Spectroscopy from the valence-space density matrix renormalization group

PAINT 2024

Progress on Ab Initio Nuclear Theory

February 28th, 2024

Tichai *et al.*, PLB (2023)

Tichai *et al.* (2024)

DMRG collaboration

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Outline

Theme:
Scalable *ab initio* simulations from tensor network approaches.

IMSRG and hybrid schemes

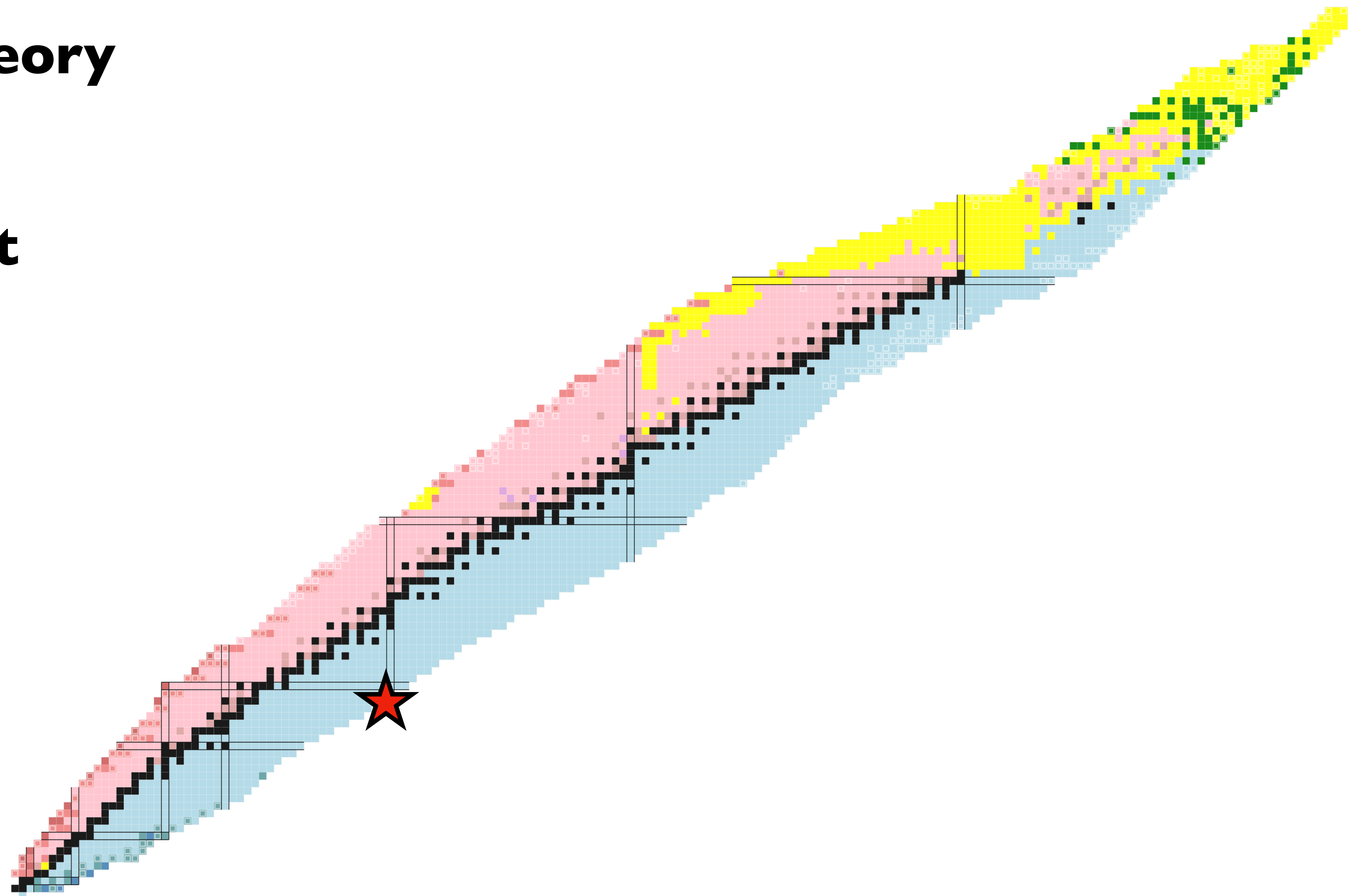
Density matrix renormalization group

Quantum information theory

Nuclear correlations

Many-body entanglement

Perspectives

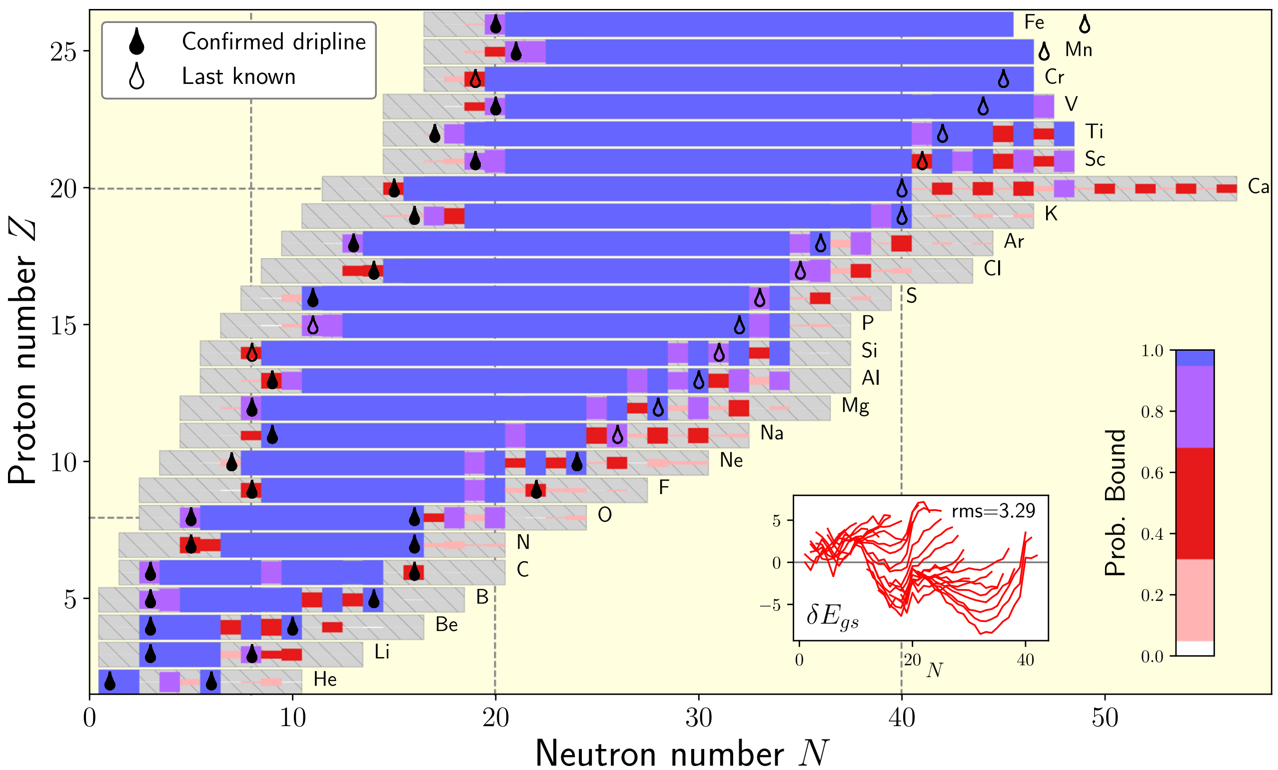


Part I

The valence-space density matrix renormalization group

Advantages of the IMSRG

Global study of ~700 nuclei from IMSRG(2)



Stroberg *et al.*, PRL (2021)

see talks by
Matthias, Ragnar and Heiko!

- **Mild scaling** with system size
- Non-perturbative resummation
- **Flexibility**: enables for targeting diverse set of observables
- **Unitary transformation:** easy interface with other methods
- Successfully **merged** with with many techniques in the past

(In-medium)
RPA, GCM, NCSM, …

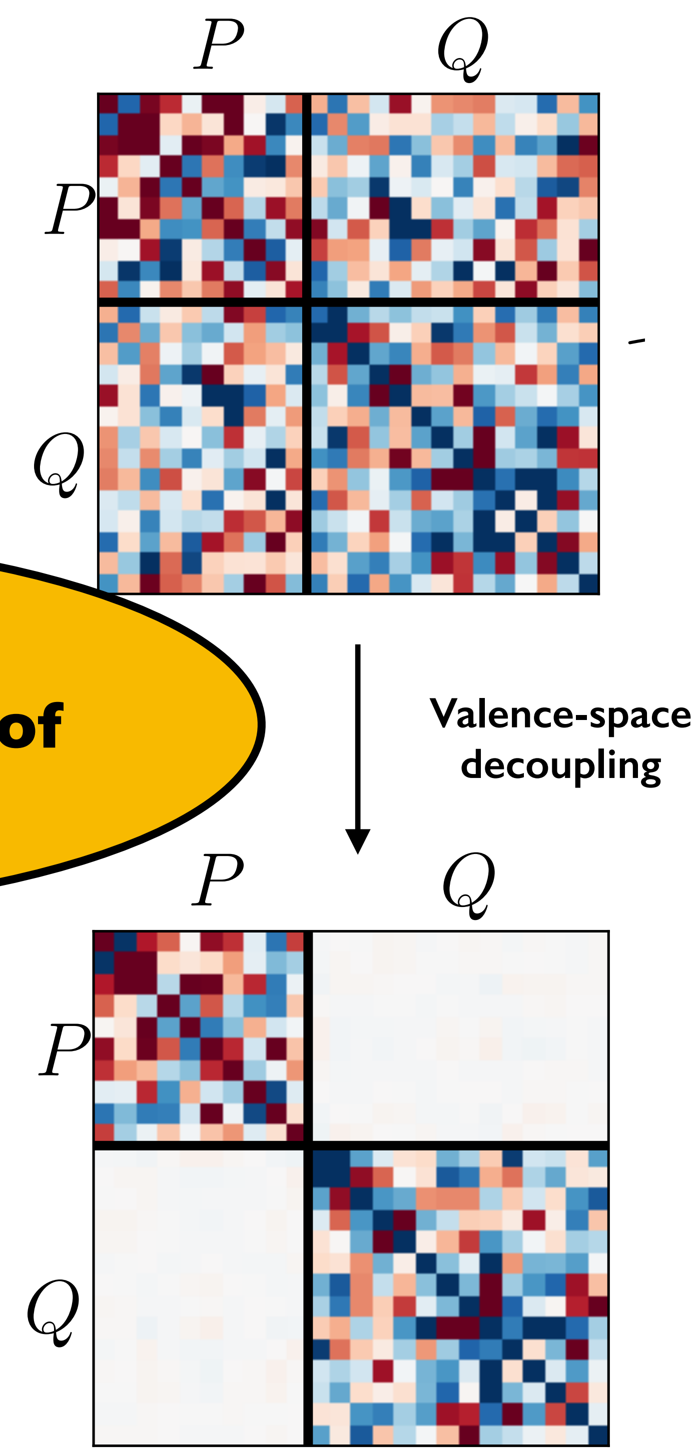
The valence-space IMSRG

- Non-perturbative decoupling of particle-hole excitations from valence space

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

- Large no-core problem mapped to tractable active-space pr
- Many-body observables shell-model diagonalization
- Simple access to low-lying spectroscopy
- Benefits from extensive machinery from shell-model developers

<u>Challenge:</u>
Computational cost of diagonalization



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

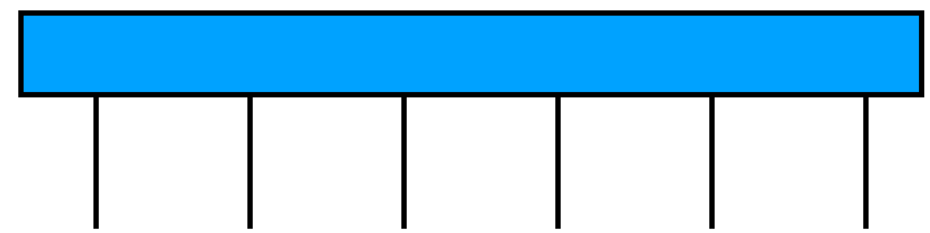
Wave-function representations

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

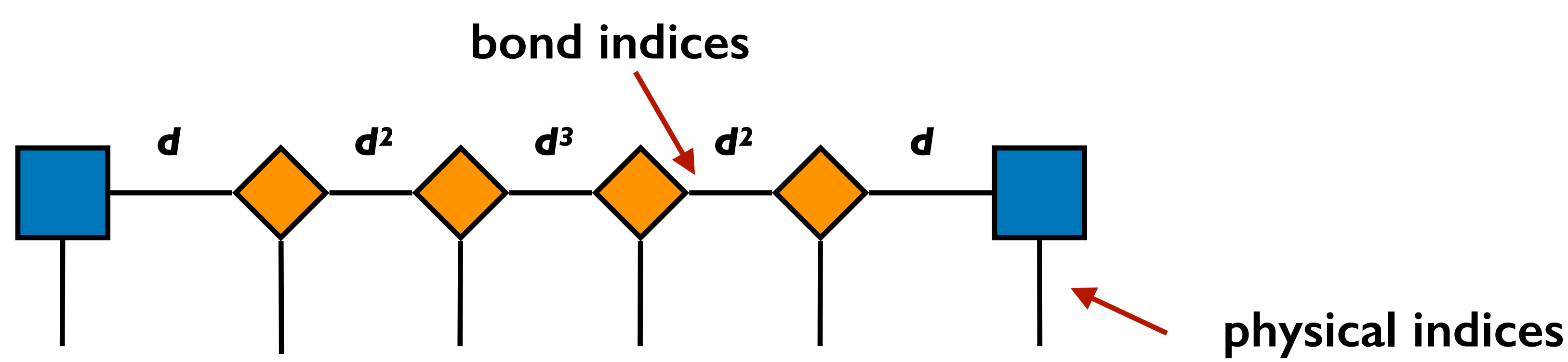
complexity d^N

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

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



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



$$|\Psi\rangle = \sum_{p_1 \dots p_N} \sum_{\alpha_1 \dots \alpha_N} A^{\alpha_1}_{p_1} A^{\alpha_1 \alpha_2}_{p_2} \cdots A^{\alpha_{N-1} \alpha_N}_{p_{N-1}} A^{\alpha_N}_{p_N} |p_1 \cdots p_N\rangle$$

- **Approximate MPS representation obtained by limiting intermediate summation**

$\longrightarrow$ **bond dimension M**

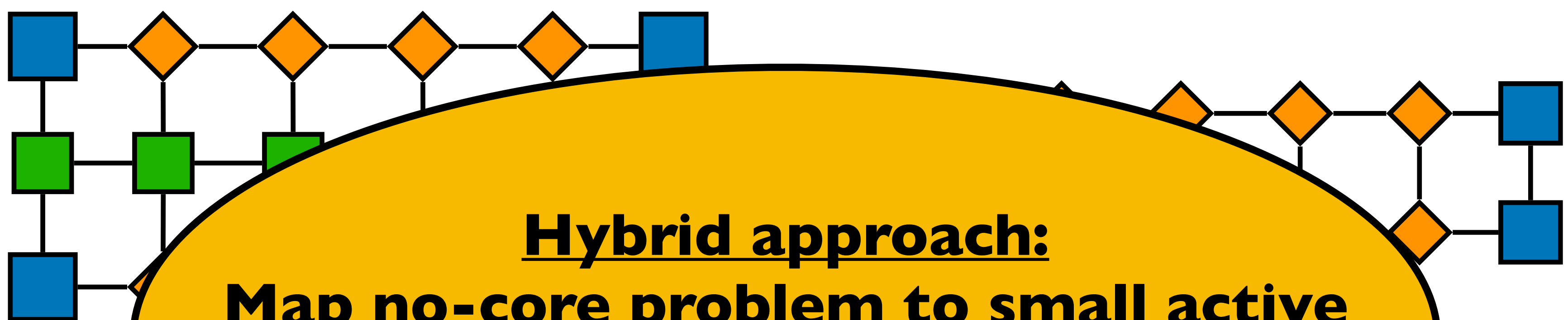
Density matrix renormalization group

White, PRL (1991)

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

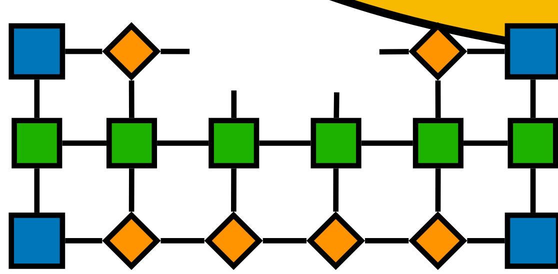
- Rewriting expectation value in terms of MPS factors yields tensor network

Schollwöck, Ann. Phys. (2011)

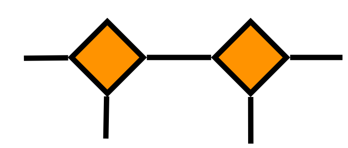


Hybrid approach:
Map no-core problem to small active space (IMSRG) and find variational approximation (DMRG)!

- DMRG sweeps: t factors



Removal of two neighbouring sites

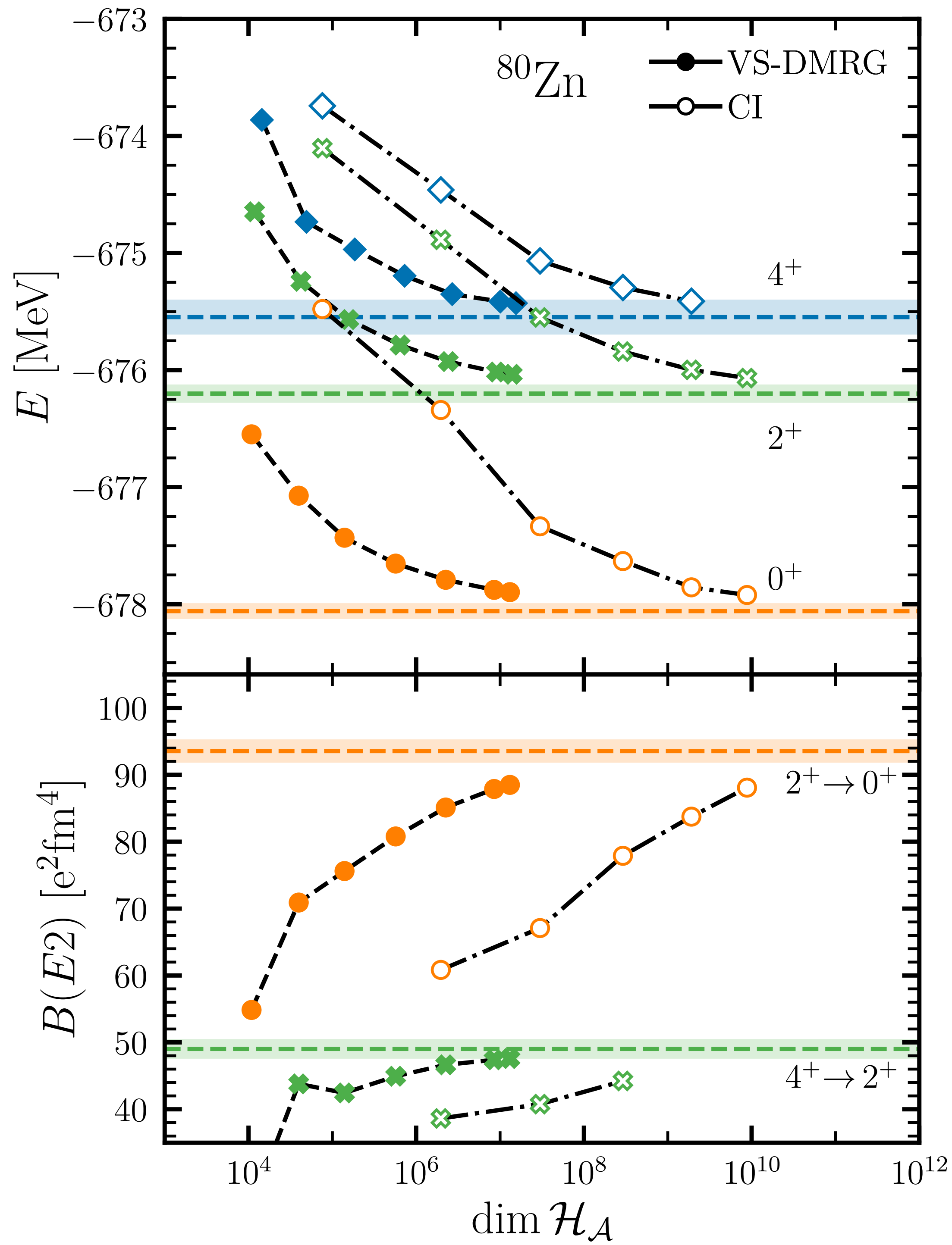


Construction of two-site tensor

- Limited by the number of orbitals and required bond dimension

DMRG vs. CI: Many-body convergence

DMRG/CI energies vs. effective dimension of H_A



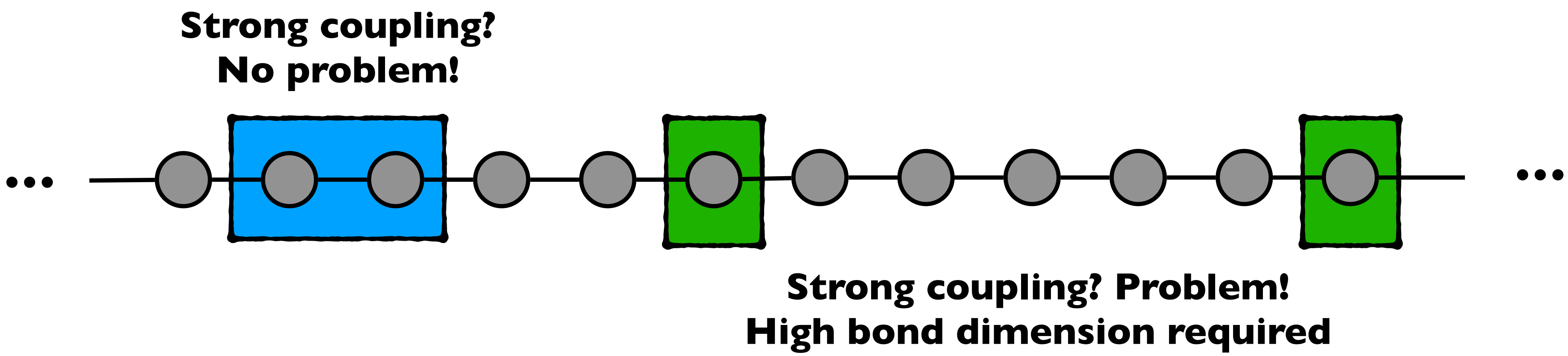
Tichai *et al.* (2024)

- **DMRG: economic representation of the many-body wave function**
- **Slow convergence of binding energies in CI calculations**
- **Robust convergence of DMRG energies at large bond dimension**
- **B(E2) transition: more systematic convergence pattern compared to CI**
- **DMRG does extend CI capacities**

Orbital ordering

- Ordering problem: which arrangement yields most rapid convergence?

Presence of long-range correlations problematic



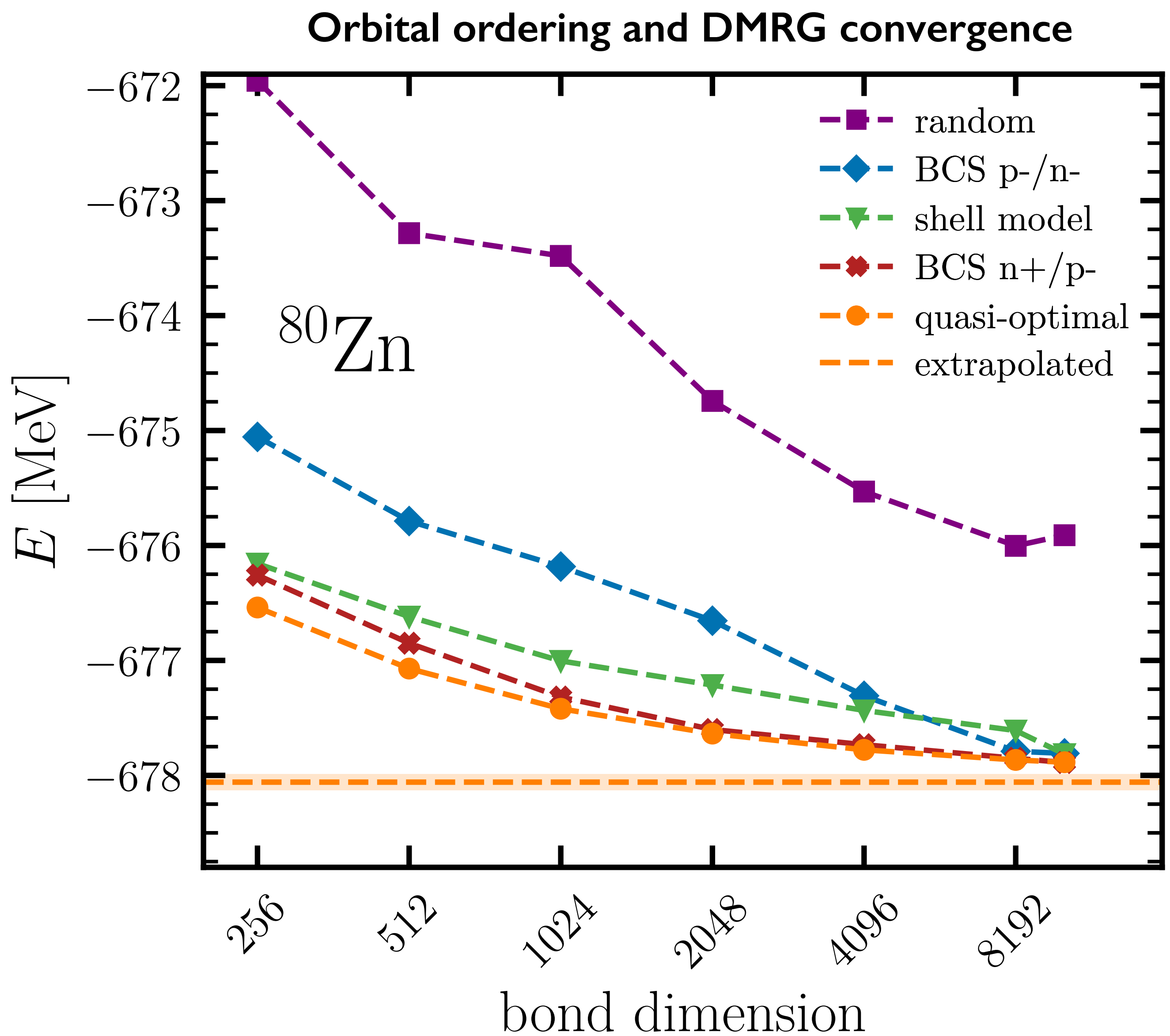
- 'Bad encodings': MPS must have large bond dimension to capture correlations

- Finding best ordering is complicated and requires exhausting all $N!$ possibilities

- Microscopic understanding of nuclear correlations can guide heuristics

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

The role of the DMRG topology



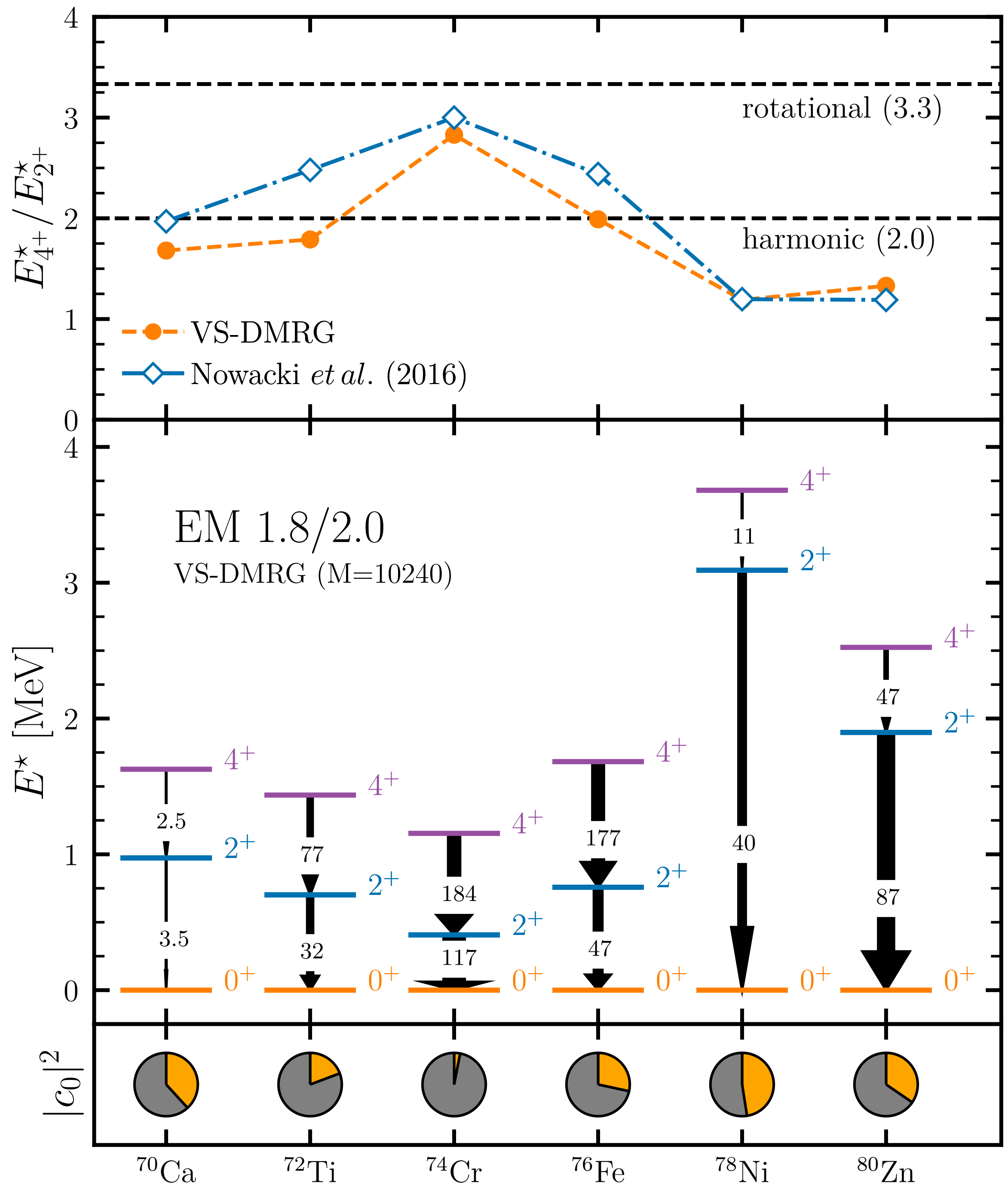
- **Random ordering gives bad results being trapped in local minimum**
- **BCS ordering: time-reversed states next to each other (m_j, $-m_j$)**
- **Arrangement of j multiplets significantly impacts convergence**
- **Stable convergence of shell-model ordering but 500 keV off at large M**
- **Quasi-optimal ordering gives consistently best results**

$$\{\nu : s_{1/2}\, d_{3/2}\, d_{5/2}\, g_{7/2}\, g_{9/2};\ \pi : f_{7/2}\, f_{5/2}\, p_{3/2}\, p_{1/2}\}$$

Quasi-optimal ordering

Transitional nuclei at *N*=50

Spectroscopy of *N*=50 isotones



Tichai *et al.* (2024)

- **Ratios of 4⁺/2⁺ excitation energies close to rigid-rotor limit**

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

- **Increase of *B(E2)* values towards open-shell ^{74}Cr**
- **Rapid transition between single-particle-like and collective excitations**
- **Qualitative agreement with previous shell-model calculations**

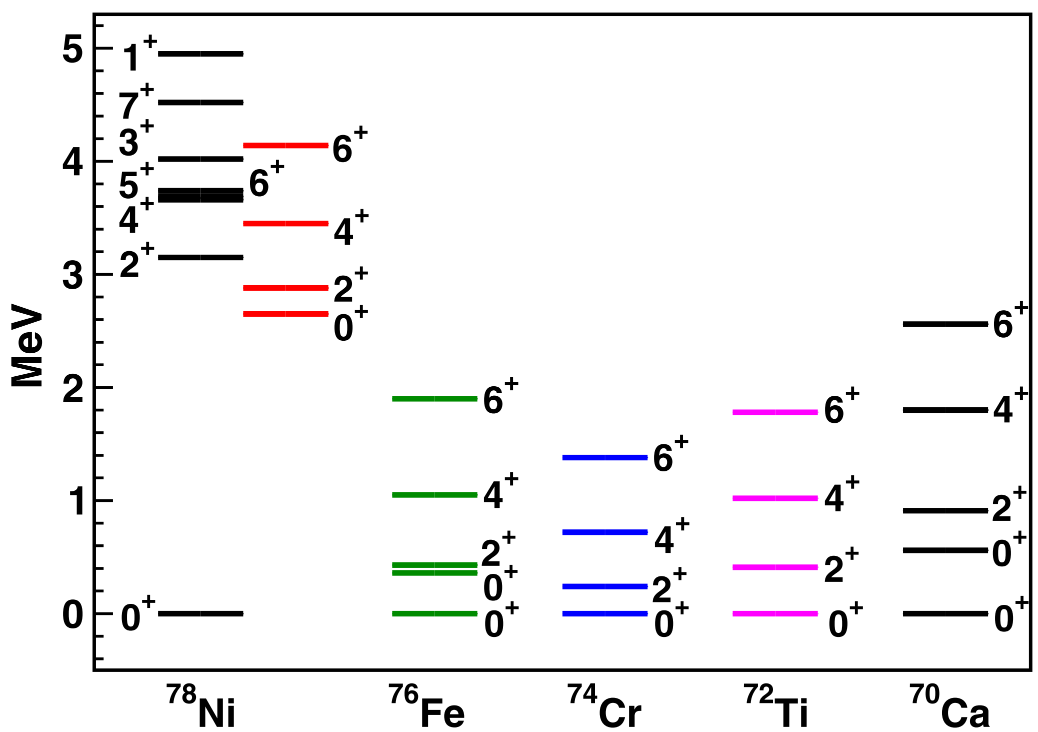
Nowacki *et al.*, PRL (2016)

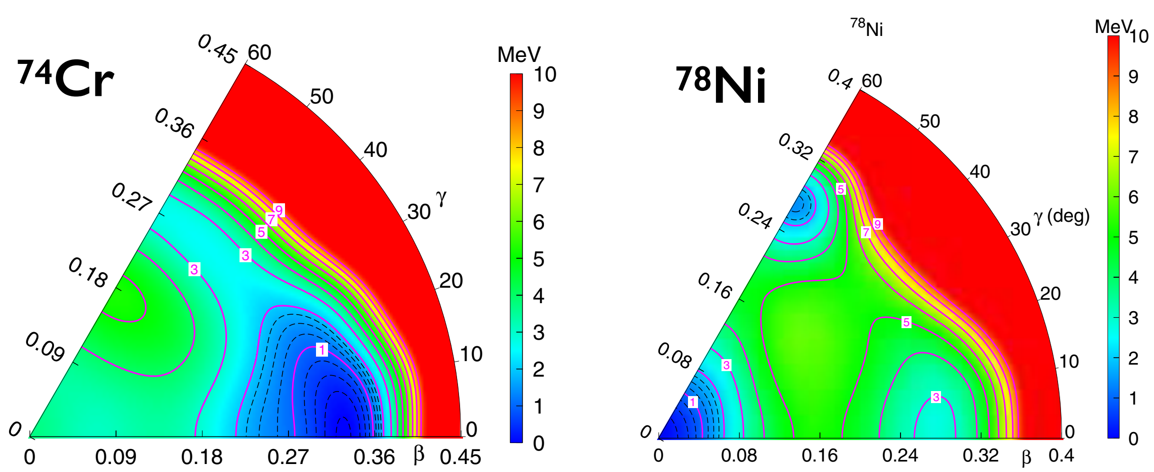
- **Island-of-inversion: very low 0p0h-component in ground state**

Future challenges: shape coexistence

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

Spectroscopy of *N=50* isotones





Nowacki *et al.*, PRL (2016)

- Emergence of excited-state rotational band in ^{78}Ni
- Second 0^+ state comes out much higher at 5 MeV: IMSRG(3) and beyond?
- Complementary perspective on deformation from valence-space HFB
- Pronounced spherical minimum in ^{78}Ni but prolate minimum in ^{74}Cr

Part II

Entanglement and nuclear phenomenology

Orbital entanglement

see also Robin, Savage, Pillet, Gu, Sun, Hagen, Papenbrock, Pérez-Obiol, Rios, Menéndez,…

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

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

(A, B two subsystems)

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

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

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

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

- Single-orbital entropy encodes nuclear correlation effects in a simple way

$$s_i = -\mathrm{Tr}\, \rho_i \log \rho_i \leq \log 2$$

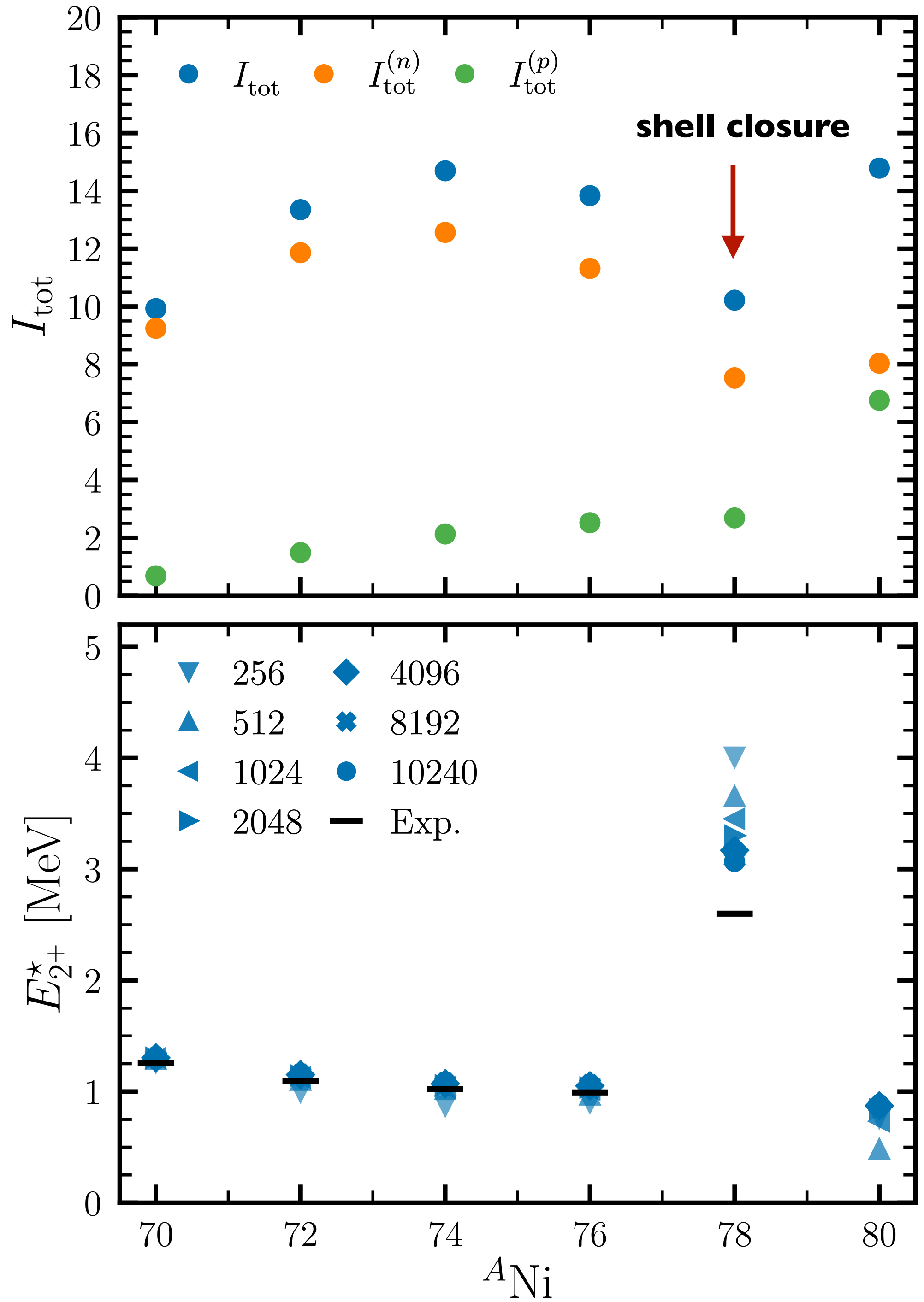
- Total correlation obtained from sum of single-orbital entropies

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

Entropies and shell structure

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

Total entropy in even-mass nickel isotopes



Tichai *et al.*, PLB (2023)

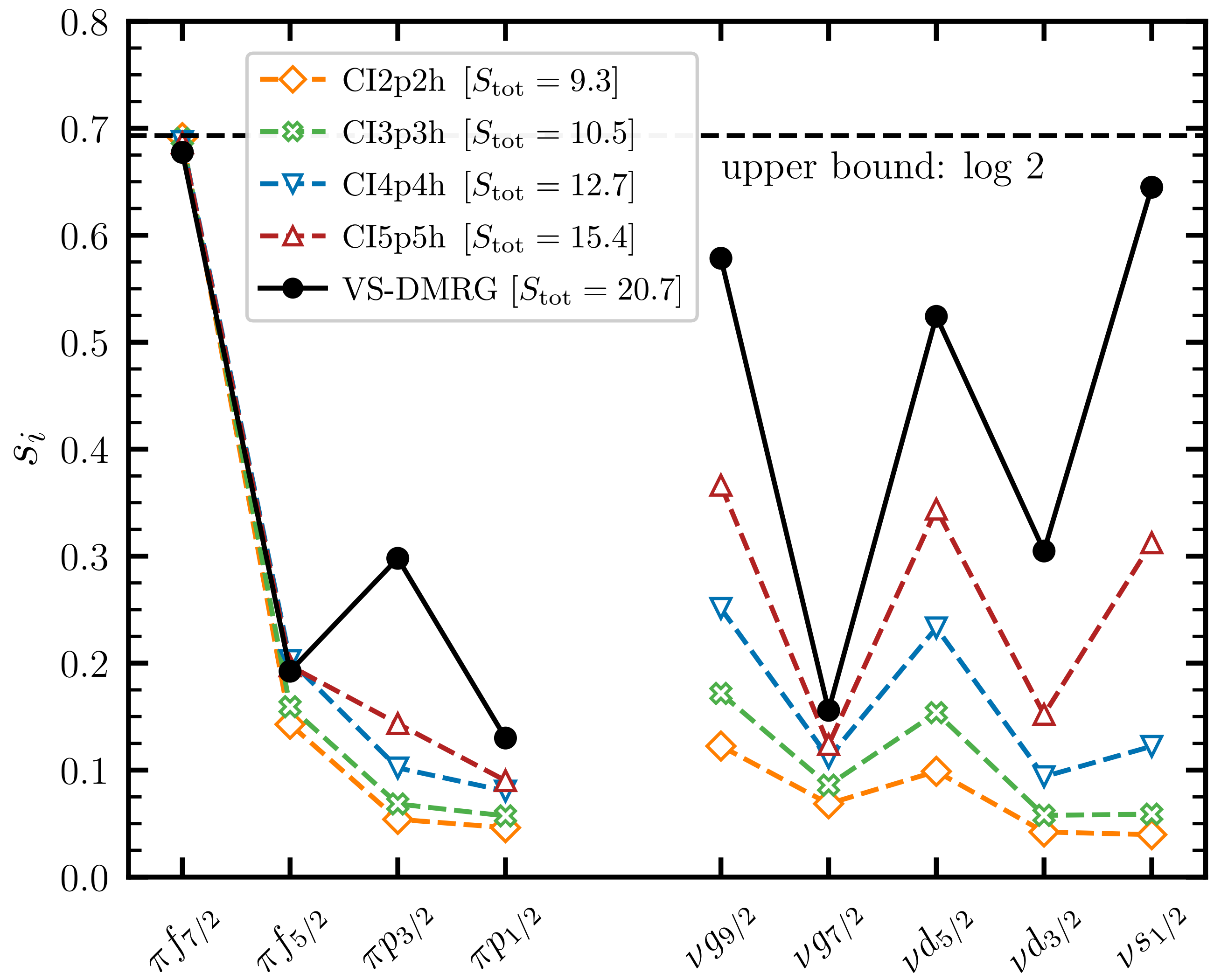
- Pronounced kink at ^{78}Ni hints at **neutron shell closure** (~ dominated by HF)
- **Larger bond dimensions** required to converge ^{78}Ni excited state
- Agreement with **conventional prediction** based on 2^+ excitation energies
- Deviation from experiment attributed to missing triples corrections: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

Total entropy is a good proxy for shell closures!

(… but non-observable and basis dependent!)

Orbital entanglement in ^{74}Cr

Entropies in DMRG and CI



Tichai *et al.* (2024)

- **Orbital correlation are only slowly built up in CI expansions**
- **Total amount of entanglement much higher in DMRG approach**
- **Subset of orbitals well captured at very low CI truncations: $f_{7/2}$**
- **Selected 6p-6h excitations (and more) are needed for high accuracy**

DMRG efficiently captures important correlations

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}

- Two-orbital-reduced density matrix encodes pairwise entanglement

$$\rho_{ij} = \begin{pmatrix} 1-\gamma_{ii}-\gamma_{jj}+\gamma_{ijij} & 0 & 0 & 0 \\ 0 & \gamma_{jj}-\gamma_{ijij} & \gamma_{ij} & 0 \\ 0 & \gamma_{ij} & \gamma_{ii}-\gamma_{ijij} & 0 \\ 0 & 0 & 0 & \gamma_{ijij} \end{pmatrix}$$

two-body density required!

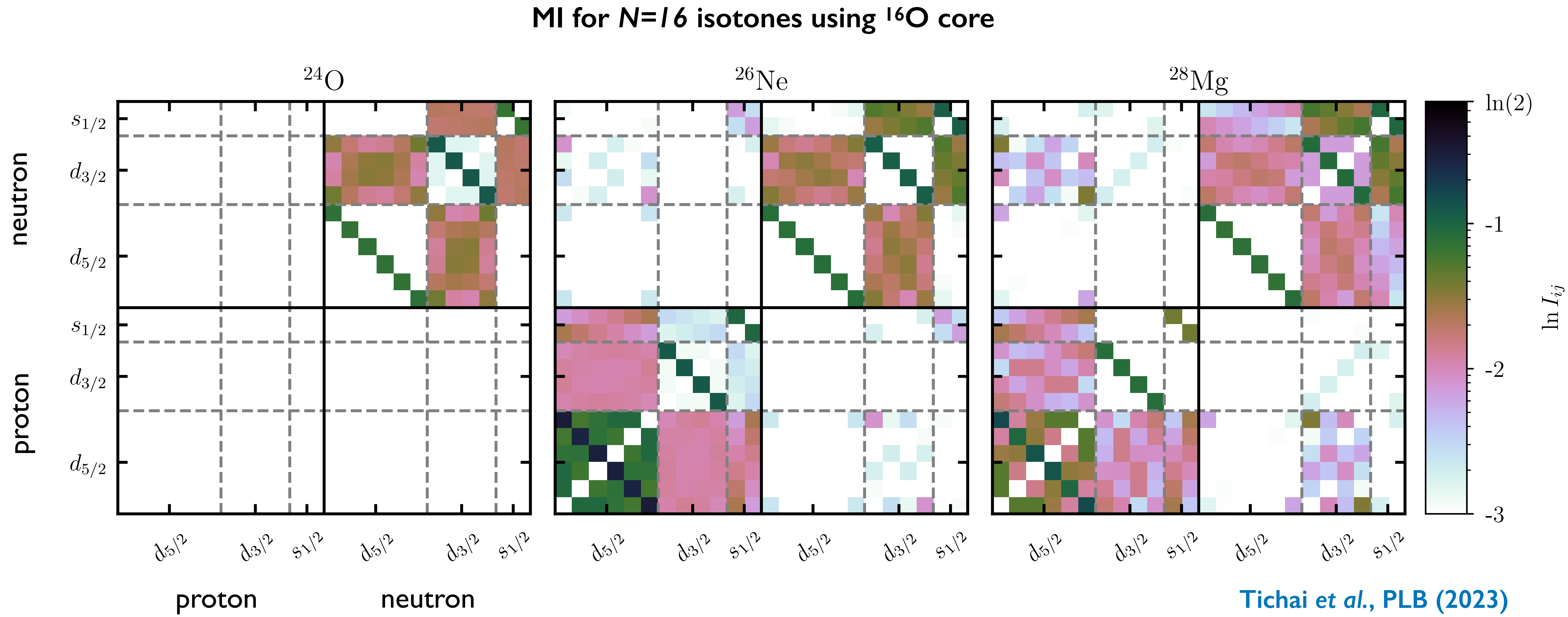
- Two-orbital entropy again obtained from two-orbital-reduced density matrix

$$s_{ij} = -\mathrm{Tr}\, \rho_{ij} \log \rho_{ij}$$

- 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.*, PLB (2023)

- Indications of BCS-type *nn*- and *pp*-pairing within the same shell (*J=0, M=0, T=1*)
- Neutron-neutron correlations affected by presence of protons
- Proton-neutron correlations suppressed but off-diagonal coupling present

Conclusions

Establish DMRG as scalable alternative to CI

- MPS representation is superior to CI representation
- Robust convergence of observables with reduced uncertainties
- VS-DMRG: novel merging of complementary *ab initio* approaches

Next steps: SU(2)-invariant … cases in heavy nuclei

Thank you for your attention!

Nuclear entanglement from quantum information theory

- Link nuclear phenomenology to QIT measures
- New perspective from orbital entanglement
- Superfluid correlations and shell closures related to entropies

Next steps: systematic understanding of collective nuclear effects