

# New Horizons for Ab Initio Nuclear Structure Theory with Chiral NN+3N Interactions

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# Ab Initio Nuclear Structure

## Nuclear Structure Observables

Low-Energy Quantum Chromodynamics

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consistent & improvable NN, 3N,... interactions

### **Chiral Effective Field Theory**

systematic low-energy effective theory of QCD

### **Low-Energy Quantum Chromodynamics**

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chiral EFT on lattice

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few-body et al.

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guided by chiral EFT

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few-body, no-core shell model, etc.

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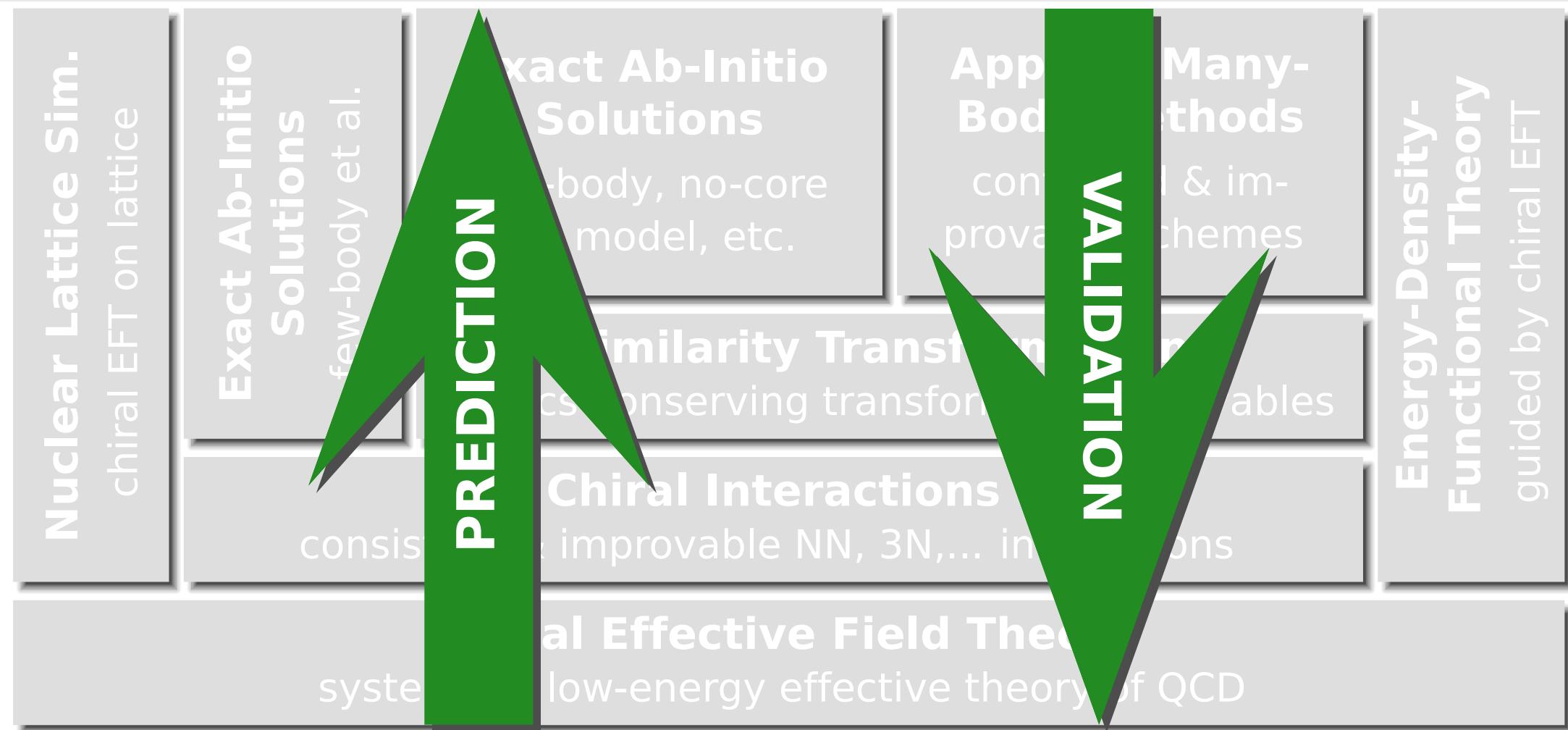
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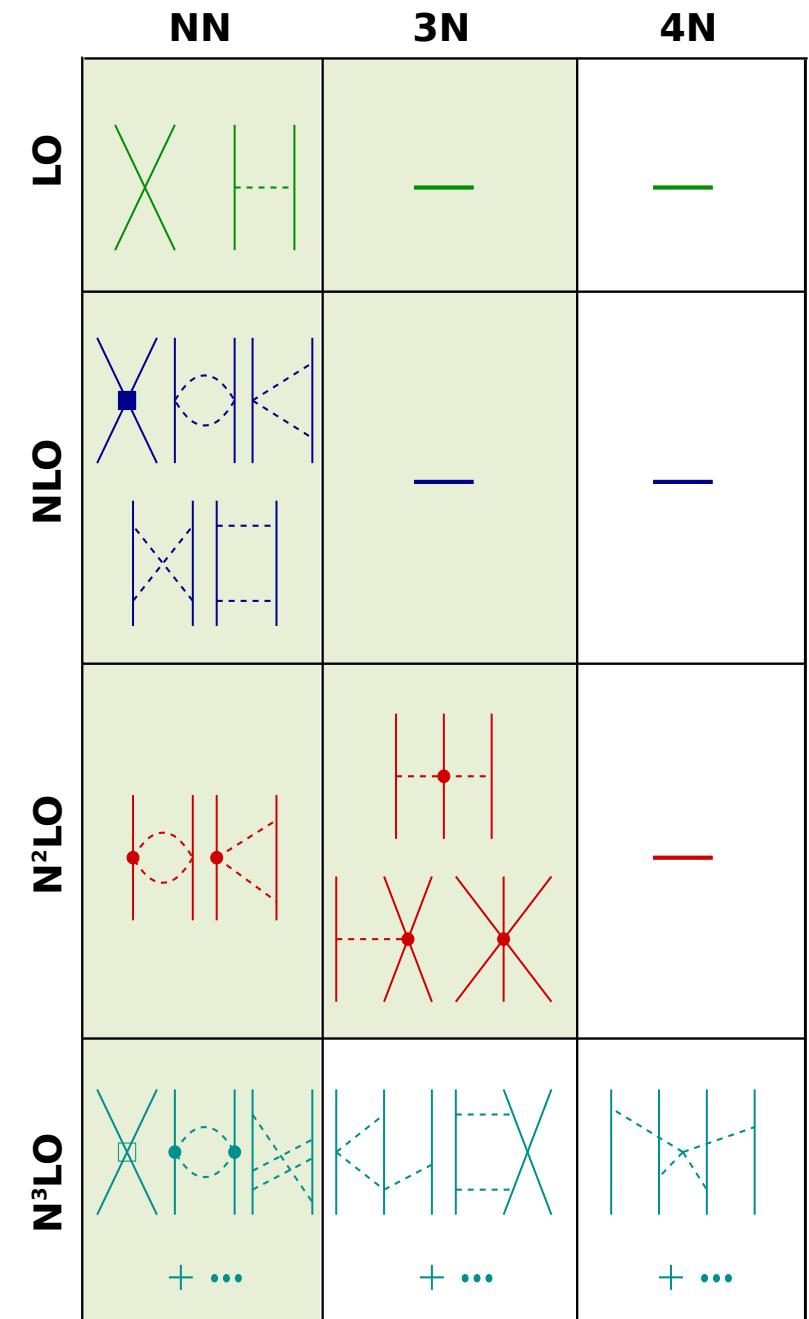
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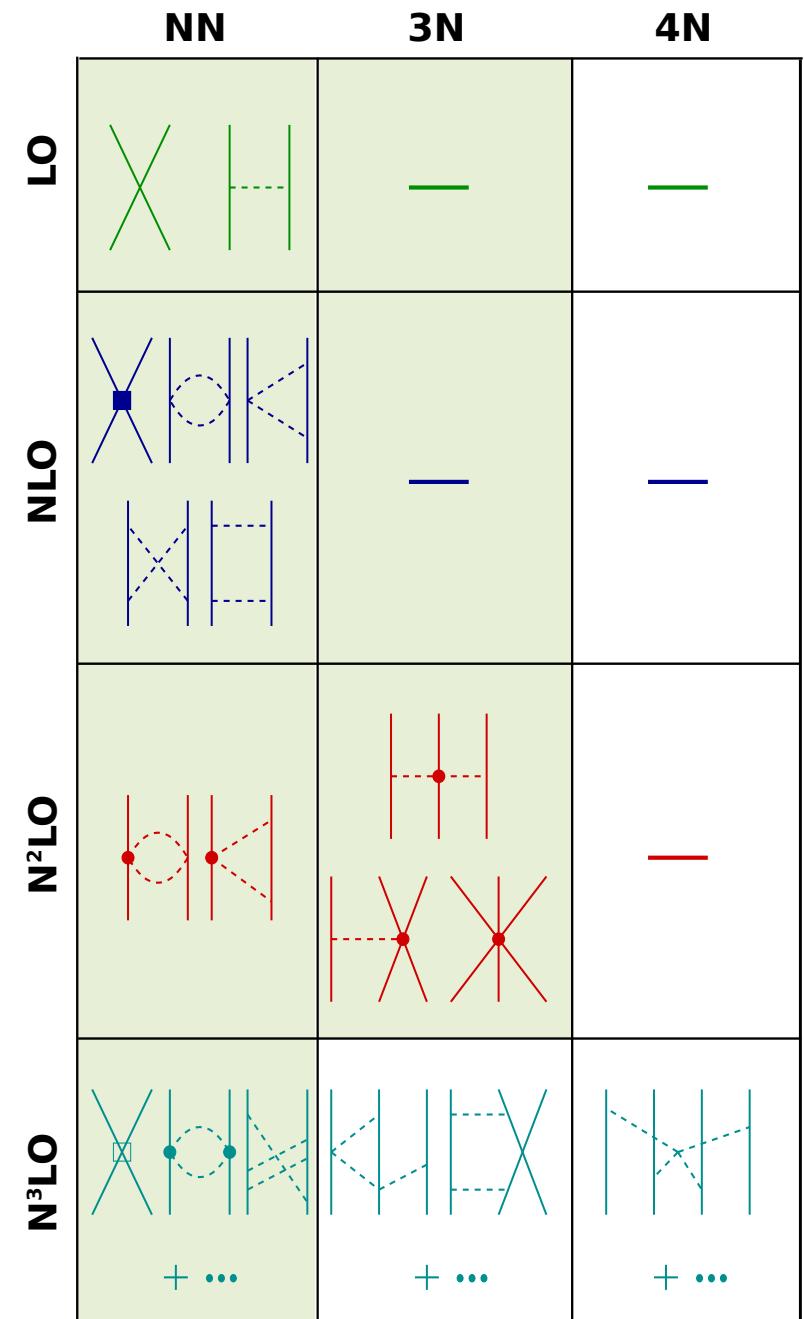
# Nuclear Interactions from Chiral EFT

- low-energy **effective field theory** for relevant degrees of freedom ( $\pi, N$ ) based on symmetries of QCD
- long-range **pion dynamics** explicitly
- short-range physics absorbed in **contact terms**, low-energy constants fitted to experiment ( $NN, \pi N, \dots$ )
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- hierarchy of **consistent NN, 3N, ... interactions** (plus currents)
- many **ongoing developments**
  - 3N interaction at  $N^3LO$
  - explicit inclusion of  $\Delta$ -resonance
  - formal issues: power counting, renormalization, cutoff choice,...



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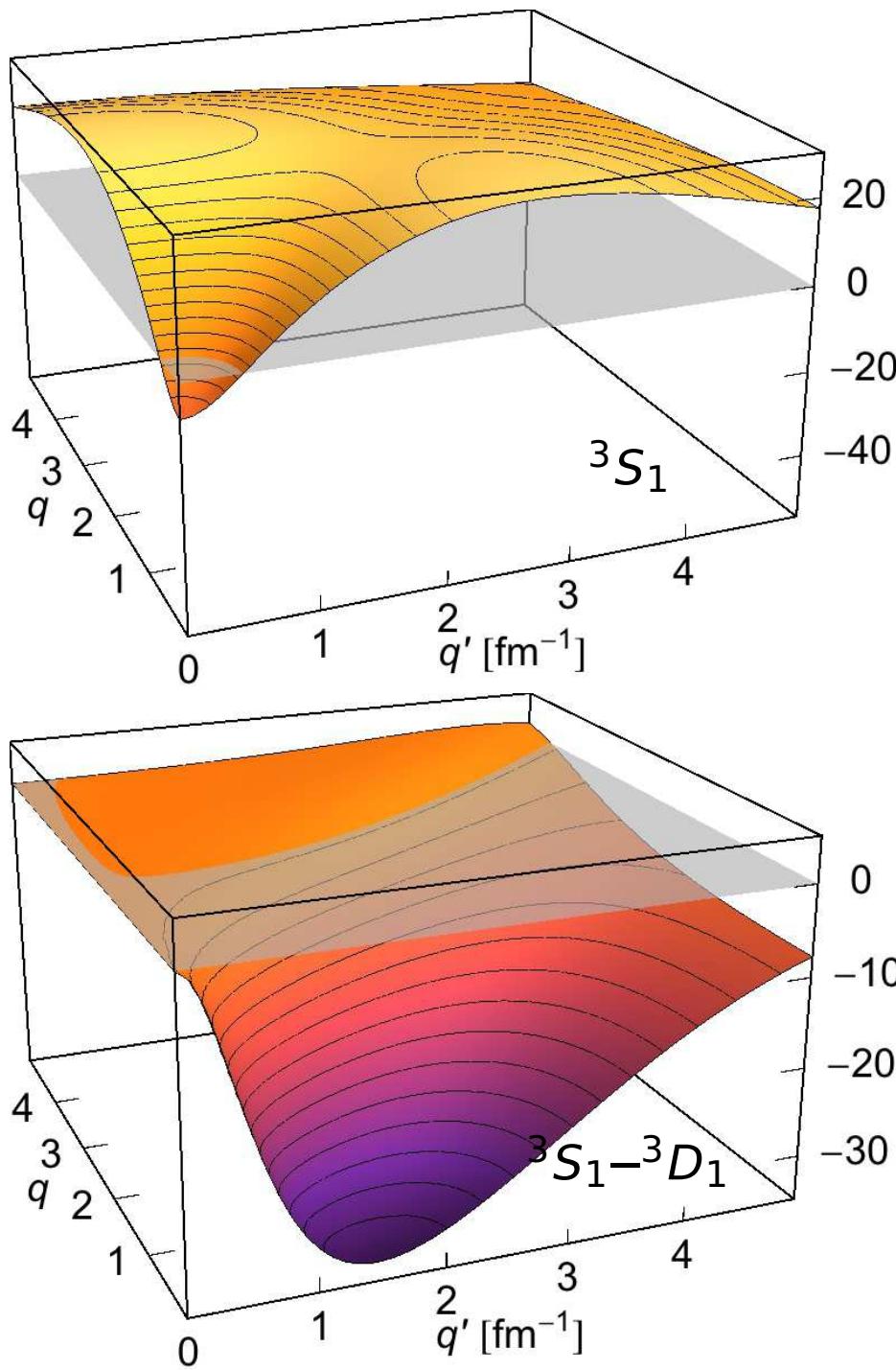
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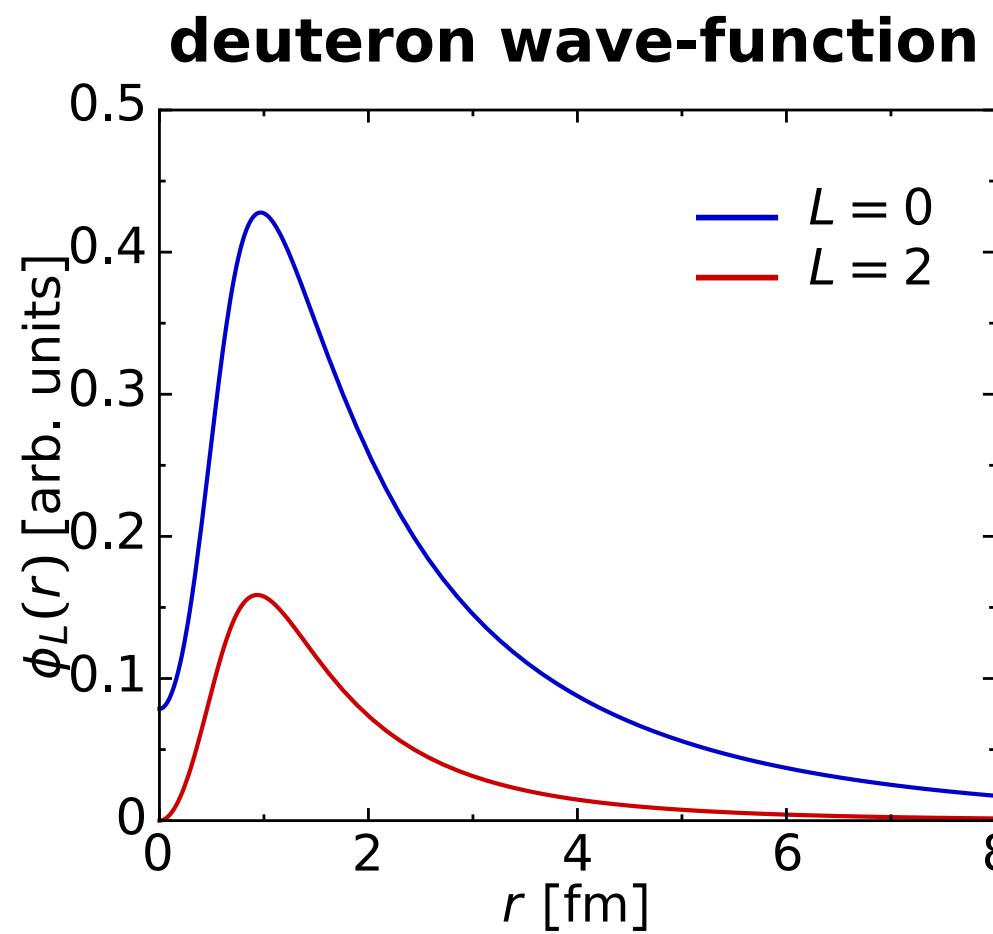
# Why Similarity Transformations?

momentum-space matrix elements



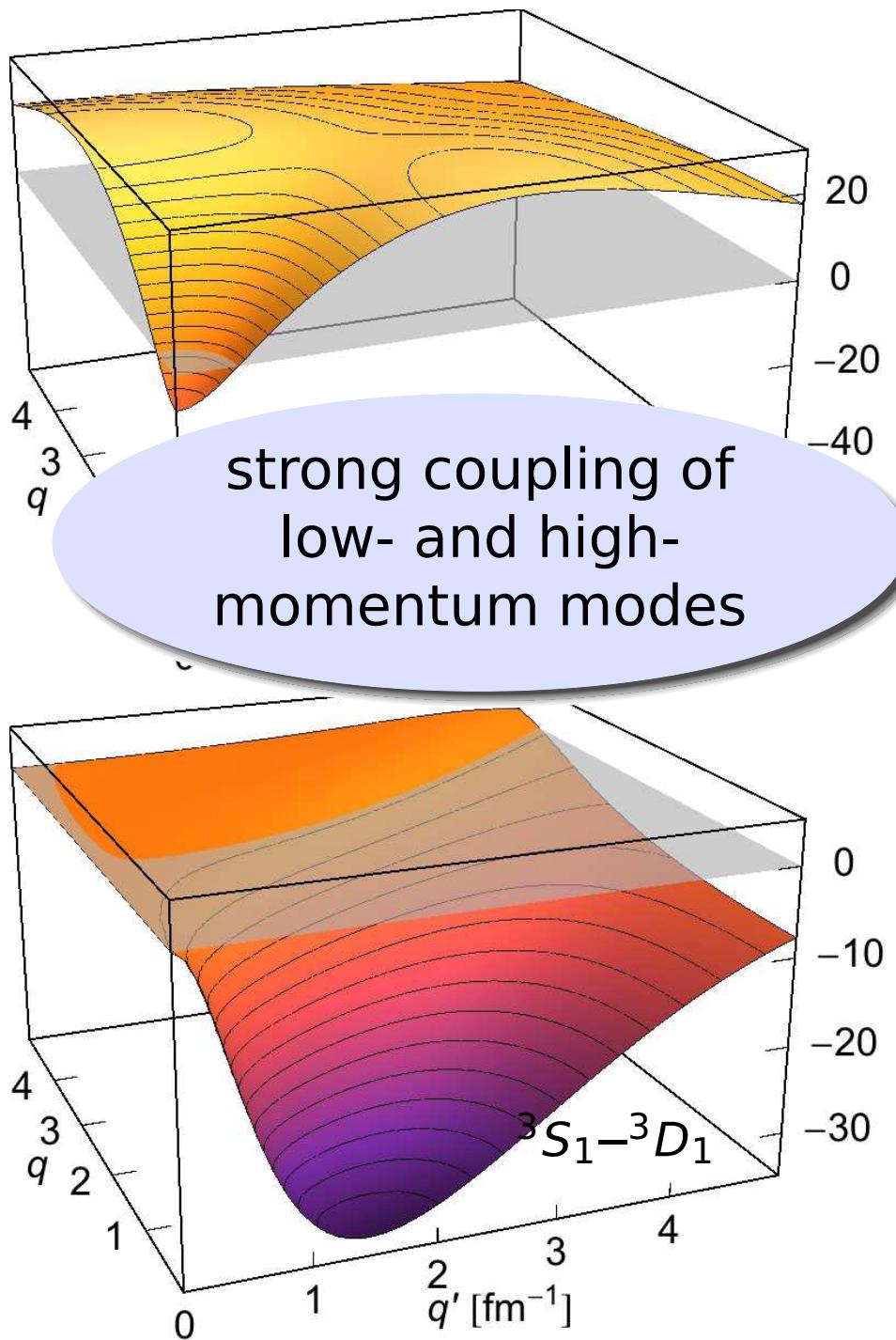
Argonne V18

$J^\pi = 1^+, T = 0$



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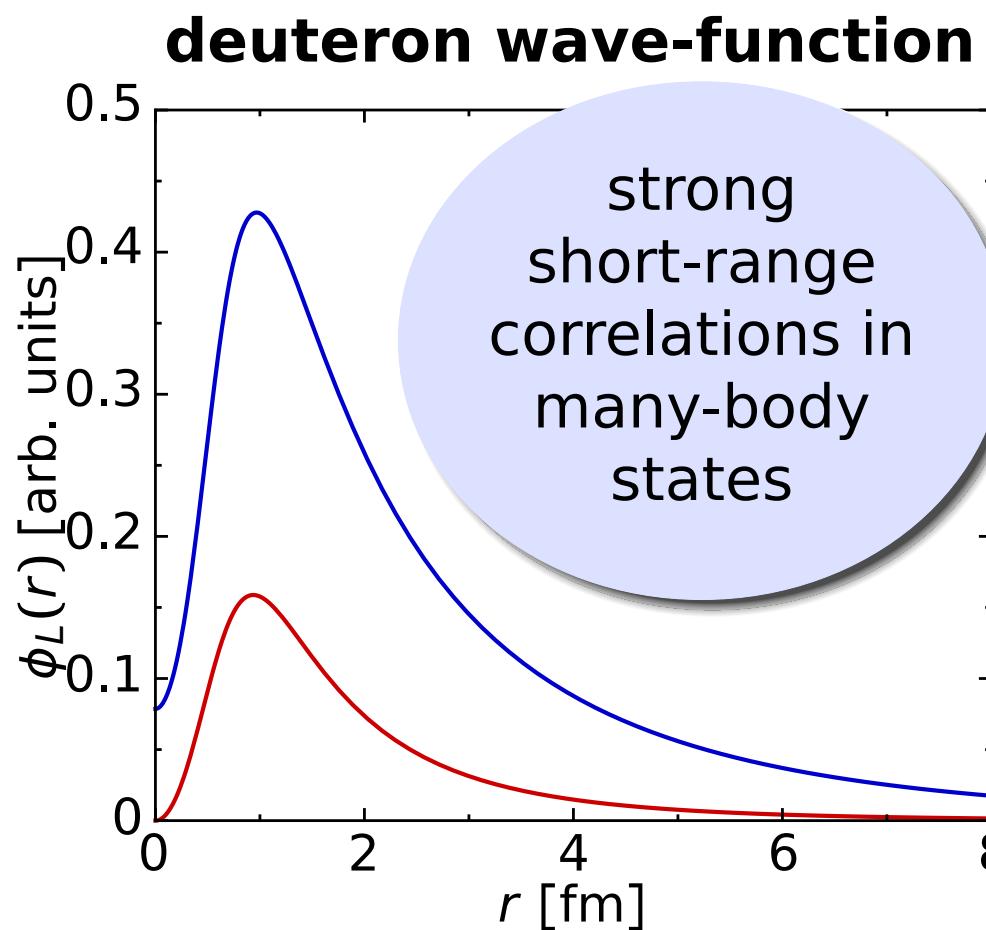


strong coupling of  
low- and high-  
momentum modes

$^3S_1 - ^3D_1$

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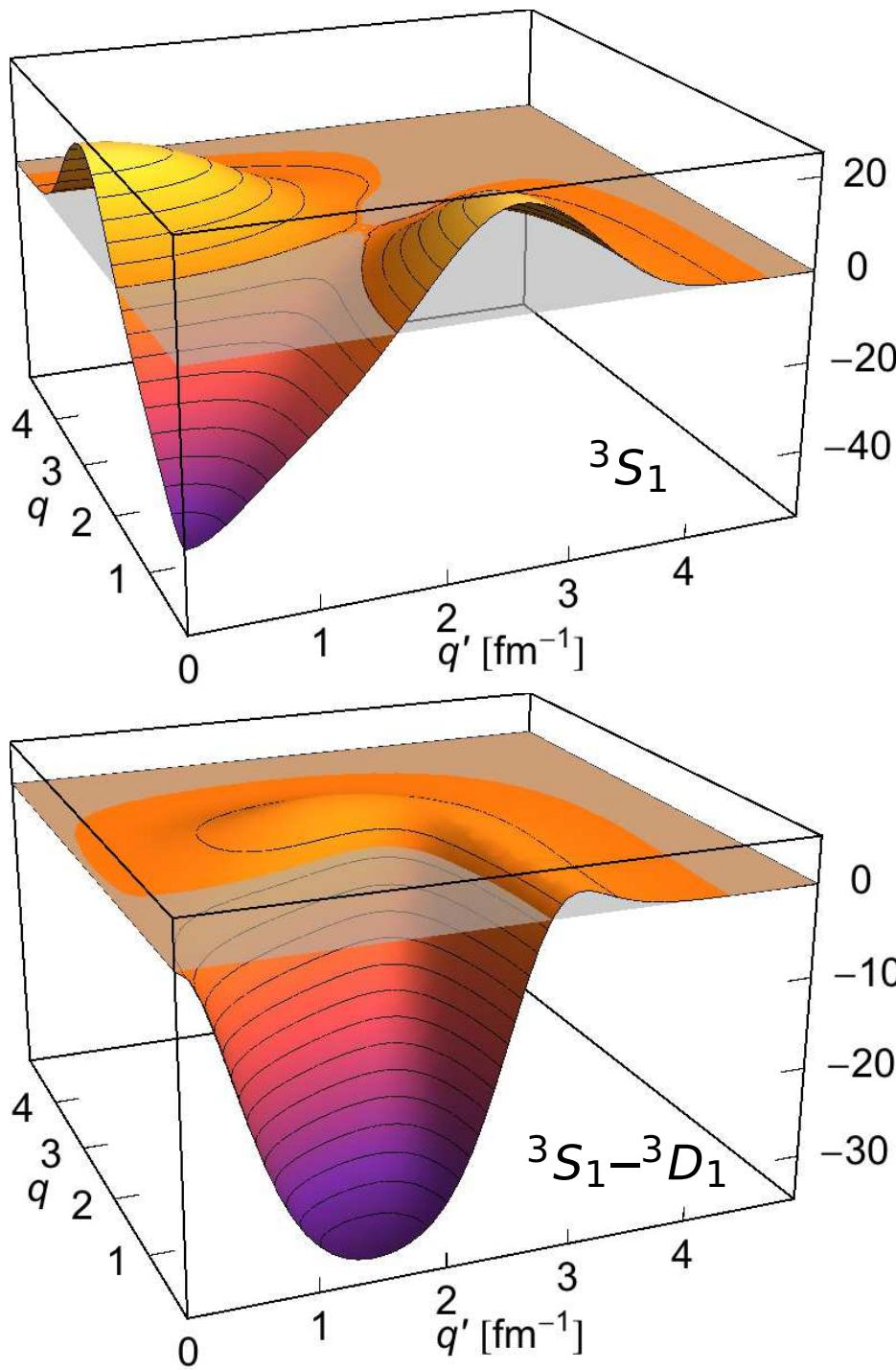


**deuteron wave-function**

strong  
short-range  
correlations in  
many-body  
states

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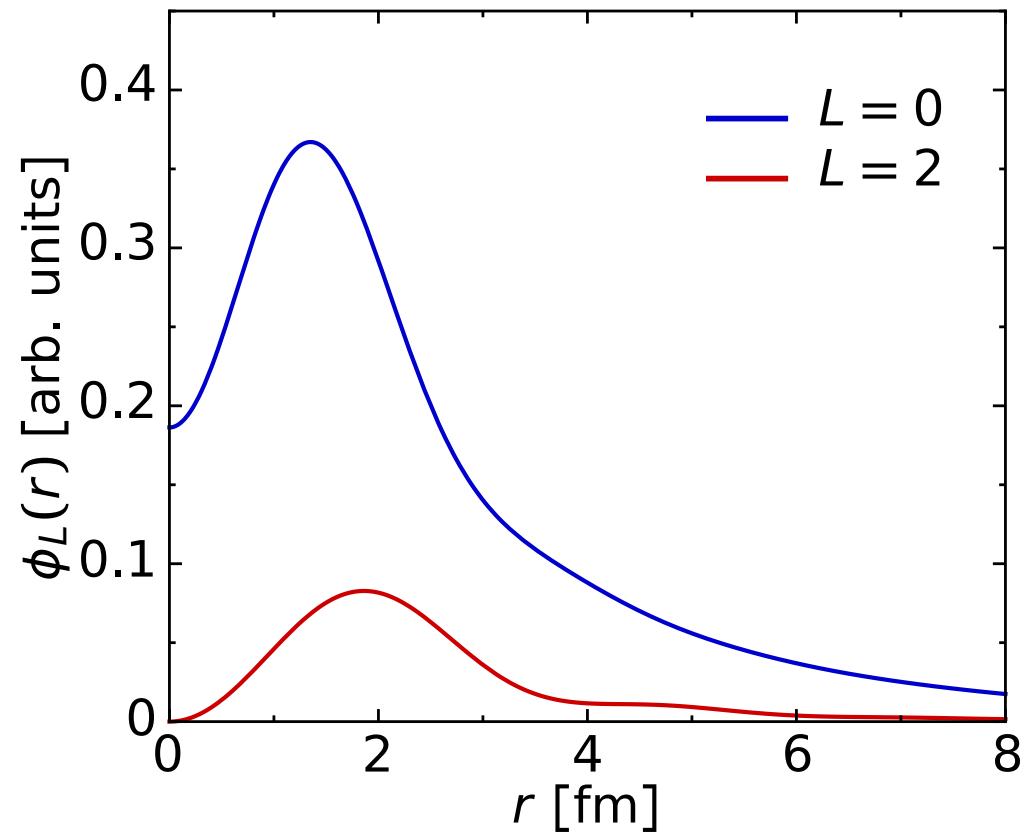


chiral N<sup>3</sup>LO

Entem & Machleidt, 500 MeV

$J^\pi = 1^+, T = 0$

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# Similarity Renormalization Group

continuous transformation driving  
**Hamiltonian to band-diagonal form**  
with respect to a chosen basis

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

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

- **evolution equations** for  $\tilde{H}_\alpha$  and  $U_\alpha$  depending on generator  $\eta_\alpha$

$$\frac{d}{d\alpha} \tilde{H}_\alpha = [\eta_\alpha, \tilde{H}_\alpha]$$

$$\frac{d}{d\alpha} U_\alpha = -U_\alpha \eta_\alpha$$

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

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

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simplicity and flexibility  
are great advantages of  
the SRG approach

other transformation  
approaches (UCOM,  $V_{\text{low}k}$ )  
follow as special cases

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

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

# SRG Evolution of Matrix Elements

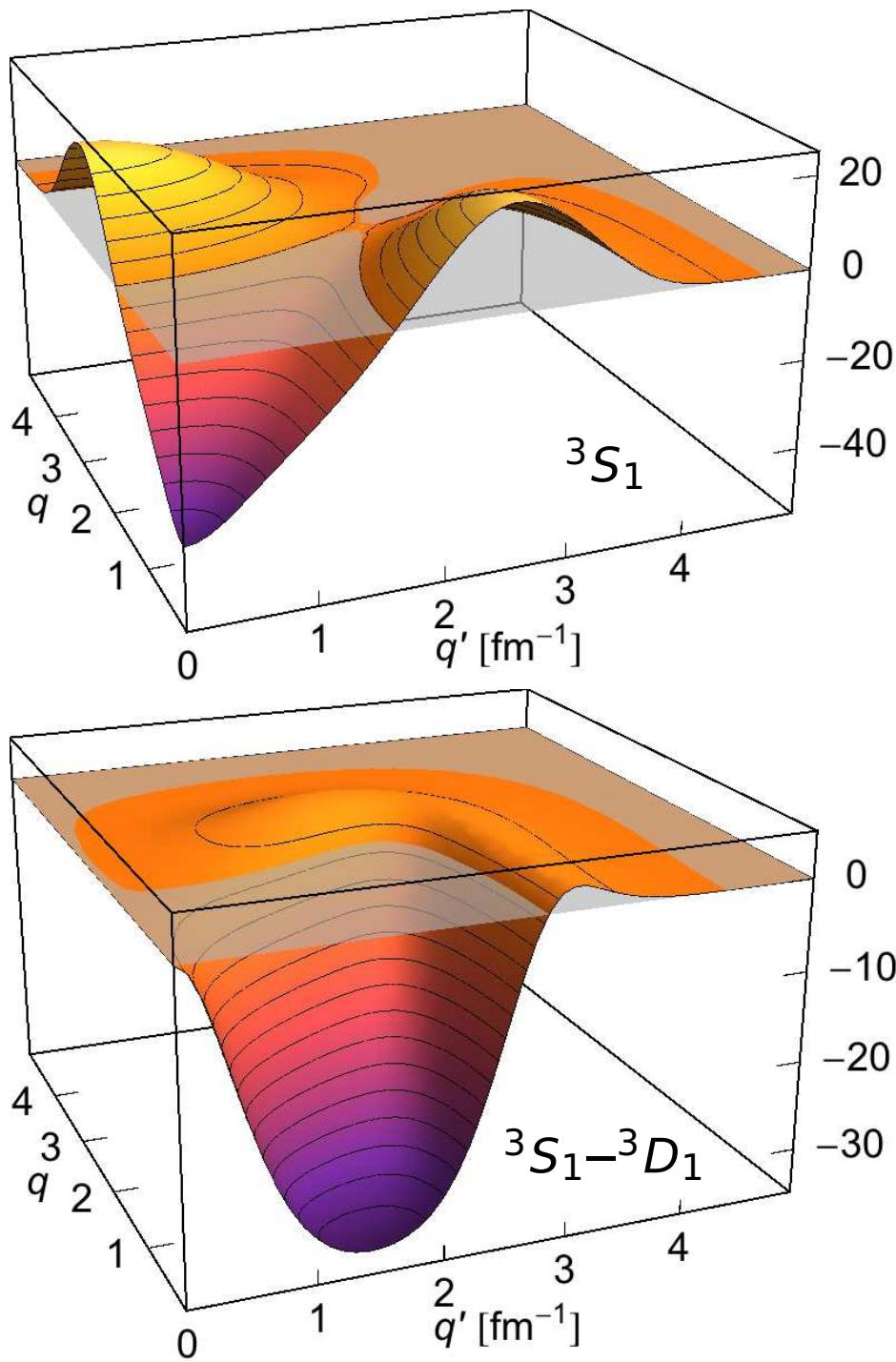
- convert Fock-space operator equations into **coupled evolution equations for matrix elements** in  $n$ -body Hilbert space
  - $n = 2$ : relative HO states  $|E(LS)J^\pi T\rangle$  or momentum states  $|q(LS)J^\pi T\rangle$
  - $n = 3$ : antisymmetrized Jacobi-coordinate HO states:  $|Eij^\pi T\rangle$
- system of **coupled evolution equations** for each  $(J^\pi T)$ -block

$$\frac{d}{d\alpha} \langle Eij^\pi T | \tilde{H}_\alpha | E'i'J^\pi T \rangle = (2\mu)^2 \sum_{E'', i''}^{E_{\text{SRG}}} \sum_{E''', i'''}^{E_{\text{SRG}}} [$$
$$\langle Eij^\pi T | T_{\text{int}} | E''i''J^\pi T \rangle \langle E''i''J^\pi T | \tilde{H}_\alpha | E'''i'''J^\pi T \rangle \langle E'''i'''J^\pi T | \tilde{H}_\alpha | E'i'J^\pi T \rangle$$
$$- 2 \langle Eij^\pi T | \tilde{H}_\alpha | E''i''J^\pi T \rangle \langle E''i''J^\pi T | T_{\text{int}} | E'''i'''J^\pi T \rangle \langle E'''i'''J^\pi T | \tilde{H}_\alpha | E'i'J^\pi T \rangle$$
$$+ \langle Eij^\pi T | \tilde{H}_\alpha | E''i''J^\pi T \rangle \langle E''i''J^\pi T | \tilde{H}_\alpha | E'''i'''J^\pi T \rangle \langle E'''i'''J^\pi T | T_{\text{int}} | E'i'J^\pi T \rangle]$$

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

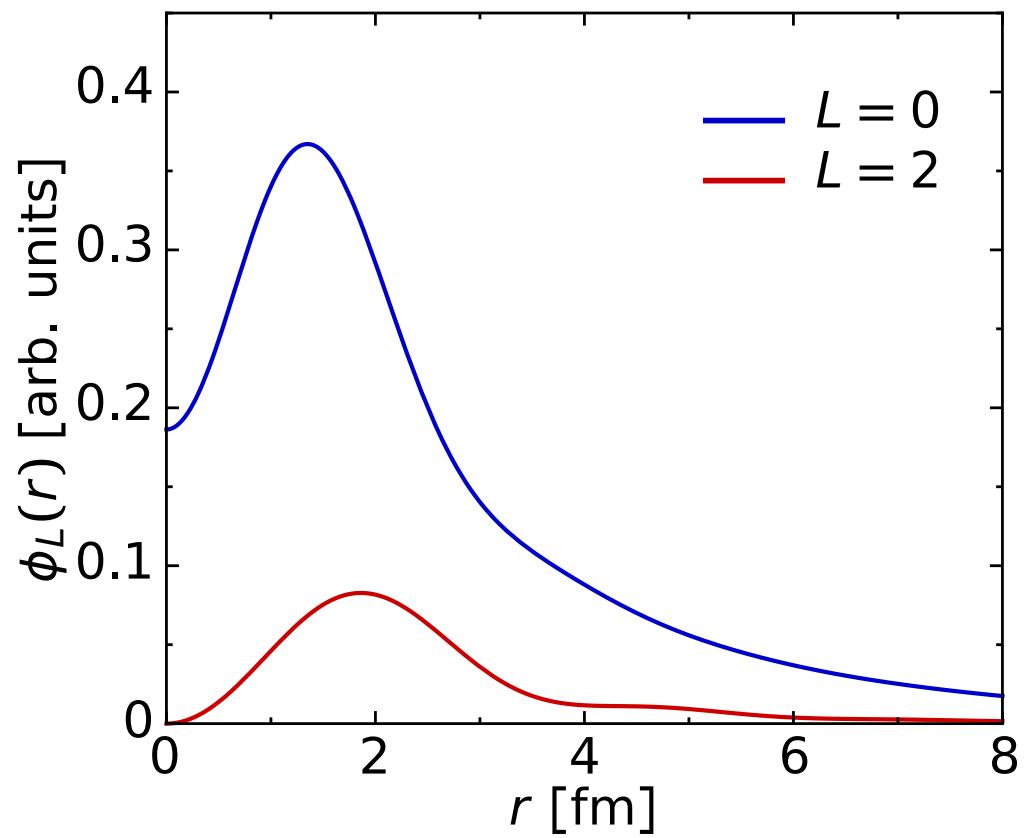
# SRG Evolution in Two-Body Space

momentum-space matrix elements



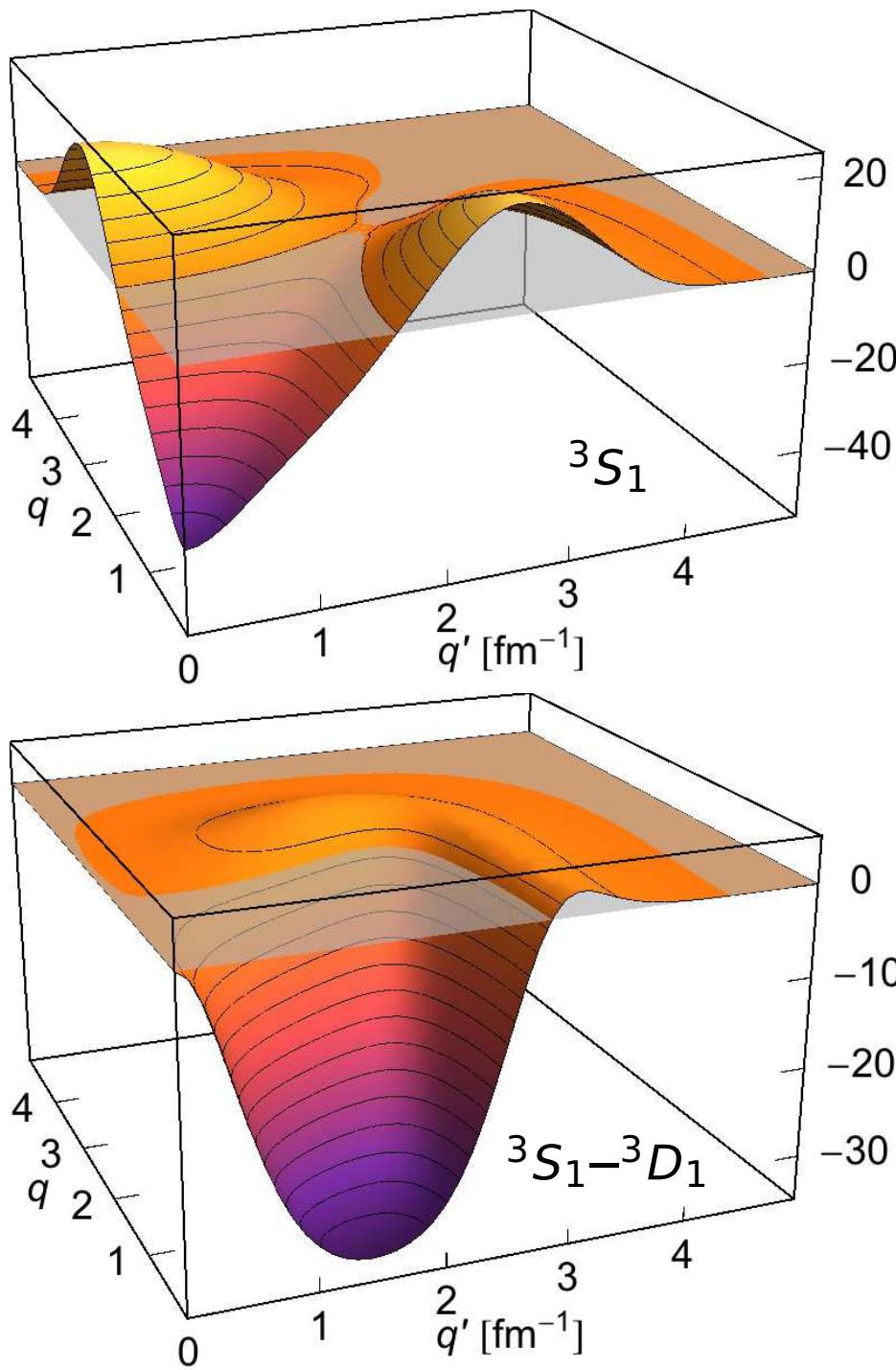
chiral NN  
Entem & Machleidt. N<sup>3</sup>LO, 500 MeV  
 $J^\pi = 1^+, T = 0$

**deuteron wave-function**



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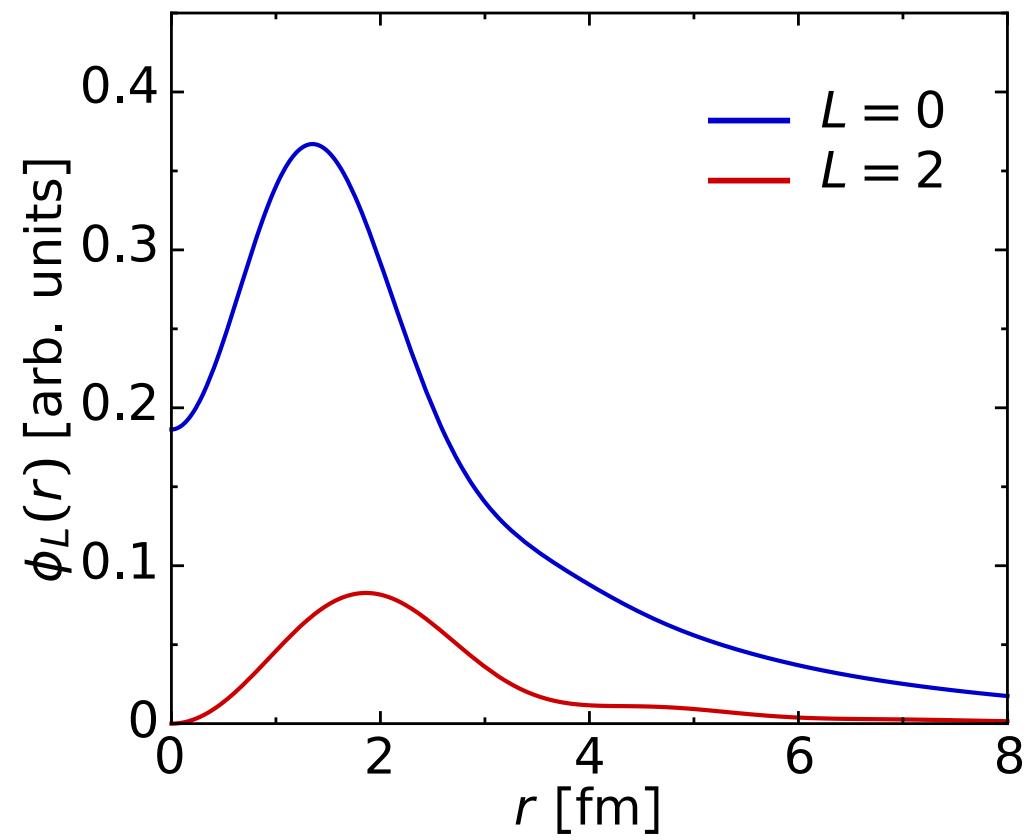


$$\alpha = 0.000 \text{ fm}^4$$

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

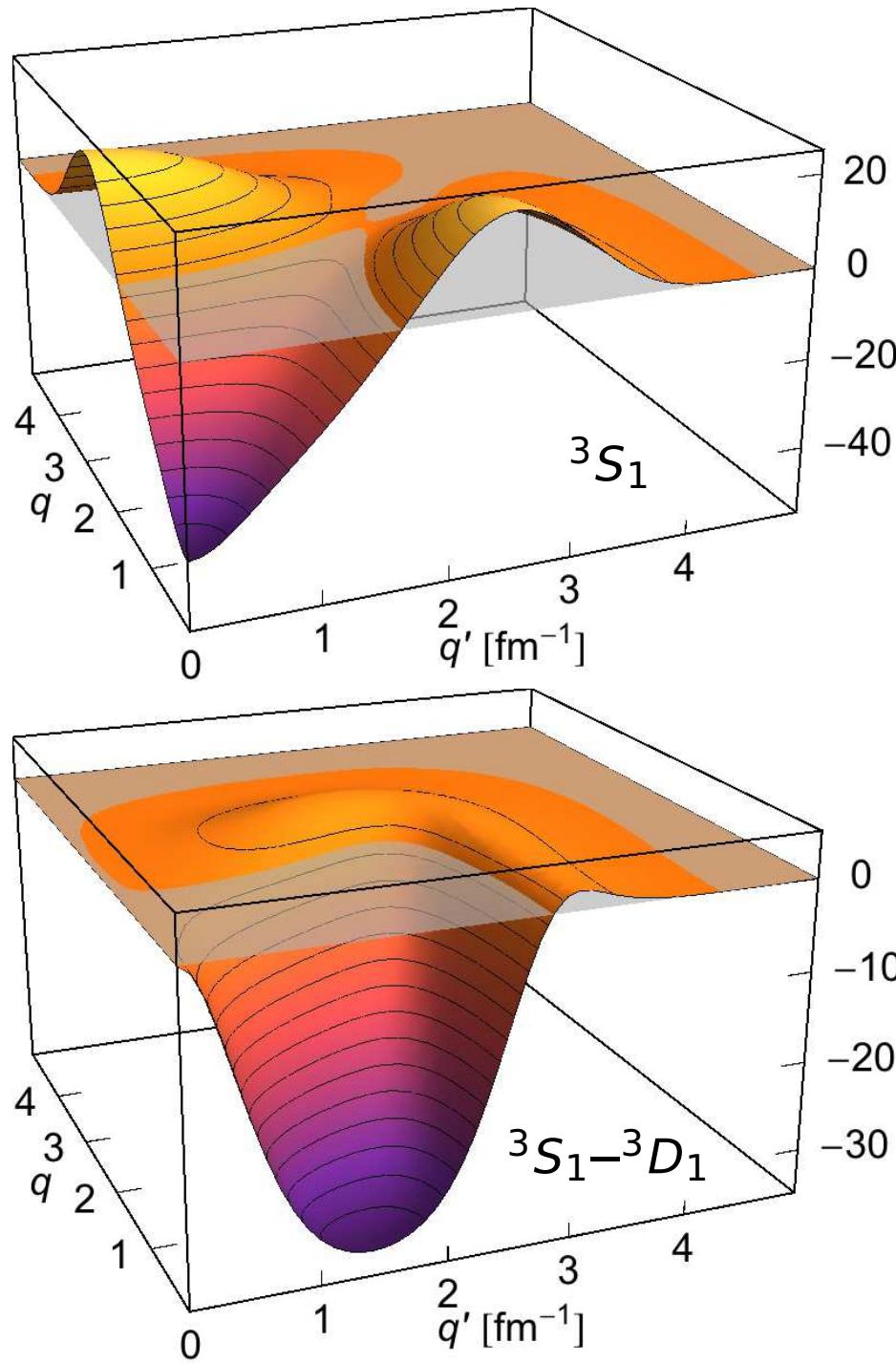
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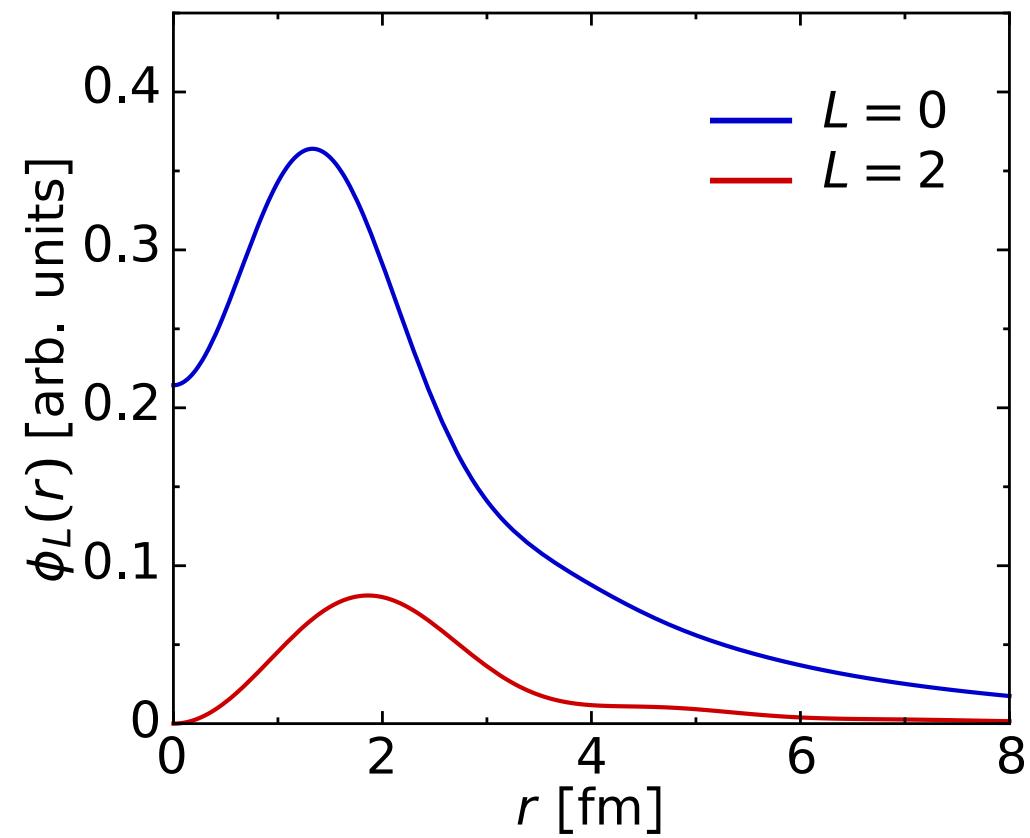


$$\alpha = 0.002 \text{ fm}^4$$

$$\Lambda = 4.73 \text{ fm}^{-1}$$

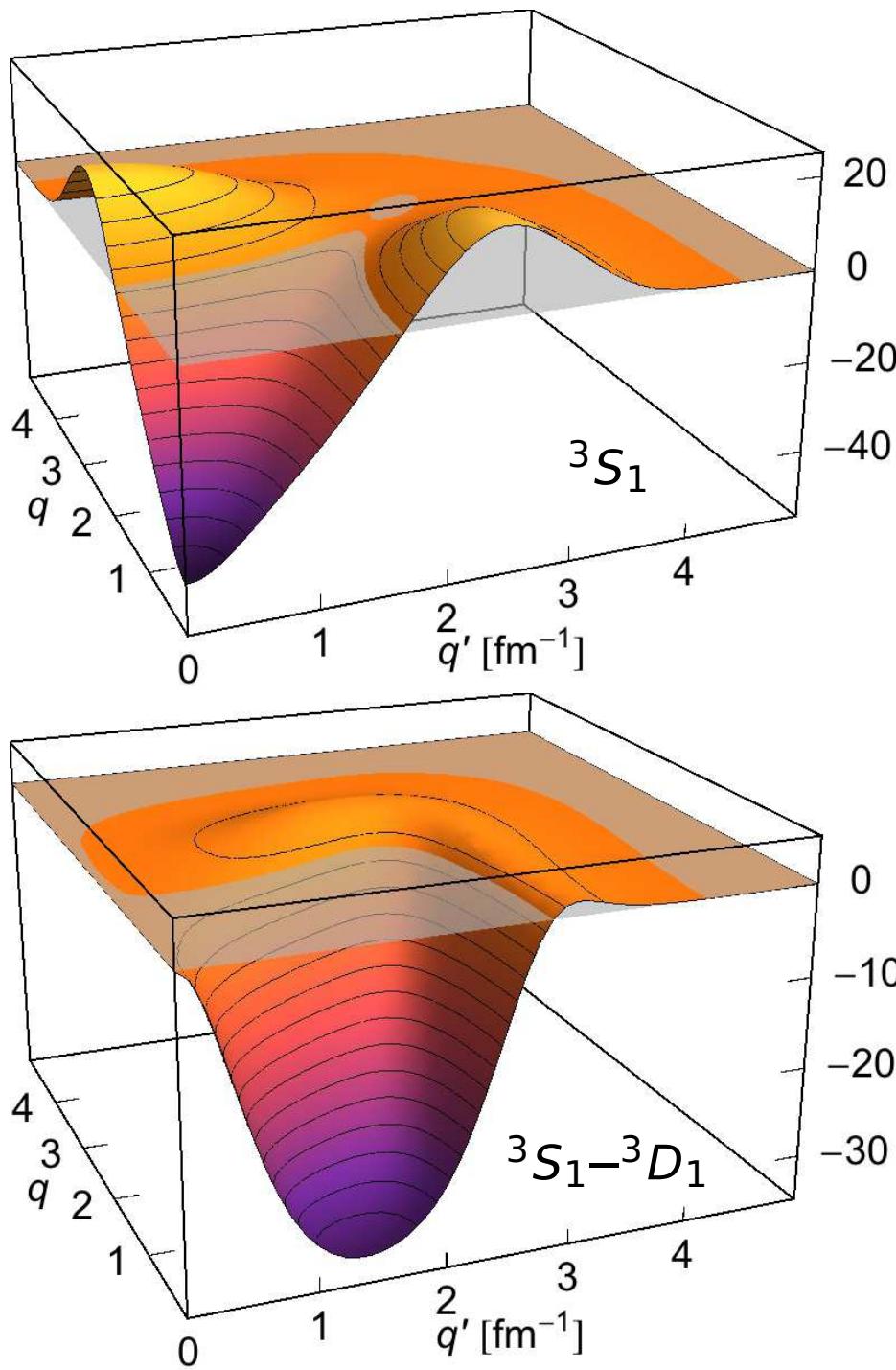
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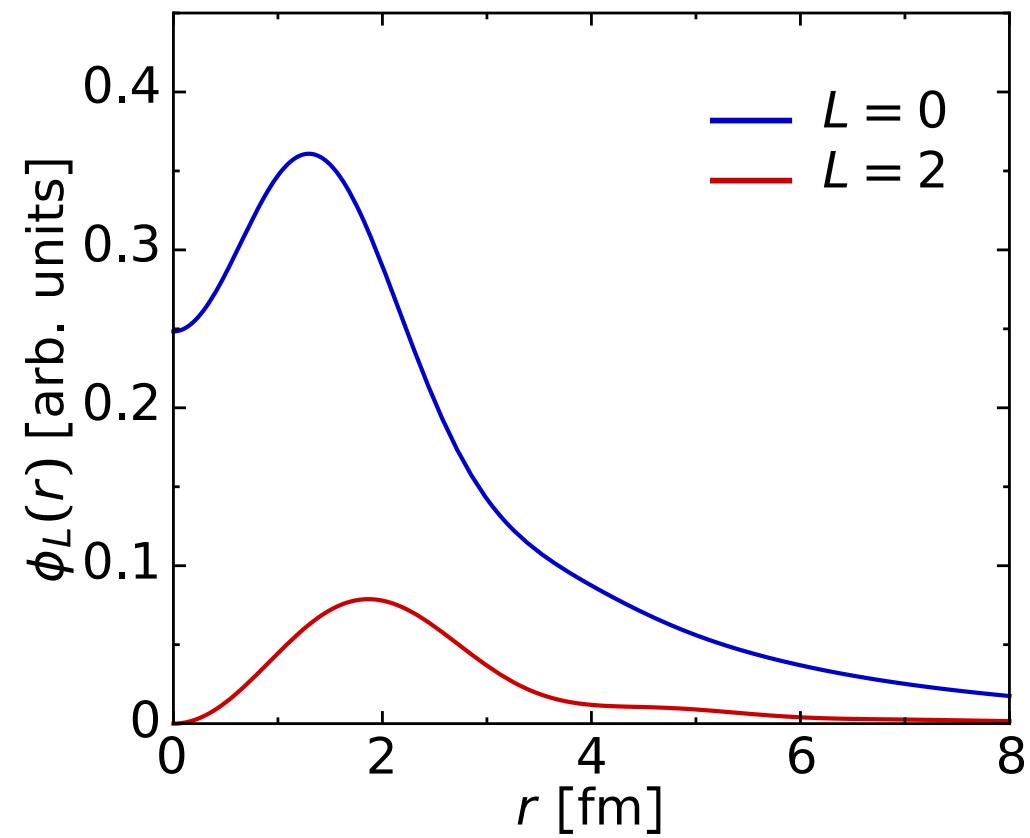


$$\alpha = 0.005 \text{ fm}^4$$

$$\Lambda = 3.76 \text{ fm}^{-1}$$

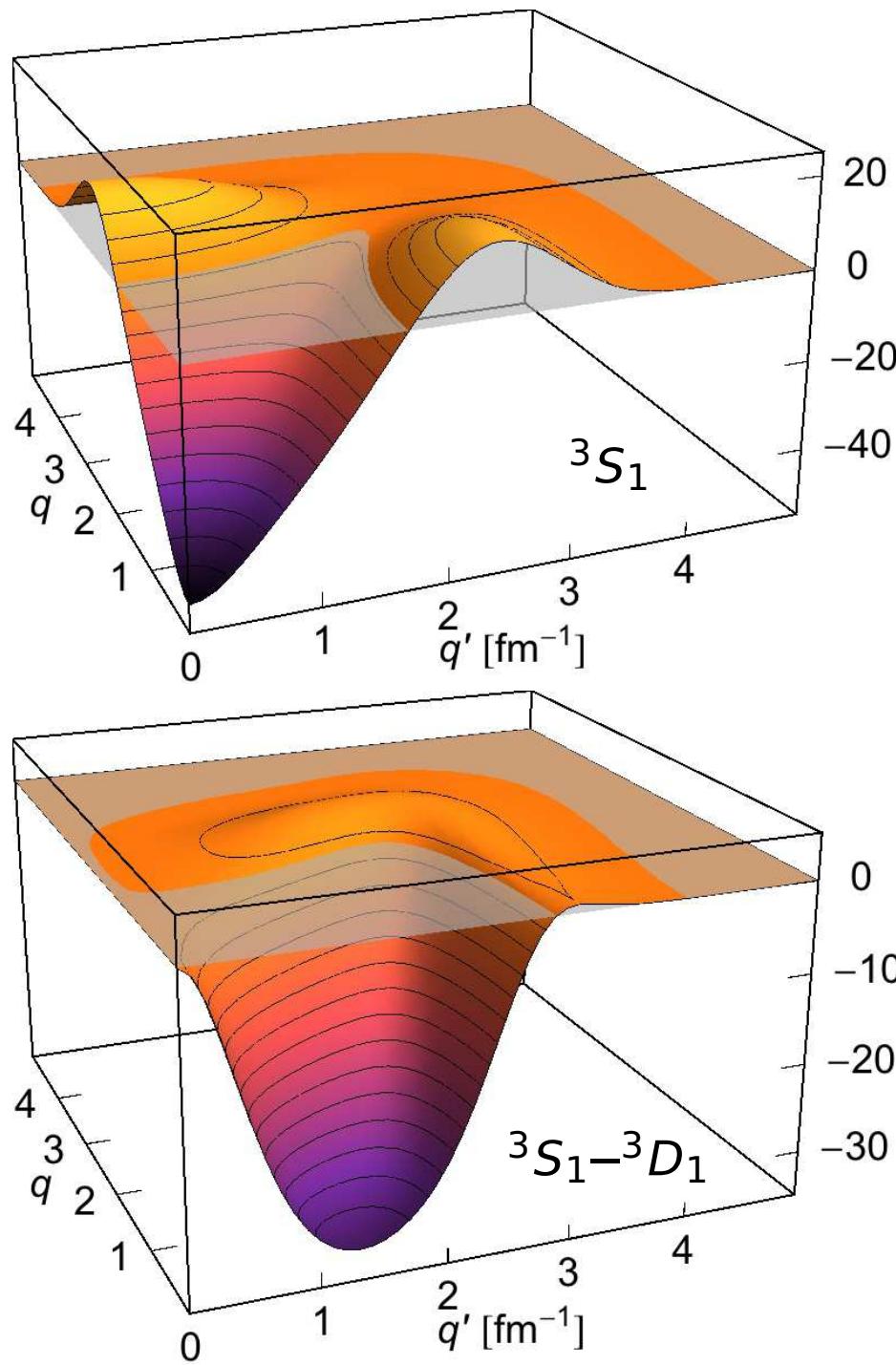
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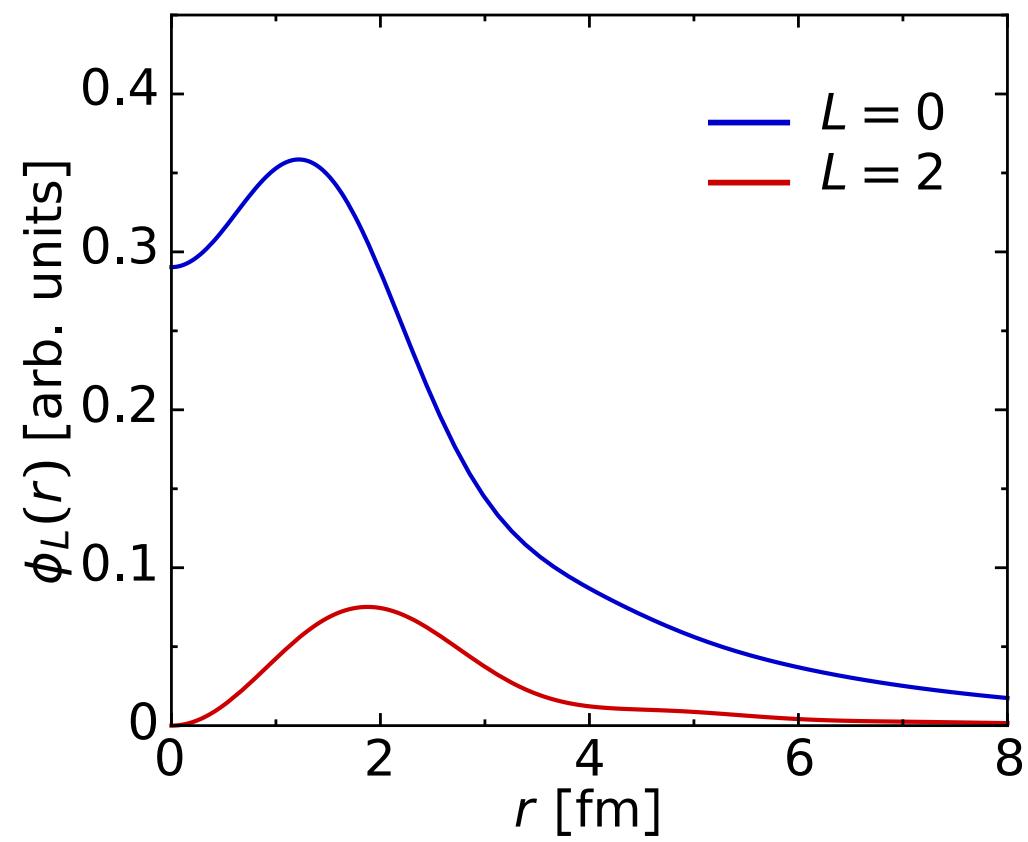


$$\alpha = 0.010 \text{ fm}^4$$

$$\Lambda = 3.16 \text{ fm}^{-1}$$

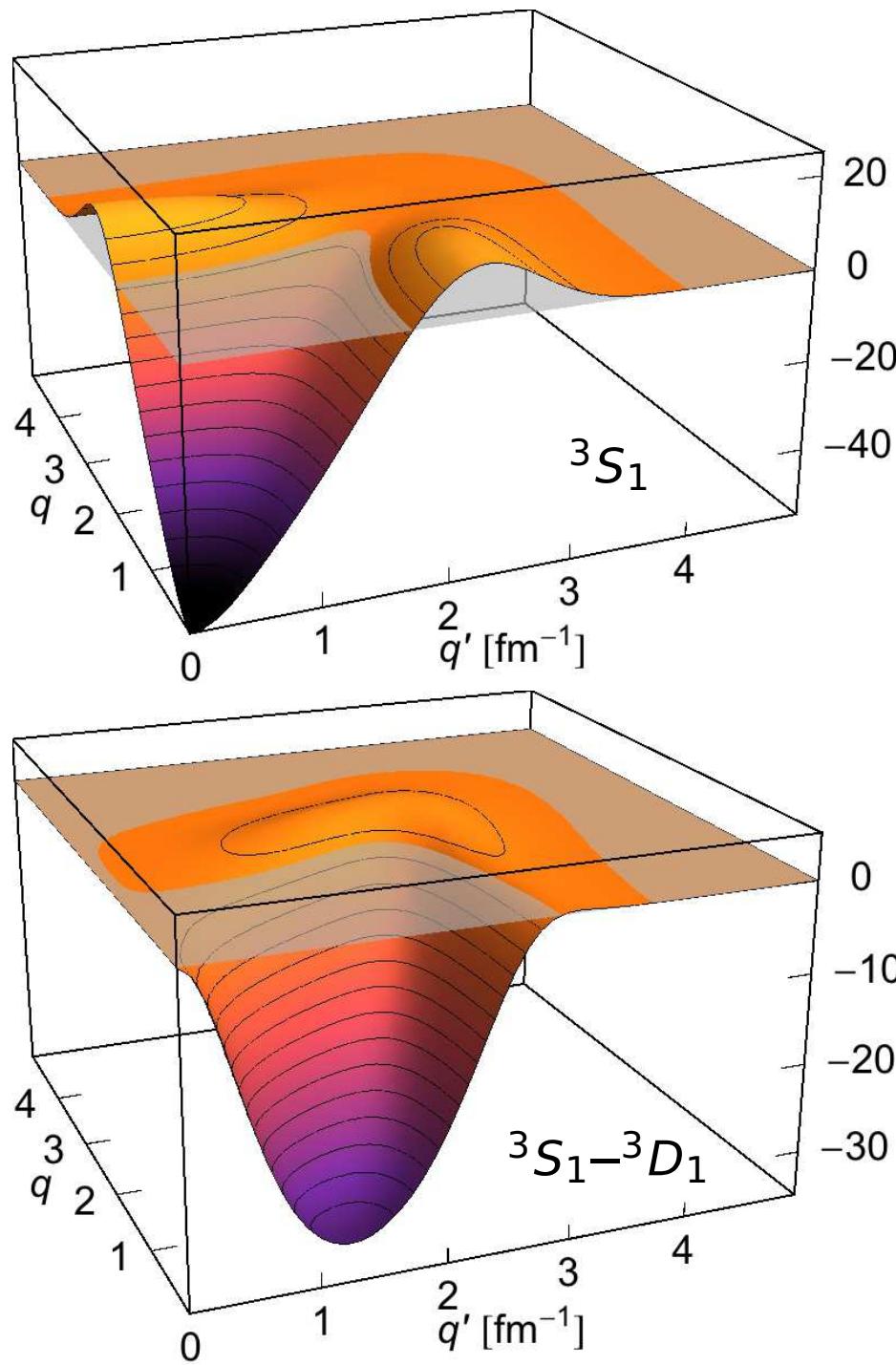
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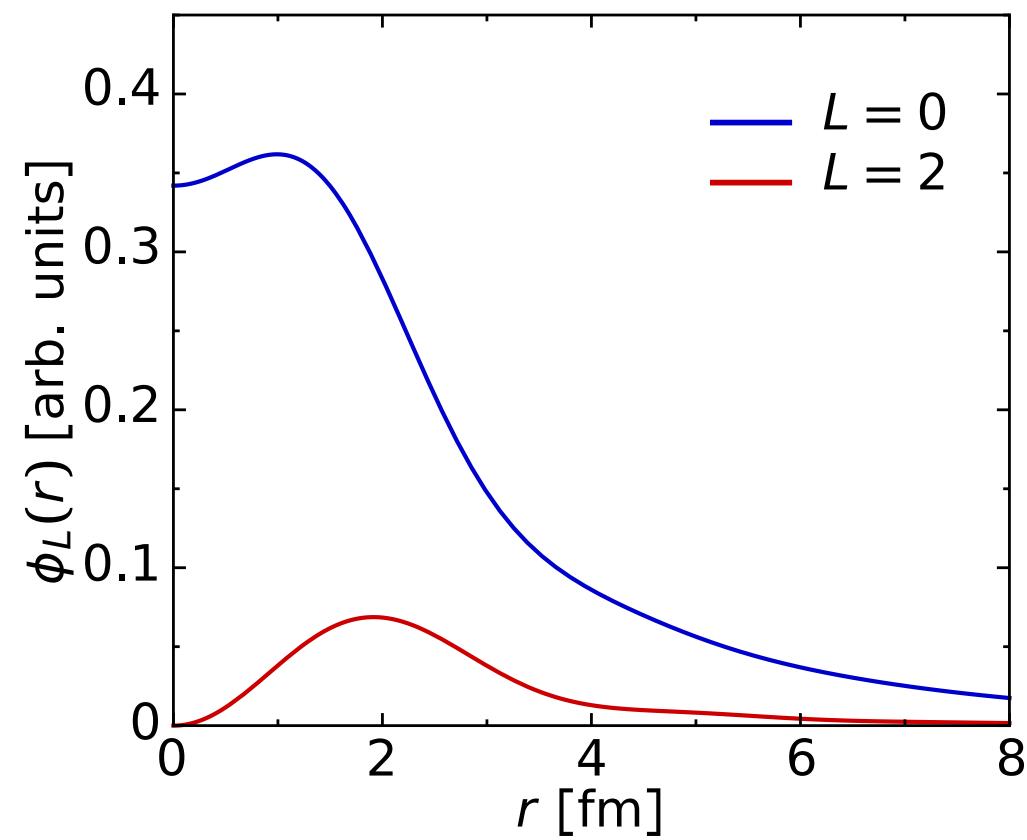


$$\alpha = 0.020 \text{ fm}^4$$

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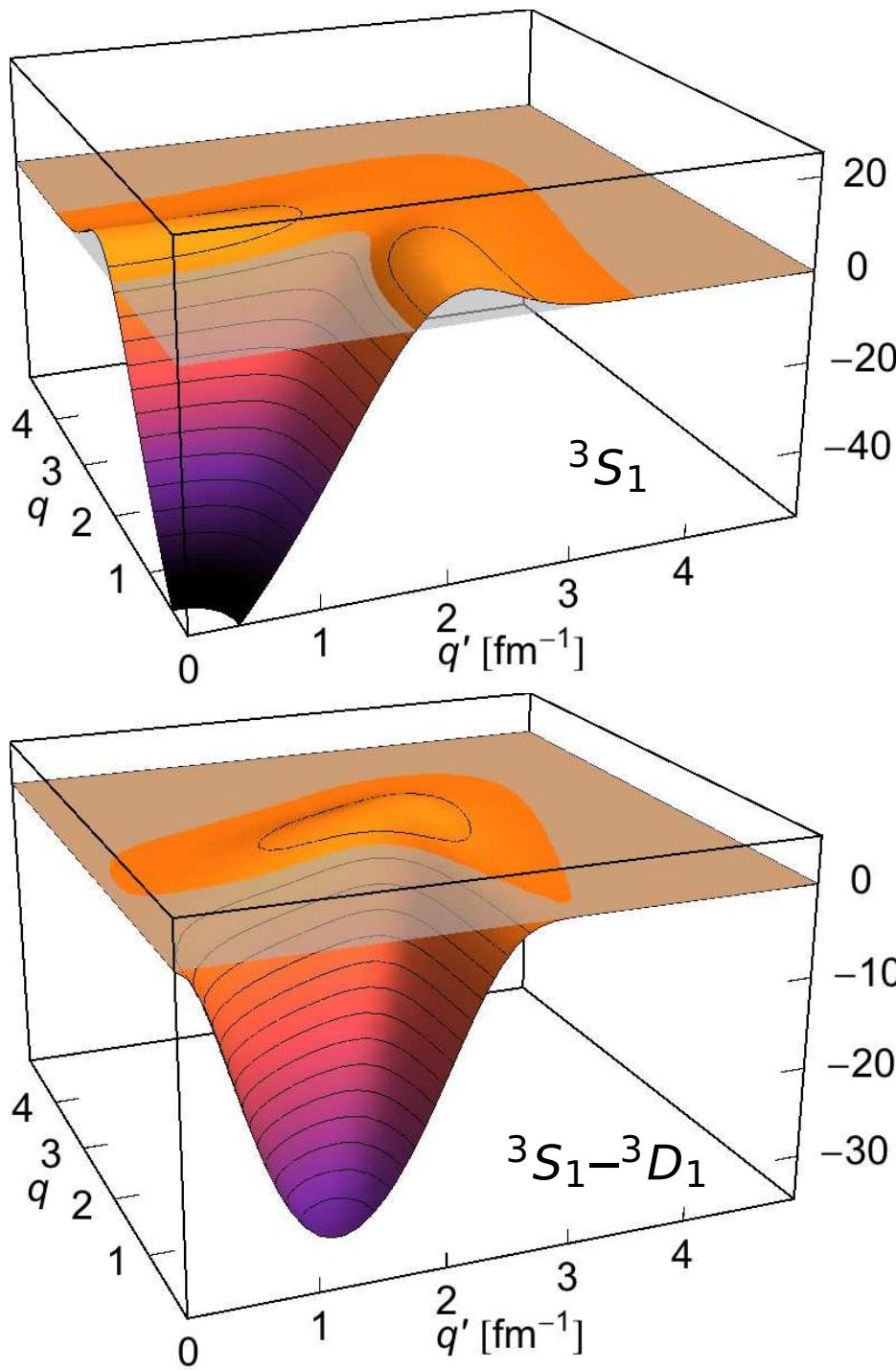
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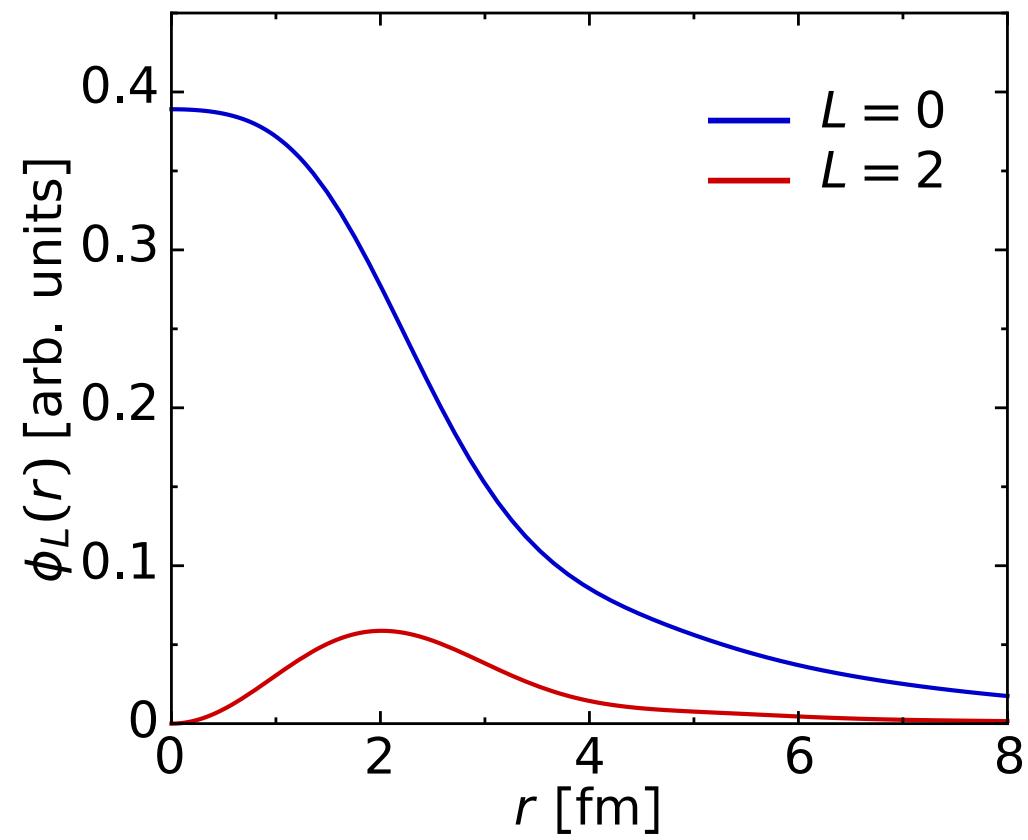


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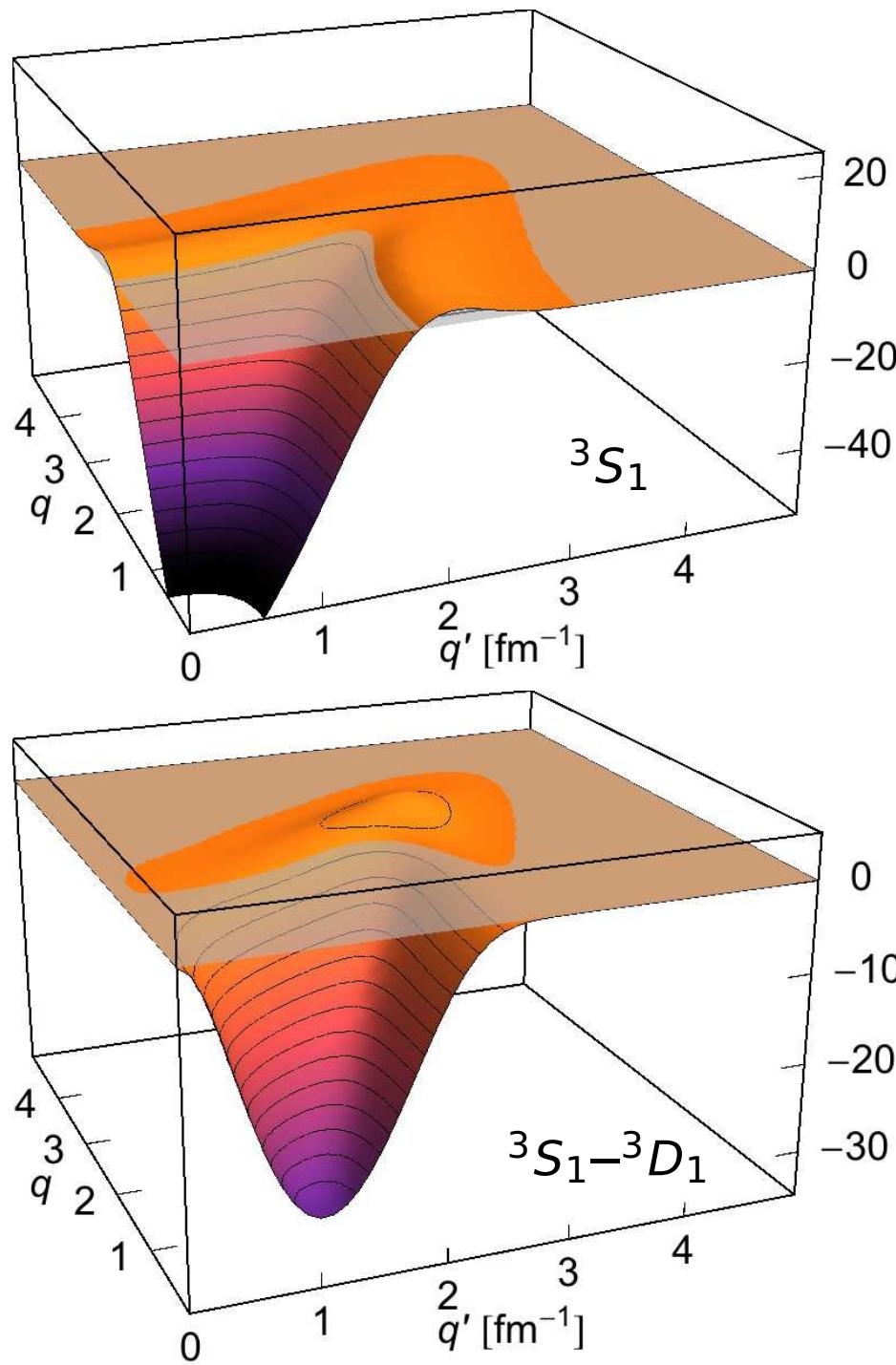
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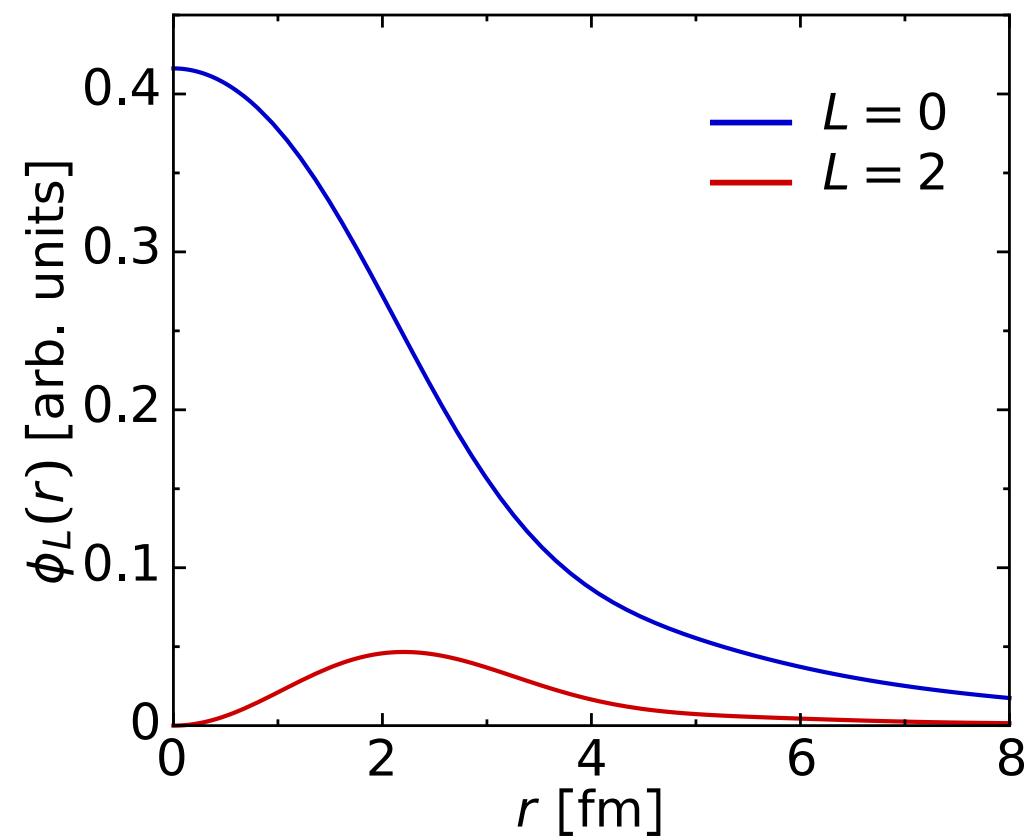


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$$\Lambda = 1.88 \text{ fm}^{-1}$$

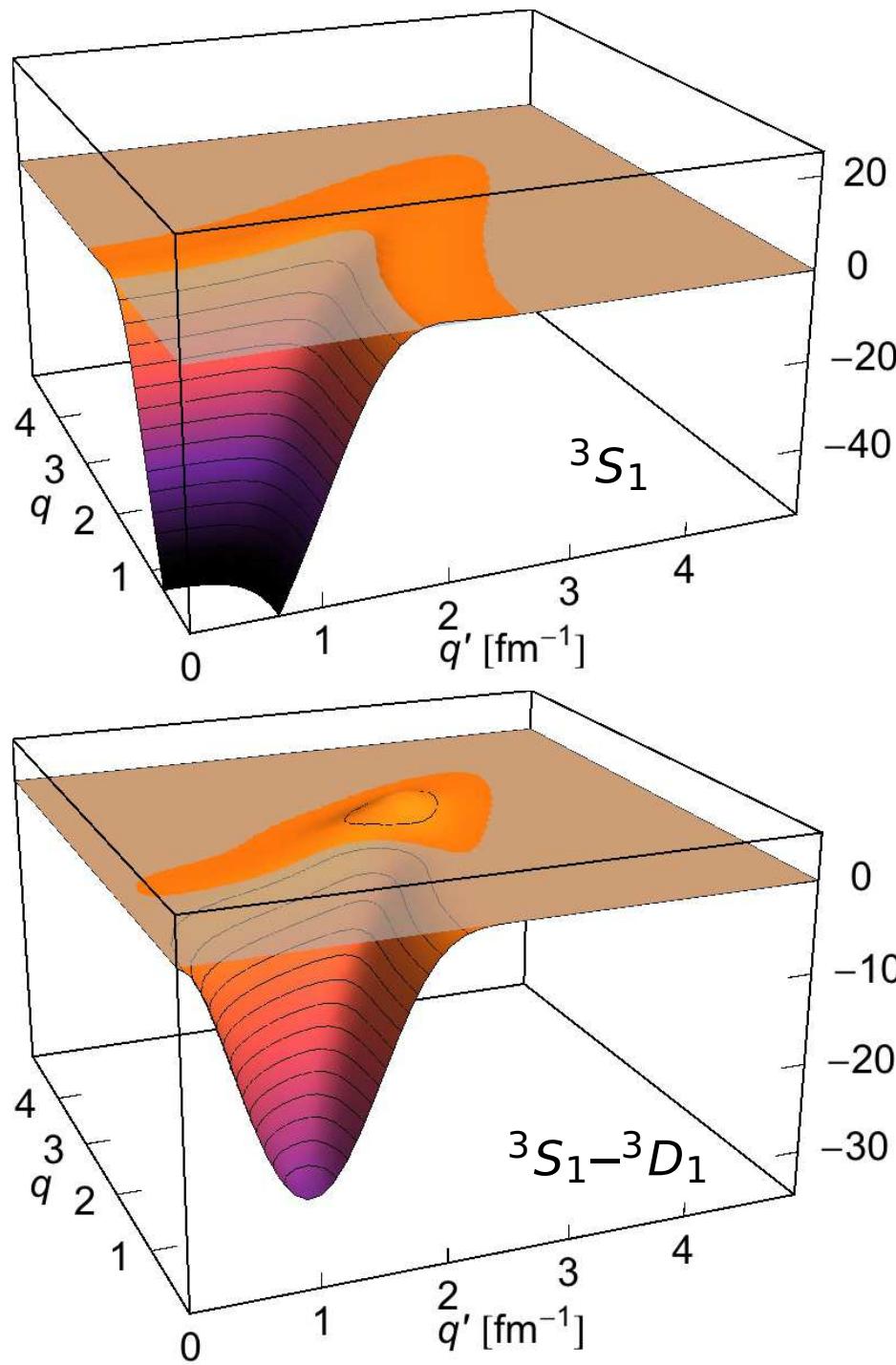
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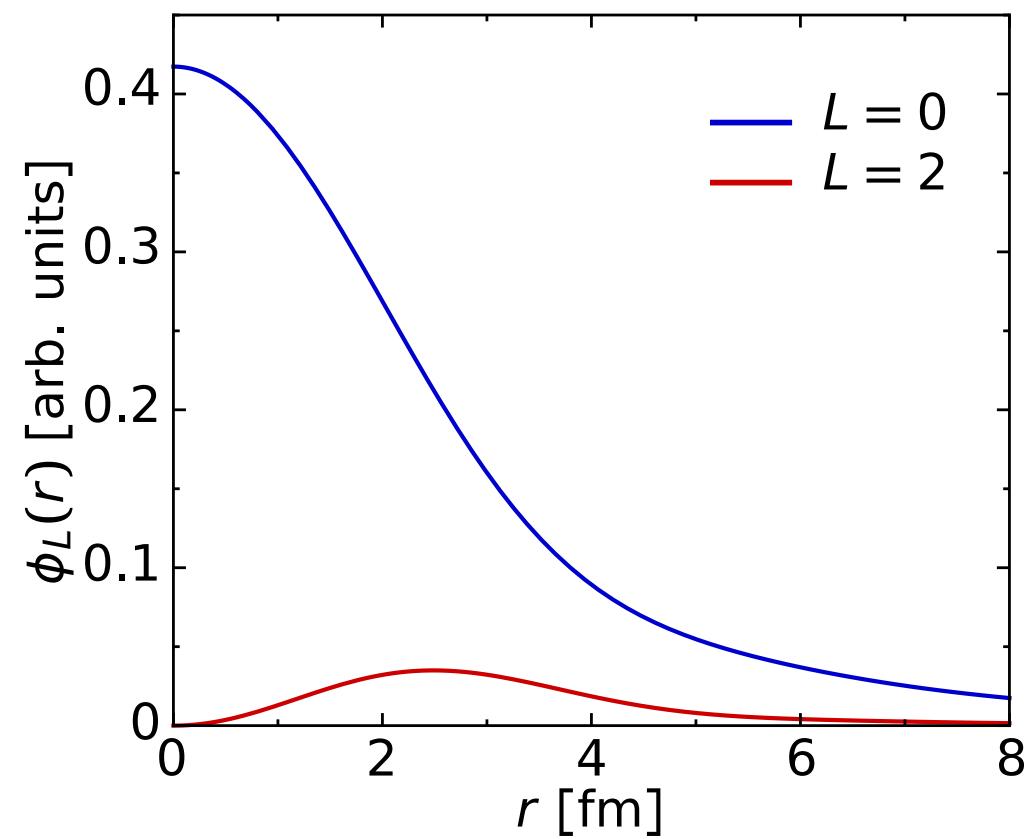


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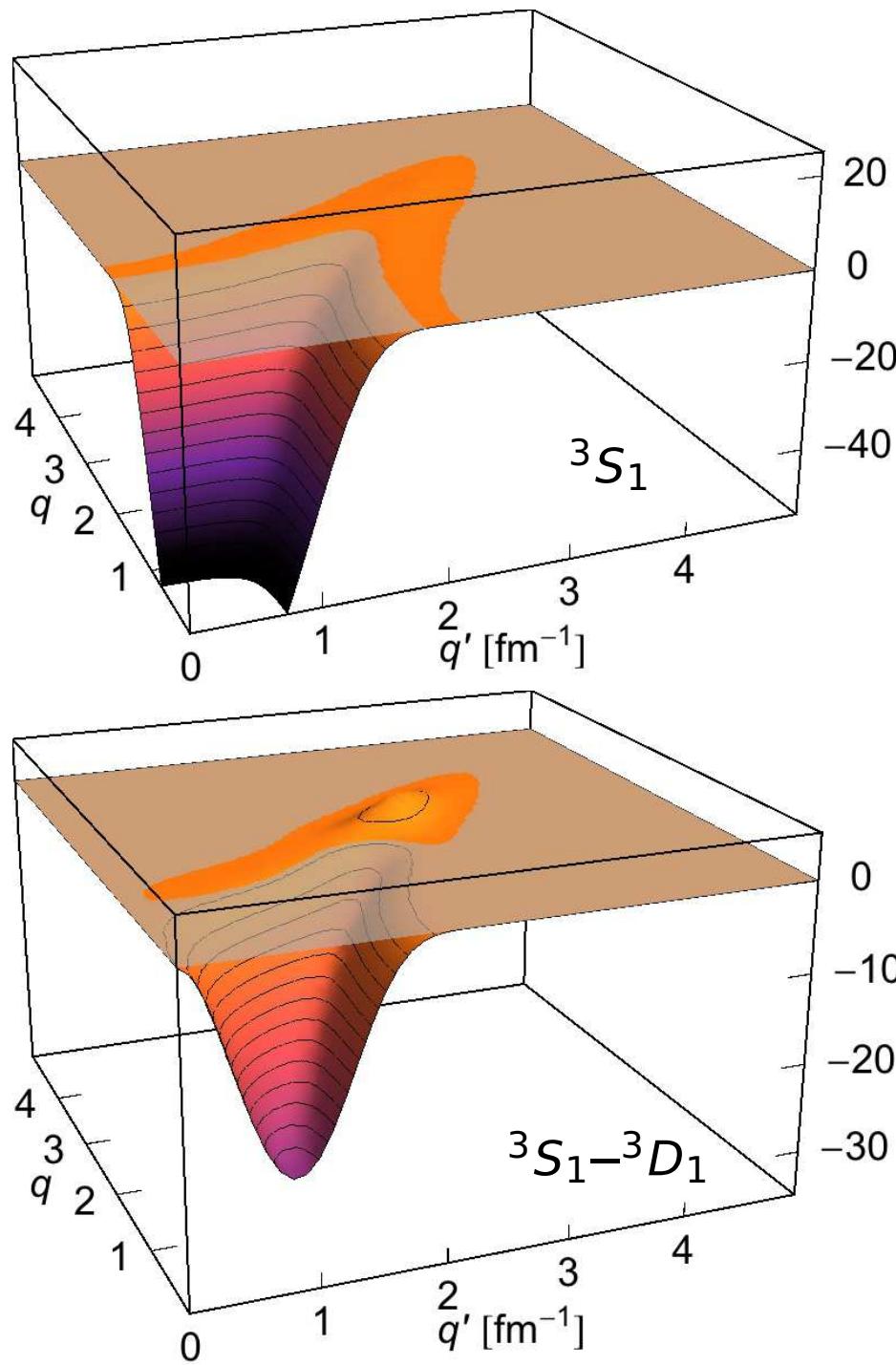
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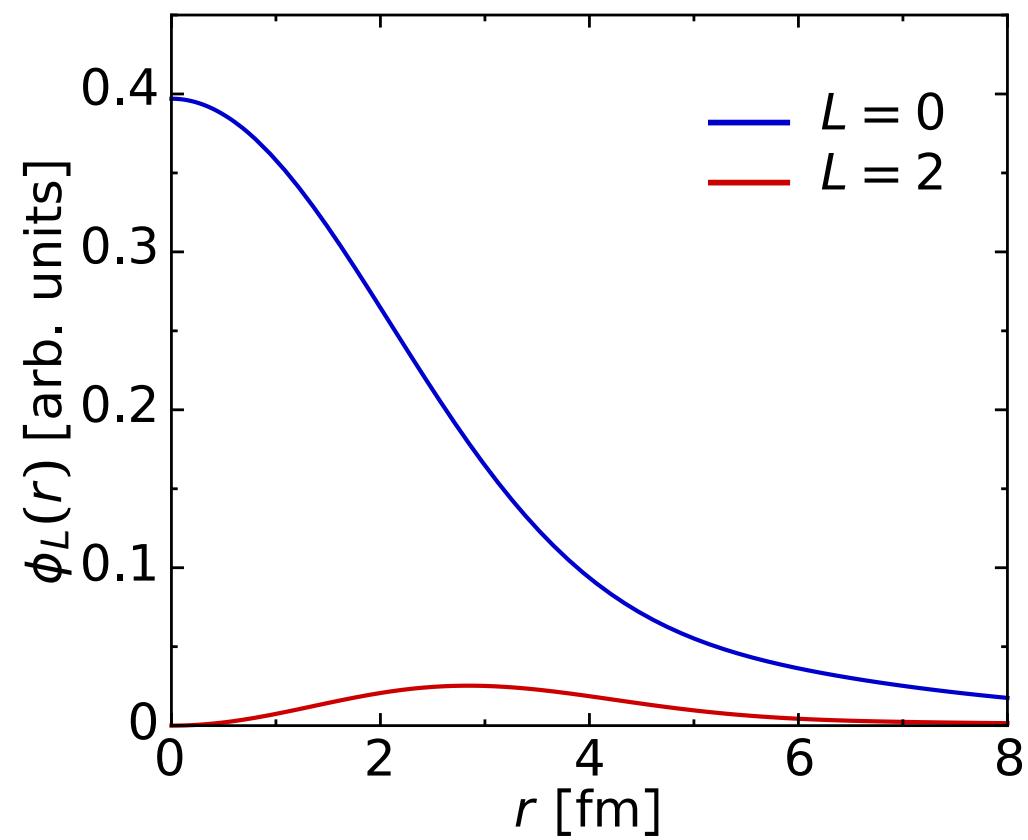


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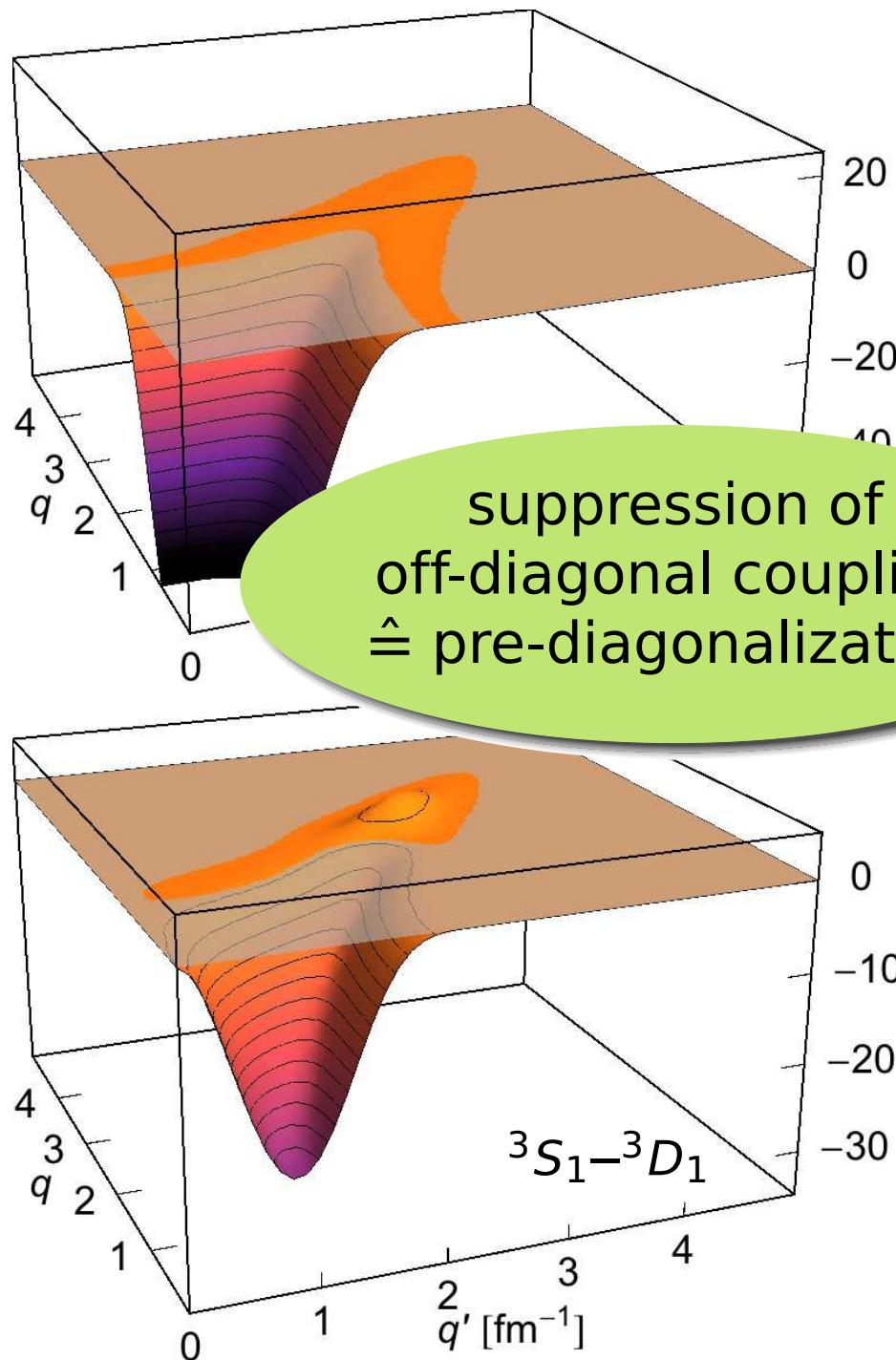
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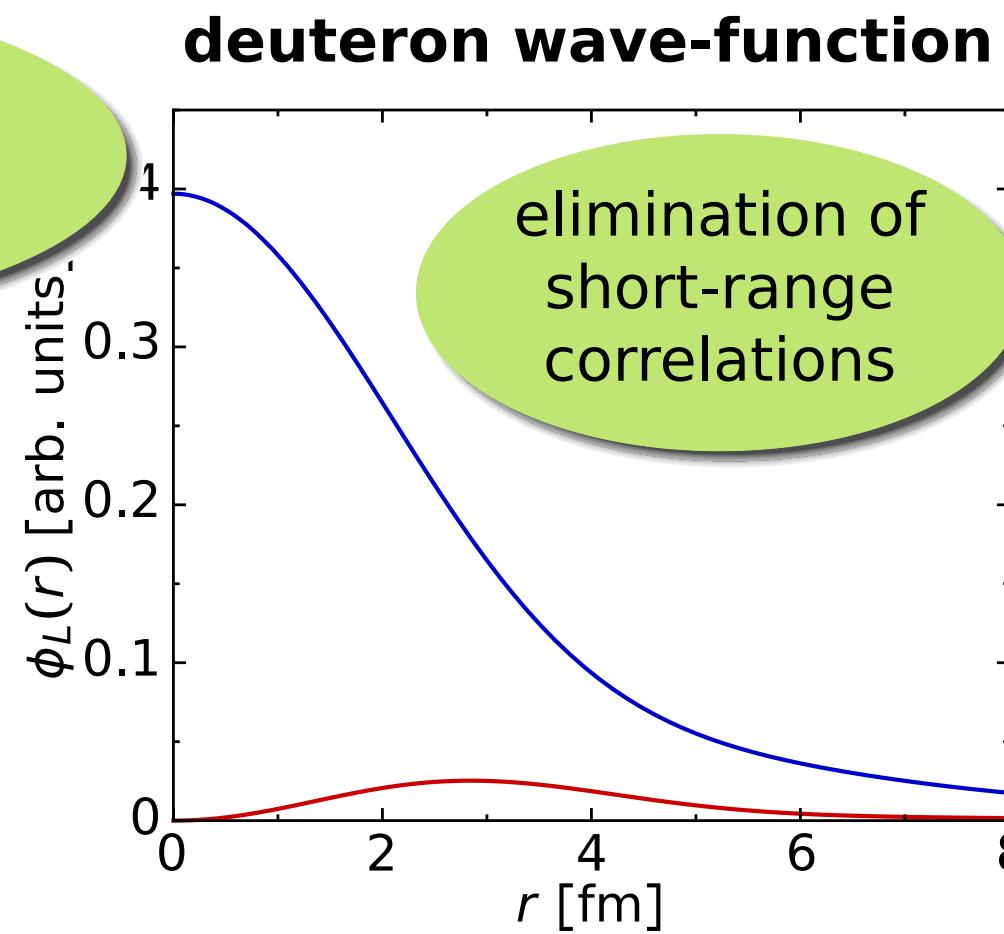
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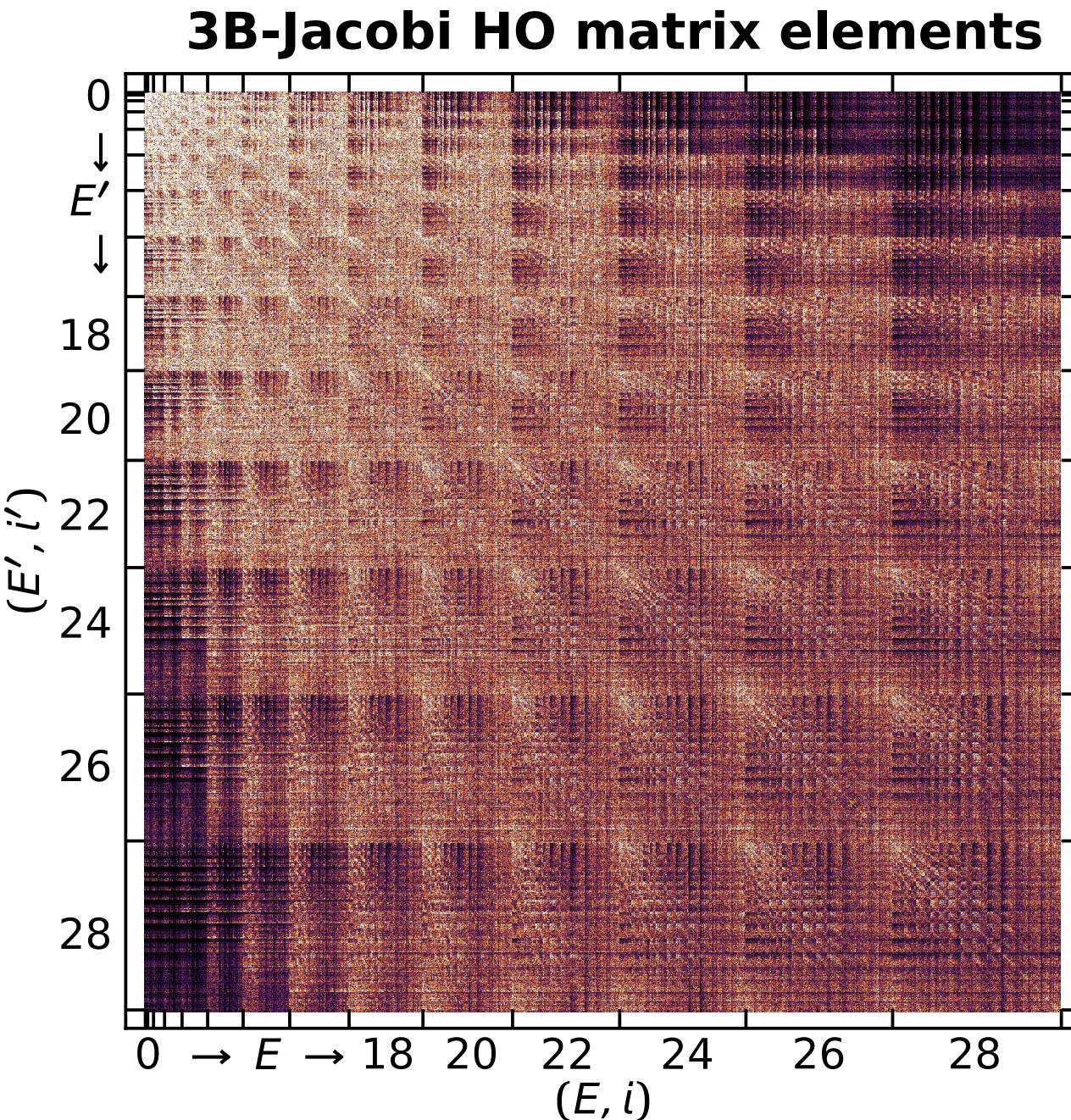
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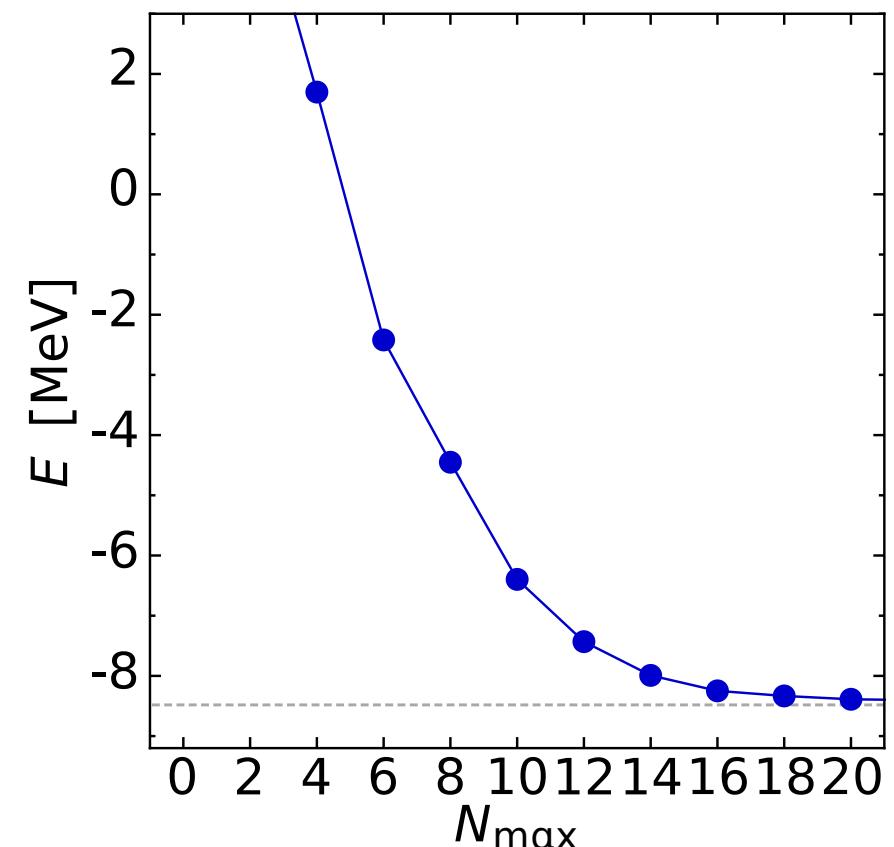


chiral NN+3N

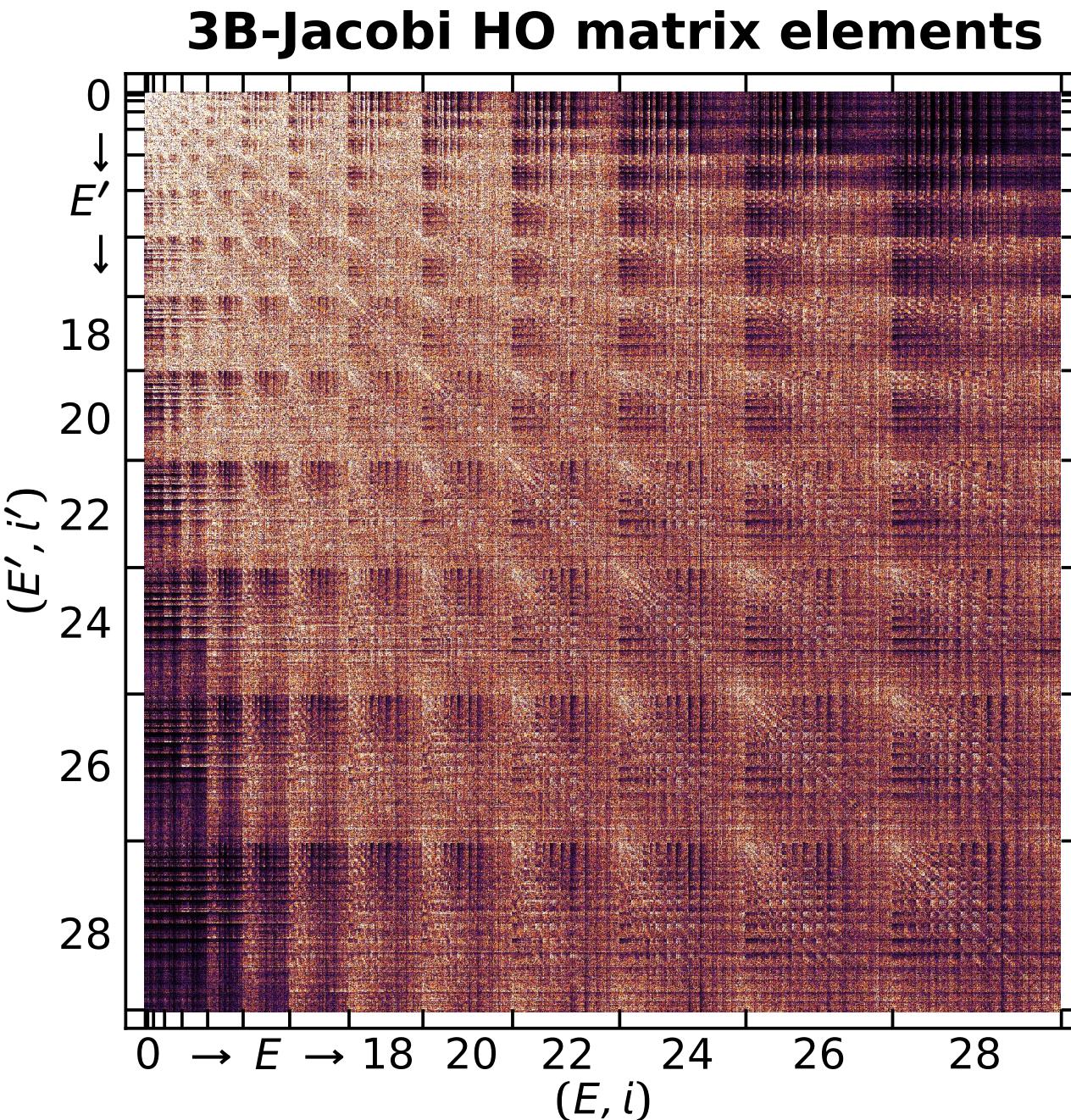
$N^3LO + N^2LO$ , triton-fit, 500 MeV

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

**NCSM ground state  ${}^3H$**



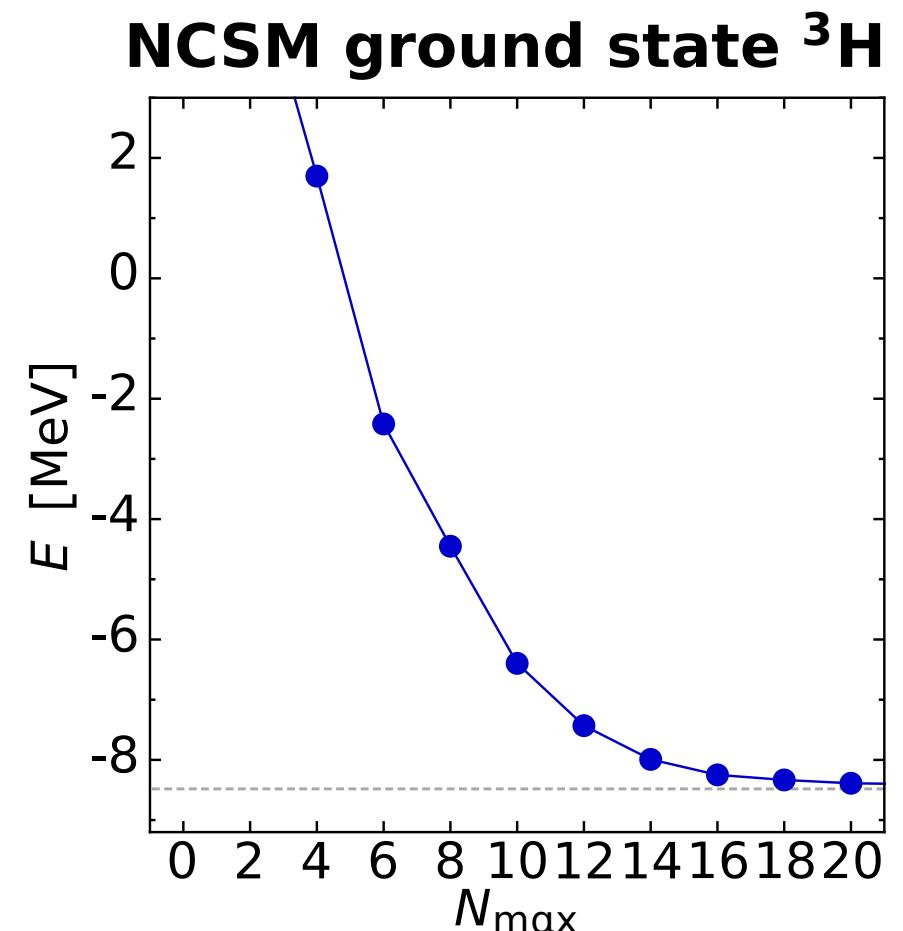
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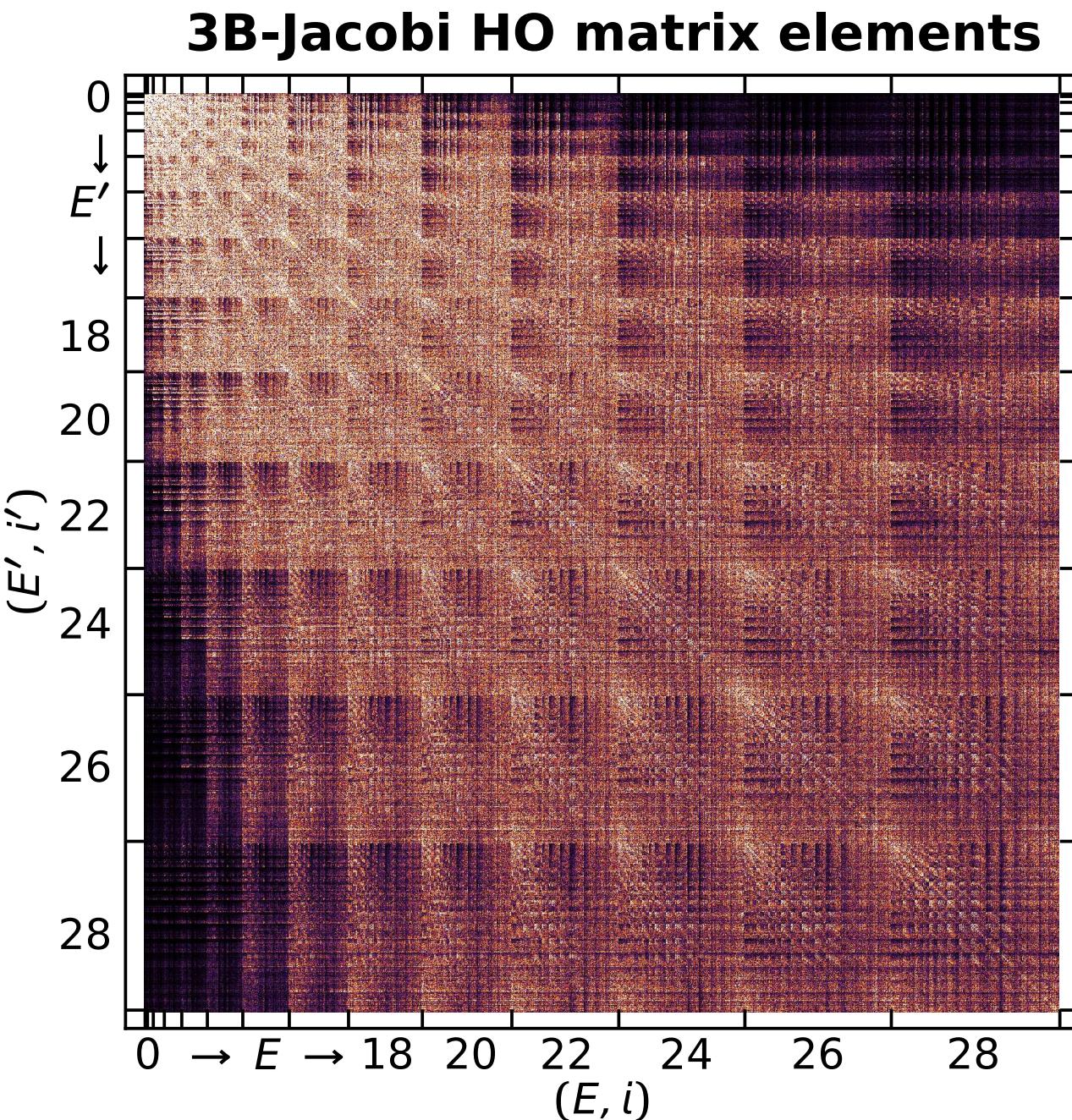
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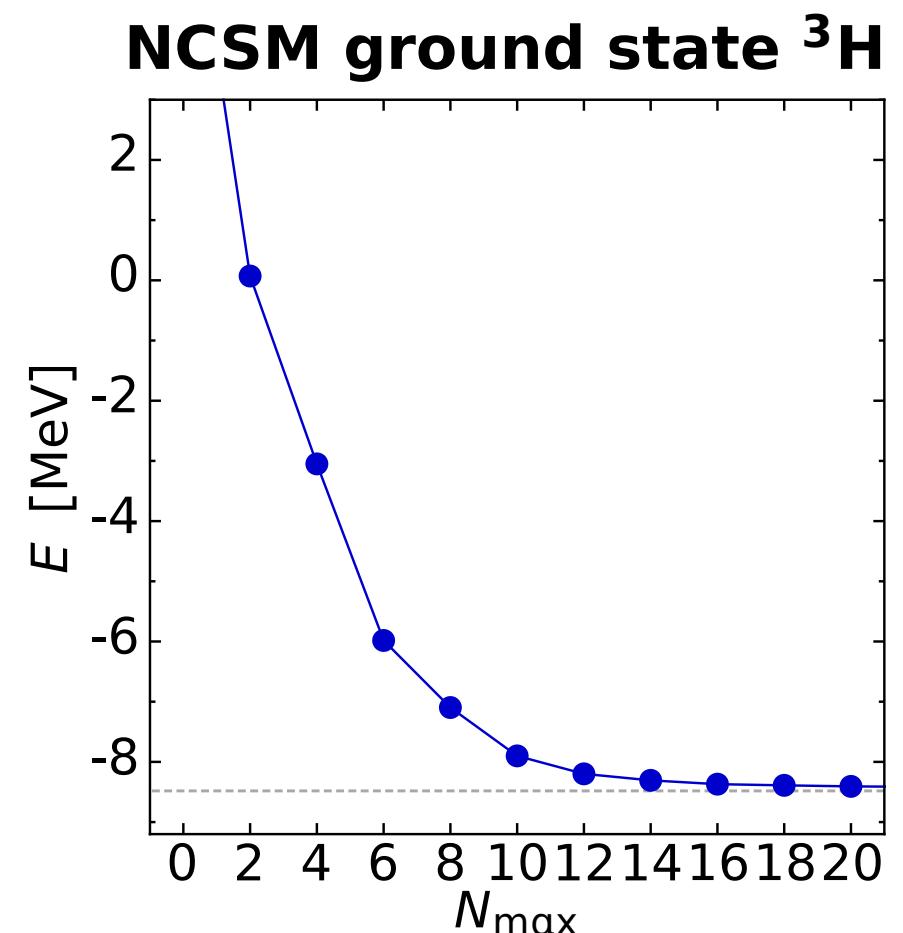
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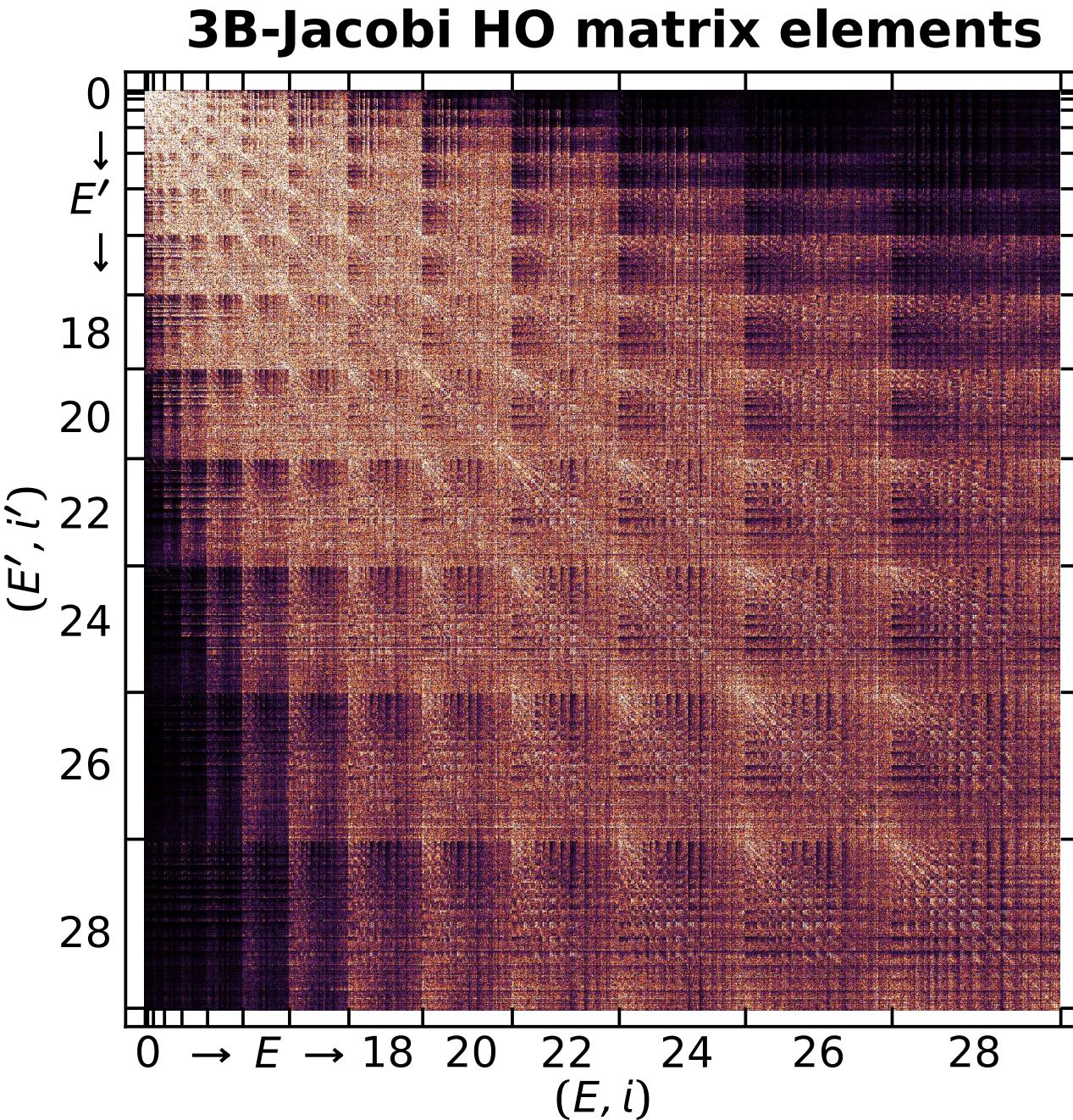
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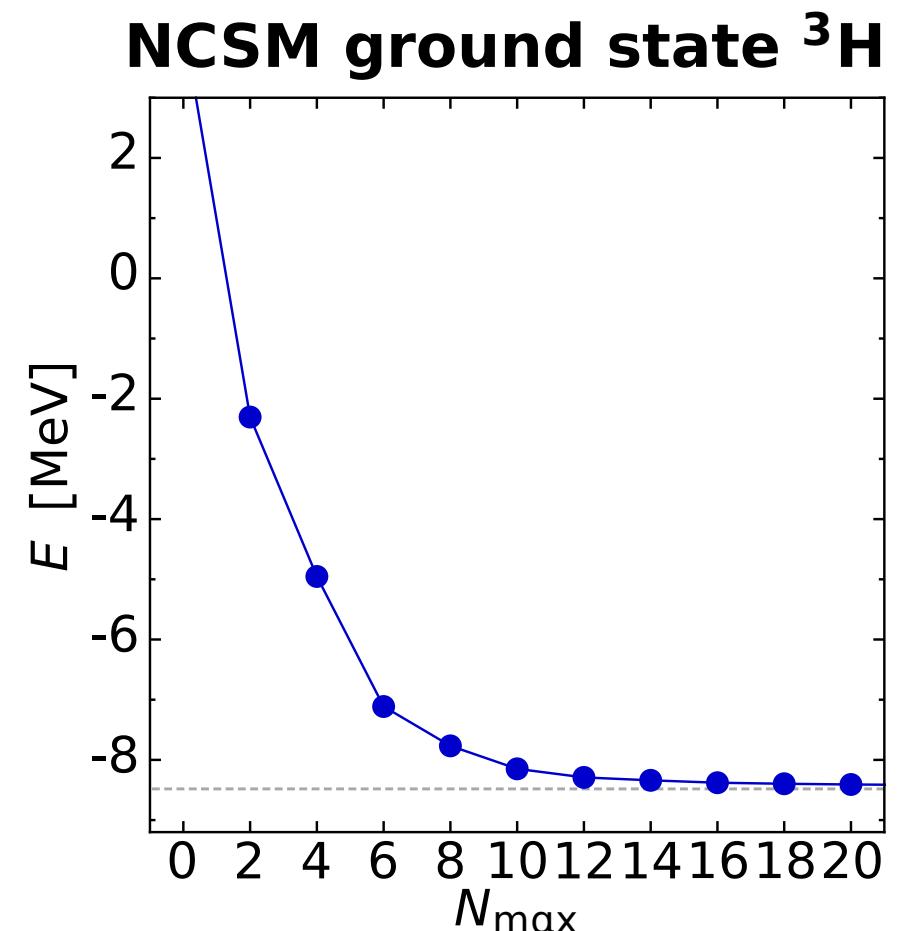
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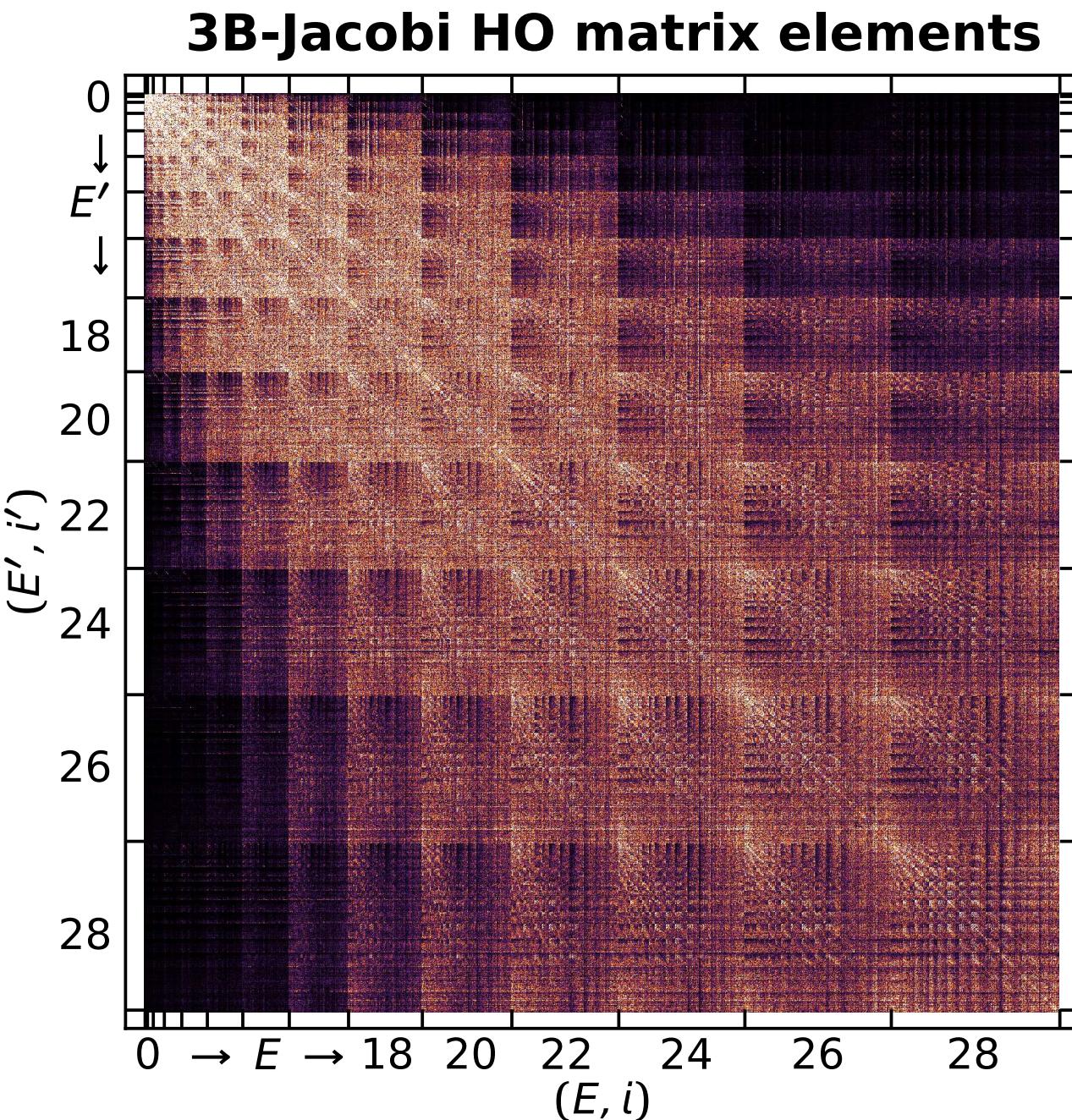
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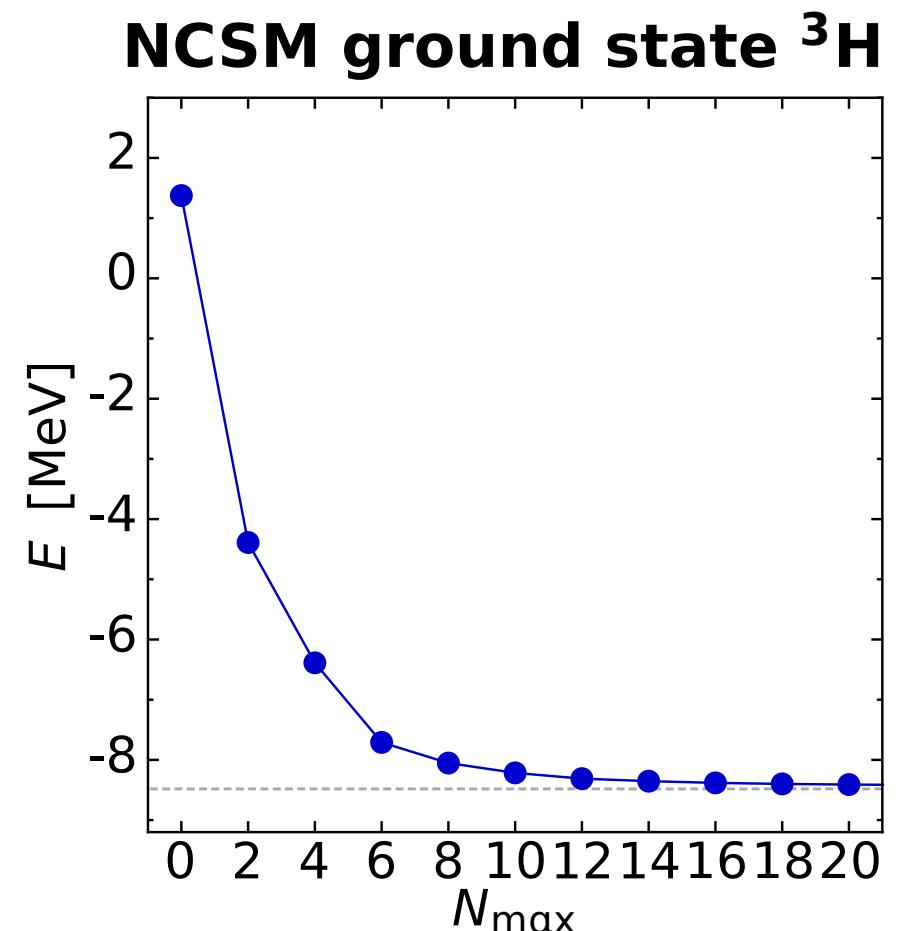
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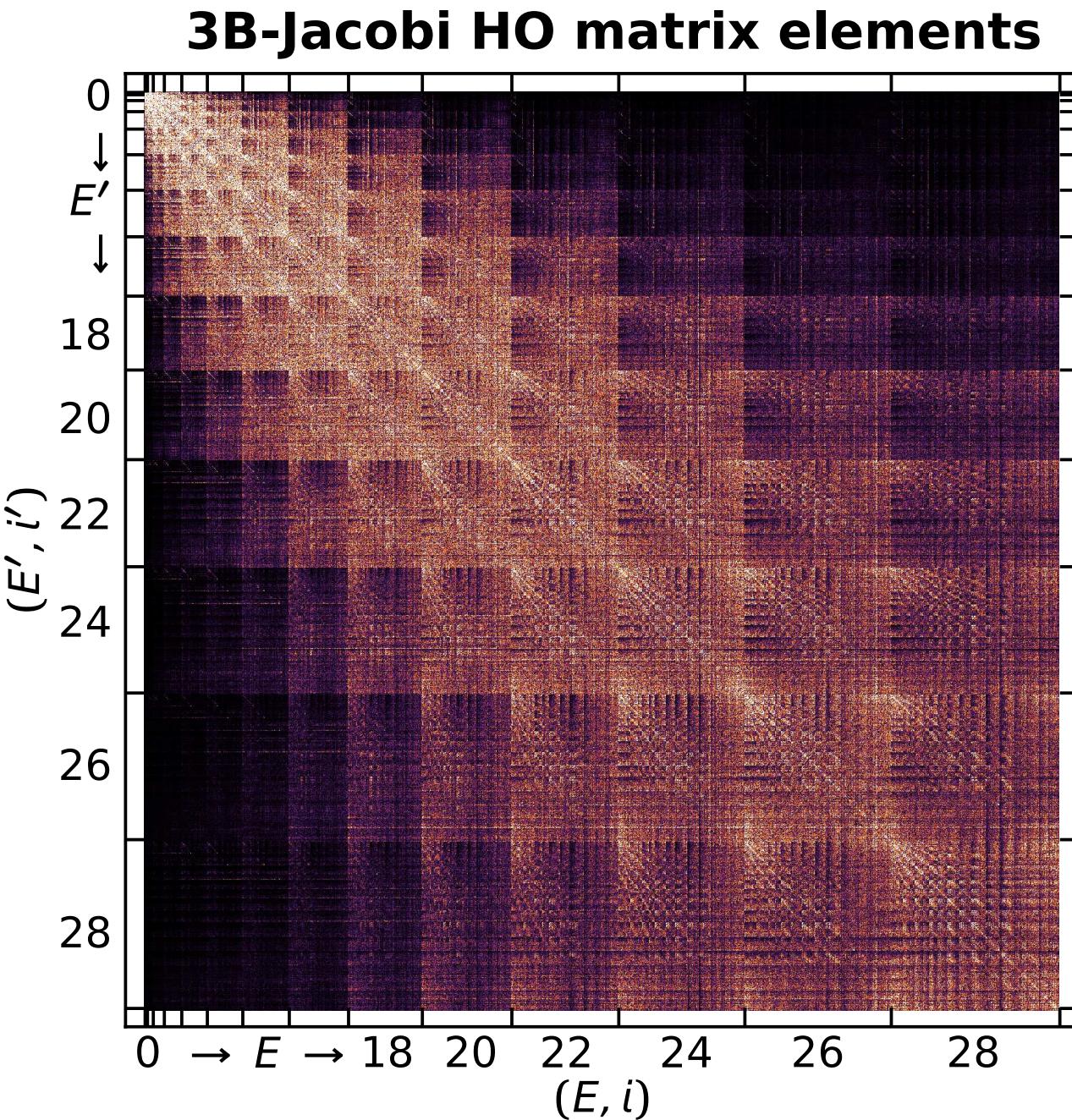
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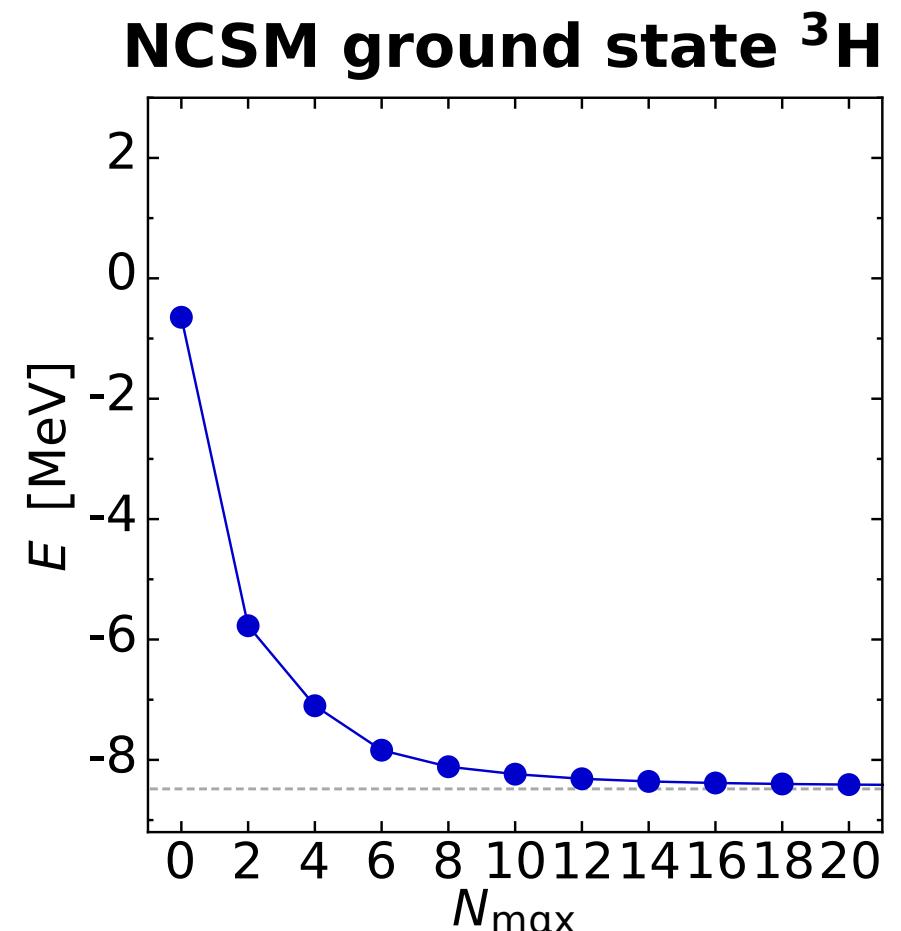
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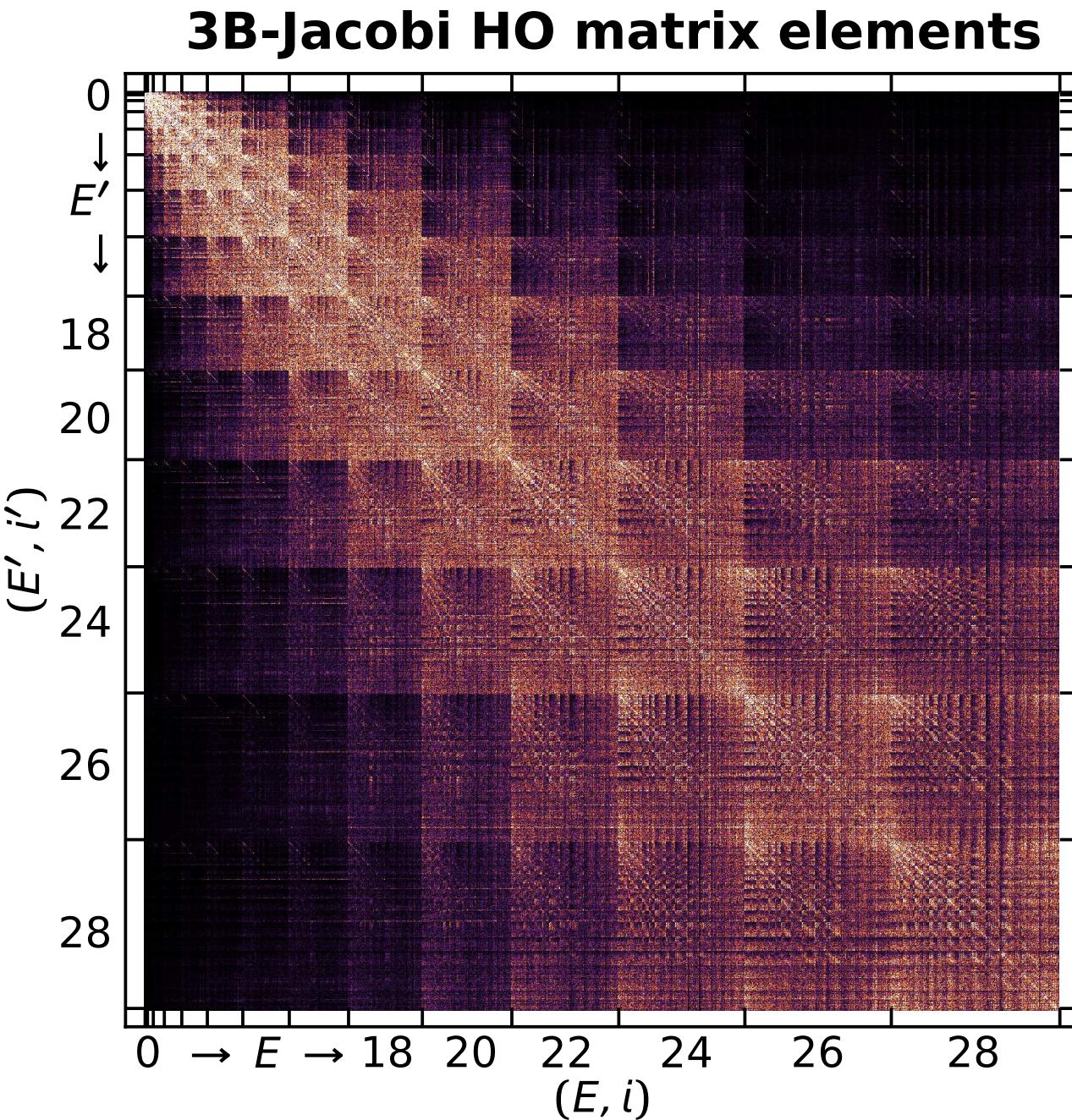
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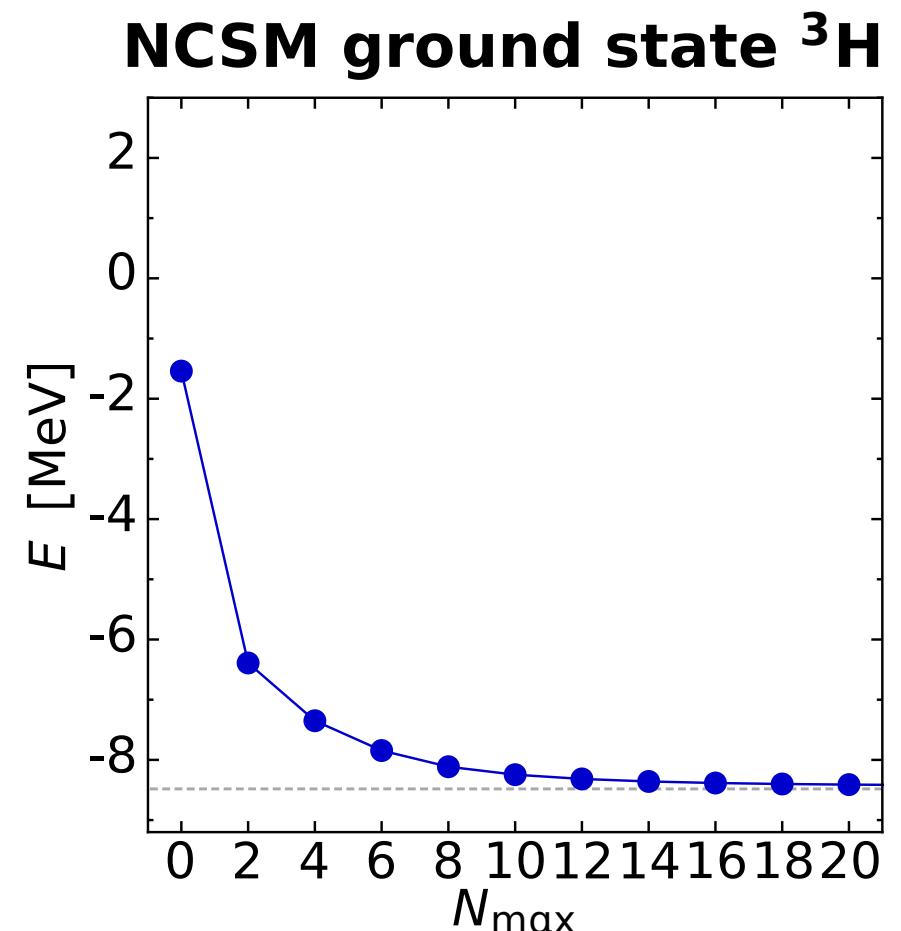
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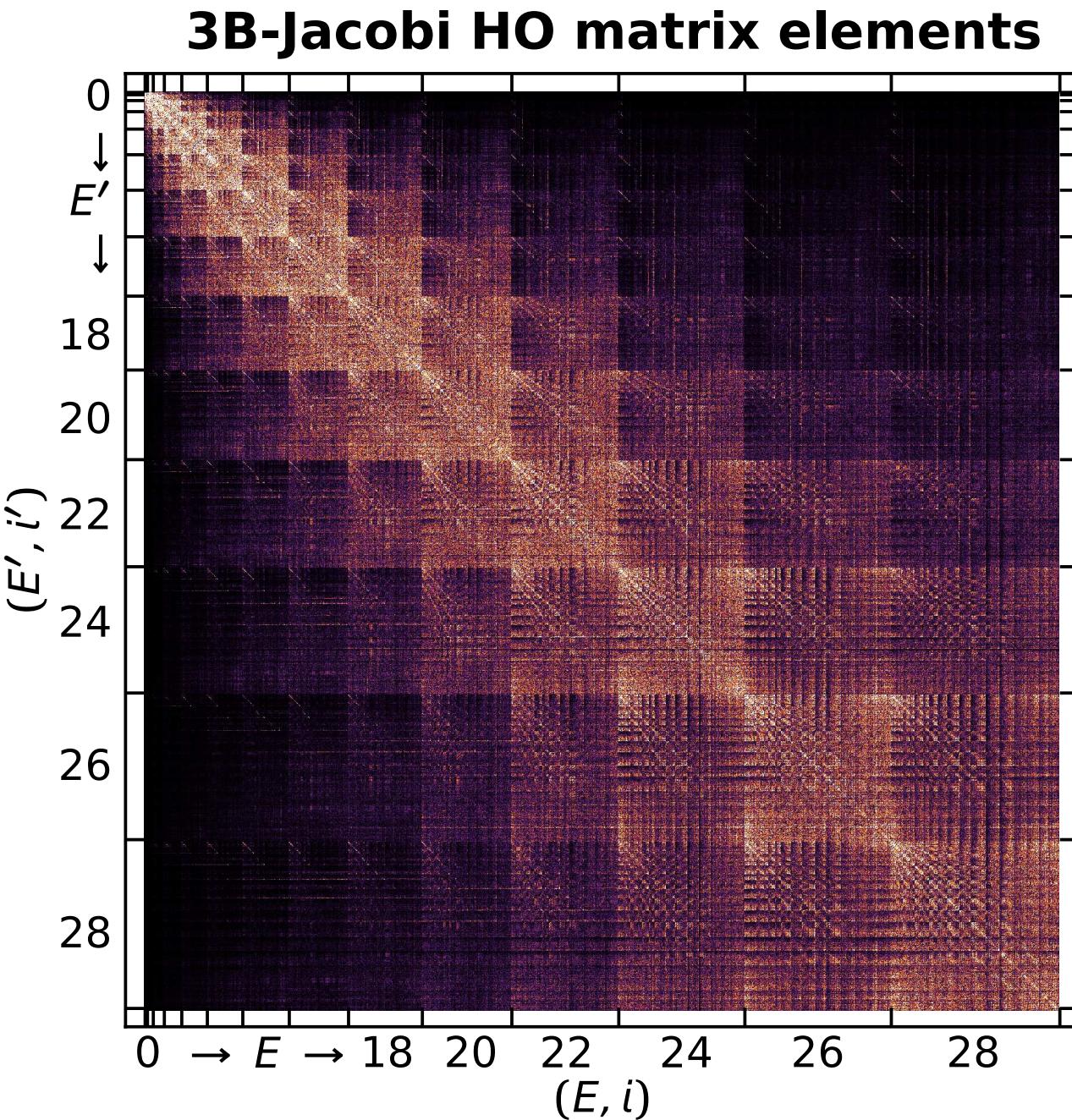
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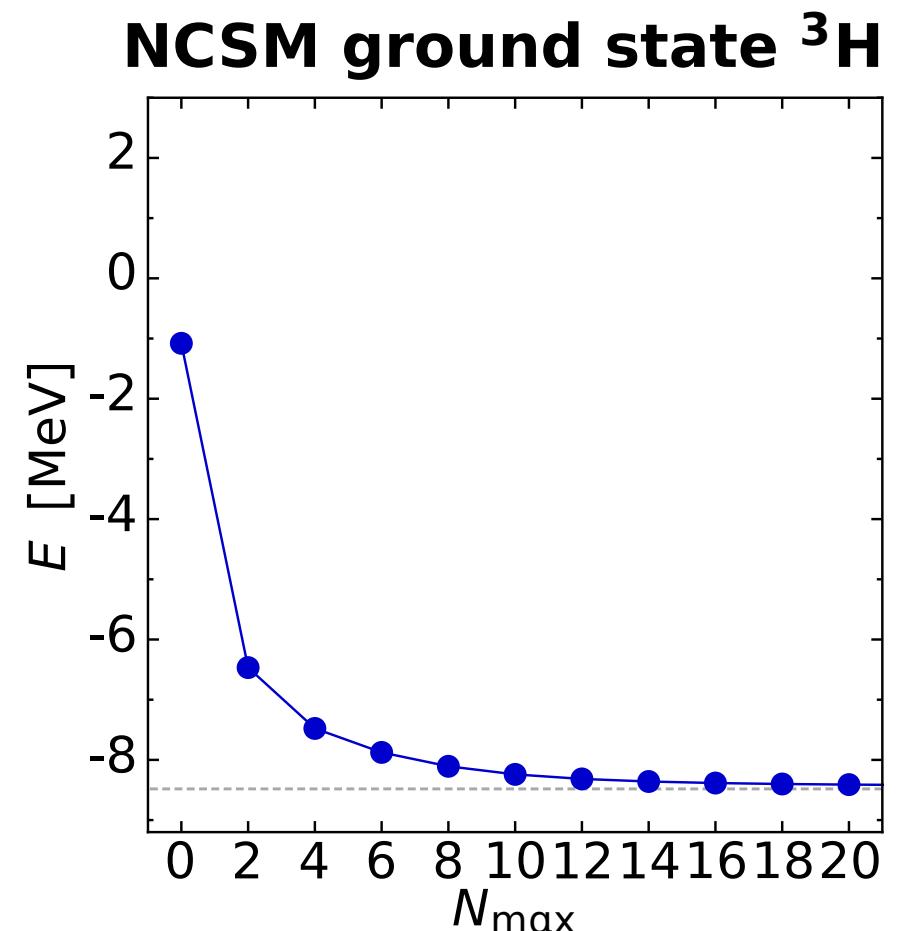
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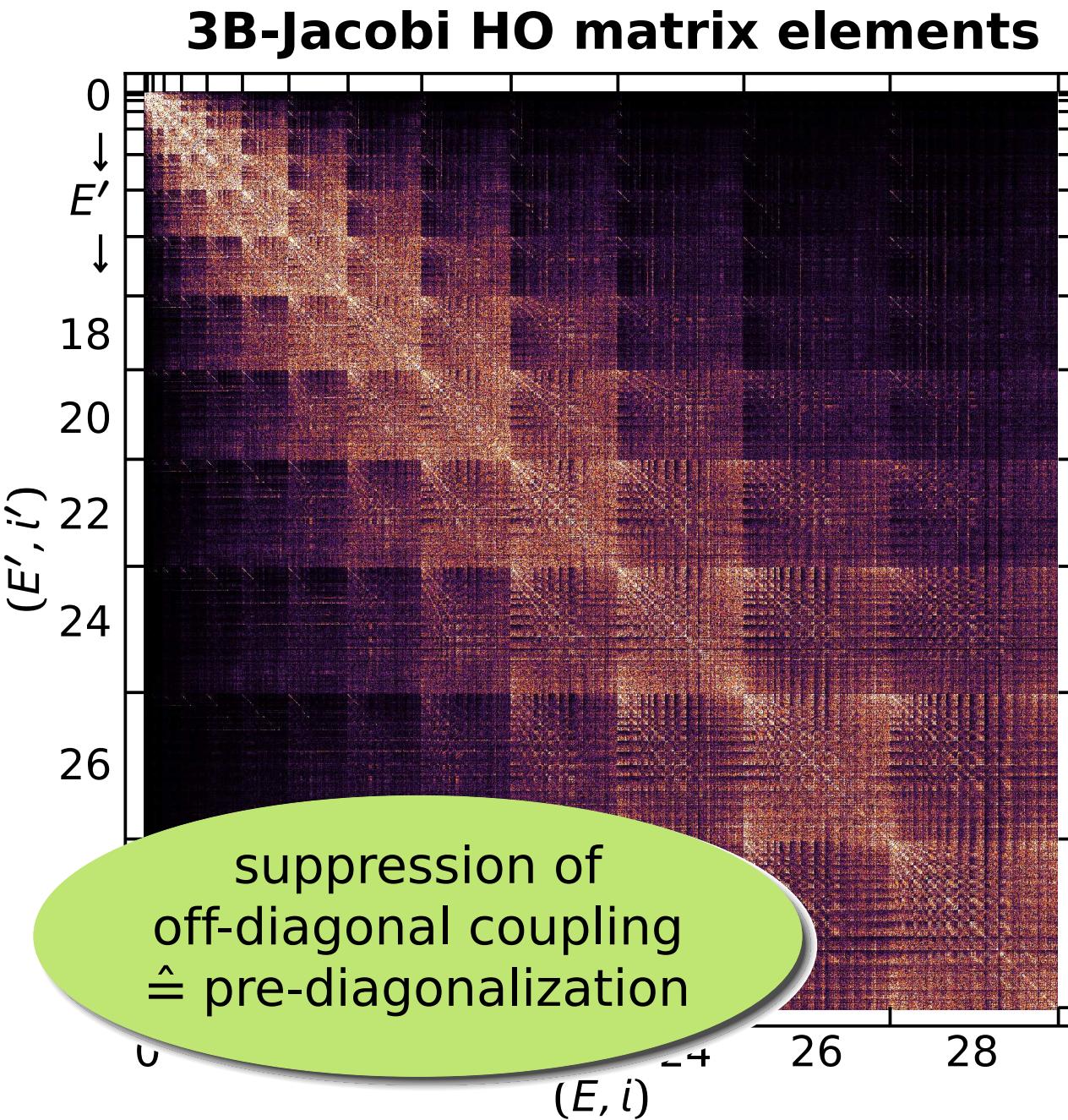
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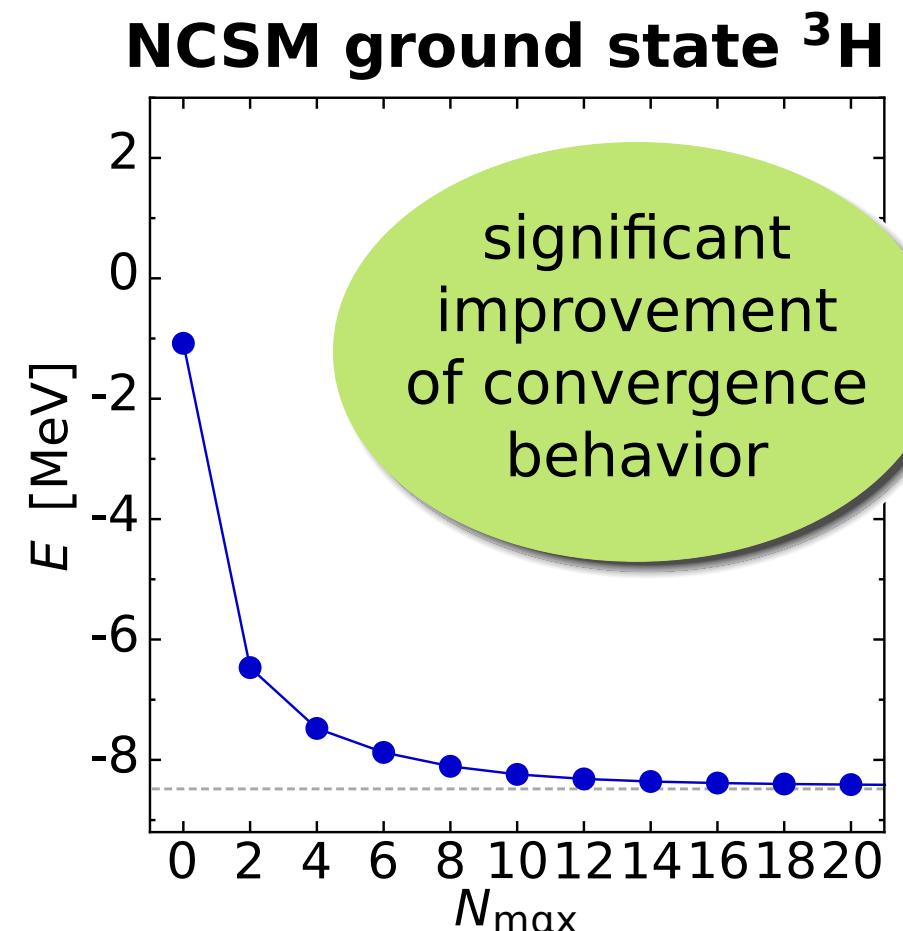
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# Calculations in $A$ -Body Space

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

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

- **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** is formally unitary and conserves  $A$ -body energy eigenvalues (independent of  $\alpha$ )
  - $\alpha$ -dependence of eigenvalues of **cluster-truncated Hamiltonian** measures impact of discarded induced many-body terms

# Calculations in $A$ -Body Space

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

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

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- $\alpha$ -dependence of eigenvalues **α-miltonian** measures impact of  $\alpha$ -variation provides a **diagnostic tool** to assess the omitted induced many-body interactions

# Ab Initio Nuclear Structure

## Nuclear Structure Observables

**Nuclear Lattice Sim.**

chiral EFT on lattice

**Exact Ab-Initio Solutions**  
few-body et al.

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few-body, no-core shell model, etc.

**Approx. Many-Body Methods**

controlled & improvable schemes

**Energy-Density-Functional Theory**  
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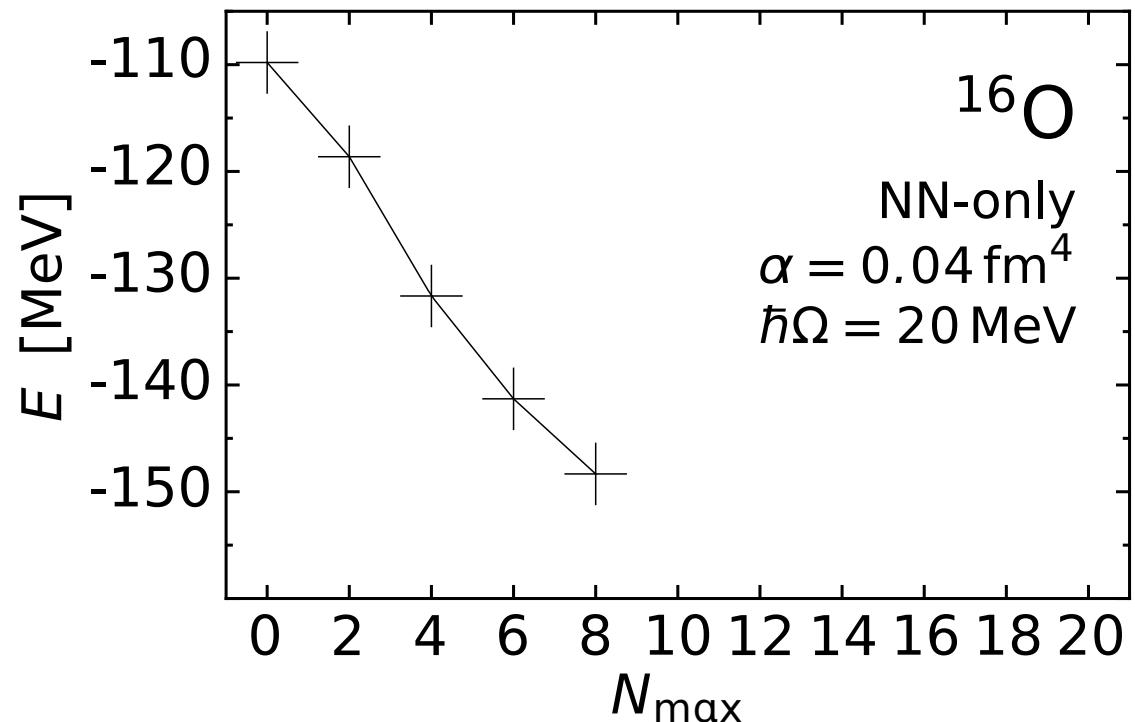
# No-Core Shell Model (NCSM)

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

- construct matrix representation of Hamiltonian using a **basis of HO Slater determinants** truncated w.r.t. HO excitation energy  $N_{\max}\hbar\Omega$
- solve **large-scale eigenvalue problem** for a few extremal eigenvalues
- **all relevant observables** can be computed from the eigenstates
- range of applicability limited by **factorial growth** of basis with  $N_{\max}$  &  $A$
- 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  $E_{3\max} = 16$

# Importance Truncated NCSM

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

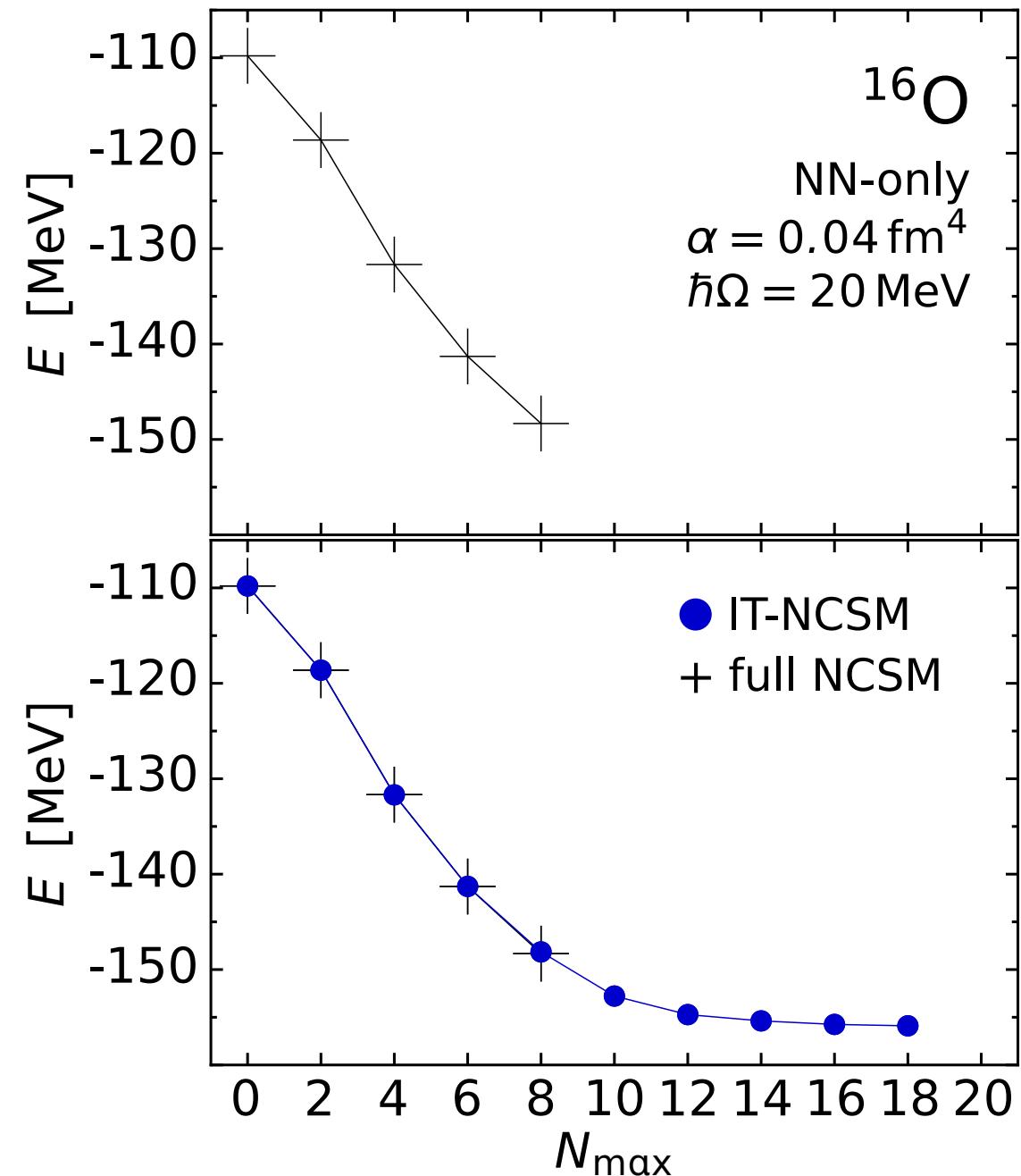


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## Importance Truncation

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



# Importance Truncation: General Idea

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

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

- 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  $|\Psi_{\text{ref}}^{(m)}\rangle$
- a posteriori **threshold extrapolation** and **perturbative correction** used to recover contributions from discarded basis states

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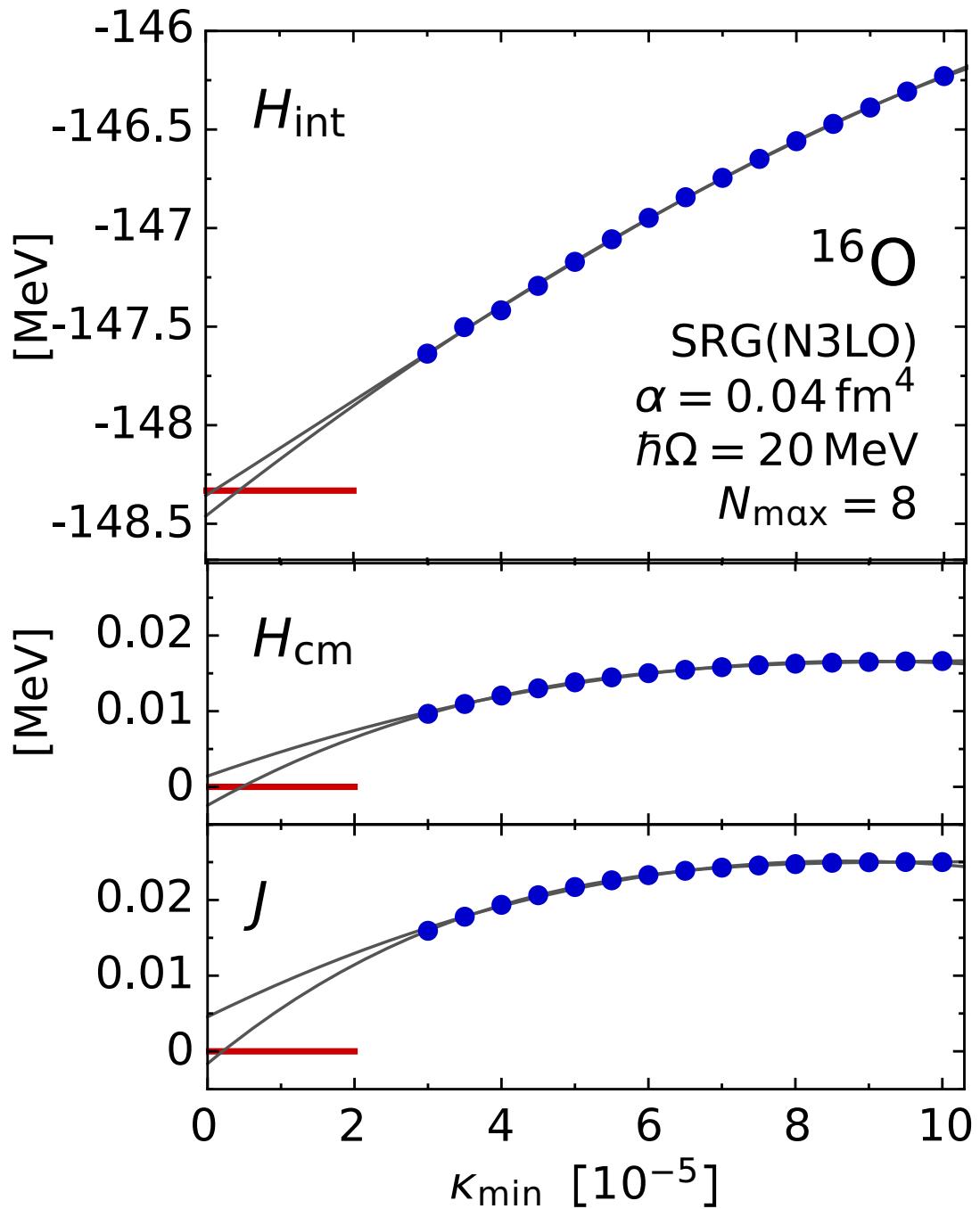
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for  $\kappa_{\min} \rightarrow 0$  the full NCSM model space and thus the **exact solution is recovered**

# 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**  $\kappa_{\min} \rightarrow 0$  of observables to account for effect of excluded configurations

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# A Tale of Three Hamiltonians

## Initial Hamiltonian

- NN: chiral interaction at N<sup>3</sup>LO (Entem & Machleidt, 500 MeV)
- 3N: chiral interaction at N<sup>2</sup>LO ( $c_D, c_E$  from <sup>3</sup>H 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 initial Hamiltonian and keep two- and three-body terms

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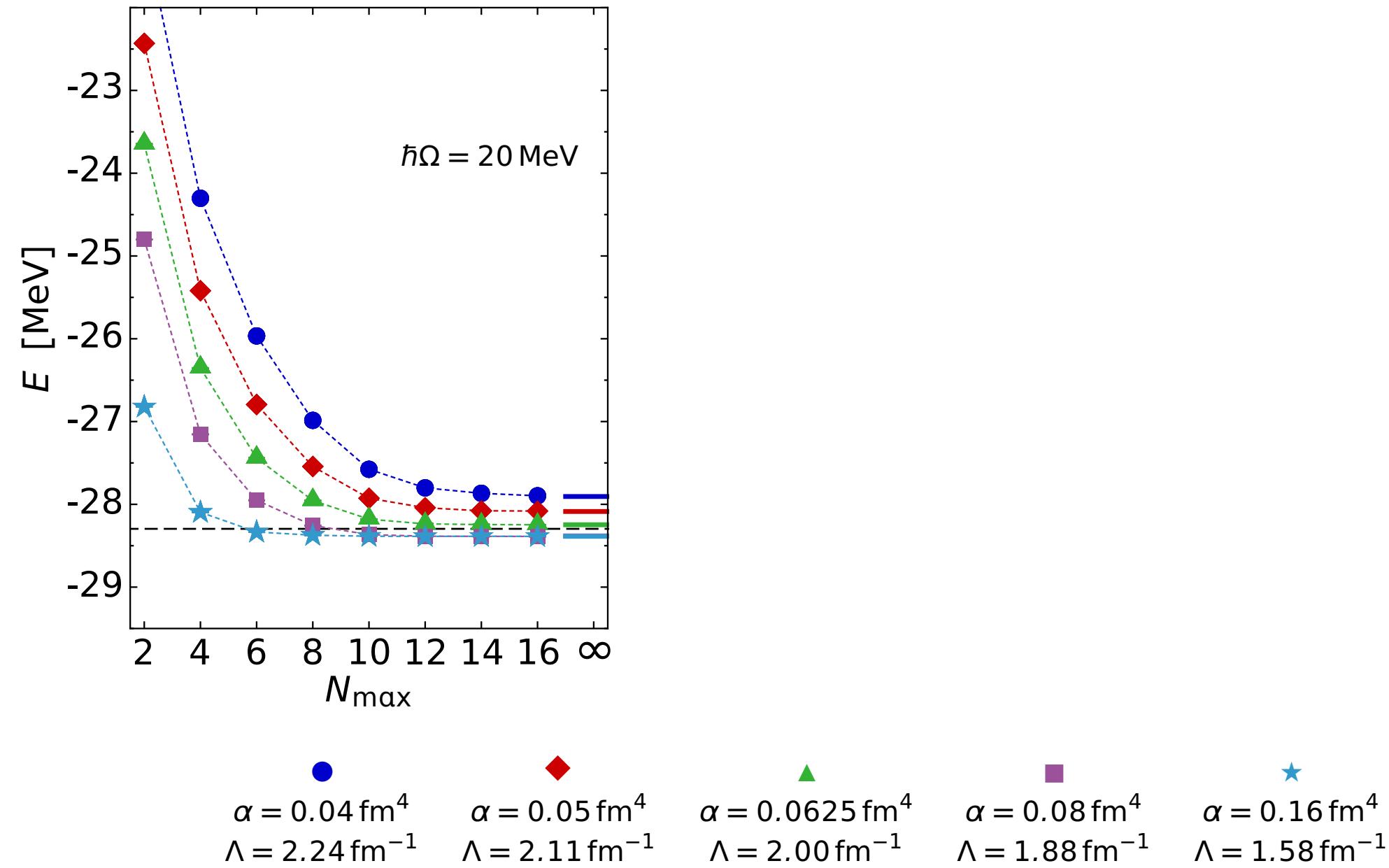
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$\alpha$ -variation provides a **diagnostic tool** to assess the contributions of omitted many-body interactions

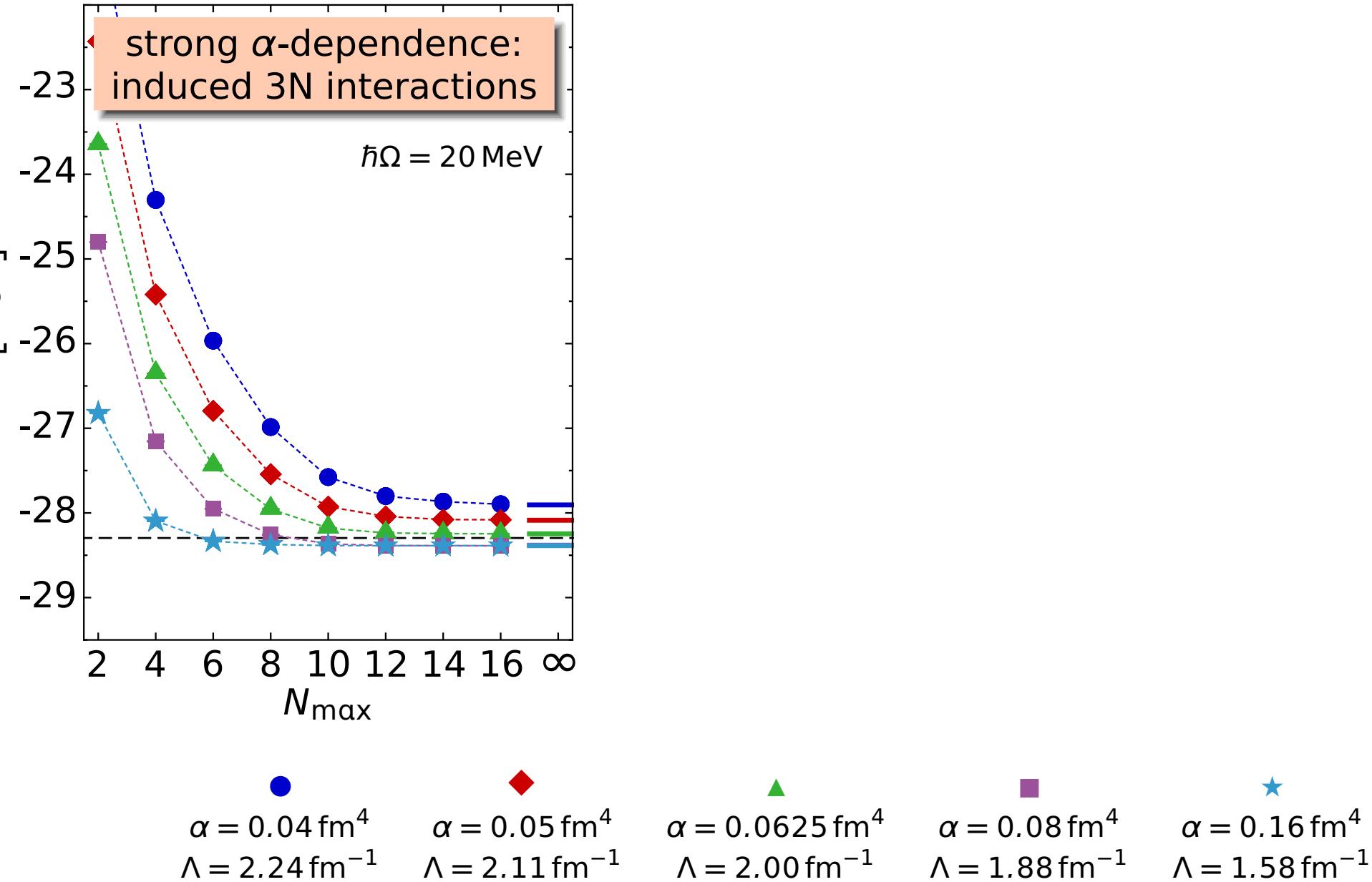
# $^4\text{He}$ : Ground-State Energies

**NN only**

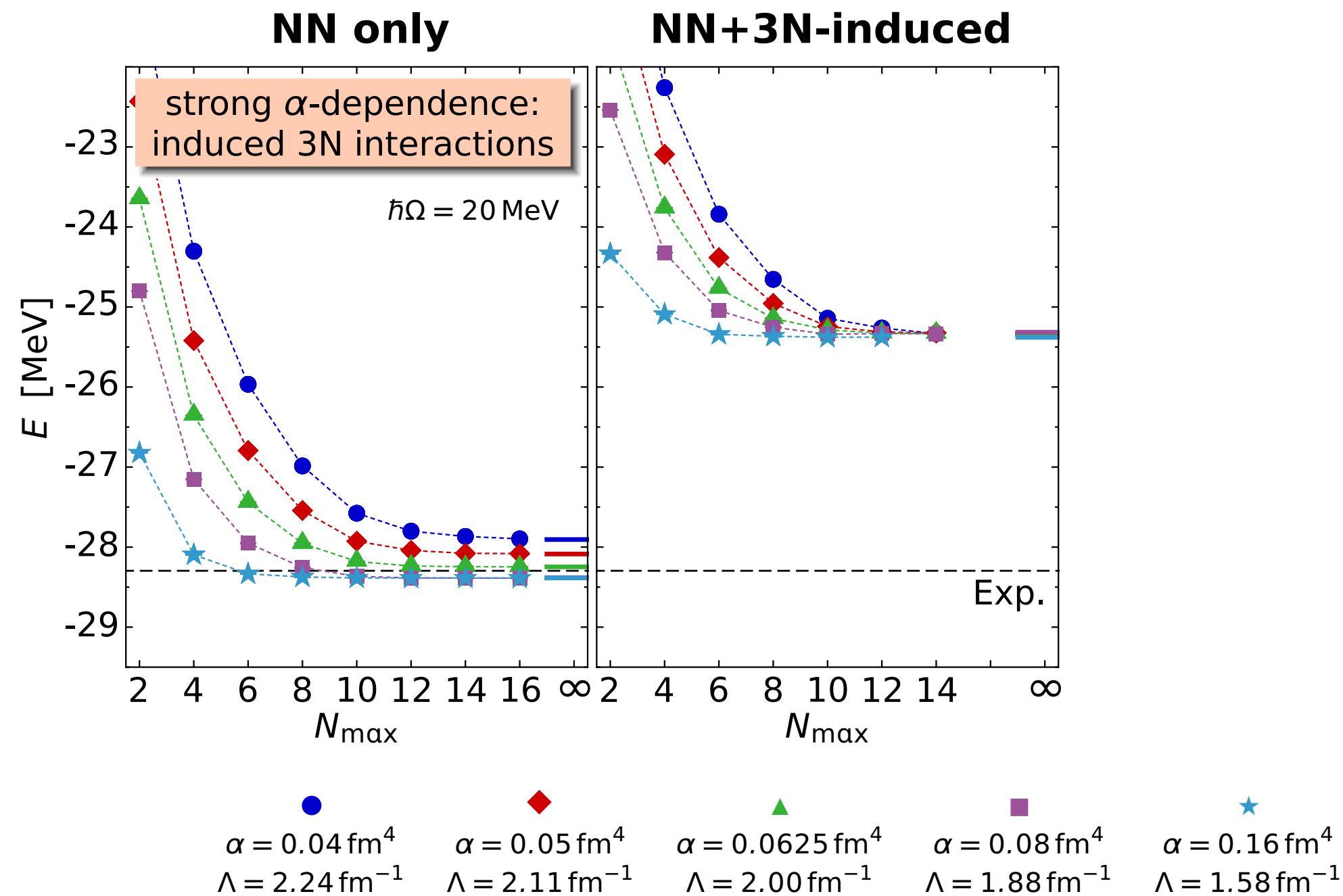


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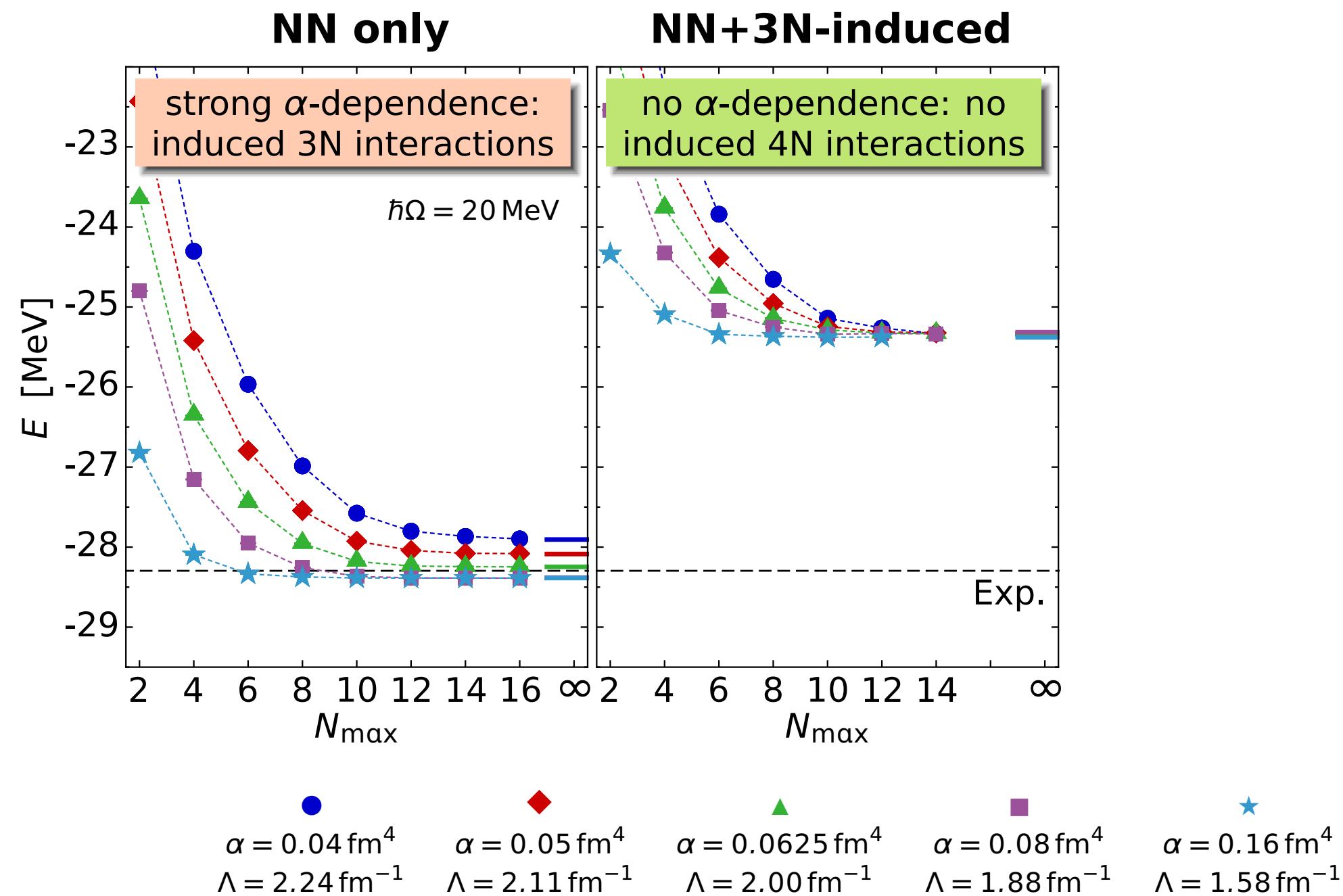
**NN only**



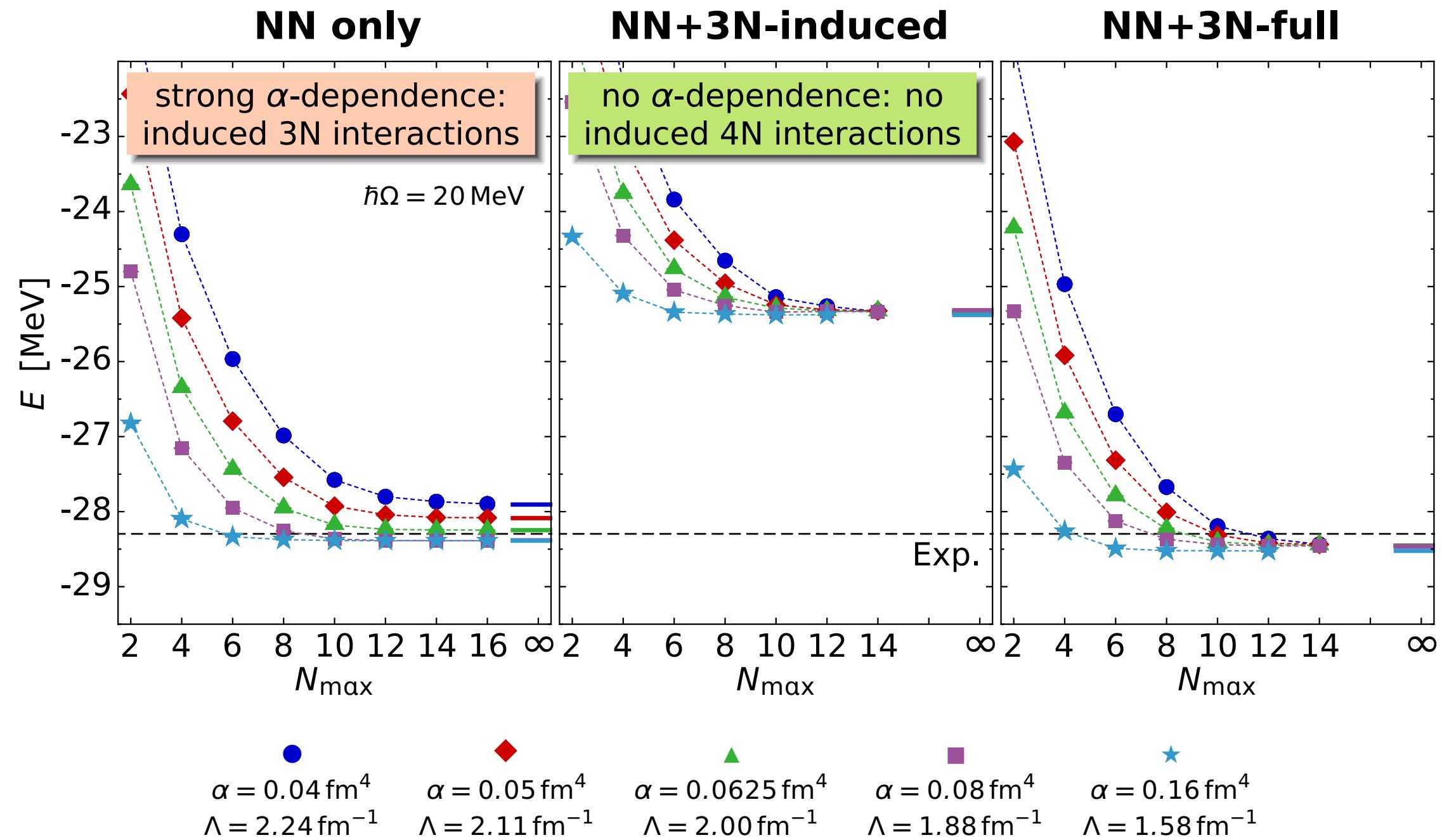
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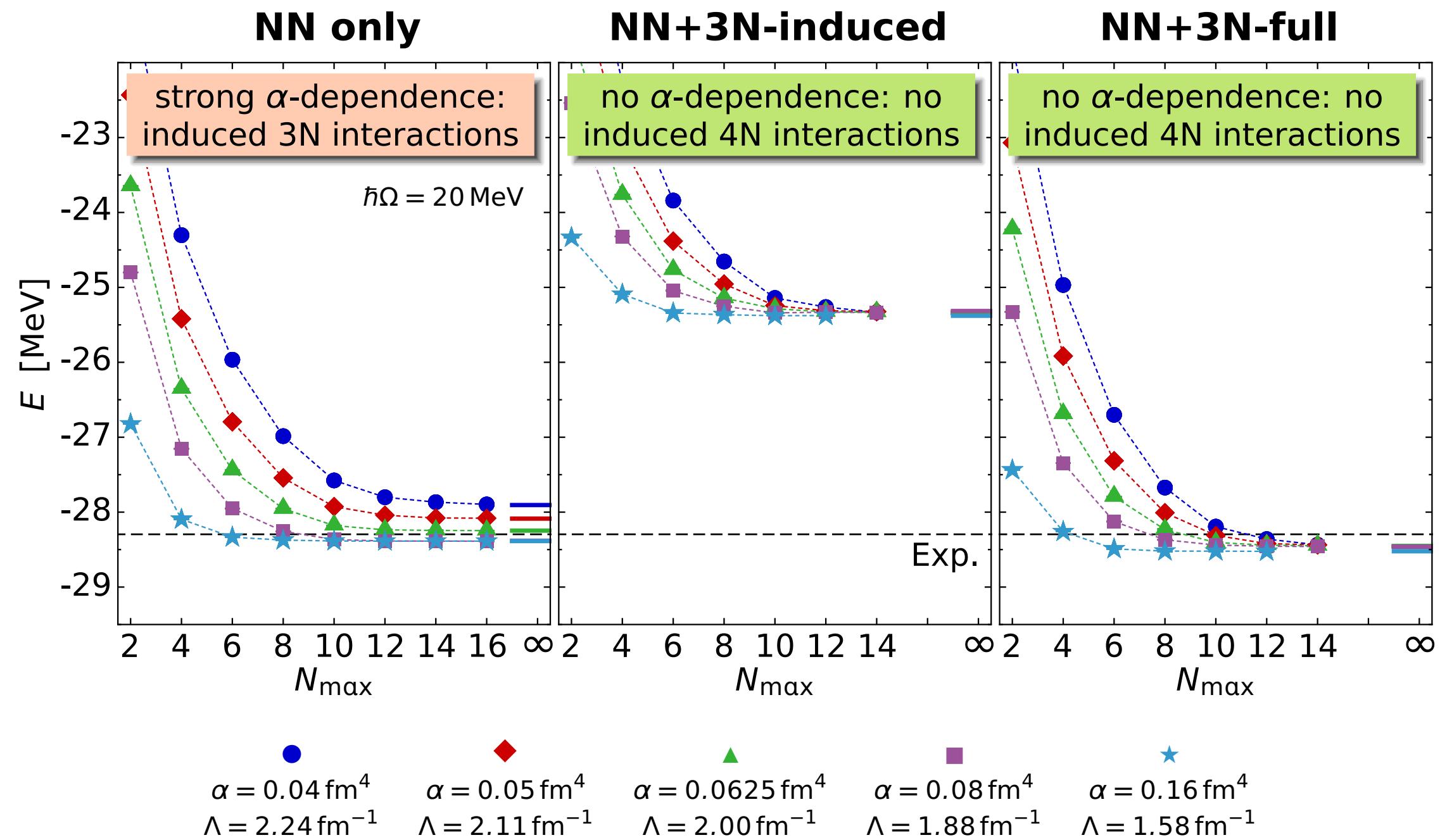
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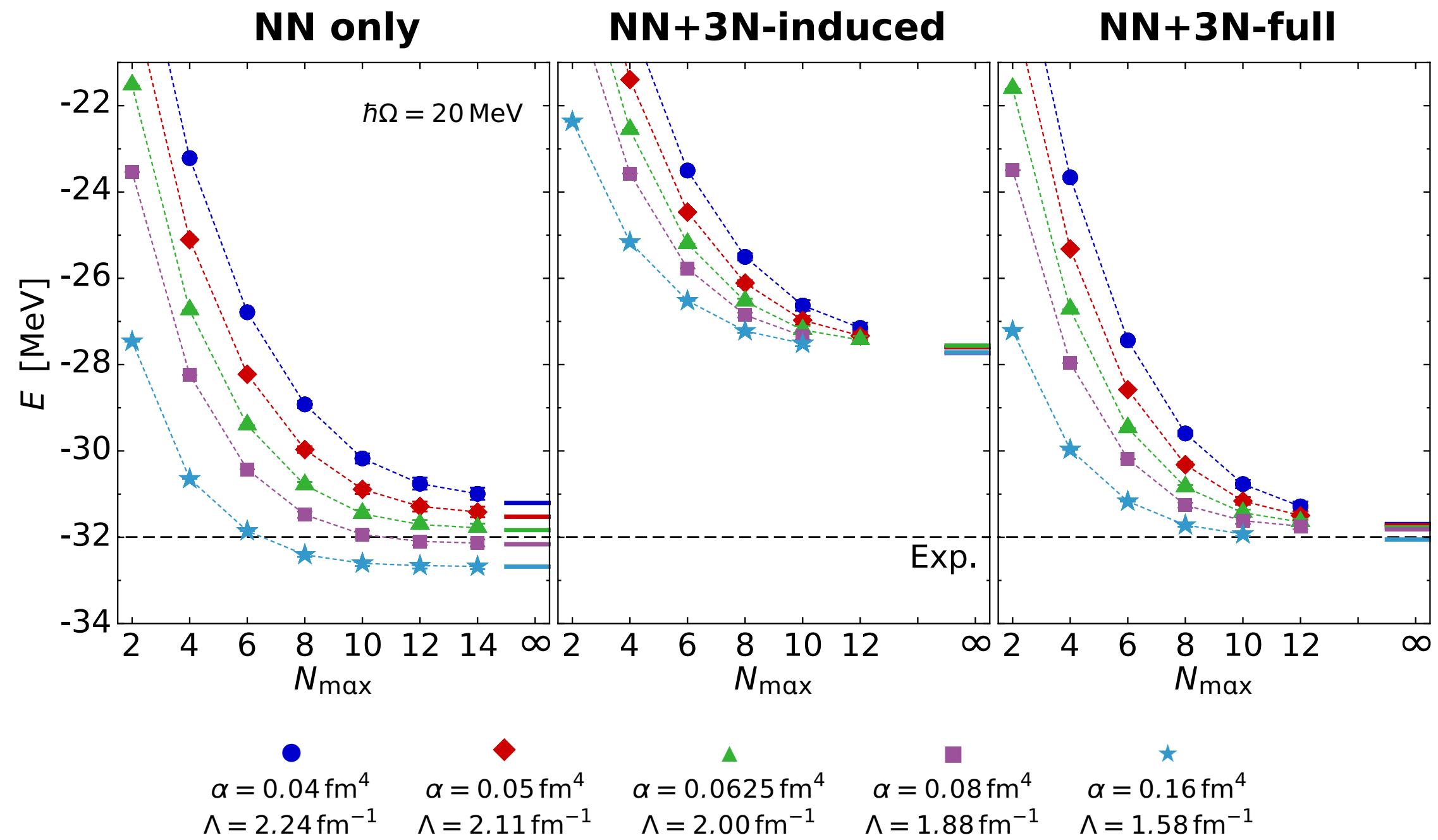
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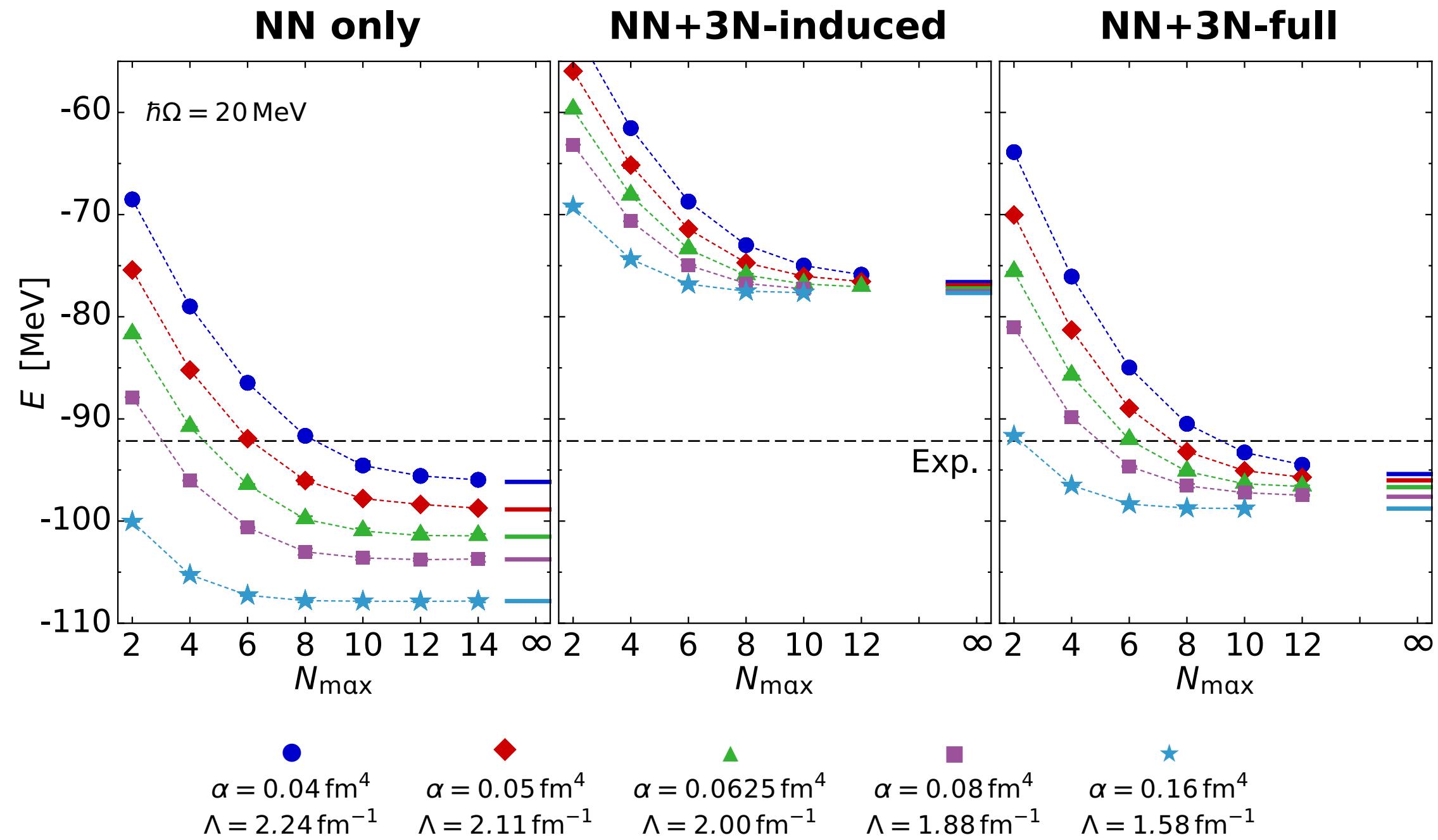
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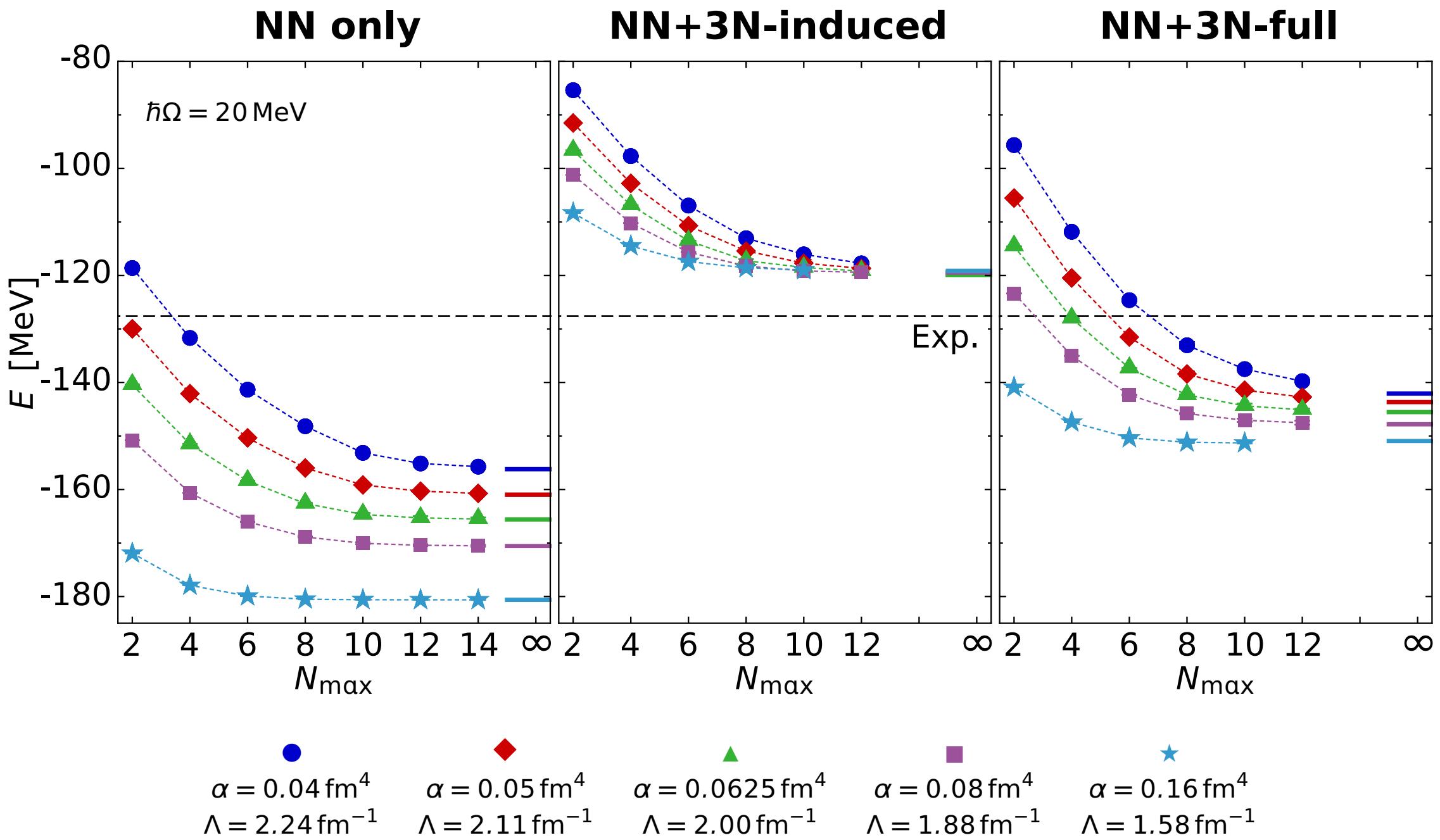
# $^6\text{Li}$ : Ground-State Energies



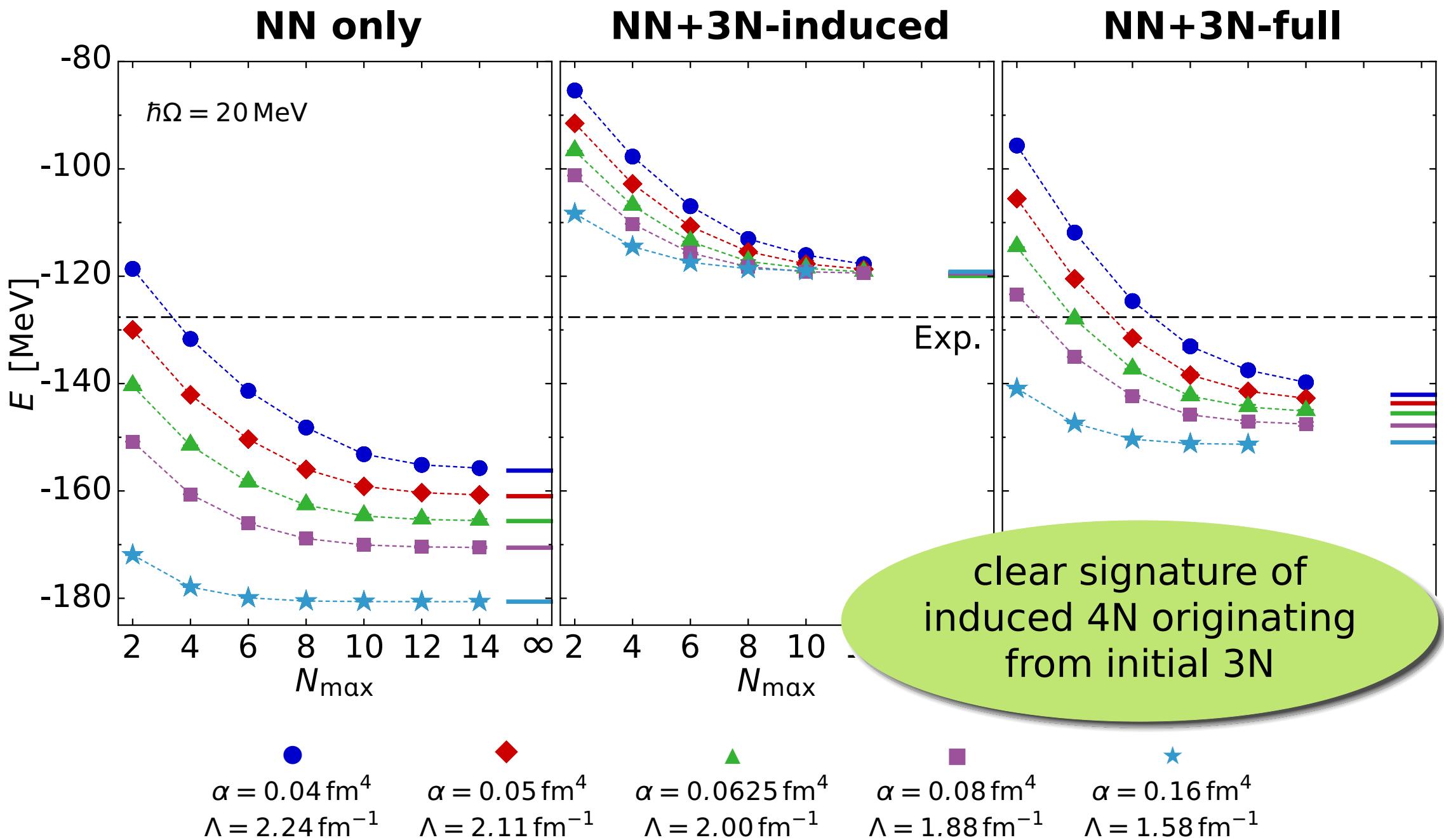
# $^{12}\text{C}$ : Ground-State Energies



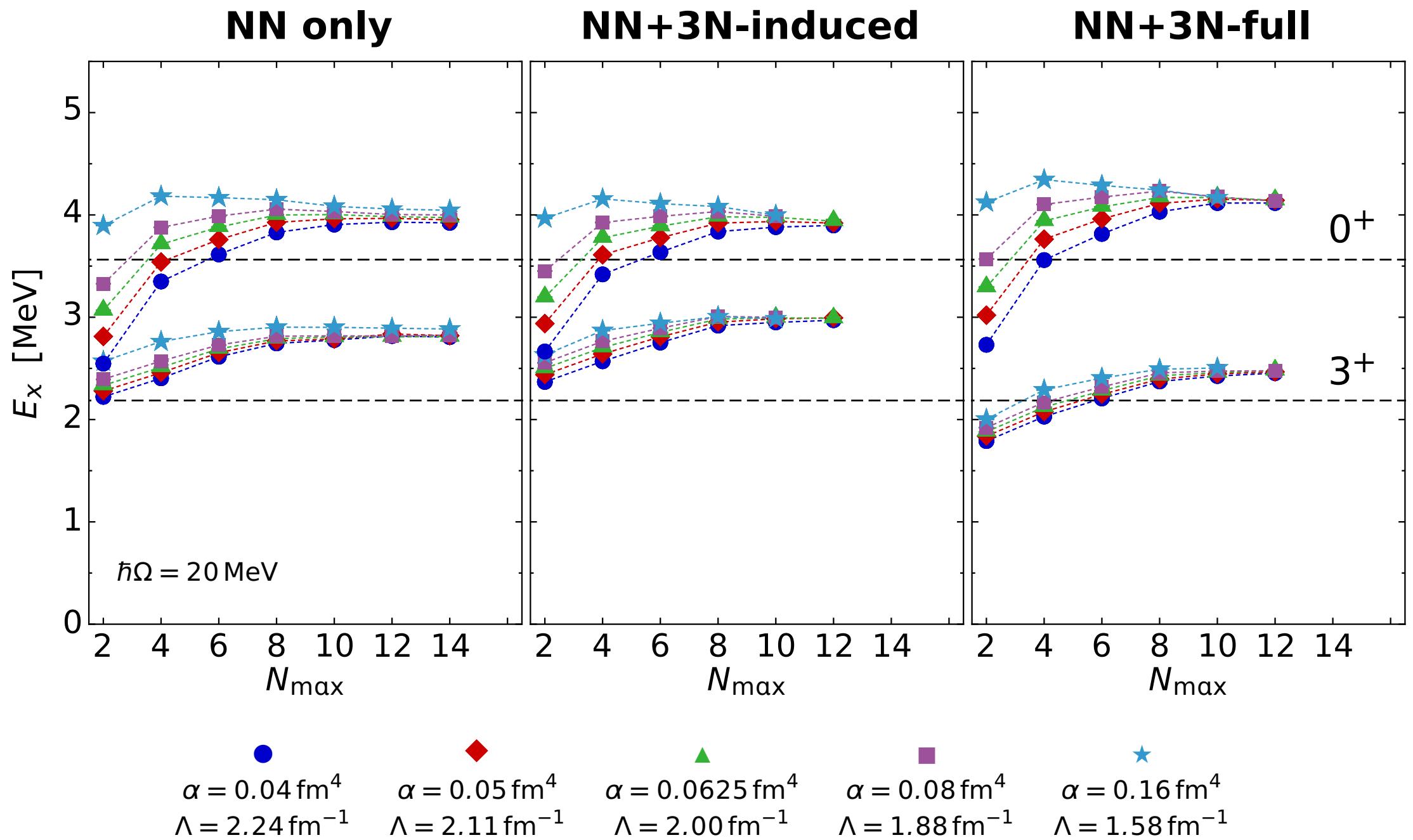
# $^{16}\text{O}$ : Ground-State Energies



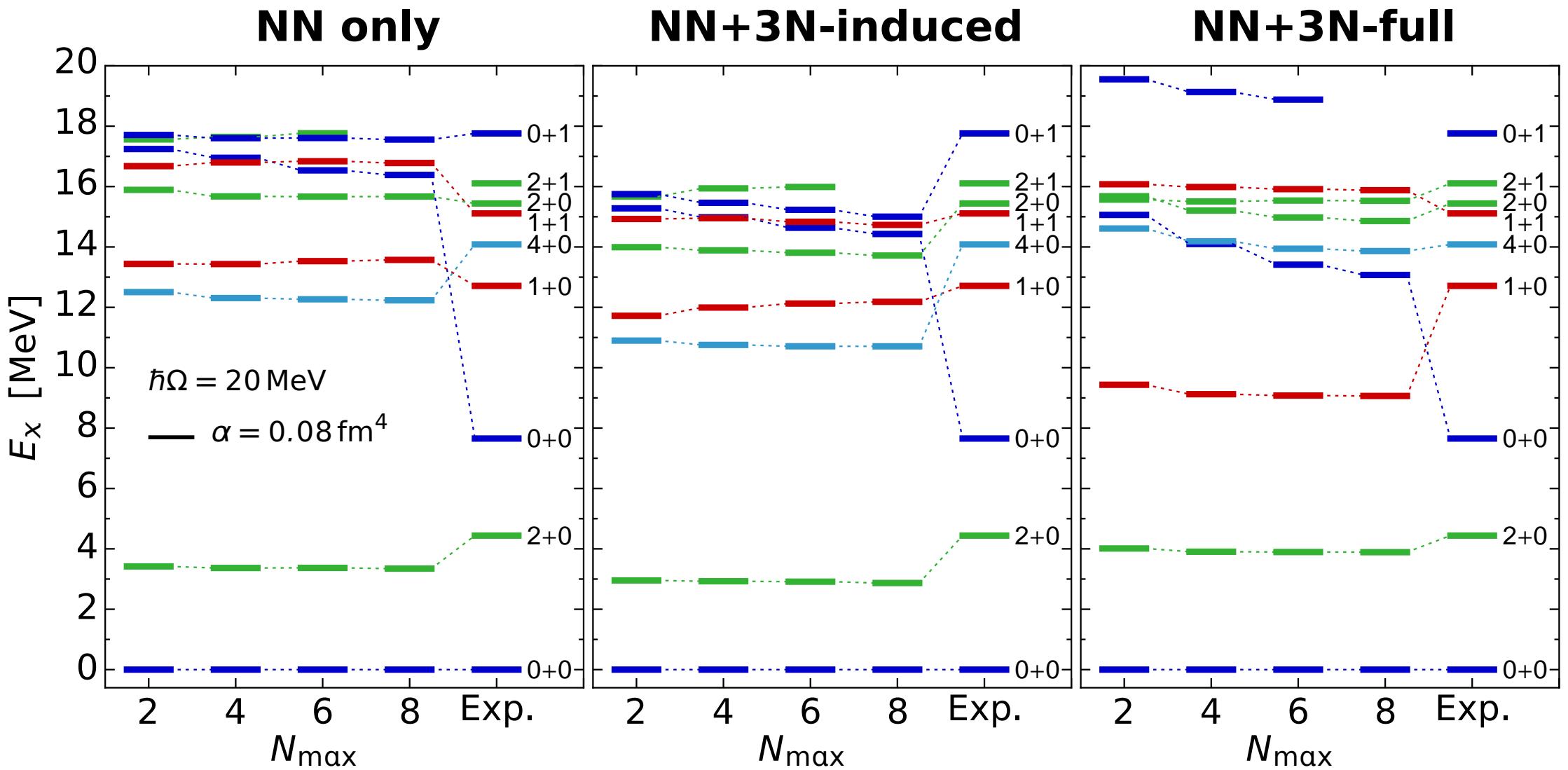
# $^{16}\text{O}$ : Ground-State Energies



# $^6\text{Li}$ : Excitation Energies

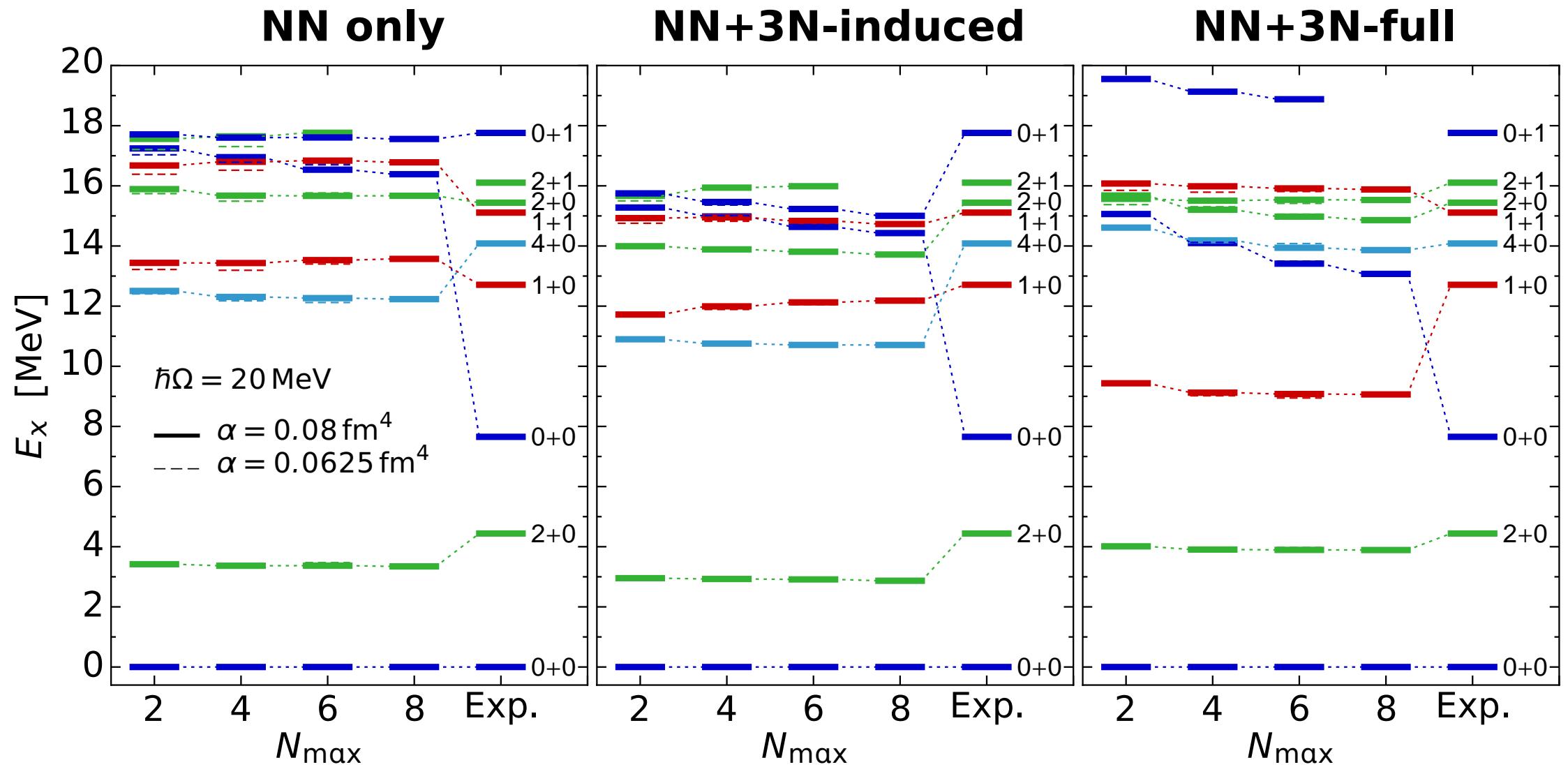


# Spectroscopy of $^{12}\text{C}$



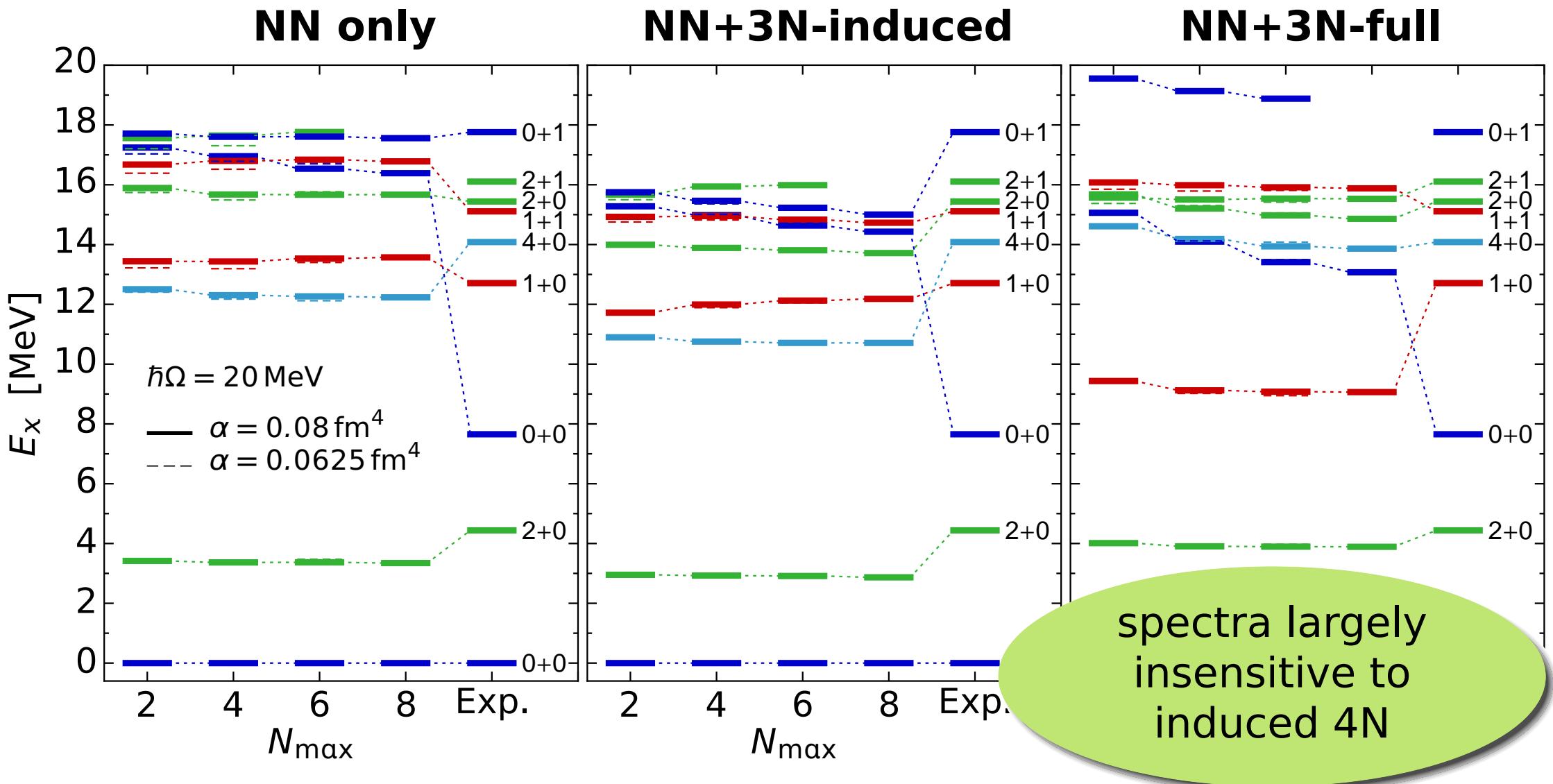
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# Where do we go from here?

- beyond the lightest nuclei, **SRG-induced 4N contributions** affect the absolute energies, but not the excitation energies
- with the inclusion of the leading 3N interaction we already obtain a **very reasonable description** of spectra (and ground states)

## SRG Transformation

- Which parts of the initial 3N cause the induced 4N contributions ?
- Can we find alternative SRG generators with suppressed induced 4N ?

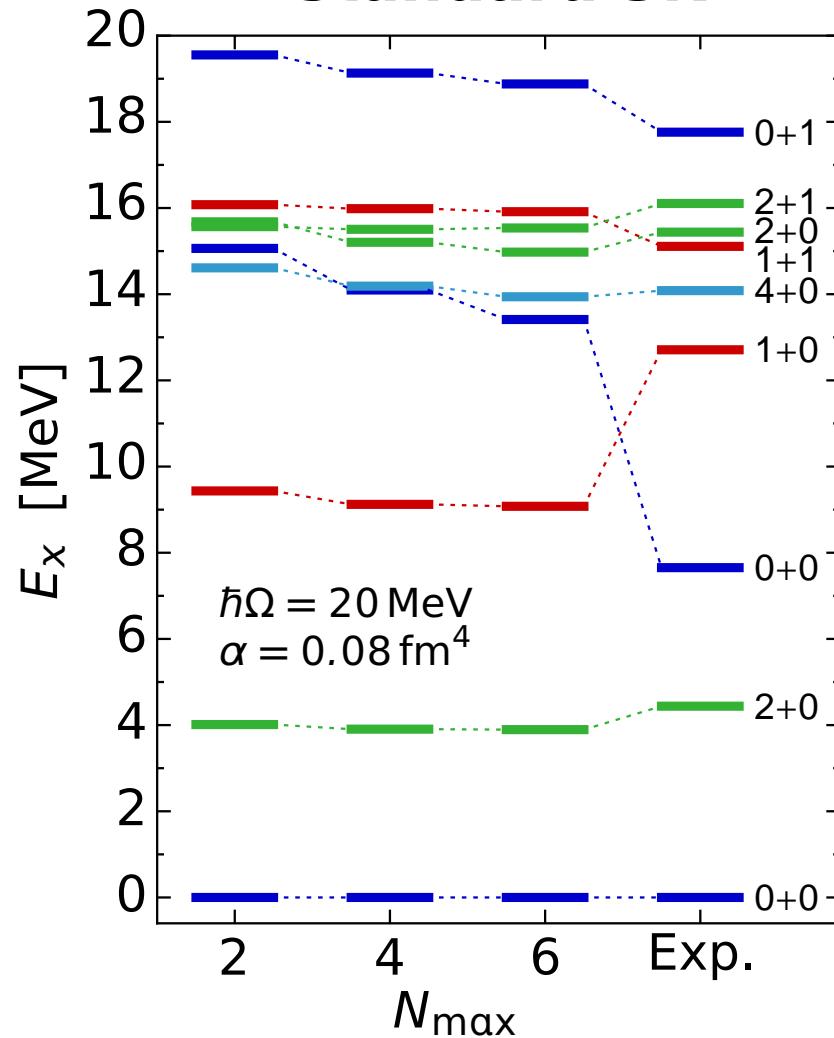
## Chiral NN+3N Interactions

- How sensitive is the spectroscopy on specifics of the 3N interaction (cutoff,  $c_i$ 's) ?
- How does the inclusion of the subleading 3N terms affect the picture ?

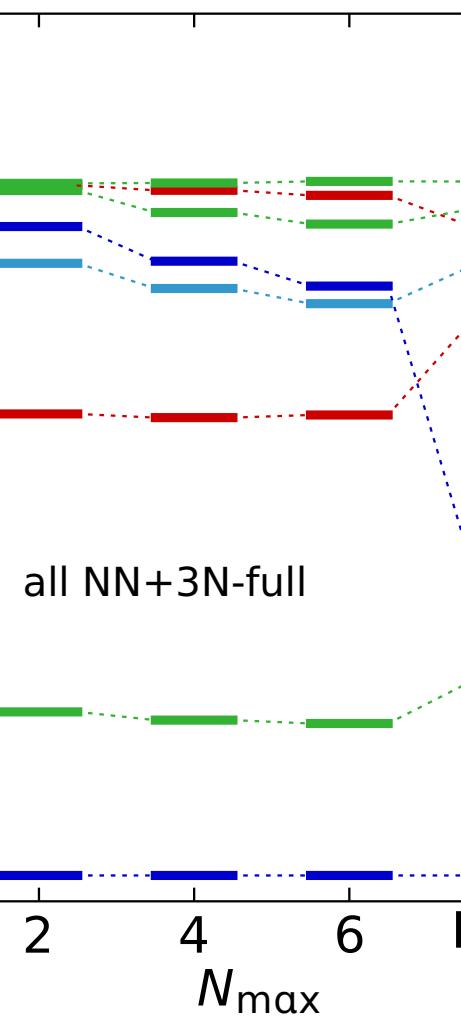
# Sensitivity on Initial $3\text{N} - {}^{12}\text{C}$

modified 3N interaction with  
shifted  $c_i$   
**400 MeV cutoff**

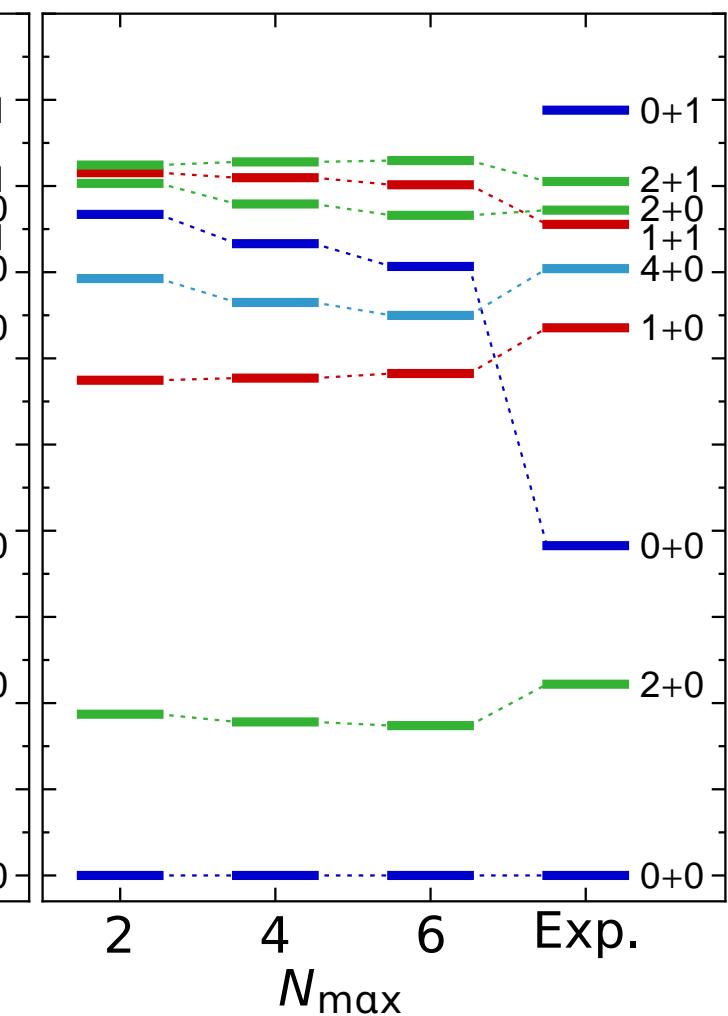
**standard 3N**



**shifted  $c_i$**



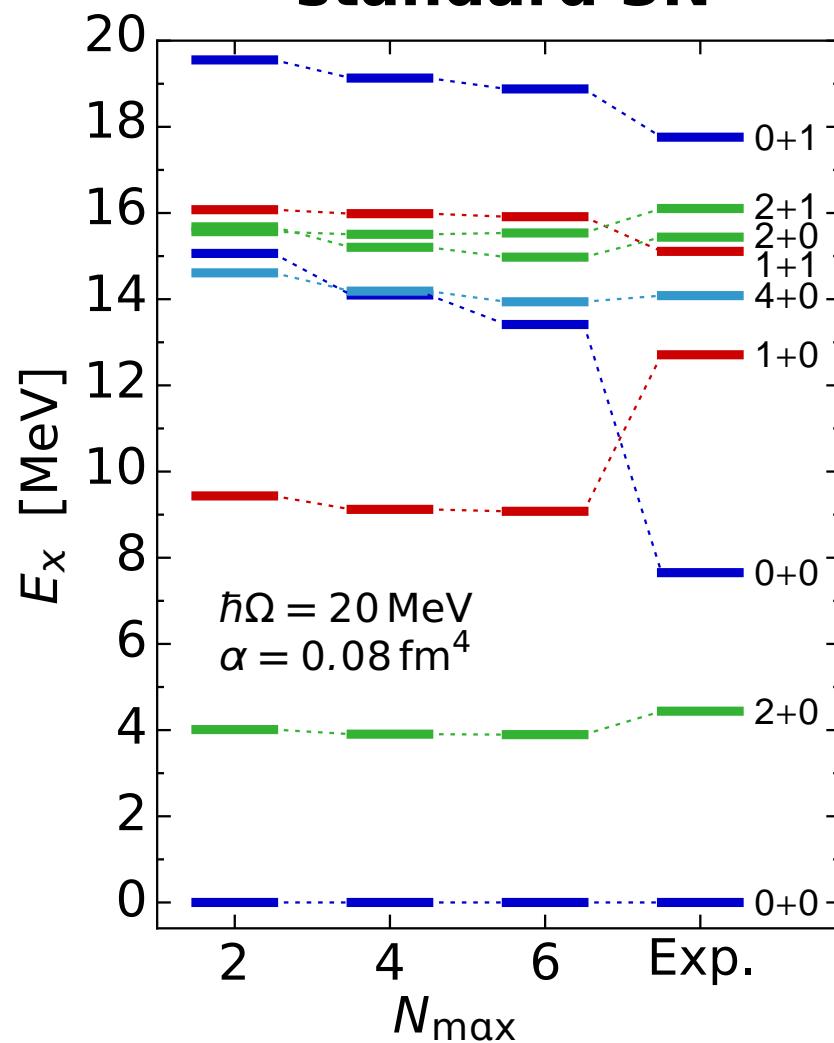
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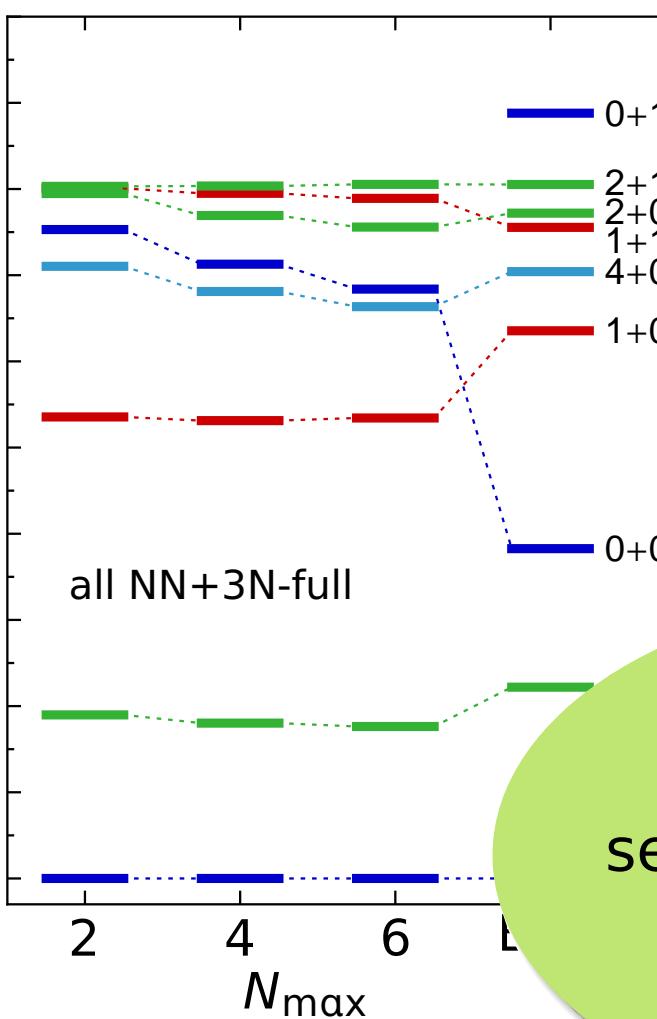
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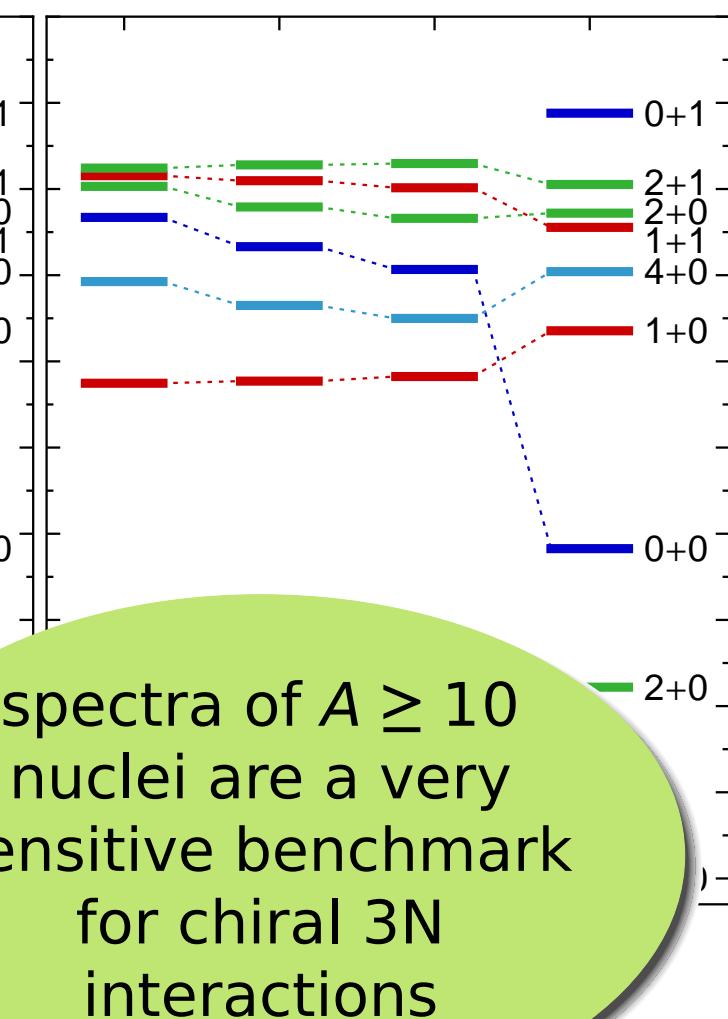
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spectra of  $A \geq 10$   
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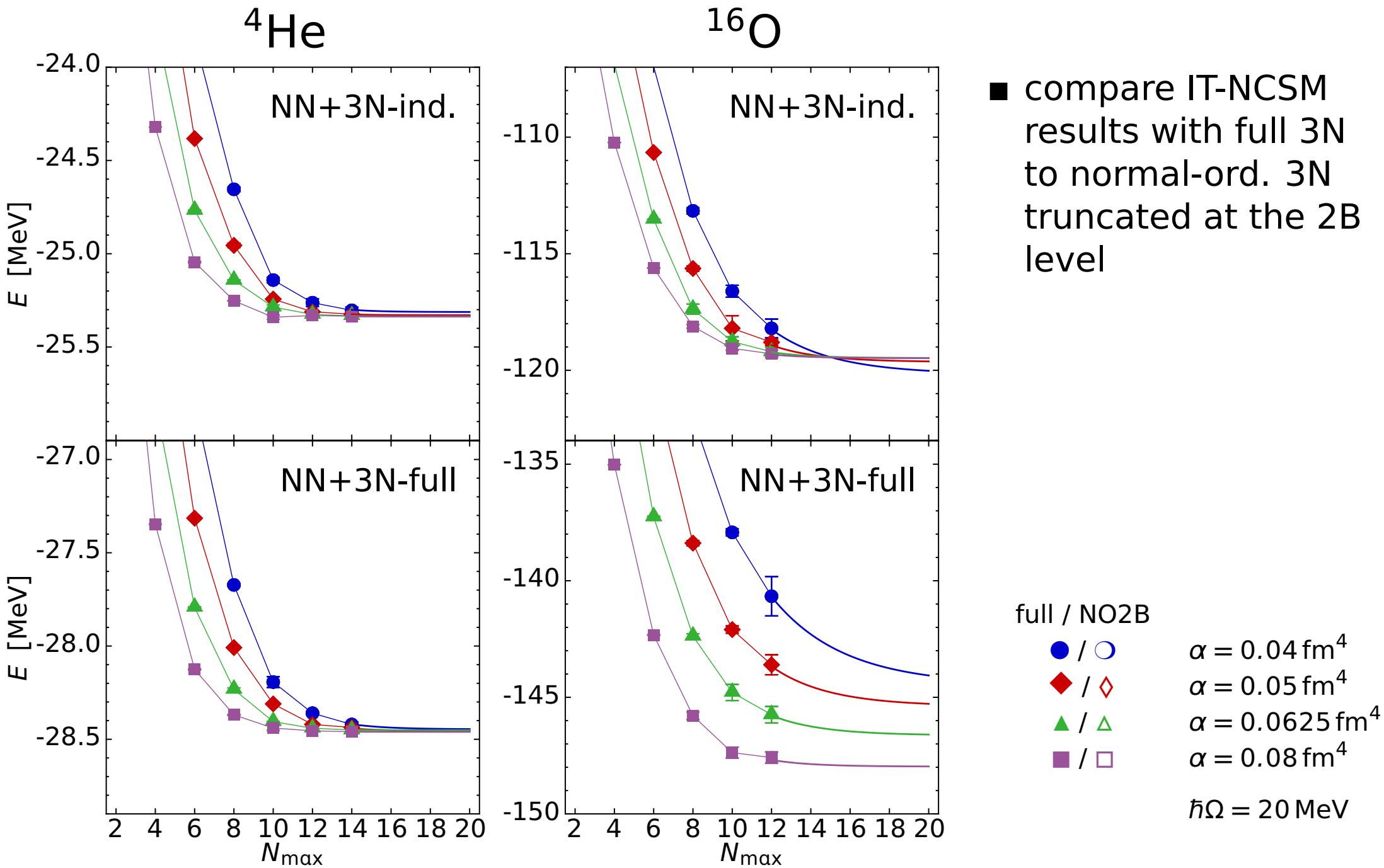
# Normal-Ordered 3N Interaction

- **motivation**: avoid the formal and computational complications of including a full 3N interaction into the many-body calculation
- **idea**: write the 3N operator in normal-ordered form with respect to an A-body reference Slater-determinant ( $0\hbar\Omega$  state)

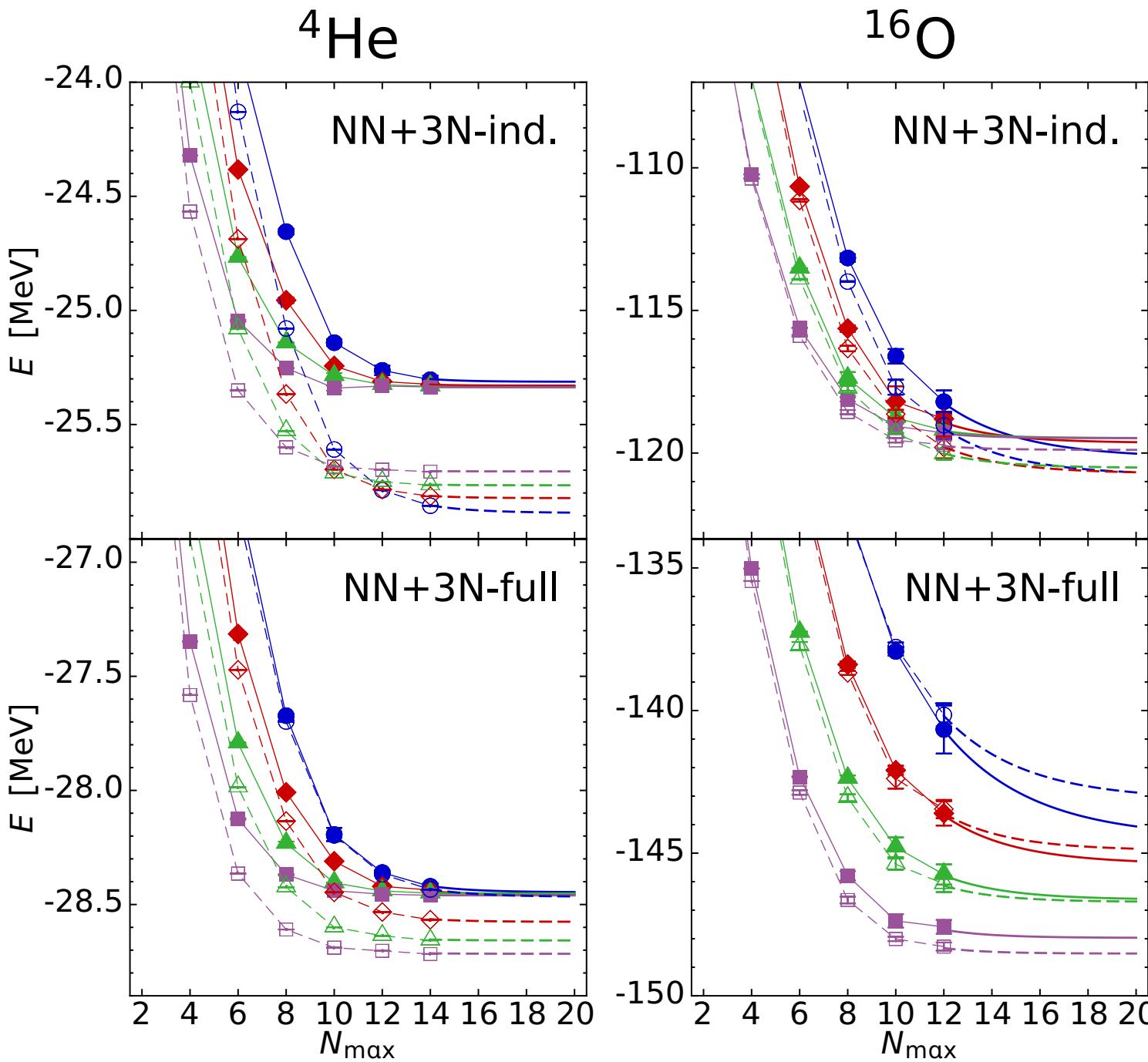
$$\begin{aligned} V_{3N} &= \sum V_{ooooo}^{3N} a_o^\dagger a_o^\dagger a_o^\dagger a_o a_o a_o \\ &= W_{oo}^{0B} + \sum W_{ooo}^{1B} \{a_o^\dagger a_o\} + \sum W_{oooo}^{2B} \{a_o^\dagger a_o^\dagger a_o a_o\} \\ &\quad + \sum W_{ooooo}^{3B} \{a_o^\dagger a_o^\dagger a_o^\dagger a_o a_o a_o\} \end{aligned}$$

- **question**: if we keep only the normal-ordered 0B, 1B & 2B terms, how well does this approximation work ?

# Benchmark of Normal-Ordered 3N



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- compare IT-NCSM results with full 3N to normal-ord. 3N truncated at the 2B level

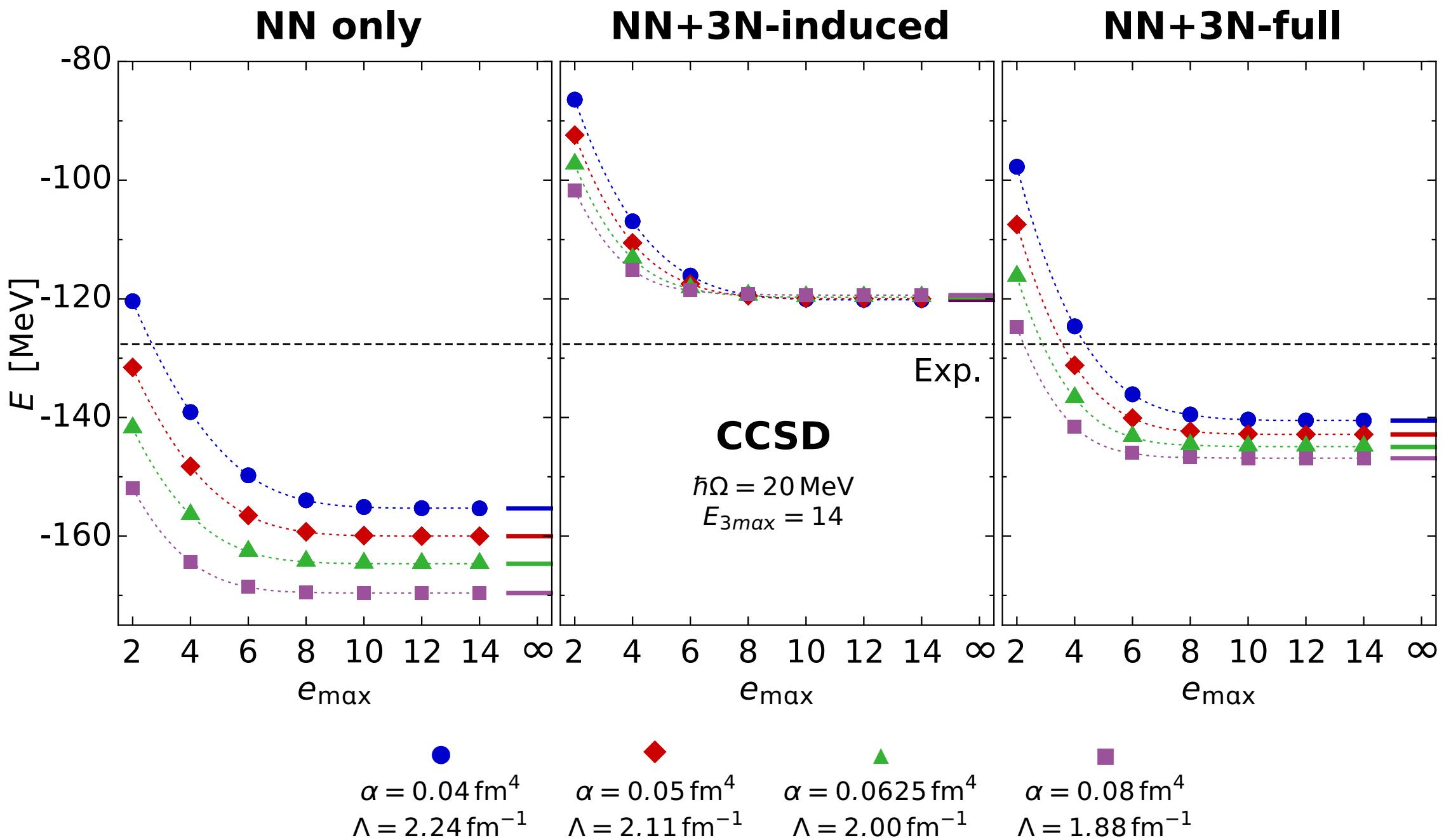
- typical deviations up to 2% for  ${}^4\text{He}$  and 1% for  ${}^{16}\text{O}$

full / NO2B

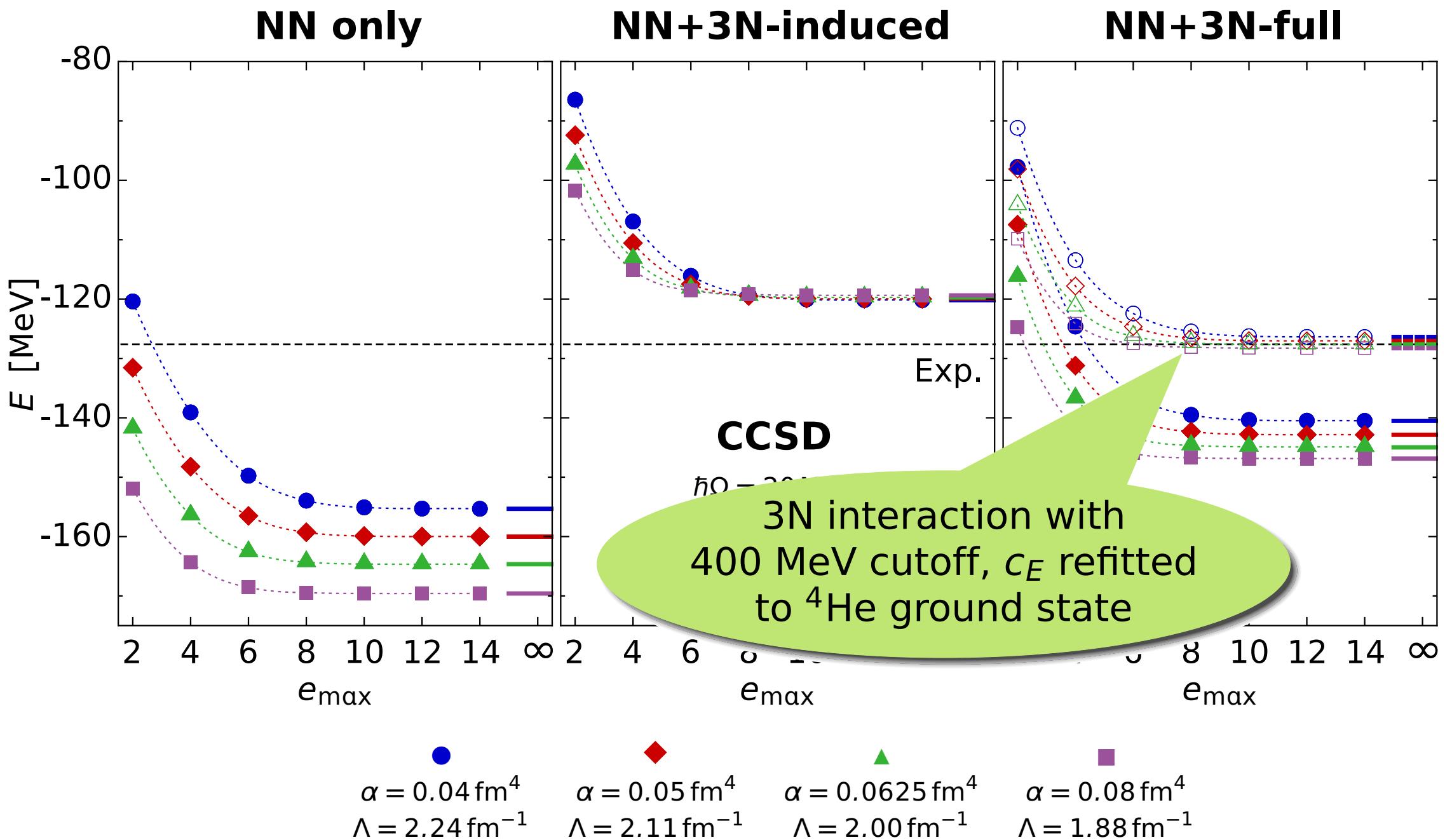
- |       |                                |
|-------|--------------------------------|
| ● / ○ | $\alpha = 0.04 \text{ fm}^4$   |
| ◆ / ◇ | $\alpha = 0.05 \text{ fm}^4$   |
| ▲ / △ | $\alpha = 0.0625 \text{ fm}^4$ |
| ■ / □ | $\alpha = 0.08 \text{ fm}^4$   |

$$\hbar\Omega = 20 \text{ MeV}$$

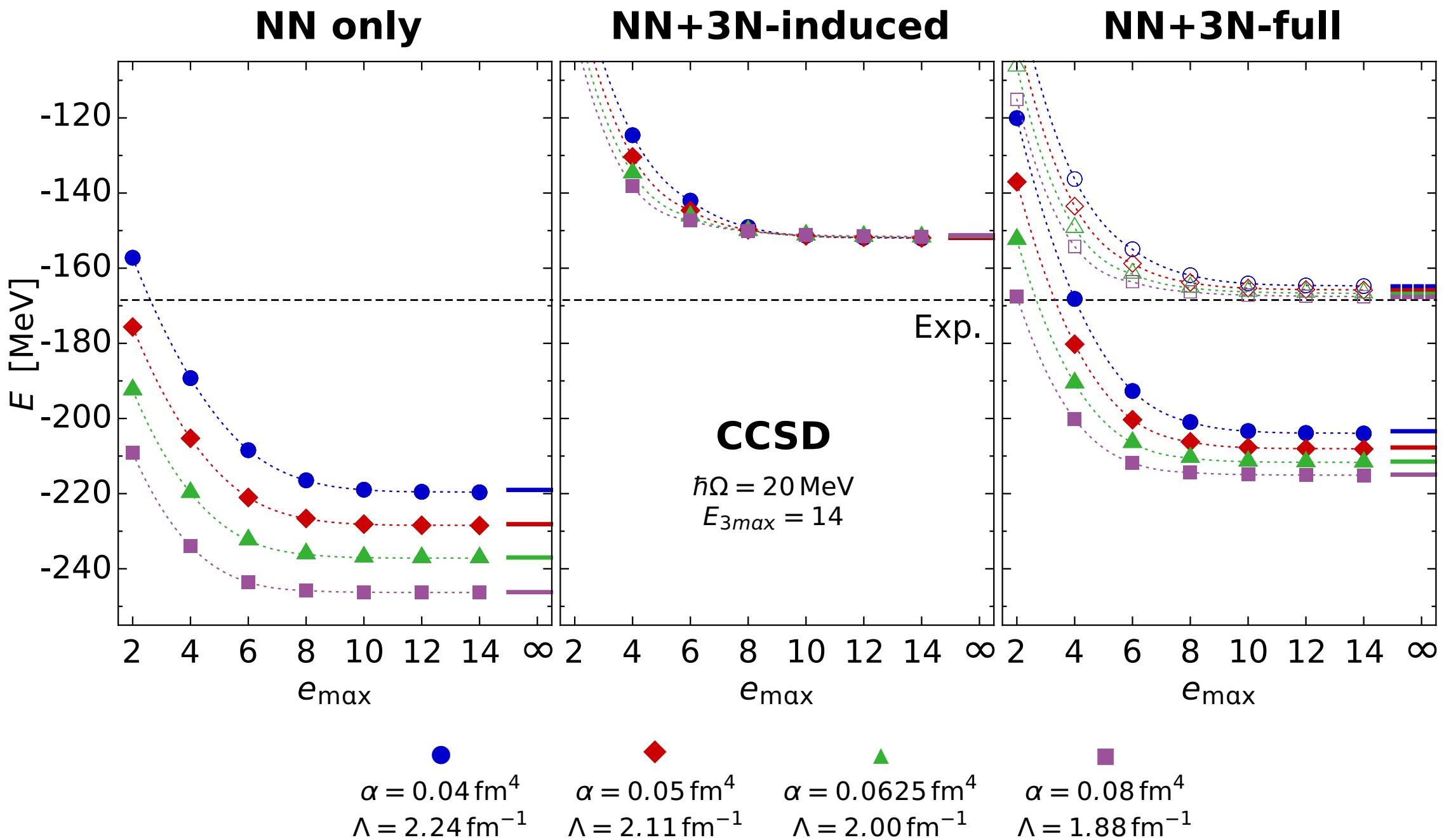
# $^{16}\text{O}$ : Coupled-Cluster with 3N<sub>NO2B</sub>



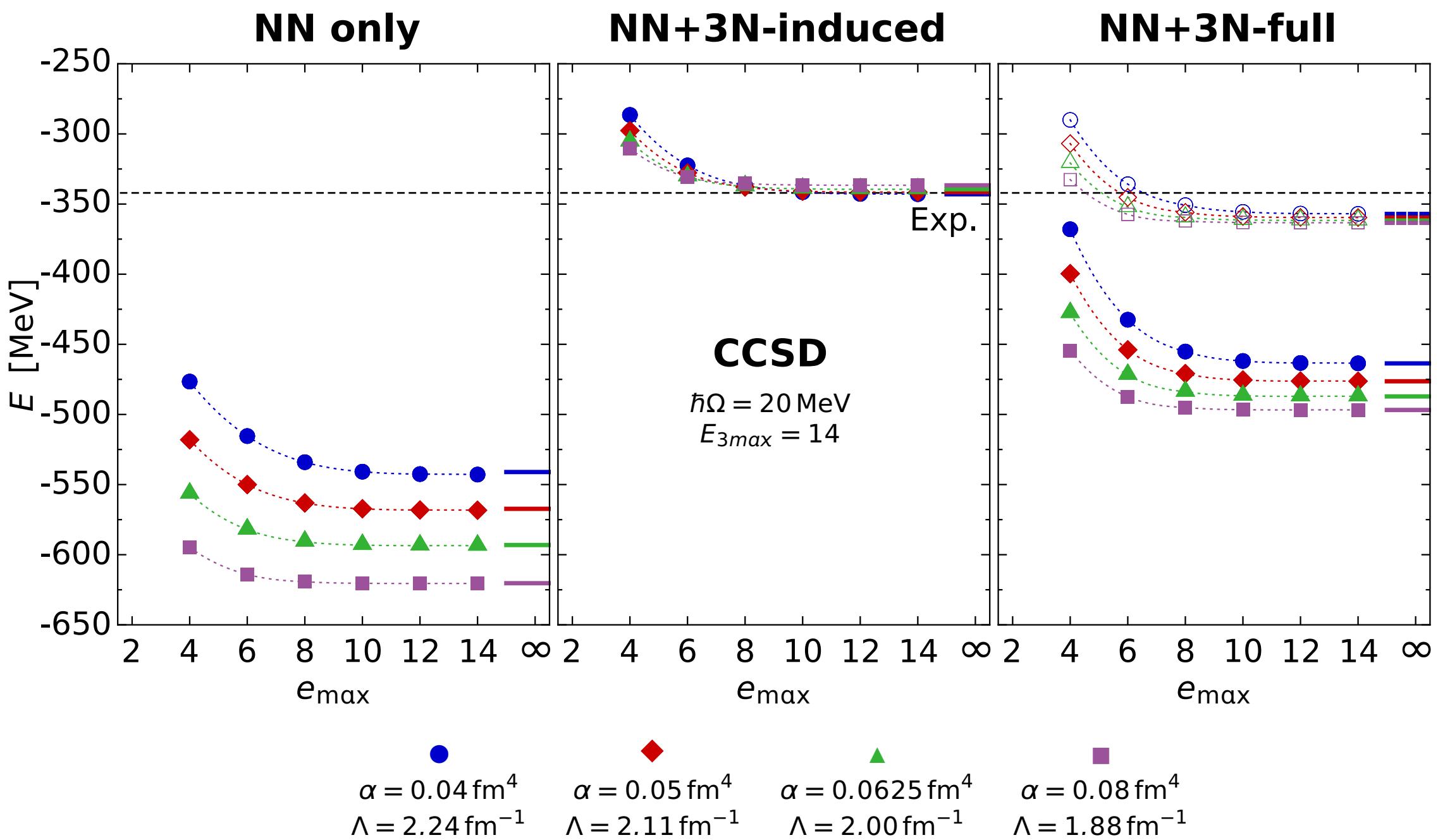
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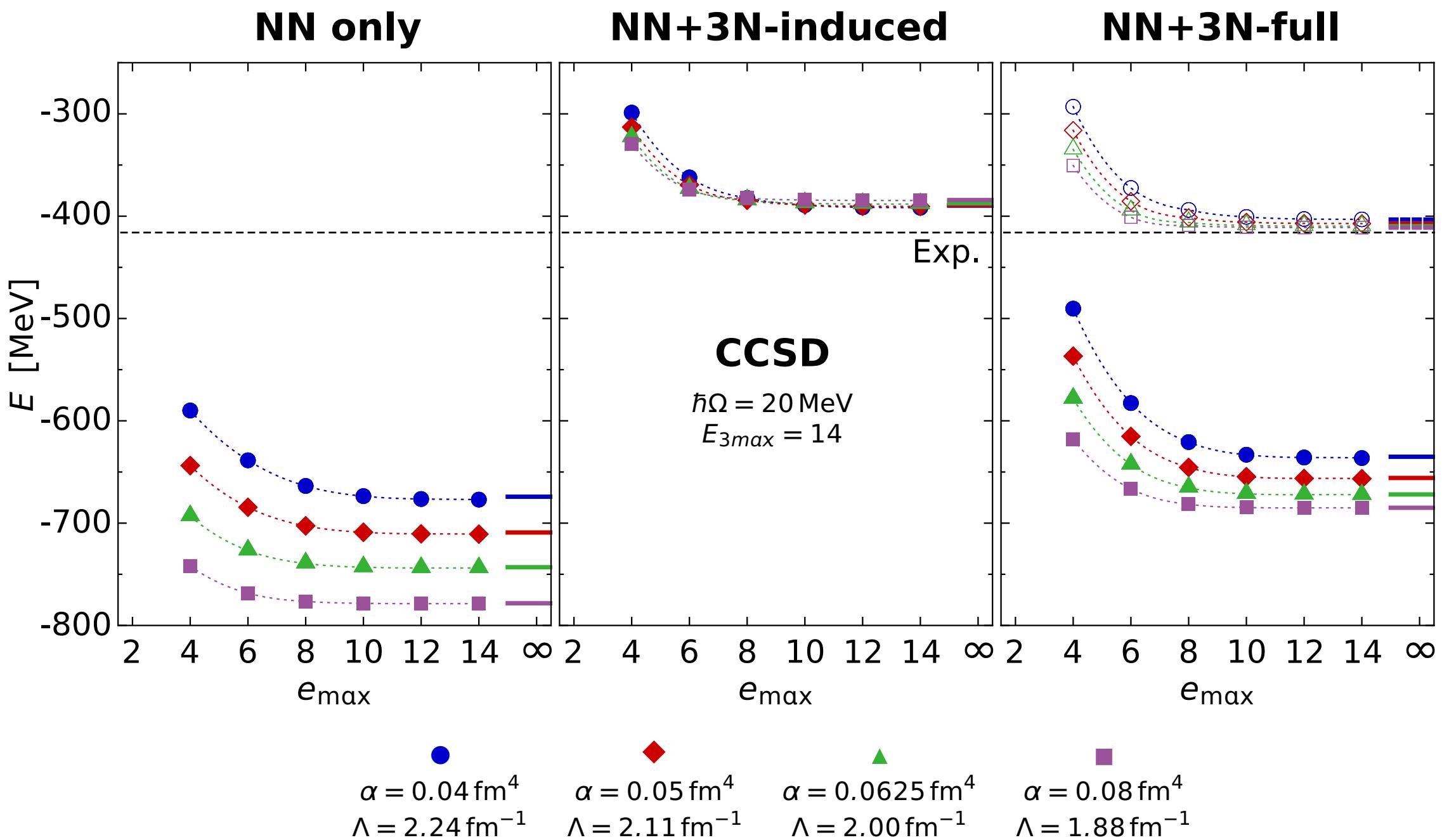
# $^{24}\text{O}$ : Coupled-Cluster with 3N<sub>NO2B</sub>



# $^{40}\text{Ca}$ : Coupled-Cluster with $3\text{N}_{\text{NO2B}}$



# $^{48}\text{Ca}$ : Coupled-Cluster with 3N<sub>NO2B</sub>



# Conclusions

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- new era of **ab-initio nuclear structure and reaction theory** connected to QCD via chiral EFT
  - chiral EFT as universal starting point... some issues remain
- consistent **inclusion of 3N interactions** in similarity transformations & many-body calculations
  - breakthrough in computation & handling of 3N matrix elements
- **innovations in many-body theory**: extended reach of exact methods & improved control over approximations
  - versatile toolbox for different observables & mass ranges
- many **exciting applications** ahead...

# Epilogue

## ■ thanks to my group & my collaborators

- **S. Binder, A. Calci**, B. Erler, E. Gebrerufael,  
A. Günther, H. Krutsch, **J. Langhammer**,  
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- **P. Navrátil**

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- S. Quaglioni

LLNL Livermore, USA

- P. Piecuch

Michigan State University, USA

- C. Forssén

Chalmers University, Sweden

- H. Feldmeier, T. Neff

GSI Helmholtzzentrum

- H. Hergert

Ohio State University, USA

- P. Papakonstantinou

IPN Orsay, F



Deutsche  
Forschungsgemeinschaft  
**DFG**

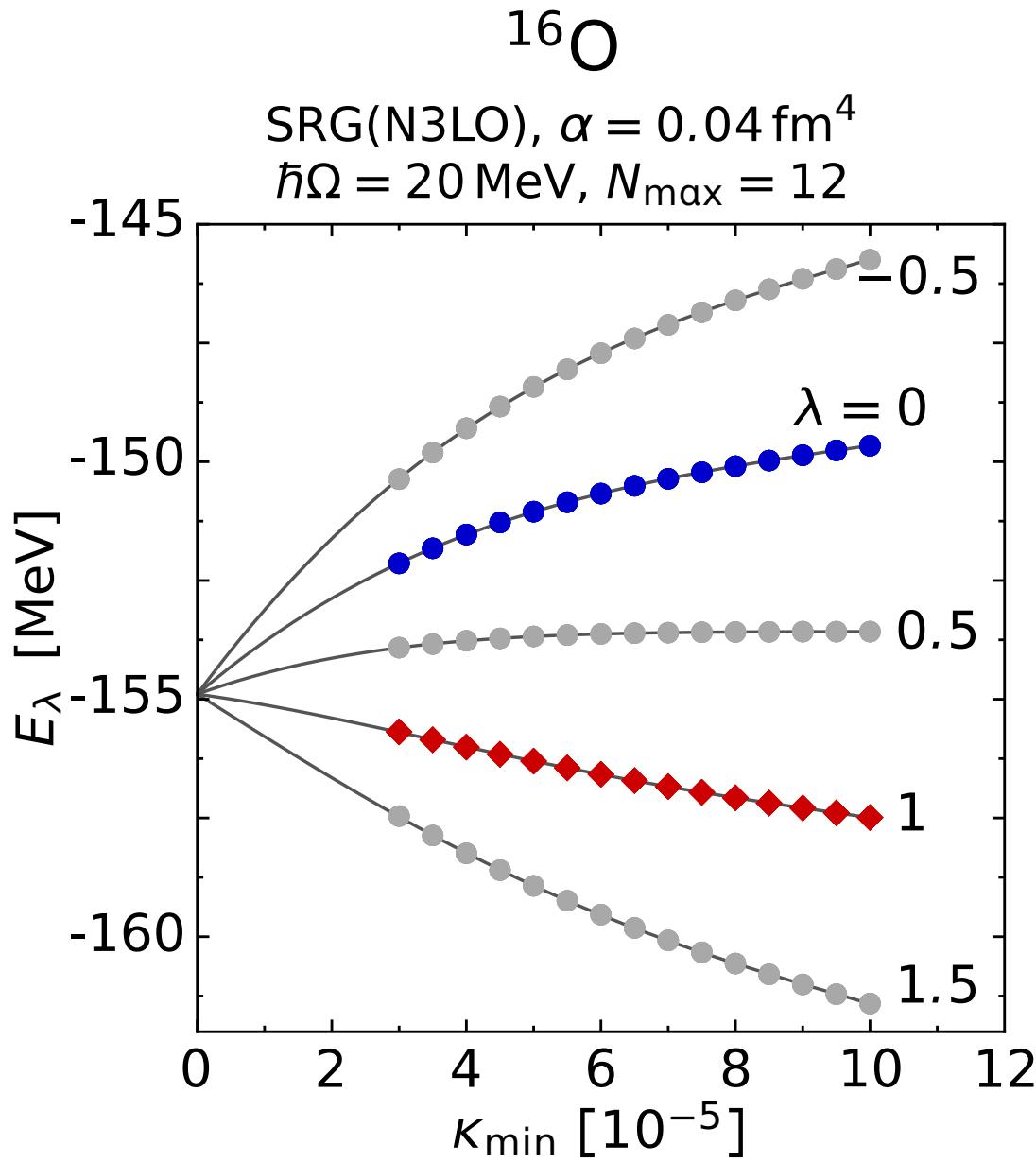


 **LOEWE** – Landes-Offensive  
zur Entwicklung Wissenschaftlich-  
ökonomischer Exzellenz



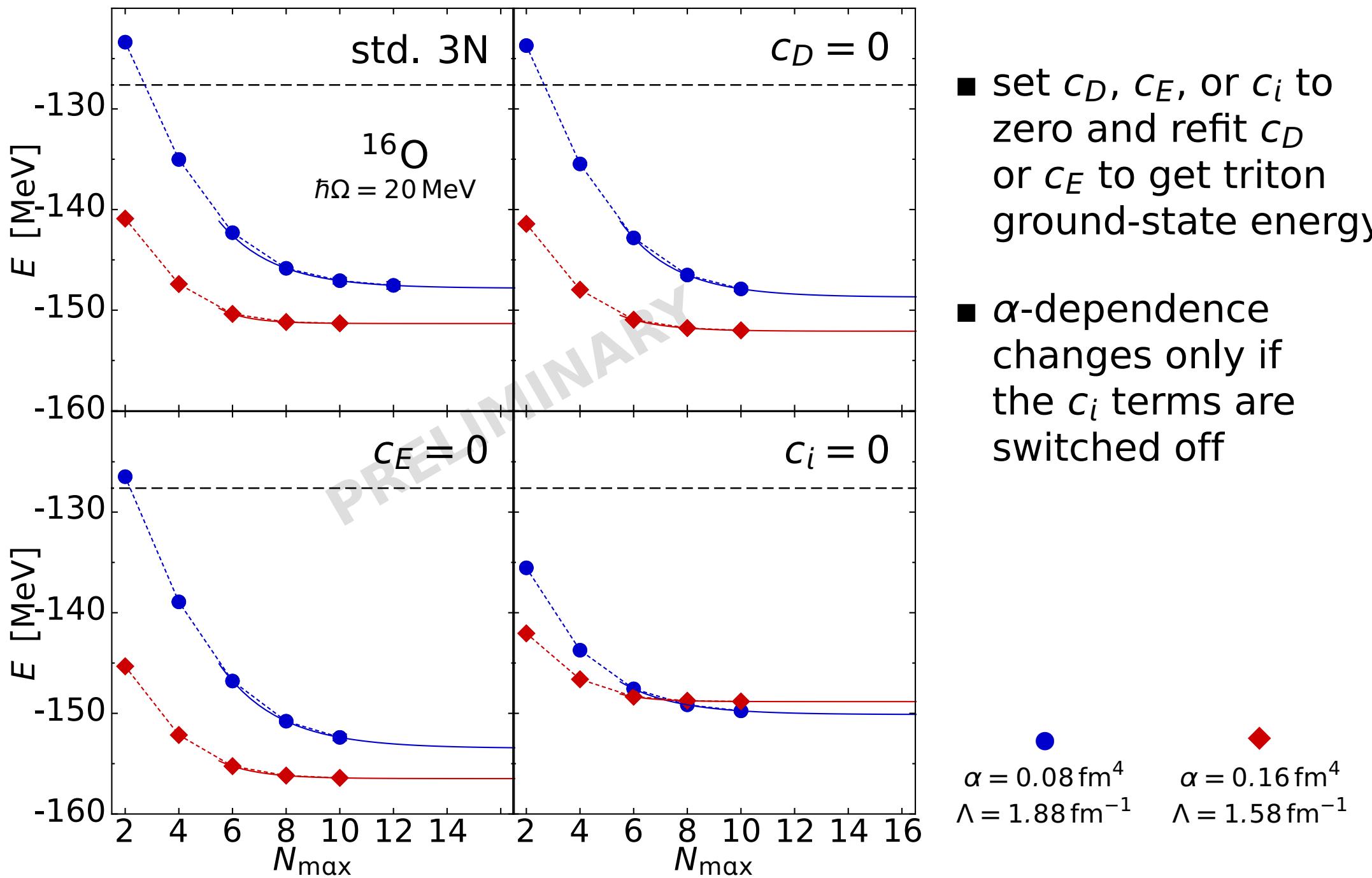
# Supplements

# Constrained Threshold Extrapolation

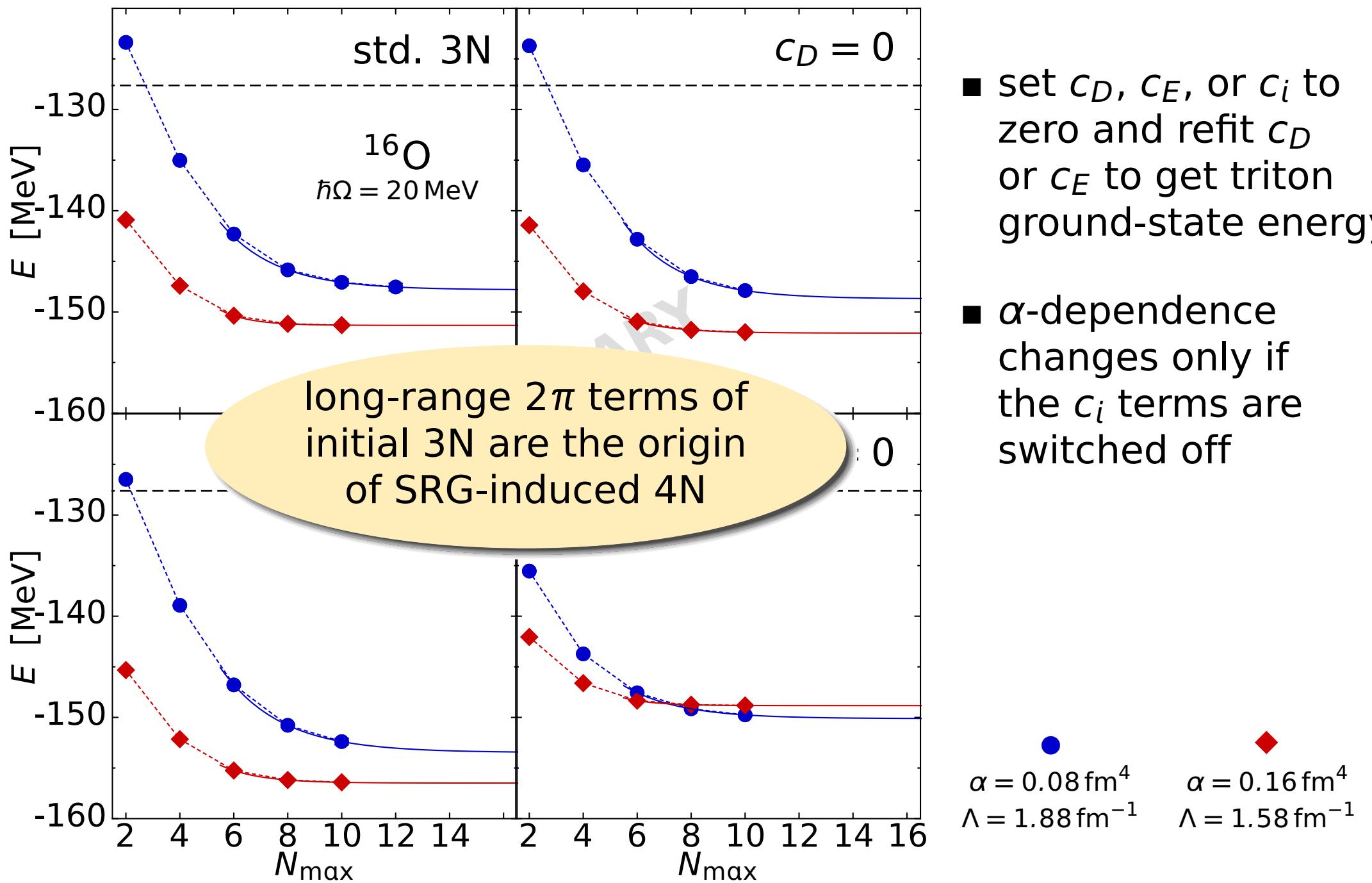


- estimate energy contribution of **excluded states** perturbatively  $\rightarrow \Delta_{\text{excl}}(\kappa_{\min})$
- **simultaneous fit** of combined energy  
$$E_\lambda(\kappa_{\min}) = E_{\text{int}}(\kappa_{\min}) + \lambda \Delta_{\text{excl}}(\kappa_{\min})$$
for set of  $\lambda$ -values with the constraint  $E_\lambda(0) = E_{\text{extrap}}$
- **robust threshold extrapolation** with error bars determined by variation of fit function

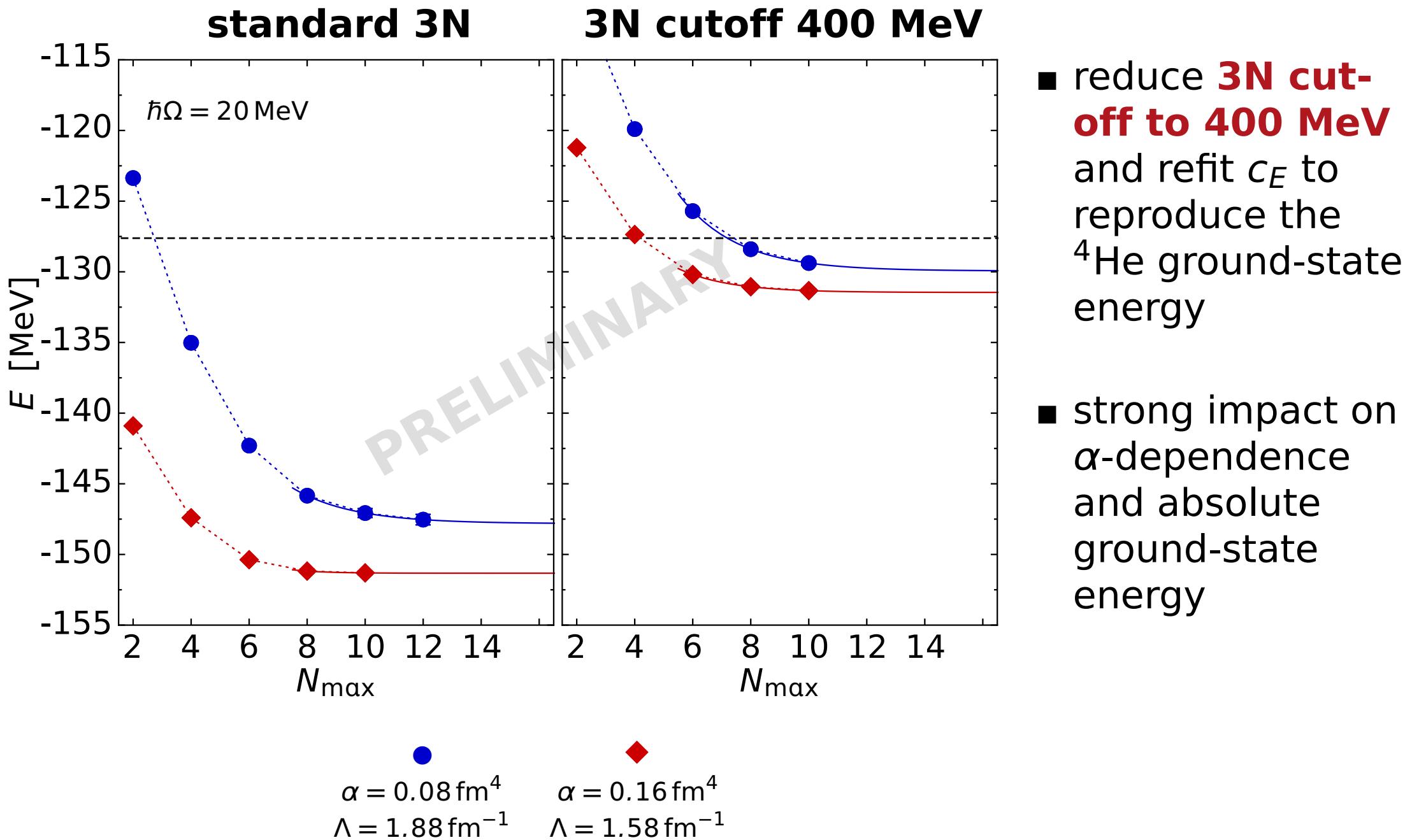
# Origin of SRG-Induced 4N Terms



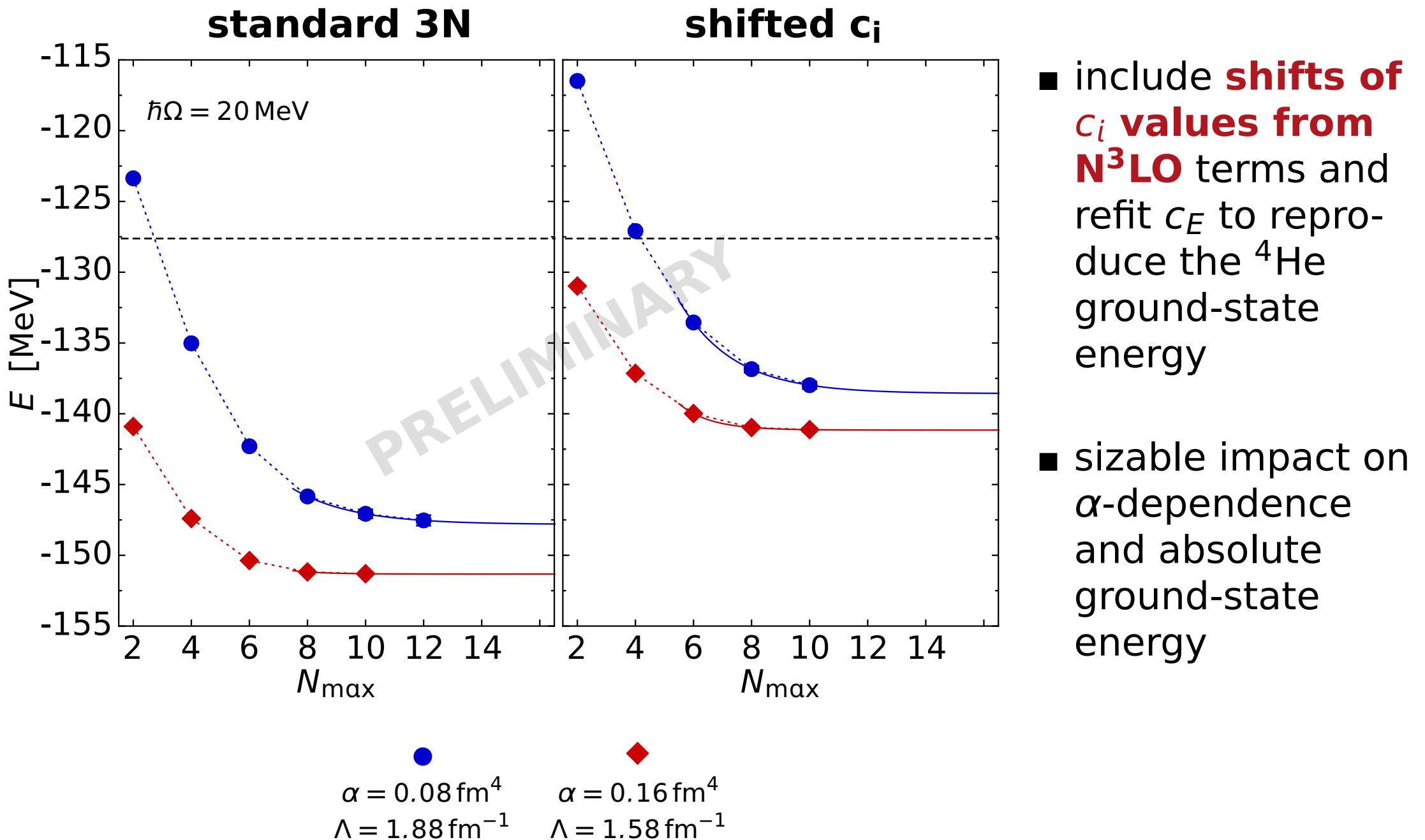
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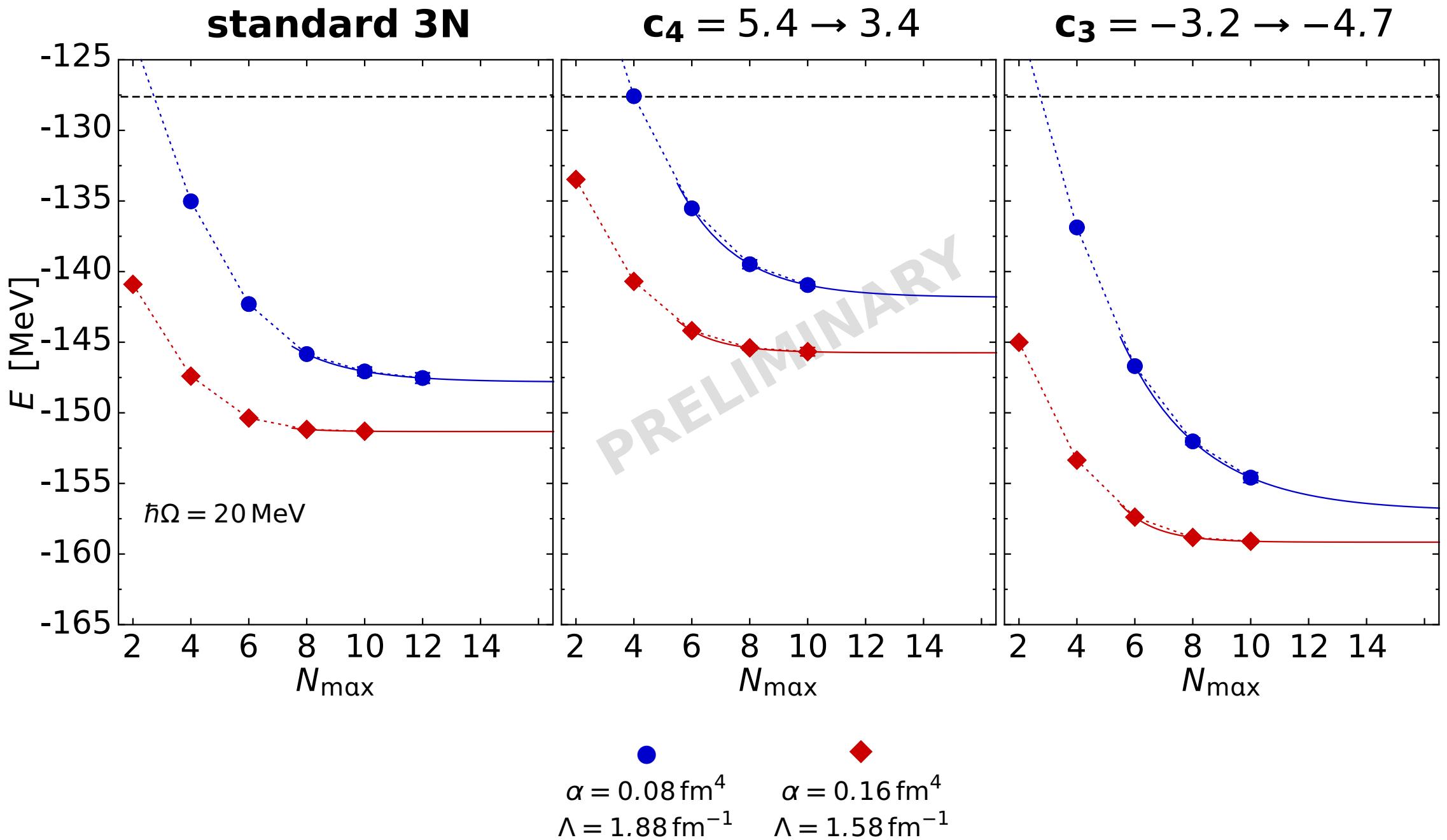
# Sensitivity on 3N Cutoff: $^{16}\text{O}$



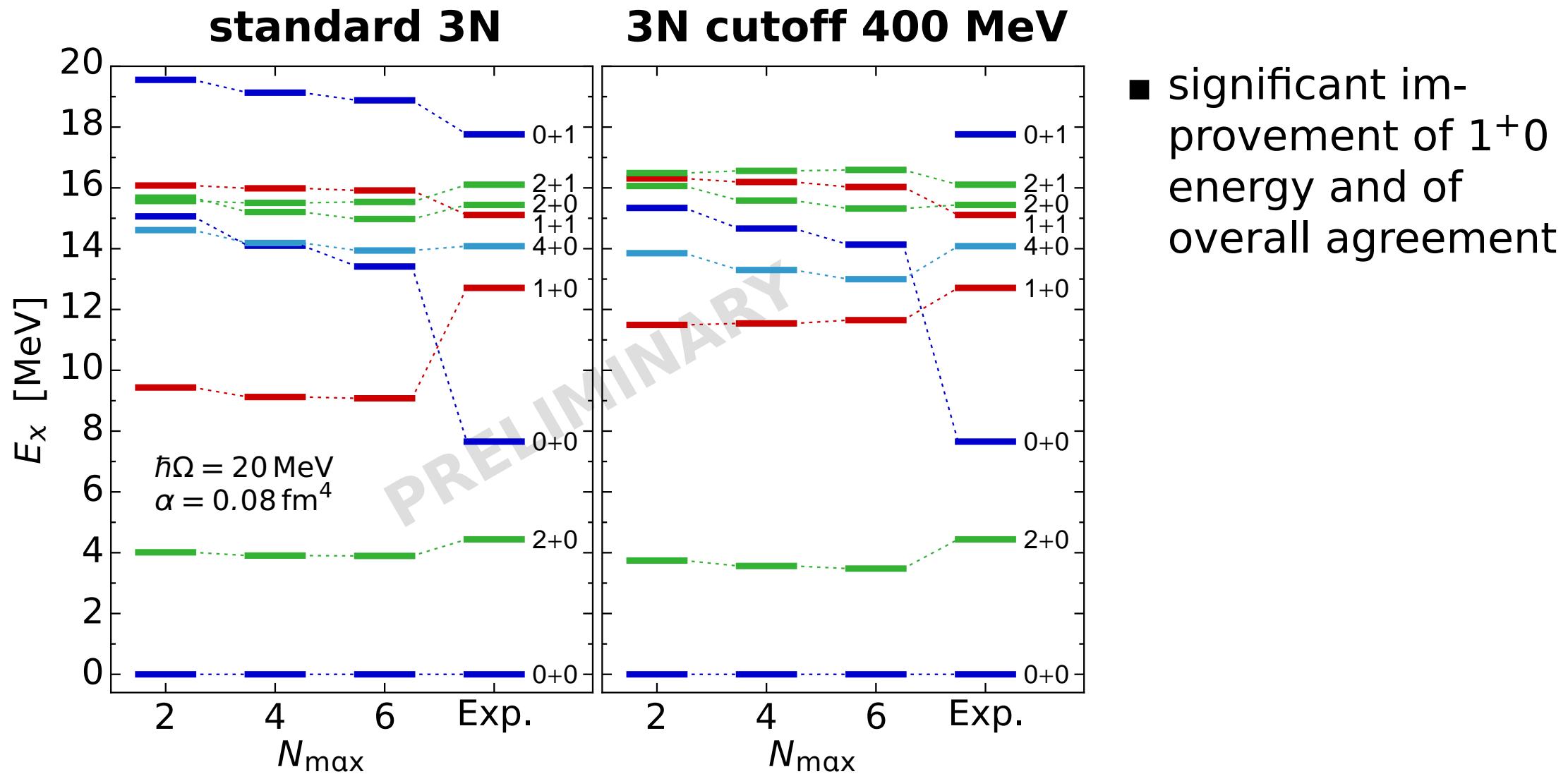
# Sensitivity on $c_i$ Shift: $^{16}\text{O}$



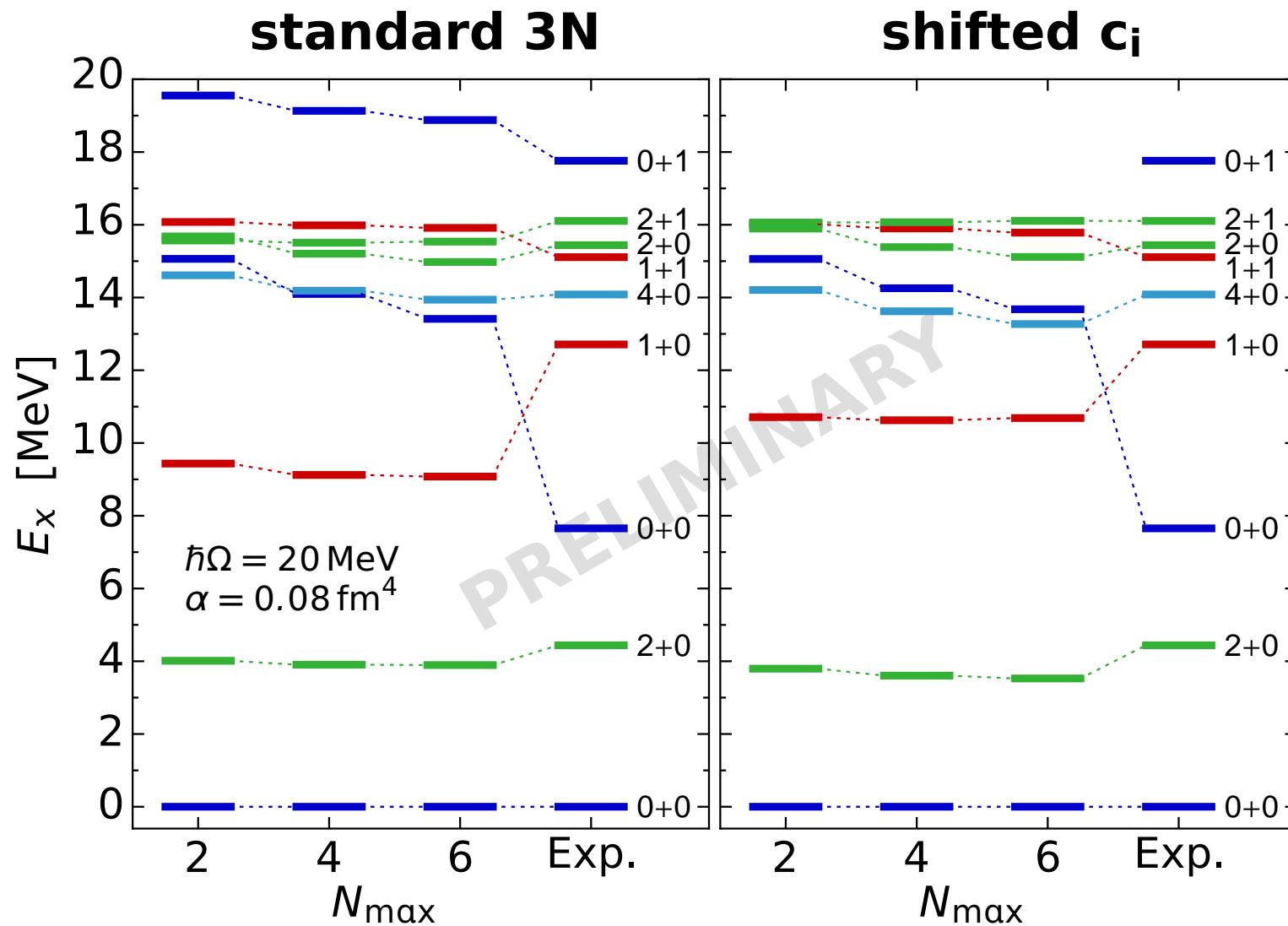
# Sensitivity on $c_3$ & $c_4$ : $^{16}\text{O}$



# Sensitivity on 3N Cutoff: $^{12}\text{C}$

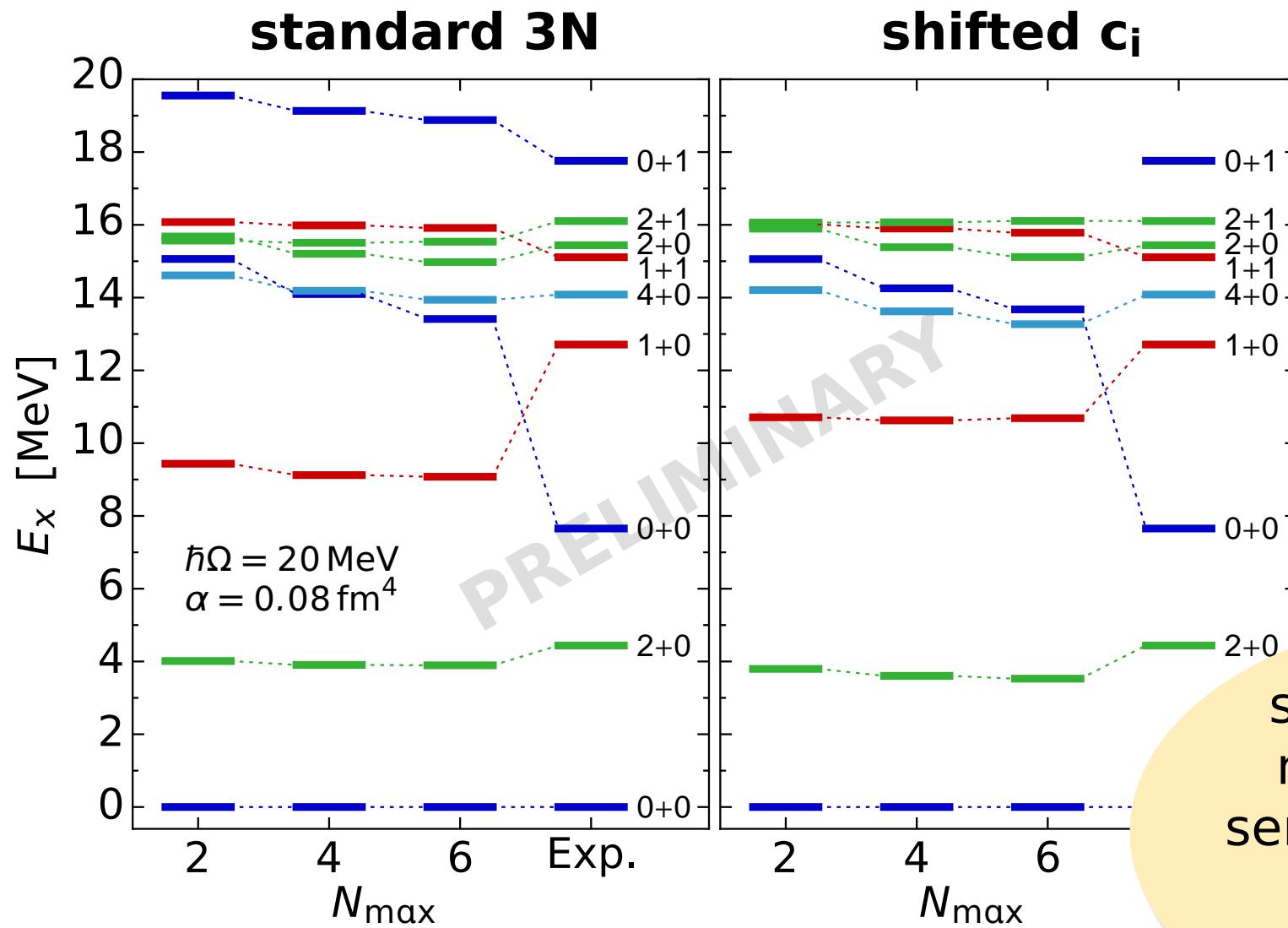


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