Ab Initio Nuclear Structure with SRG-Evolved NN plus 3N Interactions

Robert Roth
Institut für Kernphysik

TECHNISCHE UNIVERSITÄT DARMSTADT

From QCD to Nuclear Structure

Nuclear Structure

Low-Energy QCD

From QCD to Nuclear Structure

Nuclear Structure

NN+3N Interaction from Chiral EFT

Low-Energy QCD

- chiral EFT based on the relevant degrees of freedom & symmetries of QCD
- provides consistent NN & 3N interaction plus currents
- in the following:
  - NN at N^3LO (Entem & Machleidt, 500 MeV)
  - 3N at N^2LO (low-energy constants c_D & c_E from triton fit)

From QCD to Nuclear Structure

Nuclear Structure

Unitarily Transformed Hamiltonian

- adapt Hamiltonian to truncated low-energy model space
  - tame short-range correlations
  - improve convergence behavior
- transform Hamiltonian & observables consistently
- conserve experimentally constrained few-body properties

NN+3N Interaction from Chiral EFT

Low-Energy QCD

From QCD to Nuclear Structure

Nuclear Structure

Exact & Approx. Many-Body Methods

Unitarily Trans-formed Hamiltonian

NN+3N Interaction from Chiral EFT

Low-Energy QCD

- 'exact' solution of the many-body problem for light & inter-mediate masses (NCSM, CC,...)
- controlled approximations for heavier nuclei (HF & MBPT,...)
- all rely on restricted model spaces & benefit from unitary transformation

From QCD to Nuclear Structure

Nuclear Structure

↑

Exact & Approx. Many-Body Methods

↑

Unitarily Transformed Hamiltonian

↑

NN+3N Interaction from Chiral EFT

↑

Low-Energy QCD

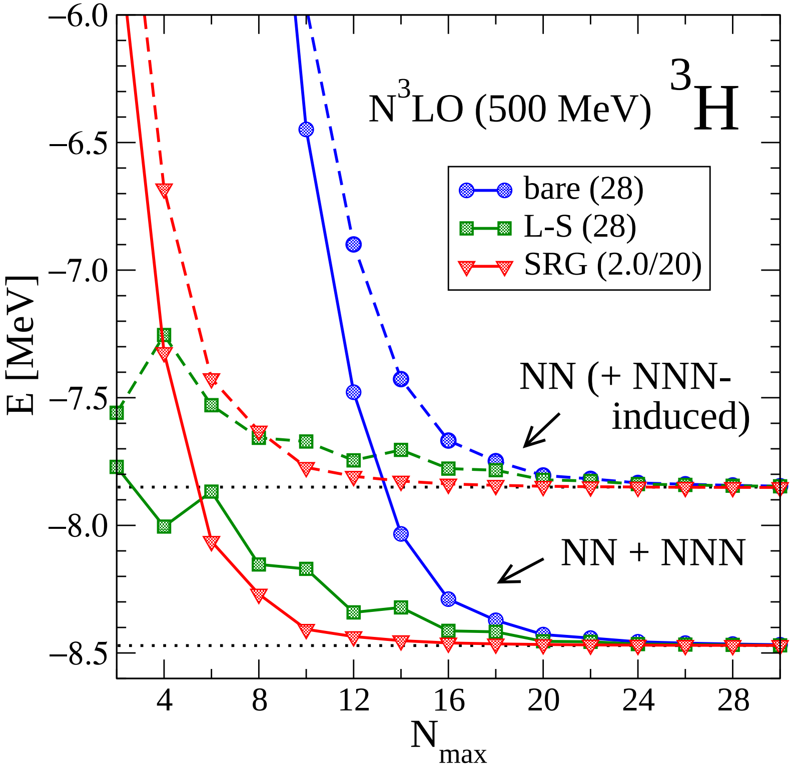
focus on consistent inclusion of chiral 3N interaction

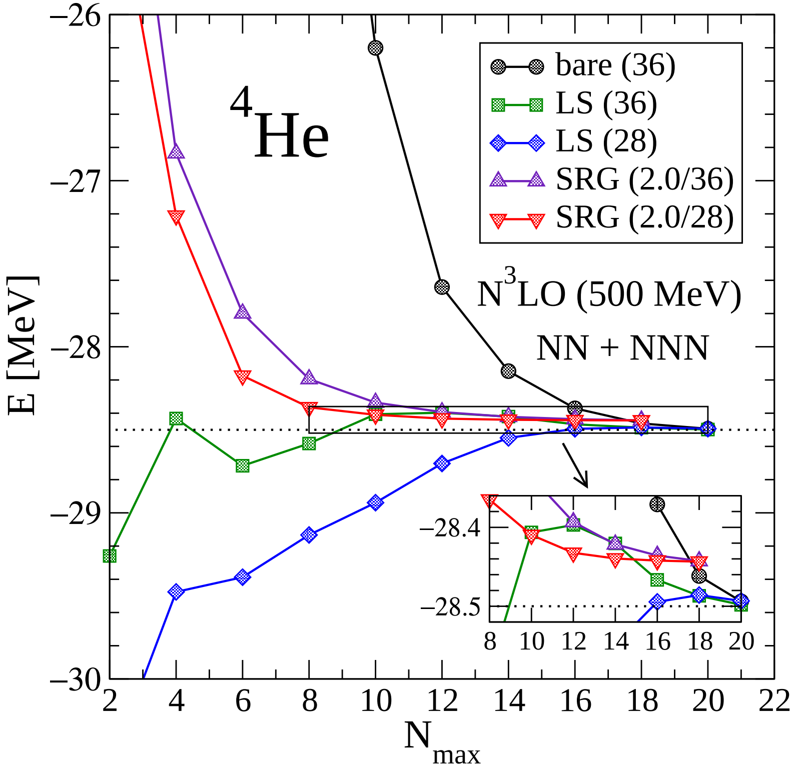
Pioneering Work

PRL 103, 082501 (2009) PHYSICAL REVIEW LETTERS week ending 21 AUGUST 2009

Evolution of Nuclear Many-Body Forces with the Similarity Renormalization Group

E. D. Jurgenson,[1] P. Navrátil,[2] and R. J. Furnstahl[1]





Overview

- **Unitarily Transformed NN+3N Hamiltonians**
  - Similarity Renormalization Group
  - consistent transformation of chiral NN+3N interactions

- **Exact Ab-Initio Calculations**
  - Importance-Truncated NCSM
  - test of SRG-transformed chiral NN+3N interactions throughout the p-shell

- **Approximate Many-Body Methods**
  - Hartree-Fock & Perturbation Theory
  - ground-state systematics throughout the nuclear chart using SRG-transformed chiral NN+3N interactions

Unitarily Transformed NN+3N Hamiltonians

Similarity Renormalization Group

Roth, Neff, Feldmeier — Prog. Part. Nucl. Phys. 65, 50 (2010)
Roth, Reinhardt, Hergert — Phys. Rev. C 77, 064033 (2008)
Hergert, Roth — Phys. Rev. C 75, 051001(R) (2007)
Roth et al. — Phys. Rev. C 72, 034002 (2005)
Roth et al. — Nucl. Phys. A 745, 3 (2004)

Similarity Renormalization Group

evolution of the **Hamiltonian to band-diagonal form** with respect to uncorrelated many-body basis

simplicity and flexibility are great advantages of the SRG approach

- **unitary transformation** of Hami

$$\widetilde{H}_\alpha = U_\alpha{}^\dagger H U_\alpha$$

- **evolution equations** for $\widetilde{H}_\alpha$ and U_α depending on generator η_α

$$\frac{d}{d\alpha}\widetilde{H}_\alpha = \left[\eta_\alpha, \widetilde{H}_\alpha\right] \qquad \frac{d}{d\alpha}U_\alpha = -U_\alpha \eta_\alpha$$

- **dynamic generator**: commutator with the operator in whose eigenbasis H shall be diagonalized

$$\eta_\alpha = (2\mu)^2 \left[T_{\text{int}}, \widetilde{H}_\alpha\right]$$

SRG Evolution of Matrix Elements

- represent operator equation in ***n*-body Jacobi HO basis** $\left|Ei J^\pi T\right\rangle$
  - $n=2$: relative LS-coupled HO states: $\left|E(LS)J^\pi T\right\rangle$
  - $n=3$: antisymmetrized Jacobi-coordinate HO states: $\left|Ei J^\pi T\right\rangle$

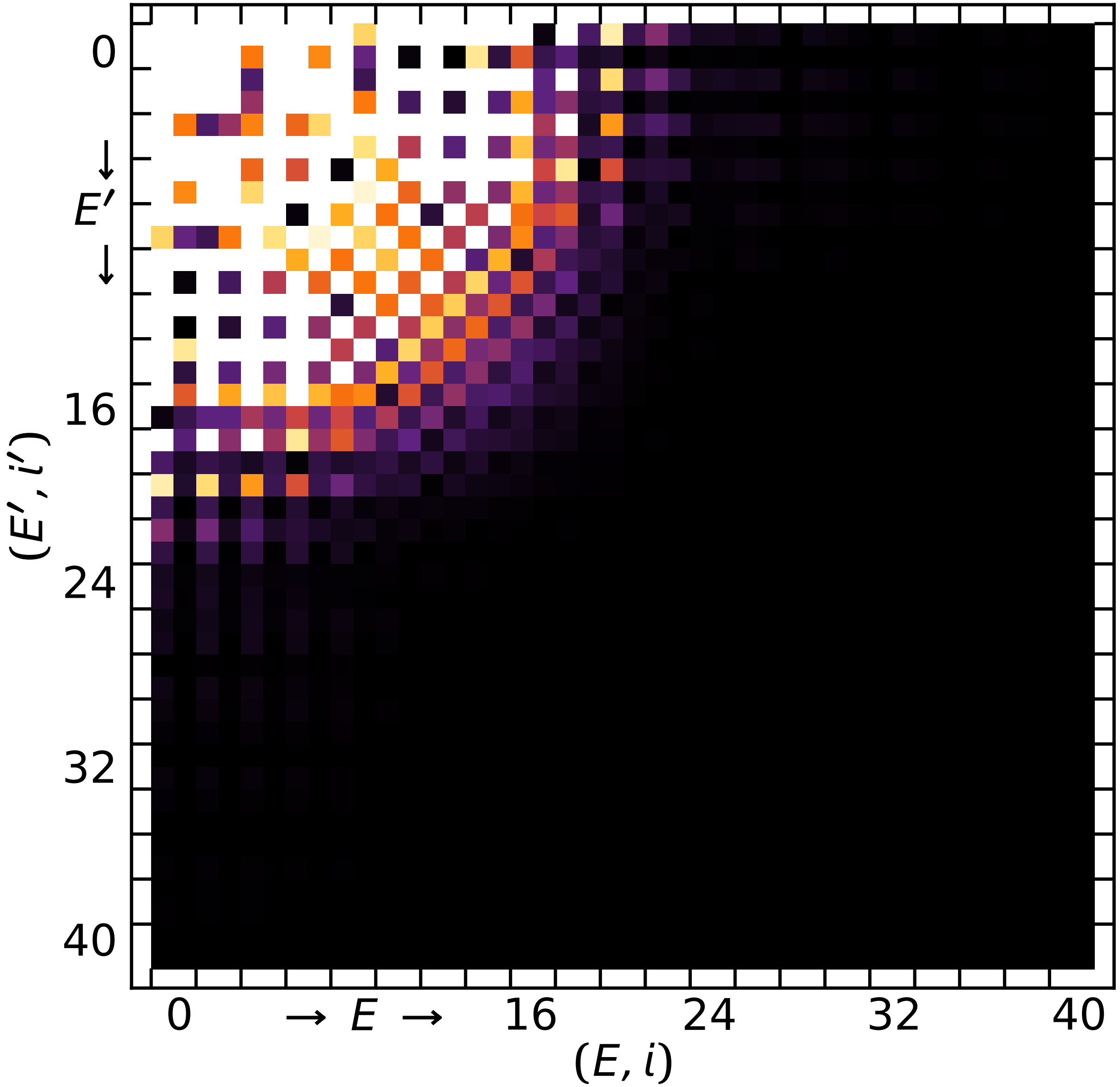
- system of **coupled evolution equations** for each $(J^\pi T)$-block

$$
\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}\alpha}\left\langle EiJ^\pi T\right|\widetilde{\mathrm{H}}_\alpha\left|E'i'J^\pi T\right\rangle = (2\mu)^2 \sum_{E'',i''}^{E_\mathrm{SRG}}\sum_{E''',i'''}^{E_\mathrm{SRG}} \Big[\\
\left\langle EiJ^\pi T\right|\mathrm{T}_\mathrm{int}\left|E''i''J^\pi T\right\rangle \left\langle E''i''J^\pi T\right|\widetilde{\mathrm{H}}_\alpha\left|E'''i'''J^\pi T\right\rangle \left\langle E'''i'''J^\pi T\right|\widetilde{\mathrm{H}}_\alpha\left|E'i'J^\pi T\right\rangle \\
-2\left\langle EiJ^\pi T\right|\widetilde{\mathrm{H}}_\alpha\left|E''i''J^\pi T\right\rangle \left\langle E''i''J^\pi T\right|\mathrm{T}_\mathrm{int}\left|E'''i'''J^\pi T\right\rangle \left\langle E'''i'''J^\pi T\right|\widetilde{\mathrm{H}}_\alpha\left|E'i'J^\pi T\right\rangle \\
+\left\langle EiJ^\pi T\right|\widetilde{\mathrm{H}}_\alpha\left|E''i''J^\pi T\right\rangle \left\langle E''i''J^\pi T\right|\widetilde{\mathrm{H}}_\alpha\left|E'''i'''J^\pi T\right\rangle \left\langle E'''i'''J^\pi T\right|\mathrm{T}_\mathrm{int}\left|E'i'J^\pi T\right\rangle \Big]
\end{aligned}
$$

- we use $E_\mathrm{SRG} = 40$ for $J \leq 5/2$ and ramp down to 24 in steps of 4 (sufficient to converge the intermediate sums for $\hbar\Omega \gtrsim 16\,\mathrm{MeV}$)

SRG Evolution in Two-Body Space

2B-Jacobi HO matrix elements

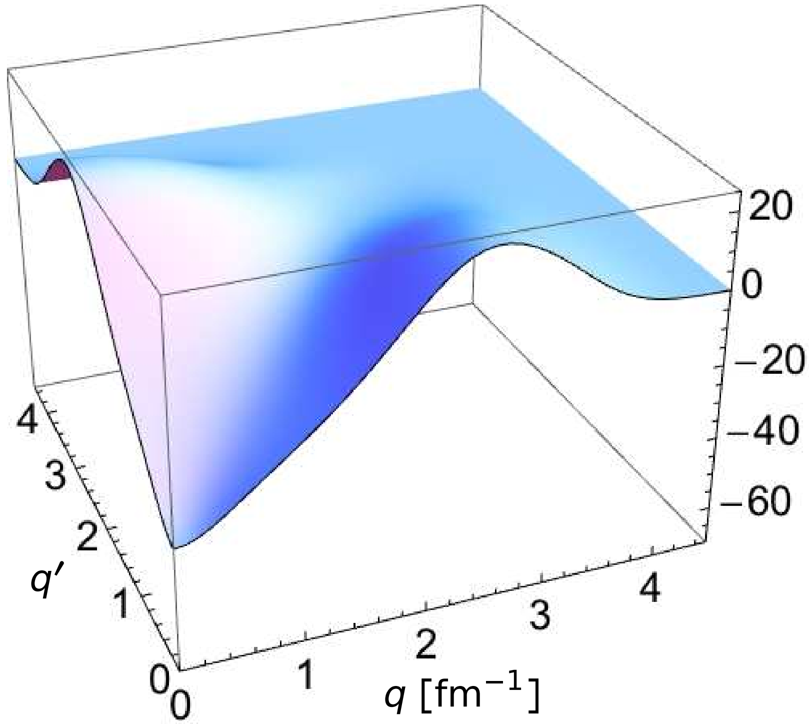


$$\alpha = 0.00\,\mathrm{fm}^4$$

$\Lambda = \infty\,\mathrm{fm}^{-1}$

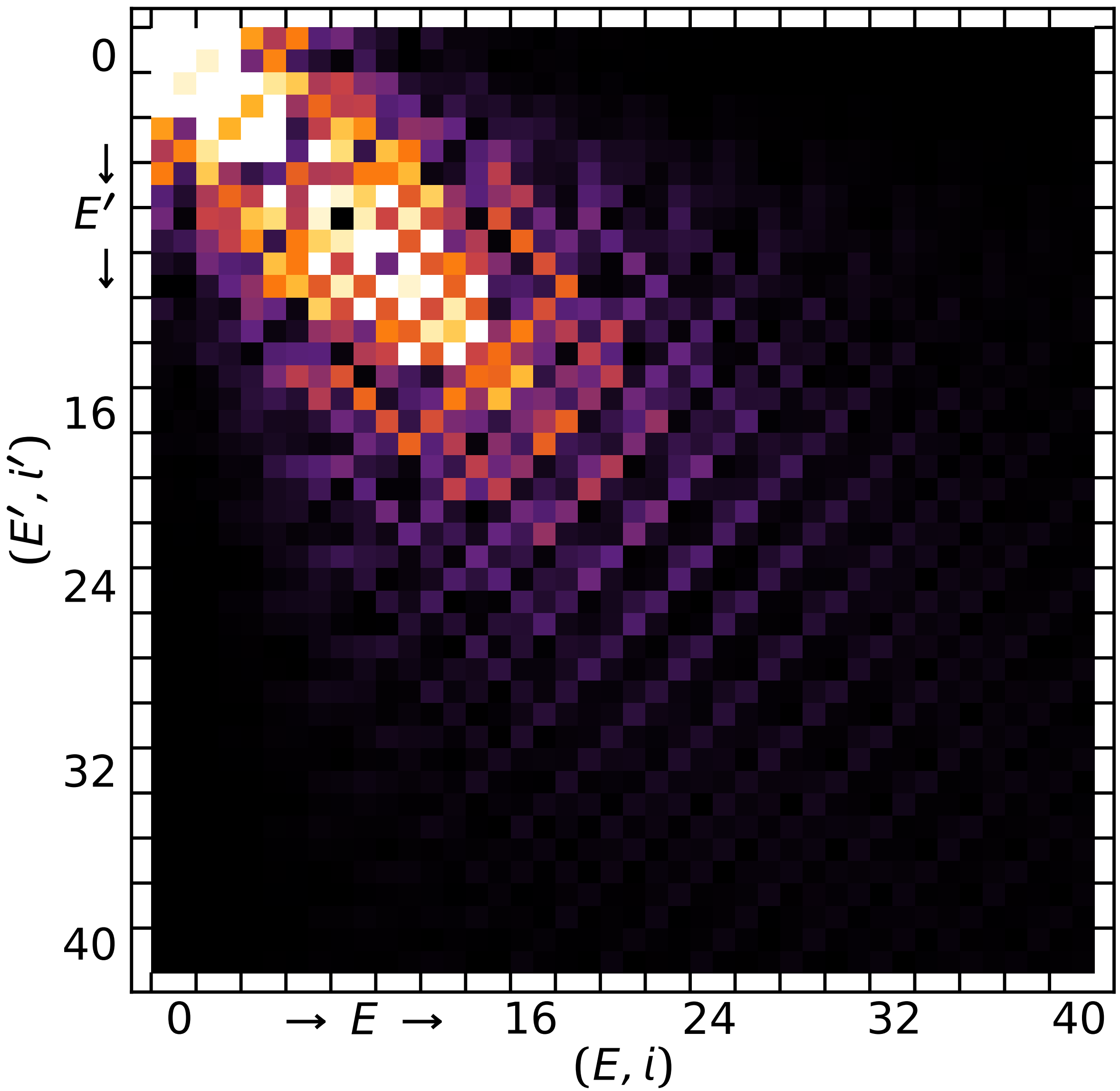
$J^\pi = 1^+, T = 0, \hbar\Omega = 28\,\mathrm{MeV}$

momentum space $^3S_1$



SRG Evolution in Two-Body Space

2B-Jacobi HO matrix elements

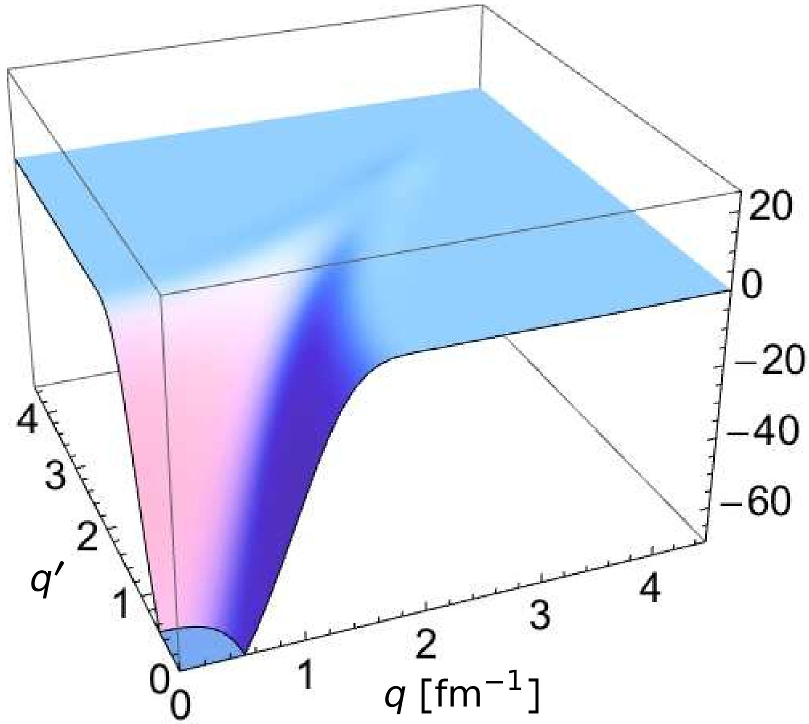


$\alpha = 0.32\,\mathrm{fm}^4$

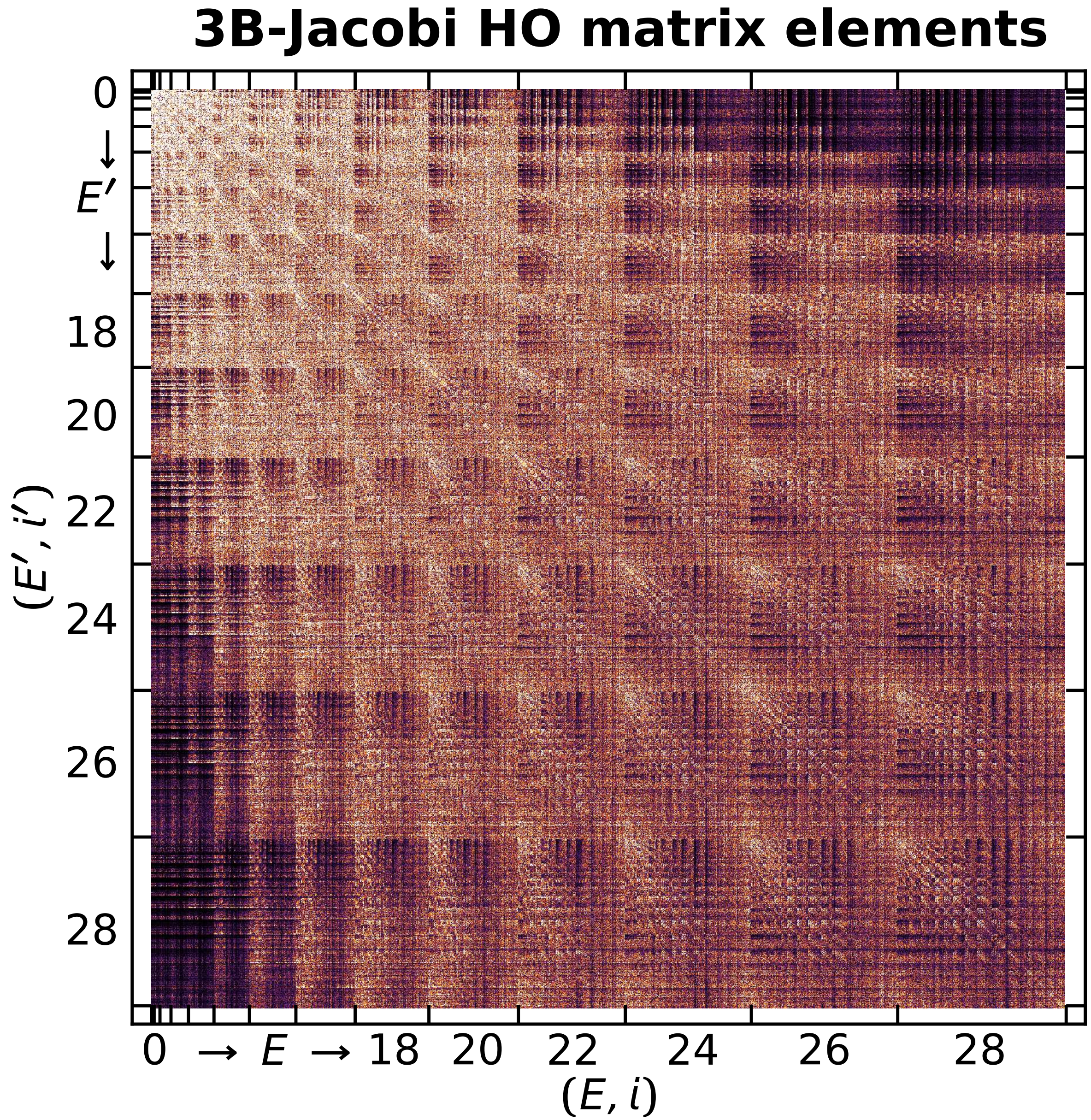
$\Lambda = 1.33\,\mathrm{fm}^{-1}$

$J^\pi = 1^+, T = 0, \hbar\Omega = 28\,\mathrm{MeV}$

momentum space $^3S_1$



SRG Evolution in Three-Body Space



$$\alpha = 0.00\,\mathrm{fm}^4$$

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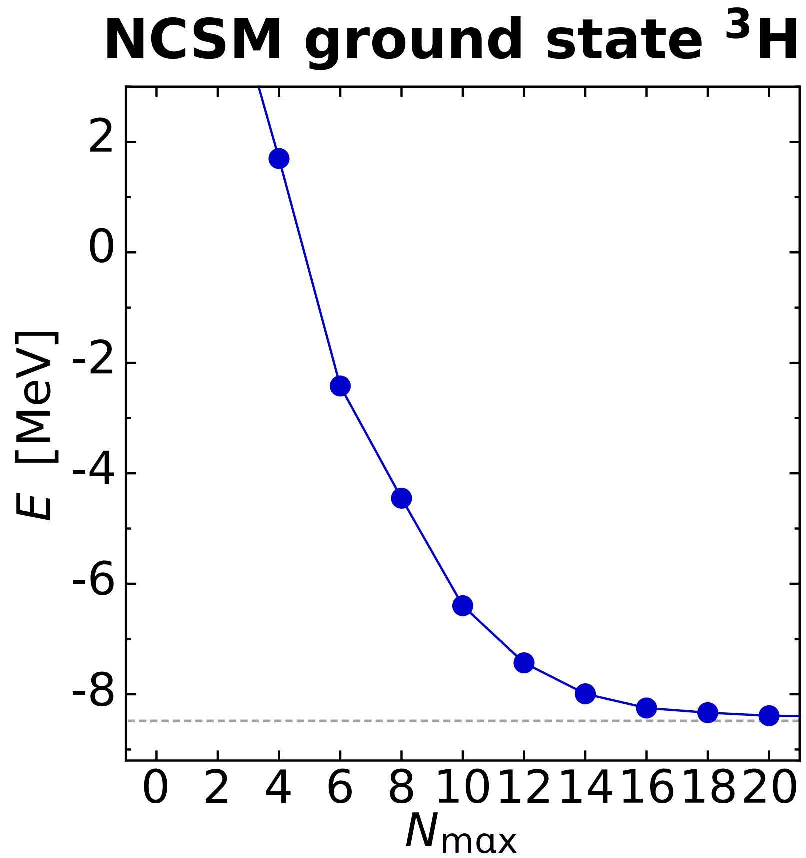
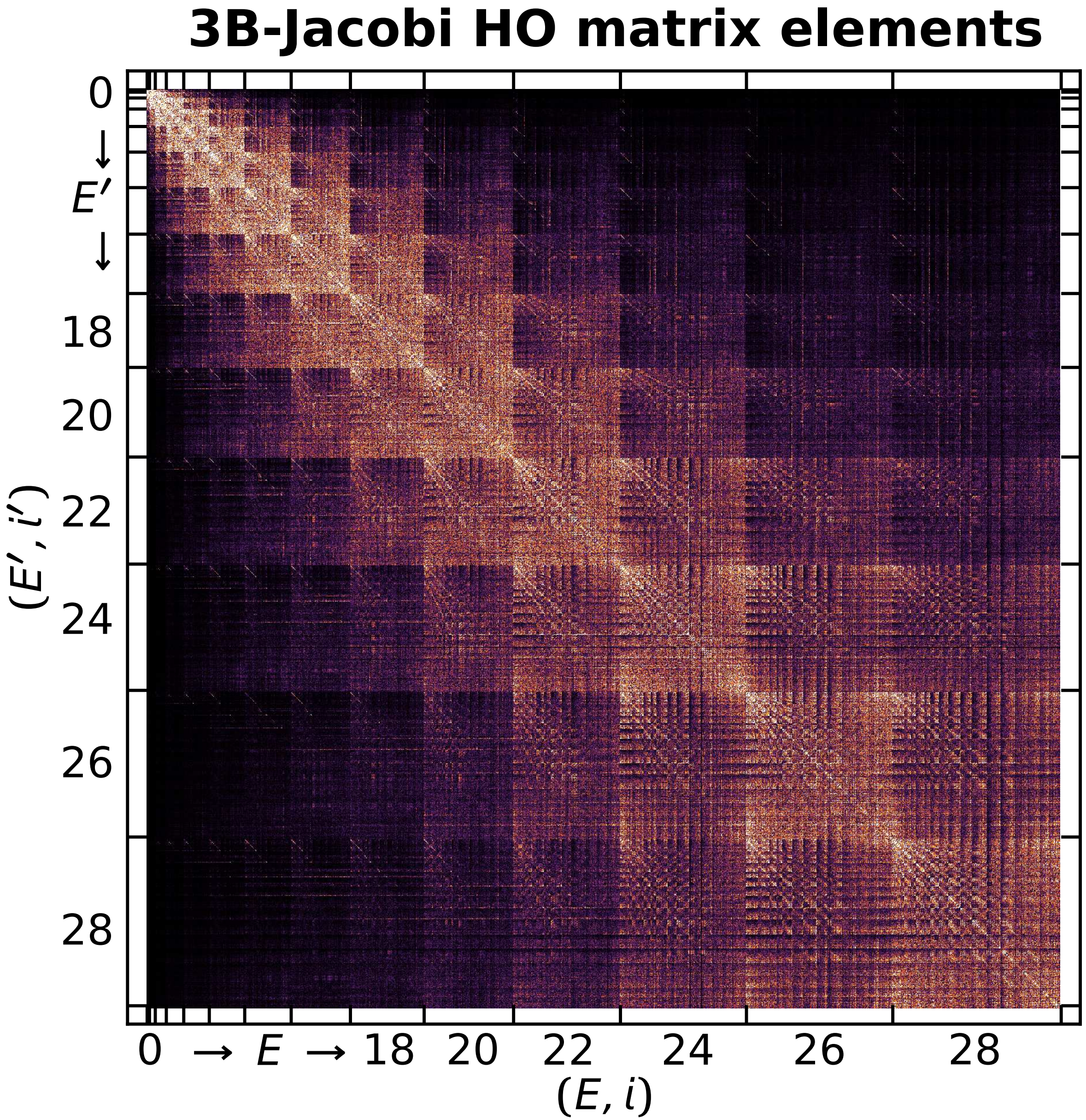
$J^\pi = \frac{1}{2}^+, T = \frac{1}{2}, \hbar\Omega = 28\,\mathrm{MeV}$



SRG Evolution in Three-Body Space



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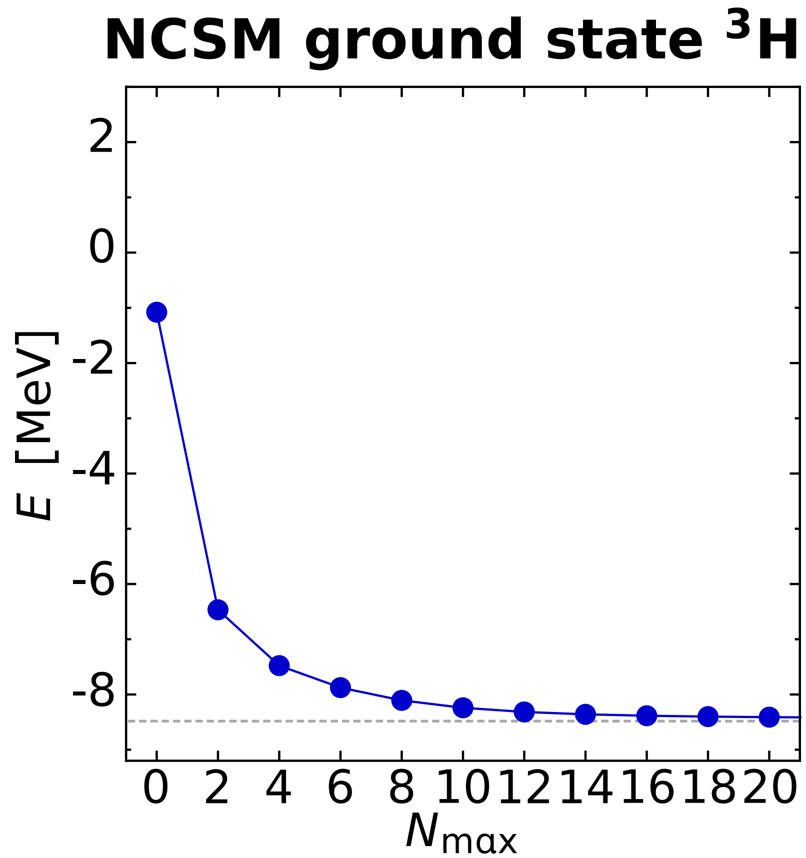


Calculations in *A*-Body Space

- **cluster decomposition**: decompose evolved Hamiltonian from 2B/3B space into irreducible *n*-body contributions $\widetilde{\mathrm{H}}_{\alpha}^{[n]}$

$$\widetilde{\mathrm{H}}_{\alpha} = \widetilde{\mathrm{H}}_{\alpha}^{[1]} + \widetilde{\mathrm{H}}_{\alpha}^{[2]} + \widetilde{\mathrm{H}}_{\alpha}^{[3]} + \ldots$$

- **cluster truncation**: can construct cluster-orders up to $n = 3$ from evolution in 2B and 3B space, have to discard $n > 3$
  - only the **full evolution in *A*-body space** conserves *A*-body energy eigenvalues and, thus, independent of α
  - α-dependence of eigenvalue… **…milto-nian** measures impact of…

α-variation provides a **diagnostic tool** to assess the contributions of omitted many-body interactions

Sounds easy, but...

❶ computation of initial 2B/3B-Jacobi HO matrix elements of chiral NN+3N interactions

- we use Petr Navratil's ManyEff code for computing 3B-Jacobi matrix elements and corresponding CFPs

❷ SRG evolution in 2B/3B space and cluster decomposition

- efficient implementation using adaptive ODE solver; largest block takes a few hours on single node

❸ transformation of 2B/3B Jacobi HO matrix elements into JT-coupled representation

- formulated transformation directly into JT-coupled scheme; highly efficient implementation; can handle $E_{3\,\mathrm{max}} = 16$ in JT-coupled scheme

❹ data management and on-the-fly decoupling in many-body codes

- invented optimized storage scheme for fast on-the-fly decoupling; can keep all matrix elements up to $E_{3\,\mathrm{max}} = 16$ in memory

Exact Ab Initio Calculations

Importance Truncated NCSM

Navrátil, Roth & Quaglioni — Phys. Rev. C 82, 034609 (2010)
Roth — Phys. Rev. C 79, 064324 (2009)
Roth, Gour & Piecuch — Phys. Lett. B 679, 334 (2009)
Roth, Gour & Piecuch — Phys. Rev. C 79, 054325 (2009)
Roth & Navrátil — Phys. Rev. Lett. 99, 092501 (2007)

Importance Truncated NCSM

NCSM is one of the most powerful and universal exact ab initio methods

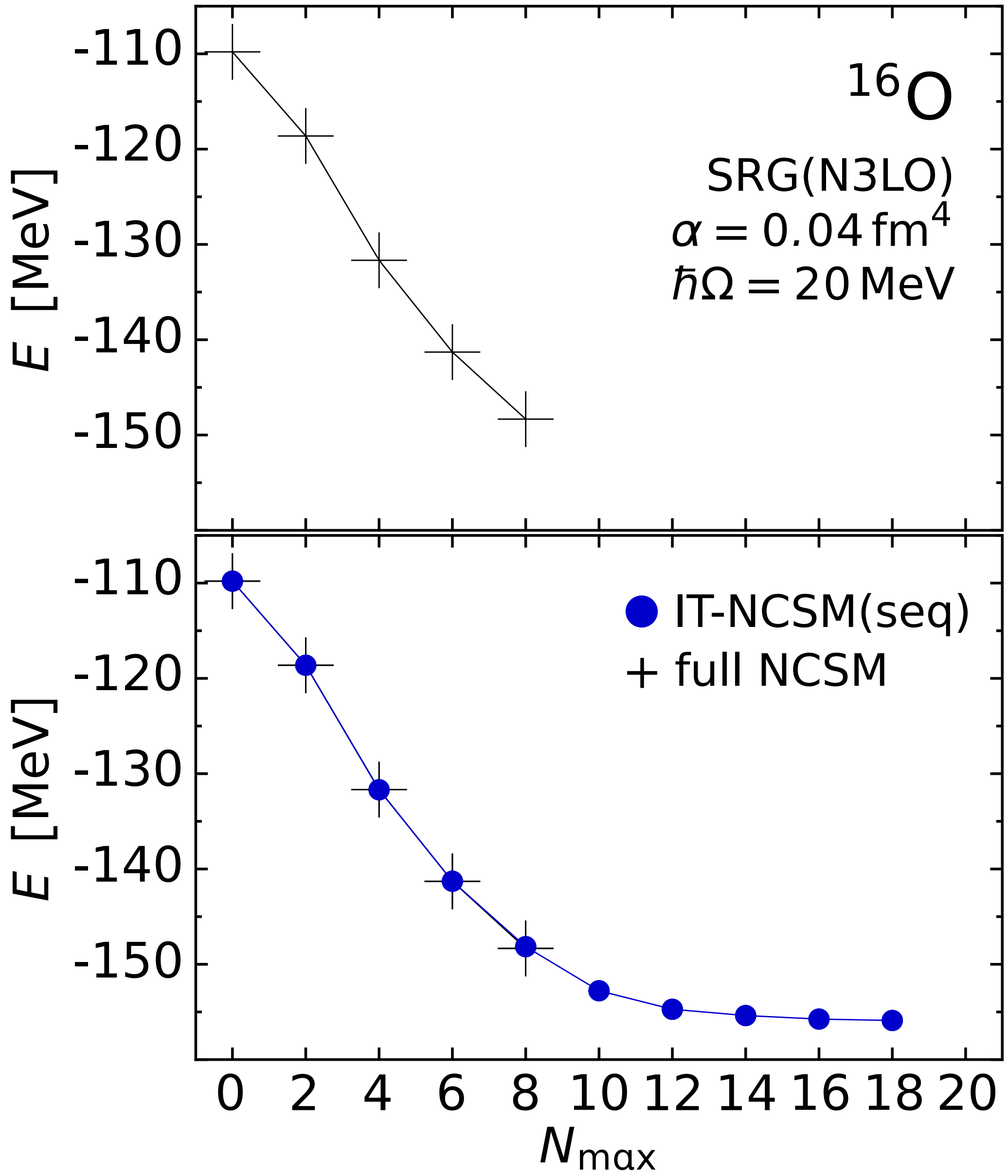
- compute low-lying eigenvalues of the Hamiltonian in a **model space of HO Slater determinants** truncated w.r.t. HO excitation energy $N_{\mathrm{max}}\hbar\Omega$
- **all relevant observables** can be computed from the eigenstates
- range of applicability limited by **factorial growth** of Slater-determinant basis with N_{max} and A
- adaptive **importance truncation** extends the range of NCSM by reducing the model space to physically relevant states
- we have developed a **parallelized IT-NCSM/NCSM code** capable of handling 3N matrix elements up to $E_{3\,\mathrm{max}} = 16$

Importance Truncated NCSM

- converged NCSM calculations essentially restricted to lower/mid p-shell
- full 10 or $12\hbar\Omega$ calculation for ^{16}O not really feasible (basis dimension > 10^{10})

Importance Truncation

reduce NCSM space to the relevant basis states using an **a priori importance measure** derived from MBPT



Importance Truncation: General Idea

- given an initial approximation $\left|\Psi_{\text{ref}}^{(m)}\right\rangle$ for the **target states**
- **measure the importance** of individual basis state $\left|\Phi_\nu\right\rangle$ via first-order multiconfigurational perturbation theory

$$\kappa_\nu^{(m)} = -\frac{\left\langle\Phi_\nu\right| \mathrm{H} \left|\Psi_{\text{ref}}^{(m)}\right\rangle}{\epsilon_\nu - \epsilon_{\text{ref}}}$$

- construct **importance truncated space** spanned by basis states with $|\kappa_\nu^{(m)}| \geq \kappa_{\min}$ and solve eigenvalue problem
- **sequential scheme**: construct importance truncated space for next $N_{\max}$ using previous eigenstates as reference $\left|\Psi_{\text{ref}}^{(m)}\right\rangle$
- a posteriori **threshold extrapolation** and **perturbative correction** used to recover contribution from discarded basis states

Applications

IT-NCSM with SRG-Evolved Chiral NN+3N Interactions

A Tale of Three Hamiltonians

- **NN only**: start with NN-only initial Hamiltonian and evolve in two-body space

$$\tilde{H}_{\alpha}^{\text{NN-only}} = T_{\text{int}} + \tilde{T}_{\text{int},\alpha}^{[2]} + \tilde{V}_{\text{NN},\alpha}^{[2]}$$

- **NN+3N-induced**: start with NN-only initial Hamiltonian and evolve in three-body space

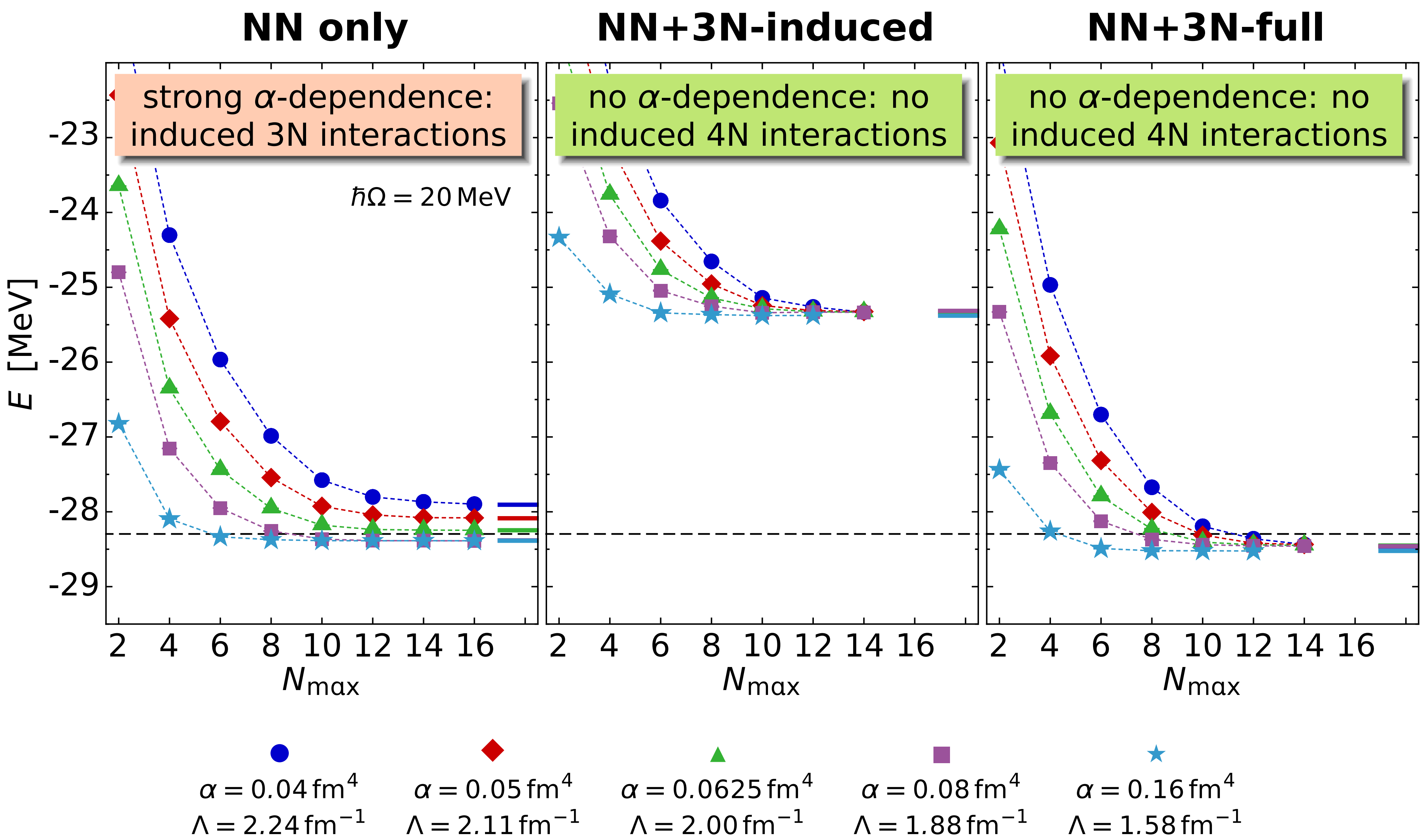
$$\tilde{H}_{\alpha}^{\text{NN+3N-induced}} = T_{\text{int}} + \tilde{T}_{\text{int},\alpha}^{[2]} + \tilde{V}_{\text{NN},\alpha}^{[2]} + \tilde{T}_{\text{int},\alpha}^{[3]} + \tilde{V}_{\text{NN},\alpha}^{[3]}$$

- **NN+3N-full**: start with NN+ … in three-body space

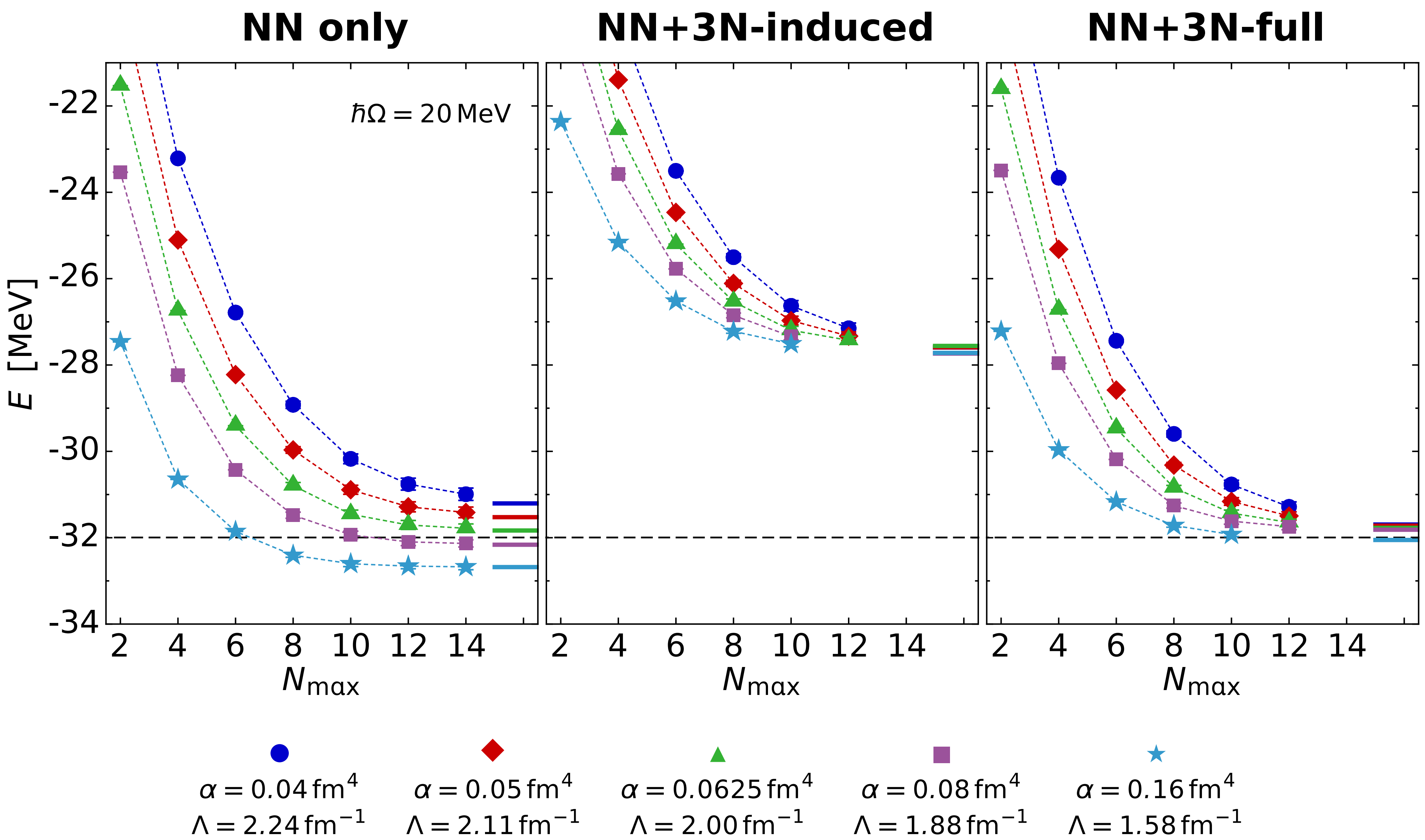
$$\tilde{H}_{\alpha}^{\text{NN+3N-full}} = T_{\text{int}} + \tilde{T}_{\text{int},\alpha}^{[\dots]} \dots$$

α-variation provides a **diagnostic tool** to assess the contributions of omitted many-body interactions

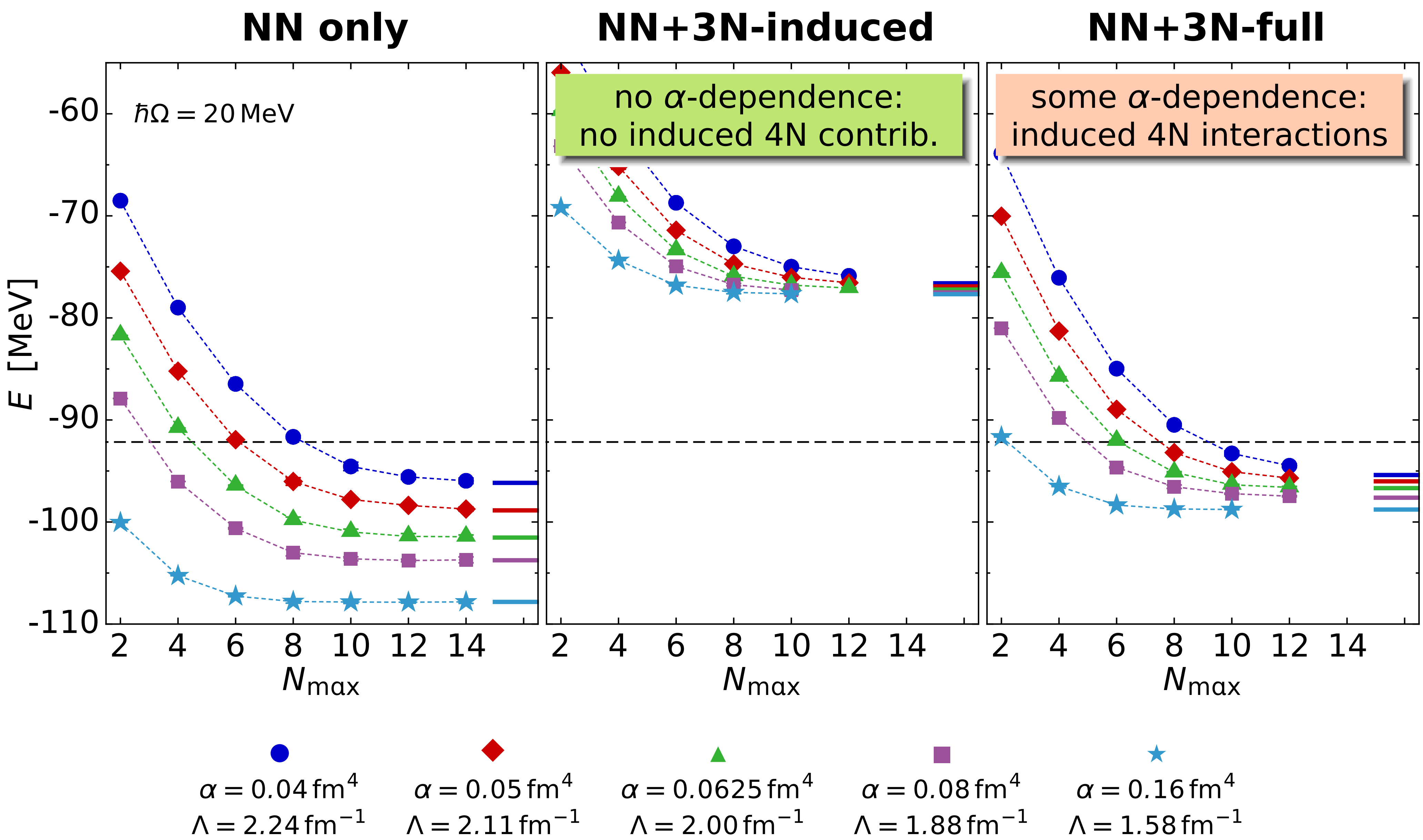
^{4}He: Ground-State Energies



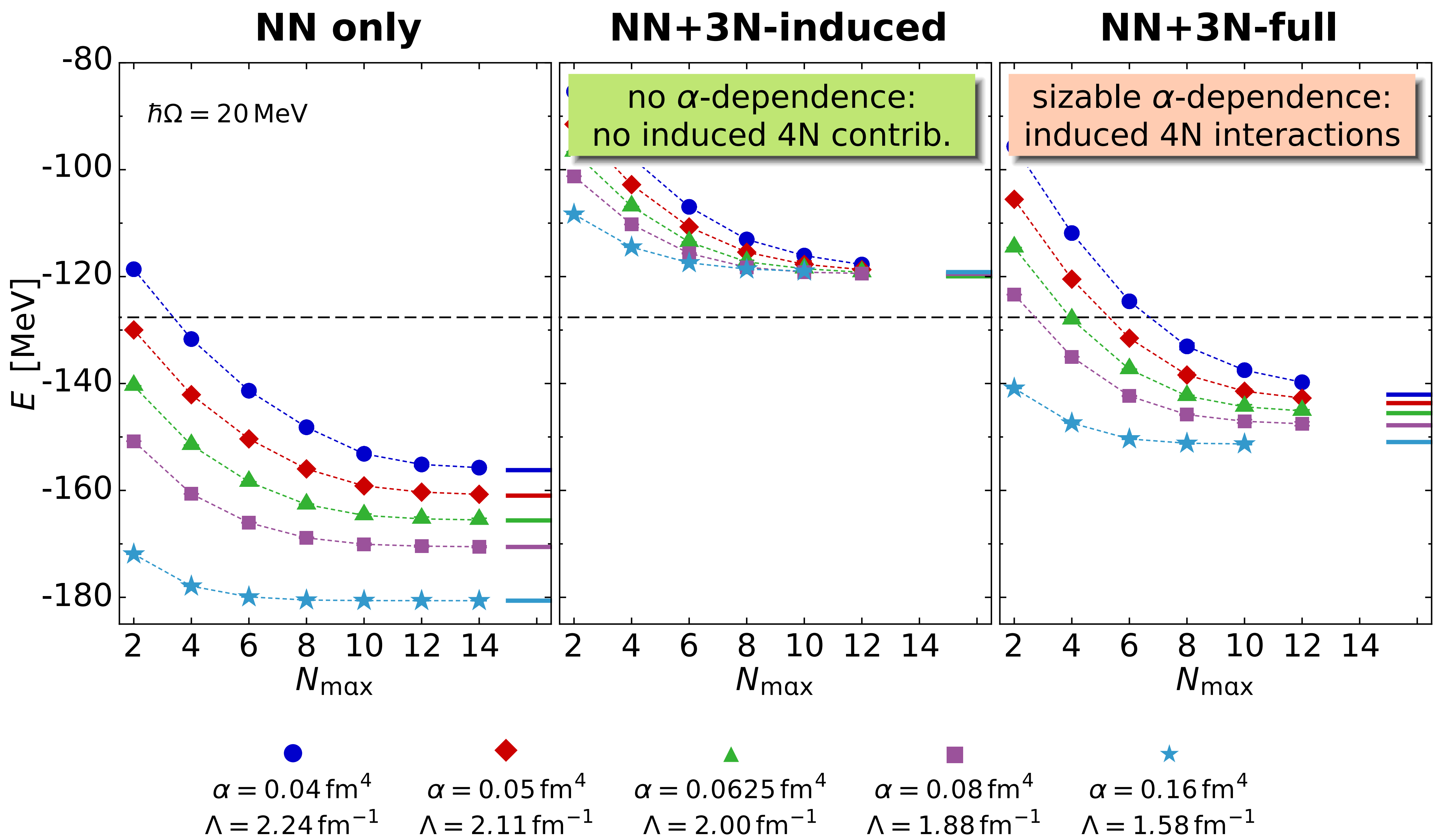
^{6}Li: Ground-State Energies



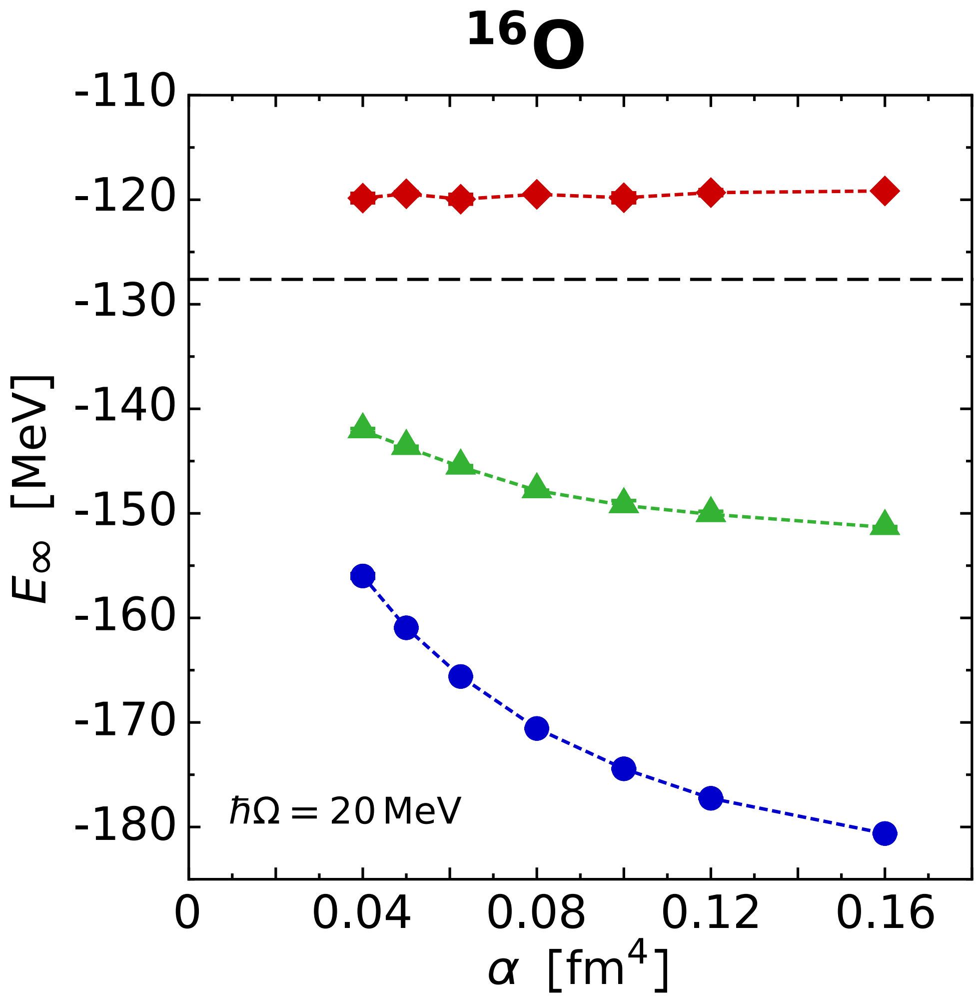
^{12}C: Ground-State Energies



^{16}O: Ground-State Energies



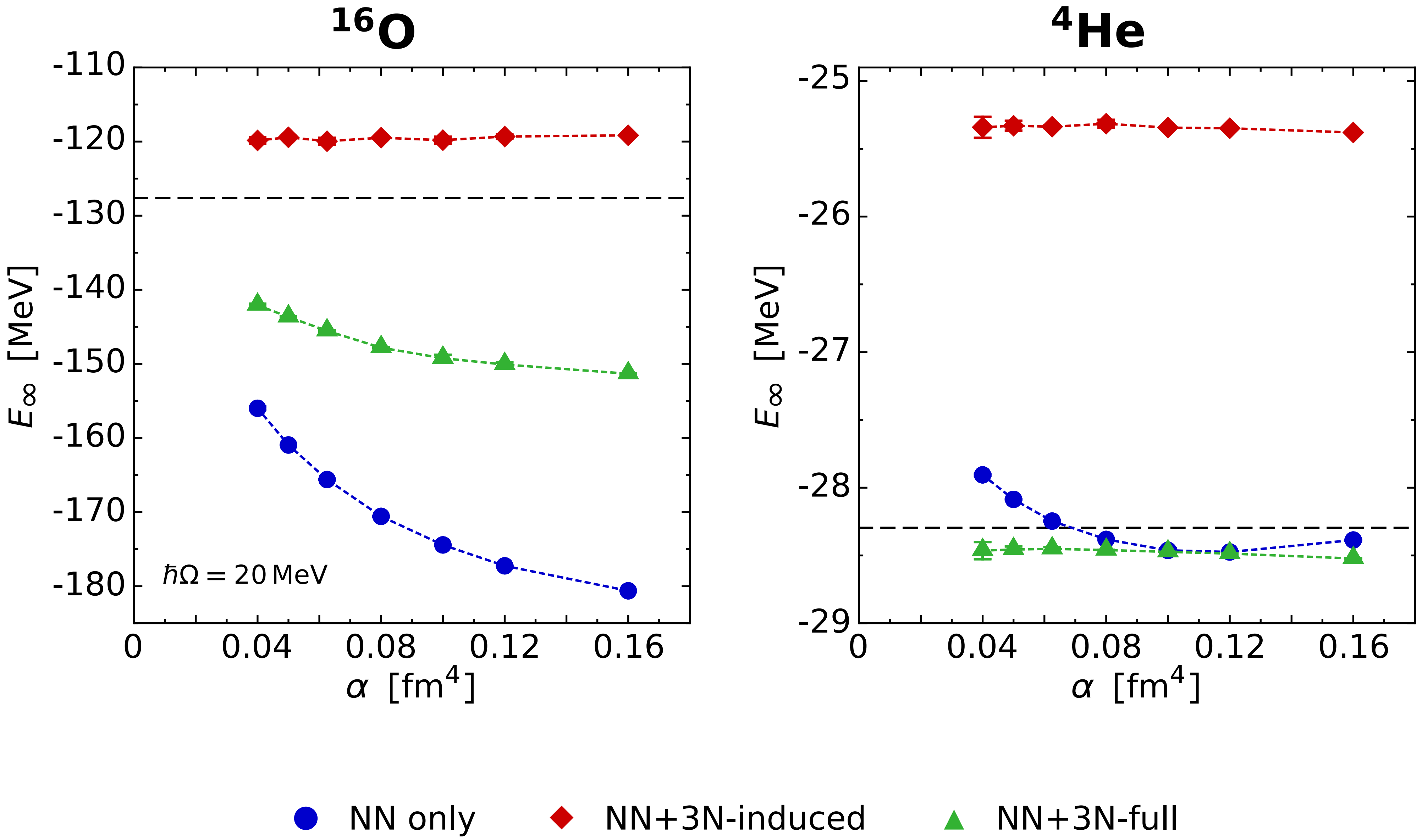
^{16}O: Energy vs. Flow Parameter



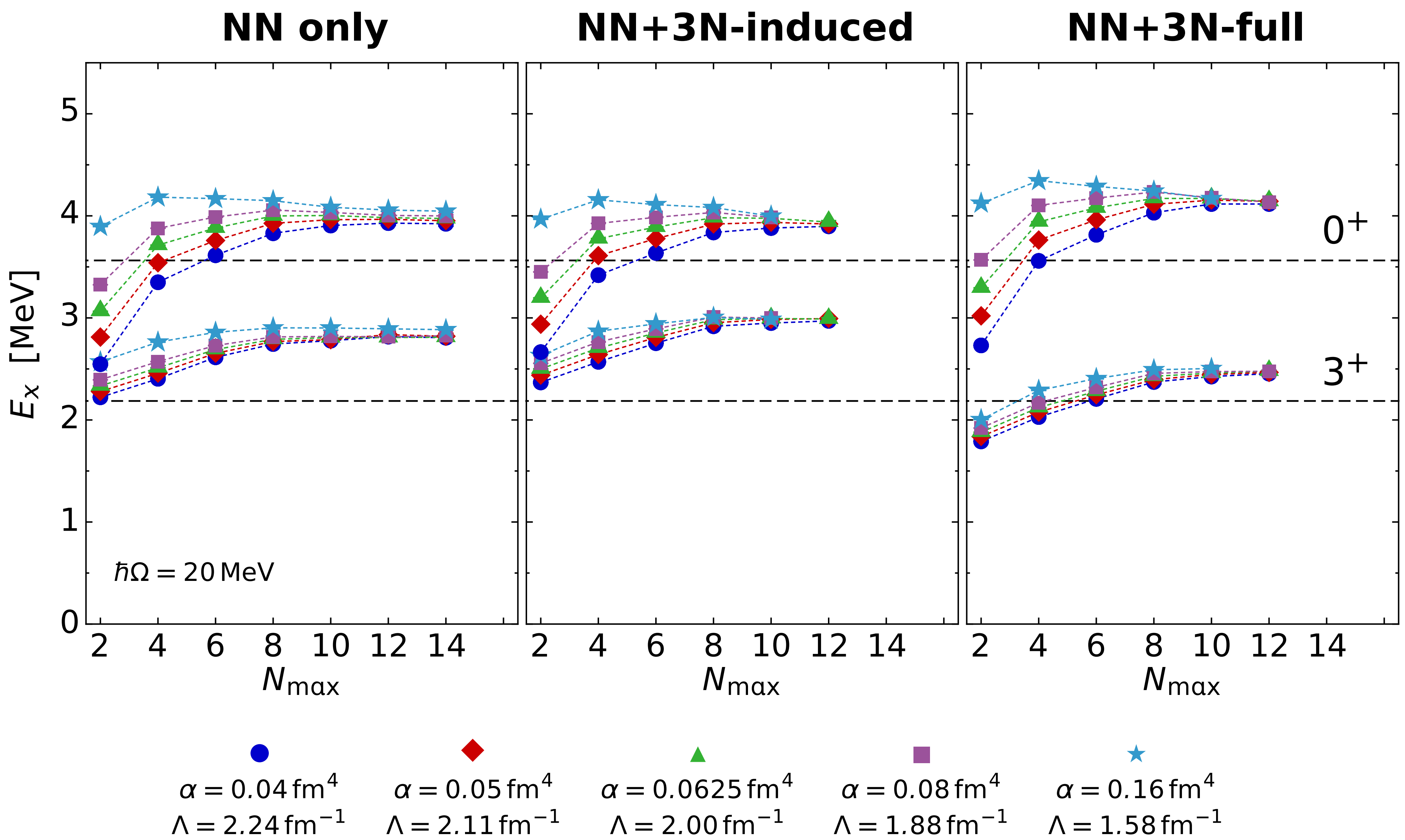
- **NN only**: strong α-dependence ➔ significant induced 3N contributions
- **NN+3N-induced**: no α-dependence ➔ all relevant induced terms from initial NN captured at 3N level
- **NN+3N-full**: sizable α-dependence ➔ additional induced terms caused by initial 3N appear at 4N level

● NN only ◆ NN+3N-induced ▲ NN+3N-full

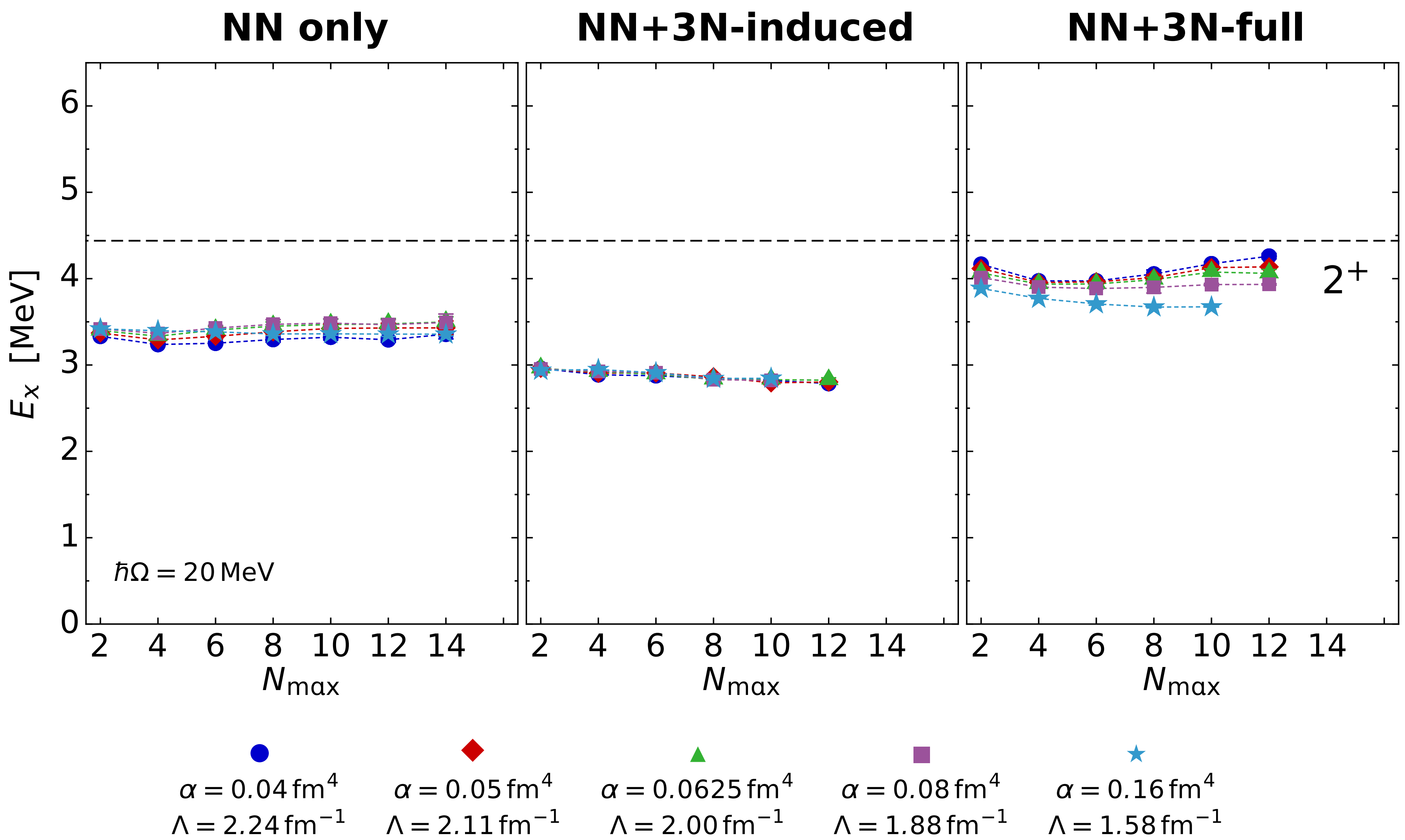
^{16}O & ^{4}He: Energy vs. Flow Parameter



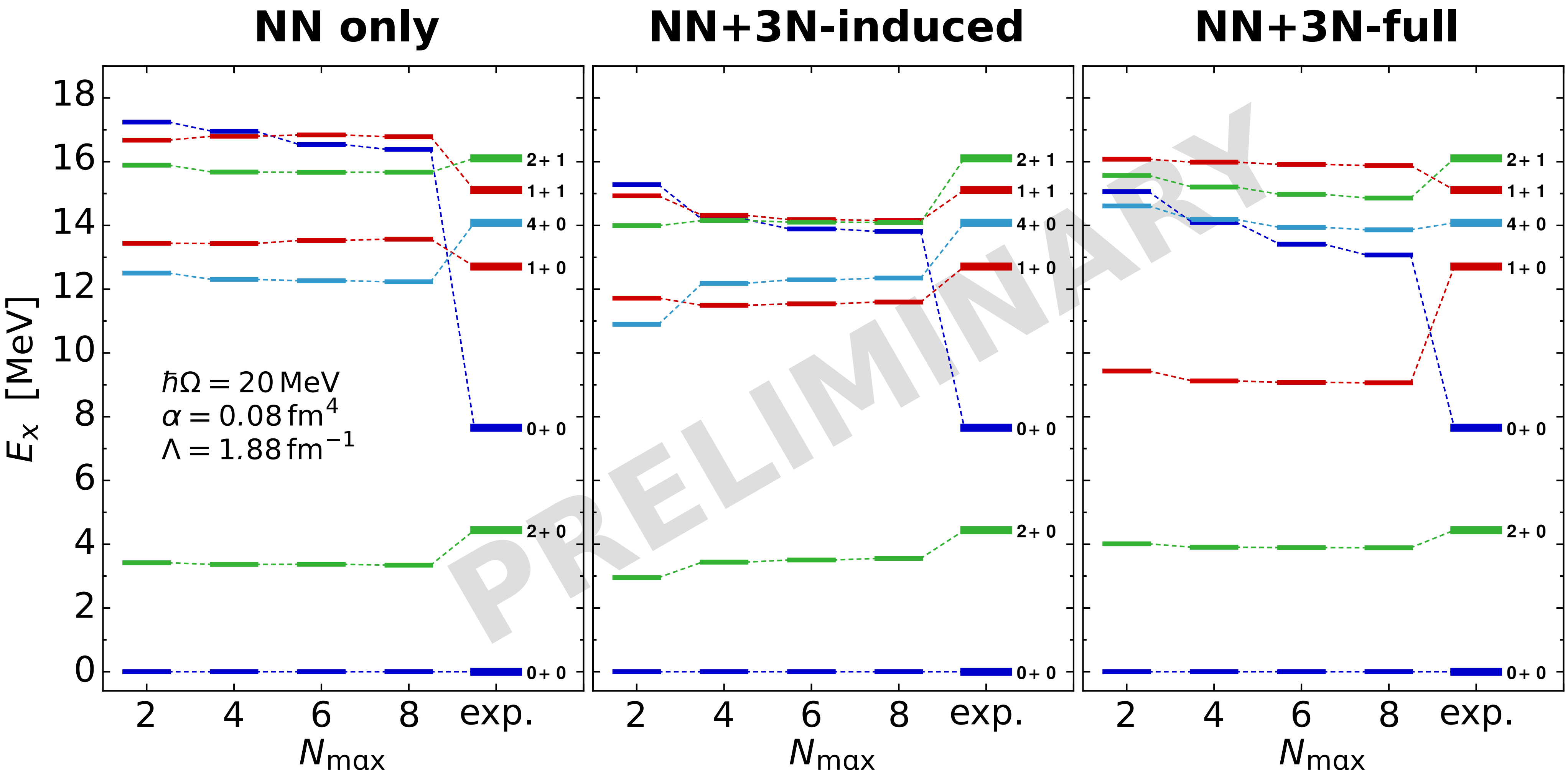
^{6}Li: Excitation Energies



^{12}C: Excitation Energies



^{12}C: Spectroscopy



- spectroscopy of heavy Carbon isotopes (e.g., ^{16}C, ^{18}C) next...

Conclusions

Conclusions

- ab initio nuclear structure calculations with consistently SRG-evolved chiral NN+3N interactions
    - consistent SRG evolution up to the 3N level
    - efficient transformation and management of JT-coupled 3N matrix elements
    - IT-NCSM with full 3N interactions up to $N_{\mathrm{max}} = 12$ (14) for all p-shell nuclei (and lower sd-shell)
- indications that induced 4N contributions resulting from initial 3N interaction become significant beyond mid-p-shell
- use modified SRG generators to suppress induced 4N contributions from the outset
- many exciting applications ahead...

Epilogue

- **thanks to my group & my collaborators**
  - **S. Binder**, **A. Calci**, B. Erler, A. Günther, M. Hild, H. Krutsch, **J. Langhammer**, P. Papakonstantinou, S. Reinhardt, F. Schmitt, C. Stumpf, R. Wirth

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DFG

HIC for FAIR
Helmholtz International Center

LOEWE – Landes-Offensive zur Entwicklung Wissenschaftlich-ökonomischer Exzellenz

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