Ab initio nuclear structure from the density matrix renormalization group

Recent Progress in Many-Body Theory XXI

Chapel Hill

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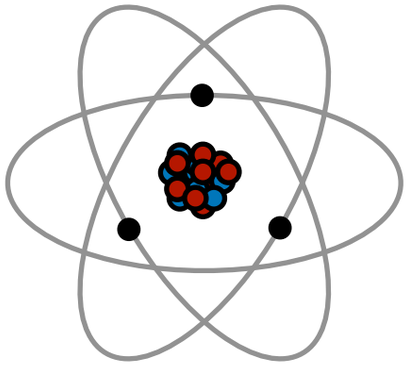


with S. Knecht, A. Kruppa, Ö. Legeza, P. Moscalina, A. Schwenk, M. Werner, G. Zarand

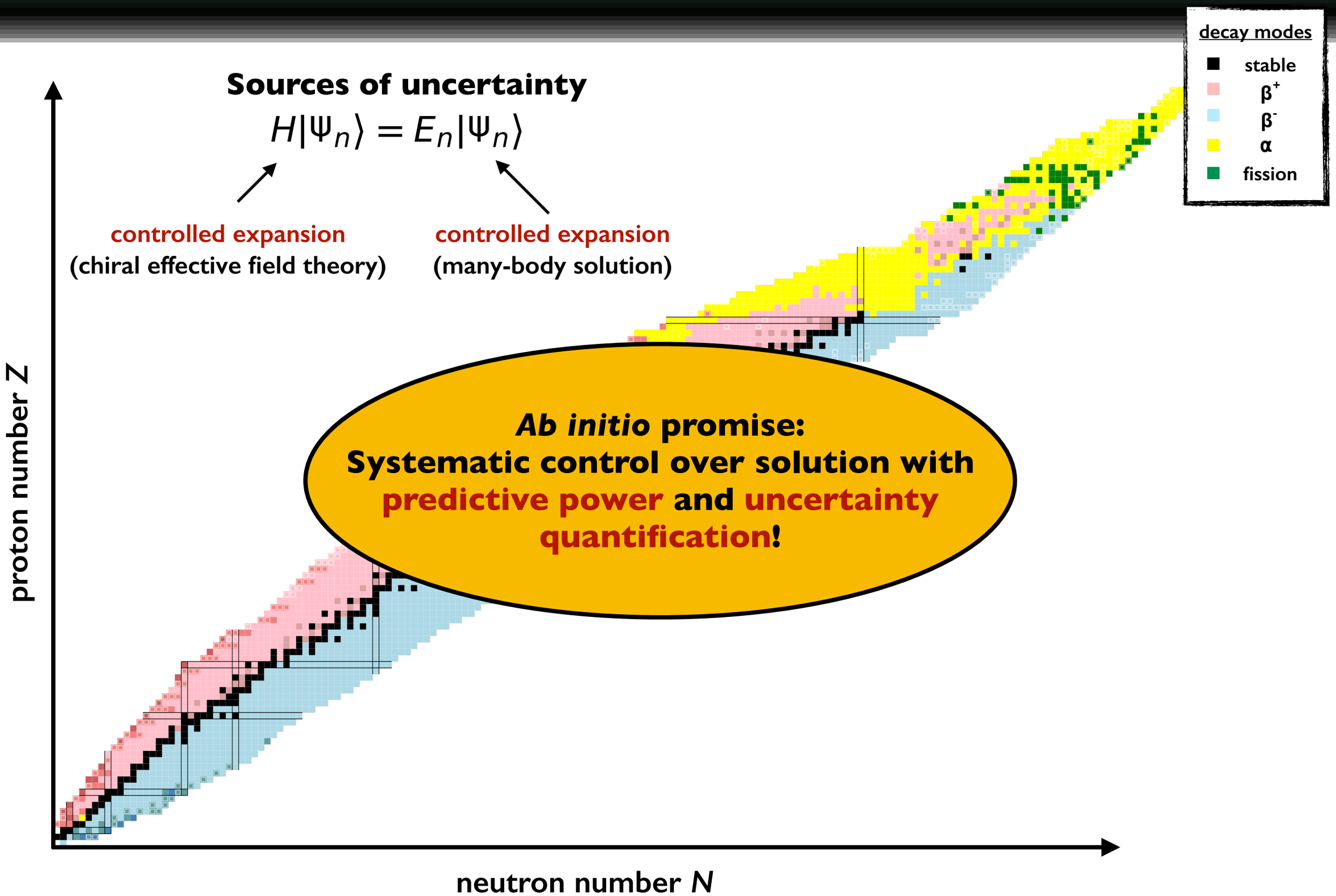
Ab initio nuclear structure

Sources of uncertainty

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

controlled expansion
(chiral effective field theory)

controlled expansion
(many-body solution)



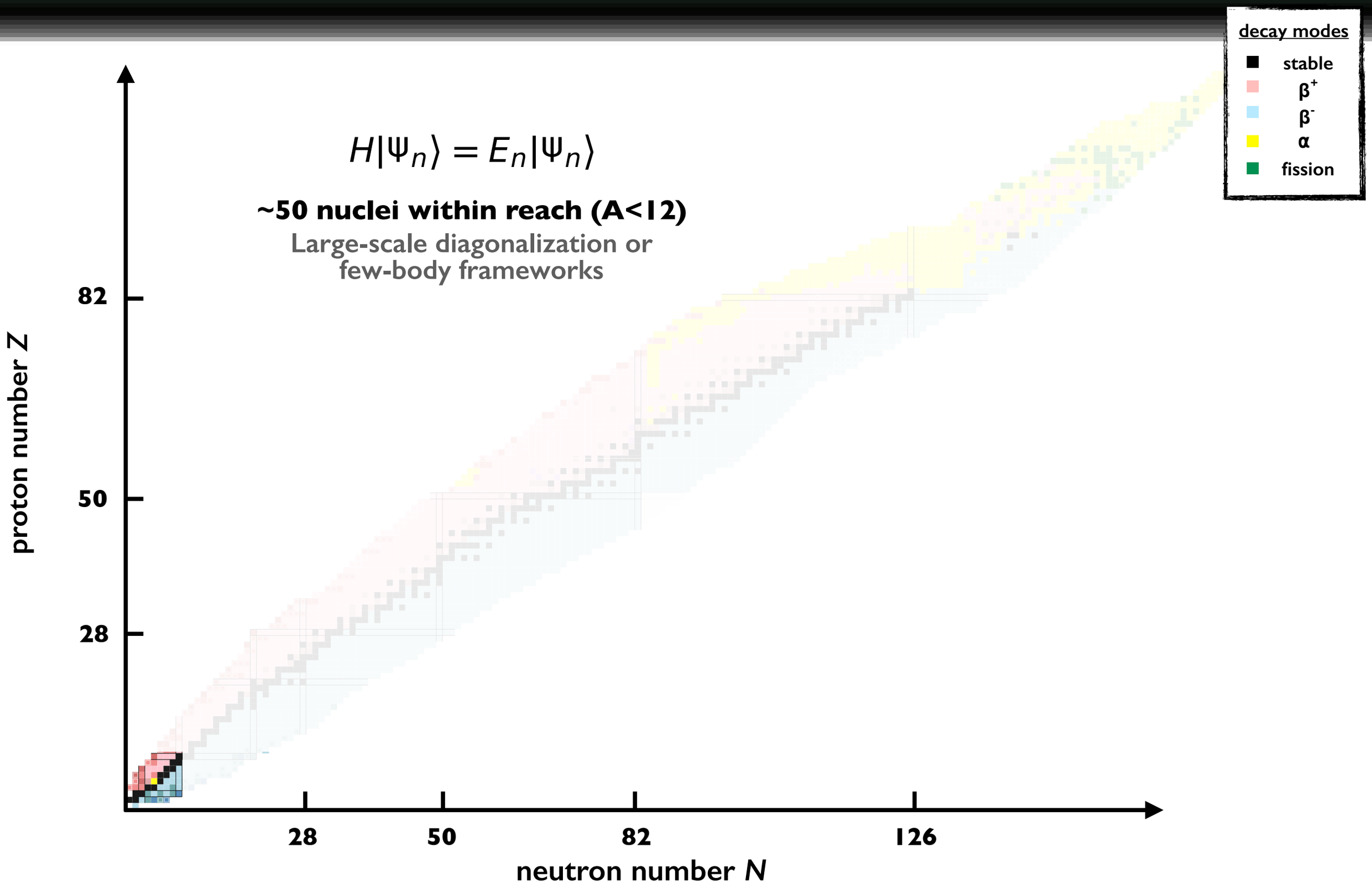
***Ab initio* promise:**
Systematic control over solution with predictive power and uncertainty quantification!

Ab initio in the early 2000's

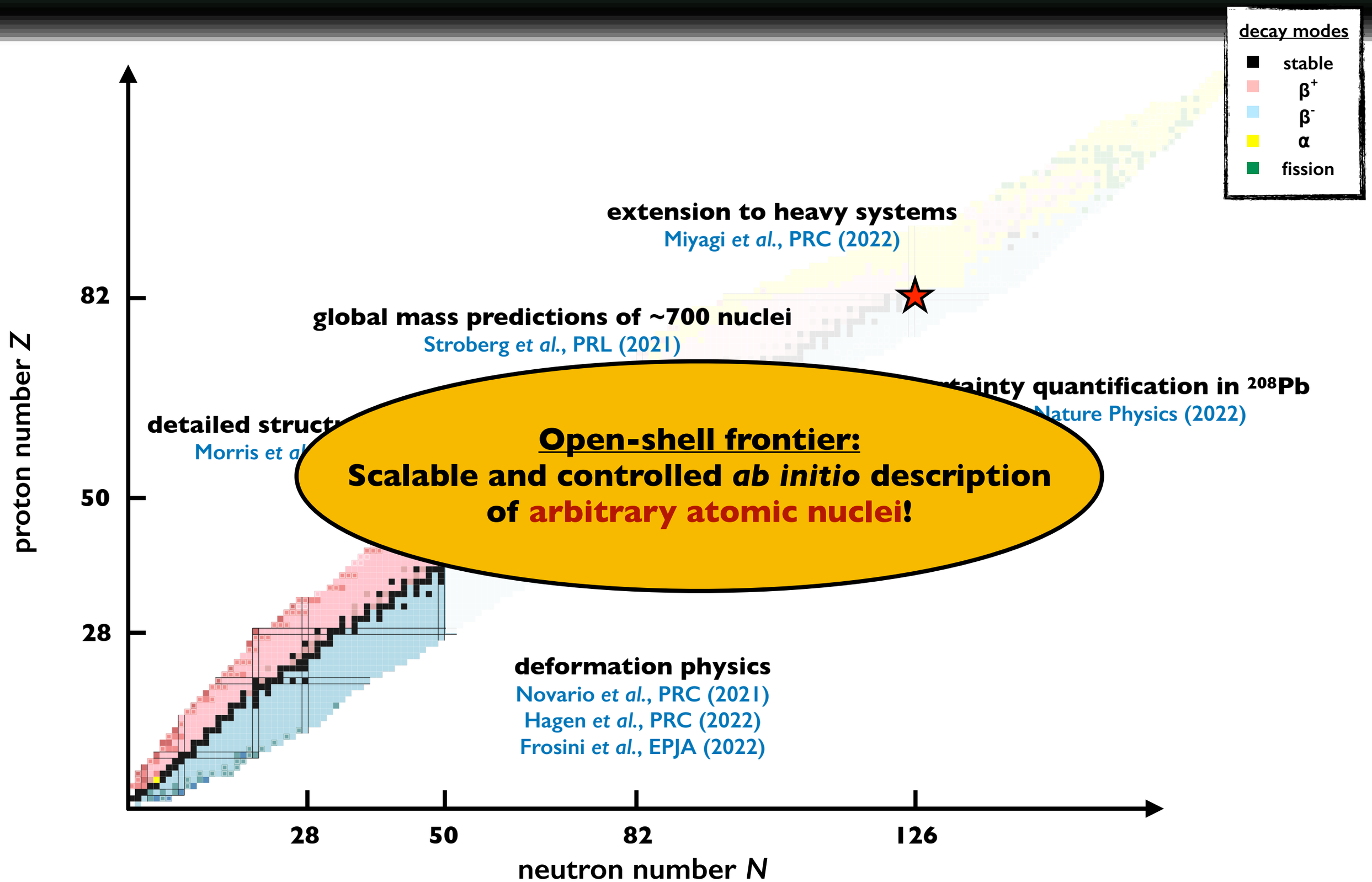
$$H|\Psi_n\rangle = E_n|\Psi_n\rangle$$

~50 nuclei within reach (A<12)

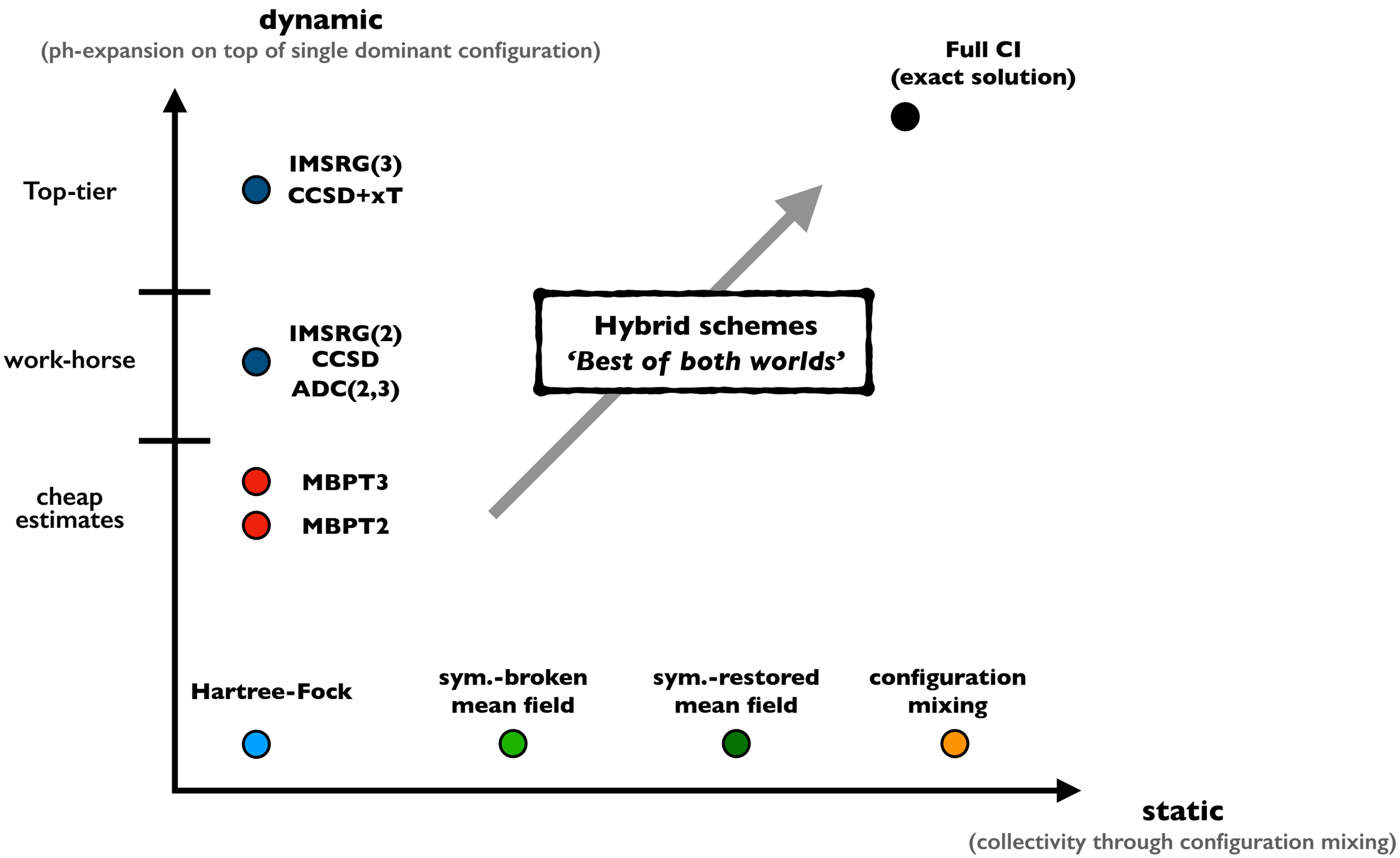
Large-scale diagonalization or few-body frameworks



Recent highlights: heavier and deformed!



Nuclear many-body approaches

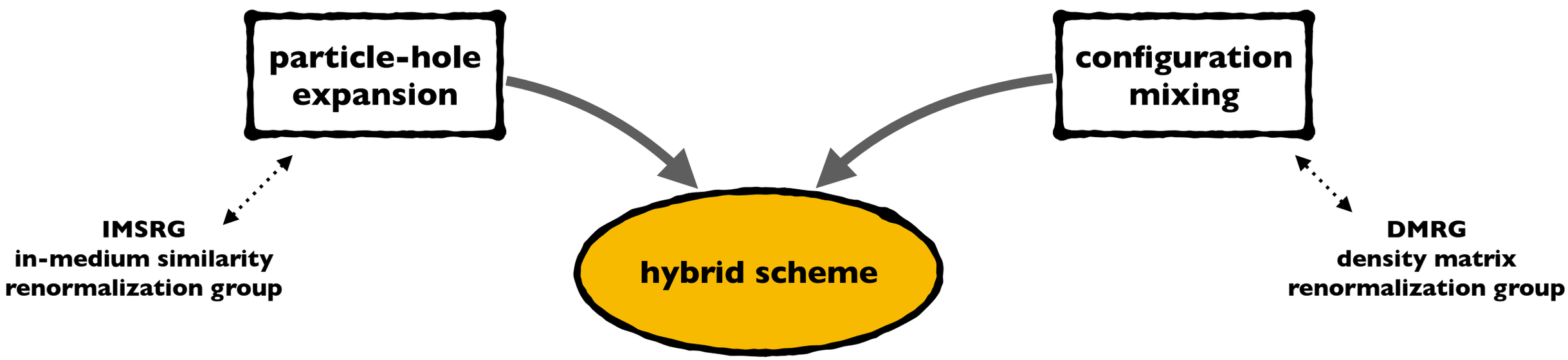


Hybrid many-body schemes

- Atomic nuclei are driven by static and dynamic correlation effects
- Challenge: static correlations require high truncation order in vertical expansion

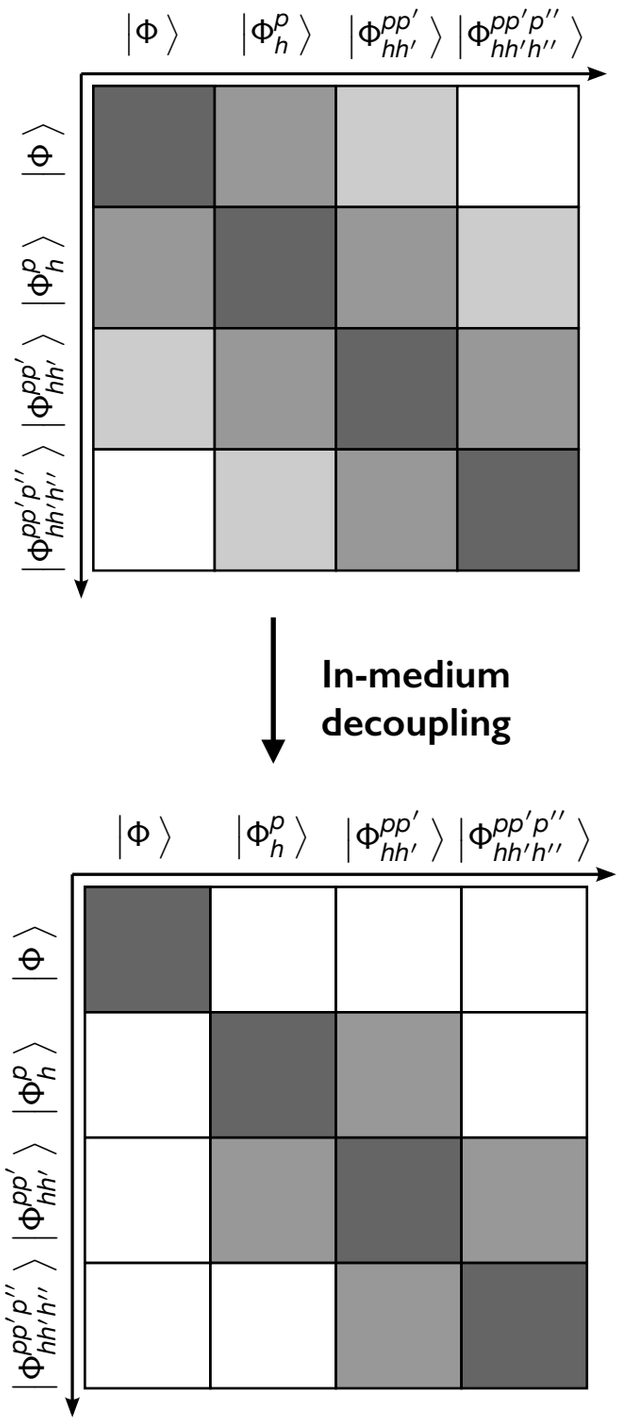
'Collectivity involves excitation of many nucleons at the same time'

- Idea: definition of hybrid schemes that combine several approaches



- Typically hybrids schemes involve multiple truncations for each component

Fundamentals of IMSRG



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

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

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

- **Reformulation as ordinary differential equation**

$$\frac{d}{ds} H(s) = [\eta(s), H(s)]$$

- **Approximation: discard induced operators**

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

- **Ground-state energy from flowing Hamiltonian**

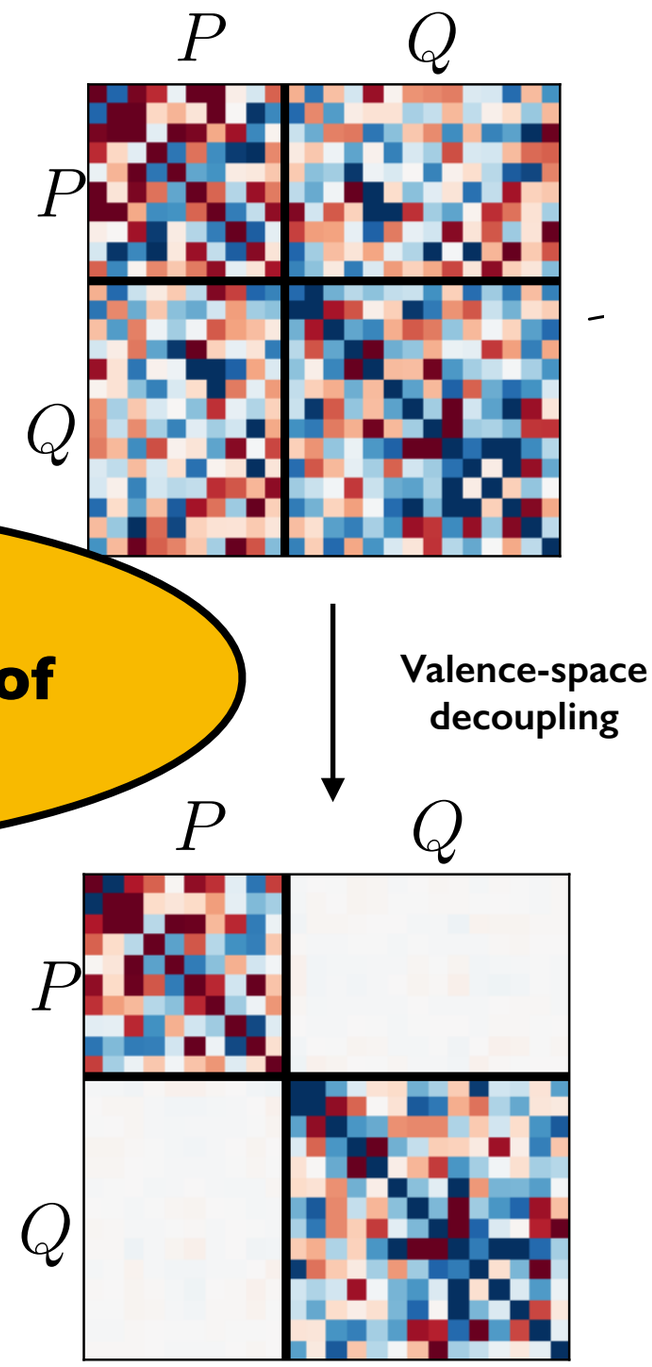
$$\lim_{s\to\infty} \langle\Phi|H(s)|\Phi\rangle = E_0$$

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

Valence-space formulation

- Modify decoupling to target valence space
- Construction of *ab-initio* inspired valence-space interactions rooted in QCD
- Non-perturbative re
correlations into acti
- Final computational step requires large-space shell-model diagonalization
- Versatility: access to diverse set of observables from shell-model codes

Challenge:
Computational cost of diagonalization



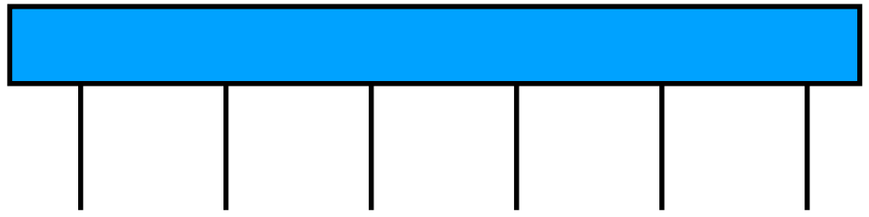
Stroberg *et al.*, Ann. Rev. Nucl. Part. Sci (2019)

Wave-function representations

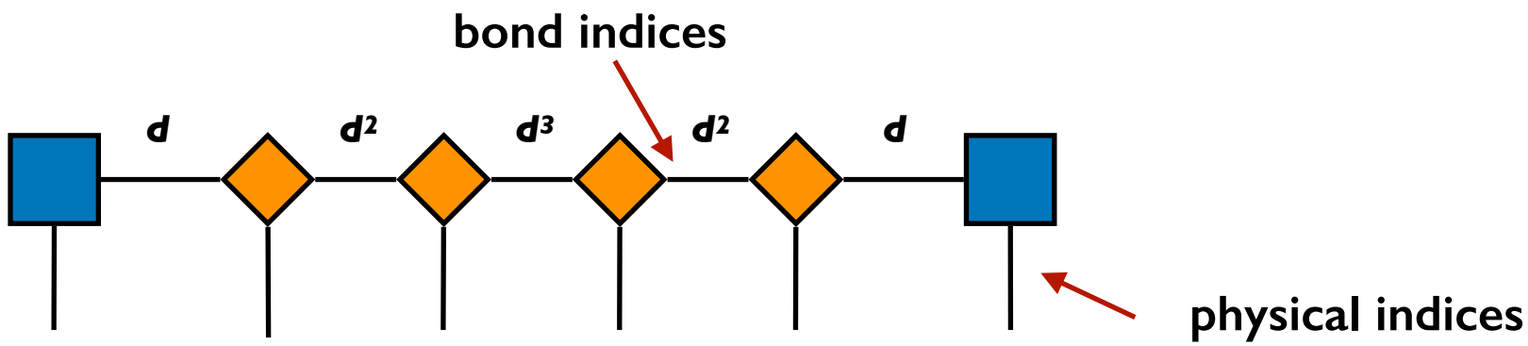
- **Many-body state is inefficiently represented in configuration interaction**

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

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



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



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

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

$\longrightarrow$ **bond dimension M**

Density matrix renormalization group

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

White, PRL (1991)

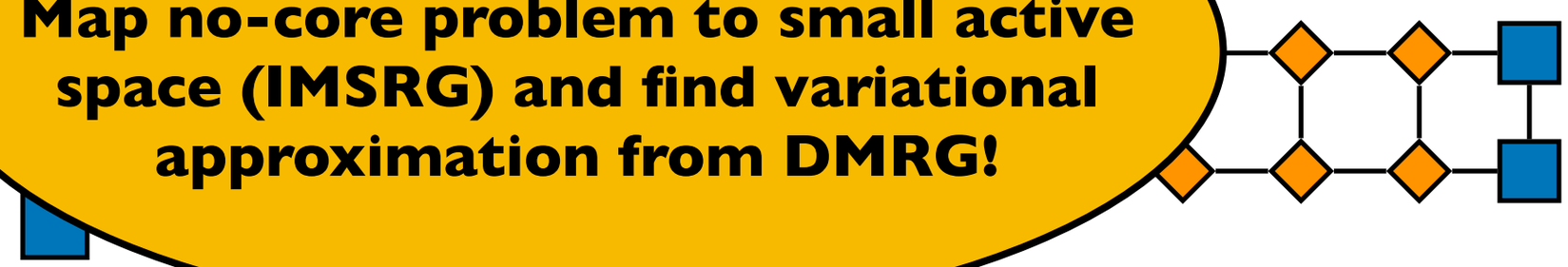
$$E = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

- Rewriting expectation val ds tensor network:

Schollwöck, Ann. Phys. (2011)

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

factorized Hamiltonian
(Matrix Product Operator)



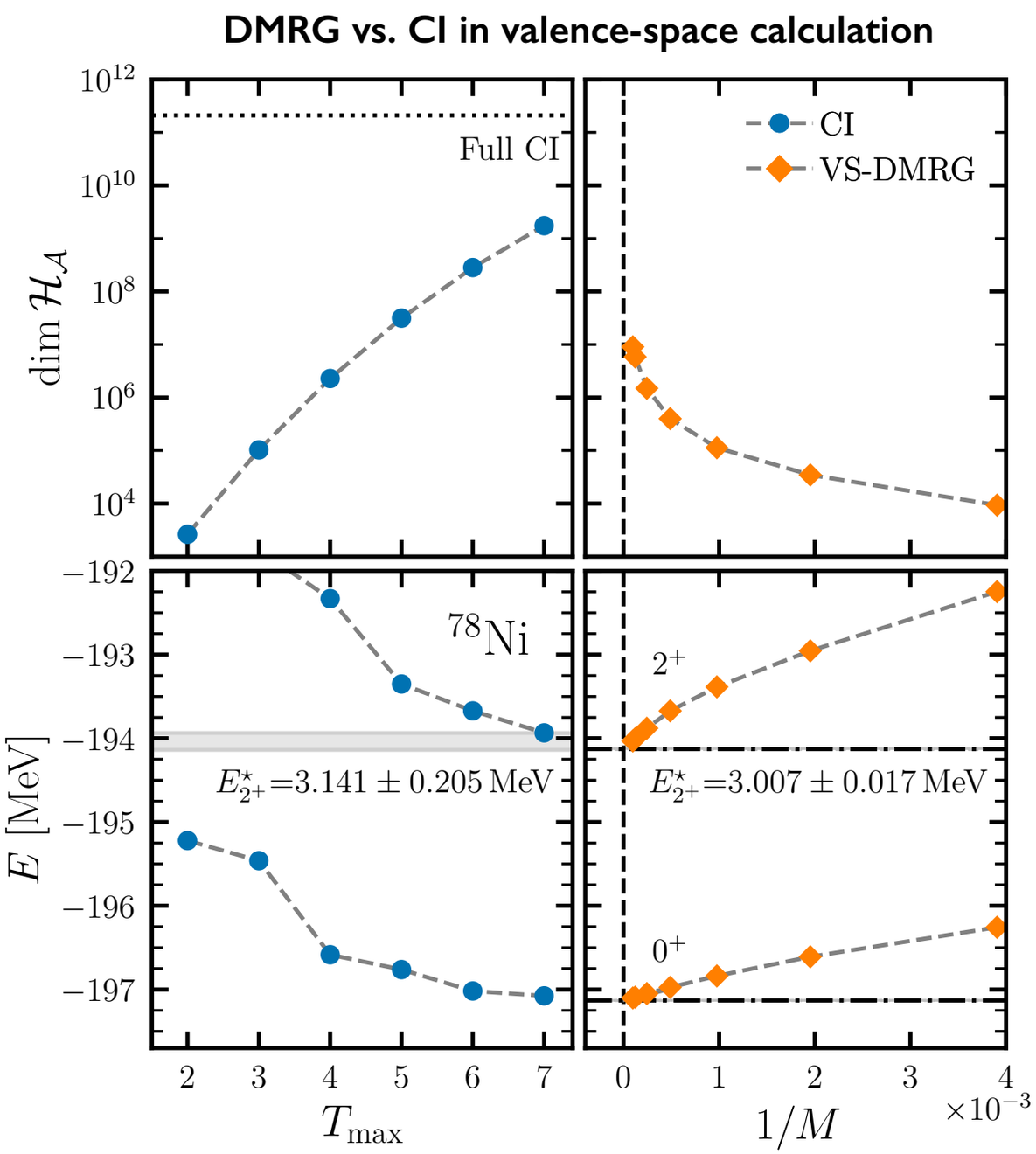
- Stationarity condition yields variational update step for factor matrices

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

- Computationally limited by the number of orbitals and required bond dimension

^{78}Ni: DMRG versus traditional CI

see also Legeza *et al.*, PRC (2015)



(particle-hole truncation)

Tichai *et al.*, 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**
- **Rigorous DRMG extrapolation in regime of quadratic convergence**

DMRG does extend CI capacities!

Entanglement measures

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)

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

- **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**

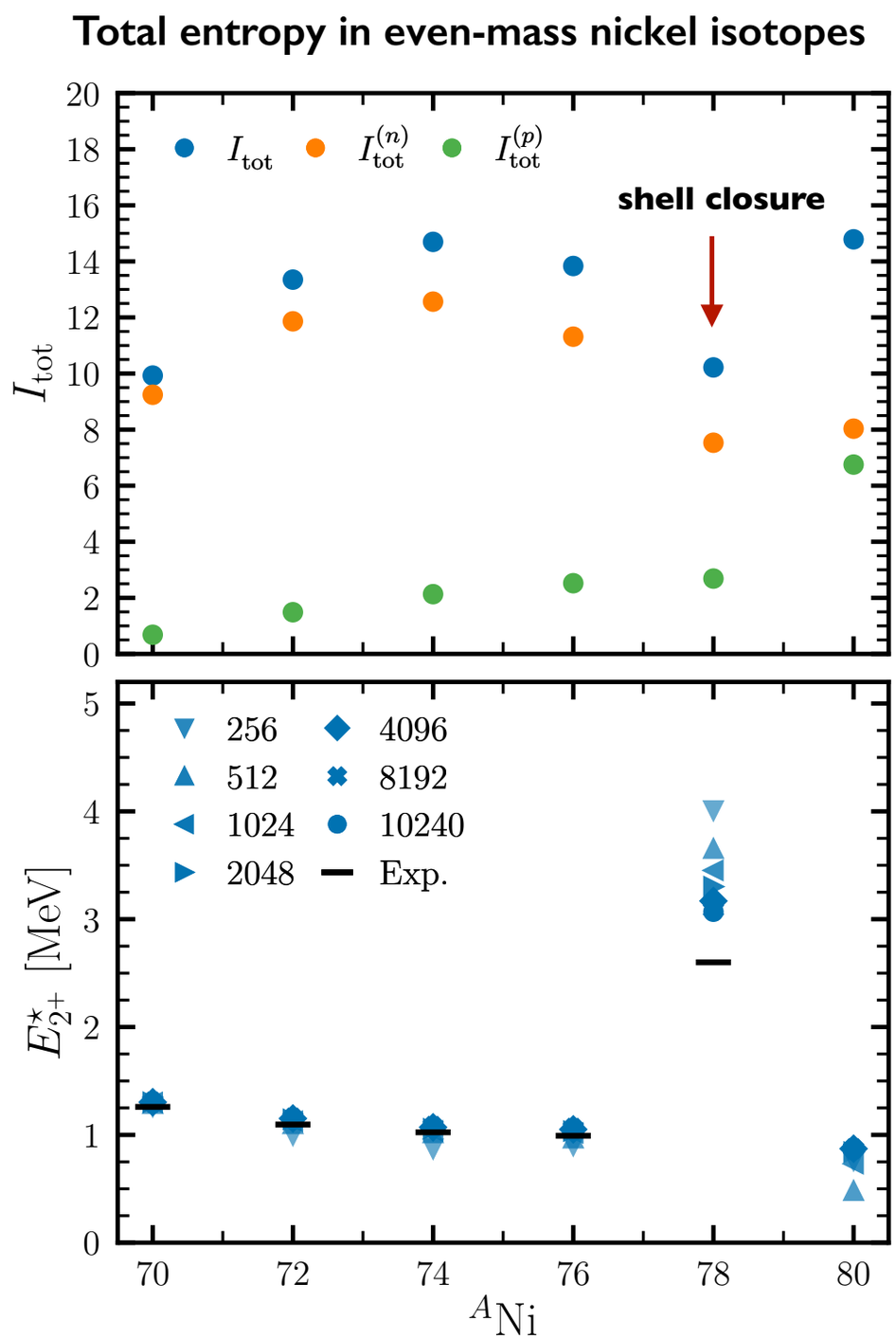
$$s_i = -\mathrm{Tr}\, \rho_i \log \rho_i$$

- **Total correlation obtained from sum of single-orbital entropies**

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

Entropies and shell structure

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



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!)

Orbital entanglement

- **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**

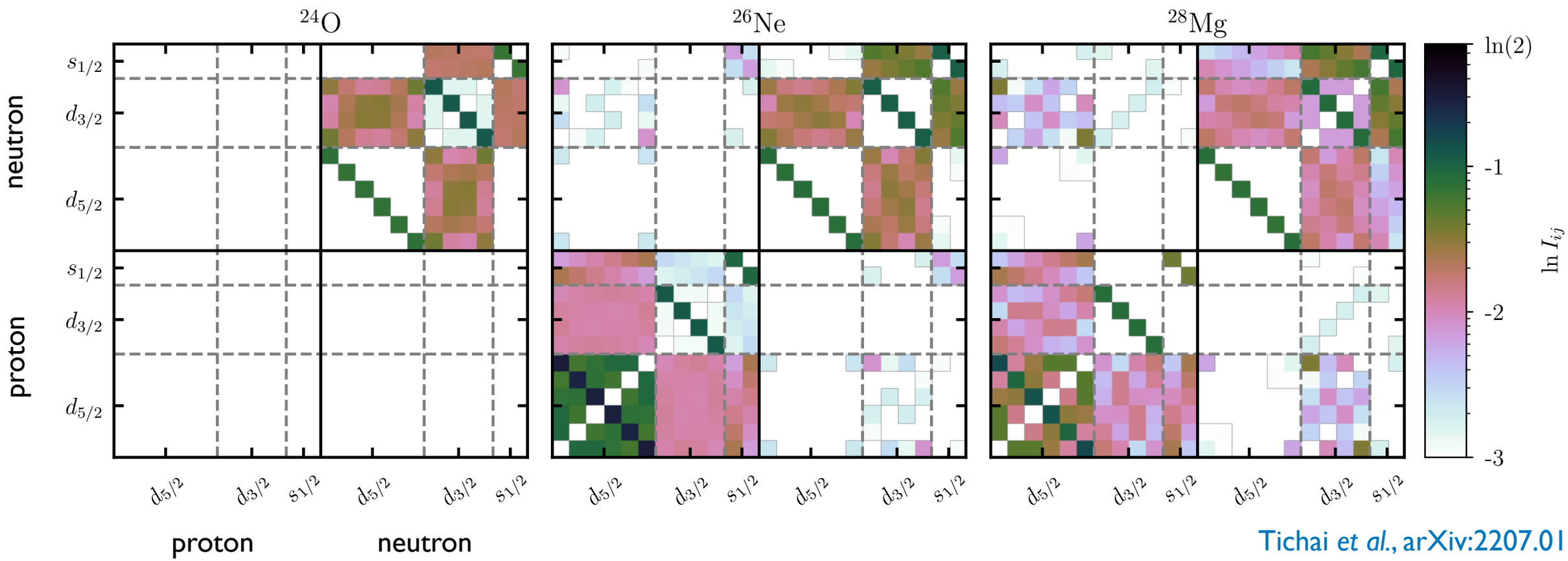
$$s_{ij} = -\mathrm{Tr}\, \rho_{ij} \log \rho_{ij}$$

- **Mutual information combines one- and two-particle entanglement**

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

Entanglement in the *sd*-shell

MI for *N=16* isotones using ^{16}O core



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**

Conclusion and outlook

More efficient wave-function parametrization

- Successful merging of DMRG approach with the valence-space IMSRG
- Significantly lower uncertainties on many-body observables in DMRG

Next steps: study of deformed systems with nuclear DMRG approach

Thank you for your attention!

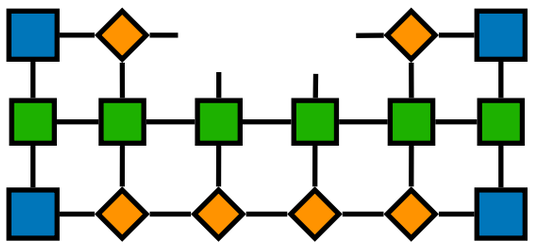
***Ab initio* perspective on nuclear correlation**

- Entropy-based correlation analysis in mid-mass *ab initio* calculations
- Emergence of shell structure from single-orbital entropies

Next steps: better understanding of higher-body nuclear correlations

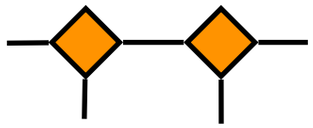
Example of an update step

Removal of two neighbouring sites



Construction of two-site tensor

site i site i+*l*

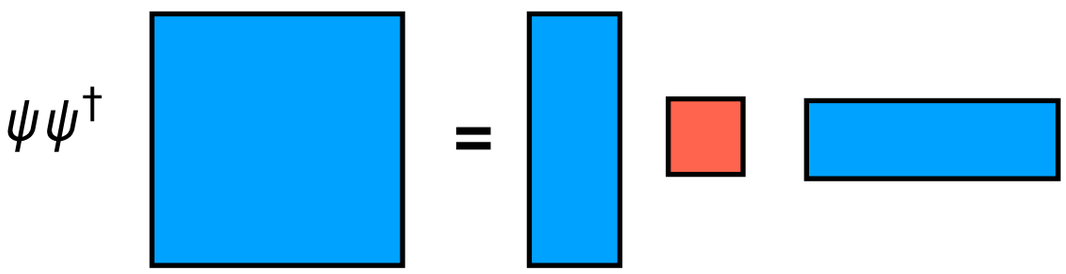


$$B^{\alpha_{i-1}\alpha_{i+1}}_{p_i p_{i+1}} = \sum_{\alpha_i} A^{\alpha_{i-1}\alpha_i}_{p_i} A^{\alpha_i\alpha_{i+1}}_{p_{i+1}}$$

<u>Macro-iterations</u> (or sweeps):
Repeat procedure by moving to the next pair of sites.
Run through orbital space until convergence.

Formation of density + truncated SVD

(number of singular values = bond dimension)



MPS update

site i site i+*l*