

Ab Initio Nuclear Structure Theory

Lecture 4: Beyond Light Nuclei

Robert Roth



TECHNISCHE
UNIVERSITÄT
DARMSTADT

Overview

■ **Lecture 1: Hamiltonian**

Prelude • Many-Body Quantum Mechanics • Nuclear Hamiltonian • Matrix Elements

■ **Lecture 2: Correlations**

Two-Body Problem • Correlations & Unitary Transformations • Similarity Renormalization Group

■ **Lecture 3: Light Nuclei**

Many-Body Problem • Configuration Interaction • No-Core Shell Model • Applications

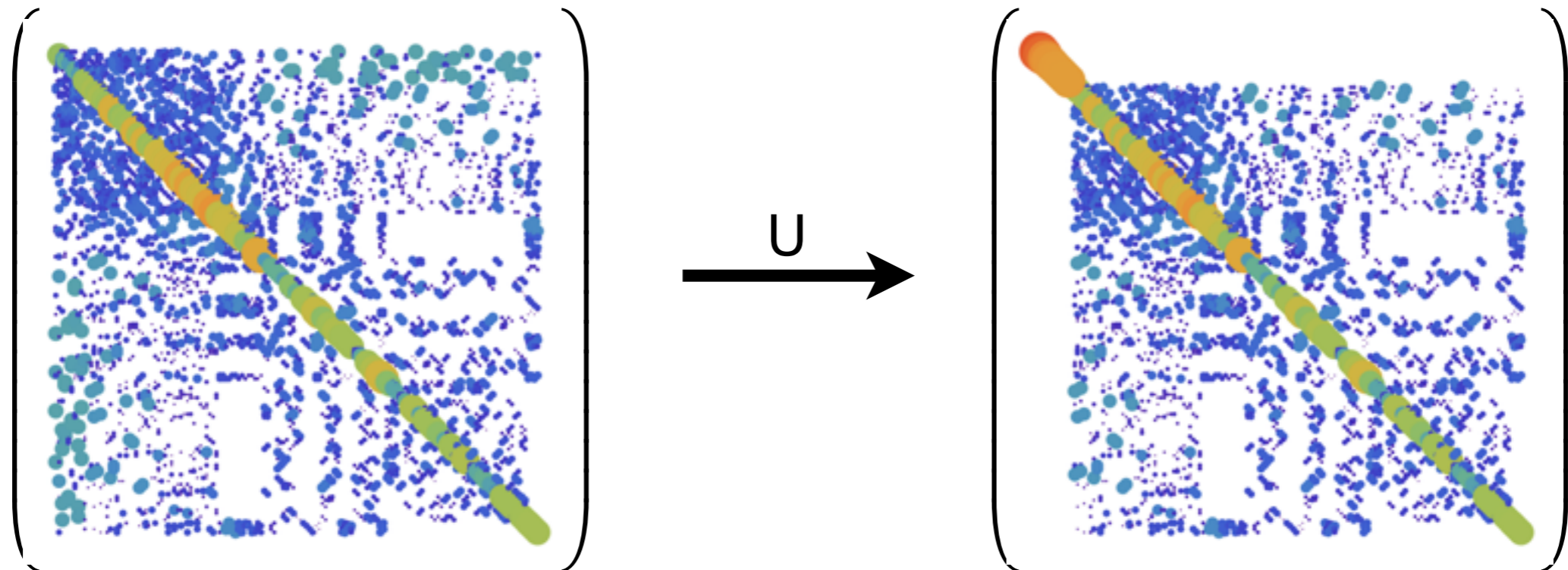
■ **Lecture 4: Beyond Light Nuclei**

Normal Ordering • Coupled-Cluster Theory • In-Medium Similarity Renormalization Group

Beyond Light Nuclei

advent of novel ab initio approaches
targeting the ground state of medium-mass nuclei
very efficiently

- **idea**: decouple reference state from particle-hole excitations by a unitary or similarity transformation of Hamiltonian



Beyond Light Nuclei

advent of novel ab initio approaches
targeting the ground state of medium-mass nuclei
very efficiently

- **idea**: decouple reference state from particle-hole excitations by a unitary or similarity transformation of Hamiltonian

Tsukiyama, Bogner, Schwenk, Hergert,...

- **In-Medium Similarity Renormalisation Group**: decouple many-body reference state from particle-hole excitations by SRG transformation

- normal-ordered A-body Hamiltonian truncated at the two-body level
- open and closed-shell nuclei can be targeted directly

Hagen, Papenbrock, Dean, Piecuch, Binder,...

- **Coupled-Cluster Theory**: ground-state is parametrised by exponential wave operator acting on single-determinant reference state

- truncation at doubles level (CCSD) with corrections for triples contributions
- directly applicable for closed-shell nuclei, equations-of-motion methods for open-shell

Normal Ordering

Particle-Hole Excitations

- short-hand notation for creation and annihilation operators

$$a_i = a_{\alpha_i} \quad a_i^\dagger = a_{\alpha_i}^\dagger$$

- define an A-body **reference Slater determinant**

$$|\Phi\rangle = |\alpha_1 \alpha_2 \dots \alpha_A\rangle = a_1^\dagger a_2^\dagger \dots a_A^\dagger |0\rangle$$

and construct arbitrary Slater determinants through **particle-hole excitations** on top of the reference state

$$\begin{aligned} |\Phi_a^\rho\rangle &= a_\rho^\dagger a_a |\Phi\rangle \\ |\Phi_{ab}^{\rho q}\rangle &= a_\rho^\dagger a_q^\dagger a_b a_a |\Phi\rangle \\ &\vdots \end{aligned}$$

index convention: a, b, c, \dots : hole states, occupied in reference state
 p, q, r, \dots : particle states, unoccupied in reference states
 i, j, k, \dots : all states

Normal Ordering

- a string of creation and annihilation operators is in **normal order** with respect to a specific reference state, if all
 - creation operators are on the left
 - annihilation operators are on the right
- standard particle-hole operators are normal ordered with respect to the vacuum state as reference state

$$a_i^\dagger a_j, \quad a_i^\dagger a_j^\dagger a_l a_k, \quad a_i^\dagger a_j^\dagger a_k^\dagger a_n a_m a_l, \dots$$

- **normal-ordered product** of string of operators

$$\{a_n a_i^\dagger \cdots a_m a_j^\dagger\} = \text{sgn}(\pi) a_i^\dagger a_j^\dagger \cdots a_n a_m$$

- defining property of a normal-ordered product: **expectation value with the reference state always vanishes**

$$\langle \Phi | \{ \dots \} | \Phi \rangle = 0$$

Normal Ordering with A-Body Reference

- in particle-hole formulation with respect to an **A-body reference Slater determinant** things are more complicated

	particle states	hole states
creation operators	$a_p^\dagger, a_{q'}^\dagger, \dots$	a_a, a_b, \dots
annihilation operators	a_p, a_q, \dots	$a_{a'}^\dagger, a_{b'}^\dagger, \dots$

- redefinition of creation and annihilation operators necessary to guarantee vanishing reference expectation value

$$\langle \Phi | \{ \dots \} | \Phi \rangle = 0$$

- starting from an operator string in vacuum normal order one has to **reorder to arrive at reference normal order**
 - “brute force” using the anticommutation relations for fermionic creation and annihilation operators
 - “elegantly” using Wick’s theorem and contractions...

Normal-Ordered Hamiltonian

- **second quantized Hamiltonian** in vacuum normal order

$$H = \frac{1}{4} \sum_{ijkl} \langle ij | T_{\text{int}} + V_{NN} | kl \rangle a_i^\dagger a_j^\dagger a_l a_k + \dots$$

normal-ordered two-body approximation: discard residual normal-ordered three-body part

- **normal-ordered Hamiltonian** with respect to reference state

$$H = E + \sum_{ij} f_j^i \{a_i^\dagger a_j\} + \frac{1}{4} \sum_{ijkl} \Gamma_{kl}^{ij} \{a_i^\dagger a_j^\dagger a_l a_k\} + \frac{1}{36} \sum_{ijkimn} W_{lmn}^{ijk} \{a_i^\dagger a_j^\dagger a_k^\dagger a_n a_m a_l\}$$

$$E = \frac{1}{2} \sum_{ab} \langle ab | T_{\text{int}} + V_{NN} | ab \rangle + \frac{1}{6} \sum_{abc} \langle abc | V_{3N} | abc \rangle$$

$$f_j^i = \sum_a \langle ai | T_{\text{int}} + V_{NN} | aj \rangle + \frac{1}{2} \sum_{ab} \langle abi | V_{3N} | abj \rangle$$

$$\Gamma_{kl}^{ij} = \langle ij | T_{\text{int}} + V_{NN} | kl \rangle + \sum_a \langle aij | V_{3N} | akl \rangle$$

$$W_{lmn}^{ijk} = \langle ijk | V_{3N} | lmn \rangle$$

Coupled-Cluster Theory

Coupled-Cluster Ansatz

- coupled-cluster ground state parametrized by **exponential of particle-hole excitation operators** acting on reference state

$$|\Psi_{CC}\rangle = \exp(T) |\Phi\rangle = \exp(T_1 + T_2 + \dots + T_A) |\Phi\rangle$$

- with the **n-particle-n-hole excitation operators** with unknown amplitudes

$$T_1 = \sum_{a,p} t_a^p \{a_p^\dagger a_a\}$$

$$T_2 = \sum_{ab,pq} t_{ab}^{pq} \{a_p^\dagger a_q^\dagger a_b a_a\}$$

⋮

- need to **truncate the excitation operator** at some small particle-hole order, defining different levels of coupled-cluster approximations

T_1

CCS

$T_1 + T_2$

CCSD

$T_1 + T_2 + T_3$

CCSDT

Coupled-Cluster Equations

- insert the coupled-cluster ansatz into the **A-body Schrödinger equation** and manipulate

$$H_{\text{int}} |\Psi_{\text{CC}}\rangle = E |\Psi_{\text{CC}}\rangle \quad \Rightarrow \quad \exp(-T) H_{\text{int}} \exp(T) |\Phi\rangle = E |\Phi\rangle$$

to obtain Schrödinger-like equation for a **similarity-transformed Hamiltonian**

$$\mathcal{H} |\Phi\rangle = E |\Phi\rangle \quad \text{with} \quad \mathcal{H} = \exp(-T) H_{\text{int}} \exp(T)$$

- note: this is **not a unitary transformation** and therefore the transformed Hamiltonian is non-hermitian
 - as a result approximations will be non-variational
- similarity transformation of the Hamiltonian can be expanded in a **Baker–Campbell–Hausdorff series**, which **terminates at finite order**
 - CCSD with a two-body Hamiltonian terminates after order T^4

CCSD Equations

- project the Schrödinger-like equation onto the reference state, 1p1h states, and 2p2h states to obtain **CCSD energy and amplitude equations**

$$\langle \Phi | \mathcal{H} | \Phi \rangle = E_{\text{CCSD}}$$

$$\langle \Phi_a^\rho | \mathcal{H} | \Phi \rangle = 0$$

$$\langle \Phi_{ab}^{\rho q} | \mathcal{H} | \Phi \rangle = 0$$

- after BCH-expansion these are **coupled non-linear algebraic equations** for the amplitudes $t_a^\rho, t_{ab}^{\rho q}$ and the CCSD energy
- for large-scale calculations use **spherical formulation**, where particle-hole operators are coupled to $J=0$
- full CCSDT is too expensive, various **non-iterative triples corrections** are being used to include triples contributions
- coupled-cluster with **explicit 3N interactions** can be done and was used to test the NO2B approximation

CCSD Equations for Amplitudes

$$\begin{aligned}
 \Delta E^{(\text{CCSD})} = & \quad + \frac{(EA)}{4} \sum_{abij} v_{ab}^{ij} t_{ij}^{ab} + \sum_{ai} f_a^i t_i^a + \frac{(EC)}{2} \sum_{abij} v_{ab}^{ij} t_i^a t_j^b \\
 & \quad + f_i^a + \sum_{ck} f_c^k t_{ik}^{ac} + \frac{(SBb)}{2} \sum_{cdk} v_{cd}^{ak} t_{ik}^{cd} - \frac{(SBc)}{2} \sum_{ckl} v_{ic}^{kl} t_{kl}^{ac} \\
 & \quad + \sum_c f_c^a t_i^c - \sum_i f_i^k t_k^a + \sum_{ck} v_{ic}^{ak} t_k^c - \frac{(SDa)}{2} \sum_{cdkl} v_{cd}^{kl} t_{kl}^{ad} t_i^c \\
 & \quad - \frac{(SDb)}{2} \sum_{cdkl} v_{cd}^{kl} t_{il}^{cd} t_k^a + \sum_{cdkl} v_{cd}^{kl} t_{li}^{da} t_k^c - \sum_{ck} f_c^k t_i^c t_k^a \\
 & \quad + \sum_{cdk} v_{cd}^{ak} t_i^c t_k^d - \sum_{ckl} v_{ic}^{kl} t_k^a t_l^c - \sum_{cdkl} v_{cd}^{kl} t_k^a t_i^c t_l^d \\
 & = 0, \quad \forall a, i
 \end{aligned}$$

$$\begin{aligned}
 & \quad + v_{ij}^{ab} + \hat{P}_{ab} \sum_c f_c^b t_{ij}^{ac} - \hat{P}_{ij} \sum_k f_j^k t_{ik}^{ab} \\
 & \quad + \frac{(DBc)}{2} \sum_{cd} v_{cd}^{ab} t_{ij}^{cd} + \frac{(DBd)}{2} \sum_k v_{ij}^{kl} t_{kl}^{ab} + \hat{P}_{ab} \hat{P}_{ij} \sum_{ck} v_{cj}^{kb} t_{ik}^{ac} \\
 & \quad + \frac{(DCa)}{4} \sum_{cdkl} v_{cd}^{kl} t_{ij}^{cd} t_{kl}^{ab} + \hat{P}_{ij} \sum_{cdkl} v_{cd}^{kl} t_{ik}^{ac} t_{jl}^{bd} \\
 & \quad - \frac{(DCc)}{2} \hat{P}_{ij} \sum_{cdkl} v_{cd}^{kl} t_{ik}^{dc} t_{lj}^{ab} - \frac{(DCd)}{2} \hat{P}_{ab} \sum_{cdkl} v_{cd}^{kl} t_{lk}^{ac} t_{ij}^{db} \\
 & \quad + \hat{P}_{ij} \sum_c v_{cj}^{ab} t_i^c - \hat{P}_{ab} \sum_k v_{ij}^{kb} t_k^a - \hat{P}_{ij} \sum_{ck} f_c^k t_{kj}^{ab} t_i^c \\
 & \quad - \hat{P}_{ab} \sum_{ck} f_c^k t_{ij}^{cb} t_k^a + \hat{P}_{ab} \hat{P}_{ij} \sum_{cdk} v_{cd}^{ak} t_{kj}^{db} t_i^c \\
 & \quad - \hat{P}_{ab} \hat{P}_{ij} \sum_{ckl} v_{ic}^{kl} t_{lj}^{cb} t_k^a - \frac{(DEe)}{2} \hat{P}_{ab} \sum_{cdk} v_{cd}^{kb} t_{ij}^{cd} t_k^a \\
 & \quad + \frac{(DEf)}{2} \hat{P}_{ij} \sum_{ckl} v_{cj}^{kl} t_{kl}^{ab} t_i^c + \hat{P}_{ab} \sum_{cdk} v_{cd}^{ka} t_{ij}^{db} t_k^c \\
 & \quad - \hat{P}_{ij} \sum_{ckl} v_{ci}^{kl} t_{lj}^{ab} t_k^c + \sum_{cd} v_{cd}^{ab} t_i^c t_j^d + \sum_{kl} v_{ij}^{kl} t_k^a t_l^b \\
 & \quad - \hat{P}_{ab} \hat{P}_{ij} \sum_{ck} v_{cj}^{kb} t_k^a t_i^c + \frac{(DGa)}{2} \sum_{cdkl} v_{cd}^{kl} t_{kl}^{ab} t_i^c t_j^d \\
 & \quad + \frac{(DGb)}{2} \sum_{cdkl} v_{cd}^{kl} t_{ij}^{cd} t_k^a t_l^b - \hat{P}_{ab} \hat{P}_{ij} \sum_{cdkl} v_{cd}^{kl} t_{lj}^{db} t_k^a t_i^c \\
 & \quad - \hat{P}_{ij} \sum_{cdkl} v_{cd}^{kl} t_{lj}^{ab} t_k^c t_i^d - \hat{P}_{ab} \sum_{cdkl} v_{cd}^{kl} t_{ij}^{db} t_l^a t_k^c \\
 & \quad - \hat{P}_{ab} \sum_{cdk} v_{cd}^{kb} t_k^a t_i^c t_j^d + \hat{P}_{ij} \sum_{ckl} v_{cj}^{kl} t_k^a t_l^b t_i^c \\
 & \quad + \sum_{cdkl} v_{cd}^{kl} t_k^a t_l^b t_i^c t_j^d = 0, \quad \forall a, b, i, j
 \end{aligned}$$

Coupled Cluster: Pros & Cons

much more efficient than ph-truncated CI

can deal with explicit 3N interaction

PRO

size extensive

very mild scaling with A

not variational

only for closed shell nuclei *

CON

other observables difficult

only for ground states *

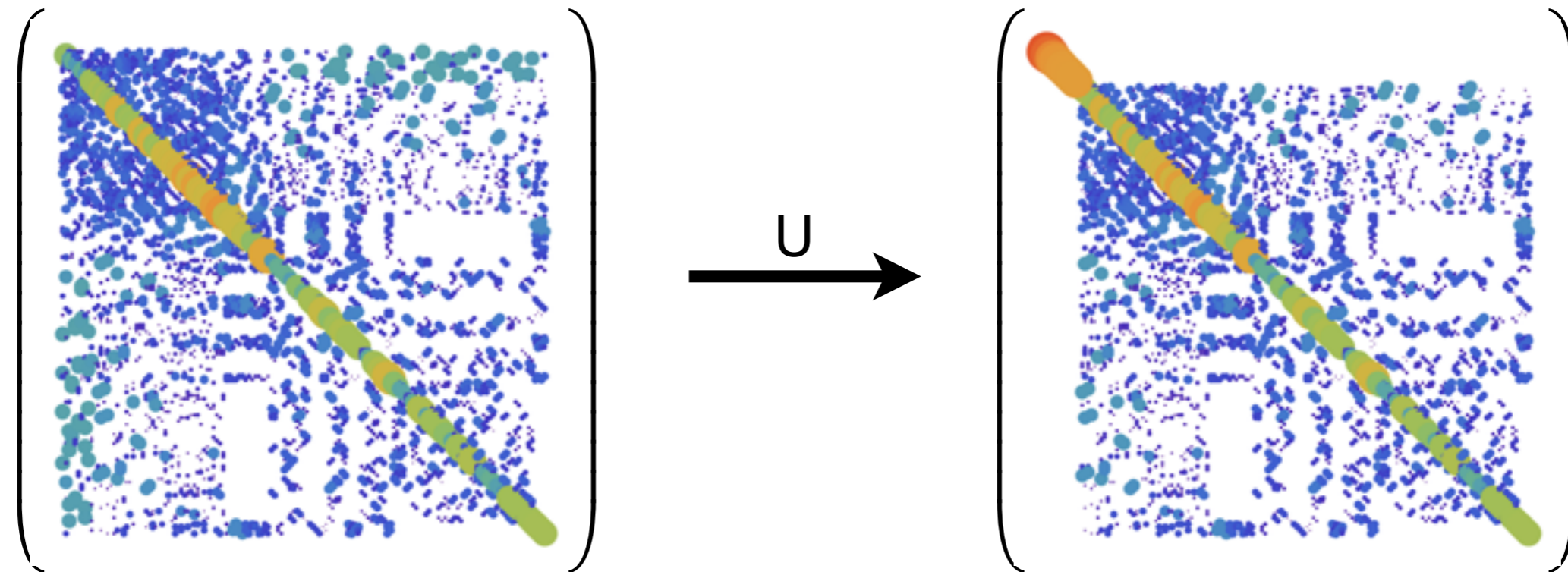
non-hermitian Hamiltonian

* equations of motion methods give access to near-closed-shell isotopes and excited states

In-Medium SRG

Decoupling in A-Body Space

- partially **diagonalize Hamilton matrix** through a unitary transformation and read-off eigenvalues from the diagonal



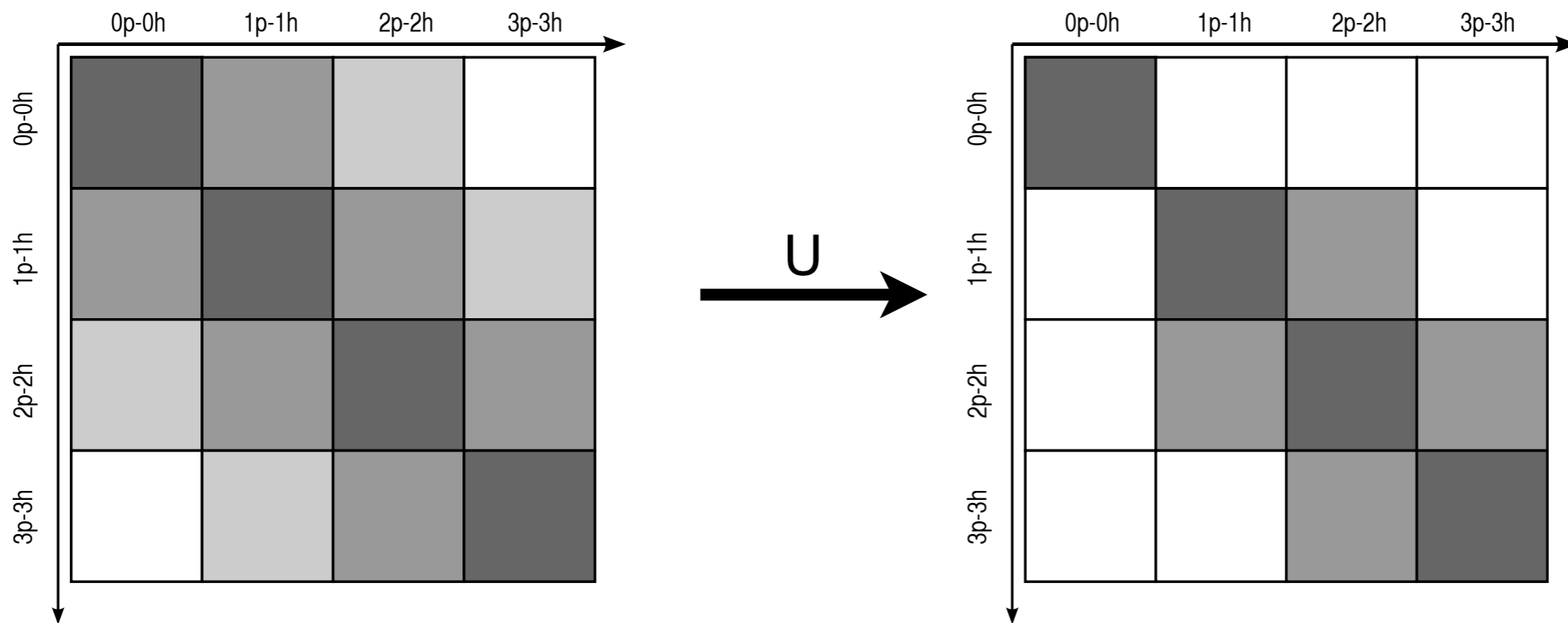
- **continuous unitary transformation** of many-body Hamiltonian

$$H_\alpha = U_\alpha^\dagger H U_\alpha$$

morphs the initial Hamilton matrix ($\alpha = 0$) to diagonal form ($\alpha \rightarrow \infty$)

Decoupling in A-Body Space

- partially **diagonalize Hamilton matrix** through a unitary transformation and read-off eigenvalues from the diagonal



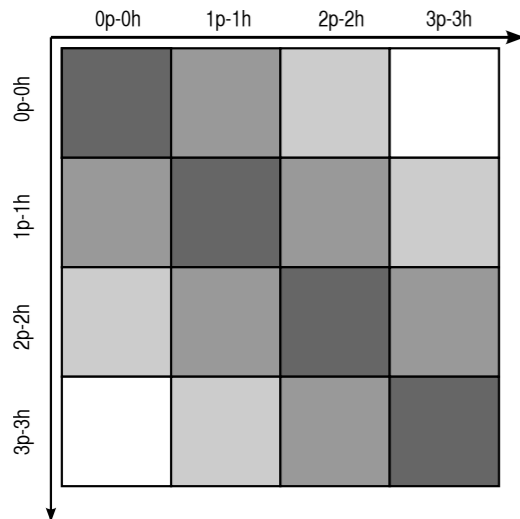
- continuous unitary transformation** of many-body Hamiltonian

$$H_\alpha = U_\alpha^\dagger H U_\alpha$$

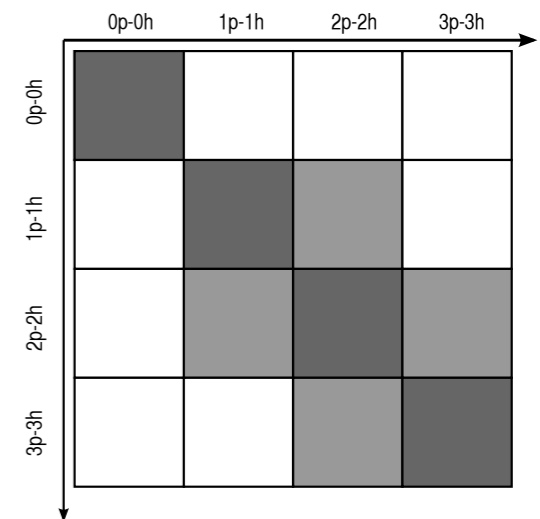
morphs the initial Hamilton matrix ($\alpha = 0$) to diagonal form ($\alpha \rightarrow \infty$)

In-Medium SRG

Tsukiyama, Bogner, Schwenk, Hergert,...



use SRG flow equations for normal-ordered Hamiltonian to decouple many-body reference state from excitations



- **flow equation** for Hamiltonian

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

- Hamiltonian in single-reference or multi-reference **normal order**, omitting normal-ordered 3B term

$$H(s) = E(s) + \sum_{ij} f_j^i(s) \{a_i^\dagger a_j\} + \frac{1}{4} \sum_{ijkl} \Gamma_{kl}^{ij}(s) \{a_i^\dagger a_j^\dagger a_l a_k\}$$

In-Medium SRG Generators

- **Wegner**: simple, intuitive, inefficient

$$\eta = [H_d, H] = [H_d, H_{od}]$$

- **White**: efficient, problems with near degeneracies

$$\eta_2^1 = (\Delta_2^1)^{-1} n_1 \bar{n}_2 f_2^1 - [1 \leftrightarrow 2]$$

$$\eta_{34}^{12} = (\Delta_{34}^{12})^{-1} n_1 n_2 \bar{n}_3 \bar{n}_4 \Gamma_{34}^{12} - [12 \leftrightarrow 34]$$

- **Imaginary Time**: good work horse [Morris, Bogner]

$$\eta_2^1 = \text{sgn}(\Delta_2^1) n_1 \bar{n}_2 f_2^1 - [1 \leftrightarrow 2]$$

$$\eta_{34}^{12} = \text{sgn}(\Delta_{34}^{12}) n_1 n_2 \bar{n}_3 \bar{n}_4 \Gamma_{34}^{12} - [12 \leftrightarrow 34]$$

- **Brillouin**: potentially better work horse [Hergert]

$$\eta_2^1 = \langle \Phi | [H, \{a_1^\dagger a_2\}] | \Phi \rangle$$

$$\eta_{34}^{12} = \langle \Phi | [H, \{a_1^\dagger a_2^\dagger a_4 a_3\}] | \Phi \rangle$$

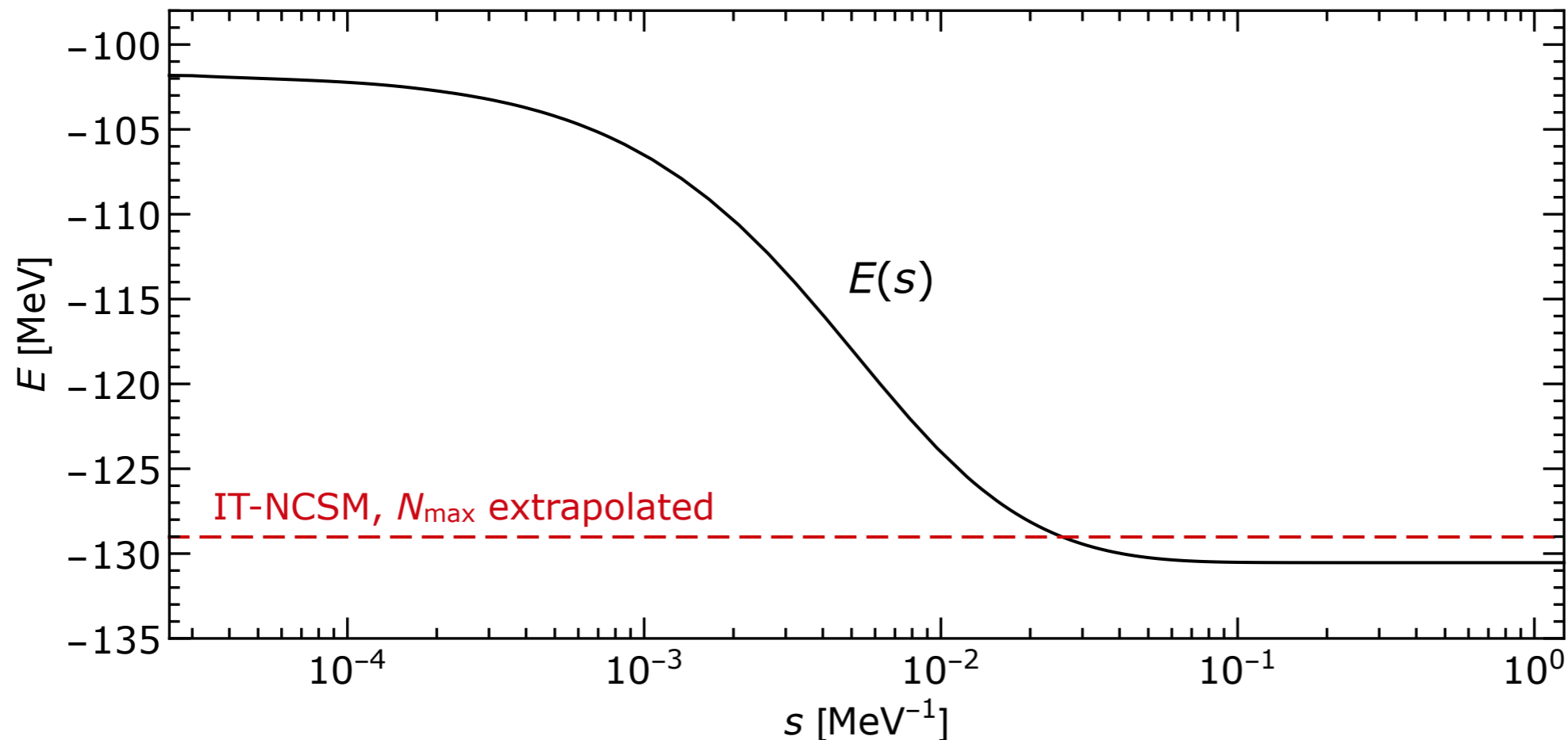
Flow-Equations for Matrix Elements

$$\frac{dE}{ds} = \sum_{ab} (n_a - n_b) \left(\eta_b^a f_a^b - f_b^a \eta_a^b \right) + \frac{1}{4} \sum_{abcd} \left(\eta_{cd}^{ab} \Gamma_{ab}^{cd} - \Gamma_{cd}^{ab} \eta_{ab}^{cd} \right) n_a n_b \bar{n}_c \bar{n}_d$$

$$\begin{aligned} \frac{d}{ds} f_2^1 &= \sum_a \left(\eta_a^1 f_2^a - f_a^1 \eta_2^a \right) + \sum_{ab} \left(\eta_b^a \Gamma_{a2}^{b1} - f_b^a \eta_{a2}^{b1} \right) (n_a - n_b) \\ &+ \frac{1}{2} \sum_{abcdef} \left(\eta_{bc}^{1a} \Gamma_{2a}^{bc} - \Gamma_{bc}^{1a} \eta_{2a}^{bc} \right) (n_a \bar{n}_b \bar{n}_c + \bar{n}_a n_b n_c) \end{aligned}$$

$$\begin{aligned} \frac{d}{ds} \Gamma_{34}^{12} &= \sum_a \left(\eta_a^1 \Gamma_{34}^{a2} + \eta_a^2 \Gamma_{34}^{1a} - \eta_3^a \Gamma_{a4}^{12} - \eta_4^a \Gamma_{3a}^{12} - f_a^1 \eta_{34}^{a2} - f_a^2 \eta_{34}^{1a} + f_3^a \eta_{a4}^{12} + f_4^a \eta_{3a}^{12} \right) \\ &+ \frac{1}{2} \sum_{ab} \left(\eta_{ab}^{12} \Gamma_{34}^{ab} - \Gamma_{ab}^{12} \eta_{34}^{ab} \right) (1 - n_a - n_b) \\ &+ \sum_{ab} (n_a - n_b) \left(\left(\eta_{3b}^{1a} \Gamma_{4a}^{2b} - \Gamma_{3b}^{1a} \eta_{4a}^{2b} \right) - \left(\eta_{3b}^{2a} \Gamma_{4a}^{1b} - \Gamma_{3b}^{2a} \eta_{4a}^{1b} \right) \right) \end{aligned}$$

In-Medium SRG: Single Reference



^{16}O

chiral NN+3N

$\Lambda_{3N}=400$ MeV

$\alpha=0.08$ fm⁴

$\hbar\Omega=20$ MeV

$e_{\max}=12$

$N_{\max}=0$ reference

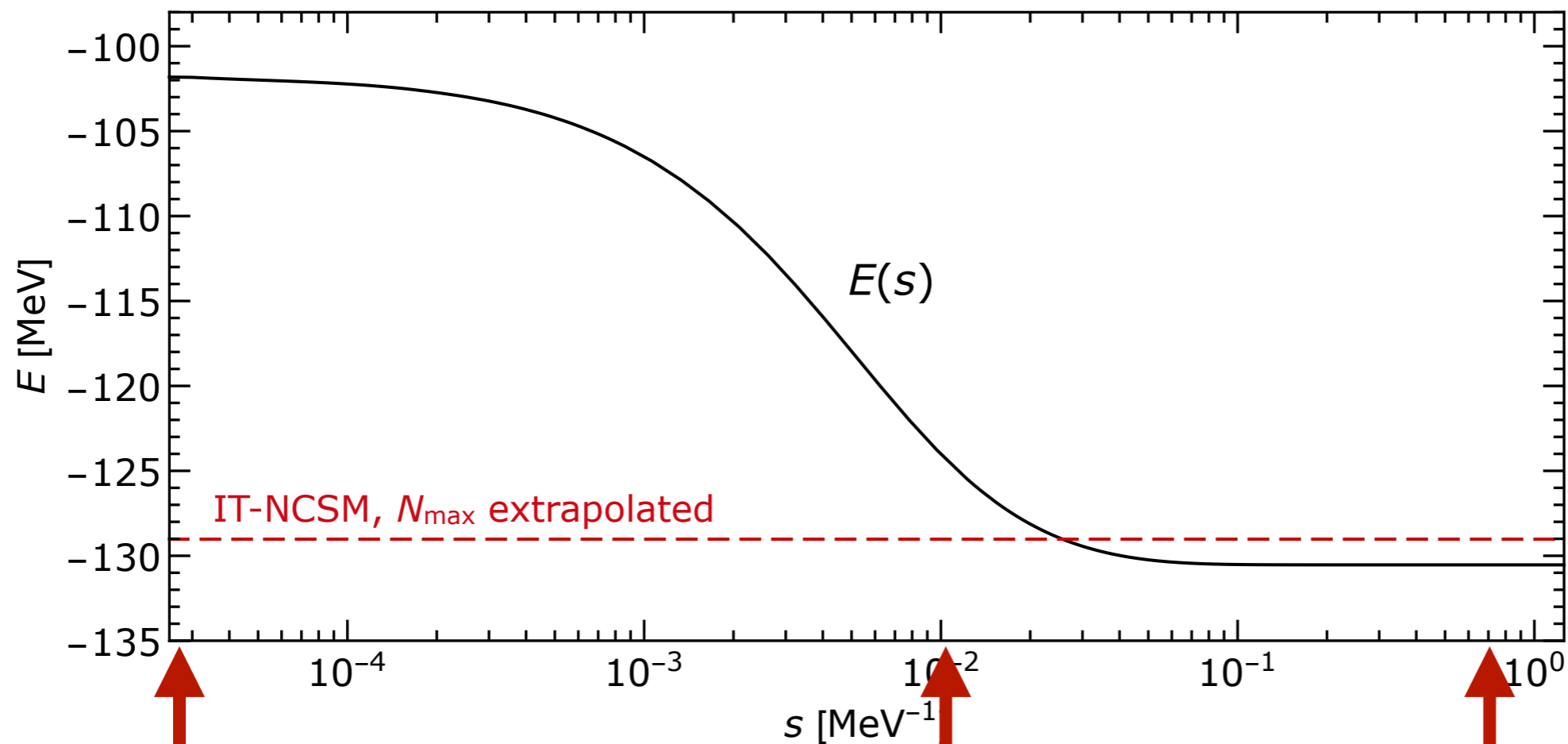
HF basis

- zero-body piece of the flowing Hamiltonian gives **ground-state energy** when full decoupling is reached

$$E(s) = \langle \Phi_{\text{ref}} | H(s) | \Phi_{\text{ref}} \rangle$$

- truncation of flow equations destroys unitarity, induced many-body terms

In-Medium SRG: Single Reference



^{16}O

chiral NN+3N

$\Lambda_{3N}=400$ MeV

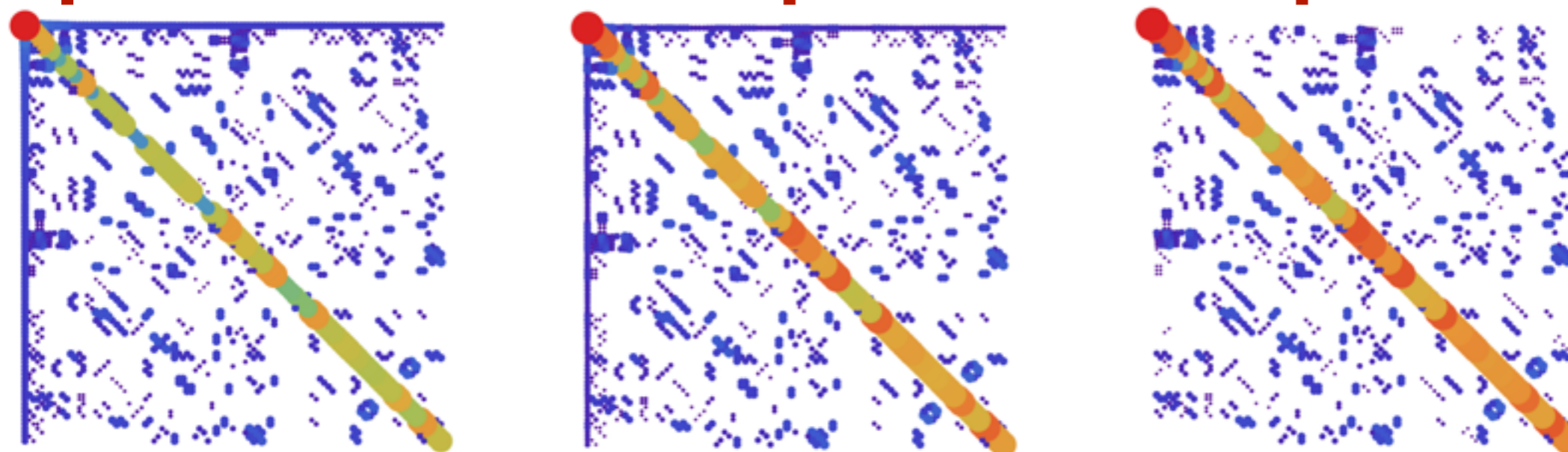
$\alpha=0.08$ fm⁴

$\hbar\Omega=20$ MeV

$e_{\max}=12$

$N_{\max}=0$ reference

HF basis



Hamilton
matrix in
 $N_{\max}=2$
space

Merging NCSM and IM-SRG

**NCSM:
Reference State**

- 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

**IM-SRG:
Many-Body Decoupling**

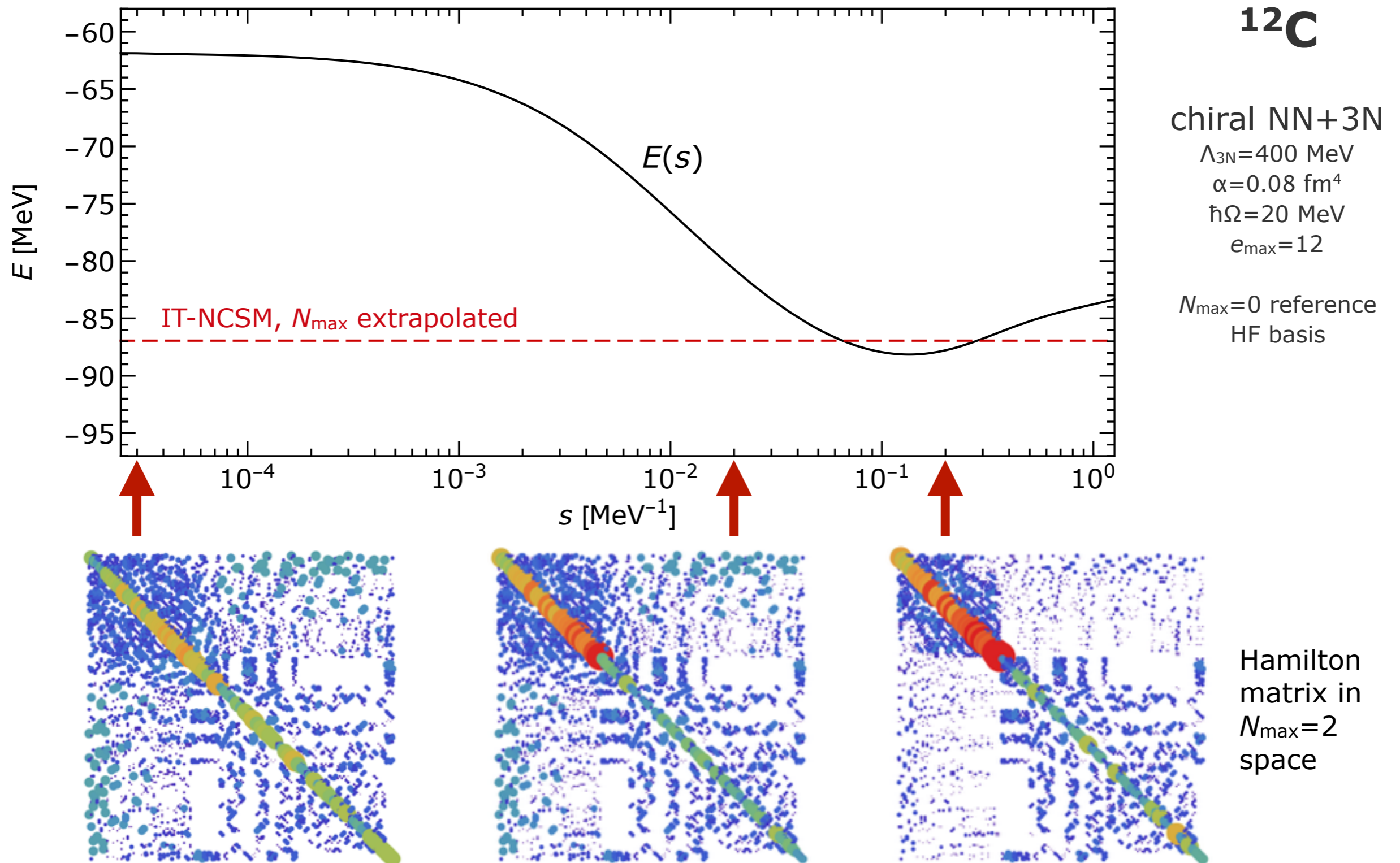
- IM-SRG evolution of multi-reference normal-ordered Hamiltonian (and other operators)
- decoupling of particle-hole excitations, i.e., pre-diagonalization in A -body space

**NCSM:
Observables**

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

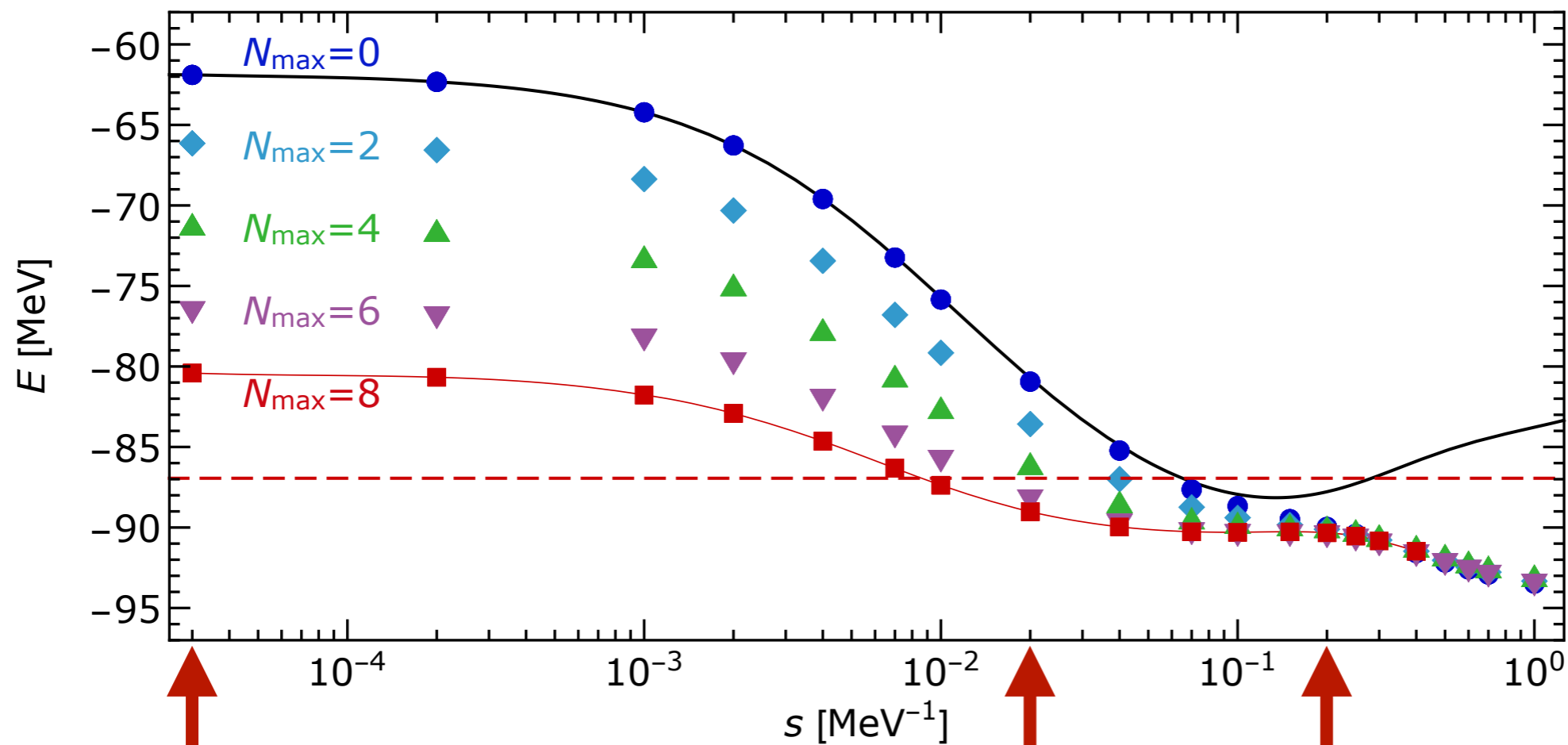
In-Medium SRG: Multi Reference

Gebrerufael et al., arXiv:1610.05254



In-Medium SRG: Multi Reference

Gebrerufael et al., arXiv:1610.05254



^{12}C

chiral NN+3N

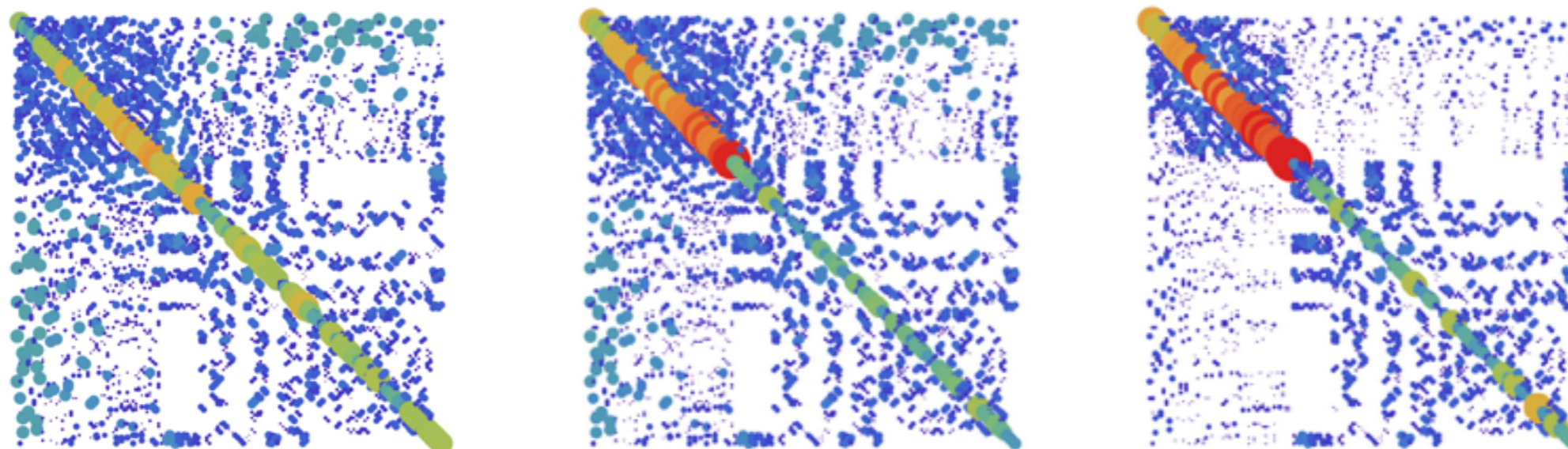
$\Lambda_{3N}=400$ MeV

$\alpha=0.08$ fm⁴

$\hbar\Omega=20$ MeV

$e_{\max}=12$

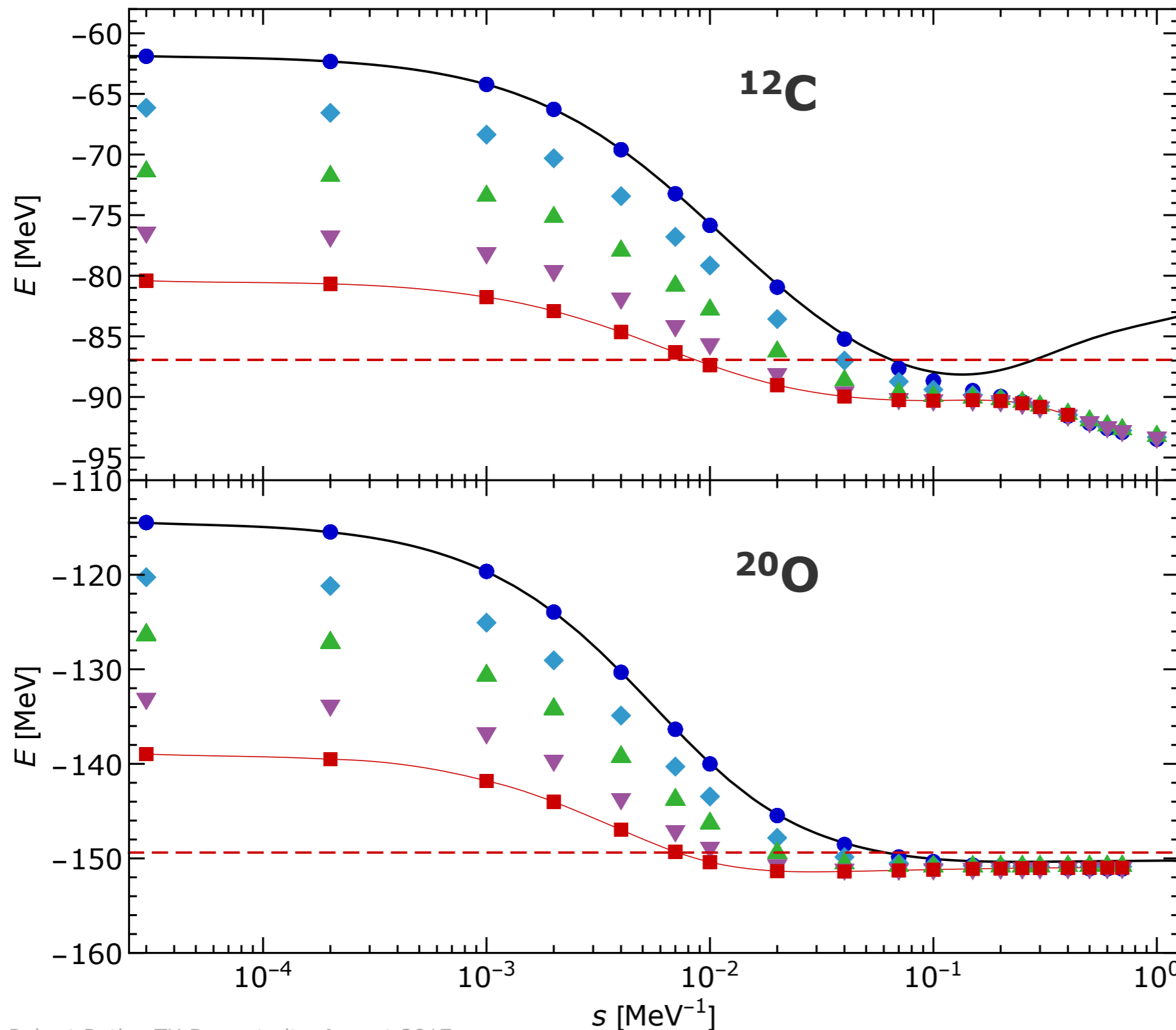
$N_{\max}=0$ reference
 HF basis



Hamilton
 matrix in
 $N_{\max}=2$
 space

Flow: Ground-State Energy

Gebrerufael et al., arXiv:1610.05254



- NCSM convergence is drastically improved
- $N_{\text{max}}=0$ eigenvalues deviated from $E(s)$
- identify plateau in s before induced terms blow up

chiral NN+3N

$\Lambda_{3N}=400$ MeV

$\alpha=0.08$ fm⁴

$\hbar\Omega=20$ MeV

$e_{\text{max}}=12$

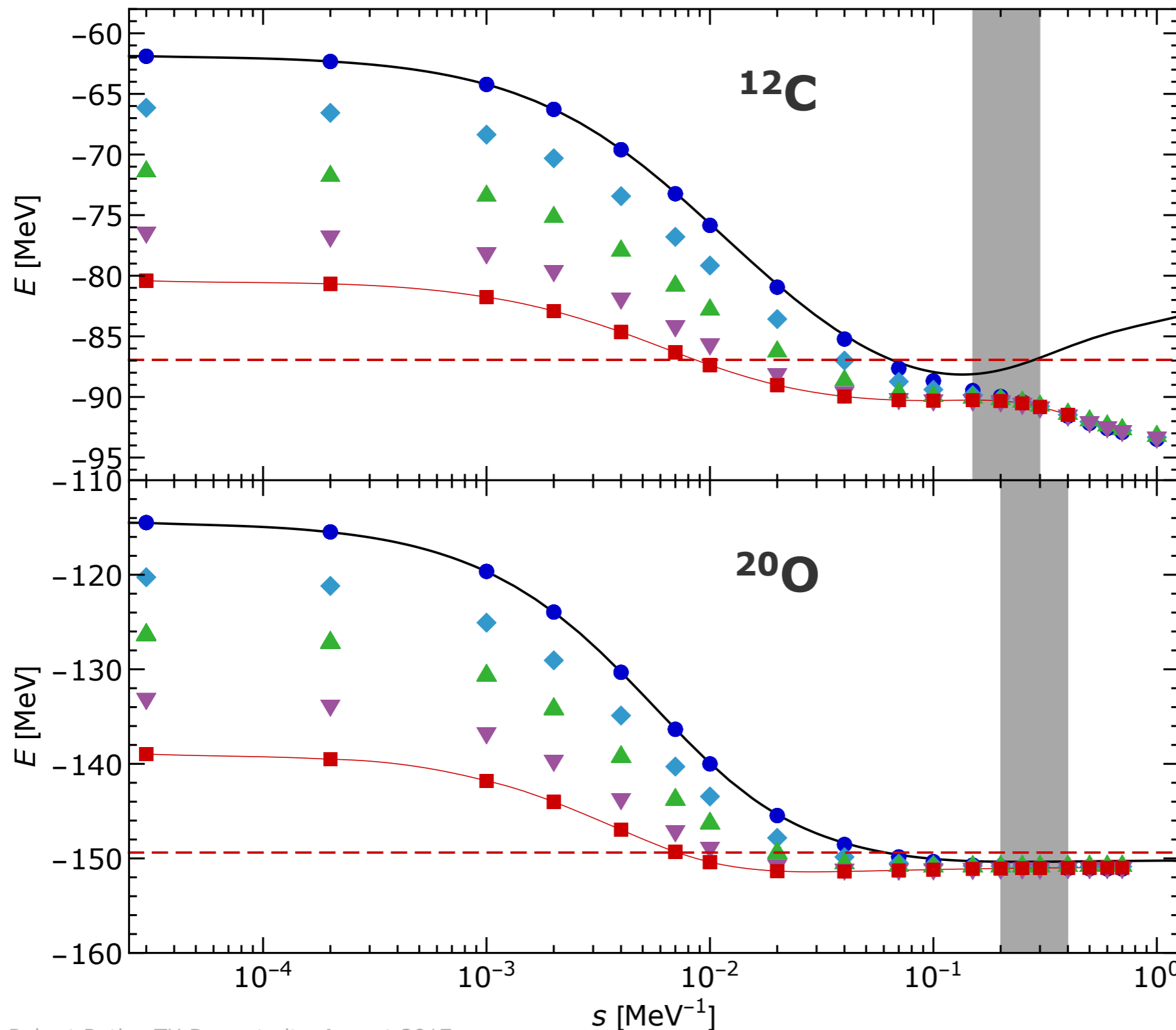
HF basis

$N_{\text{max}}=0$ reference state

$N_{\text{max}}=0, 2, 4, 6, 8$

Flow: Ground-State Energy

Gebrerufael et al., arXiv:1610.05254



- NCSM convergence is drastically improved
- $N_{\text{max}}=0$ eigenvalues deviated from $E(s)$
- identify plateau in s before induced terms blow up

chiral NN+3N

$\Lambda_{3N}=400$ MeV

$\alpha=0.08$ fm 4

$\hbar\Omega=20$ MeV

$e_{\text{max}}=12$

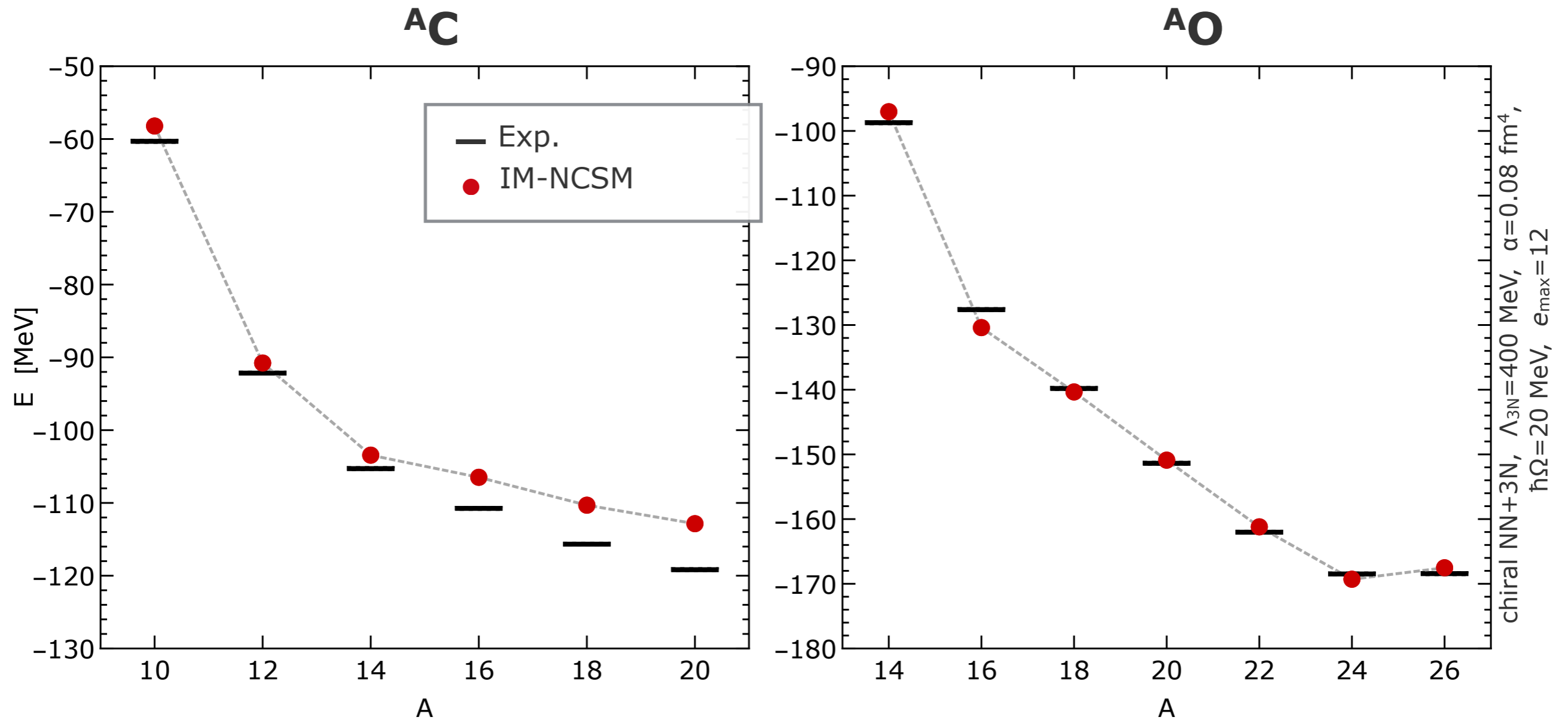
HF basis

$N_{\text{max}}=0$ reference state

$N_{\text{max}}=0, 2, 4, 6, 8$

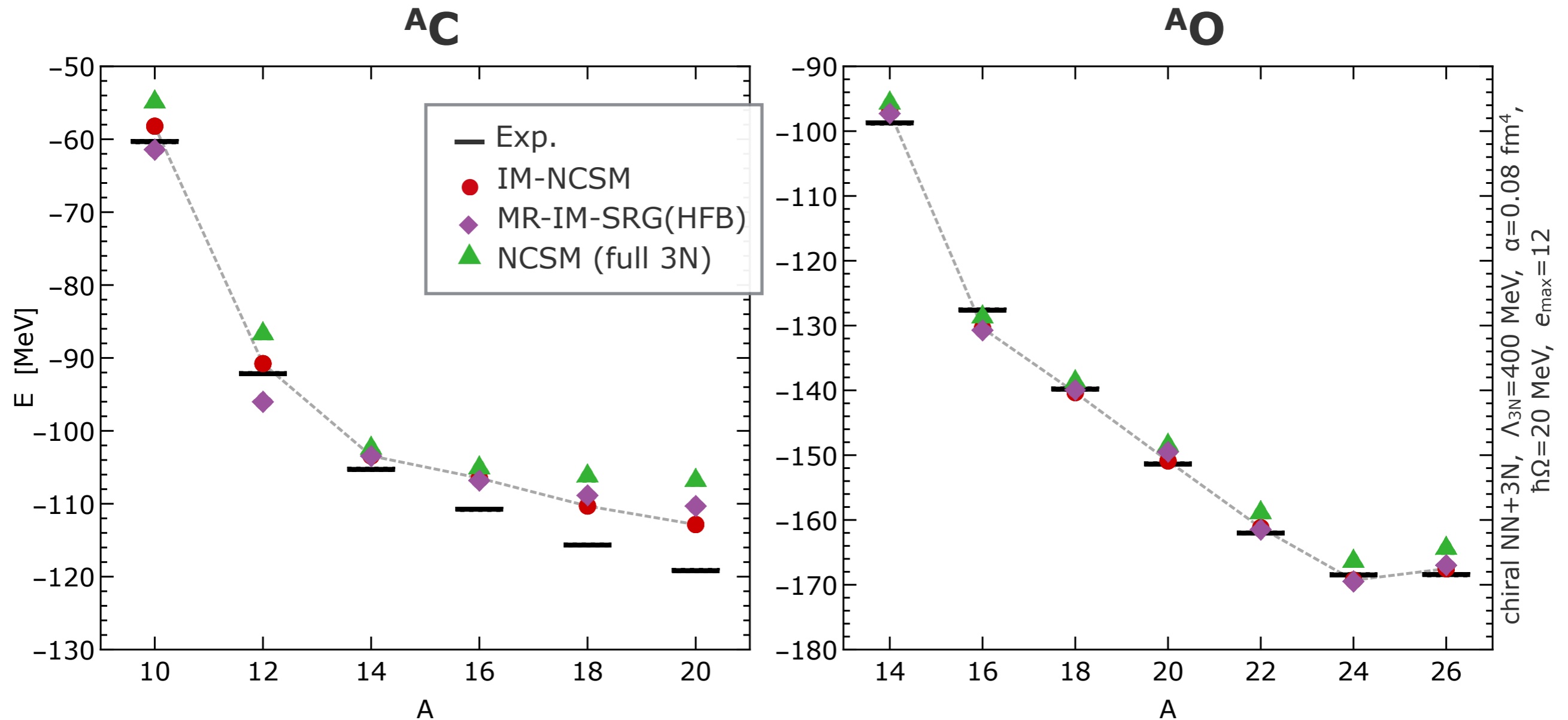
IM-NCSM: Ground-State Energies

Gebrerufael et al., arXiv:1610.05254



IM-NCSM: Ground-State Energies

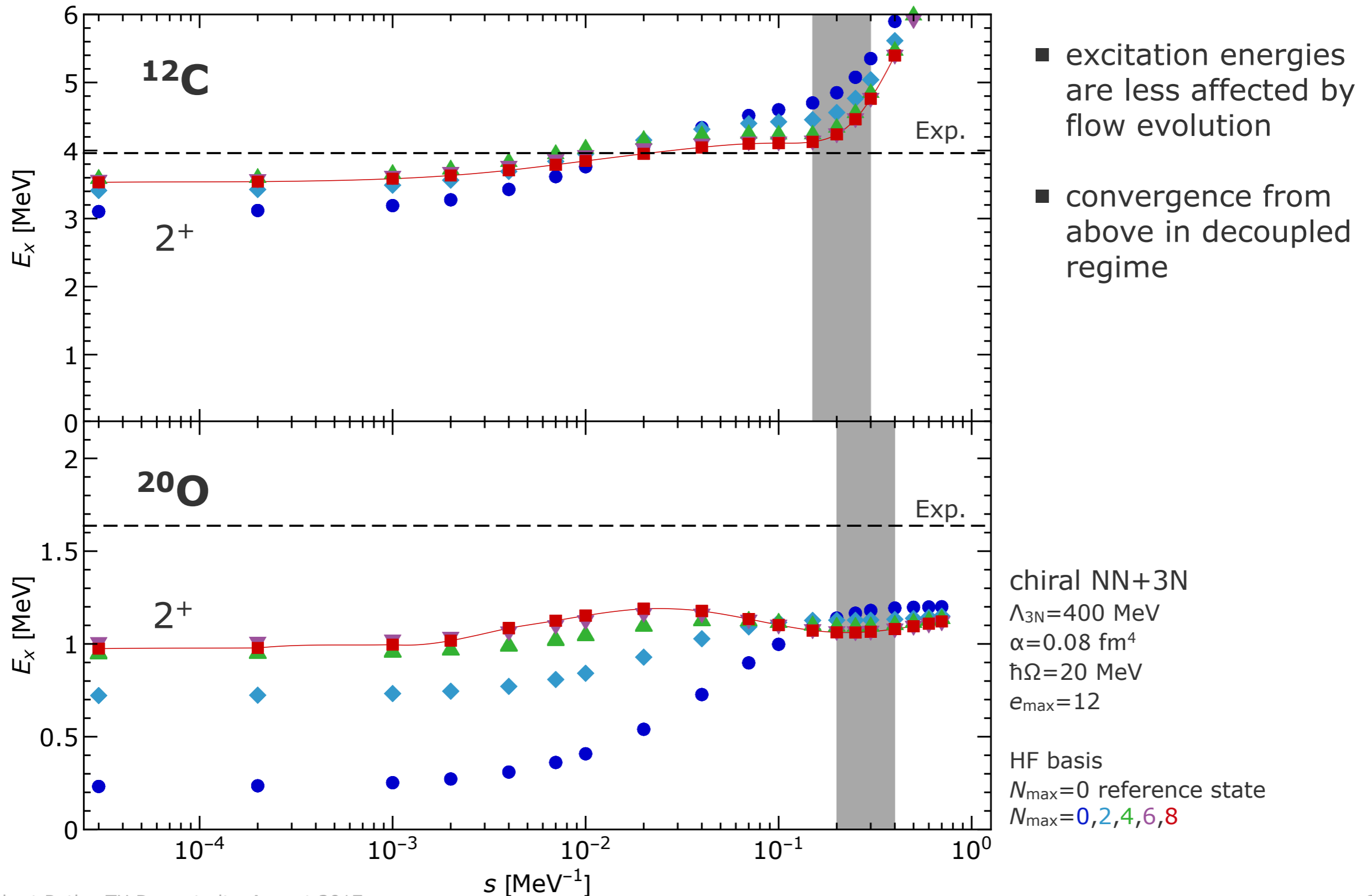
Gebrerufael et al., arXiv:1610.05254



- good agreement with NCSM within uncertainties expected from omission of normal-ordered many-body terms
- ¹²C shows surprisingly large spread among methods

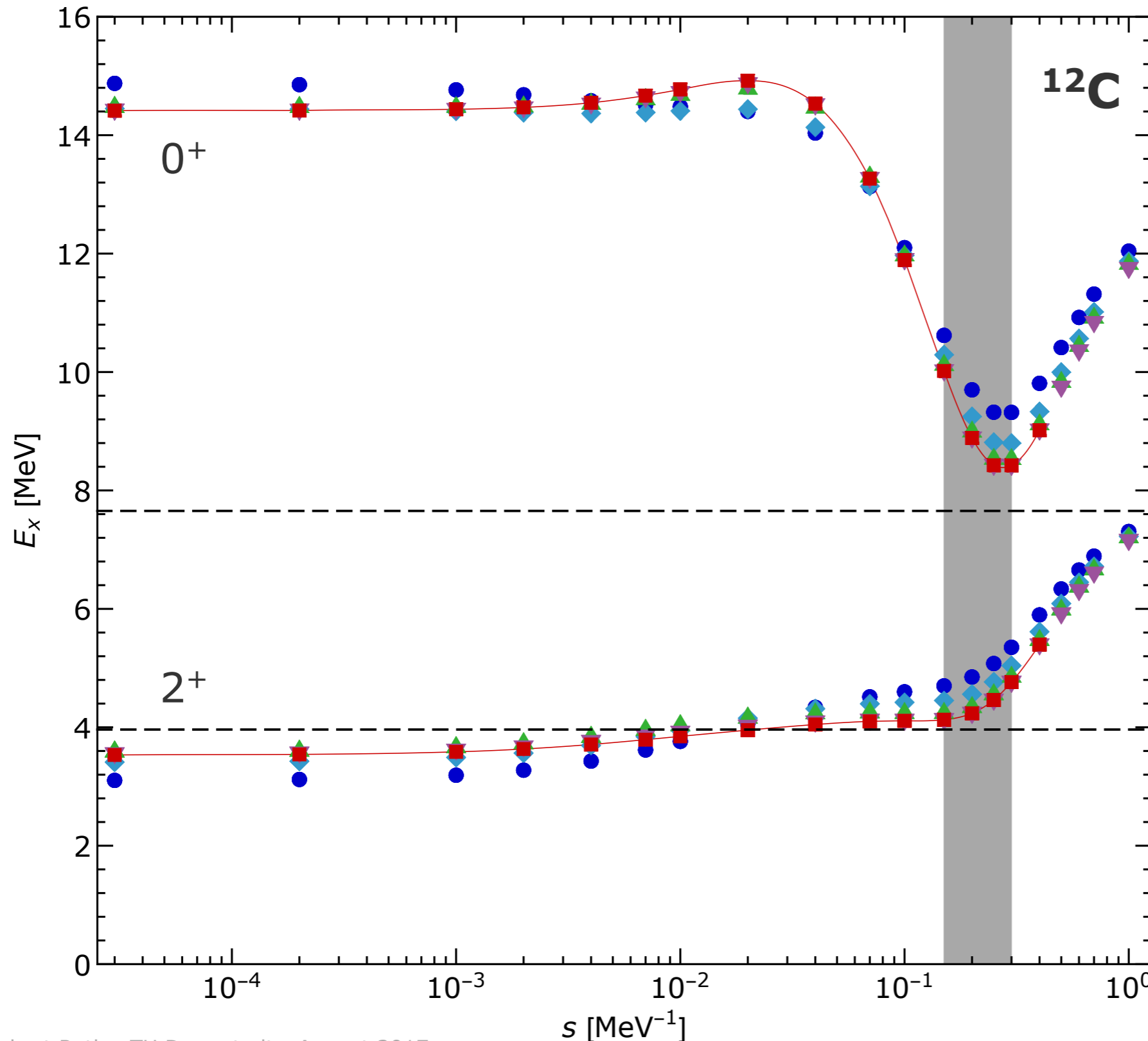
Flow: 2^+ Excitation Energy

Gebrerufael et al., arXiv:1610.05254



Flow: 0^+ Excitation Energy

Gebrerufael et al., arXiv:1610.05254



- excited 0^+ state behaves differently
- excitation energy drops by ~ 5 MeV in decoupling regime
- no stable result before induced many-body terms blow up

chiral NN+3N

$\Lambda_{3N}=400$ MeV

$\alpha=0.08$ fm⁴

$\hbar\Omega=20$ MeV

$e_{\max}=12$

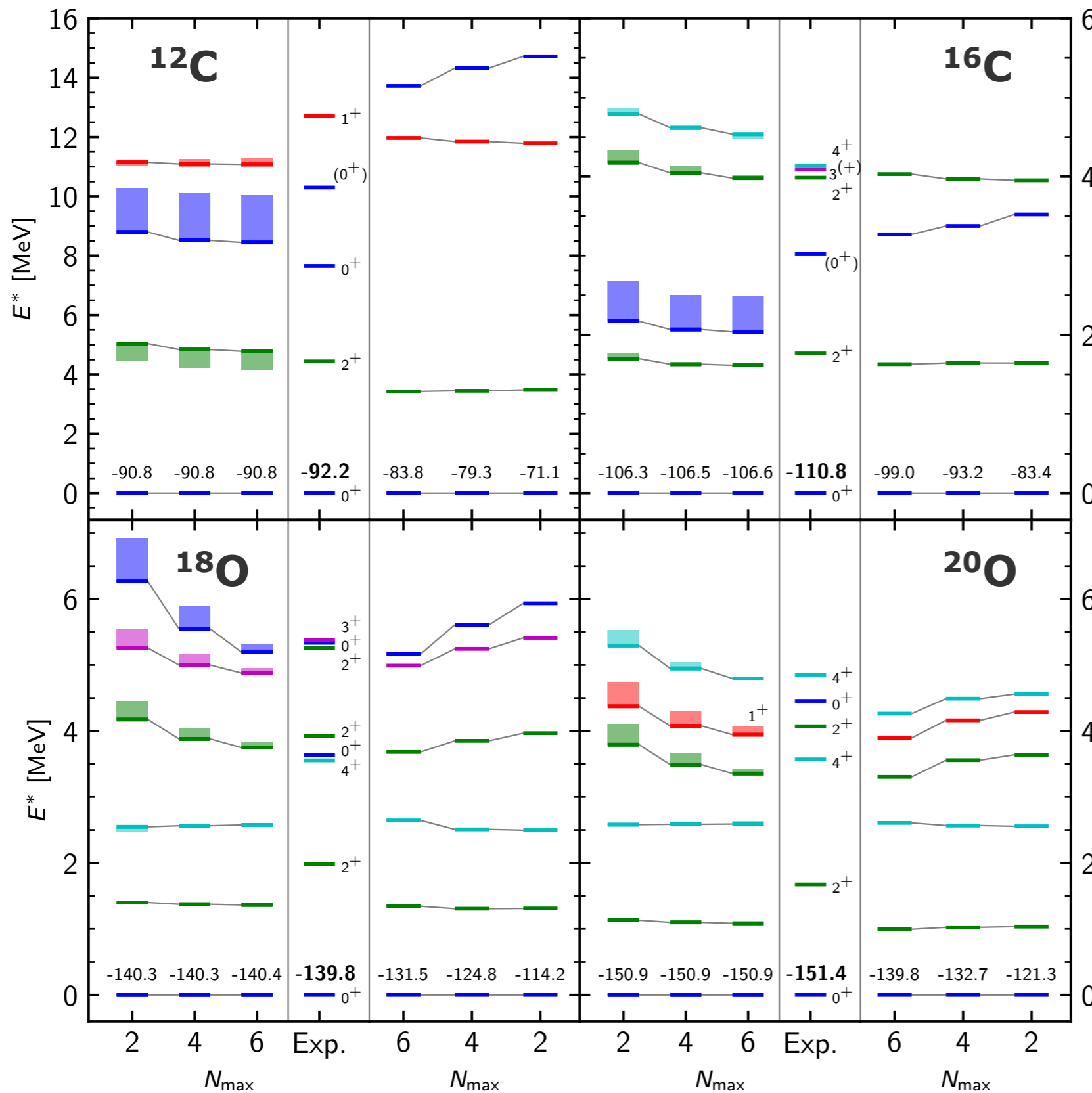
HF basis

$N_{\max}=0$ reference state

$N_{\max}=0, 2, 4, 6, 8$

IM-NCSM: Excitation Spectra

Gebrerufael et al., arXiv:1610.05254



- IM-NCSM and direct NCSM in excellent agreement for converged states
- first excited 0^+ states in ^{12}C and ^{16}C differ

chiral NN+3N
 $\Lambda_{3N}=400$ MeV
 $\alpha=0.08$ fm⁴
 $\hbar\Omega=16$ MeV
 $e_{\text{max}}=12$
 HF basis

In-Medium SRG: Pros & Cons

flexibility of generators

much more efficient than ph-truncated CI

straight-forward extension to open-shell nuclei

PRO

size extensive

very mild scaling with A

hermitian Hamiltonian

easy access to other observables

bridge to shell model

not variational

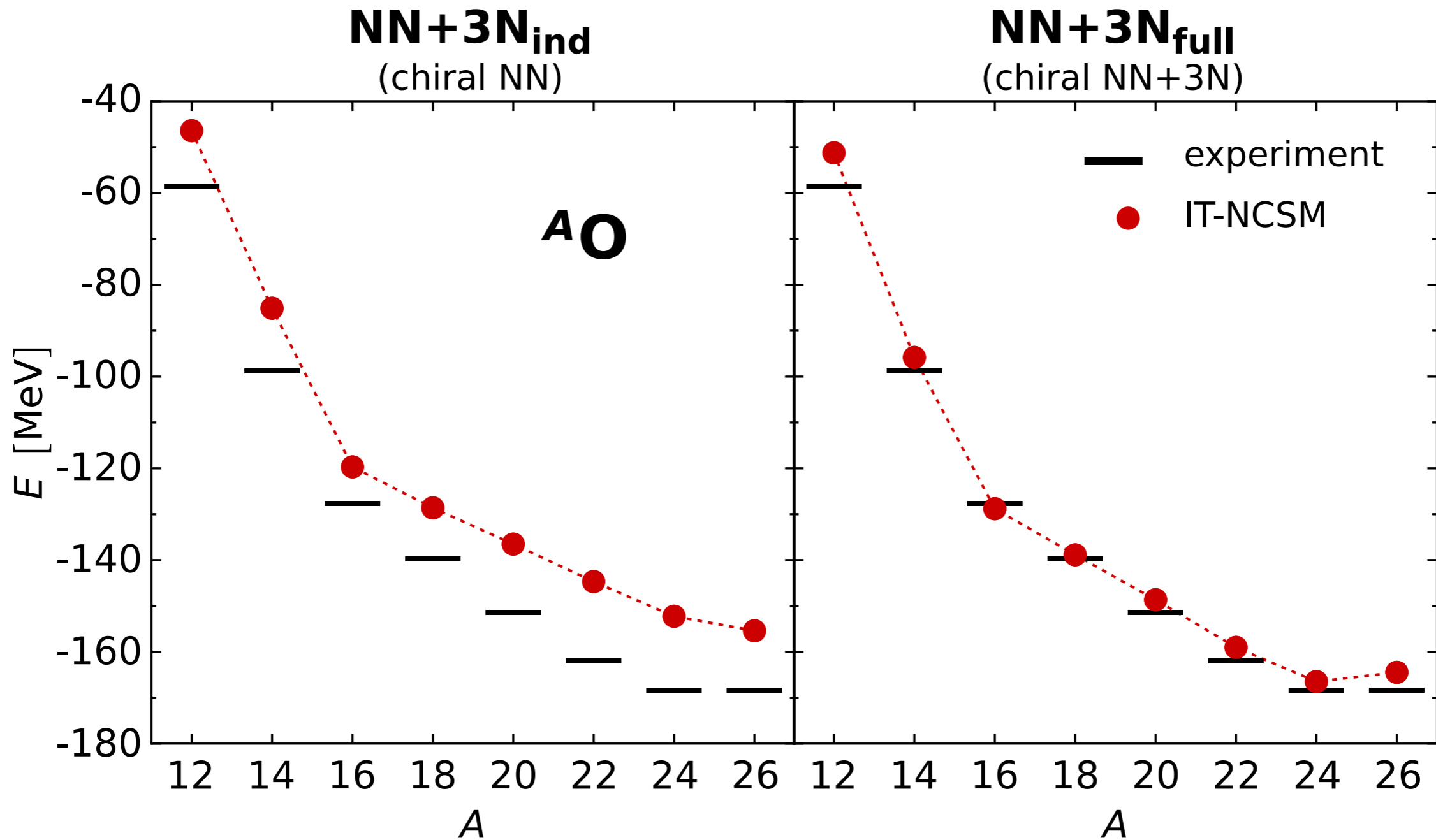
CON

NO3B needs some work

Applications for Medium-Mass Nuclei

Ground States of Oxygen Isotopes

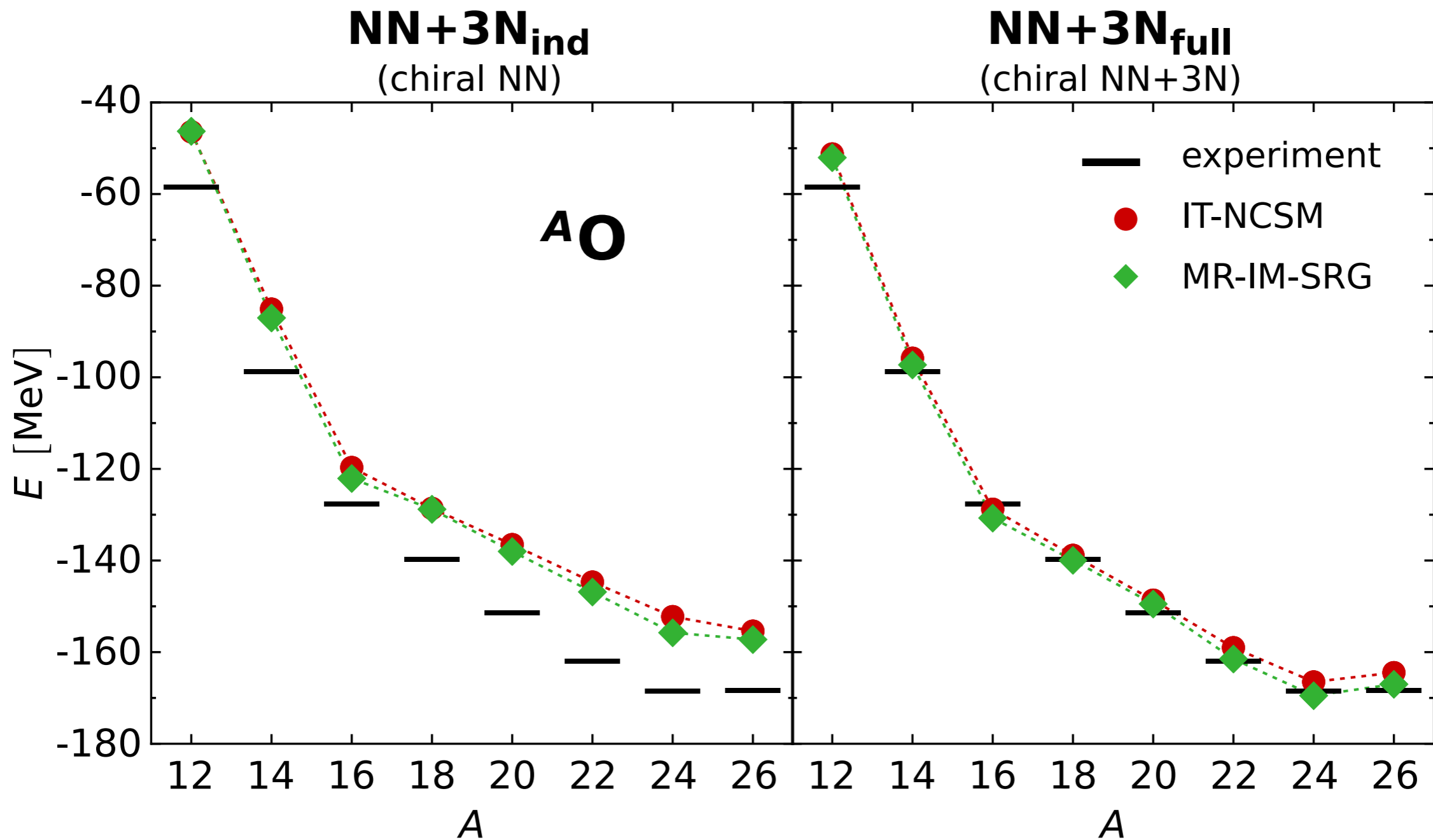
Hergert et al., PRL 110, 242501 (2013)



$$\Lambda_{3N} = 400 \text{ MeV}, \quad \alpha = 0.08 \text{ fm}^4, \quad E_{3\text{max}} = 14, \quad \text{optimal } h\Omega$$

Ground States of Oxygen Isotopes

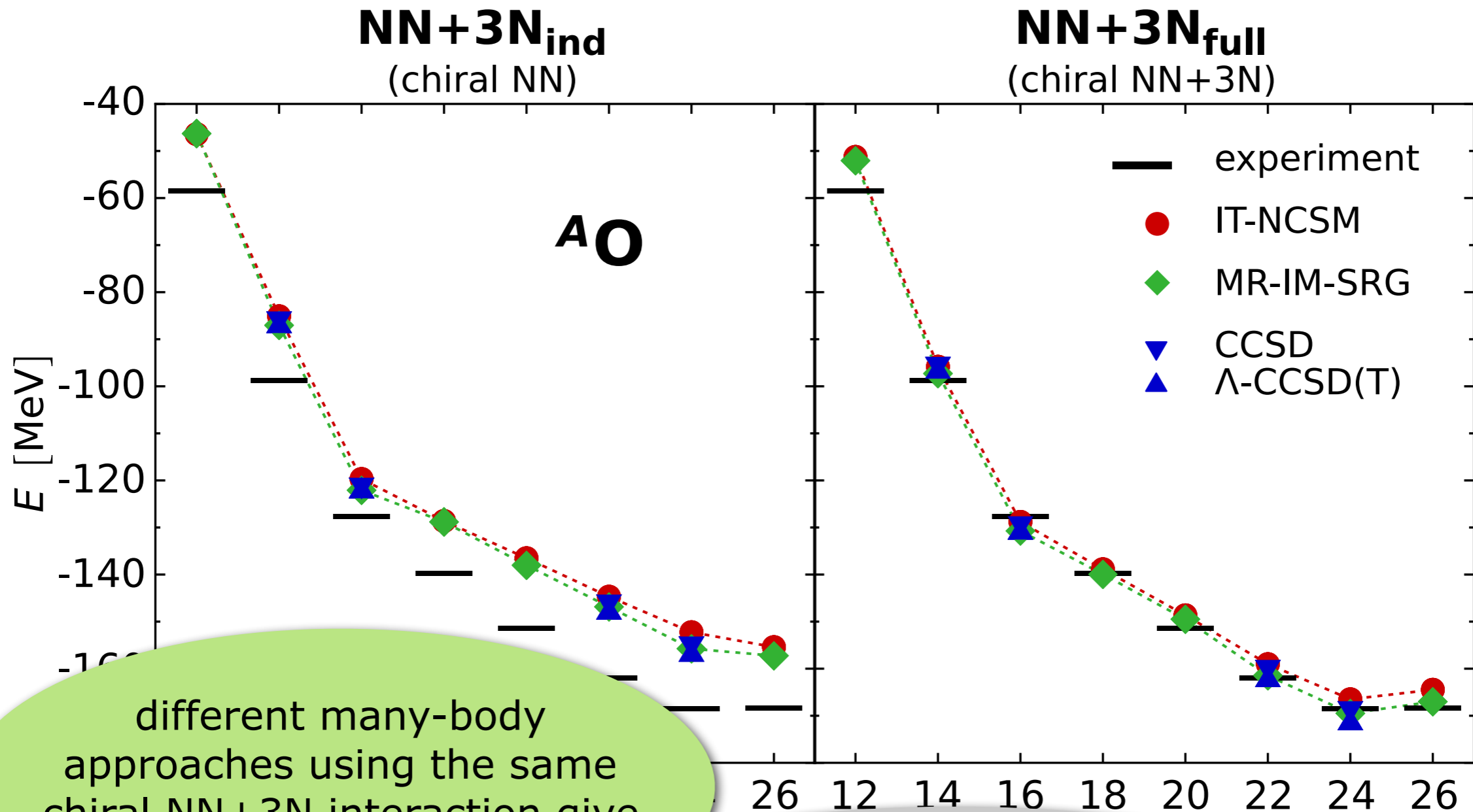
Hergert et al., PRL 110, 242501 (2013)



$$\Lambda_{3N} = 400 \text{ MeV}, \quad \alpha = 0.08 \text{ fm}^4, \quad E_{3\text{max}} = 14, \quad \text{optimal } h\Omega$$

Ground States of Oxygen Isotopes

Hergert et al., PRL 110, 242501 (2013)

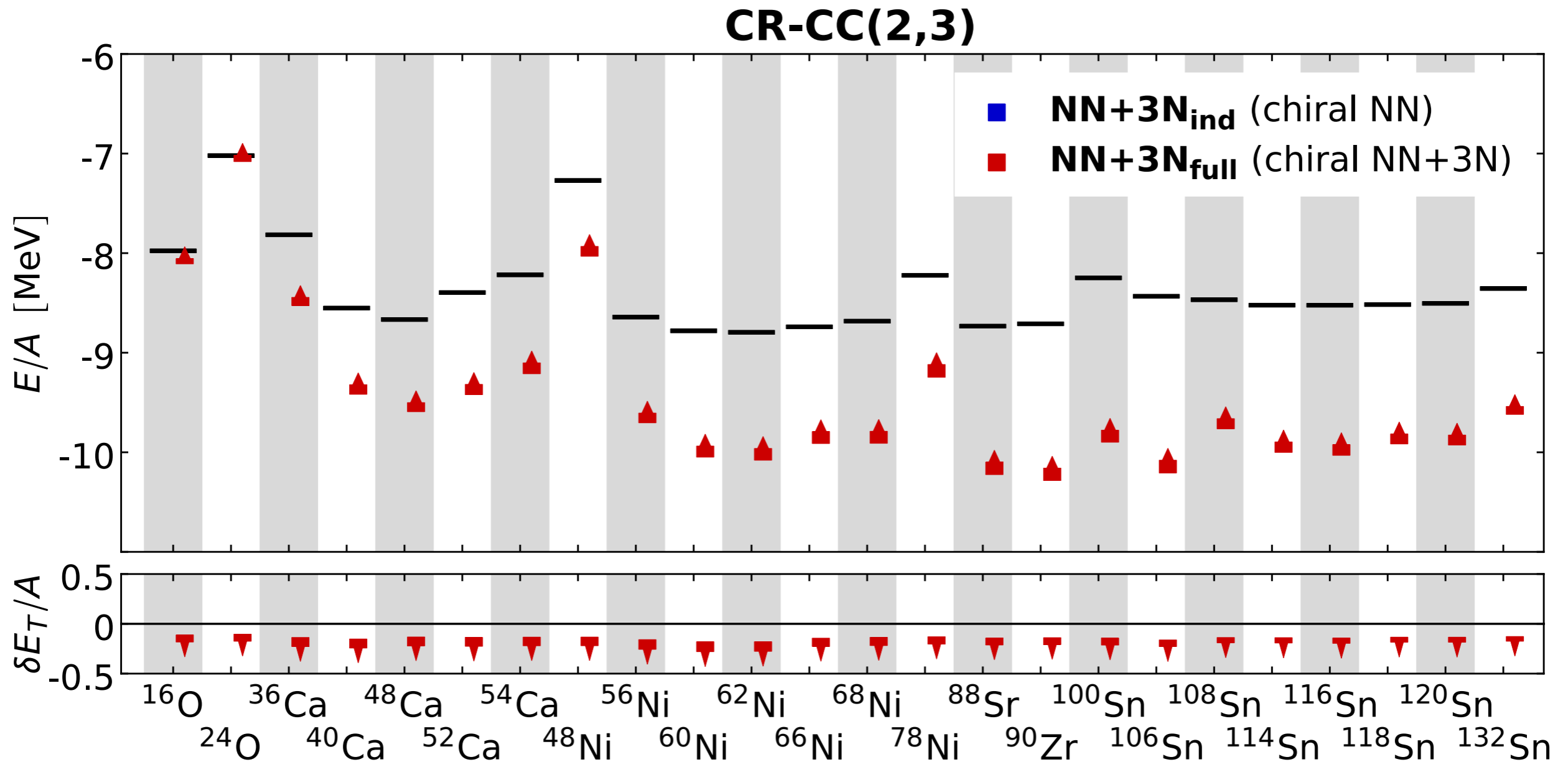


different many-body approaches using the same chiral NN+3N interaction give consistent results

minor differences are understood in terms of uncertainties due to truncations

Towards Heavy Nuclei - Ab Initio

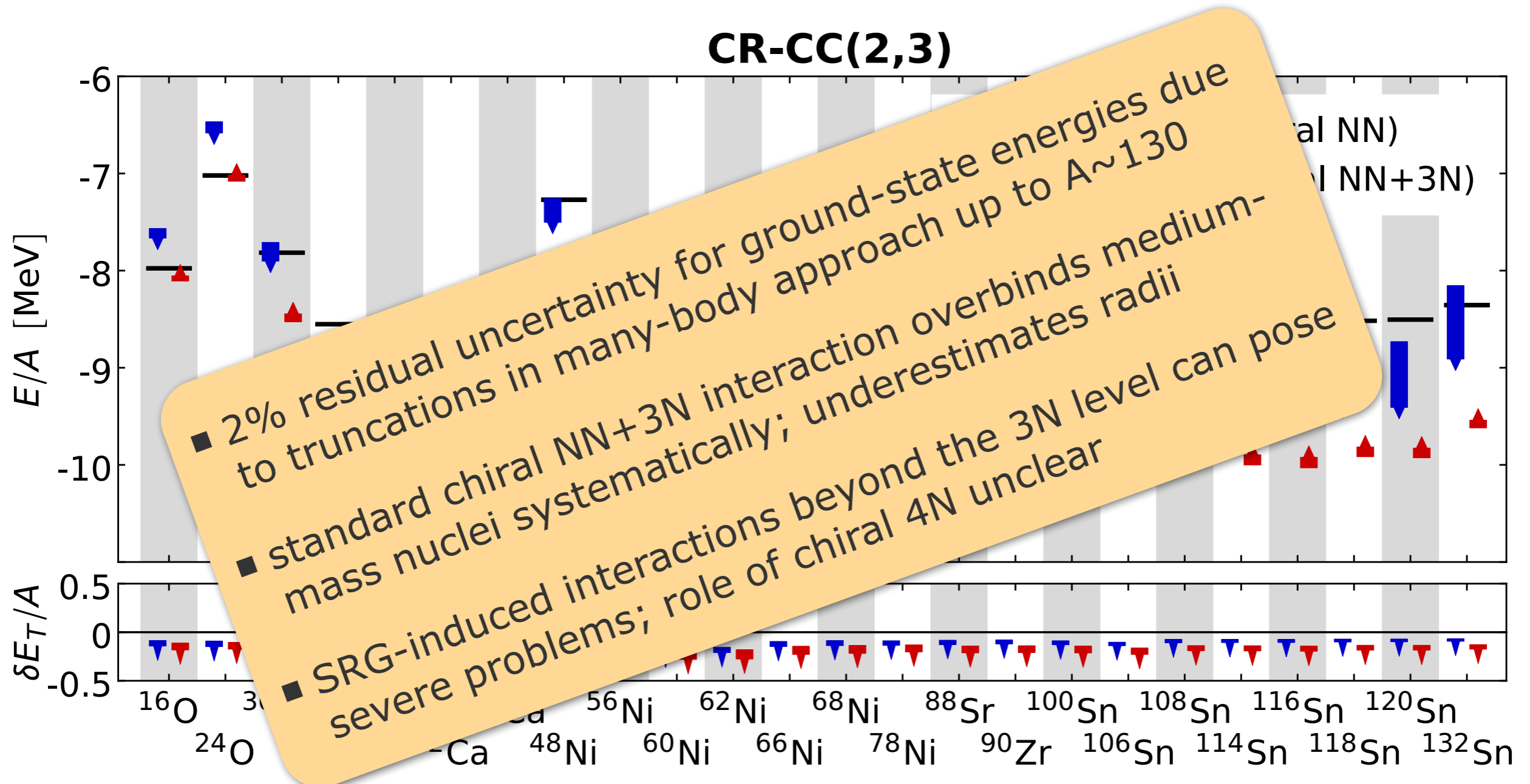
Binder et al., PLB 736, 119 (2014)



$$\Lambda_{3N} = 400 \text{ MeV}, \quad \alpha = 0.08 \rightarrow 0.04 \text{ fm}^4, \quad E_{3\text{max}} = 18, \quad \text{optimal } h\Omega$$

Towards Heavy Nuclei - Ab Initio

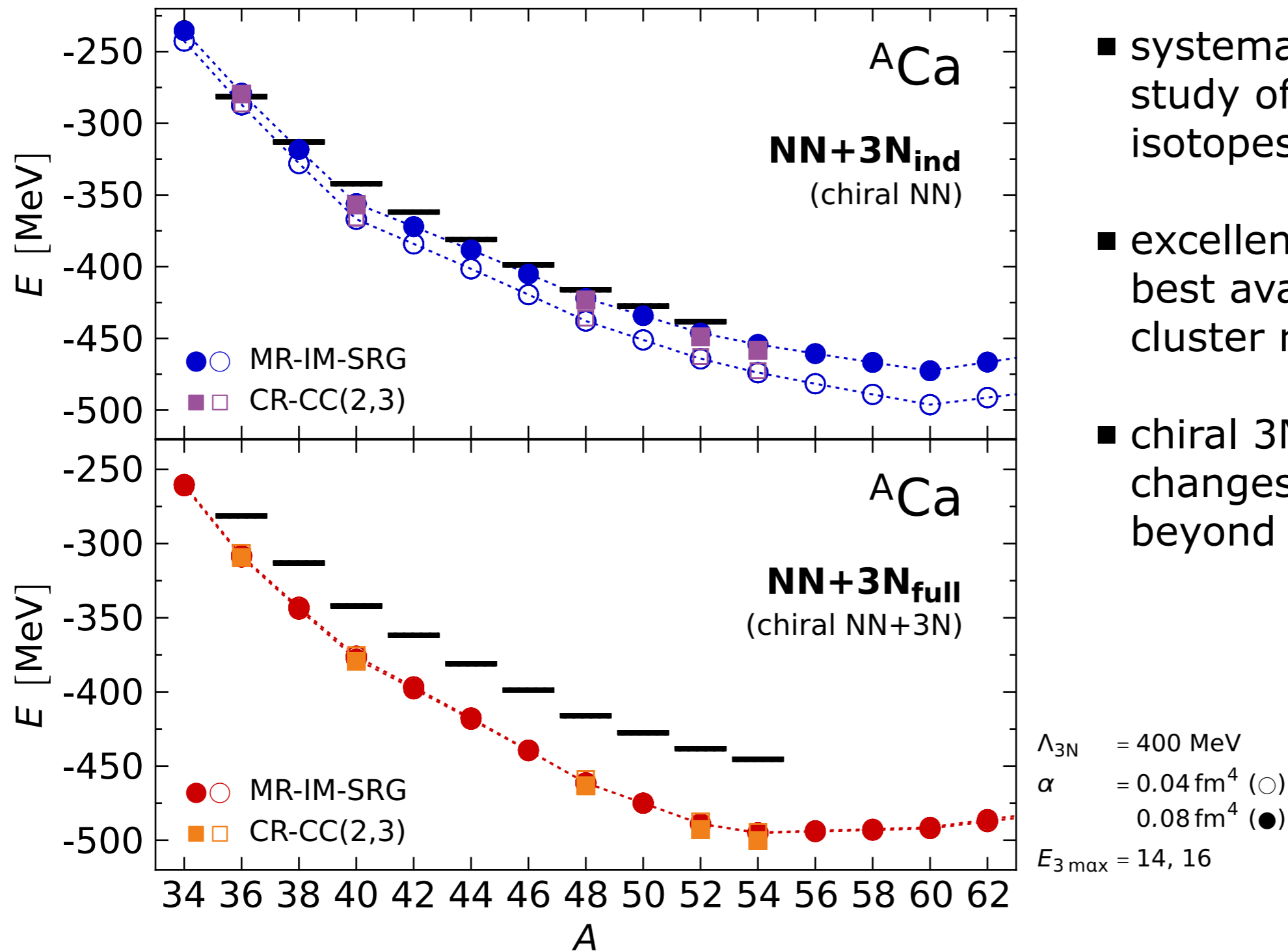
Binder et al., PLB 736, 119 (2014)



$$\Lambda_{3N} = 400 \text{ MeV}, \quad \alpha = 0.08 \rightarrow 0.04 \text{ fm}^4, \quad E_{3 \text{ max}} = 18, \quad \text{optimal } h\Omega$$

Open-Shell Medium-Mass Nuclei

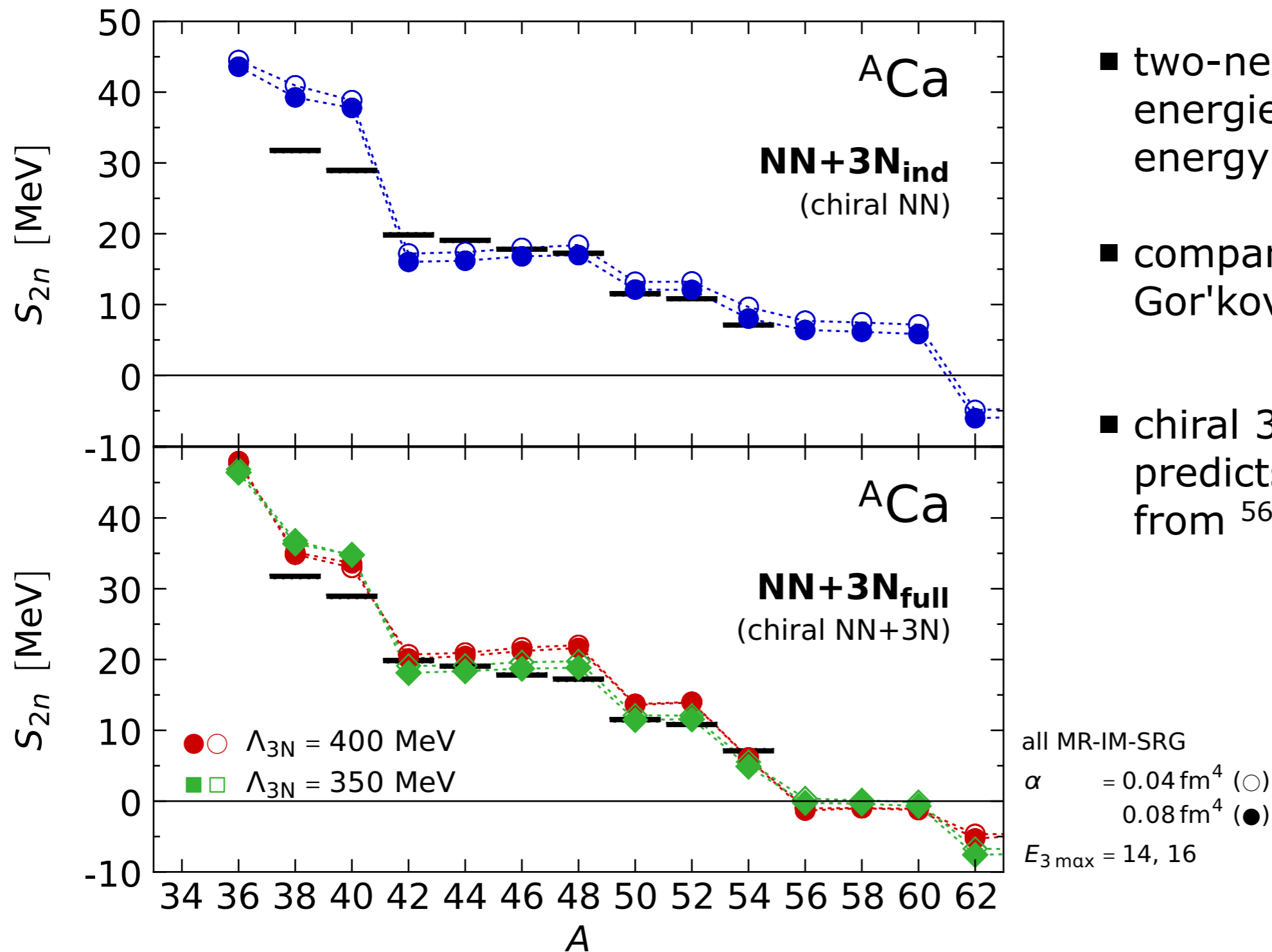
Hergert et al., PRC 90, 041302(R) (2014)



- systematic MR-IM-SRG study of even Ca and Ni isotopes
- excellent agreement with best available coupled-cluster results
- chiral 3N interaction changes behavior at and beyond ^{54}Ca

Open-Shell Medium-Mass Nuclei

Hergert et al., PRC 90, 041302(R) (2014)



- two-neutron separation energies hide overall energy shift

- compares well to updated Gor'kov-GF results

[priv. comm. V. Soma]

- chiral 3N interaction predicts flat "drip-region" from ^{56}Ca to ^{60}Ca

Conclusions

Ab Initio Frontiers

■ **ab initio theory is entering new territory...**

- **QCD frontier**
nuclear structure connected systematically to QCD via chiral EFT
- **precision frontier**
precision spectroscopy of light nuclei, including current contributions
- **mass frontier**
ab initio calculations up to heavy nuclei with quantified uncertainties
- **open-shell frontier**
extend to medium-mass open-shell nuclei and their excitation spectrum
- **continuum frontier**
include continuum effects and scattering observables consistently
- **strangeness frontier**
ab initio predictions for hyper-nuclear structure & spectroscopy

...providing a coherent theoretical framework for nuclear structure & reaction calculations

Epilogue

■ thanks to my group and my collaborators

- S. Alexa, E. Gebrerufael, T. Hüther, L. Mertes, S. Schulz, H. Spielvogel, C. Stumpf, A. Tichai, K. Vobig, R. Wirth
Technische Universität Darmstadt
- P. Navrátil, A. Calci
TRIUMF, Vancouver
- S. Binder
Oak Ridge National Laboratory
- H. Hergert
NSCL / Michigan State University
- J. Vary, P. Maris
Iowa State University
- S. Quaglioni
Lawrence Livermore National Laboratory
- E. Epelbaum, H. Krebs & the LENPIC Collaboration
Universität Bochum, ...



Deutsche
Forschungsgemeinschaft

DFG



Exzellente Forschung für
Hessens Zukunft

