No-Core Shell Model

and Related Areas (NCSM*)

Lecture 3: Beyond Light Nuclei

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Overview

- **Lecture 1: Hamiltonian**

  Prelude • Nuclear Hamiltonian • Matrix Elements • Two-Body Problem • Correlations & Unitary Transformations

- **Lecture 2: Light Nuclei**

  Similarity Renormalization Group • Many-Body Problem • Configuration Interaction • No-Core Shell Model • Hypernuclei

- **Lecture 3: Beyond Light Nuclei**

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

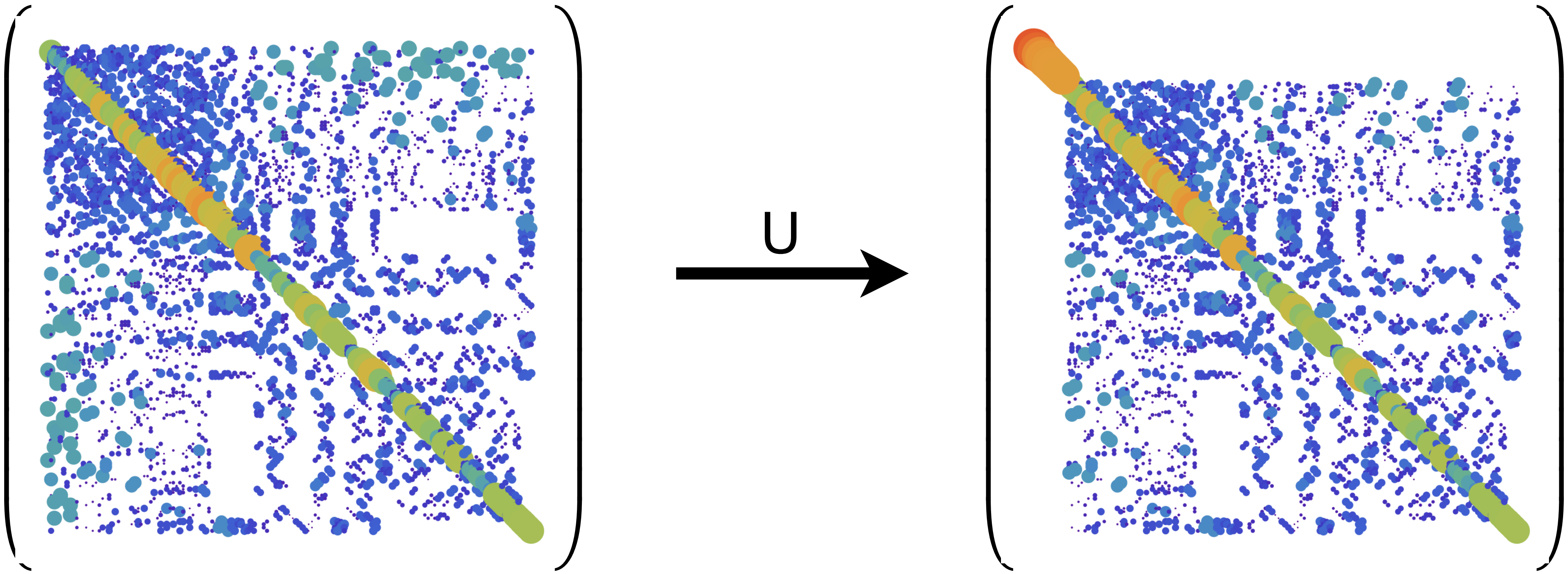
- **Hands-On: Do-It-Yourself NCSM**

  Three-Body Problem • Numerical SRG Evolution • NCSM Eigenvalue Problem • Lanczos Algorithm

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
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- **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

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

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

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

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

$$|\Phi_a^p\rangle = a_p^\dagger a_a |\Phi\rangle$$
$$|\Phi_{ab}^{pq}\rangle = a_p^\dagger a_q^\dagger a_b a_a |\Phi\rangle$$
$$\vdots$$

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

$$a_i^\dagger a_j \,, \qquad a_i^\dagger a_j^\dagger a_l a_k \,, \qquad a_i^\dagger a_j^\dagger a_k^\dagger a_n a_m a_l \,, \ldots$$

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

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

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

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

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	$a^\dagger_p, a^\dagger_q, \ldots$	$a_a, a_b, \ldots$
annihilation operators	$a_p, a_q, \ldots$	$a^\dagger_a, a^\dagger_b, \ldots$

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

$$\langle\Phi|\,\{\ldots\}\,|\Phi\rangle = 0$$

- 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

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

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

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

$$H = E + \sum_{ij} f^i_j\, \{a_i^\dagger a_j\} + \frac{1}{4}\sum_{ijkl} \Gamma^{ij}_{kl}\, \{a_i^\dagger a_j^\dagger a_l a_k\} + \cancel{\frac{1}{36}\sum_{ijklmn} W^{ijk}_{lmn}\, \{a_i^\dagger a_j^\dagger a_k^\dagger a_n a_m a_l\}}$$

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

$$f^i_j = \sum_{a}\langle ai|\, T_{\text{int}} + V_{NN}\, |aj\rangle + \frac{1}{2}\sum_{ab}\langle abi|\, V_{3N}\, |abj\rangle$$

$$\Gamma^{ij}_{kl} = \langle ij|\, T_{\text{int}} + V_{NN}\, |kl\rangle + \sum_{a}\langle aij|\, V_{3N}\, |akl\rangle$$

$$W^{ijk}_{lmn} = \langle ijk|\, V_{3N}\, |lmn\rangle$$

Coupled-Cluster Theory

Coupled-Cluster Ansatz

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

$$|\Psi_{CC}\rangle = \exp(\mathrm{T})\,|\Phi\rangle = \exp(\mathrm{T}_1 + \mathrm{T}_2 + \cdots \mathrm{T}_A)\,|\Phi\rangle$$

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

$$\mathrm{T}_1 = \sum_{a,p} t_a^p \;\{a_p^\dagger a_a\}$$

$$\mathrm{T}_2 = \sum_{ab,pq} t_{ab}^{pq} \;\{a_p^\dagger a_q^\dagger a_b a_a\}$$

$$\vdots$$

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

T_1	CCS
$\mathrm{T}_1 + \mathrm{T}_2$	CCSD
$\mathrm{T}_1 + \mathrm{T}_2 + \mathrm{T}_3$	CCSDT

Coupled-Cluster Equations

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

$$\mathrm{H}_{\mathrm{int}}\,|\Psi_{\mathrm{CC}}\rangle = E\,|\Psi_{\mathrm{CC}}\rangle \qquad \Rightarrow \qquad \exp(-T)\,\mathrm{H}_{\mathrm{int}}\exp(T)\;|\Phi\rangle = E\,|\Phi\rangle$$

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

$$\mathcal{H}\;|\Phi\rangle = E\,|\Phi\rangle \qquad \text{with} \qquad \mathcal{H} = \exp(-T)\,\mathrm{H}_{\mathrm{int}}\exp(T)$$

- 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**

$$\langle\Phi|\,\mathcal{H}\,|\Phi\rangle = E_{\text{CCSD}}$$
$$\langle\Phi^{p}_{a}|\,\mathcal{H}\,|\Phi\rangle = 0$$
$$\langle\Phi^{pq}_{ab}|\,\mathcal{H}\,|\Phi\rangle = 0$$

- after BCH-expansion these are **coupled non-linear algebraic equations** for the amplitudes t^{p}_{a}, t^{pq}_{ab} 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

$$\Delta E^{(\mathrm{CCSD})} = \overset{(EA)}{+} \frac{1}{4}\sum_{abij} v^{ij}_{ab}\, t^{ab}_{ij} \overset{(EB)}{+} \sum_{ai} f^{i}_{a}\, t^{a}_{i} \overset{(EC)}{+} \frac{1}{2}\sum_{abij} v^{ij}_{ab}\, t^{a}_{i}\, t^{b}_{j}$$

$$\begin{aligned}
&\overset{(SA)}{+} f^{a}_{i} \overset{(SBa)}{+} \sum_{ck} f^{k}_{c}\, t^{ac}_{ik} \overset{(SBb)}{+} \frac{1}{2}\sum_{cdk} v^{ak}_{cd}\, t^{cd}_{ik} \overset{(SBc)}{-} \frac{1}{2}\sum_{ckl} v^{kl}_{ic}\, t^{ac}_{kl} \\
&\overset{(SCa)}{+} \sum_{c} f^{a}_{c}\, t^{c}_{i} \overset{(SCb)}{-} \sum_{i} f^{k}_{i}\, t^{a}_{k} \overset{(SCc)}{+} \sum_{ck} v^{ak}_{ic}\, t^{c}_{k} \overset{(SDa)}{-} \frac{1}{2}\sum_{cdkl} v^{kl}_{cd}\, t^{ad}_{kl}\, t^{c}_{i} \\
&\overset{(SDb)}{-} \frac{1}{2}\sum_{cdkl} v^{kl}_{cd}\, t^{cd}_{il}\, t^{a}_{k} \overset{(SDc)}{+} \sum_{cdkl} v^{kl}_{cd}\, t^{da}_{li}\, t^{c}_{k} \overset{(SEa)}{-} \sum_{ck} f^{k}_{c}\, t^{c}_{i}\, t^{a}_{k} \\
&\overset{(SEb)}{+} \sum_{cdk} v^{ak}_{cd}\, t^{c}_{i}\, t^{d}_{k} \overset{(SEc)}{-} \sum_{ckl} v^{kl}_{ic}\, t^{a}_{k}\, t^{c}_{l} \overset{(SF)}{-} \sum_{cdkl} v^{kl}_{cd}\, t^{a}_{k}\, t^{c}_{i}\, t^{d}_{l} \\
&= 0\,,\ \forall\, a,i
\end{aligned}$$

$$\begin{aligned}
&\overset{(DA)}{+} v^{ab}_{ij} \overset{(DBa)}{+} \hat{P}_{ab} \sum_{c} f^{b}_{c}\, t^{ac}_{ij} \overset{(DBb)}{-} \hat{P}_{ij} \sum_{k} f^{k}_{j}\, t^{ab}_{ik} \\
&\overset{(DBc)}{+} \frac{1}{2}\sum_{cd} v^{ab}_{cd}\, t^{cd}_{ij} \overset{(DBd)}{+} \frac{1}{2}\sum_{k} v^{kl}_{ij}\, t^{ab}_{kl} \overset{(DBe)}{+} \hat{P}_{ab}\,\hat{P}_{ij} \sum_{ck} v^{kb}_{cj}\, t^{ac}_{ik} \\
&\overset{(DCa)}{+} \frac{1}{4}\sum_{cdkl} v^{kl}_{cd}\, t^{cd}_{ij}\, t^{ab}_{kl} \overset{(DCb)}{+} \hat{P}_{ij} \sum_{cdkl} v^{kl}_{cd}\, t^{ac}_{ik}\, t^{bd}_{jl} \\
&\overset{(DCc)}{-} \frac{1}{2}\hat{P}_{ij} \sum_{cdkl} v^{kl}_{cd}\, t^{dc}_{ik}\, t^{ab}_{lj} \overset{(DCd)}{-} \frac{1}{2}\hat{P}_{ab} \sum_{cdkl} v^{kl}_{cd}\, t^{ac}_{lk}\, t^{db}_{ij} \\
&\overset{(DDa)}{+} \hat{P}_{ij} \sum_{c} v^{ab}_{cj}\, t^{c}_{i} \overset{(DDb)}{-} \hat{P}_{ab} \sum_{k} v^{kb}_{ij}\, t^{a}_{k} \overset{(DEa)}{-} \hat{P}_{ij} \sum_{ck} f^{k}_{c}\, t^{ab}_{kj}\, t^{c}_{i} \\
&\overset{(DEb)}{-} \hat{P}_{ab} \sum_{ck} f^{k}_{c}\, t^{cb}_{ij}\, t^{a}_{k} \overset{(DEc)}{+} \hat{P}_{ab}\,\hat{P}_{ij} \sum_{cdk} v^{ak}_{cd}\, t^{db}_{kj}\, t^{c}_{i} \\
&\overset{(DEd)}{-} \hat{P}_{ab}\,\hat{P}_{ij} \sum_{ckl} v^{kl}_{ic}\, t^{cb}_{lj}\, t^{a}_{k} \overset{(DEe)}{-} \frac{1}{2}\hat{P}_{ab} \sum_{cdk} v^{kb}_{cd}\, t^{cd}_{ij}\, t^{a}_{k} \\
&\overset{(DEf)}{+} \frac{1}{2}\hat{P}_{ij} \sum_{ckl} v^{kl}_{cj}\, t^{ab}_{kl}\, t^{c}_{i} \overset{(DEg)}{+} \hat{P}_{ab} \sum_{cdk} v^{ka}_{cd}\, t^{db}_{ij}\, t^{c}_{k} \\
&\overset{(DEh)}{-} \hat{P}_{ij} \sum_{ckl} v^{kl}_{ci}\, t^{ab}_{lj}\, t^{c}_{k} \overset{(DFa)}{+} \sum_{cd} v^{ab}_{cd}\, t^{c}_{i}\, t^{d}_{j} \overset{(DFb)}{+} \sum_{kl} v^{kl}_{ij}\, t^{a}_{k}\, t^{b}_{l} \\
&\overset{(DFc)}{-} \hat{P}_{ab}\,\hat{P}_{ij} \sum_{ck} v^{kb}_{cj}\, t^{a}_{k}\, t^{c}_{i} \overset{(DGa)}{+} \frac{1}{2}\sum_{cdkl} v^{kl}_{cd}\, t^{ab}_{kl}\, t^{c}_{i}\, t^{d}_{j} \\
&\overset{(DGb)}{+} \frac{1}{2}\sum_{cdkl} v^{kl}_{cd}\, t^{cd}_{ij}\, t^{a}_{k}\, t^{b}_{l} \overset{(DGc)}{-} \hat{P}_{ab}\,\hat{P}_{ij} \sum_{cdkl} v^{kl}_{cd}\, t^{db}_{lj}\, t^{a}_{k}\, t^{c}_{i} \\
&\overset{(DGd)}{-} \hat{P}_{ij} \sum_{cdkl} v^{kl}_{cd}\, t^{ab}_{lj}\, t^{c}_{k}\, t^{d}_{i} \overset{(DGe)}{-} \hat{P}_{ab} \sum_{cdkl} v^{kl}_{cd}\, t^{db}_{ij}\, t^{a}_{l}\, t^{c}_{k} \\
&\overset{(DHa)}{-} \hat{P}_{ab} \sum_{cdk} v^{kb}_{cd}\, t^{a}_{k}\, t^{c}_{i}\, t^{d}_{j} \overset{(DHb)}{+} \hat{P}_{ij} \sum_{ckl} v^{kl}_{cj}\, t^{a}_{k}\, t^{b}_{l}\, t^{c}_{i} \\
&\overset{(DI)}{+} \sum_{cdkl} v^{kl}_{cd}\, t^{a}_{k}\, t^{b}_{l}\, t^{c}_{i}\, t^{d}_{j} = 0\,, \quad \forall\, a,b,i,j
\end{aligned}$$

Coupled Cluster: Pros & Cons

PRO

- much more efficient than ph-truncated CI
- can deal with explicit 3N interaction
- size extensive
- very mild scaling with A

CON

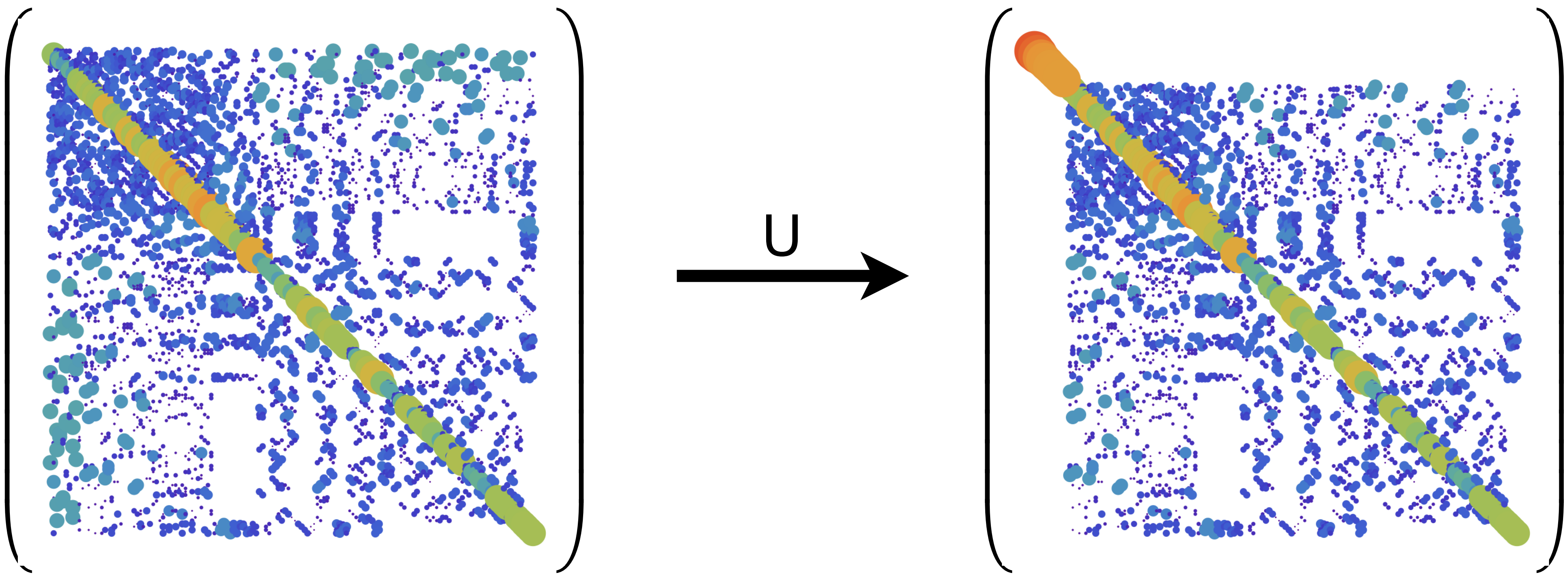
- not variational
- only for closed shell nuclei *
- other observables difficult
- only for ground states *
- non-hermititan Hamiltonian

* 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 ($\alpha \to \infty$)

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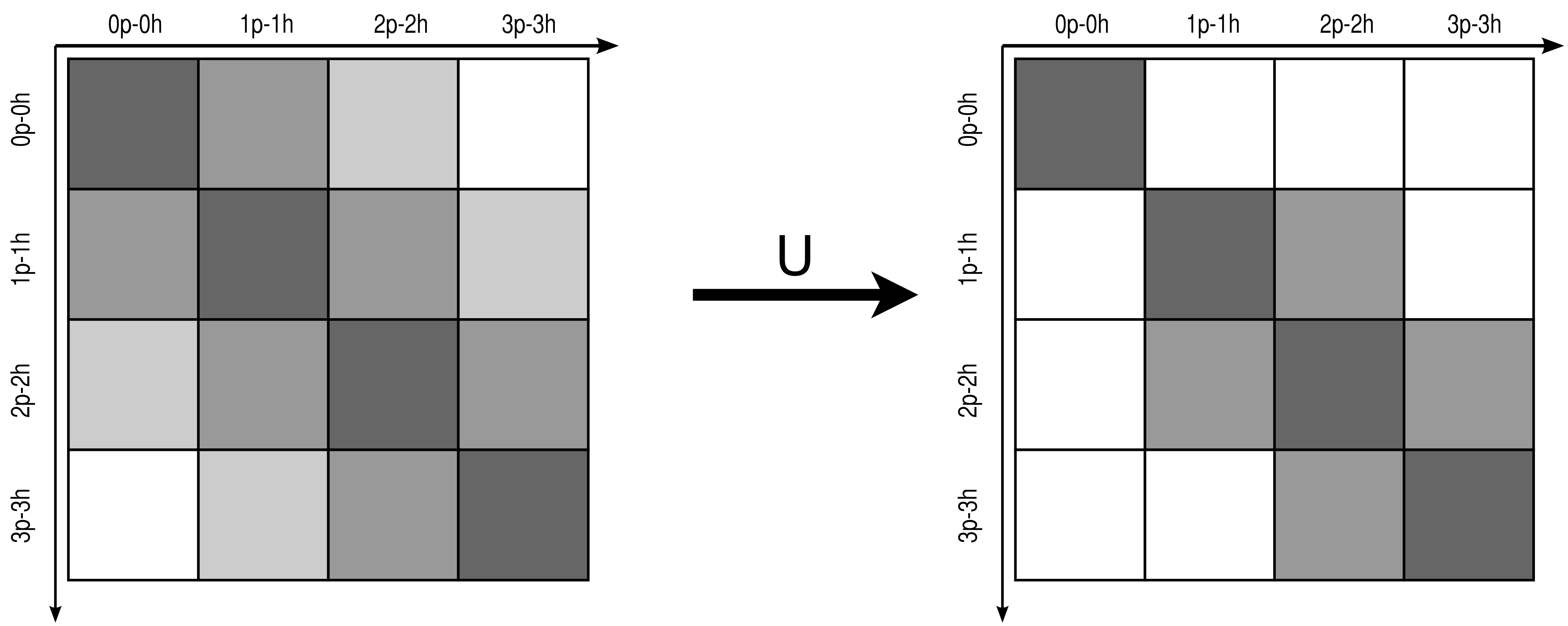

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In-Medium SRG

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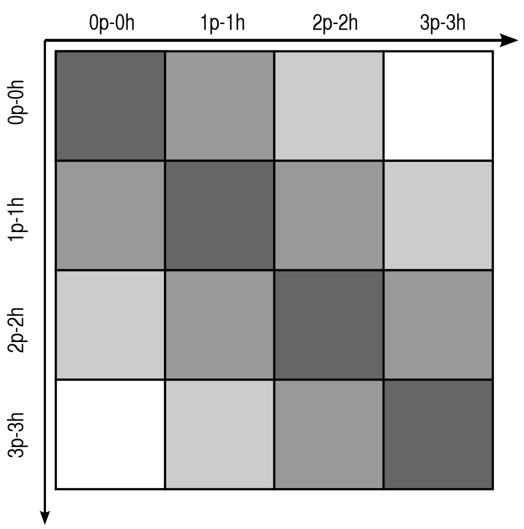
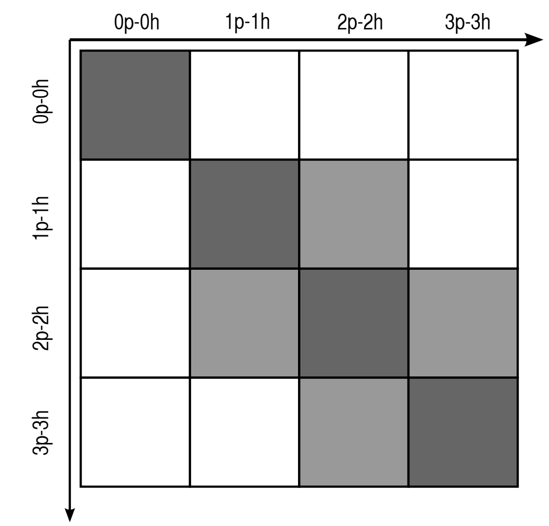


use SRG flow equations for normal-ordered Hamiltonian to decouple many-body reference state from excitations



- **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

$$\mathrm{H}(s) = E(s) + \sum_{ij} f^i_j(s)\ \{a^\dagger_i a_j\} + \frac{1}{4}\sum_{ijkl} \Gamma^{ij}_{kl}(s)\ \{a^\dagger_i a^\dagger_j a_l a_k\}$$

In-Medium SRG Generators

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

$$\eta = \left[H_\mathrm{d}, H\right] = \left[H_\mathrm{d}, H_\mathrm{od}\right]$$

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

$$\eta^1_2 = (\Delta^1_2)^{-1}\, n_1 \bar{n}_2\, f^1_2 - [1 \longleftrightarrow 2]$$

$$\eta^{12}_{34} = (\Delta^{12}_{34})^{-1}\, n_1 n_2 \bar{n}_3 \bar{n}_4\, \Gamma^{12}_{34} - [12 \longleftrightarrow 34]$$

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

$$\eta^1_2 = \mathrm{sgn}(\Delta^1_2)\, n_1 \bar{n}_2\, f^1_2 - [1 \longleftrightarrow 2]$$

$$\eta^{12}_{34} = \mathrm{sgn}(\Delta^{12}_{34})\, n_1 n_2 \bar{n}_3 \bar{n}_4\, \Gamma^{12}_{34} - [12 \longleftrightarrow 34]$$

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

$$\eta^1_2 = \langle\Phi|\,[H, \{a^\dagger_1 a_2\}]\,|\Phi\rangle$$

$$\eta^{12}_{34} = \langle\Phi|\,[H, \{a^\dagger_1 a^\dagger_2 a_4 a_3\}]\,|\Phi\rangle$$

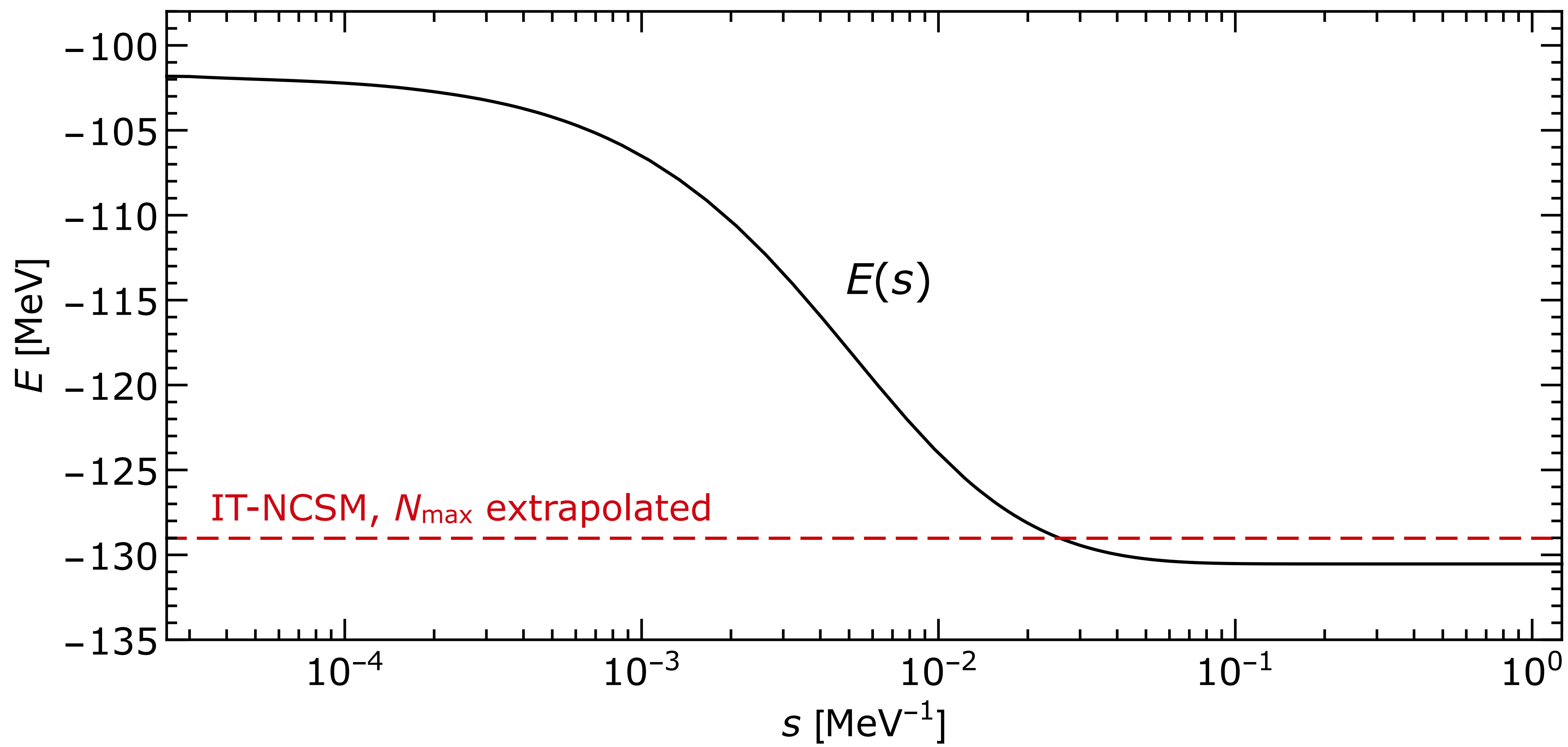
Flow-Equations for Matrix Elements

$$\frac{dE}{ds} = \sum_{ab}(n_a - n_b)\left(\eta^a_b f^b_a - f^a_b \eta^b_a\right) + \frac{1}{4}\sum_{abcd}\left(\eta^{ab}_{cd}\Gamma^{cd}_{ab} - \Gamma^{ab}_{cd}\eta^{cd}_{ab}\right) n_a n_b \bar{n}_c \bar{n}_d$$

$$\begin{aligned}\frac{d}{ds}f^1_2 = &\sum_a \left(\eta^1_a f^a_2 - f^1_a \eta^a_2\right) + \sum_{ab}\left(\eta^a_b \Gamma^{b1}_{a2} - f^a_b \eta^{b1}_{a2}\right)(n_a - n_b) \\ &+ \frac{1}{2}\sum_{abcdef}\left(\eta^{1a}_{bc}\Gamma^{bc}_{2a} - \Gamma^{1a}_{bc}\eta^{bc}_{2a}\right)(n_a \bar{n}_b \bar{n}_c + \bar{n}_a n_b n_c)\end{aligned}$$

$$\begin{aligned}\frac{d}{ds}\Gamma^{12}_{34} = &\sum_a \left(\eta^1_a \Gamma^{a2}_{34} + \eta^2_a \Gamma^{1a}_{34} - \eta^a_3 \Gamma^{12}_{a4} - \eta^a_4 \Gamma^{12}_{3a} - f^1_a \eta^{a2}_{34} - f^2_a \eta^{1a}_{34} + f^a_3 \eta^{12}_{a4} + f^a_4 \eta^{12}_{3a}\right) \\ &+ \frac{1}{2}\sum_{ab}\left(\eta^{12}_{ab}\Gamma^{ab}_{34} - \Gamma^{12}_{ab}\eta^{ab}_{34}\right)(1 - n_a - n_b) \\ &+ \sum_{ab}(n_a - n_b)\left(\left(\eta^{1a}_{3b}\Gamma^{2b}_{4a} - \Gamma^{1a}_{3b}\eta^{2b}_{4a}\right) - \left(\eta^{2a}_{3b}\Gamma^{1b}_{4a} - \Gamma^{2a}_{3b}\eta^{1b}_{4a}\right)\right)\end{aligned}$$

In-Medium SRG: Single Reference



^{16}O

chiral NN+3N
Λ_{3N}=400 MeV
α=0.08 fm^4
$\hbar\Omega$=20 MeV
e_{max}=12

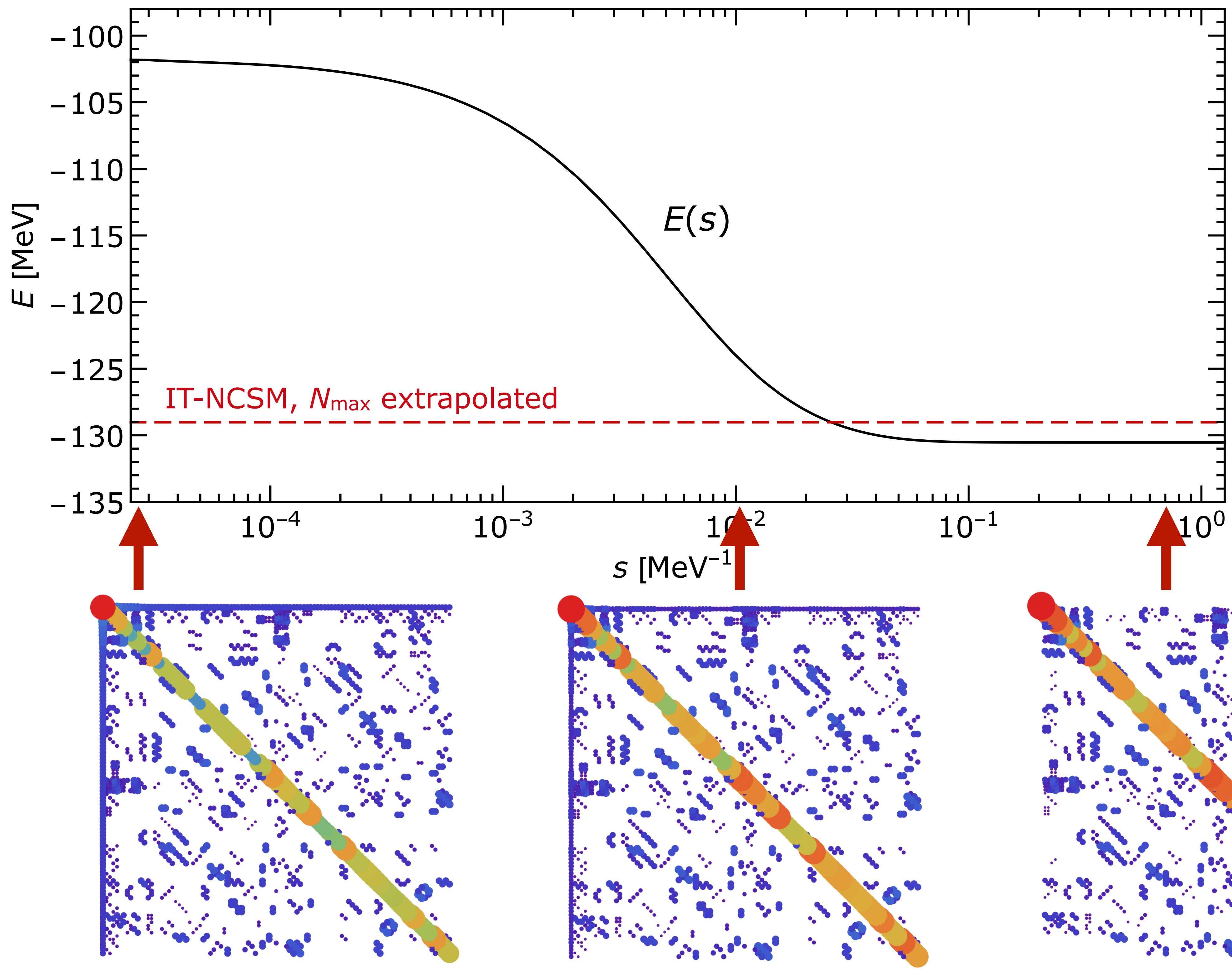
N_{max}=0 reference
HF basis

- 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



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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

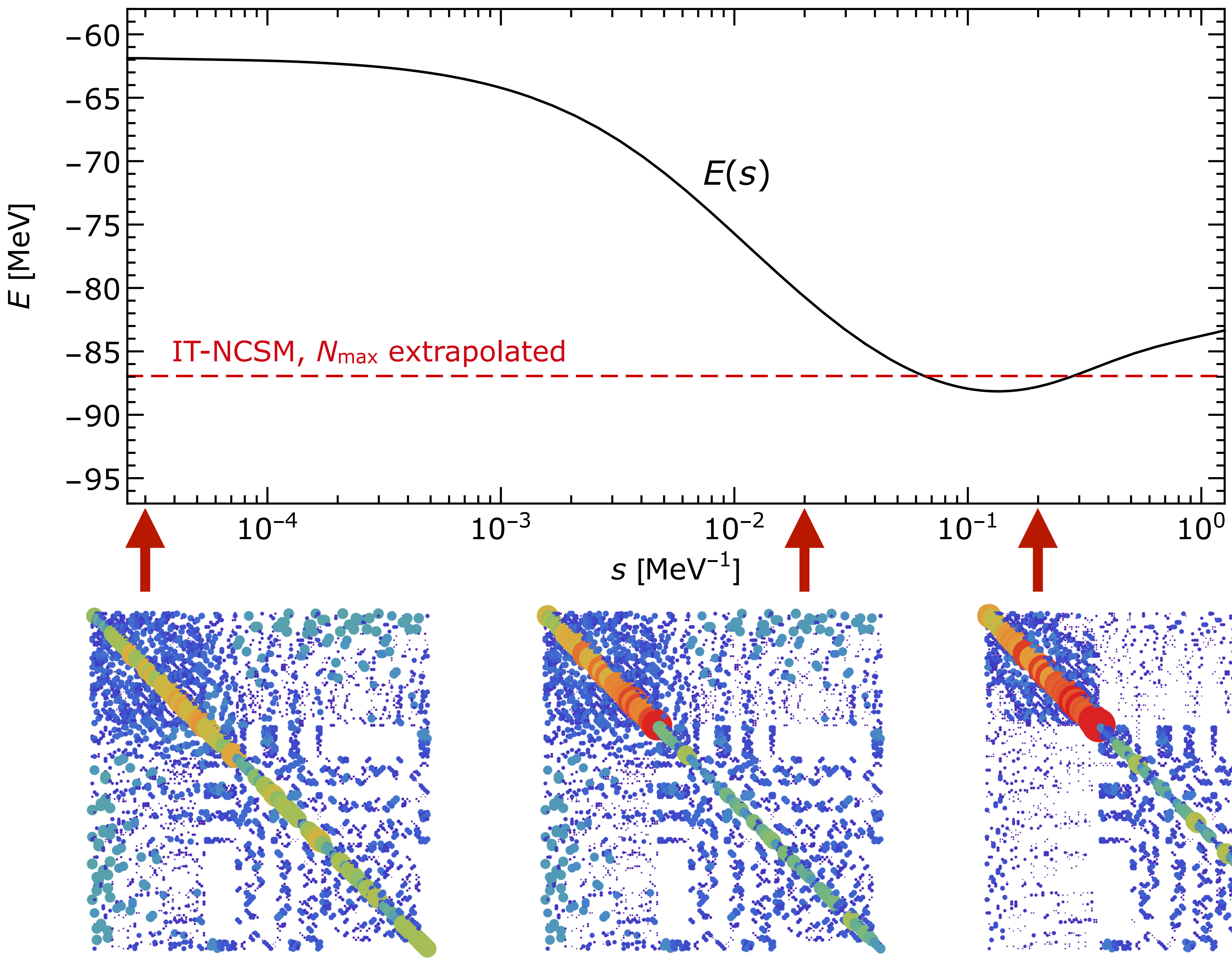
- IM-SRG evolution of multi-reference normal-ordered Hamiltonian (and other operators)
- decoupling of particle-hole excitations, i.e., pre-diagonalization in A-body space

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., PRL 118, 152503 (2017)



^{12}C

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Hamilton matrix in N_{max}=2 space

In-Medium SRG: Multi Reference

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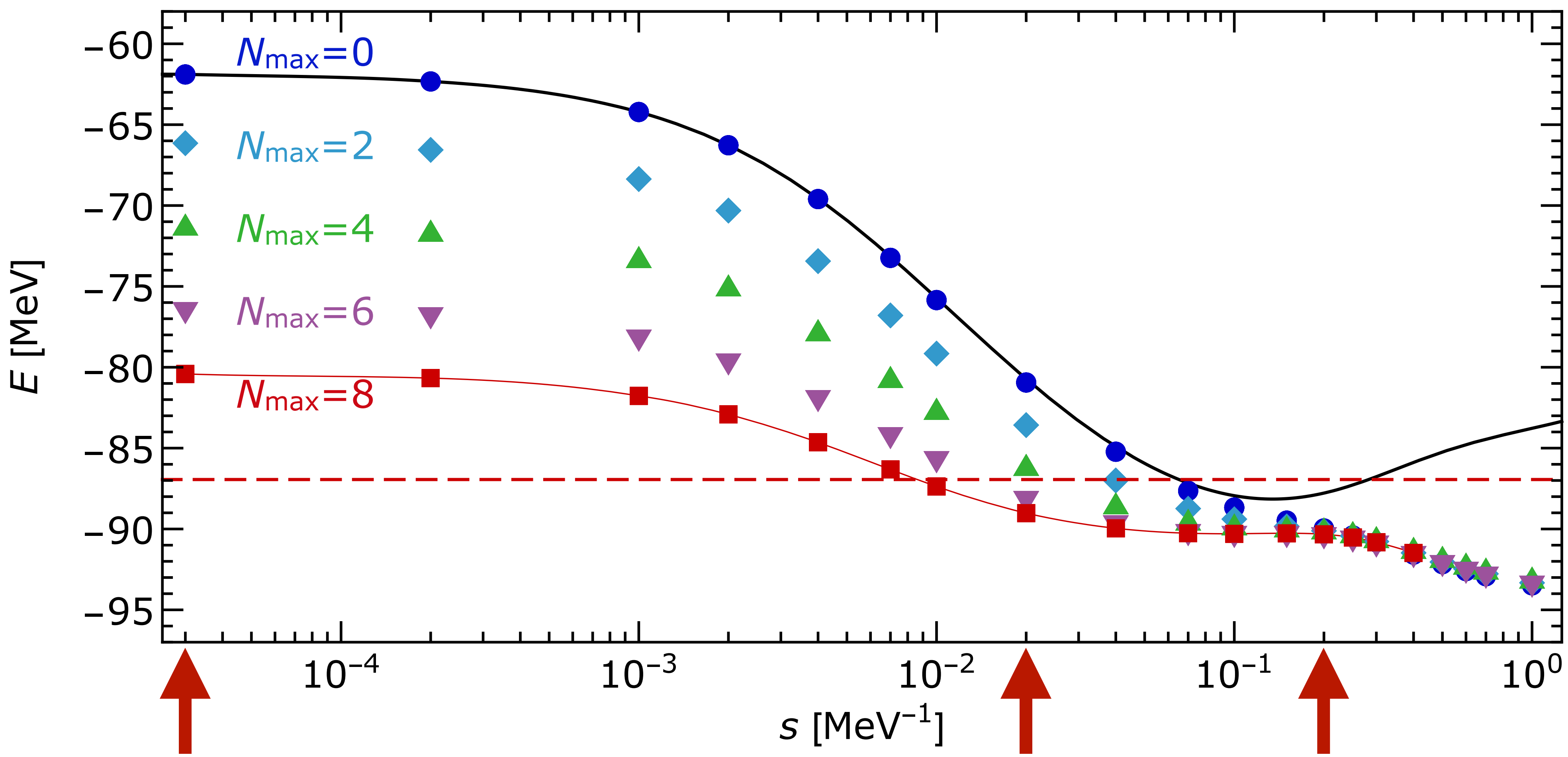

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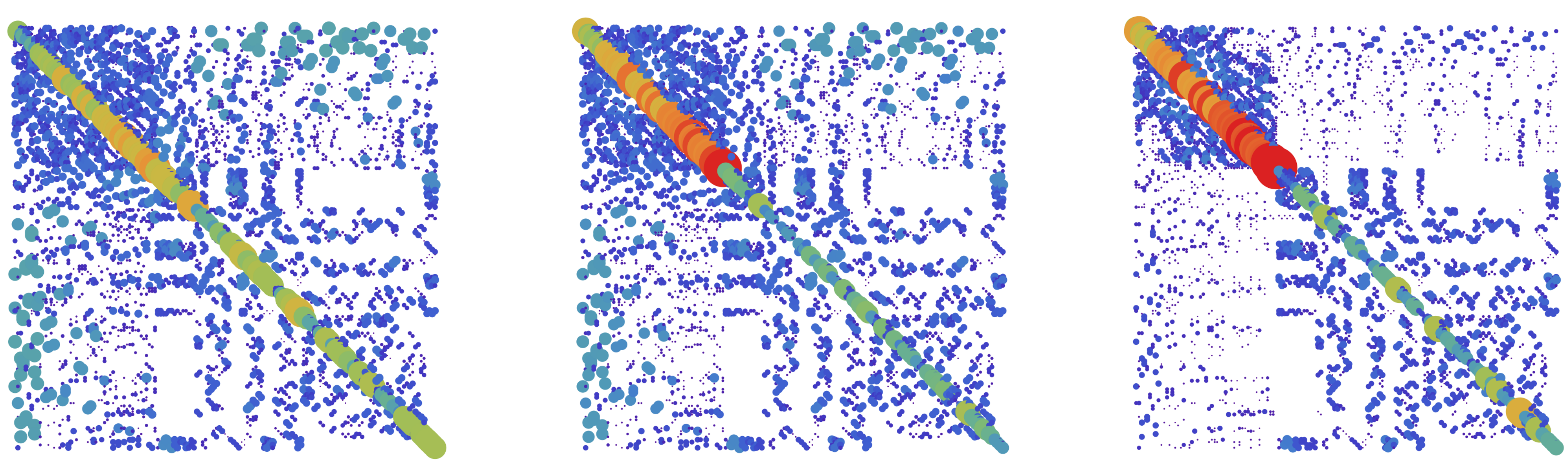
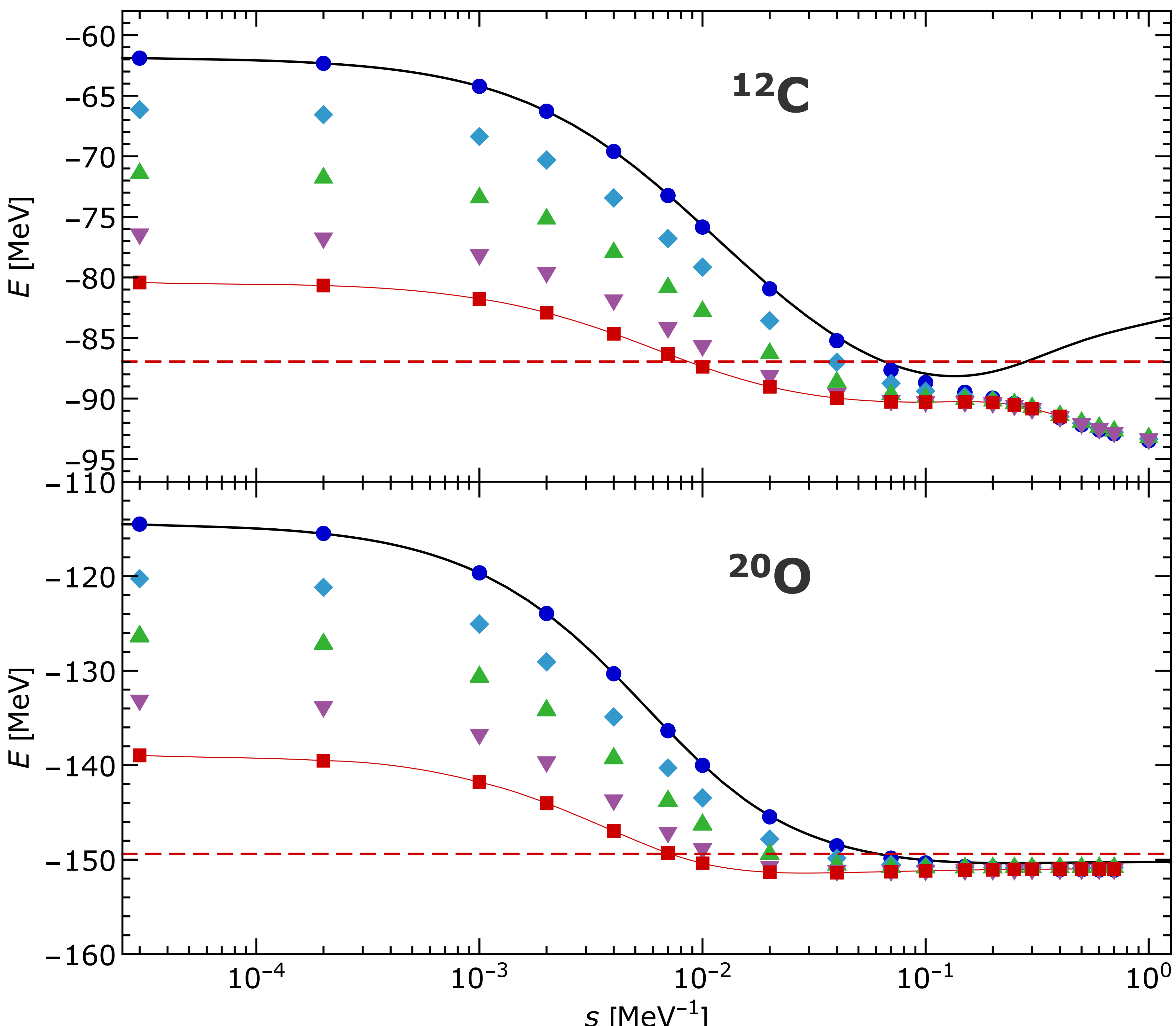


Hamilton matrix in N_{max}=2 space

Flow: Ground-State Energy

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



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

chiral NN+3N
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$\hbar\Omega$=20 MeV
e_{max}=12

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

Flow: Ground-State Energy

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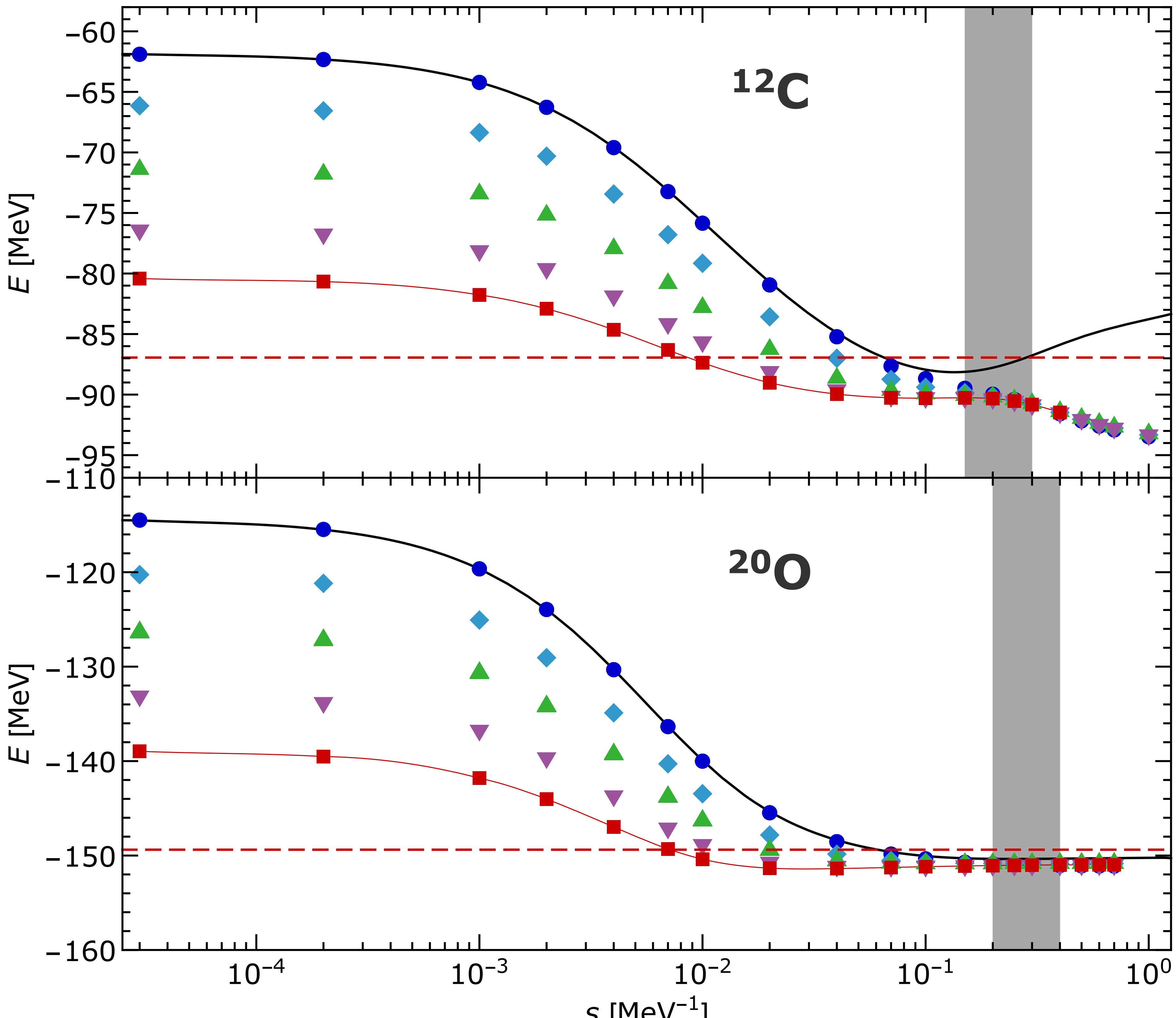

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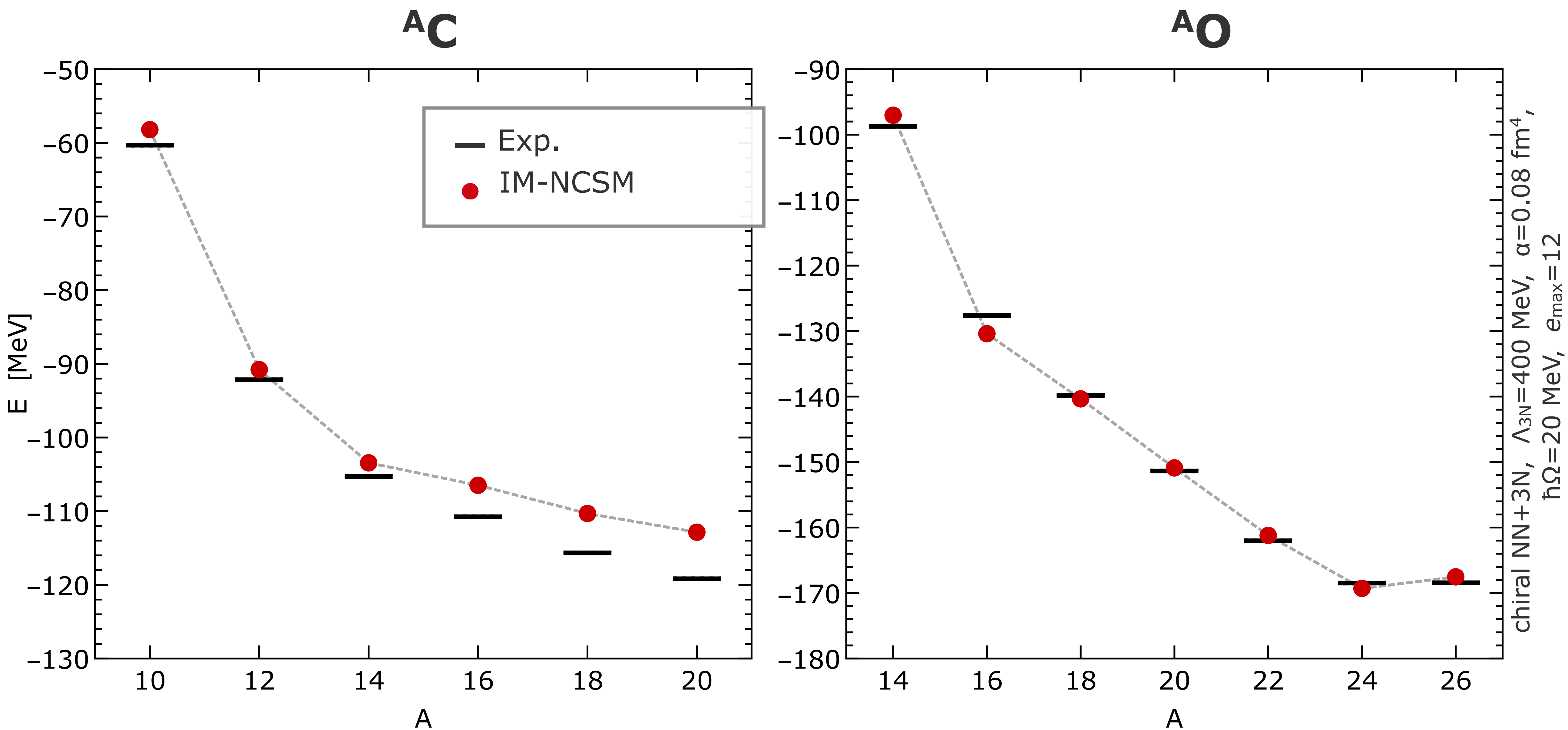
HF basis
N_{max}=0 reference state
N_{max}=0,2,4,6,8

IM-NCSM: Ground-State Energies

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



IM-NCSM: Ground-State Energies

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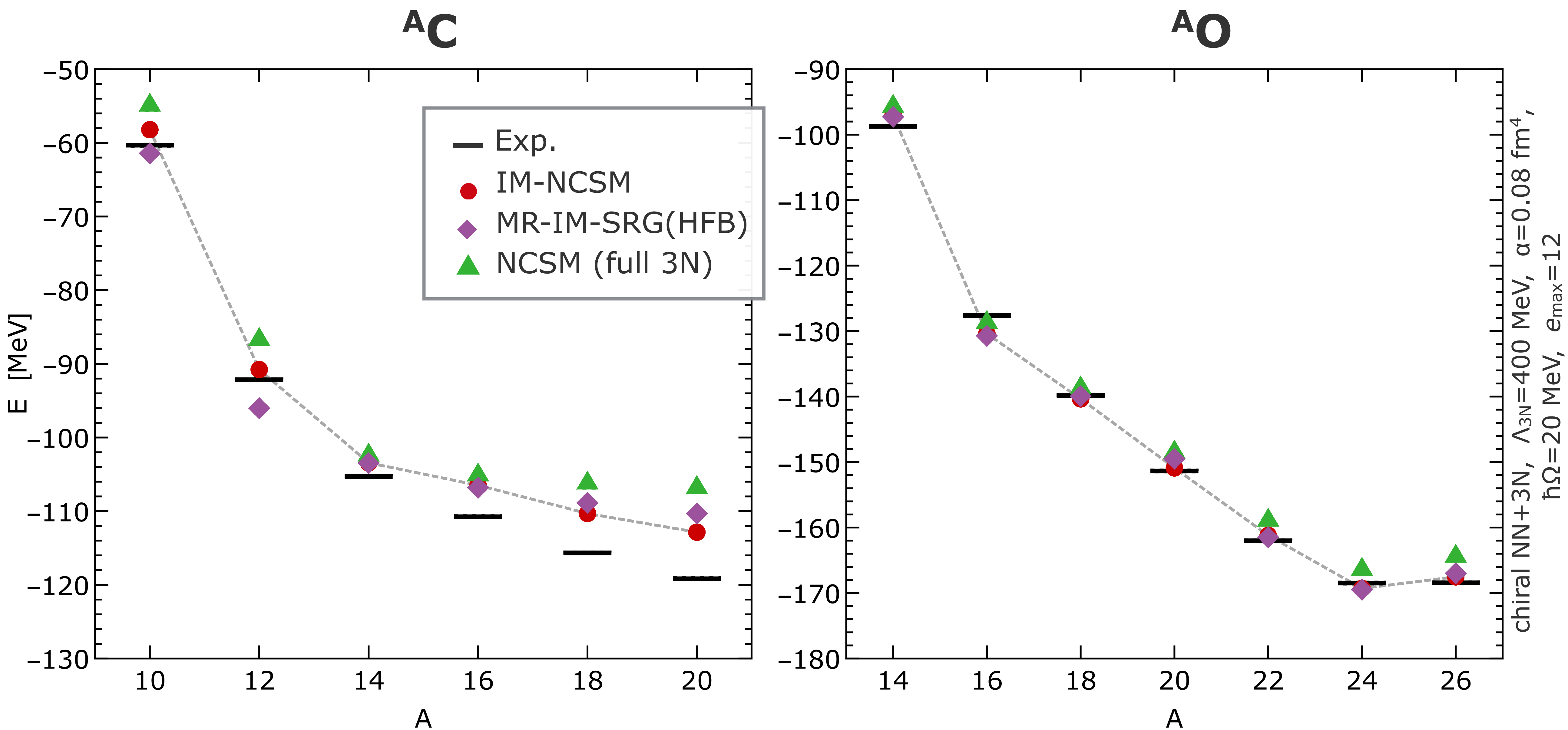
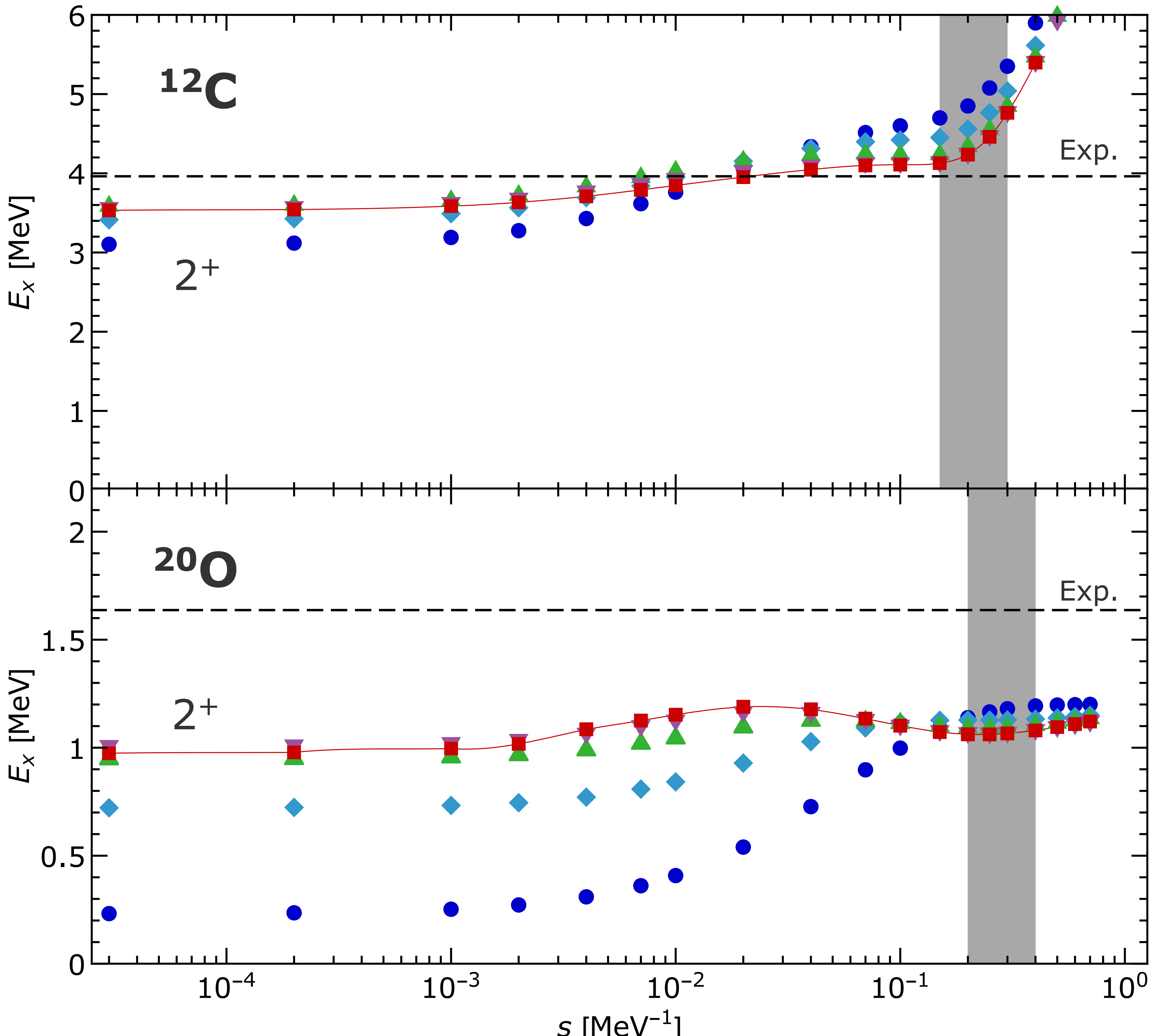


- good agreement with NCSM within uncertainties expected from omission of normal-ordered many-body terms
- ^{12}C shows surprisingly large spread among methods

Flow: 2^+ Excitation Energy

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



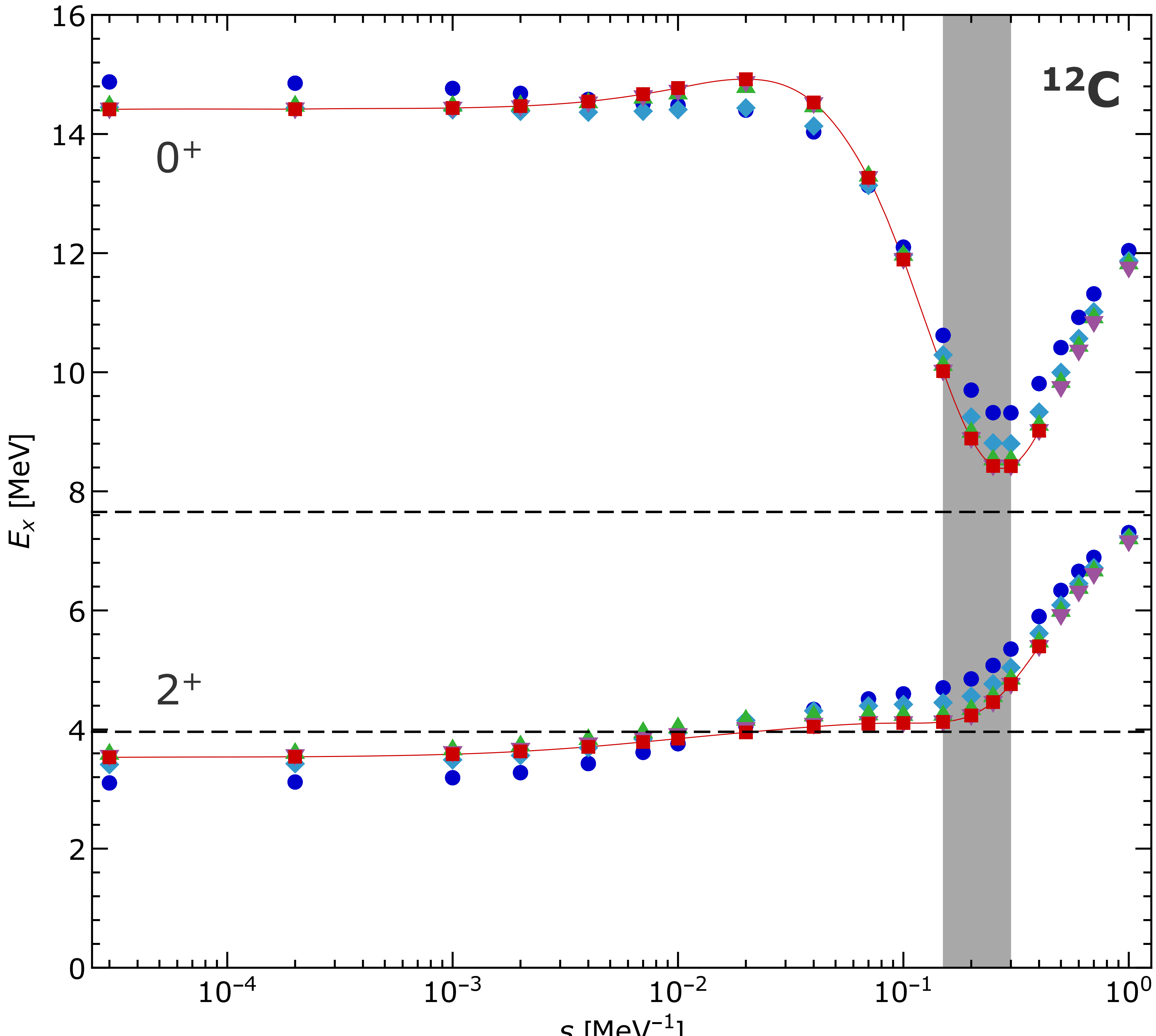
- excitation energies are less affected by flow evolution
- convergence from above in decoupled regime

chiral NN+3N
Λ_{3N}=400 MeV
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

Flow: 0+ Excitation Energy

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



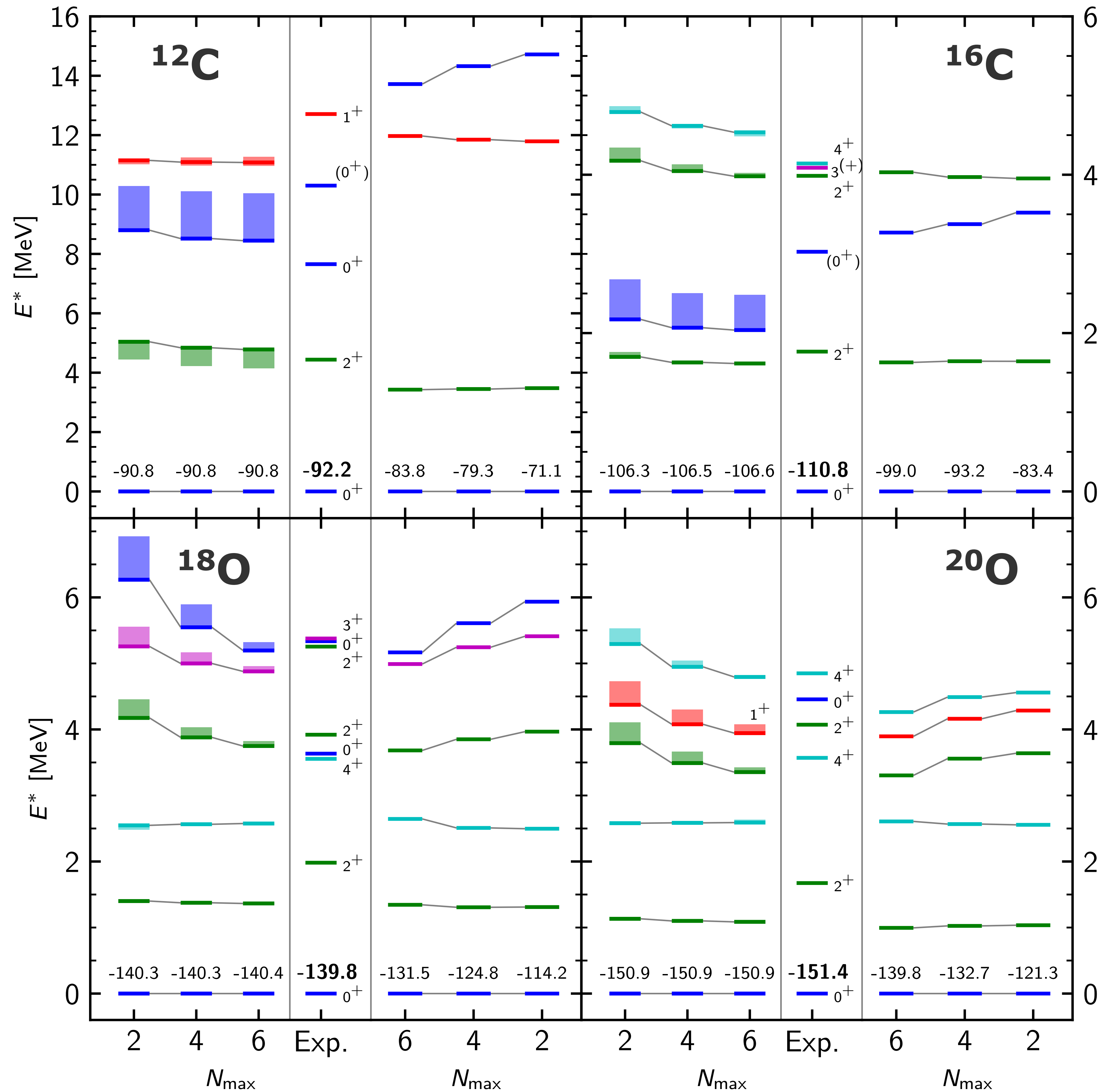
- excited 0^+ state behaves differently
- excitation energy drops by ~5 MeV in decoupling regime
- no stable result before induced many-body terms blow up

chiral NN+3N
Λ_{3N}=400 MeV
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

IM-NCSM: Excitation Spectra

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



- 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
Λ_{3N}=400 MeV
α=0.08 fm^4
$\hbar\Omega$=16 MeV
e_{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

not variational

PRO

CON

size extensive

very mild scaling with A

NO3B needs some work

hermitian Hamiltonian

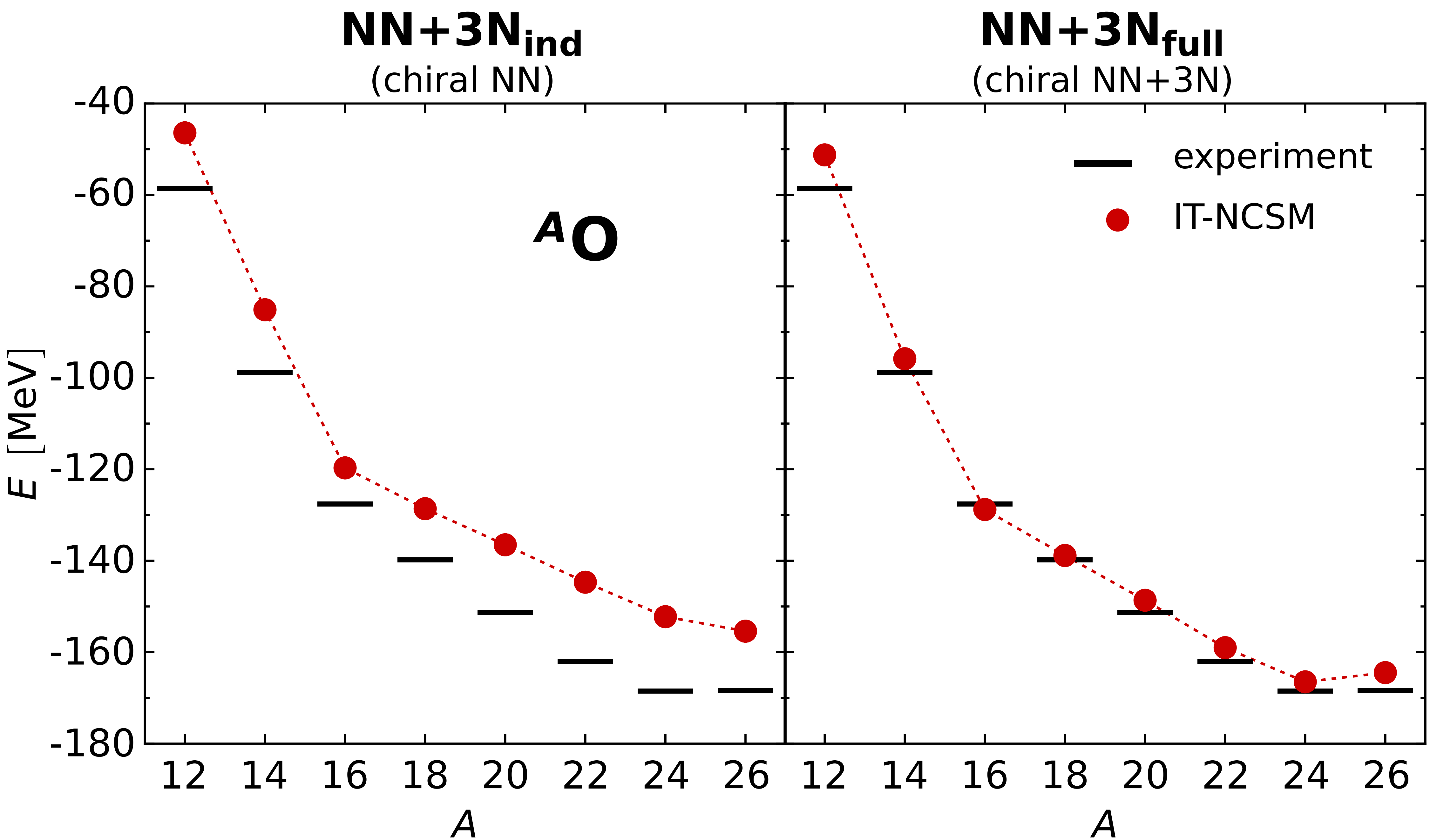
easy access to other observables

bridge to shell model

Applications for Medium-Mass Nuclei

Ground States of Oxygen Isotopes

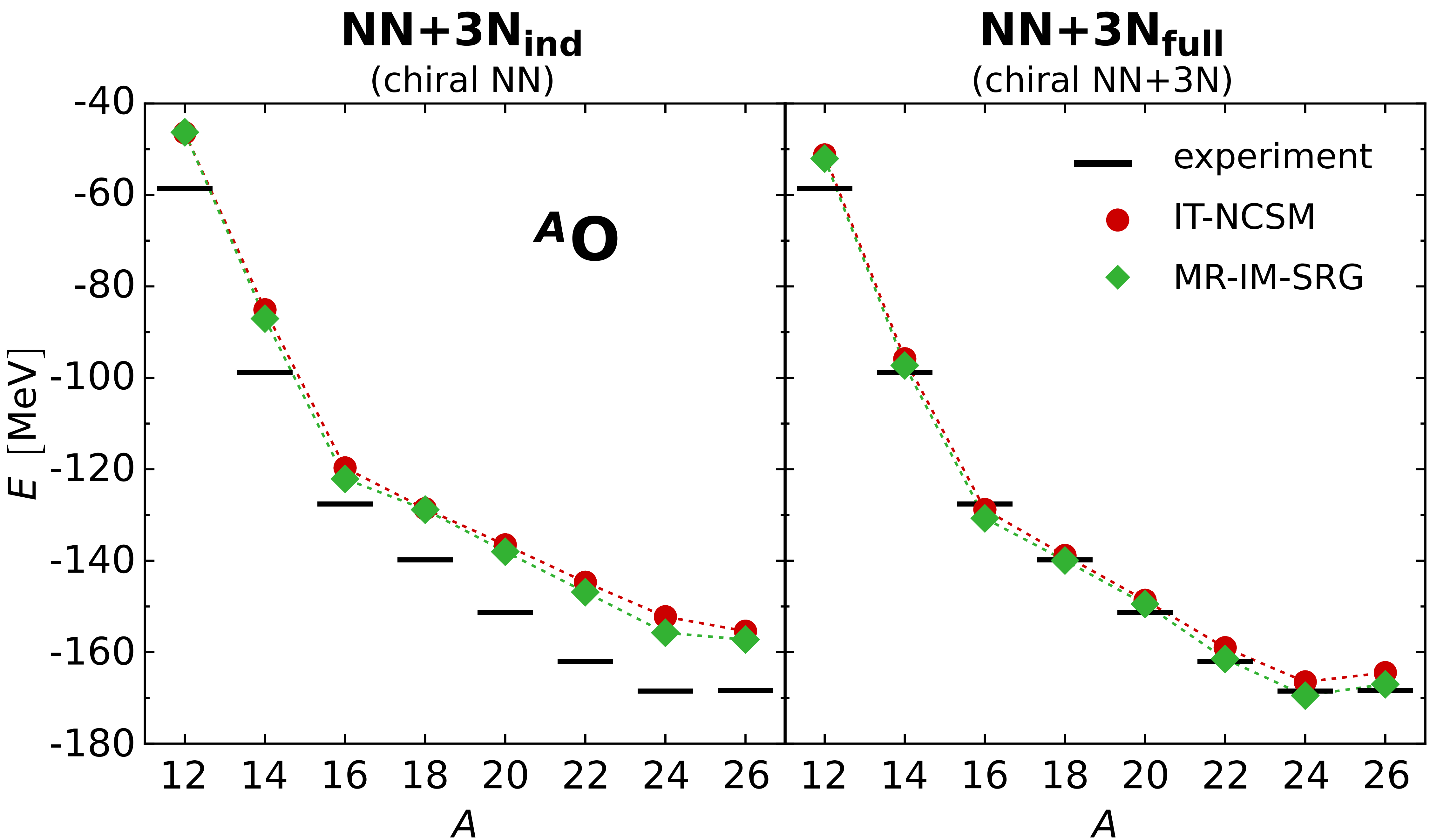
Hergert et al., PRL 110, 242501 (2013)



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

Ground States of Oxygen Isotopes

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



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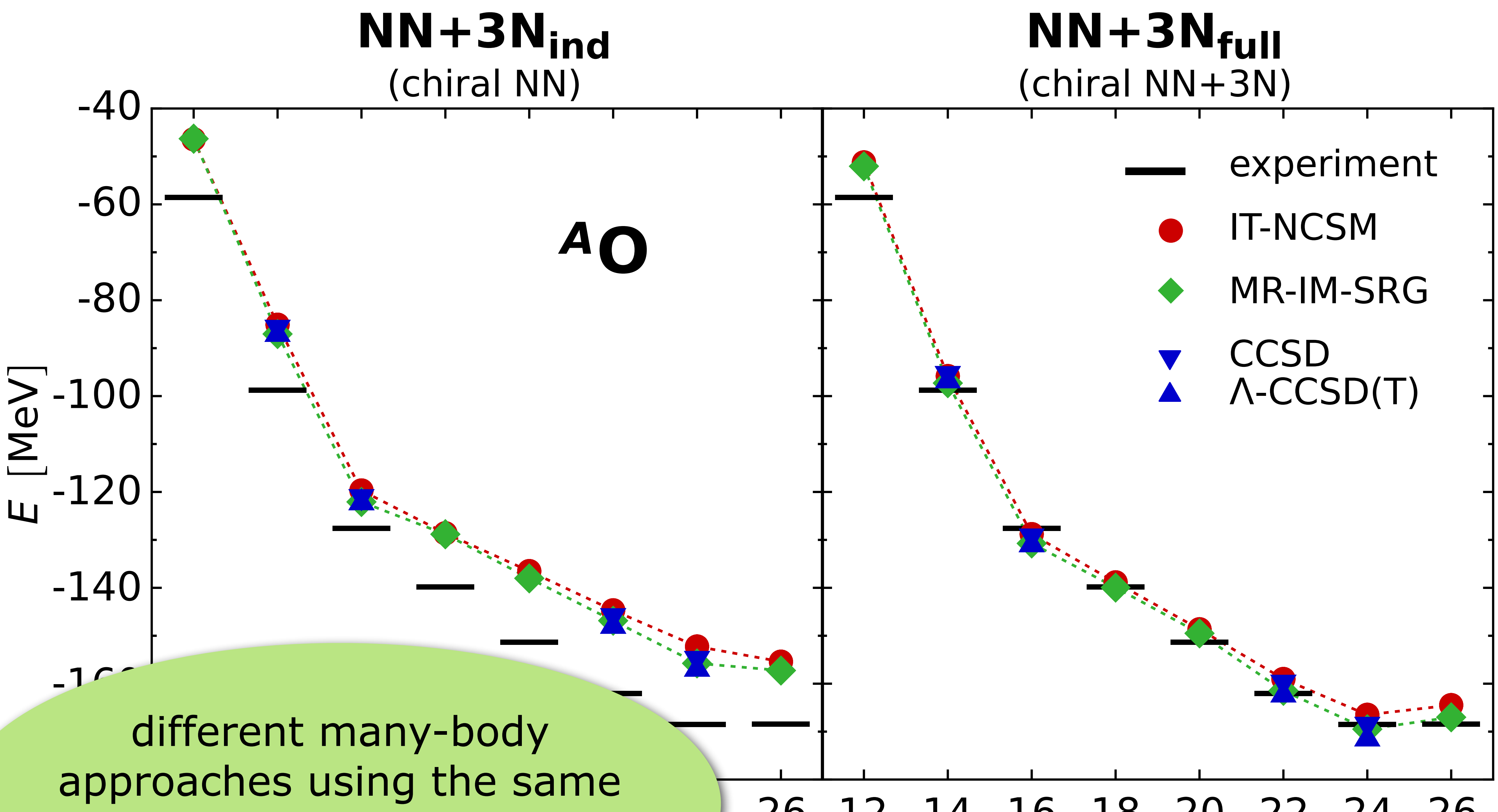
Ground States of Oxygen Isotopes

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

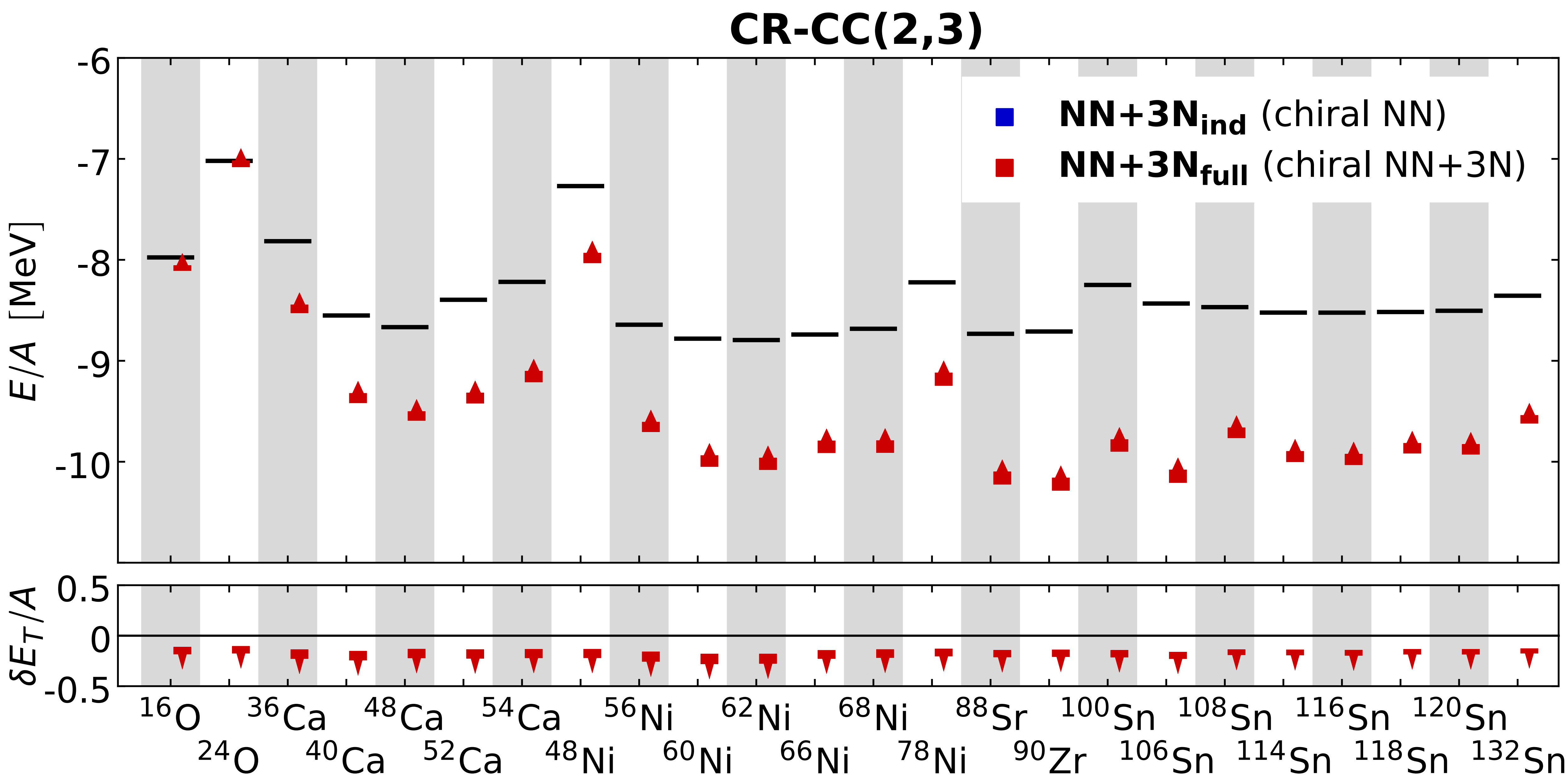


different many-body approaches using the same chiral NN+3N interaction give consistent results

minor differences are understood in terms of uncertainties due to truncations

Towards Heavy Nuclei - Ab Initio

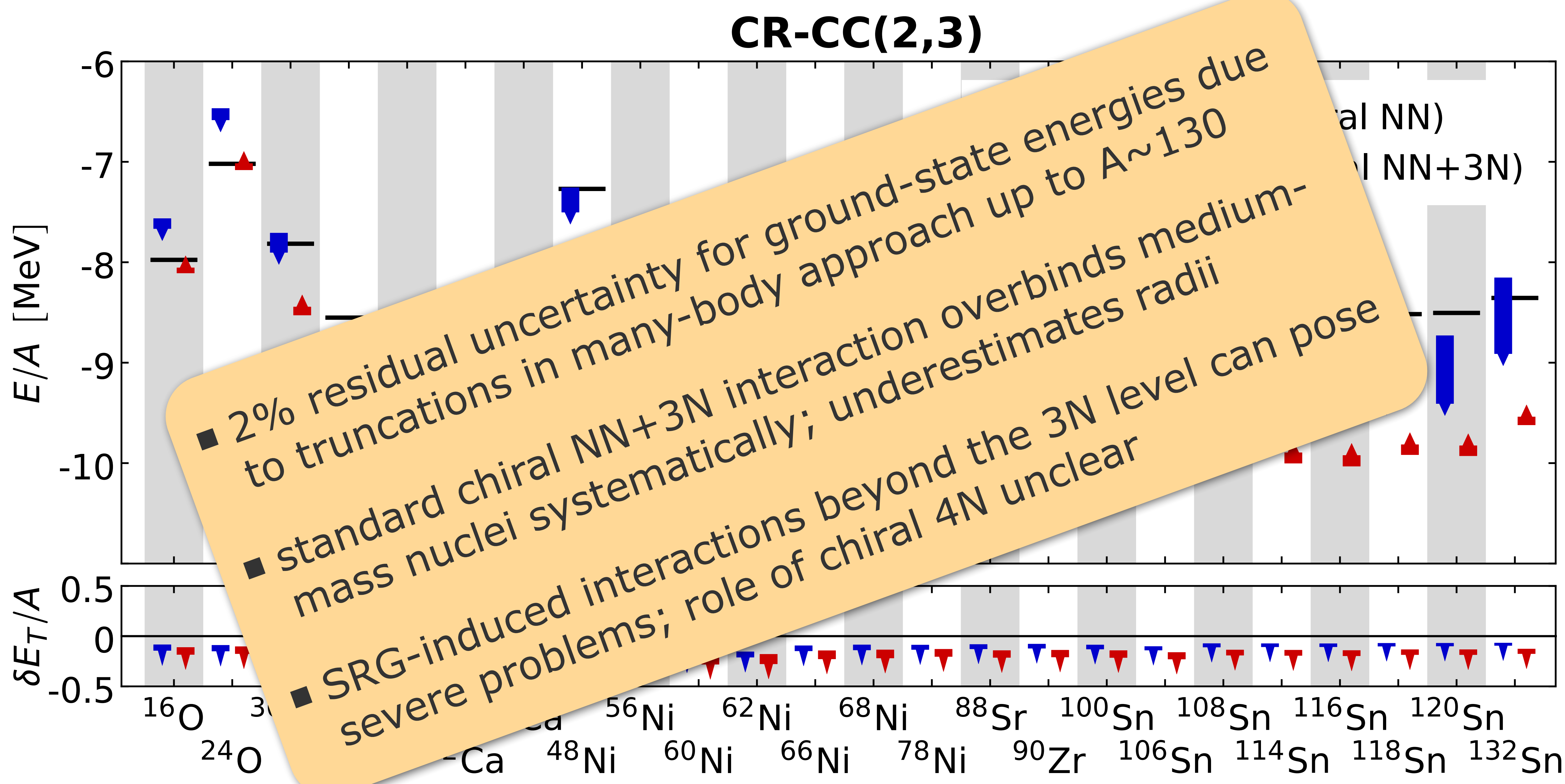
Binder et al., PLB 736, 119 (2014)



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

Towards Heavy Nuclei - Ab Initio

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

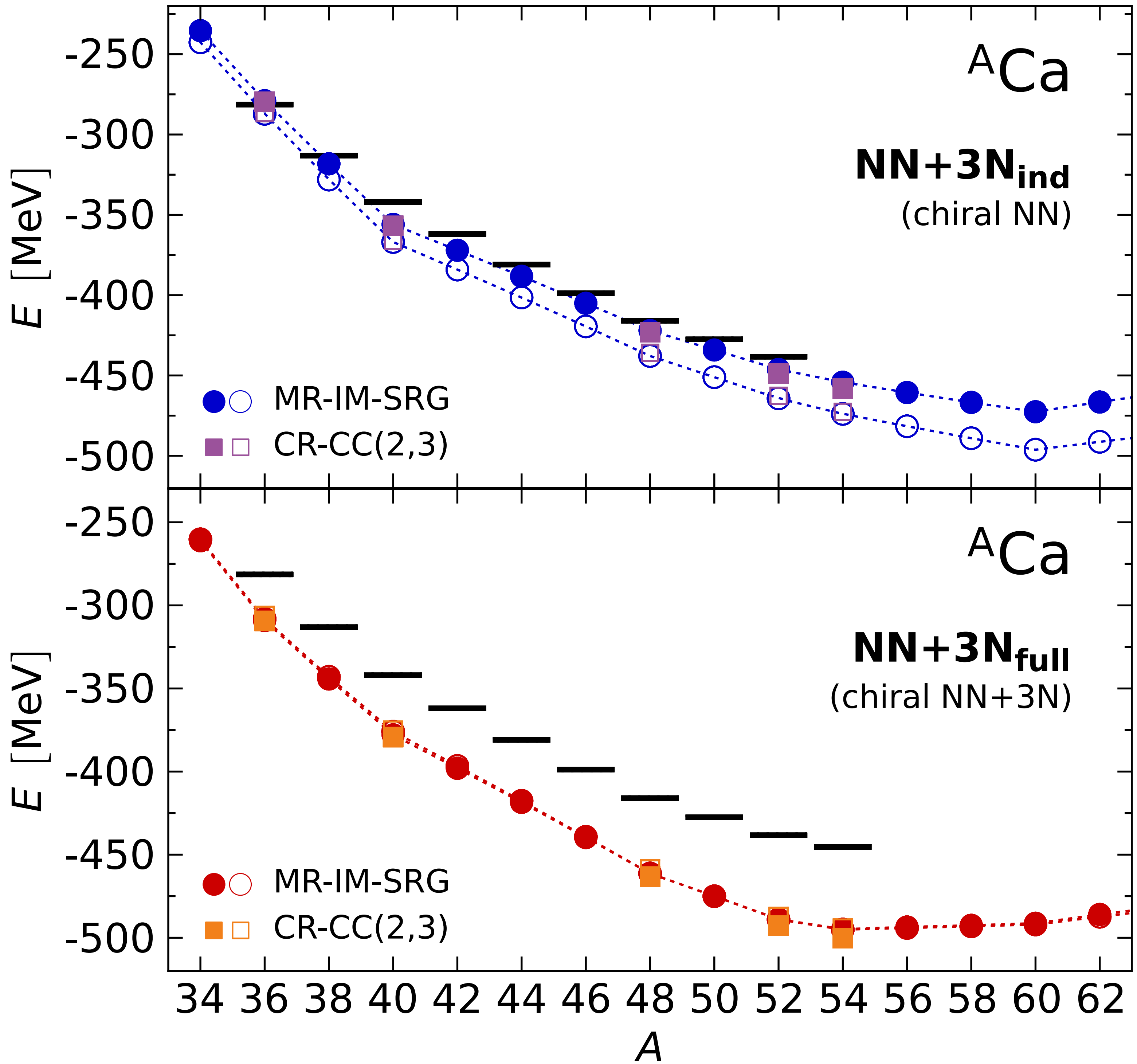


- 2% residual uncertainty for ground-state energies due to truncations in many-body approach up to A~130
- standard chiral NN+3N interaction overbinds medium-mass nuclei systematically; underestimates radii
- SRG-induced interactions beyond the 3N level can pose severe problems; role of chiral 4N unclear

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

Open-Shell Medium-Mass Nuclei

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

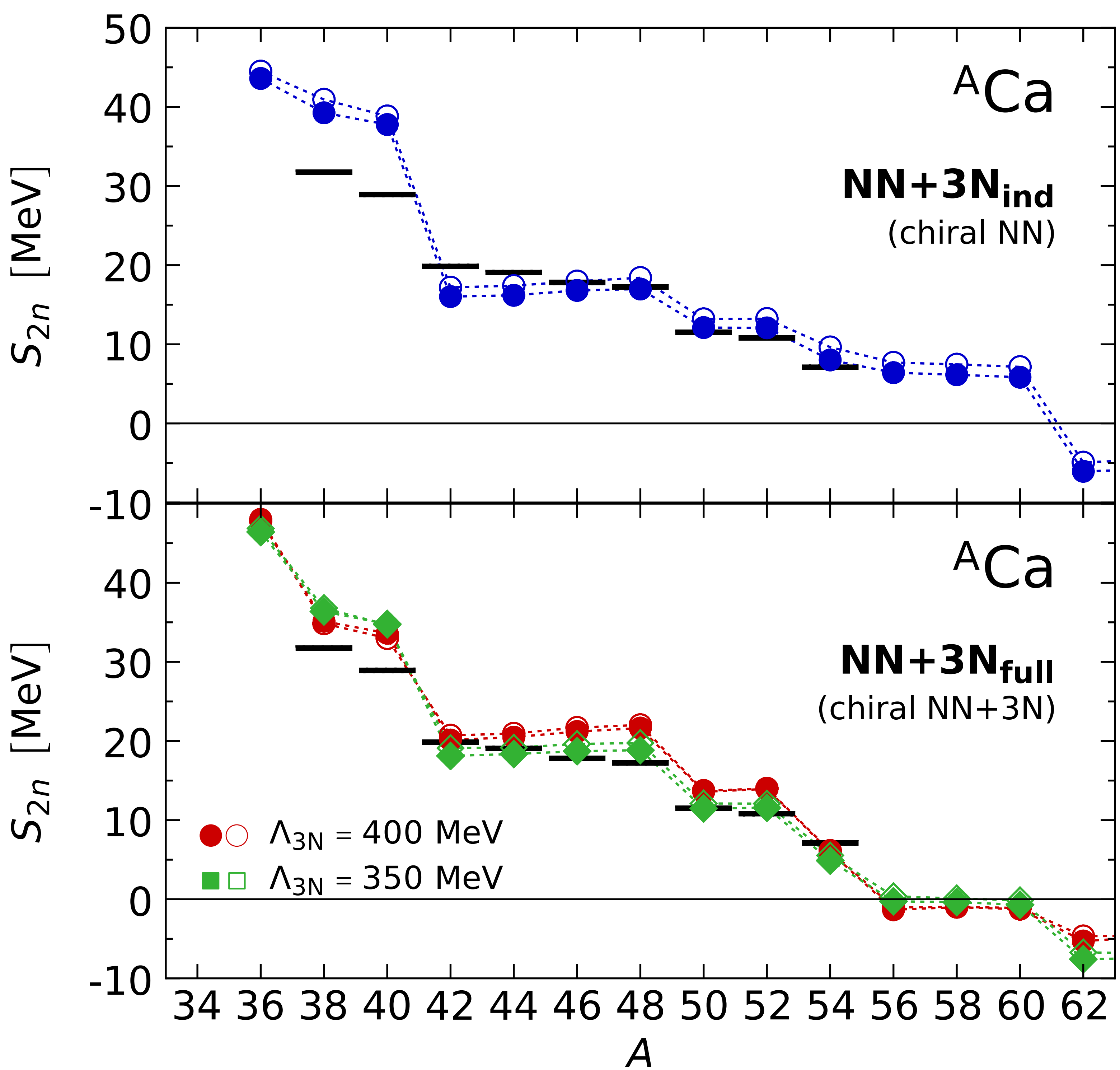


- systematic MR-IM-SRG study of even Ca and Ni isotopes
- excellent agreement with best available coupled-cluster results
- chiral 3N interaction changes behavior at and beyond ^{54}Ca

Λ_{3N} = 400 MeV
α = 0.04 fm^4 (○)
0.08 fm^4 (●)
$E_{3\,max}$ = 14, 16

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
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  - P. Navrátil, A. Calci
    TRIUMF, Vancouver
  - S. Binder
    Oak Ridge National Laboratory
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    Iowa State University
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    Universität Bochum, ...

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