Project A04:

No-Core Approaches to Medium-Mass Nuclei

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TECHNISCHE UNIVERSITÄT DARMSTADT

SFB 1245

Ab Initio No-Core Methods

No-Core Shell Model

In-Medium Similarity Renormalization Group

Many-Body Perturbation Theory

Ab Initio No-Core Methods

No-Core Shell Model

- solution of matrix eigenvalue problem in truncated many-body model space
- **universality:** all nuclei and all bound-state observables on the same footing
- **but:** limited by model-space convergence

In-Medium Similarity Renormalization Group

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In-Medium Similarity Renormalization Group

- decoupling ground-state from excitations through unitary transformation via flow equation
- **efficiency:** favorable scaling gives access to medium-mass nuclei
- **but:** limited to ground-state observables

Many-Body Perturbation Theory

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Many-Body Perturbation Theory

- power-series expansion of energies and states
- **simplicity:** low-order contributions can be evaluated very easily and efficiently
- **but:** order-by-order convergence problematic

In-Medium NCSM

NCSM
reference state

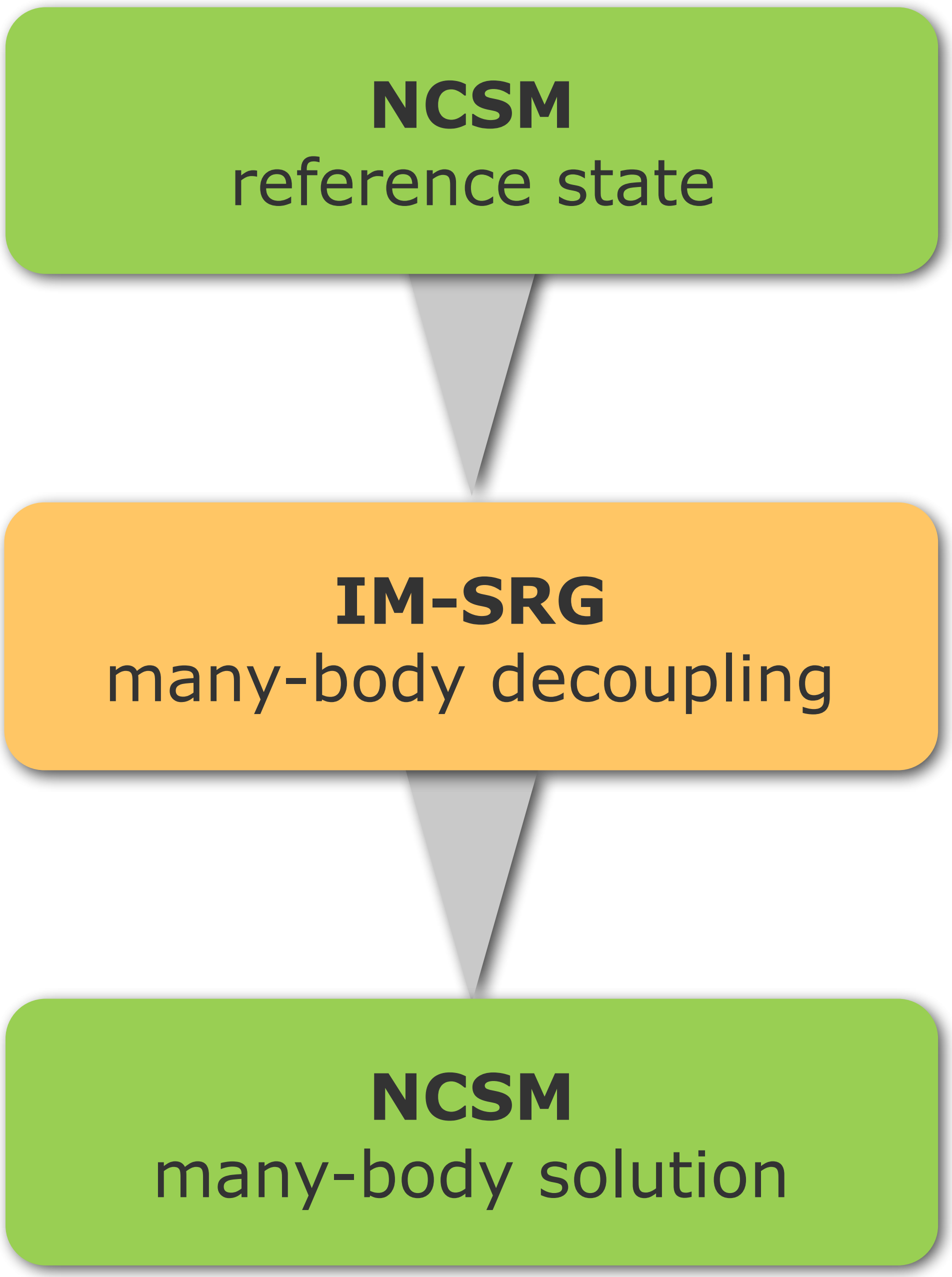
↓

IM-SRG
many-body decoupling

↓

NCSM
many-body solution

In-Medium NCSM



- ground-state from NCSM at small N_{max} as reference state for multi-reference IM-SRG
- access to all open-shell nuclei and systematically improvable

In-Medium NCSM

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reference state

IM-SRG
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- IM-SRG evolution of multi-reference normal-ordered Hamiltonian (and other operators)
- decoupling of particle-hole excitations, i.e., pre-diagonalization in many-body space

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IM-SRG
many-body decoupling

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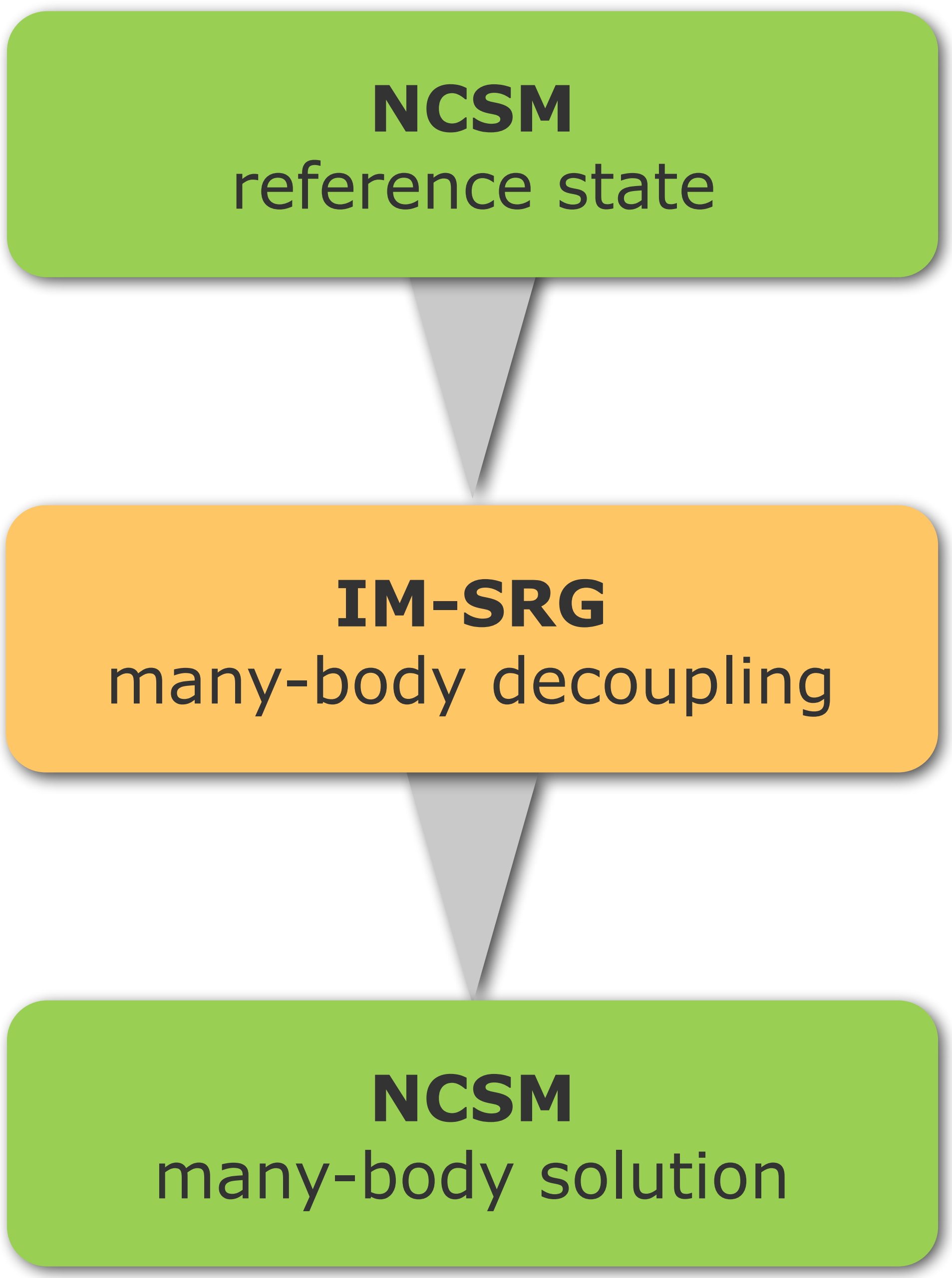
NCSM
many-body solution

- use in-medium evolved Hamiltonian for a subsequent NCSM calculation
- access to ground and excited states and full suite of observables

In-Medium NCSM

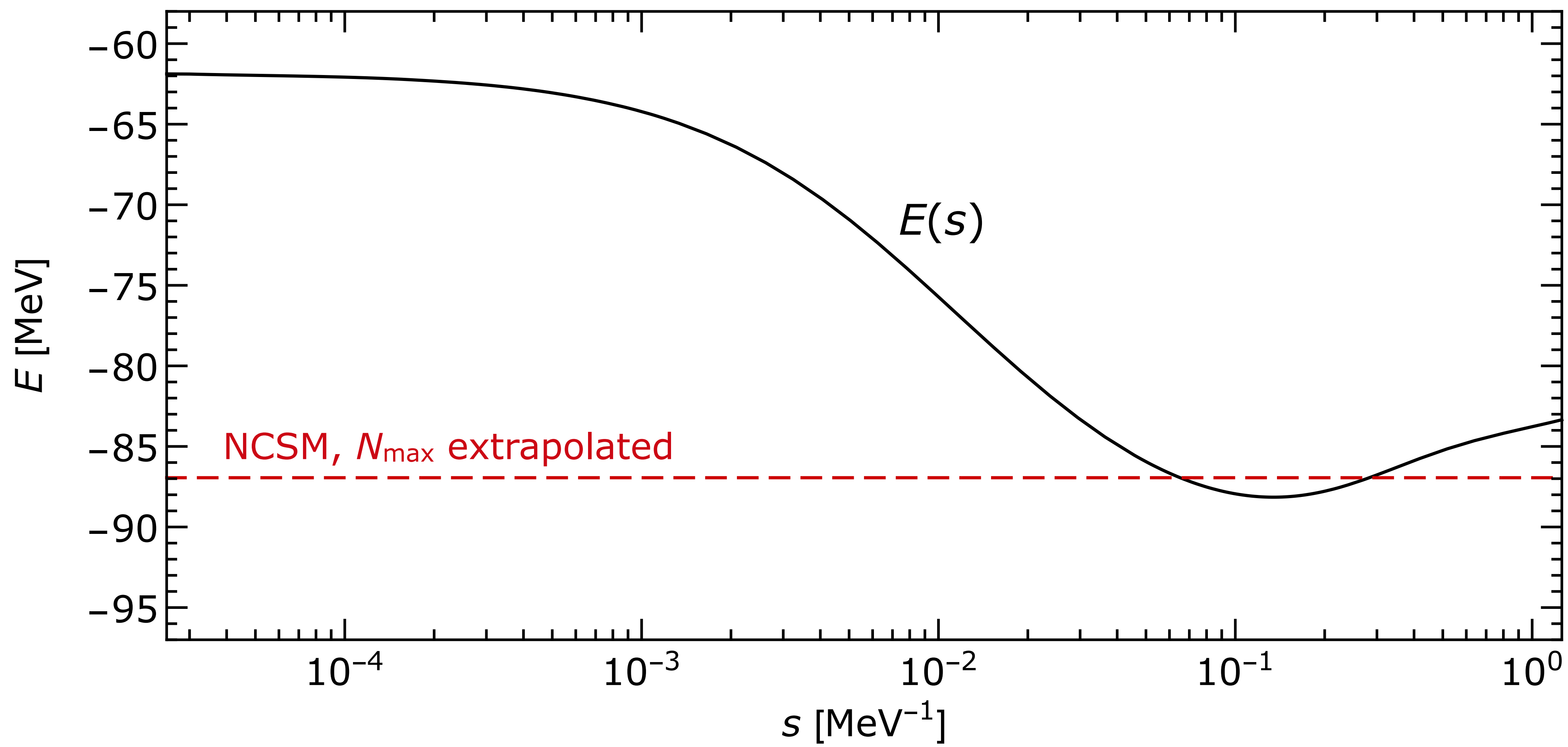


different from valence-space shell model with IM-SRG interactions

- build on explicit multi-reference formulation for nucleus of choice
- full no-core approach, all nucleons active
- all model-space truncations are converged

In-Medium SRG: Multi Reference

Gebrerufael, Vobig, Hergert, Roth; PRL 118, 152503 (2017)



^{12}C

chiral NN+3N

Λ_{3N}=400 MeV

α=0.08 fm^4

$\hbar\Omega$=20 MeV

e_{max}=12

N_{max}=0 reference

HF basis

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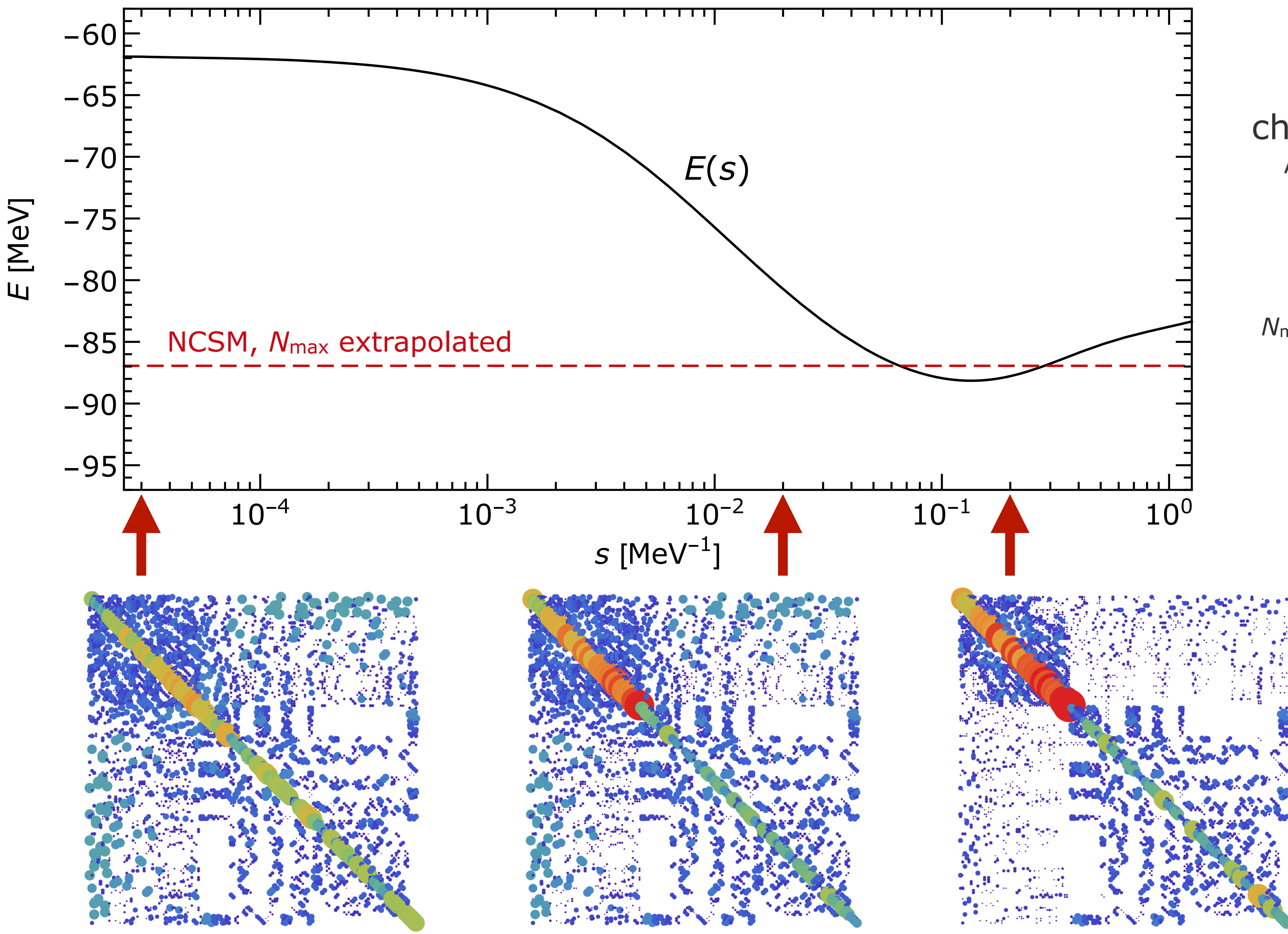

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Hamilton matrix in N_{max}=2 space

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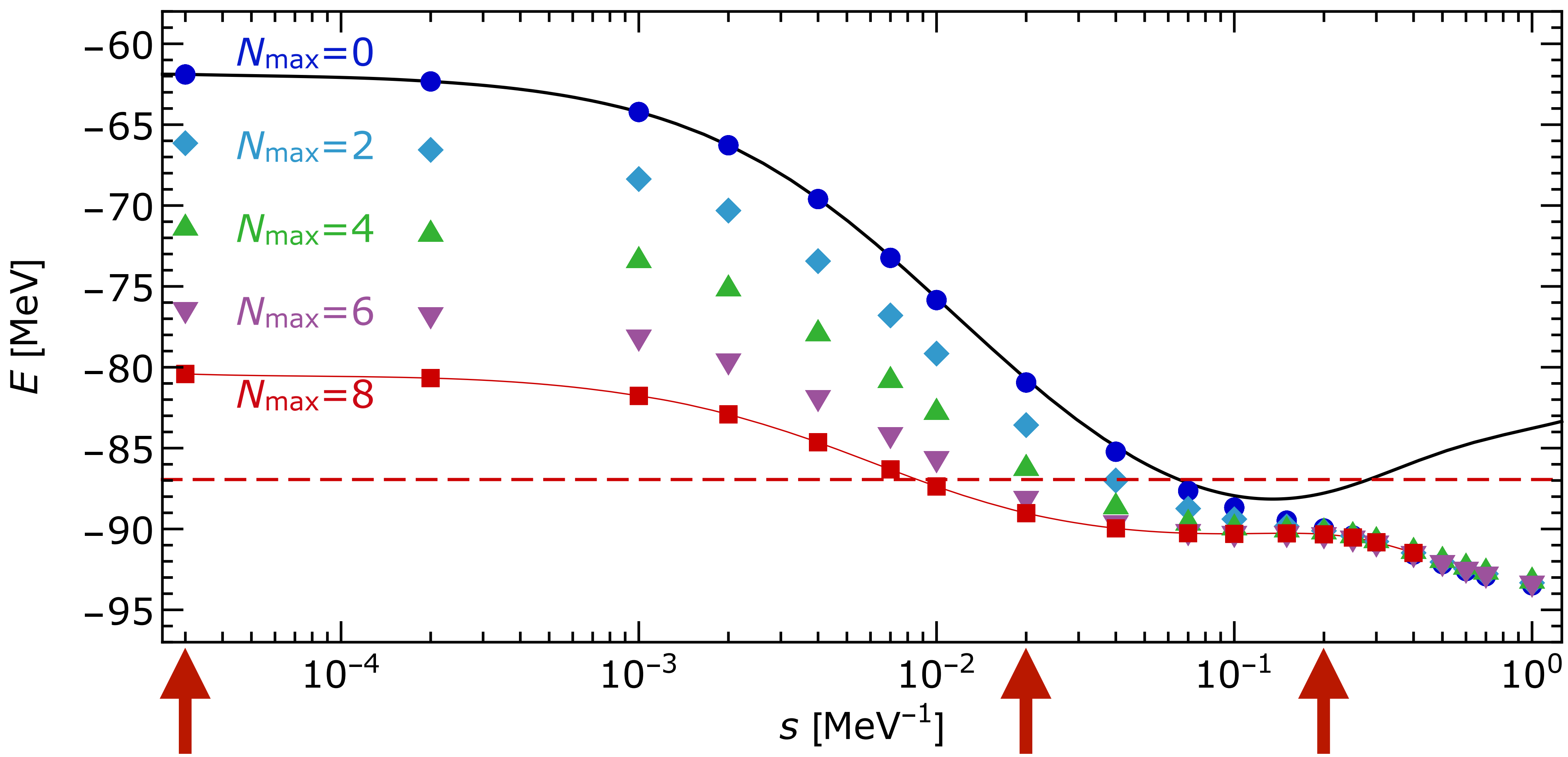

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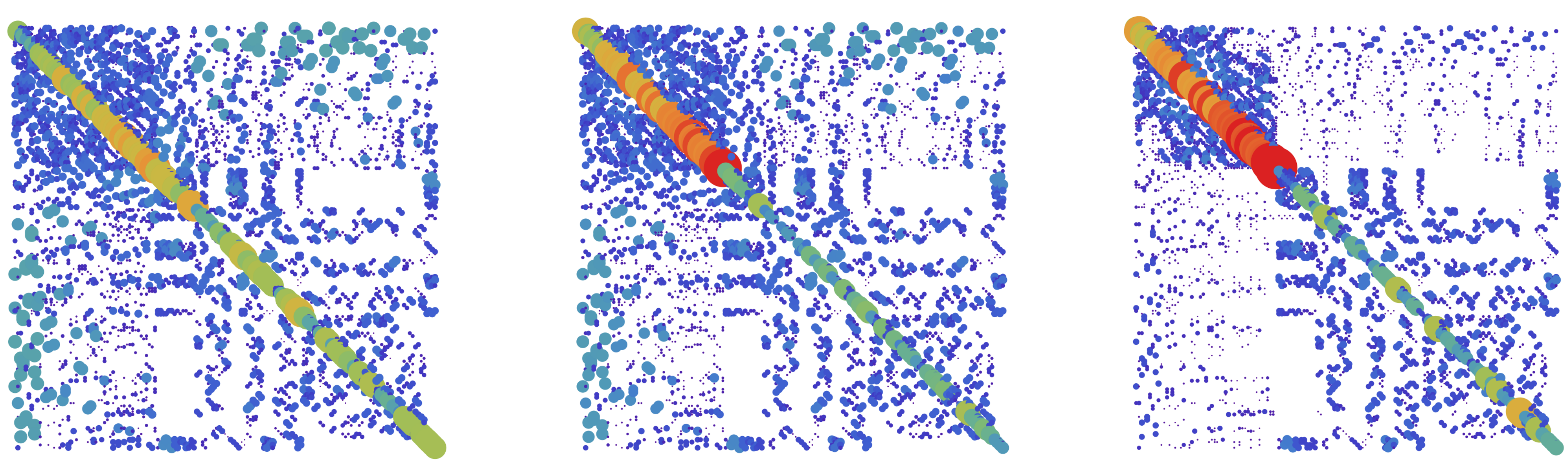
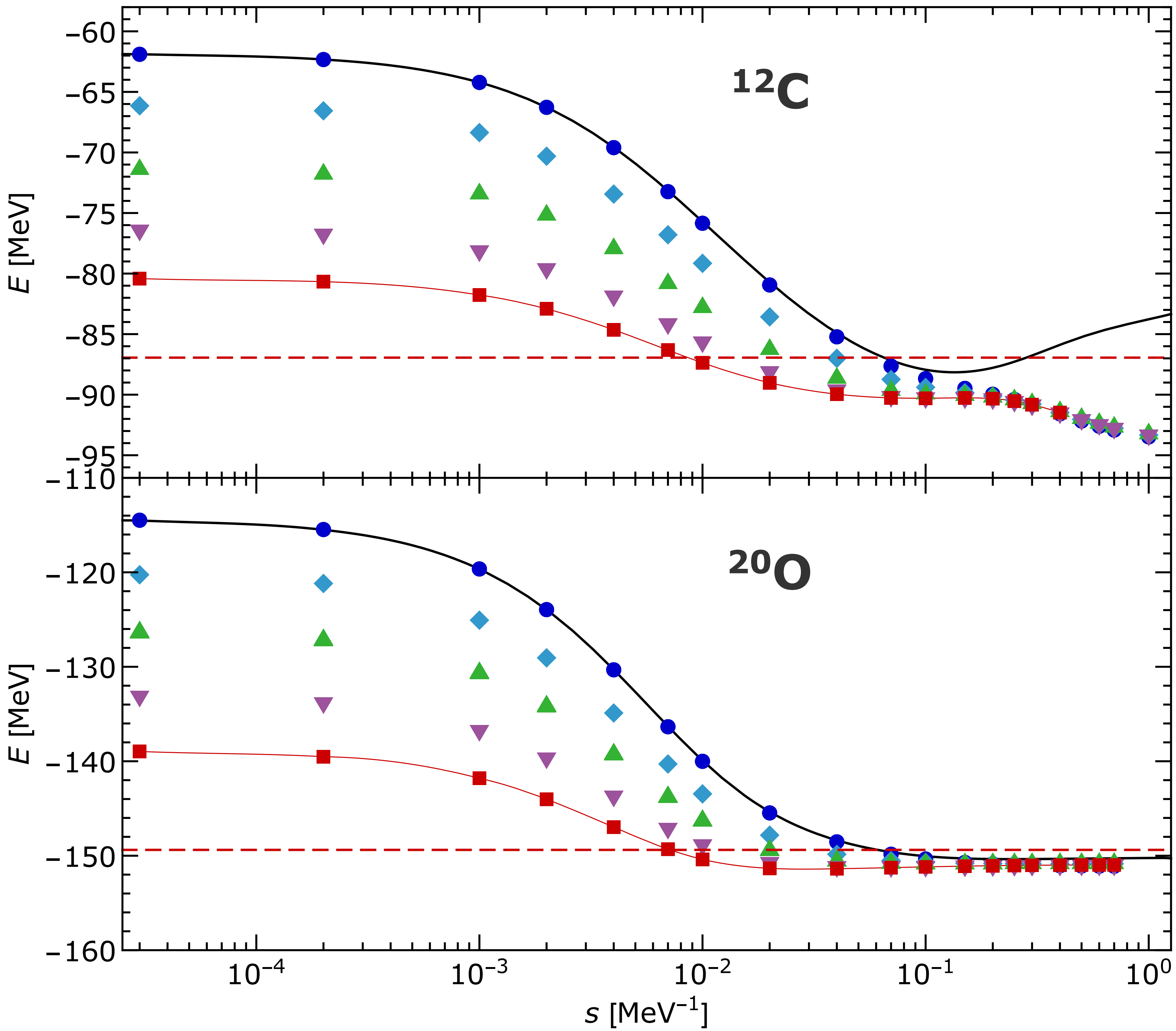


Hamilton matrix in N_{max}=2 space

Flow: Ground-State Energy

Gebrerufael, Vobig, Hergert, Roth; PRL 118, 152503 (2017)



- NCSM convergence is drastically improved
- N_{max}=0 eigenvalues deviated from $E(s)$

chiral NN+3N
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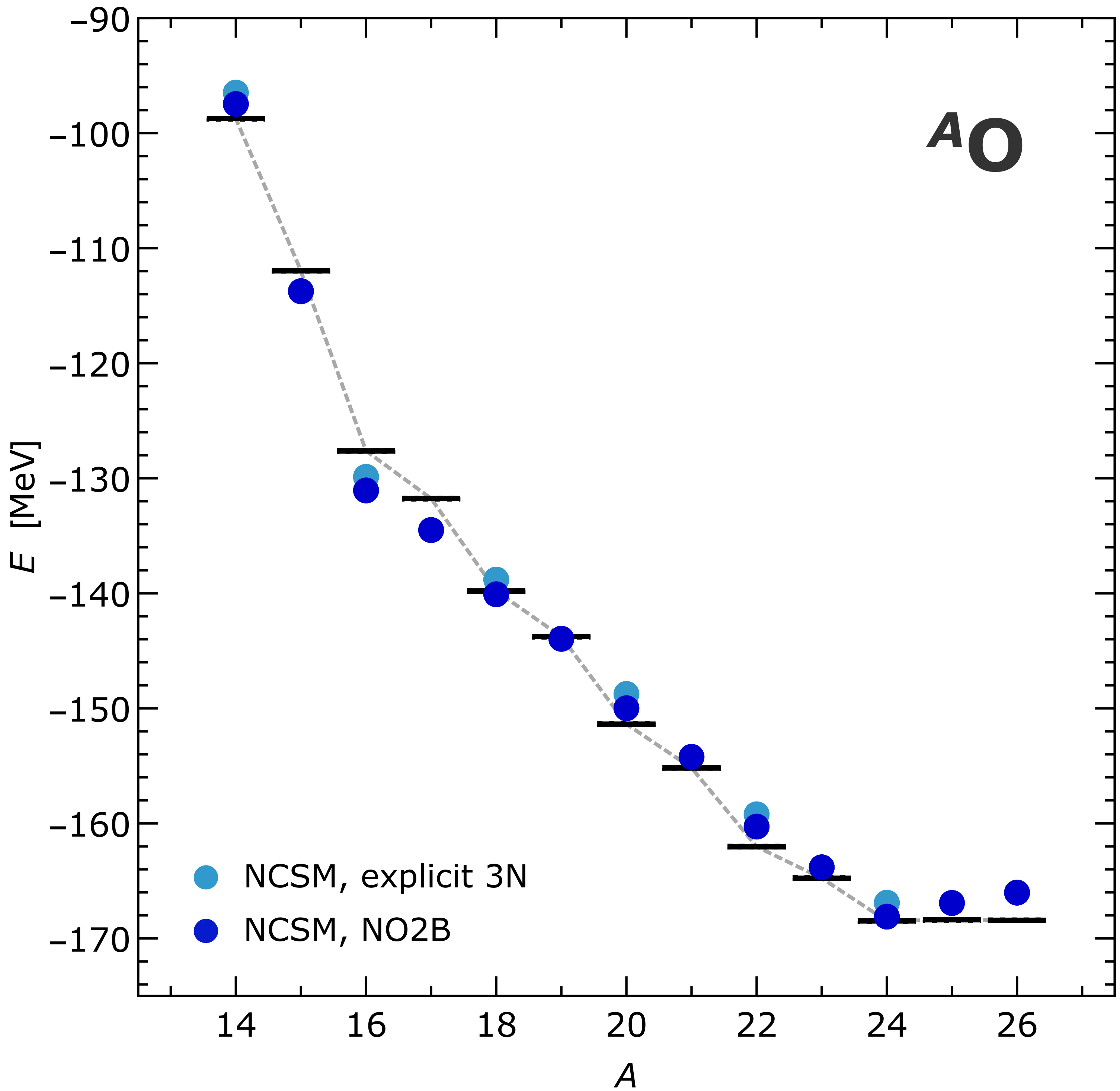
α=0.08 fm^4
$\hbar\Omega$=20 MeV
e_{max}=12

HF basis
N_{max}=0 reference state
N_{max}=0,2,4,6,8

NCSM: Oxygen Isotopes

J. Müller, A. Tichai, K. Vobig, R. Roth, in prep.



- new set of NCSM benchmark results using natural-orbital basis

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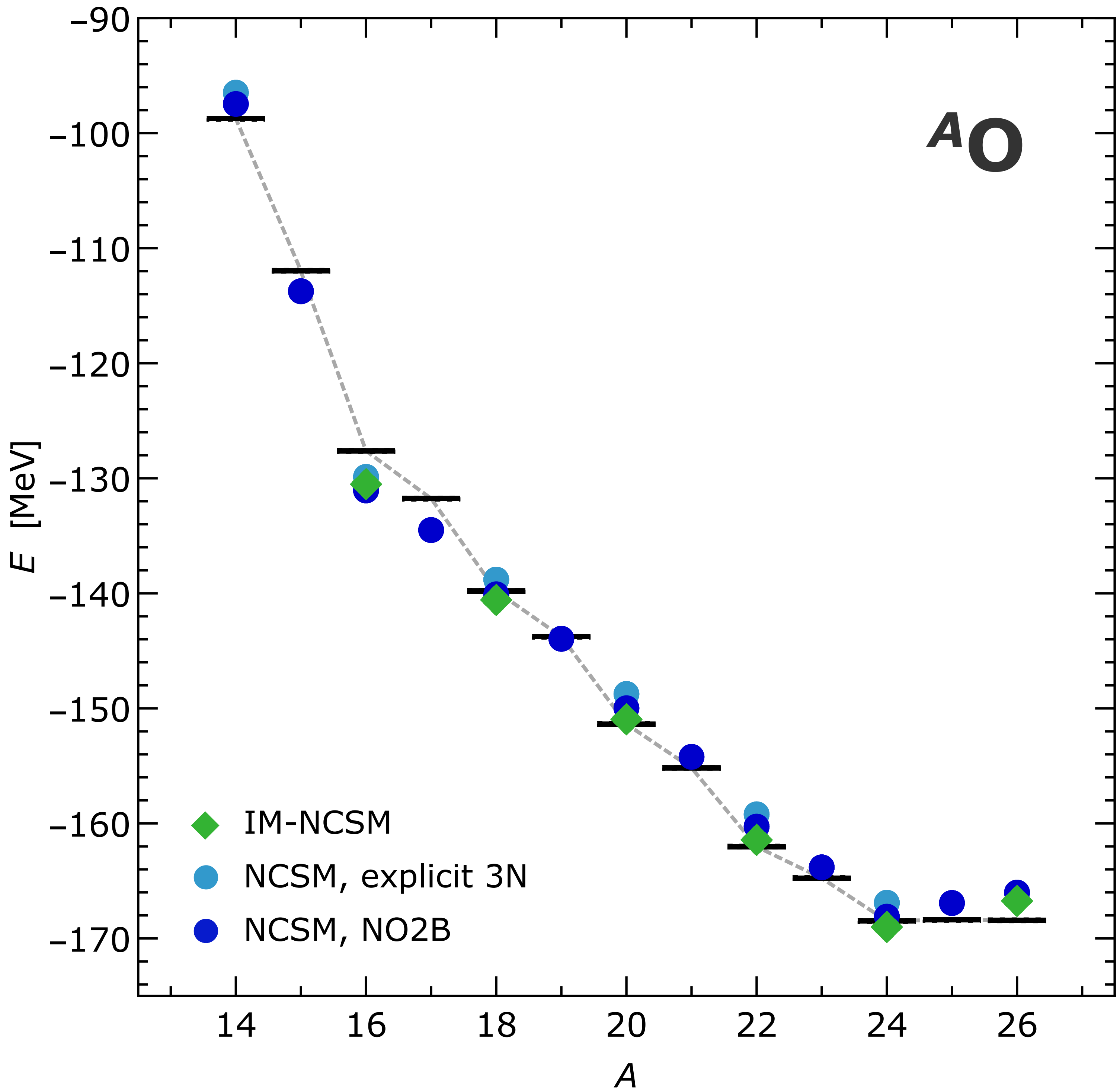
IM-NCSM: Oxygen Isotopes

Gebrerufael, et al.; PRL 118, 152503 (2017)



- excellent agreement with direct NCSM
- IM-SRG evolution limited to J=0 reference states and thus even-mass isotopes

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HF basis

N_{max}=0 reference

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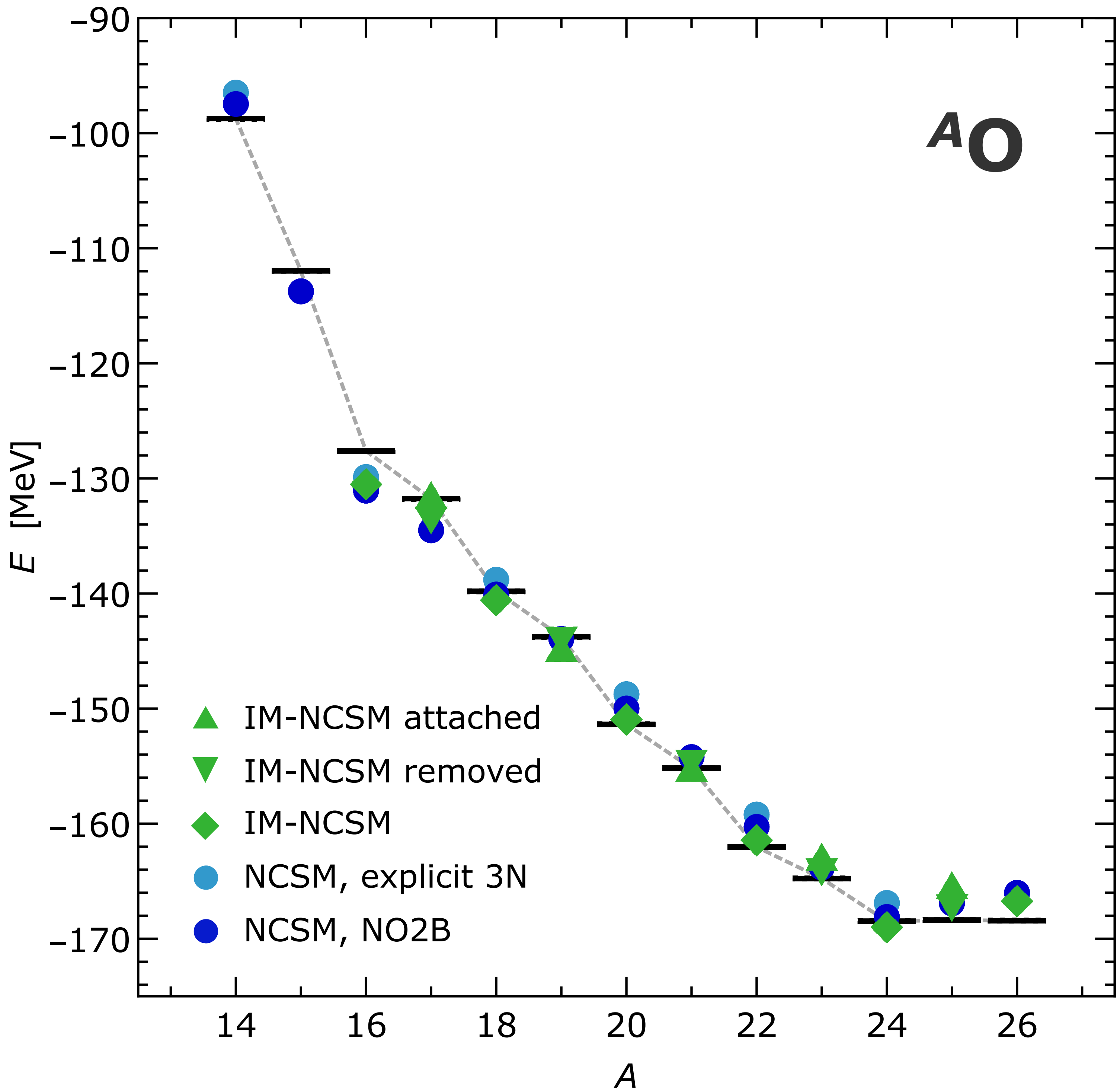

- excellent agreement with direct NCSM
- IM-SRG evolution limited to J=0 reference states and thus even-mass isotopes
- odd-mass nuclei via simple particle attachment or removal in final NCSM run

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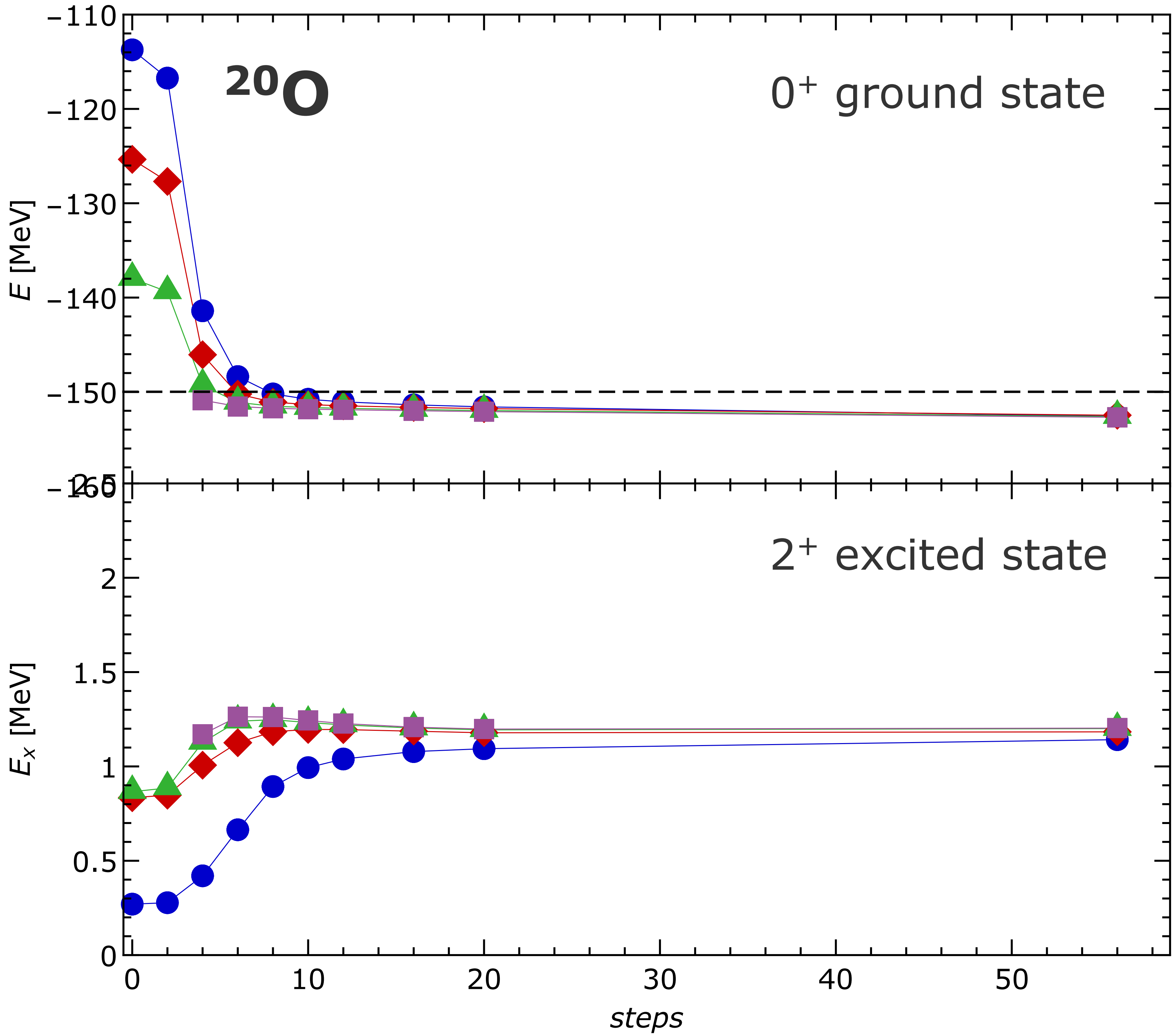
e_{max}=12

HF basis
N_{max}=0 reference

New: EM Observables

Vobig, et al.; in prep.



- excited states are obtained automatically
- rapid convergence of excitation energies

chiral NN+3N
Λ_{3N}=400 MeV
α=0.08 fm^4
$\hbar\Omega$=24 MeV
e_{max}=12

NAT basis
N_{max}=0 reference state
N_{max}=0,2,4,6

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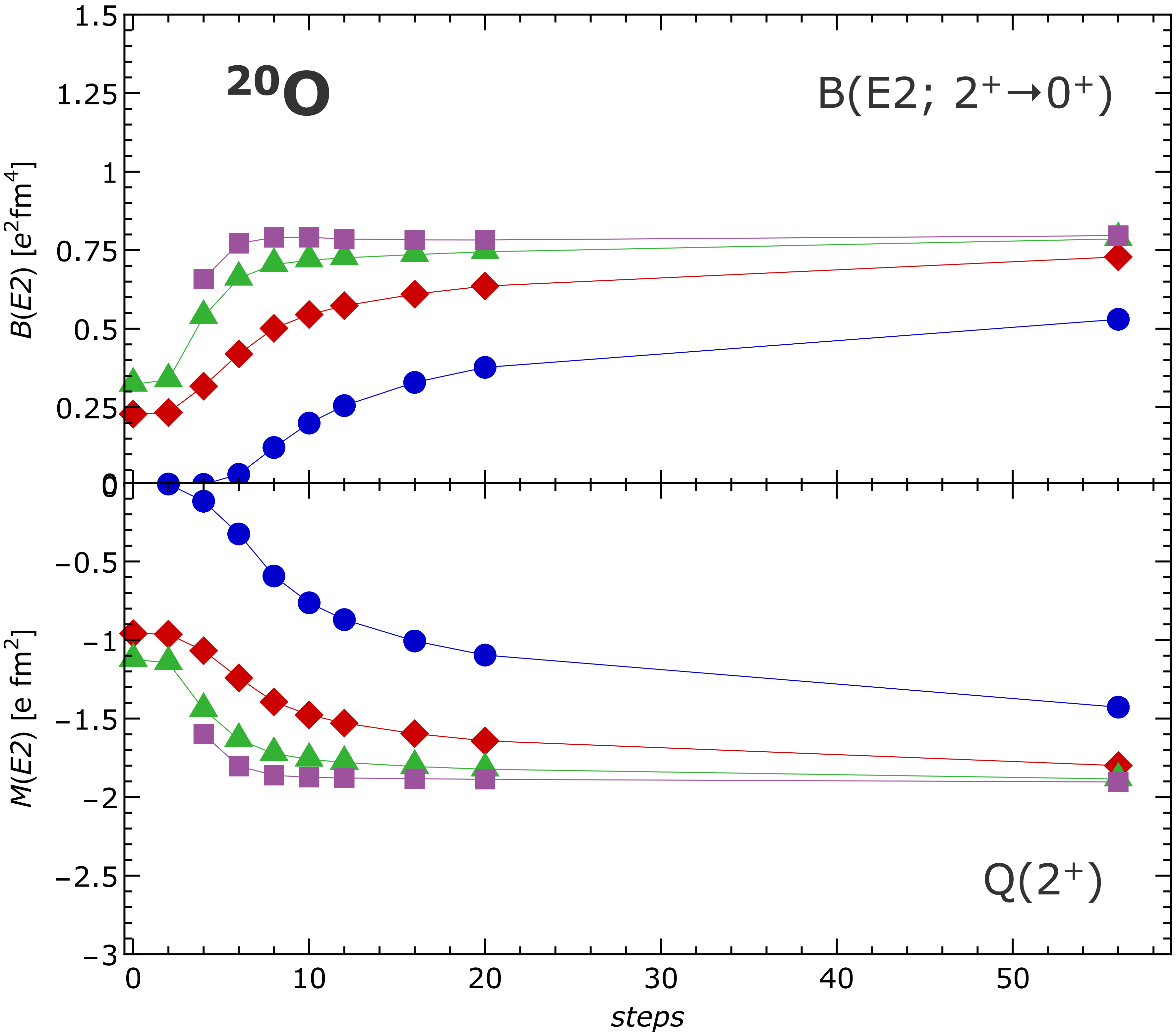

- eigenstates can be used to compute EM observables
- evolve EM operators consistently in IM-SRG
- slightly slower convergence of E2

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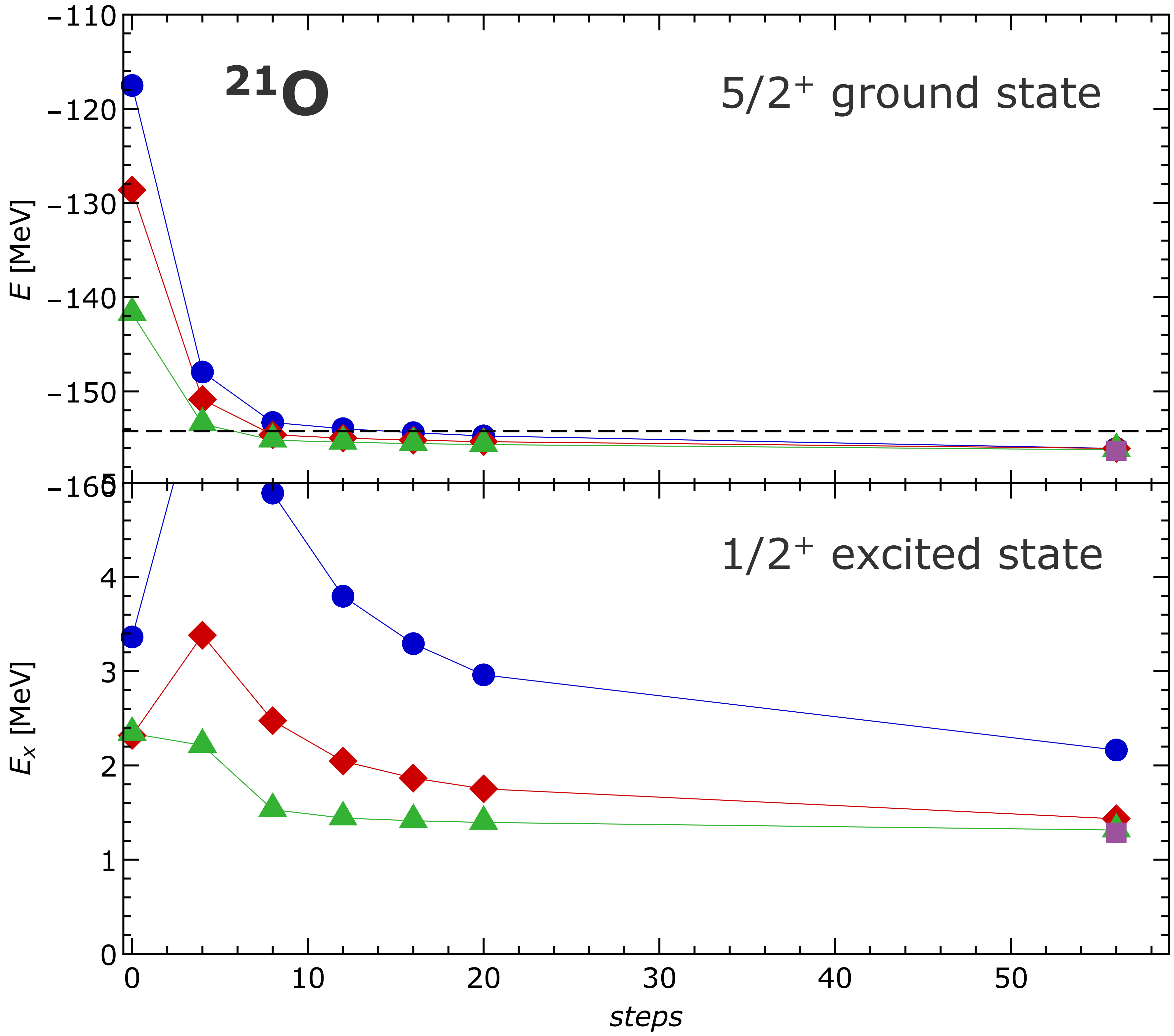
New: Odd Particle Numbers

Vobig, et al.; in prep.



- odd particle numbers treated via particle attached/removed scheme
- slightly slower convergence of excitation energies

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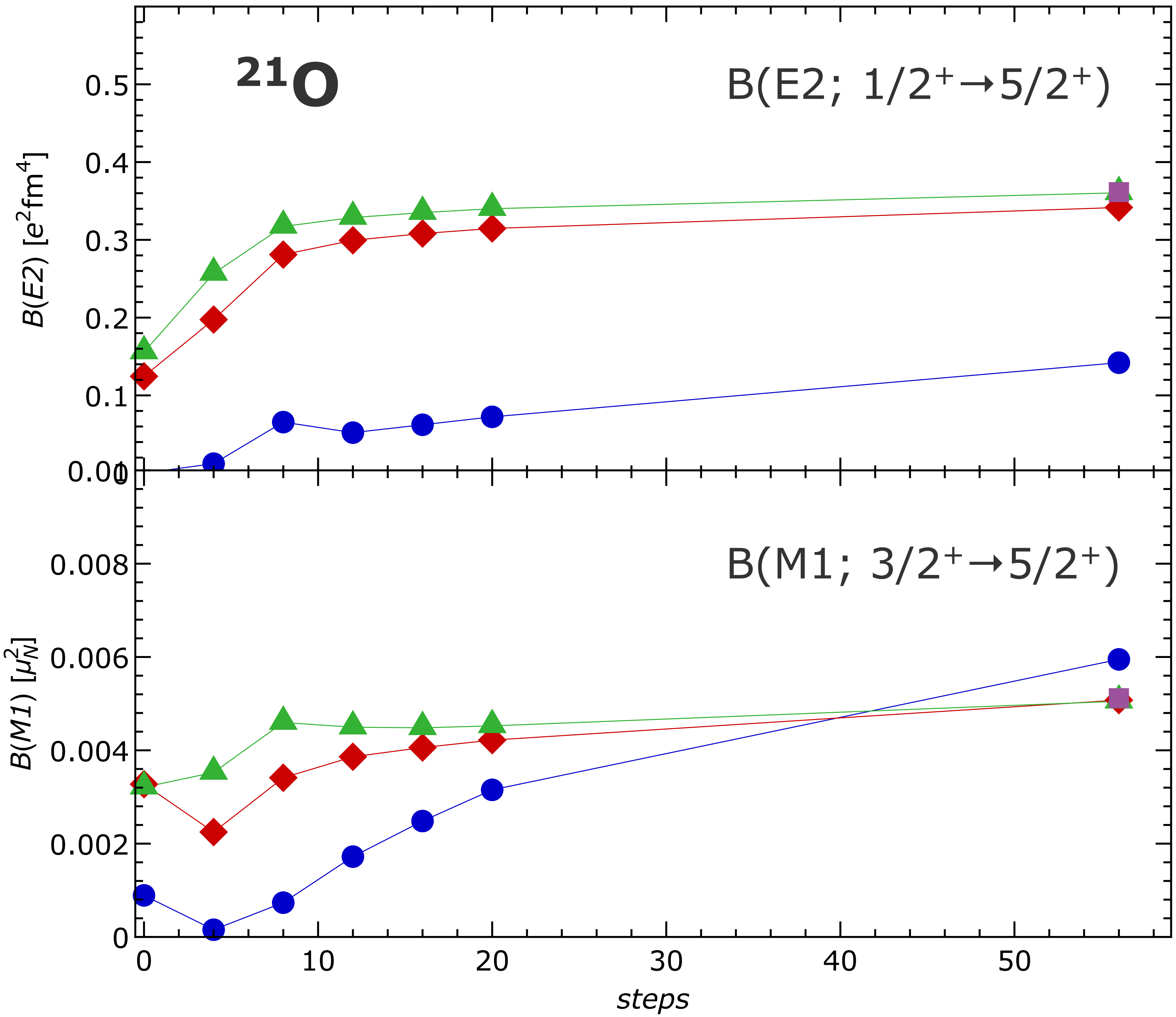

- all EM observables are accessible as well

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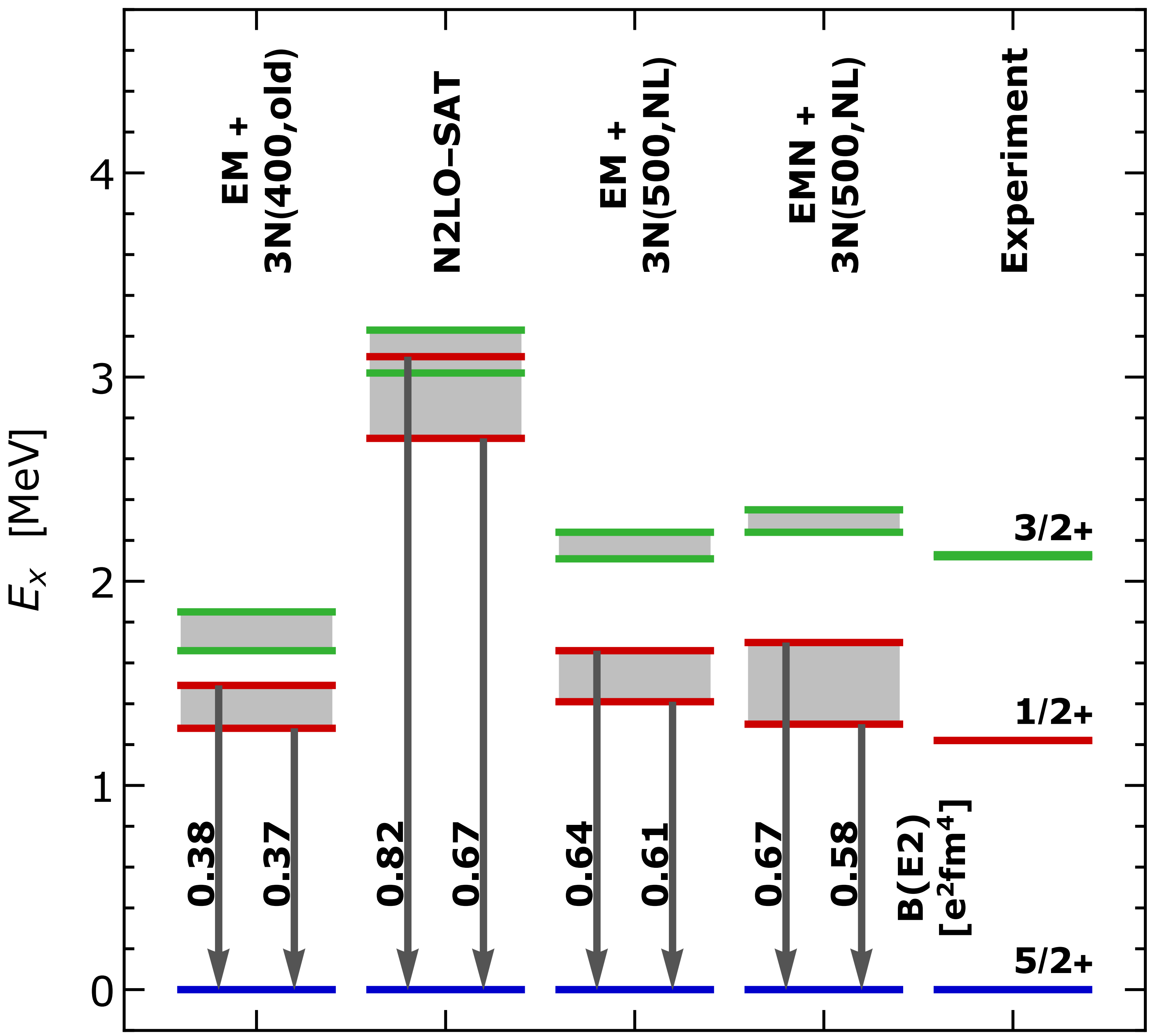
^{21}O: Collaboration with A03



- prediction of low-lying spectrum plus complete set of B(E2) and B(M1)
- different chiral NN+3N interactions
- quantification of theory uncertainties

experiment:
see talk by
Michael Mathy

Work Program: A04 Position #12

A04, position #12	Multi-reference IM-SRG for spectroscopy							
Tasks	16/1	16/2	17/1	17/2	18/1	18/2	19/1	19/2
IM-SRG+CI calculations for excitation spectra and spectroscopy of oxygen isotopes. Study of different generators and decoupling patterns, comparison to IT-NCSM and shell-model calculations.	✓							
Multi-reference IM-SRG with CI reference-state implemented and tested, study of the dependence on the reference state completed.		✓						
Comparison to ground-state calculations in the oxygen, calcium and nickel isotopic chains to previous IT-NCSM and multi-reference IM-SRG calculations.			✓					
Inclusion of non-scalar two-body operators in the multi-reference IM-SRG for a consistent inclusion of electromagnetic operators.				✓				
Multi-reference IM-SRG+CI calculations for the spectroscopy of carbon and oxygen isotopes completed. Full uncertainty quantification including chiral order-by-order systematics. Benchmark with IT-NCSM and valence-space shell model calculations.					✓	*		
Multi-reference IM-SRG+CI calculations for ground state and spectroscopy of medium-mass nuclei in the calcium and nickel mass region completed, benchmarks with shell model calculations.								

Perturbatively Improved NCSM

Tichai, Gebrerufael, Vobig, Roth; arXiv:1703.05664

NCSM
many-body solution

MBPT
convergence booster

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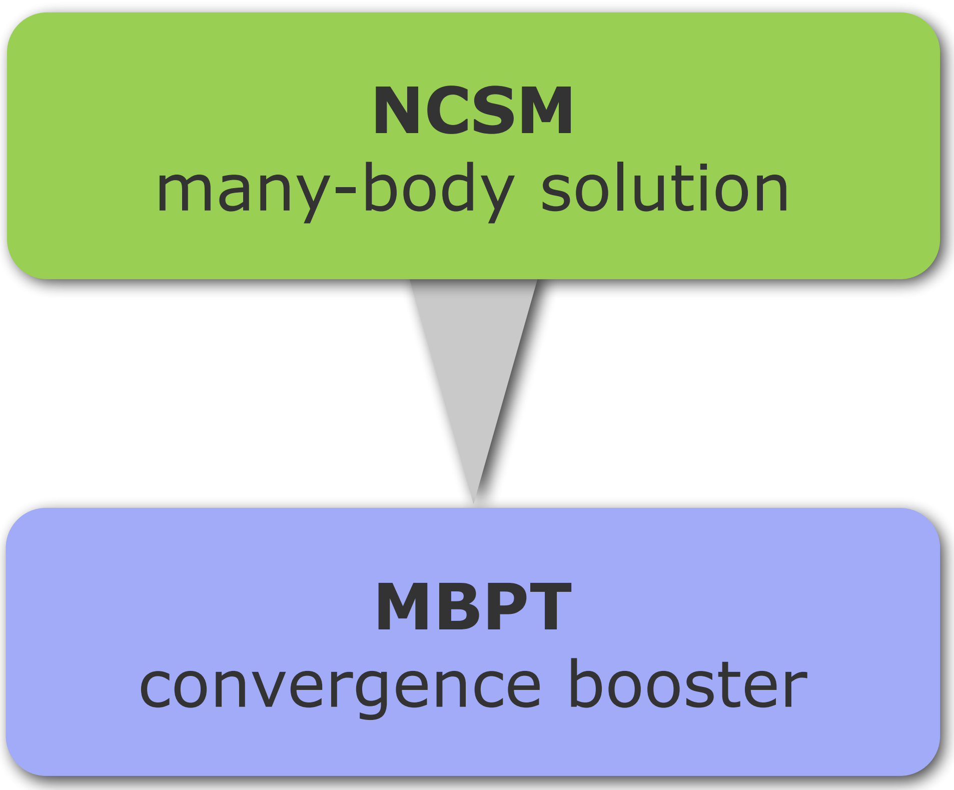

- eigenstates from NCSM at small N_{max} as unperturbed states
- access to all open-shell nuclei and systematically improvable

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many-body solution

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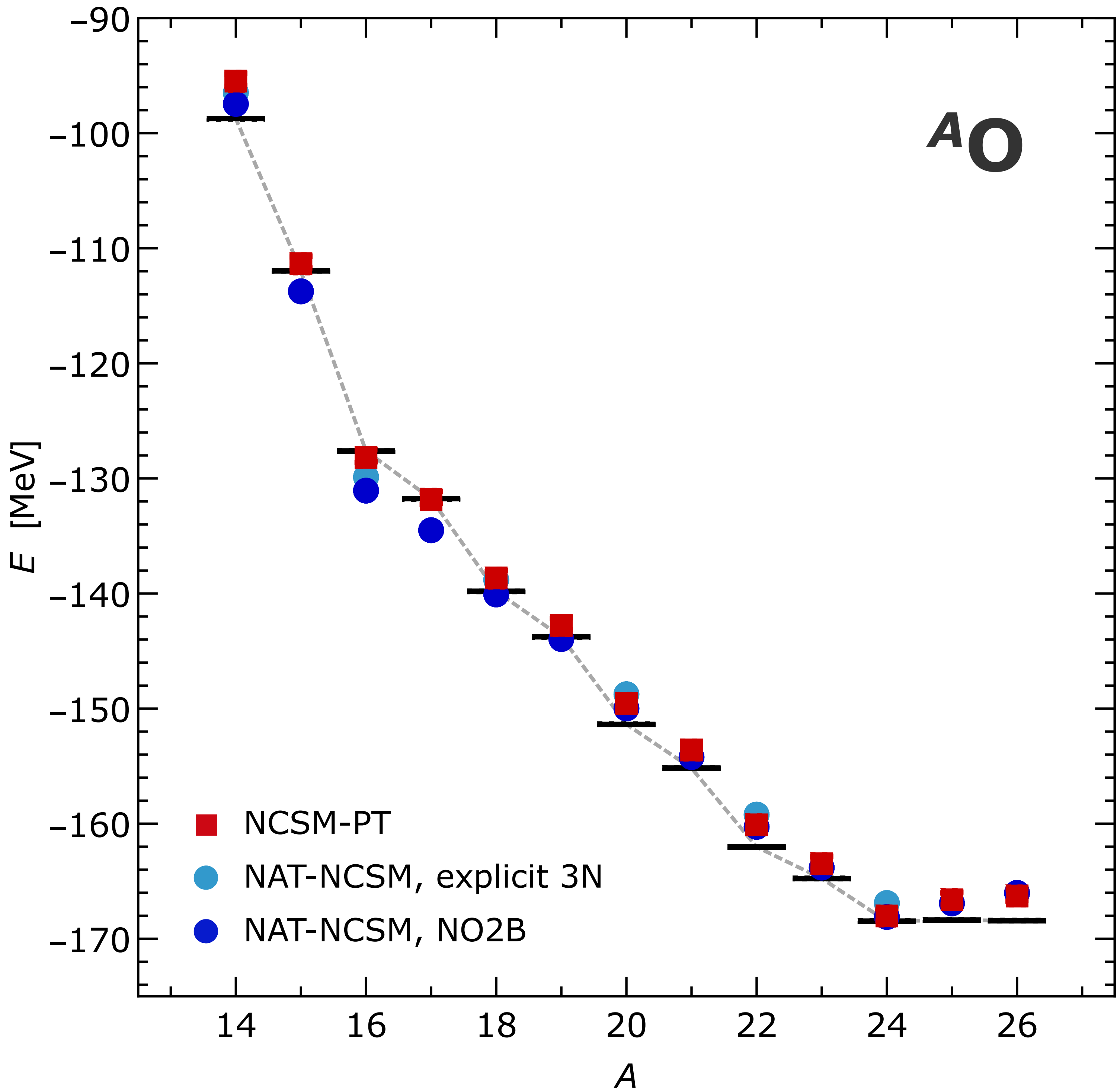
MBPT
convergence booster

- multi-configurational MBPT at second order for individual unperturbed states
- capture couplings in huge model-space through perturbative corrections

Oxygen Isotopes

Tichai, Gebrerufael, Vobig, Roth; arXiv:1703.05664



- excellent agreement with direct NCSM
- all isotopes are accessible due to simple m-scheme implementation

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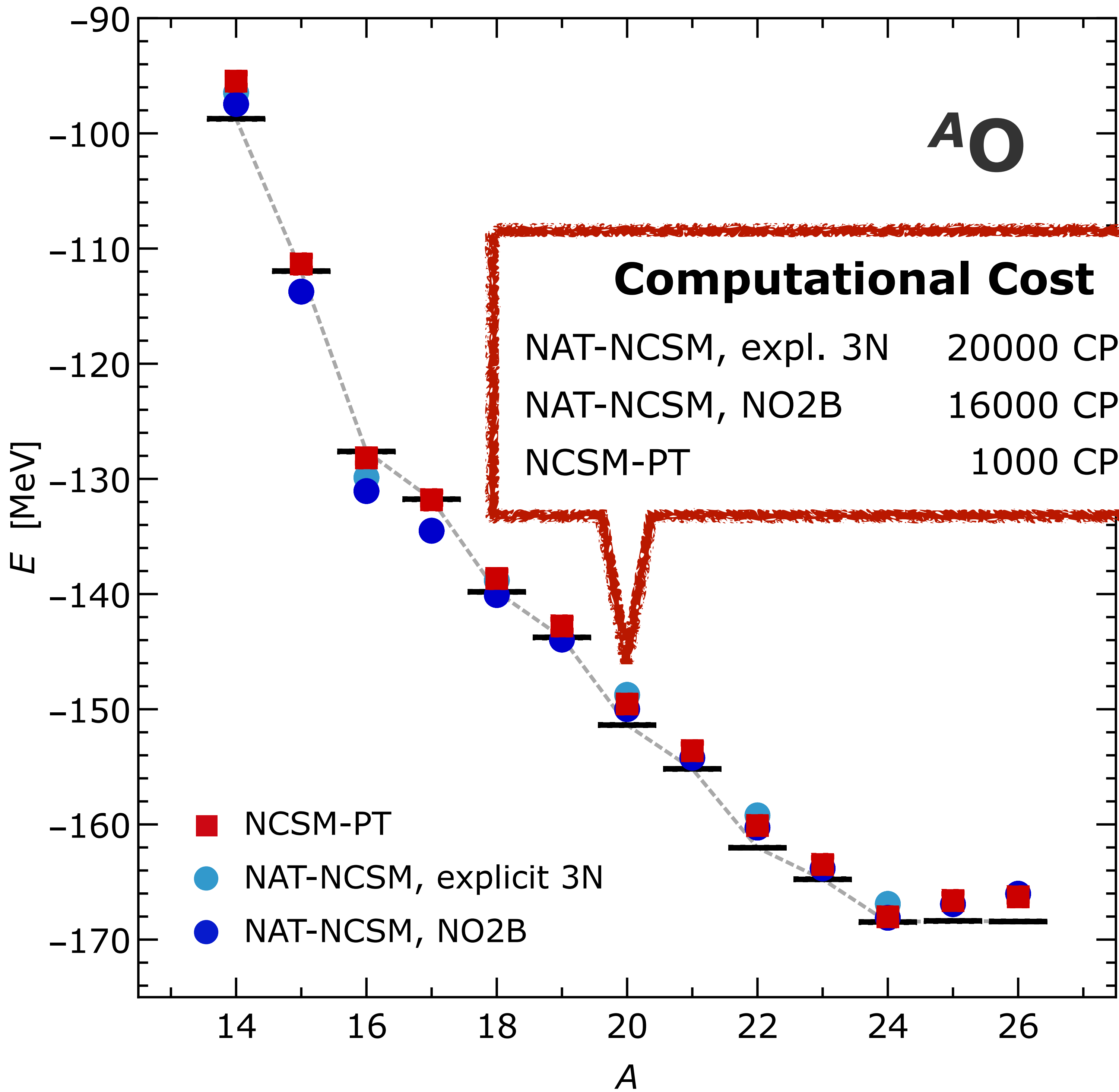

Computational Cost

NAT-NCSM, expl. 3N	20000 CPU-h
NAT-NCSM, NO2B	16000 CPU-h
NCSM-PT	1000 CPU-h

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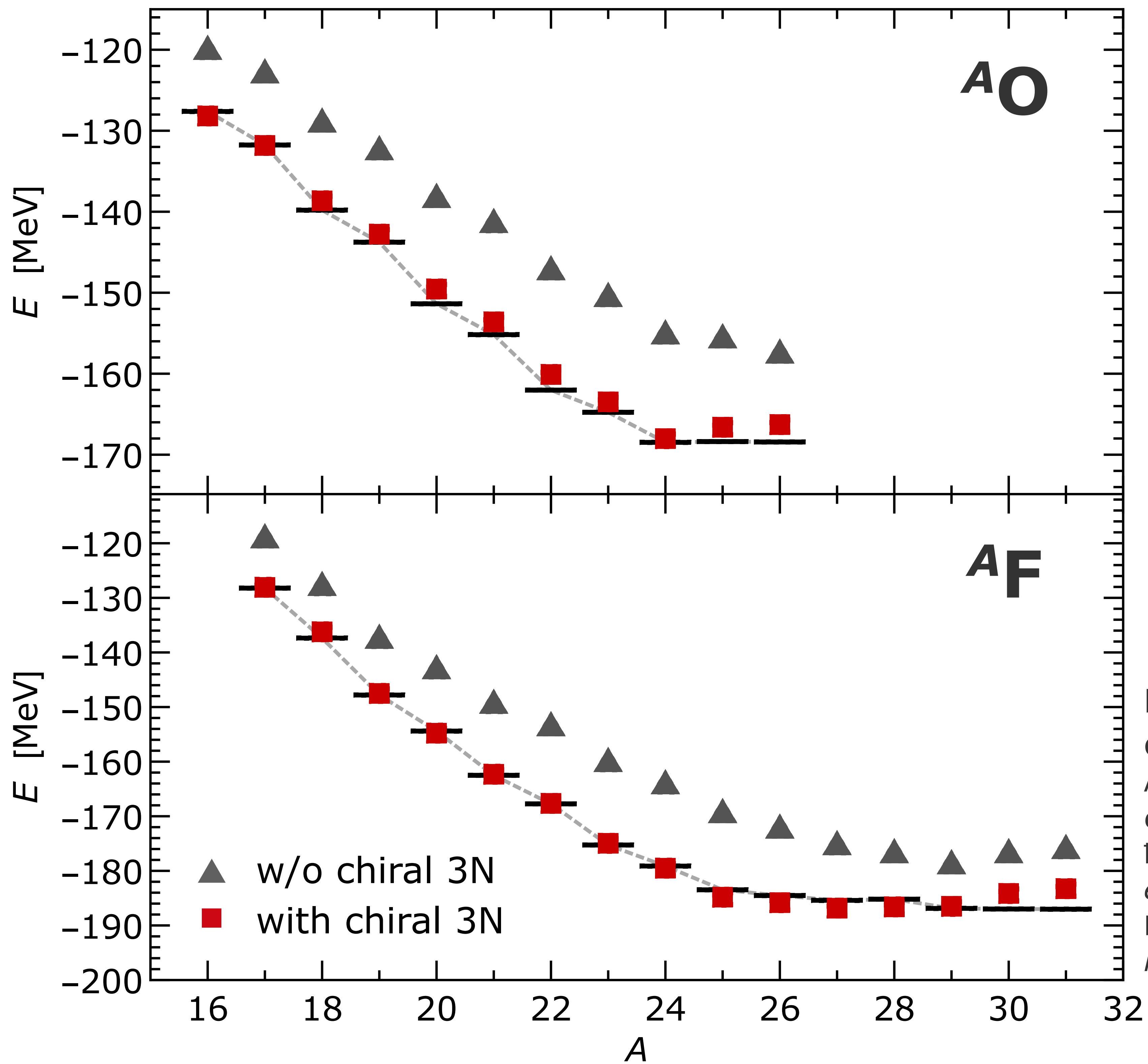
Exploring sd-Shell Phenomena

Tichai, Gebrerufael, Vobig, Roth; arXiv:1703.05664



- exploring various sd-shell phenomena, e.g., oxygen anomaly
- low computational cost enables surveys with different interactions

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