Low-rank representations of nuclear interactions

INT workshop

Tensor Networks in Many Body and Quantum Field Theory

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TECHNISCHE UNIVERSITÄT DARMSTADT

SFB 1245

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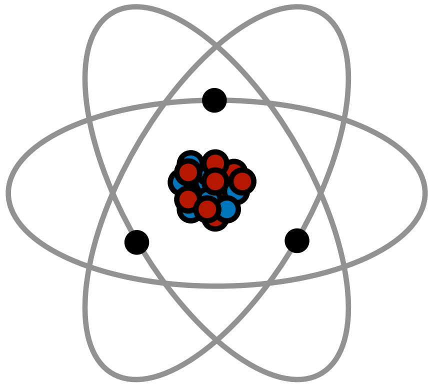


Outline

Introduction - computational challenges

I Low-rank properties of nuclear interactions

- Matrix decompositions in momentum space
- Impact on nuclear observables

II Advanced tensor formats

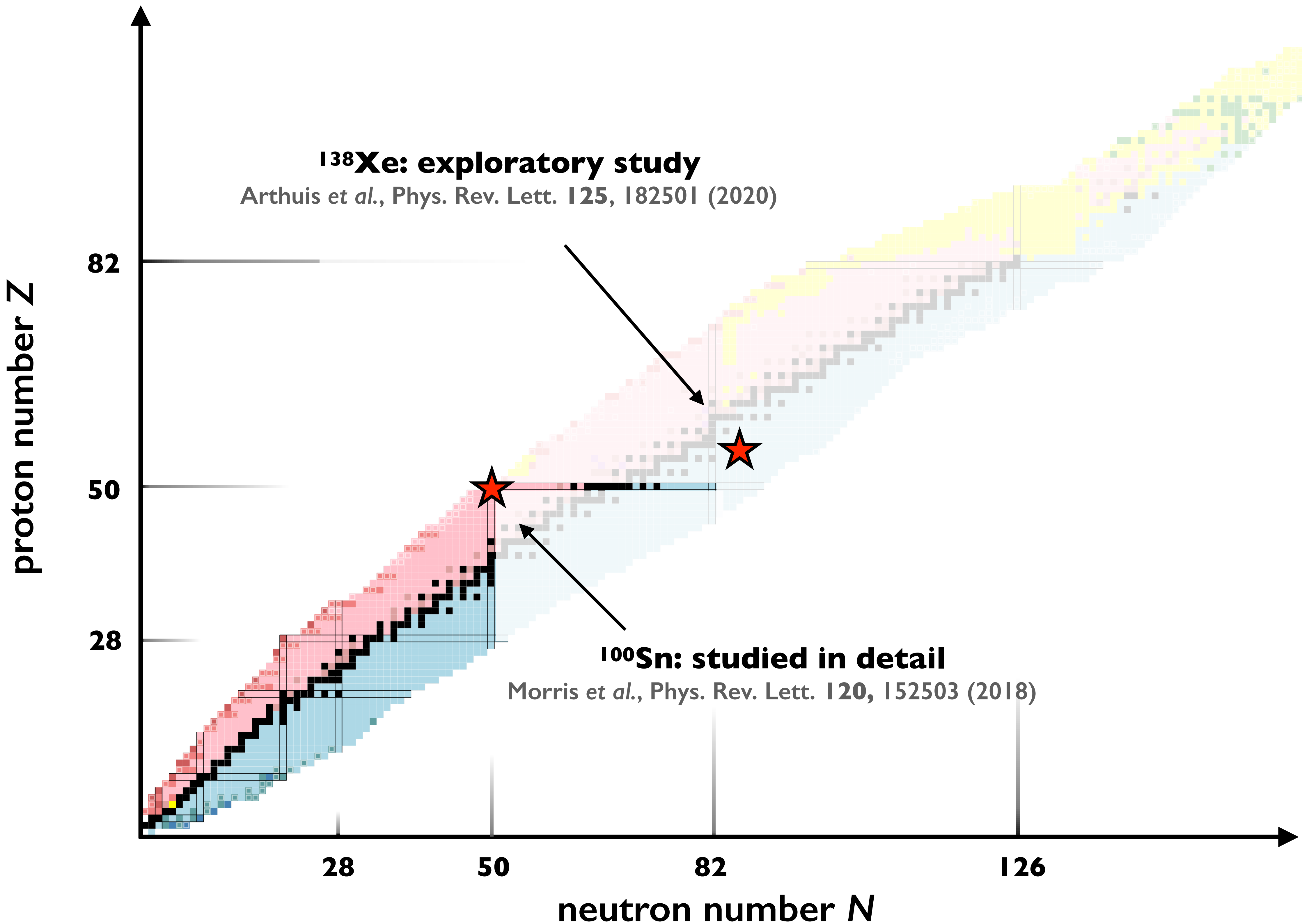
- Decompositions in single-particle bases
- Compression and accuracy

Outline

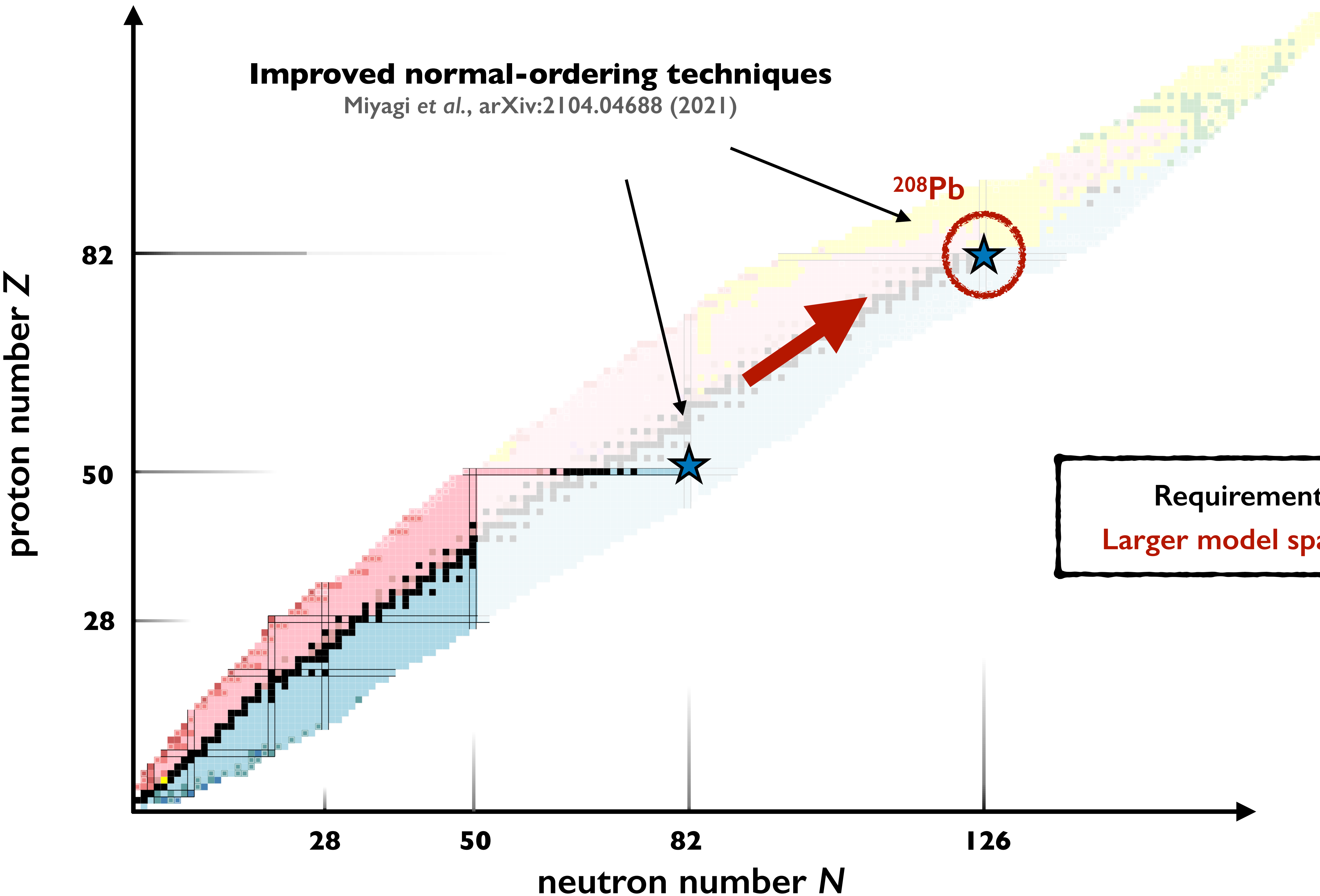
<u>Theme:</u>
How well can nuclear interaction models be compressed for given basis and tensor format?

Introduction:
Computational challenges

Current status of *ab initio* nuclear structure



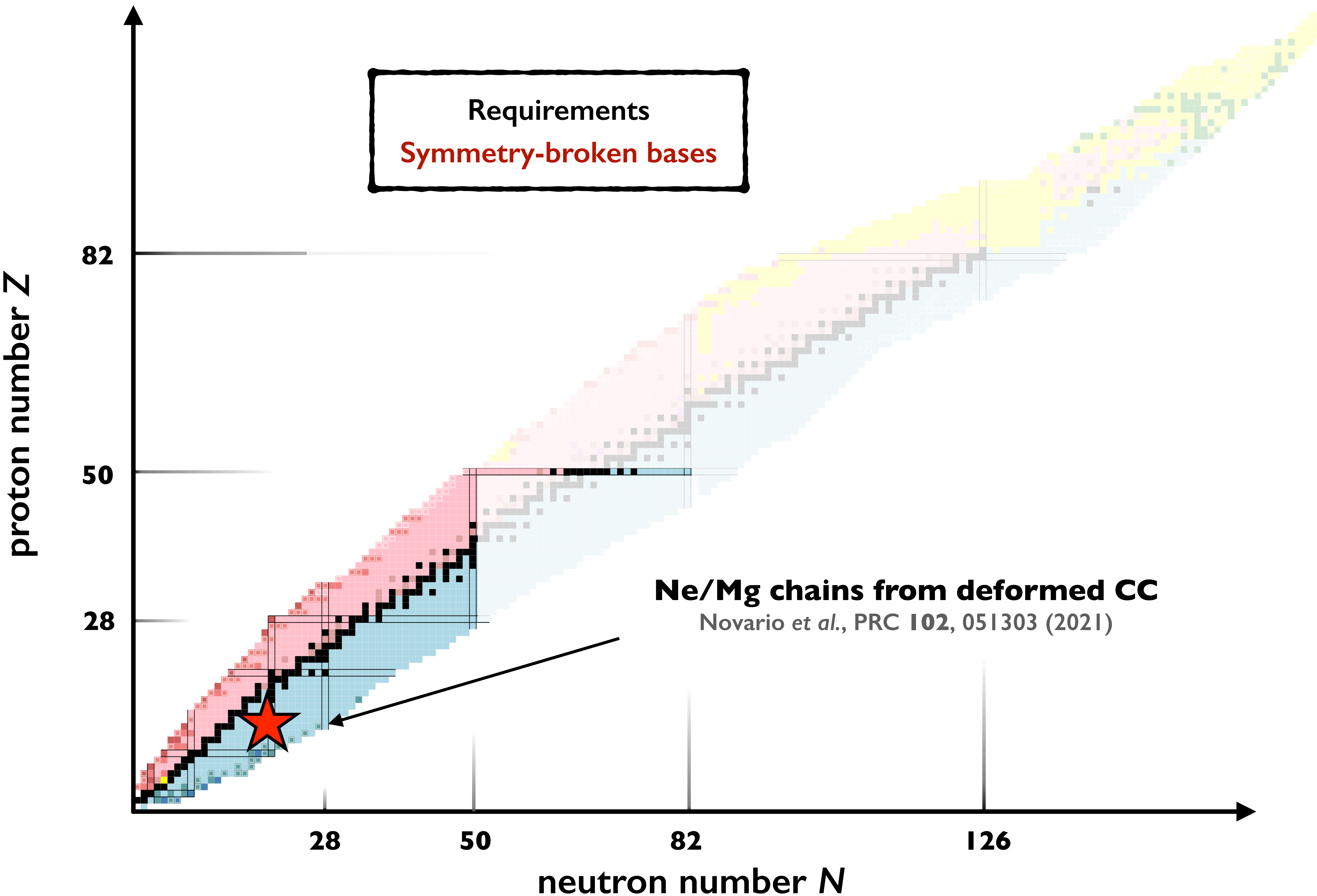
Many-body frontiers: heavy nuclei



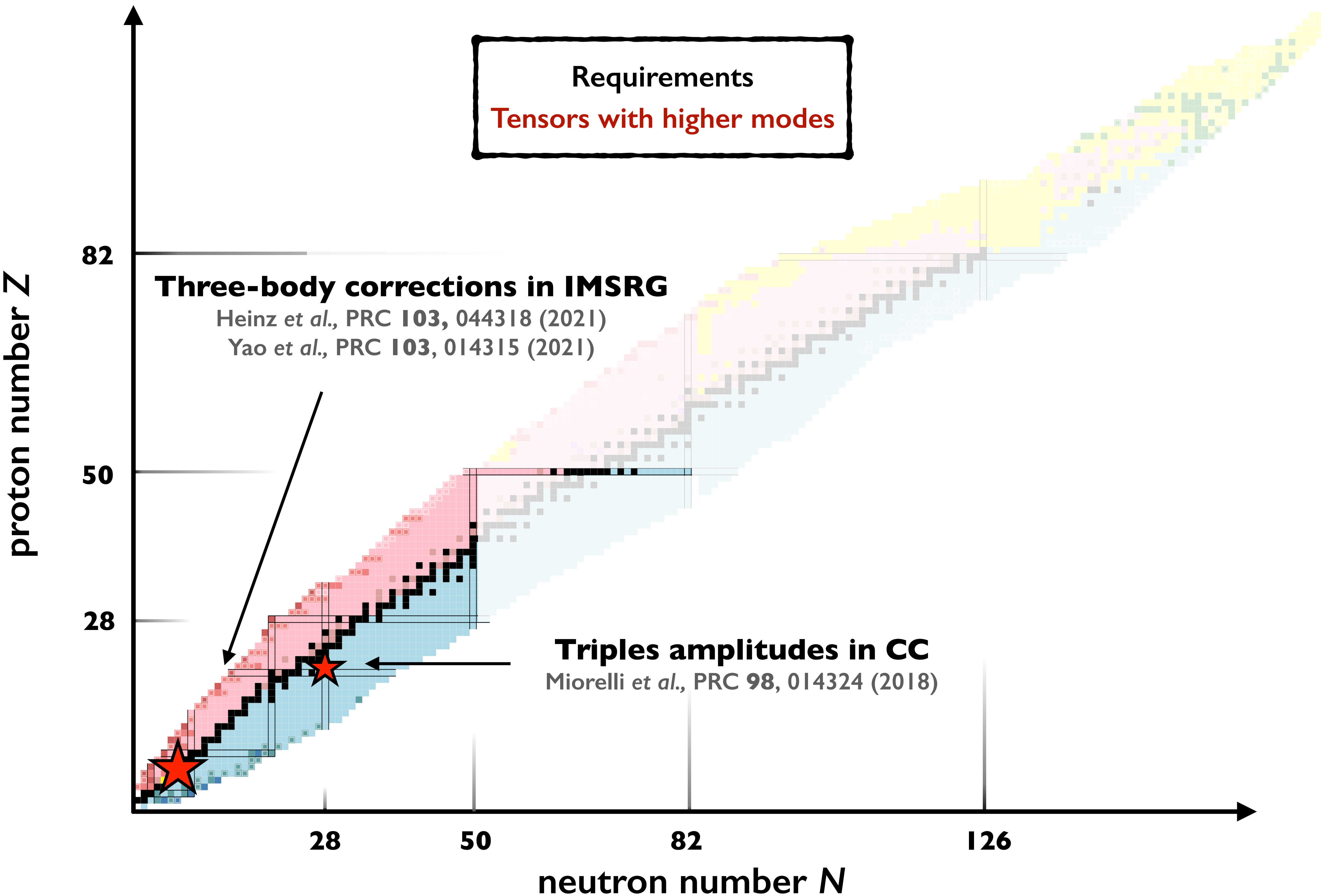
Requirements

Larger model spaces

Many-body frontiers: open-shell nuclei



Many-body frontiers: higher precision

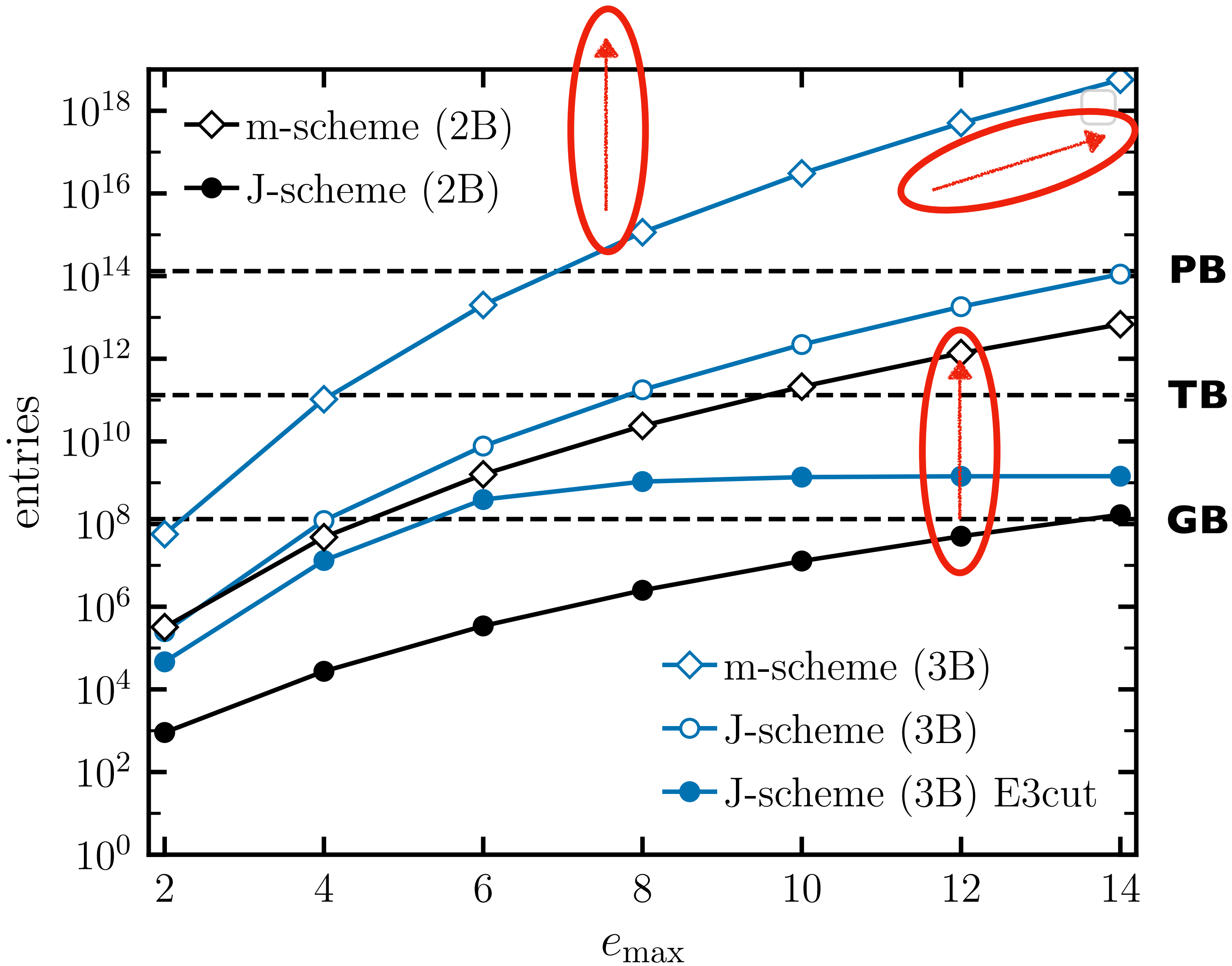


Computational implications

m-scheme: 'spin-unrestricted'
J-scheme: 'spin-restricted'

Higher precision

Better wave function representations require treatment of higher-mode tensors!



Memory scaling of many-body tensors in various bases

Heavy nuclei

Reaching convergence as a function of modelspace size is challenging in heavy nuclei!

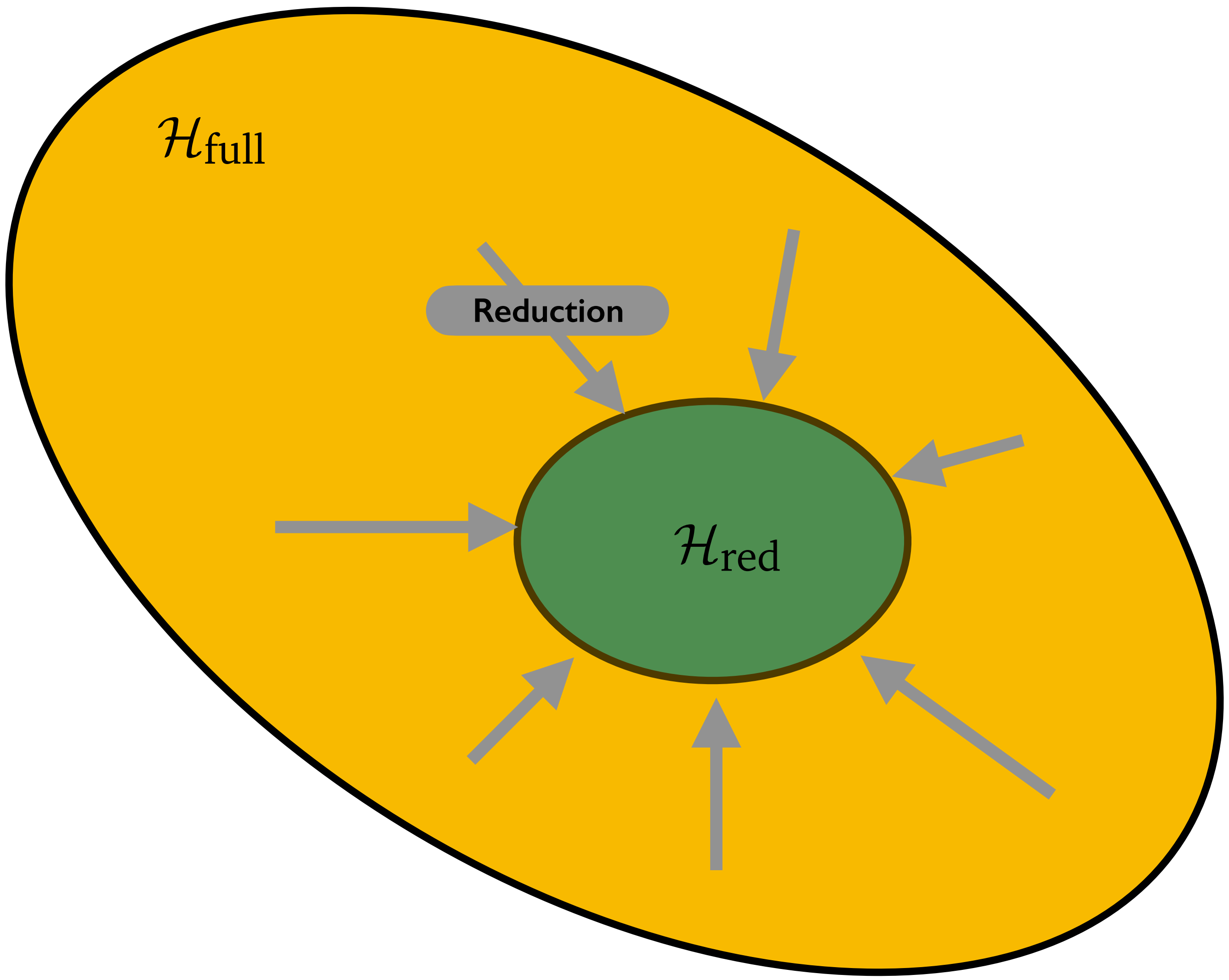
Deformation

Grasping static correlations from breaking spatial symmetries is expensive!

Fighting the exponential wall

Option I:
Subspace selection

$\mathcal{H}_{\mathrm{red}} \subset \mathcal{H}_{\mathrm{full}}$



- Solve many-body problem for selected subspace
- Gauge importance based on computationally cheap measure
- Scaling reduction in practice

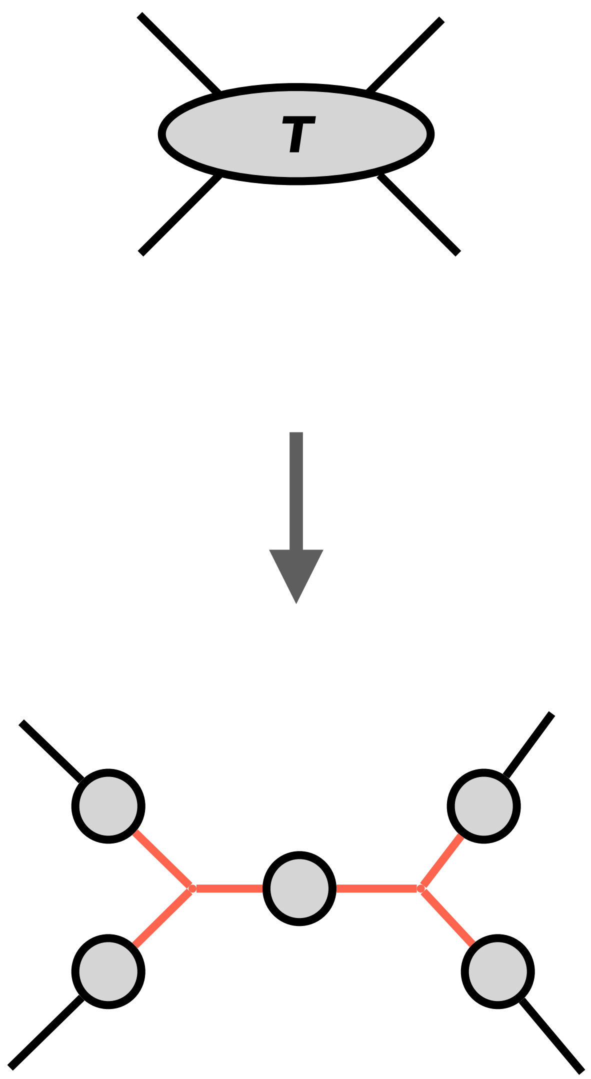
$$N^p \quad \longrightarrow \quad \alpha\, N^p$$

- Danger: potential bias from the selection procedure (typically PT)
- Many successful applications in various many-body frameworks

CI, CC, SCGF, ….

Fighting the exponential wall

Option II:
Tensor factorization



example for *tensor hypercontraction* format

- Employ different representation using decomposition techniques

- Size of rank controls accuracy of the tensor factorization

- Scaling reduction in practice

$$N^p \quad \rightarrow \quad N^{p'}$$

- Challenge I: calculation of factors can be numerically demanding

- Challenge II: taking full advantage requires reformulation of many-body approach

Part I
Revealing low-rank structure

Tichai, Arthuis, Hebeler, Heinz, Hoppe, Schwenk, arXiv:2105.03935 (2021)

Matrix decompositions

- **Prototype of a matrix factorization: singular value decomposition (SVD)**

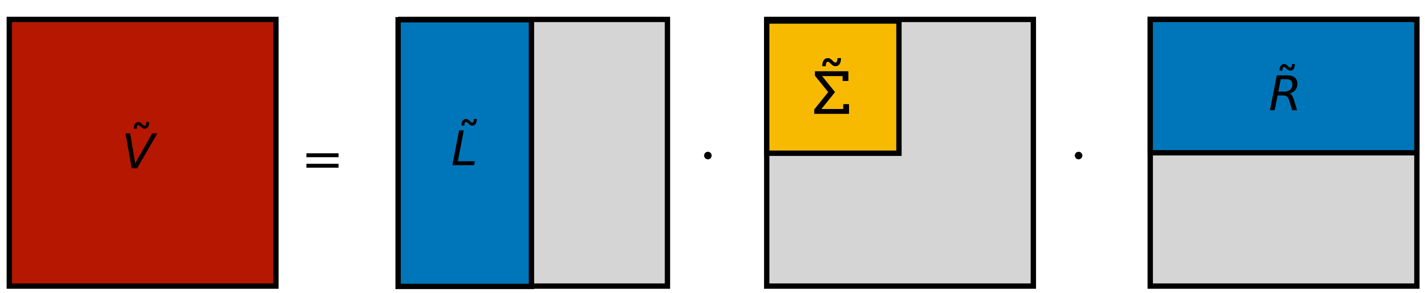
singular values (non-negative)

$$V = L \Sigma R^T \quad \text{with} \quad \Sigma = \text{diag}(s_1, \dots, s_n)$$

left/right singular vectors

- **Truncated singular valued decomposition: keep only largest singular values**

$$\tilde{V} = \tilde{L} \tilde{\Sigma} \tilde{R}^T \quad \text{with} \quad \tilde{\Sigma} = \text{diag}(s_1, \dots, s_{R_{\text{SVD}}}, 0, \dots, 0)$$



- **Key question: how many singular values do we need to keep for good accuracy?**

Intermezzo - basis representation

- Momentum-space matrix elements conserving center-of-mass momentum

(no spin/isospin for simplicity)

$$\langle \vec{k}_1 \vec{k}_2 | V_{\mathrm{NN}} | \vec{k}_3 \vec{k}_4 \rangle = \langle \vec{q} \vec{K} | V_{\mathrm{NN}} | \vec{q}\,' \vec{K}' \rangle = \delta(\vec{K} - \vec{K}') \langle \vec{q} | V_{\mathrm{NN}} | \vec{q}\,' \rangle$$

linear dimension: $\sim 10^7$

- Momentum-space matrix element are cast into partial-wave-decomposed form

$$\langle q (LS) J; T M_T | V_{\mathrm{NN}} | q' (L'S) J; T M_T \rangle$$

linear dimension: ~ 100 per channel

- Conservation of symmetries: SVDs in each of the different partial-wave channels

- Coupled channels appear when L ≠ L' and induce a 2-by-2 block structure

(e.g. deuteron $^3S_1$-$^3D_1$ channel)

$$V = \begin{pmatrix} V_{LL} & V_{LL'} \\ V_{L'L} & V_{L'L'} \end{pmatrix}$$

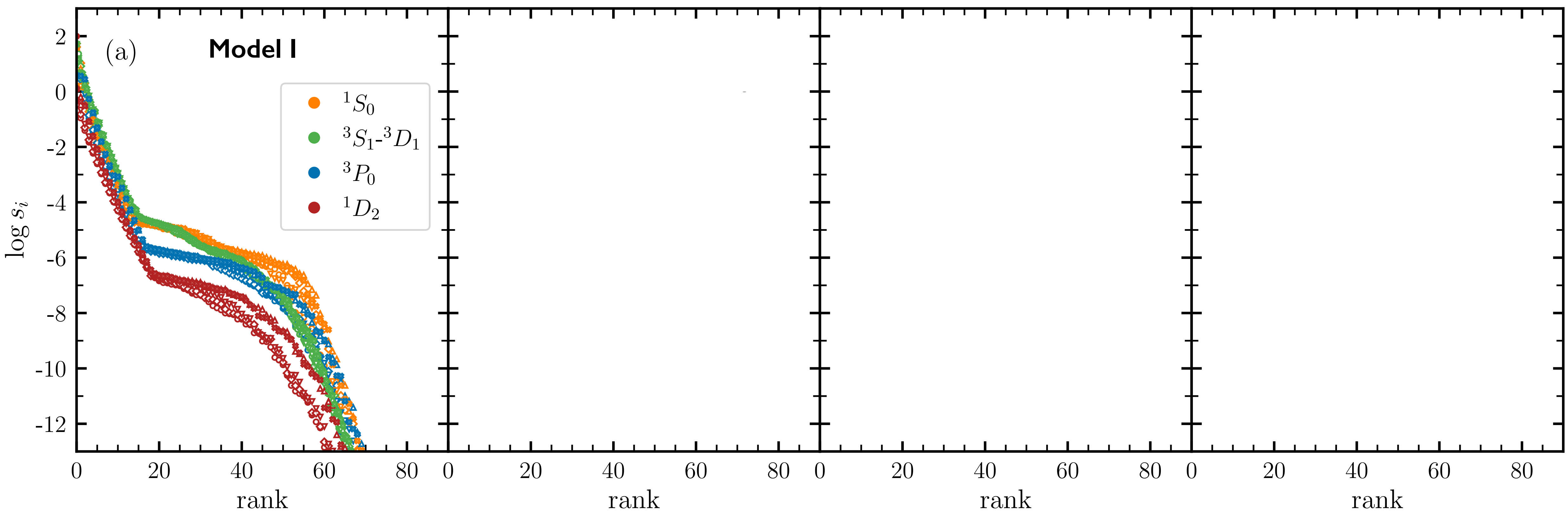
'Full' approach:
(Perform single SVD on two-by-two block matrix)

'Subblock' approach:
(Perform four SVDs on V_{ij})

Interaction benchmark

Model I	EMN 500
Model II	Δ-N²LO$_{GO}$
Model III	GT⁺@N²LO / AV18

Size of singular values vs. SVD rank



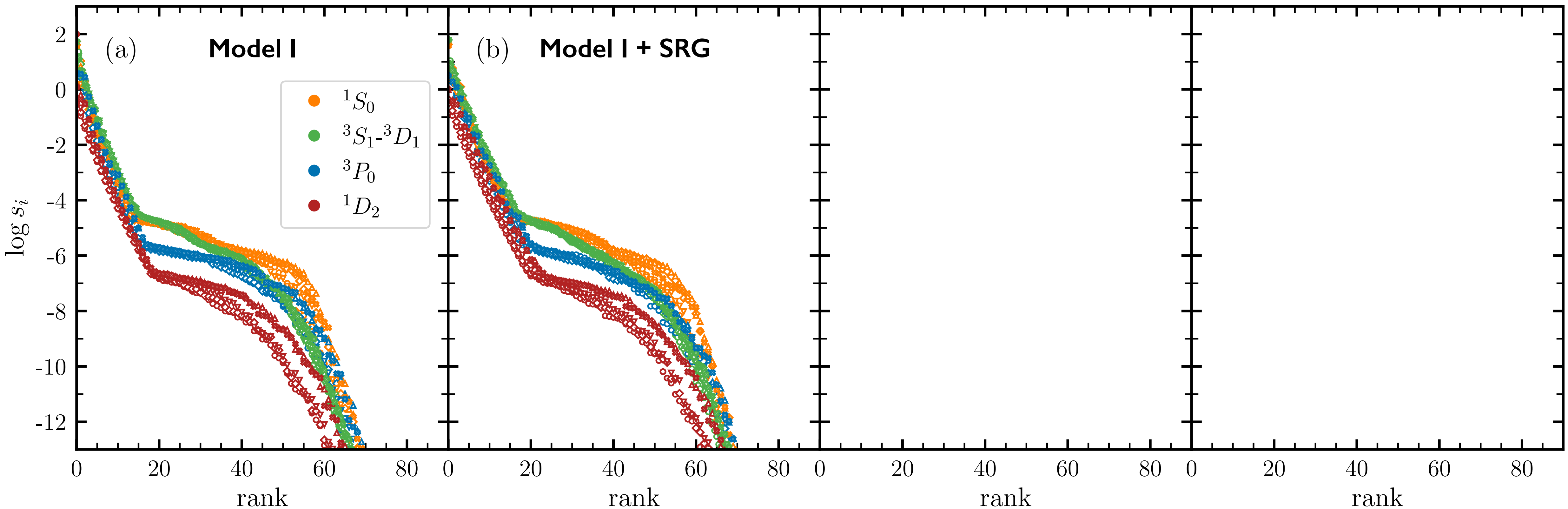
Rapid initial suppression of singular values

(R=5-10 is an excellent approximation)

Interaction benchmark

Model I	EMN 500
Model II	Δ-N^2LO_{GO}
Model III	GT^+@N^2LO / AV18

Size of singular values vs. SVD rank



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

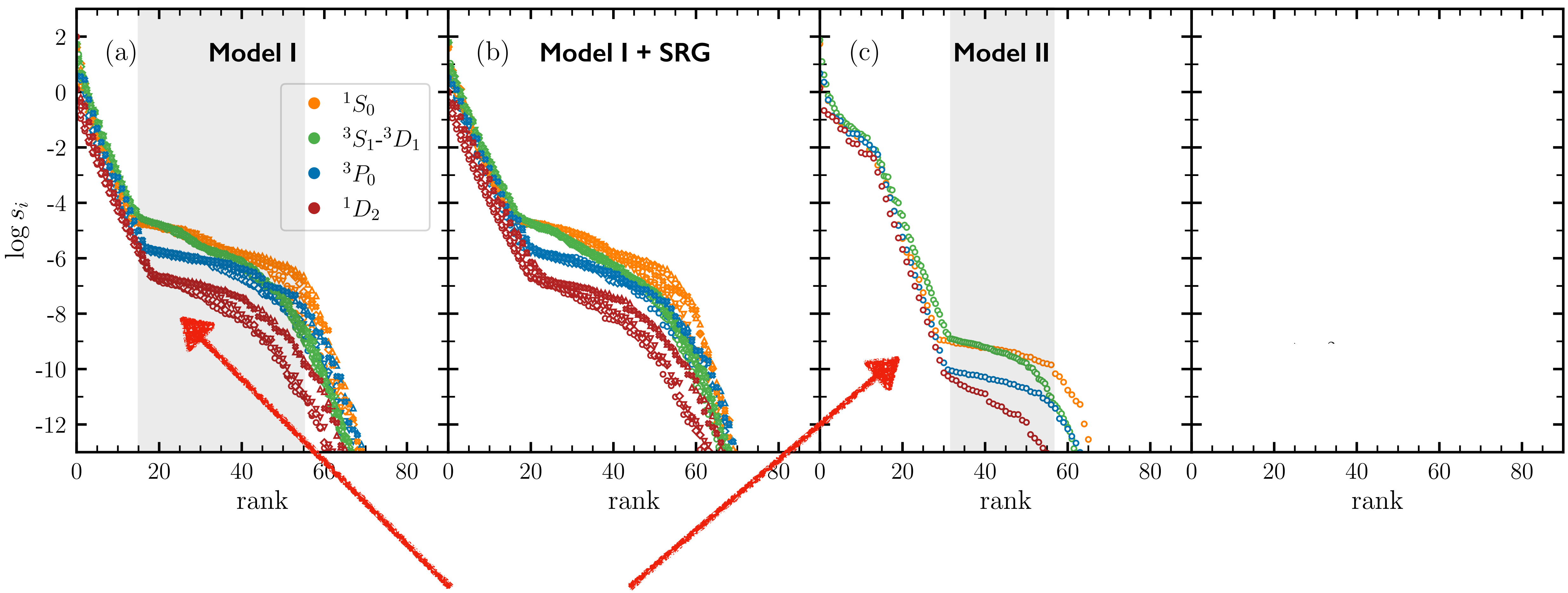
Similarity renormalization group
(see Heiko's talk!)

Singular spectrum preserved by SRG evolution

Interaction benchmark

Model I	EMN 500
Model II	Δ-N^2LO_{GO}
Model III	GT^+@N^2LO / AV18

Size of singular values vs. SVD rank

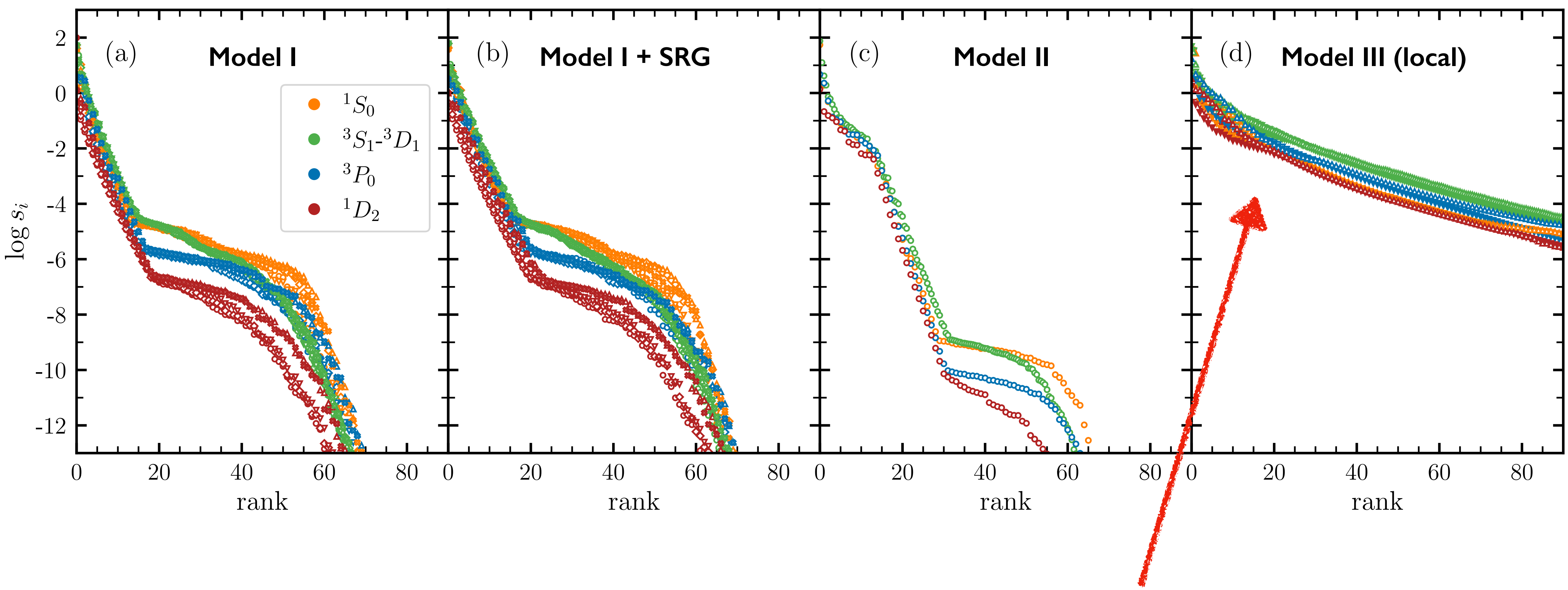


Different interactions yield different suppression details

Interaction benchmark

Model I	EMN 500
Model II	Δ-N²LO$_{GO}$
Model III	GT⁺@N²LO / AV18

Size of singular values vs. SVD rank

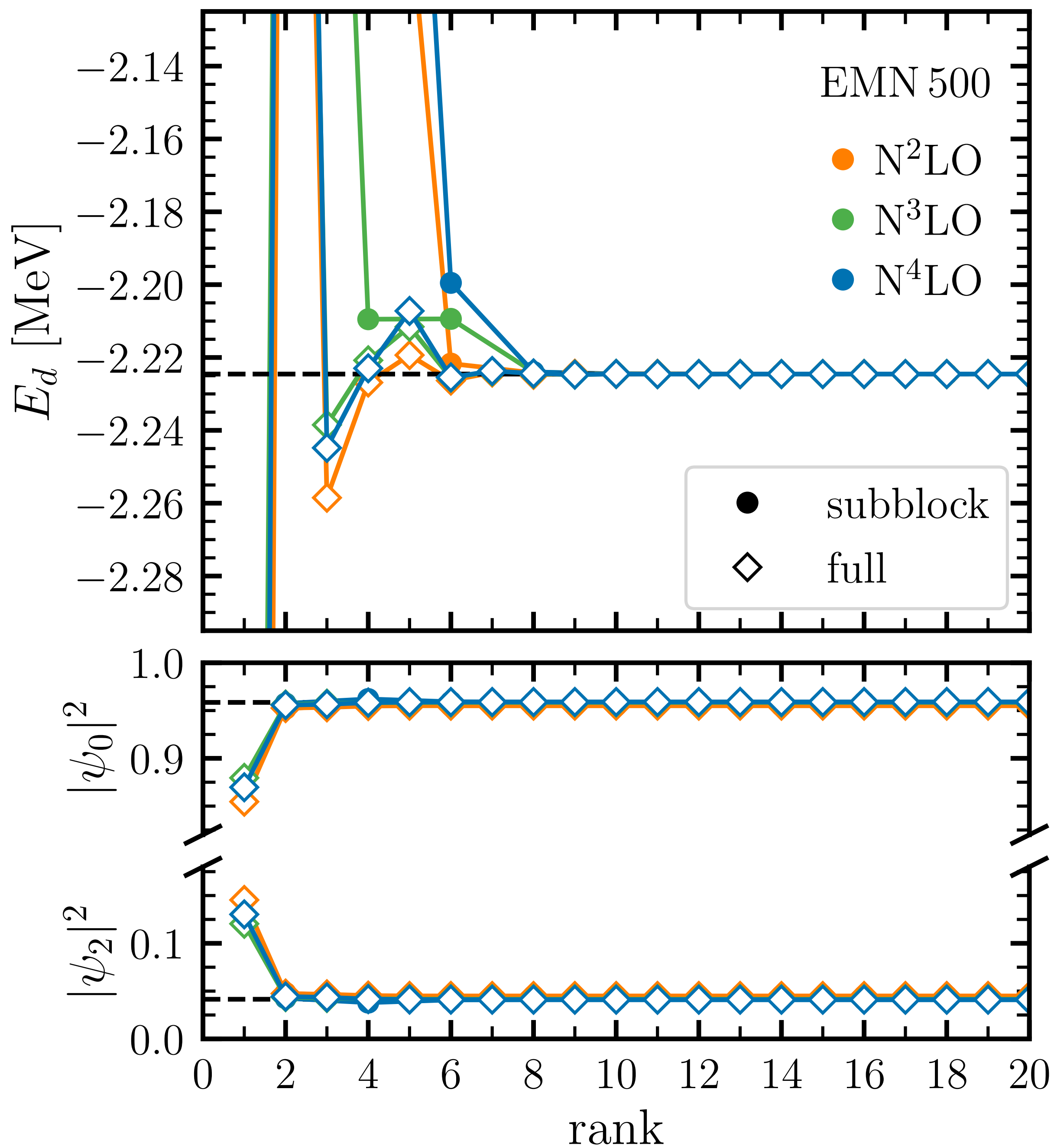


qualitatively different from model I/II

(no low-rank decomposition possible!)

Deuteron calculations

Deuteron ground-state properties vs. SVD rank

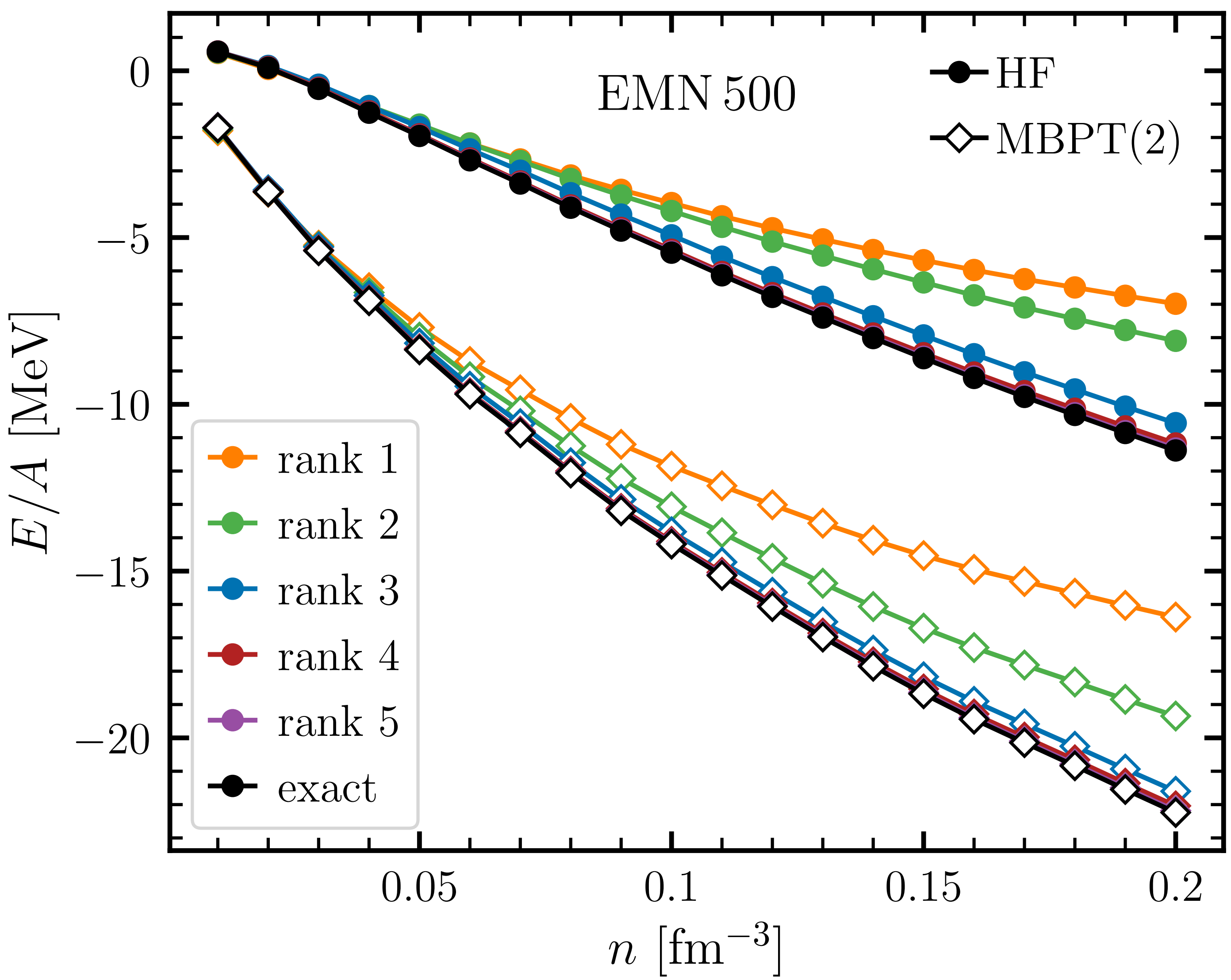


- Ground-state energy and wave function converge rapidly with SVD rank
- Chiral truncation order has no impact on the quality of results
- 1%-accuracy threshold reached at SVD ranks R=4-6
- Quality of results independent of *'decomposition mode'*

subblock vs. full

Many-body applications I - nuclear matter

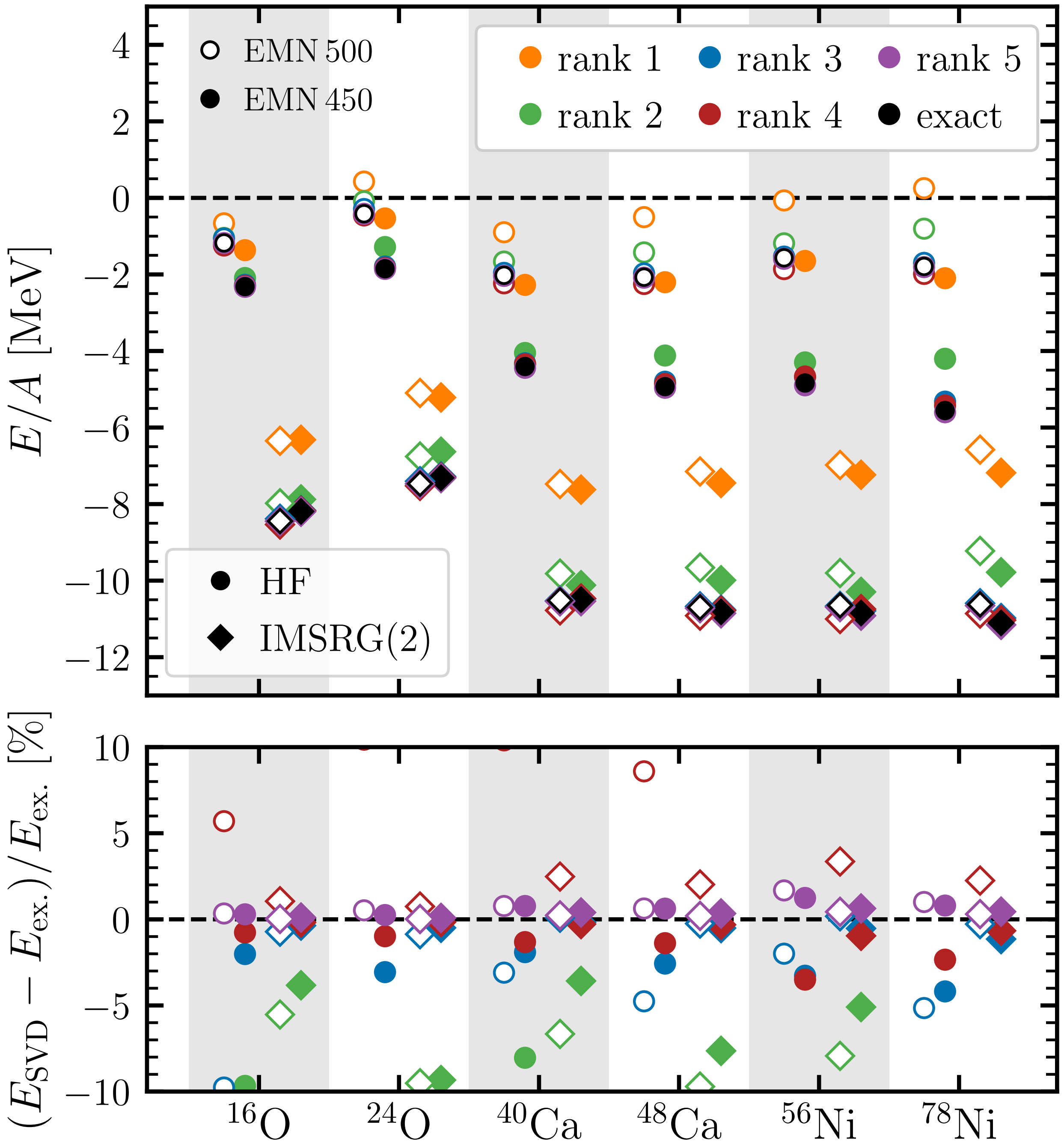
Symmetric nuclear matter vs. SVD rank



- **Systematic convergence of energy per particle with SVD rank: HF and MBPT**
- **Slightly larger error observed with increasing density but relative error is constant**
- **Rank-5 approximation yields virtually exact reproduction of untruncated calculation**
- **Lack of saturation due to missing three-nucleon forces**

Many-body applications II - finite nuclei

Large-scale medium-mass calculations vs. SVD rank



e_{max}=14, bare, EMN450/500 @ N^{3}LO

- **Systematic convergence** of energy per particle with SVD rank: HF and IMSRG(2)
- **Sub-percent accuracy** at SVD-rank 5 at both truncation levels
- ***"SVD converges more slowly"*** for harder interactions
- Potential pathology: **unbound mean-field solution** for separable case (rank one)
- Quality of low-rank SVD **independent of mass number**

Part II
Advanced tensor formats for applications in finite nuclei

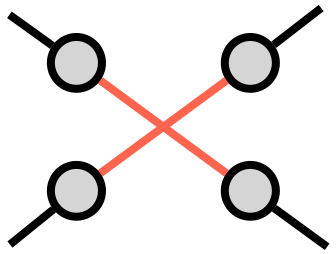
Tichai, Schutski, Scuseria, Duguet, PRC **99**, 034320 (2019)
Tichai, Ripoche, Duguet, EPJA 55:90 (2019)

Tensor formats

Hohenstein, Parrish, Martinez, Schutski, Scuseria, …

- Canonical polyadic decomposition (CPD): decoupling of all external indices

$$\tilde{T}_{k_1 k_2 k_3 k_4} = \sum_{\alpha}^{R_{\mathrm{CPD}}} X^1_{k_1\alpha} X^2_{k_2\alpha} X^3_{k_3\alpha} X^4_{k_4\alpha}$$



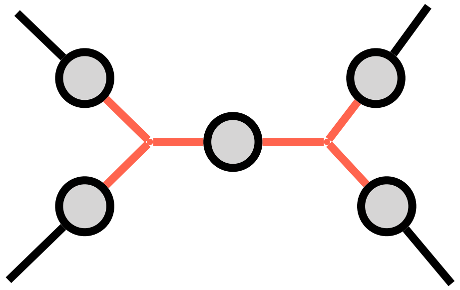
- CPD naturally extends to higher modes but is computationally demanding

$$\mathcal{O}(N^{d-1} \cdot R_{\mathrm{CPD}} \cdot n_{\mathrm{iter}})$$

- Tensor hypercontraction (THC): decoupling only among bra and ket indices

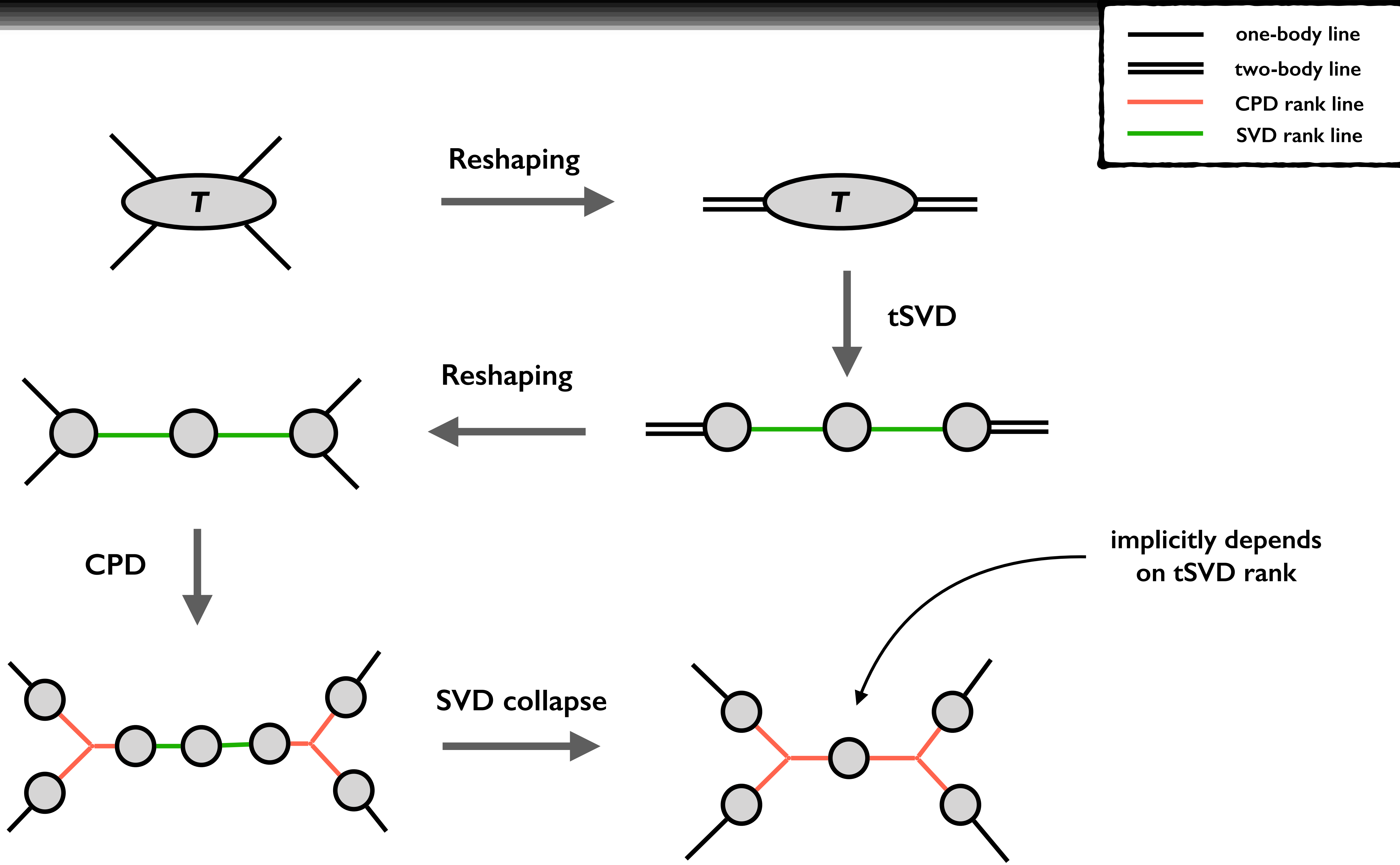
$$\tilde{T}_{k_1 k_2 k_3 k_4} = \sum_{\alpha\beta}^{R_{\mathrm{THC}}} X^1_{k_1\alpha} X^2_{k_2\alpha} W_{\alpha\beta} X^3_{k_3\beta} X^4_{k_4\beta}$$

core tensor



- Hybrid tensor format merging central ideas from tSVD and CPD

How to obtain the THC format



final THC format

Intermezzo - basis representation

- Full single-particle basis states as eigenstates of one-body operator

$$|k\rangle \equiv |n_k(l_k s_k) j_k m_{j_k} t_k\rangle$$

- Introduce spherical state via reduced index without angular-momentum projection

$$|\tilde{k}\rangle \equiv |n_k(l_k s_k) j_k t_k\rangle$$

- Employ angular-momentum coupling to obtain eigenstates of J^2 operator

$$|\tilde{k}_1 \tilde{k}_2 (JM)\rangle \equiv \sum_{m_{k_1} m_{k_2}} \left(\begin{matrix} j_{k_1} & j_{k_2} \\ m_{k_1} & m_{k_2} \end{matrix} \middle| \begin{matrix} J \\ M \end{matrix} \right) |k_1 k_2\rangle$$

- Final matrix elements are stored in angular-momentum-coupled form

$$\langle \tilde{k}_1 \tilde{k}_2 J | \tilde{O} | \tilde{k}_3 \tilde{k}_4 J \rangle = \sum_{m_{k_1} \dots m_{k_4}} \bar{o}_{k_1 k_2 k_3 k_4} \left(\begin{matrix} j_{k_1} & j_{k_2} \\ m_{k_1} & m_{k_2} \end{matrix} \middle| \begin{matrix} J \\ M \end{matrix} \right) \left(\begin{matrix} j_{k_3} & j_{k_4} \\ m_{k_3} & m_{k_4} \end{matrix} \middle| \begin{matrix} J \\ M \end{matrix} \right)$$

J-scheme matrix elements

m-scheme matrix elements

Clebsch-Gordan coefficients

THC results

- Fast convergence for most channels

$$\langle \tilde{k}_1 \tilde{k}_2 J | H_{\text{intr.}} | \tilde{k}_3 \tilde{k}_4 J \rangle$$

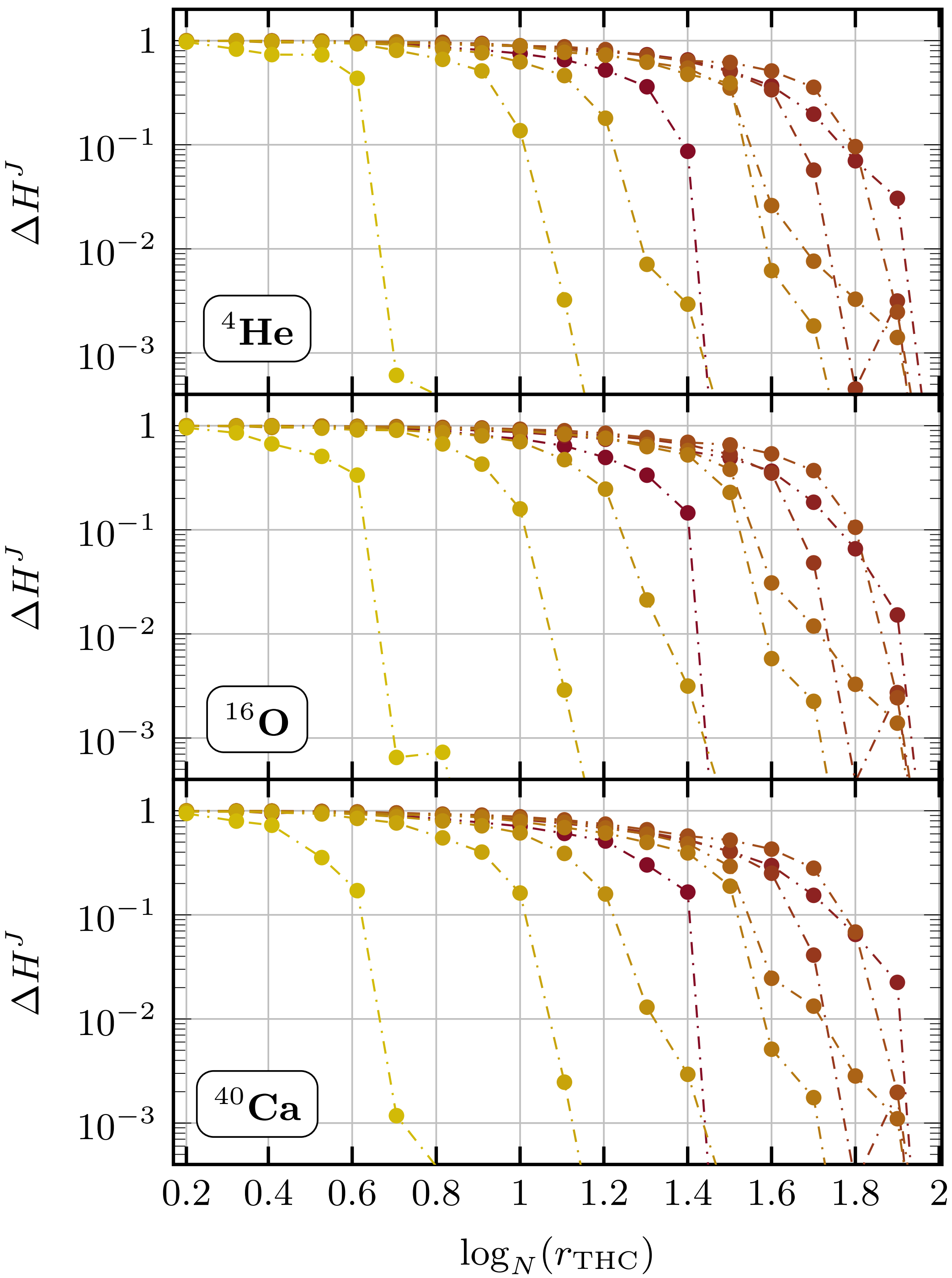
- Intermediate values of two-body angular moment converge slower

- Rapid decrease of decomposition error near critical rank

- Computationally cheaper than CPD

Next step:
Test impact of THC
on observables!

THC decomposition of matrix elements in HF basis



Tichai, Schutski, Scuseria, Duguet, PRC **99**, 034320

Energy denominators

- Perturbation theory expressions naturally involve energy denominators

$$D_{abij} = \frac{1}{\epsilon_a + \epsilon_b - \epsilon_i - \epsilon_j}$$

- Analytical CPD factorization can be obtained via inverse Laplace transform

$$D_{abij} = \int_0^\infty e^{-t(\epsilon_a + \epsilon_b - \epsilon_i - \epsilon_j)} dt$$

- Decomposition factors are obtained via numerical quadrature

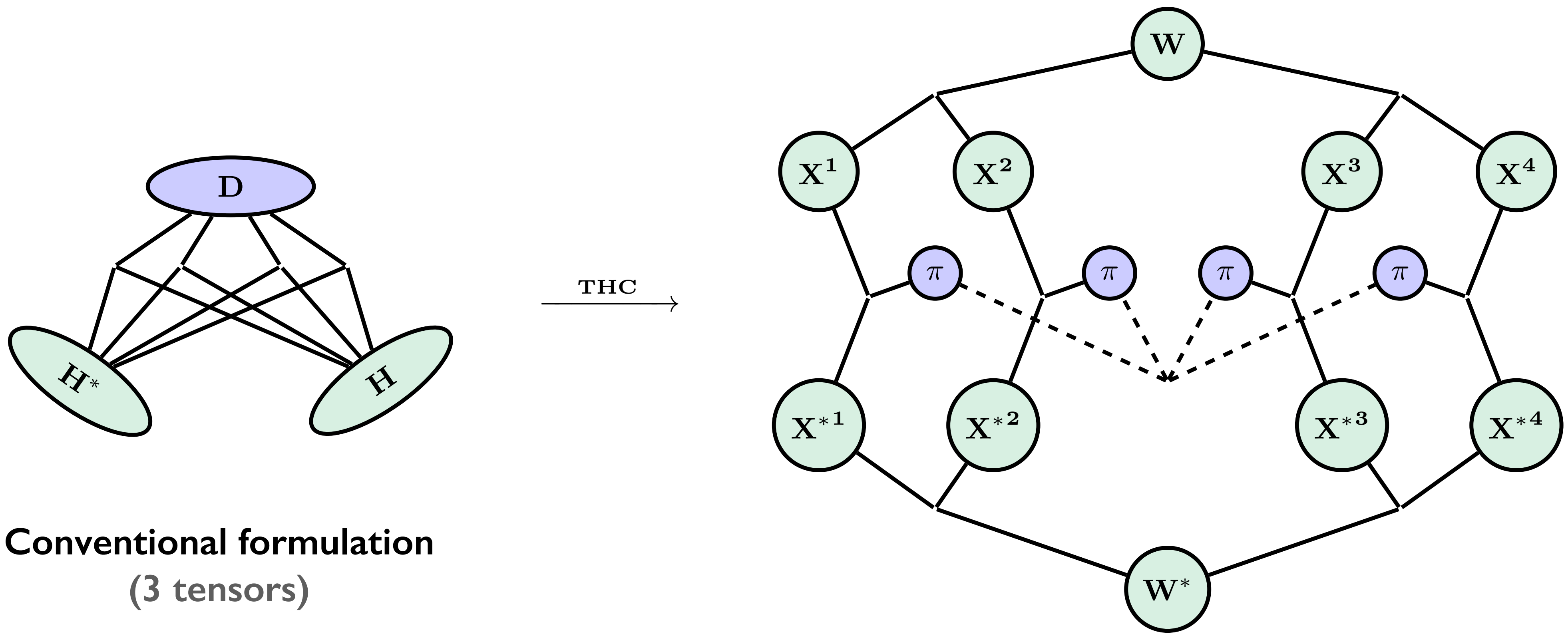
$$\tilde{D}_{abij} = \sum_s \pi_{as} \pi_{bs} \omega_s \pi_{is} \pi_{js}$$

Braess, Hackbusch,
IMA J. Numer. Anal. 25, 685 (2005)

- Integration with very high precision using constant (system-independent) mesh size

- Extension to higher-mode tensors can be done in the same way

THC-factorized MP2



Conventional formulation
(3 tensors)

Factorized formulation
(14 tensors)

- Simple MP2 tensor network replaced by more complicated factorized topology
- General feature: factorized many-body frameworks becomes more complicated

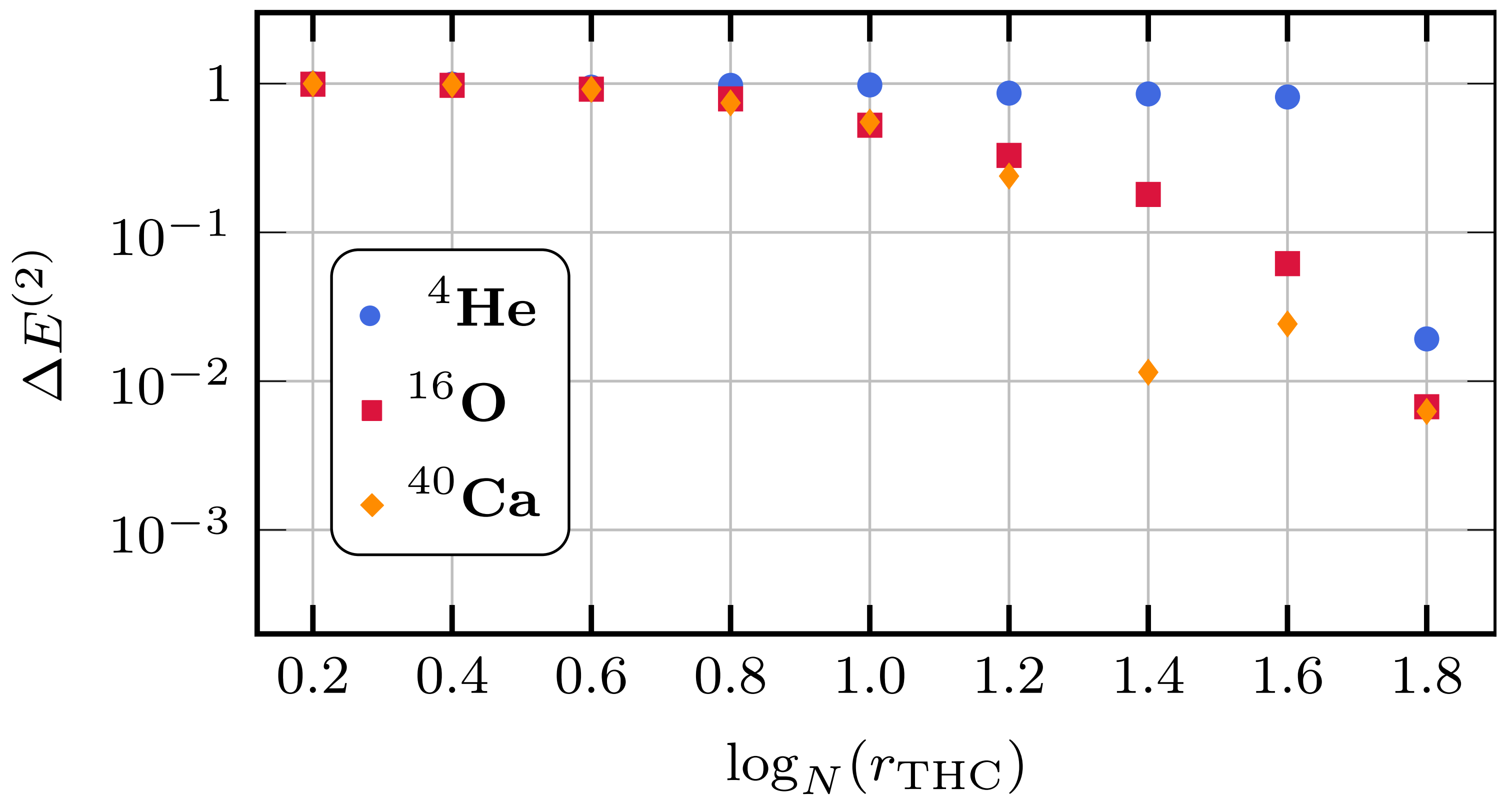
Extension to non-perturbative method non-trivial!

THC-MP2 results

Modelspace:
5 oscillator shells
140 basis functions

Tichai, Schutski, Scuseria, Duguet, PRC **99**, 034320

Error of MP2 as function of THC rank



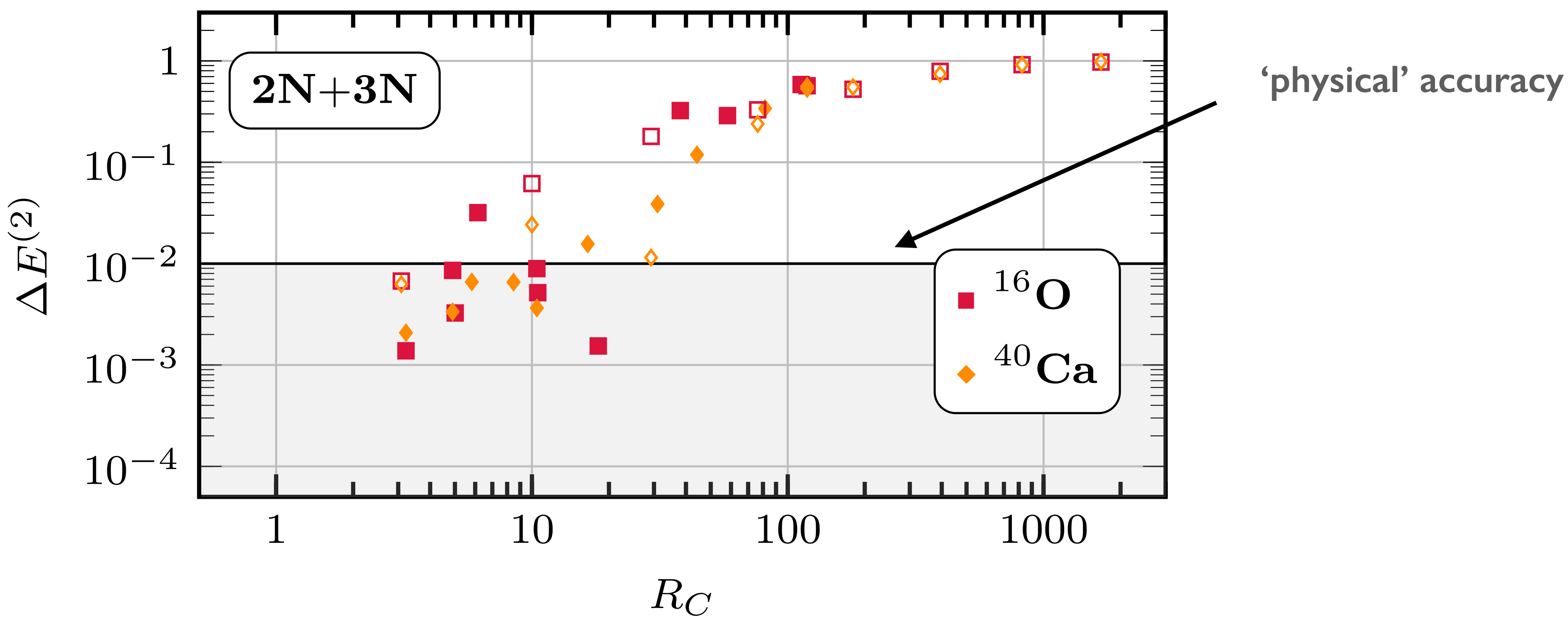
~1% error on E_0
(for soft interaction)

- **Improved accuracy** of correlation energy for higher decomposition ranks
- **Monotonic behaviour** sometimes broken and decomposition in ^{4}He induces jumps
- Correlation error vanishes when approaching the **critical THC rank** of $R_{\text{THC}} = N^2$

Compression rates

Modelspace:
5 oscillator shells
140 basis functions

Correlation between MP2 error and compression rate



- **General trend: higher precision corresponds to lower compression rates**

$$R_C = \frac{\text{full storage}}{\text{compressed storage}}$$

- **Significant compression rates obtained in high-precision regime (*ΔE* < 1%)**
- **Much larger compression rates expected in large model spaces**

Conclusions

Tensor decompositions

- Novel exciting tool to lower computational resources in nuclear theory
- Tensor formats can easily adapt to various situations/symmetries
- First applications show promising performance in nuclear physics

Future work

- Development of new tensor formats specific to nuclear theory applications
- Implementation of large-scale codes to reach larger model spaces
- Adaption of many-body toolchain to factorized tensor representations

Thanks to …

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