# Importance Truncated NCSM
with
# Chiral NN plus 3N Interactions

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# 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**

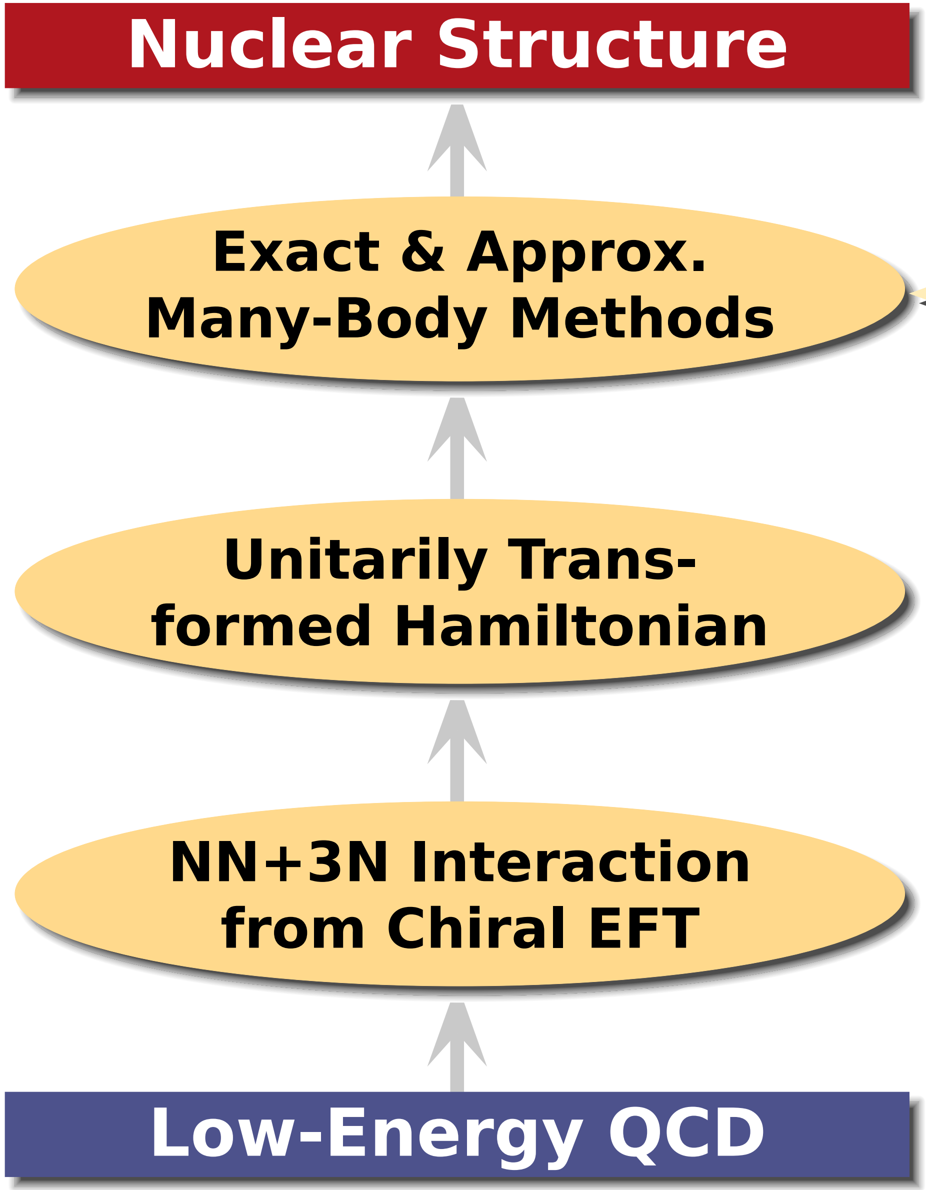
**Unitarily Transformed Hamiltonian**

**NN+3N Interaction from Chiral EFT**

**Low-Energy QCD**

- 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

# From QCD to Nuclear Structure




- ‘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 Trans-formed Hamiltonian**

↑

**NN+3N Interaction from Chiral EFT**

↑

**Low-Energy QCD**

**focus on consistent inclusion of chiral 3N interaction**

# 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 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 $U_\alpha$ depending on generator $\eta_\alpha$

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

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

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

# 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: $\left|Ei J^\pi T\right\rangle$

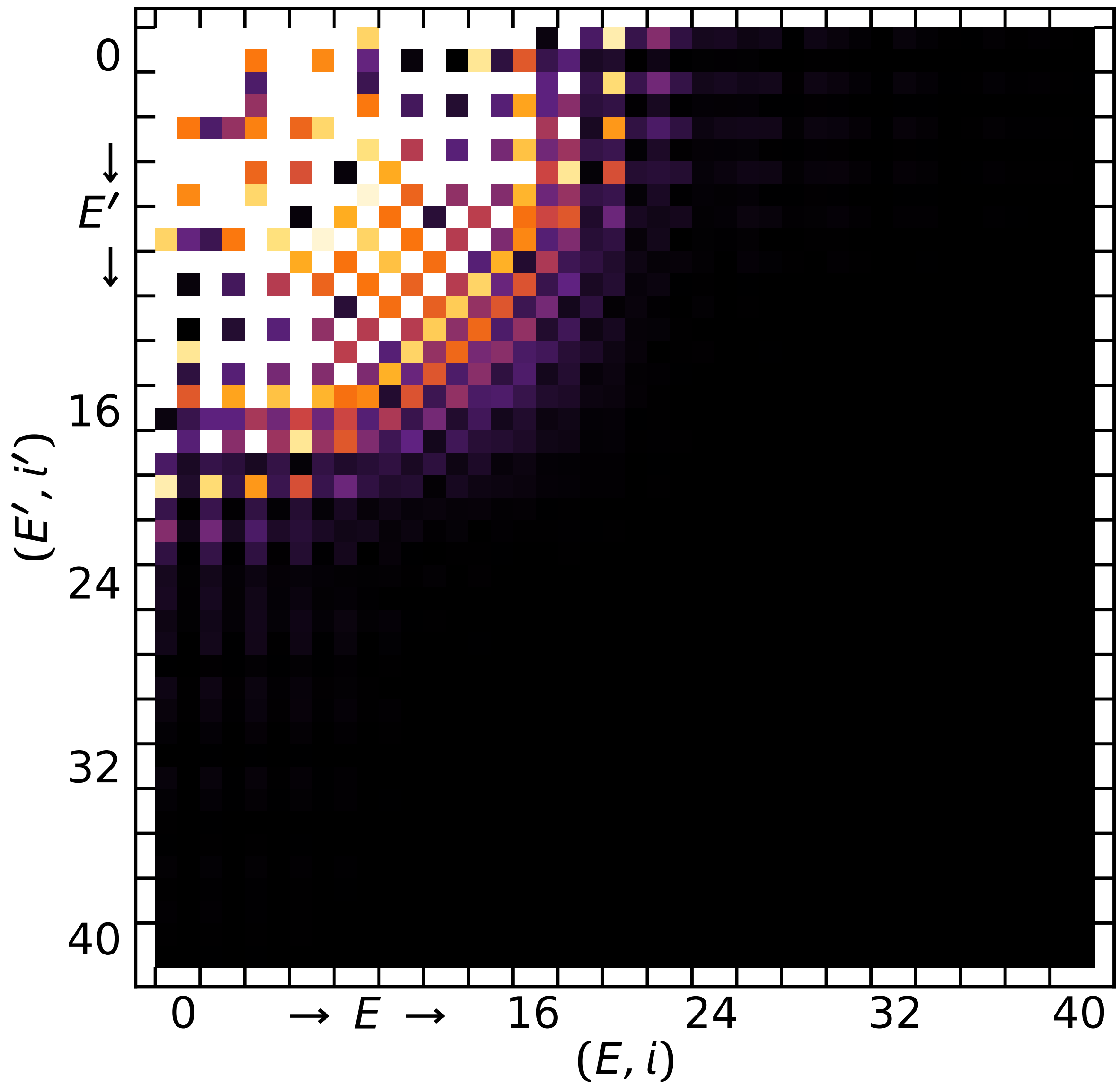
- system of **coupled evolution equations** for each $(J^\pi T)$-block

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

- 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**

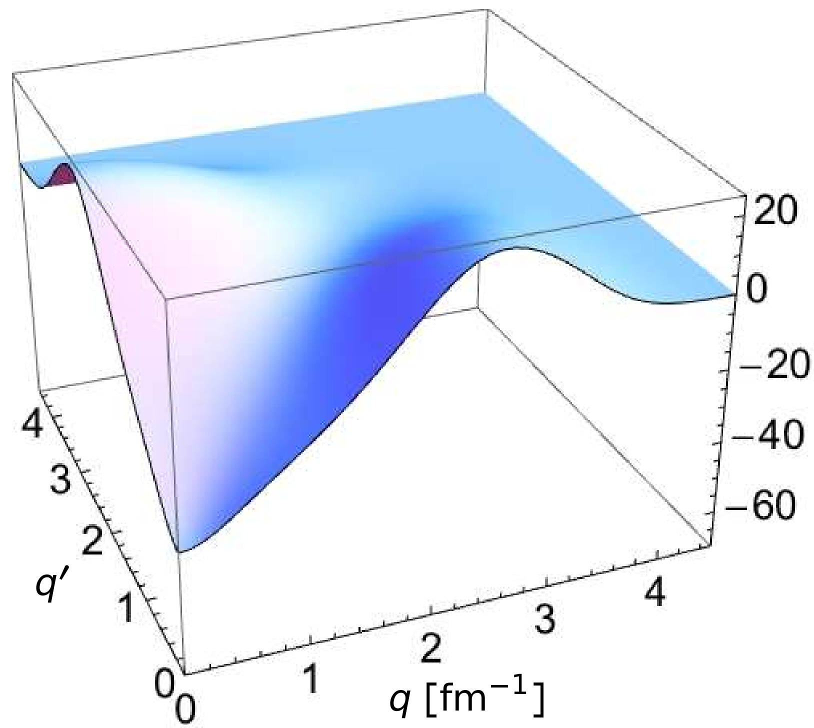



$\alpha = 0.00\,\text{fm}^4$

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

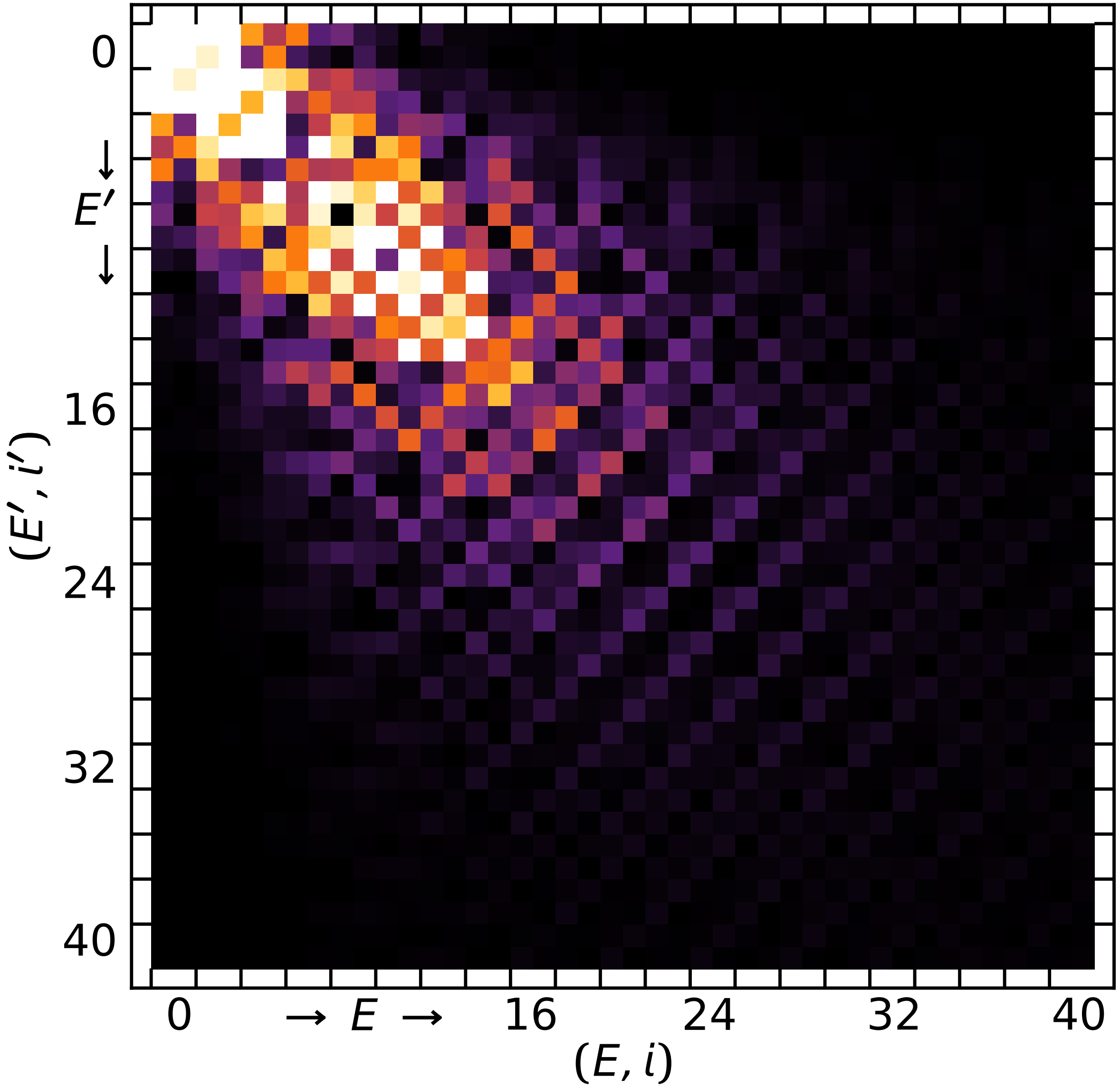
$J^\pi = 1^+, T = 0, \hbar\Omega = 28\,\text{MeV}$

**momentum space $^3S_1$**



# SRG Evolution in Two-Body Space

**2B-Jacobi HO matrix elements**




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

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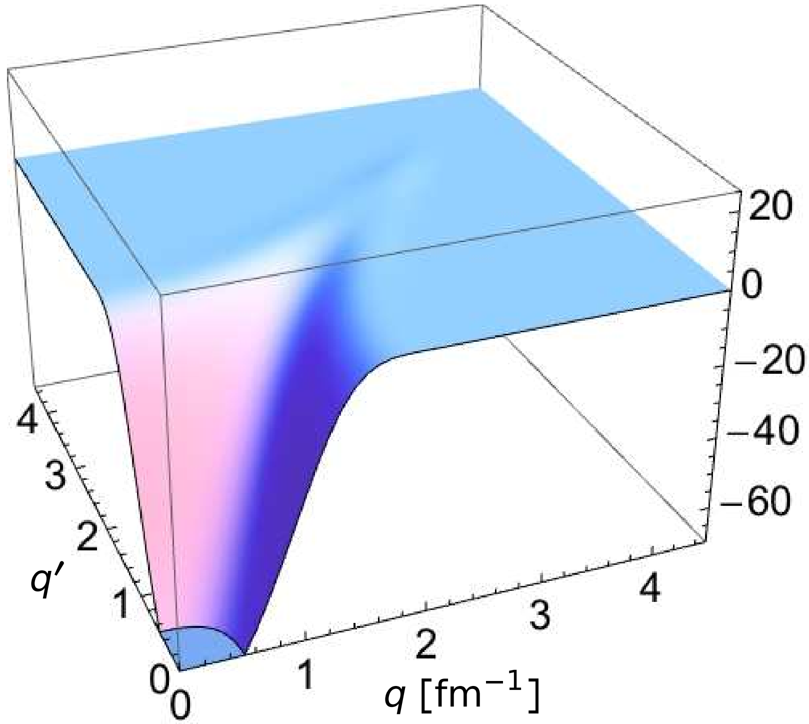
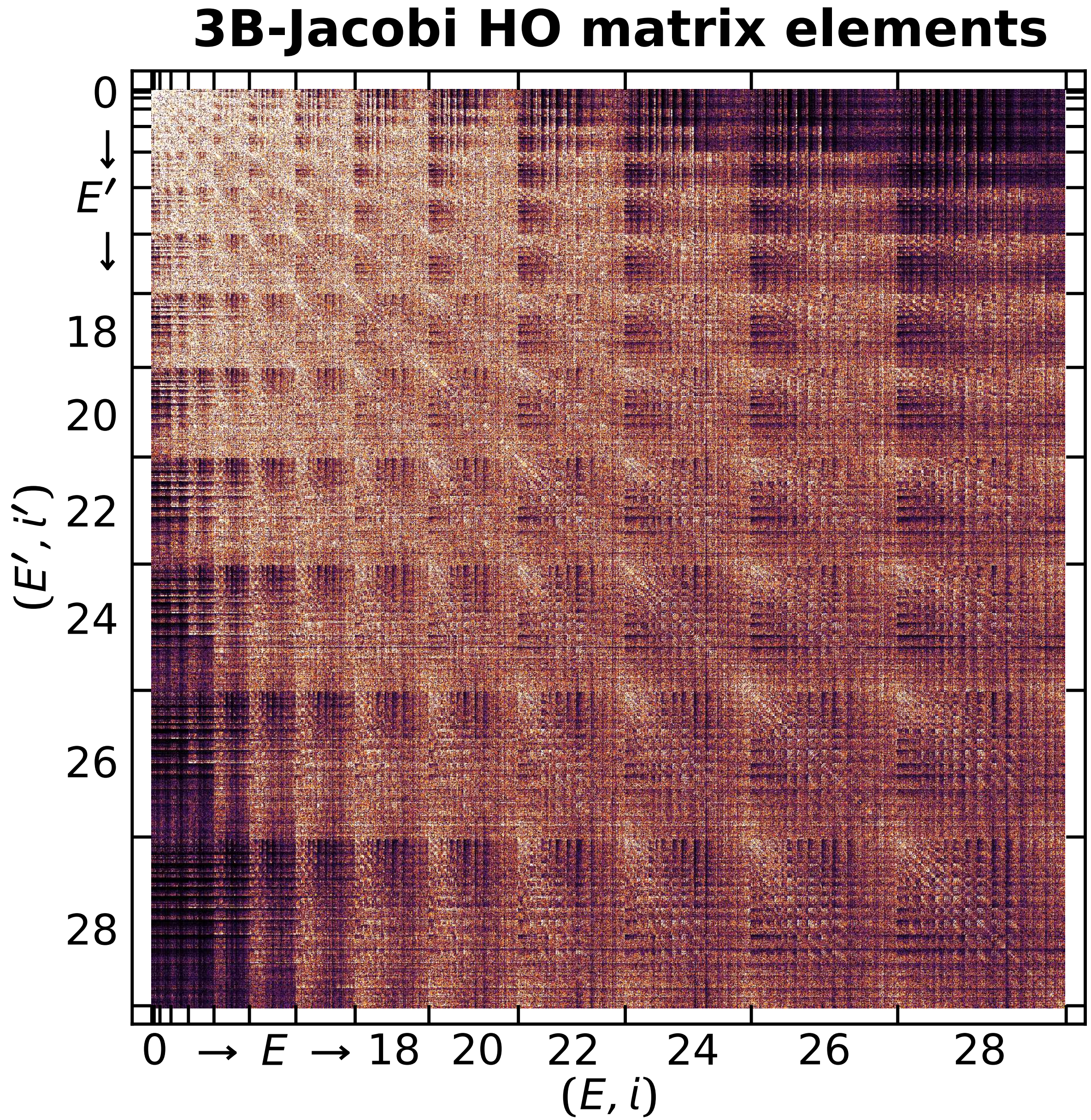
$J^\pi = 1^+, T = 0, \hbar\Omega = 28\,\mathrm{MeV}$

**momentum space** $^3S_1$



# SRG Evolution in Three-Body Space




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

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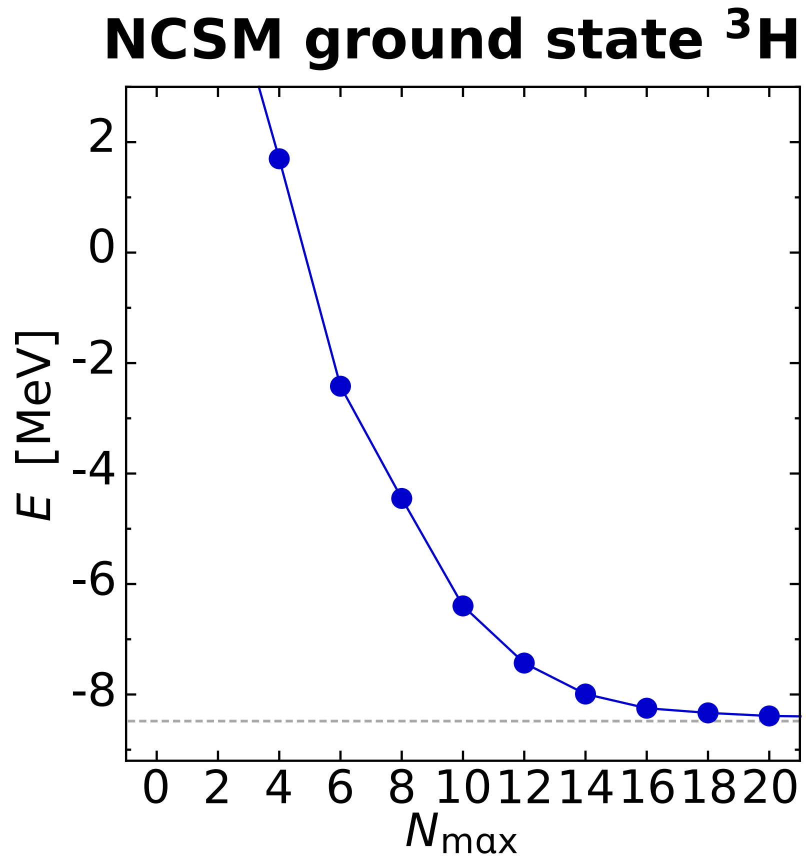
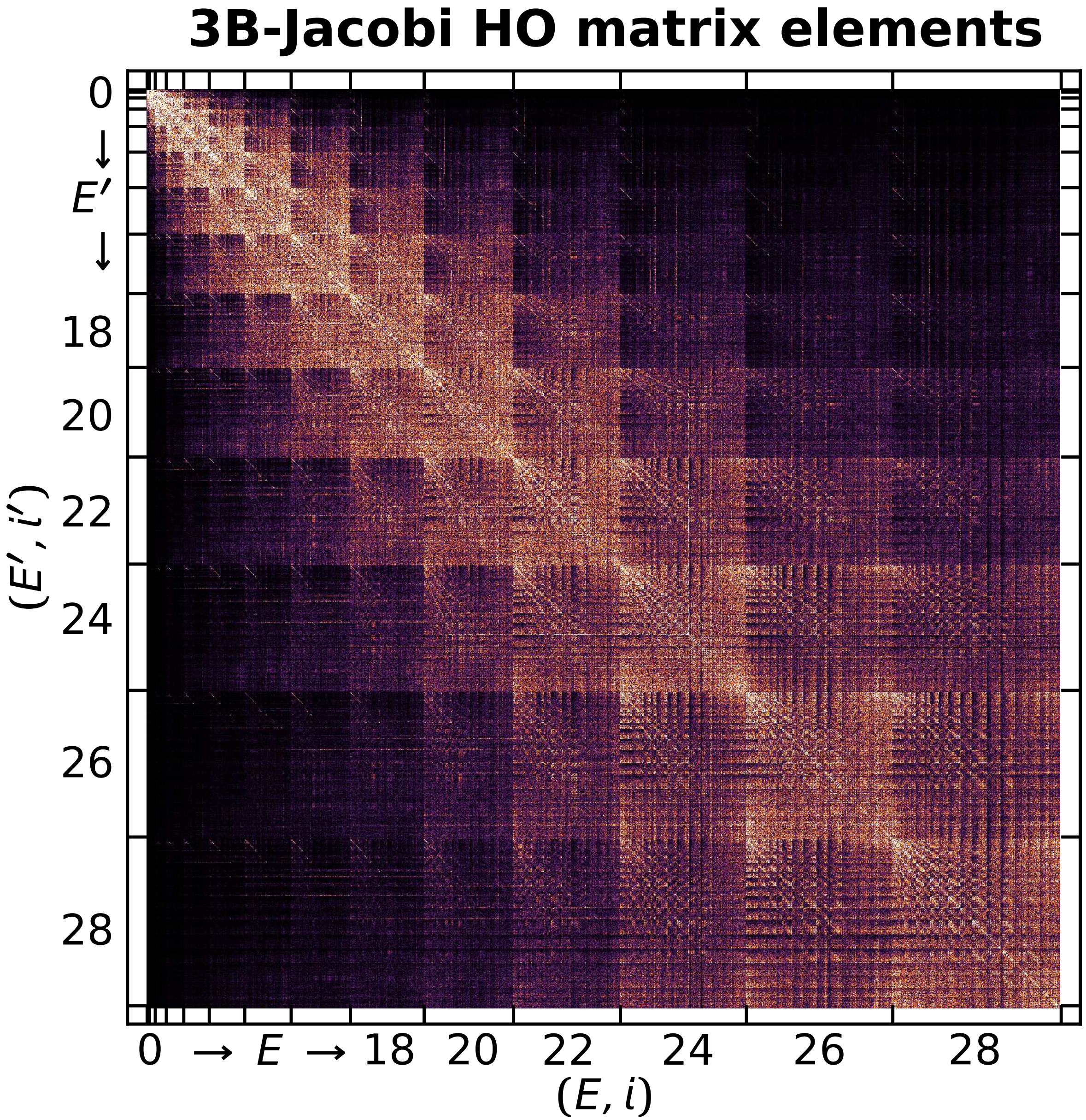
$J^\pi = \frac{1}{2}^+, T = \frac{1}{2}, \hbar\Omega = 28\,\mathrm{MeV}$



# SRG Evolution in Three-Body Space

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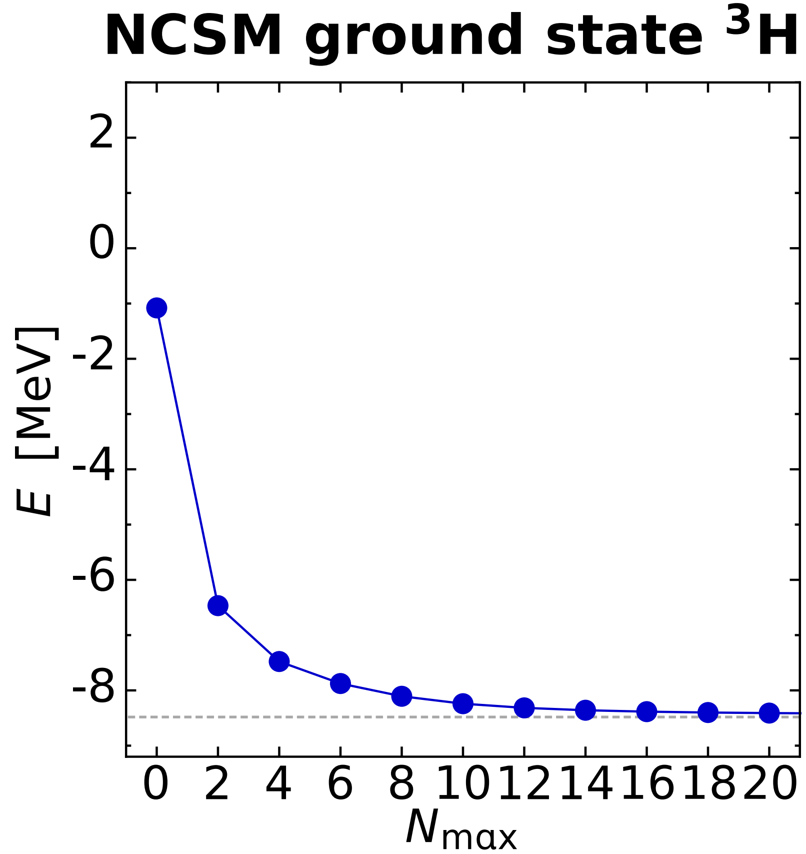
$J^\pi = \frac{1}{2}^+, T = \frac{1}{2}, \hbar\Omega = 28\,\mathrm{MeV}$



# Calculations in *A*-Body Space

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

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

- **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 $\alpha$
  - $\alpha$-dependence of eigenvalue… **…milto-nian** measures impact of…

$\alpha$-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 $E_{3\,\max} = 16$ 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 $E_{3\,\max} = 16$ in memory

Exact Ab-Initio Calculations

# Importance Truncated NCSM

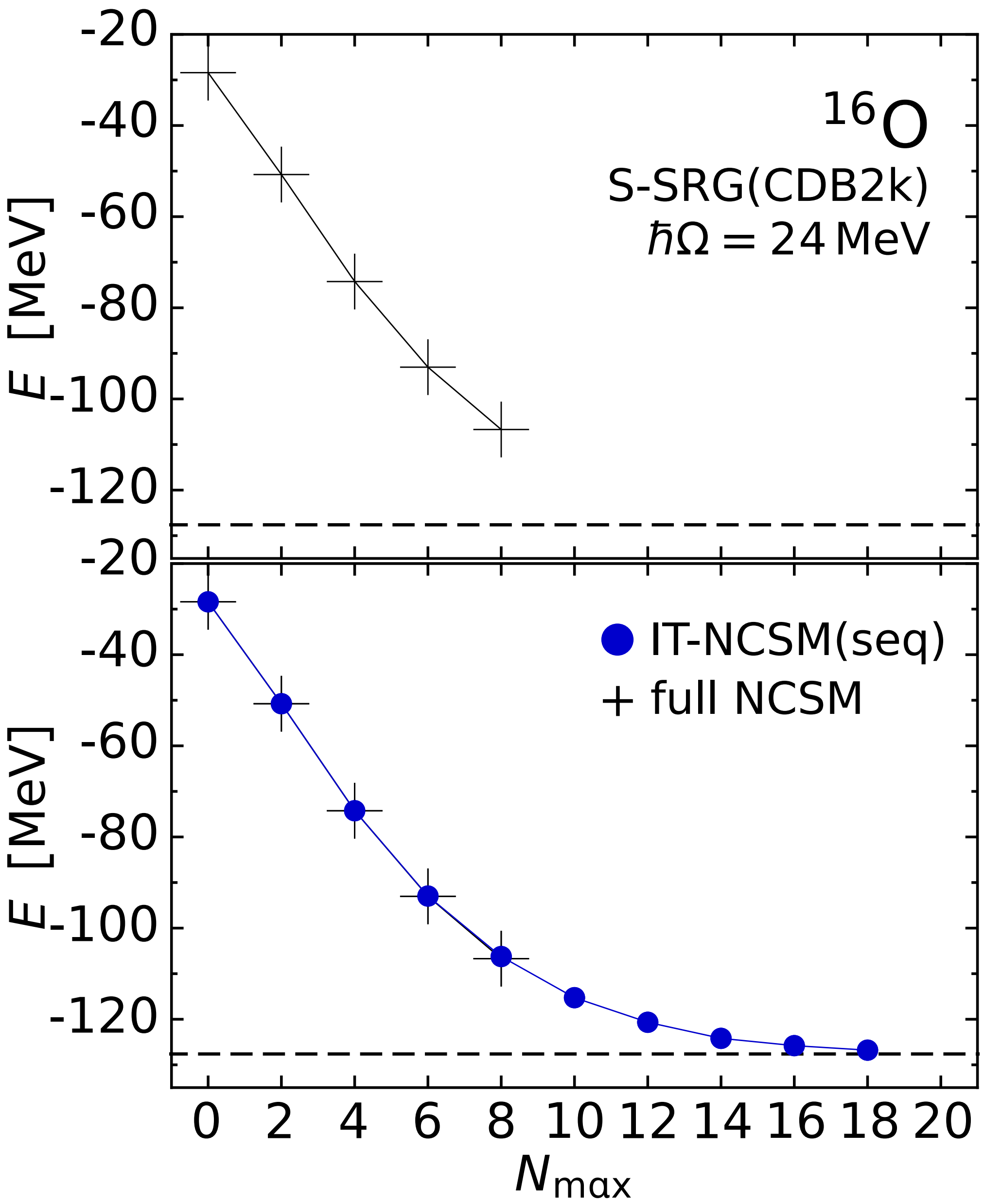

Navrátil, Roth & Quaglioni — Phys. Rev. C 82, 034609 (2010)
Roth — Phys. Rev. C 79, 064324 (2009)
Roth, Gour & Piecuch — Phys. Lett. B 679, 334 (2009)
Roth, Gour & Piecuch — Phys. Rev. C 79, 054325 (2009)
Roth & Navrátil — Phys. Rev. Lett. 99, 092501 (2007)

# Importance Truncated NCSM

- converged NCSM calculations essentially restricted to lower/mid p-shell
- full 10 or $12\hbar\Omega$ calculation for $^{16}O$ hardly 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: Basic Idea

- given a initial approximation $\left|\Psi_{\text{ref}}\right\rangle$ for the **target state** within a limited **reference space $\mathcal{M}_{\text{ref}}$**

$$\left|\Psi_{\text{ref}}\right\rangle = \sum_{\nu \in \mathcal{M}_{\text{ref}}} C_{\nu}^{(\text{ref})} \left|\Phi_{\nu}\right\rangle$$

- **measure the importance** of individual basis state $\left|\Phi_{\nu}\right\rangle \notin \mathcal{M}_{\text{ref}}$ via first-order multiconfigurational perturbation theory

$$\ldots \left\langle\Phi_{\nu}\right| \mathrm{H}_{\text{int}} \left|\Psi_{\text{ref}}\right\rangle \;/\; \ldots_{\text{ref}}$$

importance measure only probes 2p2h excitations on top of $\mathcal{M}_{\text{ref}}$ for a two-body Hamiltonian

- co… …nned by basis stat…

embed into iterative scheme to access full model space

- **solve eigenvalue problem** in … $\mathcal{M}(\kappa_{\text{min}})$ and obtain improved approxim… …get state

# Importance Truncation: Iterative Schemes

**IT-NCSM($i$) or IT-CI($i$)**

- simple iterative scheme for arbitrary model spaces

✪ start with $|\Psi_{\text{ref}}\rangle = |\Phi_0\rangle$

❶ construct importance truncated space containing up to 2p2h on top of $|\Psi_{\text{ref}}\rangle$

❷ solve eigenvalue problem

❸ use components of eigenstate with $|C_\nu| \geq C_{\min}$ as new $|\Psi_{\text{ref}}\rangle$

❹ goto ❶ (until convergence)

**IT-NCSM(seq)**

- sequential update scheme for a set of $N_{\max}\hbar\Omega$ spaces

✪ start with full NCSM eigenstate for small $N_{\max}$ as initial $|\Psi_{\text{ref}}\rangle$

❶ construct importance truncated space for $N_{\max} + 2$

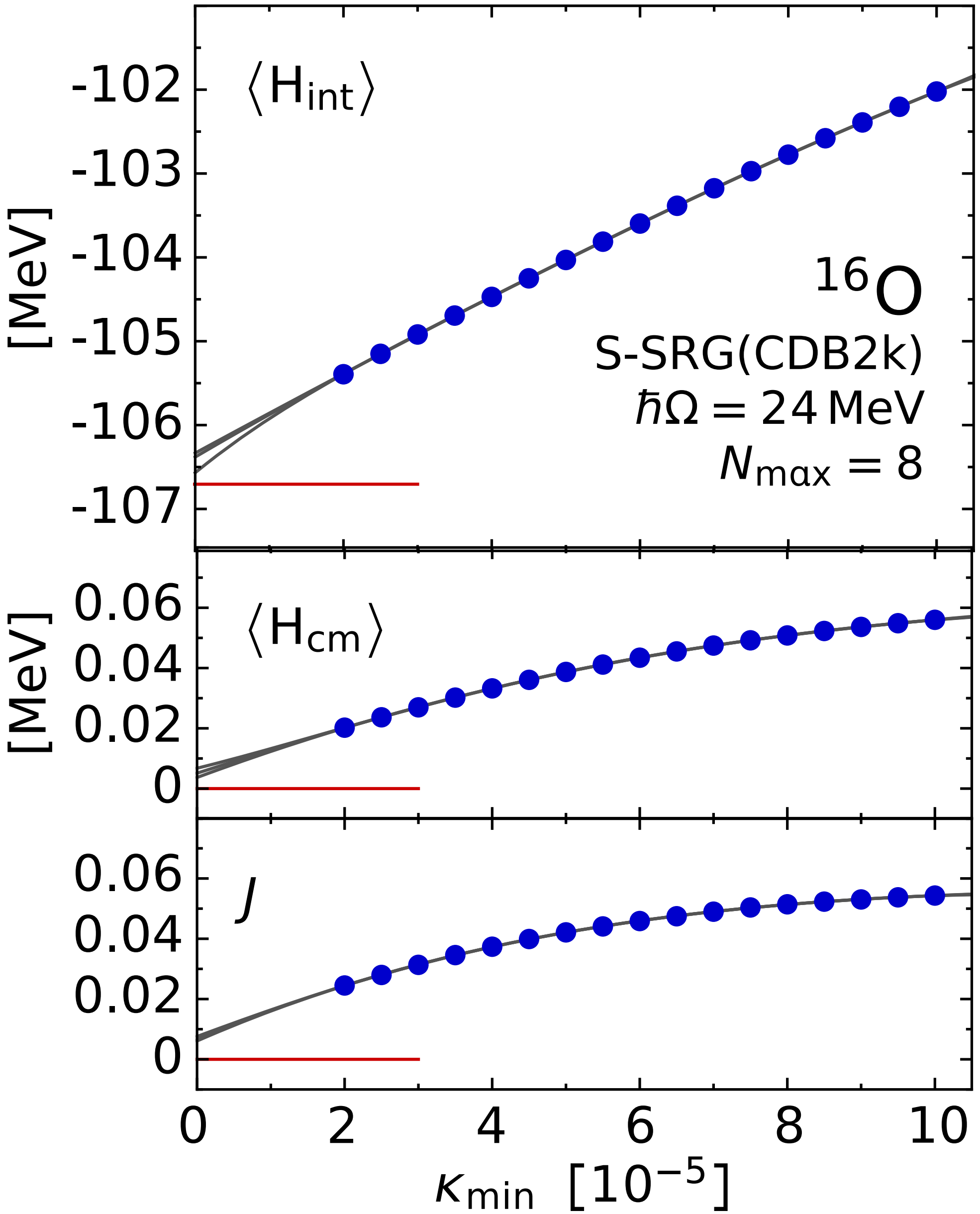
❷ solve eigenvalue problem

❸ use components of eigenstate with $|C_\nu| \geq C_{\min}$ as new $|\Psi_{\text{ref}}\rangle$

❹ goto ❶

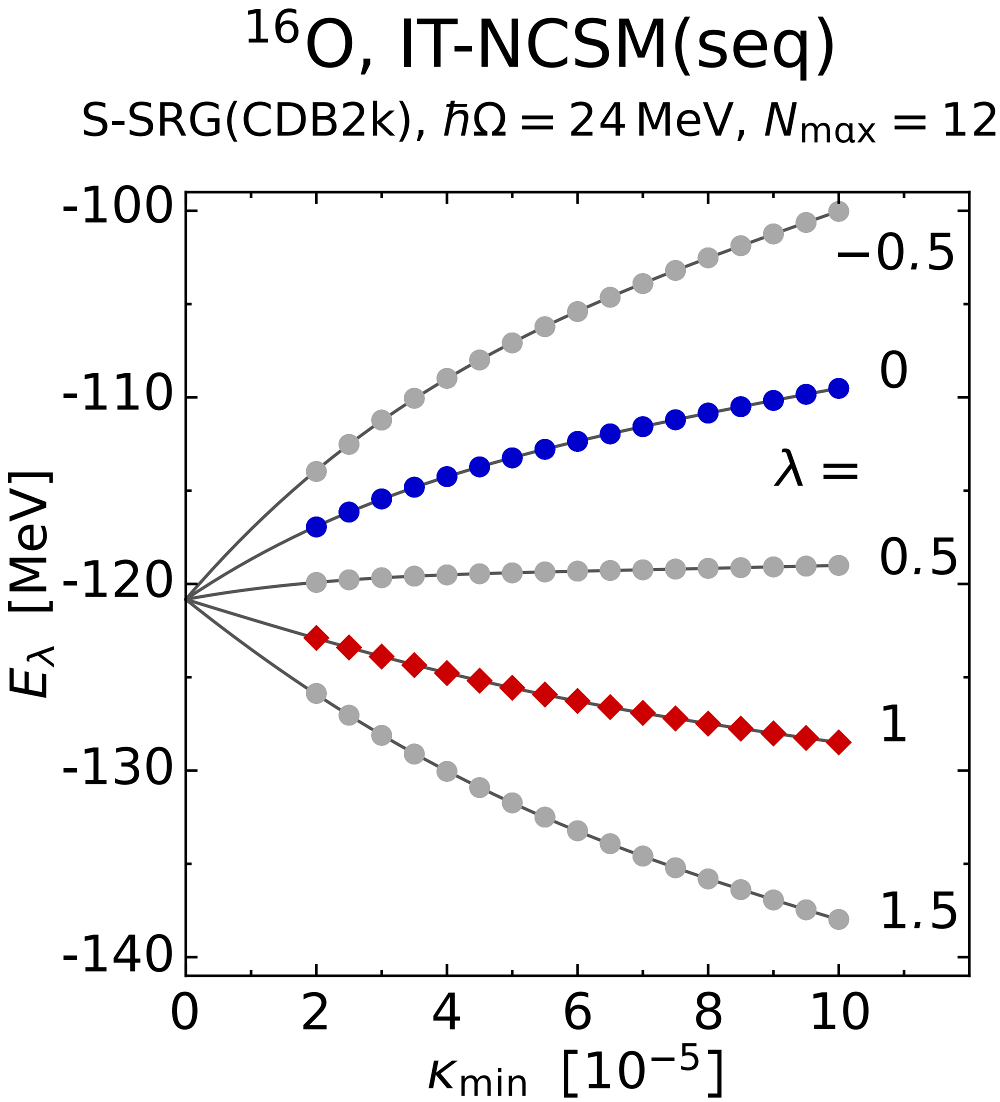
- **full NCSM space is recovered** in the limit $(\kappa_{\min}, C_{\min}) \to 0$

# Threshold Extrapolation




- do calculations for a **sequence of importance thresholds $\kappa_{min}$**
- observables show smooth threshold dependence
- systematic approach to the **full NCSM limit**
- use **a posteriori extrapolation $\kappa_{min} \to 0$** of observables to account for effect of excluded configurations

# Constrained Threshold Extrapolation




- estimate energy contribution of **excluded states** perturbatively → $\Delta_{\text{excl}}(\kappa_{\text{min}})$

- **simultaneous fit** of combined energy

$$E_\lambda(\kappa_{\text{min}}) = E_{\text{int}}(\kappa_{\text{min}}) + \lambda \Delta_{\text{excl}}(\kappa_{\text{min}})$$

  for set of $\lambda$-values with the constraint $E_\lambda(0) = E_{\text{extrap}}$

- **robust threshold extrapolation** with error bars determined by variation of fit function

# Benchmarking SRG-Evolved Chiral NN+3N Hamiltonians

# A Tale of Three Hamiltonians

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

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

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

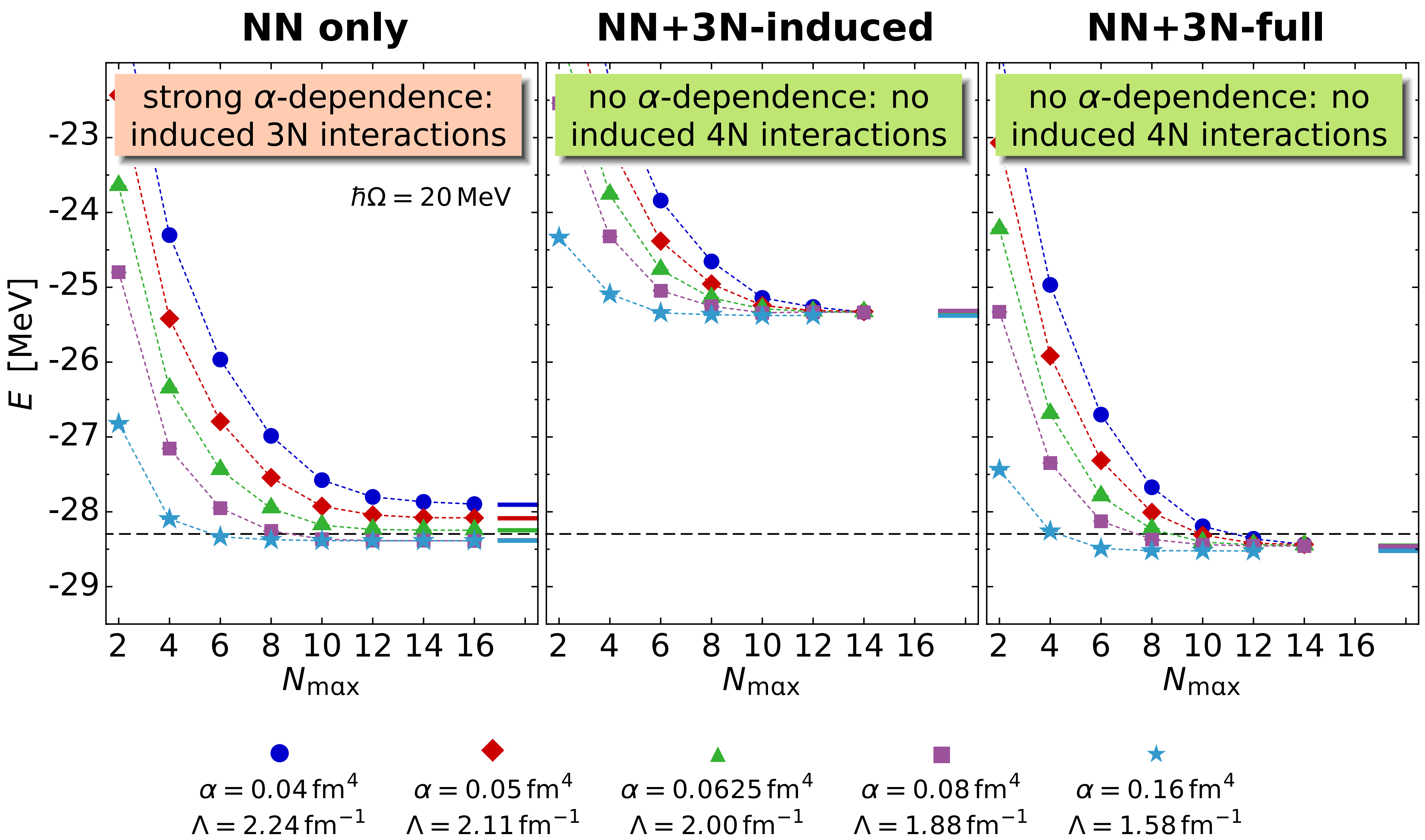
$$\widetilde{H}_\alpha^{\text{NN+3N-induced}} = T_{\text{int}} + \widetilde{T}^{[2]}_{\text{int},\alpha} + \widetilde{V}^{[2]}_{\text{NN},\alpha} + \widetilde{T}^{[3]}_{\text{int},\alpha} + \widetilde{V}^{[3]}_{\text{NN},\alpha}$$

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

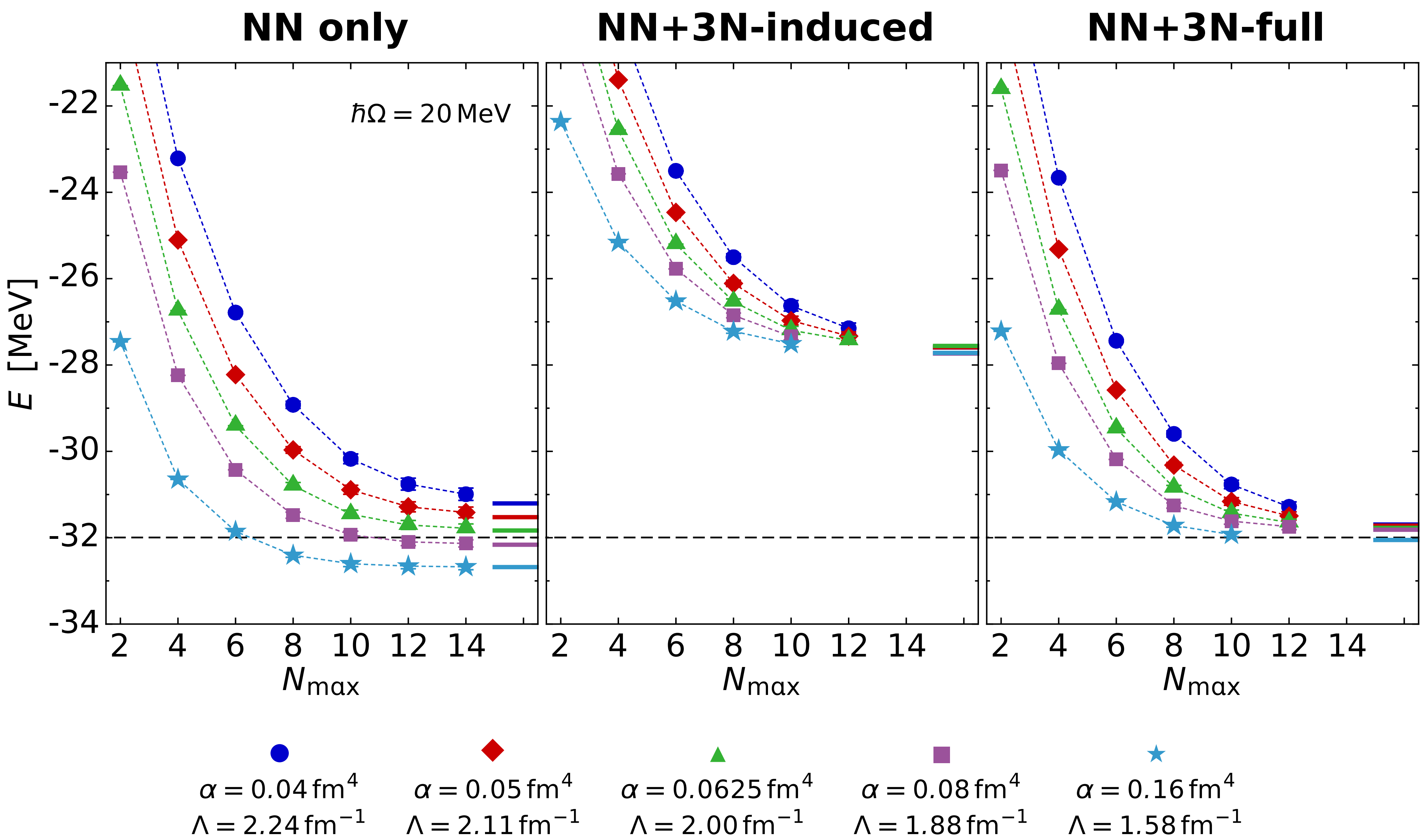
$$\widetilde{H}_\alpha^{\text{NN+3N-full}} = T_{\text{int}} + \widetilde{T}_{\text{int},\alpha} \ldots$$

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

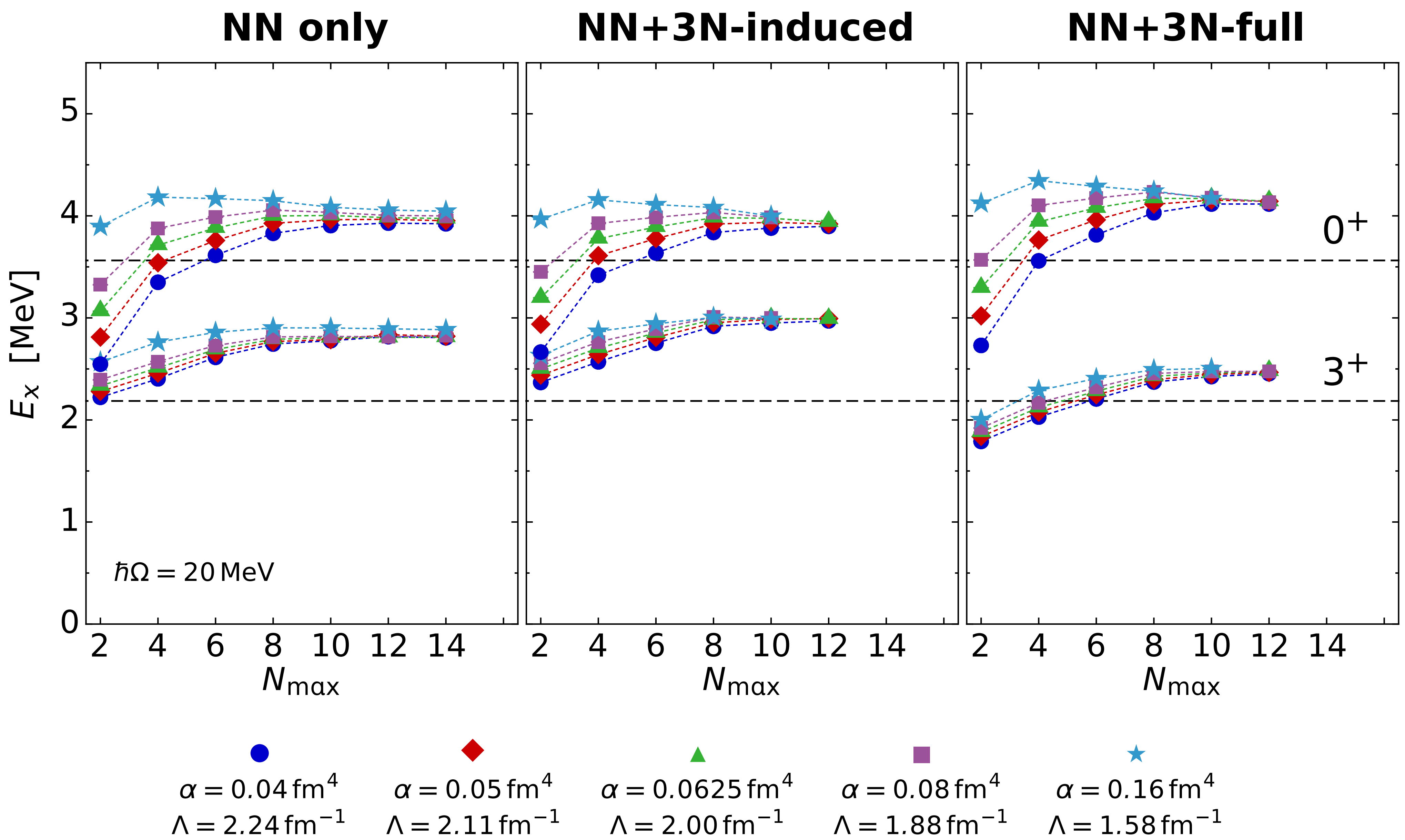
# $^{4}$He: Ground-State Energies



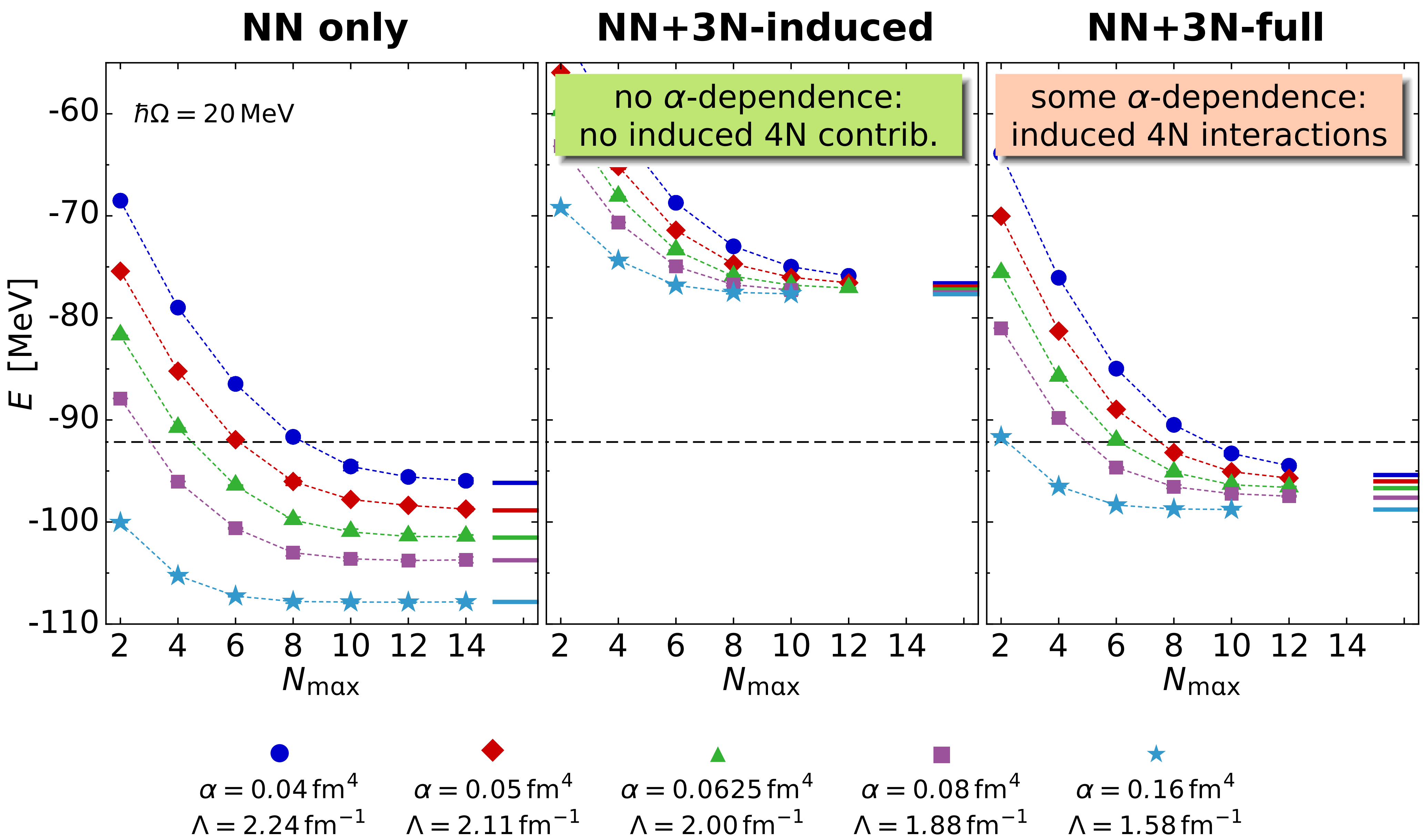
# $^6$Li: Ground-State Energies



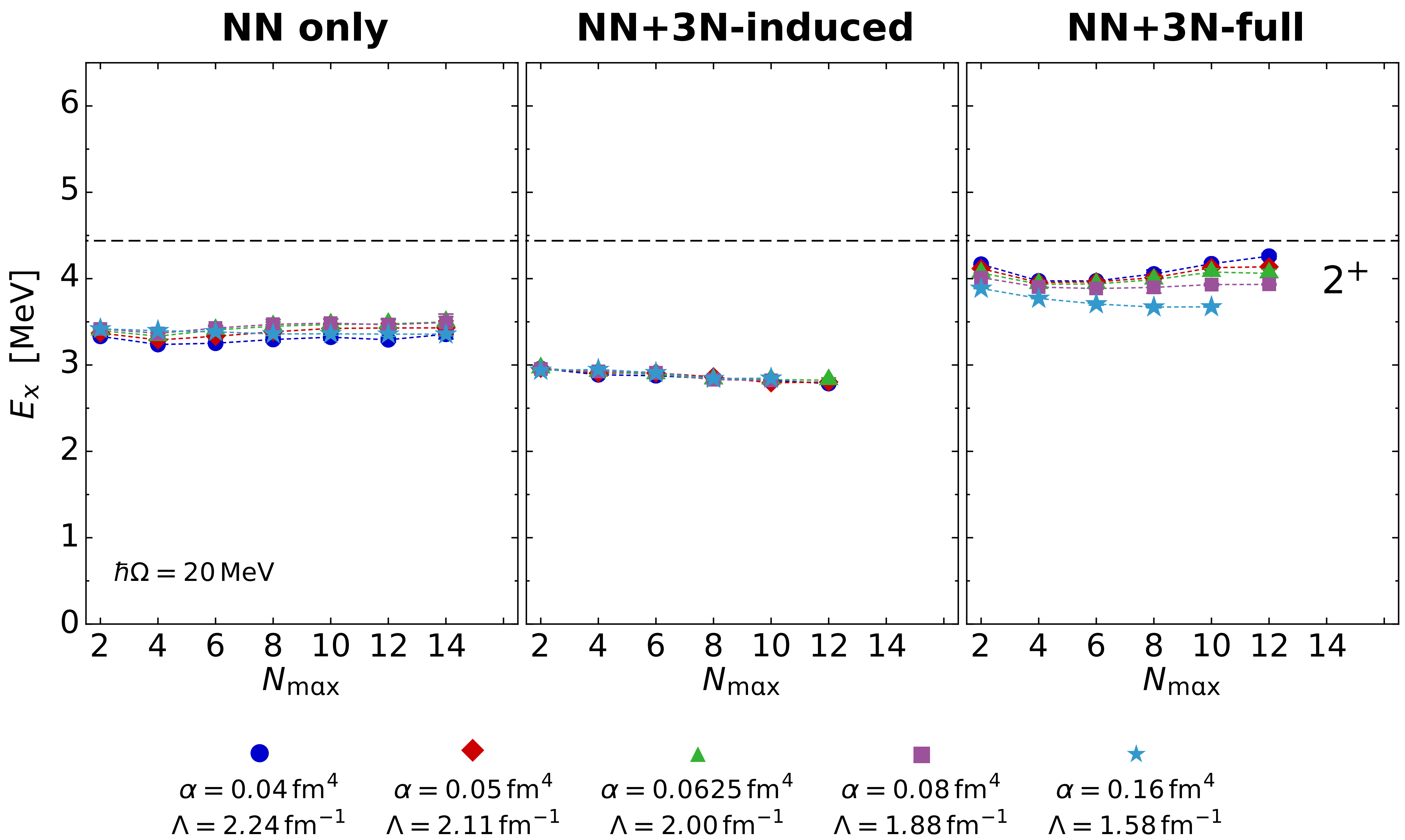
# $^{6}$Li: Excitation Energies



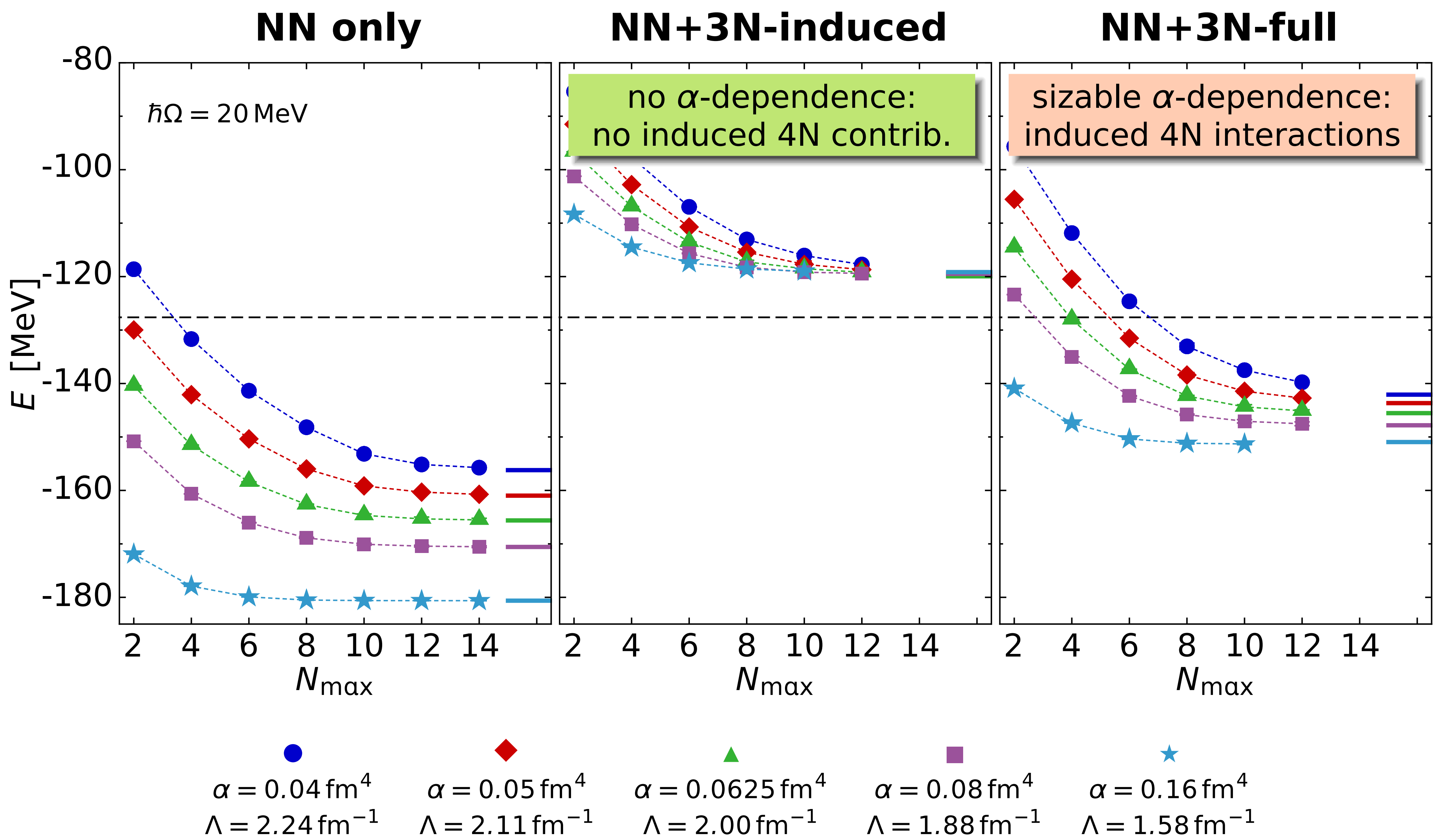
# $^{12}$C: Ground-State Energies



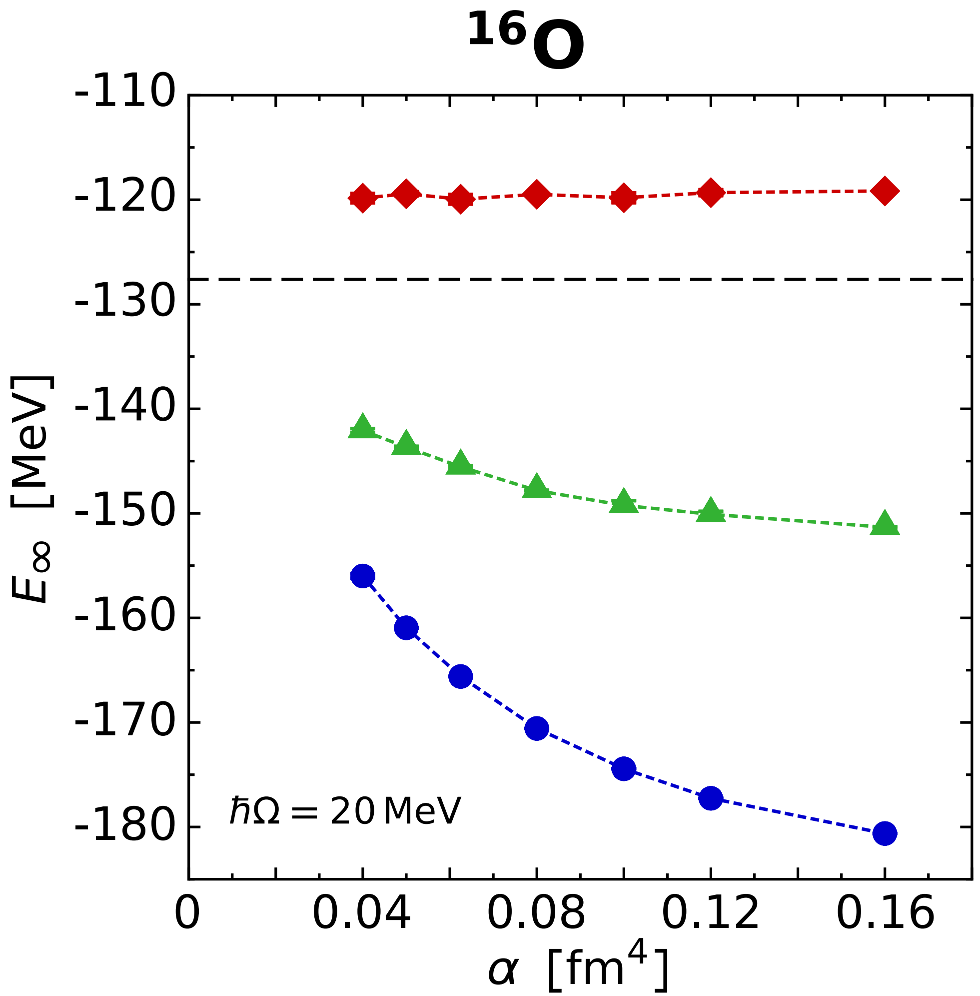
# $^{12}$C: Excitation Energies



# $^{16}$O: Ground-State Energies



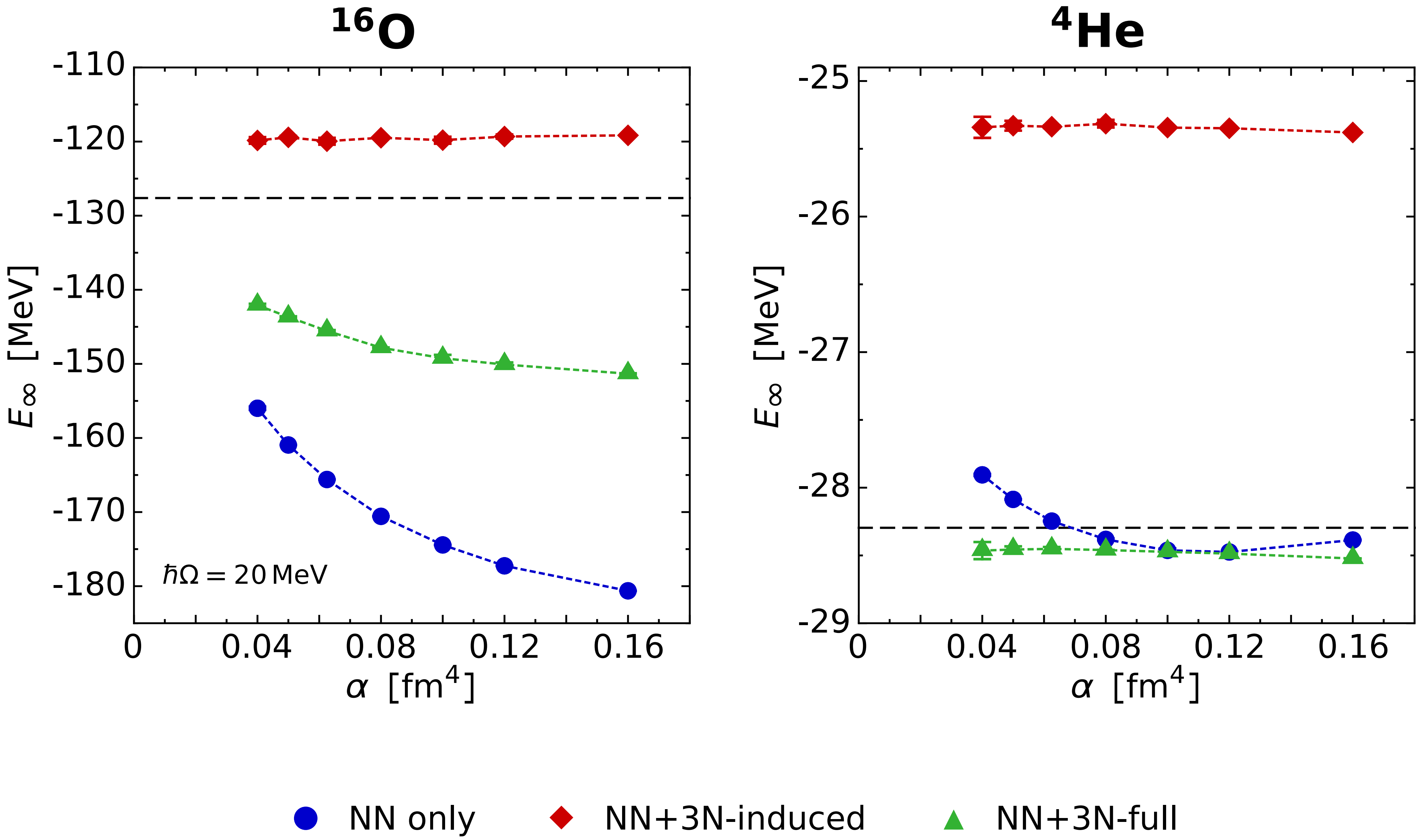
# $^{16}O$: Energy vs. Flow Parameter




- **NN only**: strong $\alpha$-dependence → significant induced 3N contributions
- **NN+3N-induced**: no $\alpha$-dependence → all relevant induced terms from initial NN captured at 3N level
- **NN+3N-full**: sizable $\alpha$-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



Approximate Many-Body Methods

# Hartree-Fock & Perturbation Theory

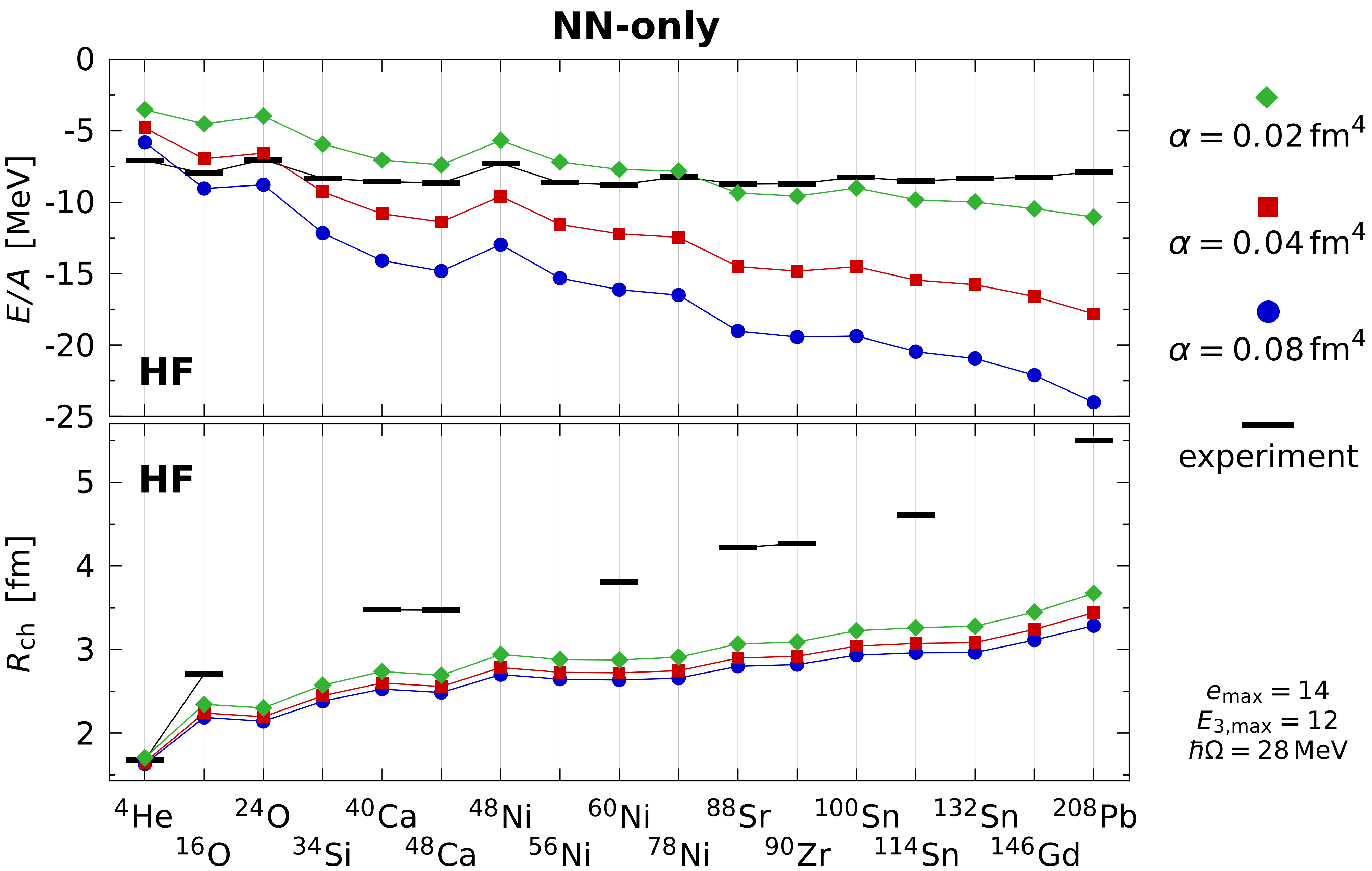
Günther, Roth, Hergert, Reinhardt — Phys. Rev. C 82, 024319 (2010)
Roth, Neff, Feldmeier — Prog. Part. Nucl. Phys. 65, 50 (2010)
Roth, Langhammer — Phys. Lett. B 683, 272 (2010)
Roth, et al. — Phys. Rev. C 73, 044312 (2006)

# Hartree-Fock & Perturbation Theory

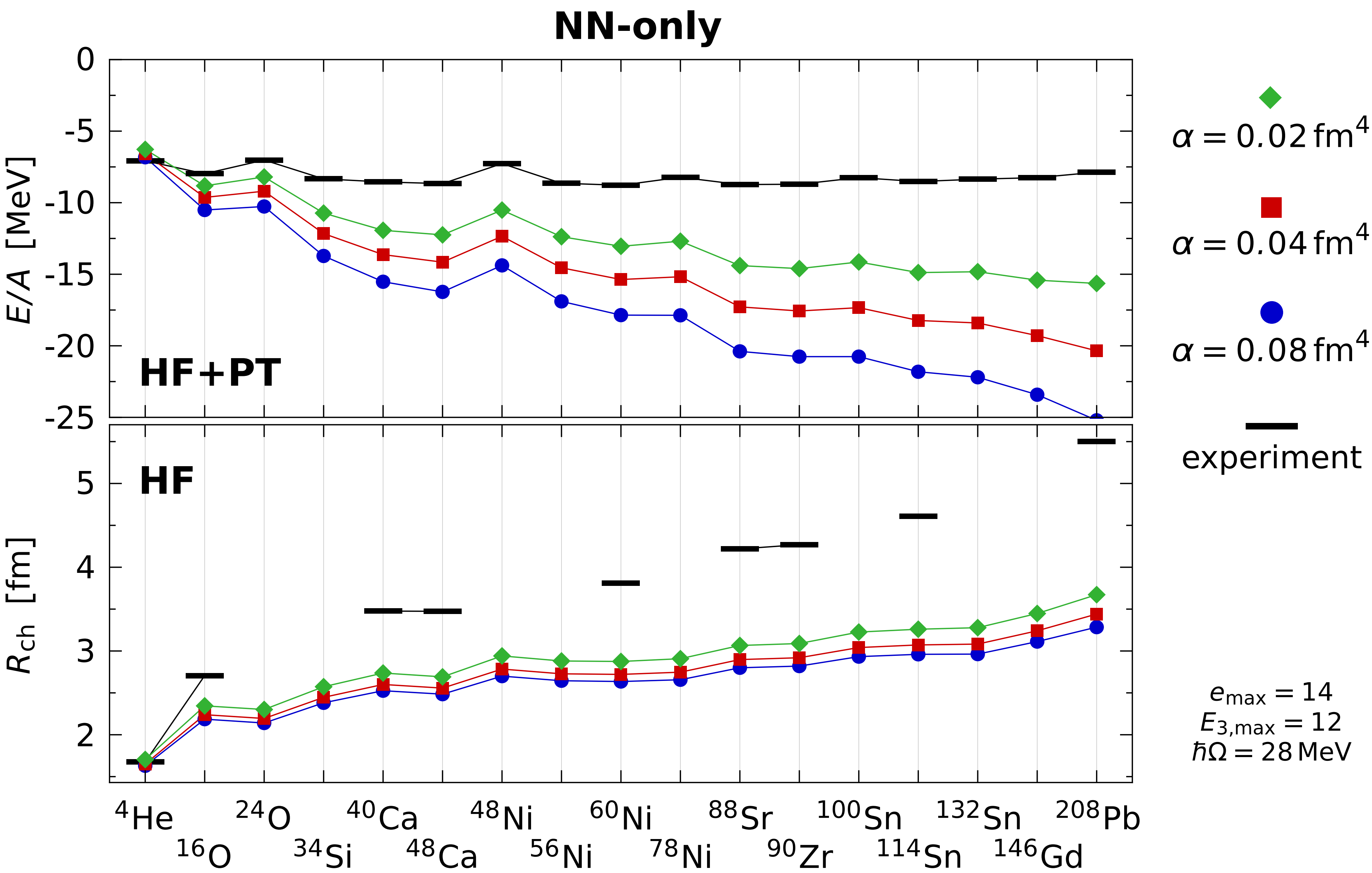
HF & PT provides information on the systematics of ground-state observables over a wide mass range

- solution of the HF equations with 3N interaction computationally simple
- second-order PT for energy with 3N interaction also straight-forward
- all following results preliminary with some limitations, but none of them will change the conclusions
  - 3N matrix elements only up to $E_{3\,\text{max}} = 12$
  - fixed oscillator frequency $\hbar\Omega = 28$ MeV
  - second-order perturbative correction includes NN contribution only

# Systematics: E/A and $R_{ch}$



# Systematics: E/A and $R_{ch}$



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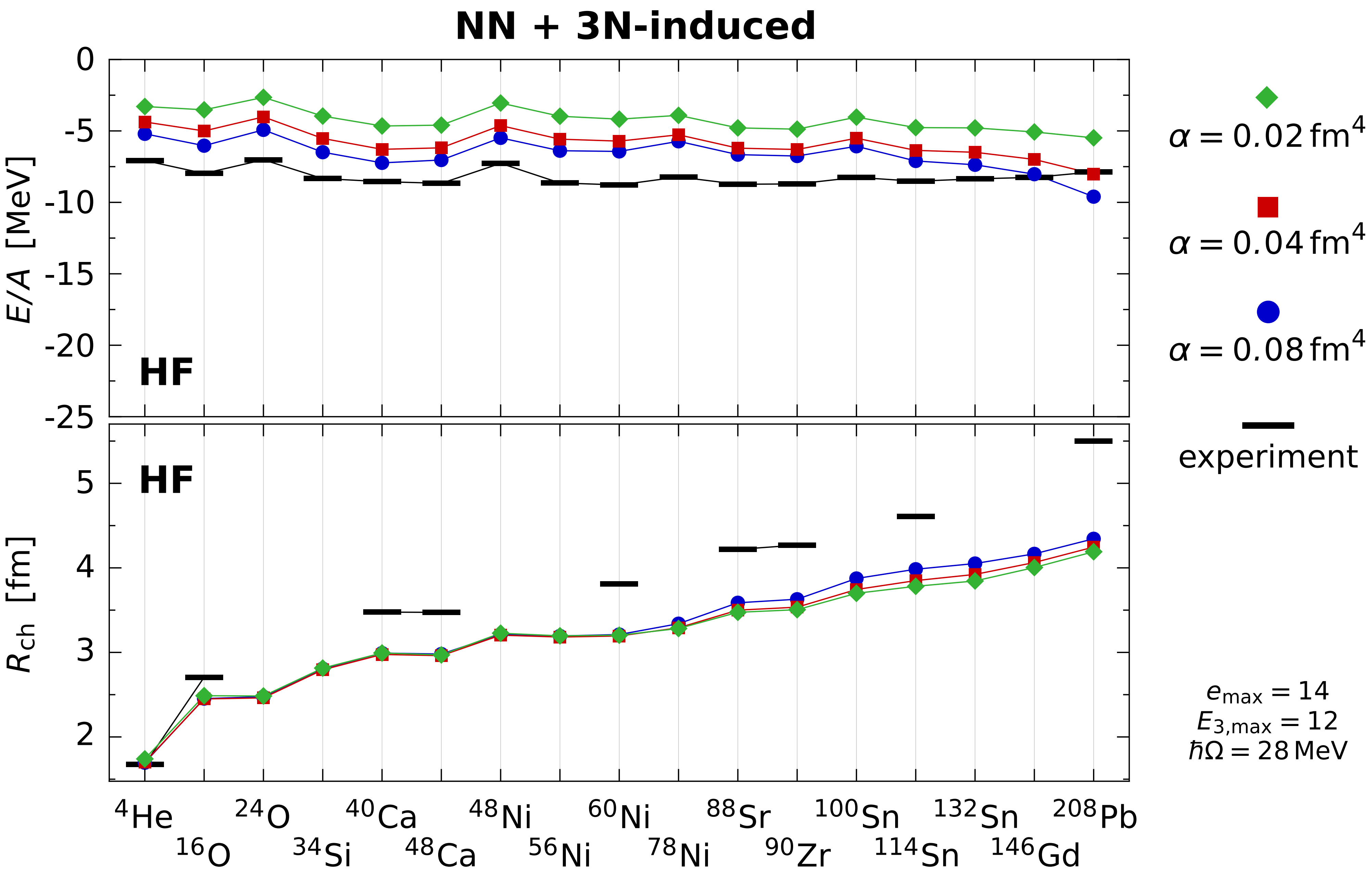

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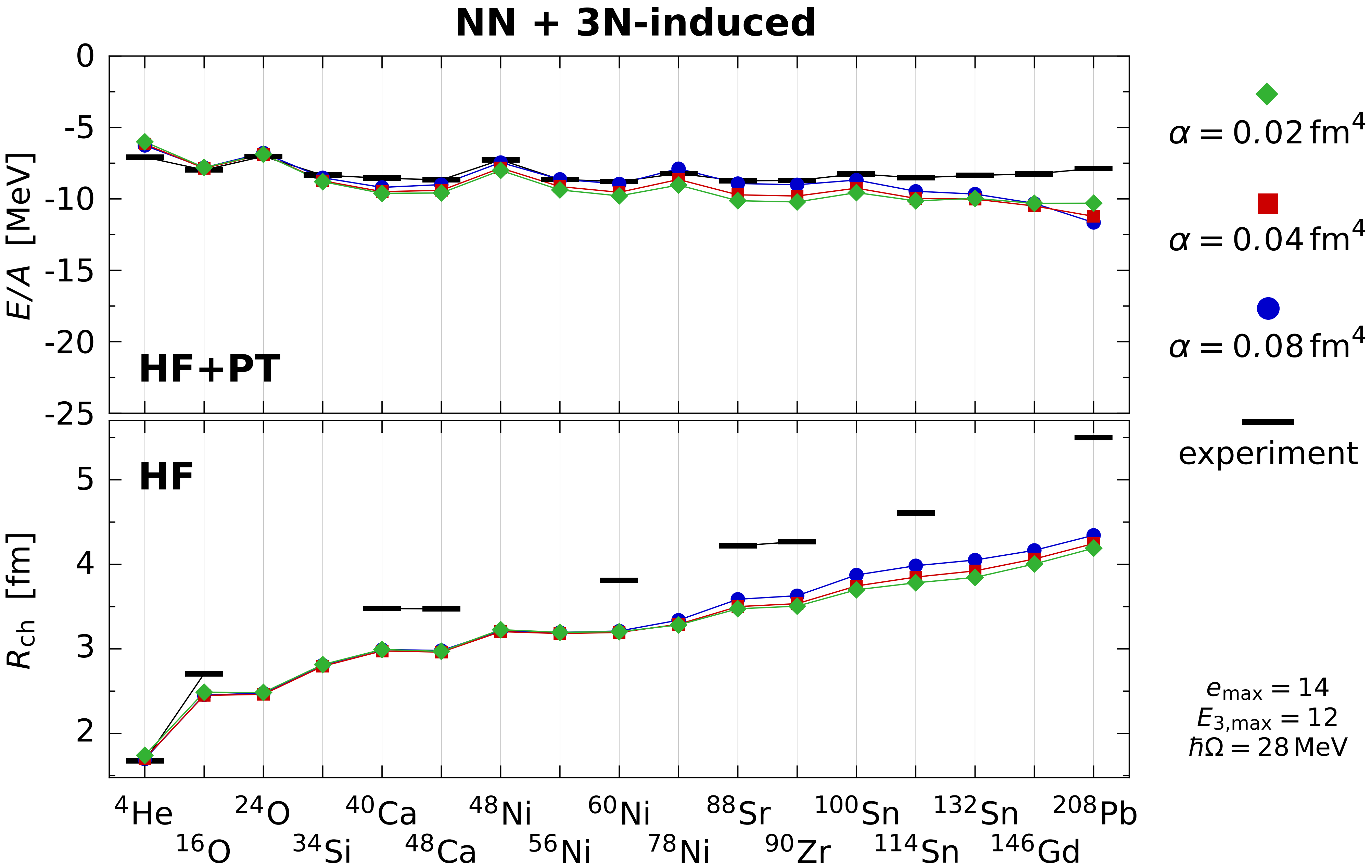

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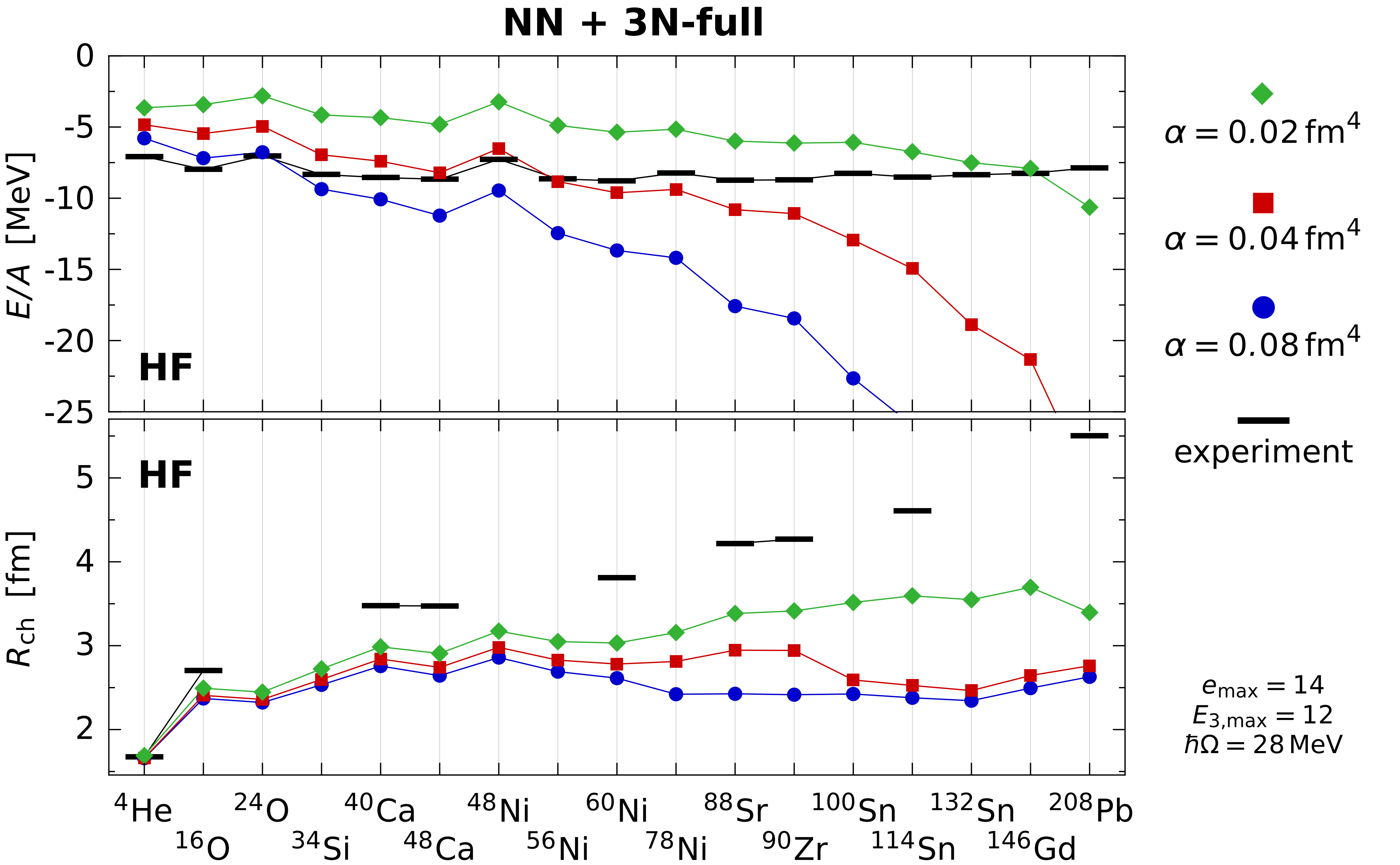

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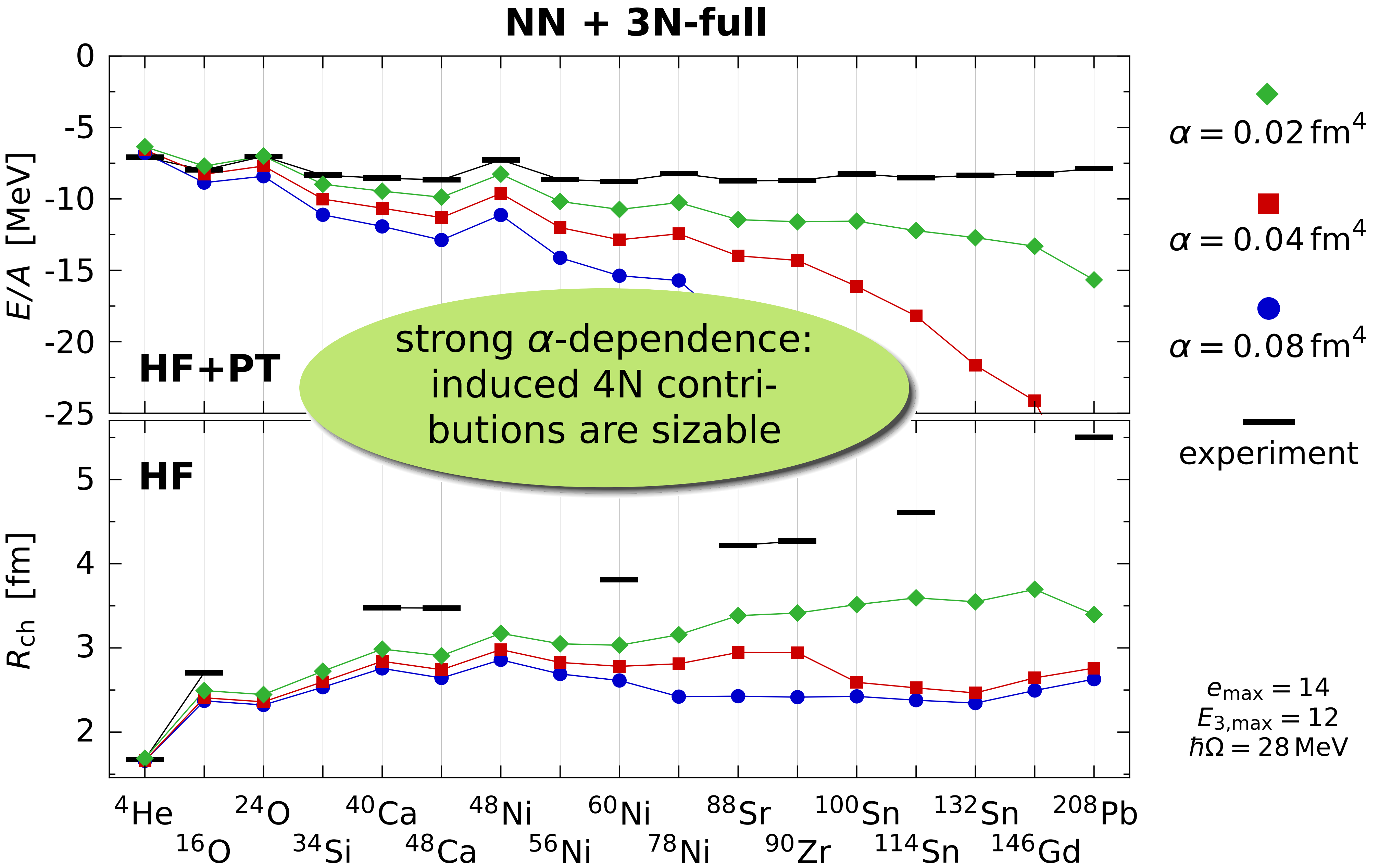

# Conclusions

# 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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