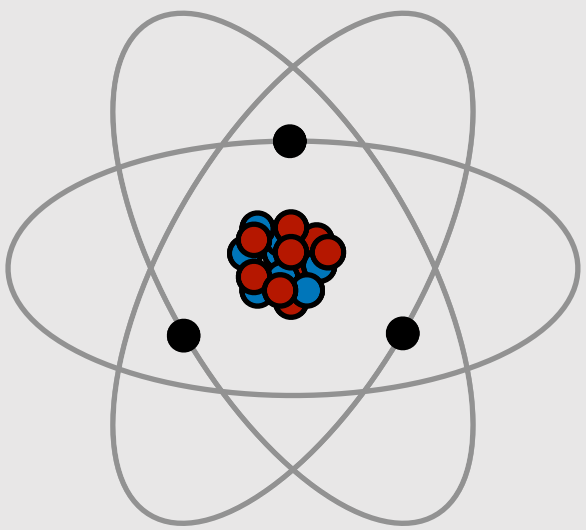
‘From Few to Many’
Recent advances in *ab initio* nuclear structure calculations

EFB25

European conference on few-body problems in physics

August 2nd, 2023



Alexander Tichai

Technische Universität Darmstadt

TECHNISCHE UNIVERSITÄT DARMSTADT

European Research Council
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SFB 1245

Scope of the talk

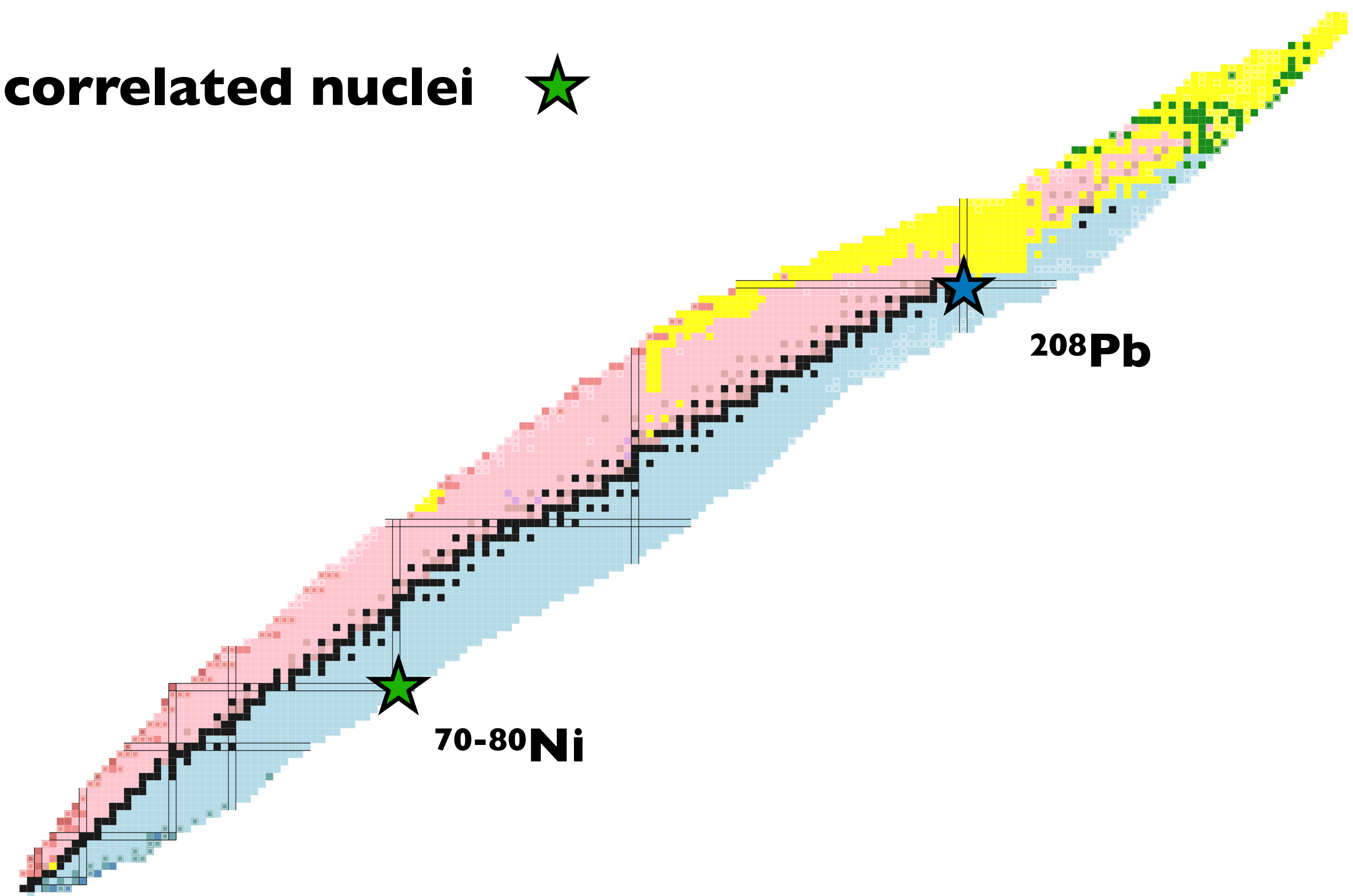
Status quo of *ab initio* nuclear structure

The road to heavy nuclei ★

Unveiling the complexity of chiral interactions

Perspectives on strongly correlated nuclei ★

Conclusions



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Status quo of *ab initio* nuclear structure

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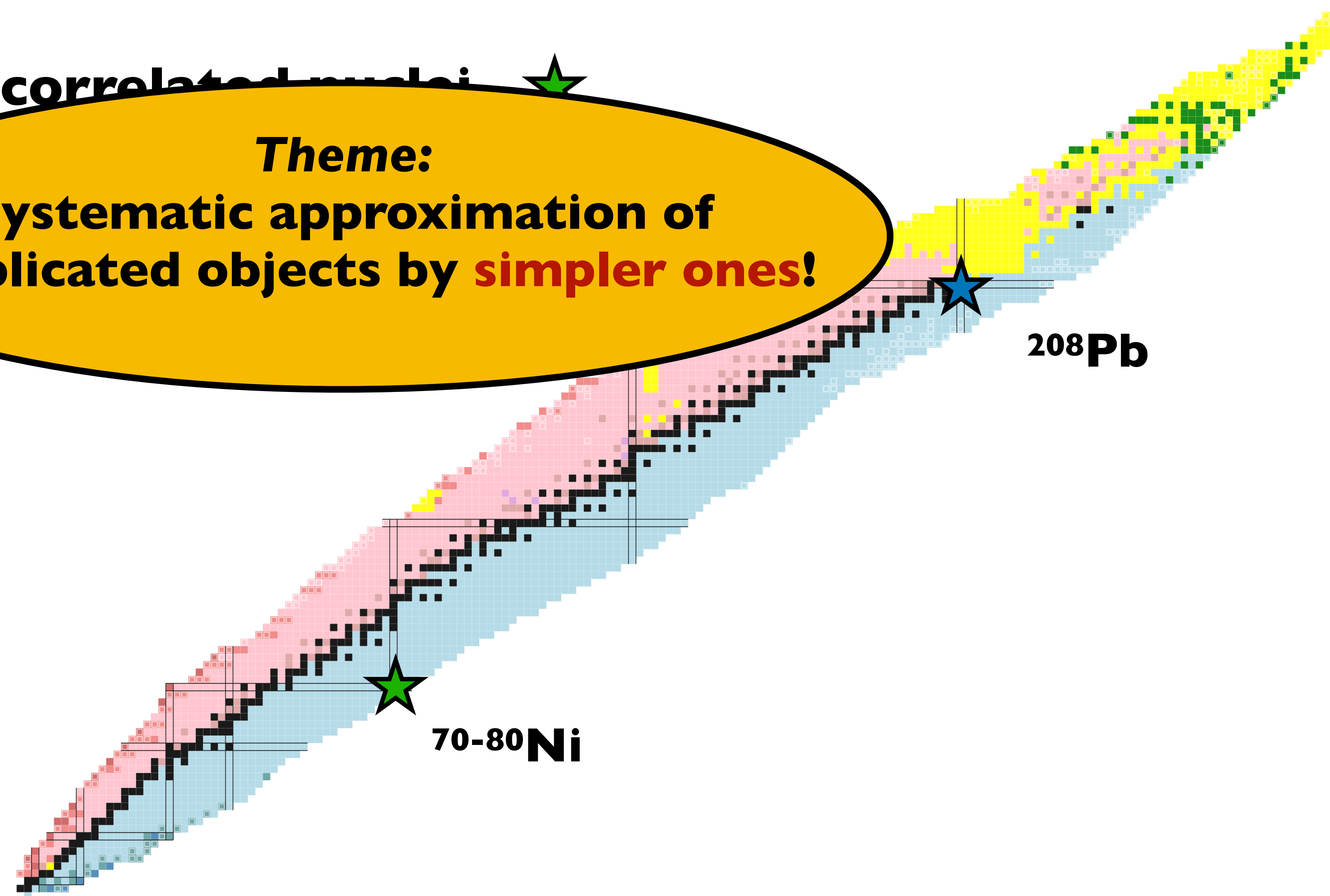
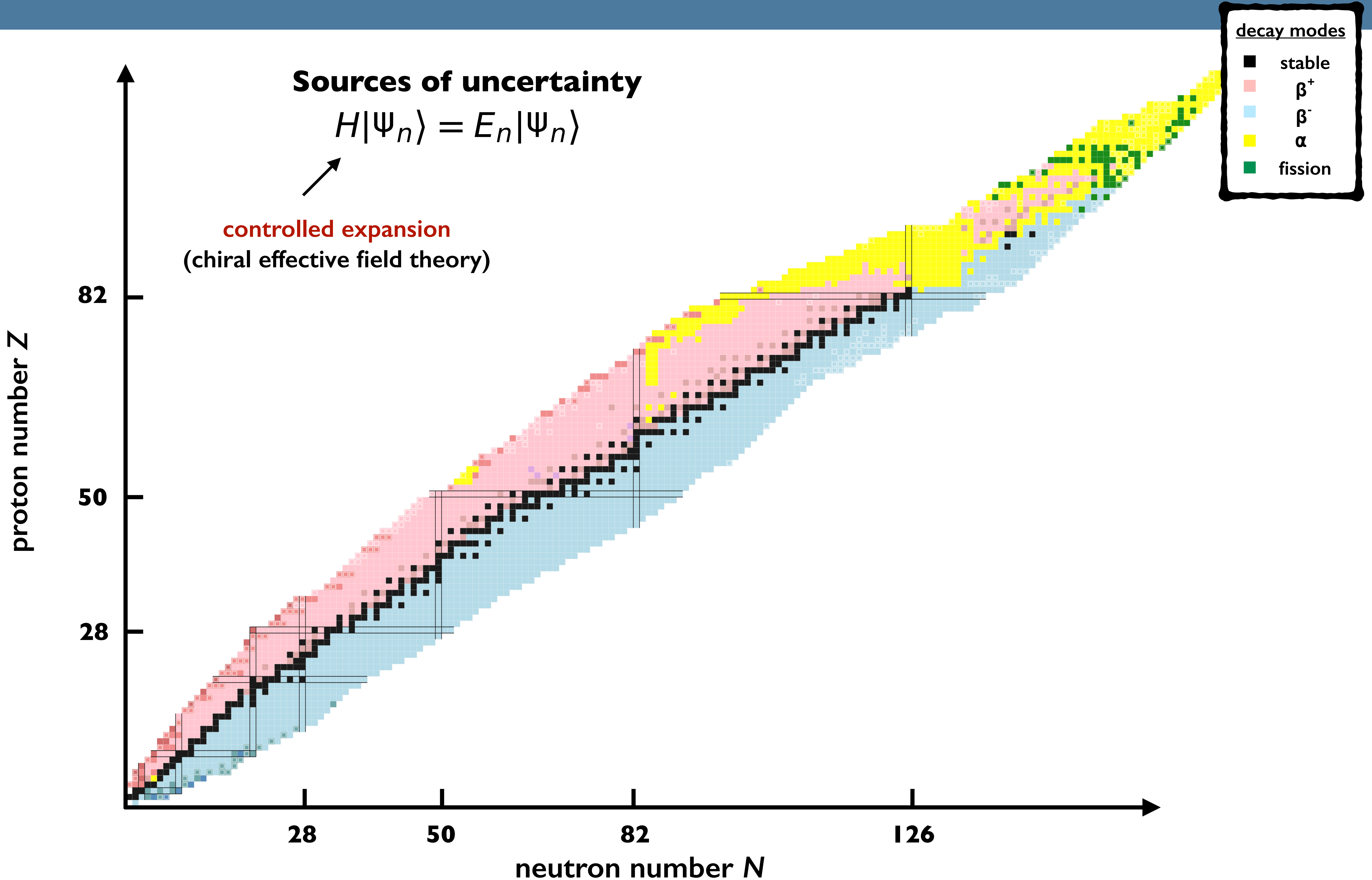
Conclusions

Theme:
Systematic approximation of complicated objects by simpler ones!



What is *ab initio* nuclear structure?



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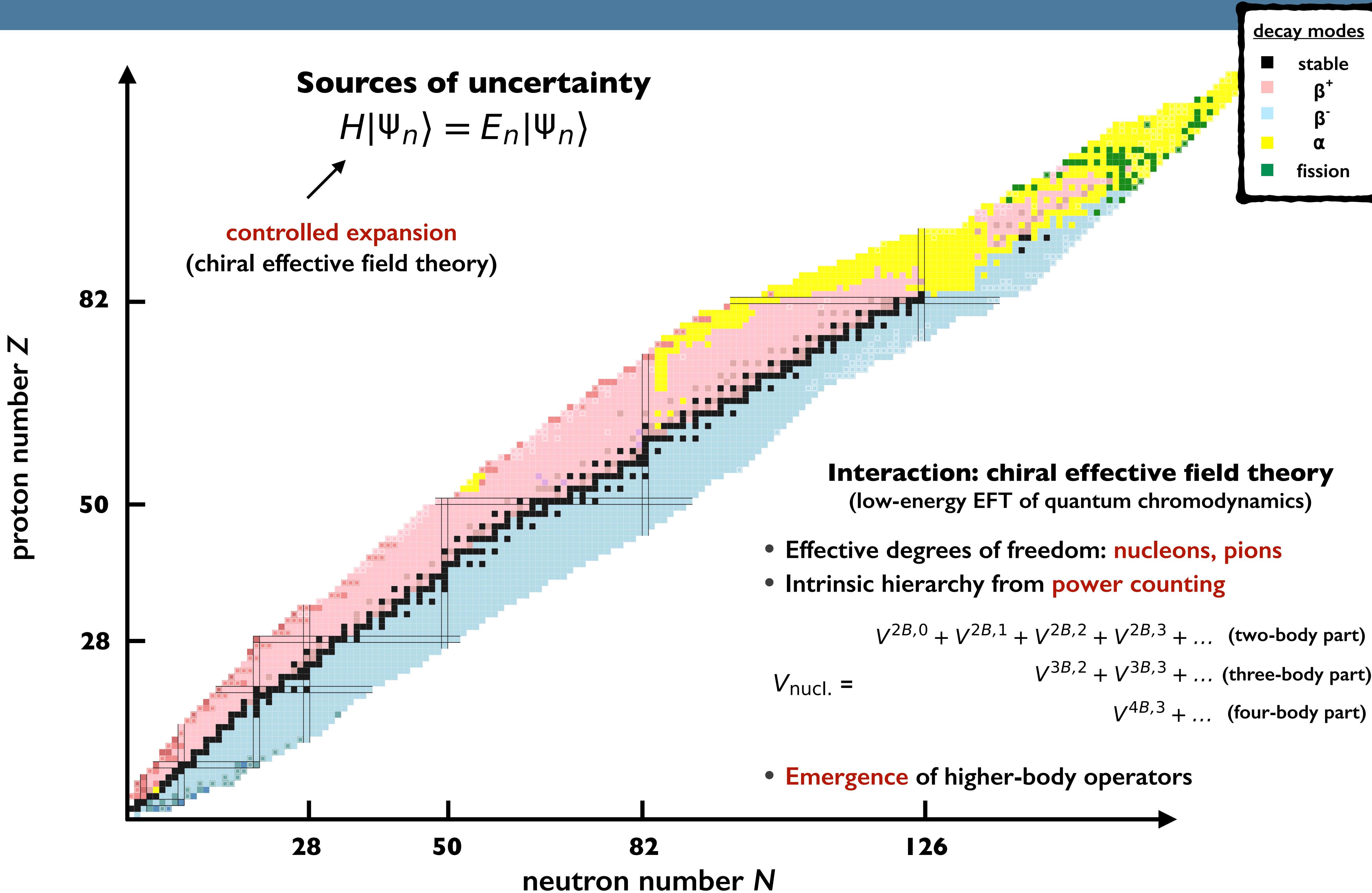

Sources of uncertainty

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

controlled expansion
(chiral effective field theory)

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

- Effective degrees of freedom: nucleons, pions
- Intrinsic hierarchy from power counting

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

- Emergence of higher-body operators

What is *ab initio* nuclear structure?

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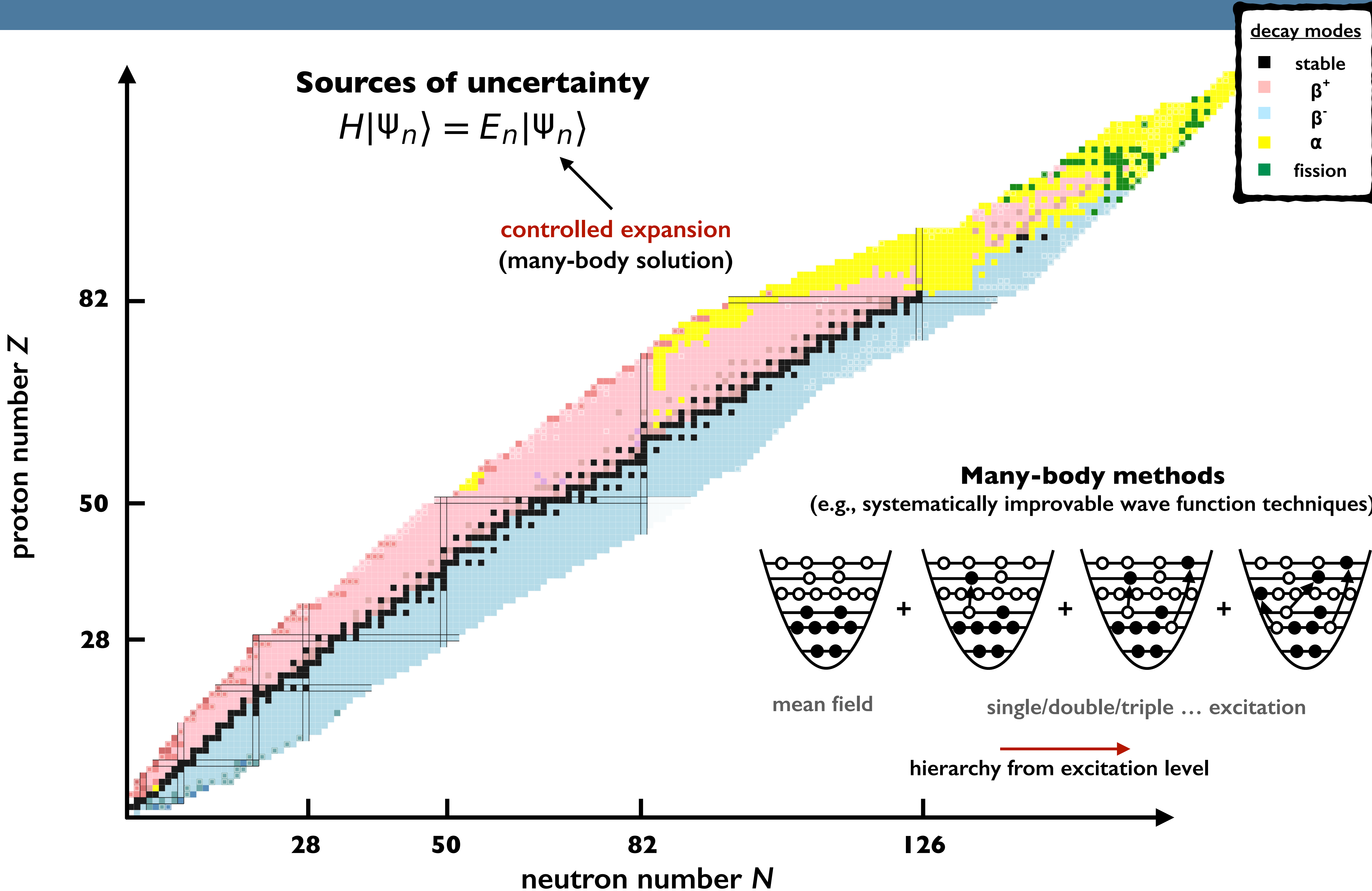
(many-body solution)



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

mean field

single/double/triple … excitation

hierarchy from excitation level

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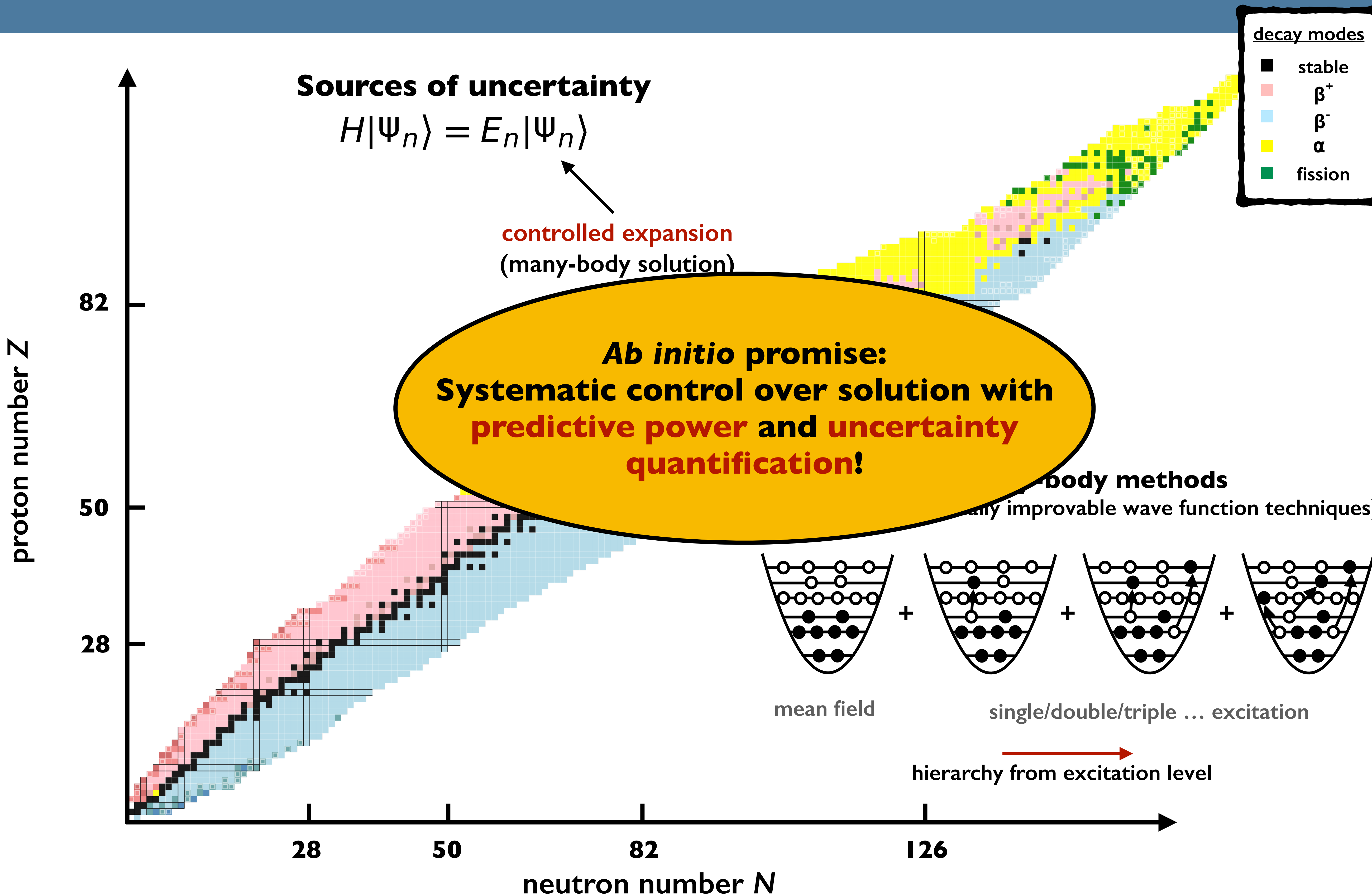

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***Ab initio* promise:**
Systematic control over solution with predictive power and uncertainty quantification!

…-body methods
(…ally improvable wave function techniques)

mean field

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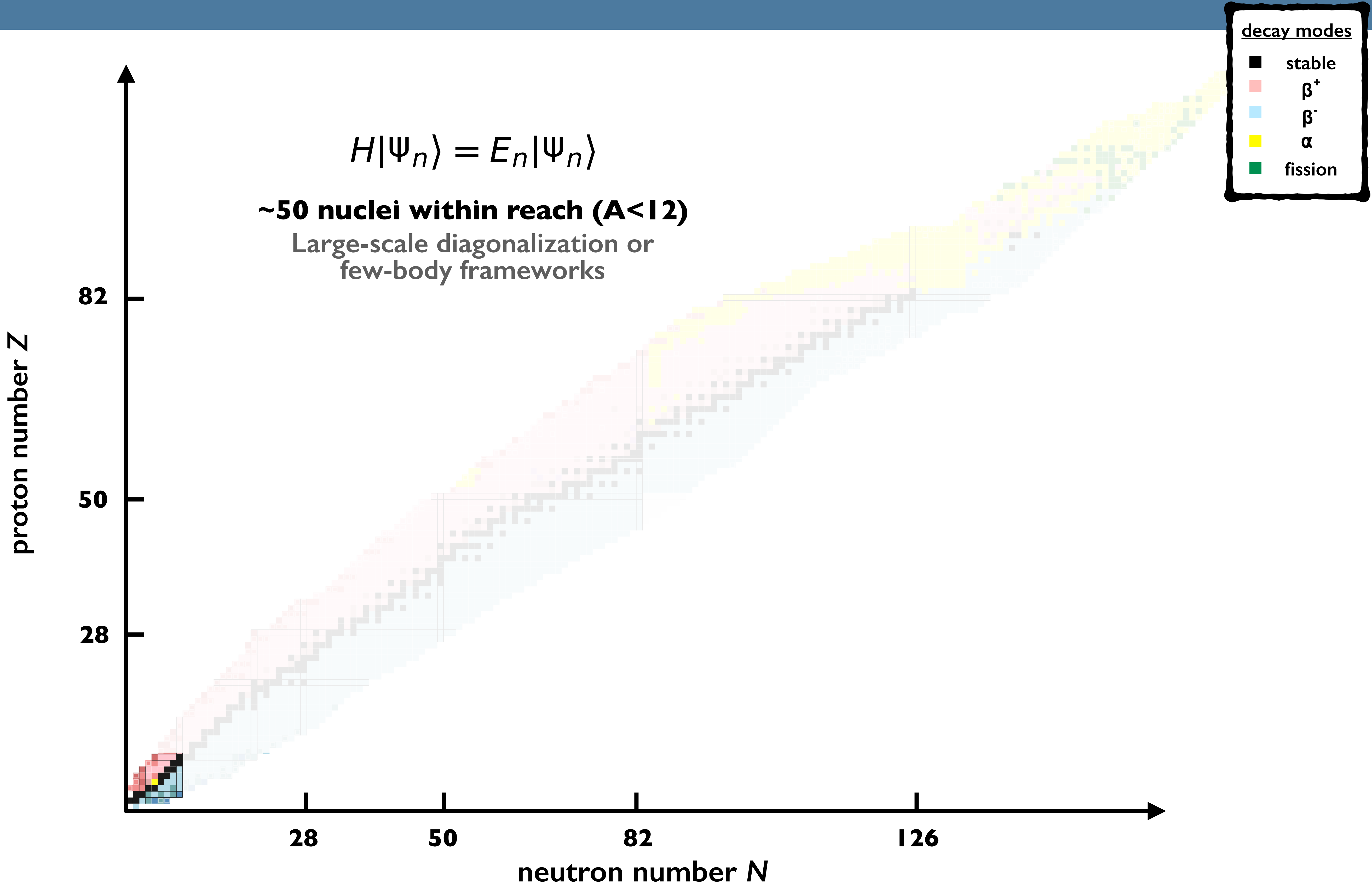
hierarchy from excitation level

Ab initio in the early 2000's ...

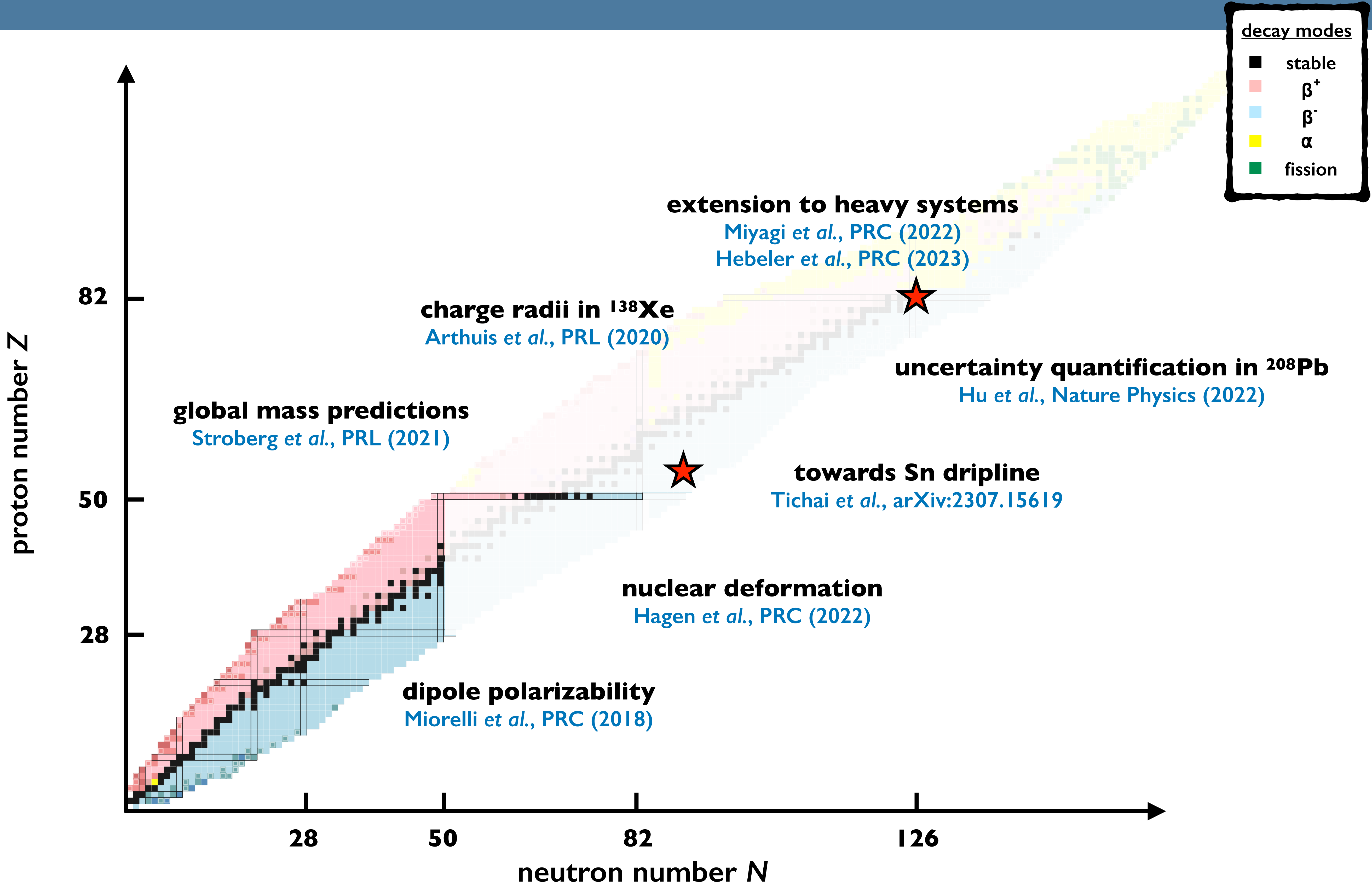


$$H|\Psi_n\rangle = E_n|\Psi_n\rangle$$

~50 nuclei within reach (A<12)

Large-scale diagonalization or few-body frameworks

… and *ab initio* today!



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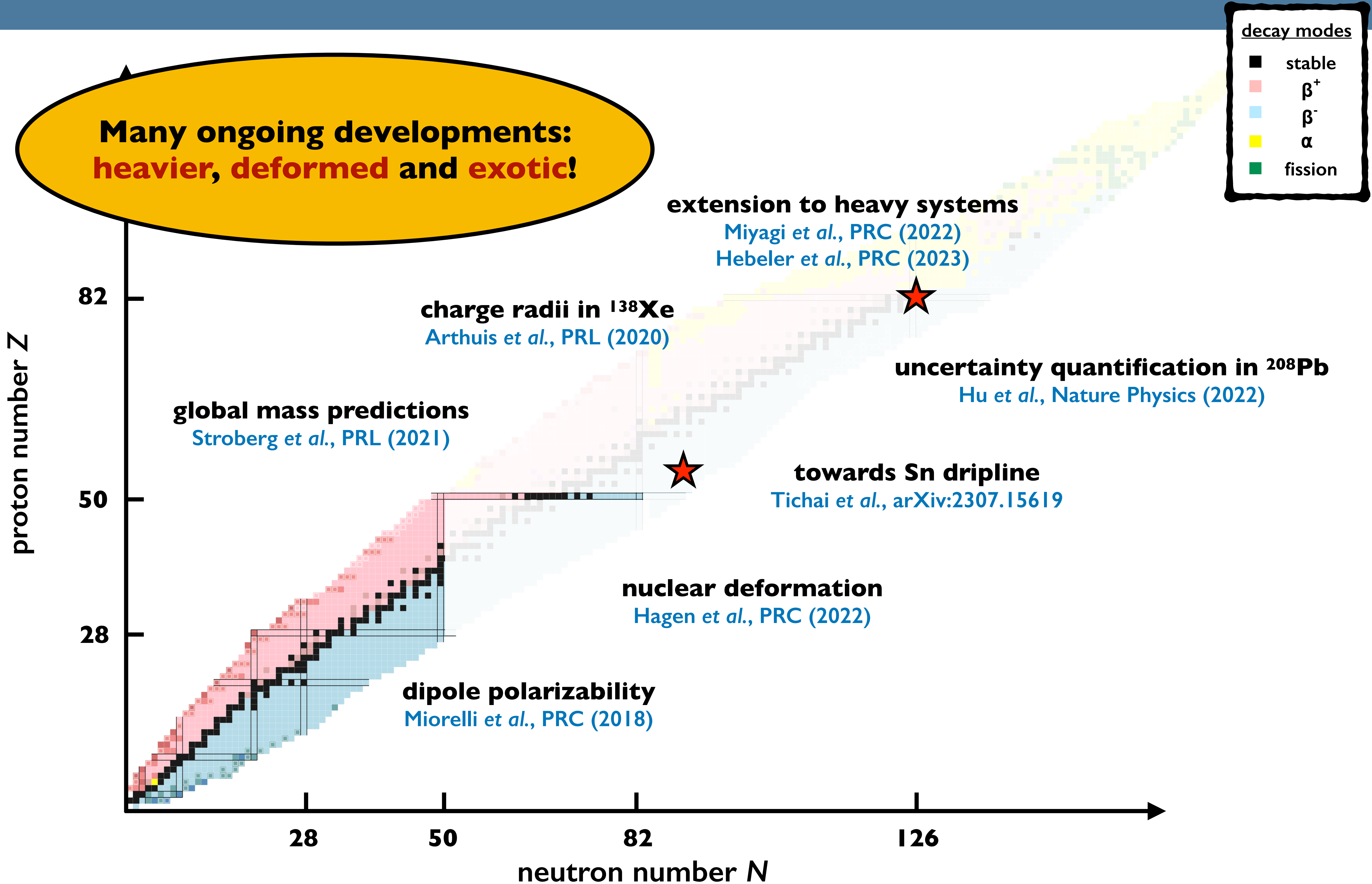

Computational challenges ahead!

- **This talk: basis-expansion approaches (alternative: lattice EFT calculation)**

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

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- **Basis: harmonic oscillator (HO) eigenstates**

$$|p\rangle = |nlm_l\rangle \otimes |sm_s\rangle \otimes |tm_t\rangle$$

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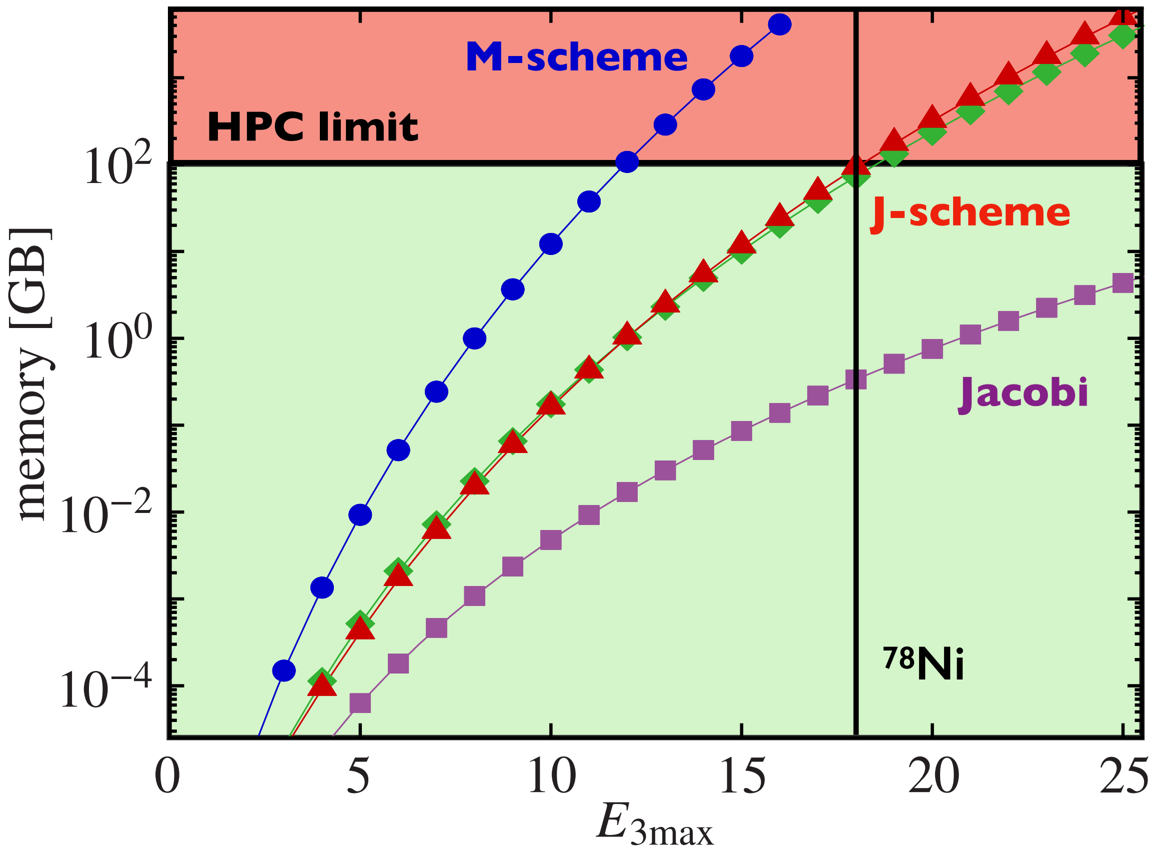
- **Challenge: excessive size of 3B operators**

$$V_{3N} = \frac{1}{36} \sum_{pqrstu} w_{pqrstu}\, c_p^\dagger c_q^\dagger c_r^\dagger c_u c_t c_s$$

Size of three-body operator



adapted from Roth *et al.*, PRC (2014)

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- **Similar problem for the encoding of a wave-function parametrization**

$$|\Psi\rangle = f(\{O_i\})$$

$$O_i \sim \sum_{\circ\cdots\circ} o_{\circ\ldots\circ}\, c_\circ^\dagger \cdots c_\circ^\dagger c_\circ \cdots c_\circ$$

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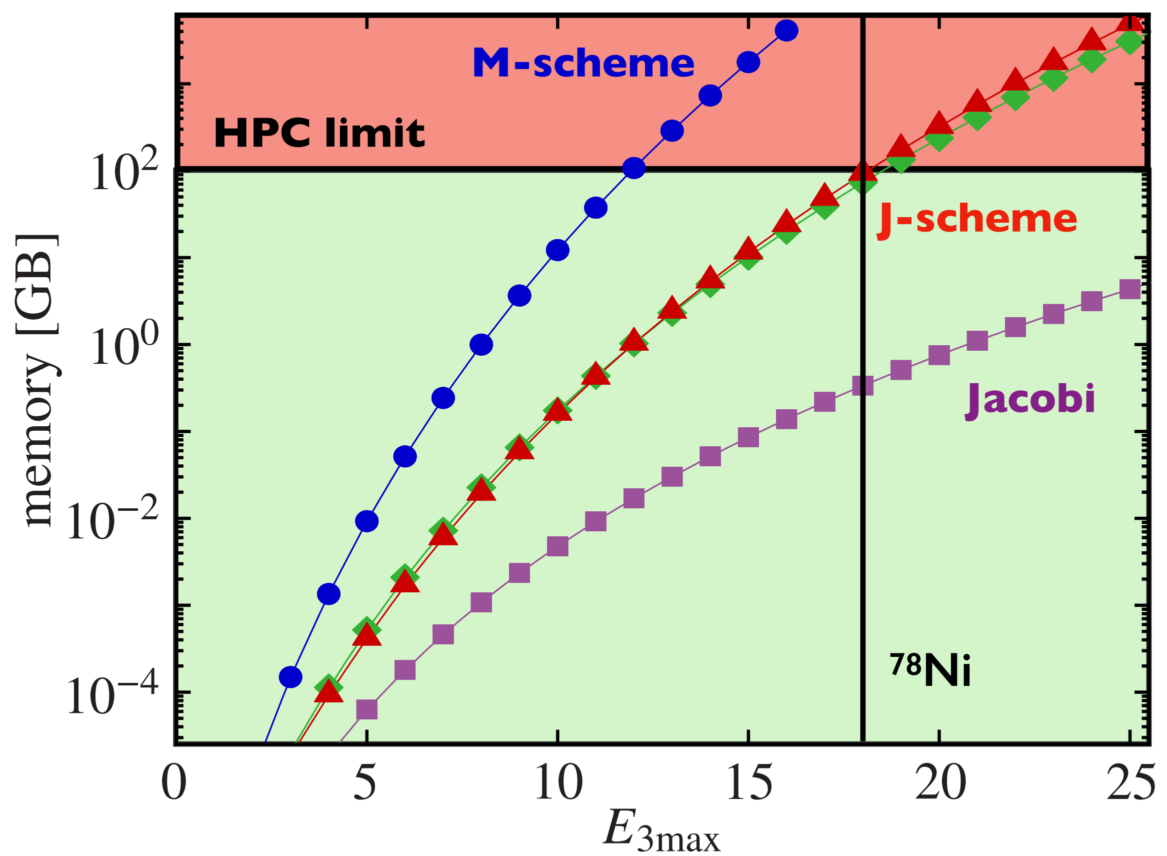

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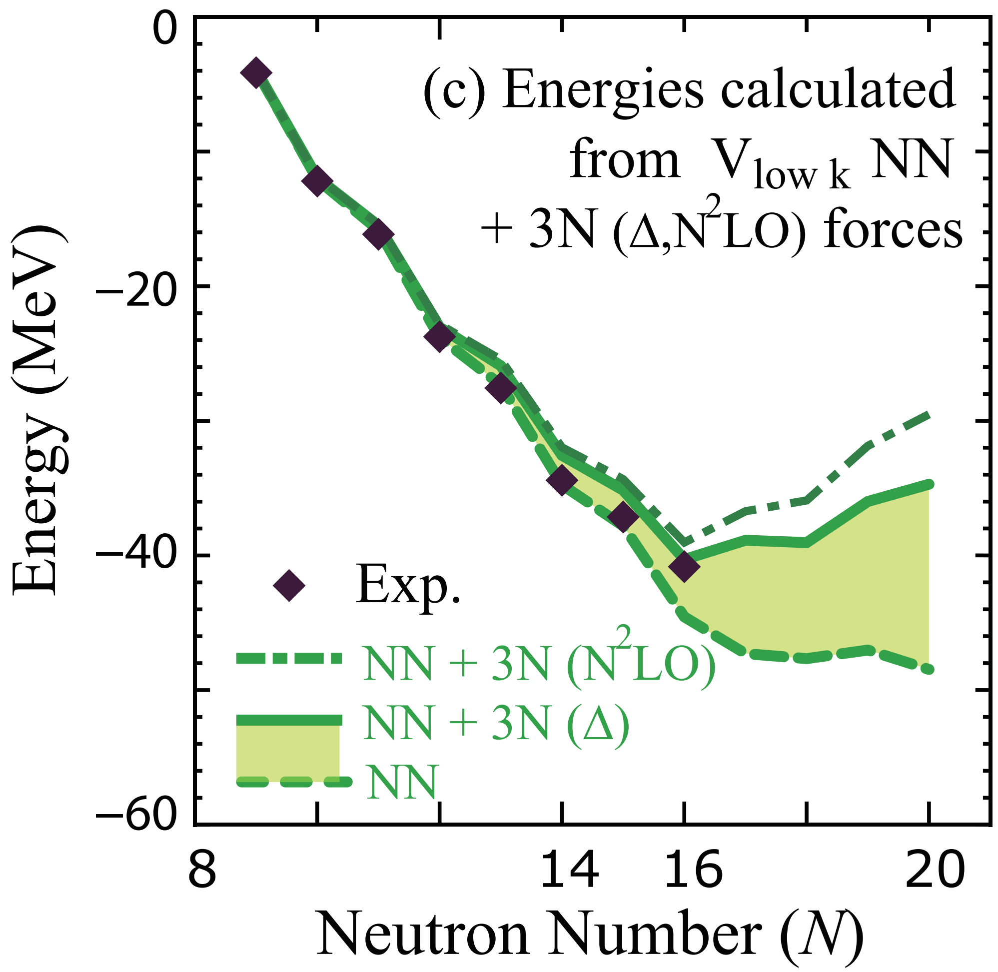
Oxygen dripline location



Otsuka *et al.*, PRL (2010)

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Key idea:
approximate representations!

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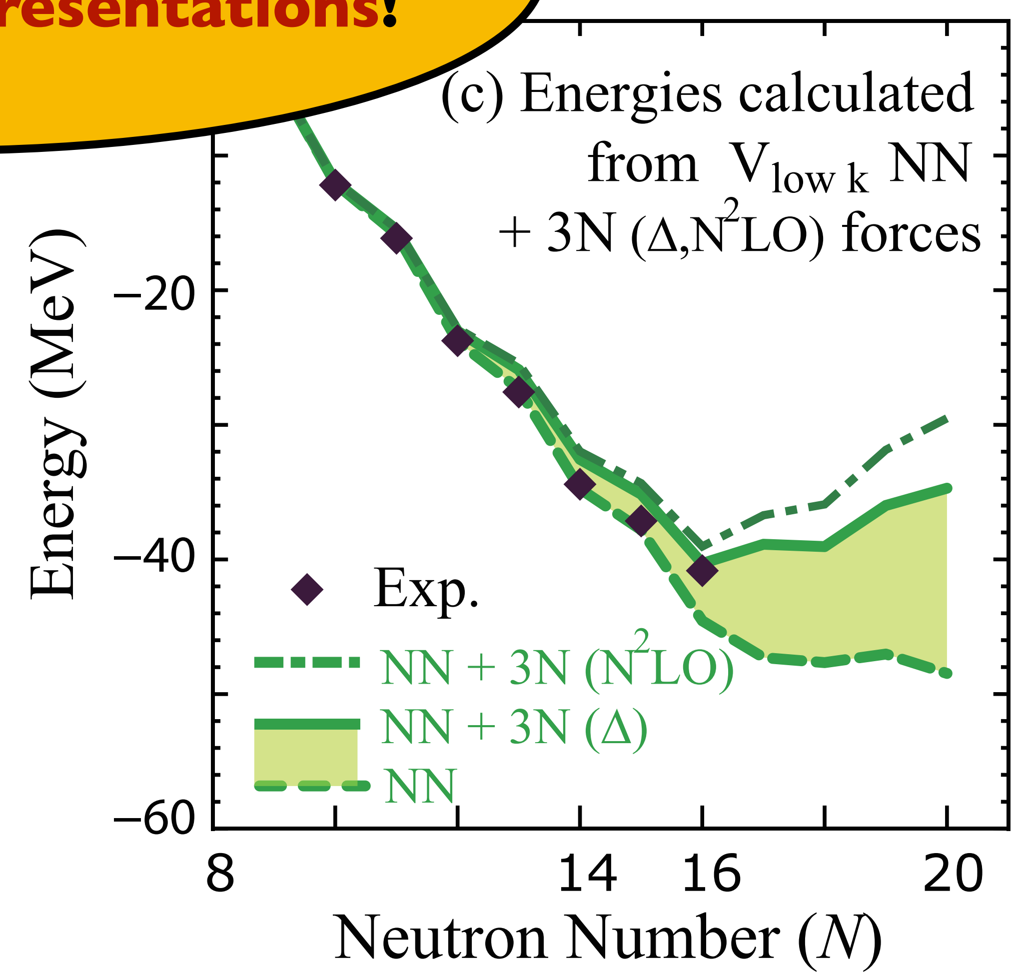

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Normal-ordering

- **Normal ordering: splitting of initial operator based on *A*-body reference state**

(typically Hartree-Fock: $|\Phi\rangle$)

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Density-dependent two-body force

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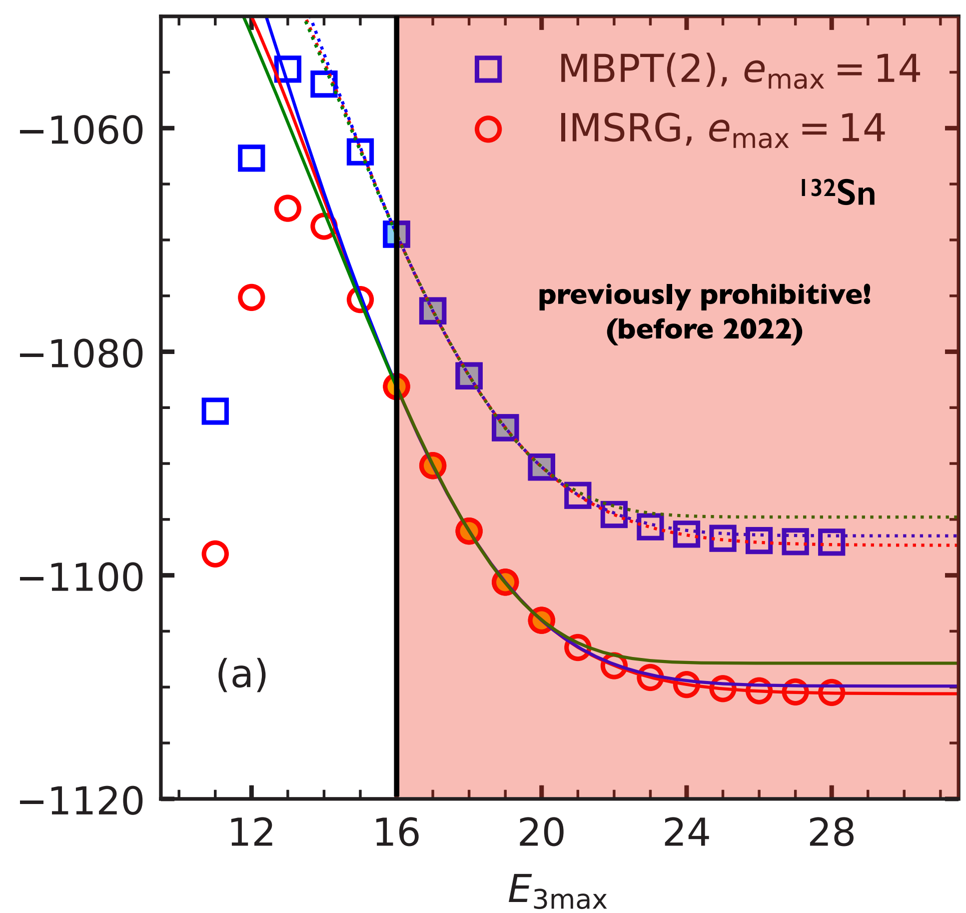
Density-dependent two-body force

- **Particle-rank reduction**: *three-body physics* with two-body operators

- **Model-space convergence gauged from truncation of three-body configurations**

$$e = 2n + l$$

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



Miyagi *et al.*, PRC (2022)

Novel normal-ordering framework

Hebeler, Durant, Hoppe, Heinz, Schwenk, Simonis, Tichai, PRC (2023)

- Fully **circumvents the storage of 3B matrix elements** in bound-state basis

Hartree-Fock density

$$\langle \vec{k}_1 \vec{k}_2 | V_{3N}^{(2B)} | \vec{k}_3 \vec{k}_4 \rangle = \int d\vec{k}_5 d\vec{k}_6 \, \rho(\vec{k}_5, \vec{k}_6) \langle \vec{k}_1 \vec{k}_2 \vec{k}_5 | V_{3N} | \vec{k}_3 \vec{k}_4 \vec{k}_6 \rangle$$

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- **In practice: partial-wave-decomposed basis**

$$|\vec{k}_1 \vec{k}_2\rangle \longrightarrow |pP, [(LS)JL_{CM}]J_{tot}T\rangle$$

dependence on center-of-mass (CM)

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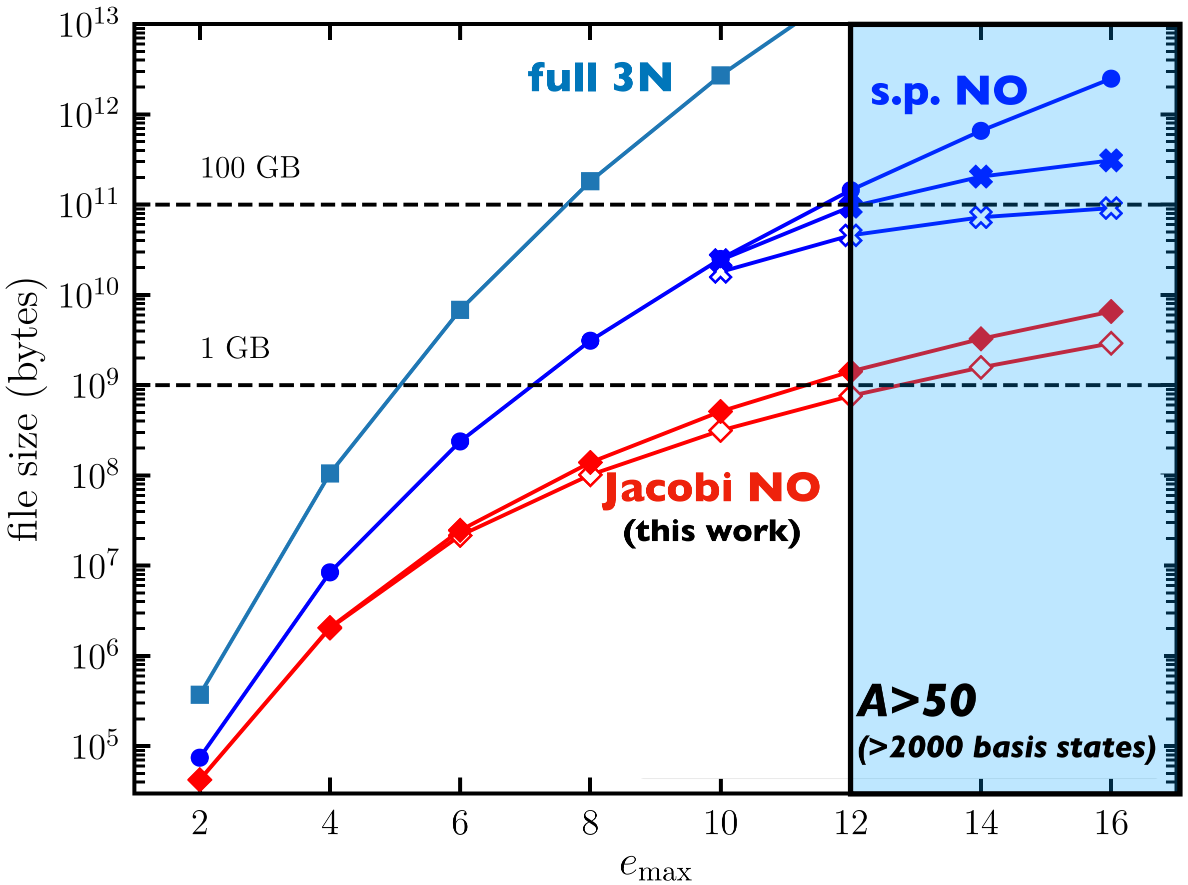
- Significantly **lowered memory requirements** compared to single-particle formulation

Storage requirements with increasing s.p. basis



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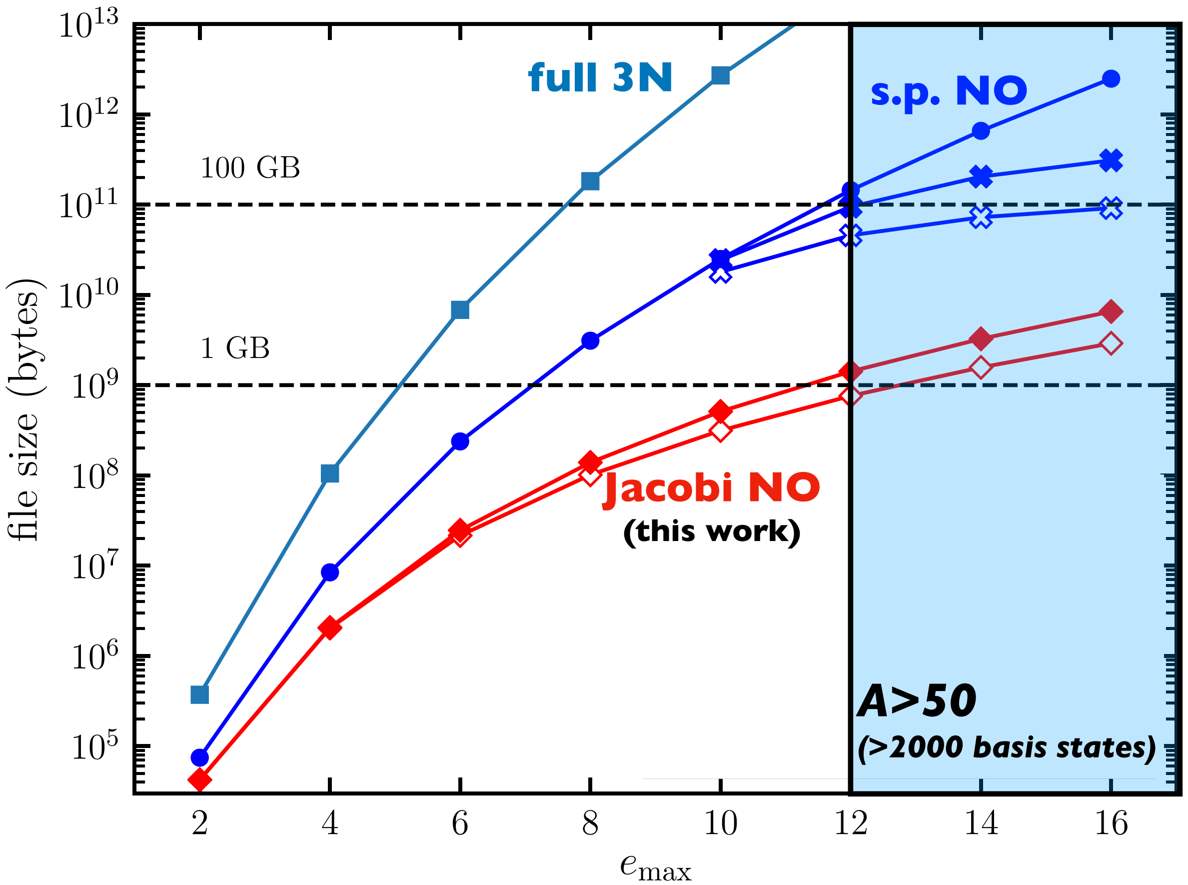
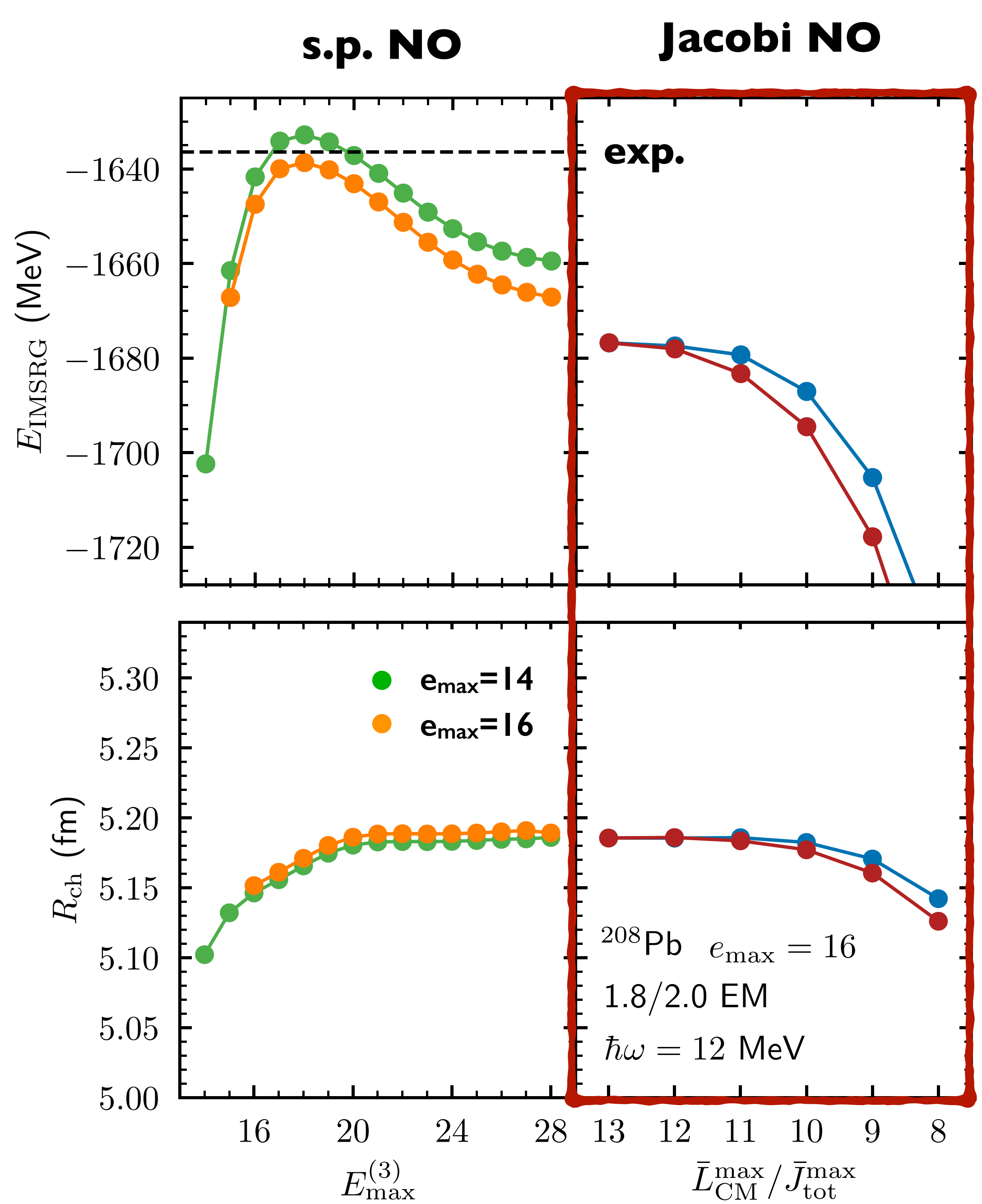
- Convergence gauged based one **new quantum numbers**

L_{CM}/J_{tot}

Storage requirements with increasing s.p. basis



^{208}Pb from first principles



Hebeler,…,Tichai *et al.*, PRC (2023)

- **Excellent agreement** between different normal-ordering frameworks

5-10 MeV difference on a 1680 MeV scale (~0.5%)!

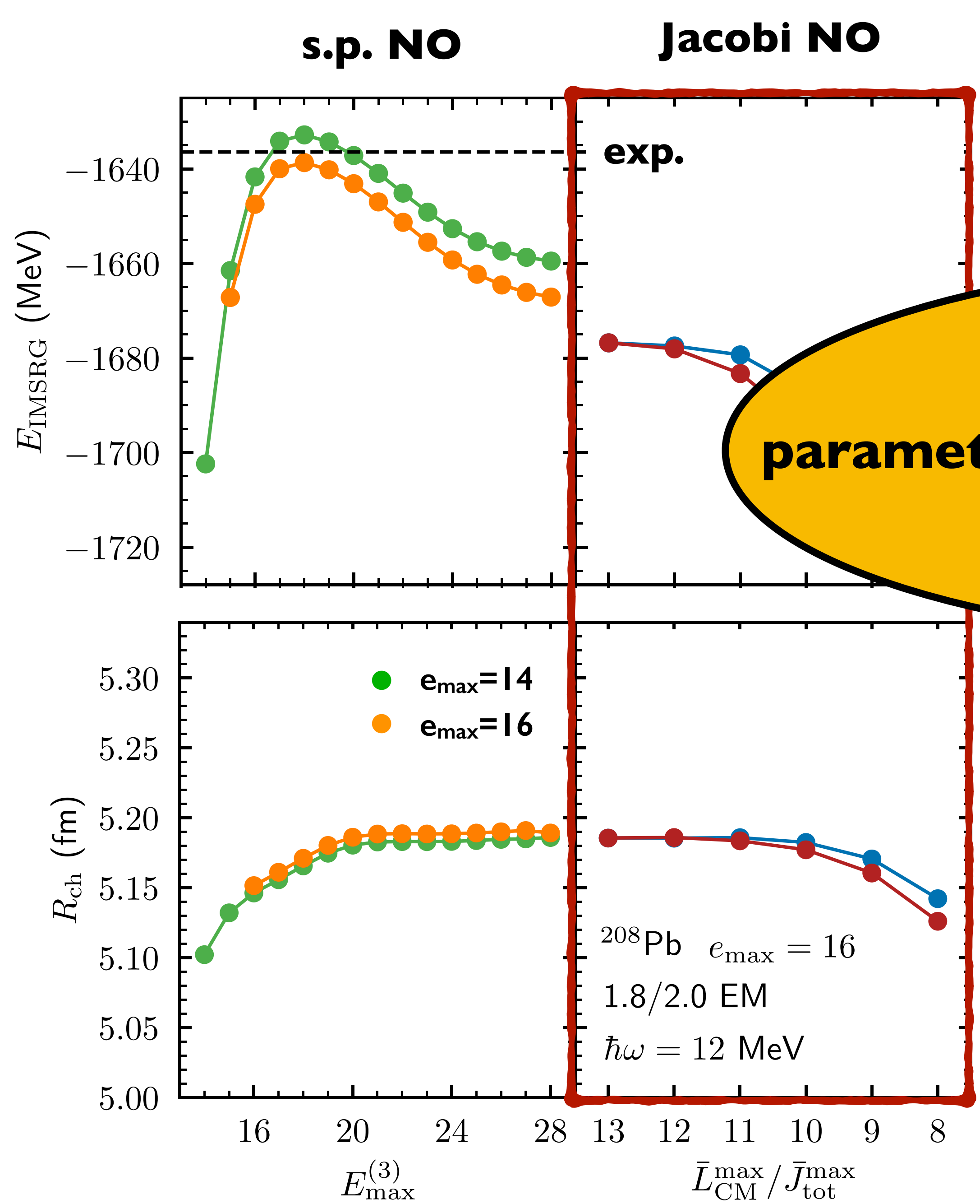
- **Monotonic convergence** as function truncation parameters L_{CM} and J_{tot}

- Novel Jacobi framework provides **alternative** at low memory cost

Heavy-mass frontier

***Ab initio* theory can target heavy nuclei in a controlled way!**

^{208}Pb from first principles



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  5-10 MeV difference on a … MeV scale (~0.5%)!

- … as function … CM and J_{tot}

Chiral EFT involves ~20 parameters (LECs), but we store billions of matrix elements …

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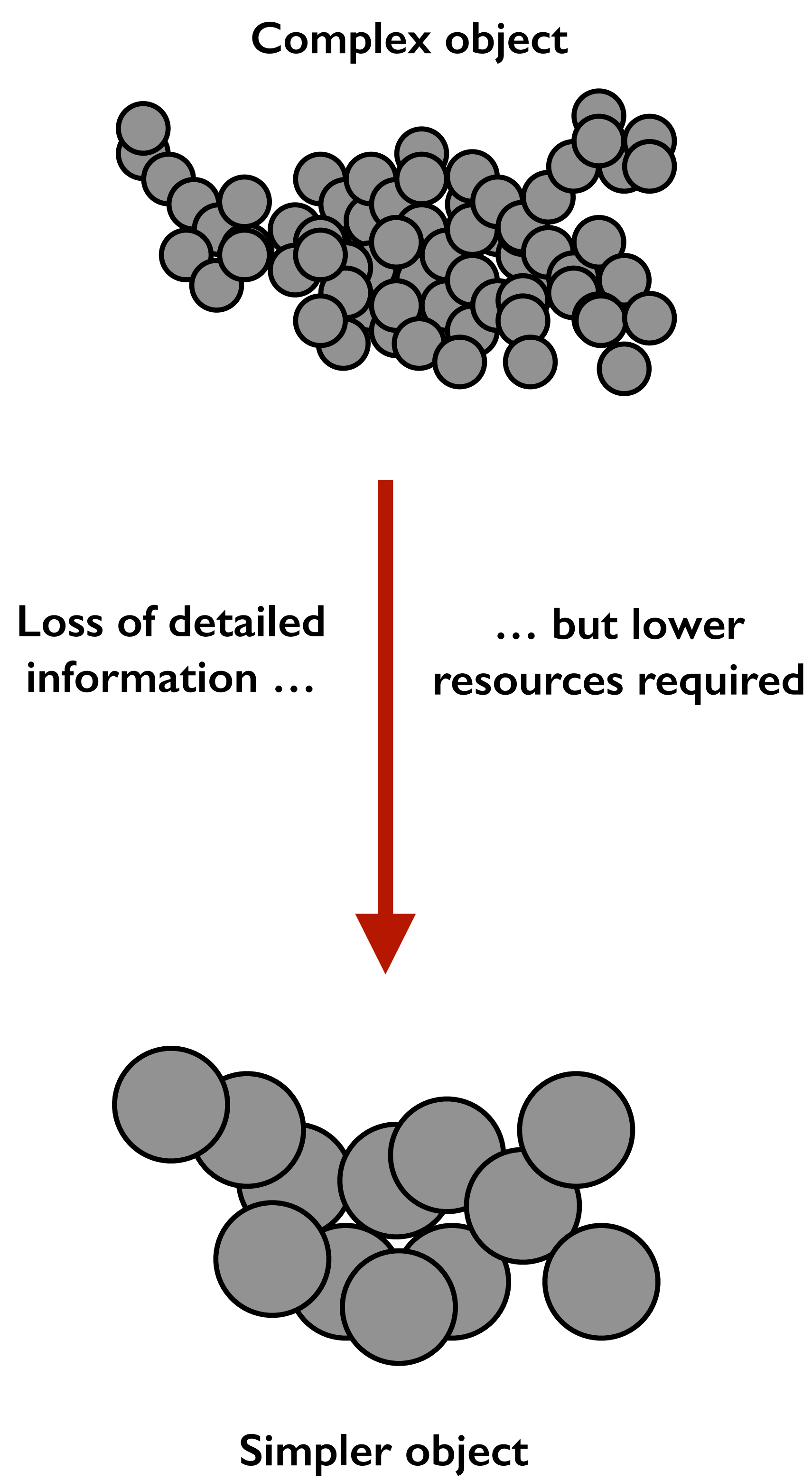
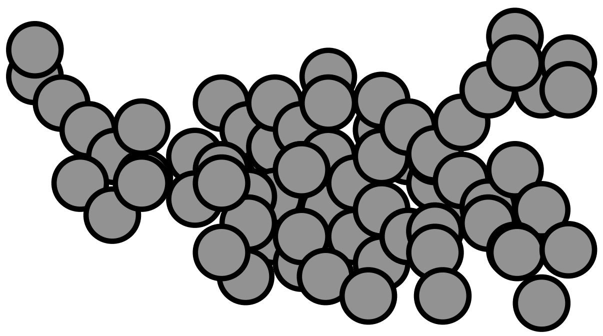
Concepts of data compression



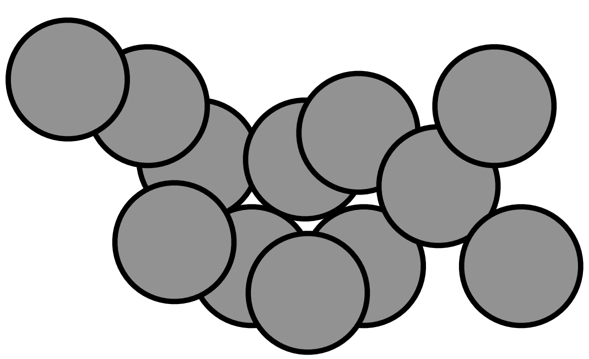
Concepts of data compression

Complex object



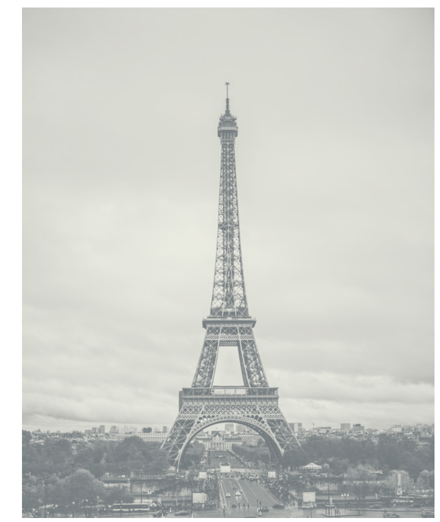
Loss of detailed information …

… but lower resources required



Simpler object

Original picture



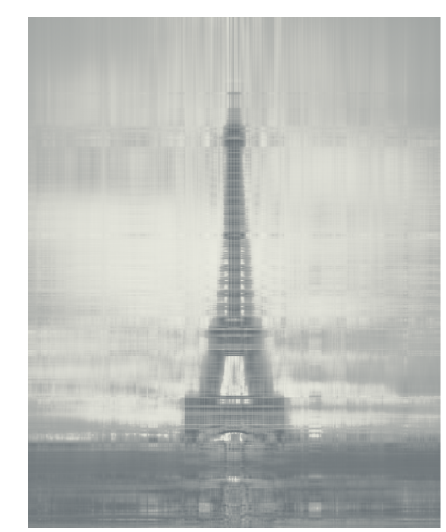
Example from image processing

791 · 640 pixels

data compression
(singular value decomposition)

30 %
(of initial file size)

9 %



3 %

Concepts of data compression

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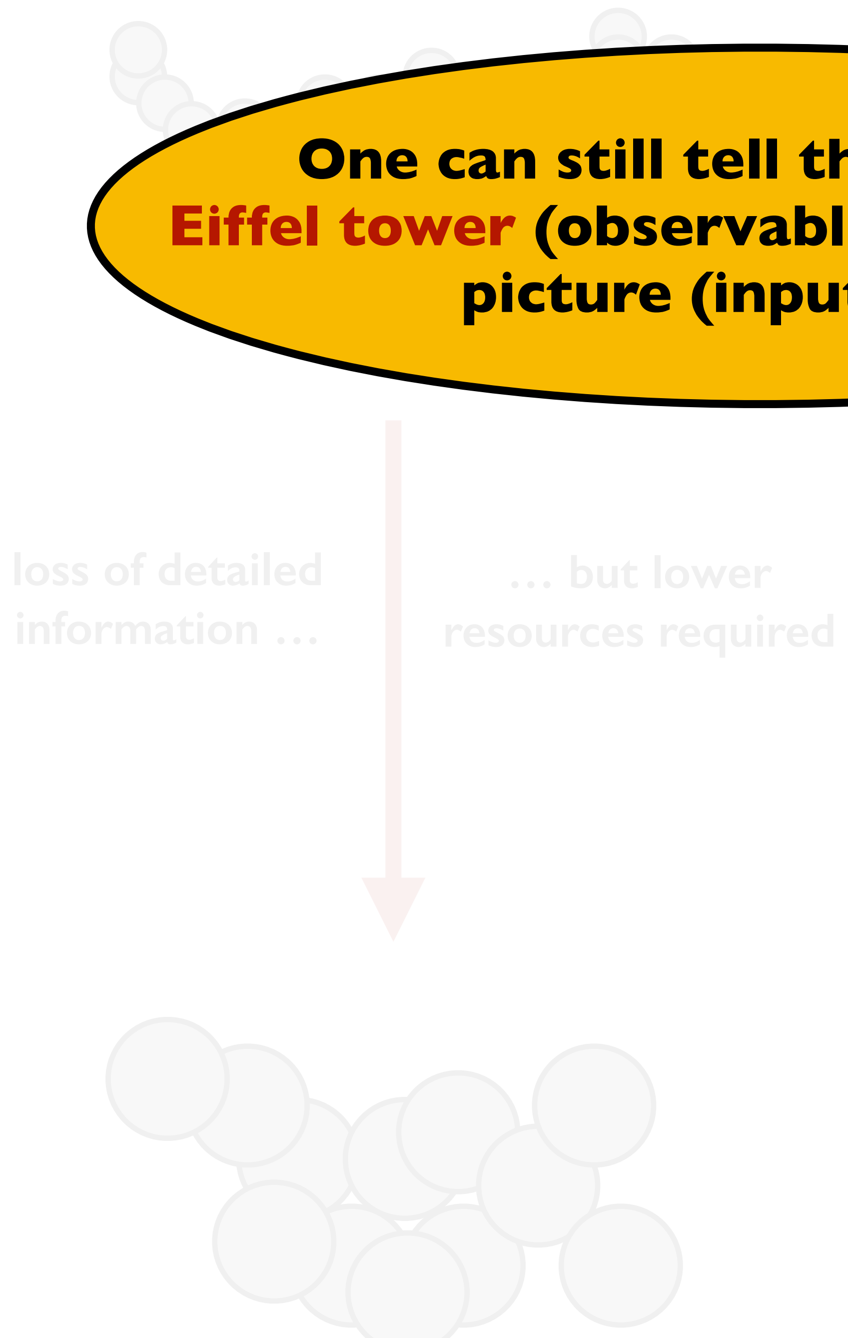
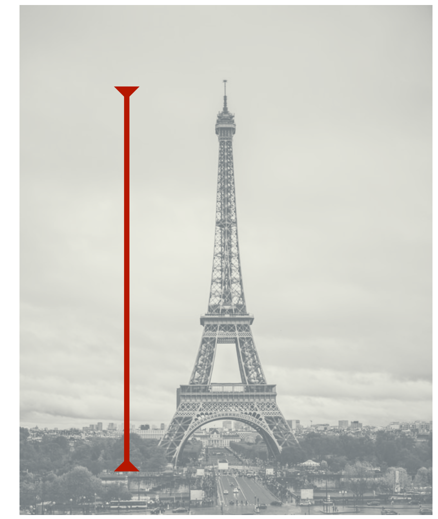


simpler object

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

Original picture



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Singular value decomposition

see also Tichai *et al.*, PRC (2018), EPJA (2018), PLB (2021), PRC (2021); Zhu *et al.* PRC (2022)

- Decomposition of matrix using singular value decomposition (SVD)

initial matrix $M = L \cdot \Sigma \cdot R^{\dagger}$

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- Important information from dominant singular values (in decreasing order)

$$\Sigma = \mathrm{diag}(s_i) \qquad s_i \geq 0$$

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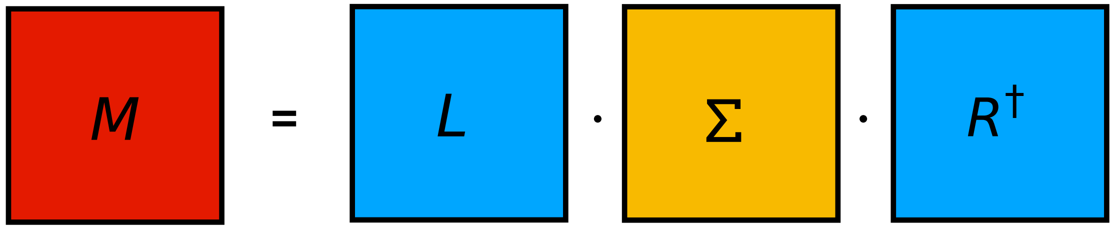

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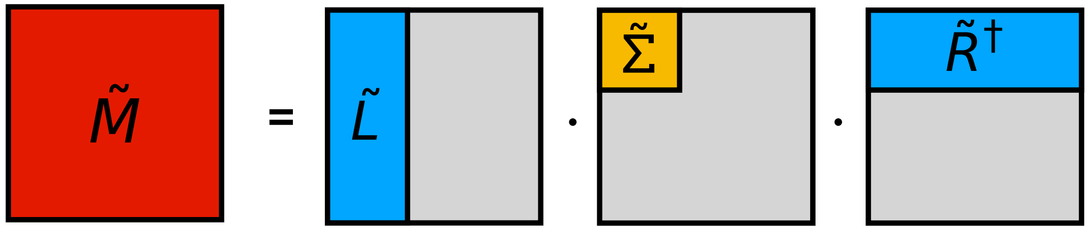
low-rank approximation



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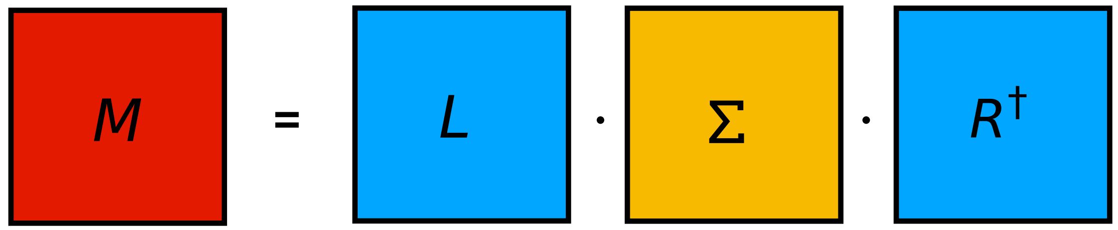

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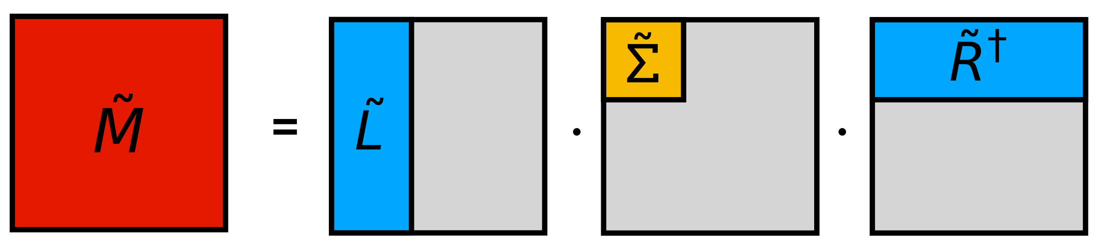

- High-resolution details can be discarded while enabling data compression

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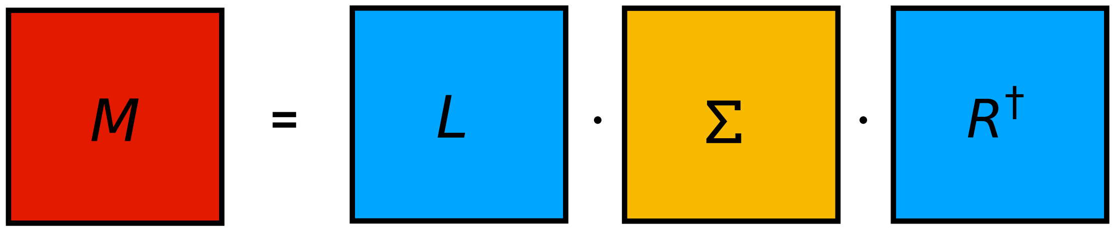

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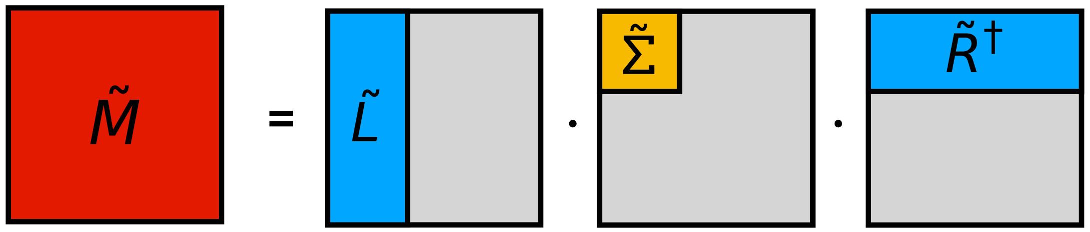

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- Validated in two-body sector: binding energies, NN phase shifts, nuclear matter, …

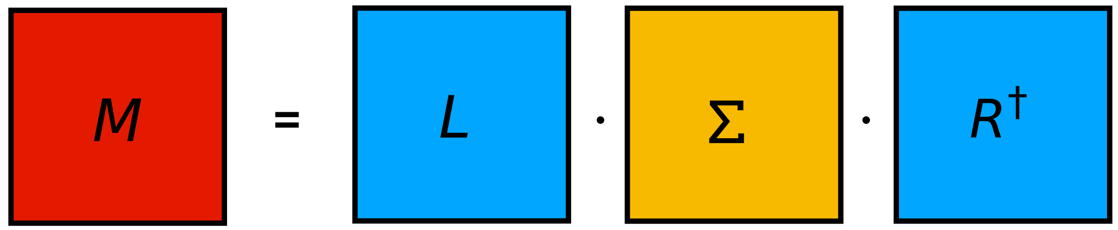
Singular value decomposition

How well does it work for **3N forces**?

see also Tichai *et al.*, PRC (2018), EPJA (... (2022)

- Decomposition of matrix using singular value decompositi...

initial matrix

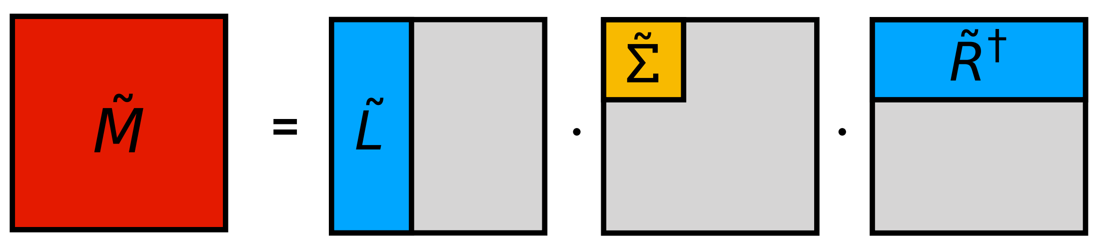


- Important information from dominant singular values (in decreasing order)

$$\Sigma = \mathrm{diag}(s_i) \qquad s_i \geq 0$$

- Low-rank approximation from truncated singular value decomposition

low-rank approximation

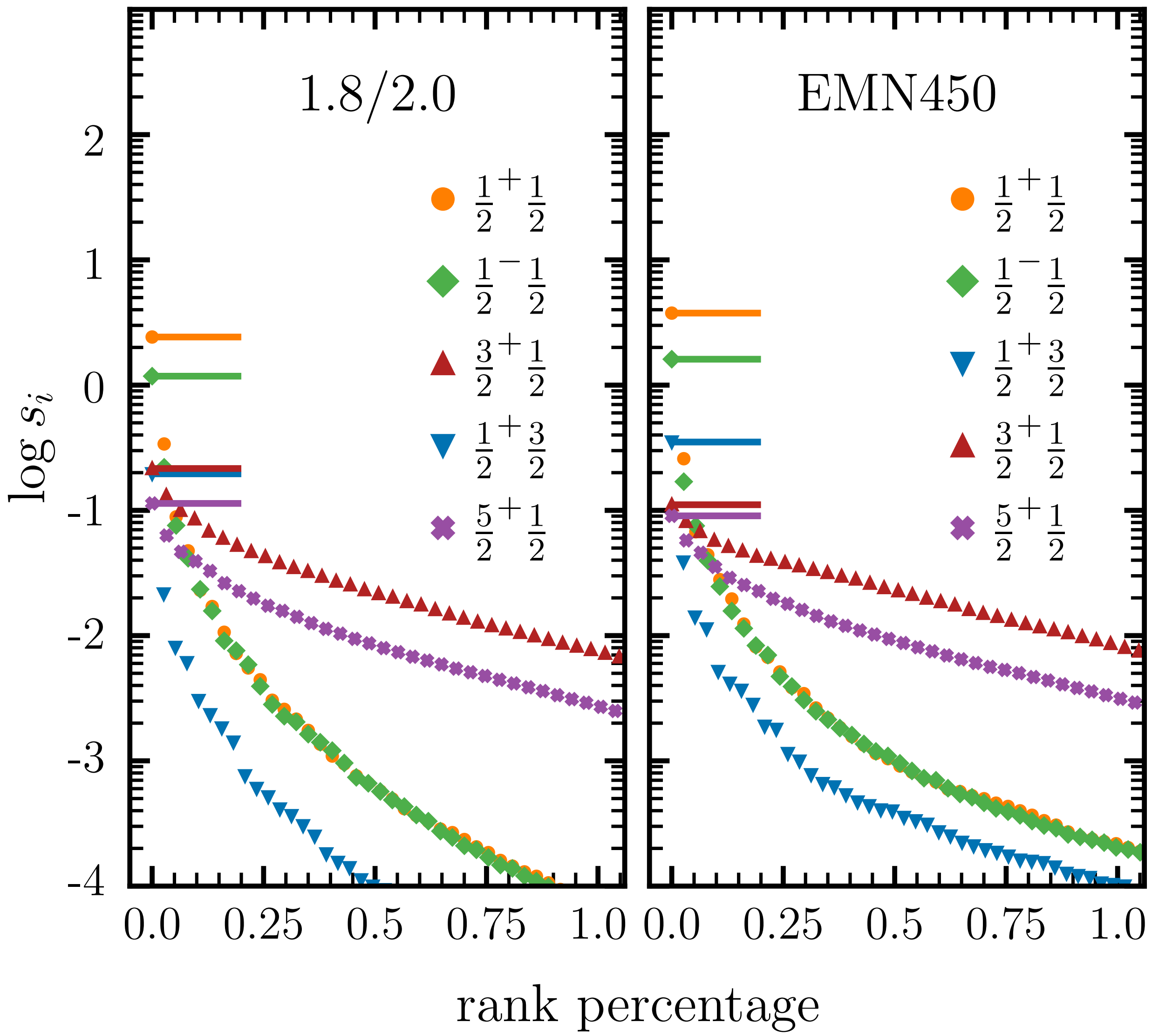


- High-resolution details can be discarded while enabling data compression

- Validated in two-body sector: binding energies, NN phase shifts, nuclear matter, …

Low-rank interactions from chiral EFT

Singular spectrum in different partial-wave channels



Tichai *et al.*, arXiv:2307.15572

- Strong **suppression of singular values** across different partial-wave channels

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

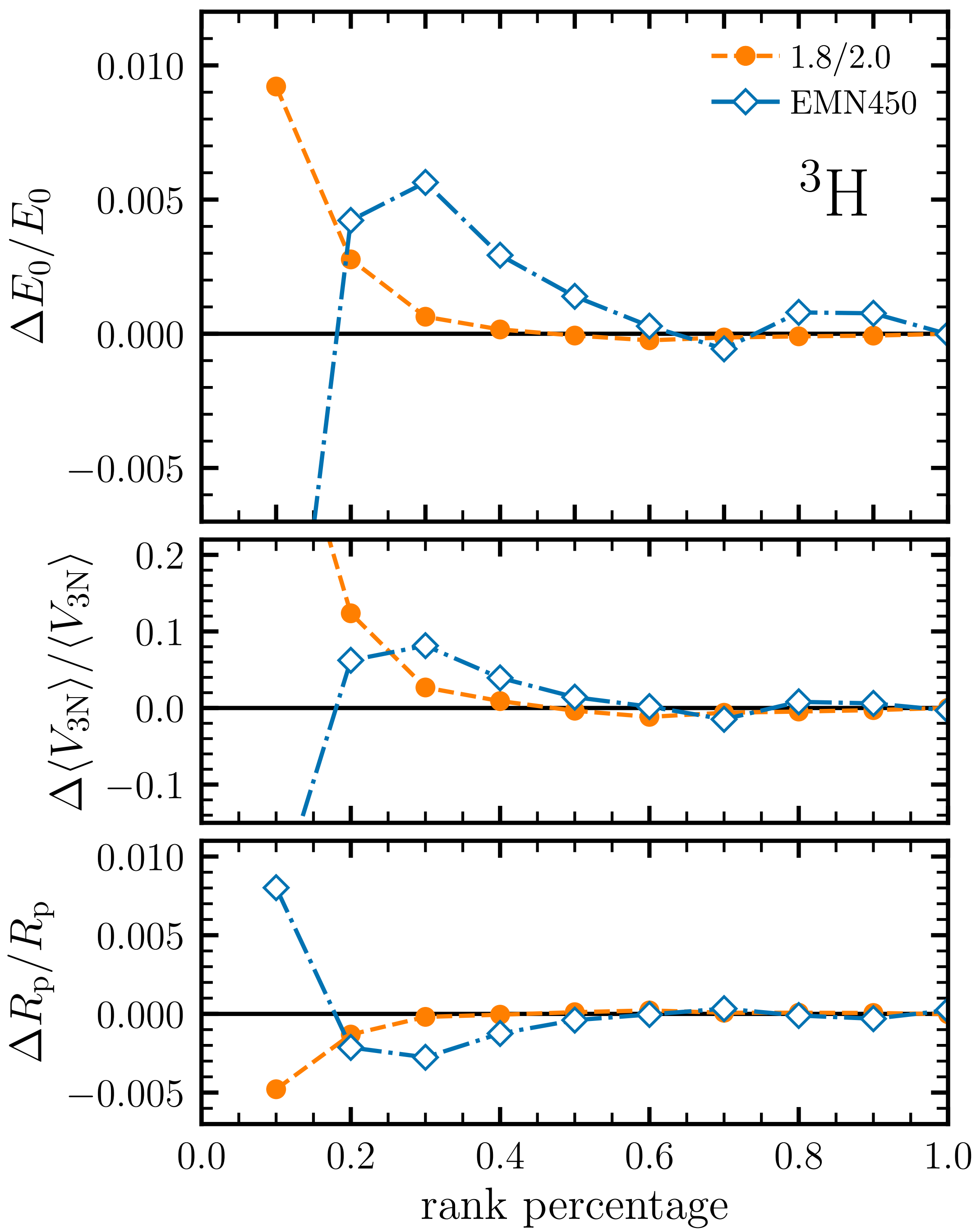
- **Higher partial waves suppressed** compared to triton channel
- Similar spectrum for parity-partner channels/isospin triplet suppressed
- Has been validated for **different chiral three-body interactions**

Chiral EFT

Singular spectrum reveals pronounced low-rank character!

Few-body calculations

Ground-state observables for ^{3}H



Tichai *et al.*, arXiv:2307.15572

- Observables from **momentum-space Fadeev solver** with full 3N force
- **Very low error** on ground-state observables for different interactions
- **1% of singular values** yield less than keV errors on ground-state energy
- Even better compression than in previous **low-rank NN studies**

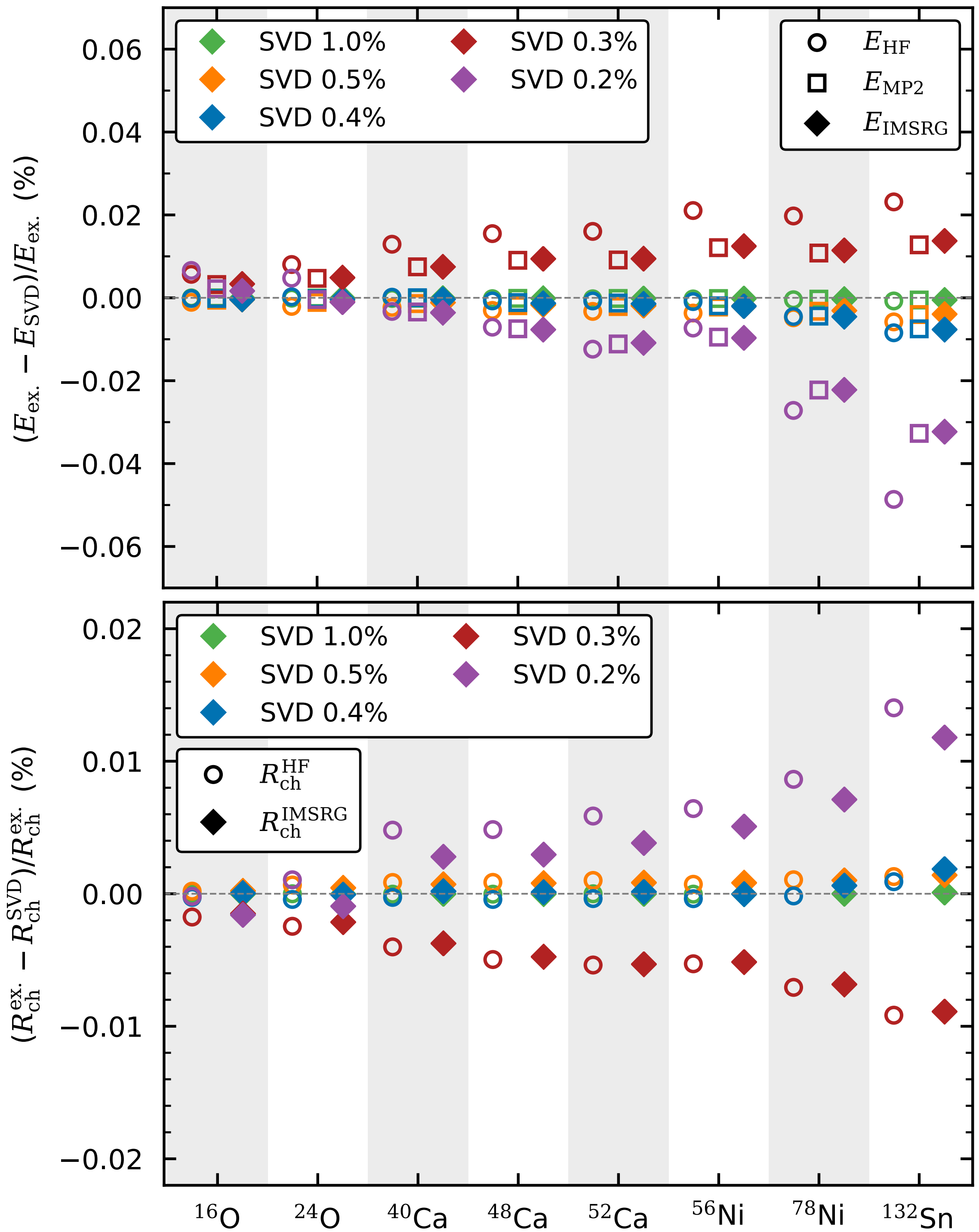
Tichai *et al.*, PLB (2021)

Few-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

- 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!

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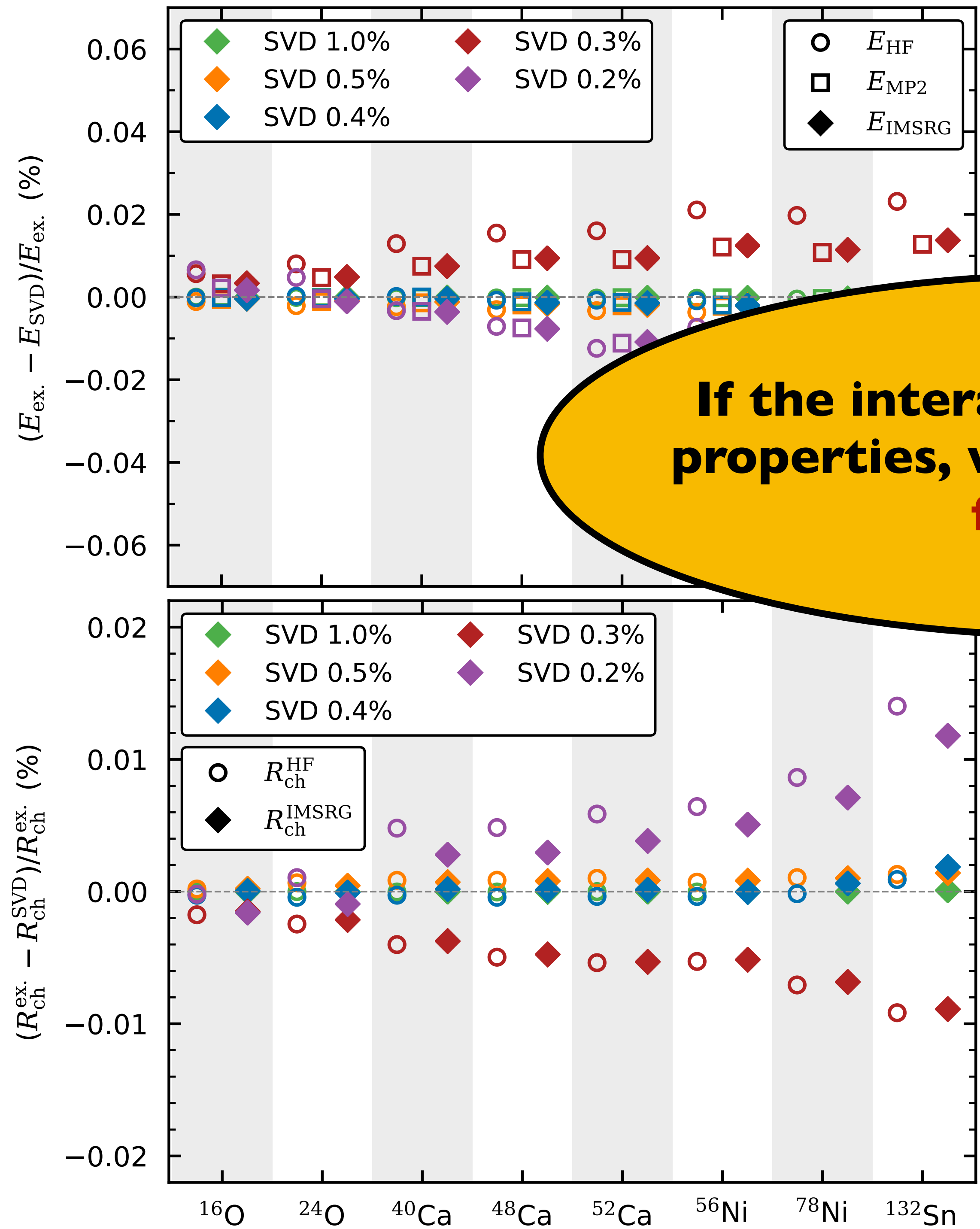

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- Matrix elements from transformation of **low-rank 3N interactions**
- **Low error on observables** from different many-body schemes
- f decomposition number

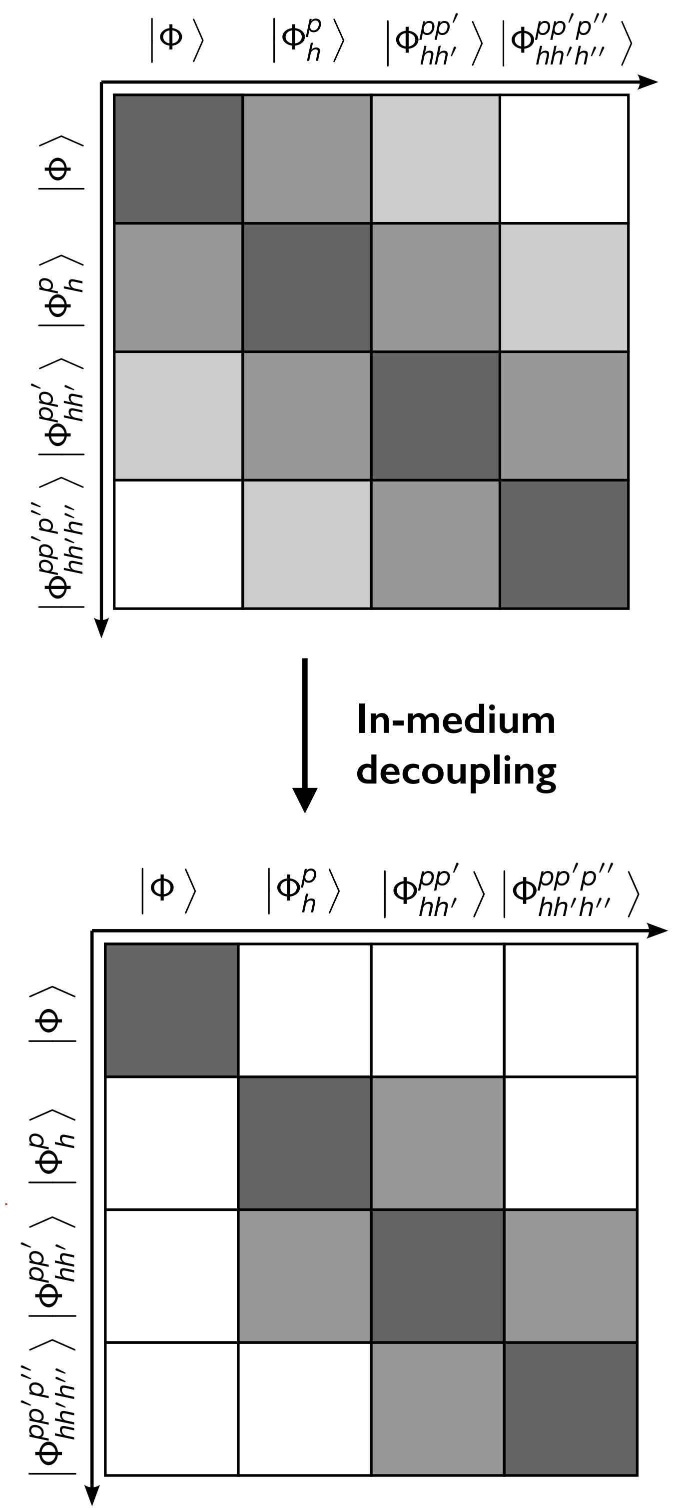
If the interaction has low-rank properties, what about the wave function?

- **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!

In-medium similarity renormalization group



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

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

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

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

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

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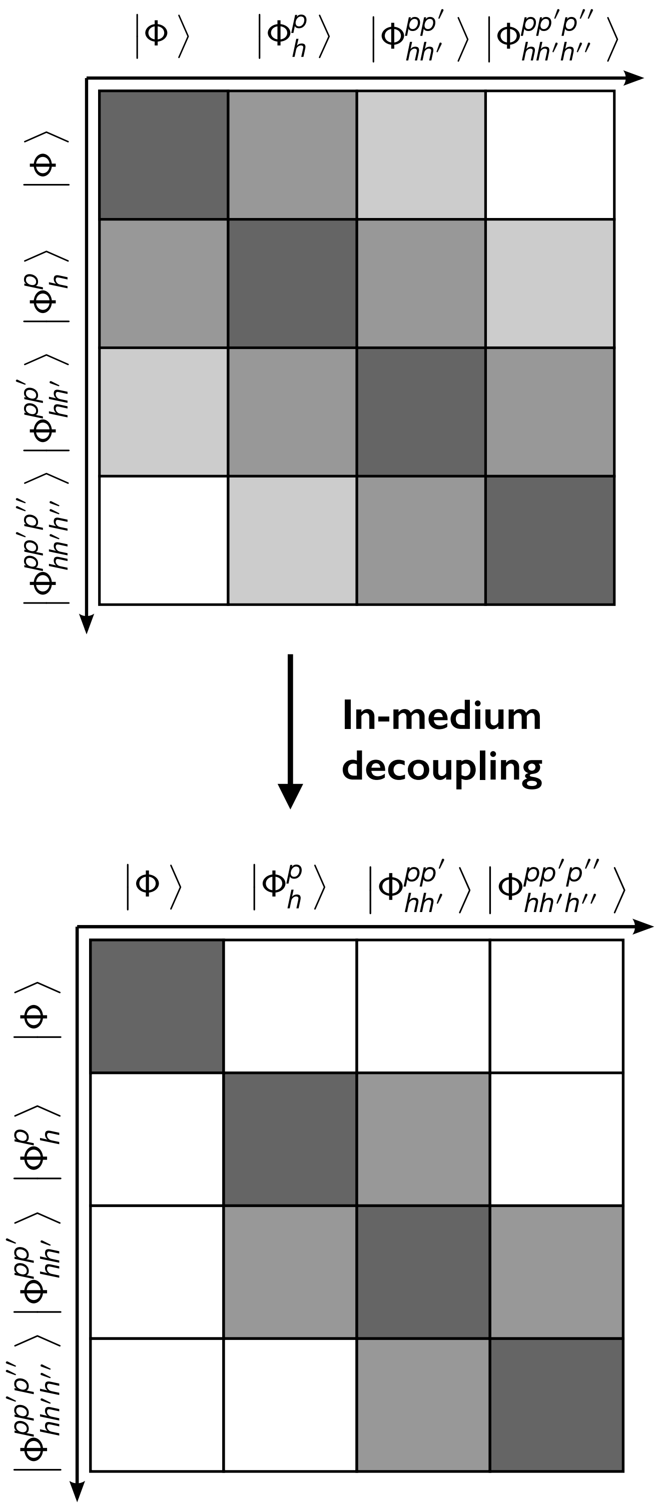

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Keep operators to *k*-body level:
IMSRG(*k*)

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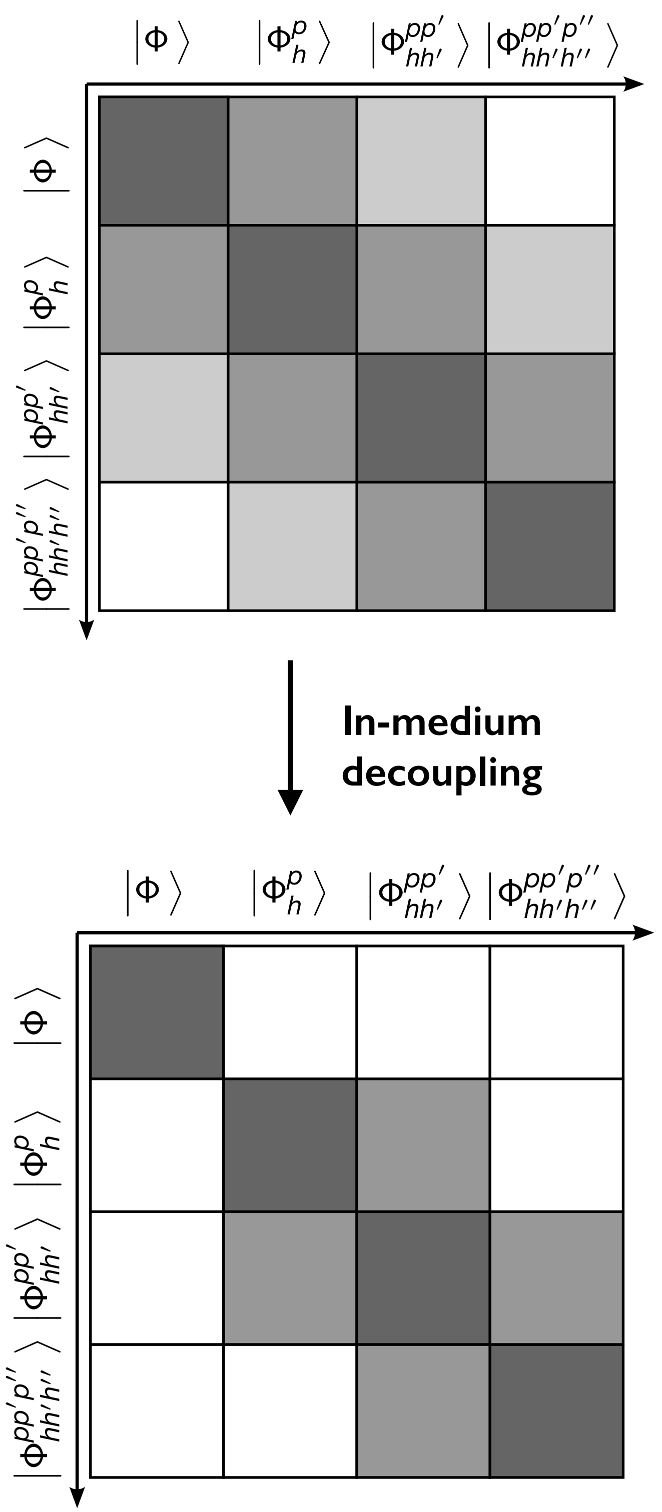

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$$\lim_{s\to\infty} \langle\Phi|H(s)|\Phi\rangle = E_0$$

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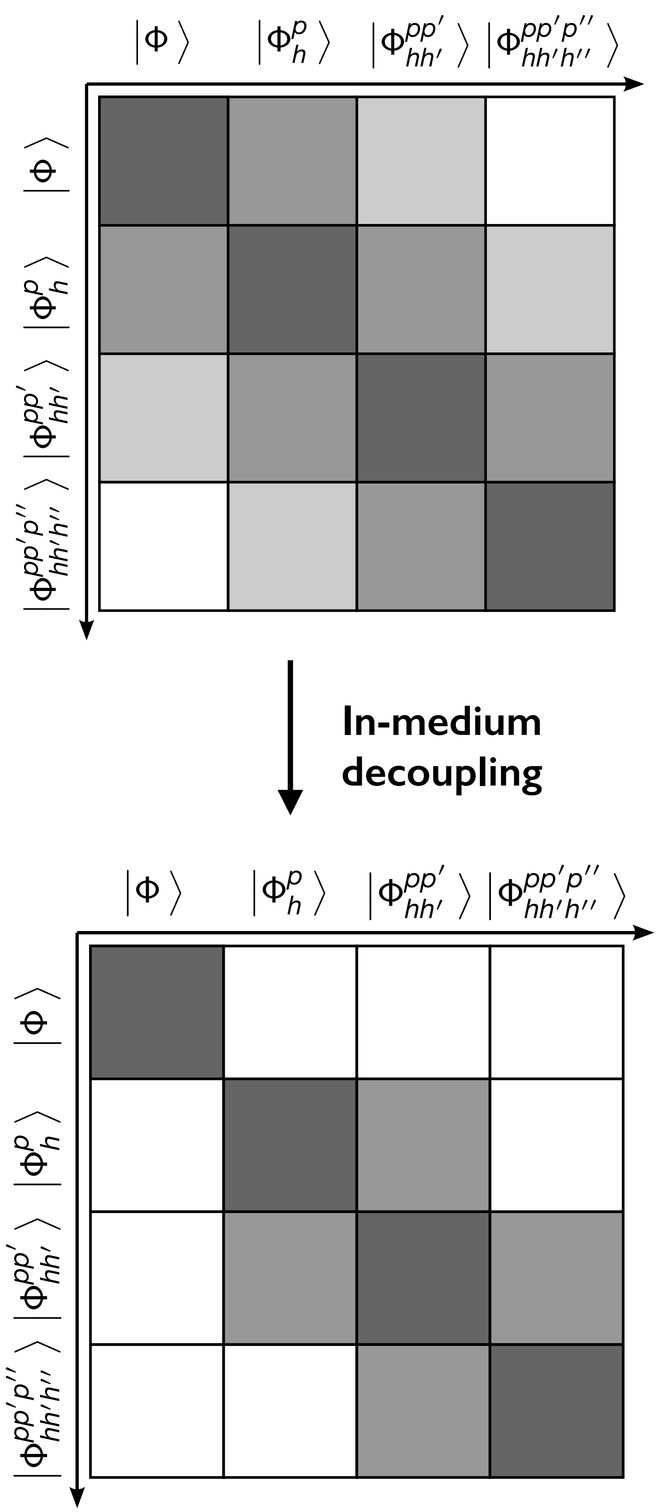

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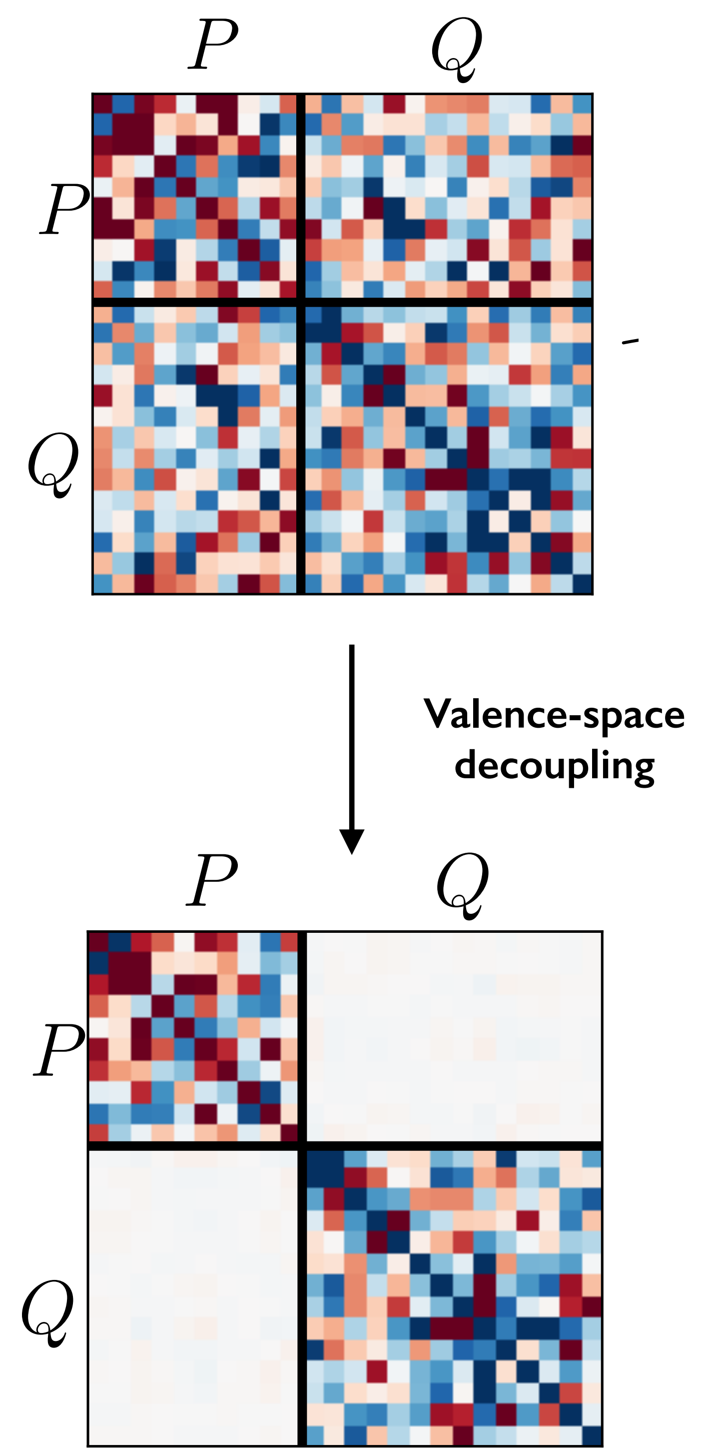
- **Versatility: generate input for other approaches**

The valence-space IMSRG

- Modify decoupling to target valence space

- Construction of *ab-initio* inspired valence-space interactions rooted in QCD



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

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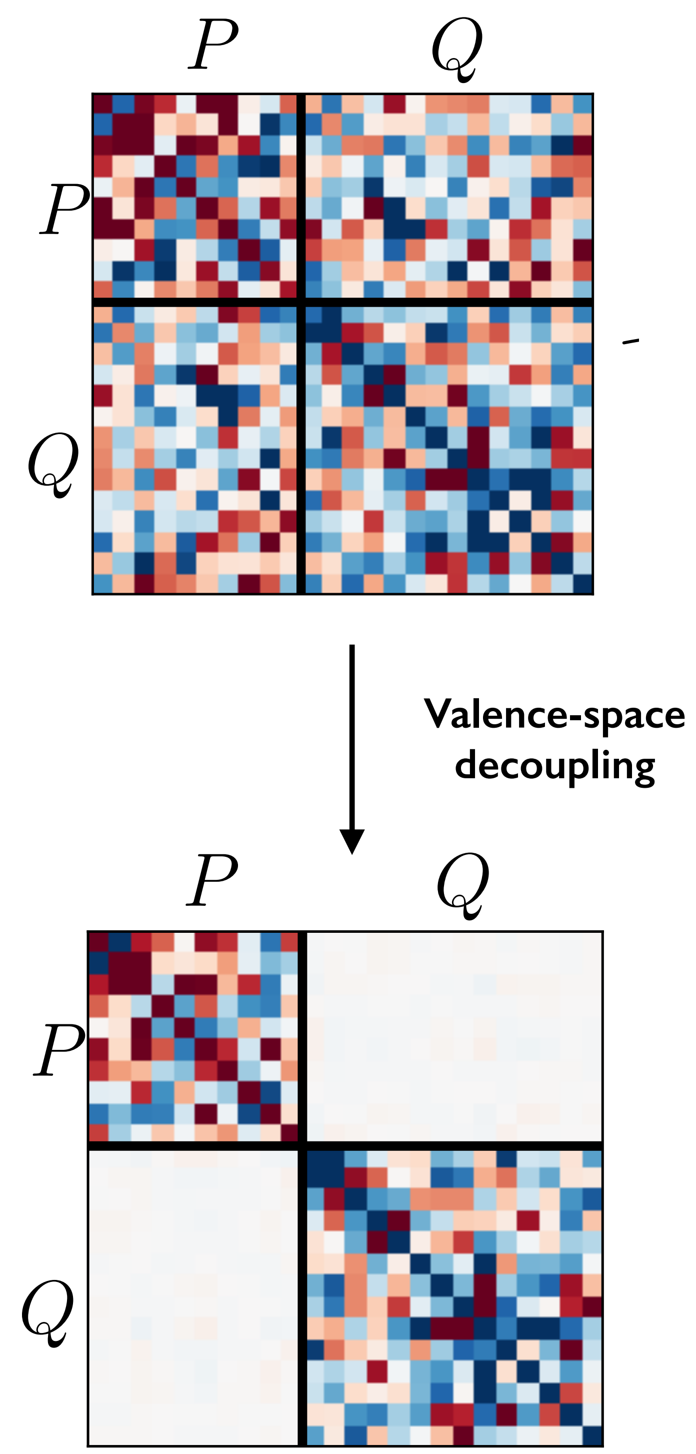

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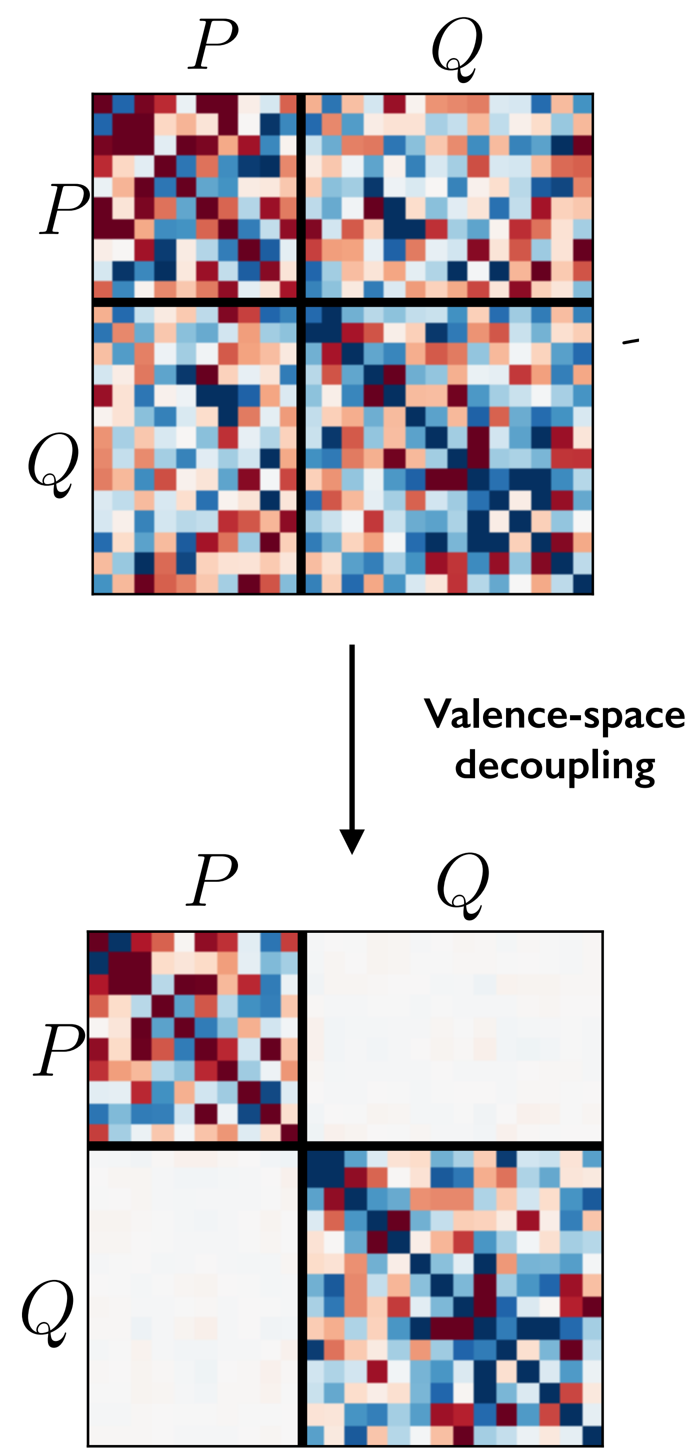

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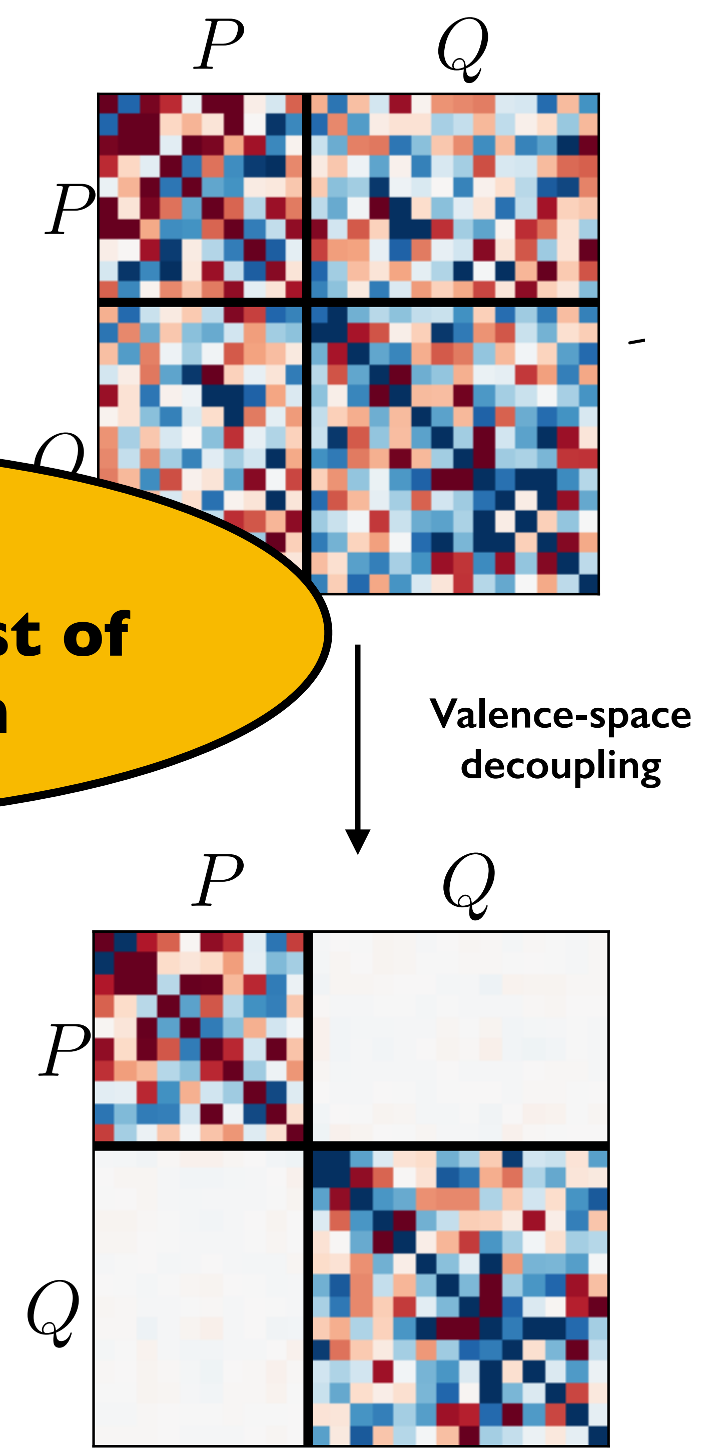
Challenge:
Computational cost of diagonalization



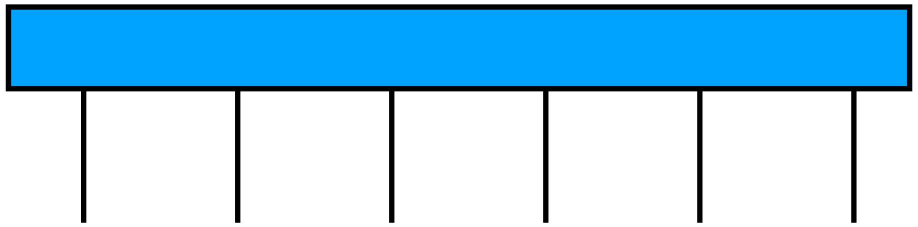
Stroberg *et al.*, Ann. Rev. Nucl. Part. Sci (2019)

Wave-function representations

- **Many-body state is inefficiently represented in configuration interaction**

complexity d^N
(d: local dimension, e.g. d=2 for s=1/2 spin chain)

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



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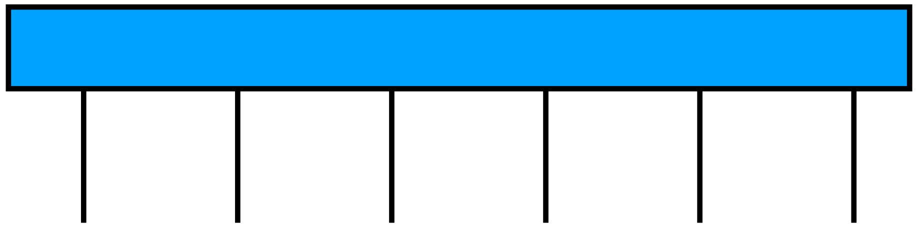
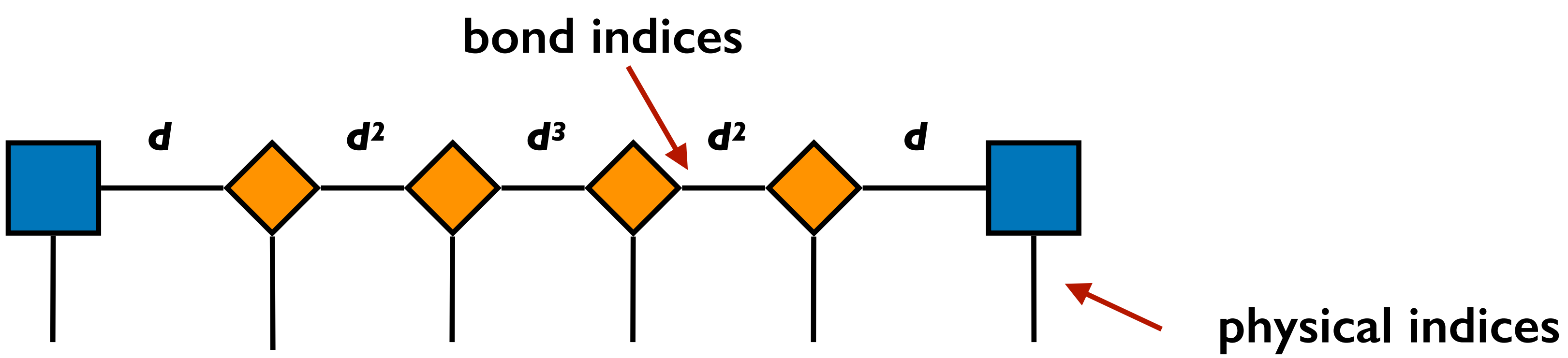


- **Exact rewriting of CI wave function using matrix product state (MPS) ansatz**



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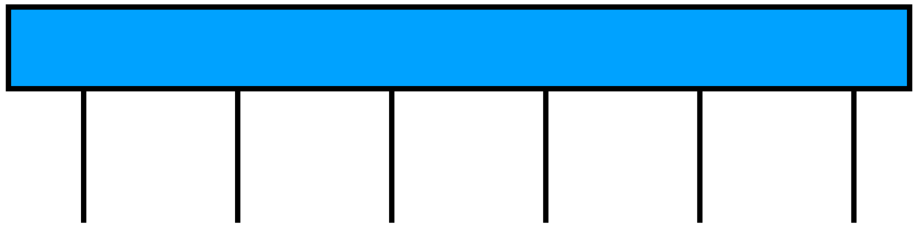

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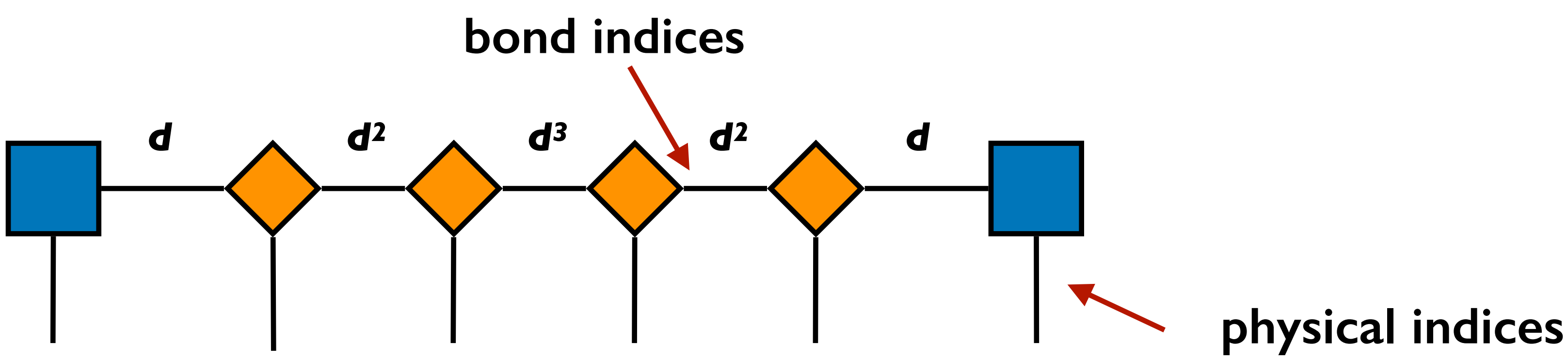

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- Approximate MPS representation obtained by limiting intermediate summation

⟶ **bond dimension M**

Density matrix renormalization group

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

White, PRL (1991)

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

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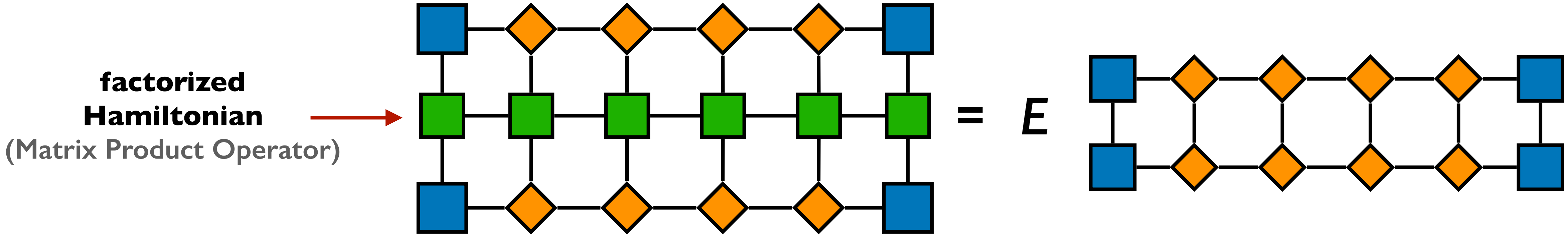
Schollwöck, Ann. Phys. (2011)



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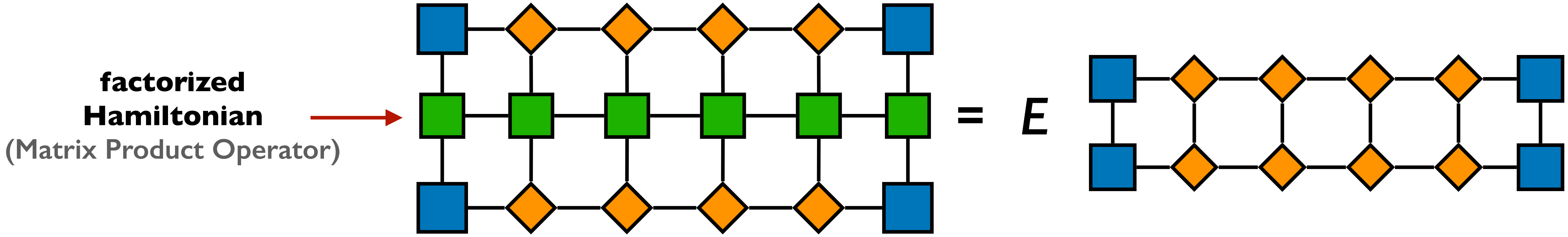

- Stationarity condition yields variational update step for factor matrices

$$\frac{\partial^2}{\partial A^{\alpha_i}_{p_{i-1}p_i} \partial A^{\alpha_{i+1}}_{p_i p_{i+1}}} \Big(\langle \Psi | H | \Psi \rangle - E \langle \Psi | \Psi \rangle \Big) = 0$$

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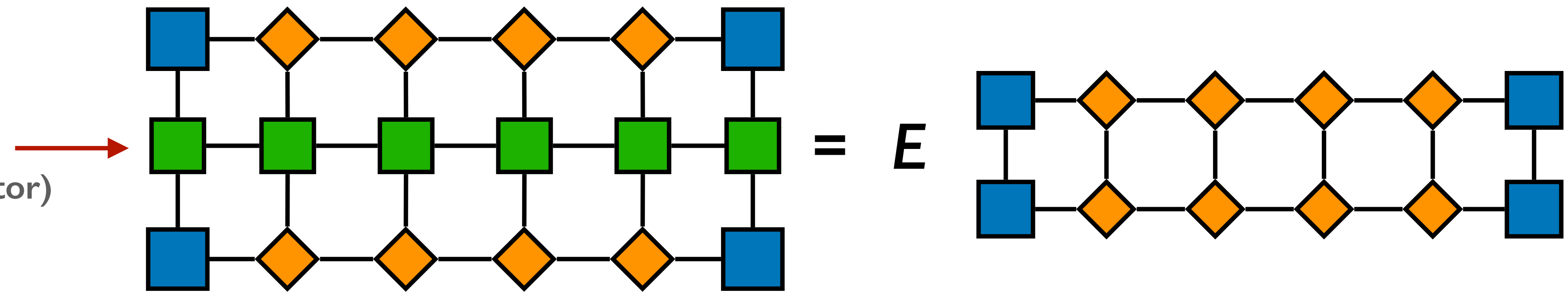

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Hybrid approach:
Map no-core problem to small active space (IMSRG) and find variational approximation (DMRG)!

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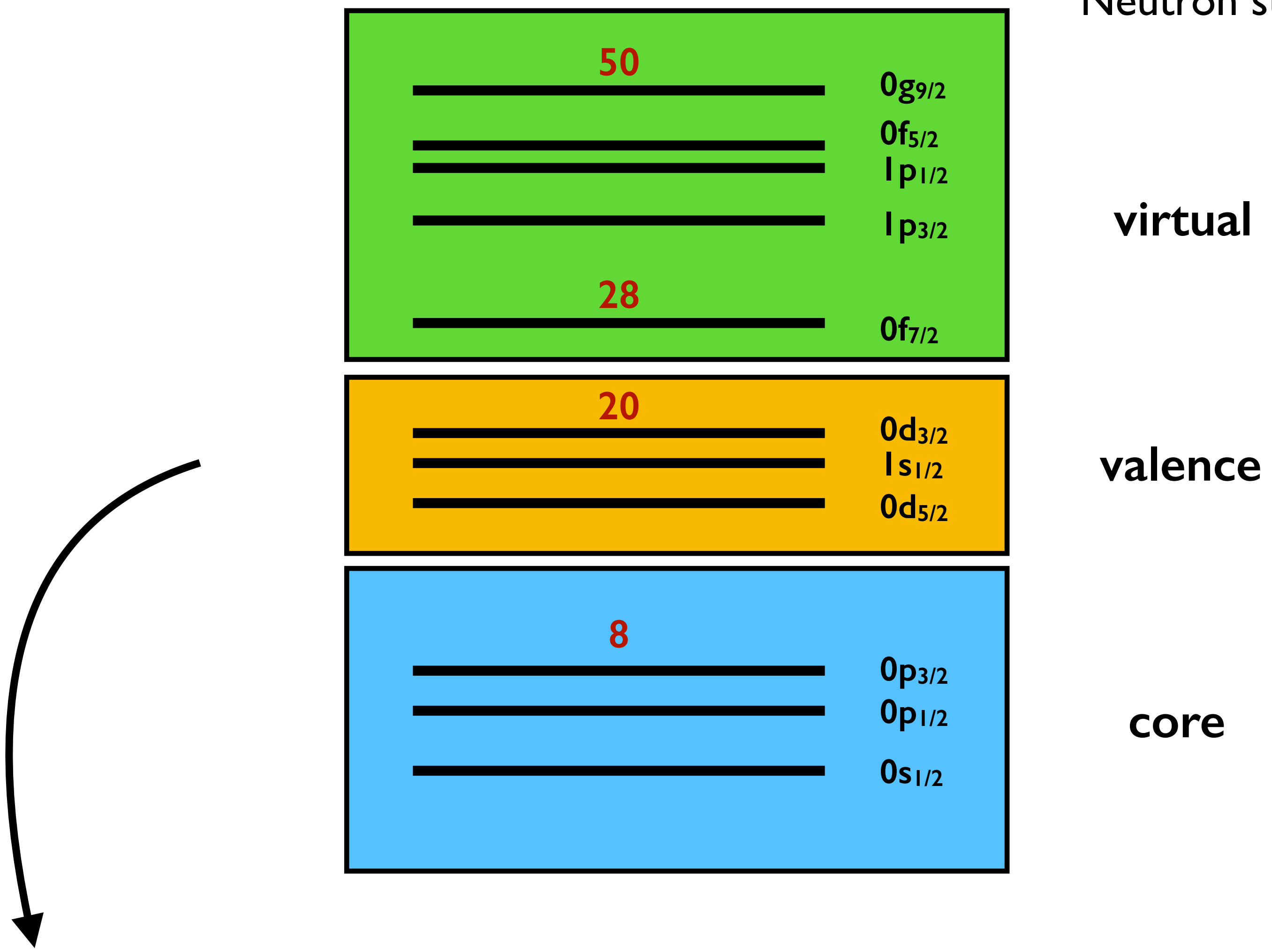
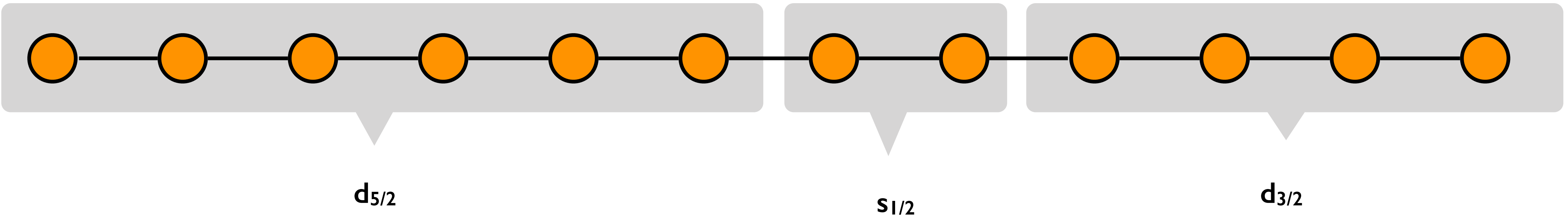
From active spaces to ‘*spin chains*’

Neutron states in *sd*-shell valence space

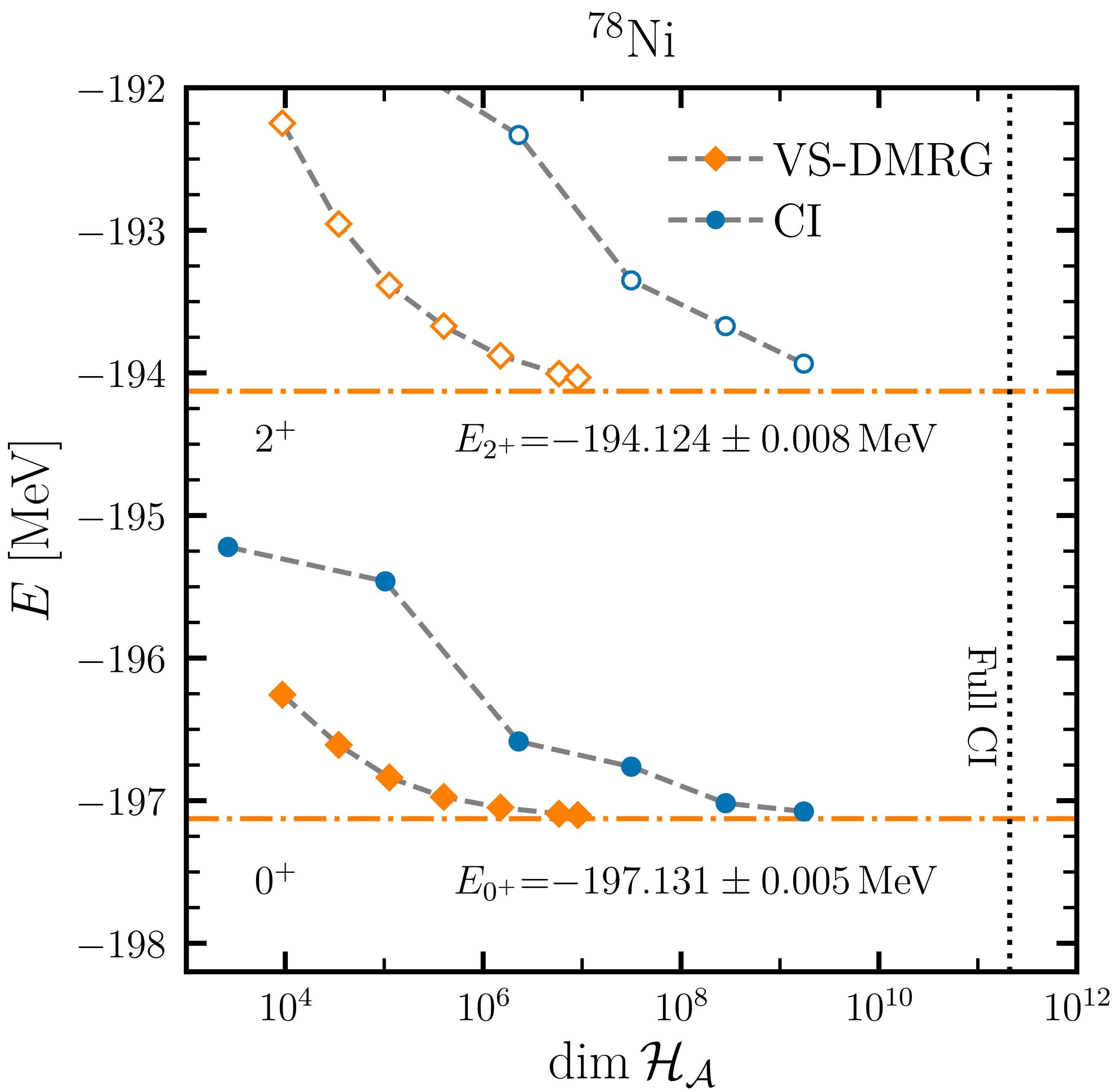


Note: optimization of orbital ordering important!



^{78}Ni: Why DMRG?

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

see also Robin et al., PRC (2021)

- **Entanglement measures** offer better understanding of (nuclear) correlation effects

Entanglement

see also Robin et al., PRC (2021)

- Entanglement measures offer better understanding of (nuclear) correlation effects

- Partition orbital space: reduced density matrices from partial trace operations

(A, B two subsystems)

$$\rho_A = \mathrm{Tr}_B\, \rho_{AB}$$

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- Orbital entanglement from **orbital-reduced density matrix**: $A=\{i\}$ and $B=\{\text{rest of basis}\}$

$$\rho_i = \begin{pmatrix} 1-\gamma_{ii} & 0 \\ 0 & \gamma_{ii} \end{pmatrix}$$

γ: reduced density matrix
(NOT orbital-reduced matrix!)

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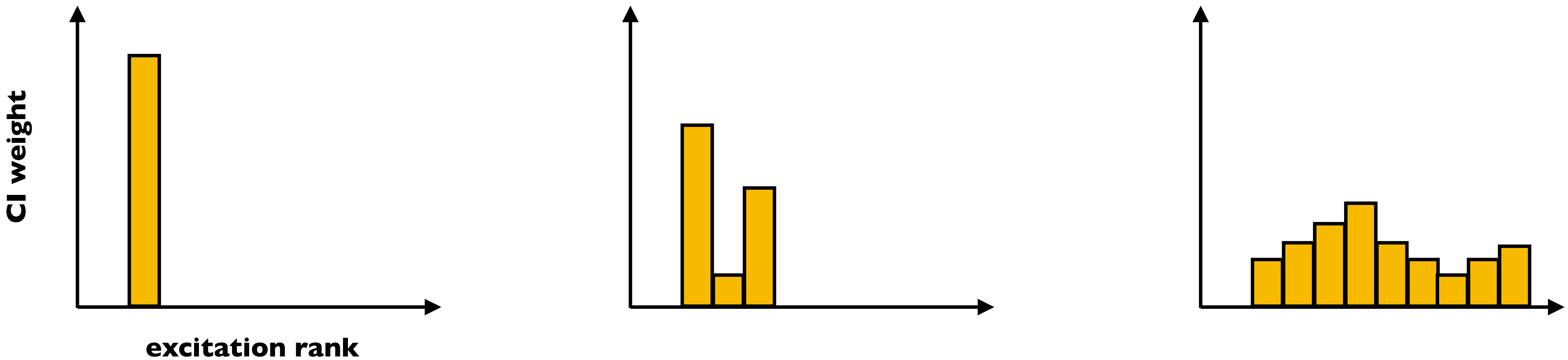
- Total correlation obtained from sum of single-orbital entropies

$$S_{\text{total}} = \sum_i s_i$$

Naive expectations

Naive picture from CI expansion



uncorrelated
(mean-field state)

weakly correlated
(HF + single/double excitations)

collective state
(complicated structure)

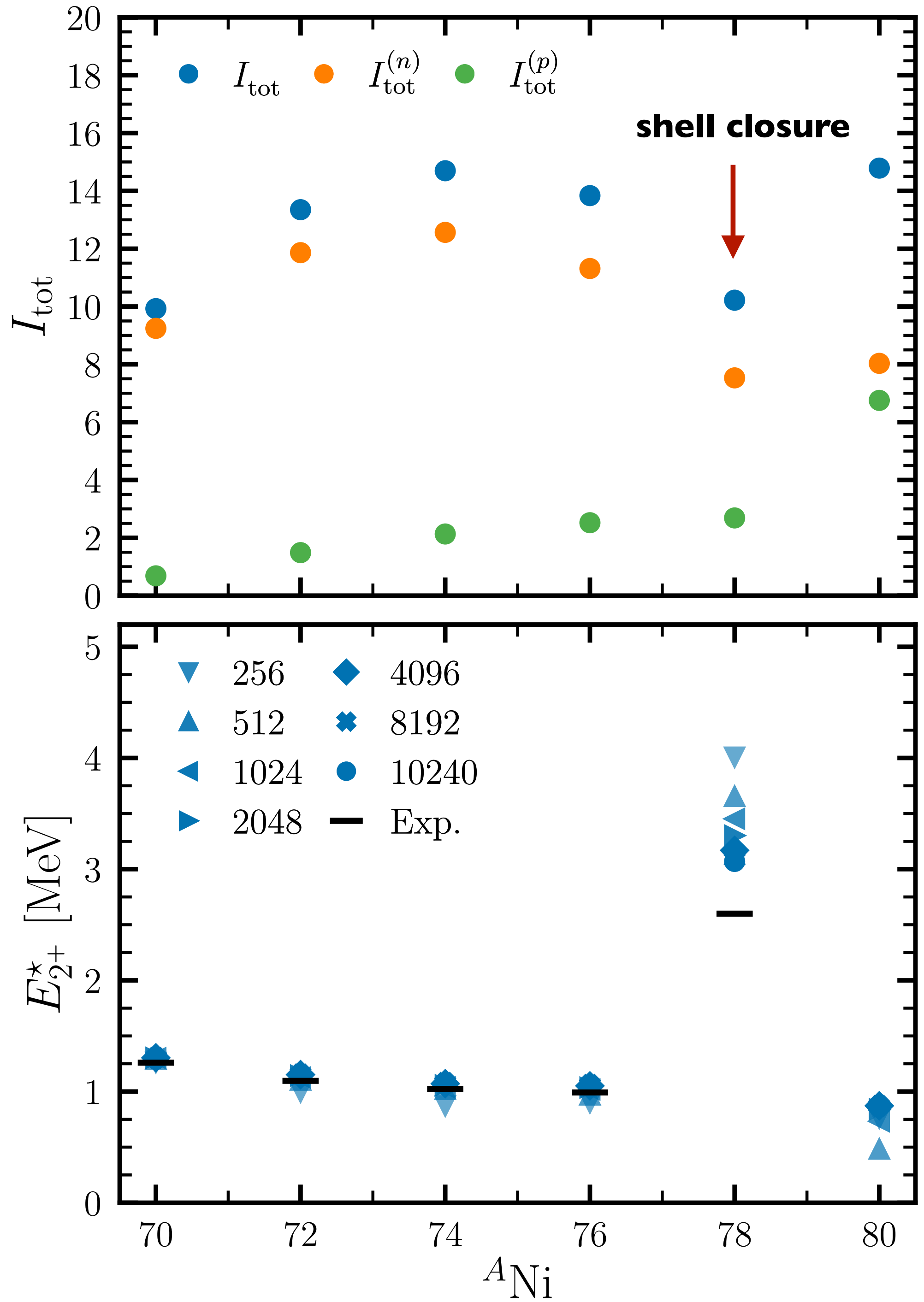
closed-shell nuclei

open-shell nuclei

Entropies and shell structure

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

Total entropy in even-mass nickel isotopes



Tichai *et al.*, arXiv:2207.01438

- Pronounced kink at ^{78}Ni hints at **neutron shell closure** (~ dominated by HF)
- **Larger bond dimensions** required to converge ^{78}Ni excited state
- Agreement with **conventional prediction** based on 2^+ excitation energies
- Deviation from experiment attributed to missing triples corrections: **IMSRG(3)**

Total entropy is a good proxy for shell closures!

(… but non-observable and basis dependent!)

Pairwise correlations

- **Better understanding of orbital correlation effects between two states**

$$\rho_{AB} = \mathrm{Tr}_C\, \rho_{ABC}$$

A = {orbit i}
B = {orbit j}
C = {rest of basis}

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- **Two-orbital-reduced density matrix encodes pairwise entanglement**

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two-body density required!

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two-body density required!

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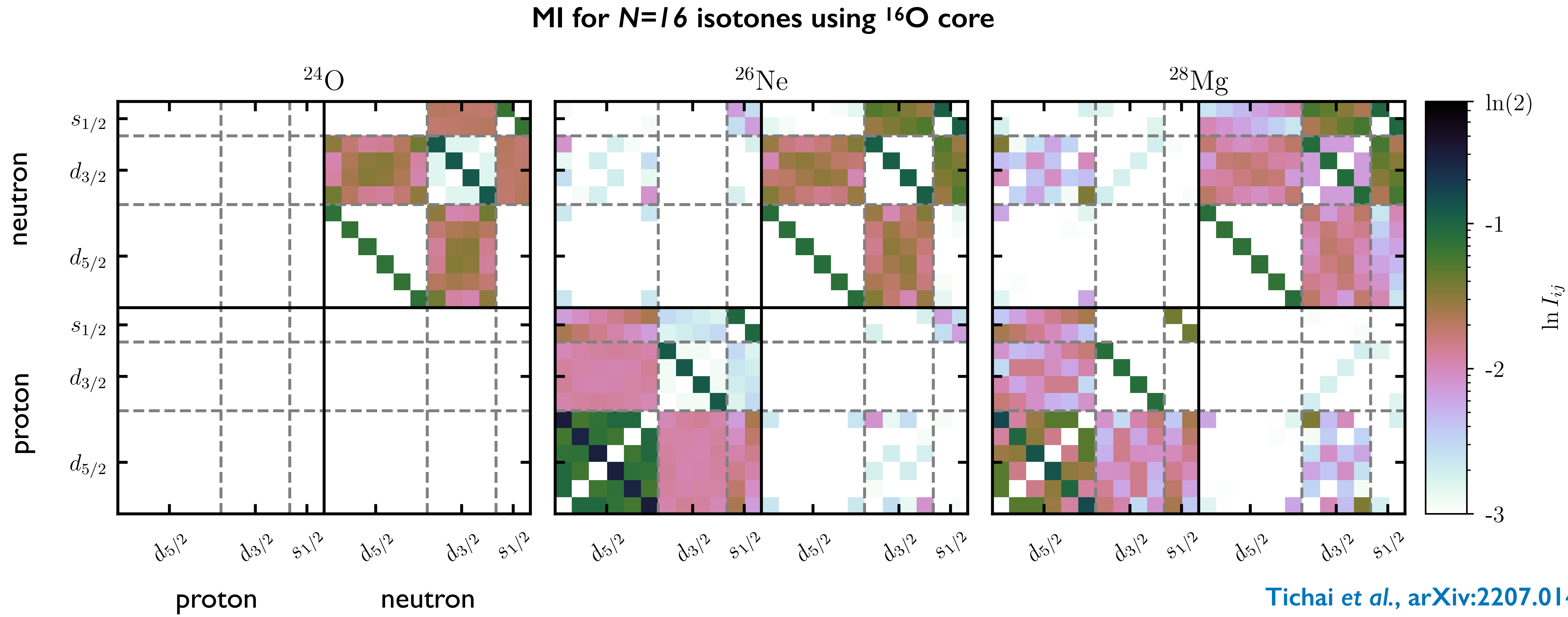
- Mutual information combines one- and two-particle entanglement

$$I_{ij} = s_i + s_j - s_{ij}$$

Mutual information in *sd*-shell nuclei



Tichai *et al.*, arXiv:2207.01438

- Vanishing MI from proton contributions in oxygen isotopes due to *sd*-shell
- Indications of BCS-type *nn*- and *pp*-pairing within the same shell (*J=0, M=0, T=1*)
- Proton-neutron correlations suppressed but off-diagonal coupling present

Conclusions

Approximations for three-nucleon forces

- Normal-ordering: complicated 3N as density dependent NN
- Singular value decomposition: complicated 3N as sum of operators
- Converged *ab initio* calculations from ^{3}H up to ^{208}Pb

Next steps: normal ordering for open-shell nuclei/leverage factorization

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Compression of wave function from DMRG

- Superior scaling properties of DMRG over diagonalization approaches
- Understanding entanglement using information-theory tools

Next steps: electromagnetic observables/large-scale DMRG runs

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Thank you for your attention!

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