Nuclear Structure with Chiral 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

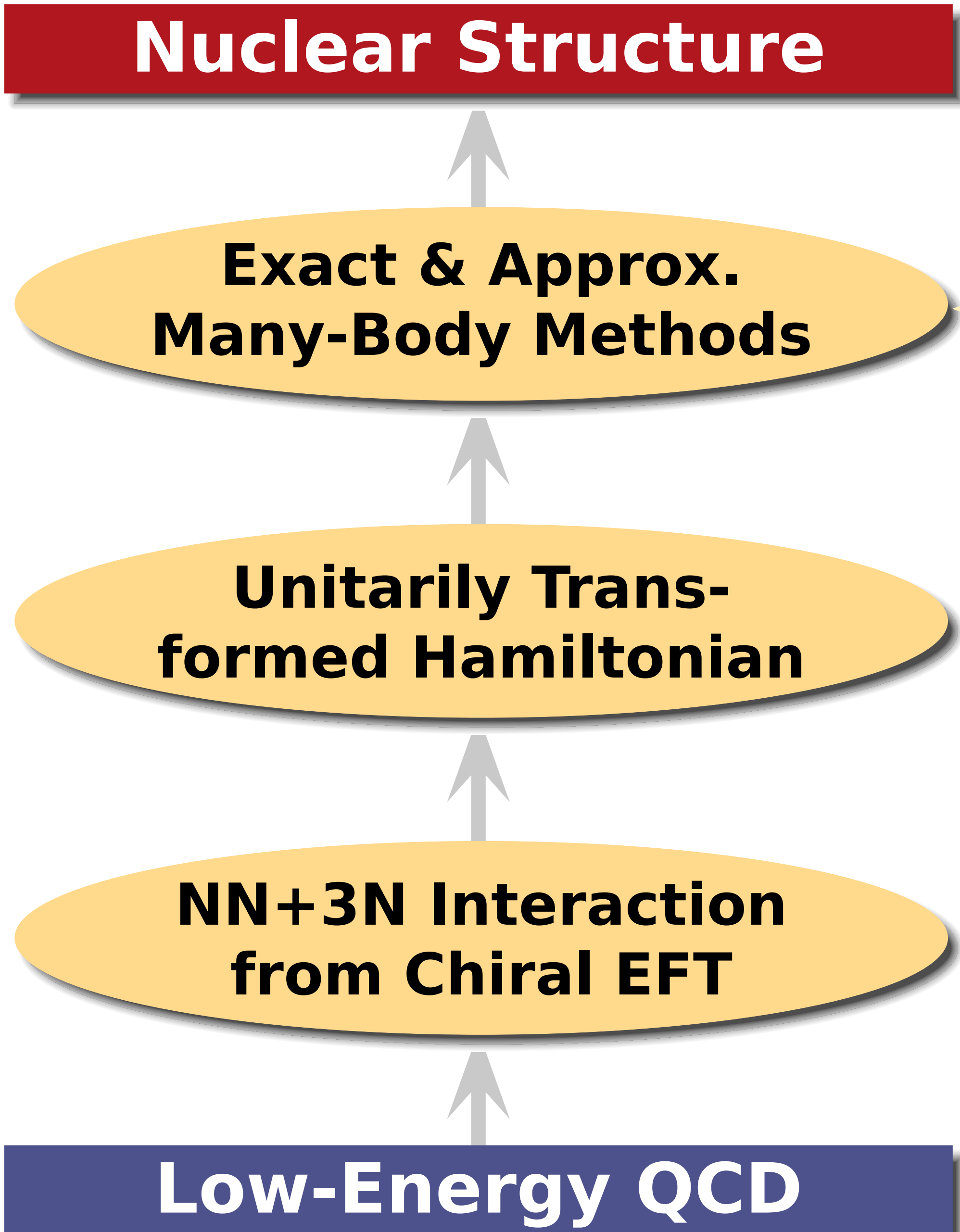
Unitarily Transformed Hamiltonian

- 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



- ‘exact’ solution of the many-body problem for light & intermediate 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

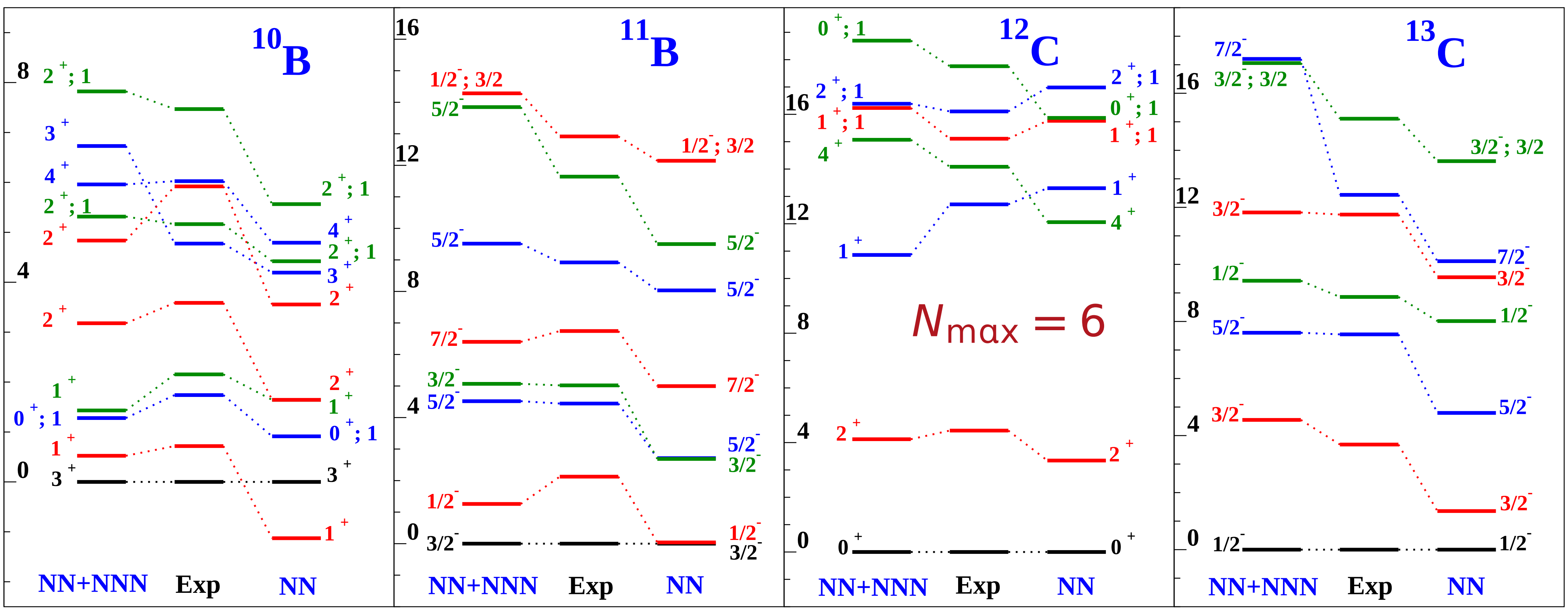
focus on consistent inclusion of chiral 3N interaction

Milestone I

PRL 99, 042501 (2007) PHYSICAL REVIEW LETTERS week ending 27 JULY 2007

Structure of $A = 10$–13 Nuclei with Two- Plus Three-Nucleon Interactions from Chiral Effective Field Theory

P. Navrátil,[1] V. G. Gueorguiev,[1,*] J. P. Vary,[1,2] W. E. Ormand,[1] and A. Nogga[3]

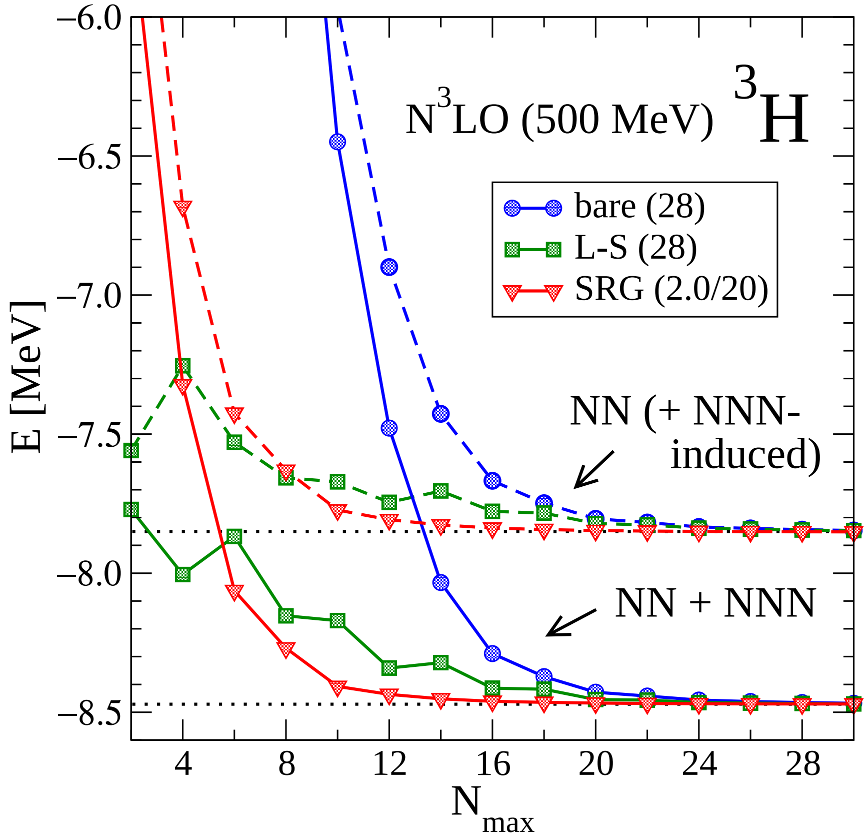


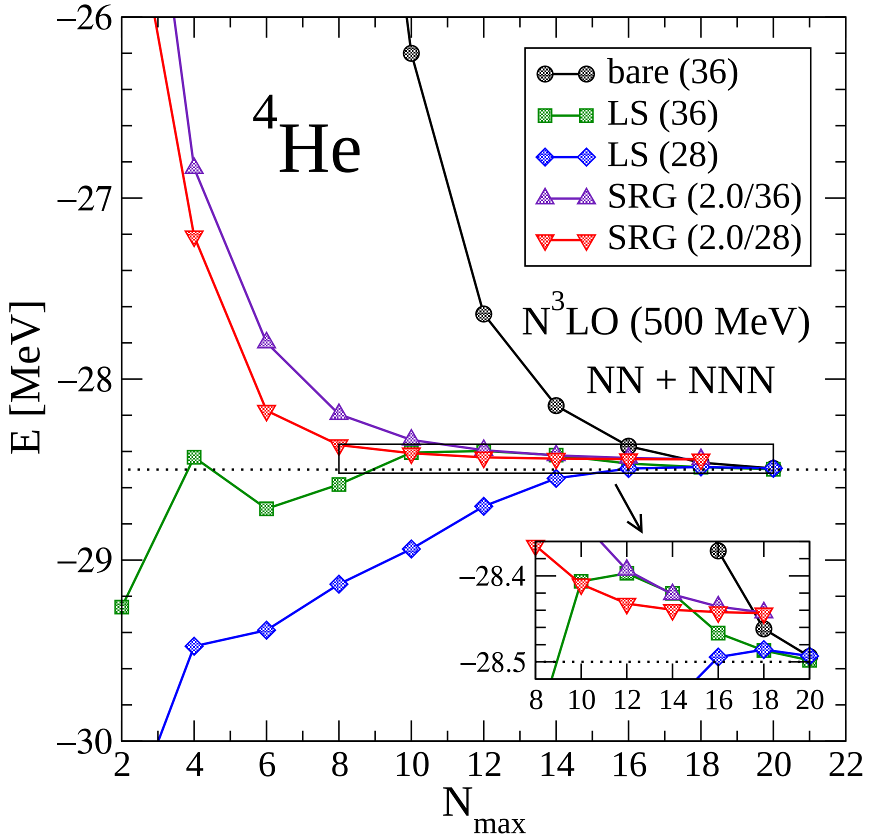
Milestone II

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
  - benchmark 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

- **unitary transformation** of Hamiltonian (and other observables)

$$\widetilde{\mathrm{H}}_\alpha = \mathrm{U}_\alpha{}^\dagger \,\mathrm{H}\, \mathrm{U}_\alpha$$

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

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

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

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

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

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

- **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

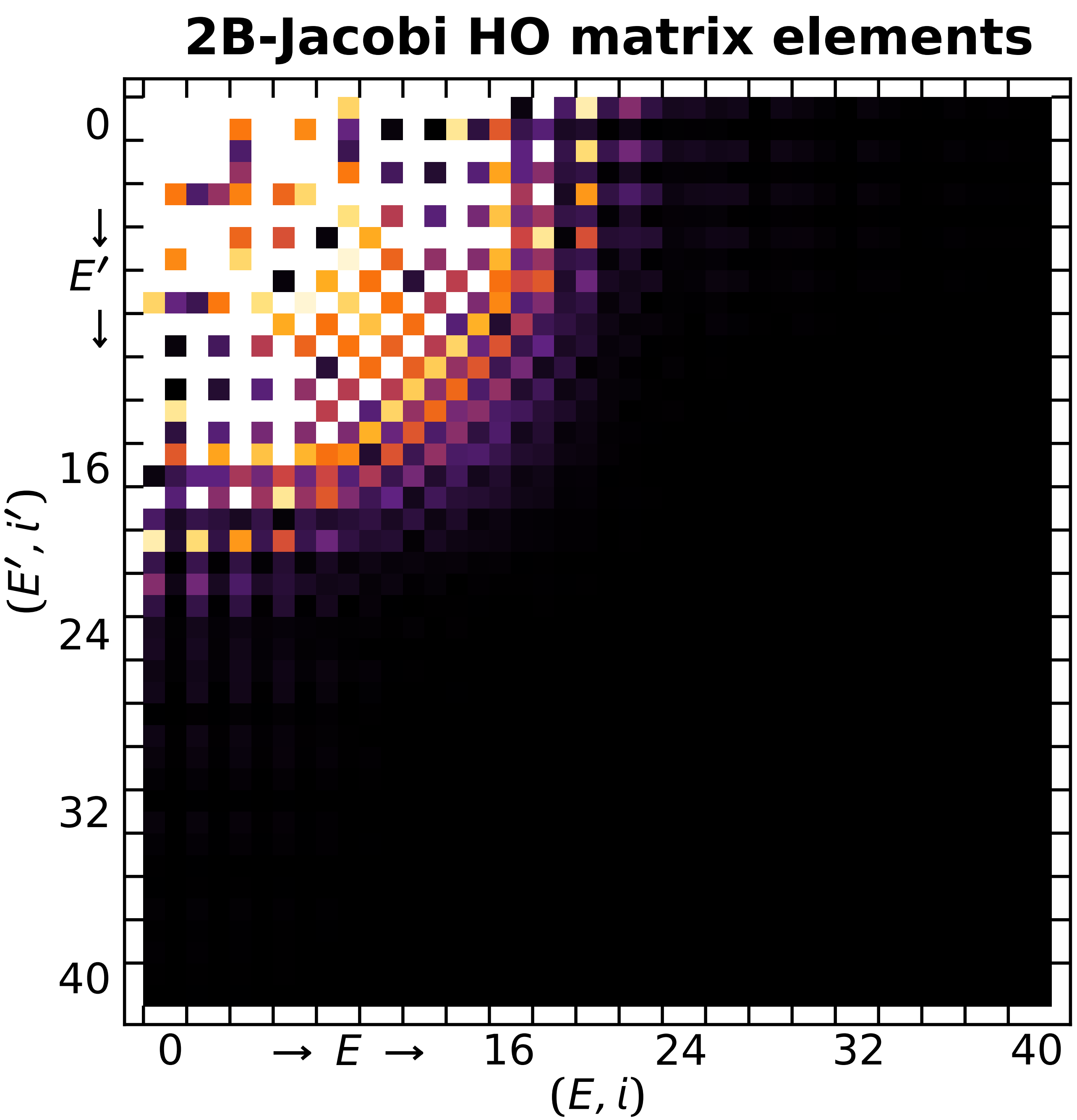
- represent operator equation in ***n*-body Jacobi HO basis** $|EiJ^{\pi}T\rangle$
  - $n = 2$: relative LS-coupled HO states: $|E(LS)J^{\pi}T\rangle$
  - $n = 3$: antisymmetrized Jacobi-coordinate HO states: $|EiJ^{\pi}T\rangle$

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

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

- we use $E_{\mathrm{SRG}} = 32$ which is sufficient to warrant convergence of intermediate sums for $\hbar\Omega \gtrsim 24\,\mathrm{MeV}$

SRG Evolution in Two-Body Space



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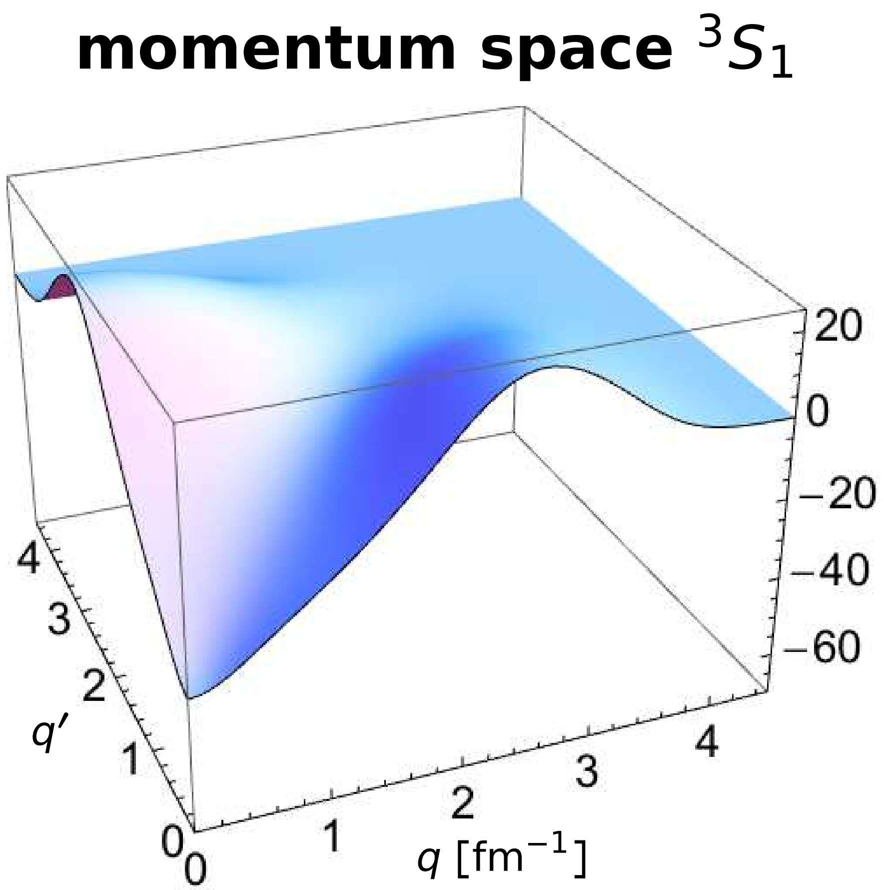
$\Lambda = \infty\,\mathrm{fm}^{-1}$

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



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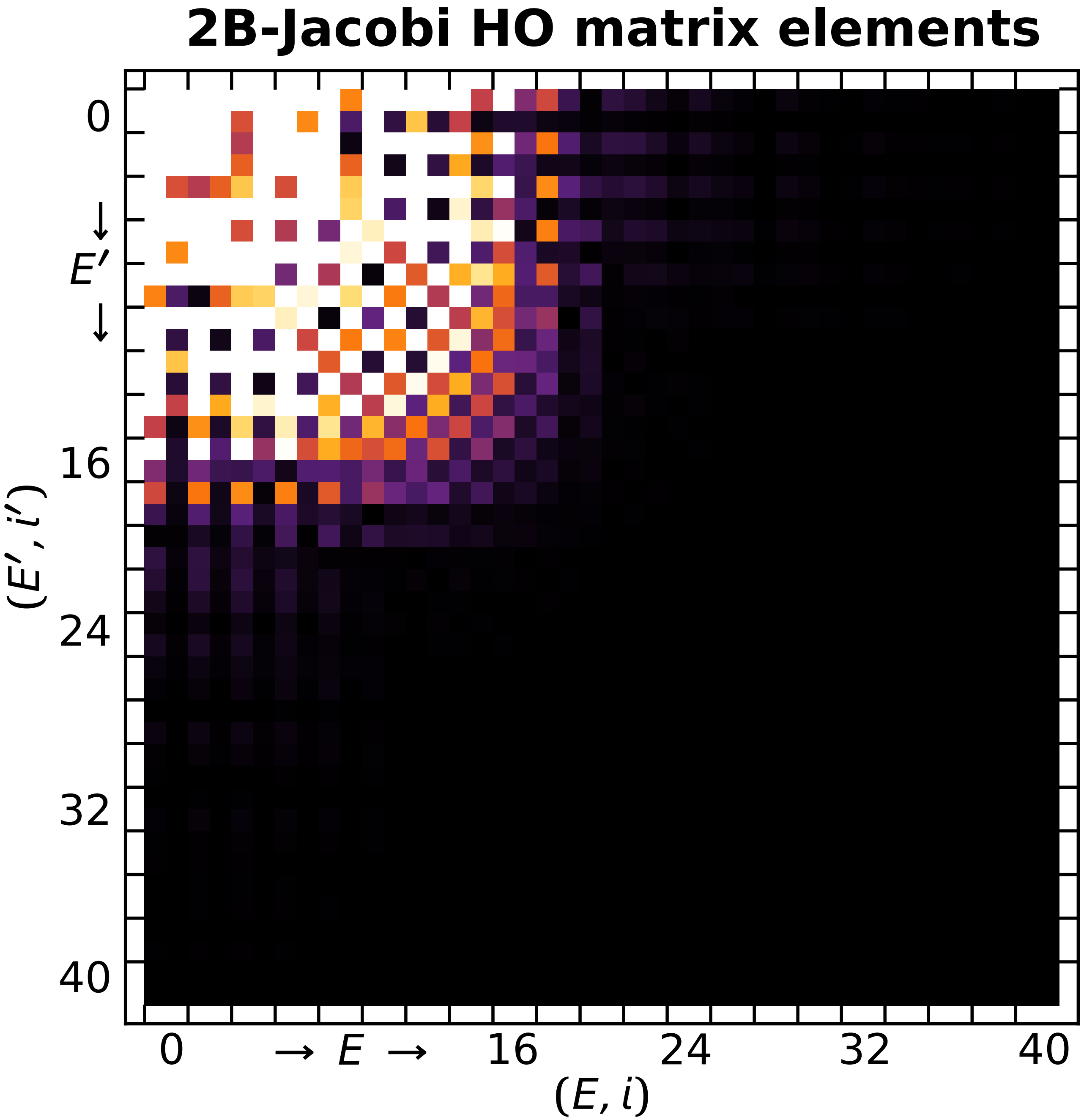

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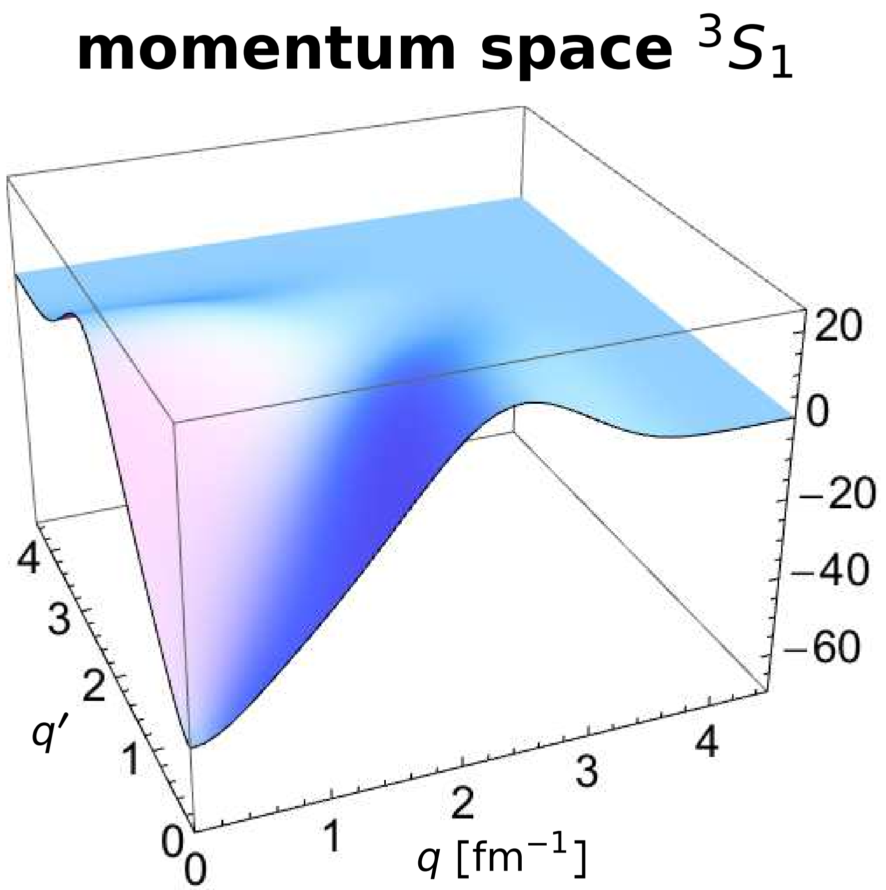

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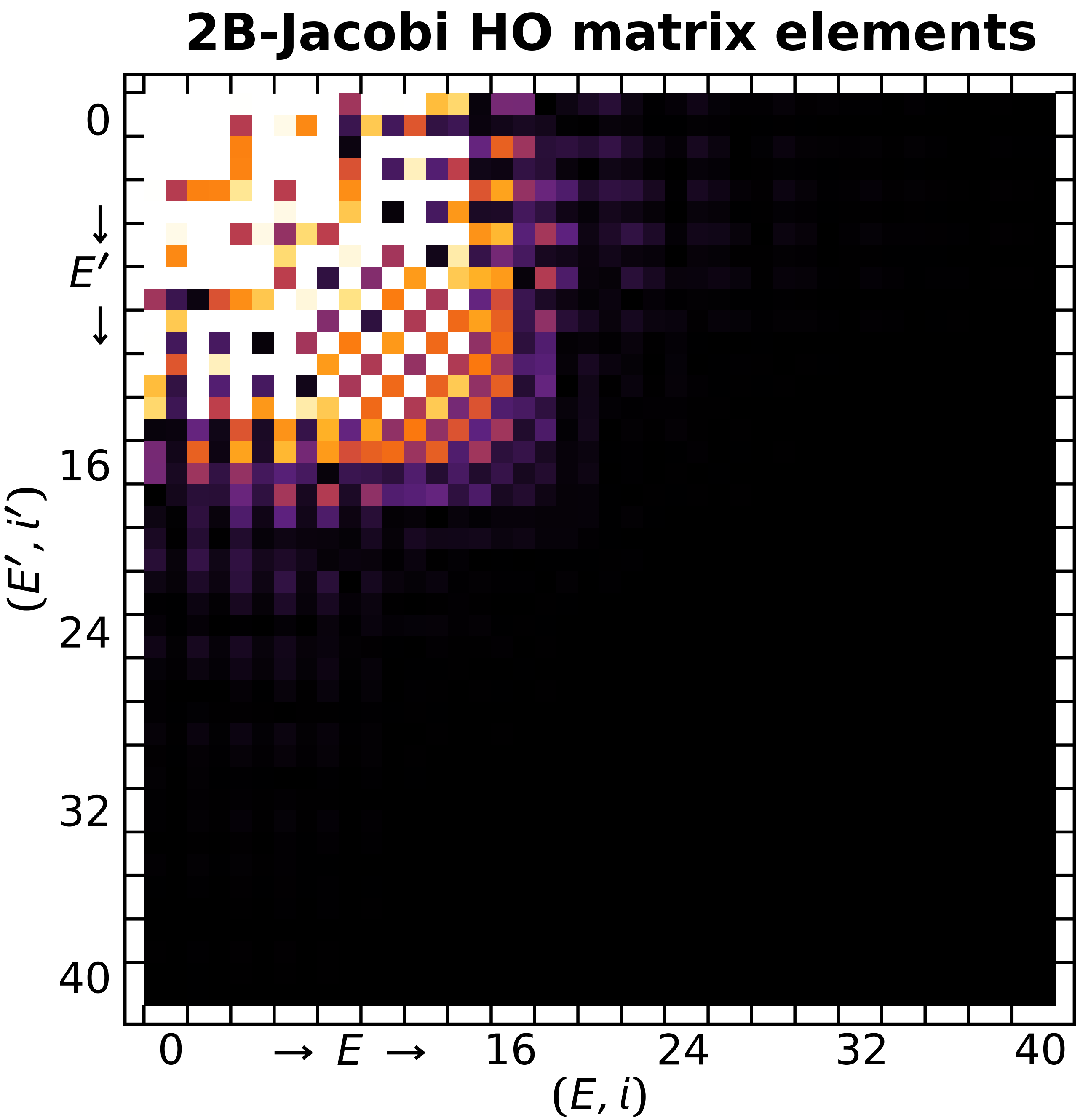

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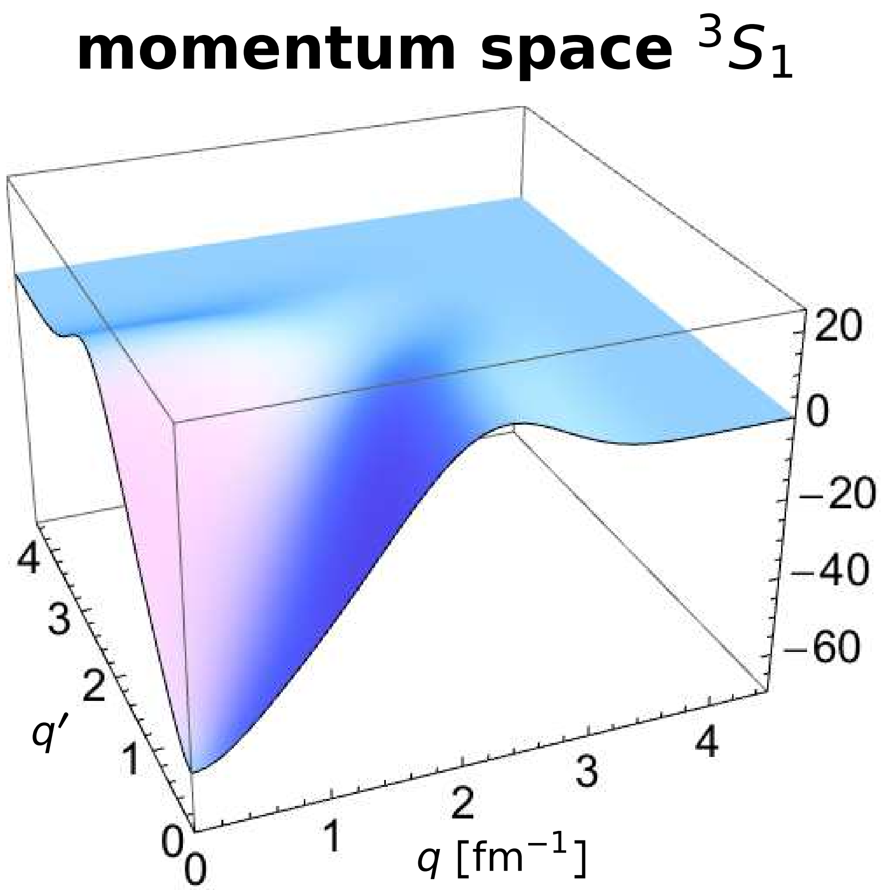

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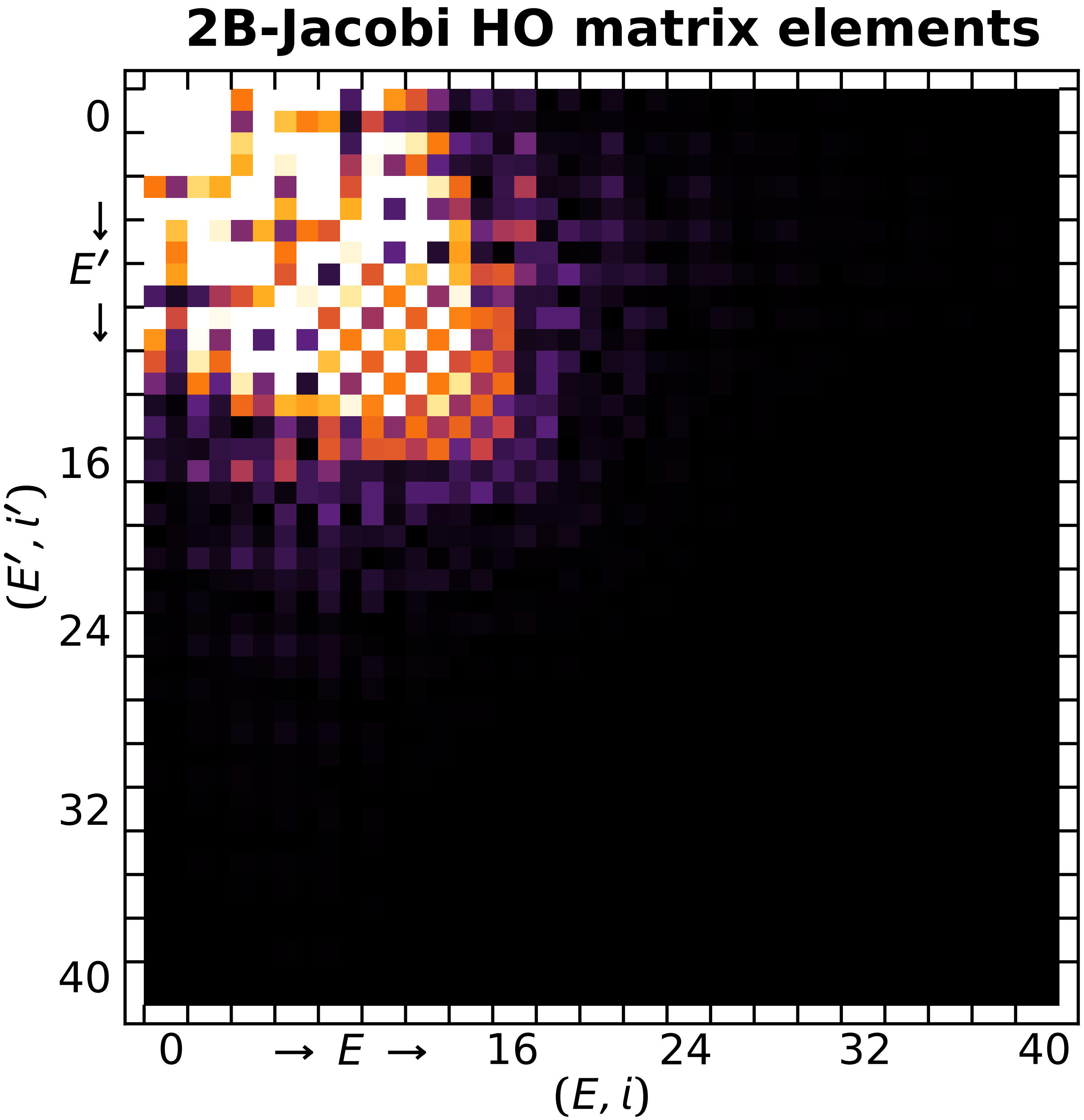

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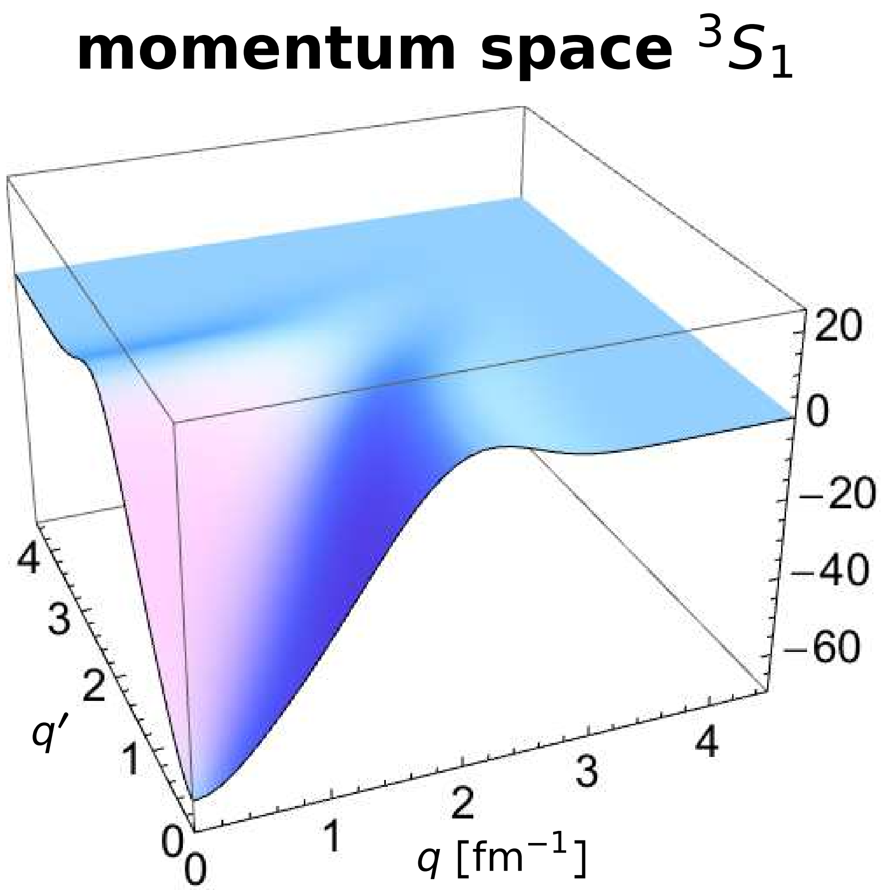

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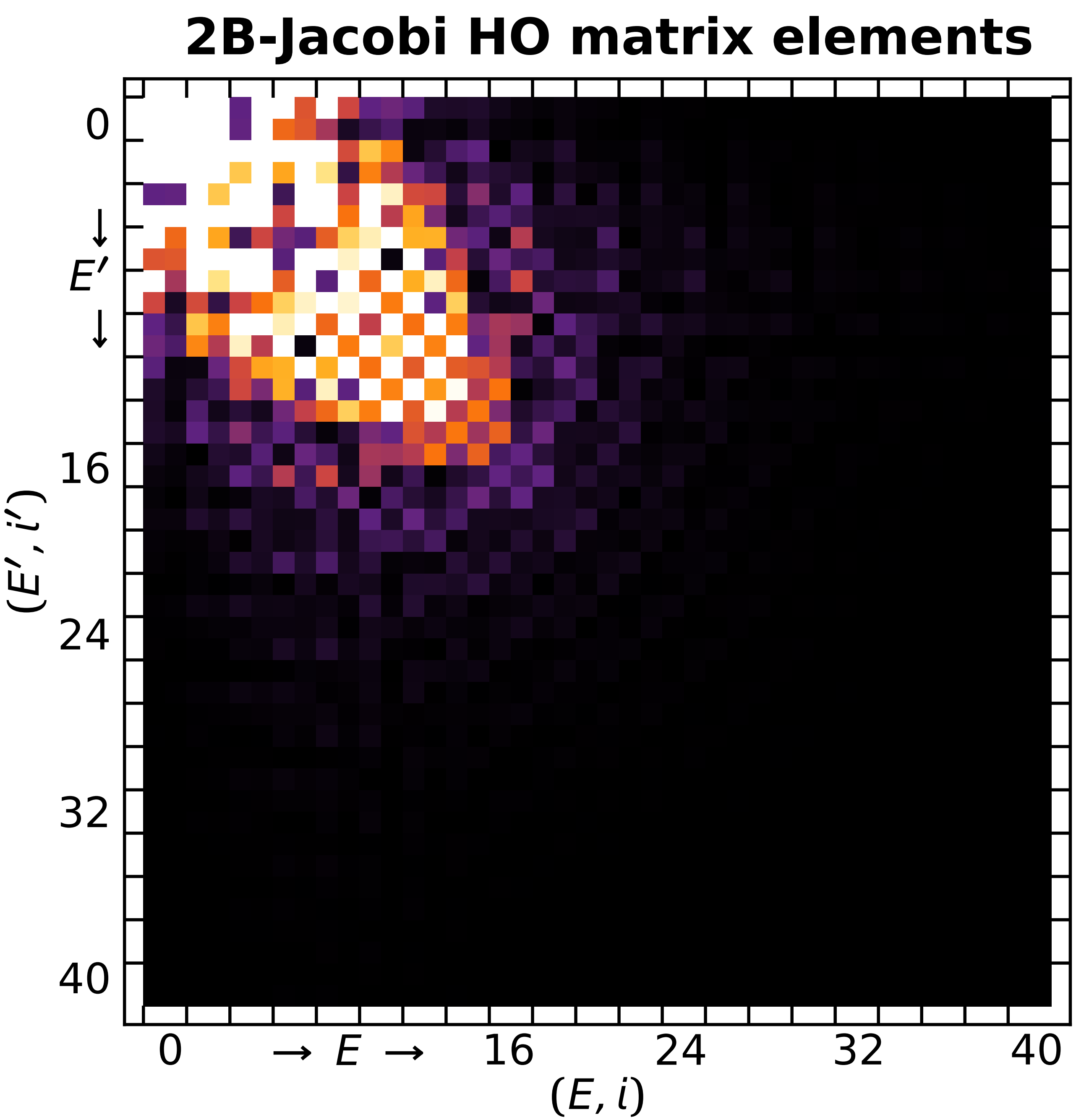

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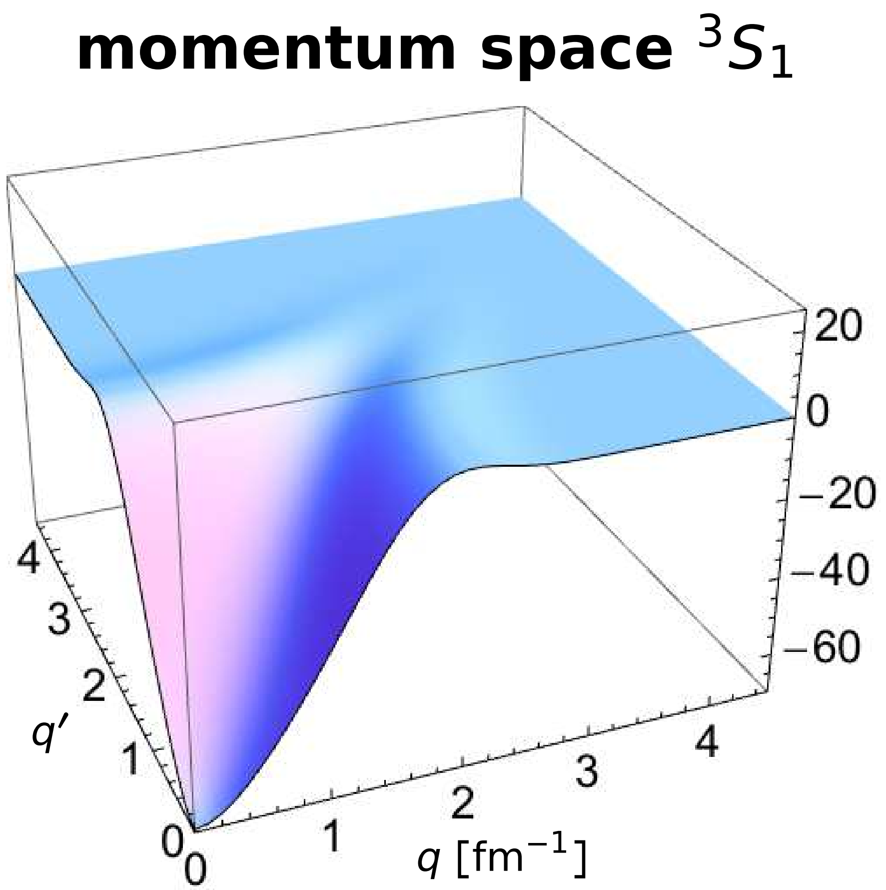
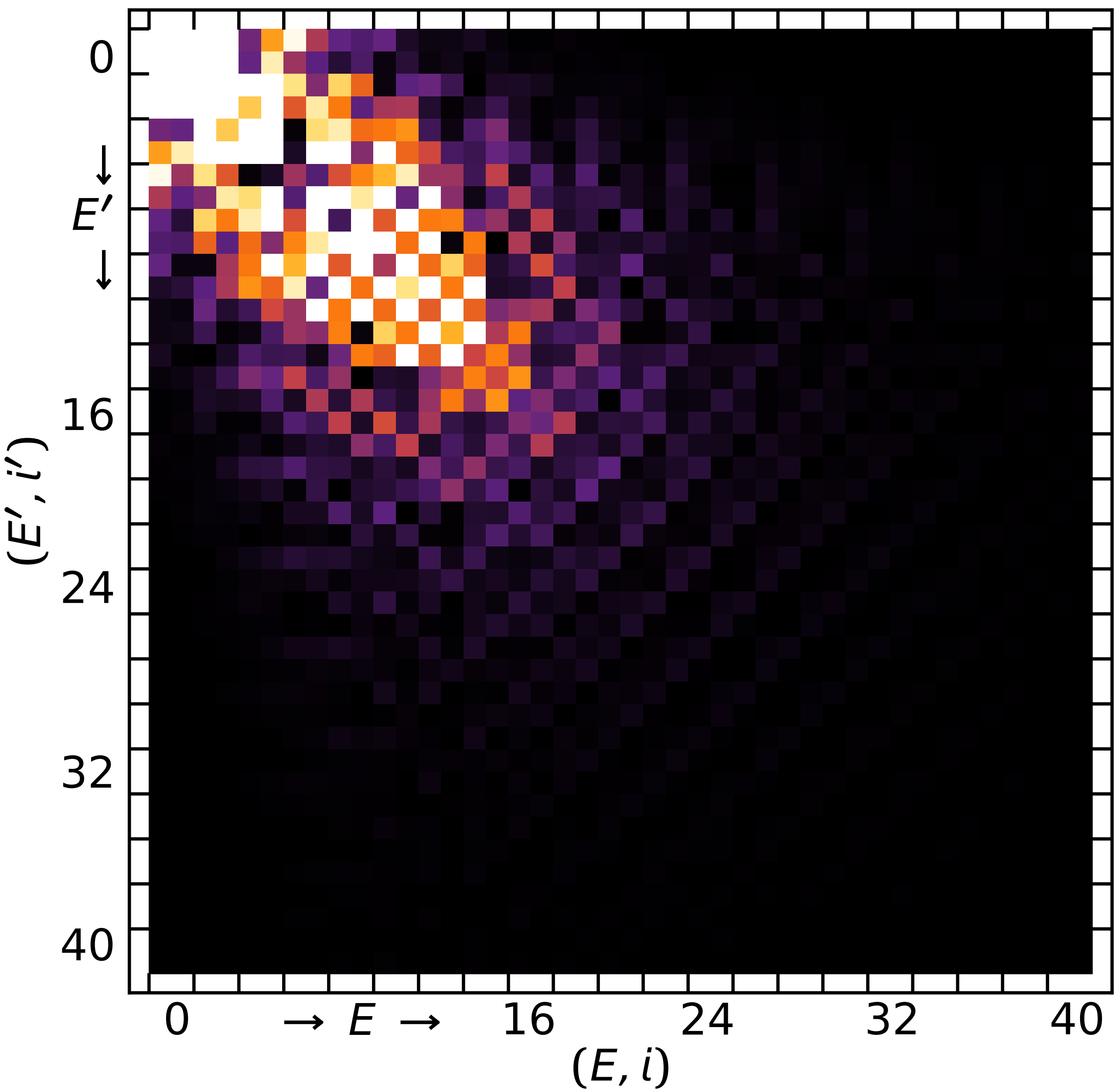


SRG Evolution in Two-Body Space

2B-Jacobi HO matrix elements



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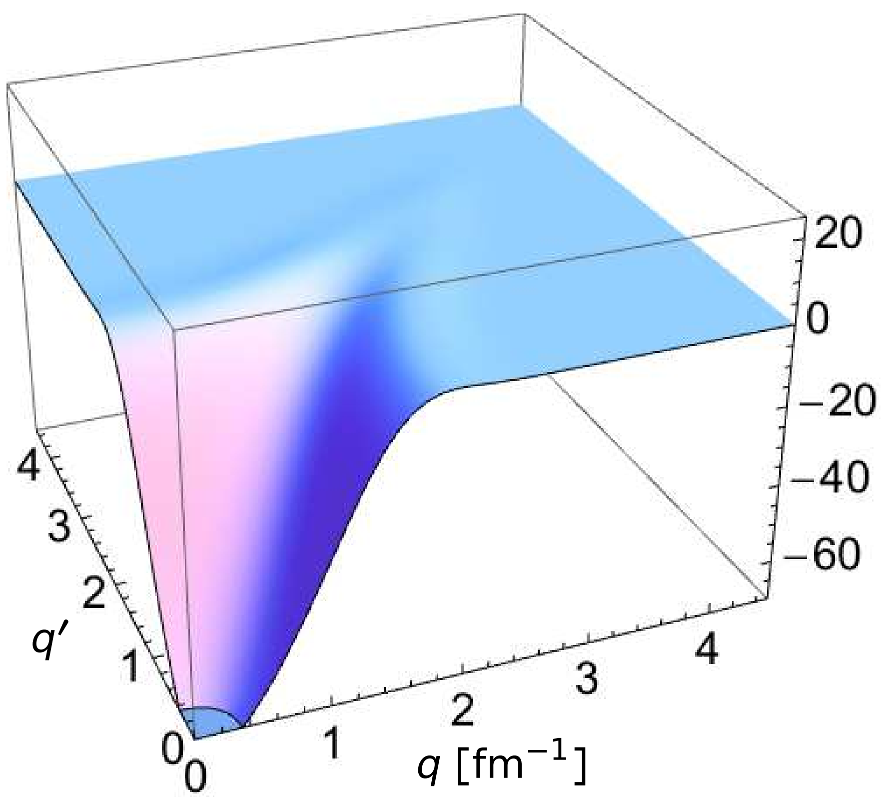
momentum space $^3S_1$



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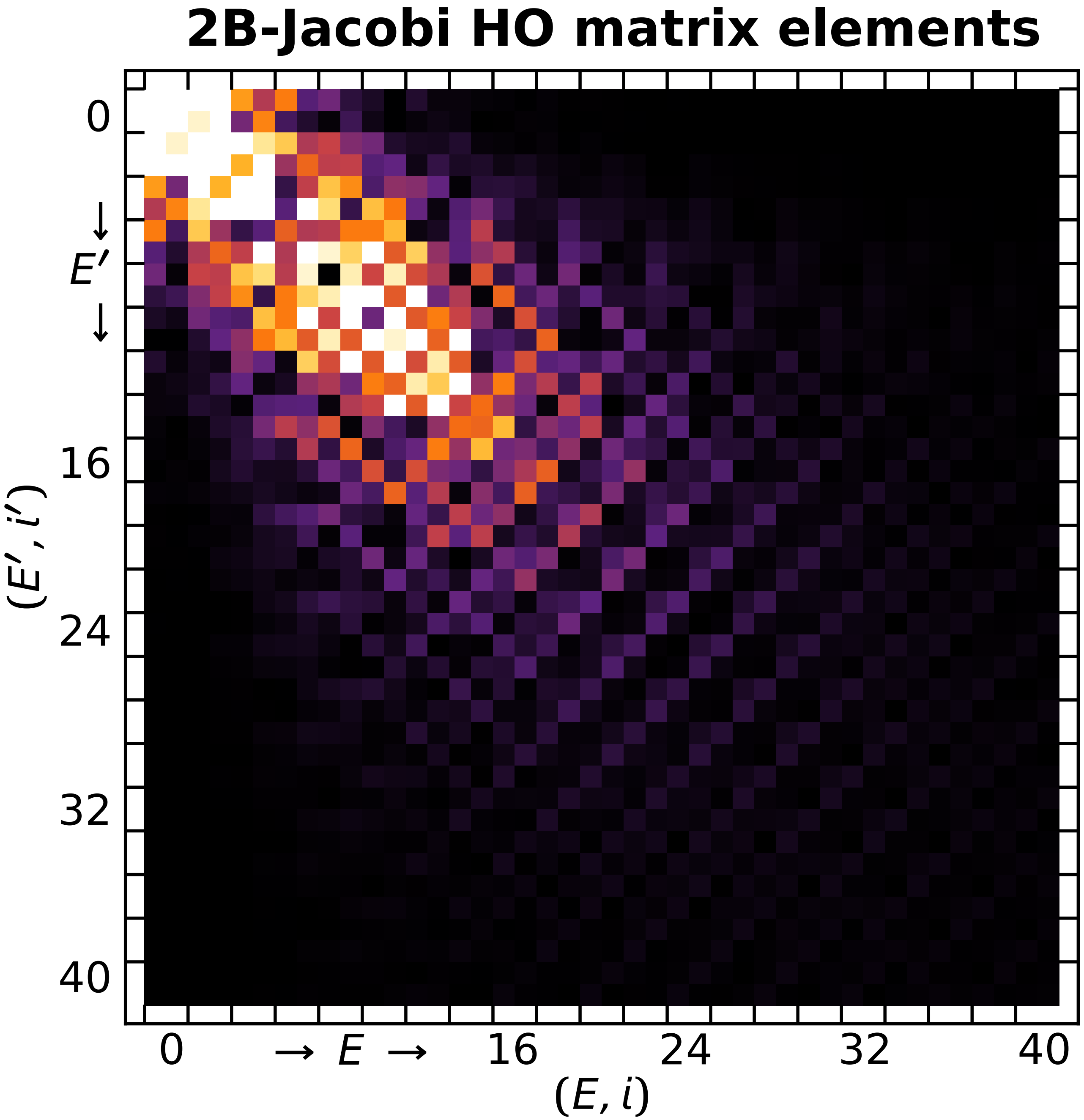

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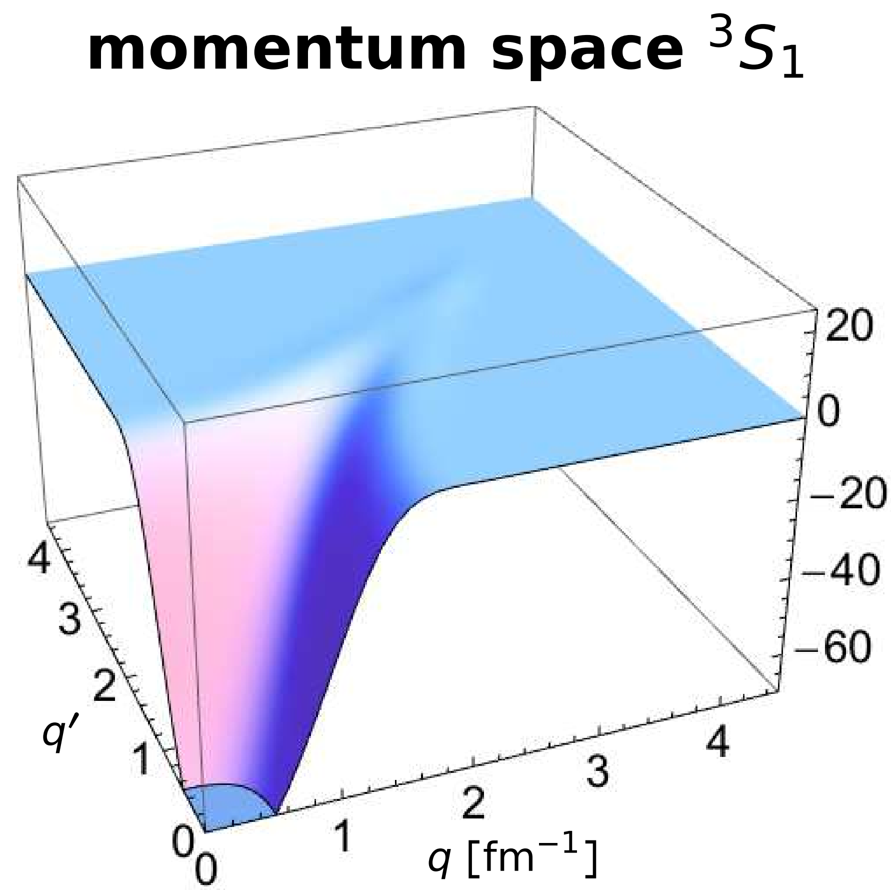

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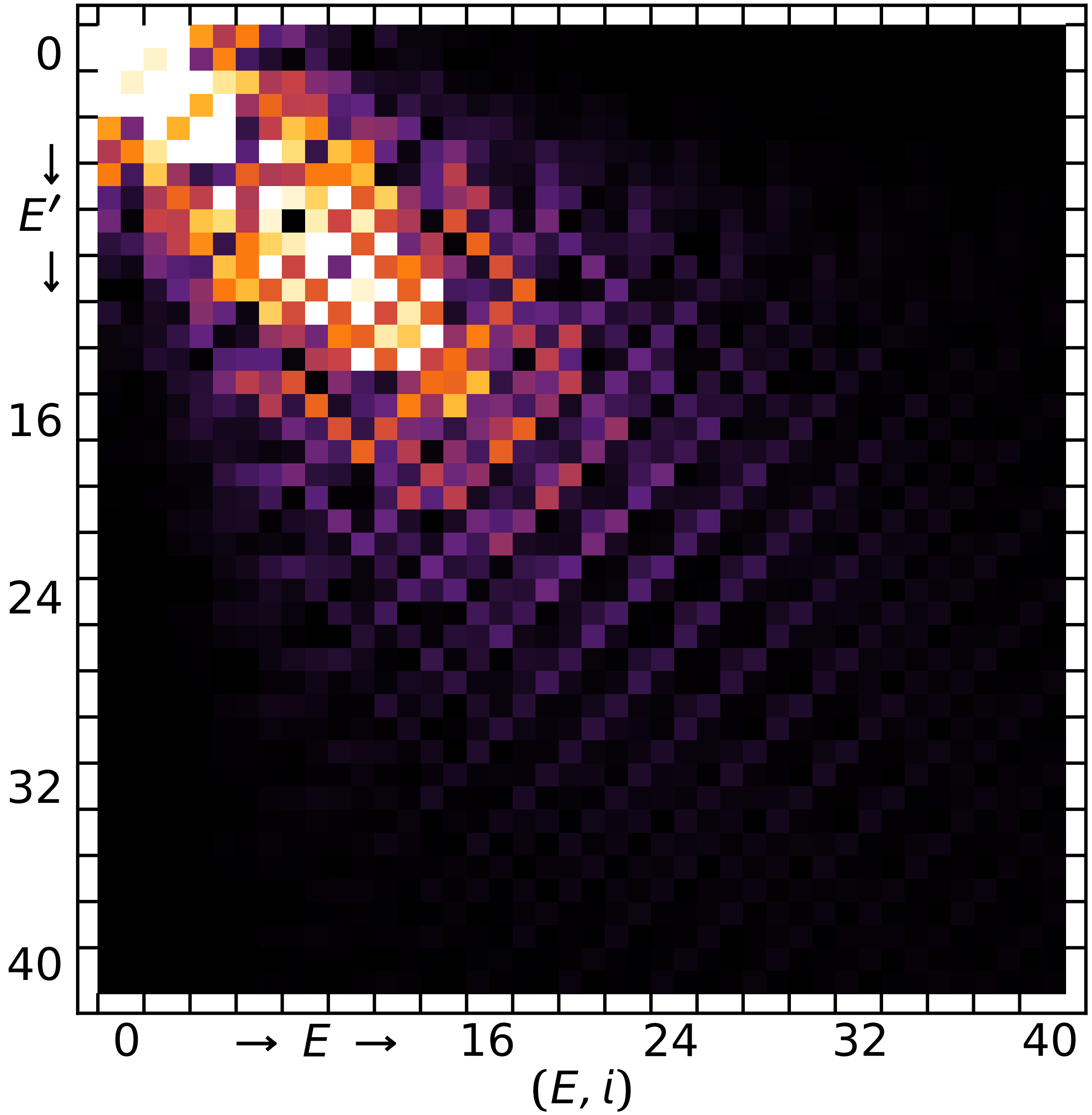

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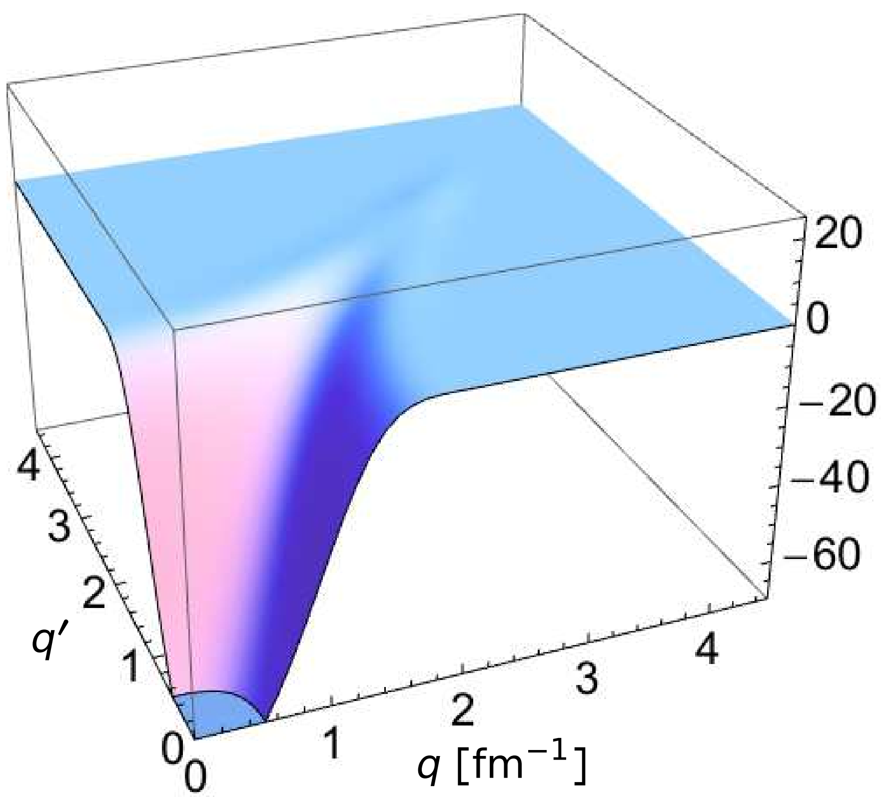

SRG Evolution in Three-Body Space

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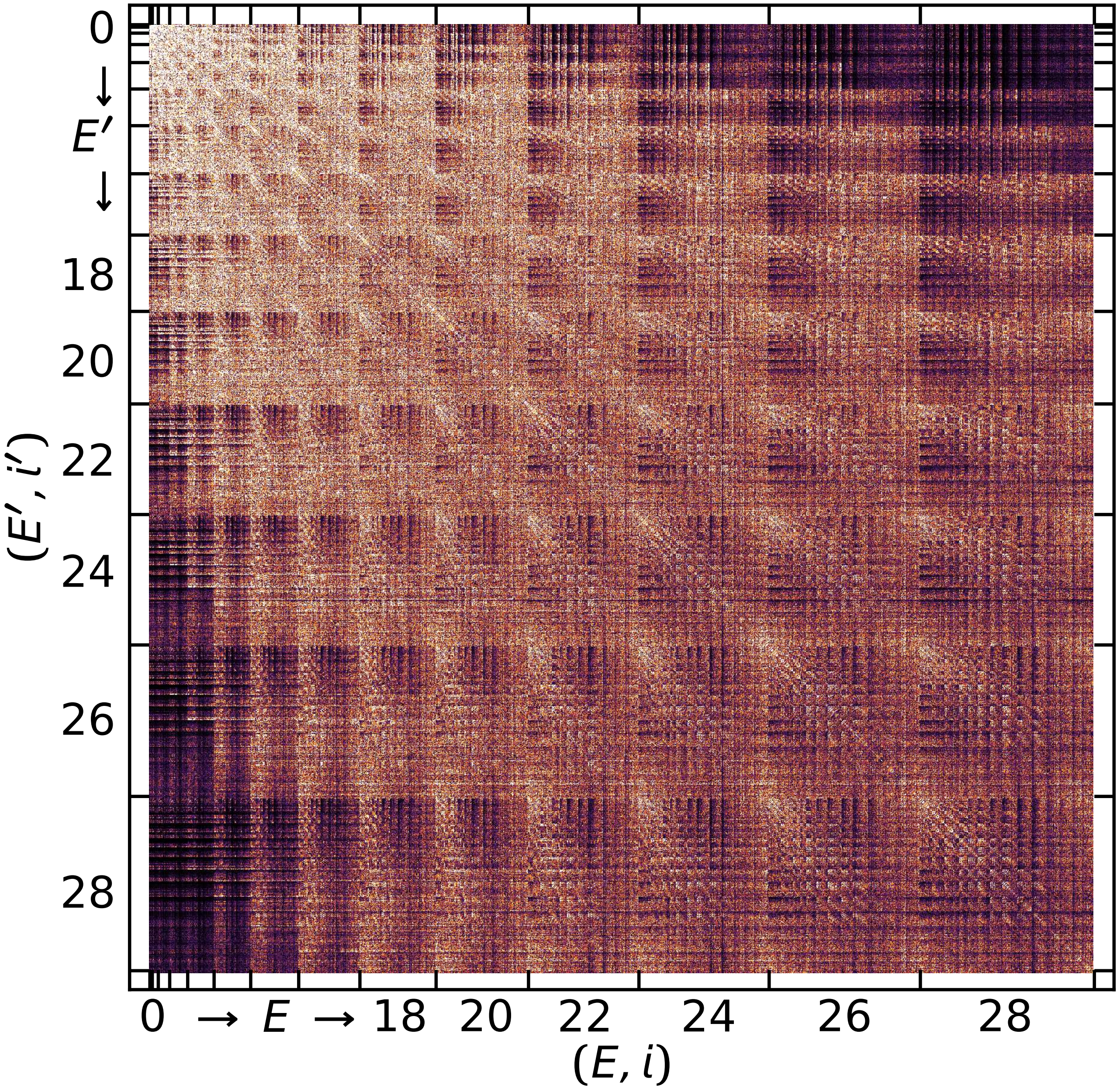

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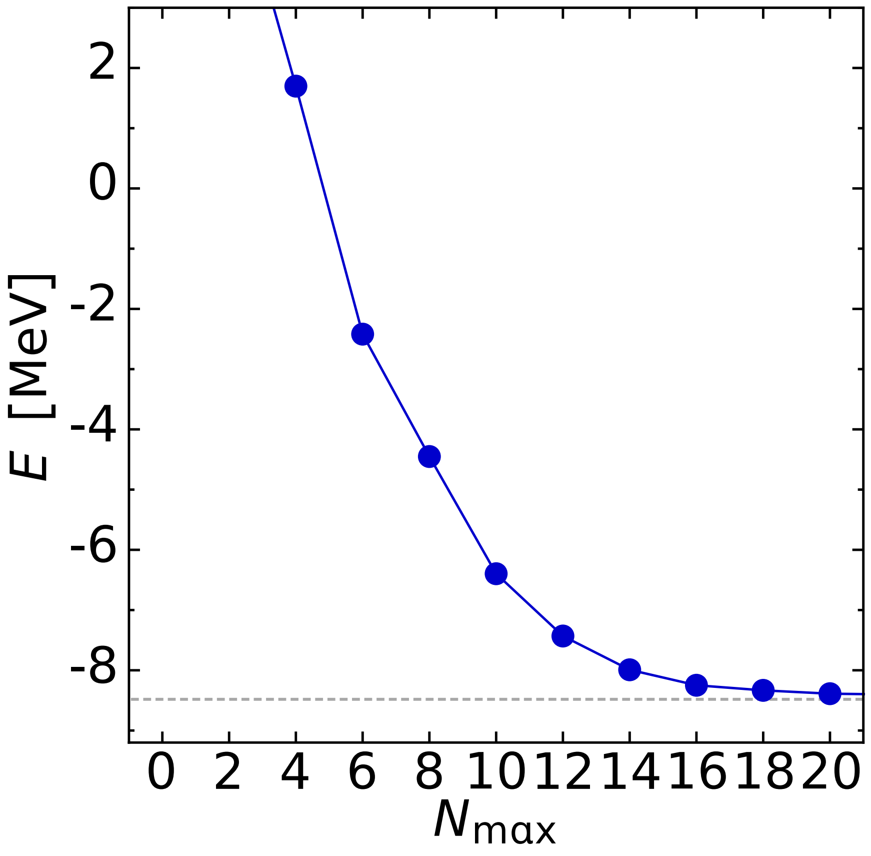

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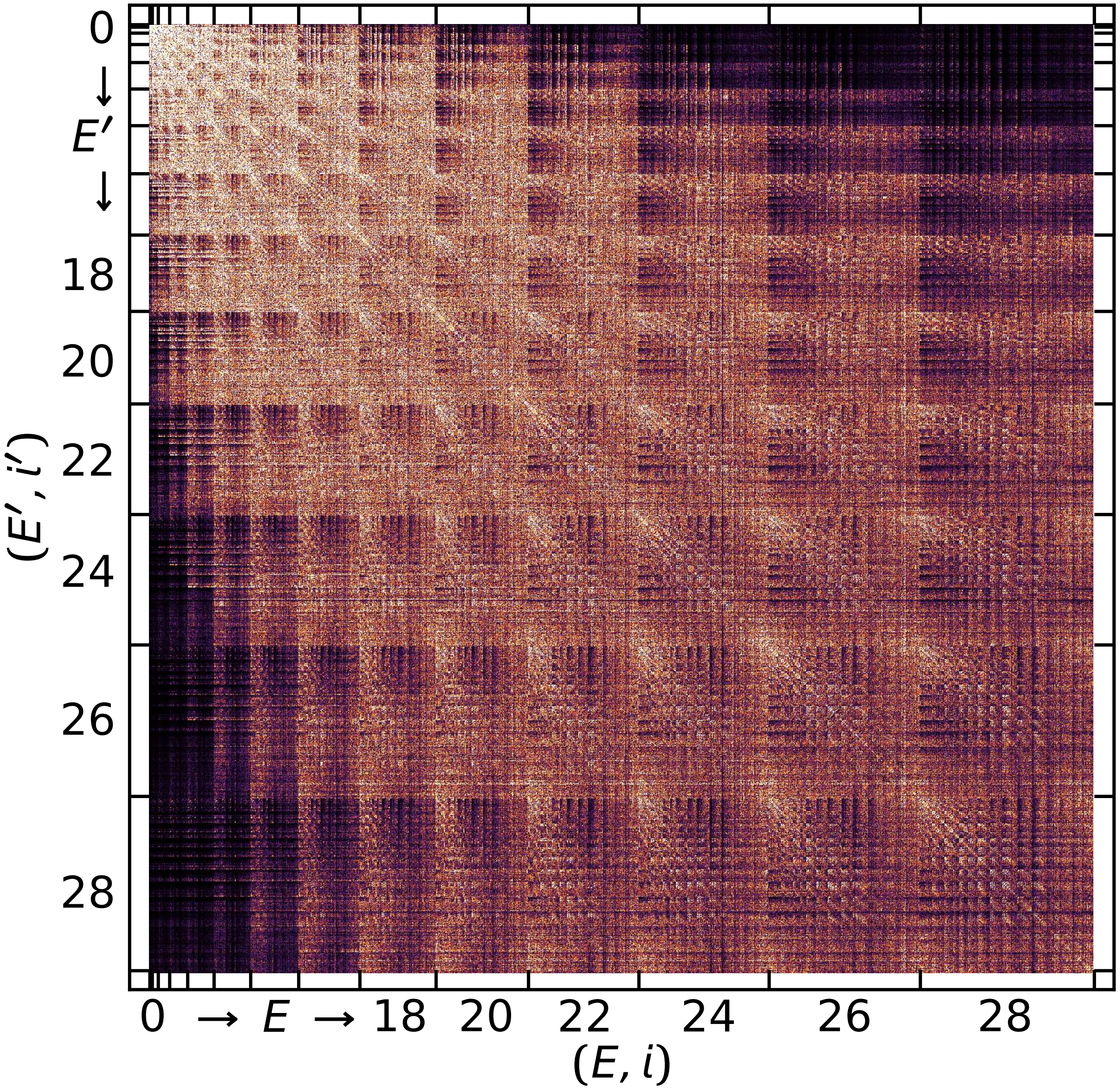

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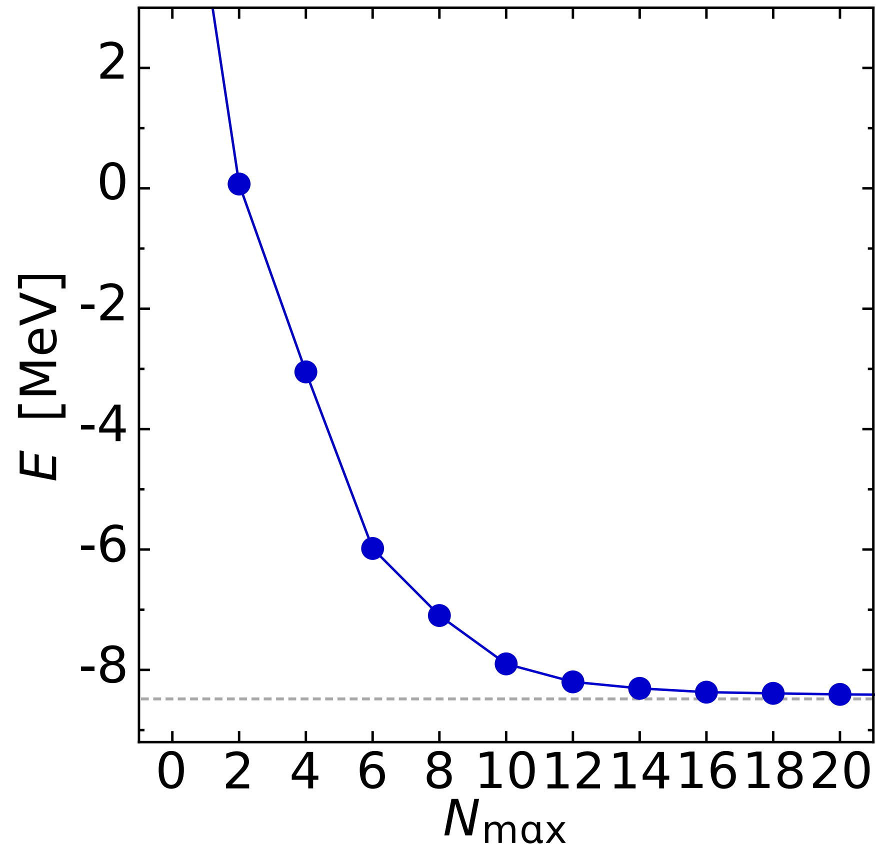

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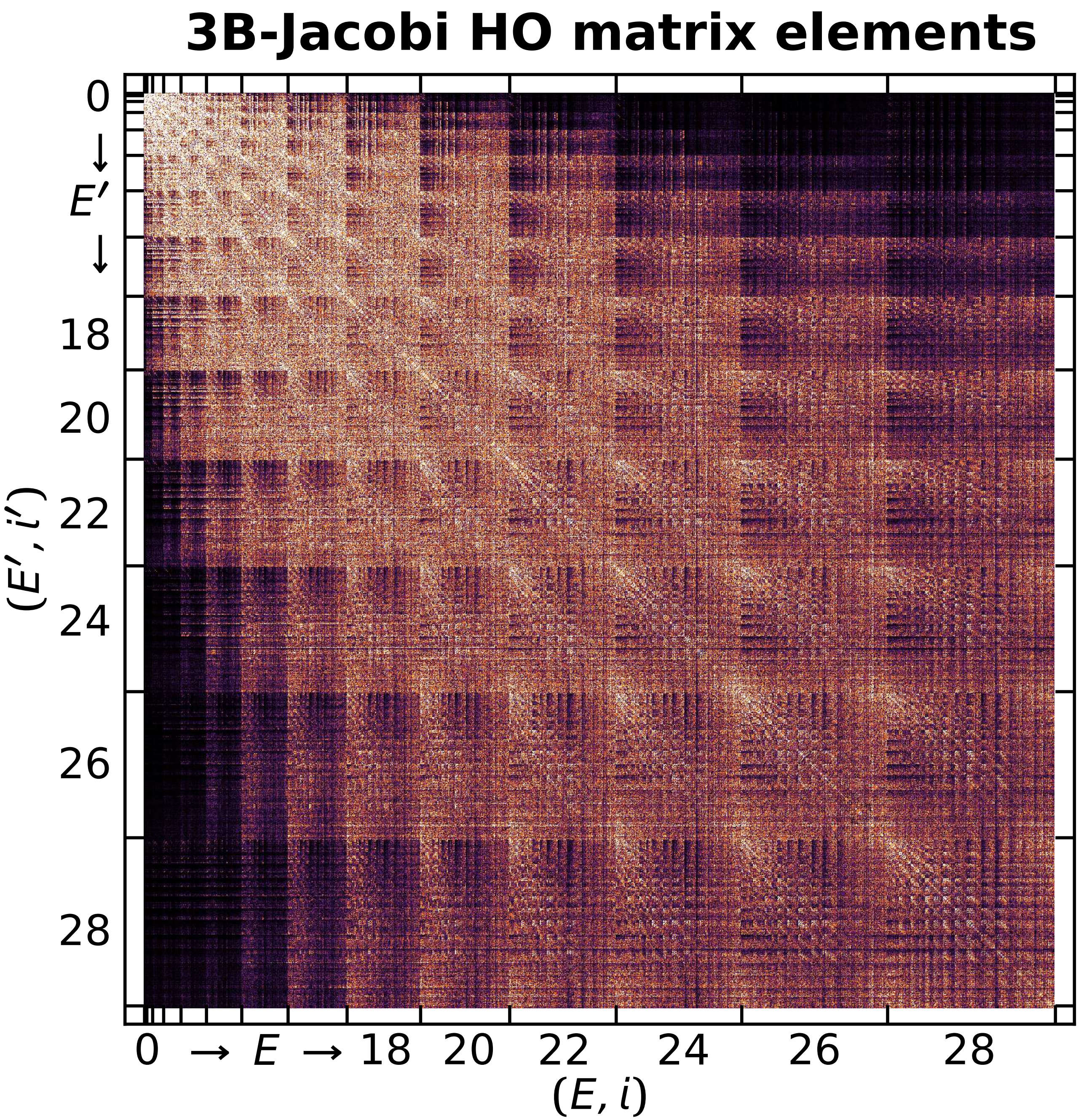

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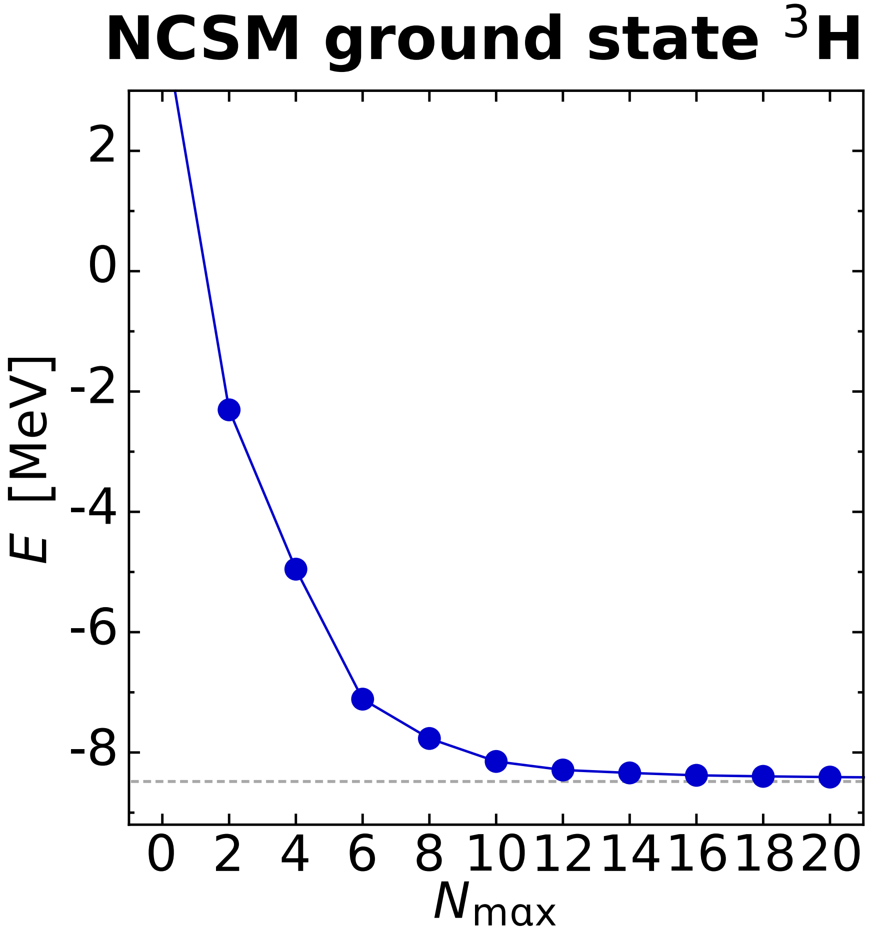

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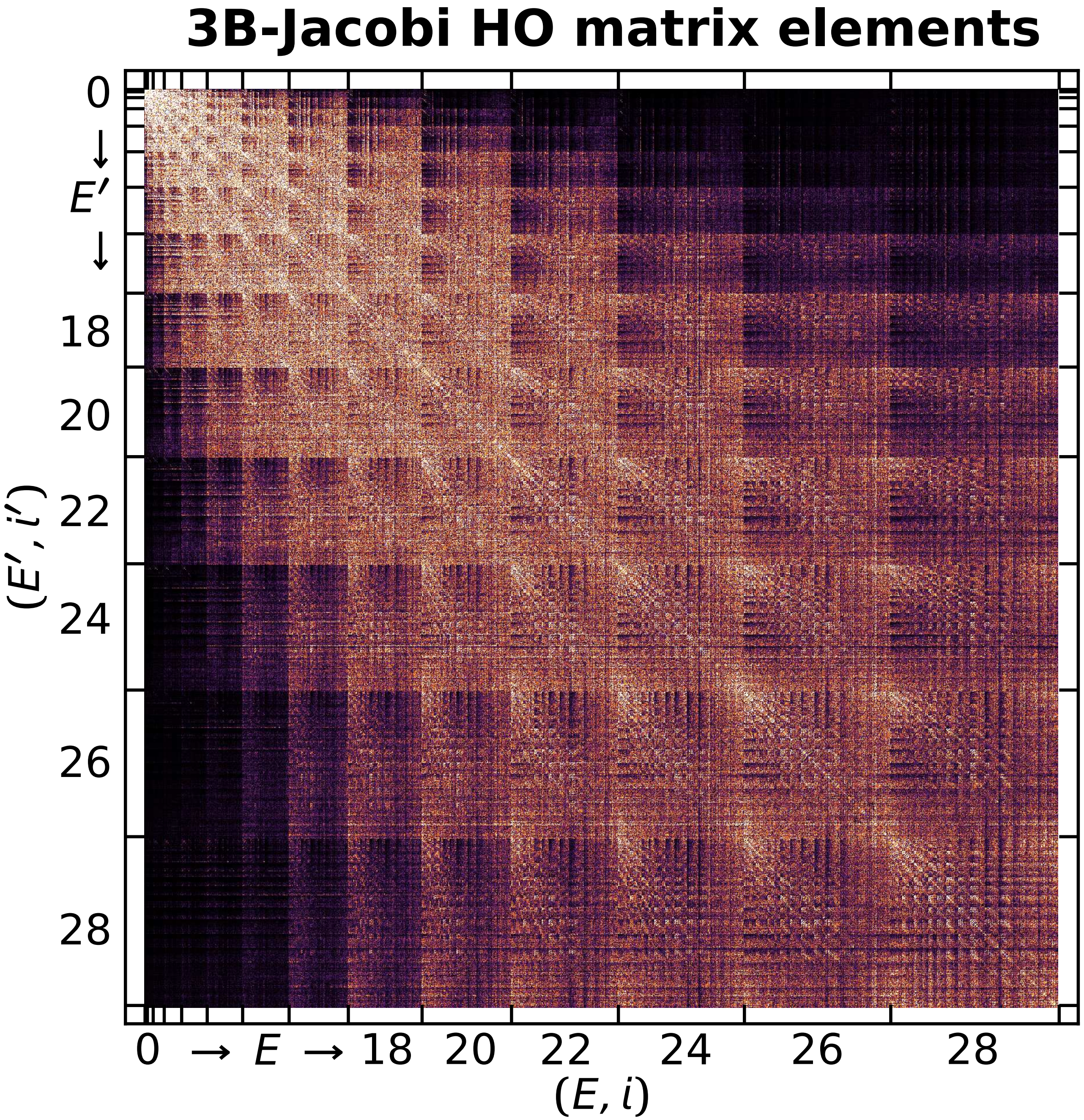

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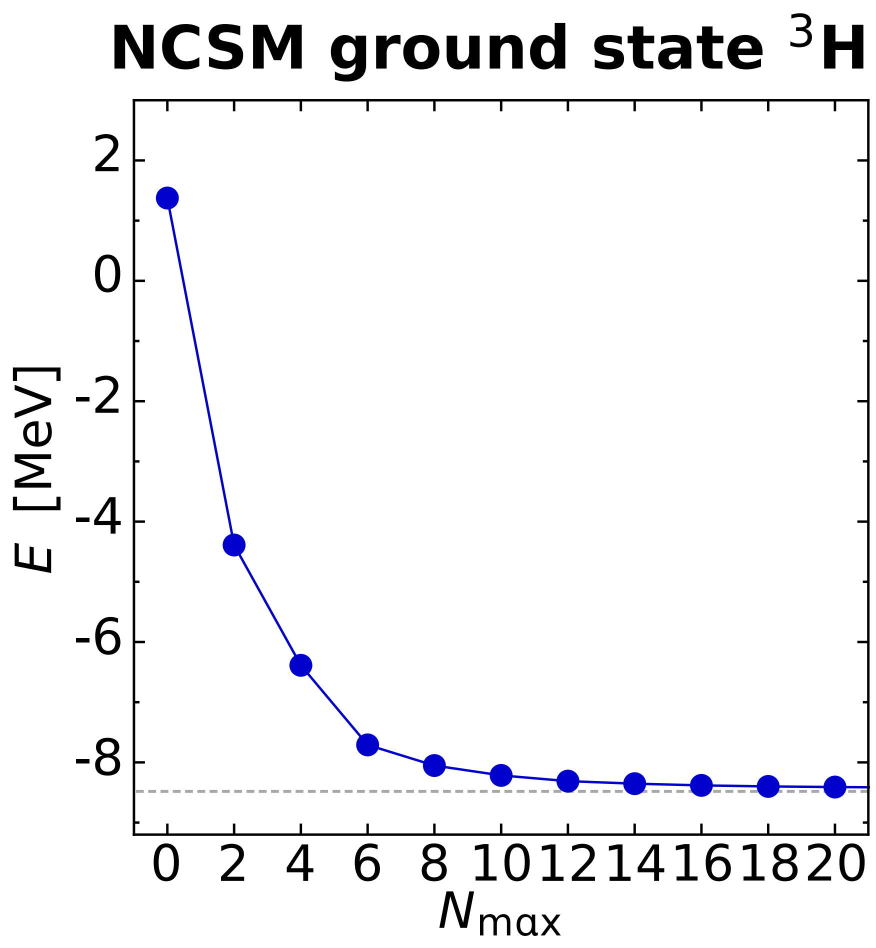

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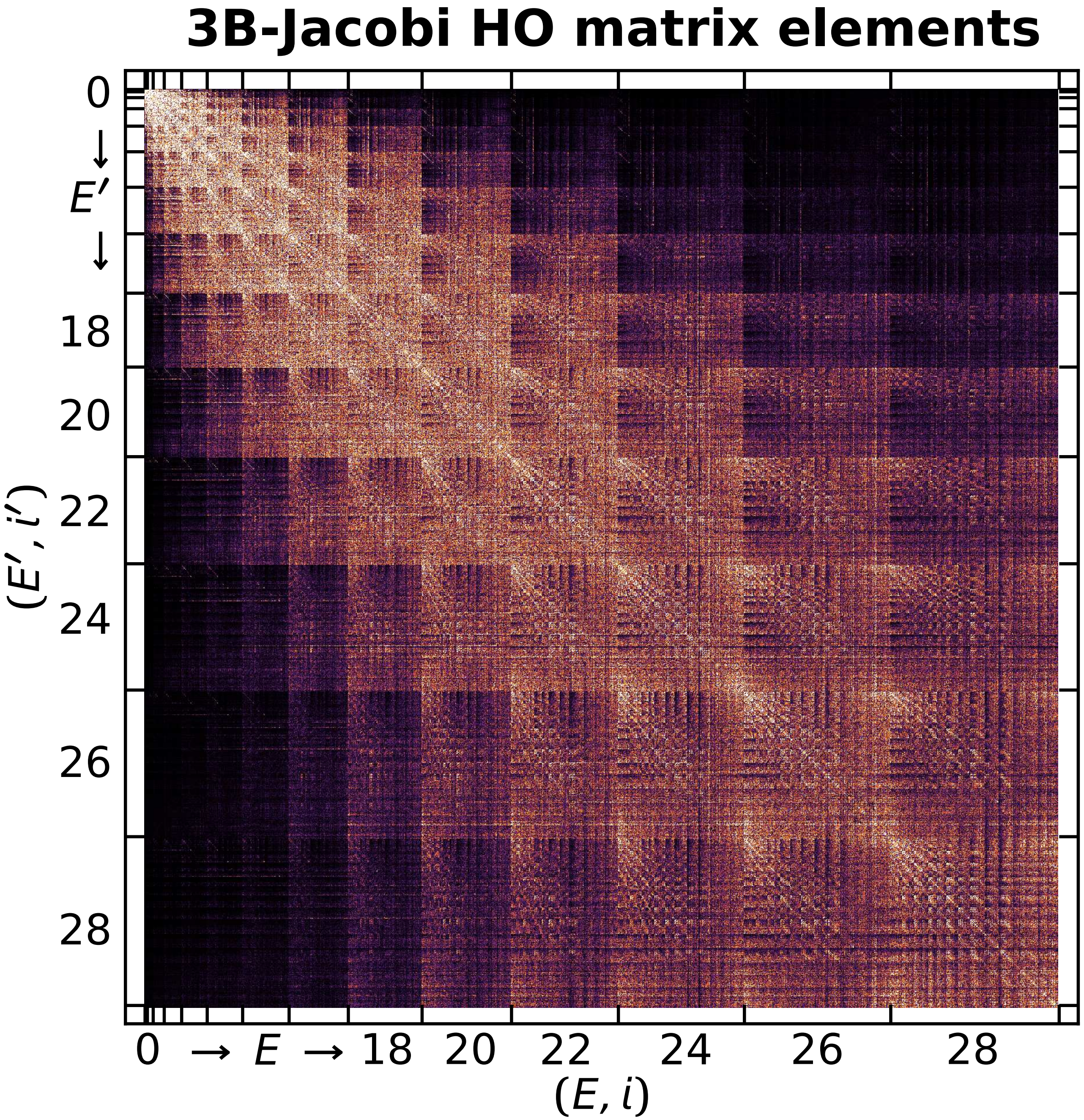

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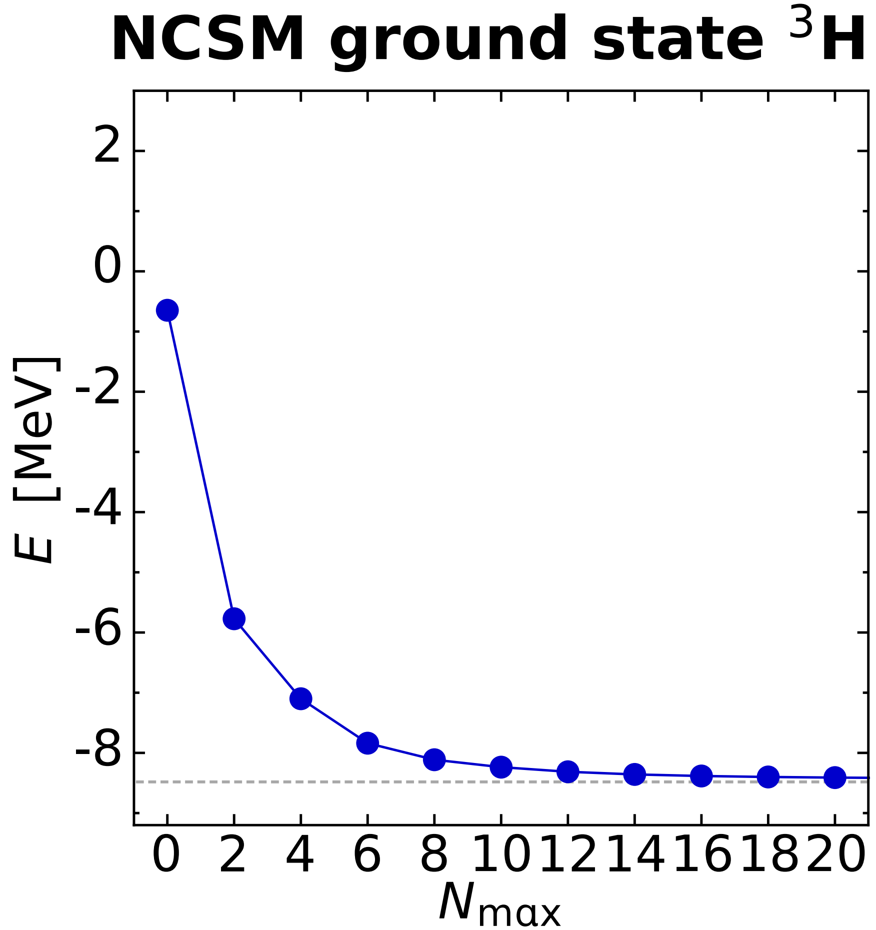

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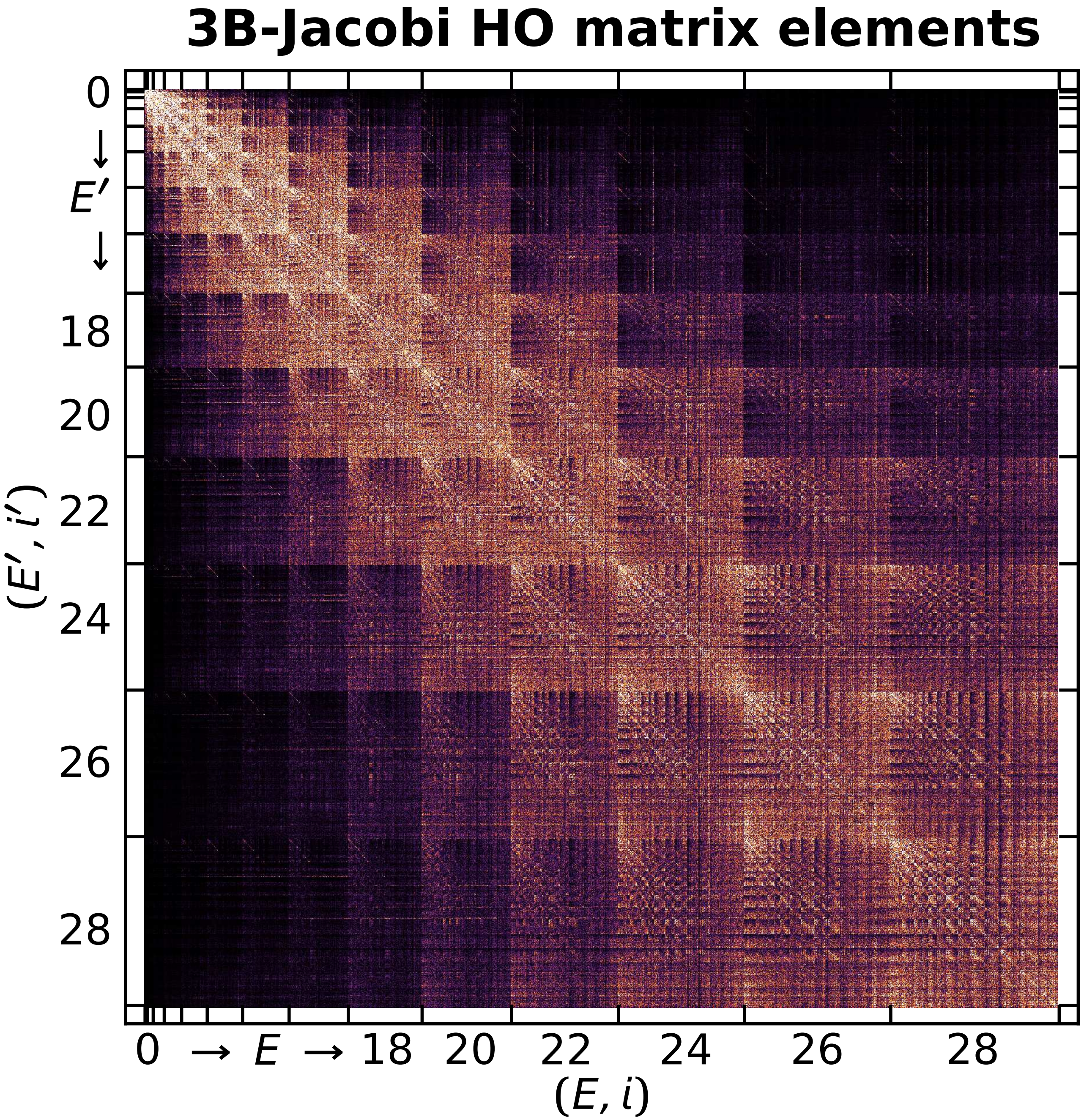

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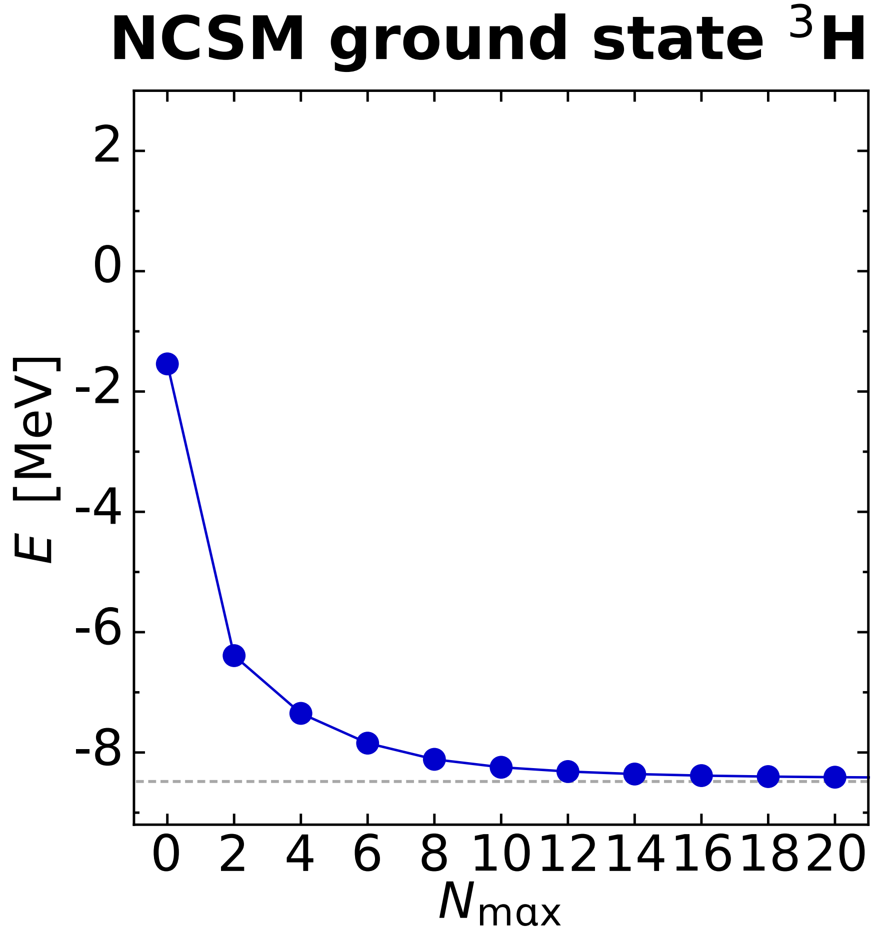
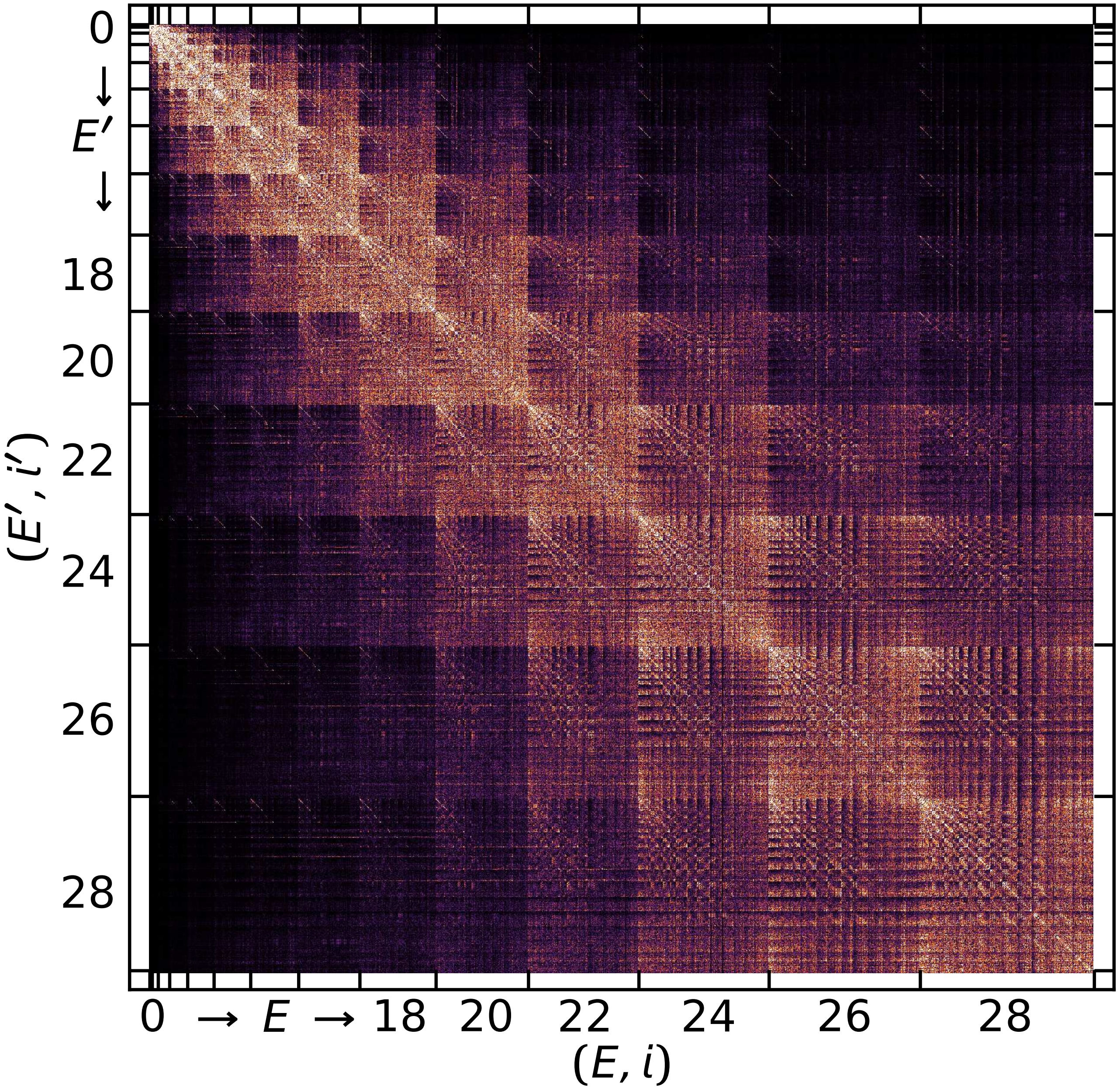


SRG Evolution in Three-Body Space

3B-Jacobi HO matrix elements



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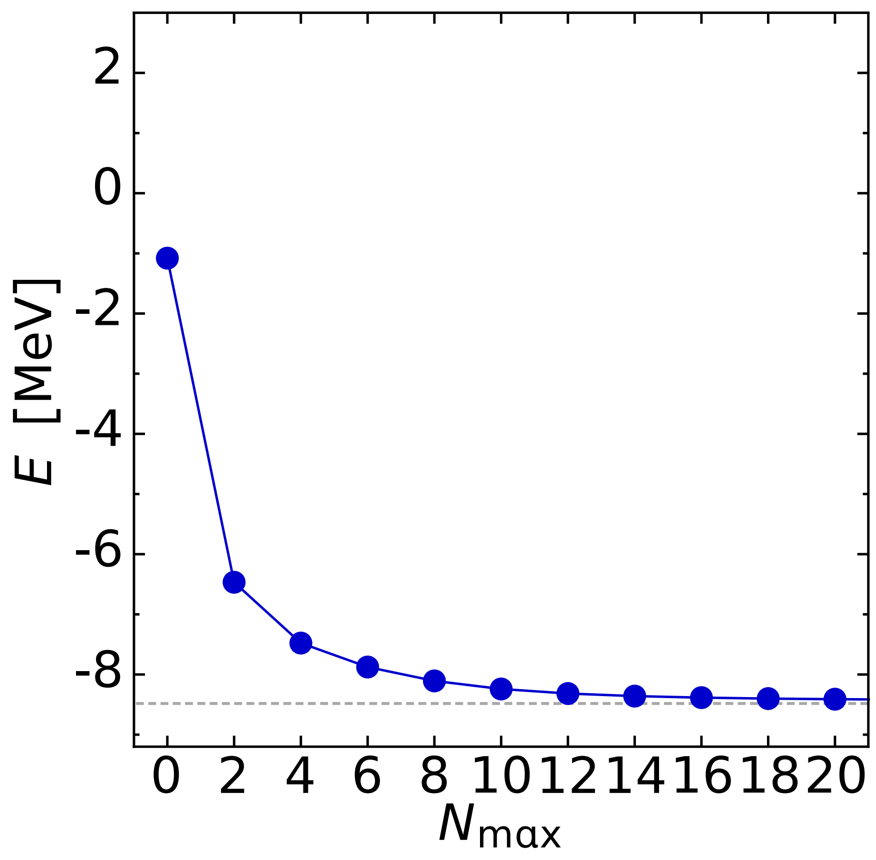

SRG Evolution in Three-Body Space

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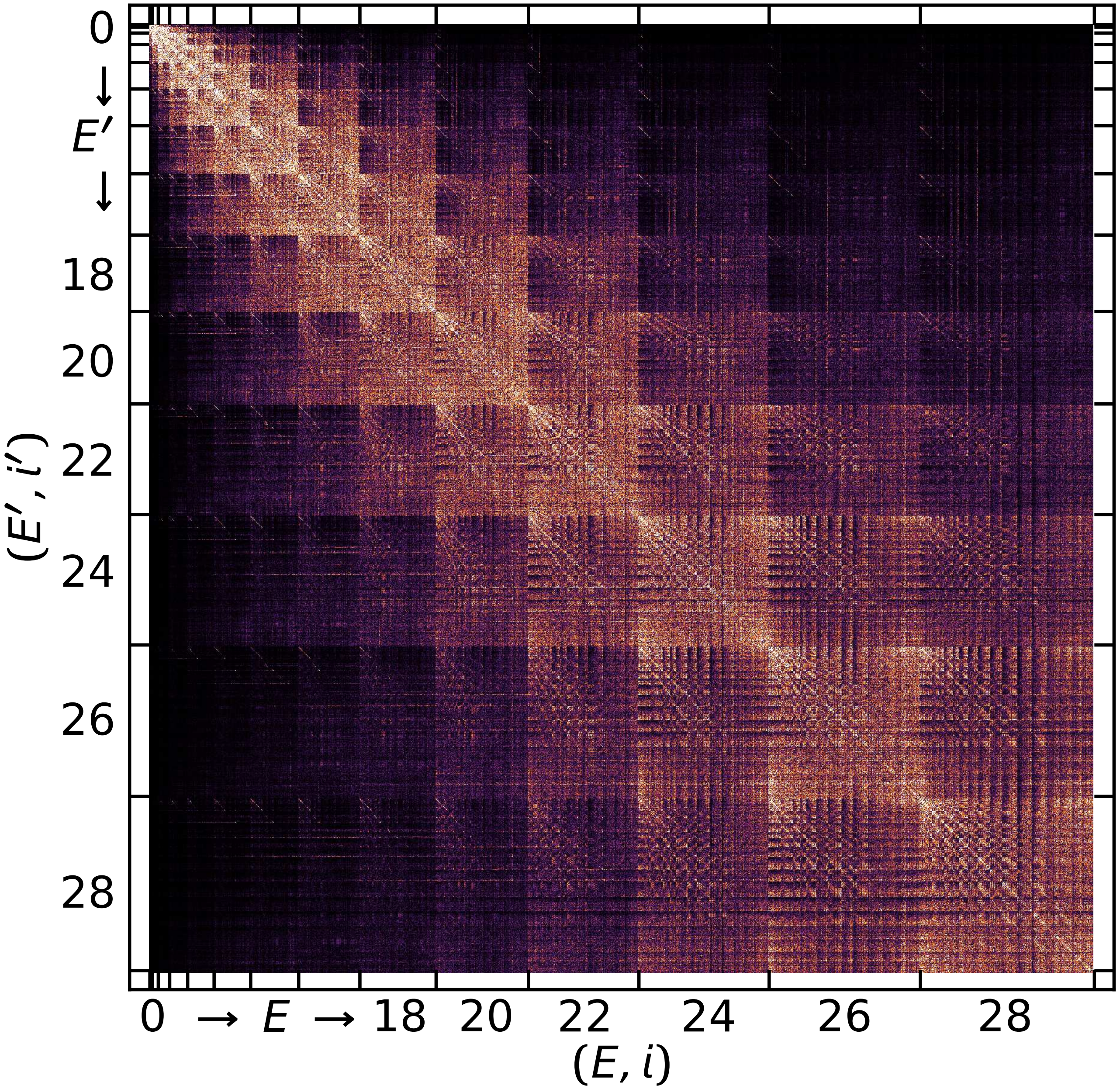

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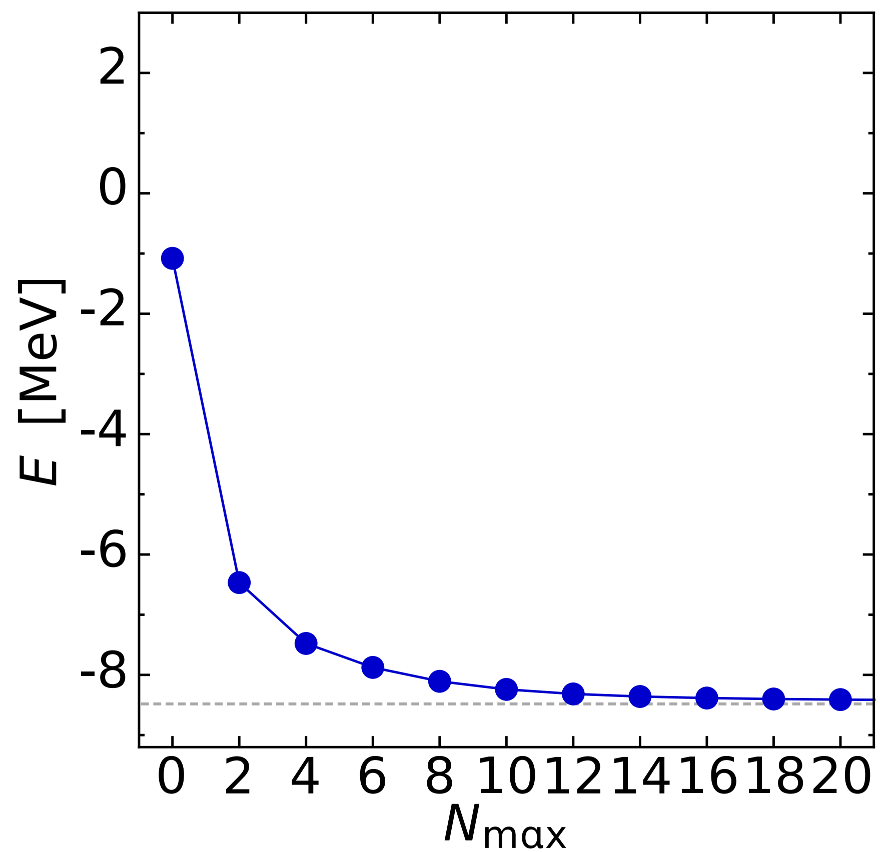

Calculations in A-Body Space

- **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 leaves A-body energy eigenvalues invariant and, thus, independent of α
  - α-dependence of eigenvalues of cluster-truncated Hamiltonian measures impact of discarded many-body contributions

Calculations in A-Body Space

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  - only the full evolution in A-body space leaves A-body energy eigenvalues invariant and, thus, independent of α
  - α-dependence of eigenvalue ... ltonian measures impact of disc...

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

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+3N initial Hamiltonian and evolve in three-body space

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

Exact Ab-Initio Calculations

Importance-Truncated NCSM

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)

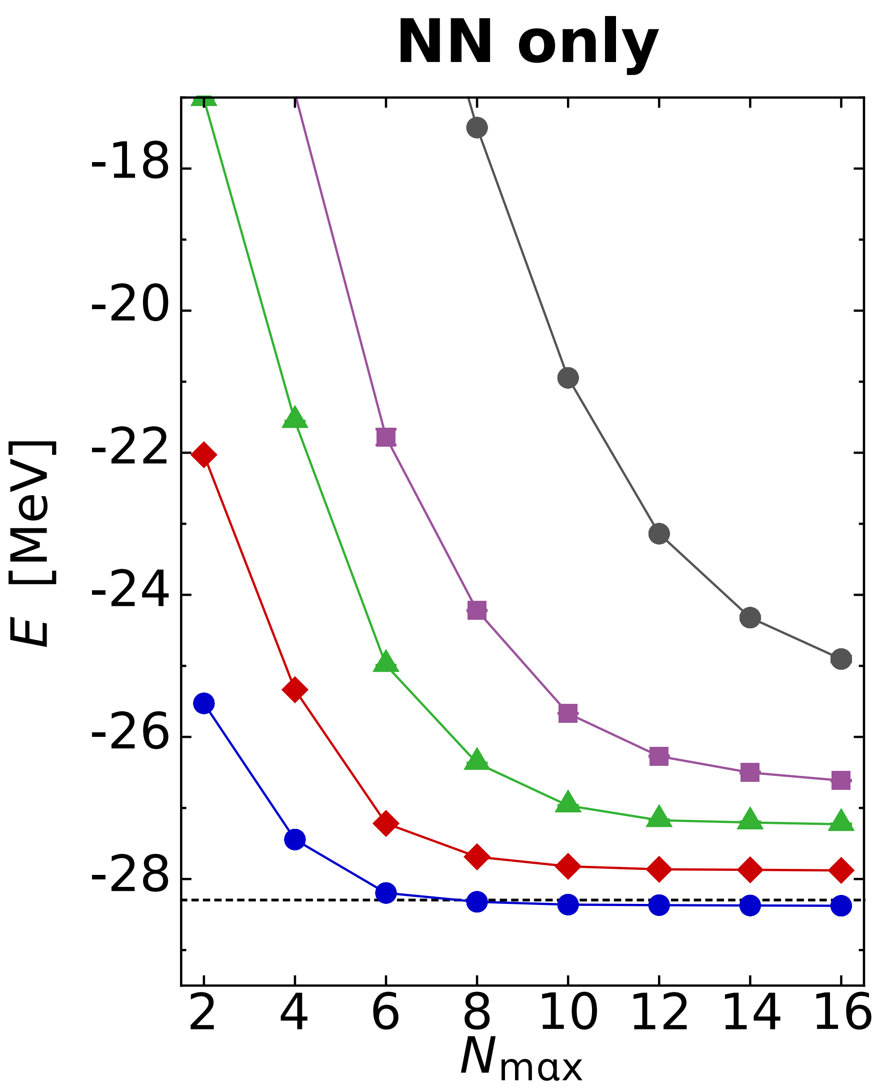
Importance-Truncated NCSM

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 $N_{\max}\hbar\Omega$
- **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 by reducing the model space to physically relevant states, contribution of discarded states included a posteriori
- we have developed a **parallelized IT-NCSM/NCSM code** capable of handling 3N matrix elements up to $E_{3\max} = 14$ or 16

^{4}He: SRG-Evolved Chiral NN+3N

$\hbar\Omega = 28\,\text{MeV}$



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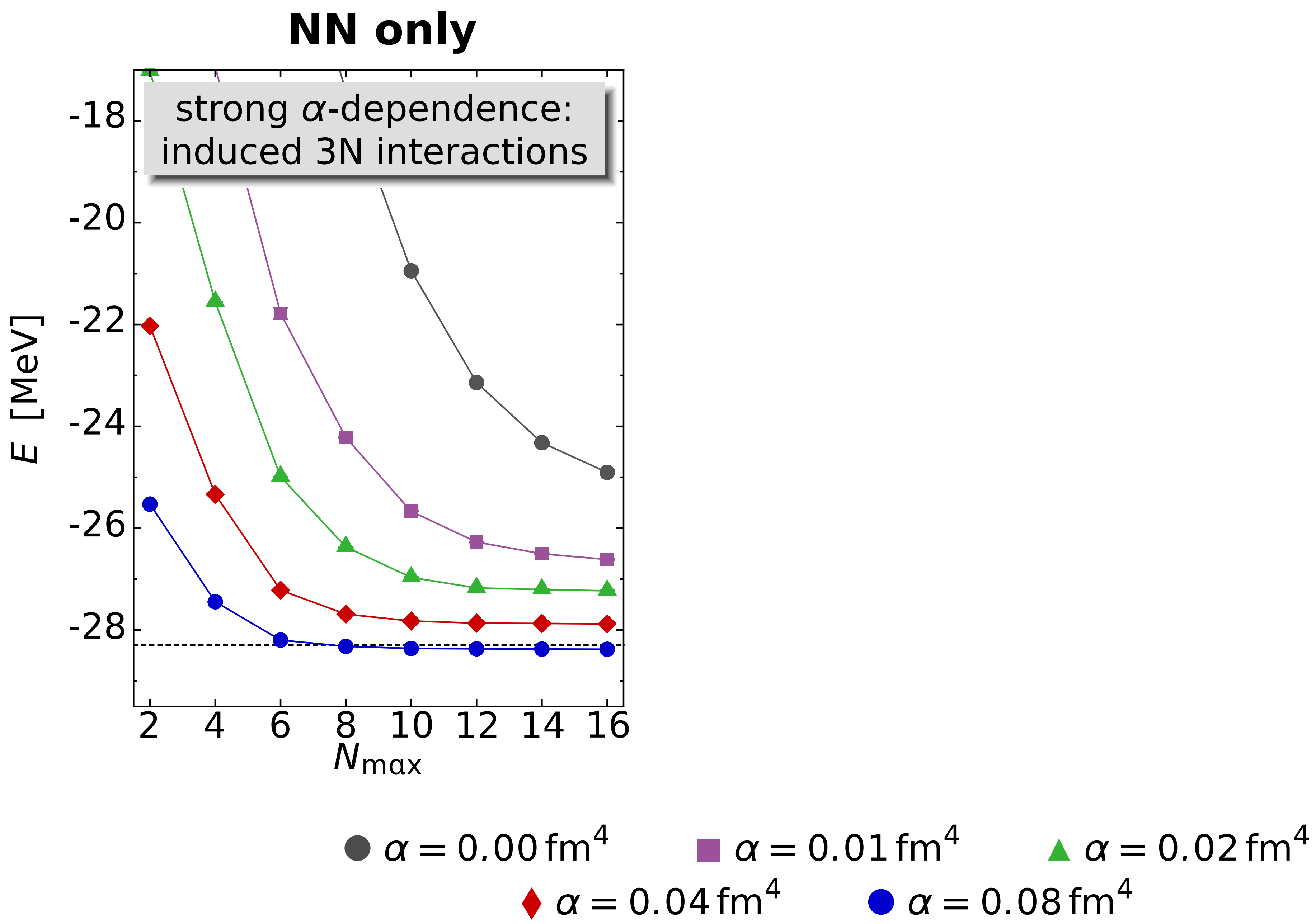
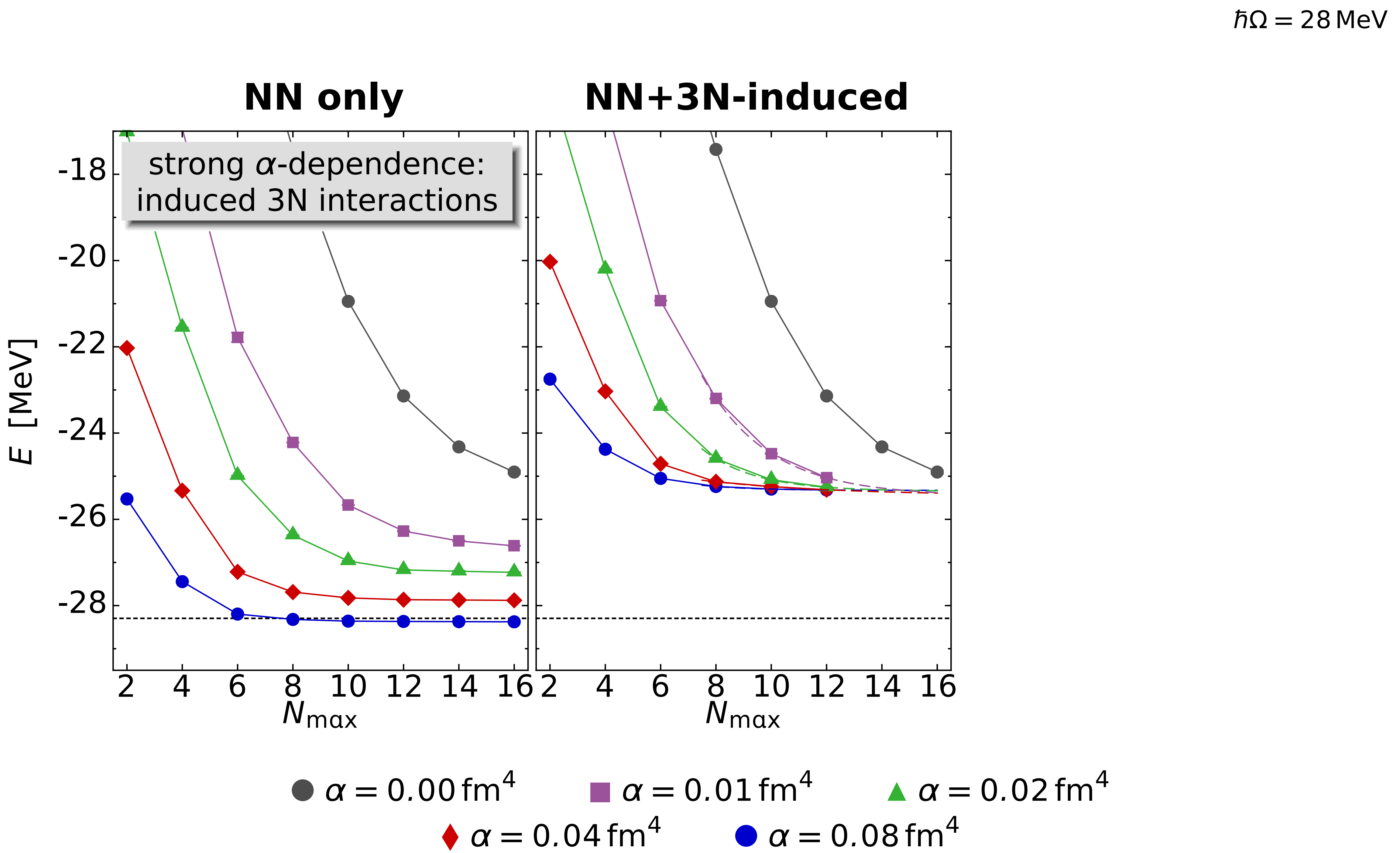
^{4}He: SRG-Evolved Chiral NN+3N

$\hbar\Omega = 28\,\mathrm{MeV}$



^{4}He: SRG-Evolved Chiral NN+3N



^{4}He: SRG-Evolved Chiral NN+3N

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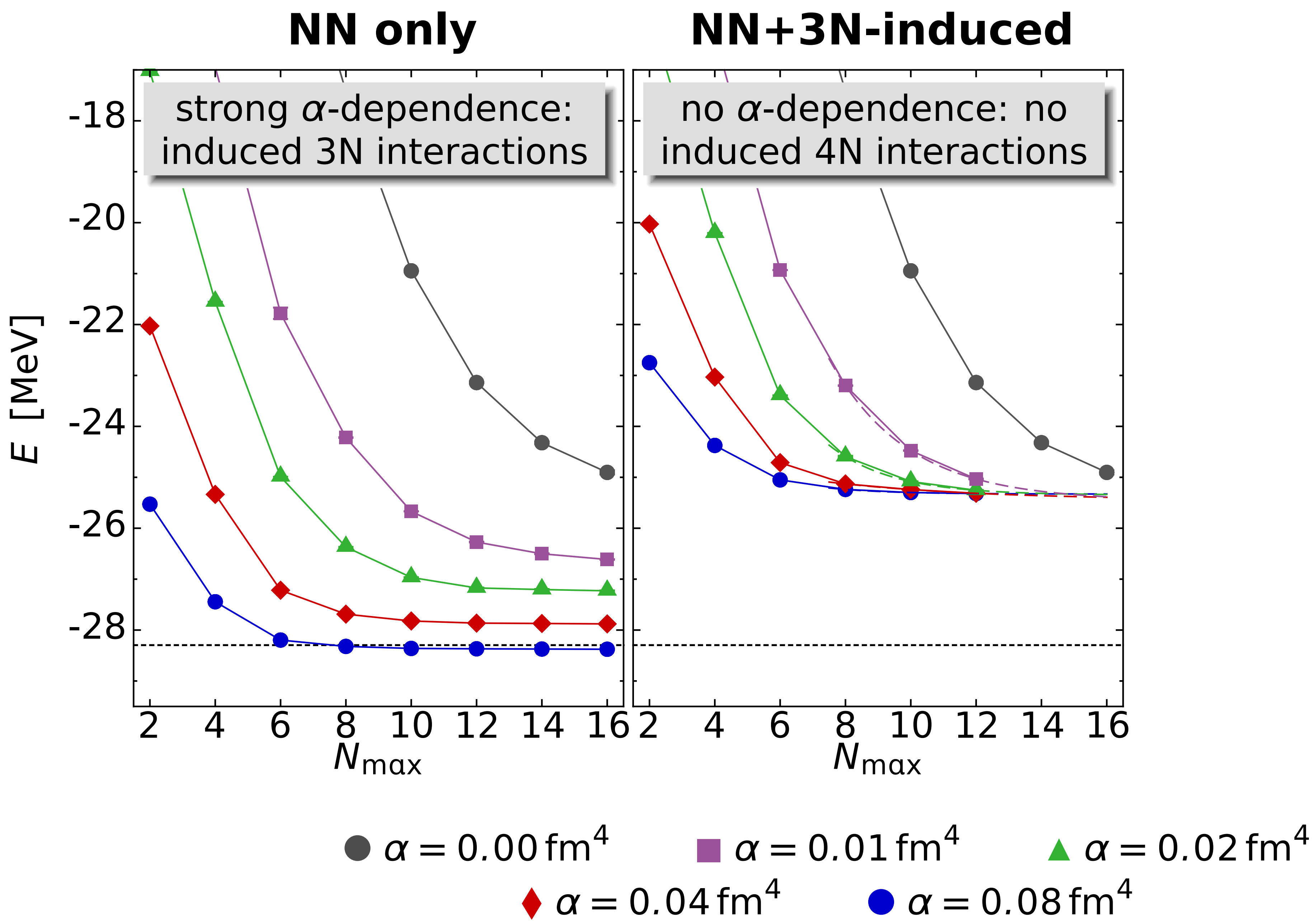
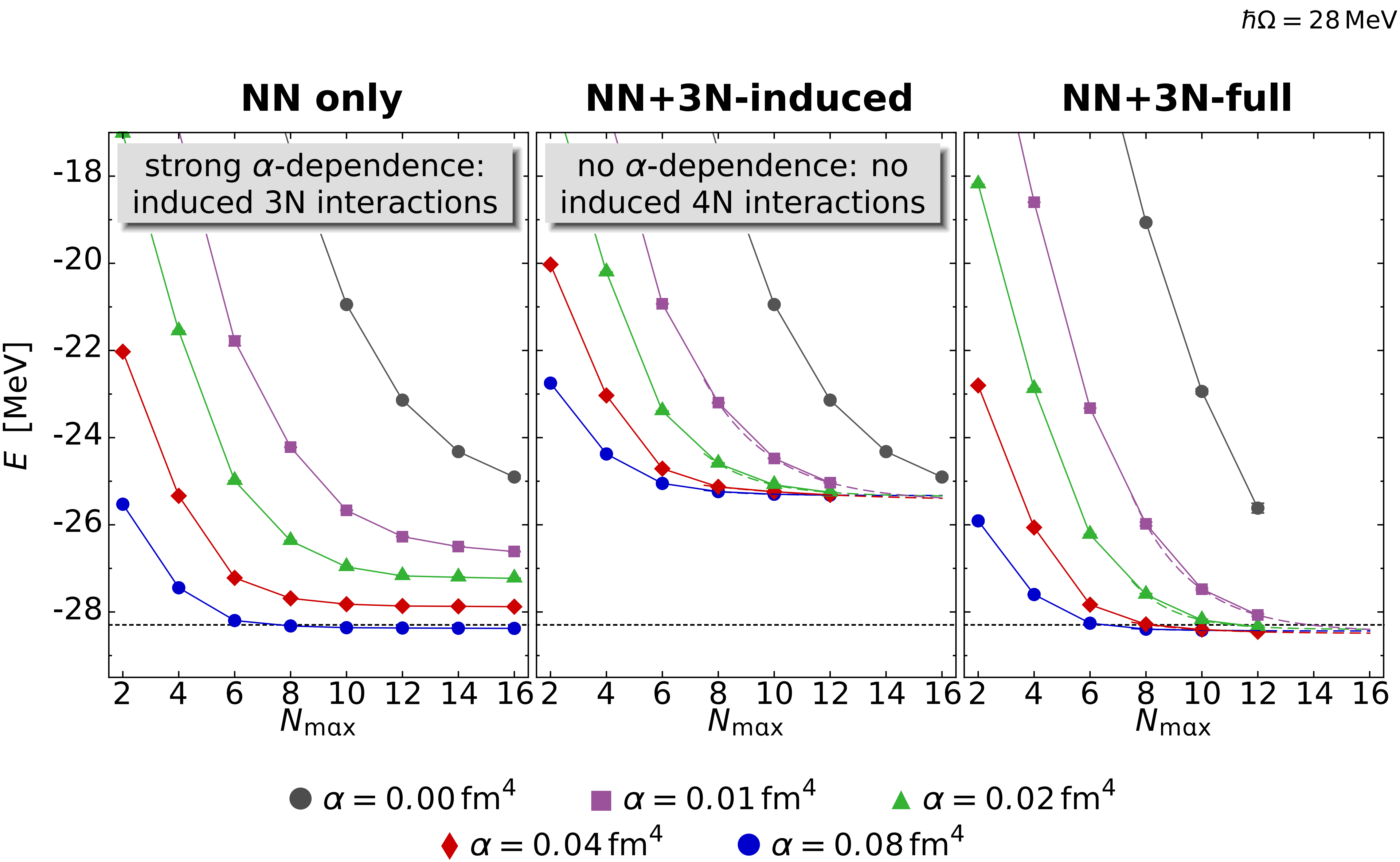
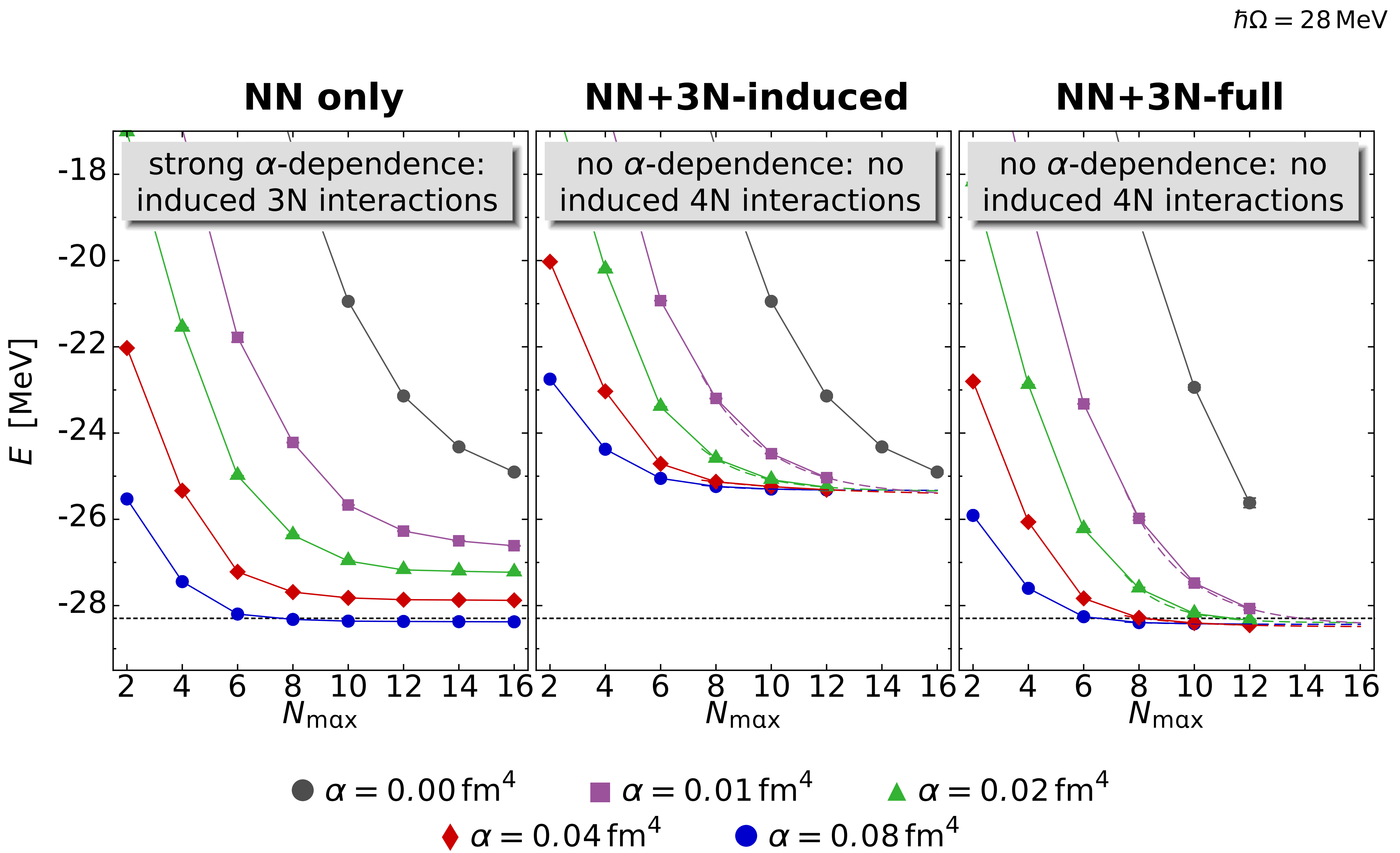


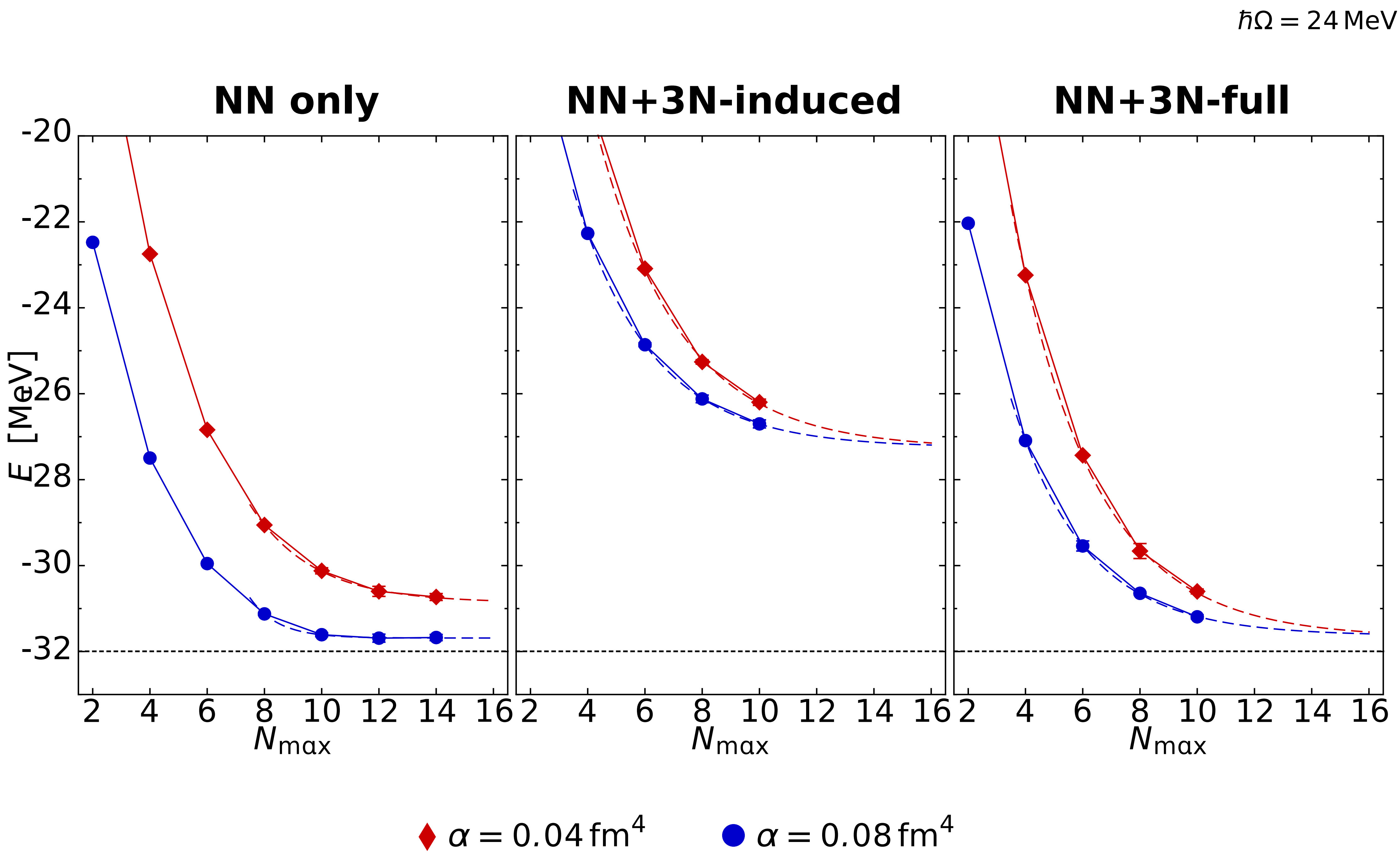
^{4}He: SRG-Evolved Chiral NN+3N



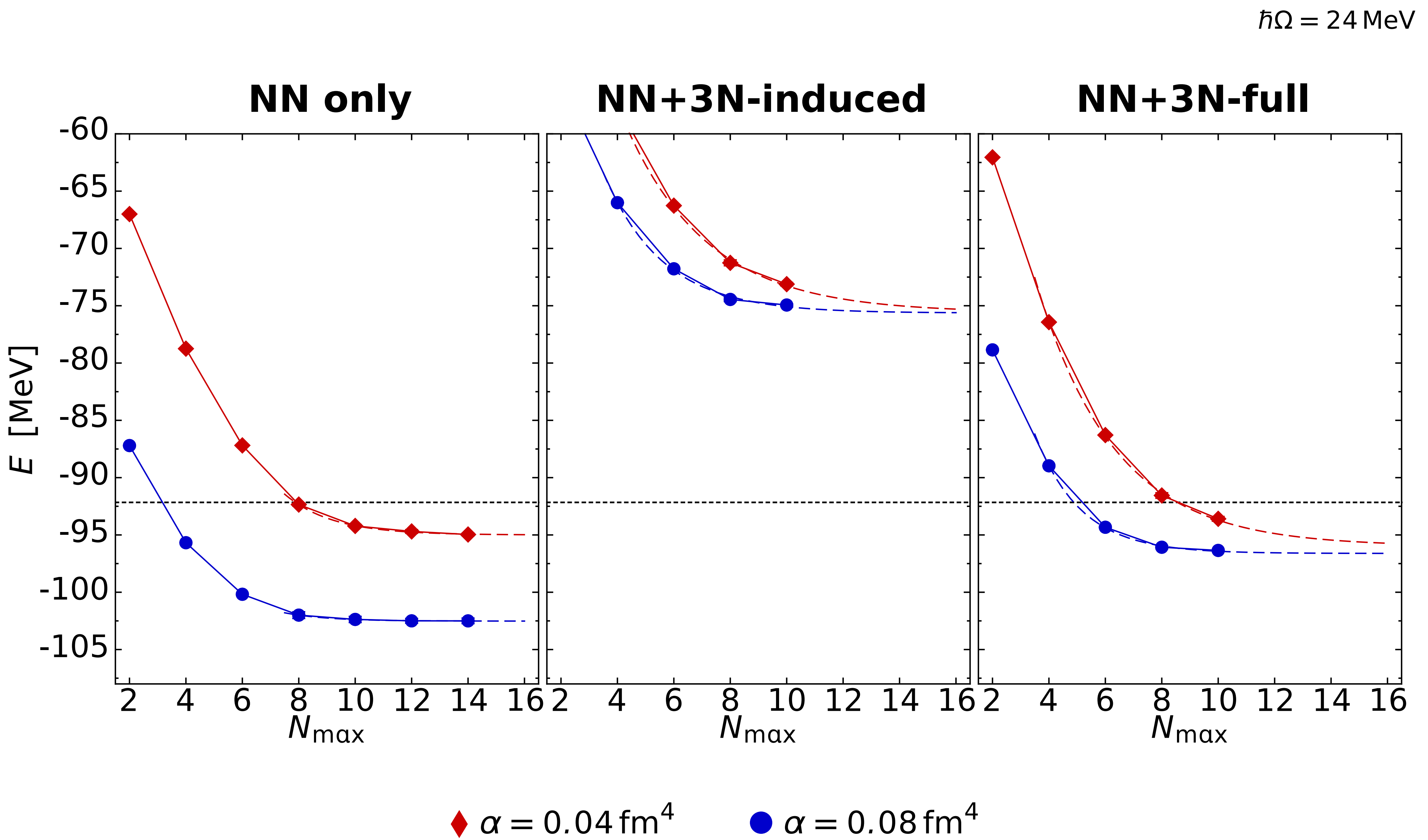
^{4}He: SRG-Evolved Chiral NN+3N



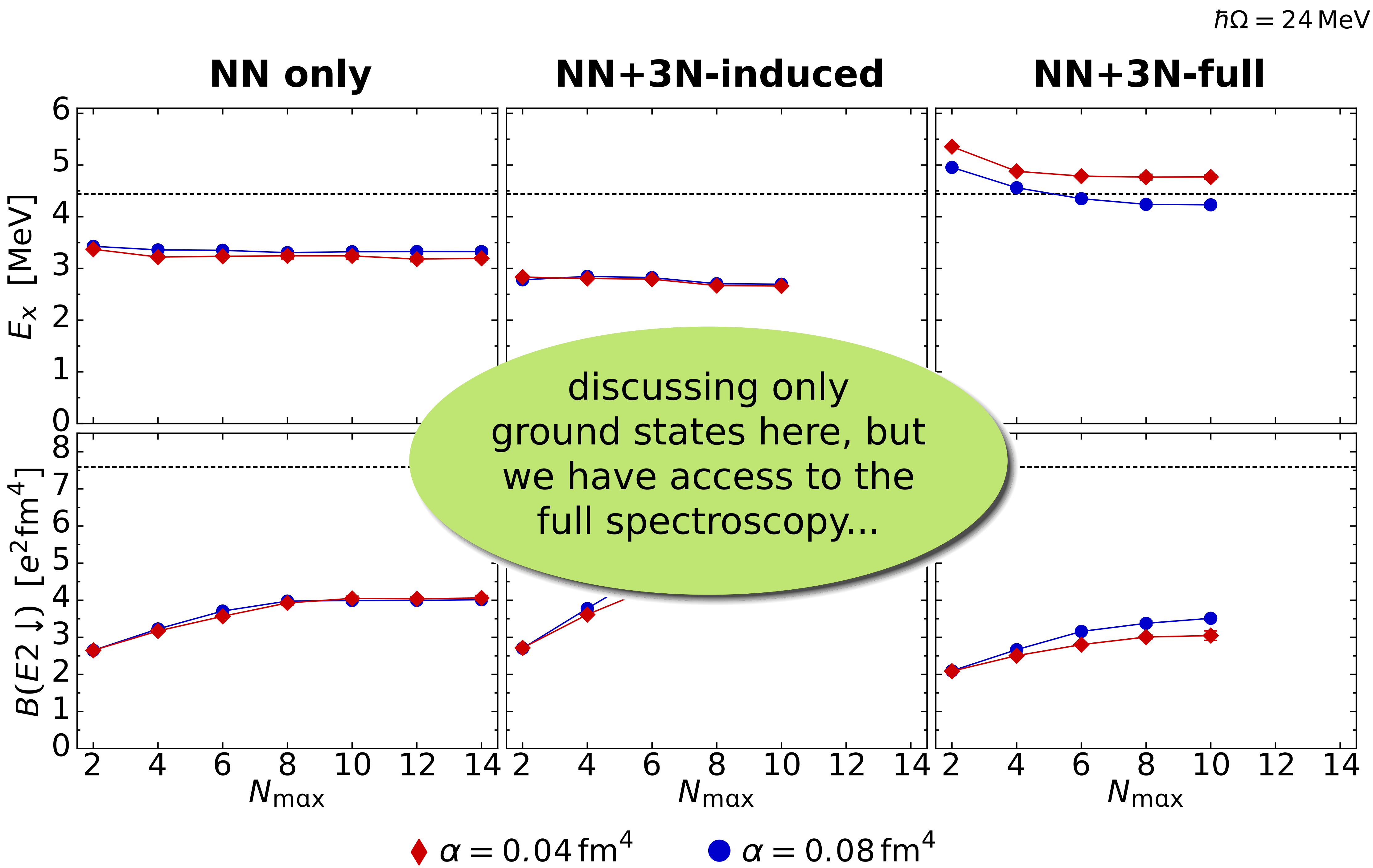
^{6}Li: SRG-Evolved Chiral NN+3N



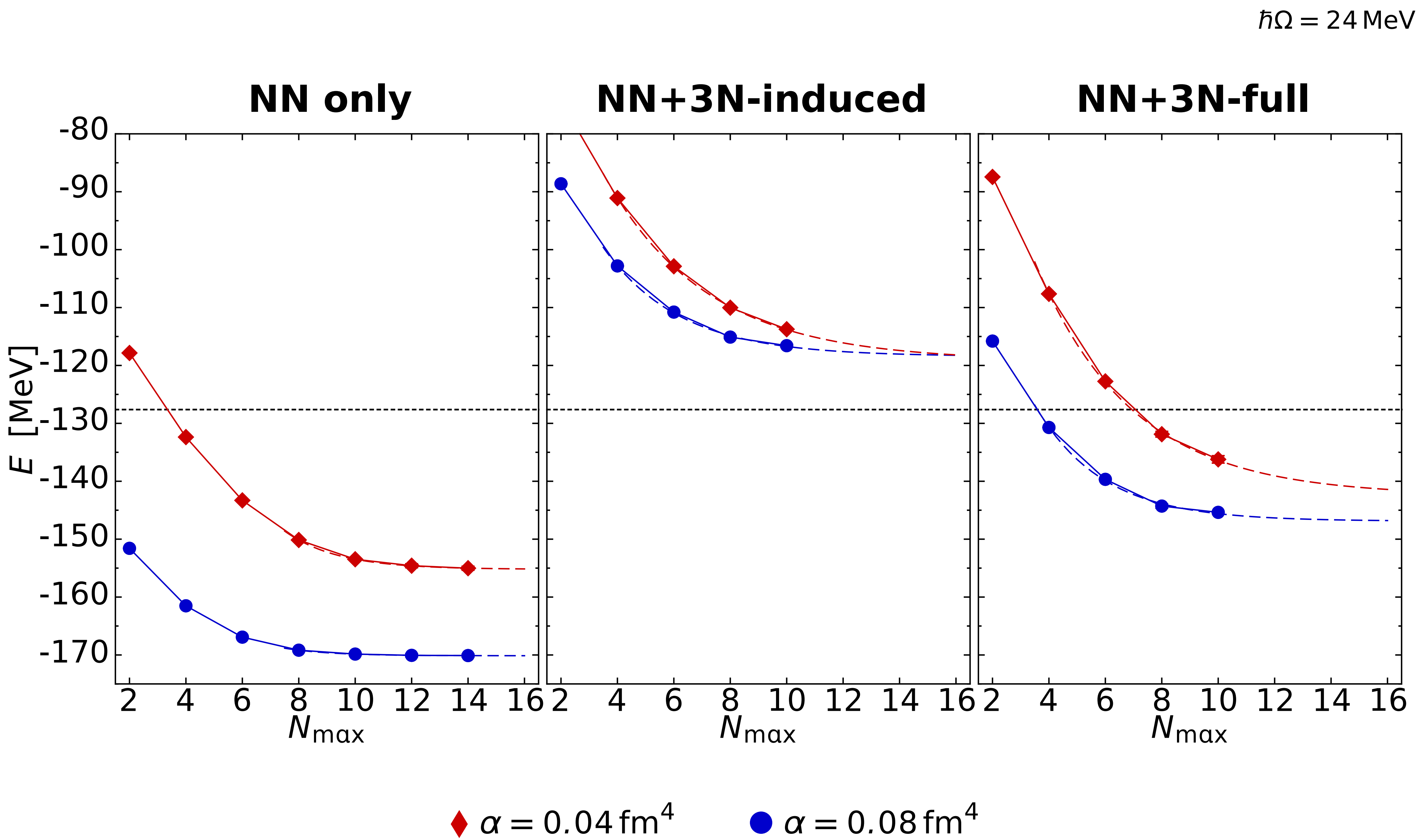
^{12}C: SRG-Evolved Chiral NN+3N



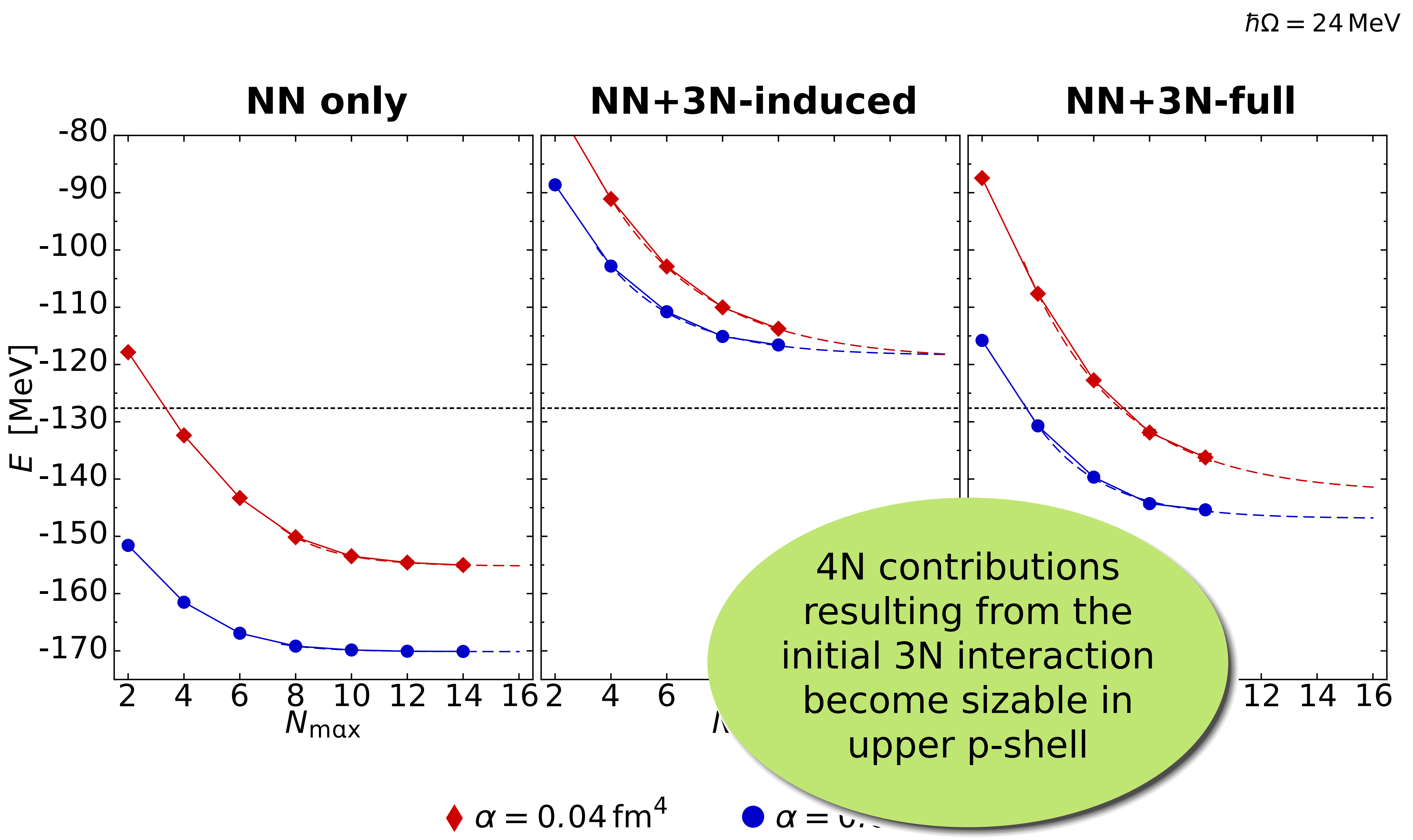
^{12}C: Spectroscopy of First 2^+ State



^{16}O: SRG-Evolved Chiral NN+3N



^{16}O: SRG-Evolved Chiral NN+3N



Approximate Many-Body Methods

Hartree-Fock & Perturbation Theory

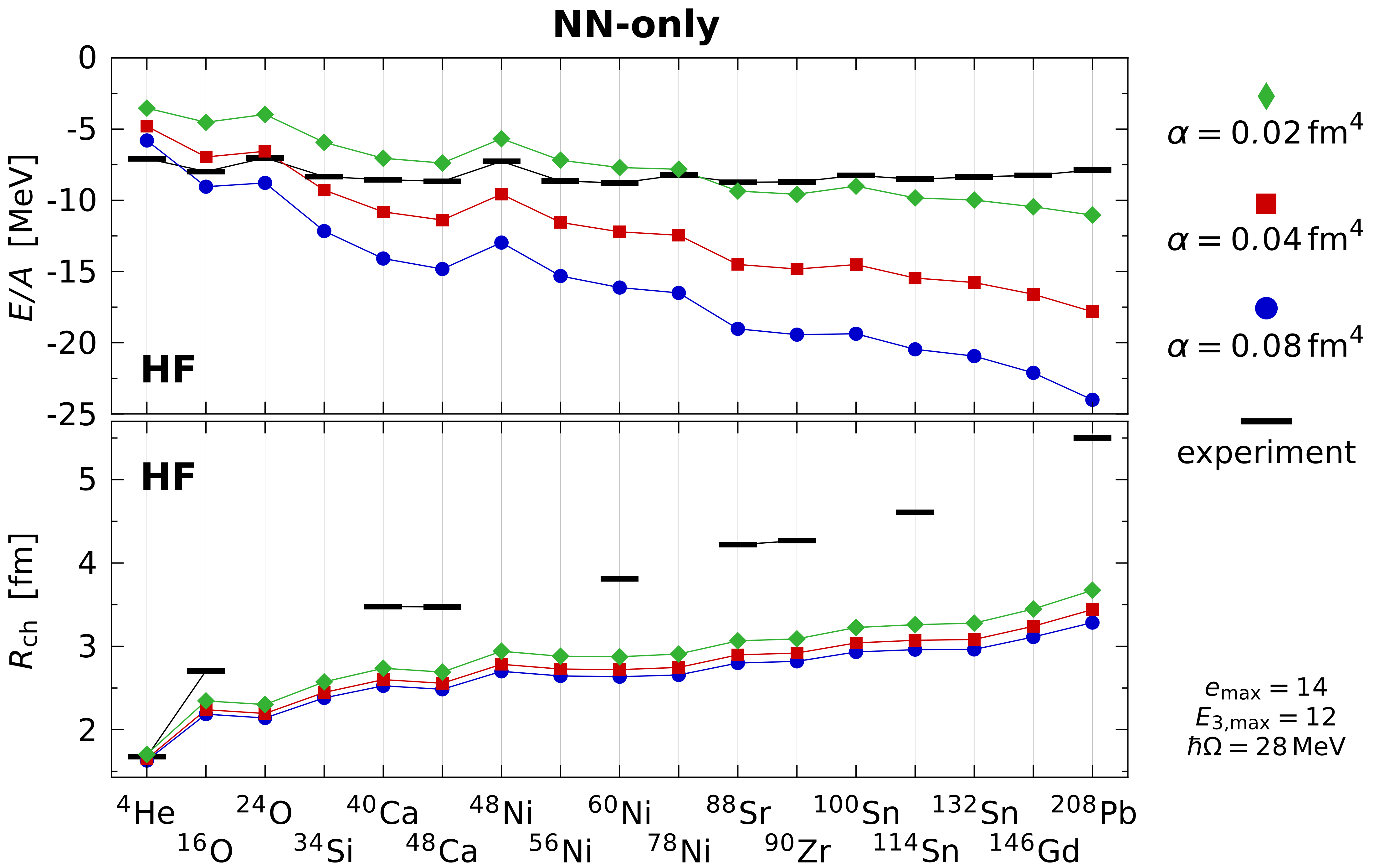
Günther, Roth, Hergert, Reinhardt — Phys. Rev. C 82, 024319 (2010)
Roth, Neff, Feldmeier — Prog. Part. Nucl. Phys. 65, 50 (2010)
Roth, Langhammer — Phys. Lett. B 683, 272 (2010)
Roth, et al. — Phys. Rev. C 73, 044312 (2006)

Hartree-Fock & Perturbation Theory

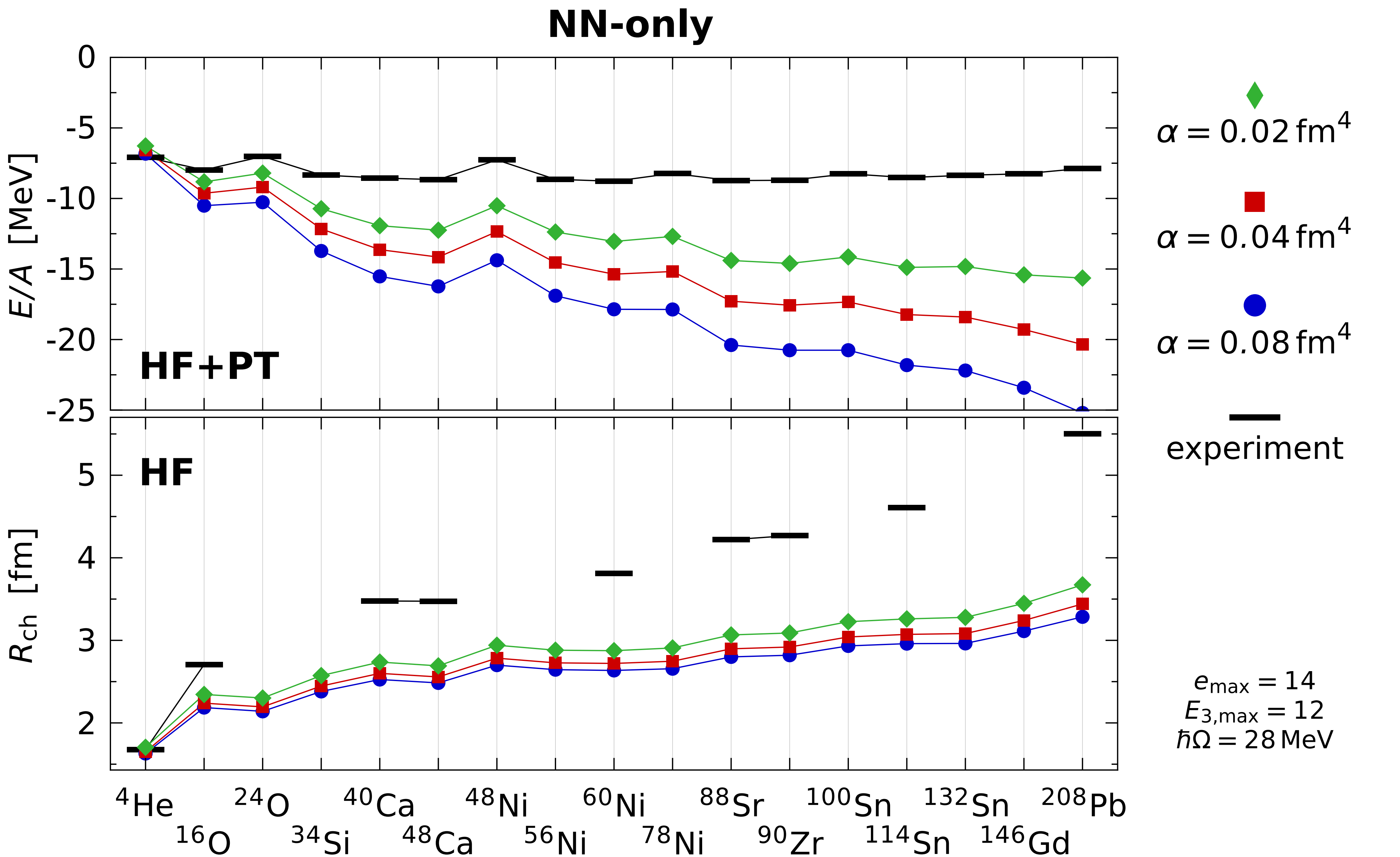
HF & PT provides information on the systematics of ground-state observables over a wide mass range

- 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 $E_{3\,\mathrm{max}} = 12$
  - fixed oscillator frequency $\hbar\Omega = 28$ MeV
  - second-order perturbative correction includes NN contribution only

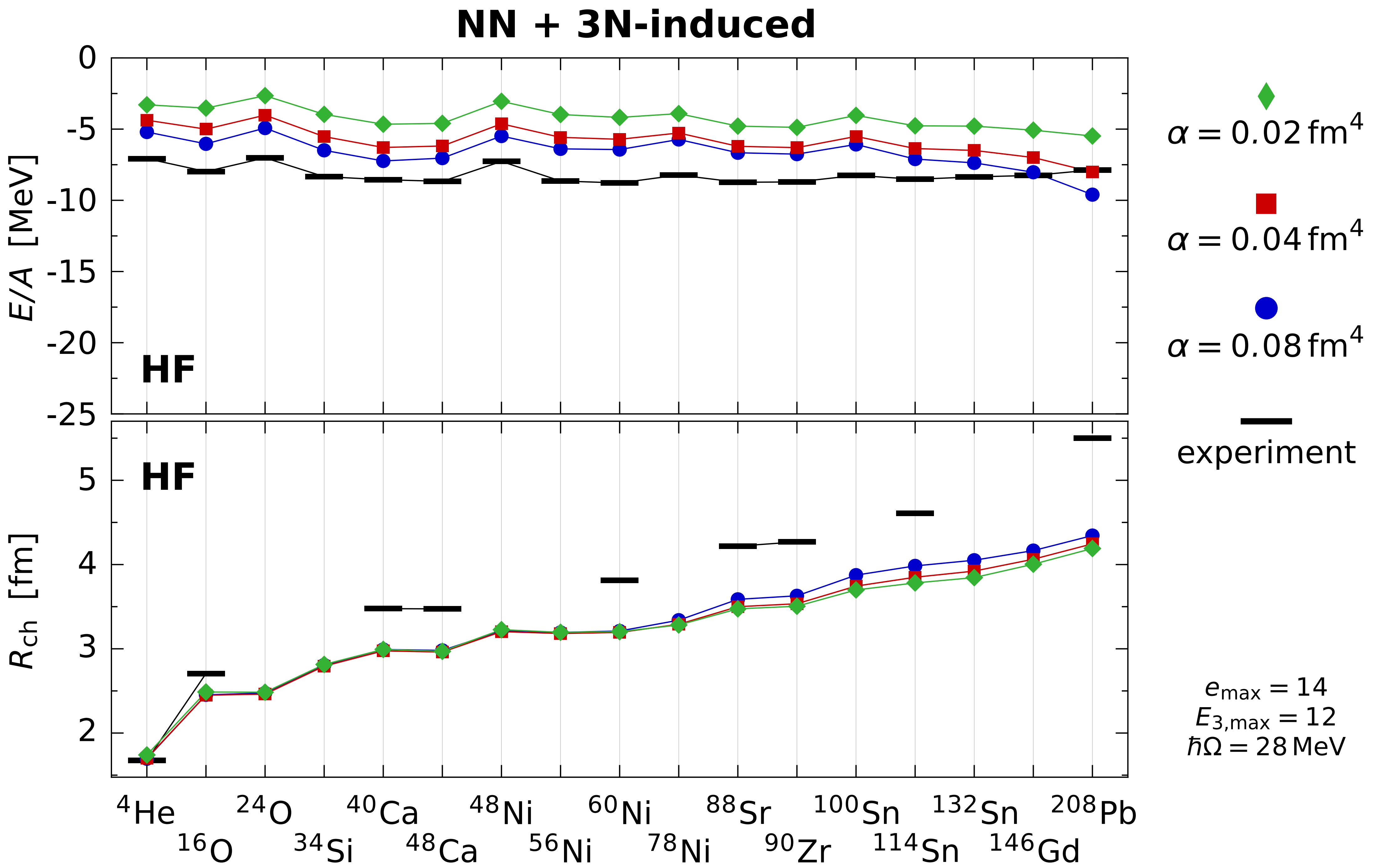
Systematics: E/A and R_{ch}



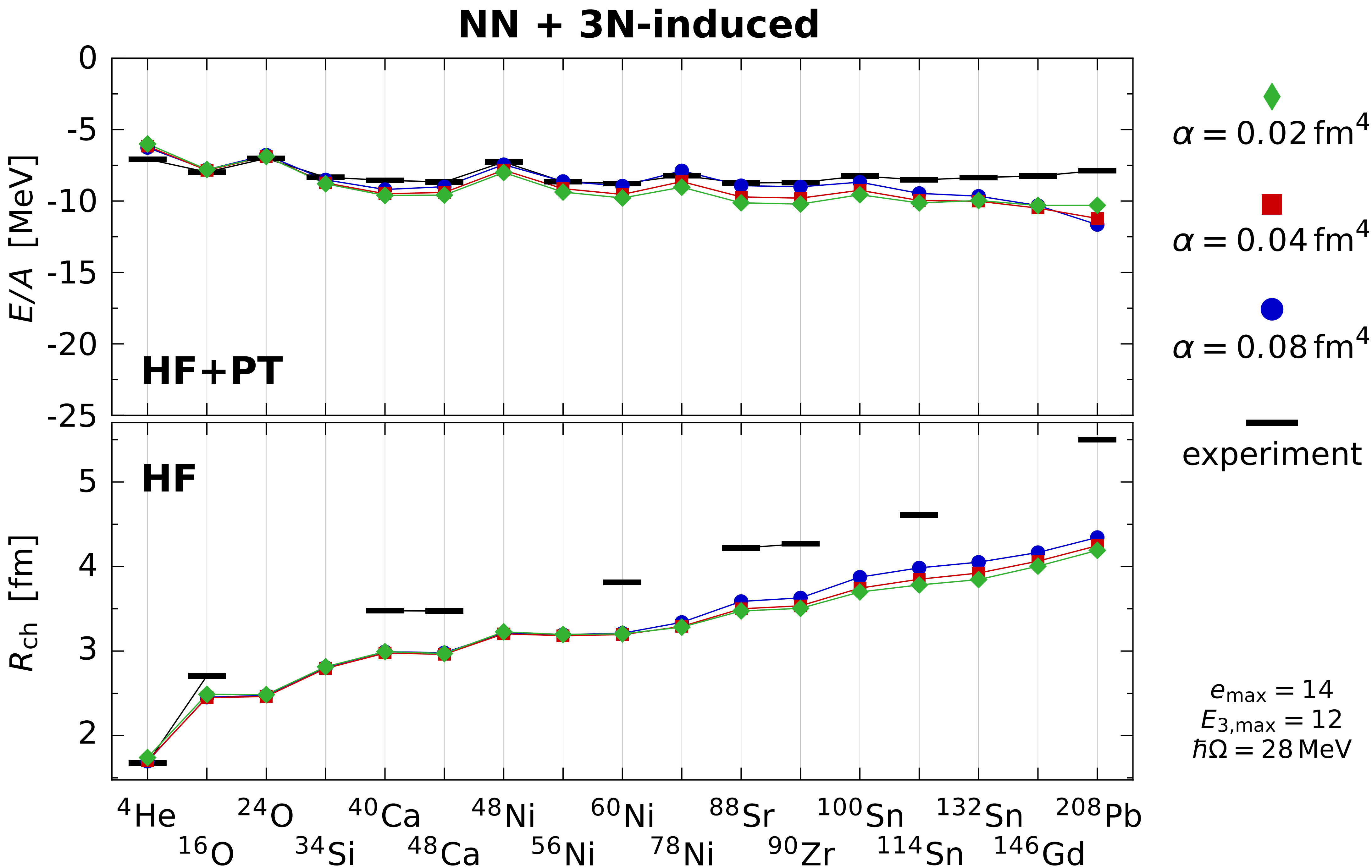
Systematics: E/A and R_{ch}



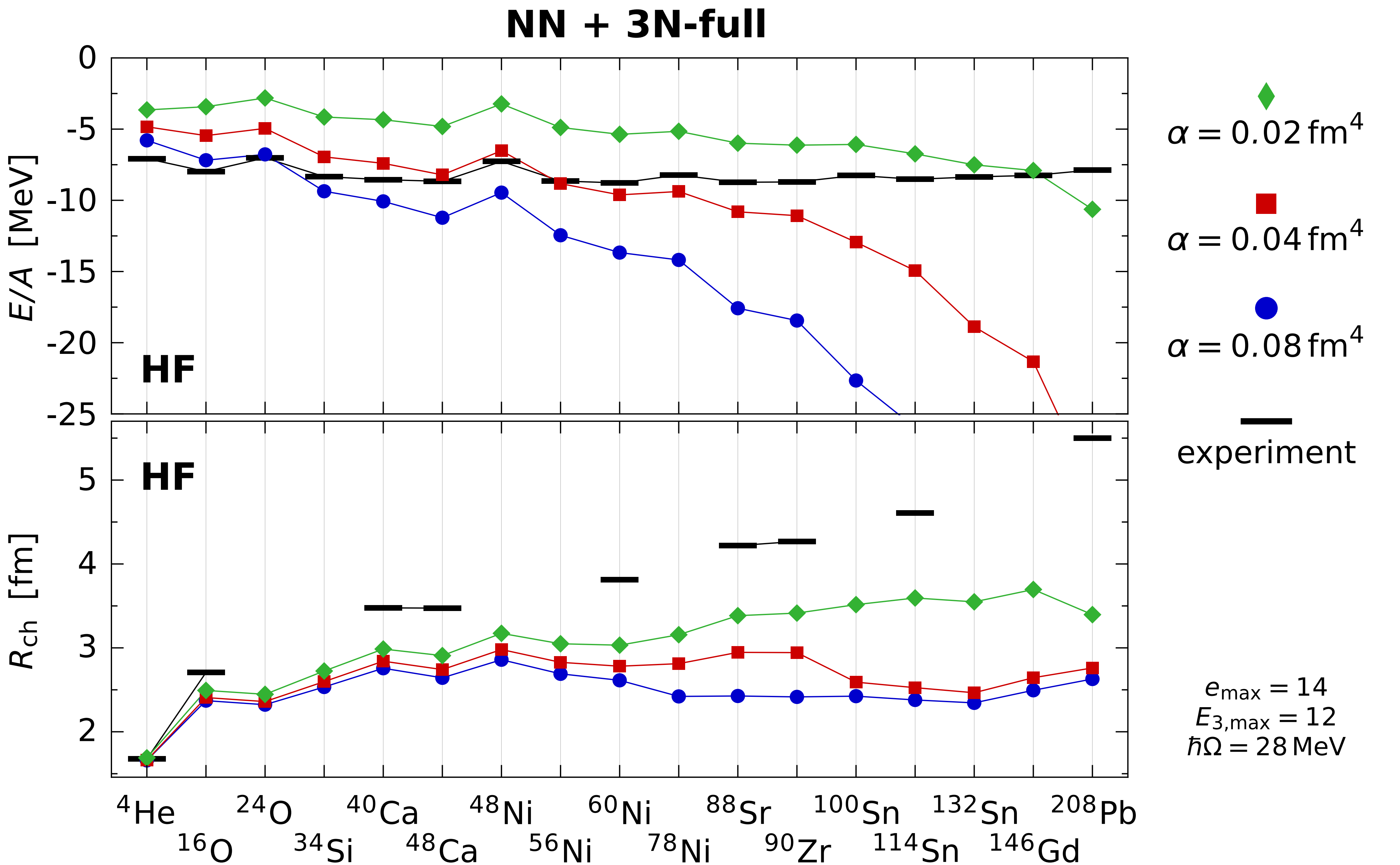
Systematics: E/A and R_{ch}



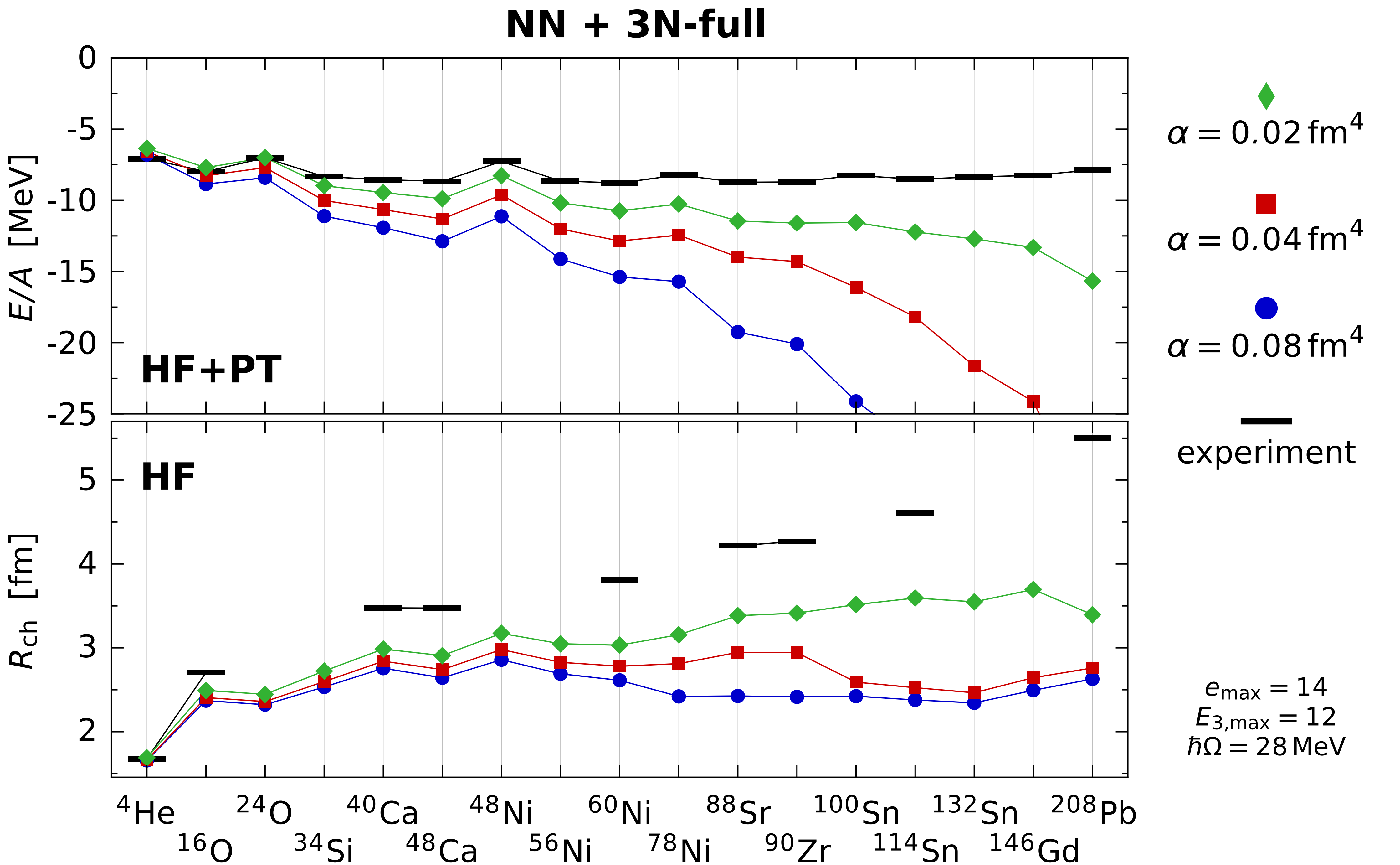
Systematics: E/A and R_{ch}



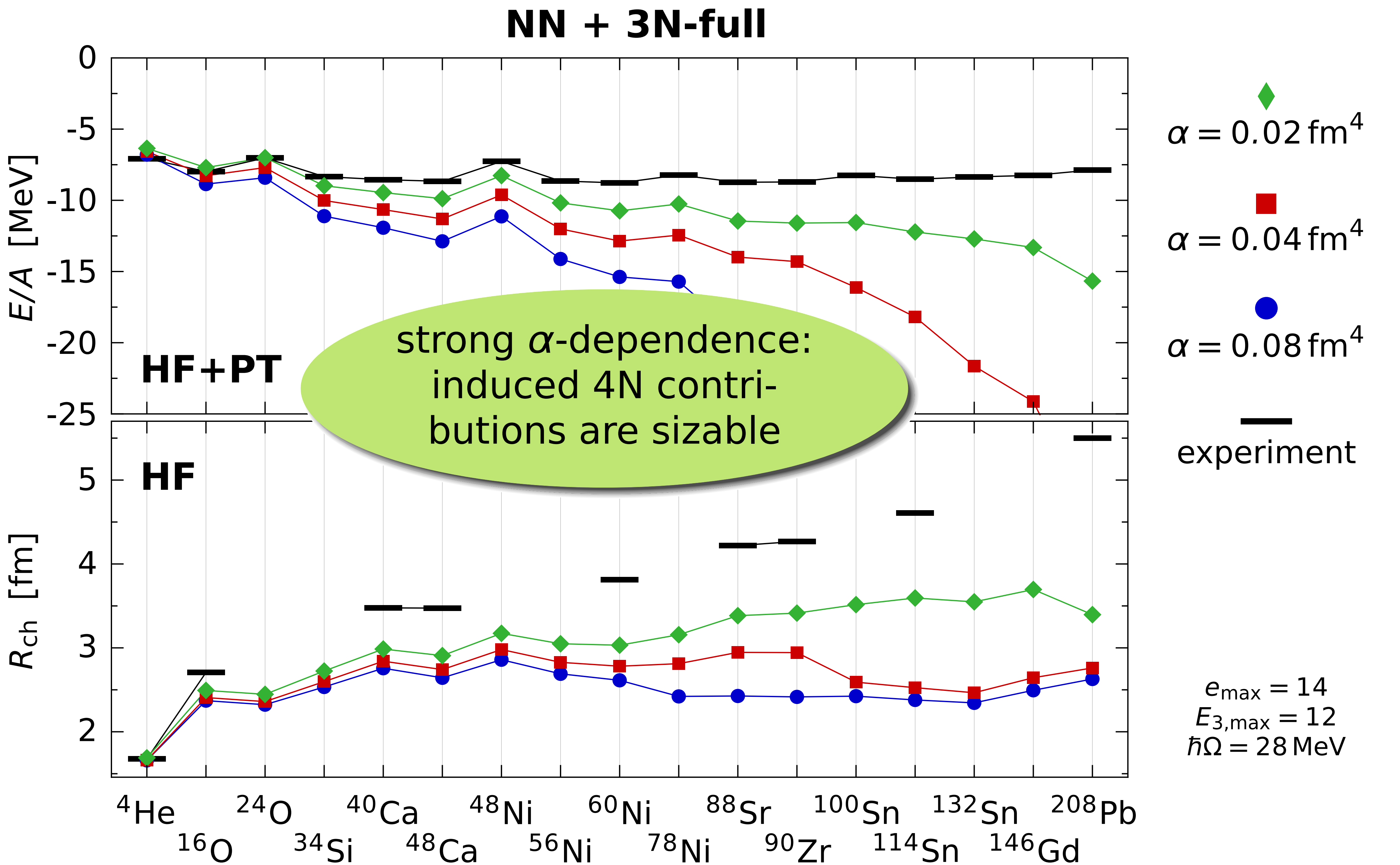
Systematics: E/A and R_{ch}



Systematics: E/A and R_{ch}



Systematics: E/A and R_{ch}



Conclusions

Conclusions

- made huge steps towards nuclear structure calculations with consistent SRG-transformed chiral NN+3N interactions
  - Similarity Renormalization Group
  - Importance-Truncated NCSM
  - Hartree-Fock & Perturbation Theory
- indications that induced 4N contributions resulting from initial 3N interaction are significant for nuclei beyond mid-p-shell
- use modified SRG generators to avoid those 4N contributions from the outset
- many exciting applications ahead...

Epilogue

- **thanks to my group & my collaborators**
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