Importance Truncated NCSM with Chiral NN+3N Interactions

Robert Roth

TECHNISCHE UNIVERSITÄT DARMSTADT

Road Map

Nuclear
Structure & Reaction Observables

Importance Truncated NCSM
ab initio studies in the p- & sd-shell

Applications to Nuclear Spectra
spectroscopy and sensitivity on 3N

Coupled Cluster Approach
systematic extension to heavy nuclei

...

Similarity Renormalization Group
pre-diagonalization of Hamiltonian by unitary transformation
computational technology for 3N matrix elements

Chiral Effective Field Theory
systematic low-energy effective theory of QCD
consistent & improvable NN, 3N,... interactions

Low-Energy Quantum Chromodynamics

Road Map

Nuclear
Structure & Reaction Observables

Importance Truncated NCSM
ab initio studies in the p- & sd-shell

Applications to Nuclear Spectra
spectroscopy and sensitivity on 3N

Coupled Cluster Approach
systematic extension to heavy nuclei

•••

Similarity Renormalization Group
pre-diagonalization of Hamiltonian by unitary transformation
computational technology for 3N matrix elements

Chiral Effective Field Theory
systematic low-energy effective theory of QCD
consistent & improvable NN, 3N,... interactions

Low-Energy Quantum Chromodynamics

Overview

- Importance Truncated NCSM
  - basic ideas & extensions
  - threshold dependence of observables
- uncertainty quantification in the IT-NCSM
  - extrapolation vs. systematic uncertainties
  - uncertainty quantification protocol
- IT-NCSM with SRG-evolved chiral NN+3N interactions
  - ground-state energies
  - induced 4N interactions and their origin
  - low-cutoff chiral 3N interaction

Importance Truncated NCSM

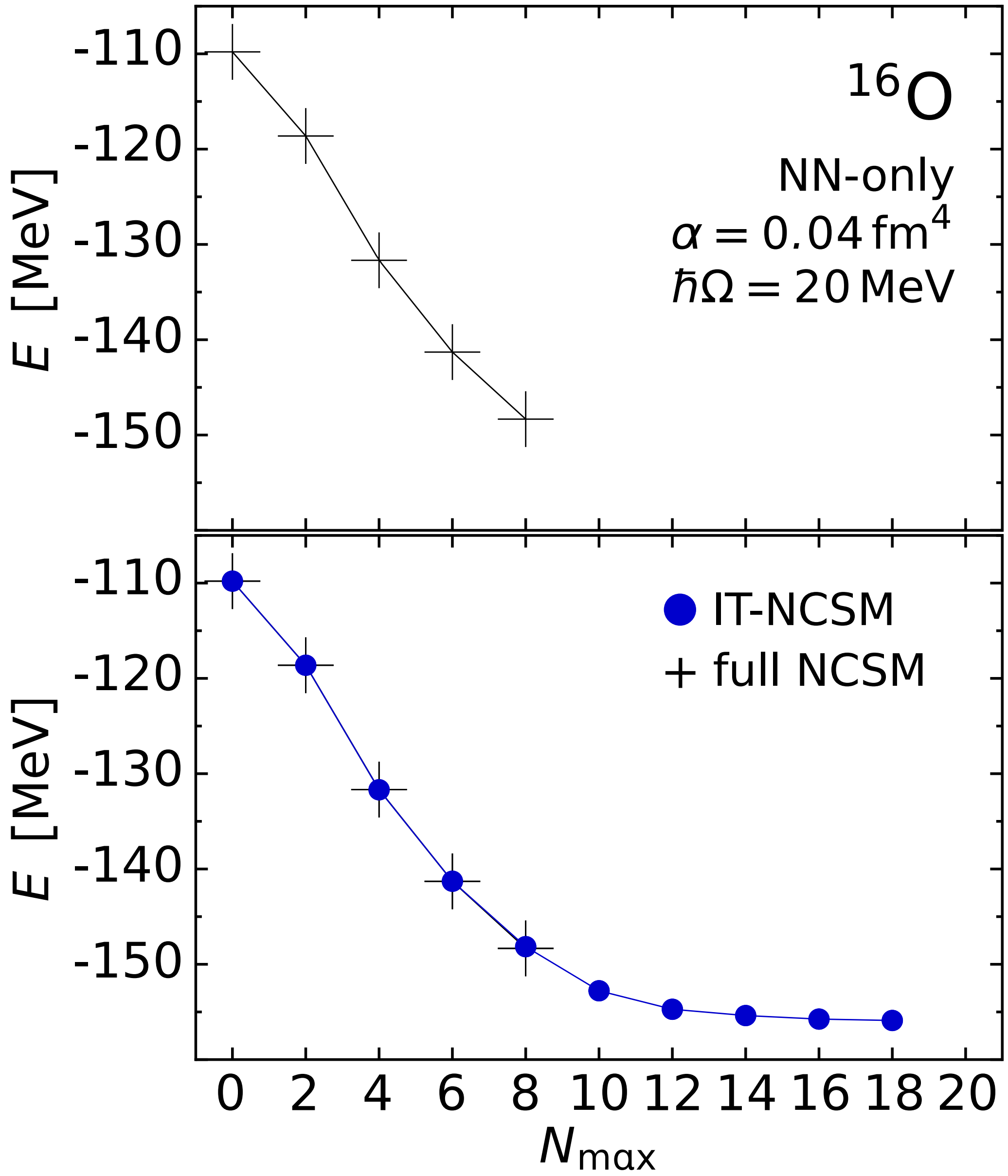
Roth, Langhammer, Calci et al. — Phys. Rev. Lett. 107, 072501 (2011)
Navrátil, Roth, Quaglioni — Phys. Rev. C 82, 034609 (2010)
Roth — Phys. Rev. C 79, 064324 (2009)
Roth, Gour & Piecuch — Phys. Lett. B 679, 334 (2009)
Roth, Gour & Piecuch — Phys. Rev. C 79, 054325 (2009)
Roth, Navrátil — Phys. Rev. Lett. 99, 092501 (2007)

Importance Truncated NCSM

- converged NCSM calculations essentially restricted to lower/mid p-shell
- full $10\hbar\Omega$ calculation for ^{16}O getting very difficult (basis dimension > 10^{10})

Importance Truncation

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



Importance Truncation: Basic Idea

- **starting point**: approximation $|\Psi_{\text{ref}}\rangle$ for the **target state** within a limited reference space $\mathcal{M}_{\text{ref}}$

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

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

$$\langle \Phi_{\nu} | H | \Psi_{\text{ref}} \rangle$$

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

- co… …m all basis states …

embed into iterative scheme to access full model space

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

Importance Truncation: Iterative Scheme

- **property of $N_{\max}$-truncated space**: step from $N_{\max}$ to $N_{\max}+2$ requires 2p2h excitations at most

- **sequential calculation** for a range of $N_{\max}\hbar\Omega$ spaces:

  ● do full NCSM calculations up to a convenient $N_{\max}$

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

  ❶ consider all states $|\Phi_\nu\rangle \notin \mathcal{M}_{\text{ref}}$ from an $N_{\max}+2$ space and add those with $|\kappa_\nu| \geq \kappa_{\min}$ to importance-truncated space $\mathcal{M}_{\text{IT}}$

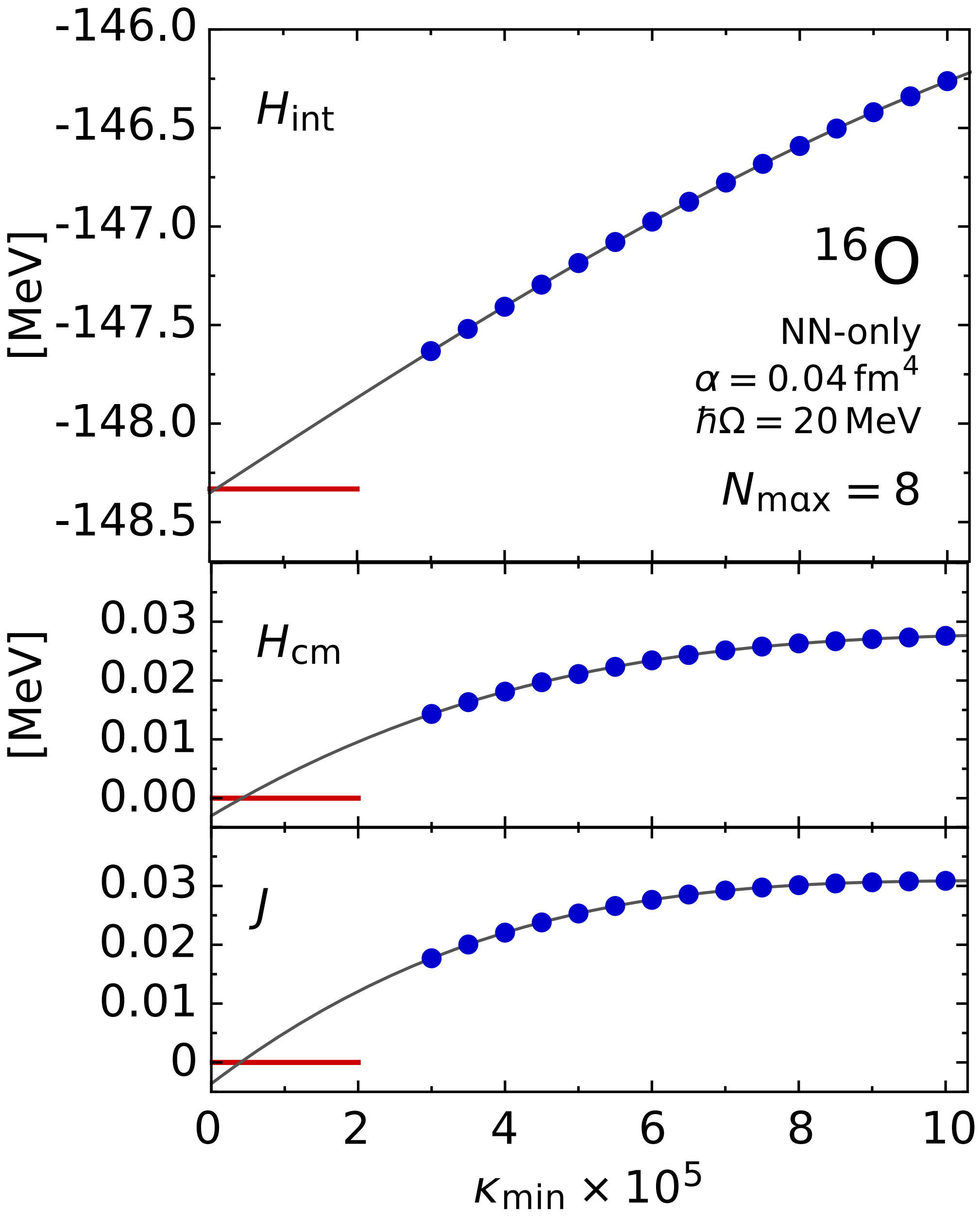
  ❷ solve eigenvalue problem in $\mathcal{M}_{\text{IT}}$

  ❸ use components of eigensta

  ❹ goto ❶

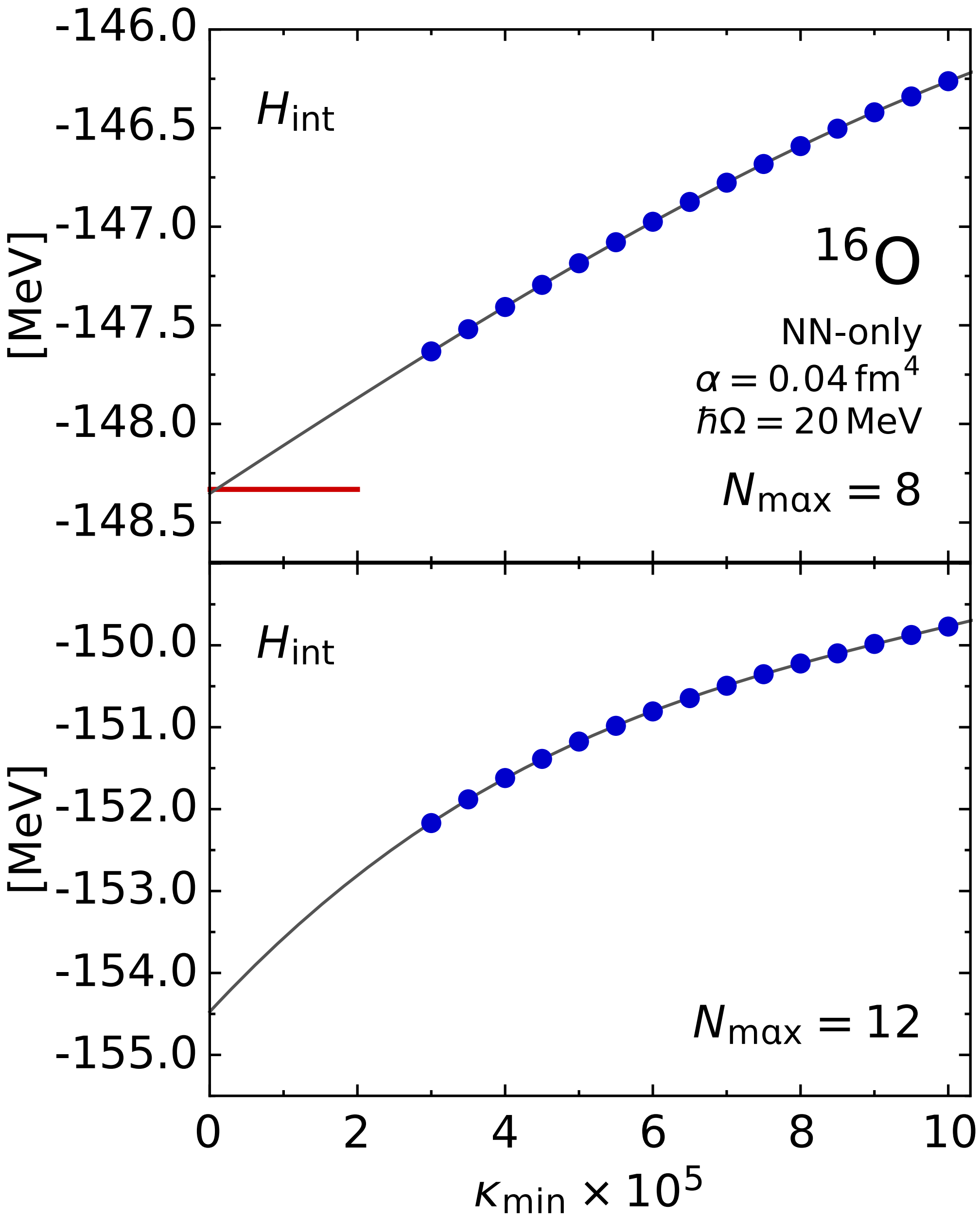
full NCSM space is recovered in the limit $(\kappa_{\min}, C_{\min}) \to 0$

Threshold Extrapolation



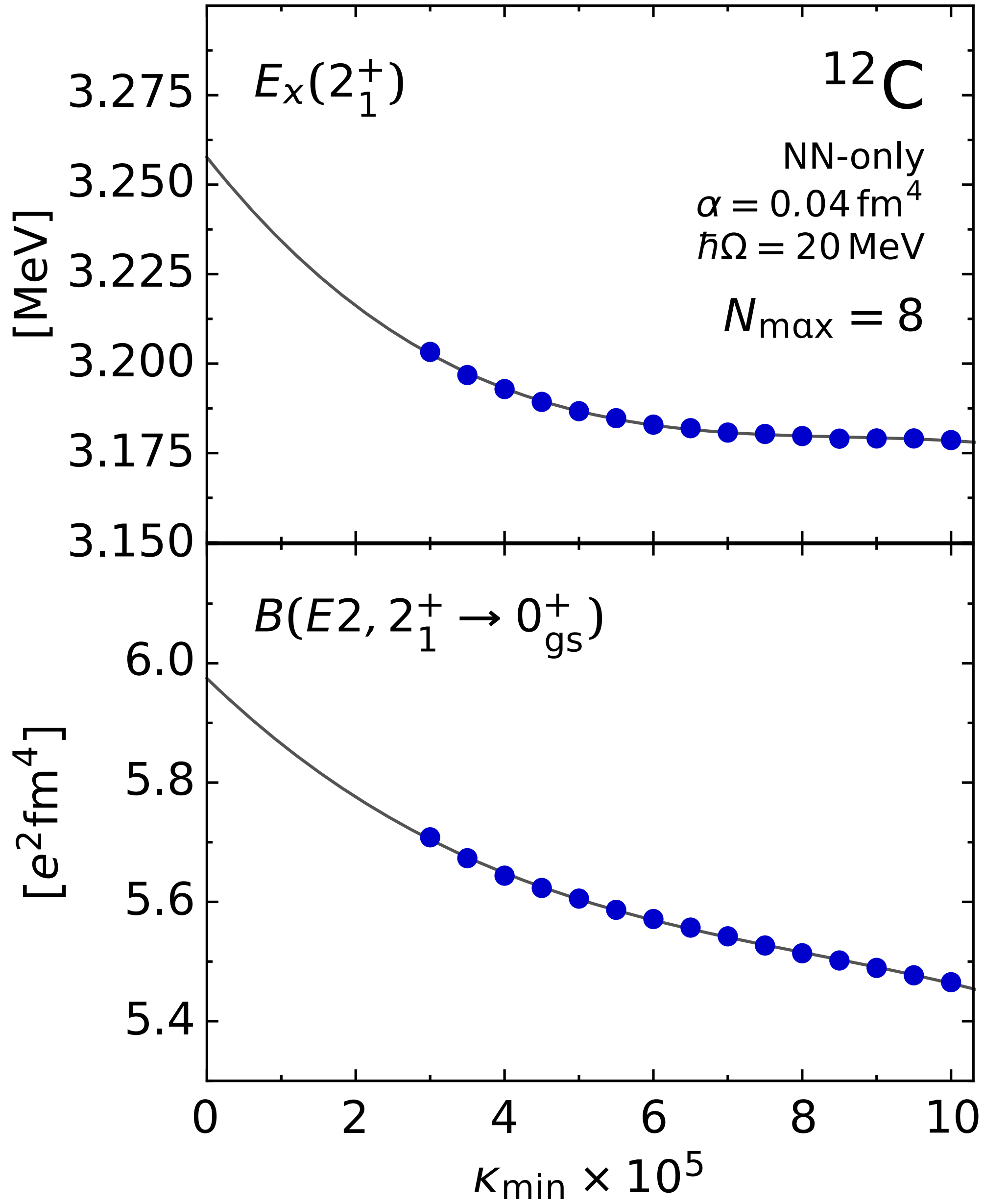
- repeat calculations for a **sequence of importance thresholds** κ_{min}
- observables show **smooth threshold dependence** and systematically approach the full NCSM limit
- use **a posteriori extrapolation** $\kappa_{min} \rightarrow 0$ of observables to account for effect of excluded configurations

Threshold Extrapolation



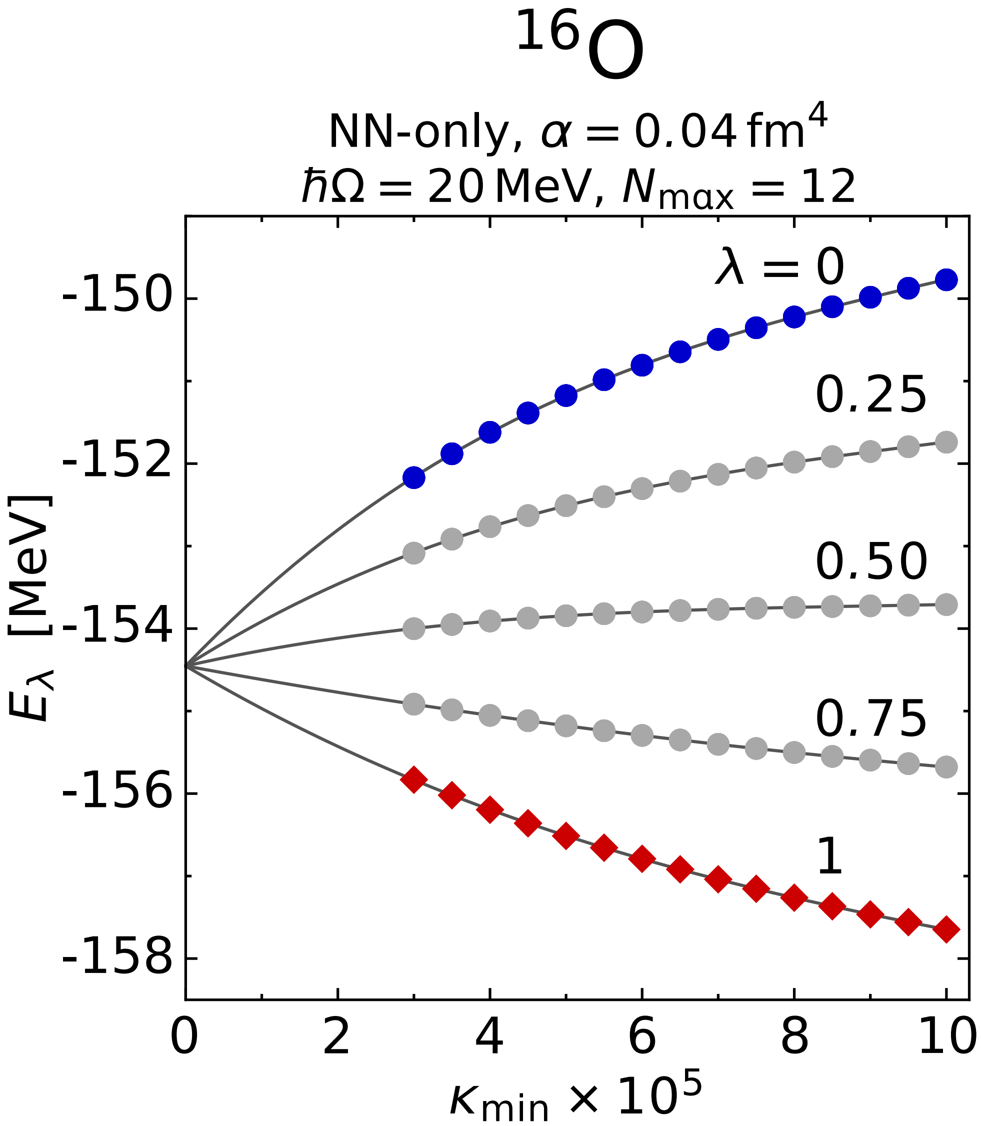
- repeat calculations for a **sequence of importance thresholds** κ_{min}
- observables show **smooth threshold dependence** and systematically approach the full NCSM limit
- use **a posteriori extrapolation** $\kappa_{min} \to 0$ of observables to account for effect of excluded configurations

Threshold Extrapolation



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

Constrained Threshold Extrapolation



- for free: importance selection gives perturbative energy correction $\Delta_{\text{excl}}(\kappa_{\text{min}})$ accounting for **excluded states**

- formal property

$$\Delta_{\text{excl}}(\kappa_{\text{min}}) \to 0 \quad \text{for} \quad \kappa_{\text{min}} \to 0$$

- auxiliary parameter λ defining a family of energy sequences

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

- **simultaneous extrapolation** for family of λ-values with constraint $E_\lambda(0) = E_{\text{extrap}}$

Importance Truncation: Extensions

Excited States

- target M lowest eigenstates simultaneously and define corresponding reference states $\left|\Psi^{(m)}_{\text{ref}}\right\rangle$ with $m = 1 \dots M$
- keep basis states with $|\kappa^{(m)}_{\nu}| \geq \kappa_{\text{min}}$ for at least one $\left|\Psi^{(m)}_{\text{ref}}\right\rangle$
- dimension of IT model space grows linearly with M

3N Interactions

- importance measure κ_{ν} includes 3N interaction explicitly
- IT-NCSM(seq) scheme does not change
- dimension of IT model space does not change significantly, but Hamilton matrix becomes denser

Uncertainty Quantification in the IT-NCSM

Two Sources of Uncertainties

Model-Space Truncation

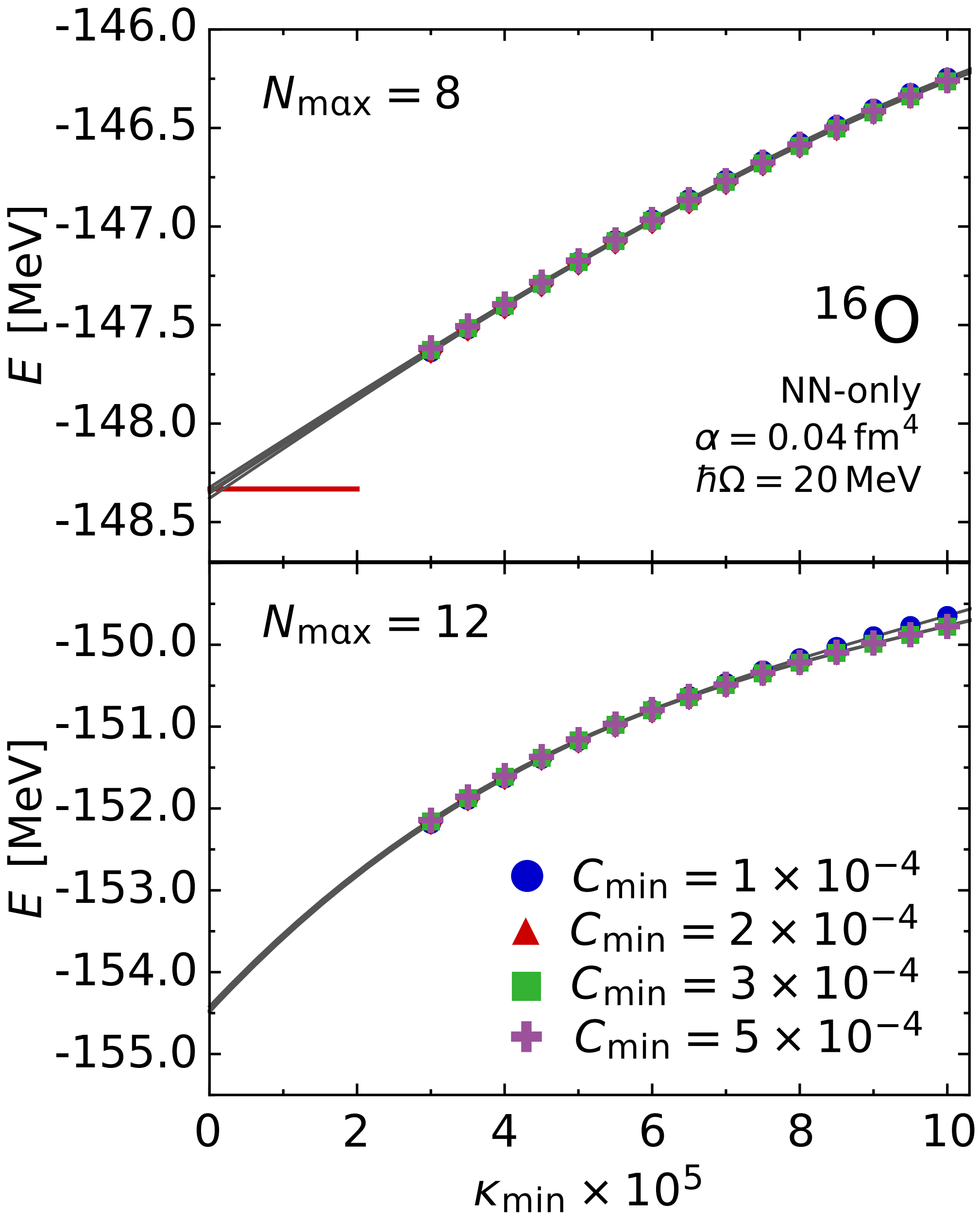
- use sequence of $N_{\max}$-truncated model spaces
- extrapolate to $N_{\max} \to \infty$ using exponential ansatz or more refined constrained extrapolation schemes
- uncertainty estimate derived from extrapolation protocol
- same **extrapolation uncertainties** as in full NCSM

Importance Truncation

- use sequence of $(C_{\min}, \kappa_{\min})$-truncated model spaces
- extrapolate to $\kappa_{\min} \to 0$ using polynomial ansatz or more refined constrained extrapolation schemes
- uncertainty estimate derived from extrapolation protocol
- **systematic uncertainty** compared to the full NCSM

- both types of uncertainties are **controlled**, well **quantified** and systematically **improvable**

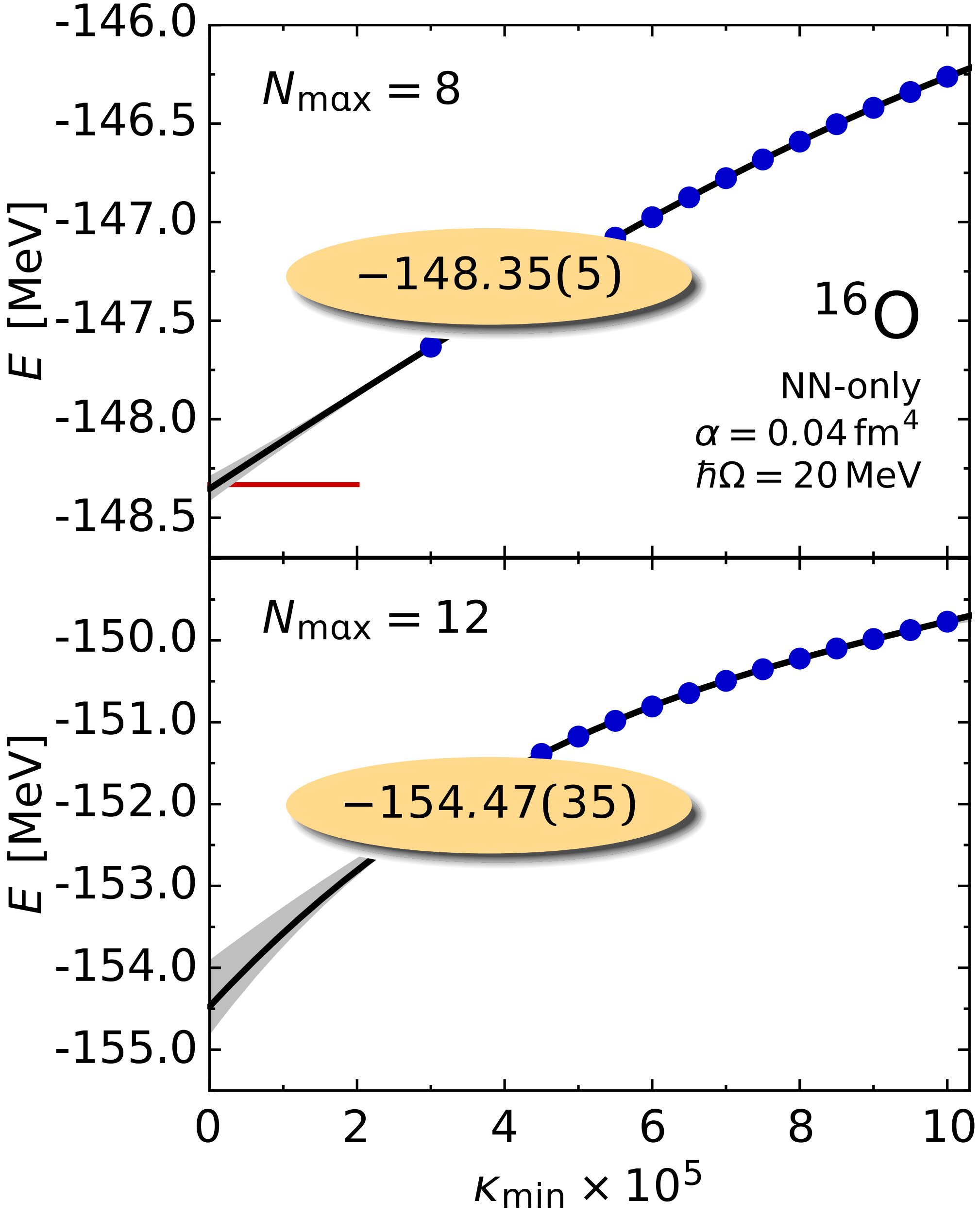
Comment on C_{min} Truncation



- **truncation of reference state** to components with $|C_\nu| \geq C_{min}$
- **technical reason**: importance selection algorithm scales with $(\dim \mathcal{M}_{ref})^2$
- typically $C_{min} = 2 \times 10^{-4}$

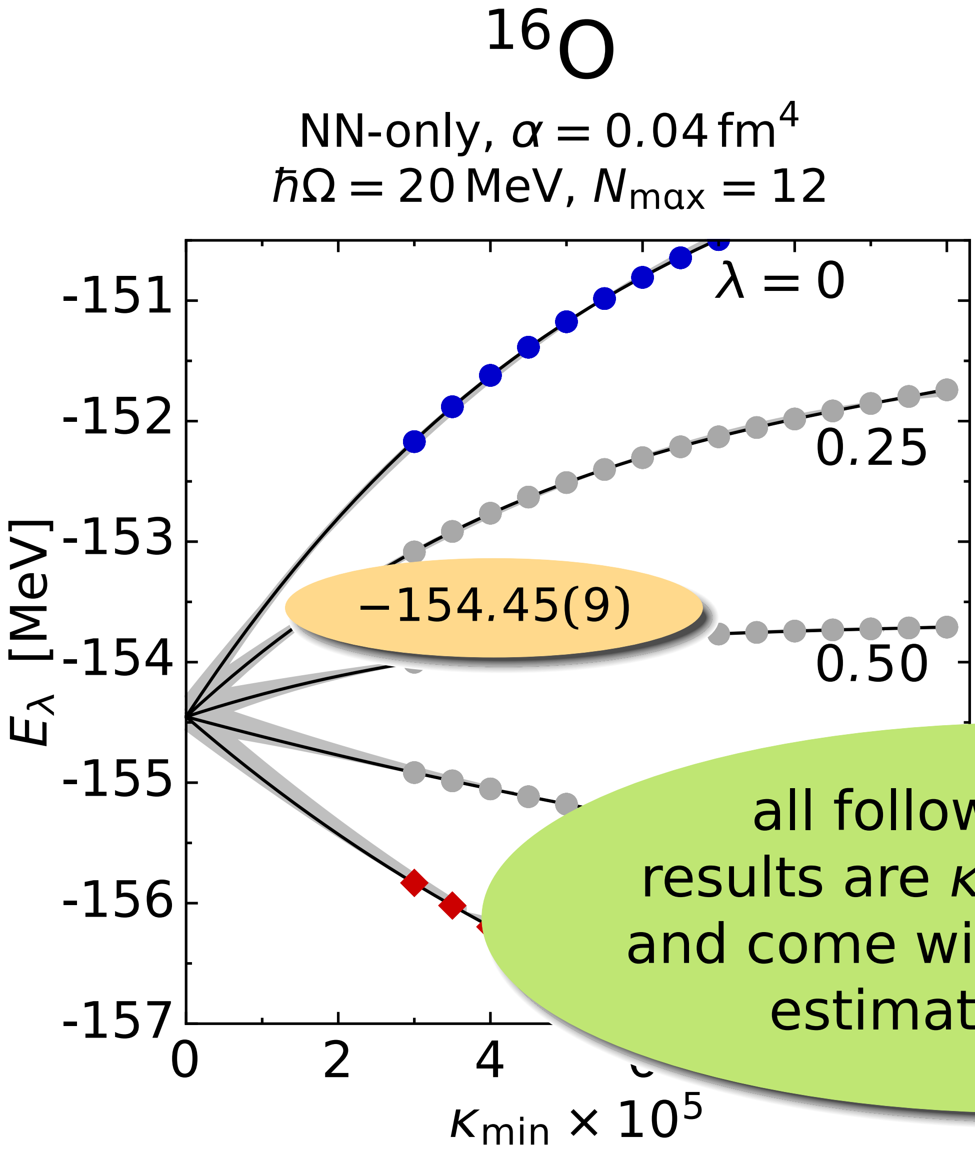
virtually no influence on threshold extrapolated energies

Protocol: Simple $\kappa_{\min}$ Extrapolation



- IT-NCSM calculations for sequence of $\kappa_{\min}$-values, typically $\kappa_{\min} = 3, 3.5, \ldots, 10 \times 10^{-5}$
- **nominal result** from extrapolation $\kappa_{\min} \to 0$ using polynomial $P_p(\kappa_{\min})$, typically order $p = 3$
- **uncertainty band** from set of alternative extrapolations
  - P_{p-1} and P_{p+1} extrapolations using full $\kappa_{\min}$-range
  - P_p extrapolations with lowest and lowest two $\kappa_{\min}$-points dropped
- nominal uncertainty from standard deviation

Protocol: Constrained κ_{min} Extrapolation



- select few λ-values to get symmetrical approach towards common $E_{extrap} = E_\lambda(\kappa_{min} = 0)$
- **nominal result** from constrained simultaneous extrapolation $\kappa_{min} \to 0$ using $P_p(\kappa_{min})$
- **uncertainty band** from set of constrained extrapolations
  - P_{p-1} and P_{p+1} extrapolations us- ... κ_{min}-range
  - ...ns with lowest and ...oints dropped
  - ...s with smallest ...λ-set dropped

all following IT-NCSM results are κ_{min} extrapolated and come with an uncertainty estimate / error bar

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

Roth, Binder, Vobig et al. — arXiv: 1112.0287

Roth, Langhammer, Calci et al. — Phys. Rev. Lett. 107, 072501 (2011)

A Tale of Three Hamiltonians

Initial Hamiltonian

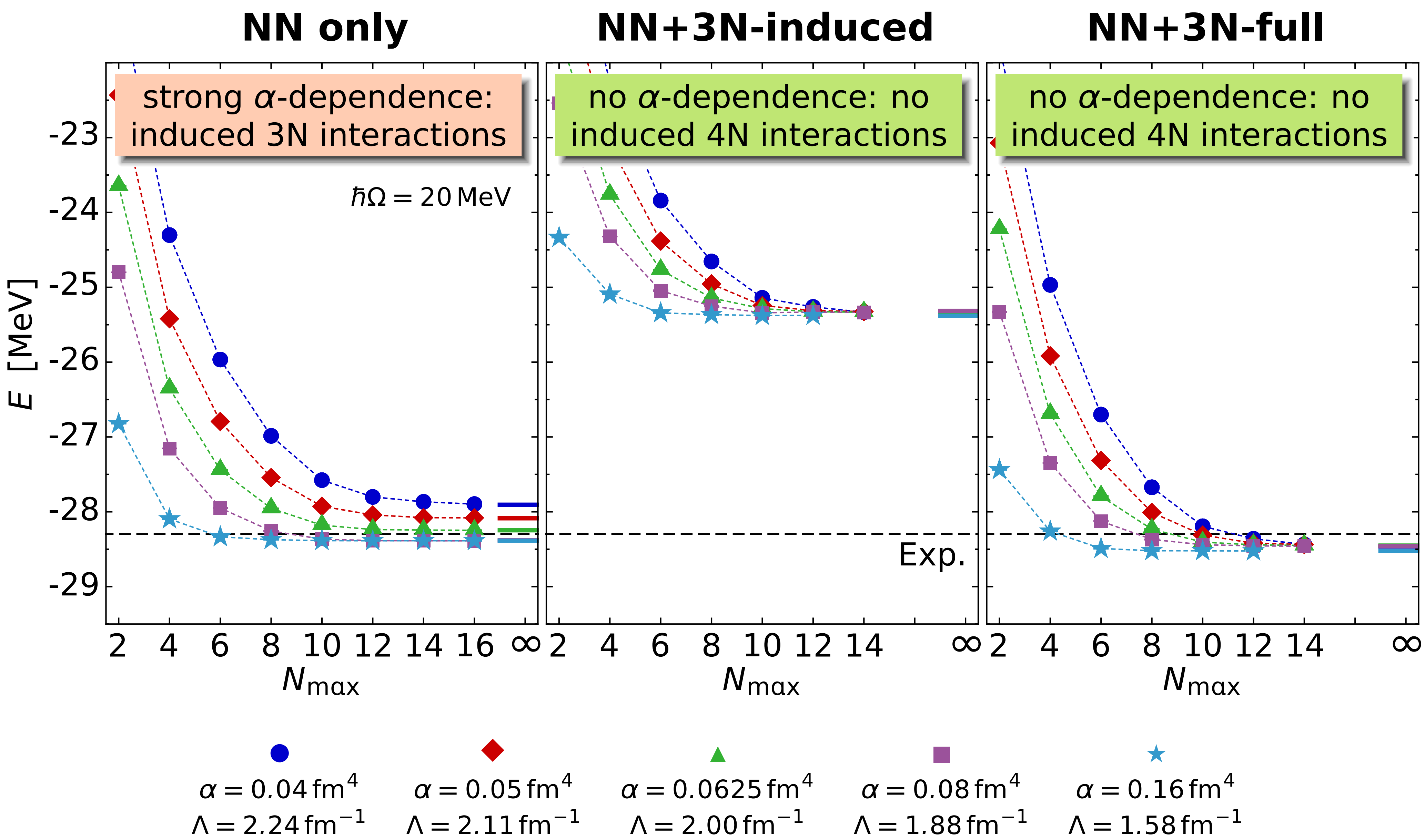
- NN: chiral interaction at N^3LO (Entem & Machleidt, 500 MeV)
- 3N: chiral interaction at N^2LO (c_D, c_E from ^3H binding & half-life)

SRG-Evolved Hamiltonians

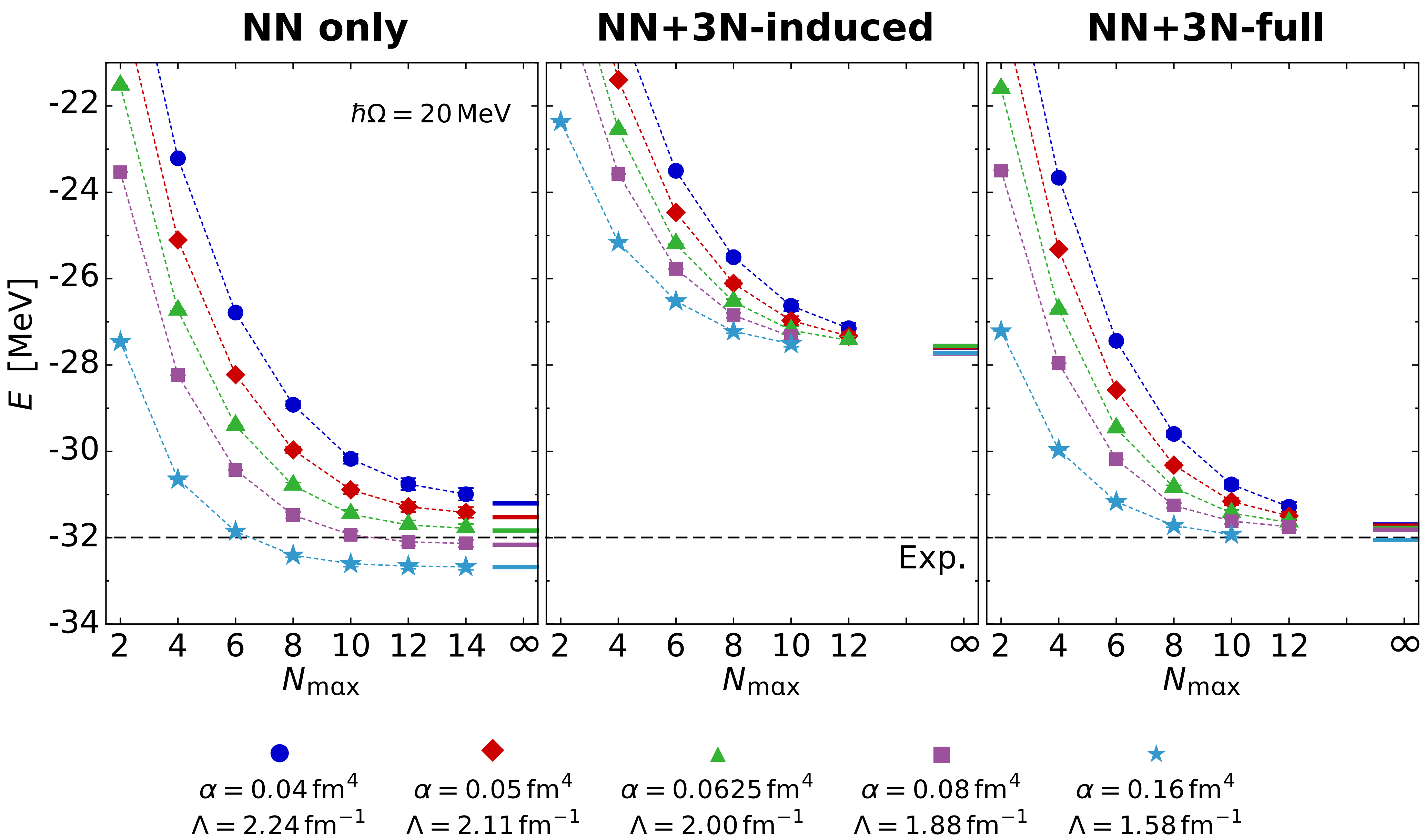
- **NN only**: start with NN initial Hamiltonian and keep two-body terms only
- **NN+3N-induced**: start with NN initial Hamiltonian and keep two- and three-body terms
- **NN+3N-full**: start with NN+3N in
two- and three-body terms

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

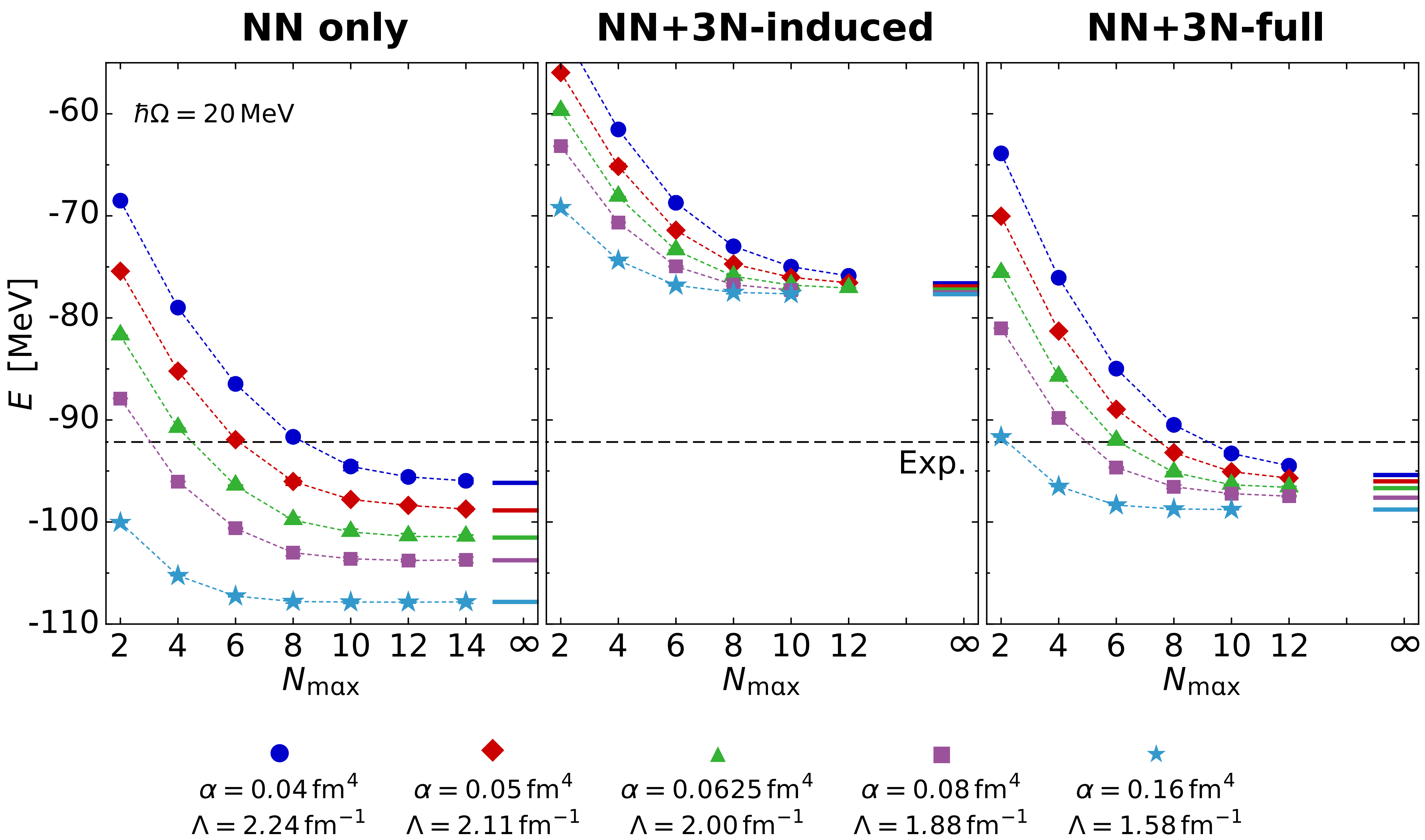
^{4}He: Ground-State Energies



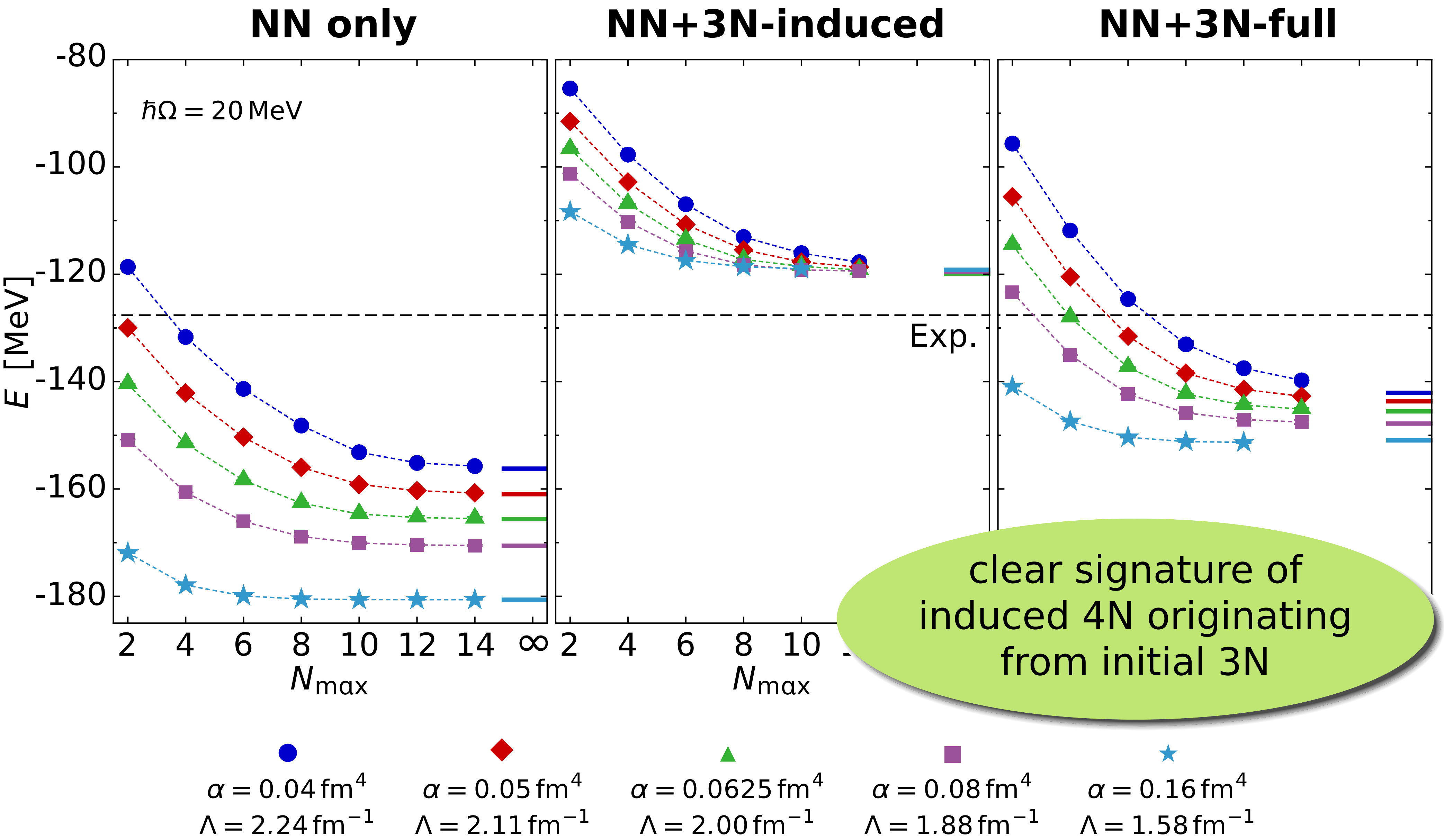
^{6}Li: Ground-State Energies



^{12}C: Ground-State Energies



^{16}O: Ground-State Energies



clear signature of induced 4N originating from initial 3N

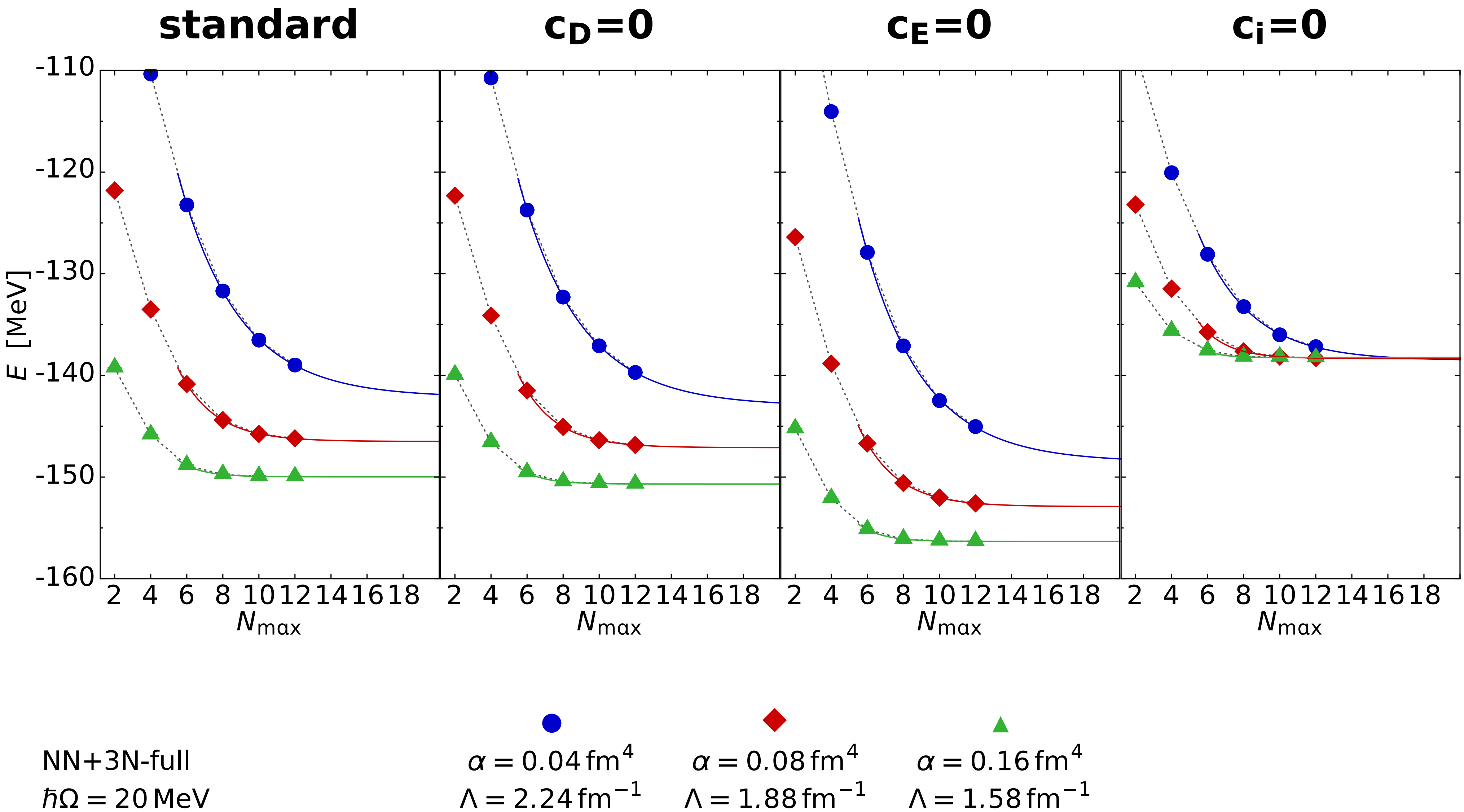
Origin of Induced 4N

- analyze the origin of the induced 4N terms by **switching off individual contributions** of the 3N interaction

	c_1	c_3	c_4	c_D	c_E
std*	$+0.81$	-3.2	$+5.4$	-0.2	$-0.240^\star$
$c_D = 0$	$+0.81$	-3.2	$+5.4$	0	$-0.205^\star$
$c_E = 0$	$+0.81$	-3.2	$+5.4$	$+1.238^\star$	0
$c_i = 0$	0	0	0	-0.2	$+0.444^\star$
$c_1 = 0$	0	-3.2	$+5.4$	-0.2	$-0.207^\star$
$c_3 = 0$	$+0.81$	0	$+5.4$	-0.2	$-0.228^\star$
$c_4 = 0$	$+0.81$	-3.2	0	-0.2	$+0.141^\star$

- refit c_E (or c_D) parameter to reproduce ^{4}He ground-state energy

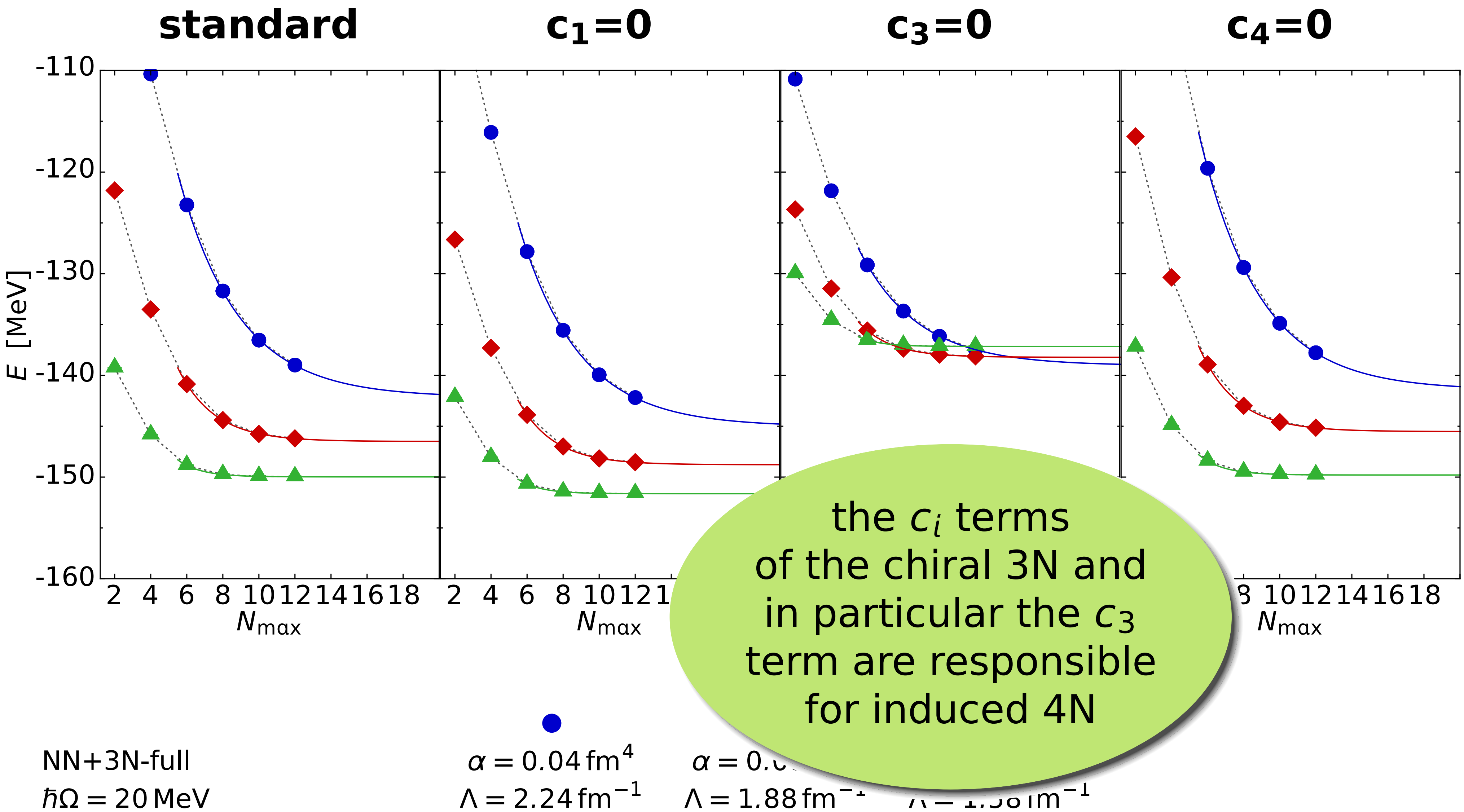
^{16}O: Origin of Induced 4N



NN+3N-full

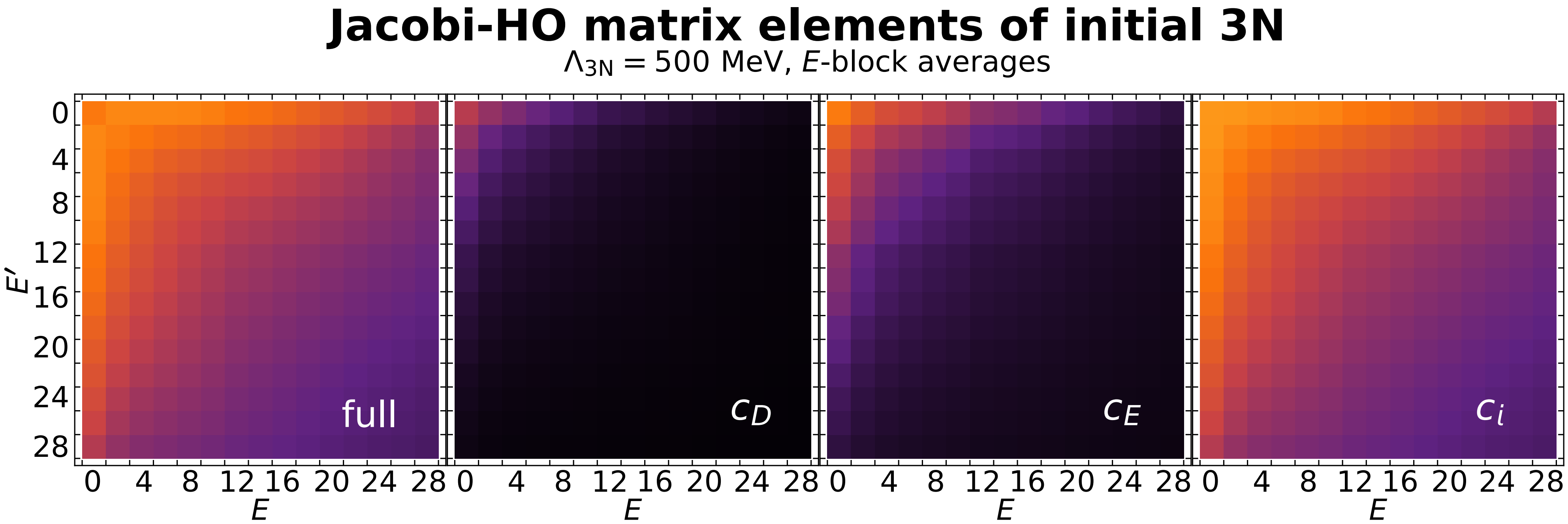
$\hbar\Omega = 20\,MeV$

^{16}O: Origin of Induced 4N



the c_i terms
of the chiral 3N and
in particular the c_3
term are responsible
for induced 4N

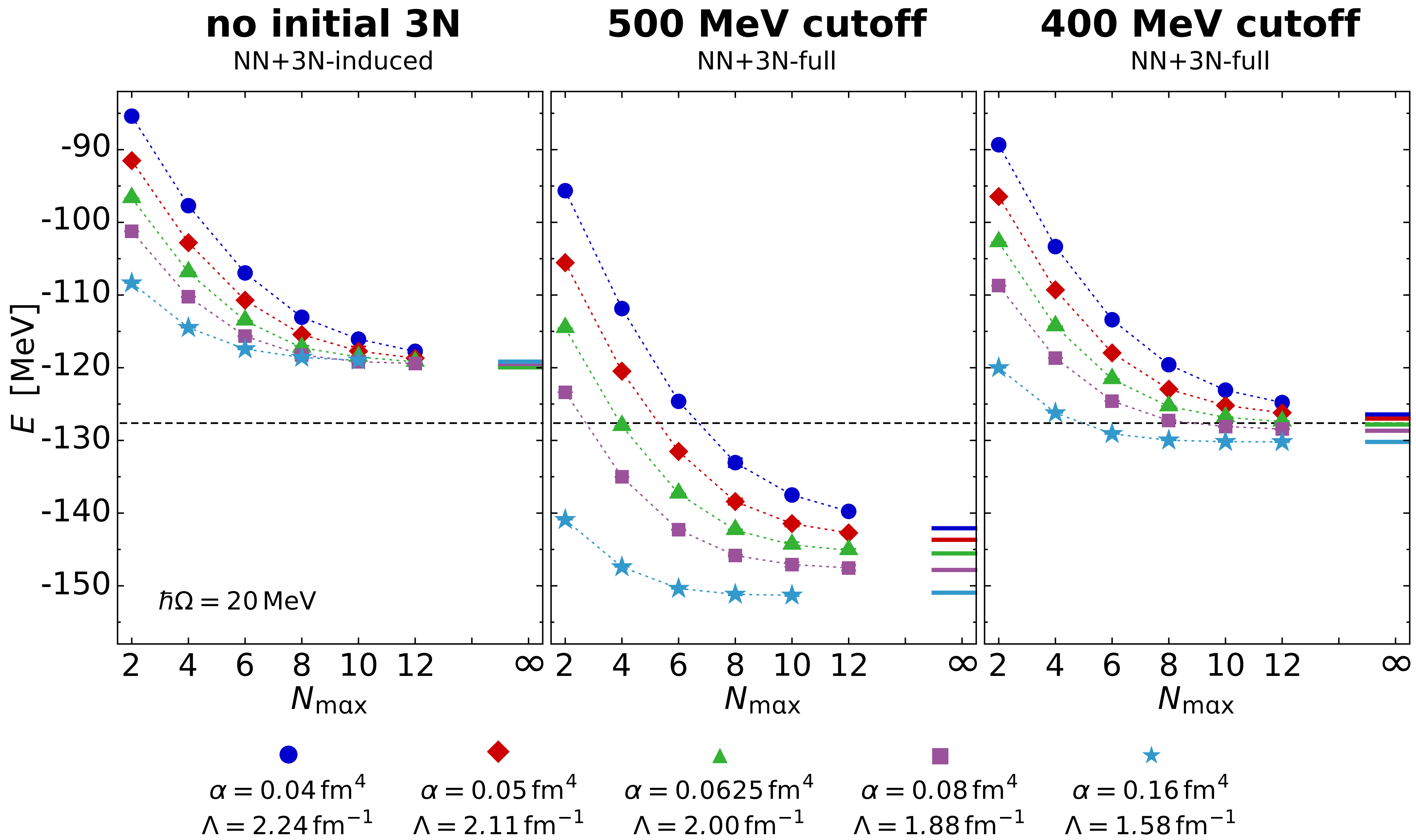
Lowering the Initial 3N Cutoff



- off-diagonal matrix elements dominated by c_i (c_3 and c_4) terms
- suppress off-diagonal matrix elements by lowering 3N cutoff Λ_{3N}

	c_1	c_3	c_4	c_D	c_E
$\Lambda_{3N} = 500$ MeV	+0.81	−3.2	+5.4	−0.2	−0.205
$\Lambda_{3N} = 400$ MeV	+0.81	−3.2	+5.4	−0.2	+0.098*

^{16}O: Lowering the Initial 3N Cutoff



Conclusions

Conclusions

- Importance-Truncated NCSM
  - powerful scheme to extend the reach of the NCSM
  - robust, universal, and efficient approach
  - controlled, quantified, and improvable uncertainties
- SRG-evolved chiral NN+3N Hamiltonians for ground states
  - induced 4N interactions become sizable in upper p-shell
  - caused by two-pion terms (c_3 in particular) of the chiral 3N
  - lowering of the initial 3N cutoff circumvents this problem
- more applications in Joachim's and Sven's talks...

Epilogue

- **thanks to my group & my collaborators**
  - **S. Binder**, **A. Calci**, B. Erler, E. Gebrerufael, A. Günther, H. Krutsch, **J. Langhammer**, S. Reinhardt, C. Stumpf, R. Trippel, K. Vobig, R. Wirth
    Institut für Kernphysik, TU Darmstadt
  - **P. Navrátil**
    TRIUMF Vancouver, Canada
  - J. Vary, P. Maris
    Iowa State University, USA
  - S. Quaglioni
    LLNL Livermore, USA
  - P. Piecuch
    Michigan State University, USA
  - H. Hergert
    Ohio State University, USA
  - P. Papakonstantinou
    IPN Orsay, F
  - C. Forssén
    Chalmers University, Sweden
  - H. Feldmeier, T. Neff
    GSI Helmholtzzentrum

JUROPA — JÜLICH FORSCHUNGSZENTRUM

LOEWE-CSC — CSC Center for Scientific Computing Frankfurt

HOPPER — NERSC

COMPUTING TIME

SFB 634

Deutsche Forschungsgemeinschaft DFG

HIC for FAIR Helmholtz International Center

LOEWE – Landes-Offensive zur Entwicklung Wissenschaftlich-ökonomischer Exzellenz

HELMHOLTZ GEMEINSCHAFT

Bundesministerium für Bildung und Forschung