Nuclear Structure with Similarity-Transformed Chiral NN+3N Interactions

Angelo Calci
Institut für Kernphysik

TECHNISCHE
UNIVERSITÄT
DARMSTADT

Outline

- Introduction
- Chiral Effective Field Theory (χEFT)
- Similarity Renormalization Group
- Transformation to $\mathcal{J}, T$-Coupled Scheme
- Importance Truncated No-Core Shell Model
- Hartree Fock
- Summary and Outlook

Outline

- **Introduction**
- Chiral Effective Field Theory (χEFT)
- Similarity Renormalization Group
- Transformation to $\mathcal{J}, T$-Coupled Scheme
- Importance Truncated No-Core Shell Model
- Hartree Fock
- Summary and Outlook

Introduction

start with many-body eigenvalue problem

$$\mathrm{H}_{\mathrm{int}}\left|\Psi_n\right\rangle = E_n\left|\Psi_n\right\rangle$$

interacti

$\mathrm{H}_{\mathrm{int}}$

body problem

ab-initio methods

- investigation and adjustment of interaction
- reference point for approximative approaches
- make predictions in low-mass regime

observables to experiment

Outline

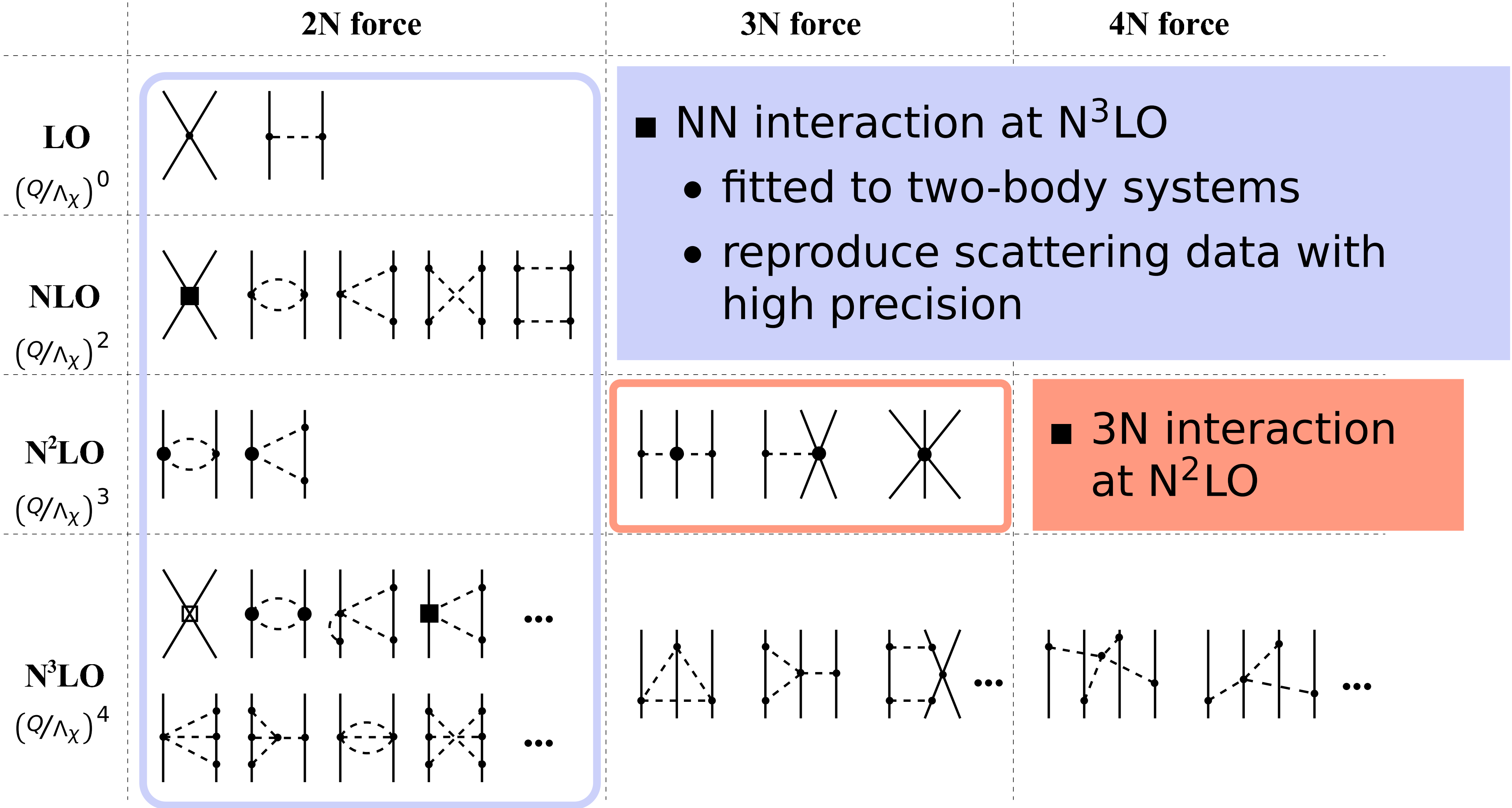
- Introduction
- **Chiral Effective Field Theory (χEFT)**
- Similarity Renormalization Group
- Transformation to $\mathcal{J}, T$-Coupled Scheme
- Importance Truncated No-Core Shell Model
- Hartree Fock
- Summary and Outlook

Chiral Effective Field Theory

- want to obtain an interaction **based on QCD** as much as possible
- Quantum Chromodynamics (QCD)
  - fundamental theory of the strong interaction
  - uses quarks and gluons as degrees of freedom
  - currently **no direct** derivation of nuclear **interaction** (non-perturbative for low-energy regime)
  - effective field theory necessary

- Chiral Effective Field Theory (χEFT)
  - considers fundamental symmetries of QCD
  - uses **nucleons** and **pions** as degrees of freedom
  - perturbative **expansion** in $\frac{Q}{\Lambda_\chi}$

Expansion in Q/Λ_χ

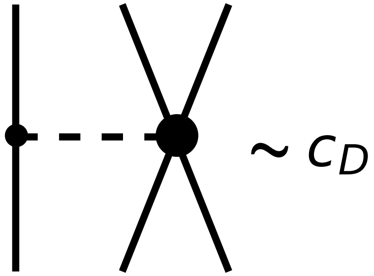


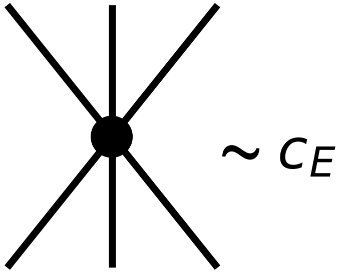
- NN interaction at N^{3}LO
  - fitted to two-body systems
  - reproduce scattering data with high precision

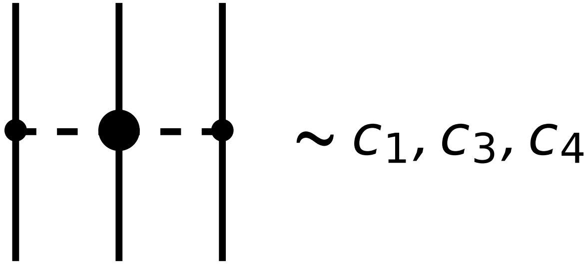
- 3N interaction at N^{2}LO

- provides **NN** and **3N interactions** in a **consistent** manner

3N Contribution at N^{2}LO


$\sim c_D$


$\sim c_E$


$\sim c_1, c_3, c_4$

one-pion exchan   pion exchange

two nucleo

required model space for (IT)-NCSM
to large to obtain converged results

⇒ apply **unitary transformation** to
accelerate convergence

low e

- c_1, c_3, c_4 fixed b
- new **LECs of 3N** interaction are $\mathbf{c_D}$ and $\mathbf{c_E}$
  - fitted to binding energy and β-decay half-life of triton

Outline

- Introduction
- Chiral Effective Field Theory (χEFT)
- **Similarity Renormalization Group**
- Transformation to $\mathcal{J}, T$-Coupled Scheme
- Importance Truncated No-Core Shell Model
- Hartree Fock
- Summary and Outlook

Similarity Renormalization Group (SRG)

accelerate convergence by **pre-diagonalizing** the Hamiltonian w.r.t. the many-body basis

- continuous **unitary transformation** of the Hamiltonian

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

- leads to **evolution equation**

$$\frac{d}{d\alpha}\widetilde{H}_\alpha = \left[\eta_\alpha, \widetilde{H}_\alpha\right] \quad \text{with} \quad \eta_\alpha = -U_\alpha^\dagger \frac{dU_\alpha}{d\alpha} = -\eta_\alpha^\dagger$$

initial value problem with $\widetilde{H}_{\alpha=0} = H_{\mathrm{int}}$

- choose the **dynamic generator**

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

advantages of SRG: **simplicity** and **flexibility**

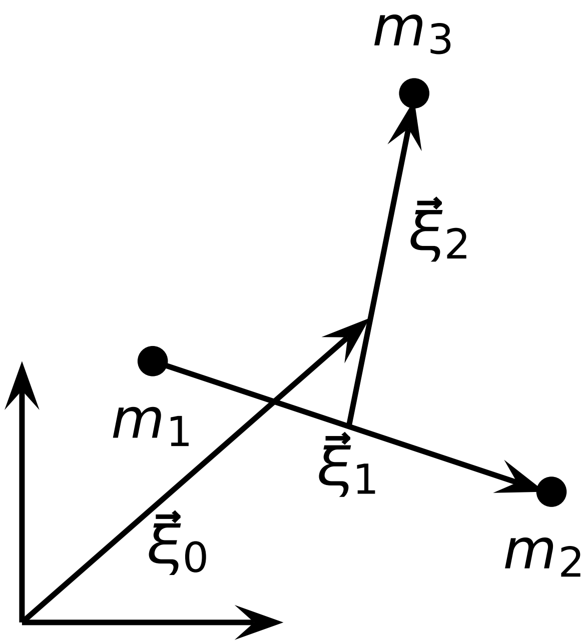
Insertion: Jacobi Coordinates

- "**relative coordinates**" for A-body system

$$\vec{\xi}_0 = \sqrt{\frac{1}{A}}\,[\vec{r}_1 + \vec{r}_2 + \ldots + \vec{r}_A]$$

$$\vec{\xi}_{n-1} = \sqrt{\frac{n-1}{n}}\,\left[\frac{1}{n-1}(\vec{r}_1 + \vec{r}_2 + \ldots + \vec{r}_{n-1}) - \vec{r}_n\right] \quad \text{with} \quad 2 \leq n \leq A$$

- for example $A = 3$:



$$\vec{\xi}_0 = \sqrt{\frac{1}{3}}\,[\vec{r}_1 + \vec{r}_2 + \vec{r}_3]$$

$$\vec{\xi}_1 = \sqrt{\frac{1}{2}}\,[\vec{r}_1 - \vec{r}_2]$$

$$\vec{\xi}_2 = \sqrt{\frac{2}{3}}\,\left[\frac{1}{2}(\vec{r}_1 + \vec{r}_2) - \vec{r}_3\right]$$

Insertion: HO Jacobi Basis

- Cartesian HO state

$$\left|n_1 l_1 m_1(\vec{r}_1), n_2 l_2 m_2(\vec{r}_2), n_3 l_3 m_3(\vec{r}_3)\right\rangle$$

where l_1 : quantum number w.r.t. $\vec{\boldsymbol{L}}_{\mathbf{1}} = \vec{\boldsymbol{r}}_{\mathbf{1}} \times \vec{\boldsymbol{p}}_{\mathbf{1}}$

l_2 : quantum number w.r.t. $\vec{\boldsymbol{L}}_{\mathbf{2}} = \vec{\boldsymbol{r}}_{\mathbf{2}} \times \vec{\boldsymbol{p}}_{\mathbf{2}}$

l_3 : quantum number w.r.t. $\vec{\boldsymbol{L}}_{\mathbf{3}} = \vec{\boldsymbol{r}}_{\mathbf{3}} \times \vec{\boldsymbol{p}}_{\mathbf{3}}$

- Jacobi HO state

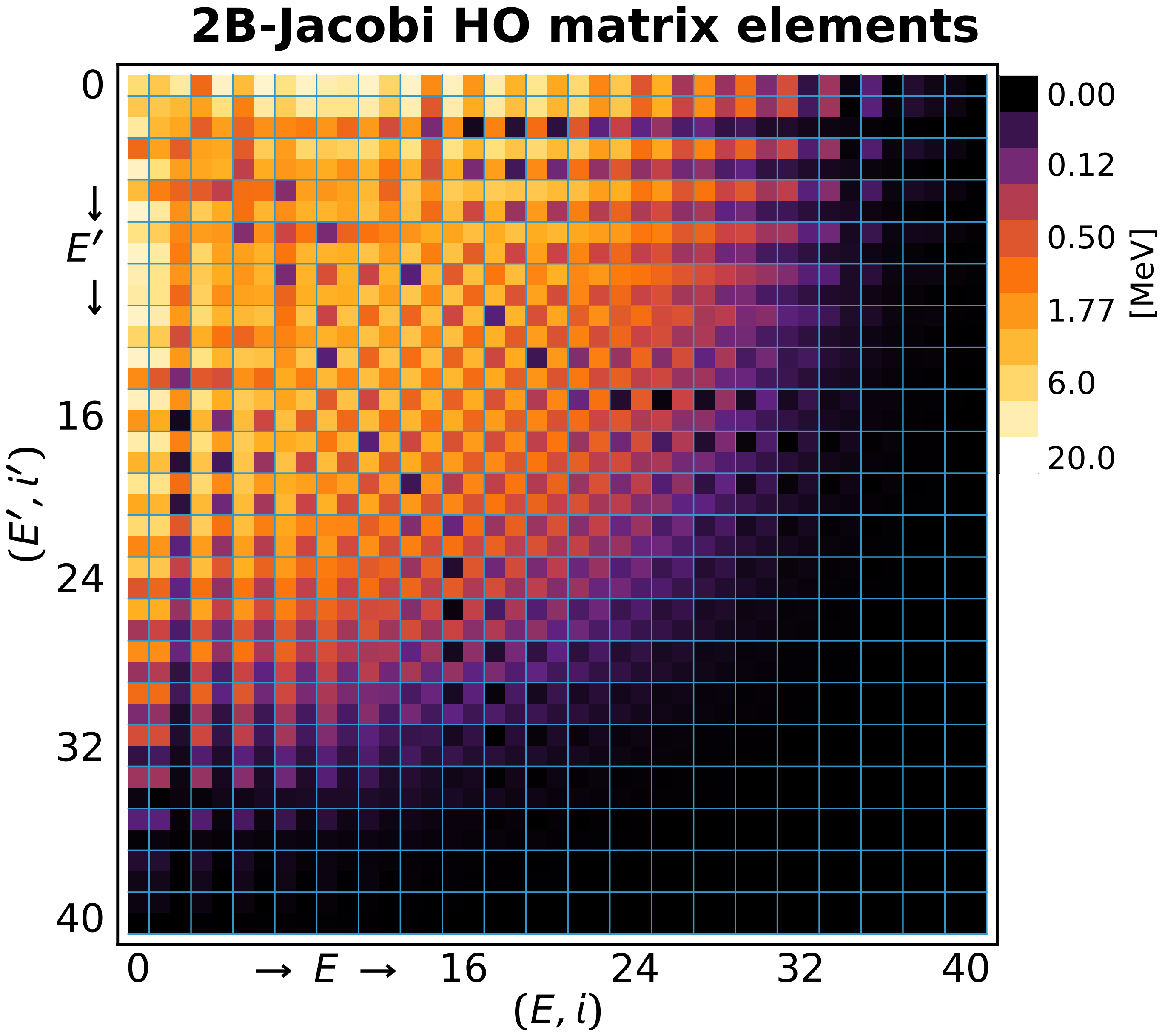
$$\left|NLM(\vec{\xi}_0), n_{12} l_{12} m_{12}(\vec{\xi}_1), \mathcal{N}_3 \mathcal{L}_3 \mathcal{M}_3(\vec{\xi}_2)\right\rangle$$

where L :

$\mathcal{L}_3$: qu

HO basis **separates** into the relevant **intrinsic** and the center of mass part

SRG Evolution in Two-Body Space

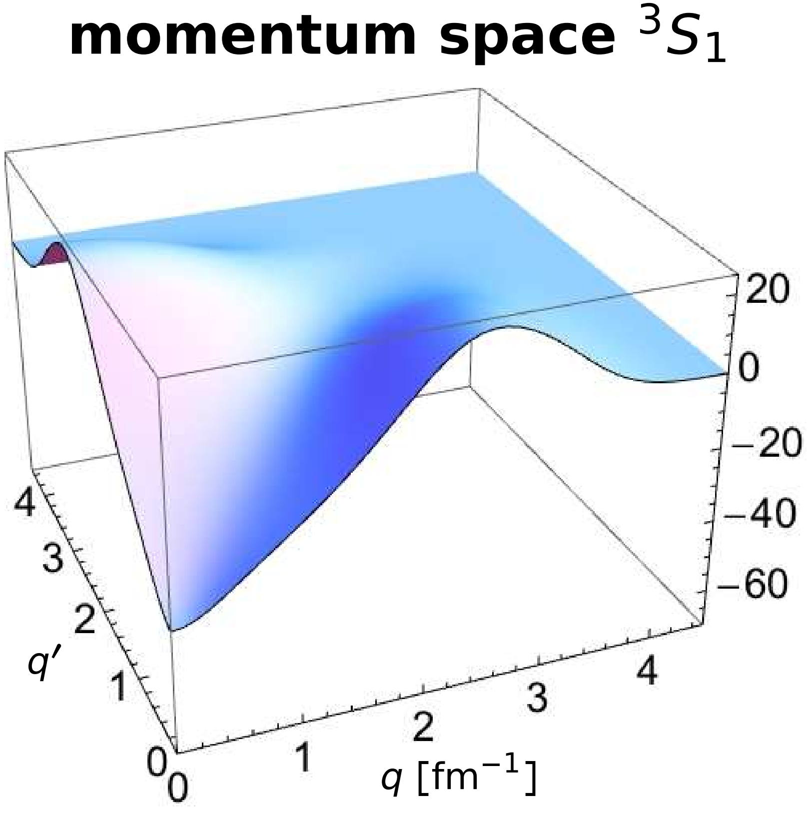


$\alpha = 0.00\,\mathrm{fm}^4$

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

$\langle E'(L'S)J^\pi T | \widetilde{\mathrm{H}}_\alpha | E(LS)J^\pi T \rangle$

$J^\pi = 1^+, T = 0, \hbar\Omega = 20\,\mathrm{MeV}$



SRG Evolution in Two-Body Space

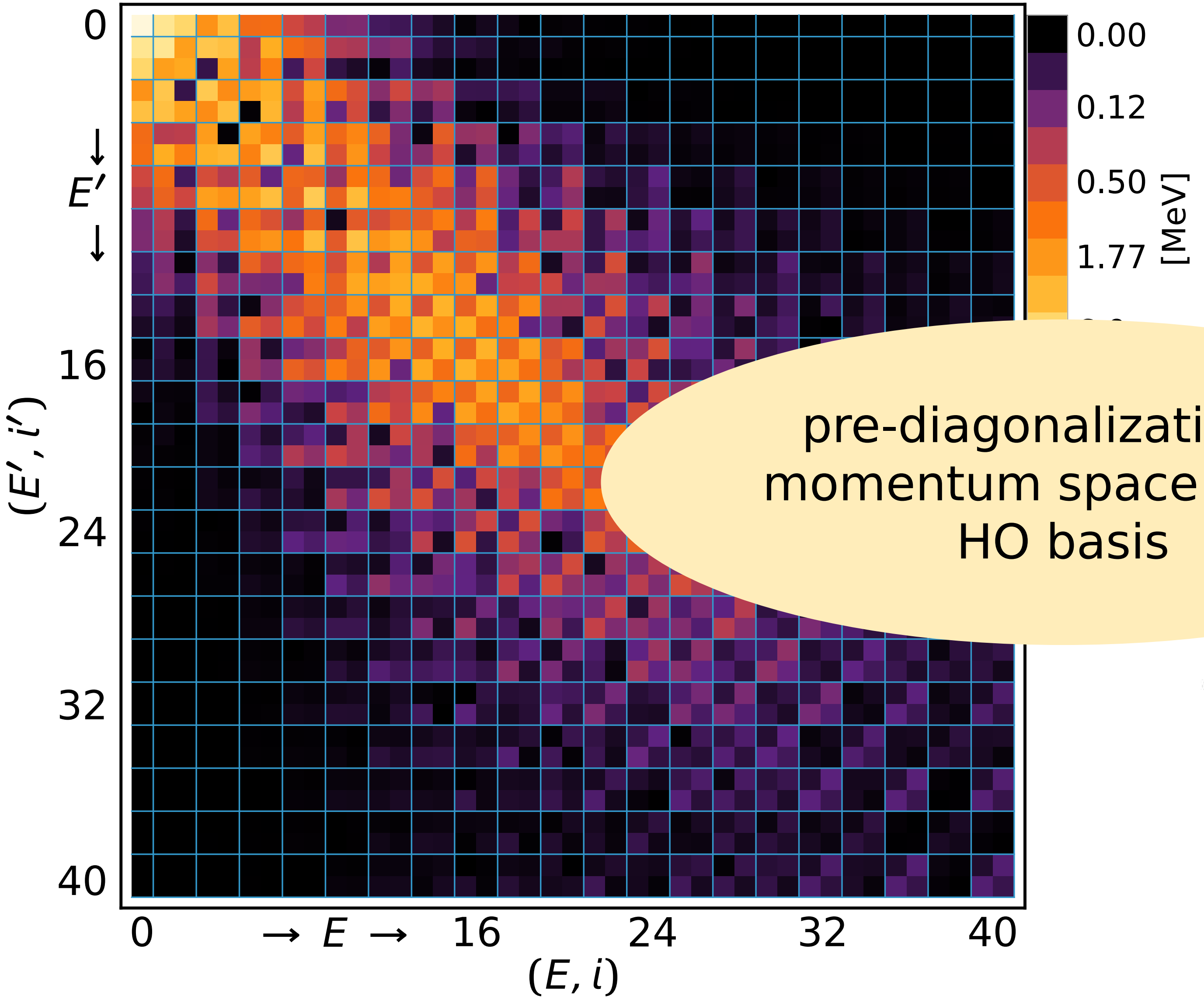
$\alpha = 0.32\,\mathrm{fm}^4$

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

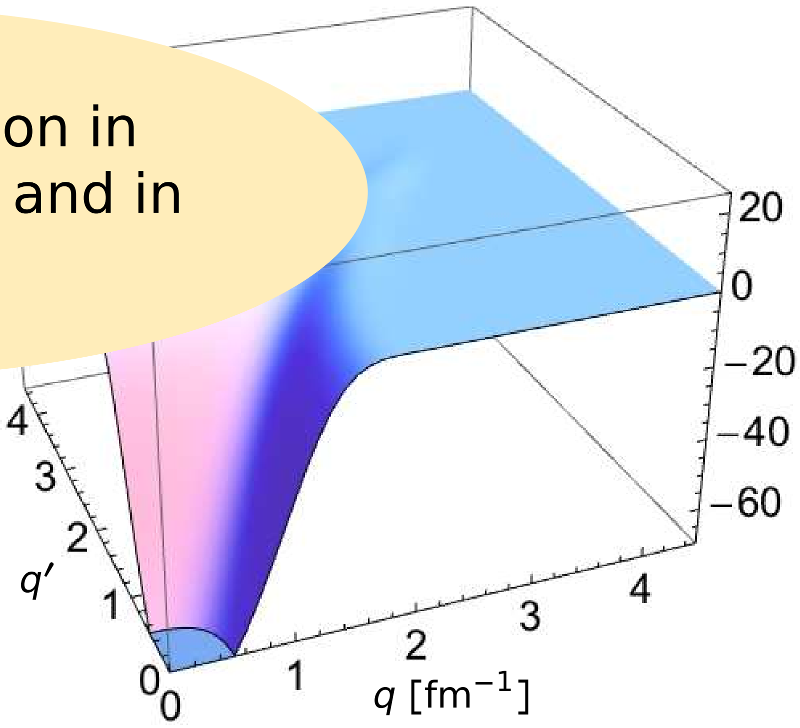
$\langle E'(L'S)J^\pi T |\, \widetilde{\mathrm{H}}_\alpha \,| E(LS)J^\pi T \rangle$

$J^\pi = 1^+, T = 0, \hbar\Omega = 20\,\mathrm{MeV}$

2B-Jacobi HO matrix elements



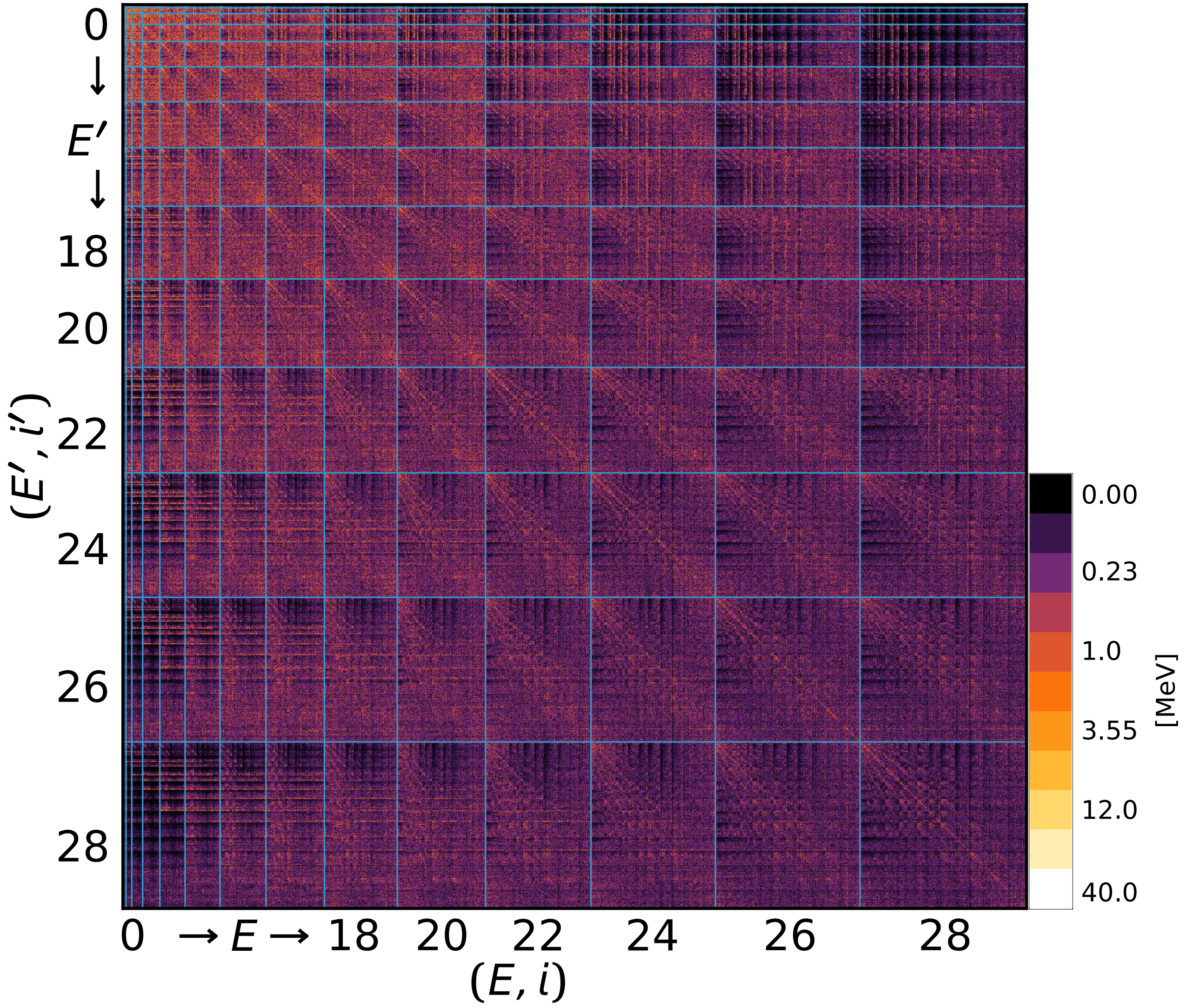
momentum space $^3S_1$



pre-diagonalization in momentum space and in HO basis

SRG Evolution in Three-Body Space

3B-Jacobi HO matrix elements



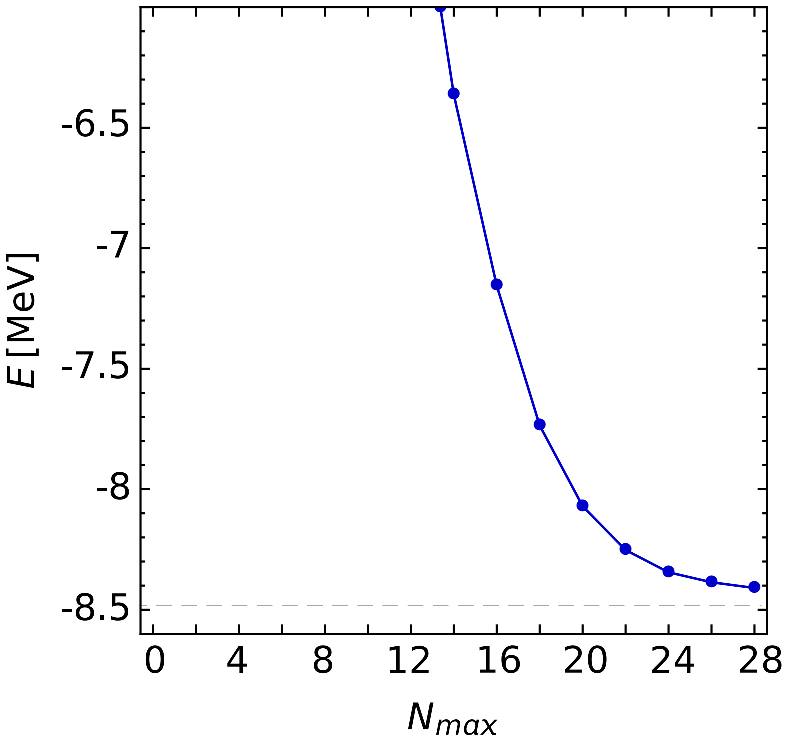
$$\alpha = 0.00\,\mathrm{fm}^4$$

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

$$\left\langle E'i'JT \right| \widetilde{\mathrm{H}}_\alpha \left| EiJT \right\rangle$$

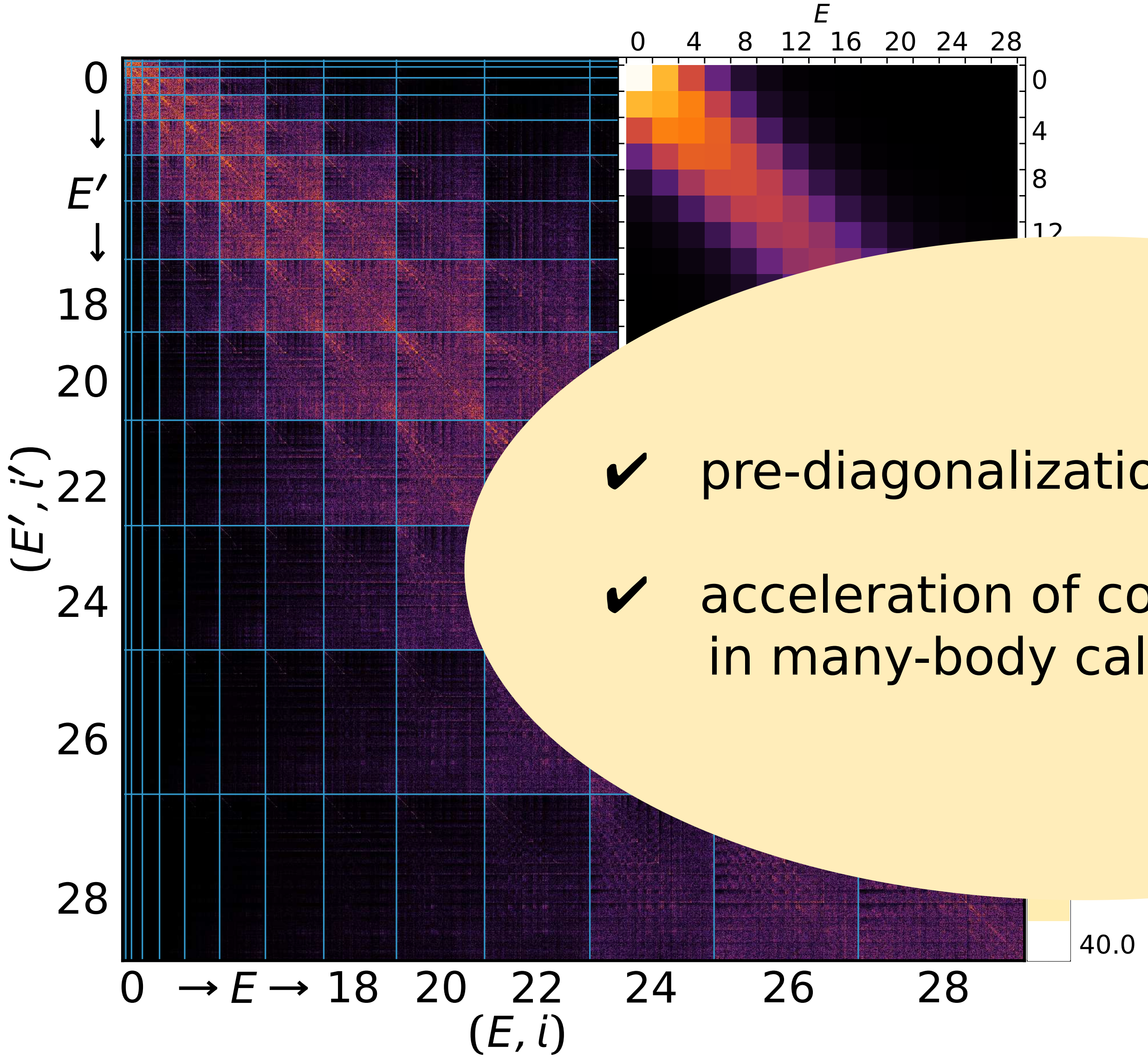
$$J^\pi = \tfrac{1}{2}^+, T = \tfrac{1}{2}, \hbar\Omega = 20\,\mathrm{MeV}$$

NCSM ground state ^{3}H



SRG Evolution in Three-Body Space

3B-Jacobi HO matrix elements



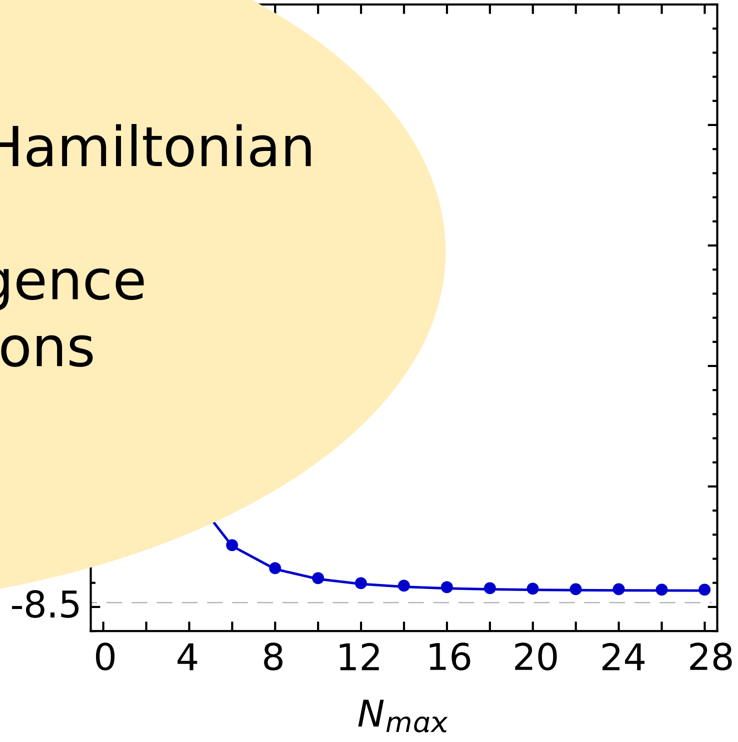
$$\alpha = 0.32\,\mathrm{fm}^4$$

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

$$\langle E'i'JT|\,\widetilde{\mathrm{H}}_\alpha\,|EiJT\rangle$$

$$J^\pi = \tfrac{1}{2}^+, T = \tfrac{1}{2}, \hbar\Omega = 20\,\mathrm{MeV}$$

CSM ground state ^{3}H



- ✔ pre-diagonalization of Hamiltonian
- ✔ acceleration of convergence in many-body calculations

Consideration of Induced Contributions

- SRG induces **irreducible** many-body **contributions**

$$\tilde{H}_\alpha^{\mathrm{NN+3N}} = T_{\mathrm{int}} + \tilde{T}^{[2]}_{\mathrm{int},\alpha} + \tilde{V}^{[2]}_{\mathrm{NN},\alpha} + \tilde{T}^{[3]}_{\mathrm{int},\alpha} + \tilde{V}^{[3]}_{\mathrm{NN},\alpha} + \tilde{V}^{[3]}_{\mathrm{3N},\alpha} + \tilde{T}^{[4]}_{\mathrm{int},\alpha} + \tilde{V}^{[4]}_{\mathrm{NN},\alpha} + \tilde{V}^{[4]}_{\mathrm{3N},\alpha} + \dots$$

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

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

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

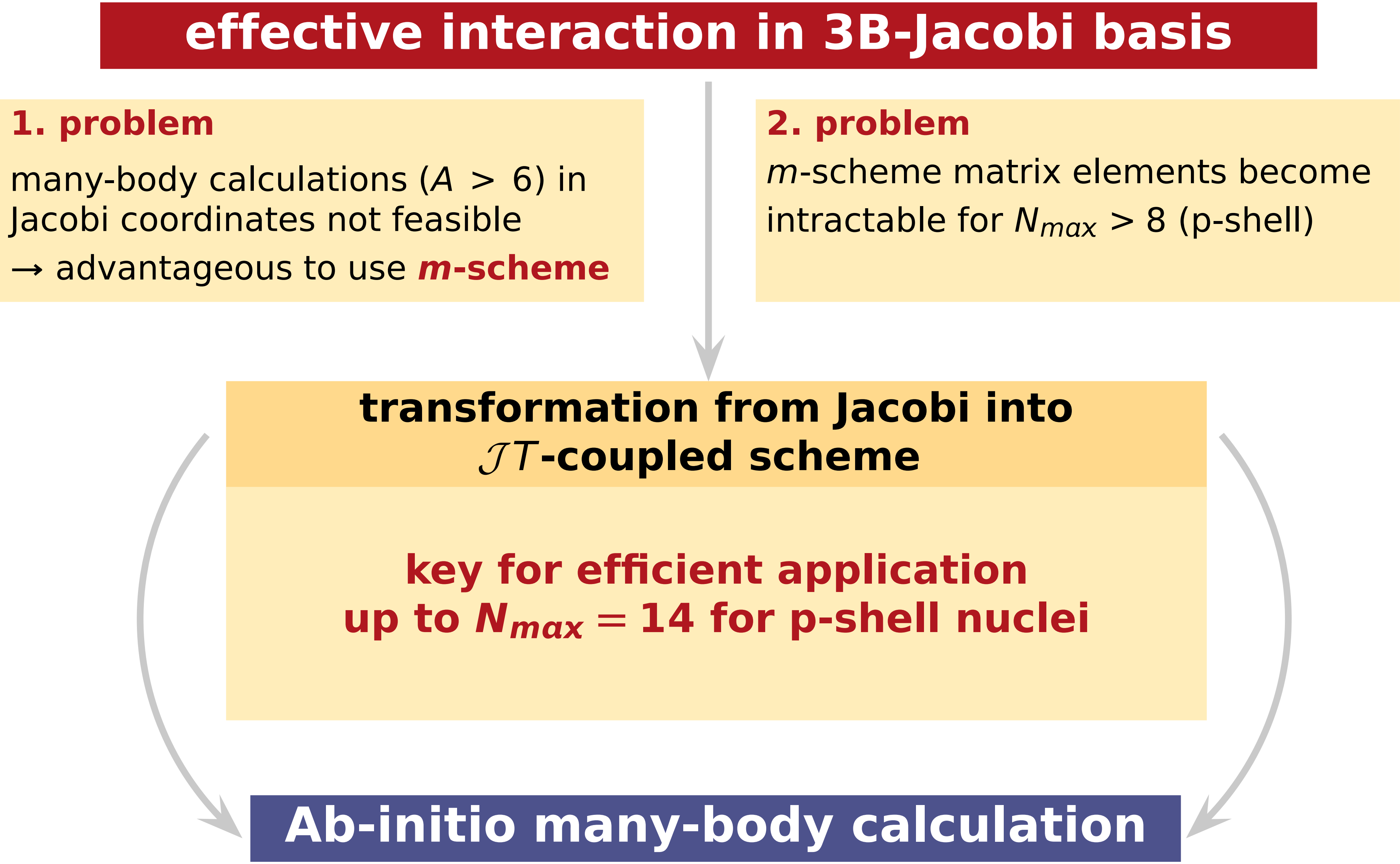
$$\tilde{H}_\alpha^{\text{NN+3N-induced}} = T_{\mathrm{int}} + \tilde{T}^{[2]}_{\mathrm{int}}$$

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

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

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

From Jacobi to $\mathcal{J}$T-coupled Scheme



effective interaction in 3B-Jacobi basis

1. problem

many-body calculations ($A > 6$) in Jacobi coordinates not feasible

→ advantageous to use ***m*-scheme**

2. problem

m-scheme matrix elements become intractable for $N_{max} > 8$ (p-shell)

transformation from Jacobi into $\mathcal{J}T$-coupled scheme

key for efficient application up to $N_{max} = 14$ for p-shell nuclei

Ab-initio many-body calculation

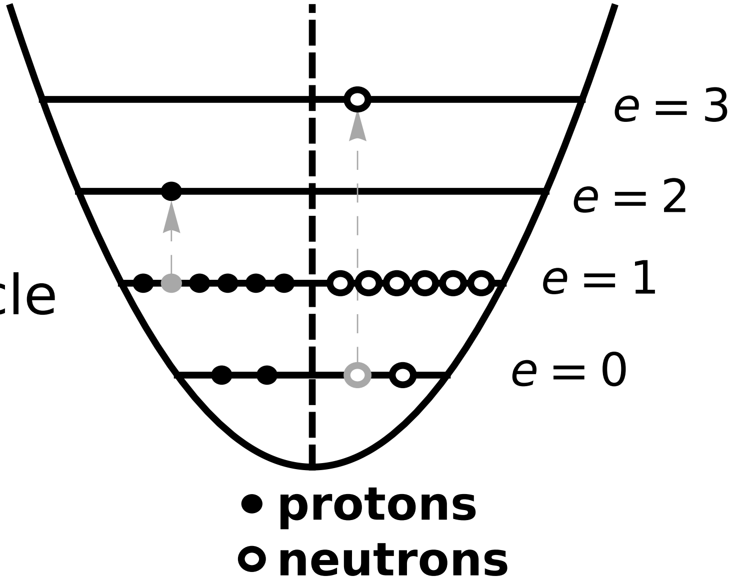
Outline

- Introduction
- Chiral Effective Field Theory (χEFT)
- Similarity Renormalization Group
- Transformation to $\mathcal{J}, T$-Coupled Scheme
- **Importance Truncated No-Core Shell Model**
- Hartree Fock
- Summary and Outlook

No-Core Schalenmodell (NCSM)

- **solving the eigenvalue problem**

$$\mathrm{H_{int}}|\Psi_n\rangle = E_n|\Psi_n\rangle$$



- **many-body basis**: Slater determinants $|\Phi_\nu\rangle$ composed of harmonic oscillator single-particle states (m-scheme)

$$\left|\Psi_n\right\rangle = \sum_\nu C_\nu^n \left|\Phi_\nu\right\rangle$$

- **model space**: spanned by *m*-scheme states $|\Phi_\nu\rangle$ with unperturbed excitation energy of up to $N_{max}\hbar\Omega$

problem

enormous increase of model space with particle number A

⇒ converged calculation limited to small A

Importance Truncated NCSM

- start with approximation $|\Psi_{\text{ref}}\rangle$ for the **target state** obtained in 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

embed into iterative scheme

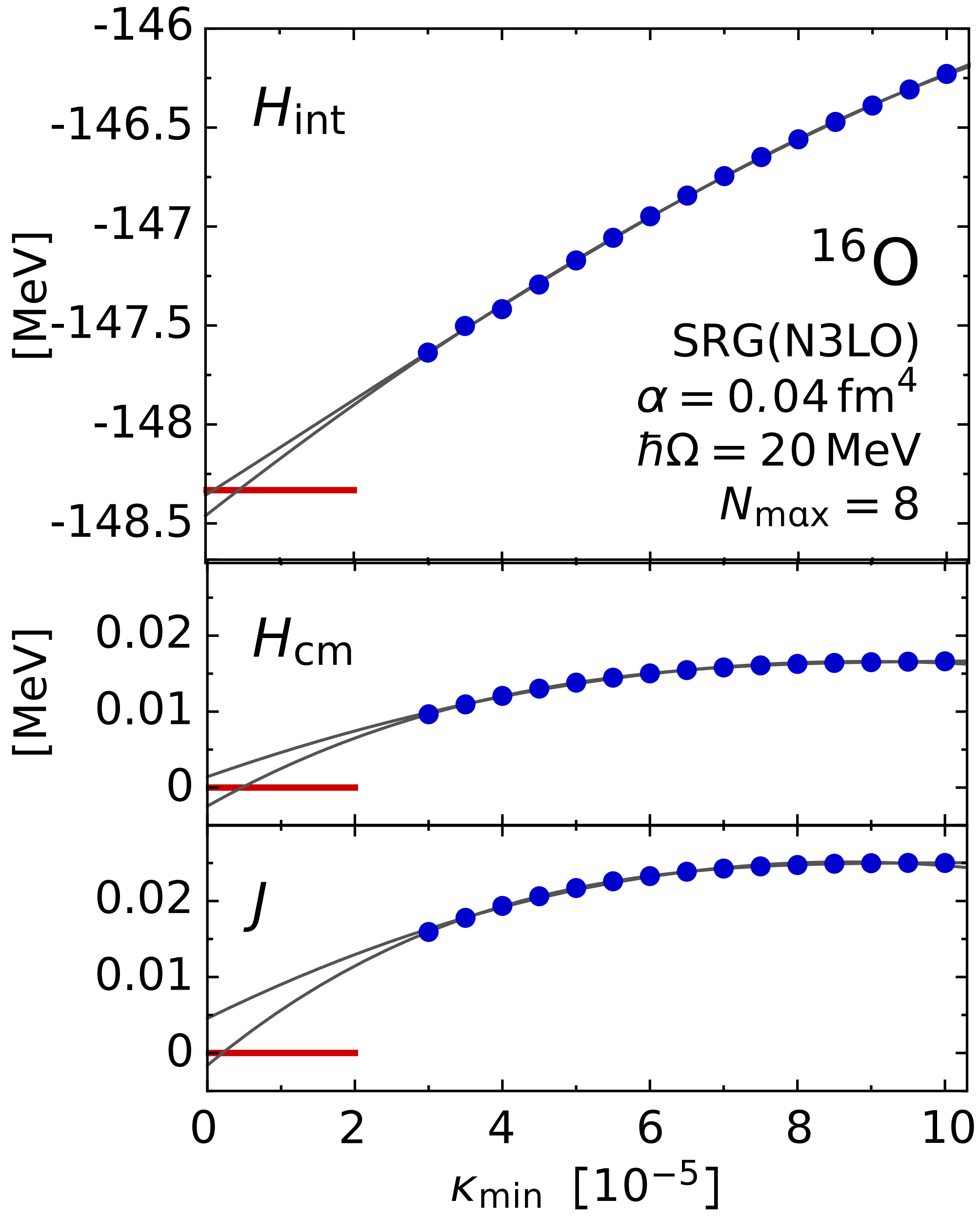
- construct **importance truncated space** $\mathcal{M}(\kappa_{\text{min}})$ spanned by basis states with $|\kappa_{\nu}| \geq \kappa_{\text{min}}$

- **solve eigenvalue problem** in importance truncated space $\mathcal{M}(\kappa_{\text{min}})$ and obtain improved approximation of target state

Importance Truncation: Iterative Scheme

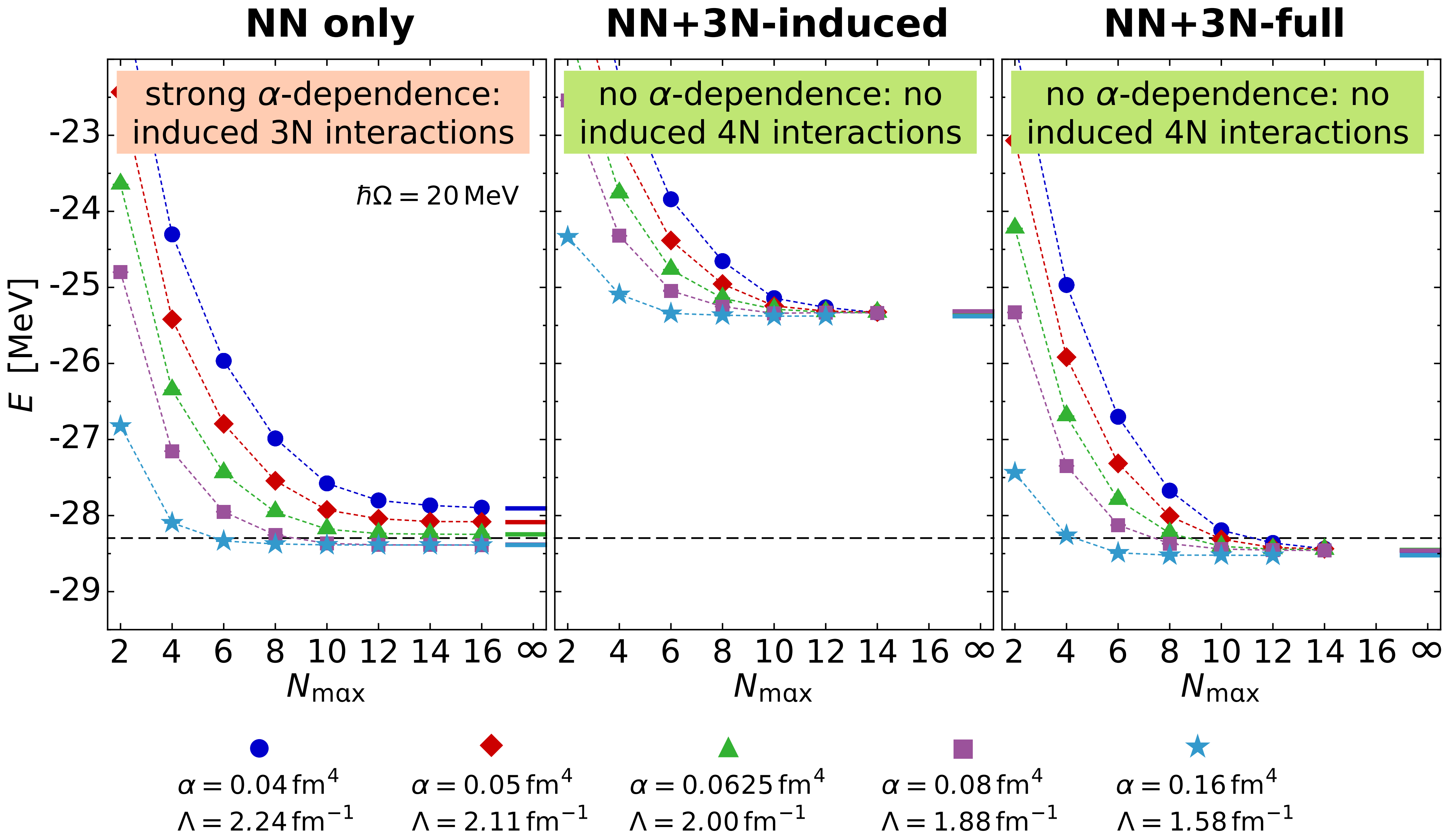
- **sequential calculation** for a range of $N_{\max}\hbar\Omega$ spaces:
  - ✪ full NCSM calculation for small $N_{\max}$ to obtain initial $|\Psi_{\text{ref}}\rangle$
  - ❶ construct importance-truncated space with $N_{\max} + 2$ of states with $|\kappa_\nu| \geq \kappa_{\min}$
  - ❷ solve eigenvalue problem
  - ❸ use eigenstate as new $|\Psi_{\text{ref}}\rangle$
  - ❹ goto ❶
- **full NCSM space is recovered** in the limit $\kappa_{\min} \to 0$

Threshold Extrapolation

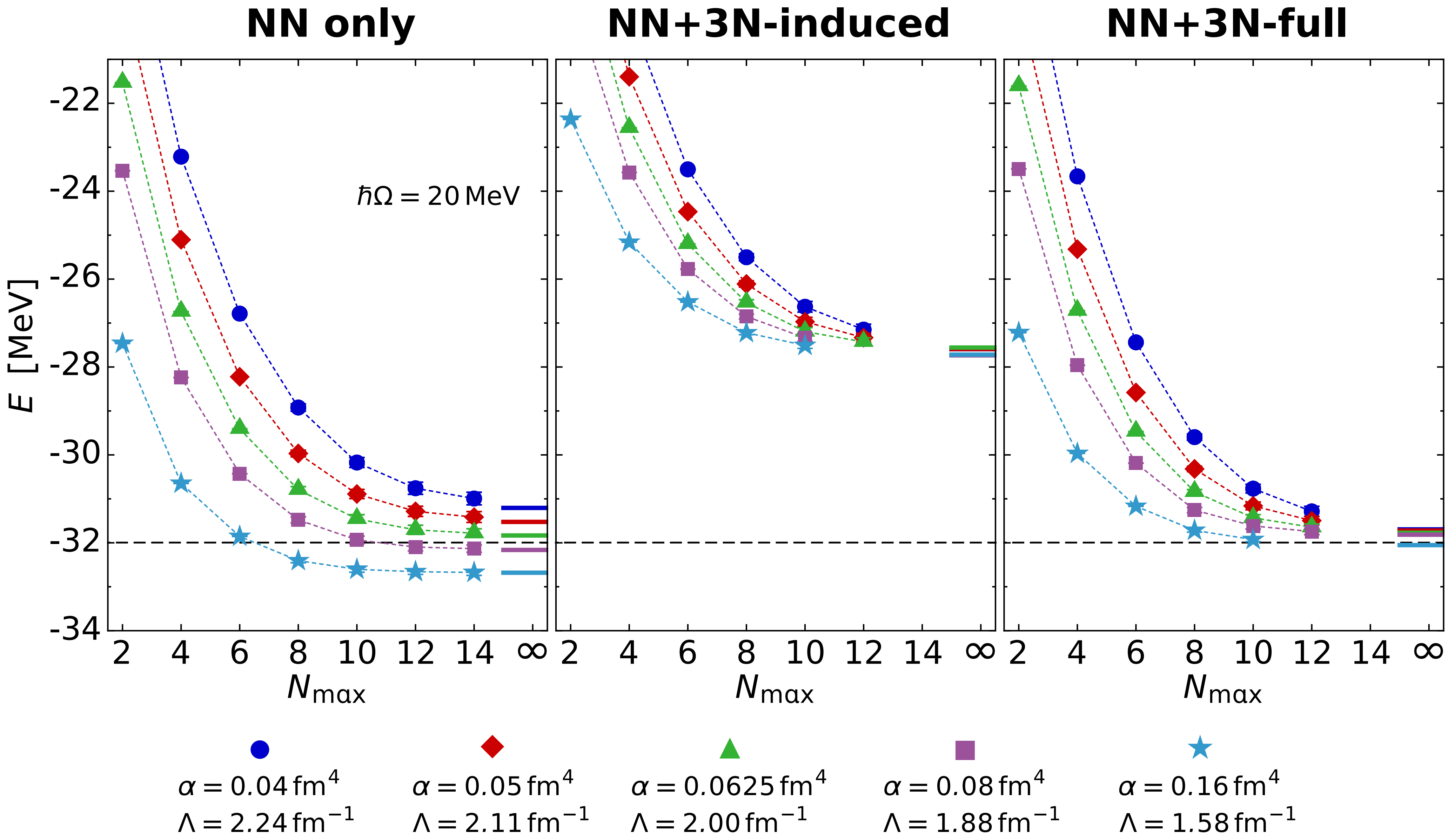


- do calculations for a **sequence of importance thresholds κ_{min}**
- observables show smooth threshold dependence
- systematic approach to the **full NCSM limit**
- use **a posteriori extrapolation** $\kappa_{\text{min}} \rightarrow 0$ of observables to account for effect of excluded configurations

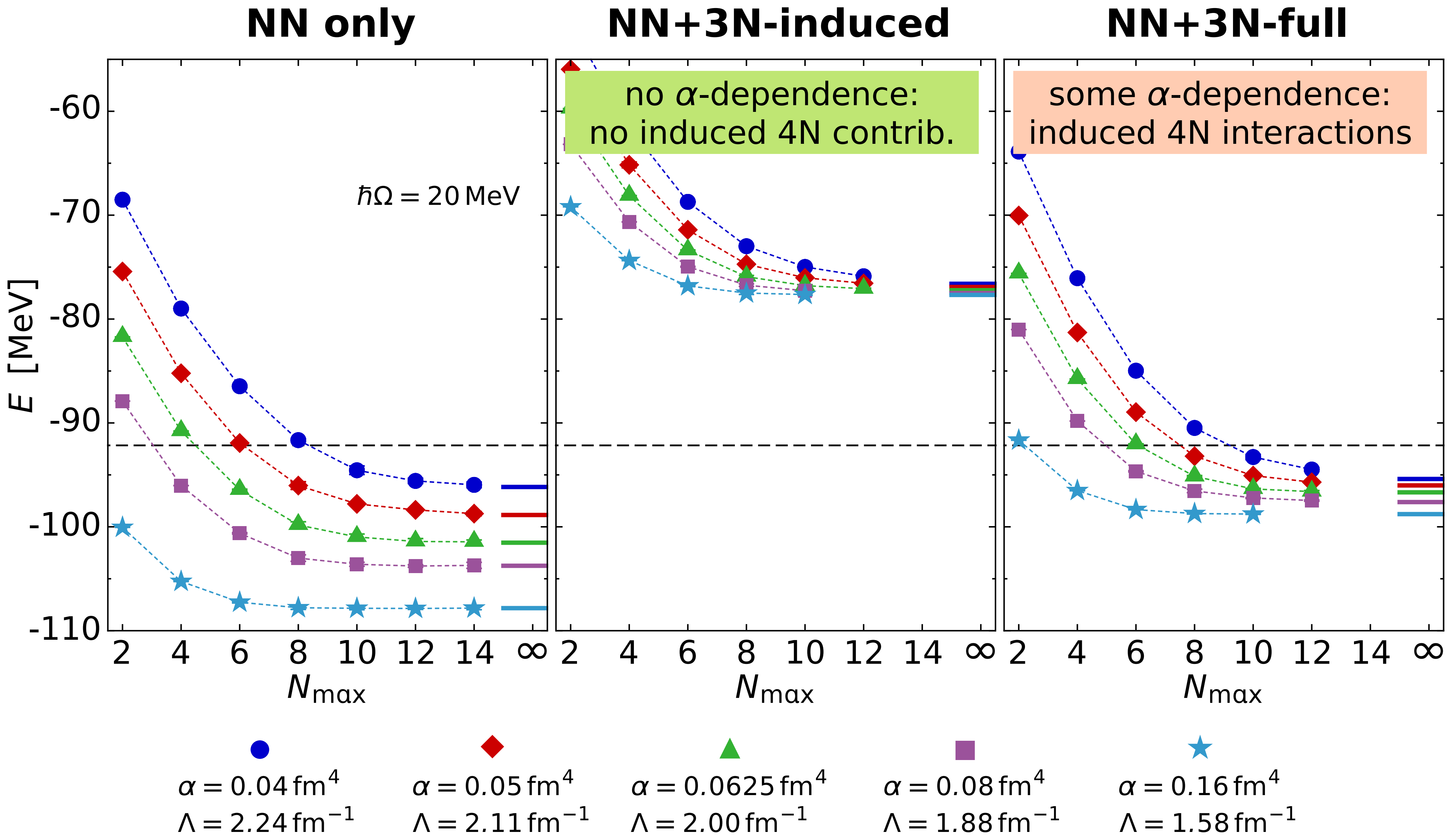
^{4}He: Ground-State Energies



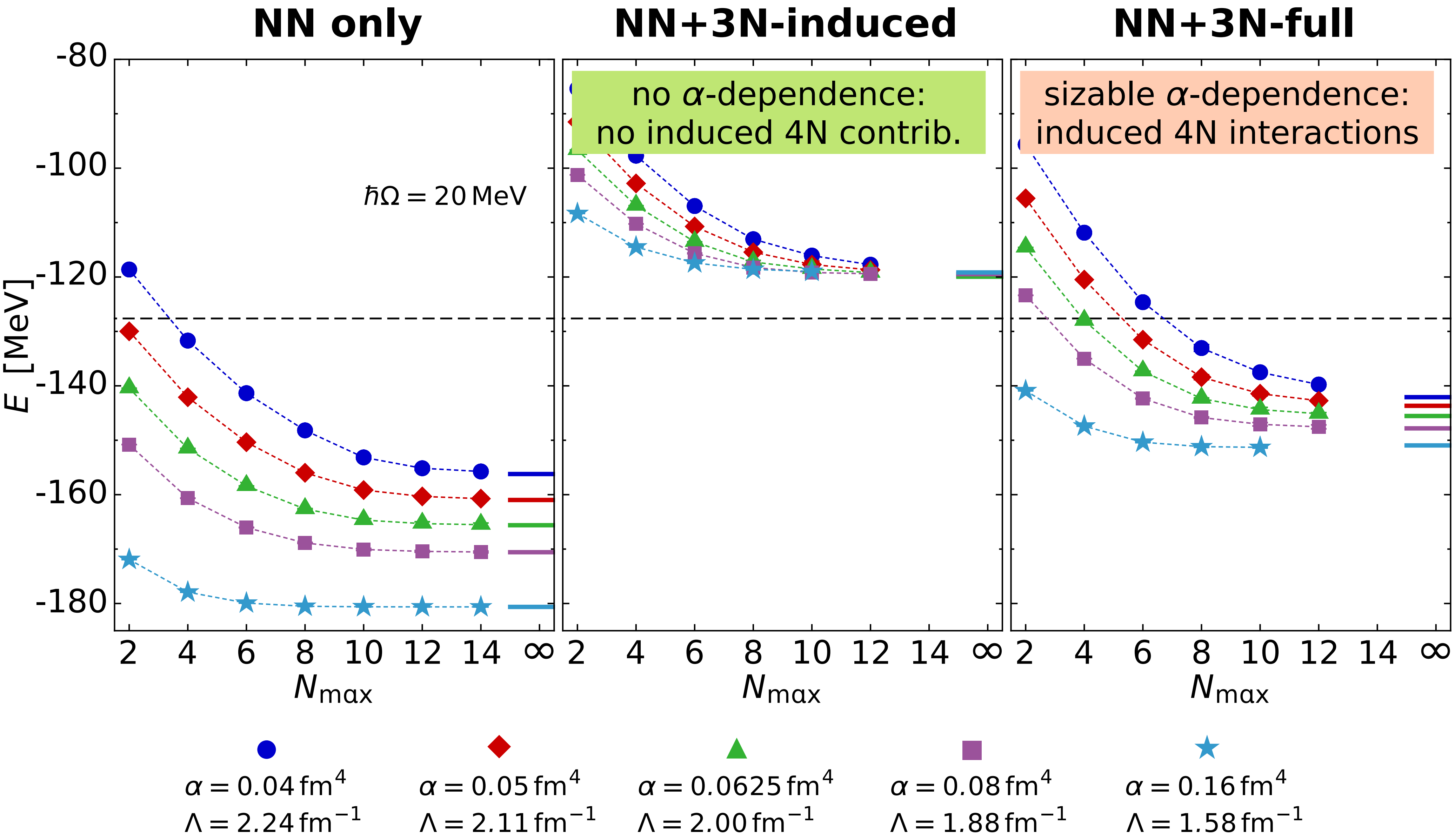
^{6}Li: Ground-State Energies



^{12}C: Ground-State Energies

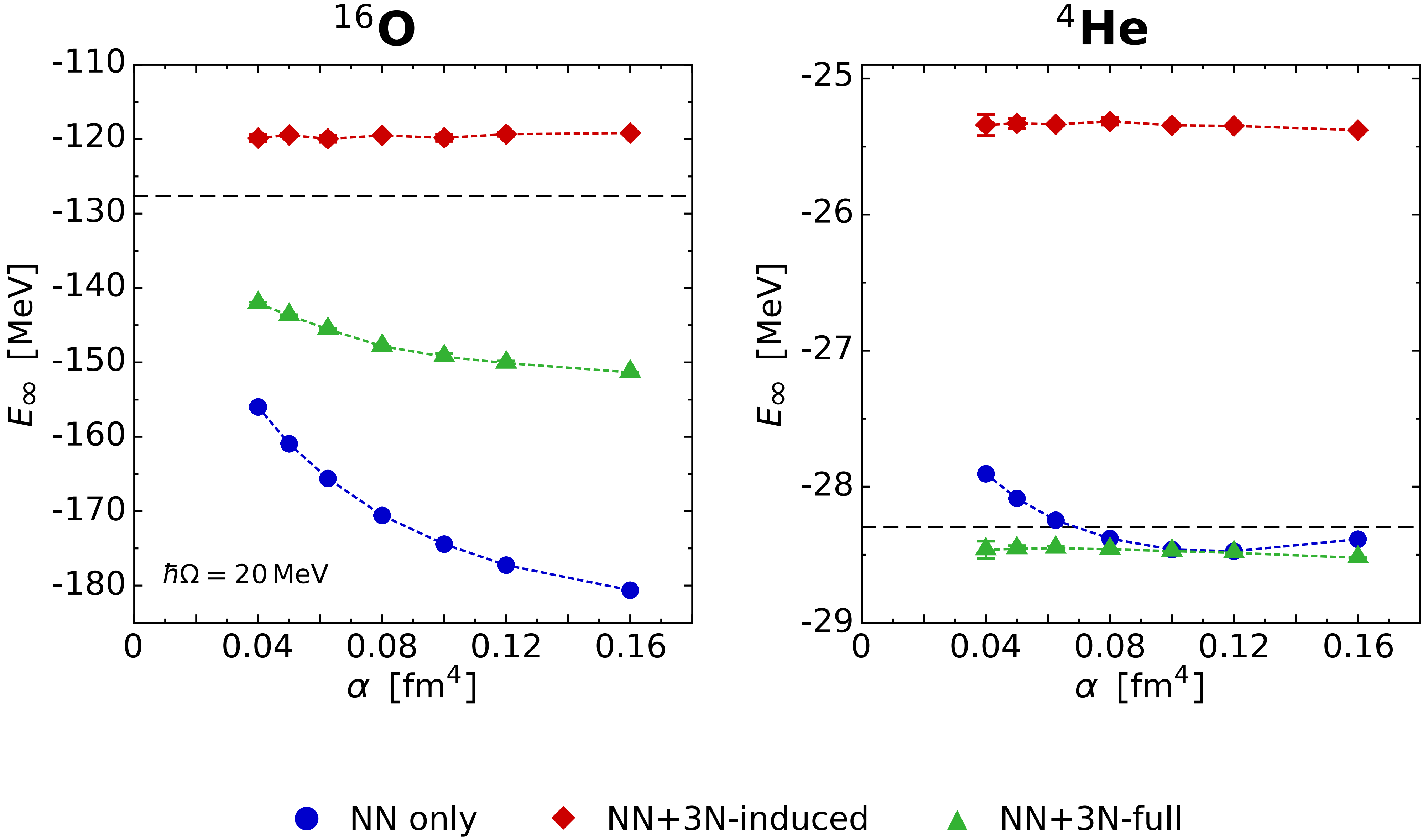


^{16}O: Ground-State Energies

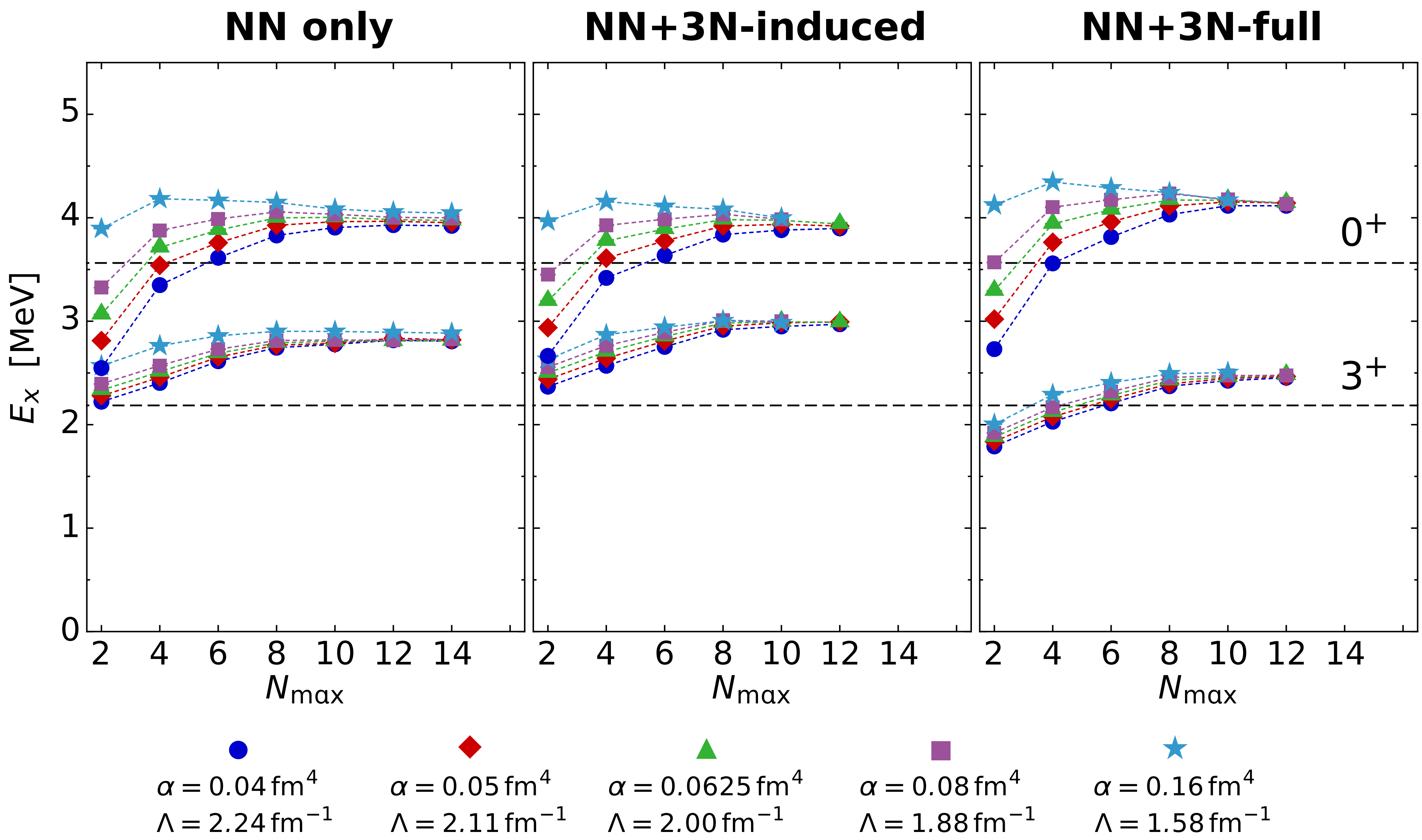

no α-dependence:
no induced 4N contrib.

sizable α-dependence:
induced 4N interactions

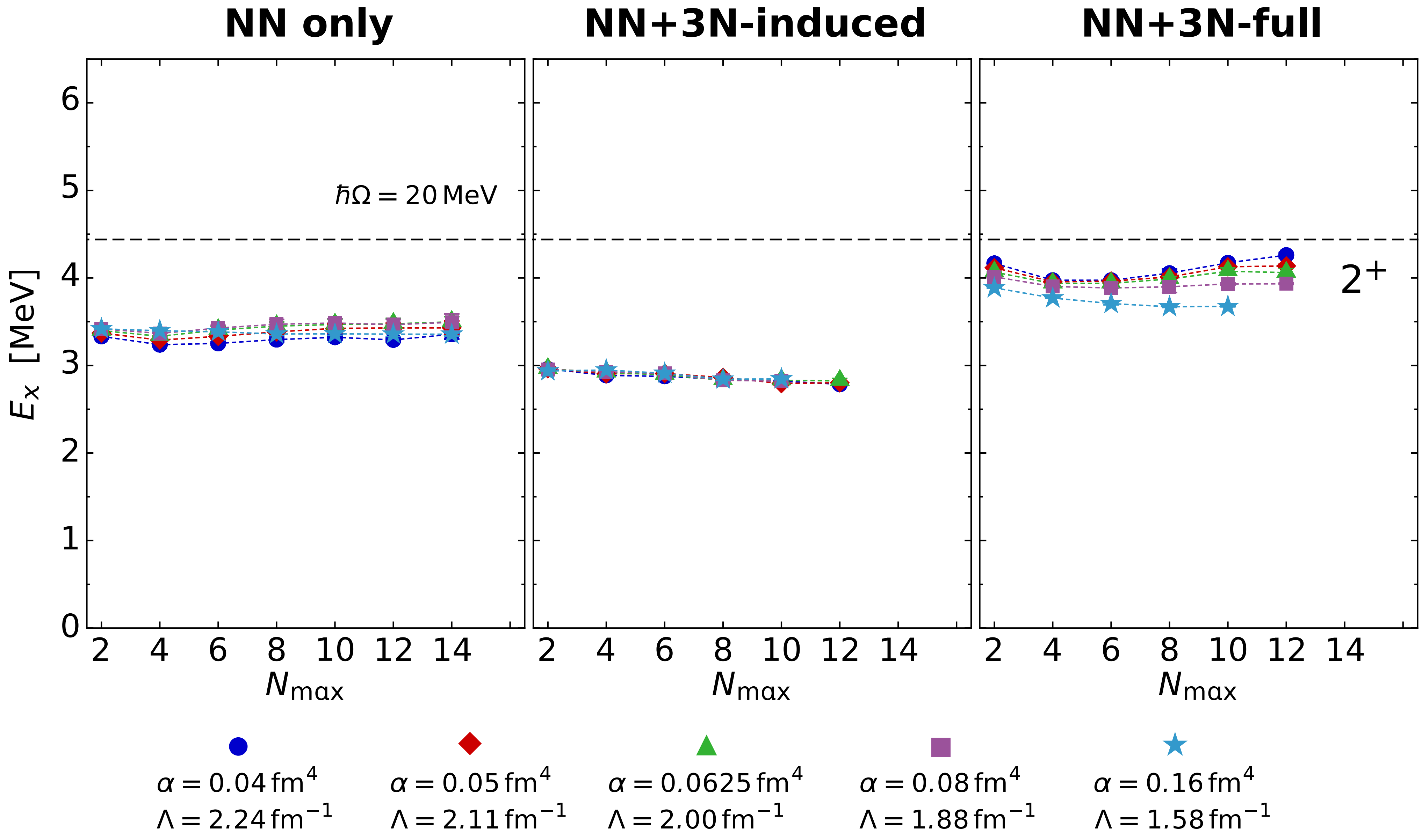
^{16}O & ^{4}He: Energy vs. Flow Parameter



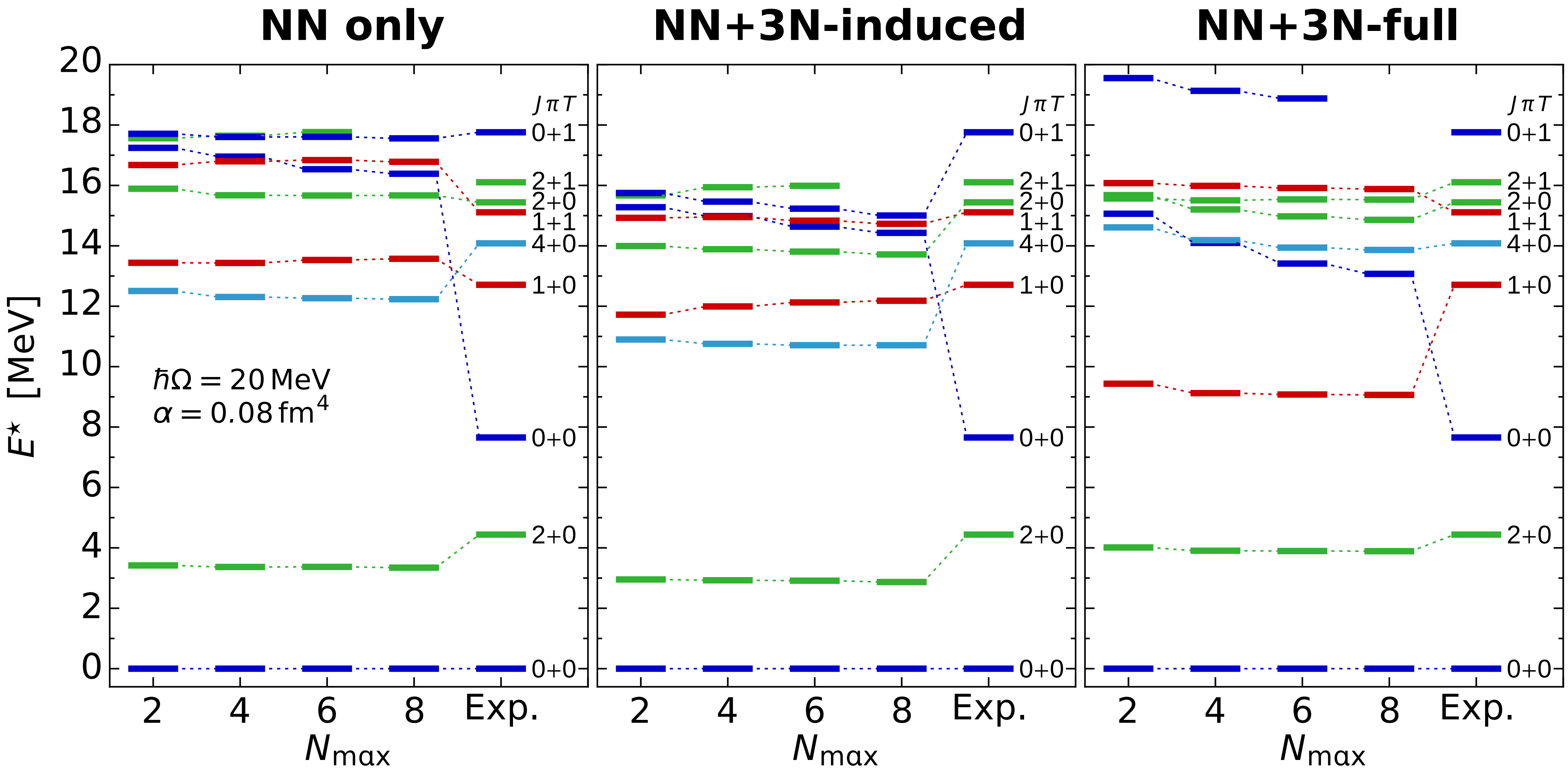
^{6}Li: Excitation Energies



^{12}C: Excitation Energies

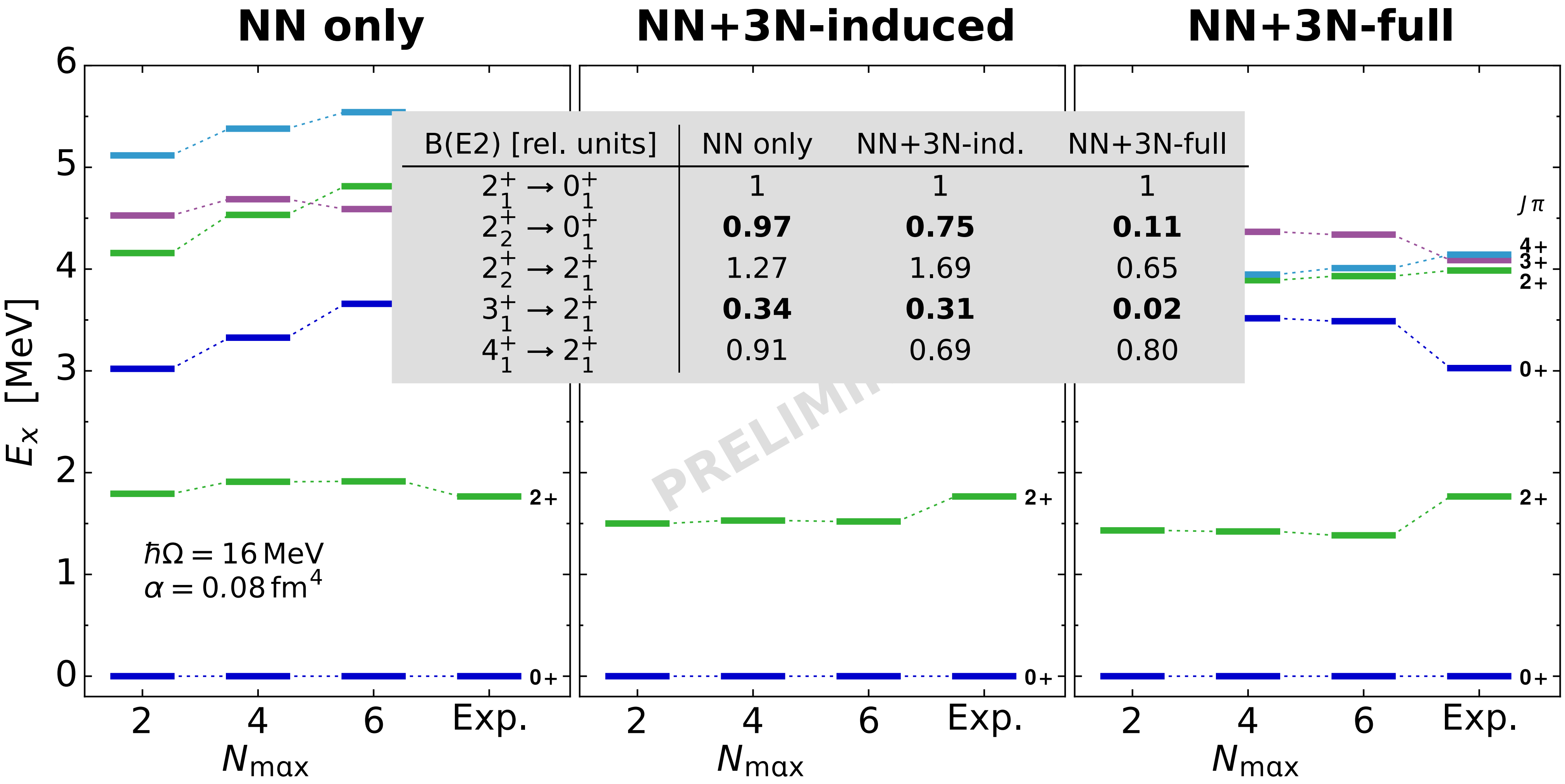


Spectroscopy of ^{12}C



- IT-NCSM gives access to **complete spectroscopy of p- and sd-shell nuclei** starting from chiral NN+3N interactions

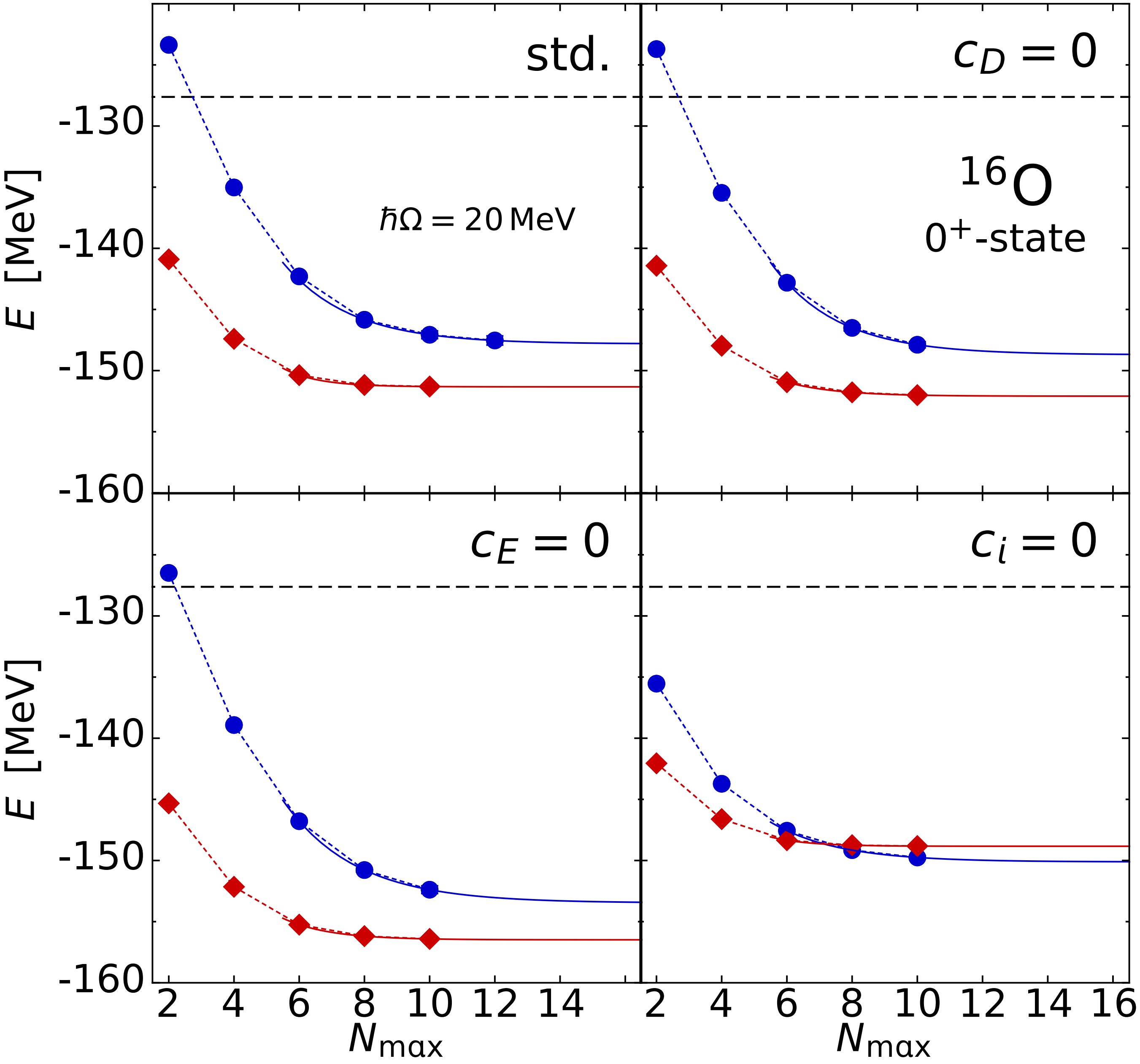
Spectroscopy of ^{16}C



B(E2) [rel. units]	NN only	NN+3N-ind.	NN+3N-full
$2^+_1 \to 0^+_1$	1	1	1
$2^+_2 \to 0^+_1$	**0.97**	**0.75**	**0.11**
$2^+_2 \to 2^+_1$	1.27	1.69	0.65
$3^+_1 \to 2^+_1$	**0.34**	**0.31**	**0.02**
$4^+_1 \to 2^+_1$	0.91	0.69	0.80

- IT-NCSM gives access to **complete spectroscopy of p- and sd-shell nuclei** starting from chiral NN+3N interactions

Origin of Induced 4N Contributions



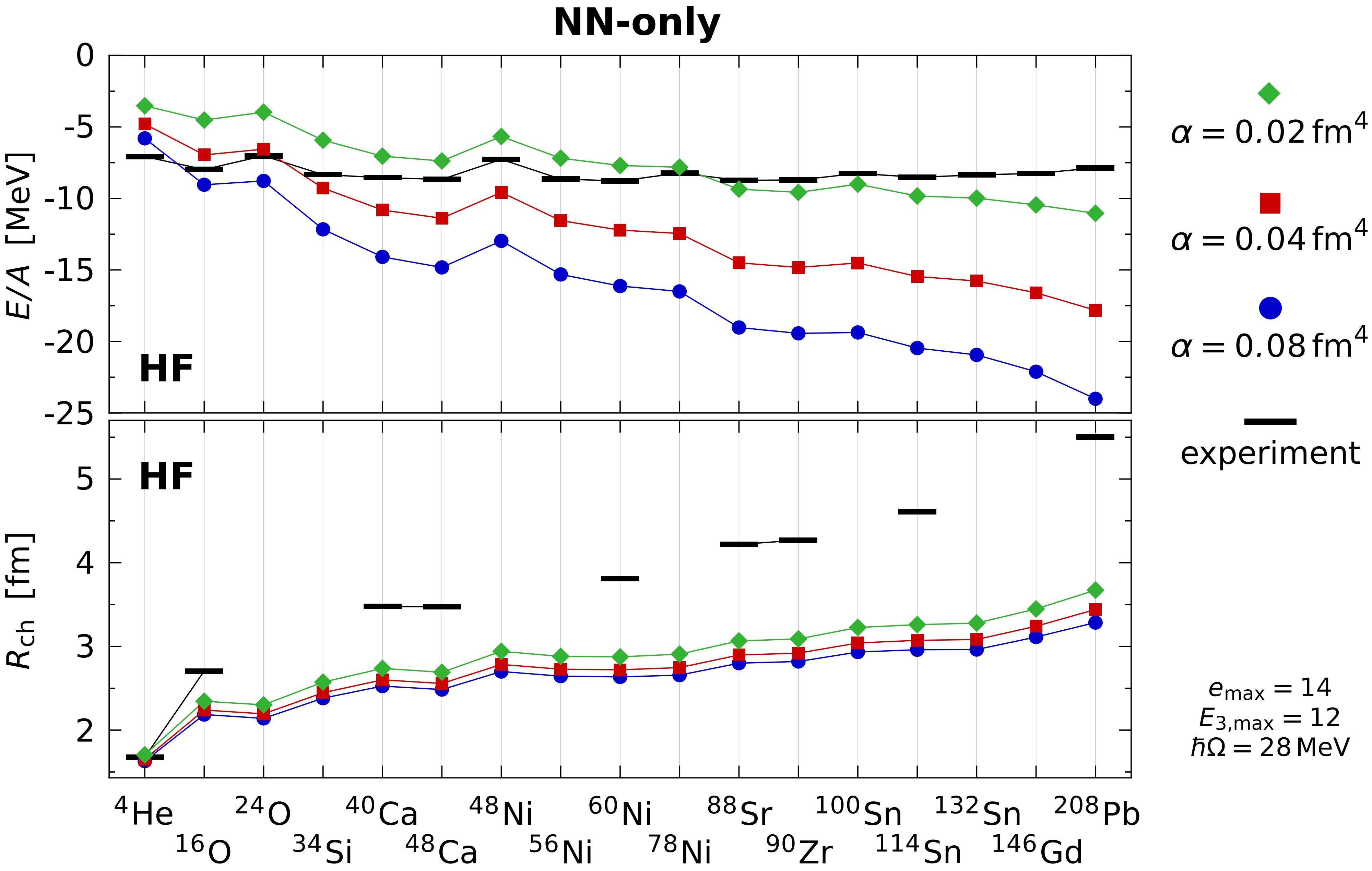
- almost same α-dependence for standard LECs and $c_D = 0$ or $c_E = 0$

⇒ **two-pion exchange** (c_i) term **induces** significant many-body **contributions**

Outline

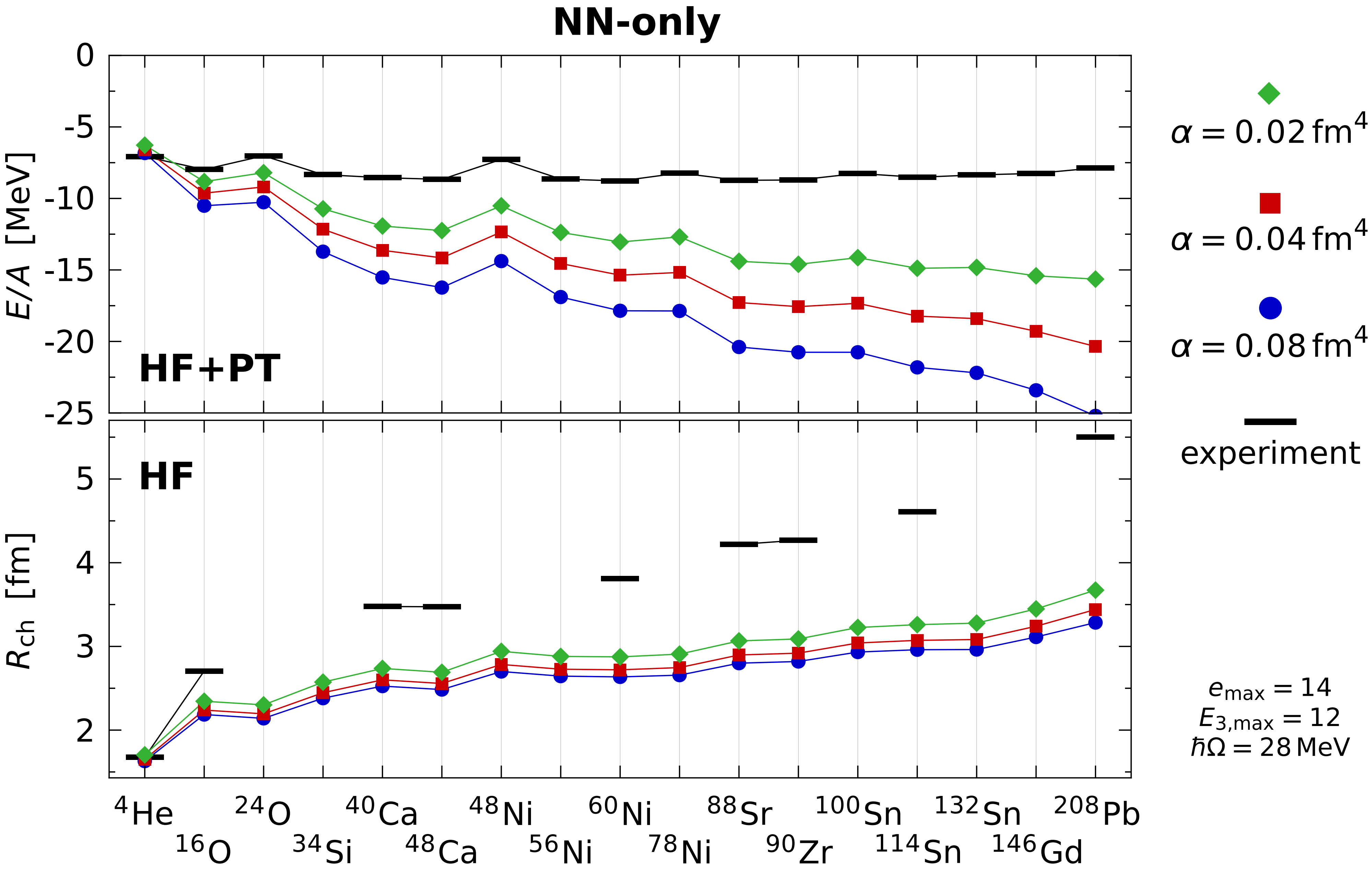
- Introduction
- Chiral Effective Field Theory (χEFT)
- Similarity Renormalization Group
- Transformation to $\mathcal{J}, T$-Coupled Scheme
- Importance Truncated No-Core Shell Model
- **Hartree Fock**
- Summary and Outlook

Systematics: E/A and R_{ch}

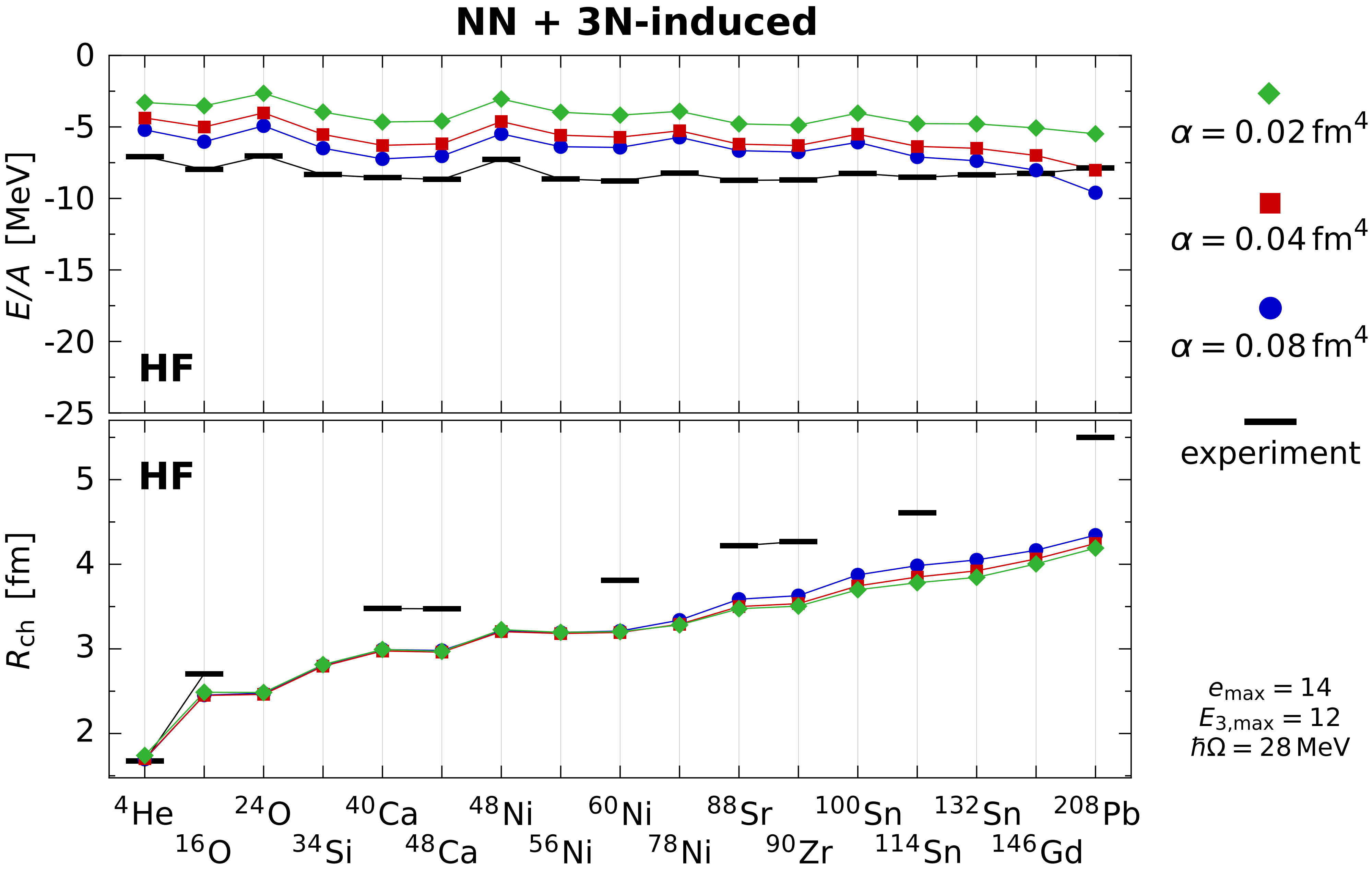


$e_{\mathrm{max}} = 14$
$E_{3,\mathrm{max}} = 12$
$\hbar\Omega = 28\,\mathrm{MeV}$

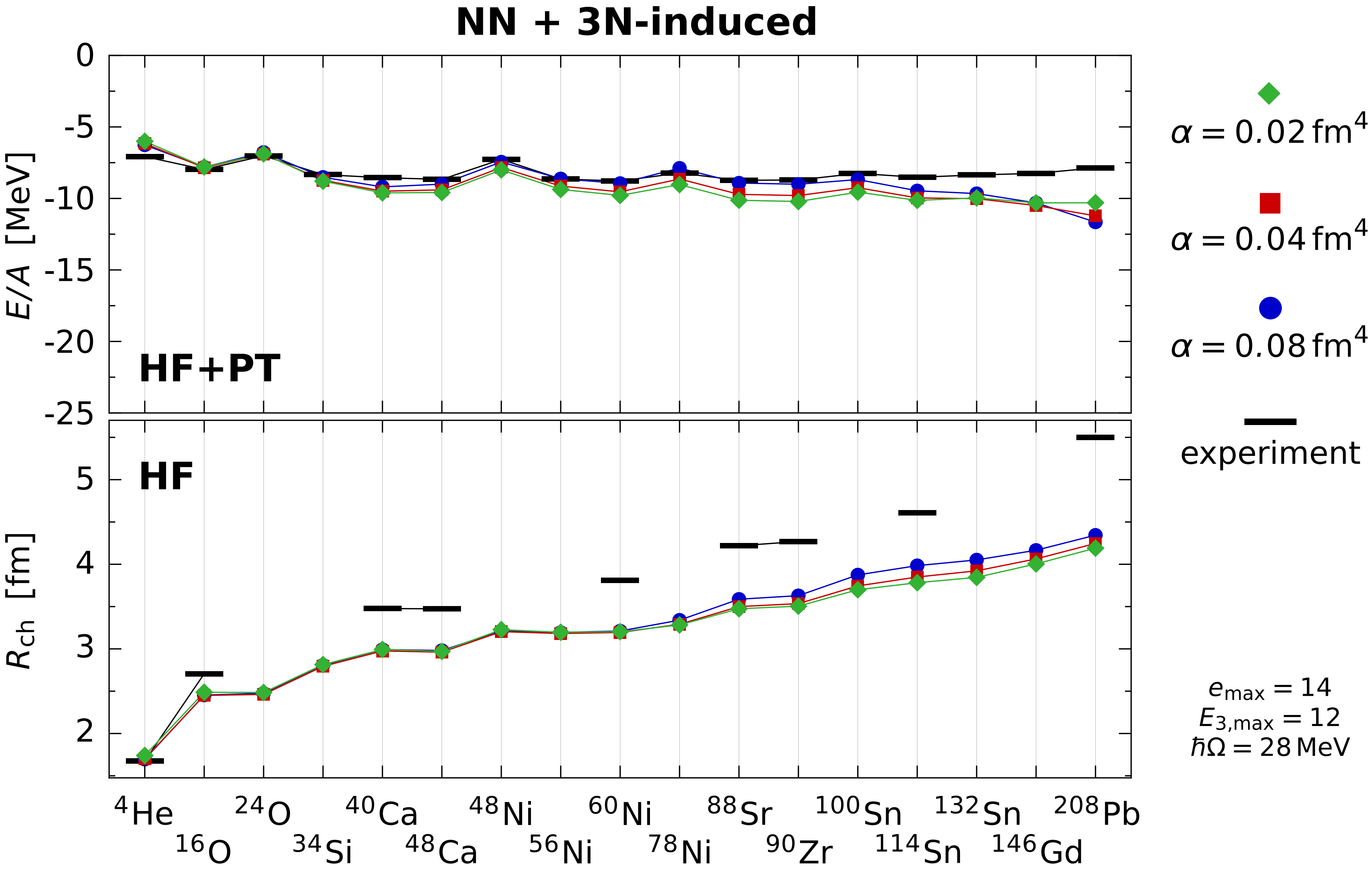
Systematics: E/A and R_{ch}



Systematics: E/A and R_{ch}

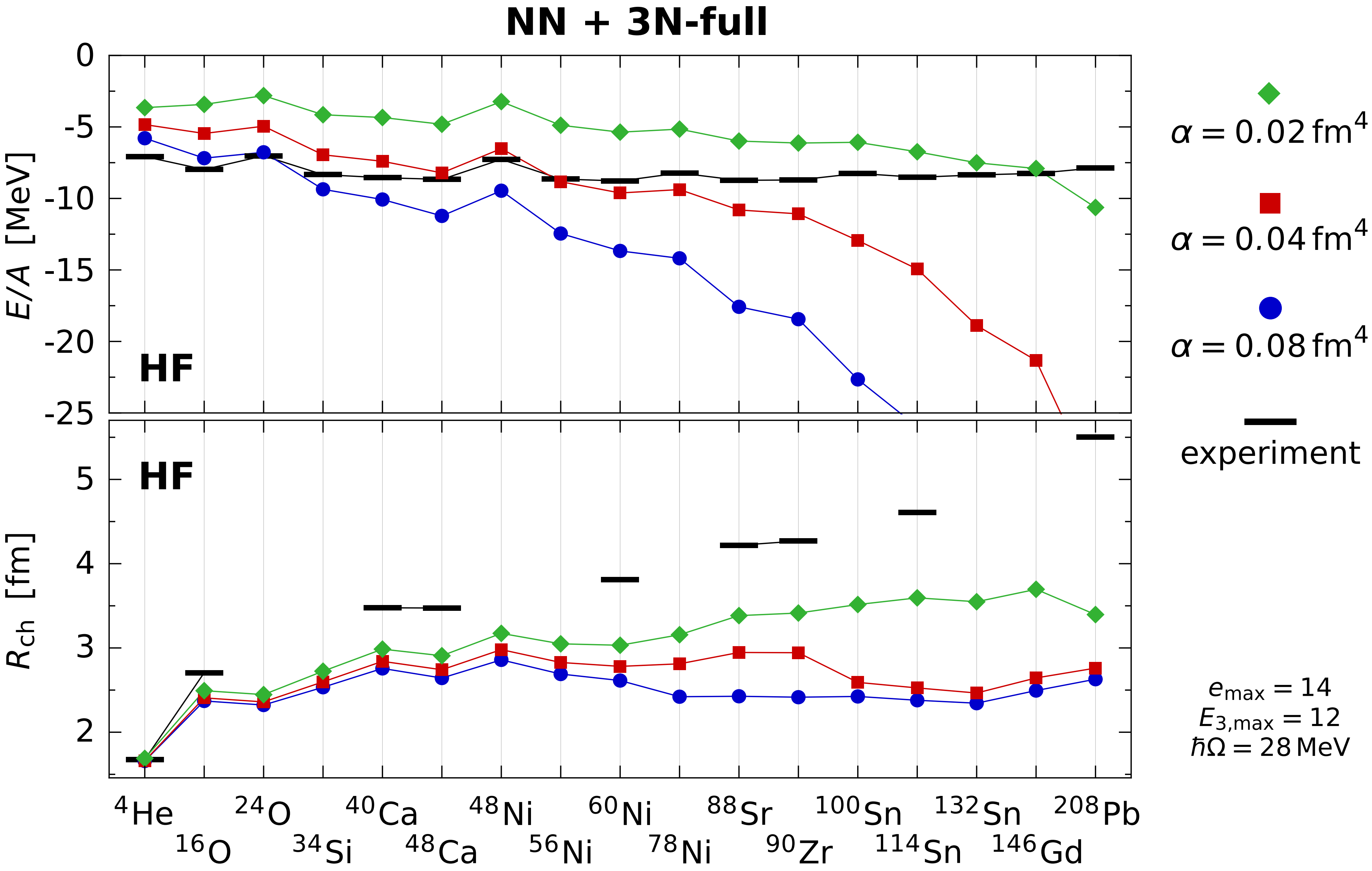


Systematics: E/A and R_{ch}



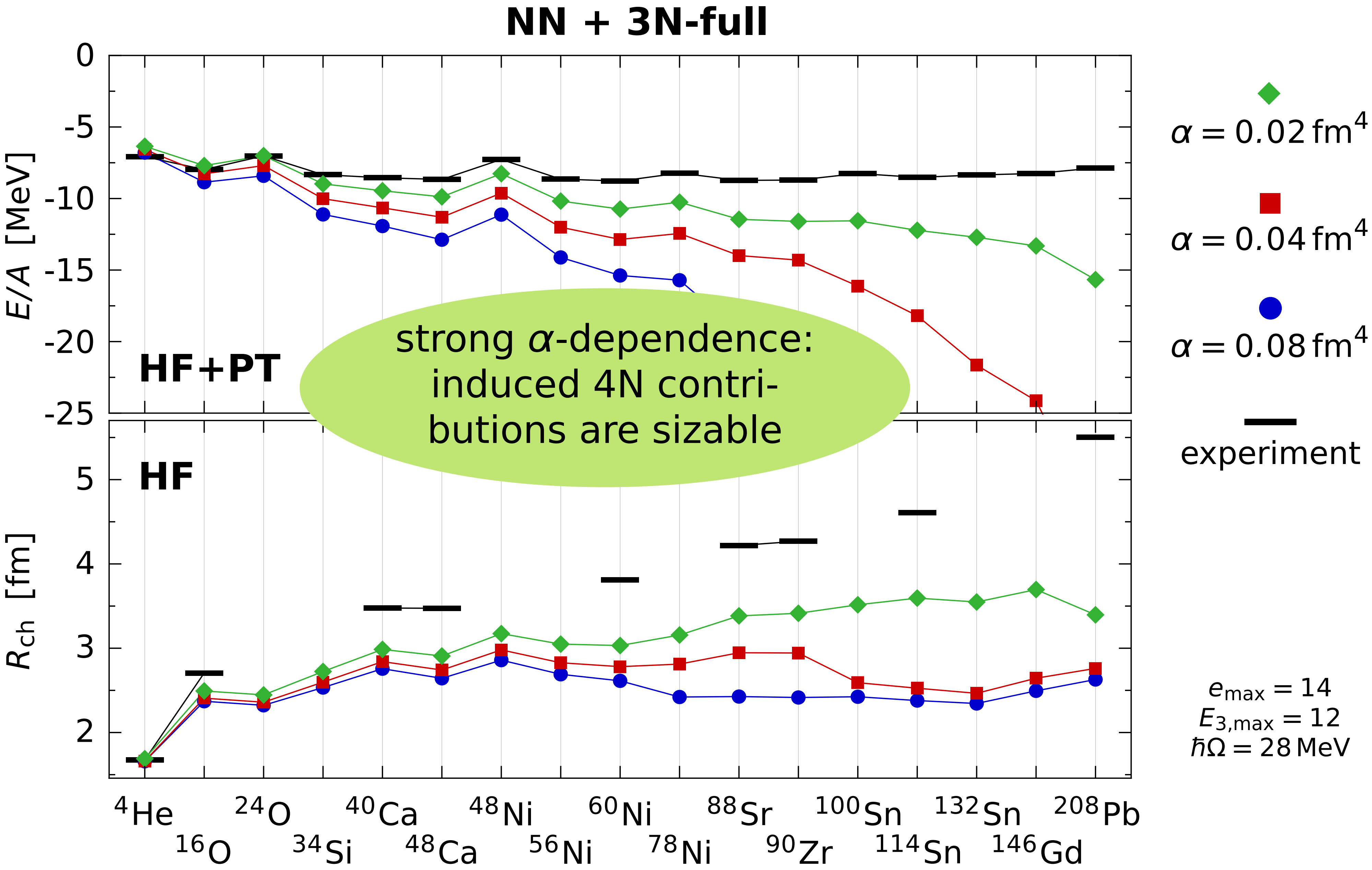
$e_{\max} = 14$
$E_{3,\max} = 12$
$\hbar\Omega = 28\,\mathrm{MeV}$

Systematics: E/A and R_{ch}



$e_{\max} = 14$
$E_{3,\max} = 12$
$\hbar\Omega = 28\,\mathrm{MeV}$

Systematics: E/A and R_{ch}



strong α-dependence: induced 4N contributions are sizable

Outline

- Introduction
- Chiral Effective Field Theory (χEFT)
- Similarity Renormalization Group
- Transformation to $\mathcal{J}, T$-Coupled Scheme
- Importance Truncated No-Core Shell Model
- Hartree Fock
- **Summary and Outlook**

Summary and Outlook

Benchmark of chiral NN+3N interactions

- consistent SRG evolution in 3B space
- efficient transformation of Jacobi matrix elements to $\mathcal{J}T$-coupled scheme
  - key for application to **$N_{max} > 8$ calculations** (p-shell)
- IT-NCSM with full chiral 3N interactions up to $N_{\text{max}} = 12$ (14) for all p-shell (and lower sd-shell) nuclei
- two-pion exchange term of 3N interaction **induces significant 4N** contributions beyond mid-p-shell

  ⇒ modify SRG generator to prevent induced 4N contributions from the beginning
- many other applications (Hartree Fock, RPA, ...)

Epilogue

- **thanks to our group & collaborators**
  - **S. Binder**, A. Blum, B. Erler, A. Günther, H. Krutsch, D. Kulawiak, **J. Langhammer**, P. Papakonstantinou, S. Reinhardt, **R. Roth**, C. Stumpf, R. Trippel, K. Vobig, R. Wirth

    Institut für Kernphysik, TU Darmstadt
  - **P. Navrátil**

    TRIUMF Vancouver, Canada
- we thank Jülich Supercomputing Centre (JSC) & LOEWE-CSC for computing time

Thank you for your attention!

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