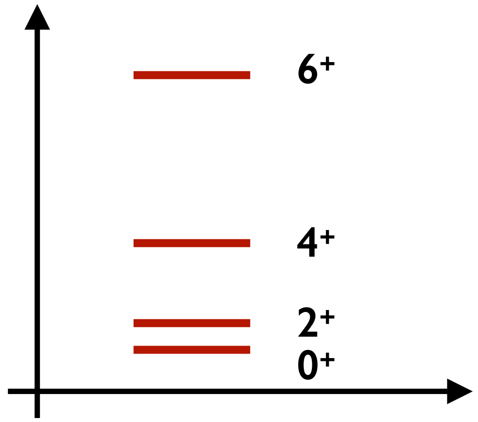


***β* = 0**

Axial deformation



***β* < 0** ***β* > 0**



rotational band (‘*yrast*’)

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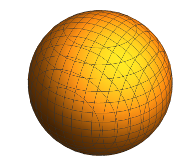
- Increased electromagnetic transitions within rotational band: B(E2) strengths

Spherical



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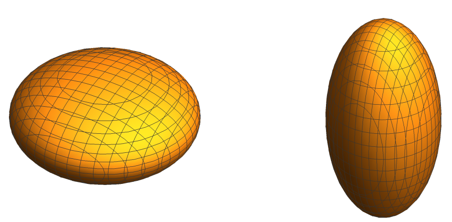
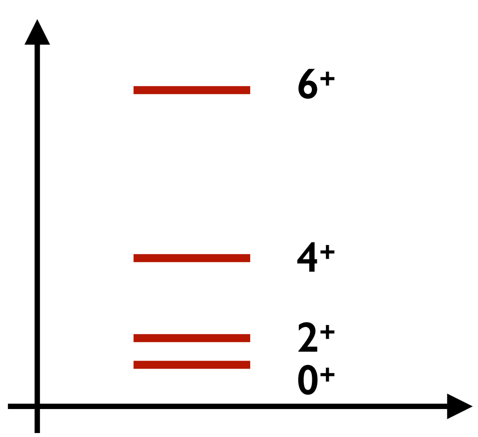
Axial deformation



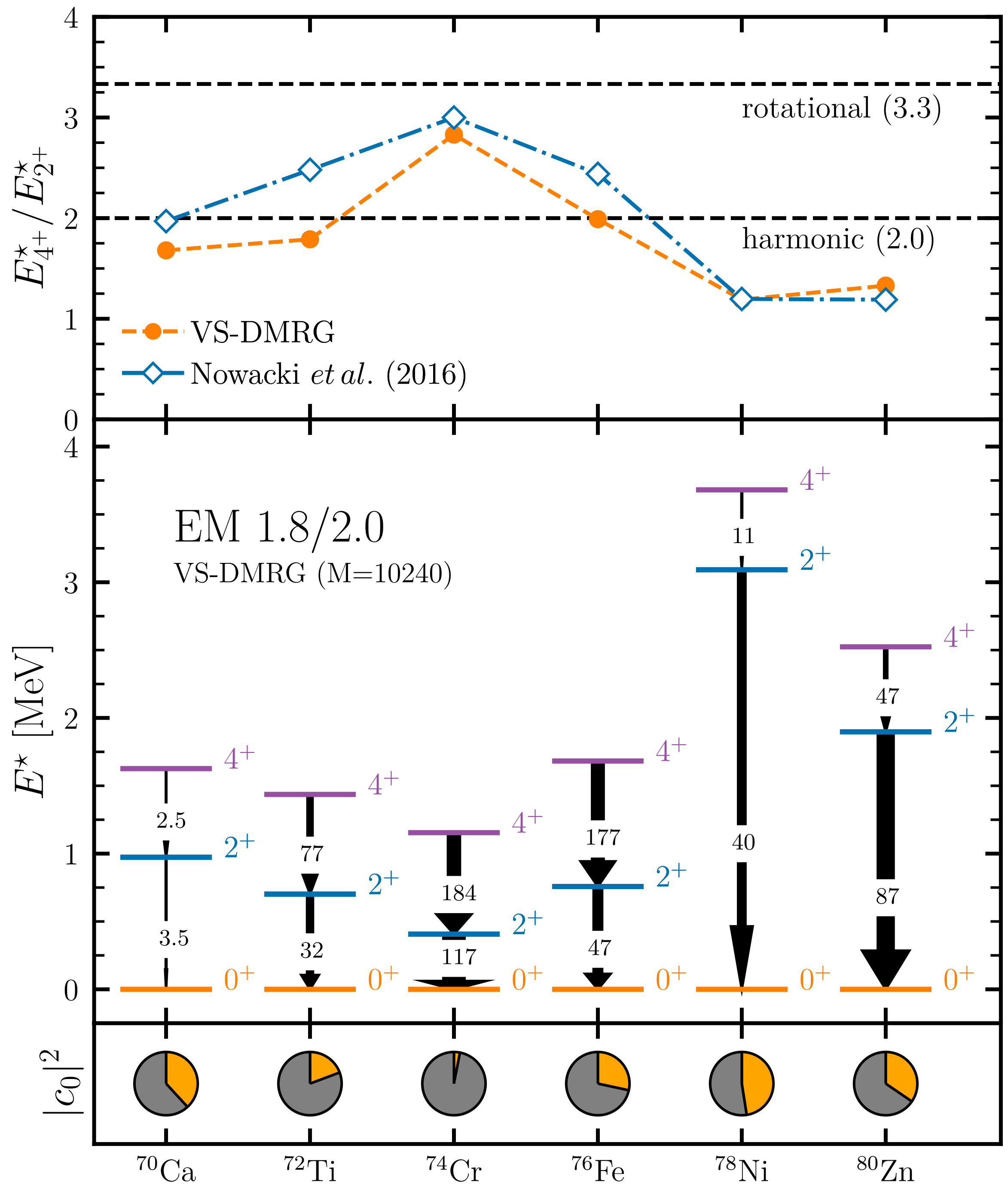
$\beta < 0$ $\beta > 0$



rotational band (‘*yrast*’)

Transitional nuclei at *N*=50

Spectroscopy of *N*=50 isotones



Tichai *et al.*, PLB (2024)

- **Onset of nuclear deformation**

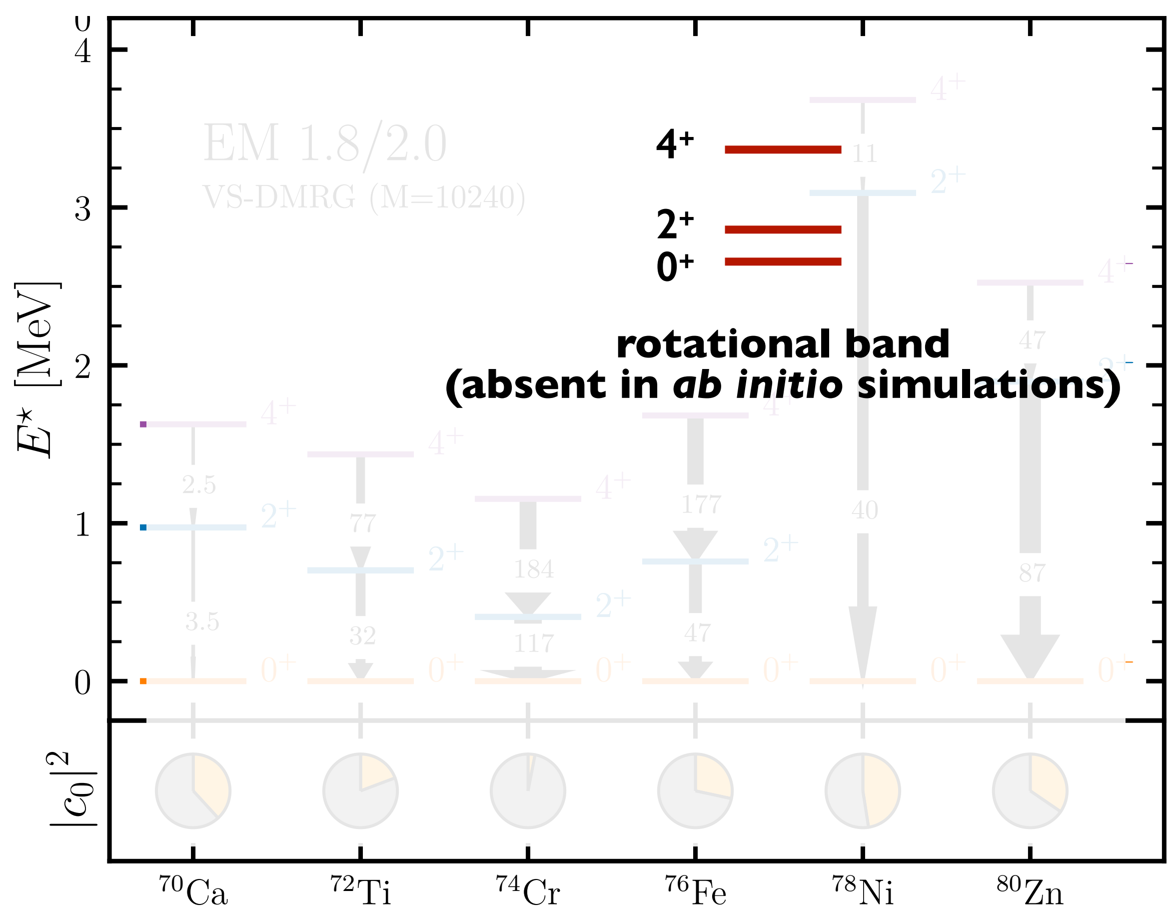
$$E^\star_{\text{rot}} \sim J(J+1) \qquad R_{42} = 10/3$$

- **Rapid transition between single-particle-like and collective excitations**

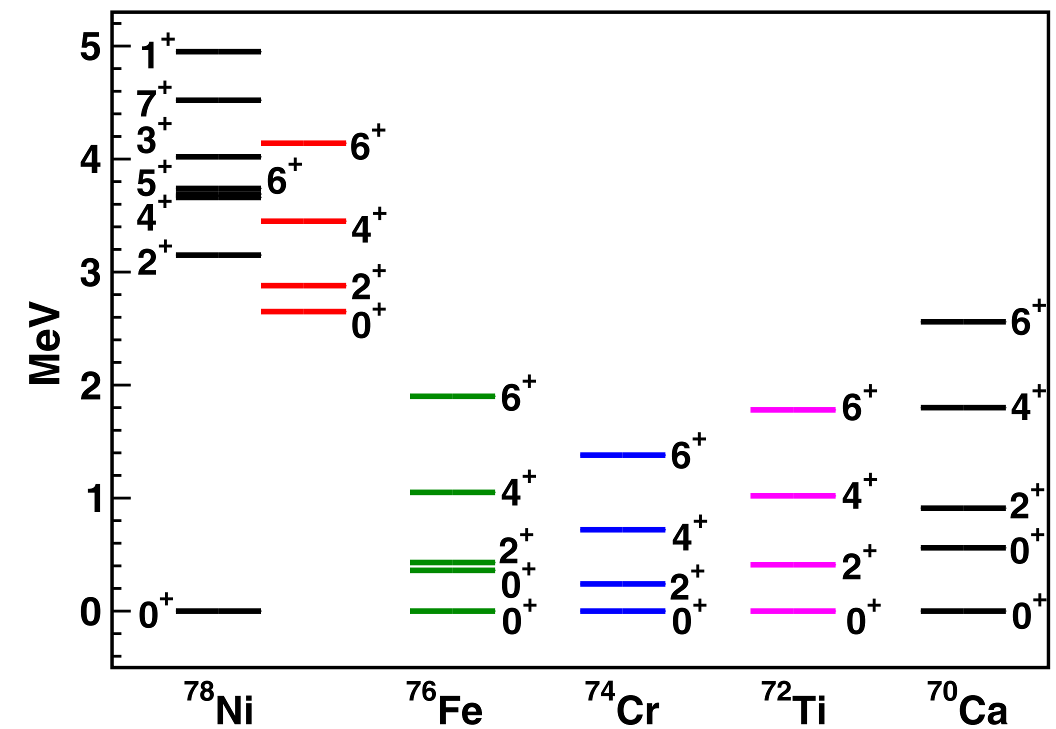
- **Qualitative agreement with previous shell-model calculations**
  Nowacki *et al.*, PRL (2016)

- **Spectroscopy: DMRG extended to electromagnetic transitions**

Transitional nuclei at *N*=50



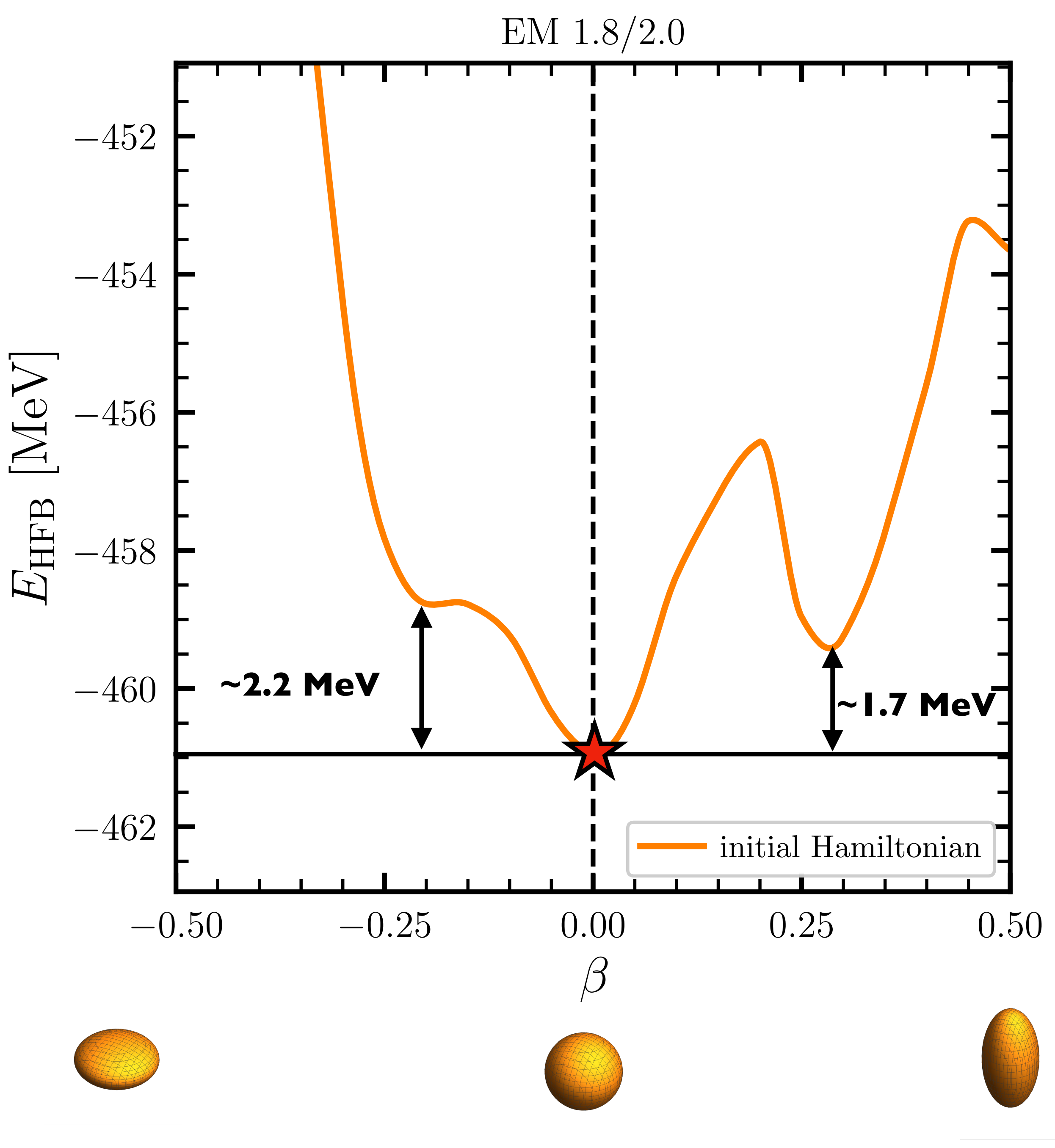
Tichai *et al.*, PLB (2024)



Nowacki *et al.*, PRL (2016)

Where is the excited rotational band?

Intrinsic structure of ^{78}Ni



- **Potential energy surface (PES) from Hartree-Fock-Bogoliubov calculation**

$$H - \lambda \cdot (Q_{20} - \langle Q_{20} \rangle)$$

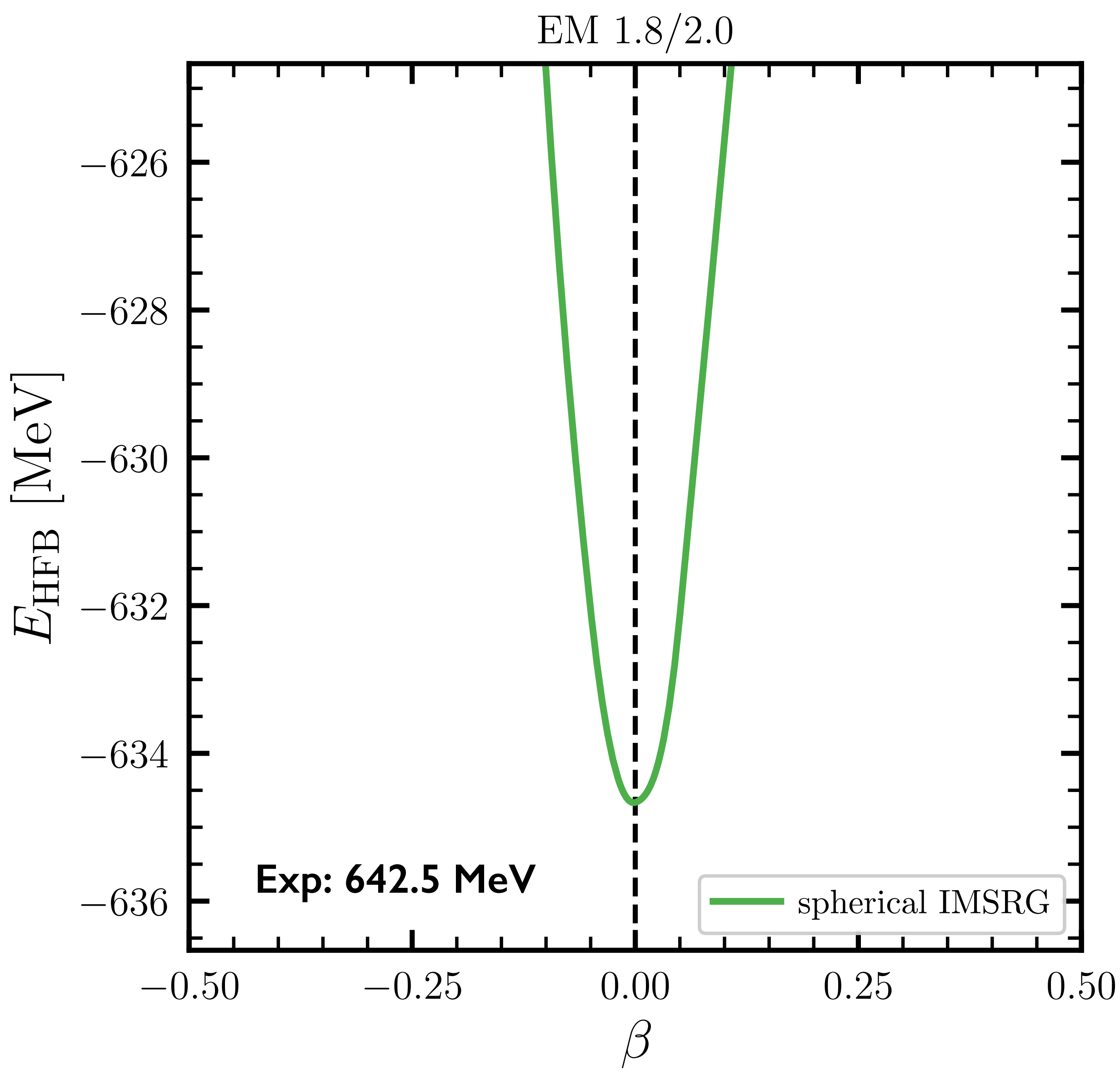
- **PES: energy as function of deformation**

$$E_{\mathrm{HFB}}(\beta)$$

- **HFB ground state breaks rotational symmetry and particle number**
- **Coexisting minimum for prolate shape**

Chiral interactions admit for deformed shapes!

Future challenges



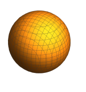
- Improvement of **bulk properties:** ground-state energy

Particle-hole correlations
(generates ~200 MeV binding)

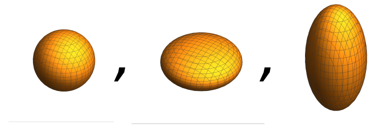
- IMSRG **destroys all intrinsic structure** of the wave function

Rotational band is gone!

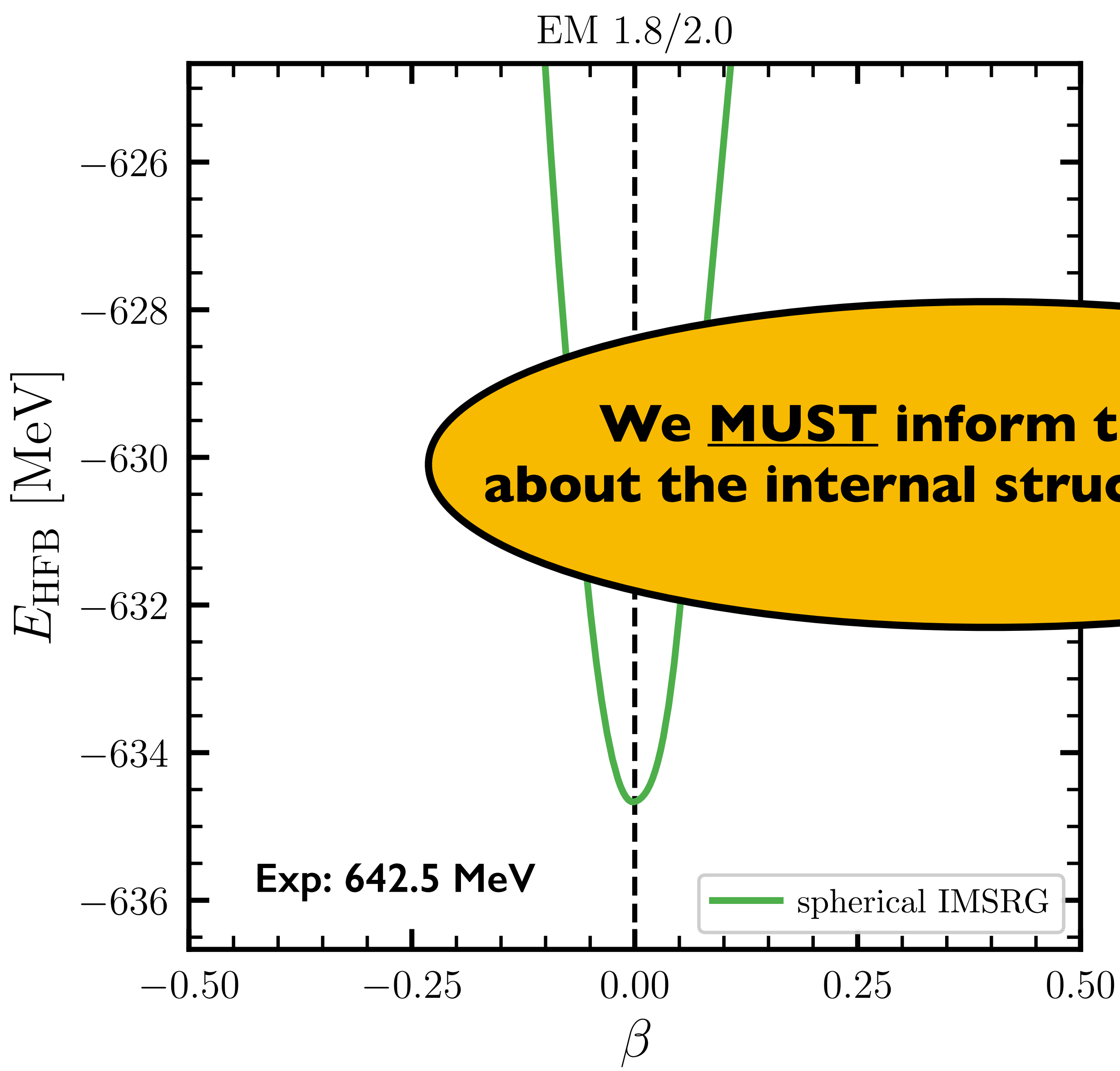
- Current IMSRG formulations:

$H_{\mathrm{IMSRG}} = f(H_{\mathrm{nucl}},$  $)$

- Next generation of IMSRG:

$H_{\mathrm{IMSRG}} = f(H_{\mathrm{nucl}},$  $, \ldots)$

Future challenges



We MUST inform the IMSRG about the internal structure (shapes)!

- Improvement of bulk properties: ground-state energy

  Particle-hole correlations
  (generates ~200 MeV binding)

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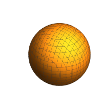
  $H_{\text{IMSRG}} = f(H_{\text{nucl}},$  $)$

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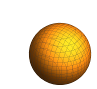
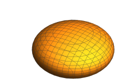
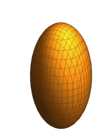
  $H_{\text{IMSRG}} = f(H_{\text{nucl}},$ , ,  $, \ldots)$

Conclusion and outlook

First-principles description of atomic nuclei

- Modern interactions via effective field theory: rooted in QCD
- Progress in many-body theory enables heavier and exotic systems
- Quantification of theory uncertainties: interaction + many-body

Major goal: controlled descriptions of structurally complex systems

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Novel frameworks in nuclear many-body theory

- Low-rank properties present in chiral interactions
- Tensor networks leverage factorized form of wave function
- Importance of nuclear deformation in open-shell nuclei

Science opportunity: link nuclear theory to heavy-ion collisions