Ab Initio Calculations of Nuclear Structure

Lecture 3: Medium-Mass Nuclei

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Overview

- **Lecture 1: Hamiltonian**

  Prelude ● Many-Body Quantum Mechanics ● 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 ● Basis Optimization

- **Lecture 3: Medium-Mass Nuclei**

  Normal Ordering ● Coupled-Cluster Theory ● In-Medium Similarity Renormalization Group ● Many-Body Perturbation Theory

- **Project: Do-It-Yourself NCSM**

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

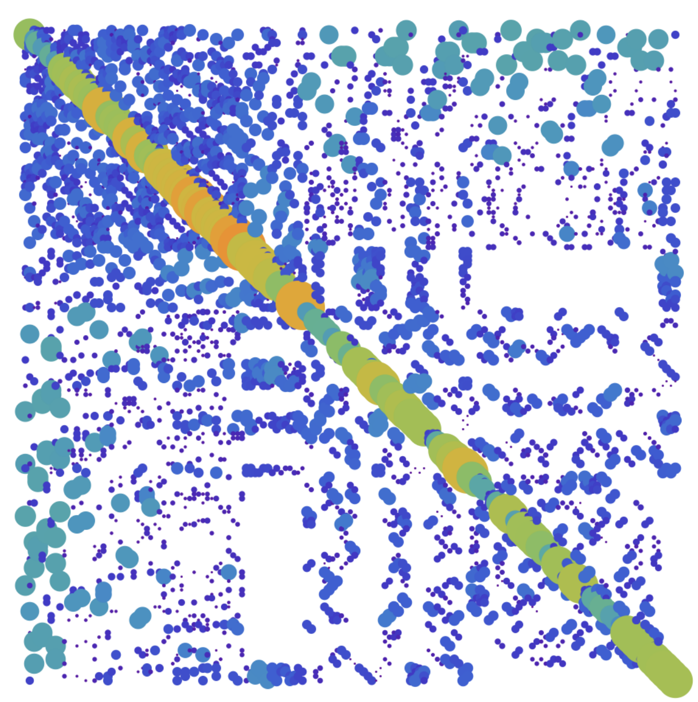
- **Lecture 4: Precision, Uncertainties, and Applications**

  Chiral Interactions for Precision Calculations ● Uncertainty Quantification ● Applications to Nuclei and Hypernuclei

No-Core Shell Model

no-core shell model is
straight-forward and powerful ab initio approach for
light nuclei (up to A≈25)

- solve eigenvalue problem of Hamiltonian represented in model space of HO Slater determinants truncated w.r.t. HO excitation energy $N_{\max}\hbar\Omega$



$$\begin{pmatrix} \cdots \end{pmatrix} \begin{pmatrix} \vdots \\ C_{i'}^{(n)} \\ \vdots \end{pmatrix} = E_n \begin{pmatrix} \vdots \\ C_{i}^{(n)} \\ \vdots \end{pmatrix}$$

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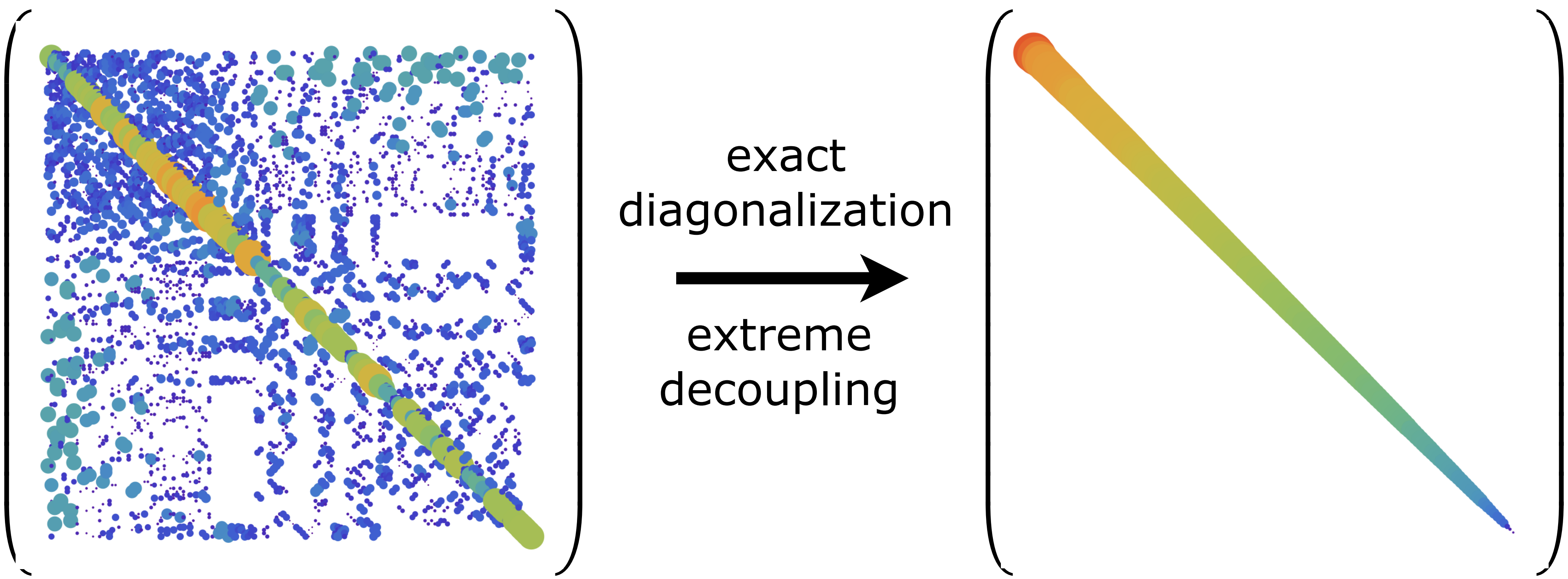
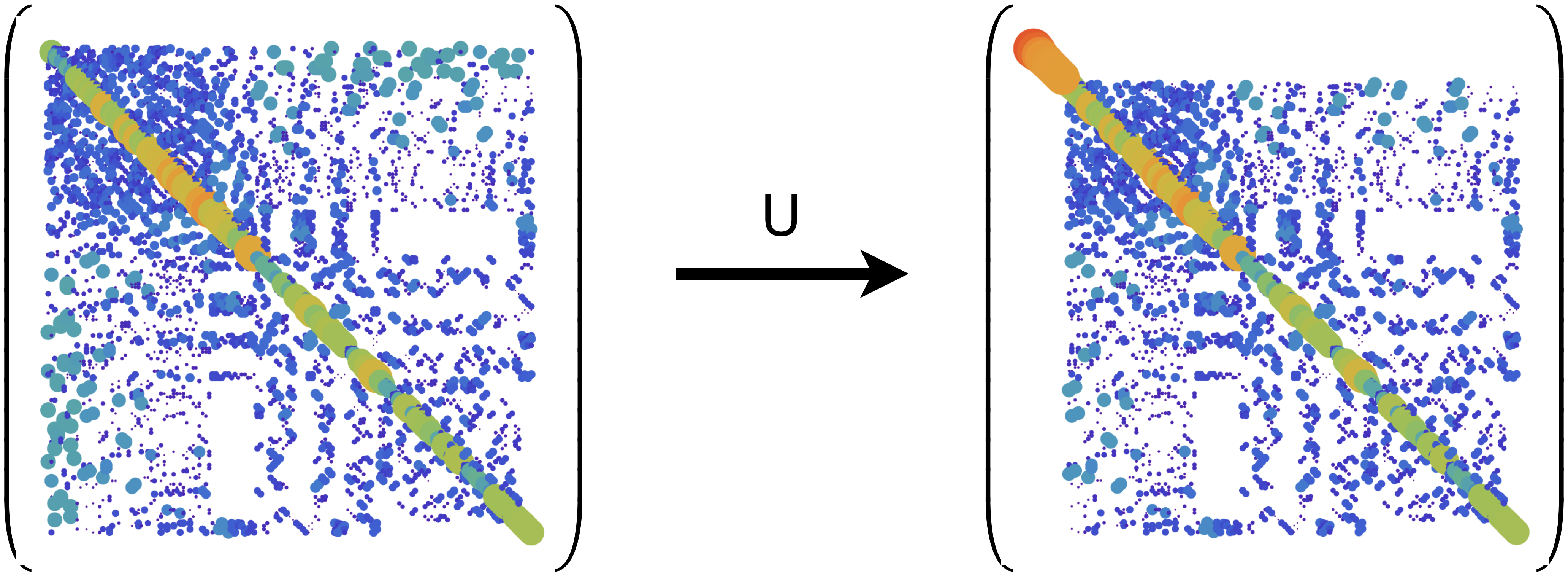


Beyond Light Nuclei

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



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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**

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

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:
$a,b,c,\dots$: 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

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

- **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**

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

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	$a^\dagger_p, a^\dagger_q, \ldots$	$a_a, a_b, \ldots$
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

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

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

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

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

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

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

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

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

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**

$$\langle\Phi|\mathcal{H}|\Phi\rangle = E_{\text{CCSD}}$$
$$\langle\Phi_a^p|\mathcal{H}|\Phi\rangle = 0$$
$$\langle\Phi_{ab}^{pq}|\mathcal{H}|\Phi\rangle = 0$$

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

$$\Delta E^{(\mathrm{CCSD})} = \overset{(EA)}{+} \frac{1}{4}\sum_{abij} v_{ab}^{ij}\, t_{ij}^{ab} \overset{(EB)}{+} \sum_{ai} f_a^i\, t_i^a \overset{(EC)}{+} \frac{1}{2}\sum_{abij} v_{ab}^{ij}\, t_i^a\, t_j^b$$

$$\overset{(SA)}{+} f_i^a \overset{(SBa)}{+} \sum_{ck} f_c^k\, t_{ik}^{ac} \overset{(SBb)}{+} \tfrac{1}{2}\sum_{cdk} v_{cd}^{ak}\, t_{ik}^{cd} \overset{(SBc)}{-} \tfrac{1}{2}\sum_{ckl} v_{ic}^{kl}\, t_{kl}^{ac}$$
$$\overset{(SCa)}{+} \sum_{c} f_c^a\, t_i^c \overset{(SCb)}{-} \sum_{i} f_i^k\, t_k^a \overset{(SCc)}{+} \sum_{ck} v_{ic}^{ak}\, t_k^c \overset{(SDa)}{-} \tfrac{1}{2}\sum_{cdkl} v_{cd}^{kl}\, t_{kl}^{ad}\, t_i^c$$
$$\overset{(SDb)}{-} \tfrac{1}{2}\sum_{cdkl} v_{cd}^{kl}\, t_{il}^{cd}\, t_k^a \overset{(SDc)}{+} \sum_{cdkl} v_{cd}^{kl}\, t_{li}^{da}\, t_k^c \overset{(SEa)}{-} \sum_{ck} f_c^k\, t_i^c\, t_k^a$$
$$\overset{(SEb)}{+} \sum_{cdk} v_{cd}^{ak}\, t_i^c\, t_k^d \overset{(SEc)}{-} \sum_{ckl} v_{ic}^{kl}\, t_k^a\, t_l^c \overset{(SF)}{-} \sum_{cdkl} v_{cd}^{kl}\, t_k^a\, t_i^c\, t_l^d$$
$$= 0\,,\ \forall\, a,i$$

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

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

Similarity Renormalization Group

Glazek, Wilson, Wegner, Perry, Bogner, Furnstahl, Hergert, Roth,...

continuous unitary transformation to pre-diagonalize the Hamiltonian with respect to a given basis

- **consistent unitary transformation** of Hamiltonian and observables

$$H_\alpha = U_\alpha^\dagger H\, U_\alpha \qquad\qquad O_\alpha = U_\alpha^\dagger O\, U_\alpha$$

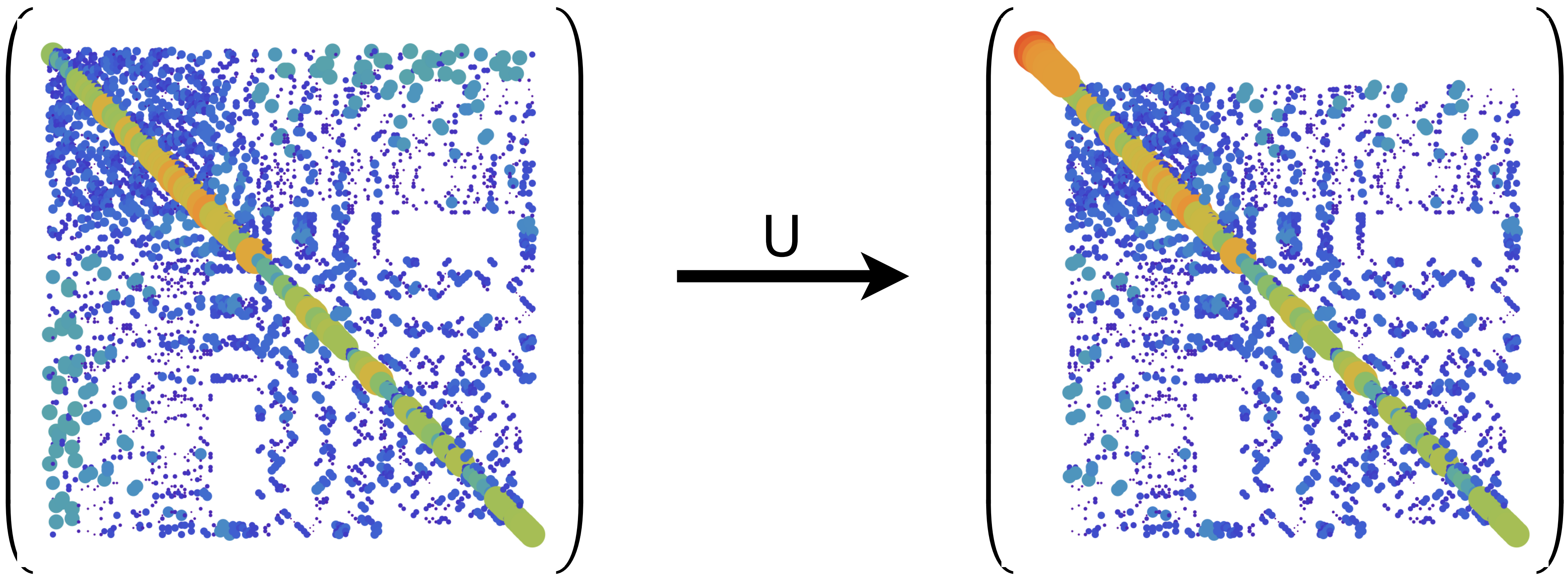
- **flow equations** for H_α and U_α with continuous **flow parameter α**

$$\frac{d}{d\alpha} H_\alpha = [\eta_\alpha, H_\alpha] \qquad \frac{d}{d\alpha} O_\alpha = [\eta_\alpha, O_\alpha] \qquad \frac{d}{d\alpha} U_\alpha = -U_\alpha \eta_\alpha$$

- the physics of the transformation is governed by the **dynamic generator η_α** and we choose an ansatz depending on the type of “pre-diaognalization” we want to achieve

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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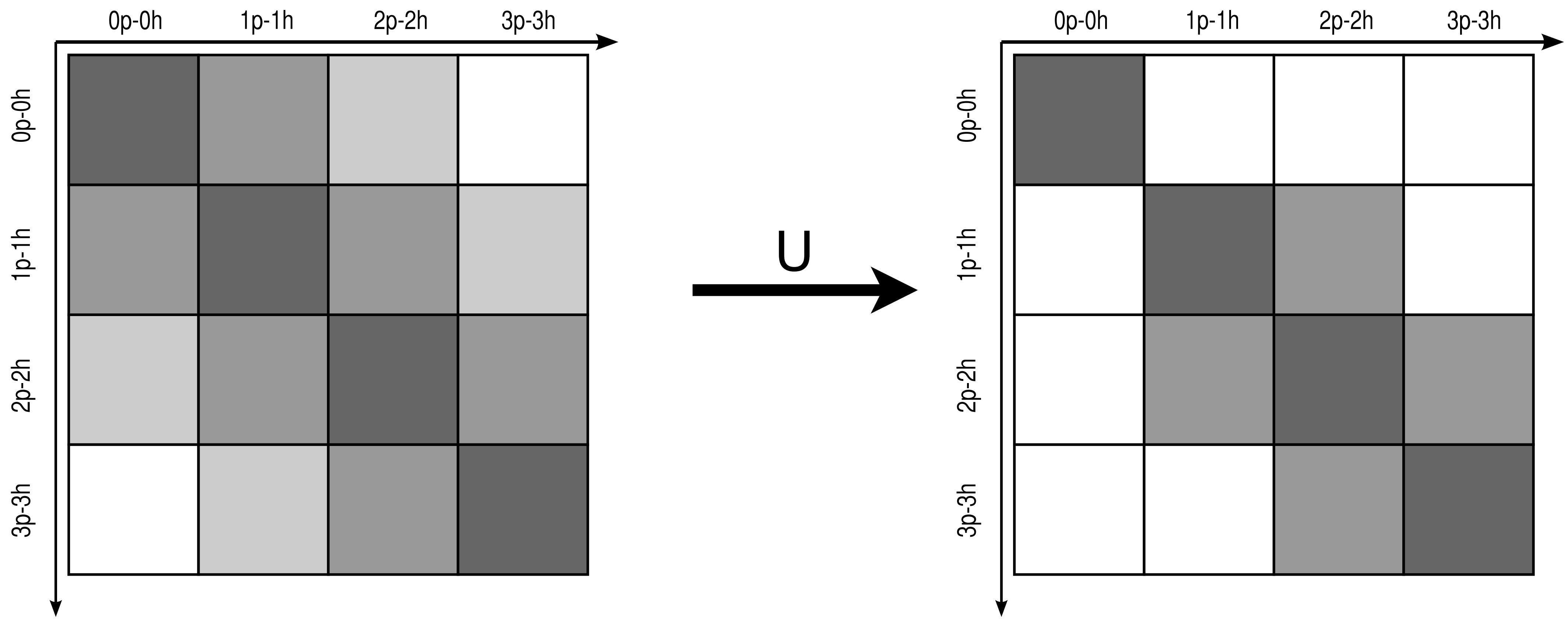

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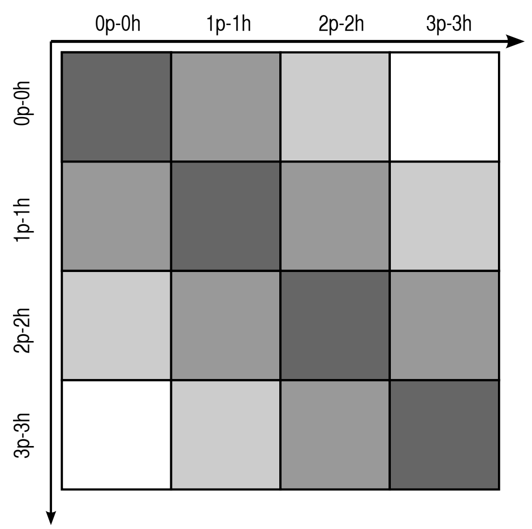
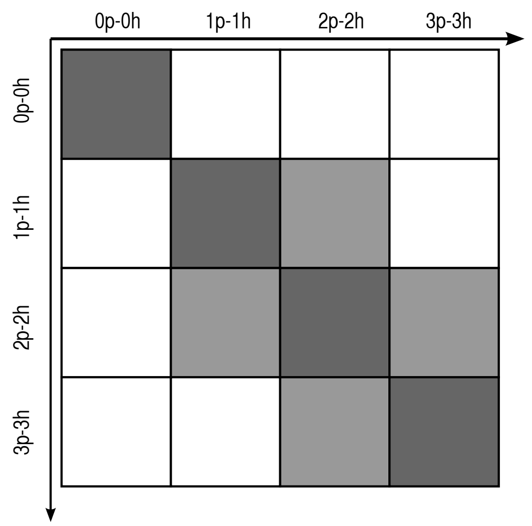
In-Medium SRG

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

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

In-Medium SRG Generators

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

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

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

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

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

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

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

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

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

$$\eta^{1}_{2} = \langle\Phi|\, [H, \{a^{\dagger}_{1} a_2\}]\, |\Phi\rangle$$

$$\eta^{12}_{34} = \langle\Phi|\, [H, \{a^{\dagger}_{1} a^{\dagger}_{2} a_4 a_3\}]\, |\Phi\rangle$$

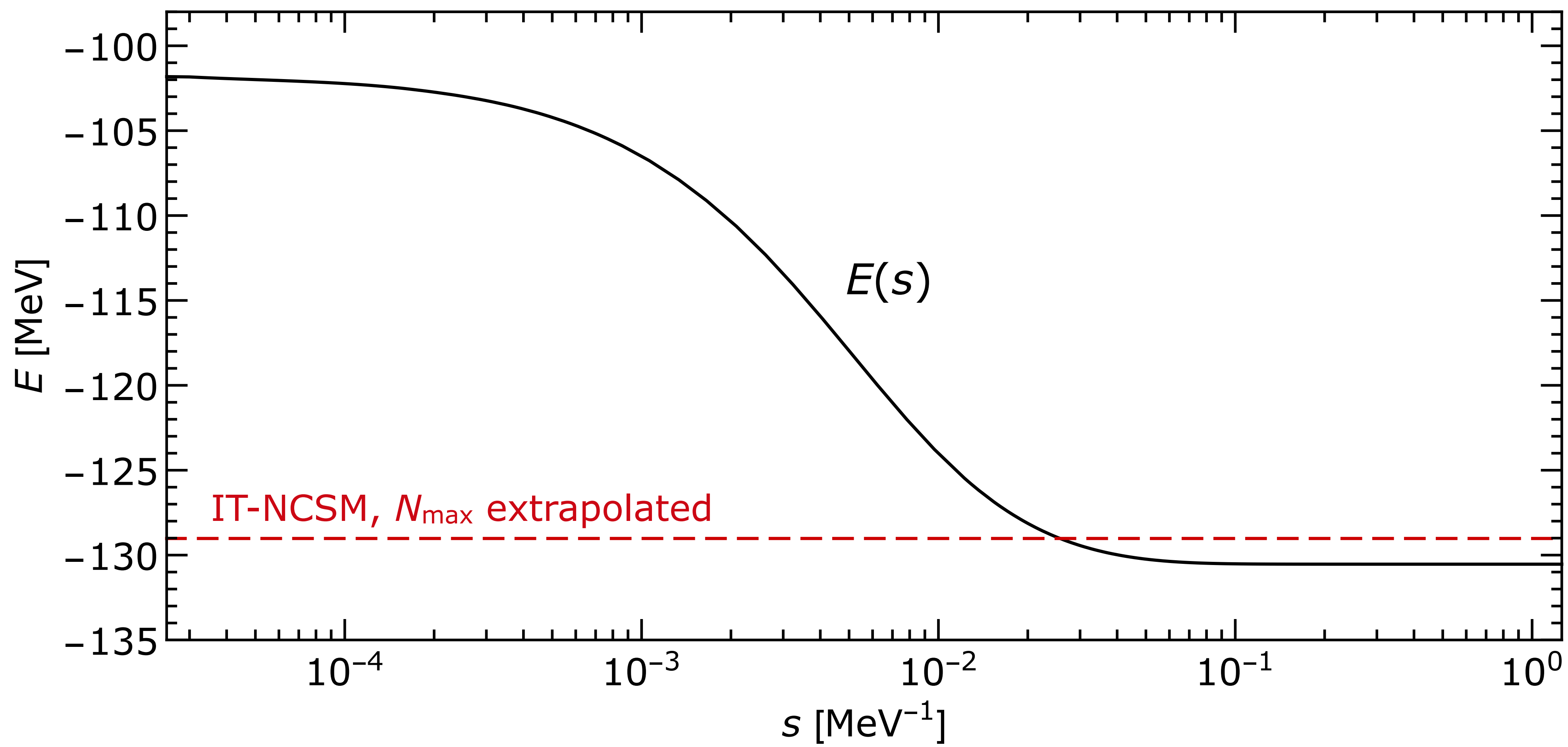
Flow-Equations for Matrix Elements

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

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

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

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

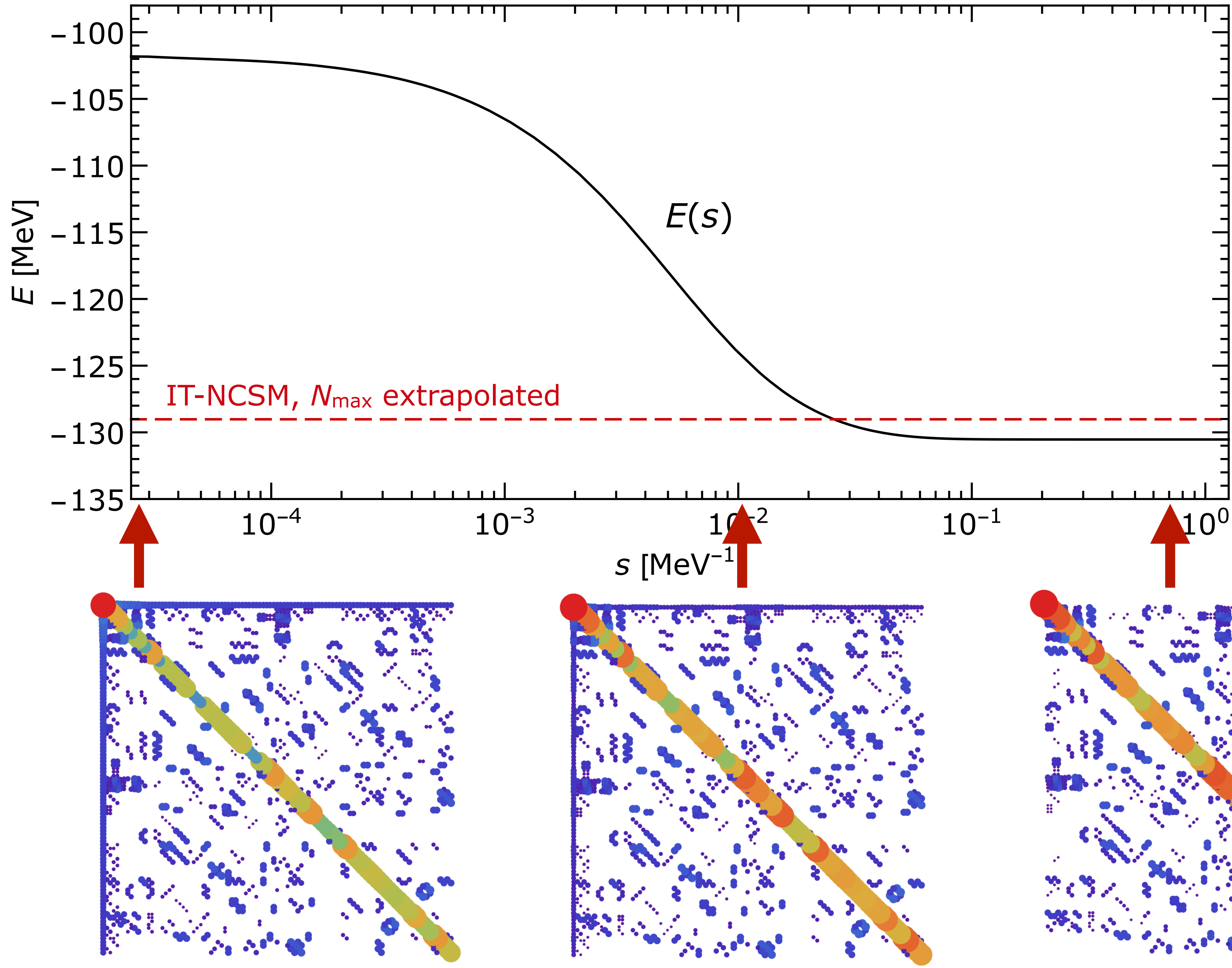
N_{max}=0 reference
HF basis

- 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



^{16}O

chiral NN+3N

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e_{max}=12

N_{max}=0 reference

HF basis

Hamilton matrix in N_{max}=2 space

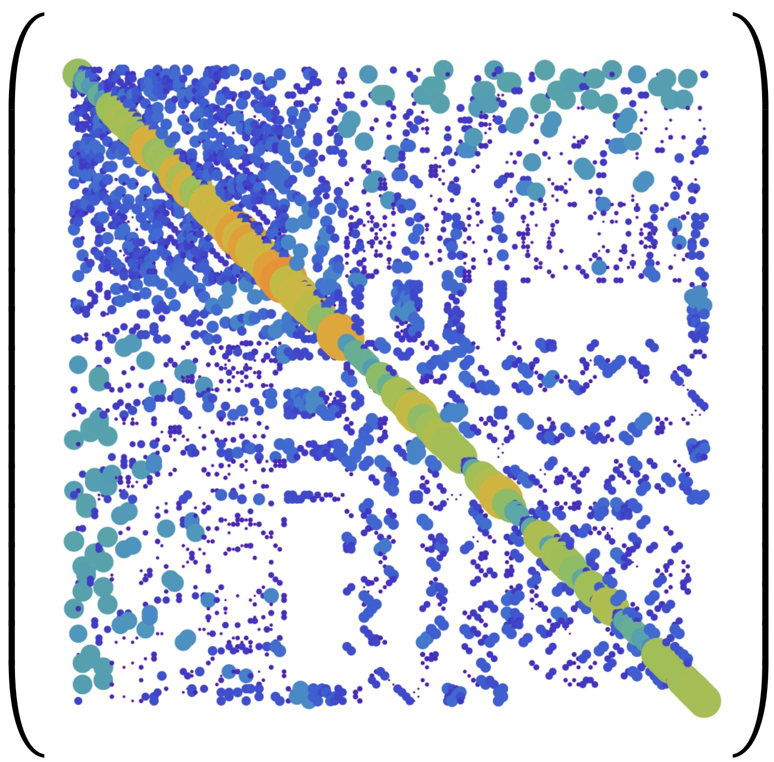
In-Medium NCSM

Multi-Reference In-Medium SRG

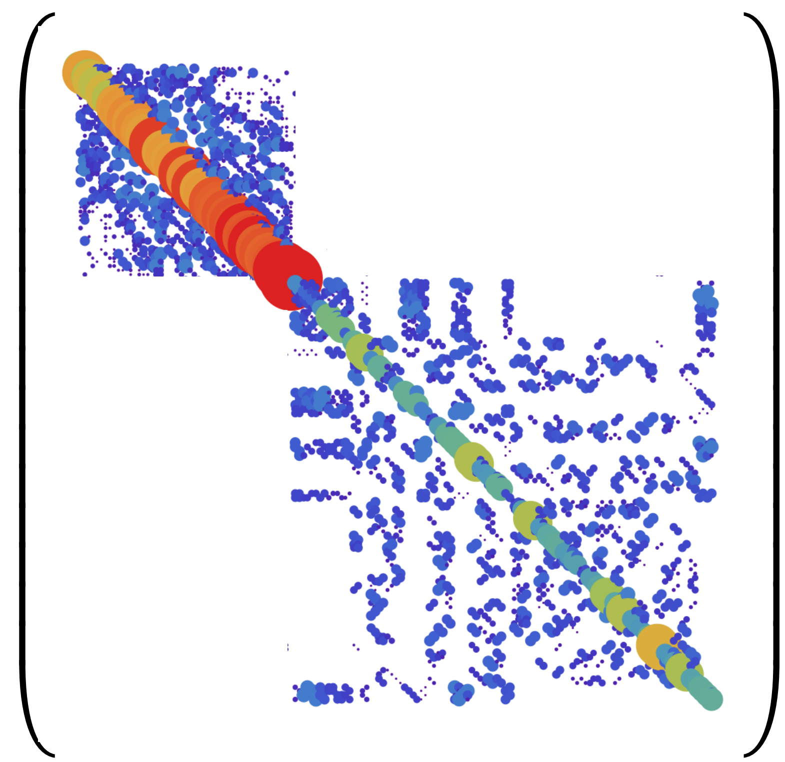
Hergert, Gebrerufael, Vobig, Mongelli, Roth,...

decouple reference state from excitations by a unitary transformation of Hamiltonian and other operators

- **idea**: use multi-reference formulation of IM-SRG to decouple reference space for rest of model space, i.e., block diagonalize *A*-body Hamiltonian



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



In-Medium NCSM

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

MR-IM-SRG
decoupling

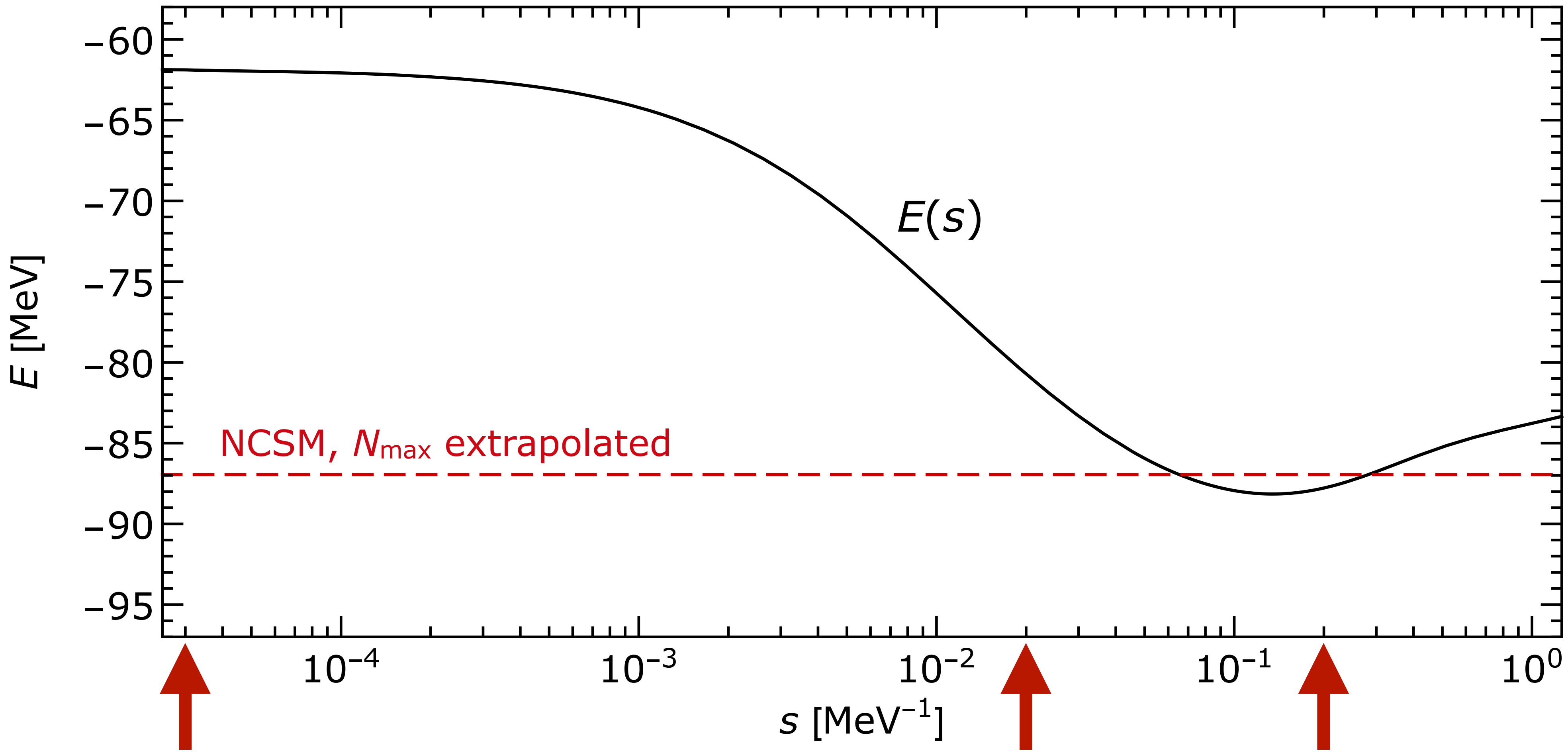
- IM-SRG evolution of multi-reference normal-ordered Hamiltonian and other operators
- decoupling of particle-hole excitations, i.e., pre-diagonalization in many-body space

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: Flow Evolution

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



^{12}C

chiral NN+3N

Λ_{3N}=400 MeV

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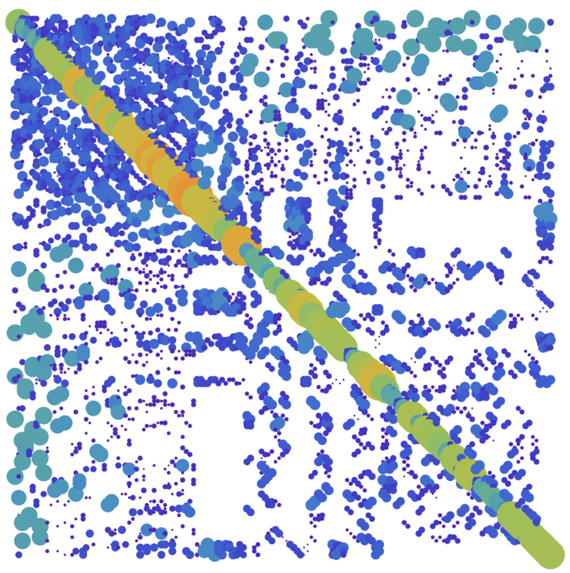
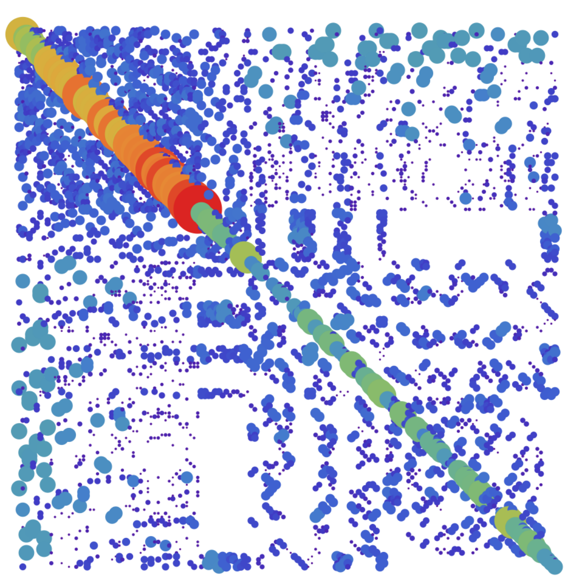
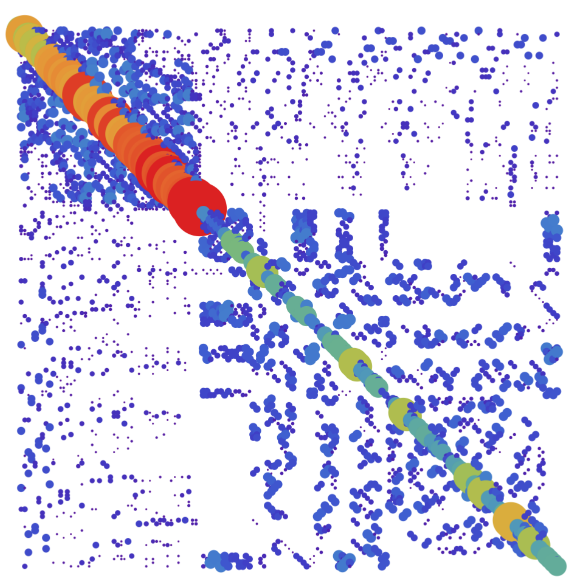
e_{max}=12

N_{max}=0 reference HF basis



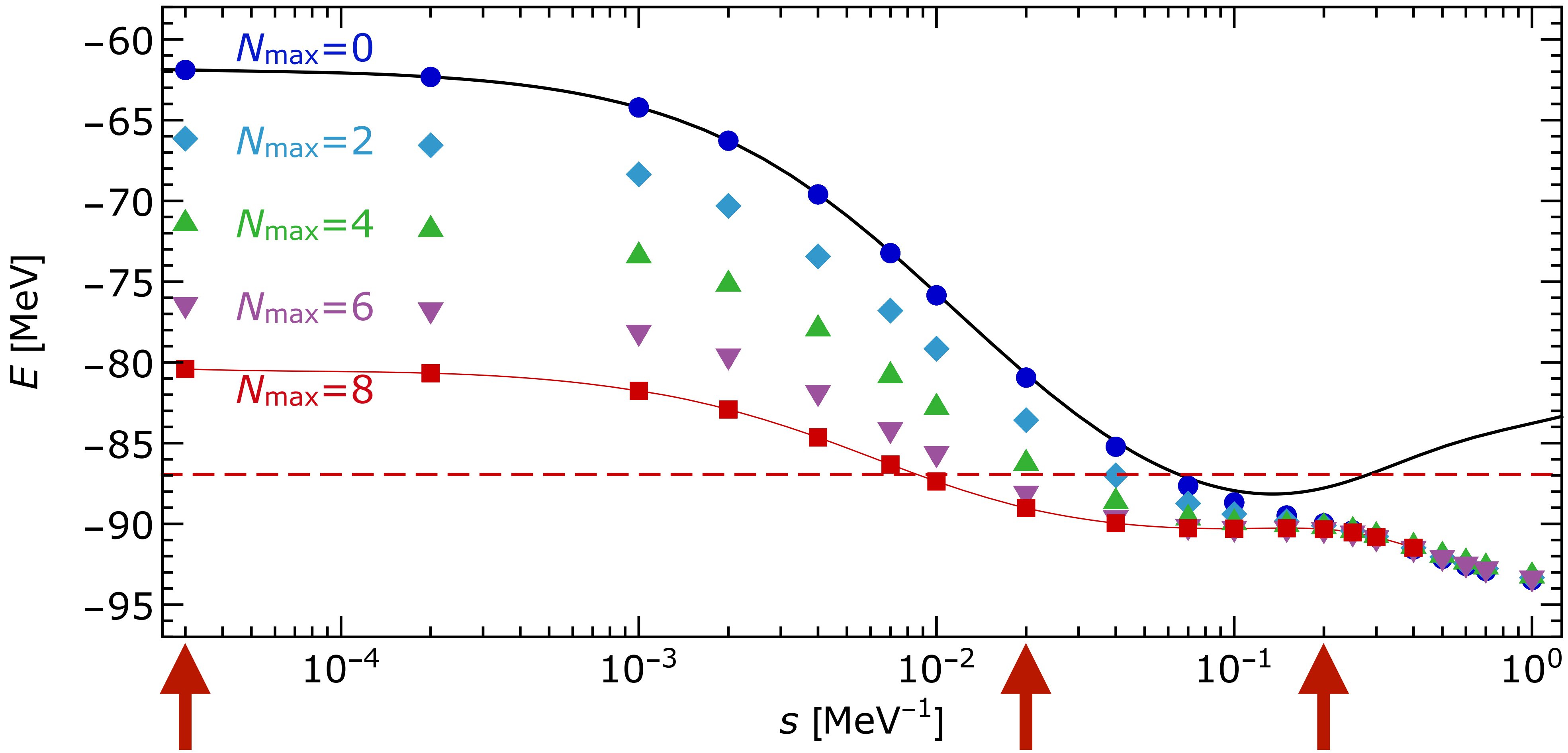




Hamilton matrix in N_{max}=2 space

In-Medium NCSM: Flow Evolution

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



^{12}C

chiral NN+3N

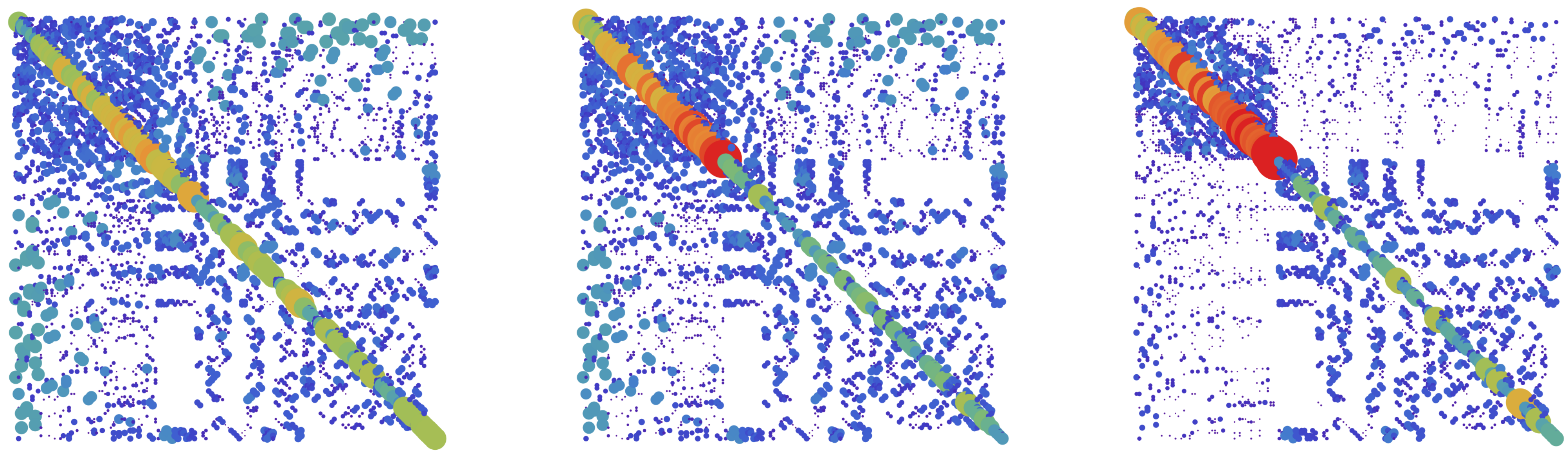
Λ_{3N}=400 MeV

α=0.08 fm⁴

ħΩ=20 MeV

e_{max}=12

N_{max}=0 reference HF basis



Hamilton matrix in N_{max}=2 space

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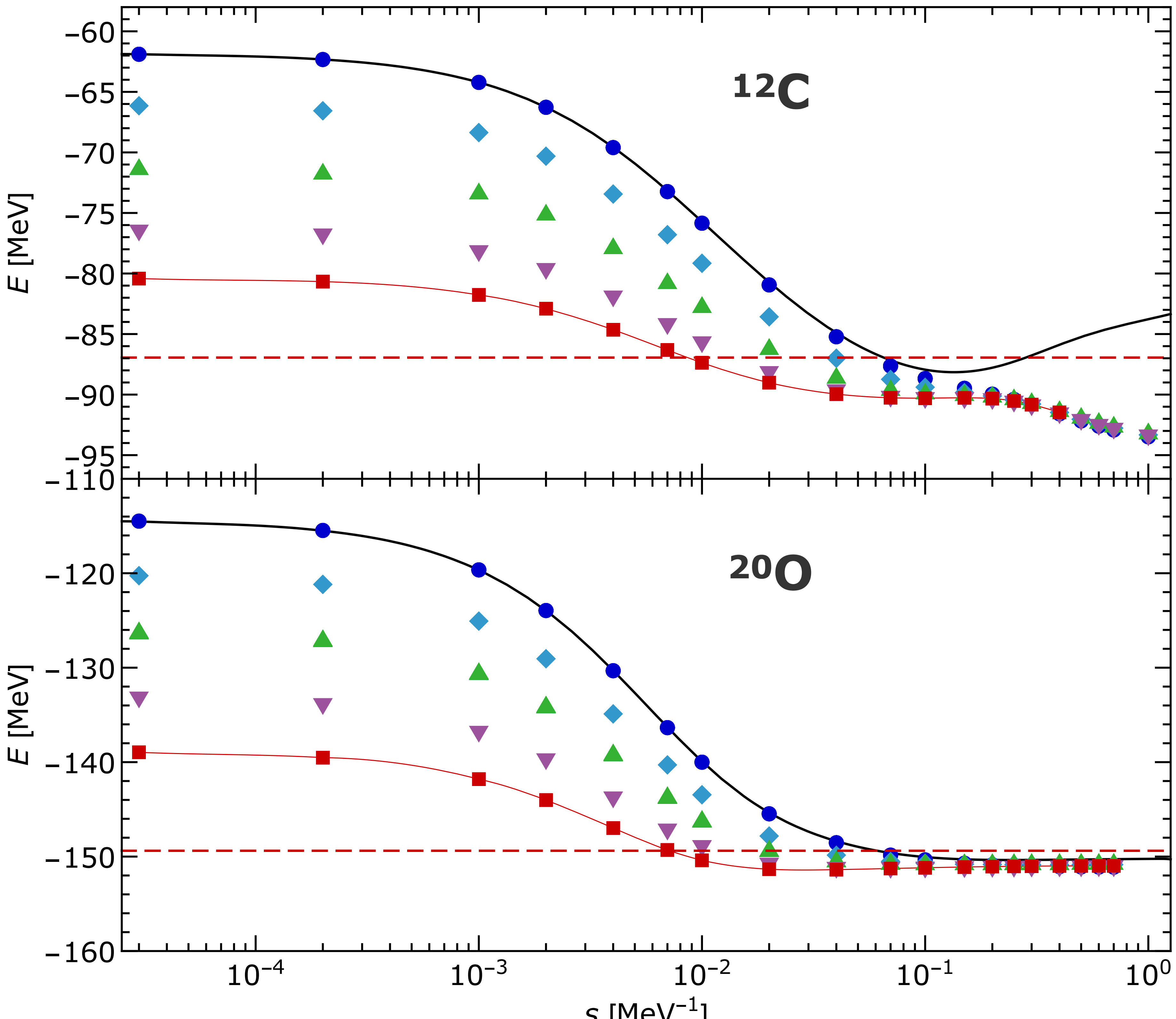


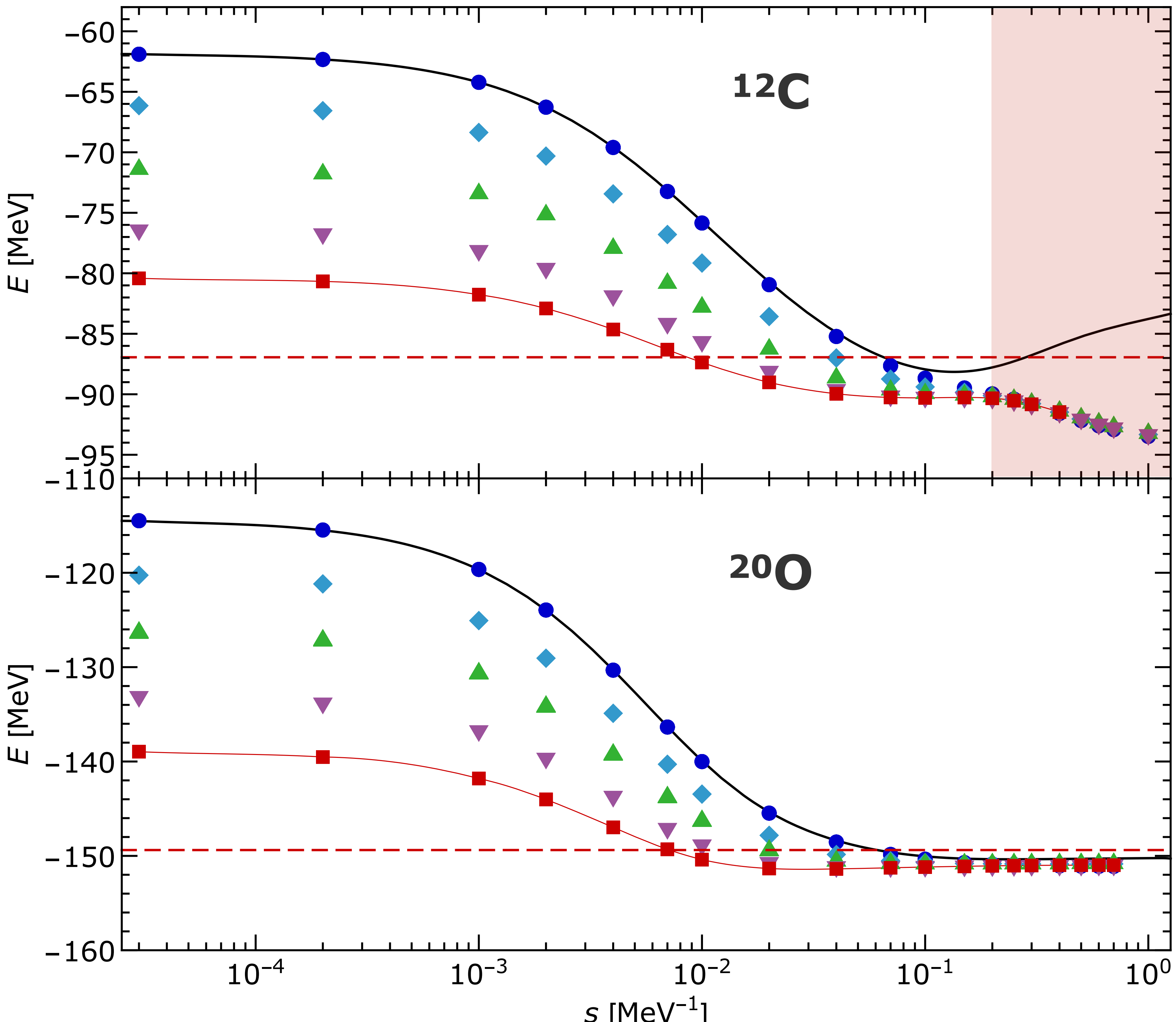
- NCSM convergence is drastically improved
- N_{max}=0 eigenvalues deviated from $E(s)$

chiral NN+3N
Λ_{3N}=400 MeV
α=0.08 fm⁴
ħΩ=20 MeV
e_{max}=12

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

In-Medium NCSM: Flow Evolution

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



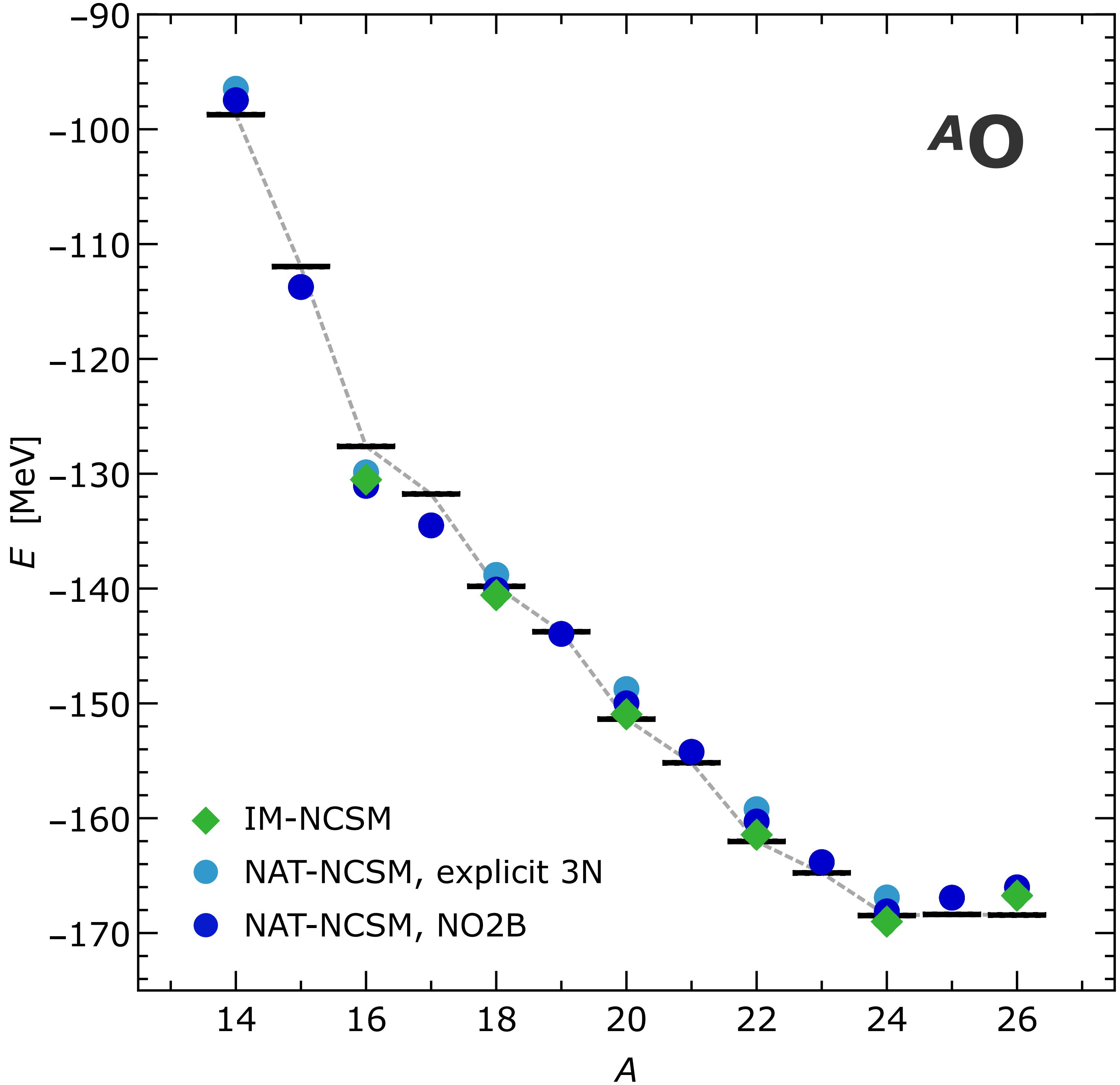
- NCSM convergence is drastically improved
- N_{max}=0 eigenvalues deviated from $E(s)$
- induced many-body contributions might affect large-s results

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: Oxygen Isotopes

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



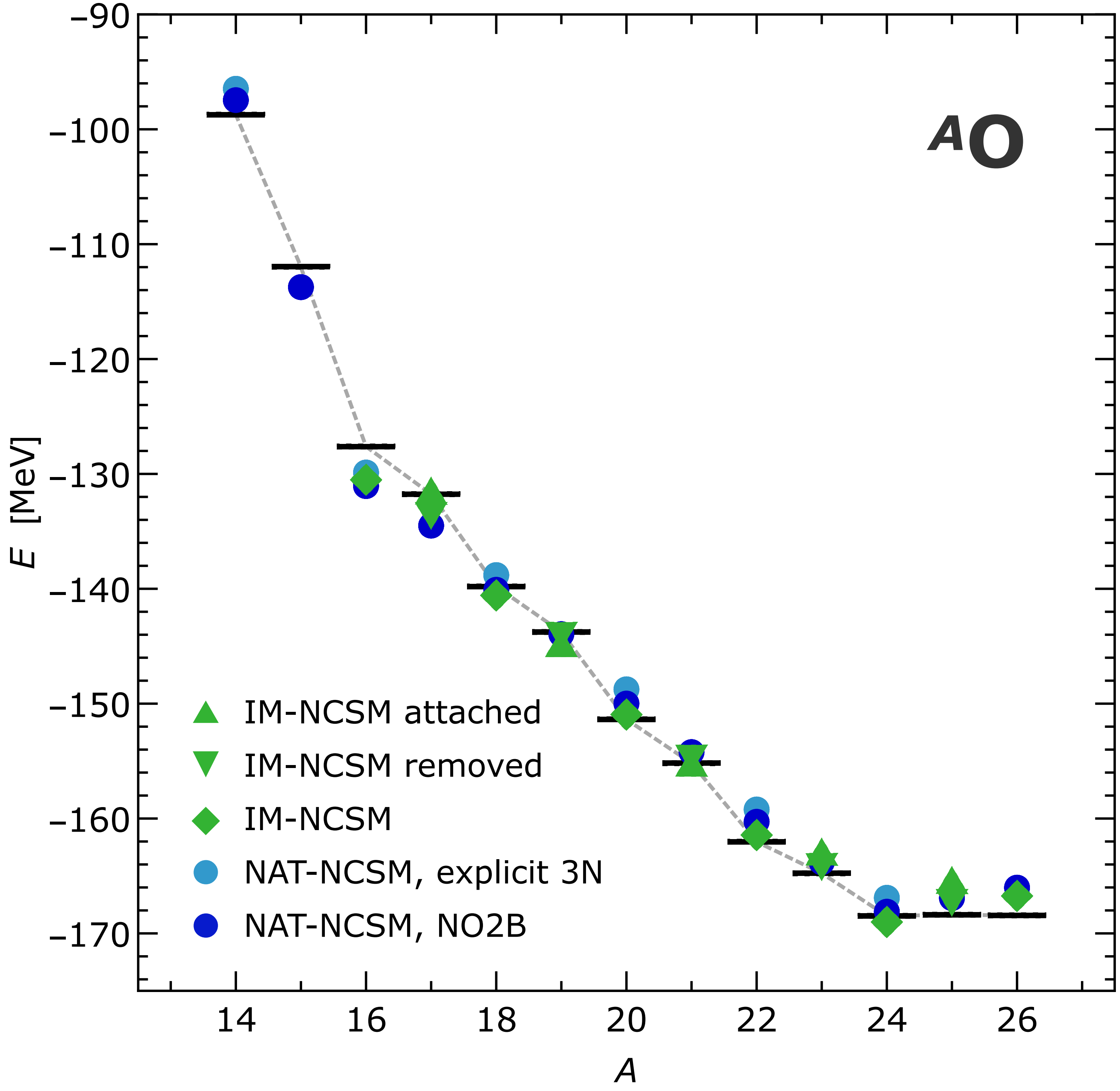
- excellent agreement with direct NCSM
- IM-SRG evolution limited to *J*=0 reference states and thus even-mass isotopes
- odd-mass nuclei via simple particle attachment or removal in final NCSM run

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

IM-NCSM: Oxygen Isotopes

Vobig, Mongelli, Roth; in prep.



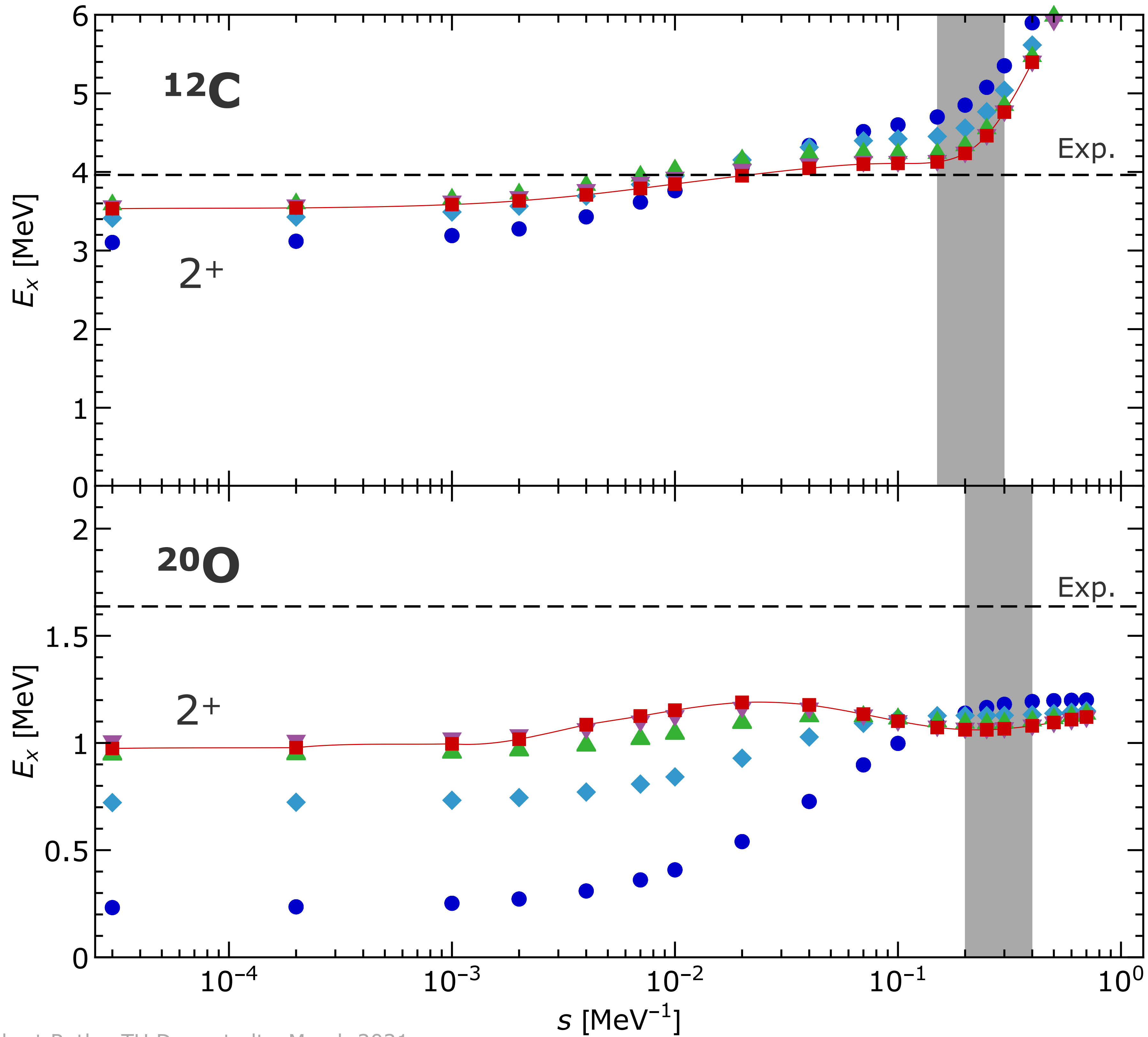
- excellent agreement with direct NCSM
- IM-SRG evolution limited to J=0 reference states and thus even-mass isotopes
- odd-mass nuclei via simple particle attachment or removal in final NCSM run

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

Flow: 2^+ Excitation Energy

Gebrerufael, Vobig, Hergert, Roth; 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

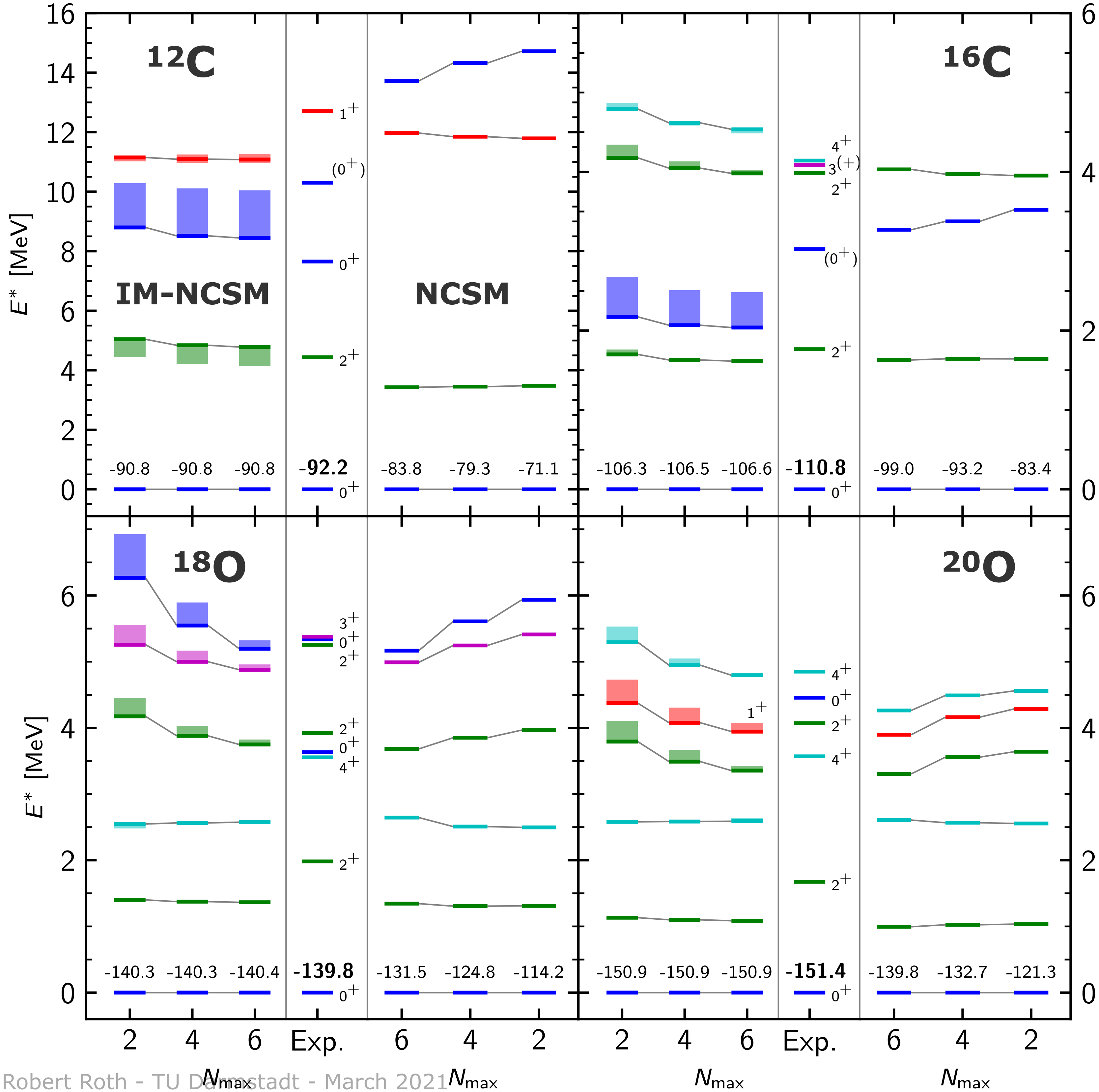
HF basis

N_{max}=0 reference state

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

IM-NCSM: Excitation Spectra

Gebrerufael, Vobig, Hergert, Roth; 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
$\hbar\Omega$=20 MeV
e_{max}=12

HF basis
N_{max}=0 reference

In-Medium SRG: Pros & Cons

PRO

- flexibility of generators
- much more efficient than ph-truncated CI
- straight-forward extension to open-shell nuclei
- size extensive
- very mild scaling with A
- hermitian Hamiltonian
- easy access to other observables
- bridge to shell model

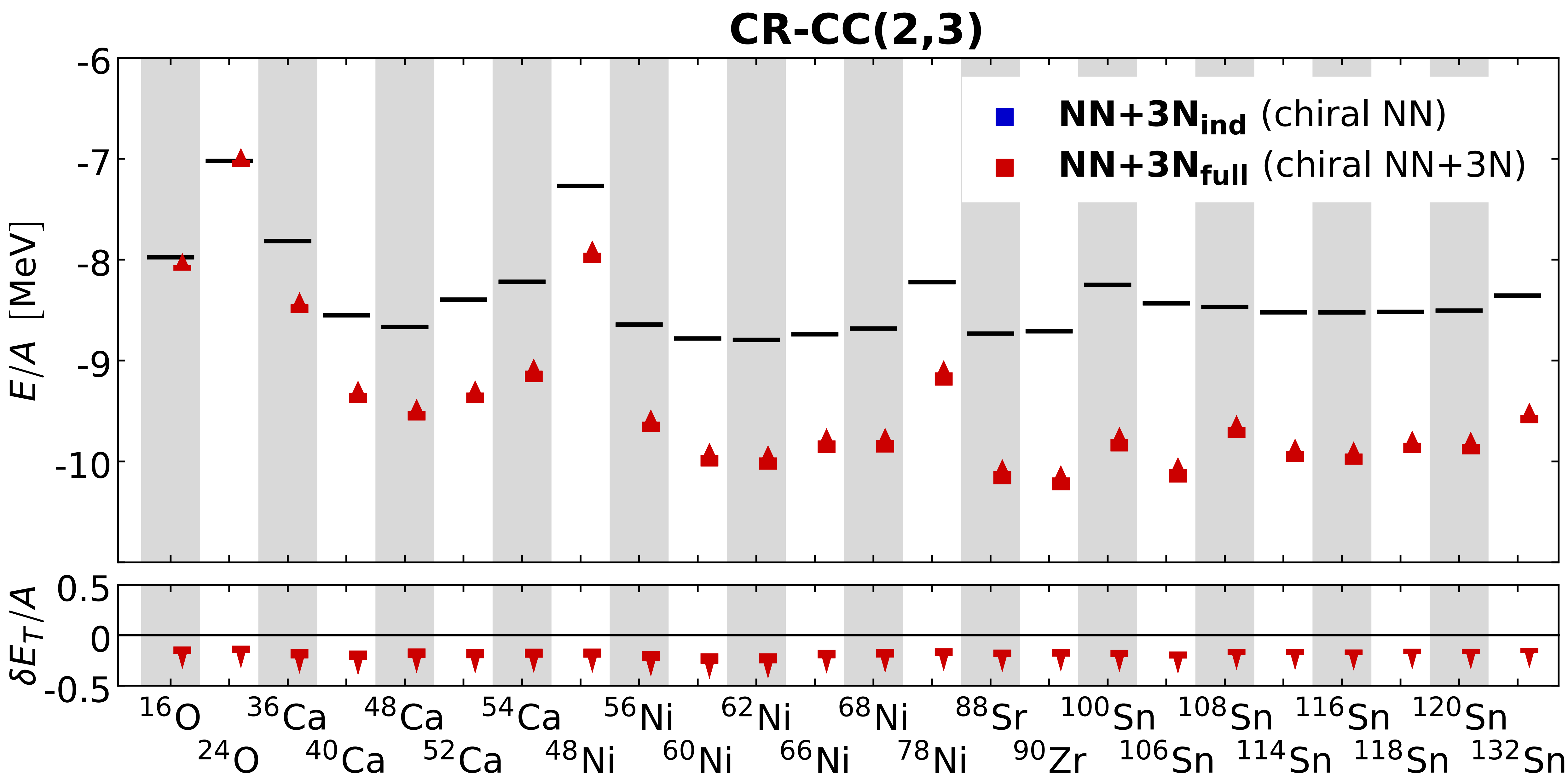
CON

- not variational
- NO3B needs some work

The Limits

Towards Heavy Nuclei - Ab Initio

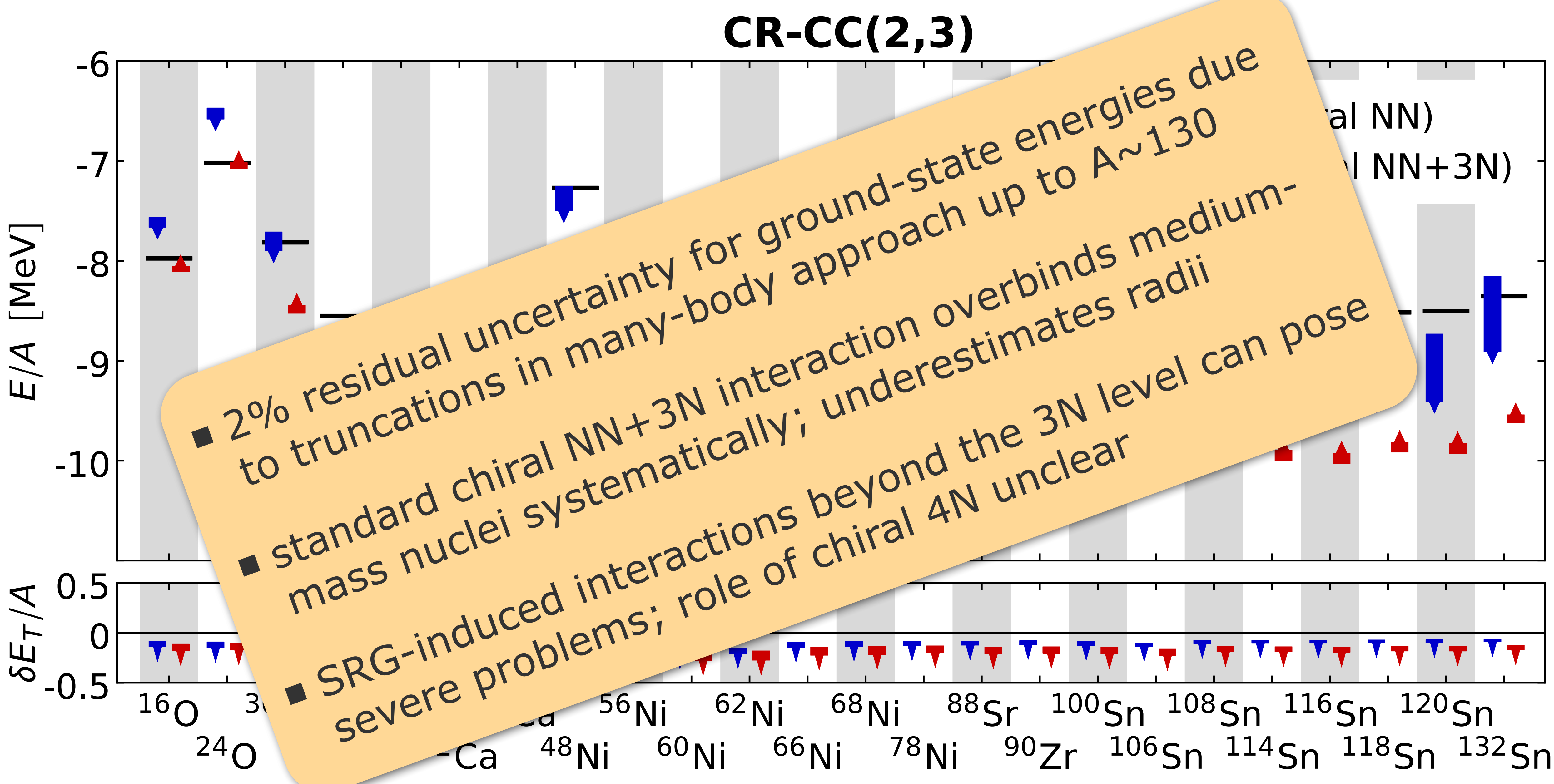
Binder et al., PLB 736, 119 (2014)



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

Towards Heavy Nuclei - Ab Initio

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

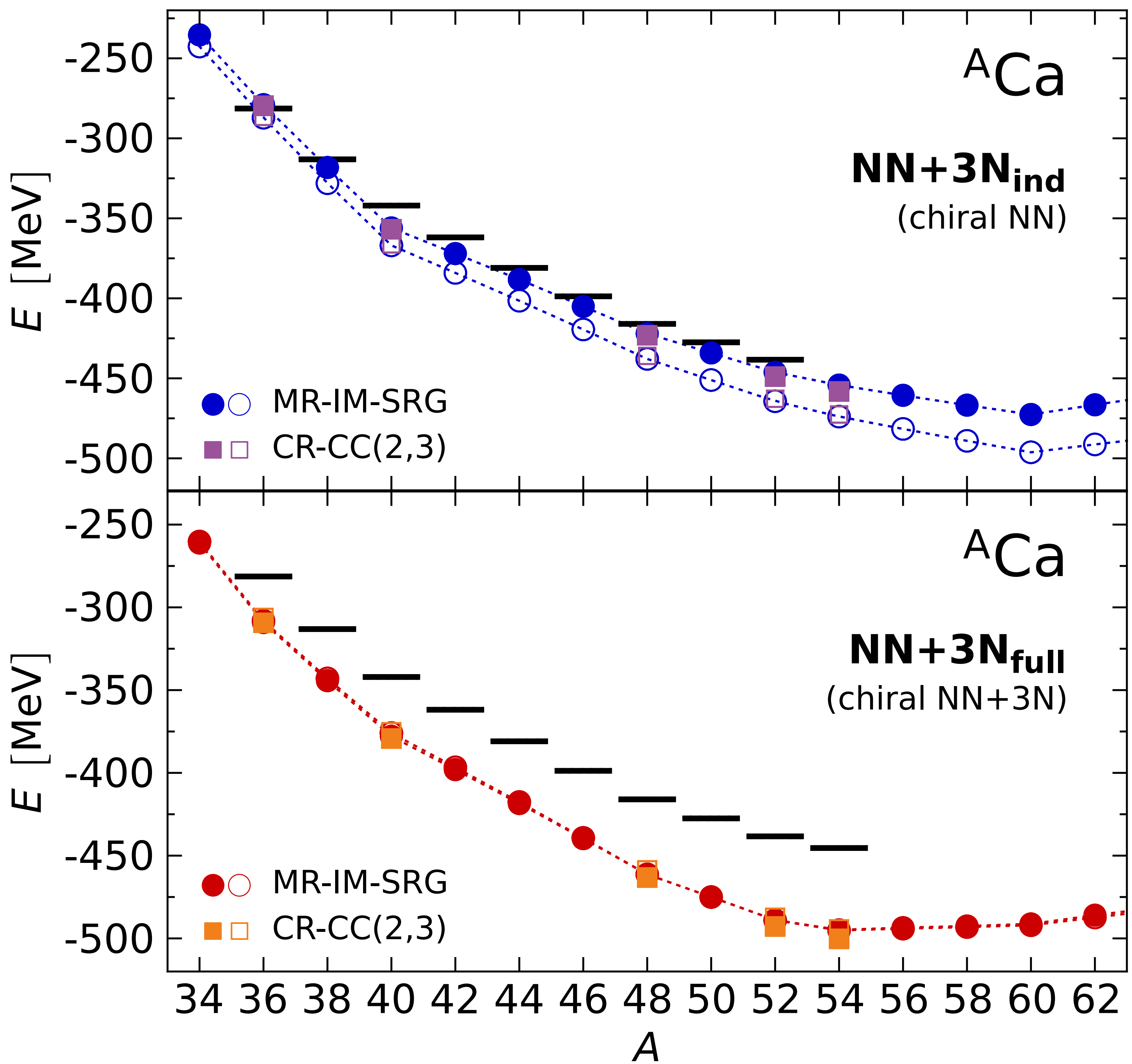


- 2% residual uncertainty for ground-state energies due to truncations in many-body approach up to A~130
- standard chiral NN+3N interaction overbinds medium-mass nuclei systematically; underestimates radii
- SRG-induced interactions beyond the 3N level can pose severe problems; role of chiral 4N unclear

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

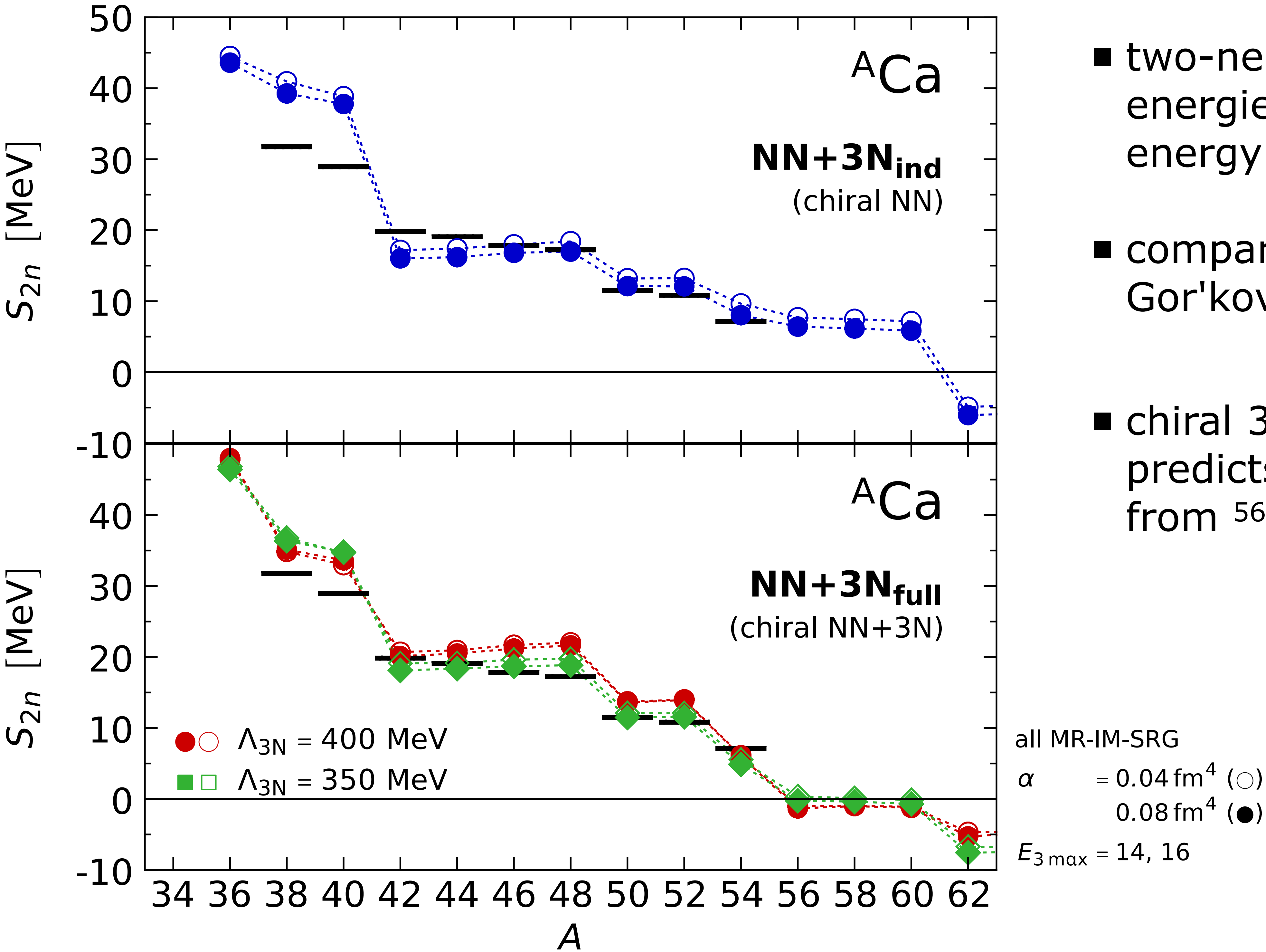
Λ_{3N} = 400 MeV

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

Many-Body Perturbation Theory

The Many Lives of MBPT

- MBPT has **turbulent history** in nuclear structure physics

- **key tool in the 1970's...**
  - valence-space shell-model interactions from MBPT
  - G-matrix, Brueckner-Hartree-Fock method

- **great depression in the 1980's...**
  - no convergence with interactions of the time (core, tensor part)
  - intruder states and multi-reference character

- **today** MBPT is coming back as...
  - auxiliary method (cf. importance truncation, natural orbital basis)
  - stand-alone many-body approach (cf. this workshop)

Single-Reference
Many-Body Perturbation Theory

Textbook MBPT

- **Rayleigh-Schrödinger perturbation theory** with partitioning defined though choice single-particle basis

$$\mathrm{H}_\lambda = \mathrm{H}_0 + \lambda \mathrm{W} \qquad \mathrm{H}_0|\Phi_n\rangle = \epsilon_n|\Phi_n\rangle$$

- power series for energy eigenvalues and eigenstates and expansion of state corrections in unperturbed basis

$$E_n = \epsilon_n + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \dots$$
$$|\Psi_n\rangle = |\Phi_n\rangle + \lambda|\Psi_n^{(1)}\rangle + \lambda^2|\Psi_n^{(2)}\rangle + \dots$$

$$|\Psi_n^{(p)}\rangle = \sum_\nu C_{n,\nu}^{(p)} \, |\Phi_\nu\rangle$$

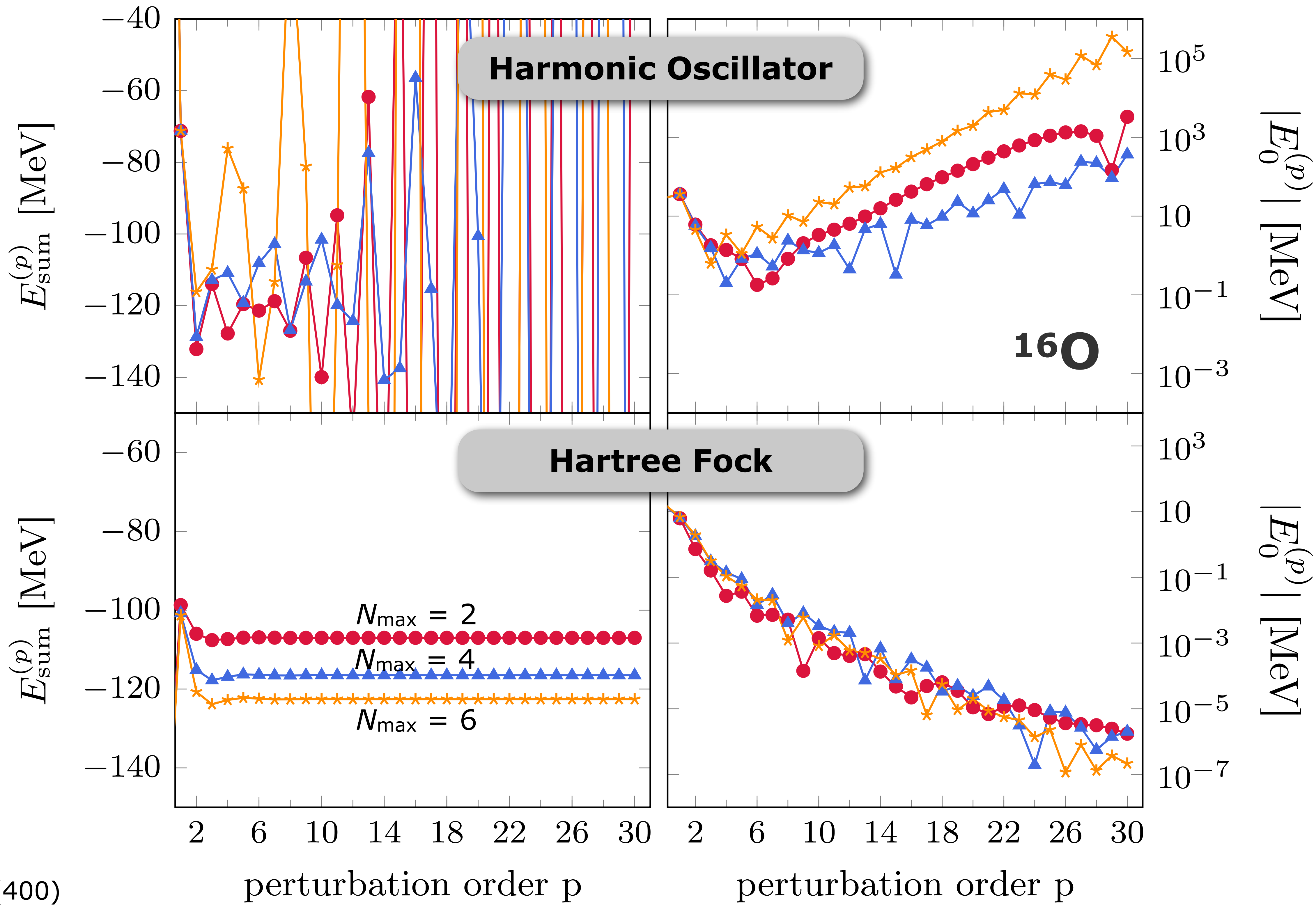
- **recursive relations for energy and state corrections** depending only on matrix elements of W in unperturbed basis

$$E_n^{(p)} = \sum_\nu \langle\Phi_n|\mathrm{W}|\Phi_\nu\rangle C_{n,\nu}^{(p-1)}$$
$$C_{n,\nu}^{(p)} = \frac{1}{\epsilon_n - \epsilon_\nu}\Big(\sum_{\nu'} \langle\Phi_\nu|\mathrm{W}|\Phi_{\nu'}\rangle C_{n,\nu'}^{(p-1)} - \sum_{j=1}^{p} E_n^{(j)} \, C_{n,\nu}^{(p-j)}\Big)$$

- evaluated at the level of many-body matrix elements **using NCSM technology**

Convergence: Single-Particle Basis

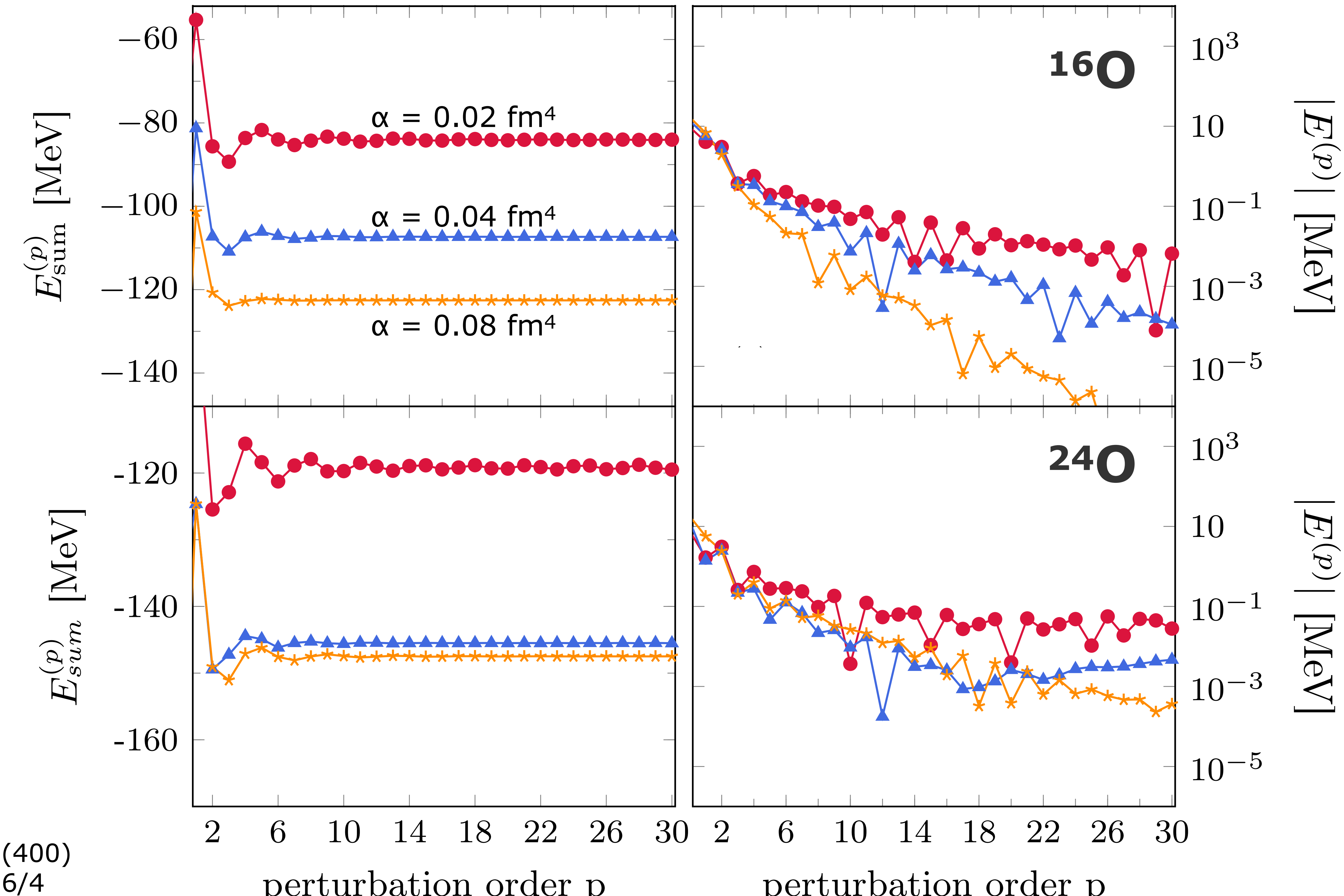
Tichai et al., PLB 756, 283 (2016)



NN+3N(400)
α = 0.08 fm⁴

Convergence: SRG Evolution

Tichai et al., PLB 756, 283 (2016)



NN+3N(400)
N_{max} = 6/4
Hartree-Fock

Low-Order MBPT

- switch to **explicit expressions** for low-order energy corrections involving summations over m-scheme single-particle states, e.g.,

$$E^{(2)} = \frac{1}{4} \sum_{a,b}^{<\epsilon_F} \sum_{m,n}^{>\epsilon_F} \frac{|\langle ab|\,\mathrm{W}\,|mn\rangle|^2}{\epsilon_a + \epsilon_b - \epsilon_m - \epsilon_n}$$

➡ **large model spaces**, truncated wrt. single-particle energy $e_{\max}$ are easily accessible

- make use of **angular-momentum** coupling for closed-shell nuclei, reducing summations to orbital indices

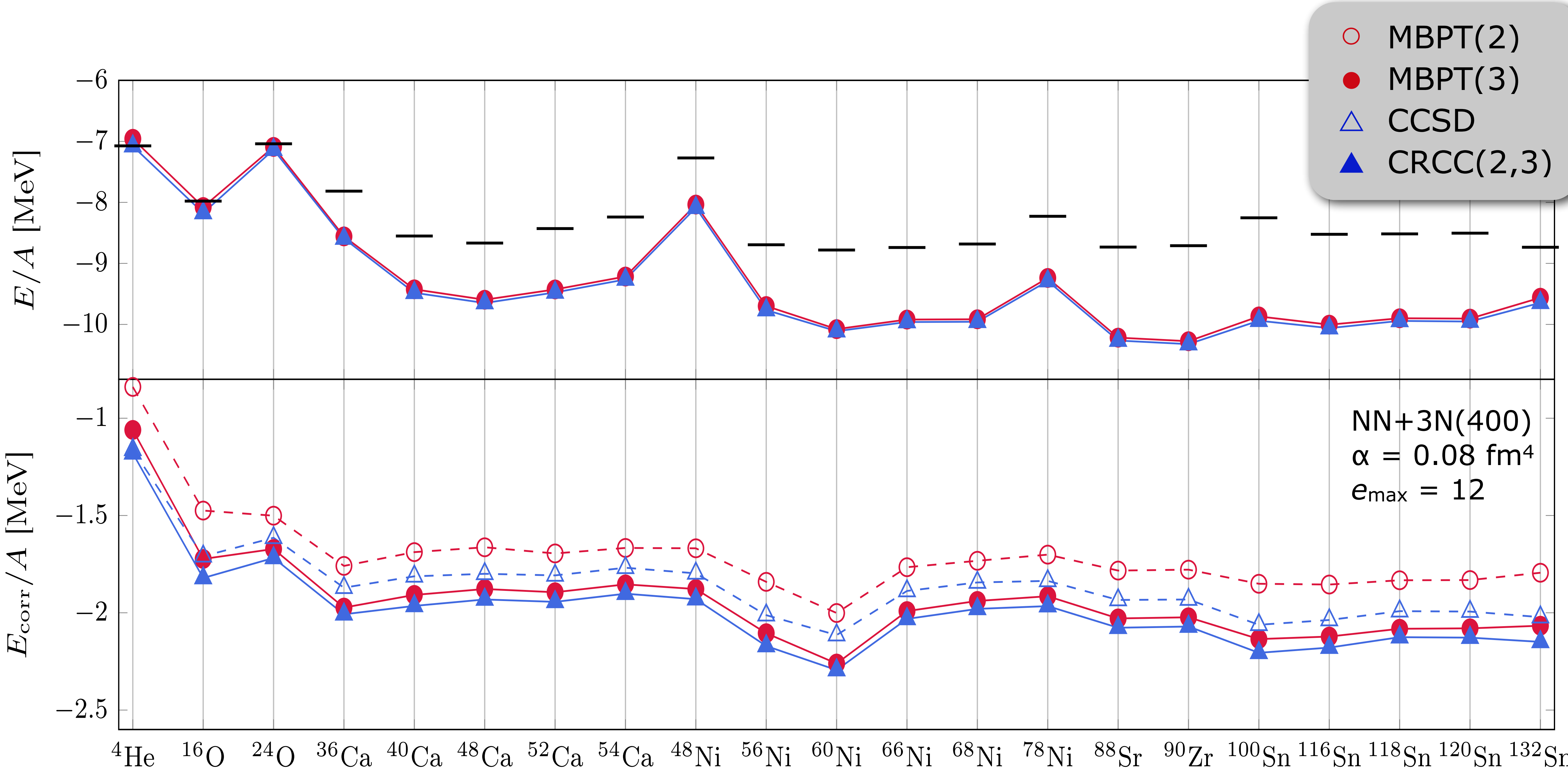
$$E^{(2)} = \frac{1}{4} \sum_{\bar{a},\bar{b}}^{<\epsilon_F} \sum_{\bar{m},\bar{n}}^{>\epsilon_F} \sum_{J} (2J+1) \frac{|\langle \bar{a}\bar{b};J|\,\mathrm{W}\,|\bar{m}\bar{n};J\rangle|^2}{\epsilon_{\bar{a}} + \epsilon_{\bar{b}} - \epsilon_{\bar{m}} - \epsilon_{\bar{n}}}$$

➡ makes evaluation of sums **much more efficient** since coupled matrix elements are directly available

- quickly gets tedious when going to higher orders…

Low-Order MBPT

Tichai et al., PLB 756, 283 (2016)



- **good agreement** of MBPT(3) ground-state energies with **advanced coupled-cluster calculations** throughout the complete mass range

Multi-Configurational Many-Body Perturbation Theory

Multi-Configurational Perturbation Theory

Tichai, Gebrerufael, Vobig, Roth; arXiv:1703.05664

- select **NCSM reference space** $\mathcal{M}_{\text{ref}}$ and solve full eigenvalue problem

$$|\Psi_n^{\text{ref}}\rangle = \sum_{\mu \in \mathcal{M}_{\text{ref}}} B_{n,\mu}^{\text{ref}} \, |\Phi_\mu\rangle$$

- define **unperturbed Hamiltonian** with reference-space eigenstates

$$\text{H}_0 = \sum_{\mu \in \mathcal{M}_{\text{ref}}} \epsilon_\mu^{\text{ref}} \, |\Psi_\mu^{\text{ref}}\rangle\langle\Psi_\mu^{\text{ref}}| + \sum_{\nu \notin \mathcal{M}_{\text{ref}}} \epsilon_\nu \, |\Phi_\nu\rangle\langle\Phi_\nu|$$

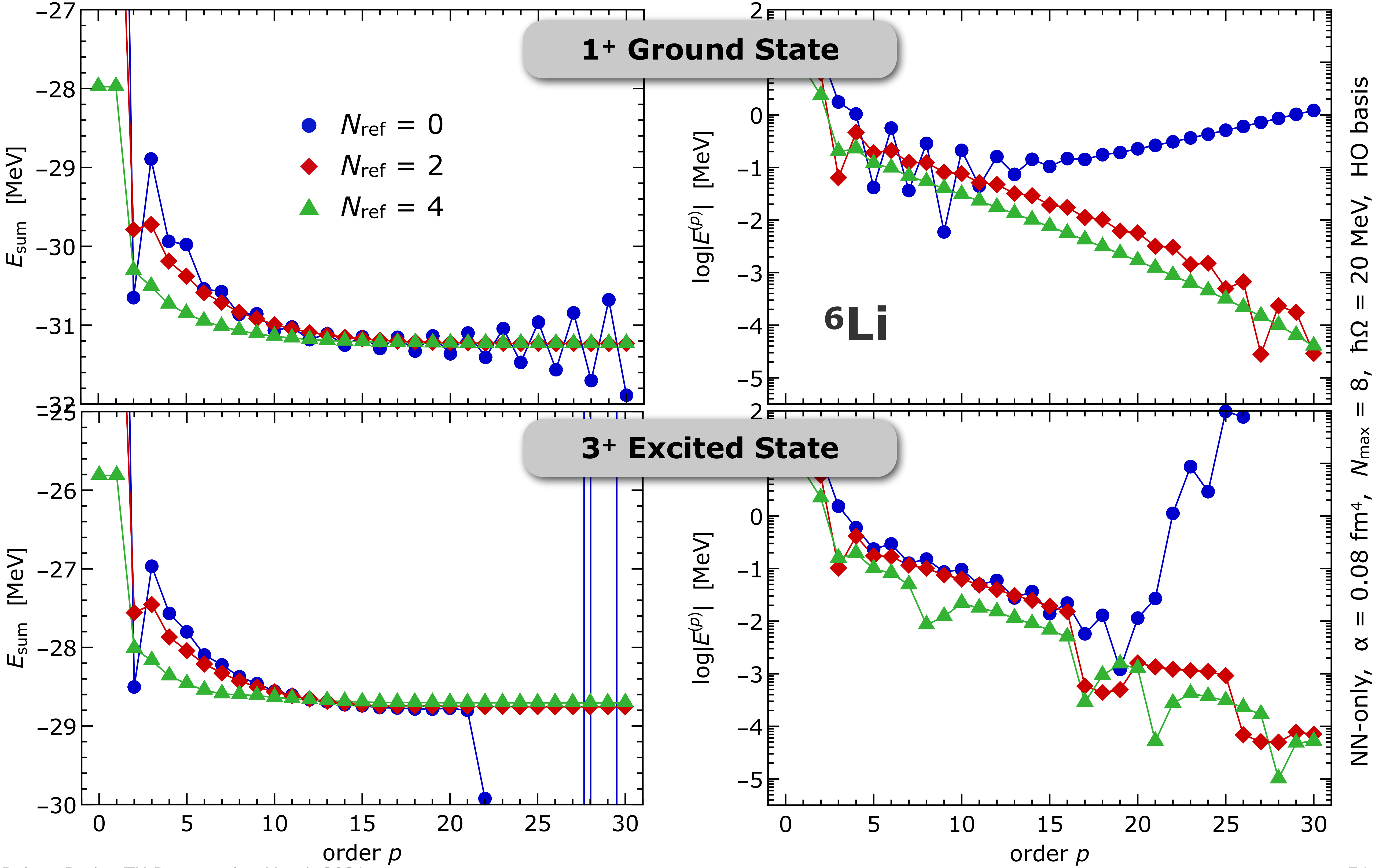
- usual MBPT derivation yields **recursive relations** for energy and state corrections

$$E_n^{(p)} = \sum_{\nu \notin \mathcal{M}_{\text{ref}}} \langle\Psi_n^{\text{ref}}|\text{W}|\Phi_\nu\rangle \, C_{n,\nu}^{(p-1)} \qquad |\Psi_n^{(p)}\rangle = \sum_{\mu \in \mathcal{M}_{\text{ref}}} D_{n,\mu}^{(p)} \, |\Psi_\mu^{\text{ref}}\rangle + \sum_{\nu \notin \mathcal{M}_{\text{ref}}} C_{n,\nu}^{(p)} \, |\Phi_\nu\rangle$$

$$C_{n,\nu}^{(p)} = \frac{1}{\epsilon_n - \epsilon_\nu}\left(\sum_{\nu' \notin \mathcal{M}_{\text{ref}}} \langle\Phi_\nu|\text{W}|\Phi_{\nu'}\rangle \, C_{n,\nu'}^{(p-1)} + \sum_{\mu \in \mathcal{M}_{\text{ref}}} \langle\Phi_\nu|\text{W}|\Psi_\mu^{\text{ref}}\rangle \, D_{n,\mu}^{(p-1)} - \sum_{j=1}^{p} E_n^{(j)} C_{n,\nu}^{(p-j)} \right)$$

$$D_{n,\mu}^{(p)} = \frac{1}{\epsilon_n - \epsilon_\mu}\left(\langle\Psi_\mu^{\text{ref}}|\text{W}|\psi_n^{(p-1)}\rangle - \sum_{j=1}^{p} E_n^{(j)} D_{n,\mu}^{(p-j)} \right)$$

Convergence: Reference Space



Perturbatively Improved NCSM

Tichai, Gebrerufael, Vobig, Roth; arXiv:1703.05664

NCSM
many-body solution

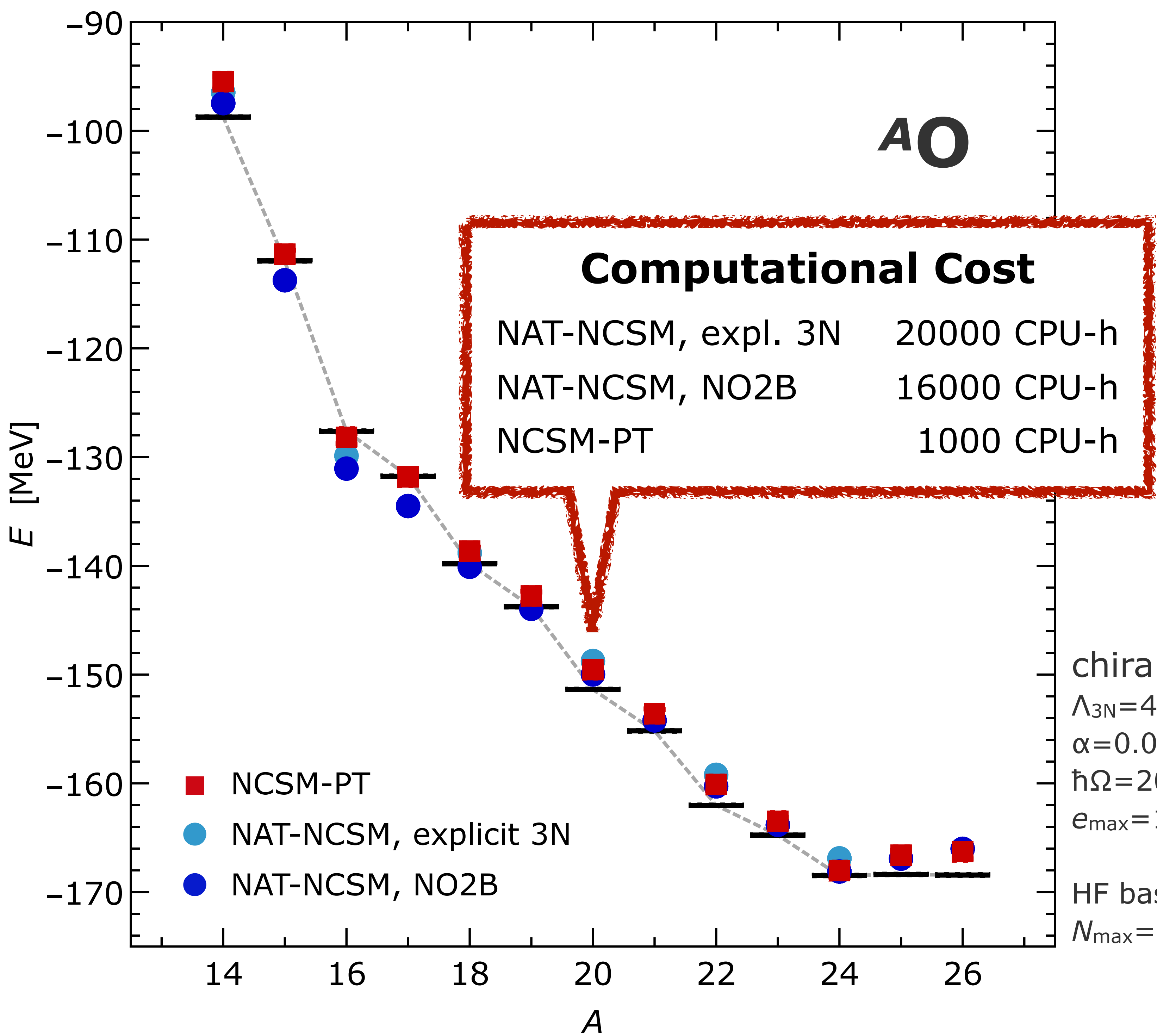
MBPT
convergence booster

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

- 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



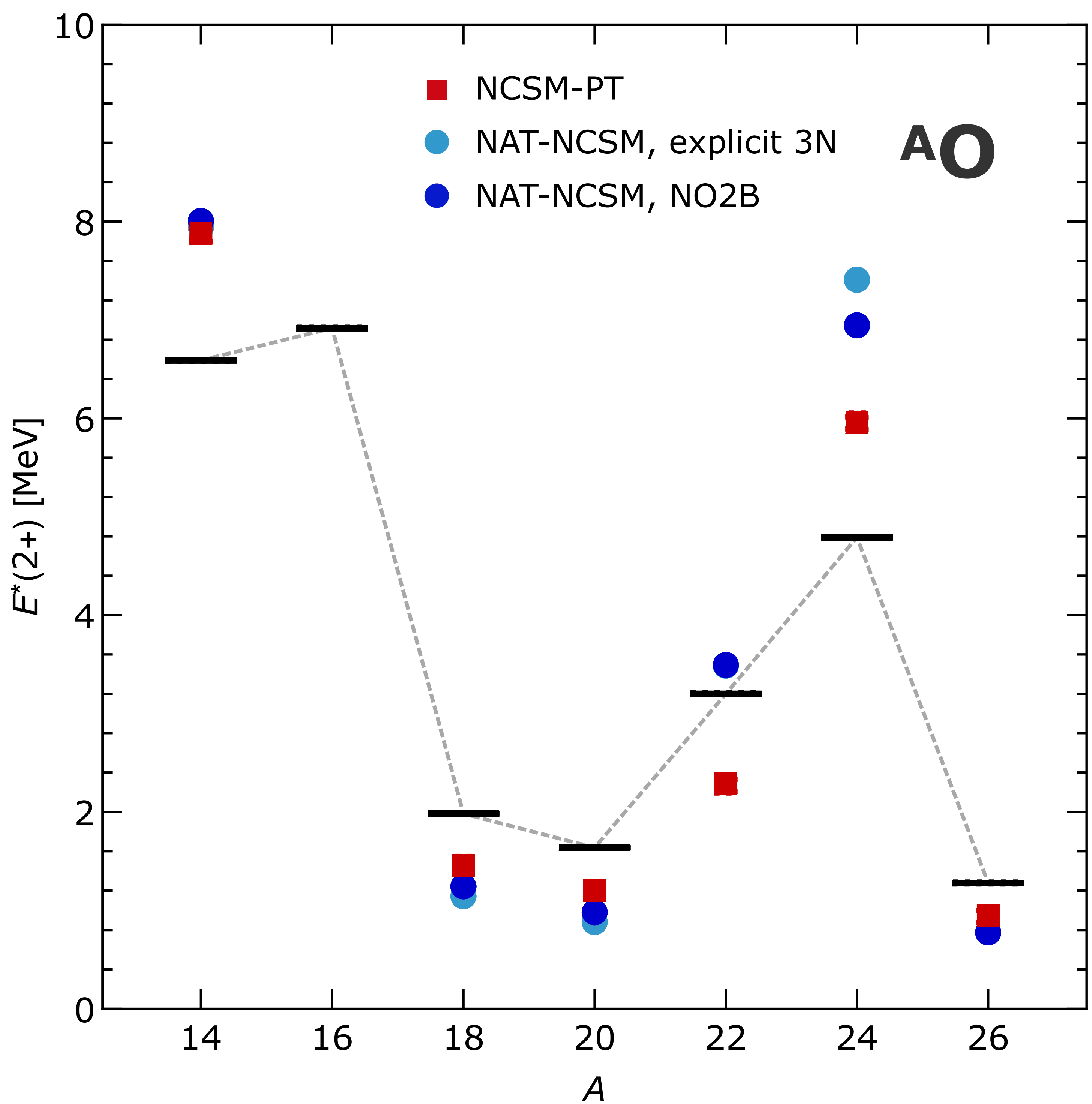
- excellent agreement with direct NCSM
- all isotopes are accessible due to simple m-scheme implementation

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

HF basis
N_{max}=2 reference

Oxygen Isotopes: Excited 2^+ States

Tichai, et al.; in prep.



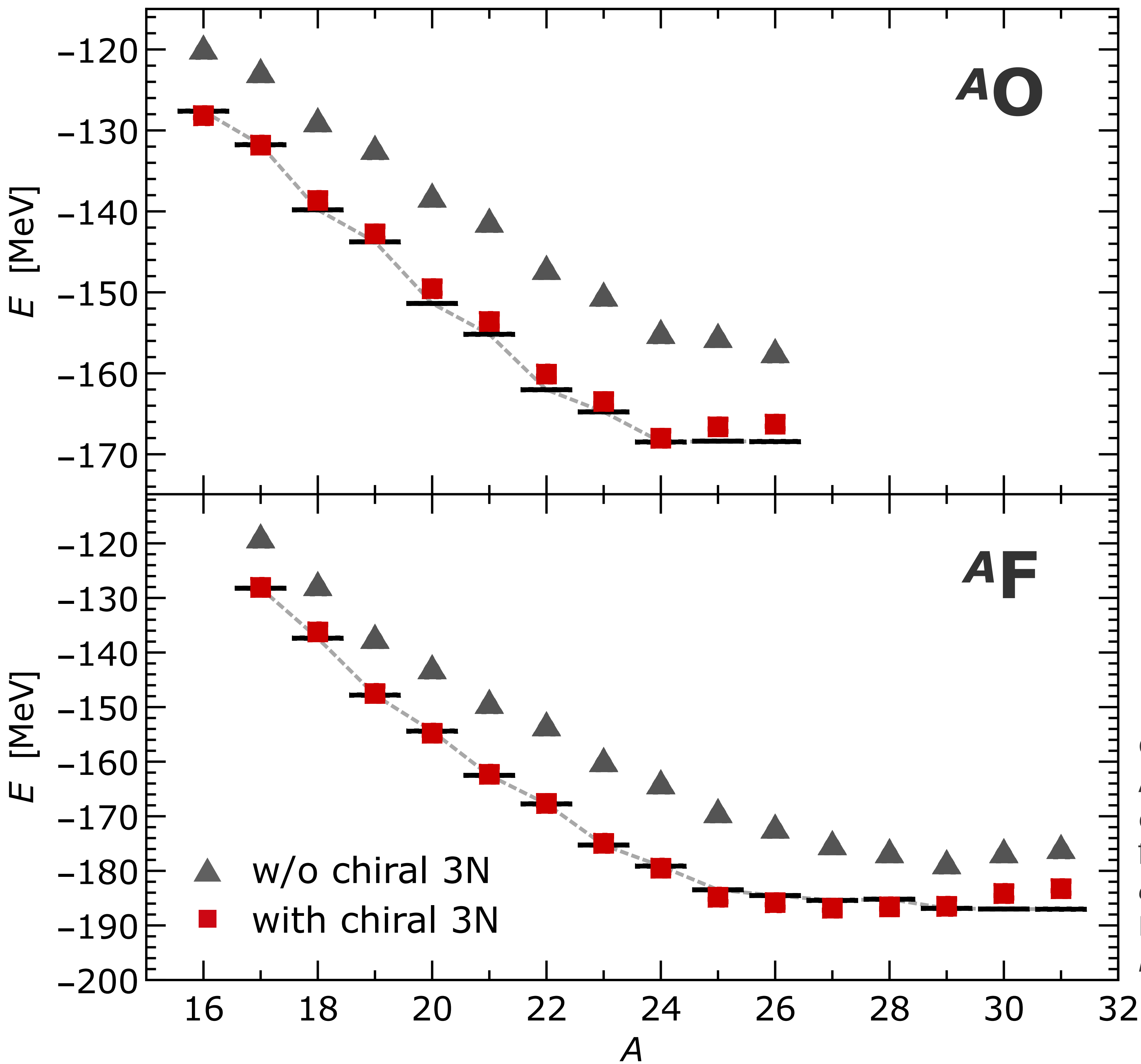
- can address excited states natively
- example: first 2^+ states in even oxygen isotopes
- excellent agreement among methods except for closed (sub-)shells ^{22}O, ^{24}O…

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

HF basis
N_{max}=2 reference

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

NCSM-PT
chiral NN+3N
Λ_{3N}=400 MeV
α=0.08 fm⁴
ħΩ=20 MeV
e_{max}=12
HF basis
N_{max}=2 reference

Overview

- **Lecture 1: Hamiltonian**

  Prelude ● Many-Body Quantum Mechanics ● 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 ● Basis Optimization

- **Lecture 3: Medium-Mass Nuclei**

  Normal Ordering ● Coupled-Cluster Theory ● In-Medium Similarity Renormalization Group ● Many-Body Perturbation Theory

- **Project: Do-It-Yourself NCSM**

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

- **Lecture 4: Precision, Uncertainties, and Applications**

  Chiral Interactions for Precision Calculations ● Uncertainty Quantification ● Applications to Nuclei and Hypernuclei