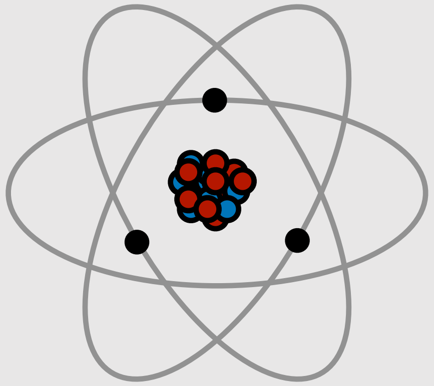
Recent advances in nuclear many-body theory

MITP workshop

Uncertainty quantification in nuclear physics

June 24th, 2024



Alexander Tichai

Technische Universität Darmstadt

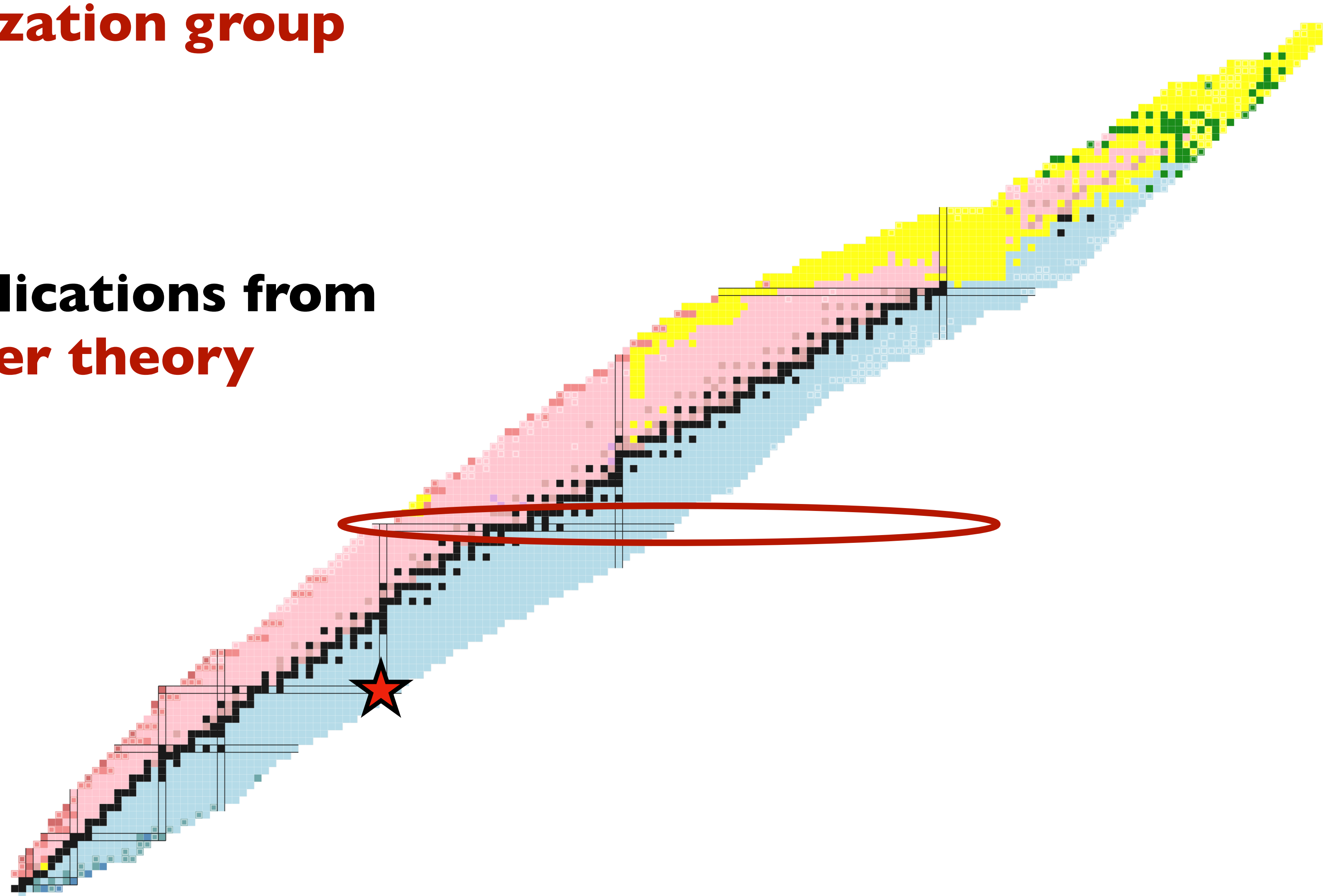
Outline

Theme:
Many-body developments with an eye on theory uncertainties.

Part I:
Structure around ^{78}Ni from the density matrix renormalization group
(Configuration mixing)

Part II:
Towards heavy-mass applications from Bogoliubov coupled cluster theory
(Symmetry breaking)

Perspectives



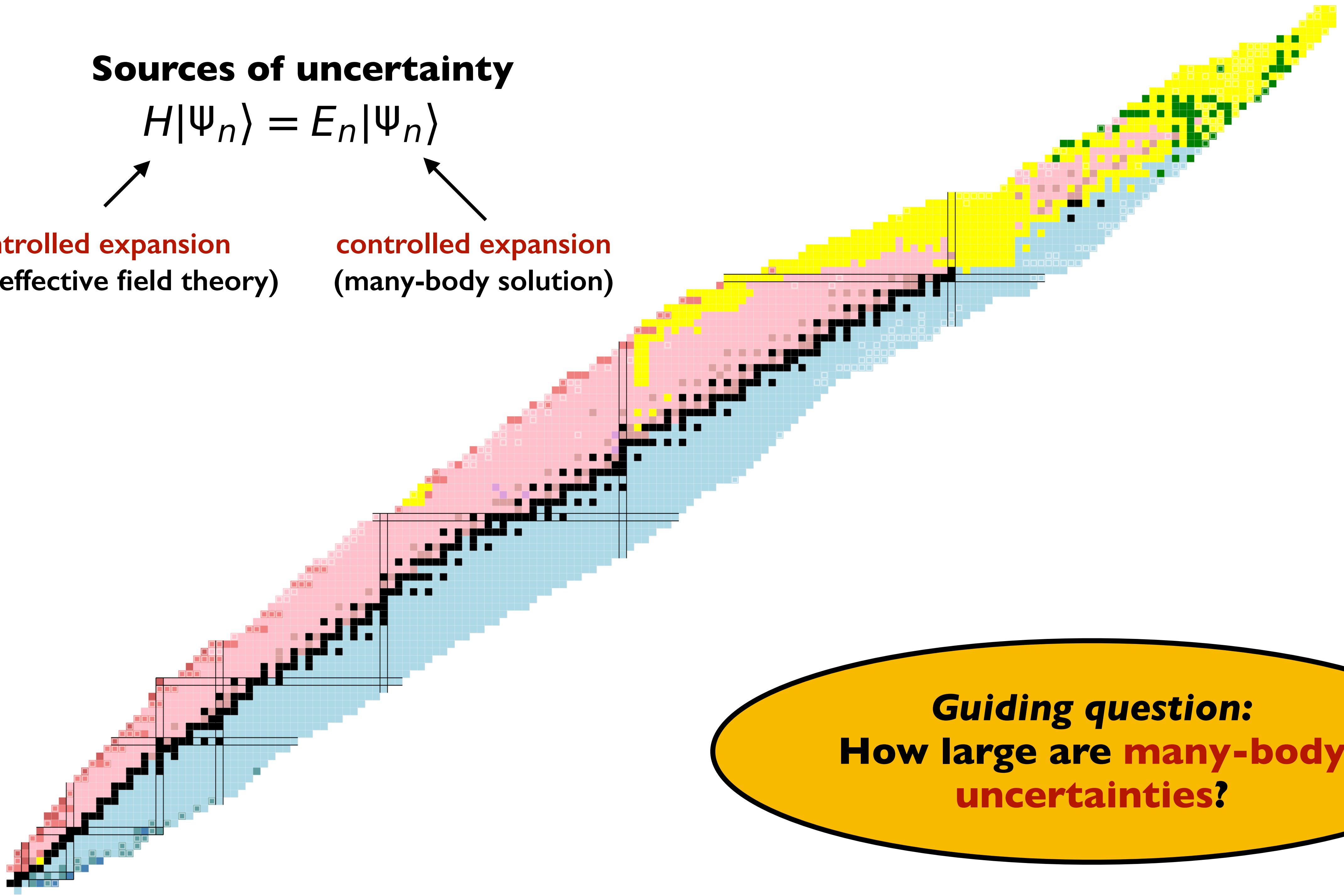
Ab initio nuclear structure

Sources of uncertainty

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

controlled expansion
(chiral effective field theory)

controlled expansion
(many-body solution)



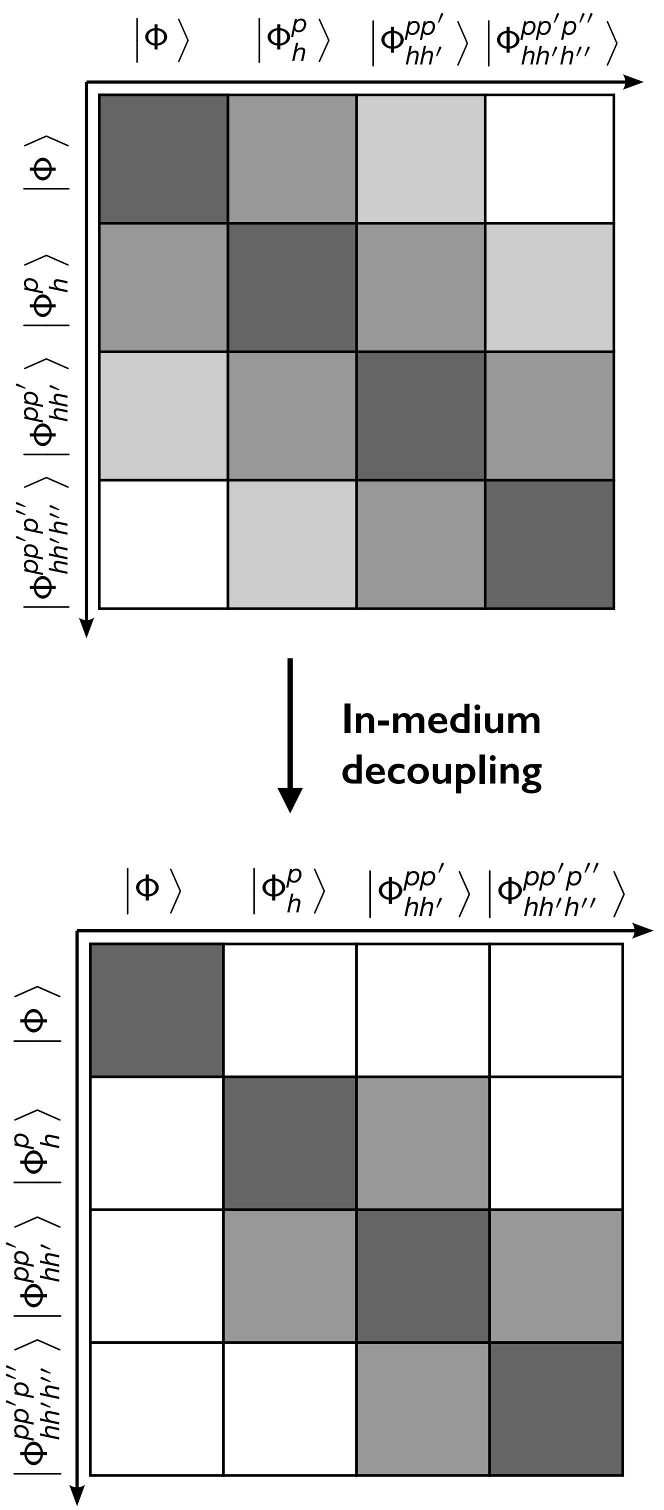
Guiding question:
How large are many-body uncertainties?

<u>Part I</u>
The nuclear density matrix renormalization group

Tichai *et al.*, PLB (2023)
Tichai *et al.*, arXiv:2402.18723

DMRG collaboration
Achim and Takayuki
K. Kapás, S. Knecht, A. Kruppa, Ö. Legeza,
P. Moca, M. Werner, G. Zarand

In-medium similarity renormalization group



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

- Input: nuclear Hamiltonian in second quantization

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

- Goal: decoupling of elementary ph-excitations

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

- 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

The valence-space IMSRG

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

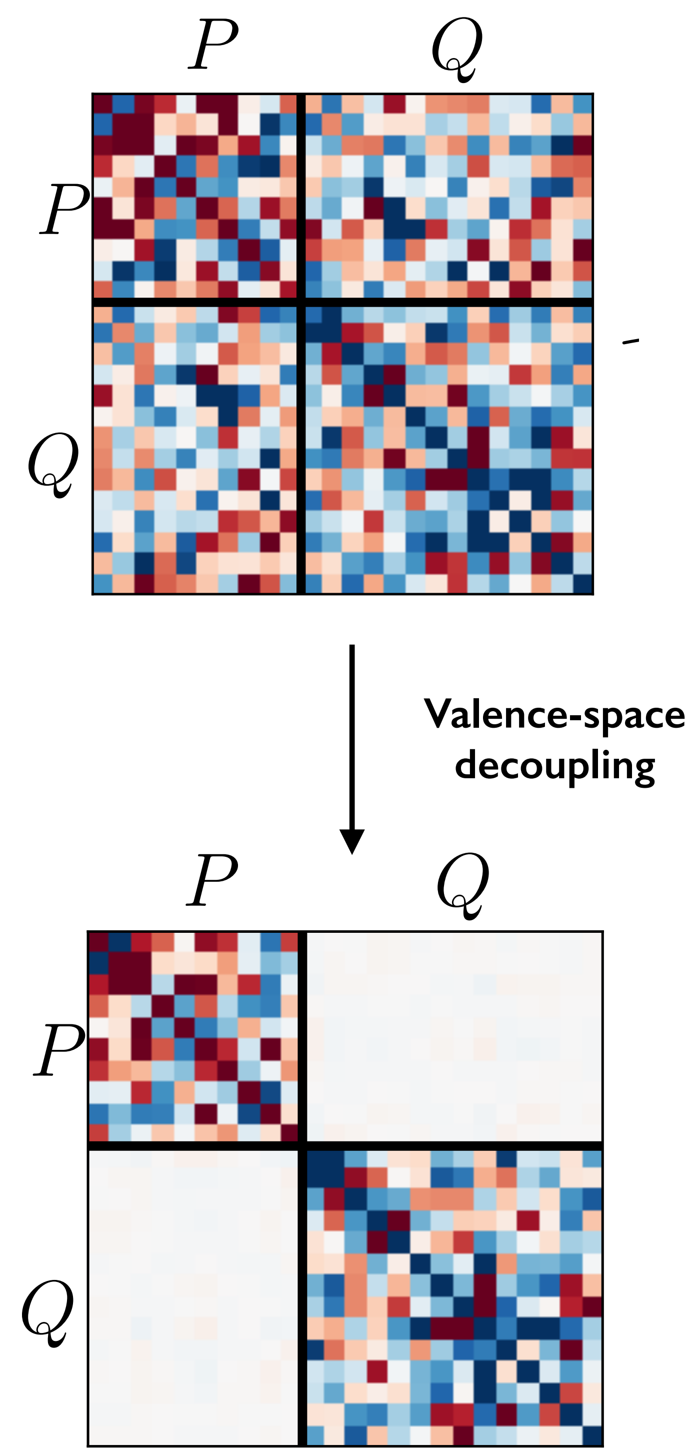
$$H(s) = U^\dagger(s)\, H\, U(s)$$

- Large no-core problem mapped to tractable active-space problem

- Many-body observables from large-space shell-model diagonalization

- Simple access of low-lying spectroscopy

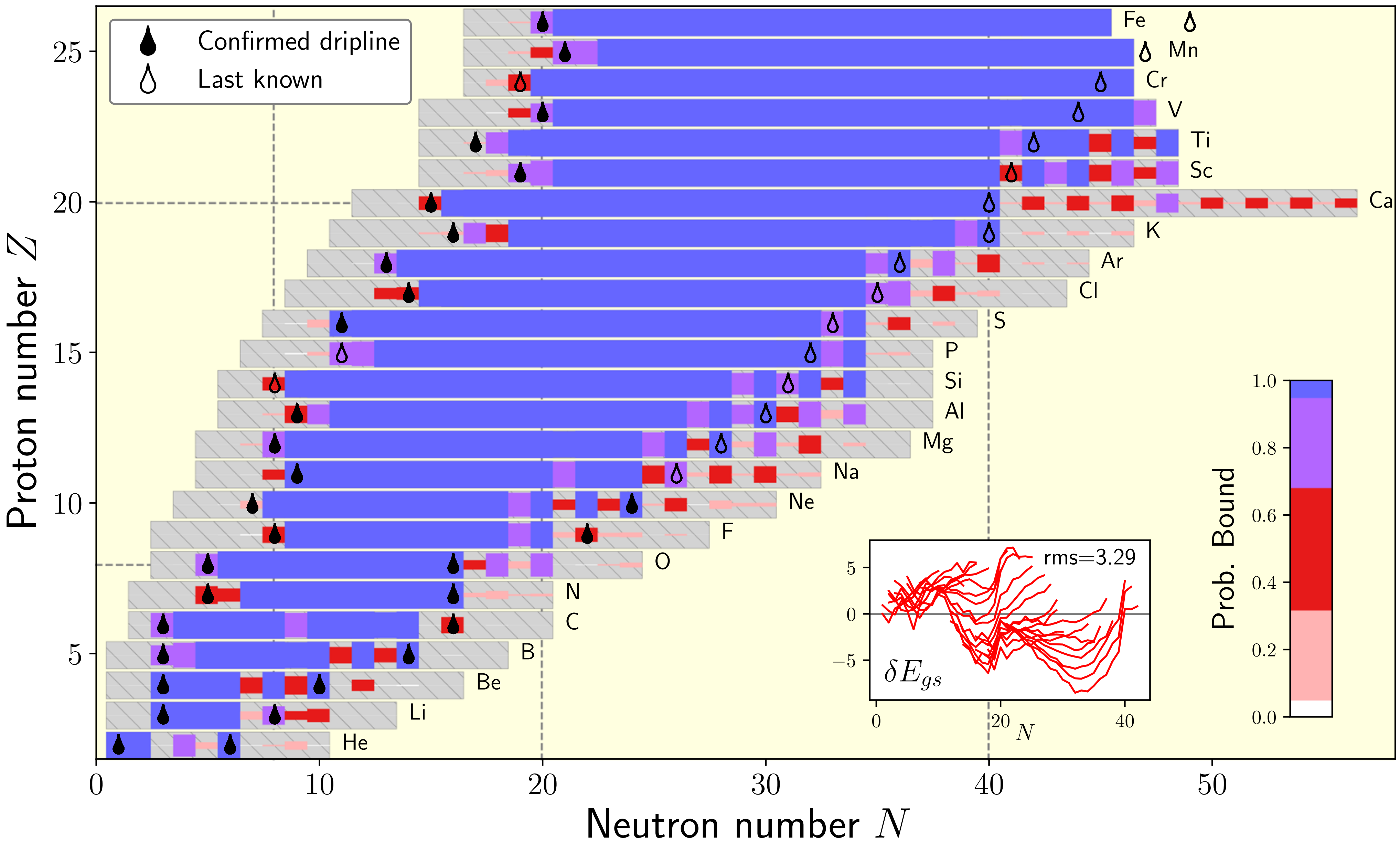
- Benefits from open-sourced shell-model machinery (kshell, Nushell, ANTOINE, …)



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

Successes of the IMSRG

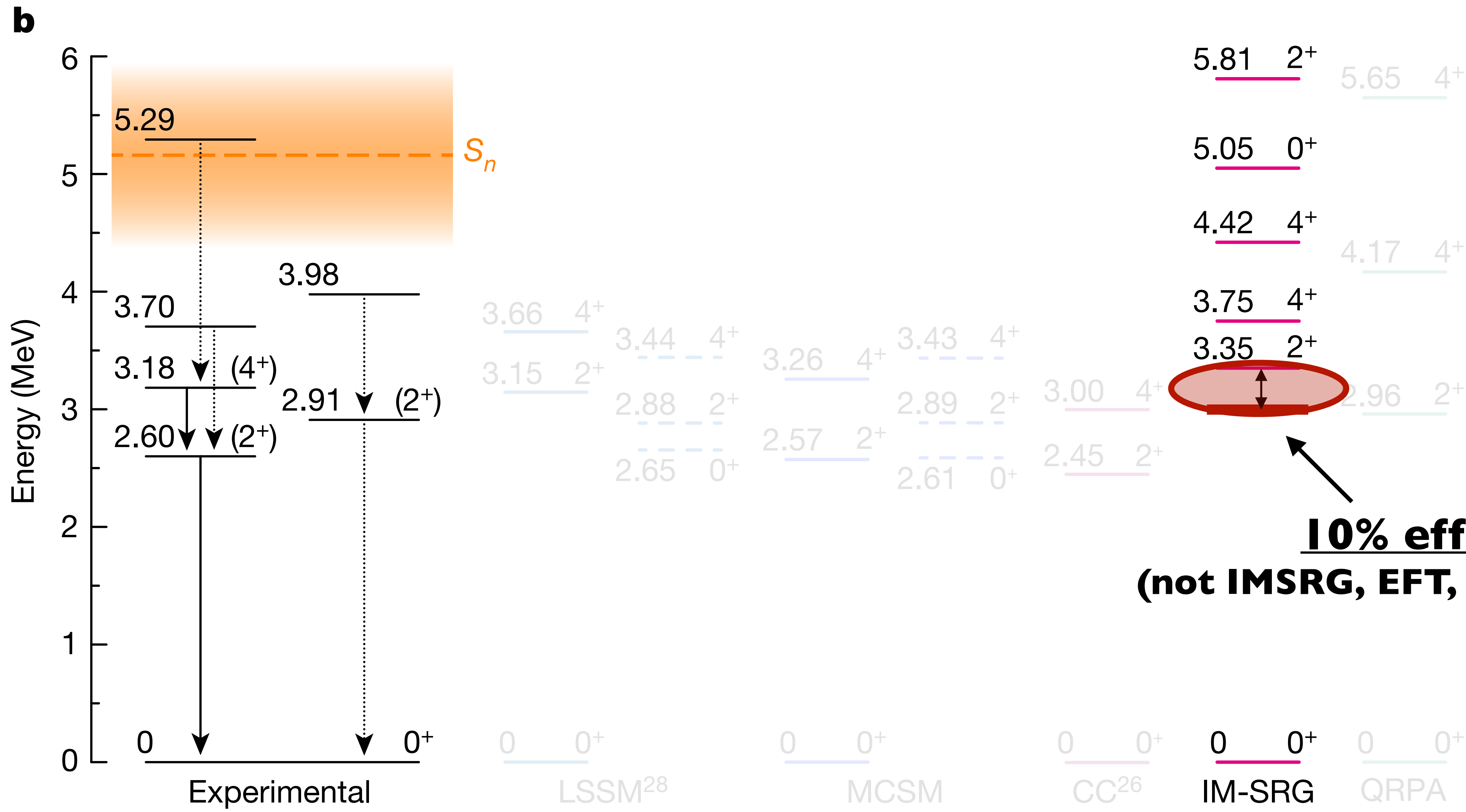
Global study of ~700 nuclei from IMSRG(2)



Stroberg *et al.*, PRL (2021)

Many-body uncertainties

Overview of low-ling spectrum in ^{78}Ni



10% effect!
(not IMSRG, EFT, model space)

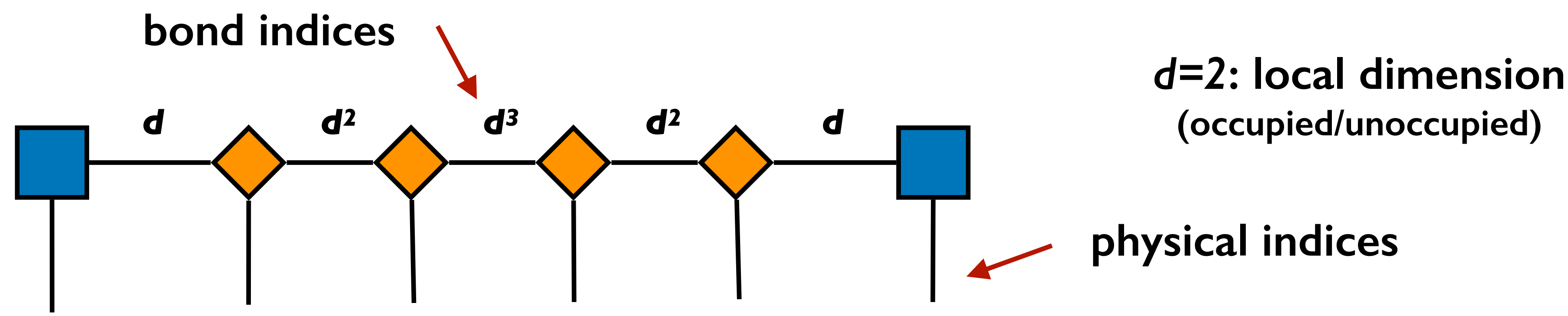
Taniuchi *et al.*, Nature (2019)

VS-IMSRG: 3.350 (50) MeV
DMRG: 3.007 (17) MeV

Density matrix renormalization group

White, PRL (1993)   Schollwöck, Annals of Physics (2011)

- **Matrix product state** (MPS) ansatz for fully correlated wave function

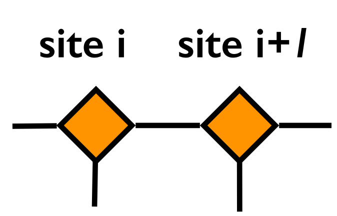


- Approximate MPS representation obtained by **limiting intermediate summation**

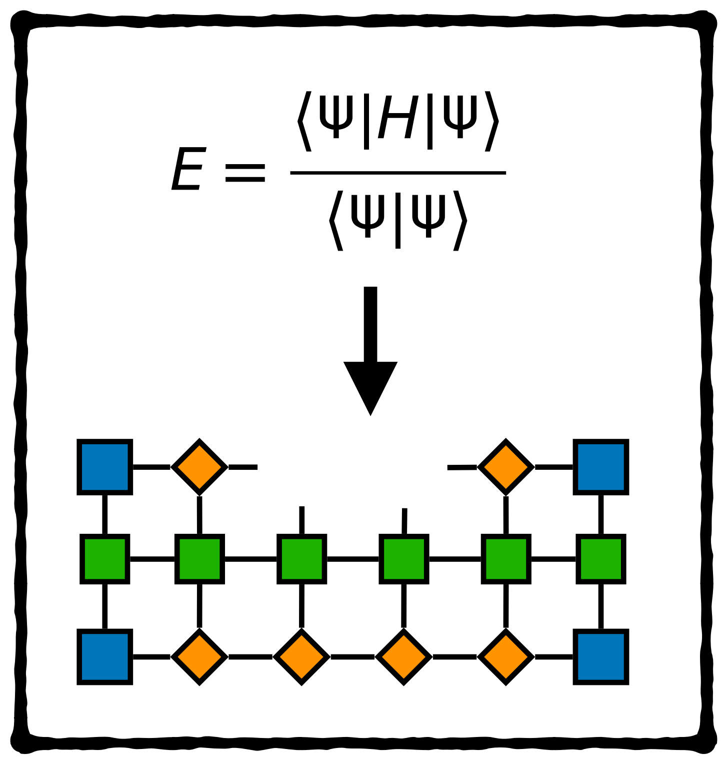
  ⟶ **bond dimension *M***

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

- **Local optimization** of two-site tensors



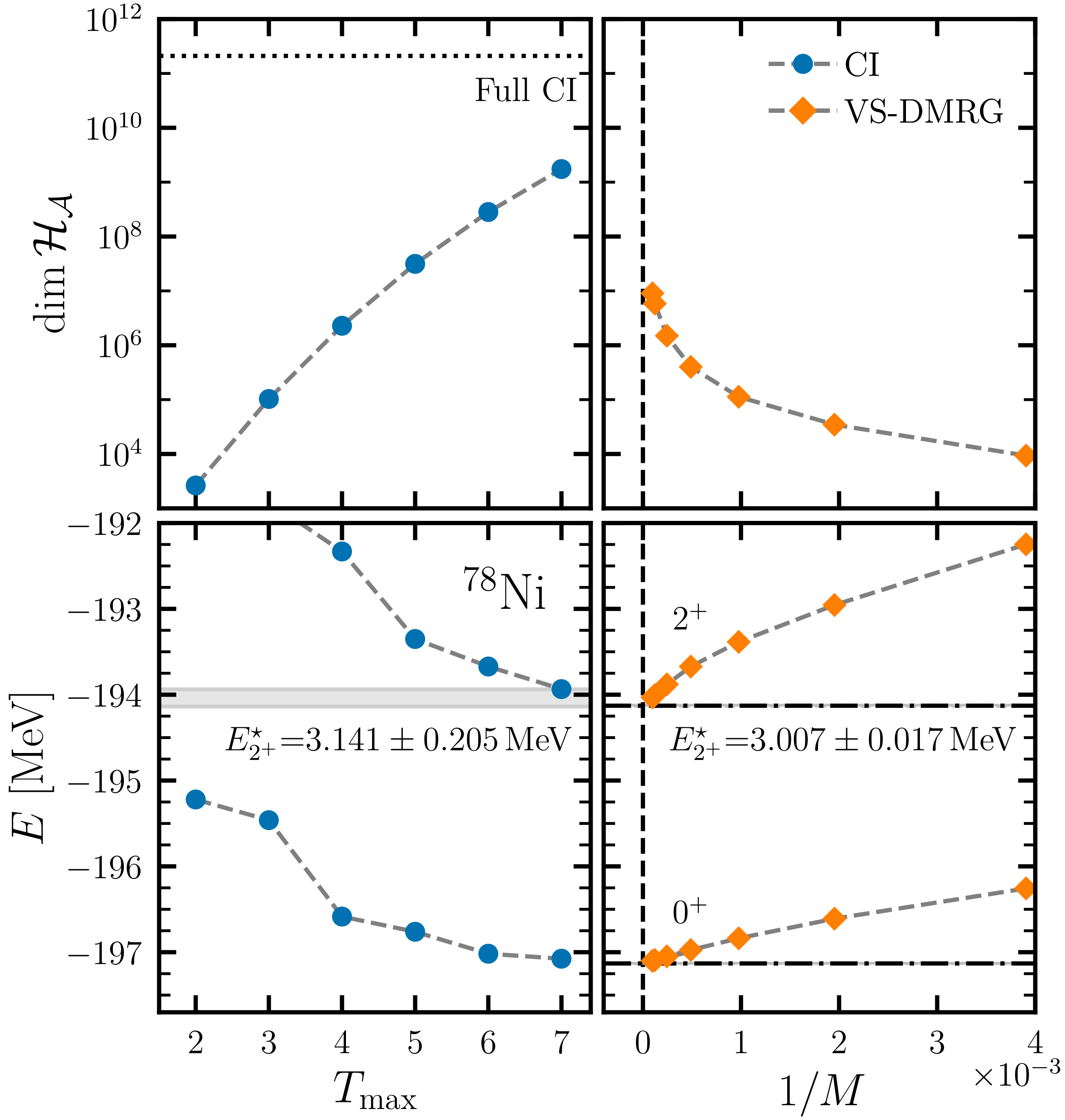
- **Efficient encoding** of nuclear correlations



Revisiting the example of ^{78}Ni

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

DMRG vs. CI in valence-space calculation



(particle-hole truncation)

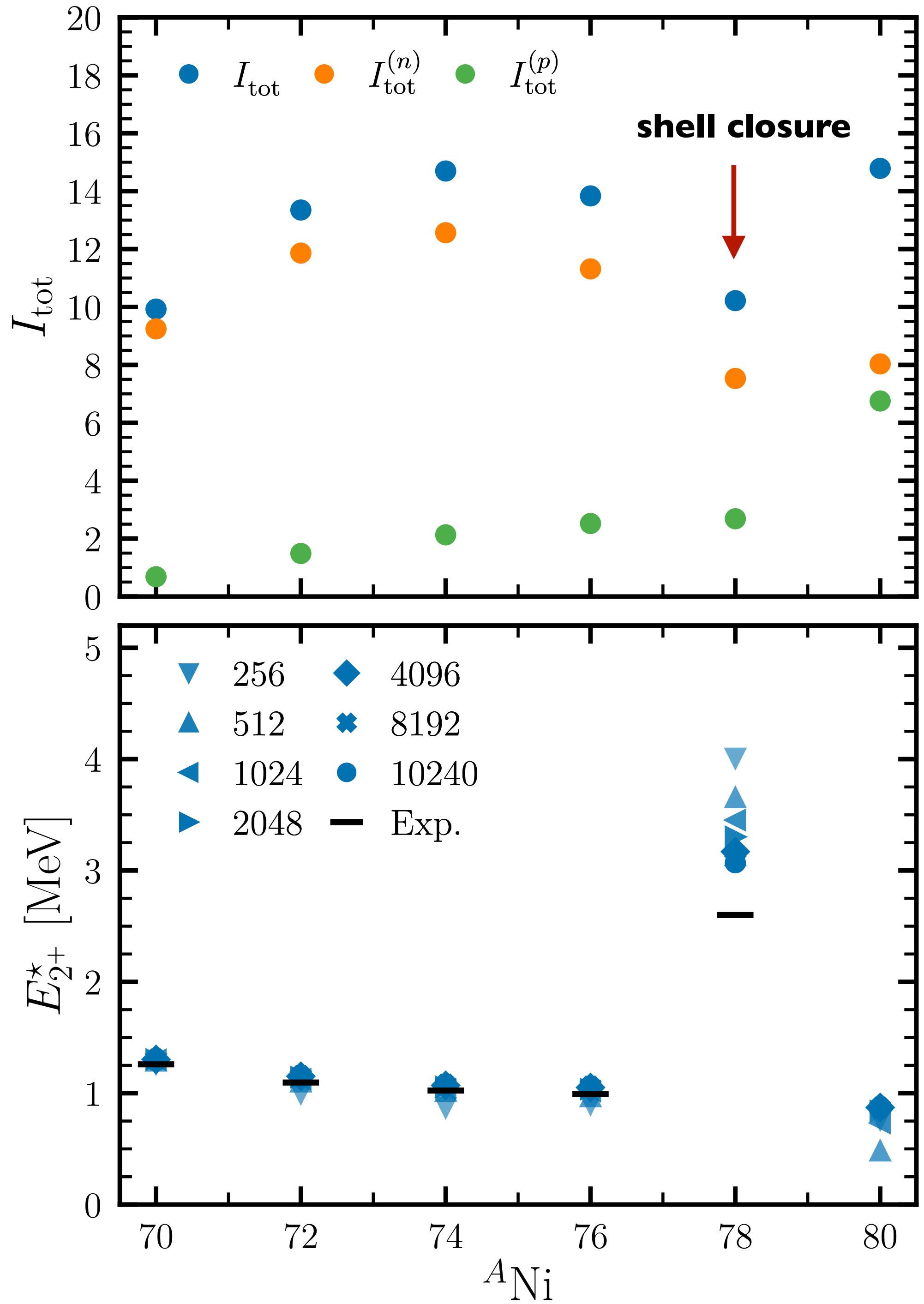
Tichai *et al.*, PLB (2023)

- **DMRG: economic representation of the many-body wave function**
- **Robust convergence of DMRG energies at large bond dimension**
- **Exact solution out of reach: ~220 billion Slater determinants**
- **Conventional diagonalization makes robust UQ impossible**

Intermezzo: Entanglement and correlations

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

Total entropy in even-mass nickel isotopes



Tichai *et al.*, PLB (2023)

- Entanglement through information science

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

- Total entropy quantifies entanglement

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

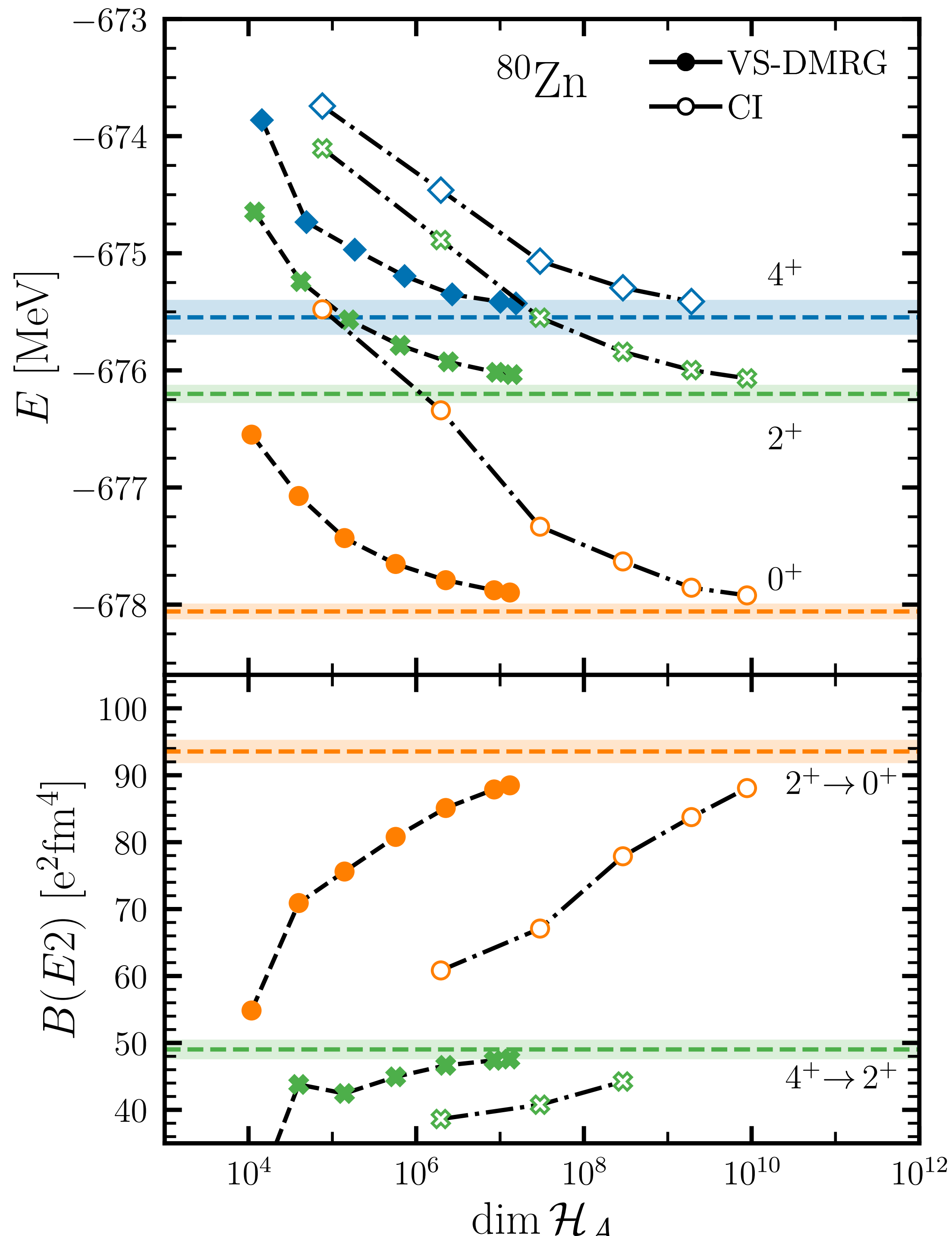
- Pronounced kink at ^{78}Ni hints at neutron shell closure (~ dominated by HF)

- Agreement with conventional prediction based on 2^+ excitation energies

Phenomenology through the eyes of information theory!

Towards spectroscopy

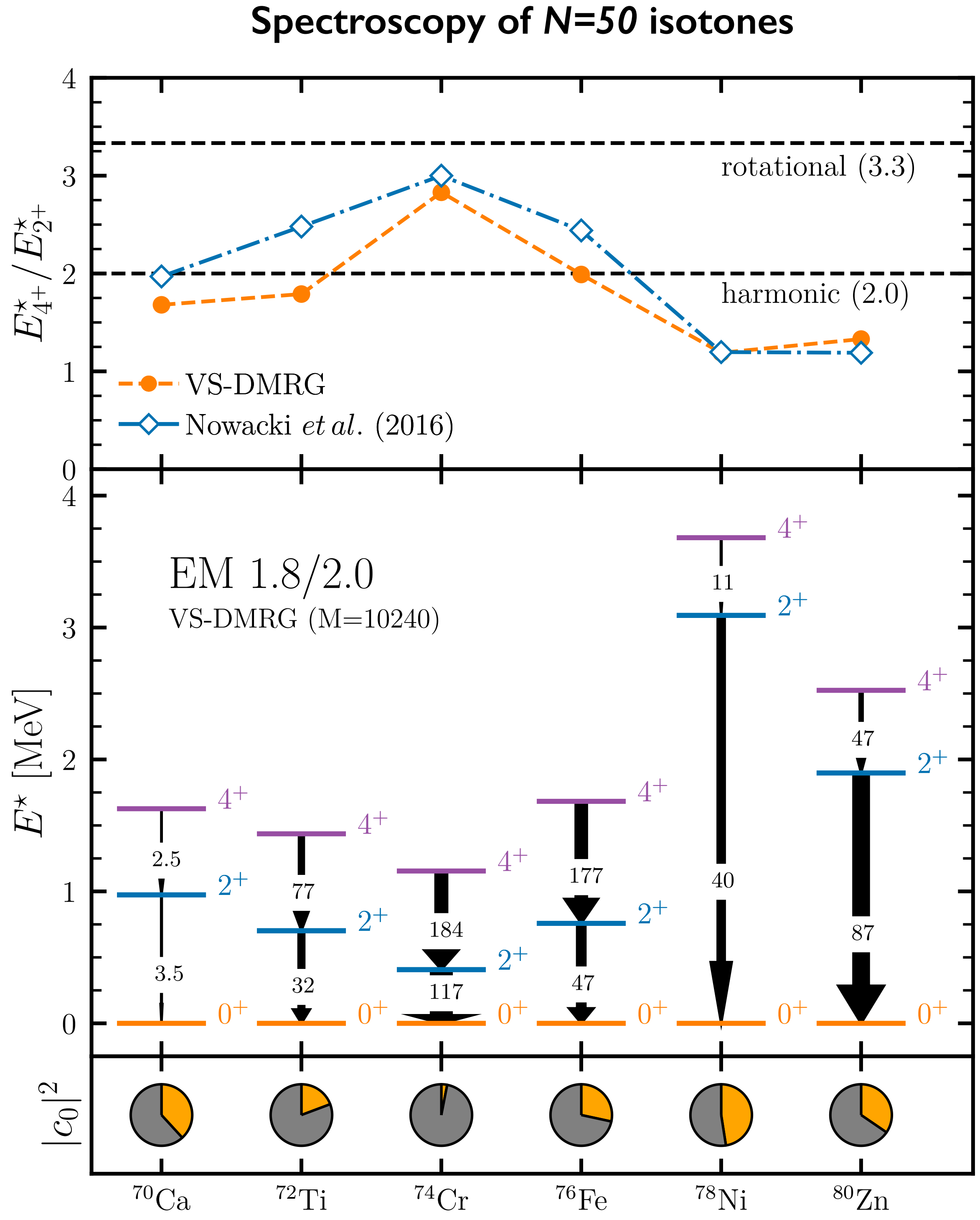
DMRG/CI observables vs. effective dimension of H_A



- **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**

Tichai *et al.*, arXiv:2402.18723

Transitional nuclei at *N*=50



Tichai *et al.*, arXiv:2402.18723

- 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

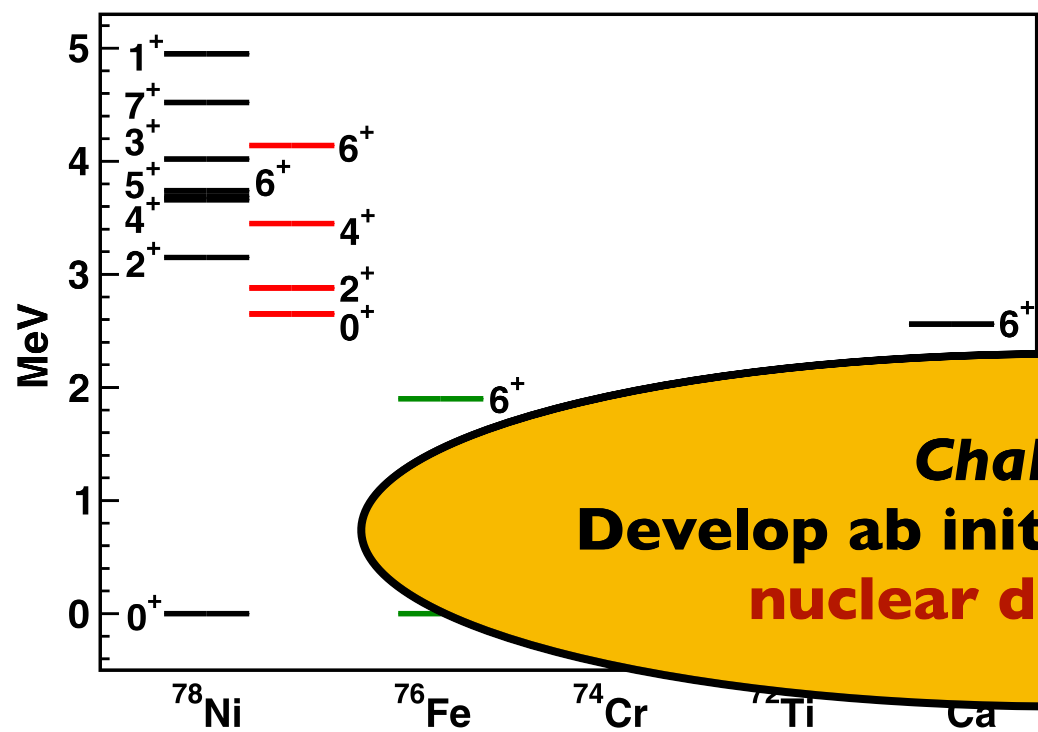
Nowacki *et al.*, PRL (2016)

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

Future challenges: shape coexistence

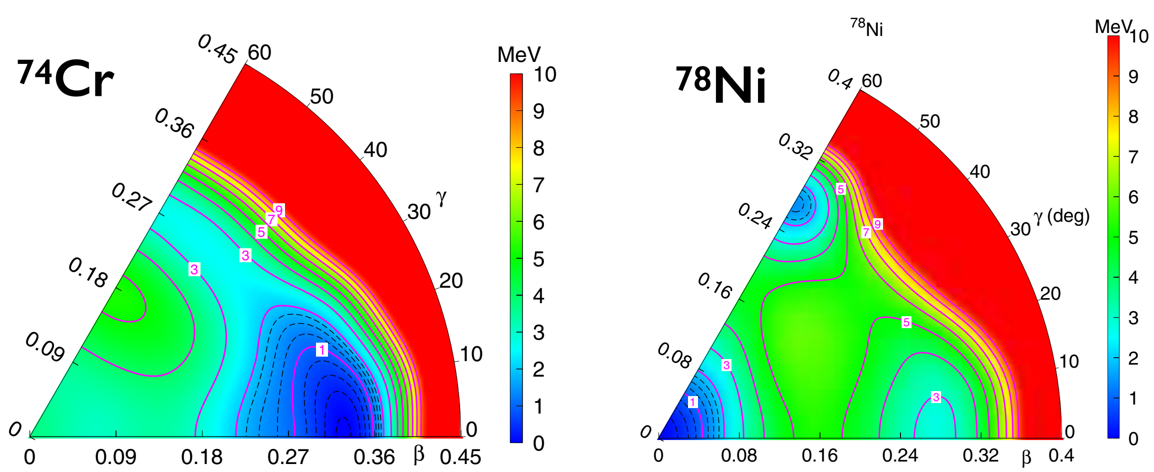
see also Taniuchi *et al.*, Nature (2019)

Spectroscopy of *N=50* isotones



- Emergence of deformed excited-state rotational band in ^{78}Ni
- Second 0^+ state comes out much higher at 5 MeV: IMSRG(3) and beyond?
- ...herical minimum in ...rolate minimum in ^{74}Cr

Challenge:
Develop ab initio machinery for nuclear deformation.



Nowacki *et al.*, PRL (2016)

Collective phenomena induce larger uncertainties!

Part II
Bogoliubov coupled cluster theory for heavy nuclei

Tichai *et al.*, PLB (2024)
Demol *et al.*, PLB (unpublished)
Vernik *et al.*, (unpublished)

BCC collaboration
Pepijn Demol, Urban Vernik, Thomas Duguet

Bogoliubov coupled cluster theory

Signoracci *et al.*, PRC (2015)

- Coupled cluster: exponential representation of ground-state wave function

$$|\Psi_{\text{BCC}}\rangle = e^{\mathcal{T}}|\Phi\rangle$$

Quasi-particle extension of standard CC theory
('CC theory for HFB states')

- Definition in terms of cluster operator with unknown cluster amplitudes

$$\mathcal{T} = \mathcal{T}_1 + \mathcal{T}_2 + \ldots + \mathcal{T}_A \qquad \mathcal{T}_2 = \frac{1}{4!}\sum_{pqrs} t_{pqrs}\beta^\dagger_p\beta^\dagger_q\beta^\dagger_r\beta^\dagger_s$$

- Similarity-transformed grand potential as core object in formalism

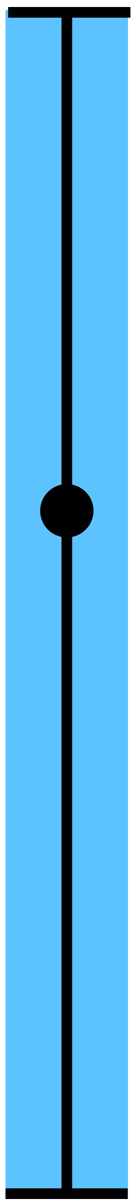
$$\tilde{\Omega} = e^{-\mathcal{T}}\Omega e^{\mathcal{T}} \qquad \Omega = H - \lambda A$$

- Determine cluster amplitudes iteratively from left-projected amplitude equation

$$\langle\Phi^{pq}|\tilde{\Omega}|\Phi\rangle = 0$$

$$\langle\Phi^{pqrs}|\tilde{\Omega}|\Phi\rangle = 0$$

(*Ad hoc*) Many-body uncertainties



- Truncation of E_{3max} for three-body matrix elements

explicit extrapolation

- Finite size of the one-body Hilbert space (e_{max})

1 - 2 % of total binding energy ↓

- Normal-ordering approximation of three-body force

2 % of total binding energy ↓↑

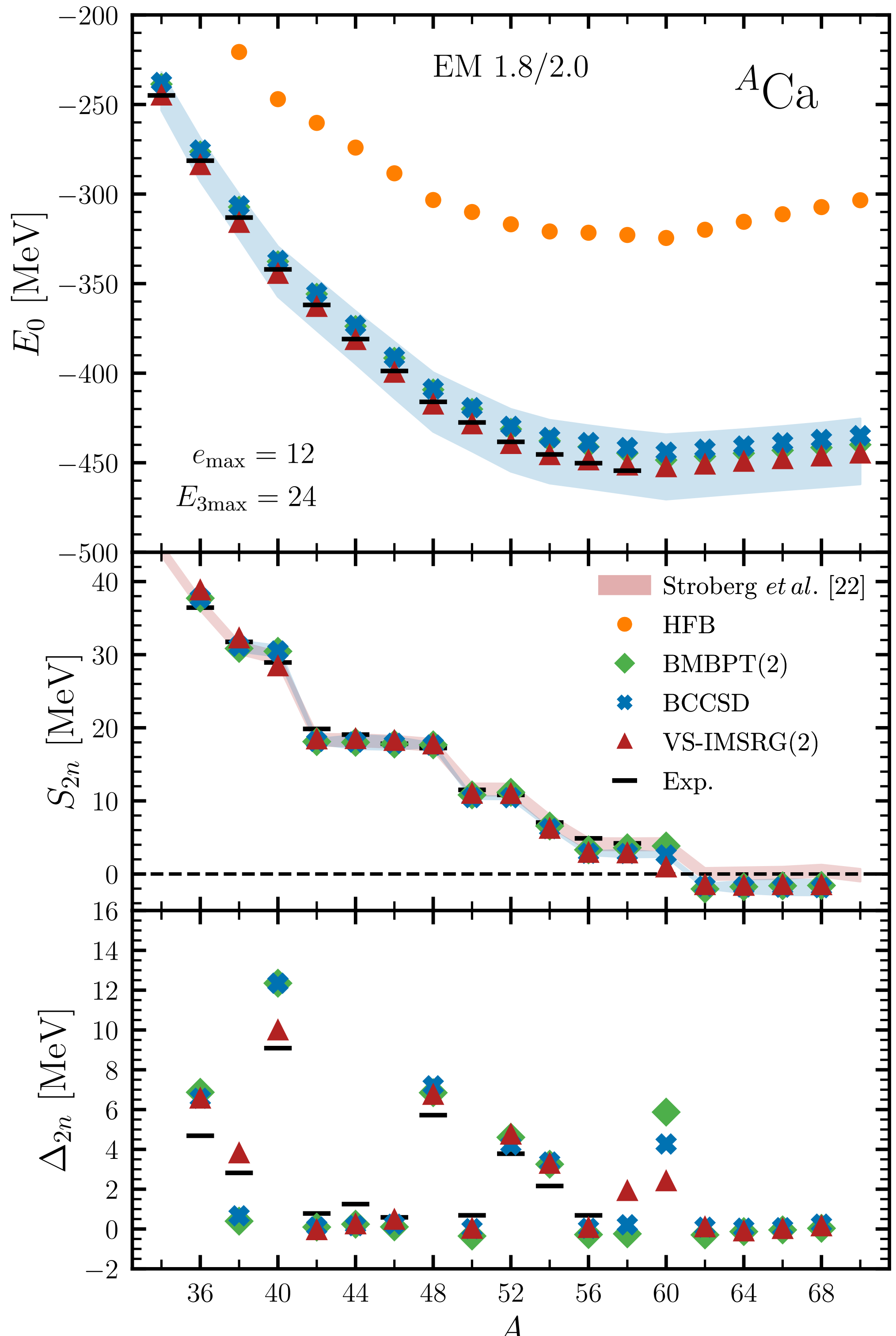
- Truncation of BCC expansion: missing T_3 amplitudes

10 % of correlation energy ↓

- Lack of particle-number projection of wave function

approximate HFB projection
(less than 3 MeV)

Validation in the calcium chain



- **Reproduction of experimental trends and VS-IMSRG predictions**
- **Consistent prediction of two-neutron separation energies**
- **Tentative drip line 'assignment' at A=60 but more neutron-rich nuclei supported within error bars**

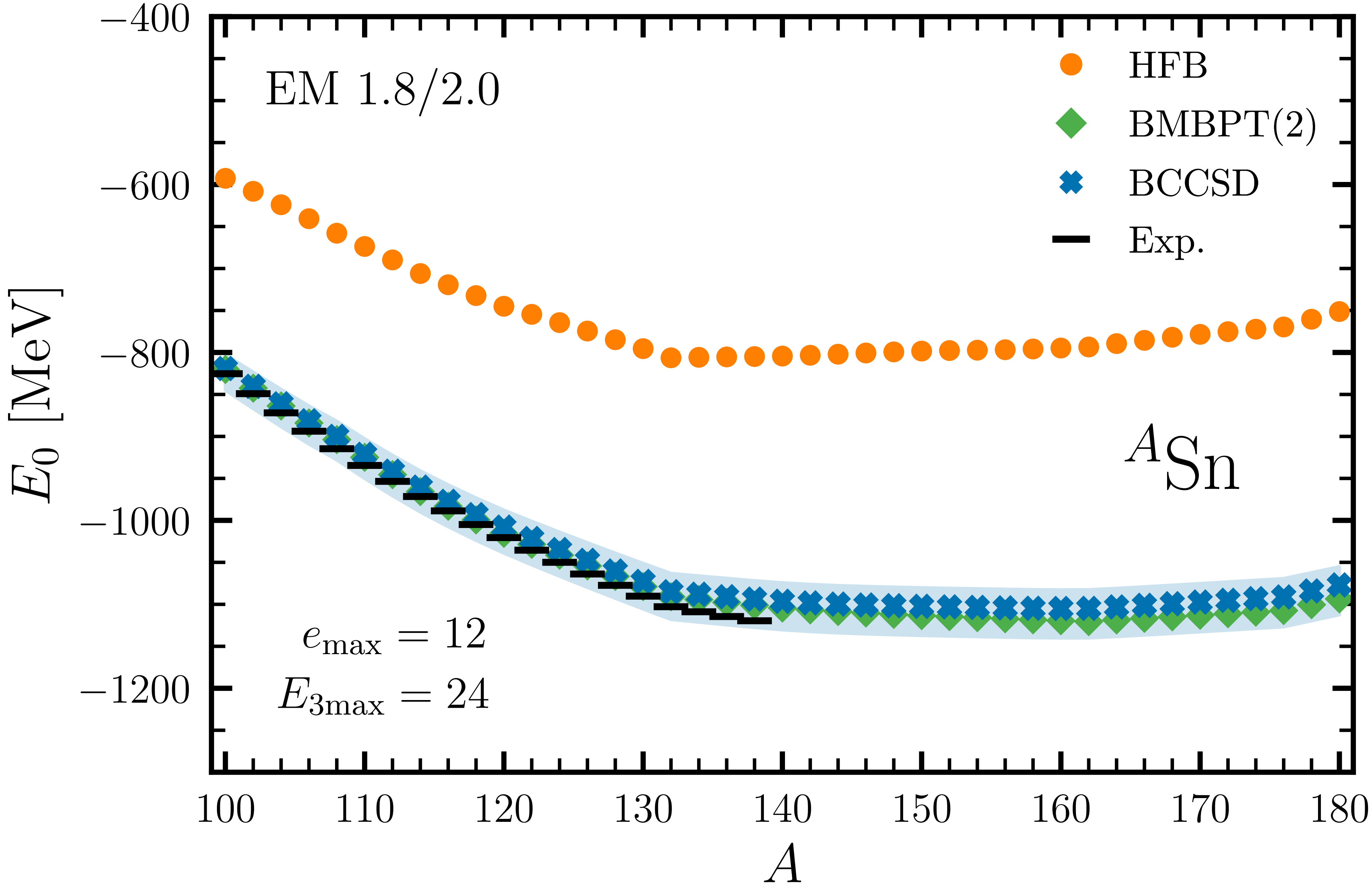
$$S_{2n}(N,Z) = E(N,Z) - E(N-2,Z)$$

- **Two-neutron shell gap serves as proxy for shell closures**

$$\Delta_{2n}(N,Z) = |S_{2n}(N,Z)| - |S_{2n}(N-2,Z)|$$

Tichai *et al.*, PLB (2024)

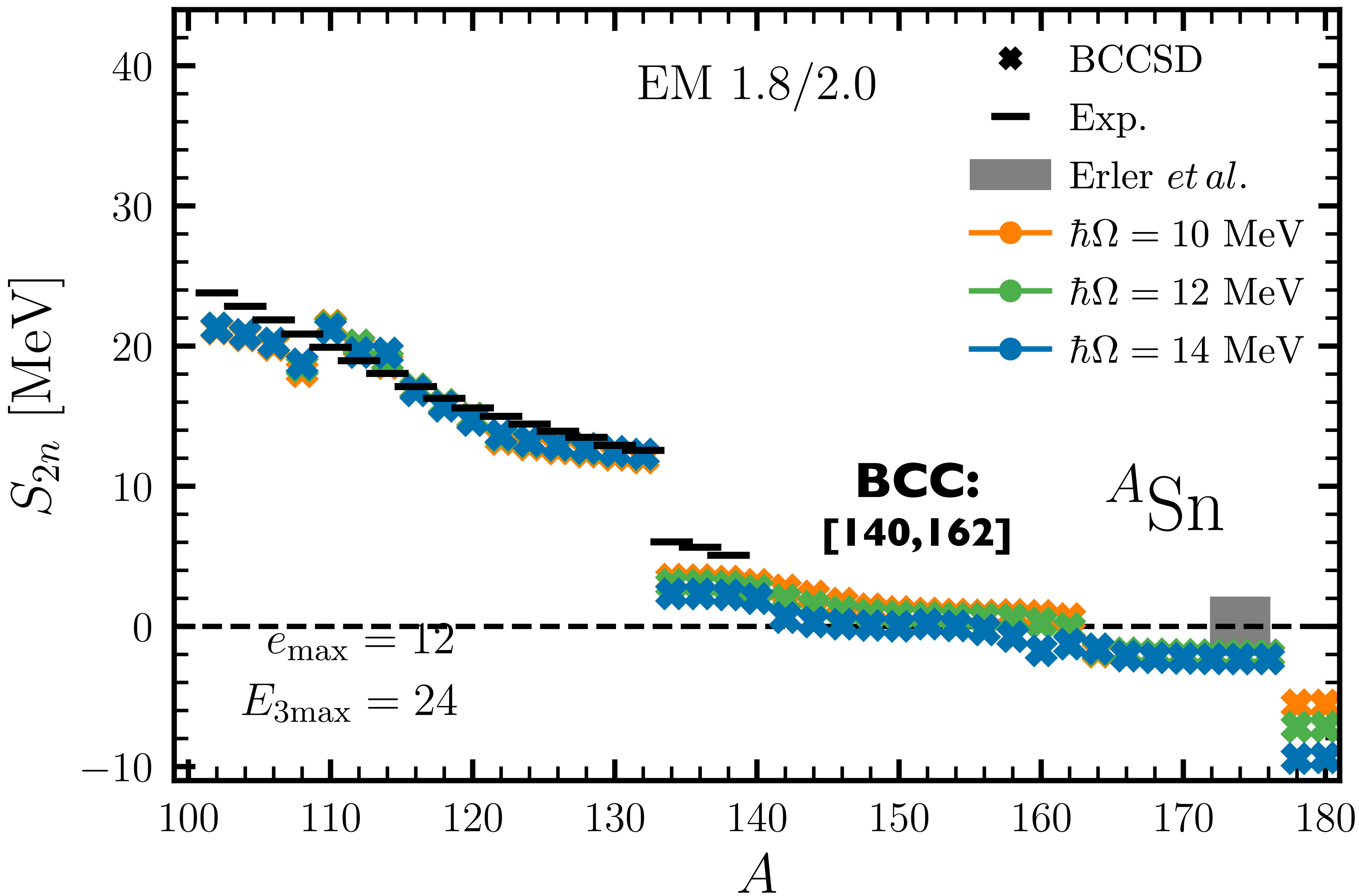
Heavy-mass frontier: tin



Heaviest open-shell *ab initio* calculations so far!
(To the best of my knowledge)

Tichai *et al.*, PLB (2024)

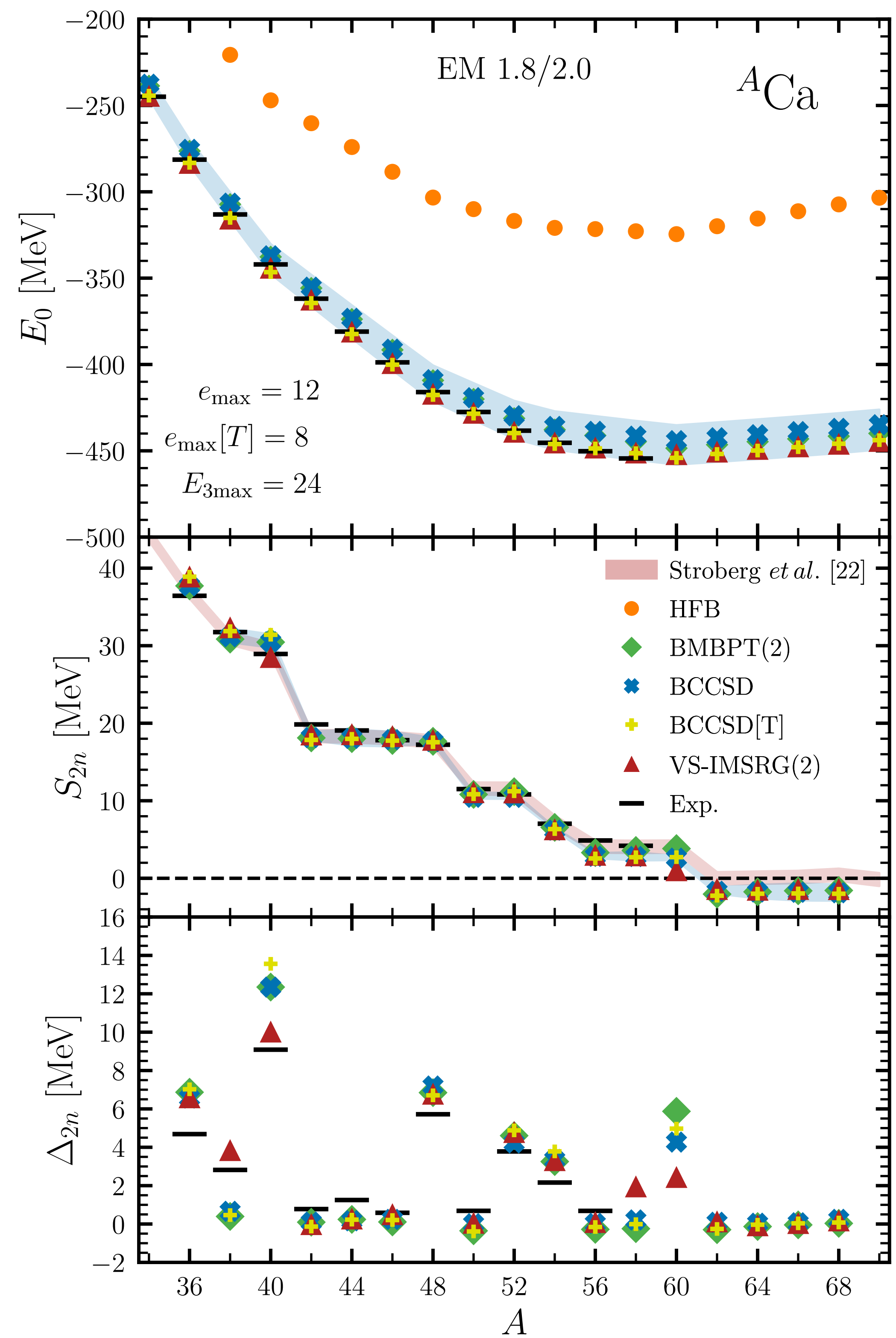
Neutron dripline in tin



UQ (many-body + interaction) needed
to quantitatively compare dripline predictions!

Tichai *et al.*, PLB (2024)

Towards higher accuracy

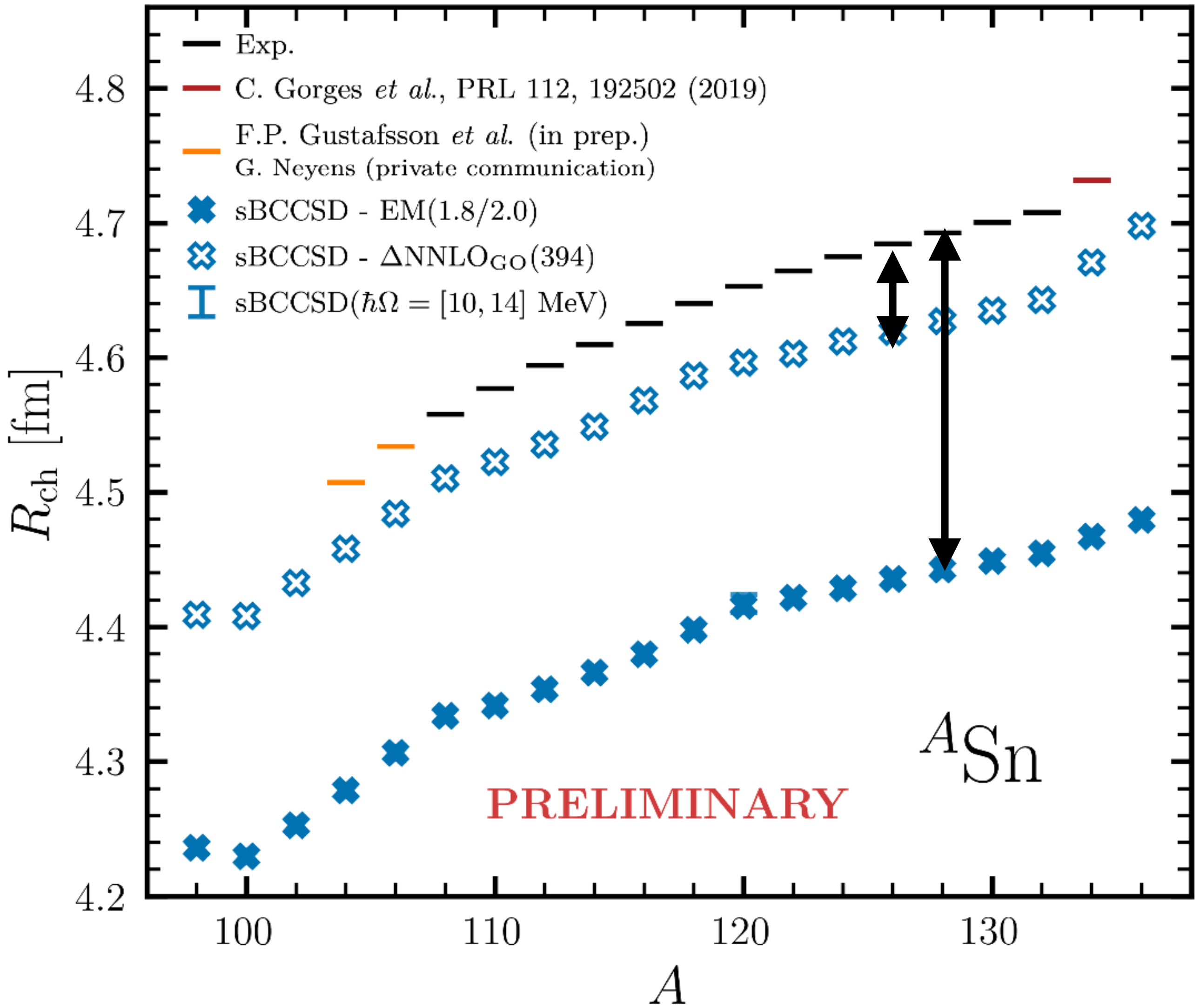


- Incorporation of **leading-order triples effects** in BCC framework
- Many-body uncertainty: triples in CC contribute **8-10 % of correlation energy**
- **Systematic improvement** towards VS-IMSRG(2) simulations
- Differential quantities remain largely unaffected in calcium isotopes
- **Two-neutron shell gap** serves as proxy for shell closures

Vernik, Demol, Tichai, Duguet (unpublished)

Radii in tin isotopes

Charge in tin isotopes



Demol, Tichai, Duguet (unpublished)

- Observables consistently calculated in BCC theory

- Well-known underproduction of charge radii from chiral EFT

  EM 1.8/2.0: ~ 5 %

  N^{2}LO$_{GO}$: ~ 1 %

- New experiment data available

  ^{134}Sn Gorges *et al.*, PRL (2019)

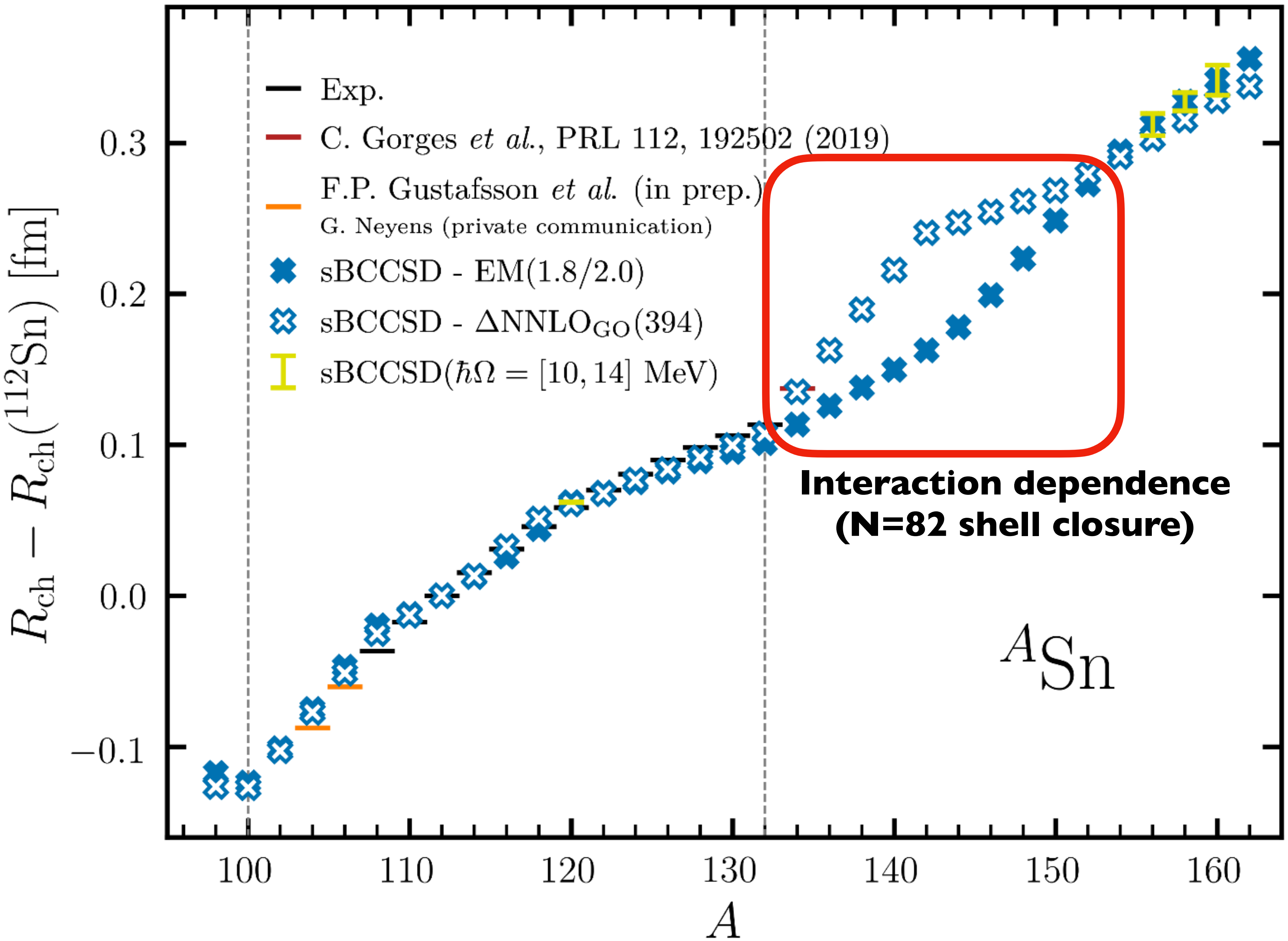
  $^{104-106}$Sn Gustafson *et al.*, (in prep.)

- New hope from novel interactions with large LECs (c_D = 7.5)

  Arthuis *et al.*, arXiv:2401.06675

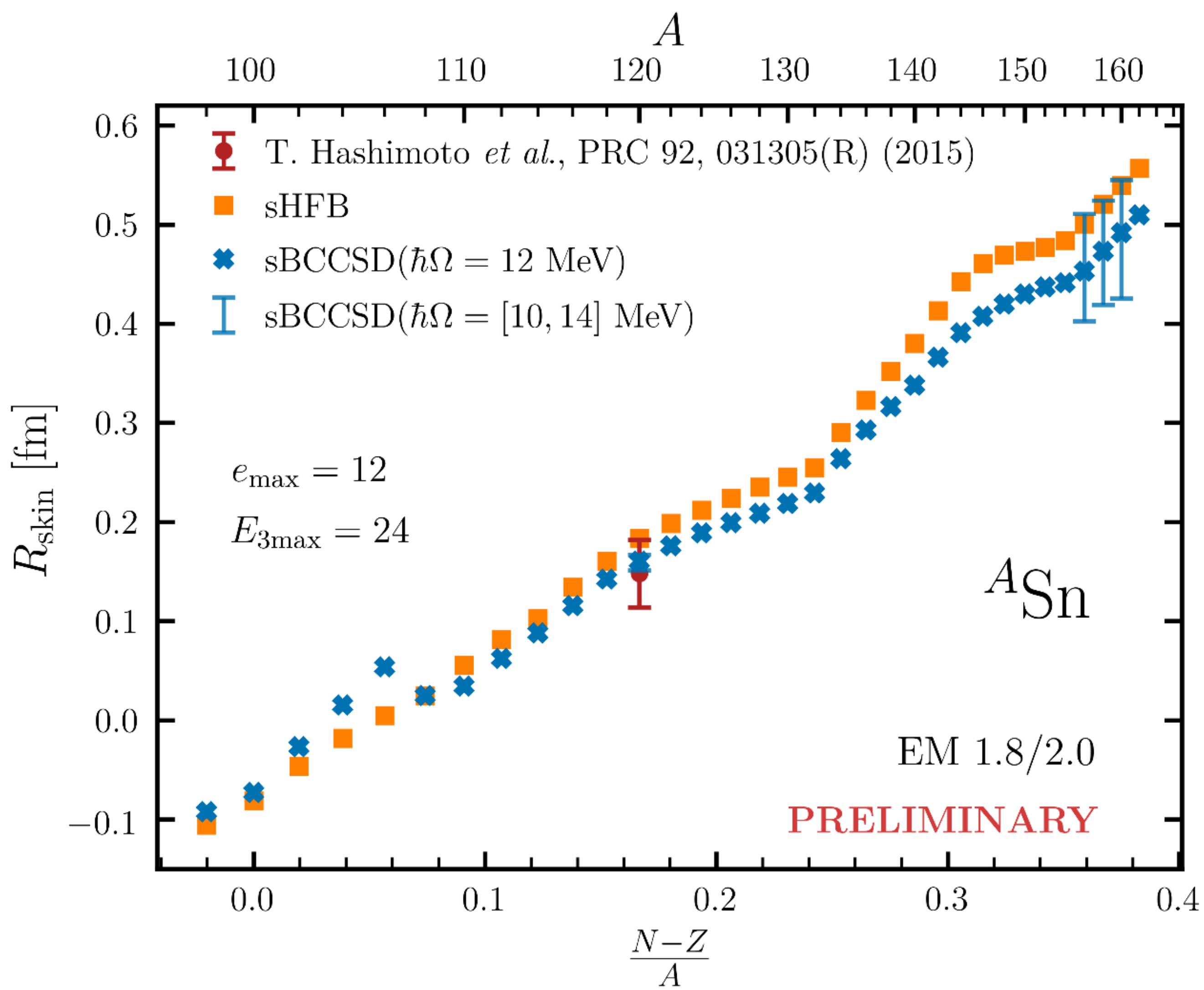
Differential charge radii

Interaction sensitivity in neutron-rich tins



Demol, Tichai, Duguet (unpublished)

Neutron skins in tin



Demol, Tichai, Duguet (to be published)

- **Correlated with slope parameter in symmetric nuclear matter**

Nuclear EOS

- **Linear dependence of neutron skins on isospin asymmetry**
- **Local variations due to nuclear shell structure**
- **Sizeable uncertainties due to incomplete model space (e_{max})**

Summary

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: explore larger spaces beyond shell model capacities

---

Heavy nuclei from Bogoliubov coupled cluster

- Extension applicable to general open-shell nuclei
- Scalable approach to heavy nuclei at mild computational cost
- New insights into interaction effects from chiral EFT

Next steps: test new set of chiral interactions for *A>100*

For discussion

- Design of robust error models for nuclear many-body uncertainties

$$\epsilon_{\text{MB}} = \epsilon_{\text{CC/IMSRG}} + \epsilon_{\text{FBS}} + \epsilon_{\text{NO2B}} + \epsilon_{\text{3B}}$$

- EFT advantage: converged predictions from ‘many’ consecutive orders available

LO $\longrightarrow$ NLO $\longrightarrow$ N^{2}LO $\longrightarrow$ N^{3}LO

versus

IMSRG(2) $\rightarrow$ IMSRG(3) $\rightarrow$ IMSRG(4)

- Different observables have different sensitivities to nuclear correlations

E_0: particle-hole correlations

B(E2): quadrupole collectivity

- Current many-body machinery must be extended to target complex structures

Deformation, clustering, halo structures, ...

- Development of many-body emulators is a highly non-trivial problem