Ab Initio Nuclear Structure Theory

with Chiral NN plus 3N Interactions

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From QCD to Nuclear Structure

Nuclear Structure

Low-Energy QCD

From QCD to Nuclear Structure

Nuclear Structure

NN+3N Interaction from Chiral EFT

Low-Energy QCD

- chiral EFT based on the relevant degrees of freedom & symmetries of QCD
- provides consistent NN & 3N interaction plus currents
- in the following:
  - NN at N^3LO (Entem & Machleidt, 500 MeV)
  - 3N at N^2LO (low-energy constants c_D & c_E from triton fit)

From QCD to Nuclear Structure

Nuclear Structure

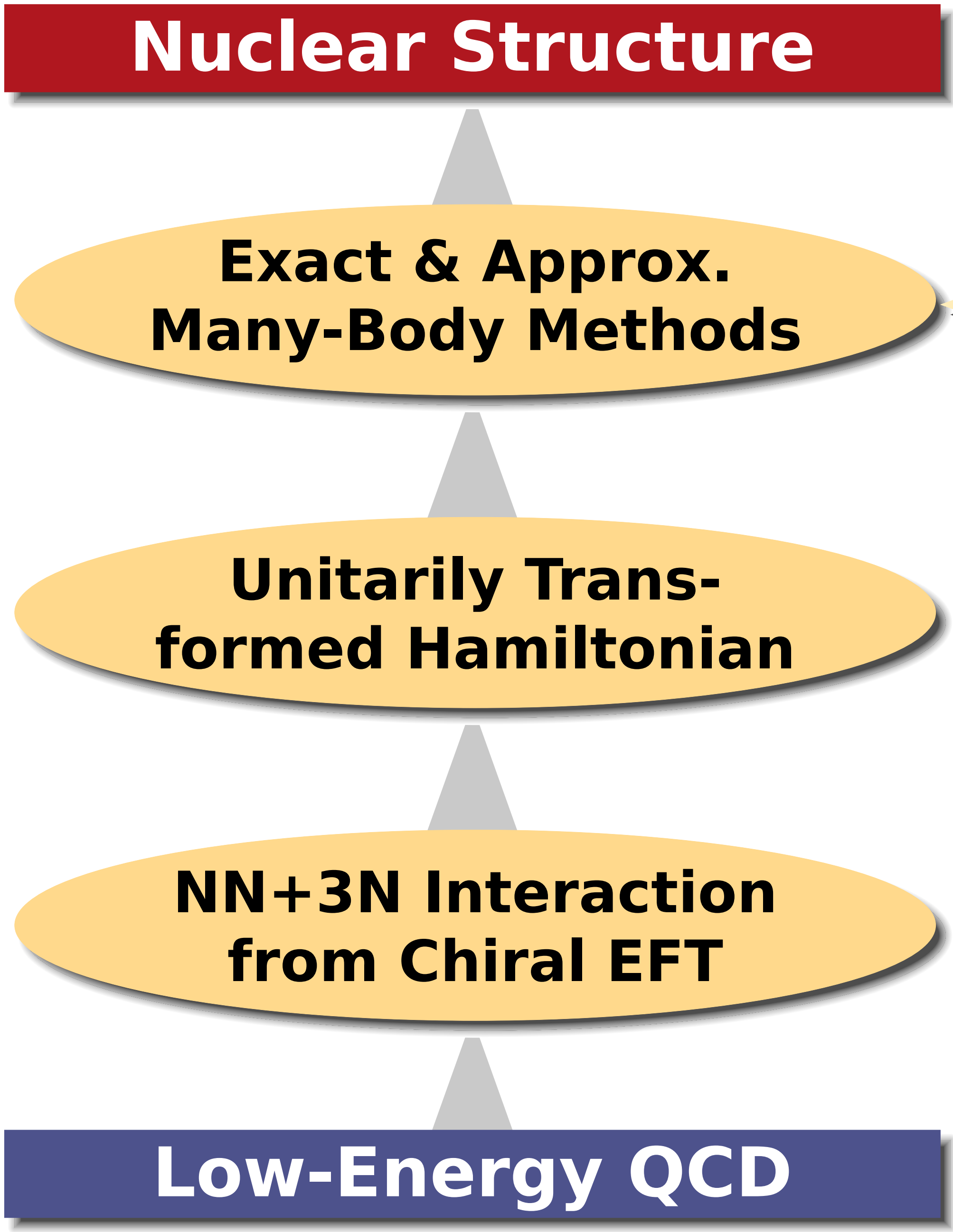
Unitarily Transformed Hamiltonian

- 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

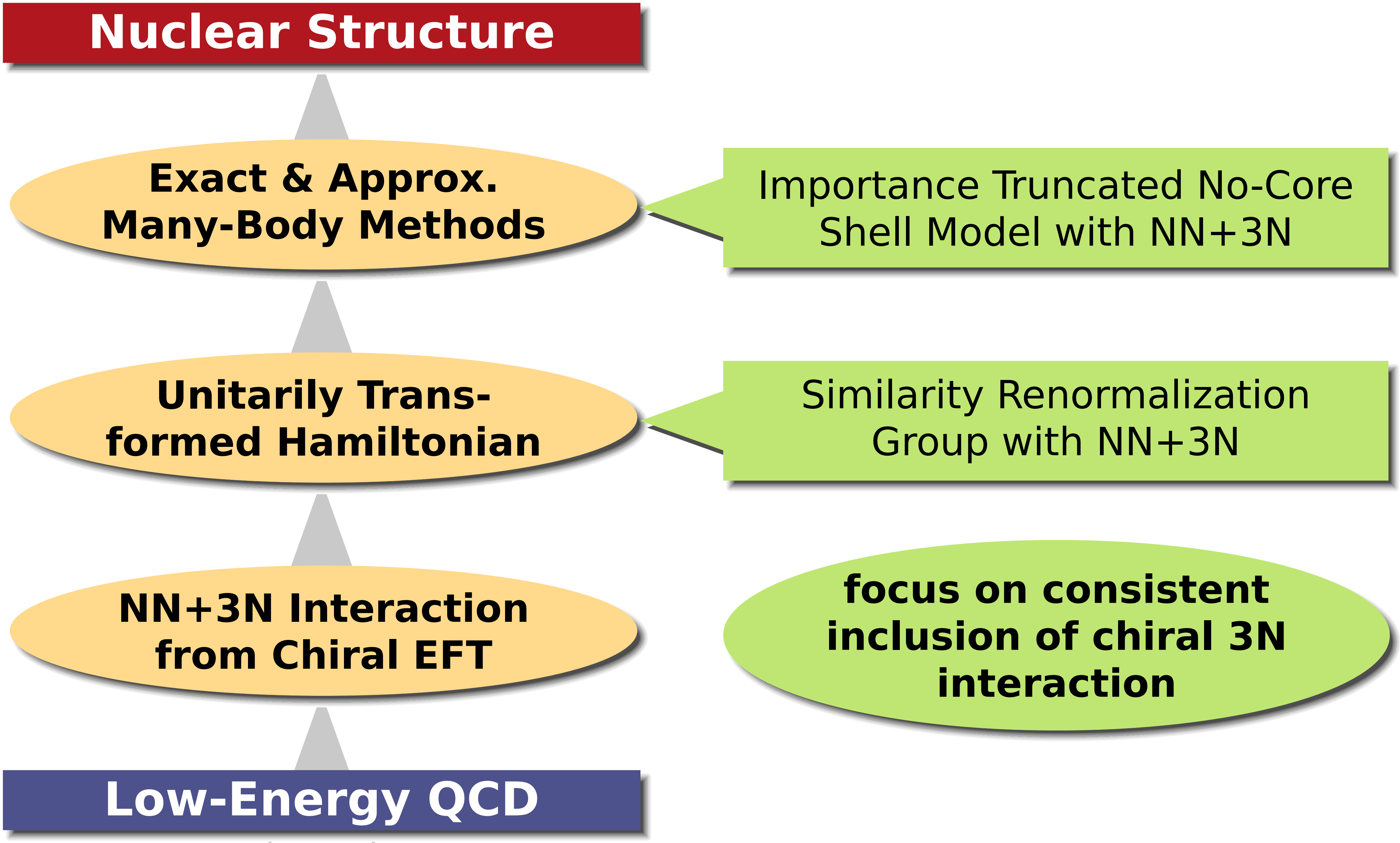
Low-Energy QCD

From QCD to Nuclear Structure



- 'exact' solution of the many-body problem for light & inter-mediate masses (NCSM, CC,...)
- controlled approximations for heavier nuclei (HF & MBPT,...)
- all rely on restricted model spaces & benefit from unitary transformation

From QCD to Nuclear Structure



Unitarily Transformed Hamiltonian

Similarity Renormalization Group

Roth et al. — Phys. Rev. Lett. (2011); arXiv:1105.3173
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)

Similarity Renormalization Group

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

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

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

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

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

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

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

Similarity Renormalization Group

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

simplicity and flexibility are great advantages of the SRG approach

- **unitary transformation** of Hami

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

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

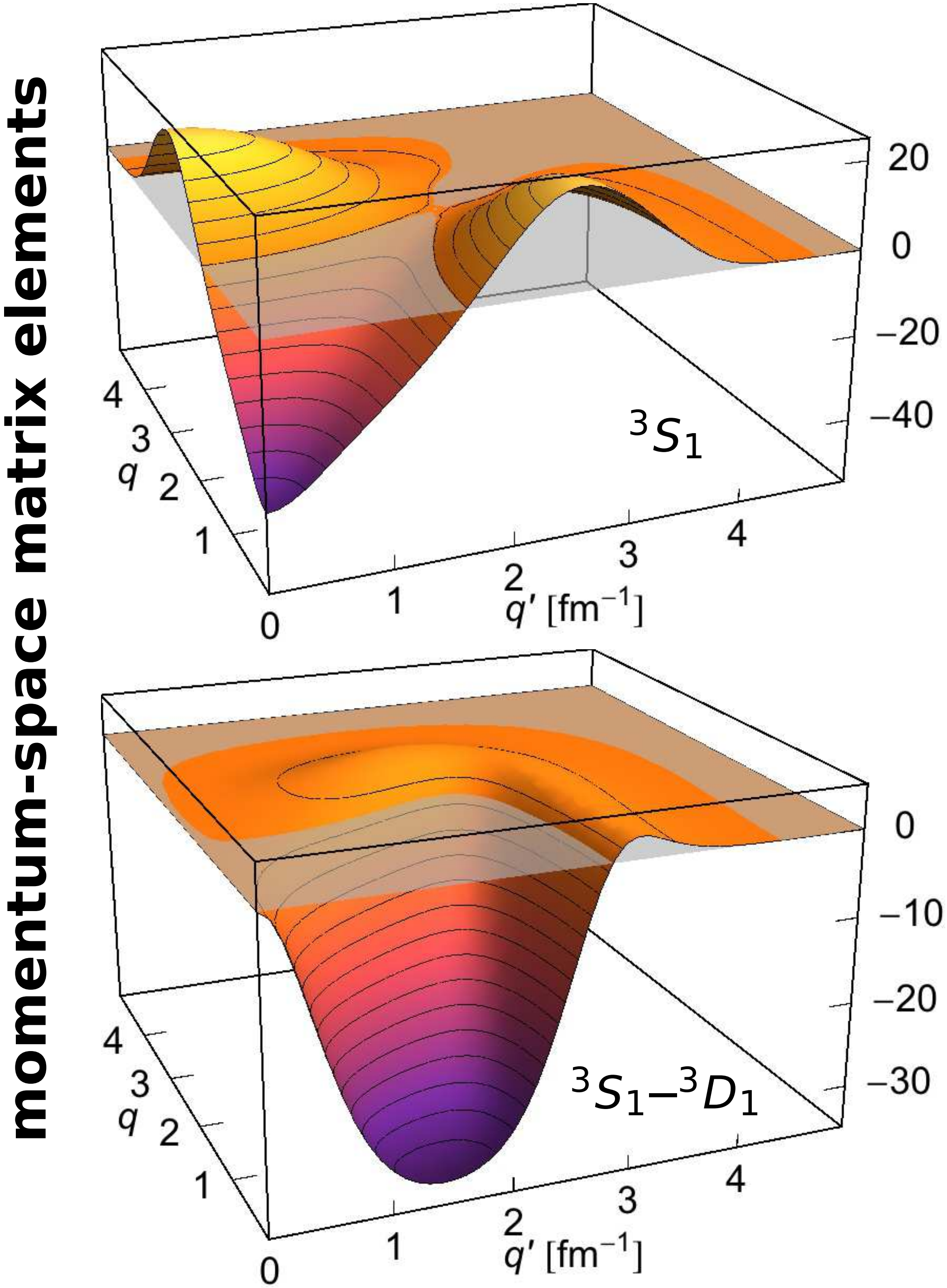
SRG Evolution of Matrix Elements

- represent operator equation in **antisym. n-body Jacobi basis**
  - $n = 2$: momentum space $\left|q(LS)JT\right\rangle$ or harmonic oscillator $\left|E(LS)J^{\pi}T\right\rangle$
  - $n = 3$: harmonic oscillator Jacobi states $\left|EiJ^{\pi}T\right\rangle$
- system of **coupled evolution equations** for each $(J^{\pi}T)$-block

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

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

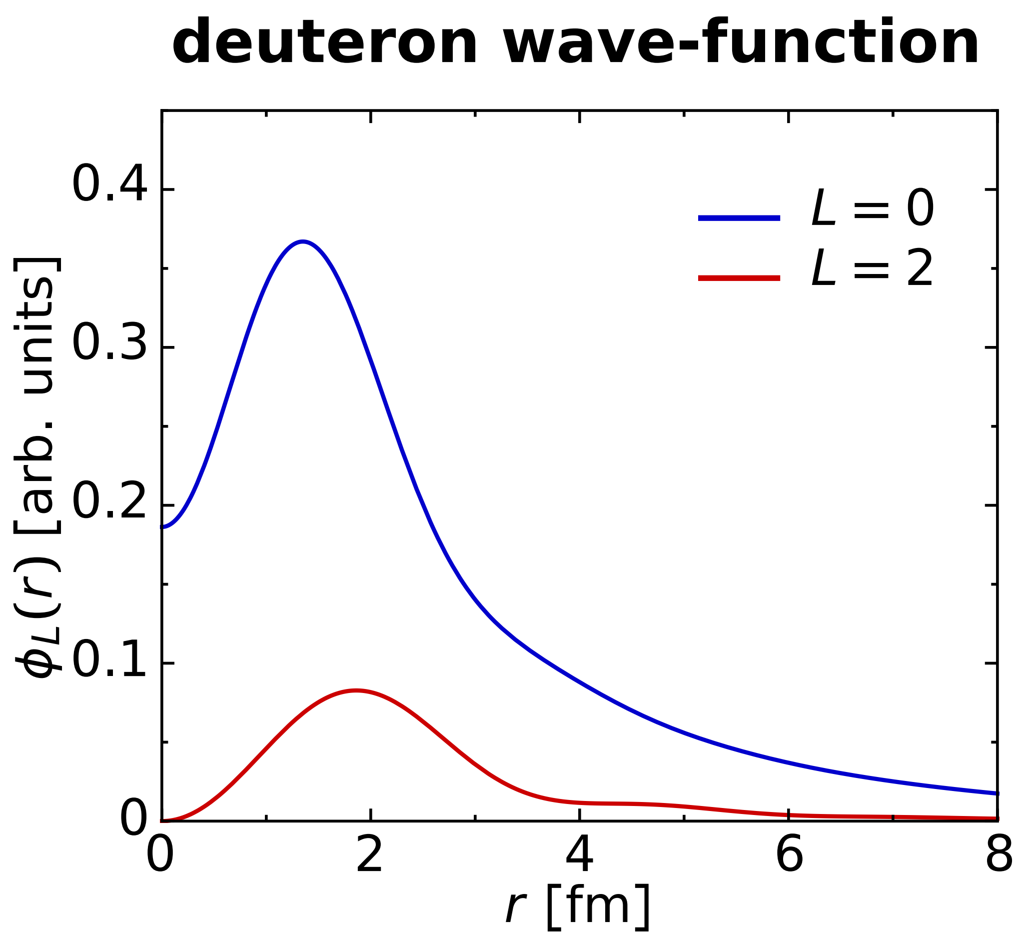
SRG Evolution in Two-Body Space



chiral NN

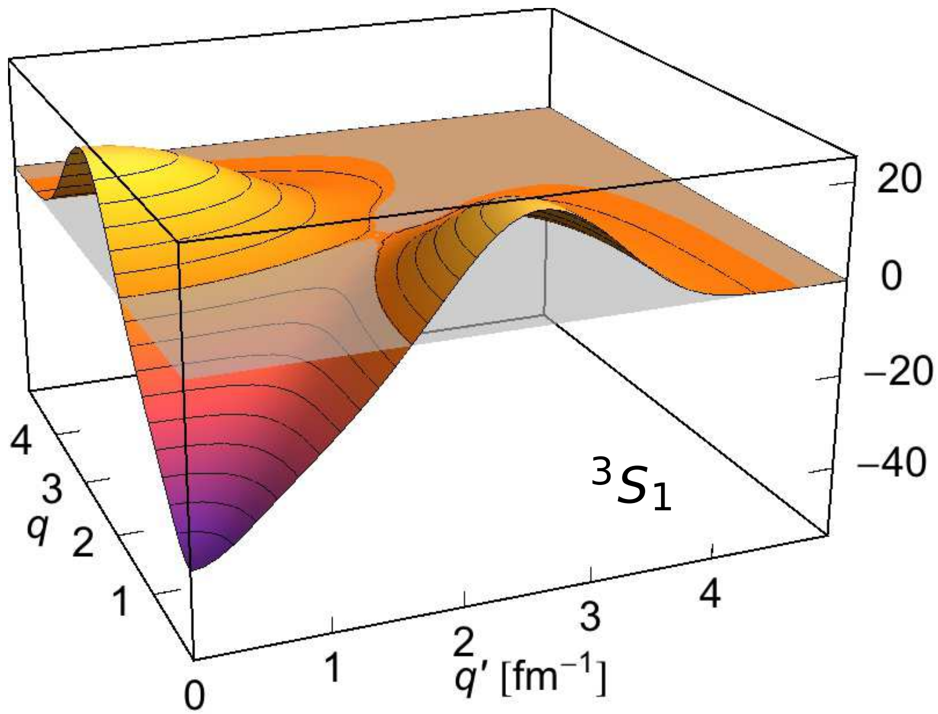
Entem & Machleidt. N^{3}LO, 500 MeV

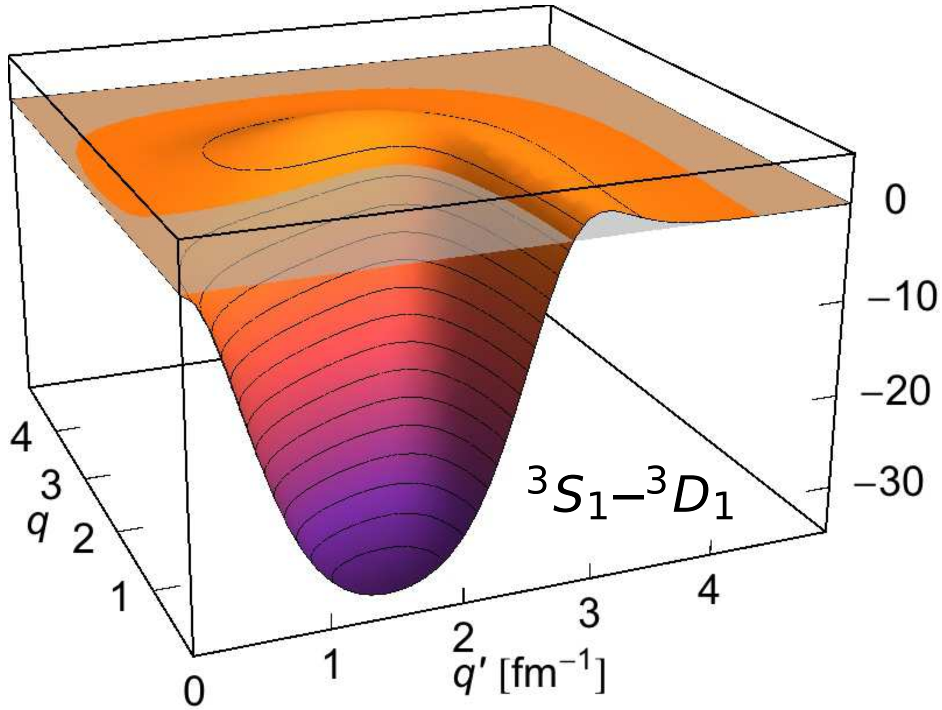
$J^\pi = 1^+, T = 0$



SRG Evolution in Two-Body Space

momentum-space matrix elements



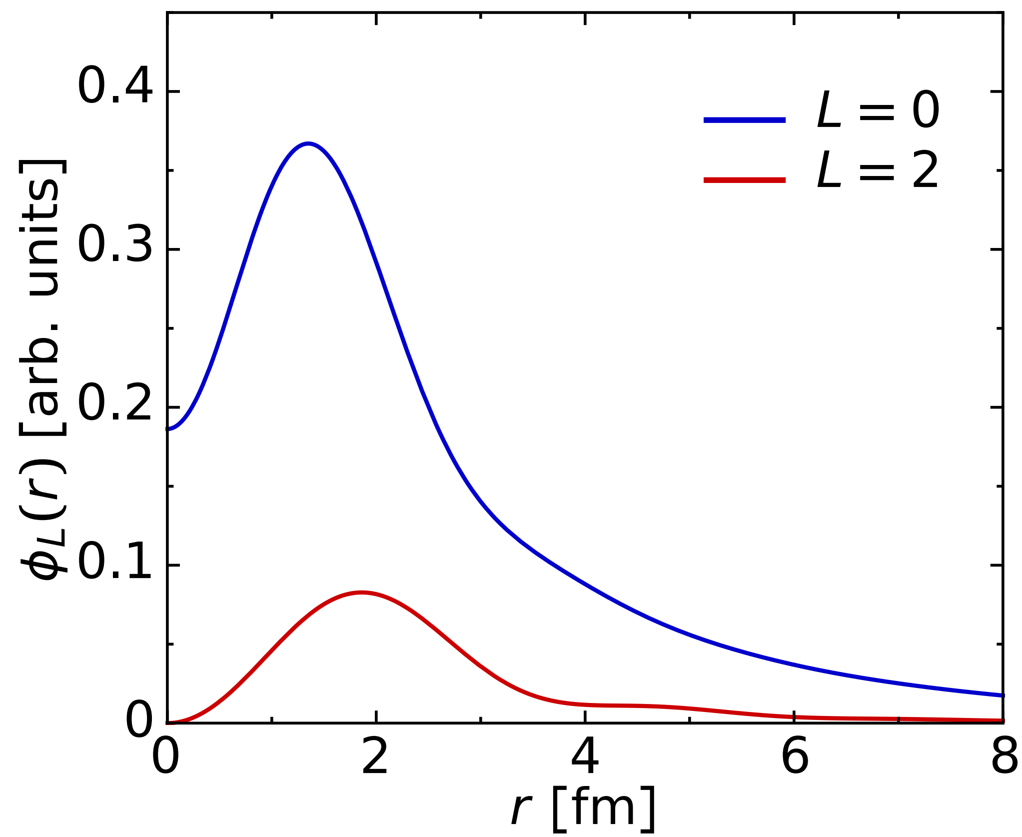


$\alpha = 0.000\,\mathrm{fm}^4$

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

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

deuteron wave-function



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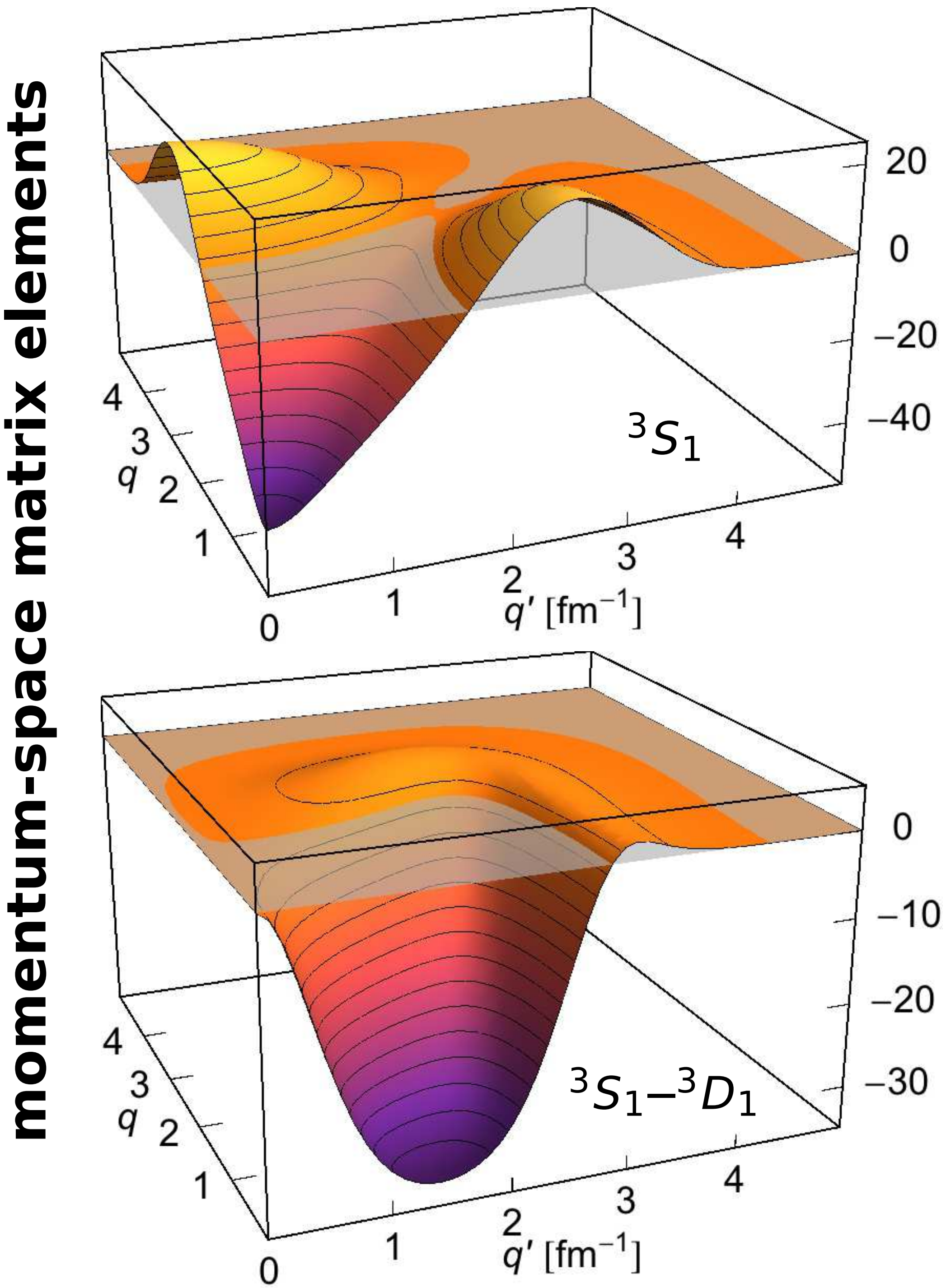
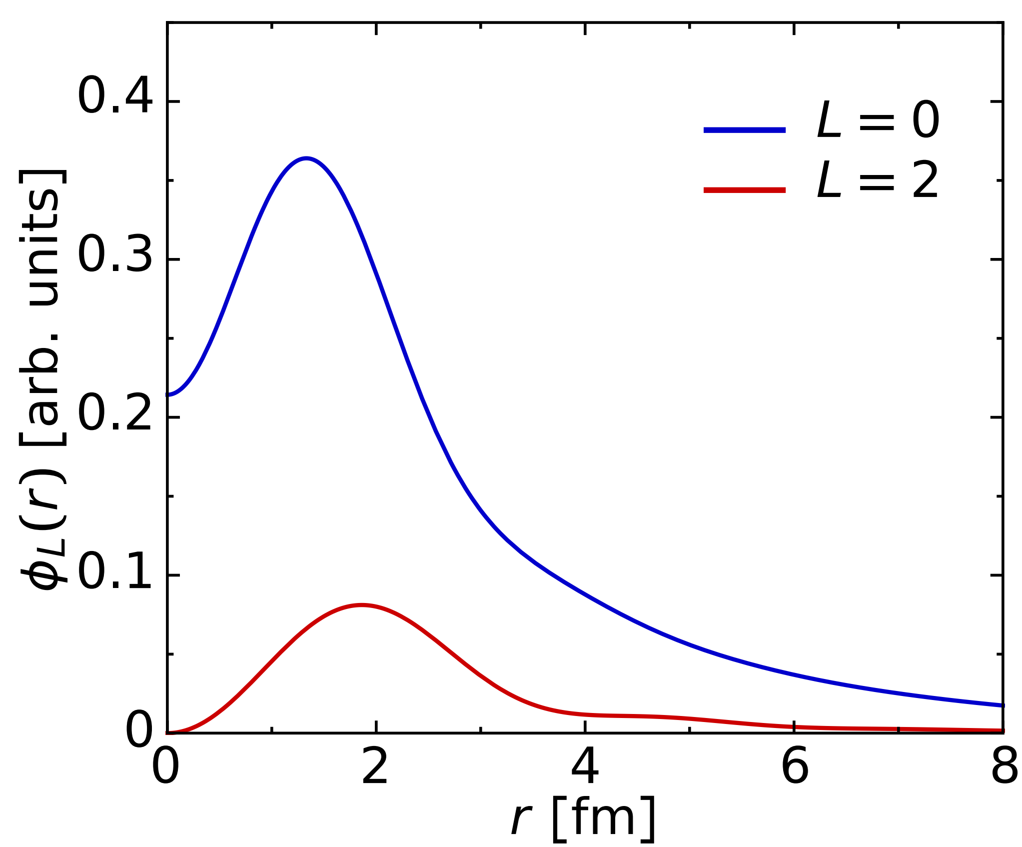


$\alpha = 0.002\,\text{fm}^4$

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

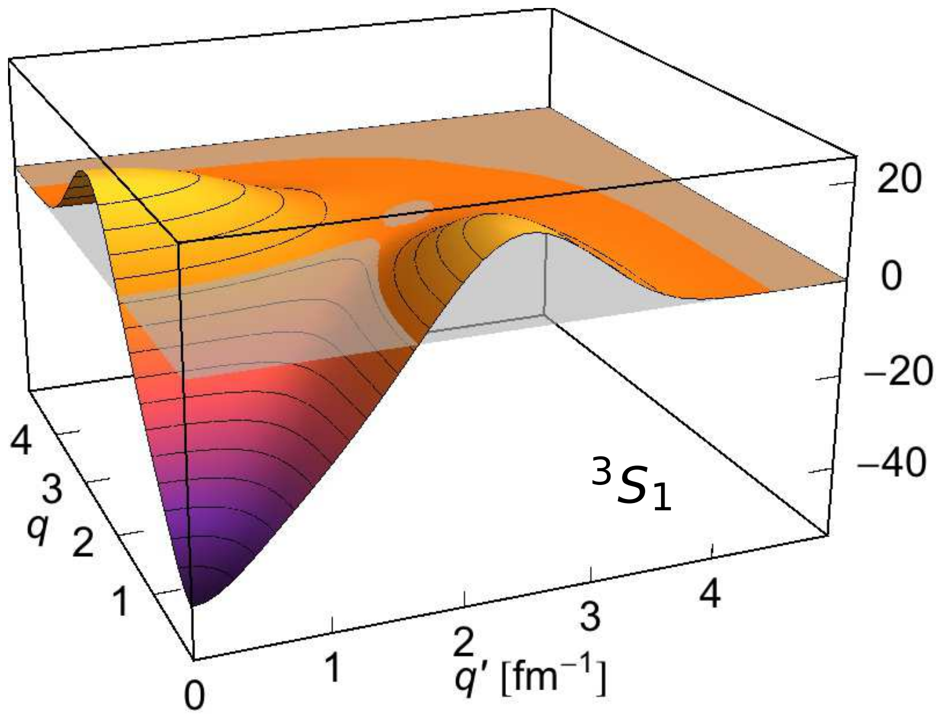
$J^\pi = 1^+, T = 0$

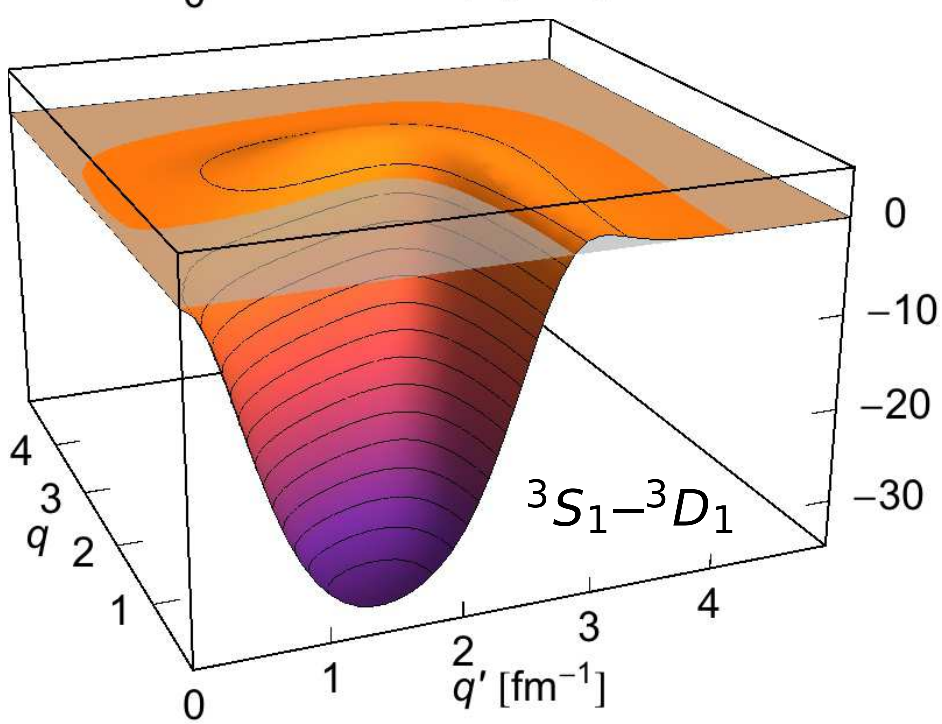
deuteron wave-function



SRG Evolution in Two-Body Space

momentum-space matrix elements



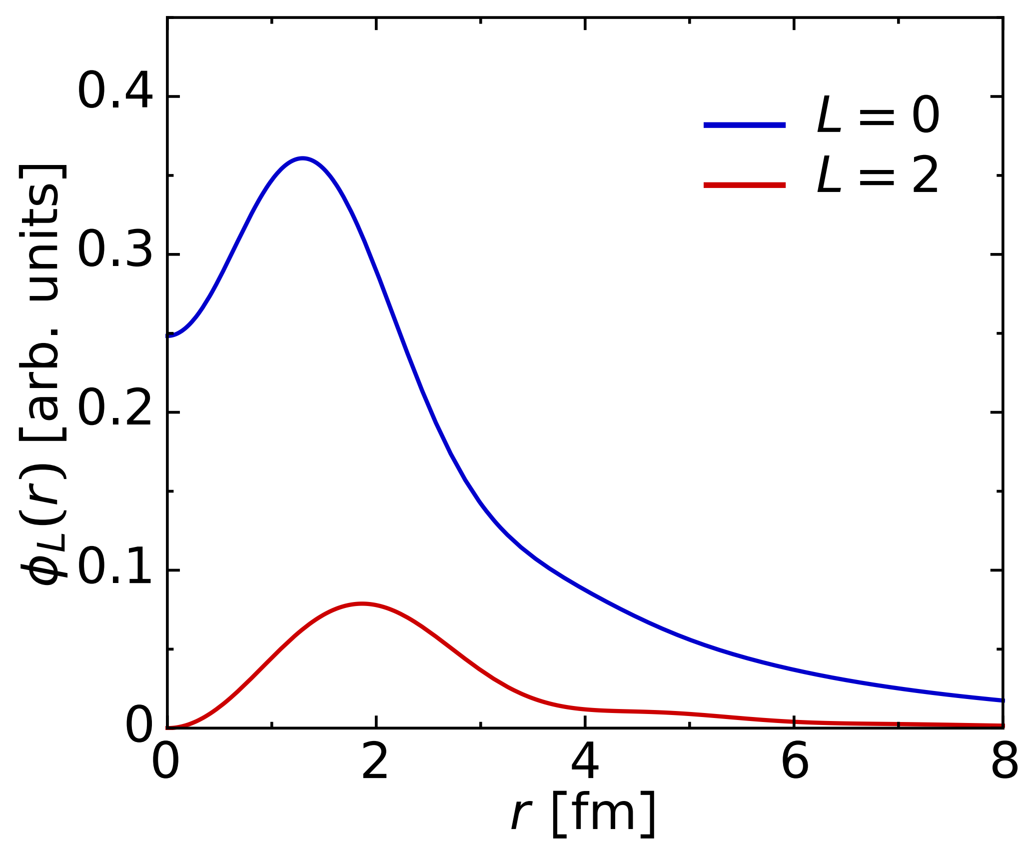


$\alpha = 0.005\,\mathrm{fm}^4$

$\Lambda = 3.76\,\mathrm{fm}^{-1}$

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

deuteron wave-function



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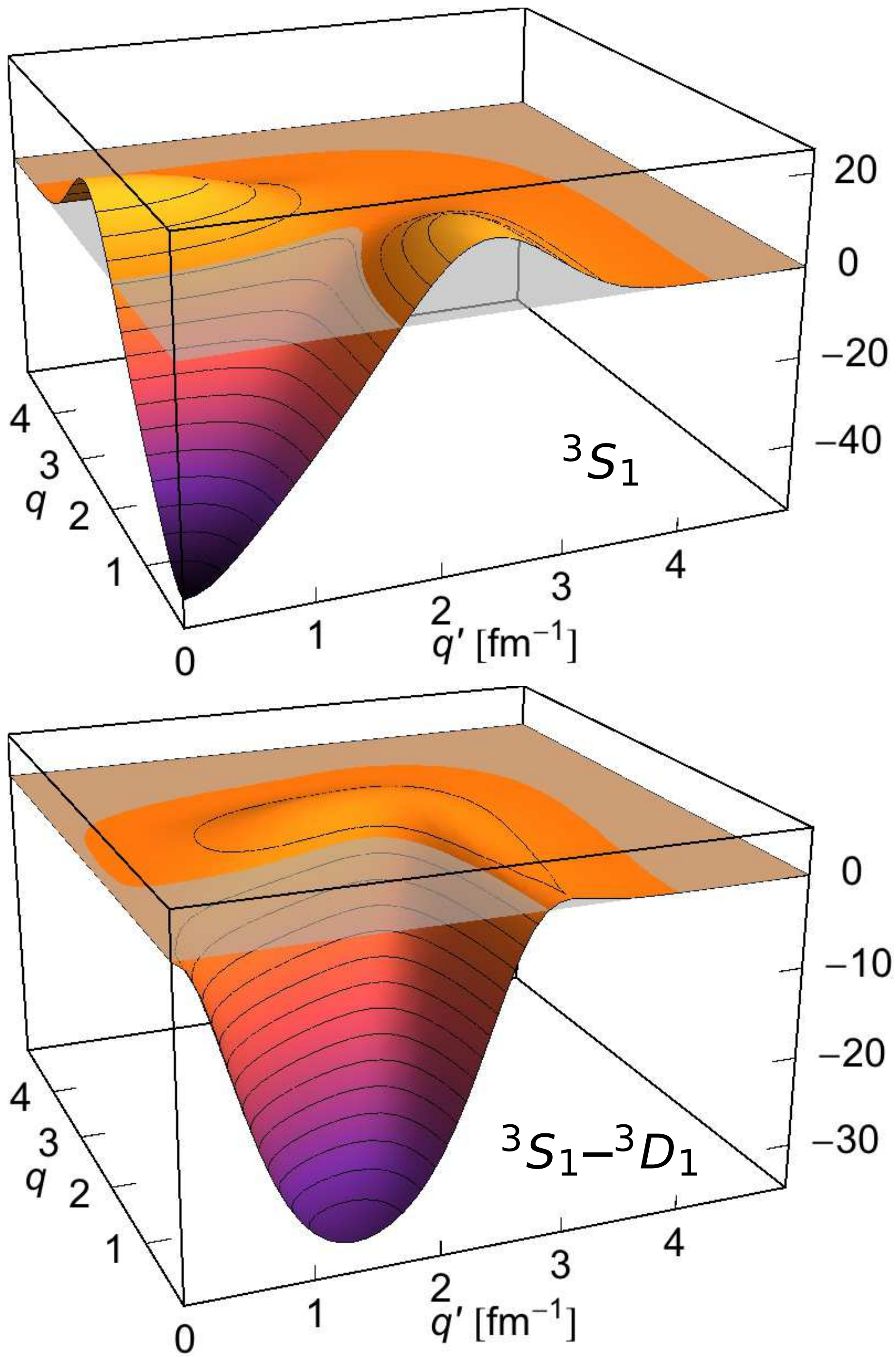

$\alpha = 0.010\,\text{fm}^4$

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

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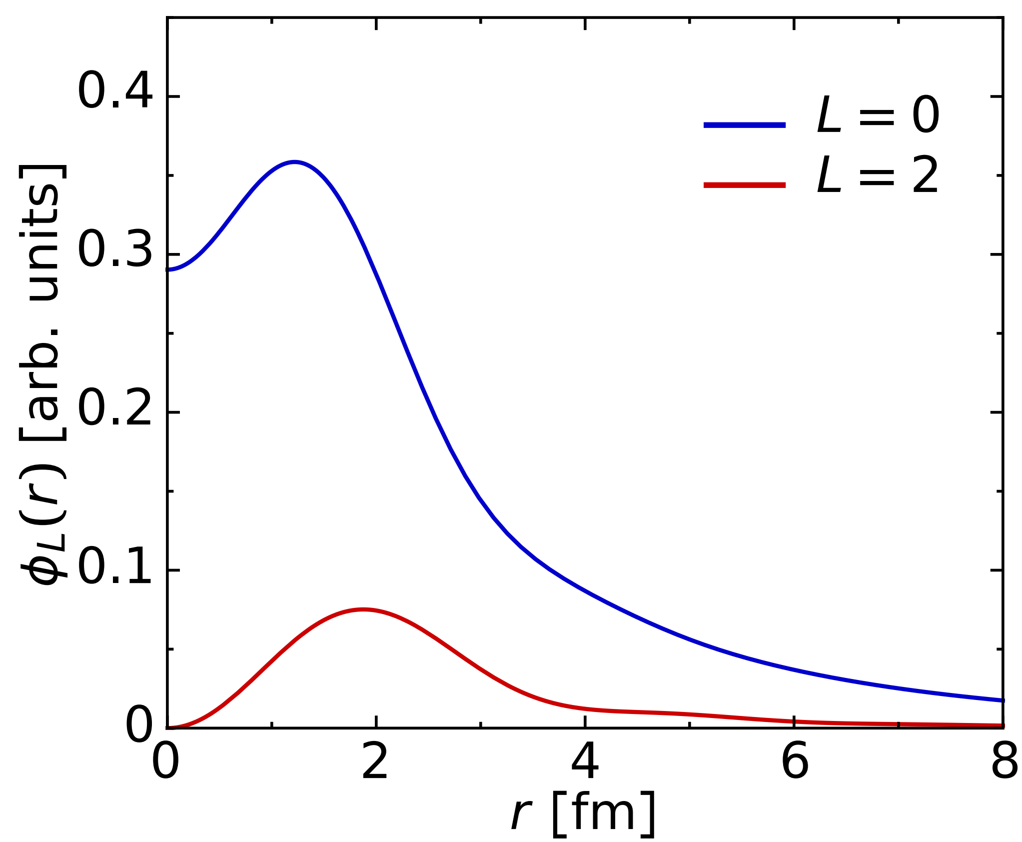

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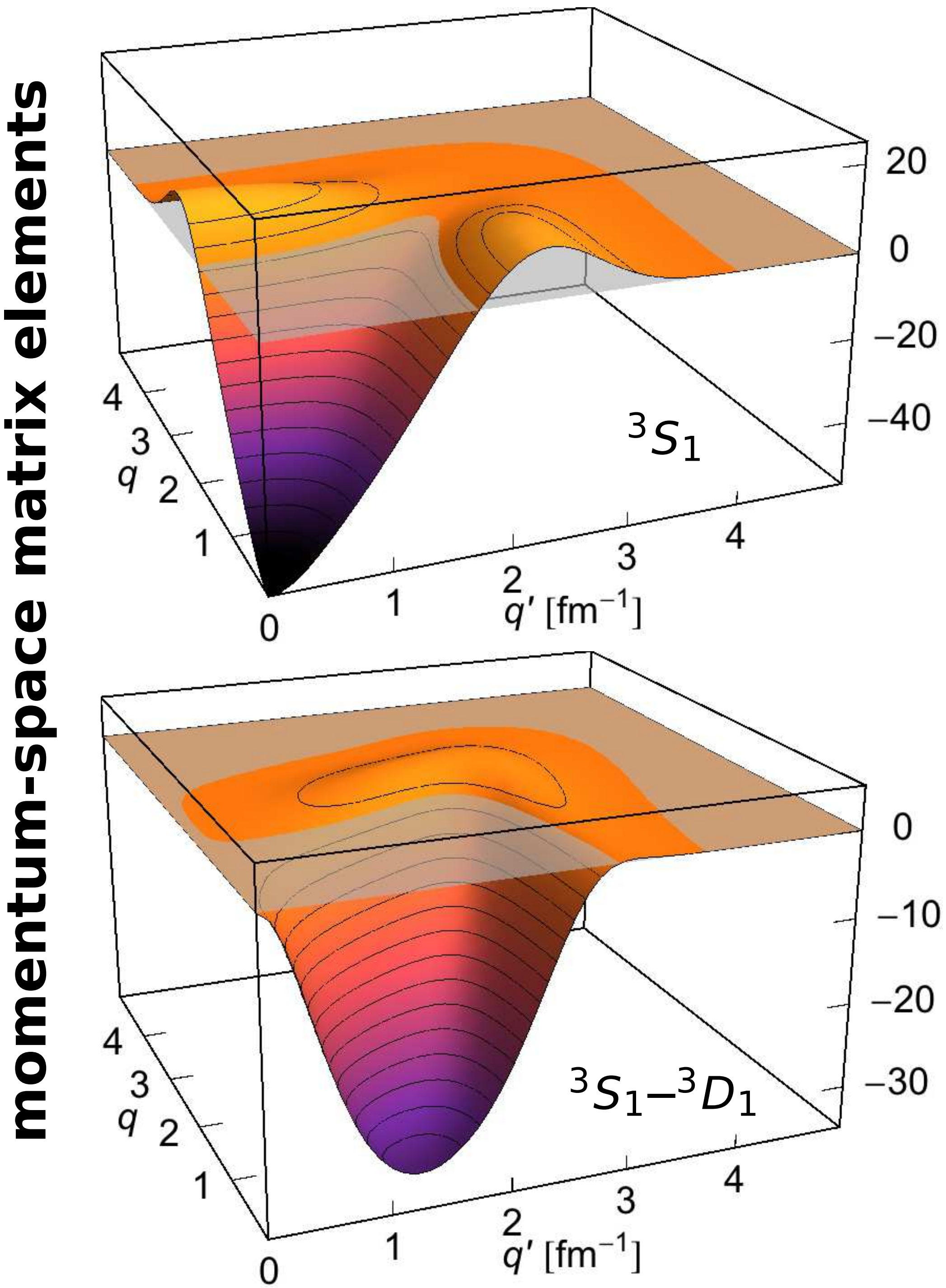

$\alpha = 0.020\,\mathrm{fm}^4$

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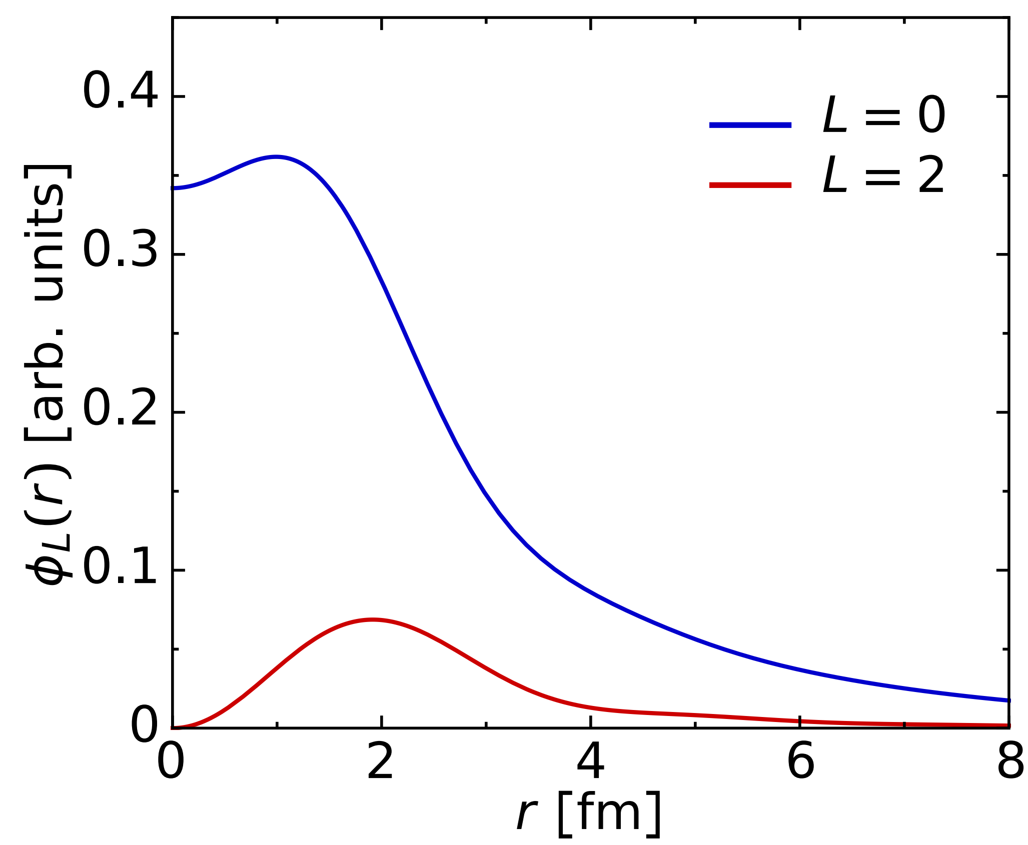
$J^\pi = 1^+, T = 0$

deuteron wave-function



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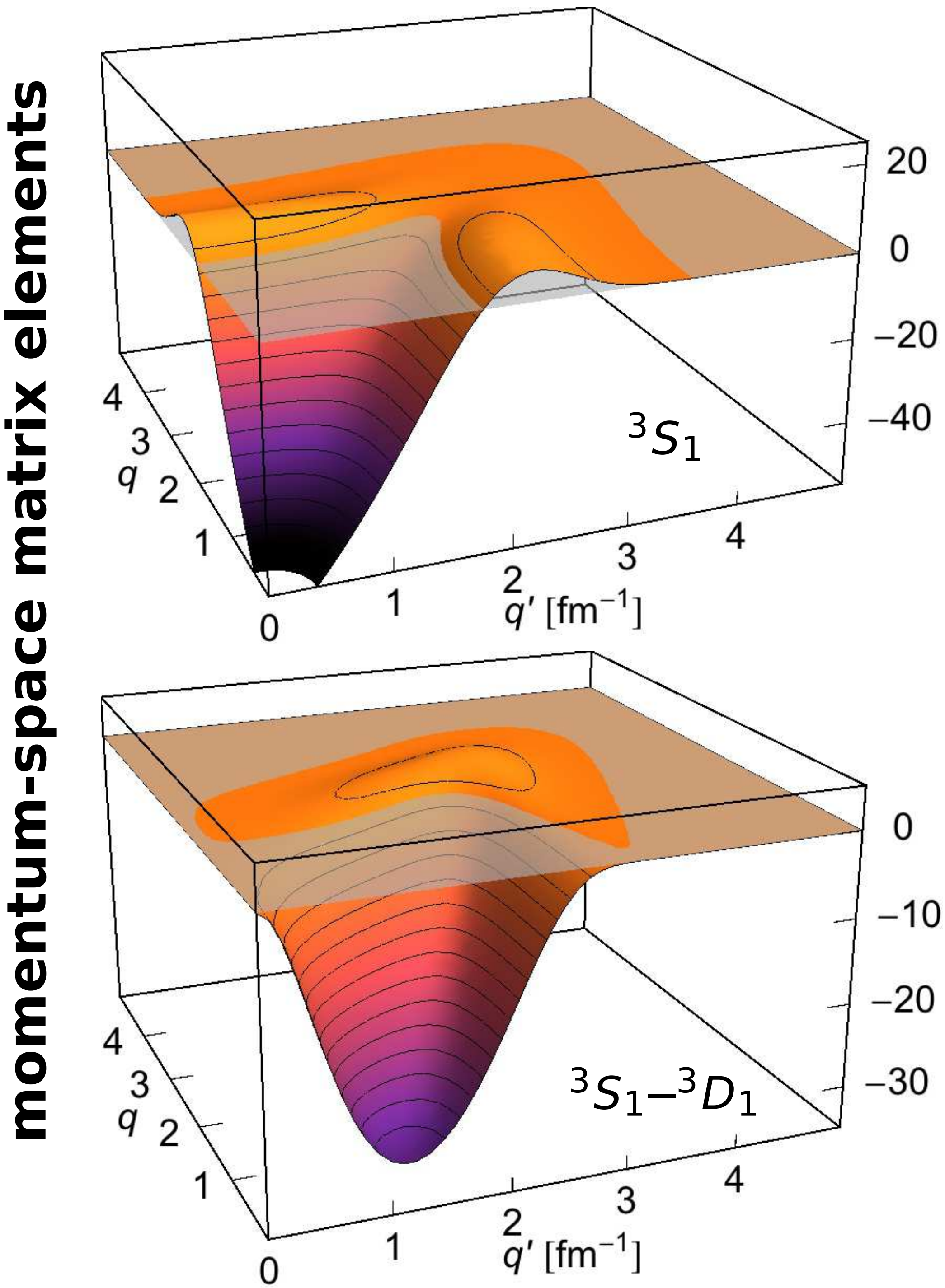

$\alpha = 0.040\,\mathrm{fm}^4$

$\Lambda = 2.24\,\mathrm{fm}^{-1}$

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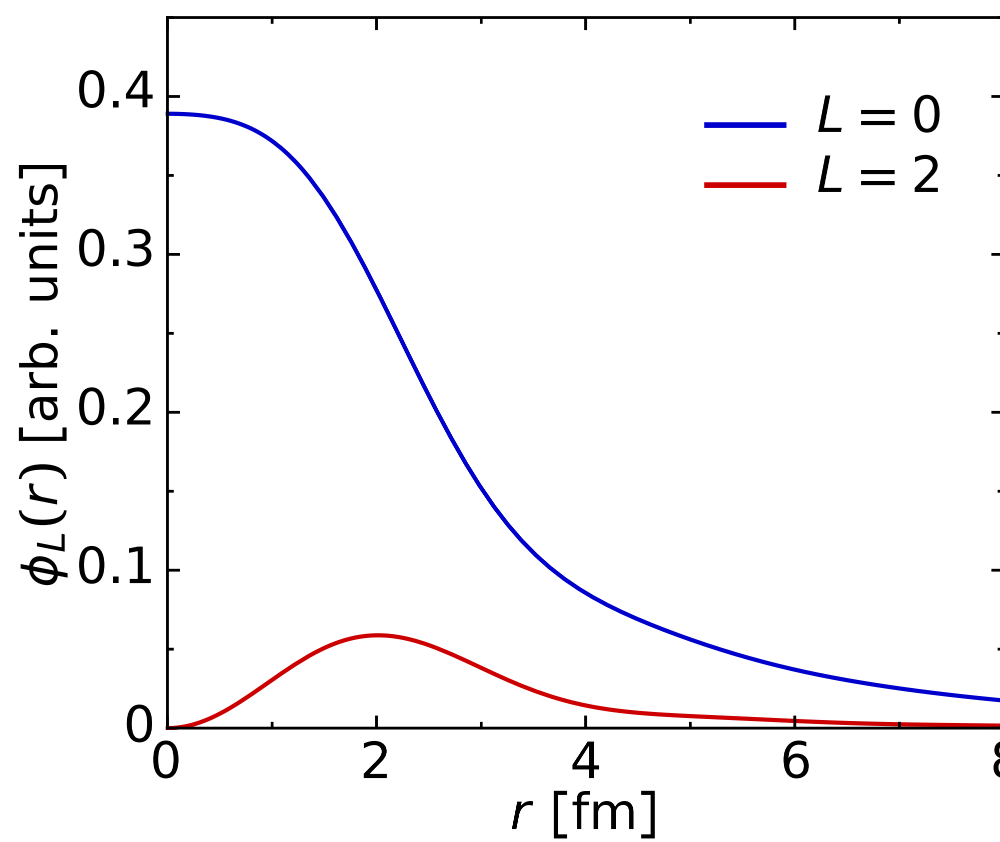

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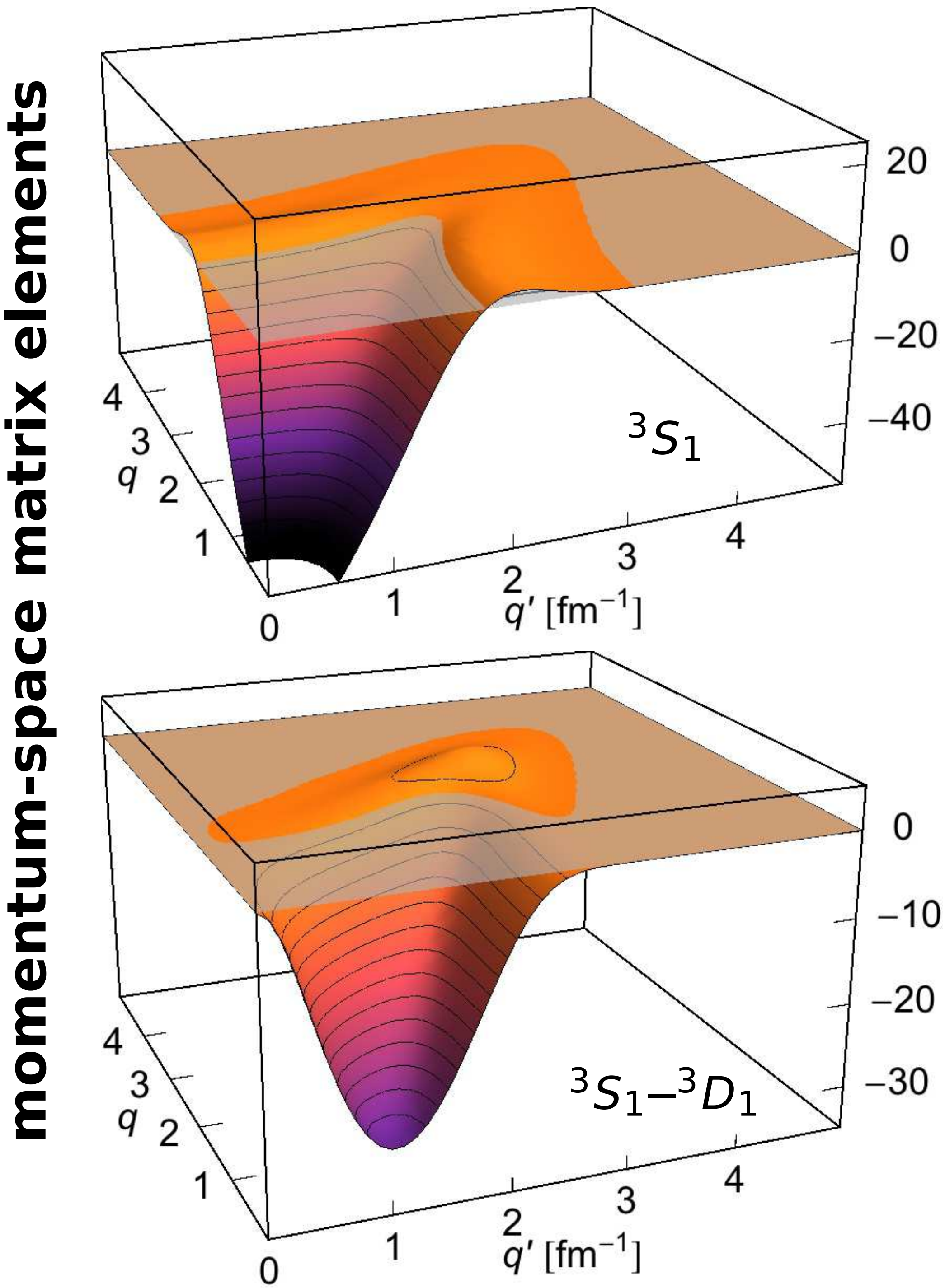

$\alpha = 0.080\,\text{fm}^4$

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

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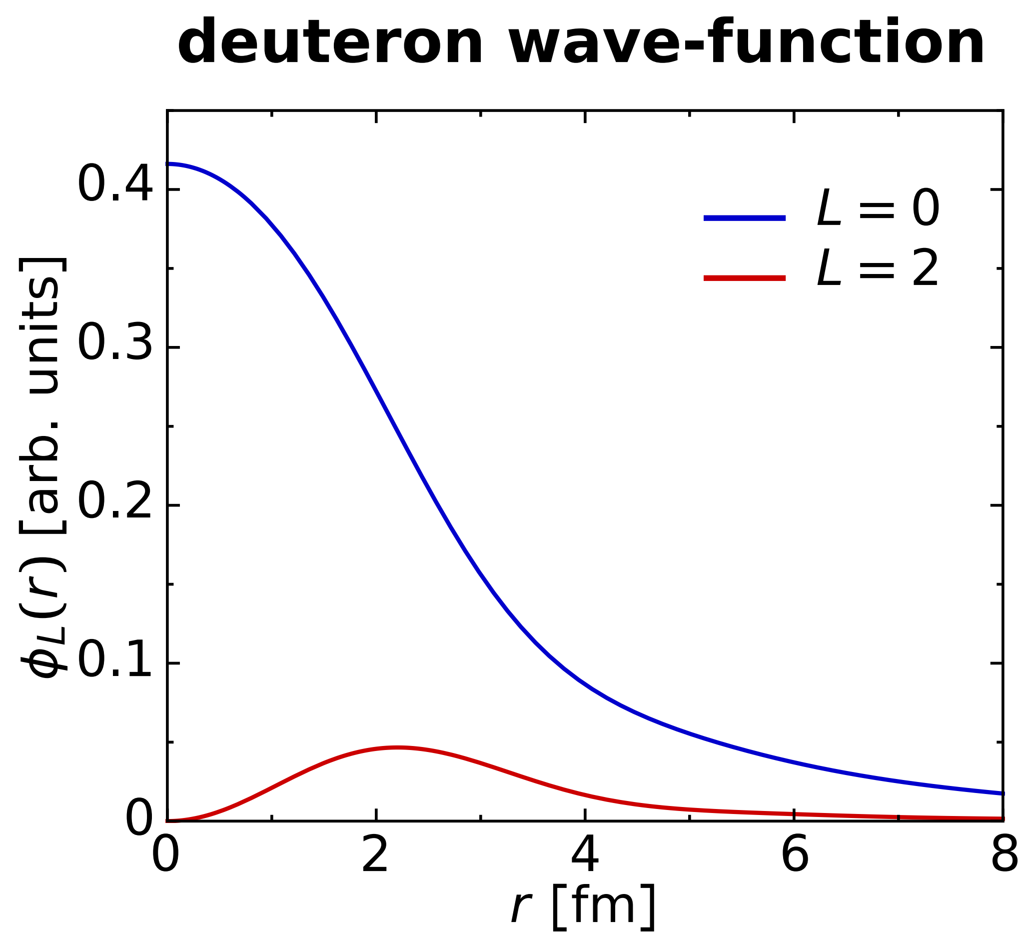

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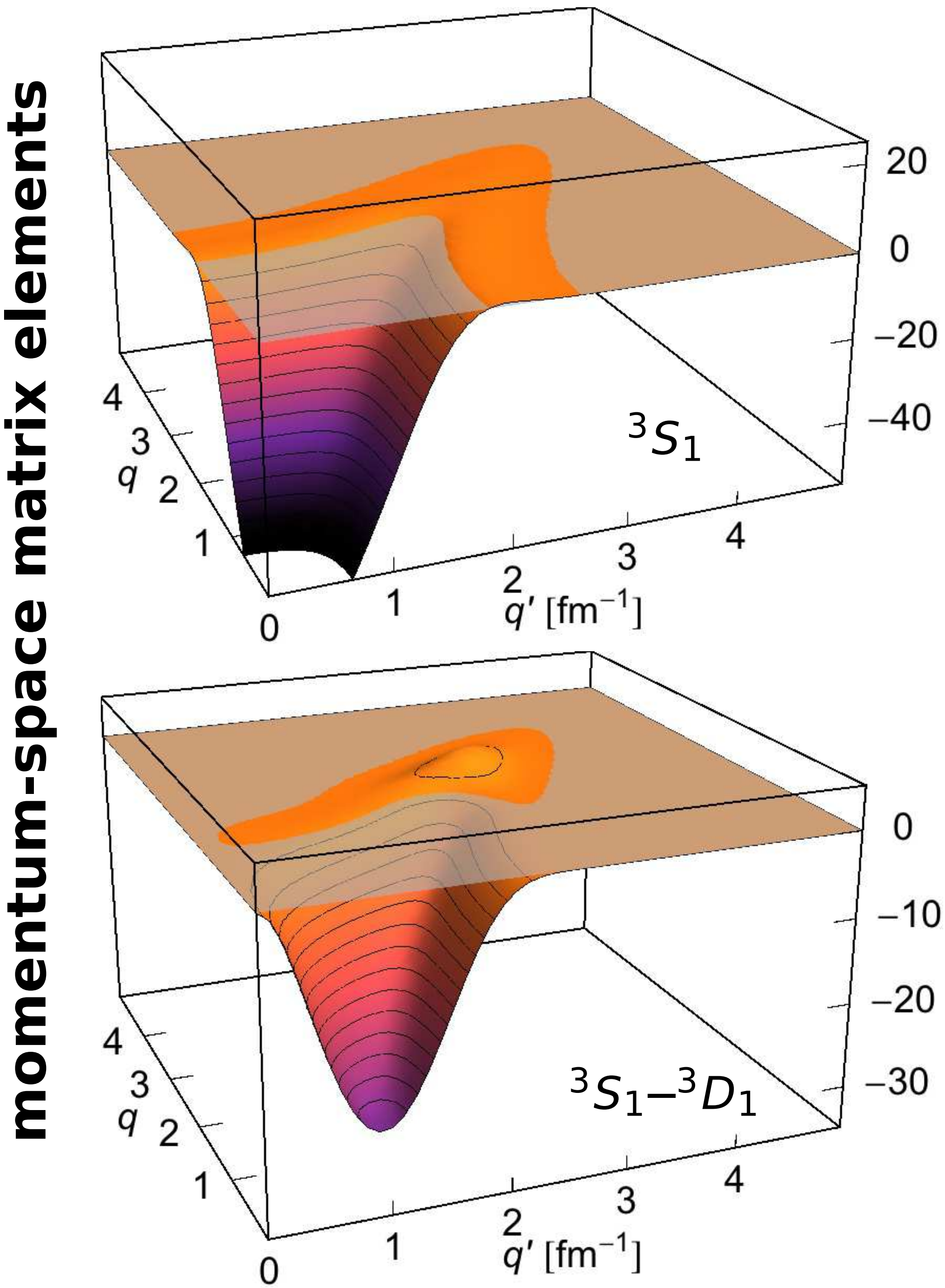

$\alpha = 0.160\,\mathrm{fm}^4$

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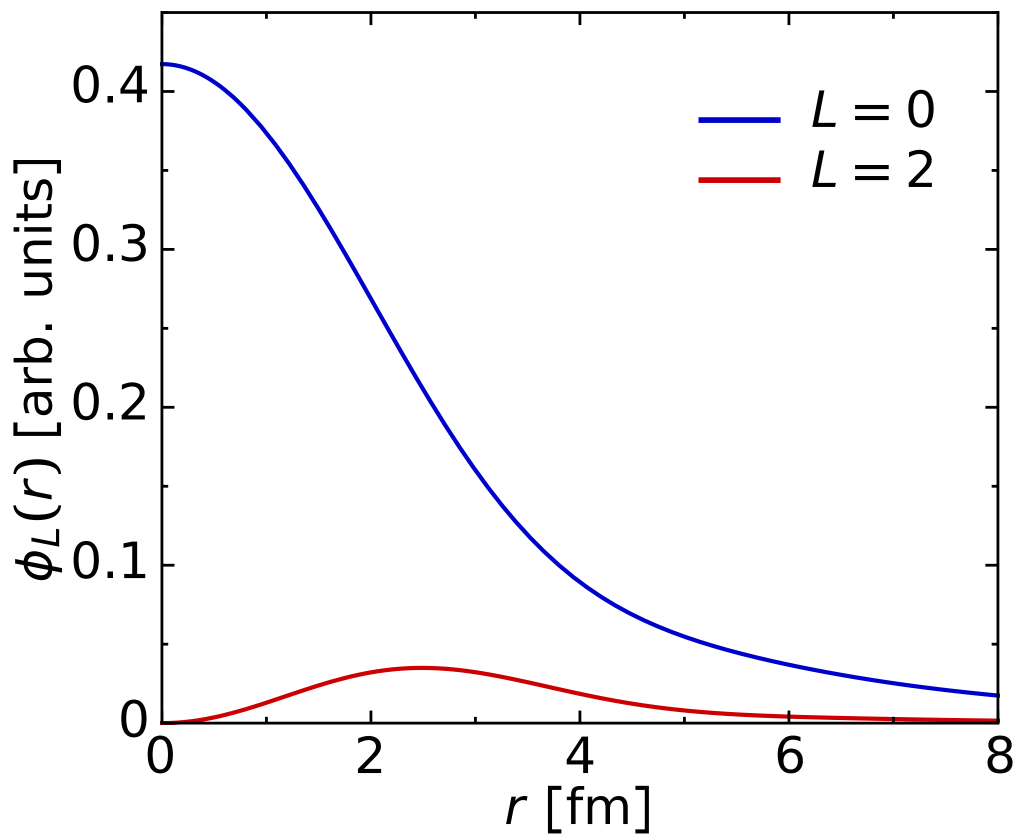
$J^\pi = 1^+, T = 0$

deuteron wave-function



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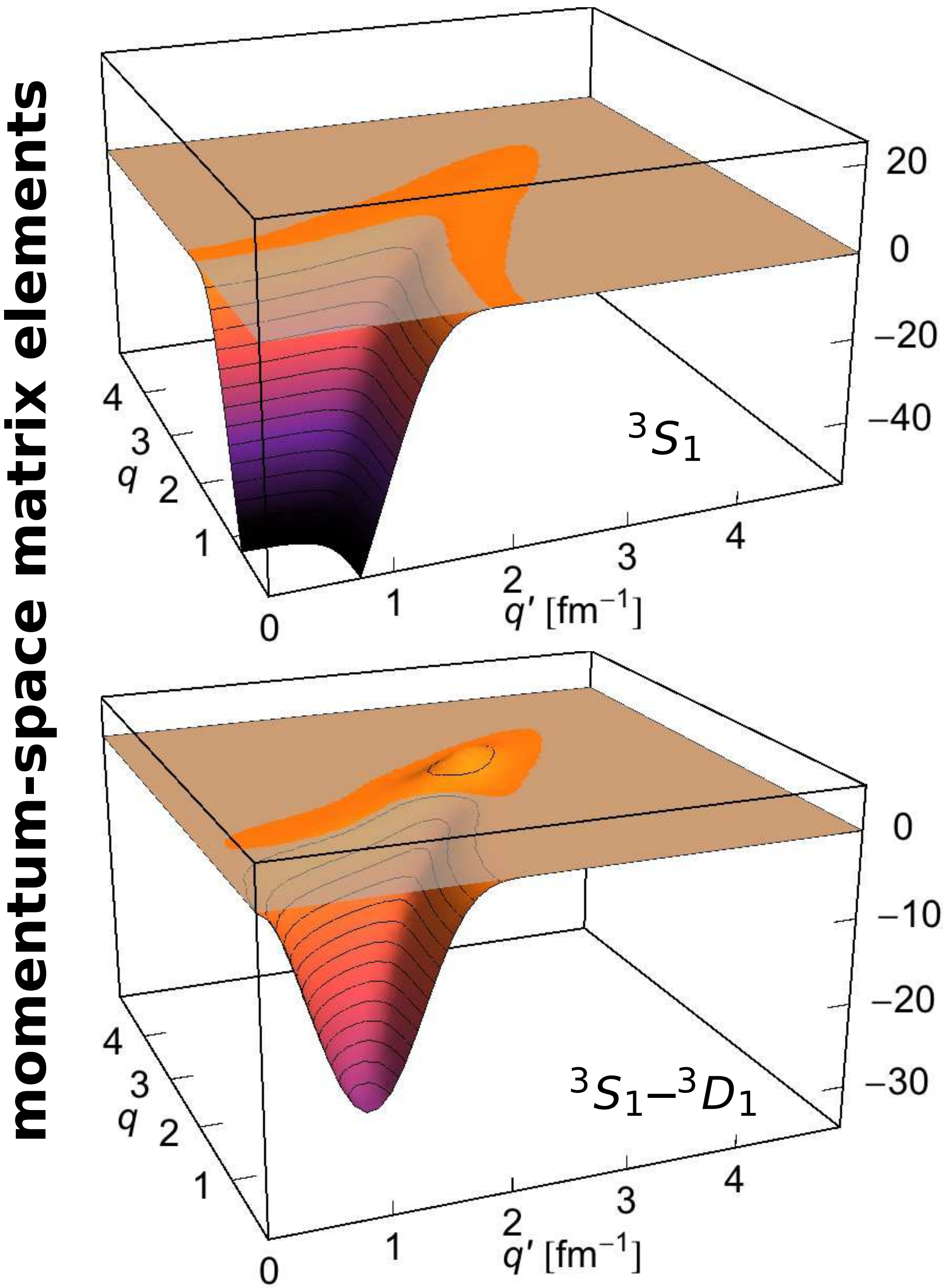
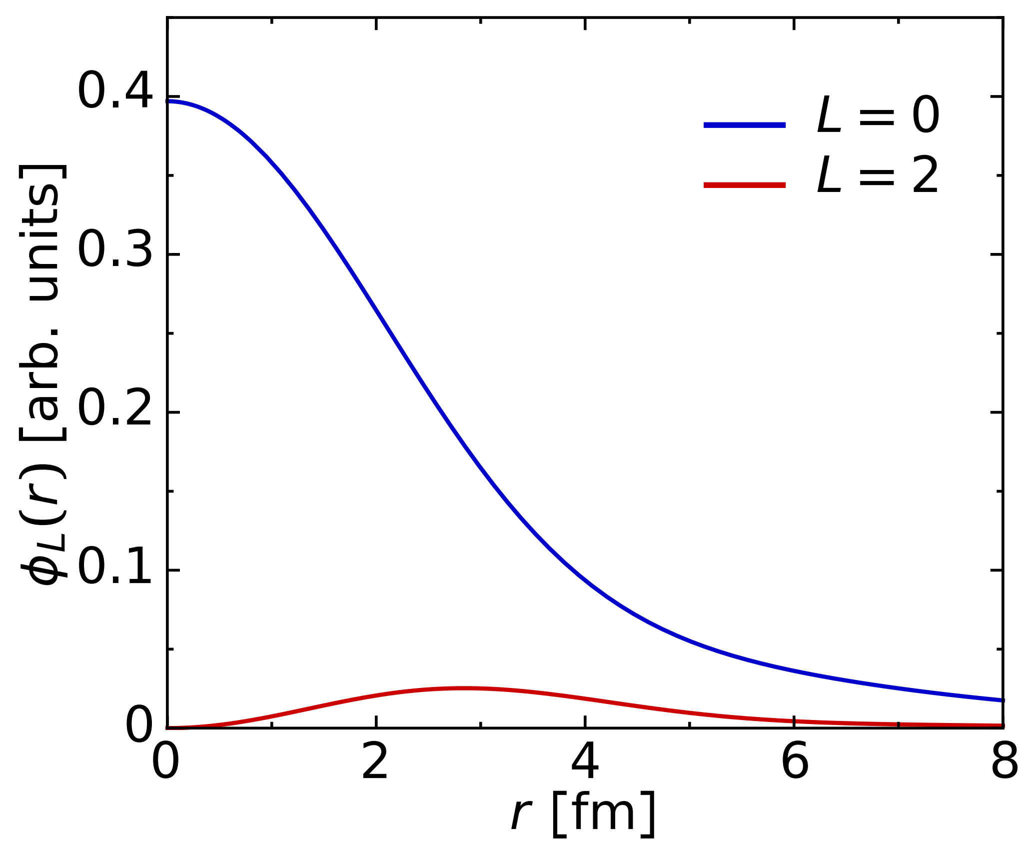


$\alpha = 0.320\,\mathrm{fm}^4$

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

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

deuteron wave-function



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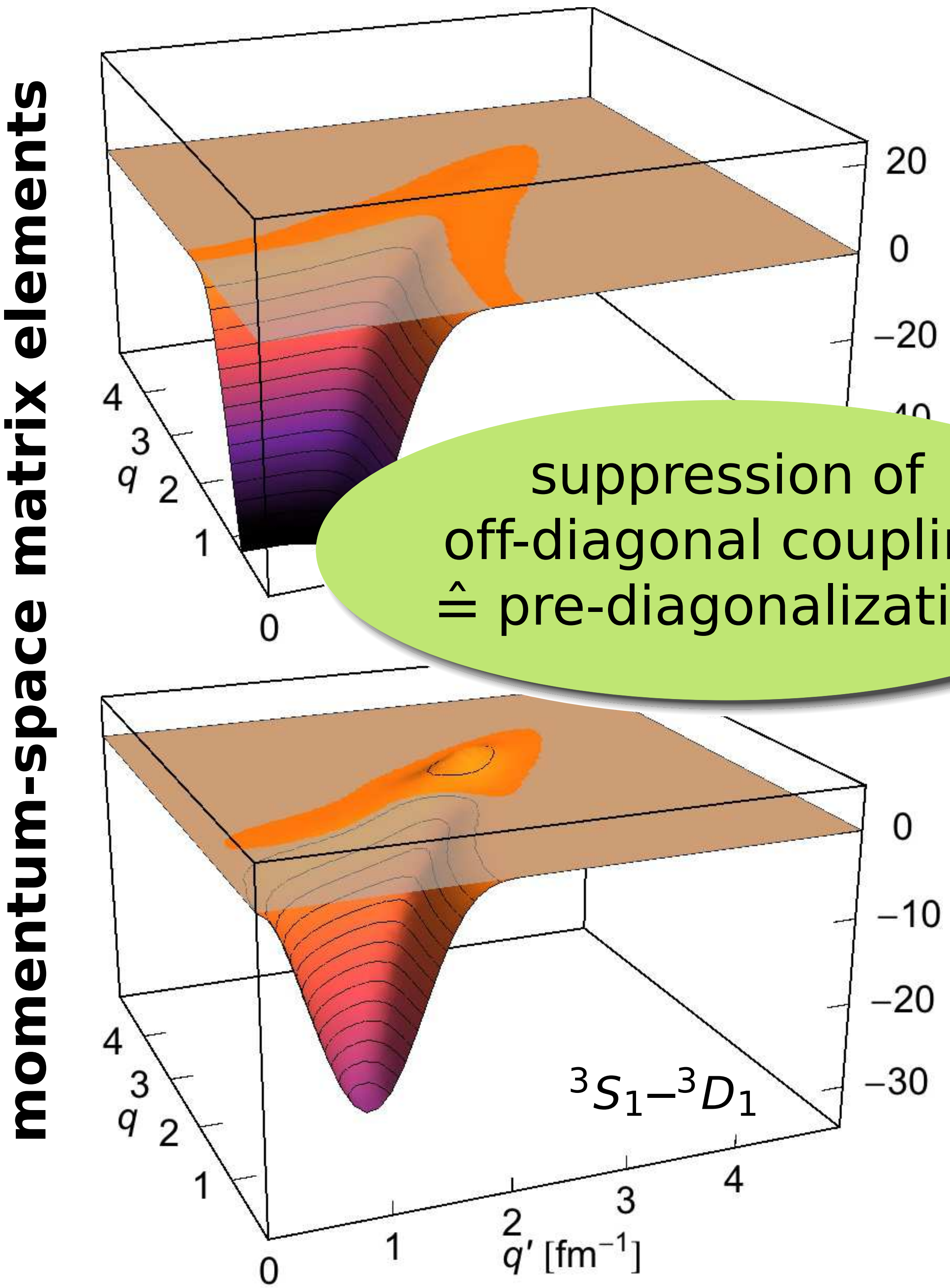
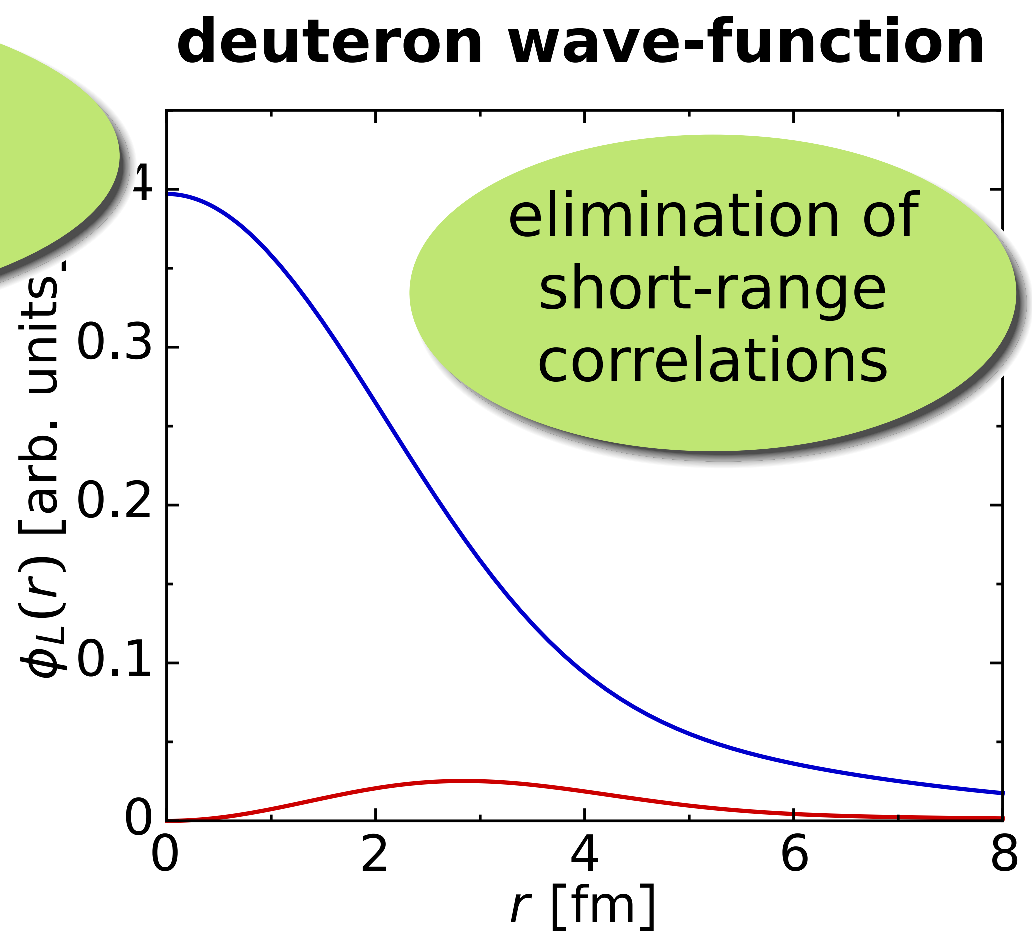
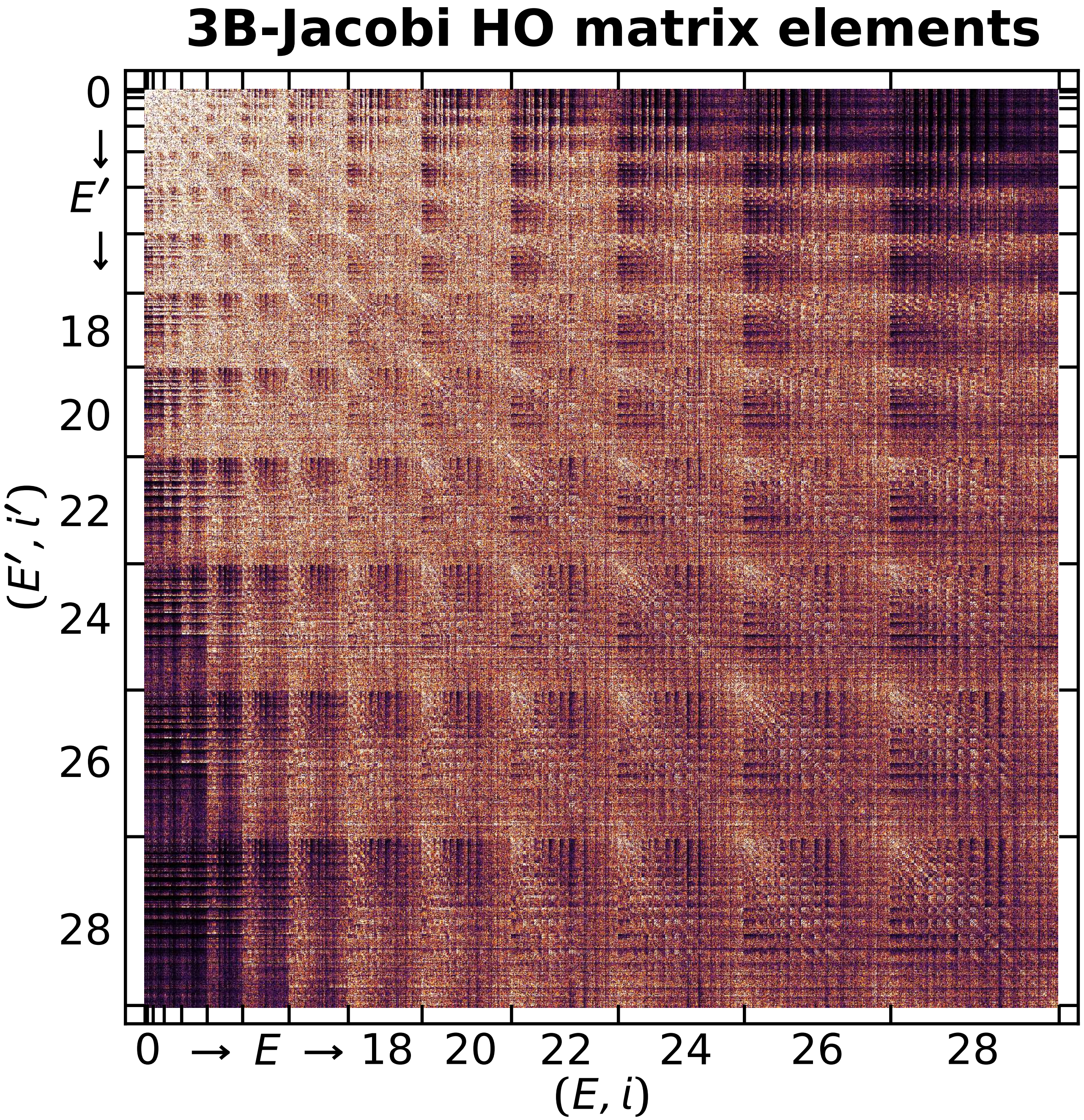


suppression of
off-diagonal coupling
≙ pre-diagonalization



elimination of
short-range
correlations

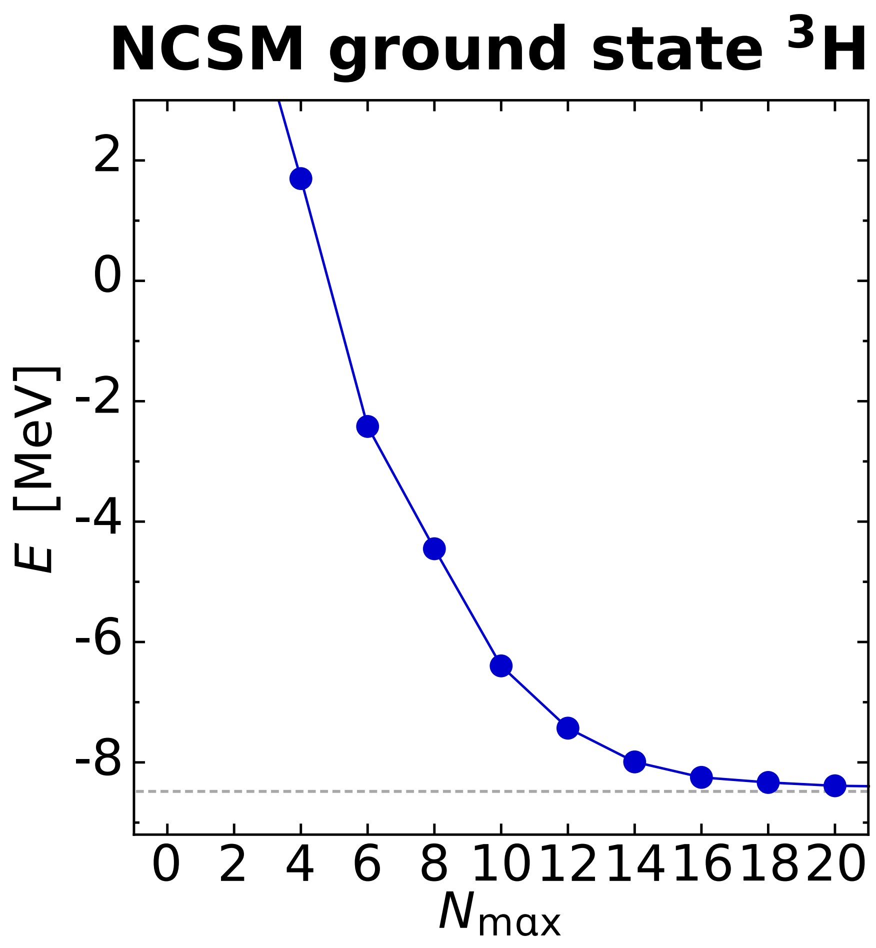
SRG Evolution in Three-Body Space



chiral NN+3N

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

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



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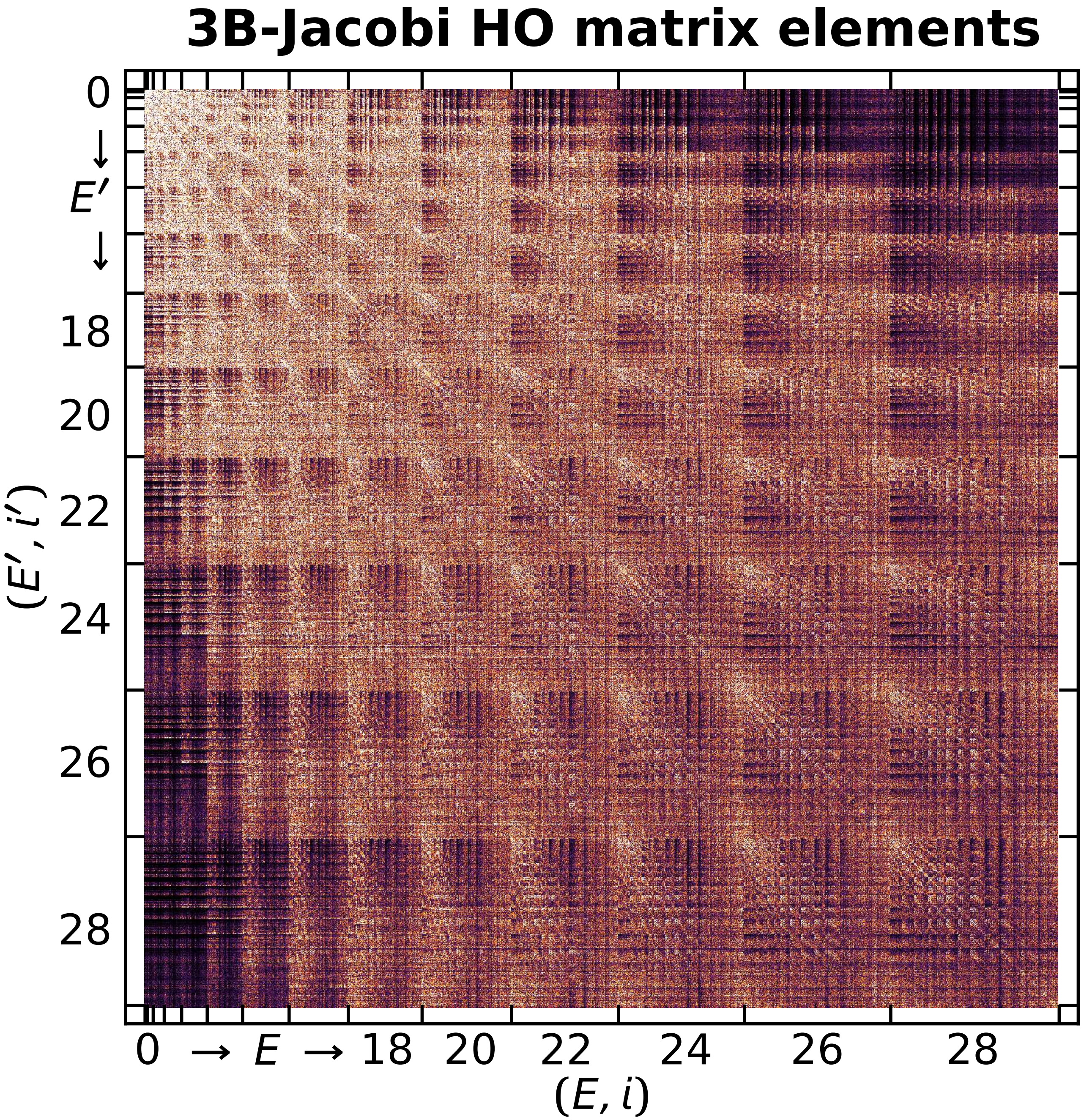

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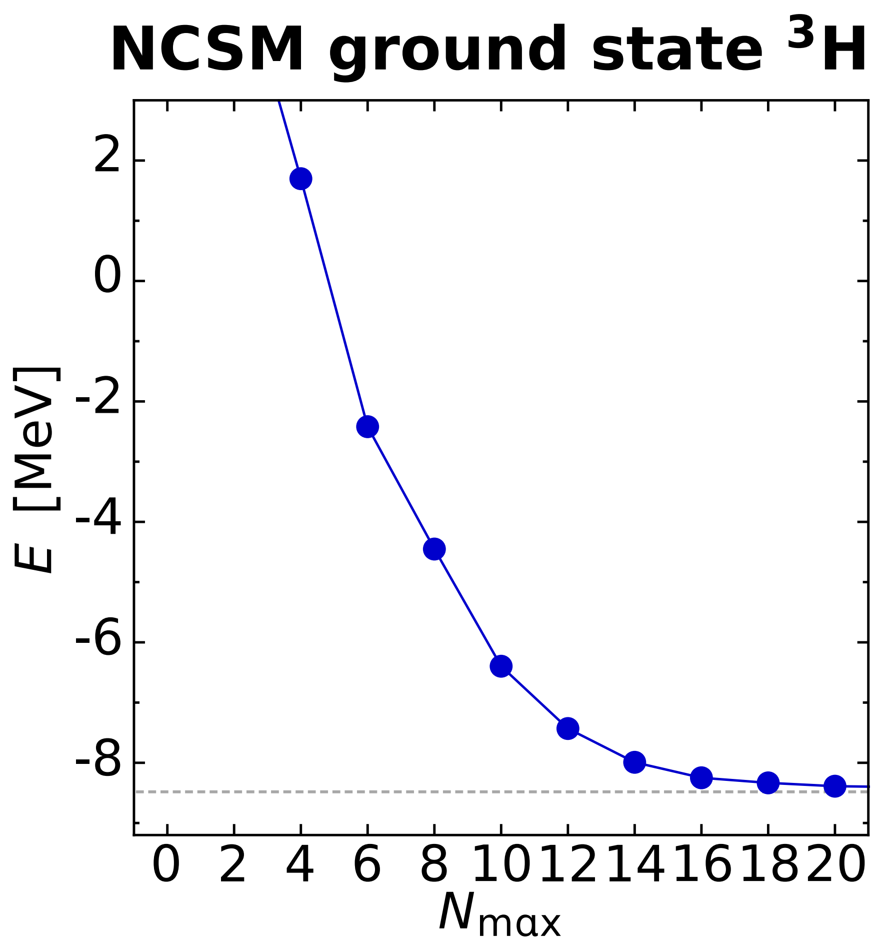

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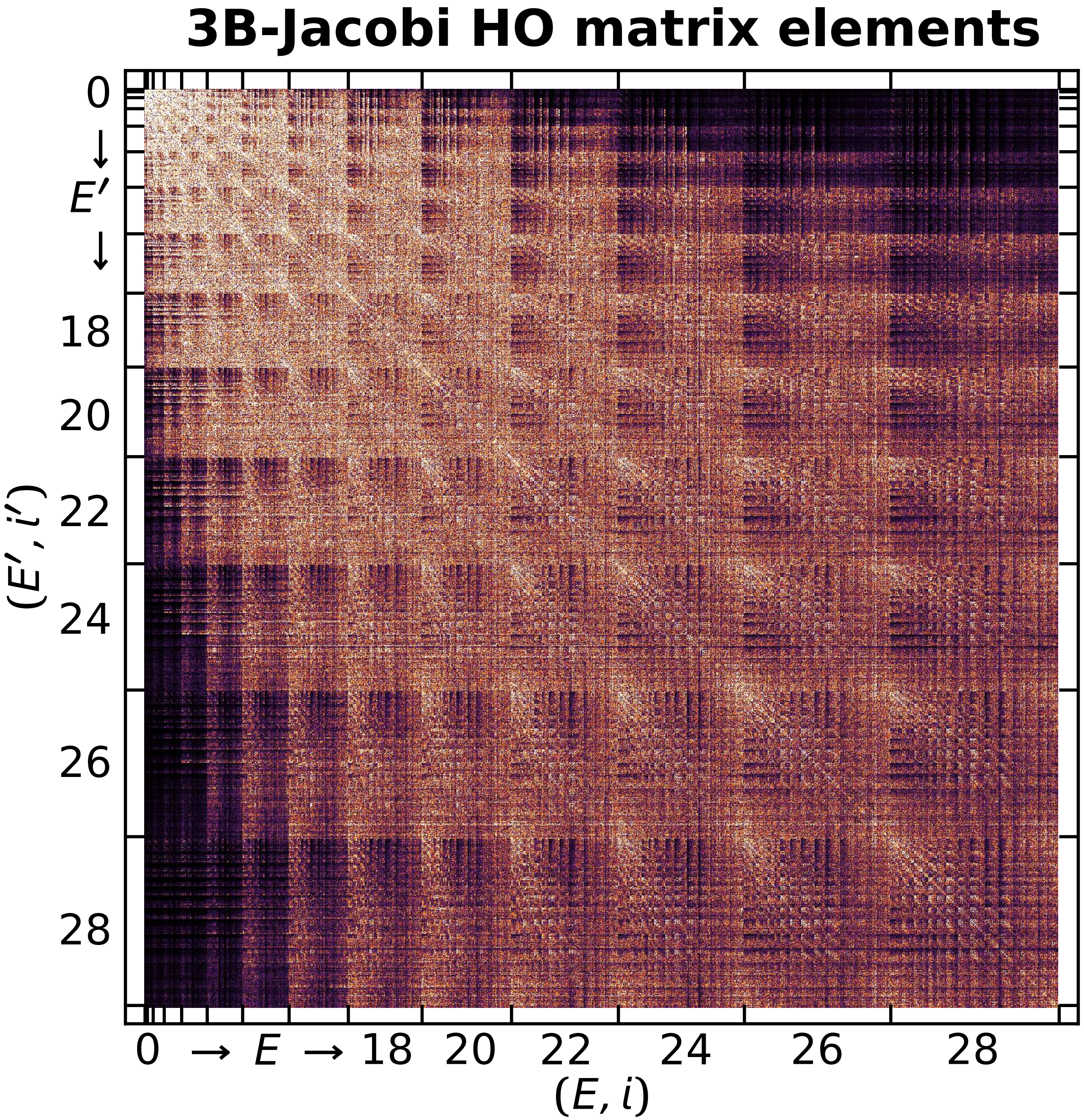

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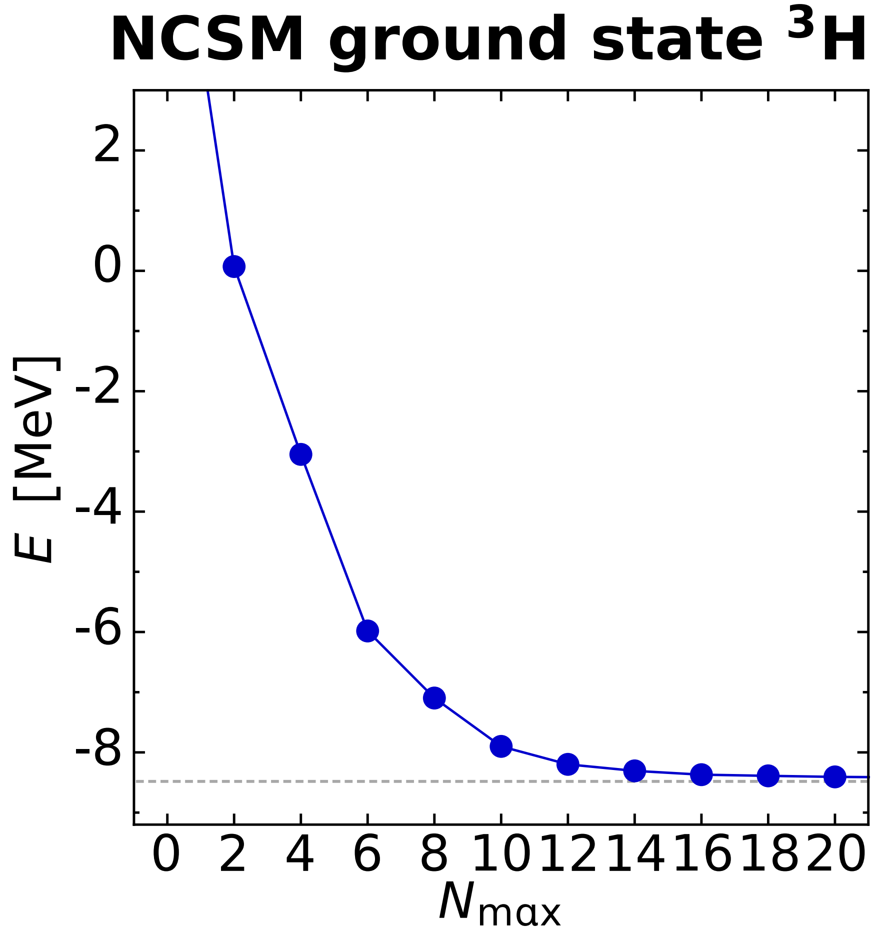

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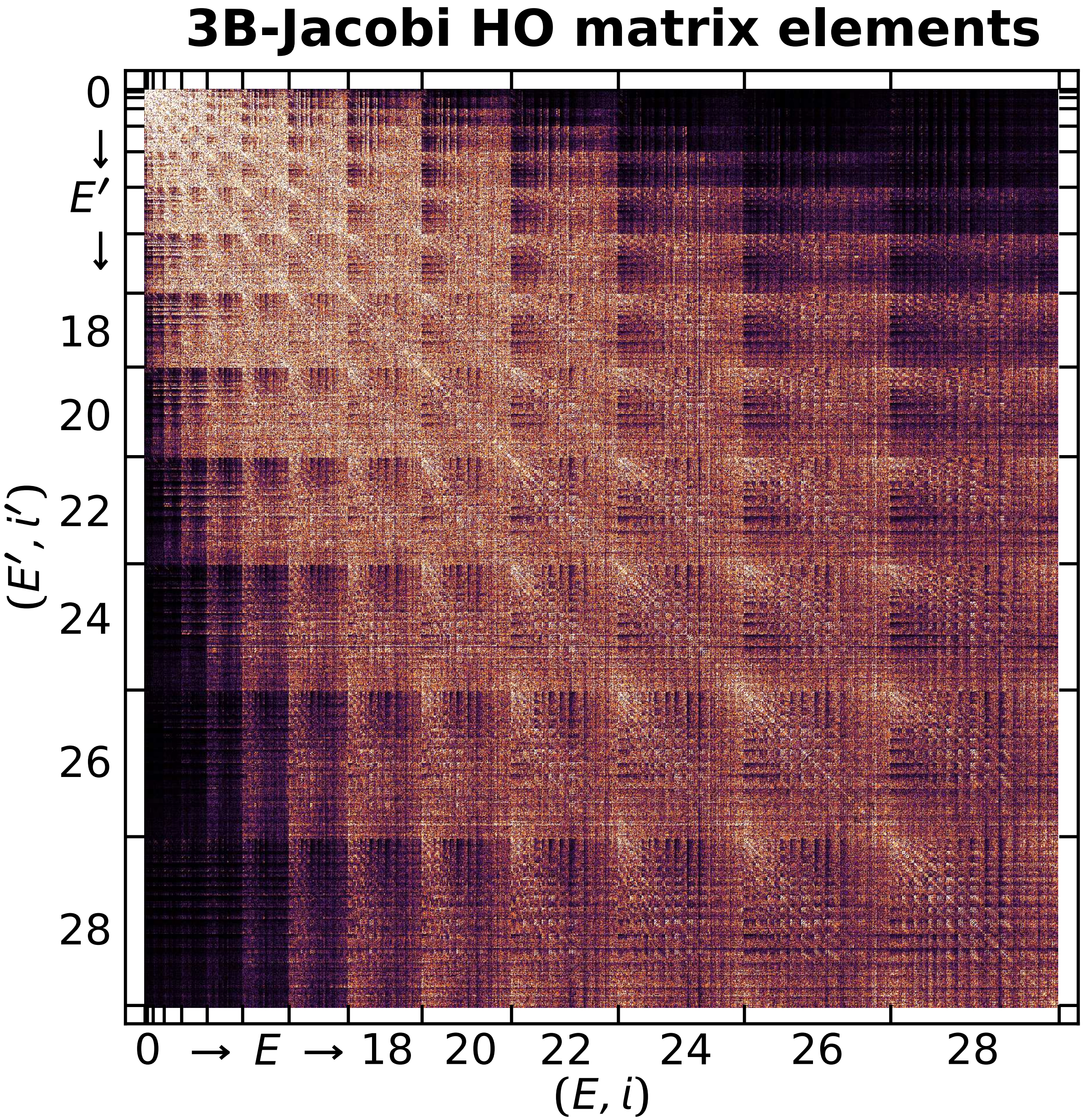

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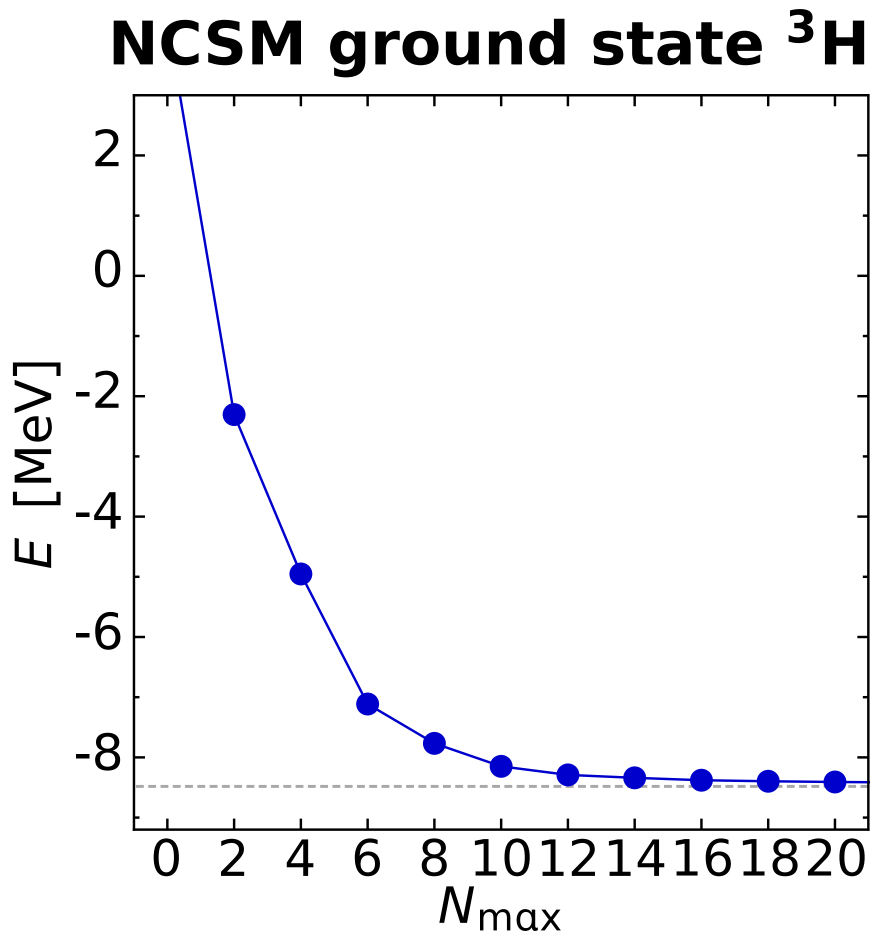

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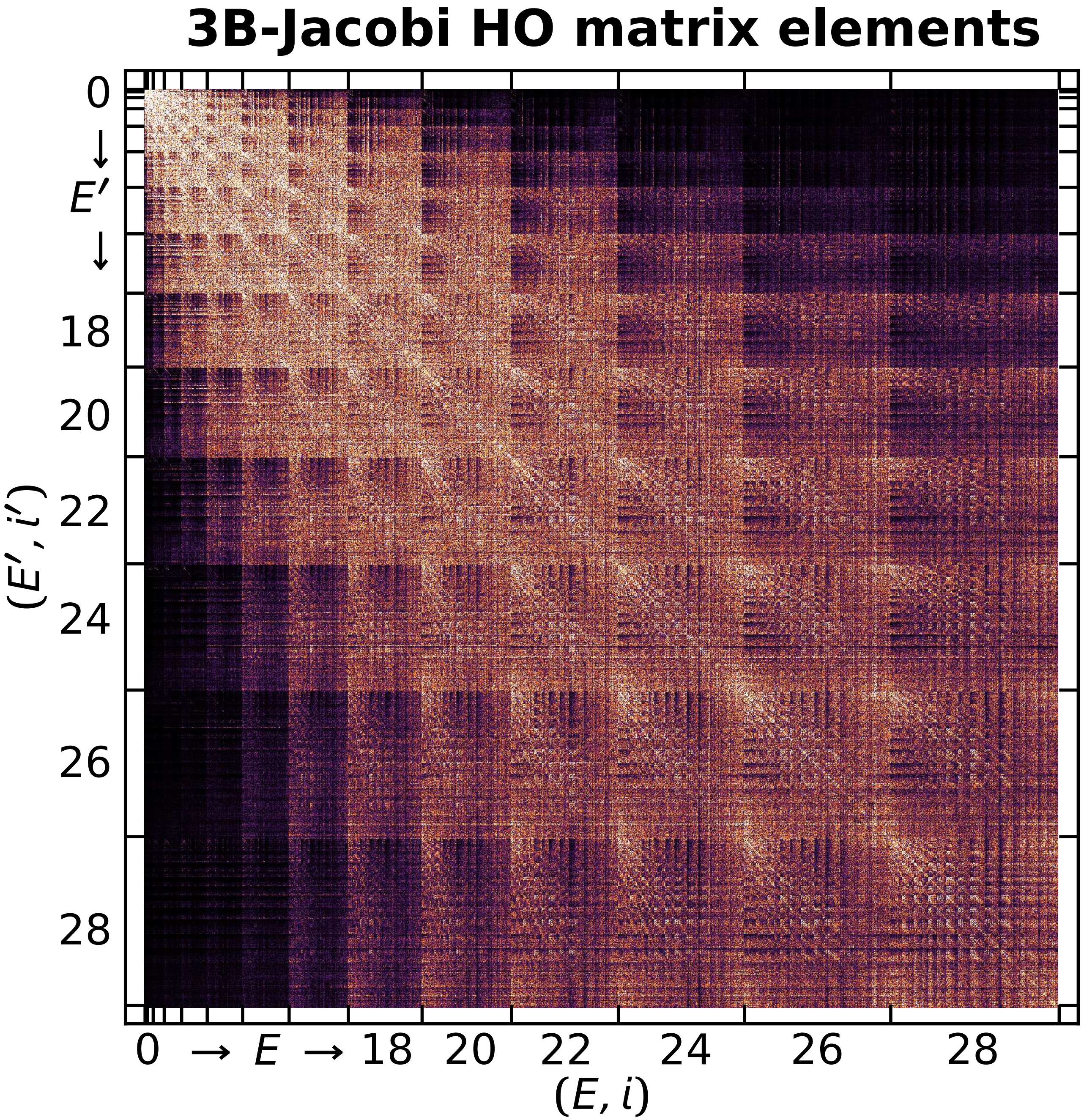

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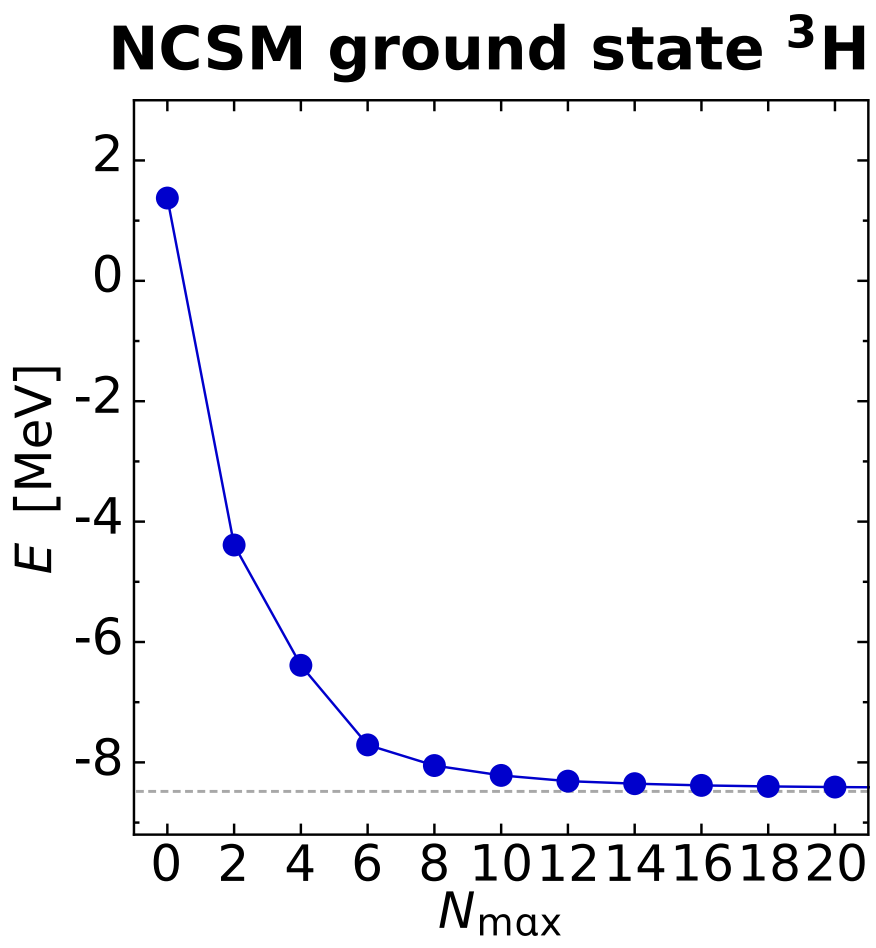

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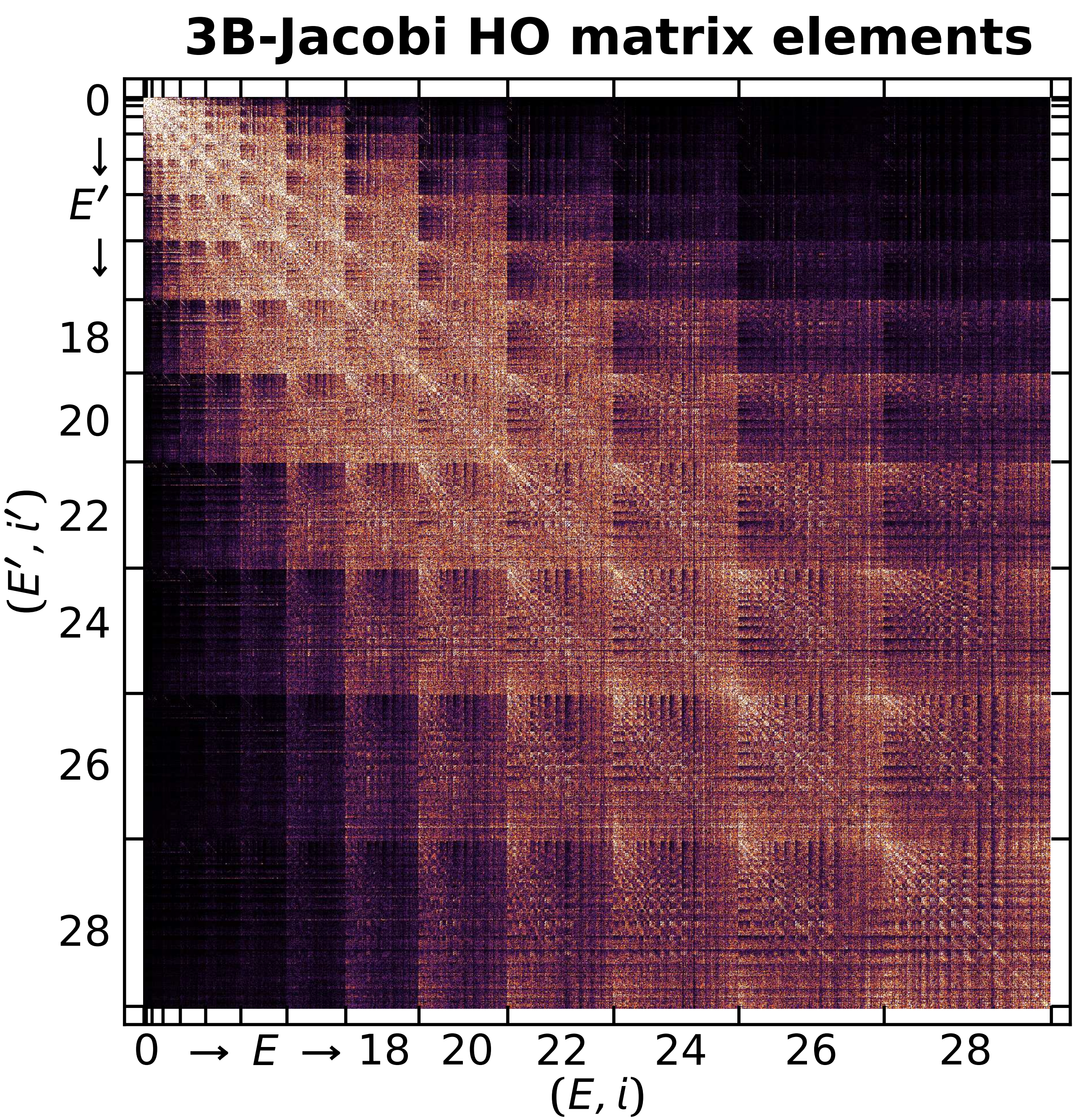

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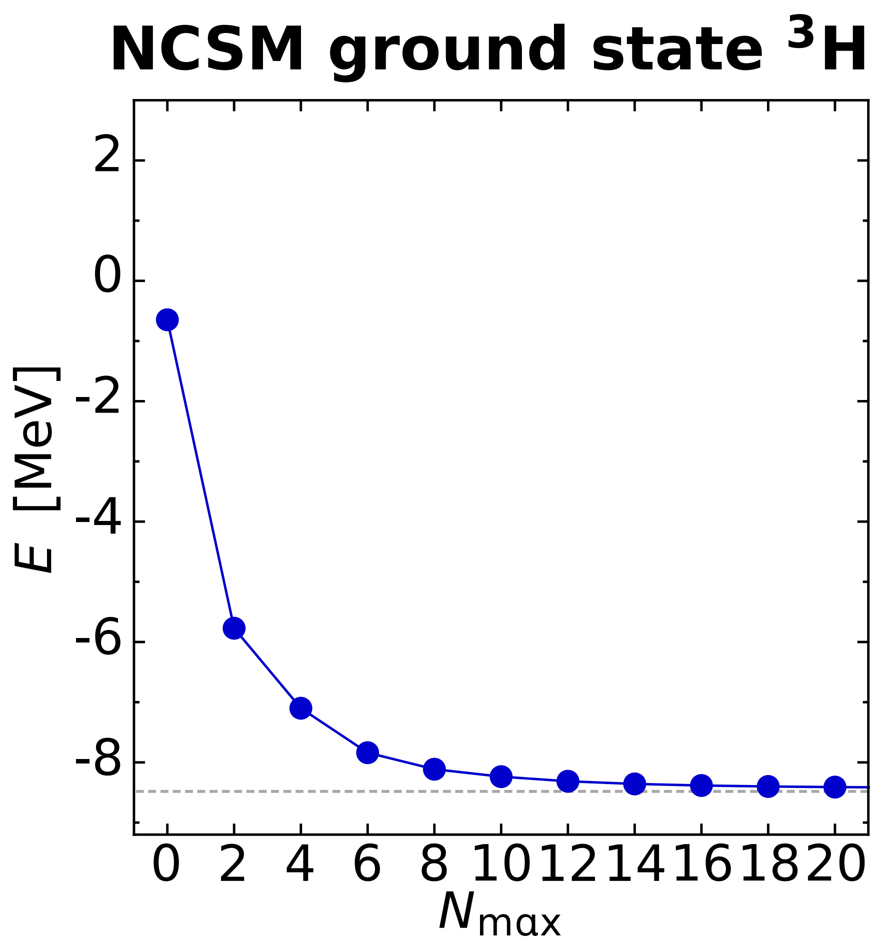

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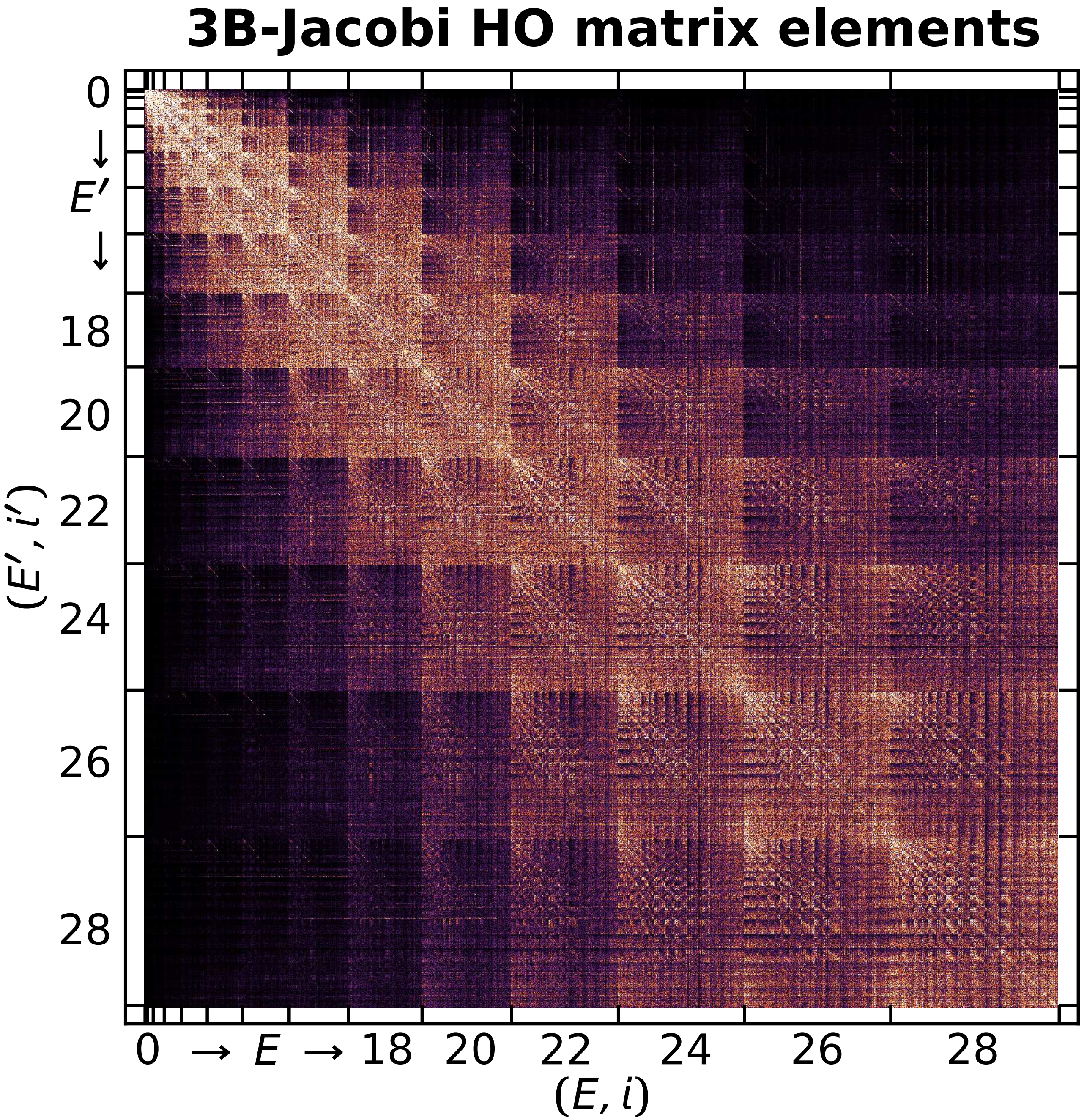

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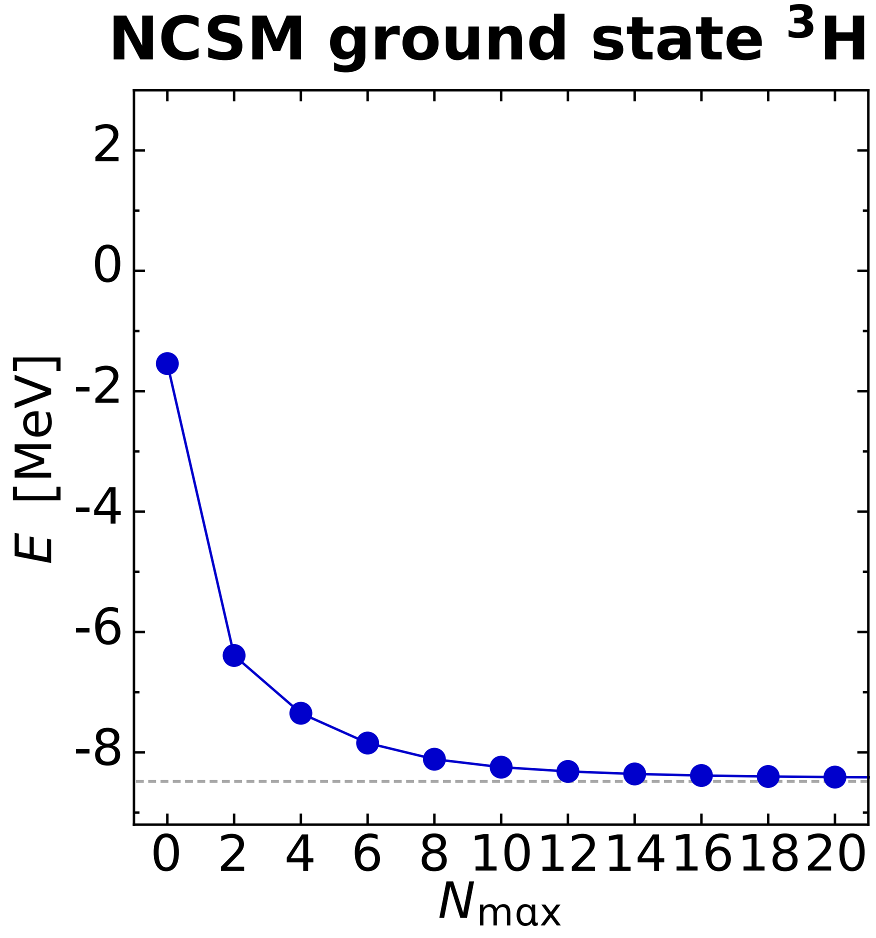

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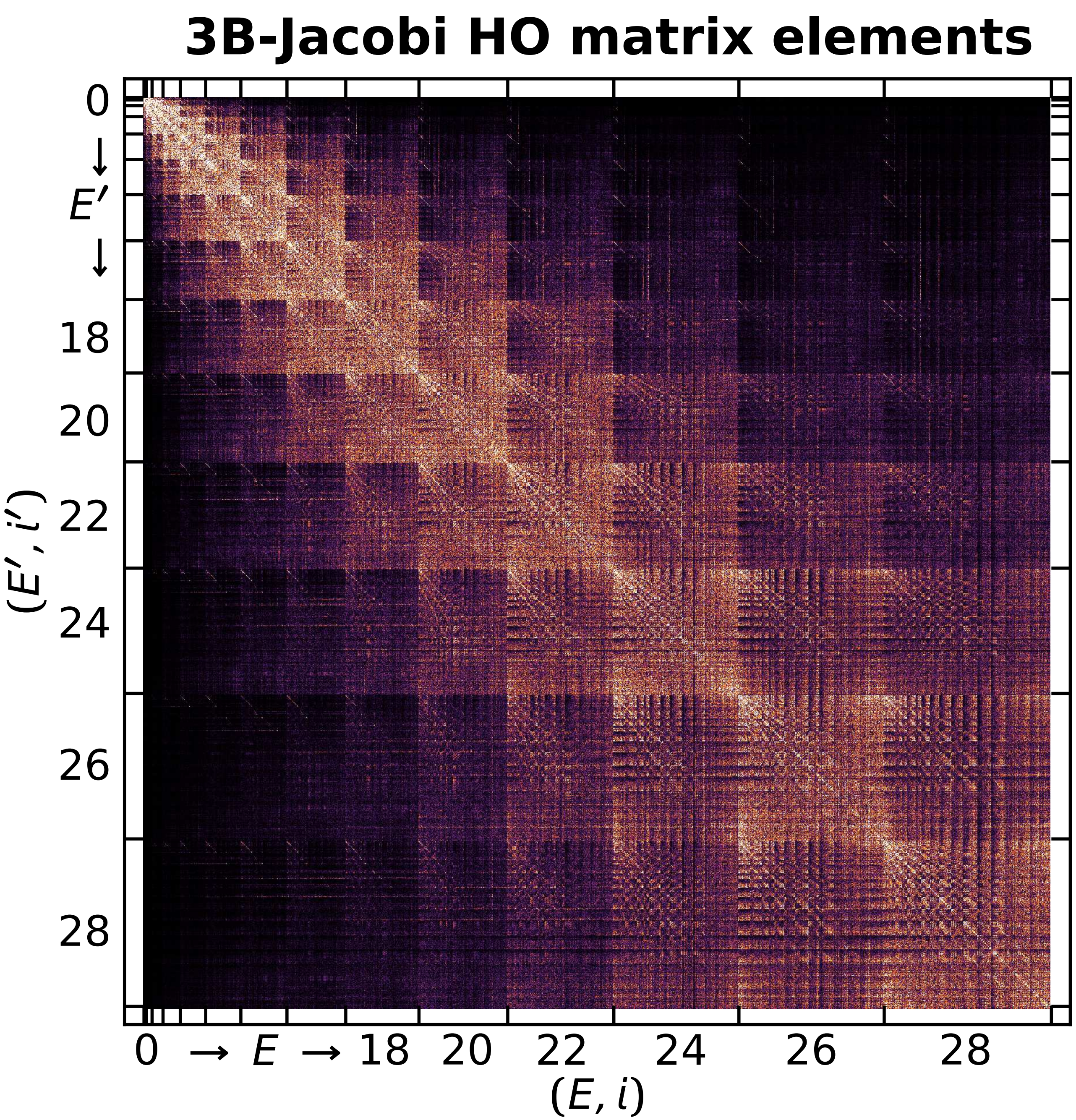

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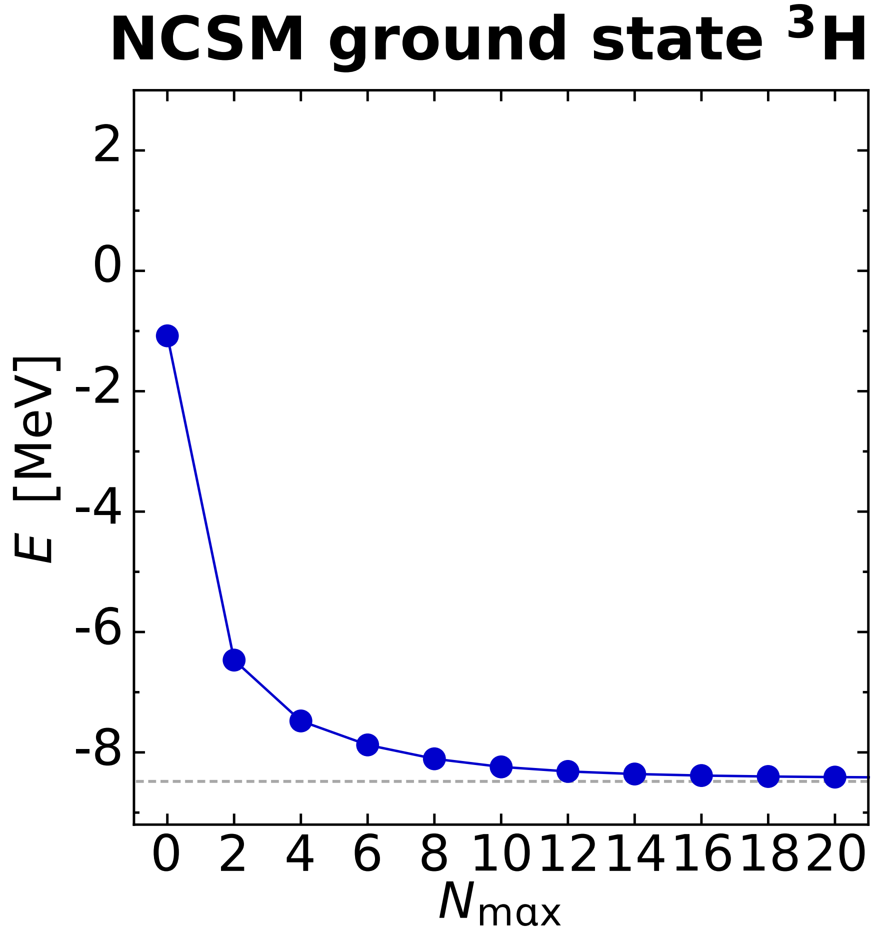

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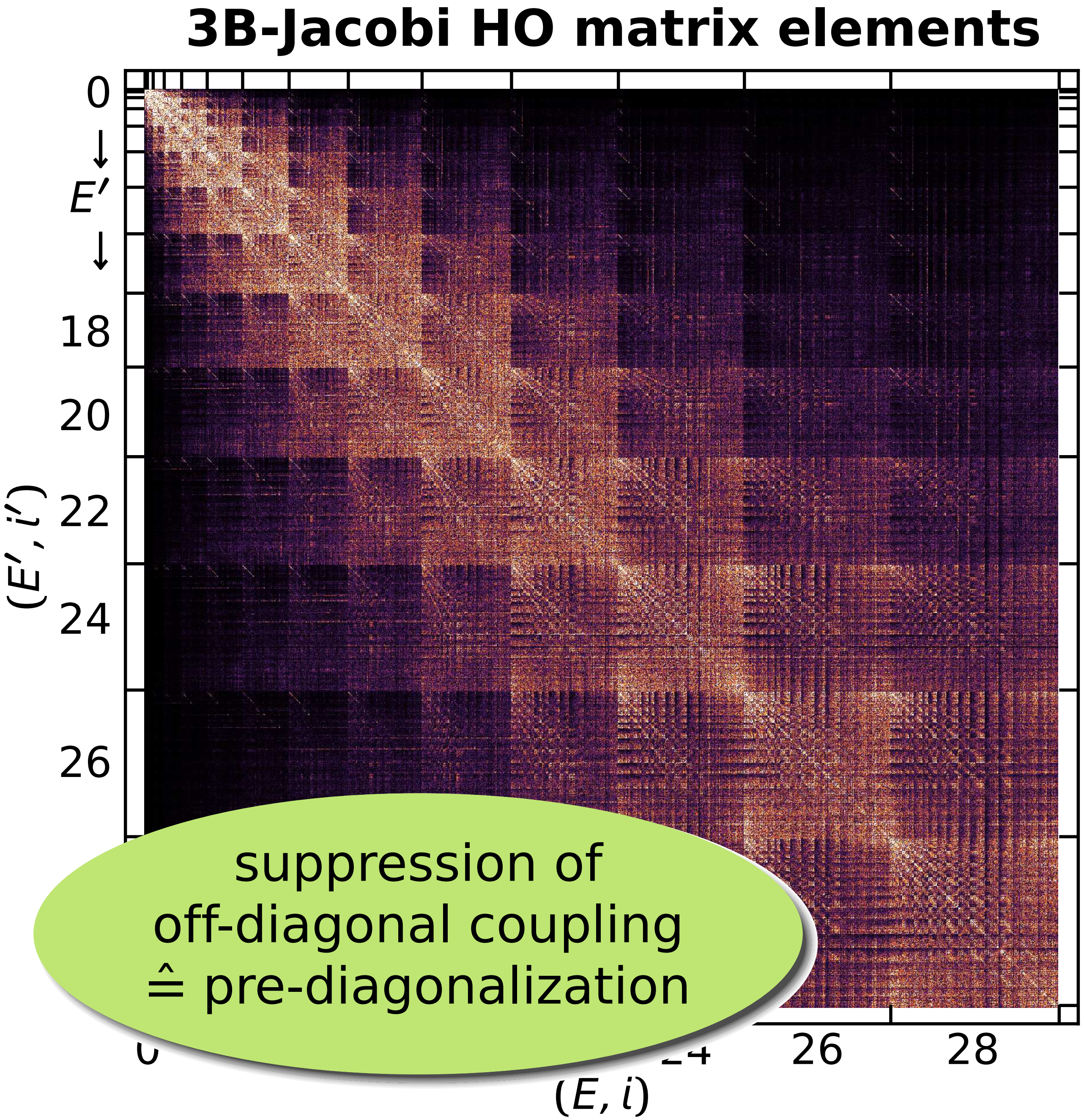

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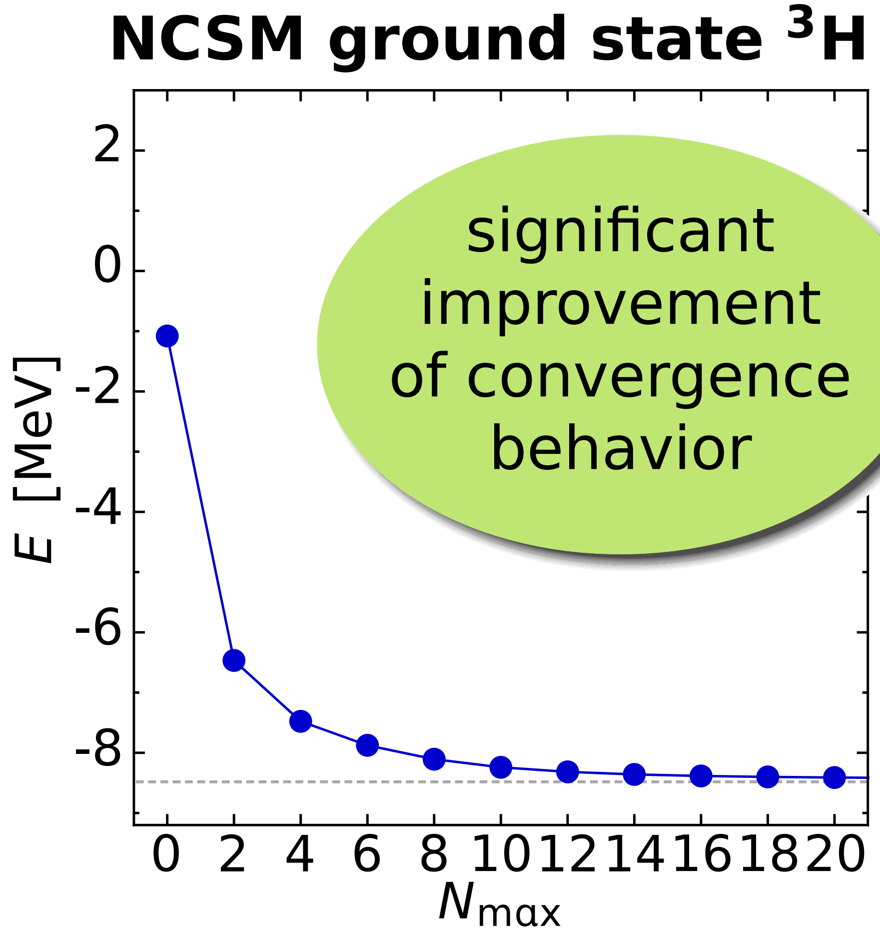


significant
improvement
of convergence
behavior

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** is formally unitary and conserves A-body energy eigenvalues (independent of α)
  - α-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 $\widetilde{\mathrm{H}}_{\alpha}^{[n]}$

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

- **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** is formally unitary and conserves *A*-body energy eigenvalues (independent of α)
  - α-dependence of eigenvalue[...] **[...]milto-nian** measures impact of [...]es

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

Sounds easy, but...

❶ computation of initial 2B/3B-Jacobi HO matrix elements of chiral NN+3N interactions

- we use Petr Navratil's ManyEff code for computing 3B-Jacobi matrix elements and corresponding CFPs

❷ SRG evolution in 2B/3B space and cluster decomposition

- efficient implementation using adaptive ODE solver & BLAS; largest block takes a few hours on single node

❸ transformation of 2B/3B Jacobi HO matrix elements into JT-coupled representation

- formulated transformation directly into JT-coupled scheme; highly efficient implementation; can handle $E_{3\,\mathrm{max}} = 16$ in JT-coupled scheme

❹ data management and on-the-fly decoupling in many-body codes

- invented optimized storage scheme for fast on-the-fly decoupling; can keep all matrix elements up to $E_{3\,\mathrm{max}} = 16$ in memory

Exact Many-Body Methods

Importance Truncated NCSM

Roth et al. — Phys. Rev. Lett. (2011); arXiv:1105.3173
Navrátil et al. — Phys. Rev. C 82, 034609 (2010)
Roth — Phys. Rev. C 79, 064324 (2009)
Roth & Navrátil — Phys. Rev. Lett. 99, 092501 (2007)

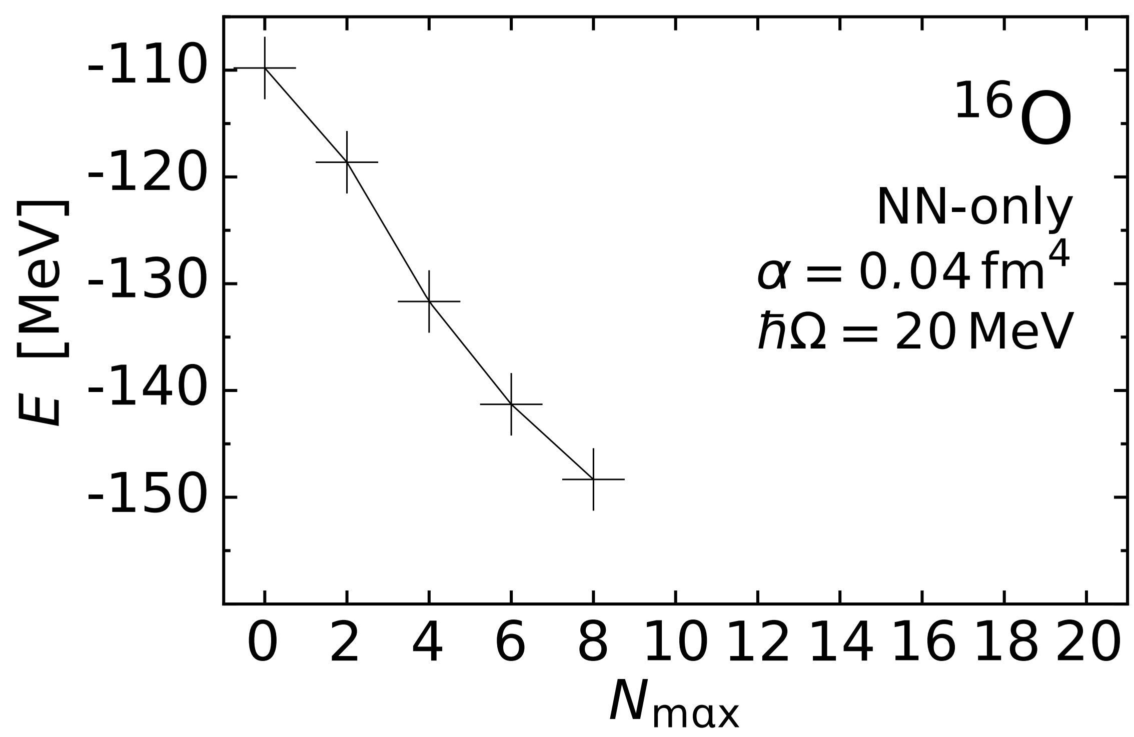
Importance Truncated NCSM

NCSM is one of the most powerful and universal ab initio many-body 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 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}O not really feasible (basis dimension > 10^{10})



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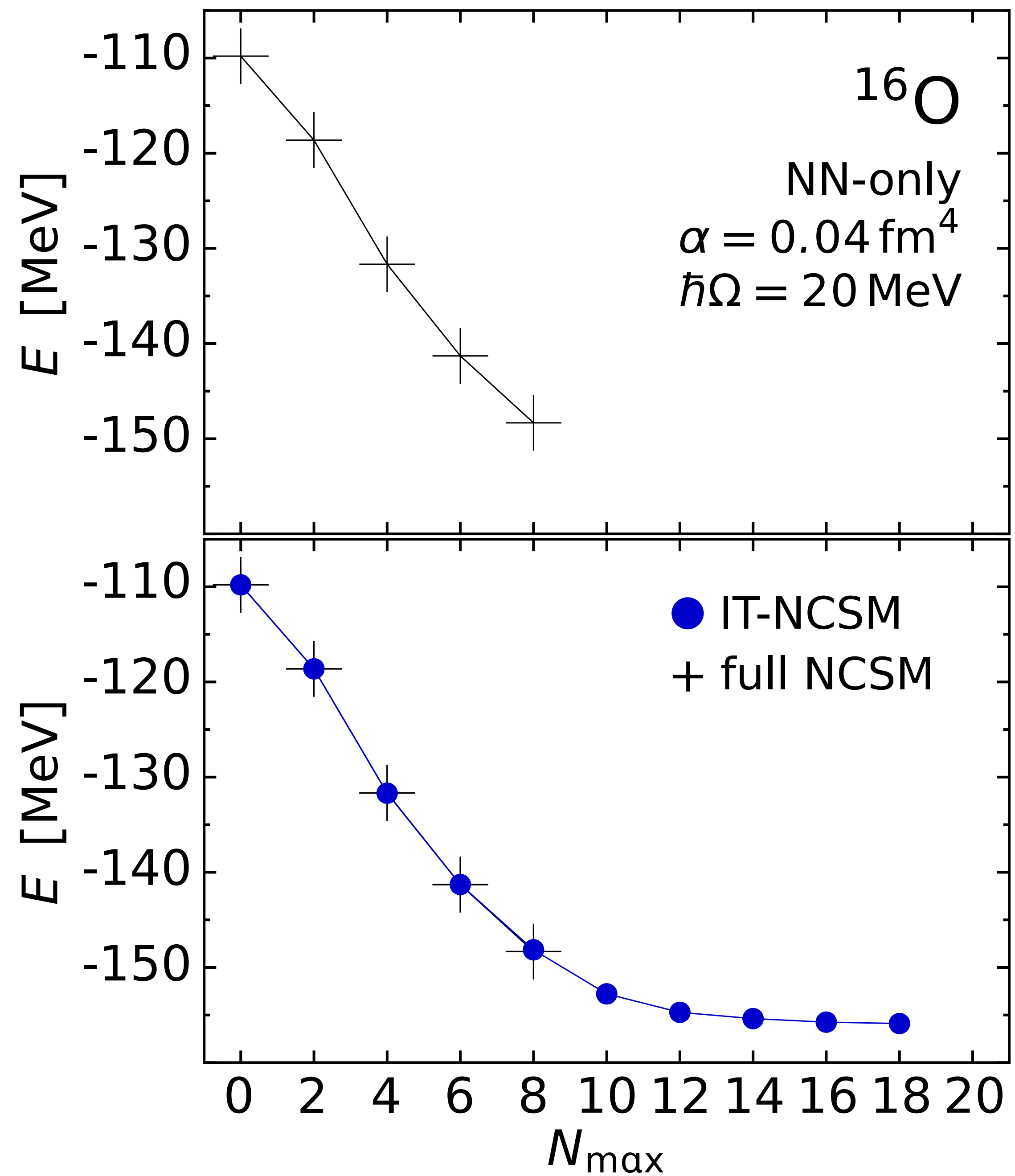
Importance Truncation

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



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-live)

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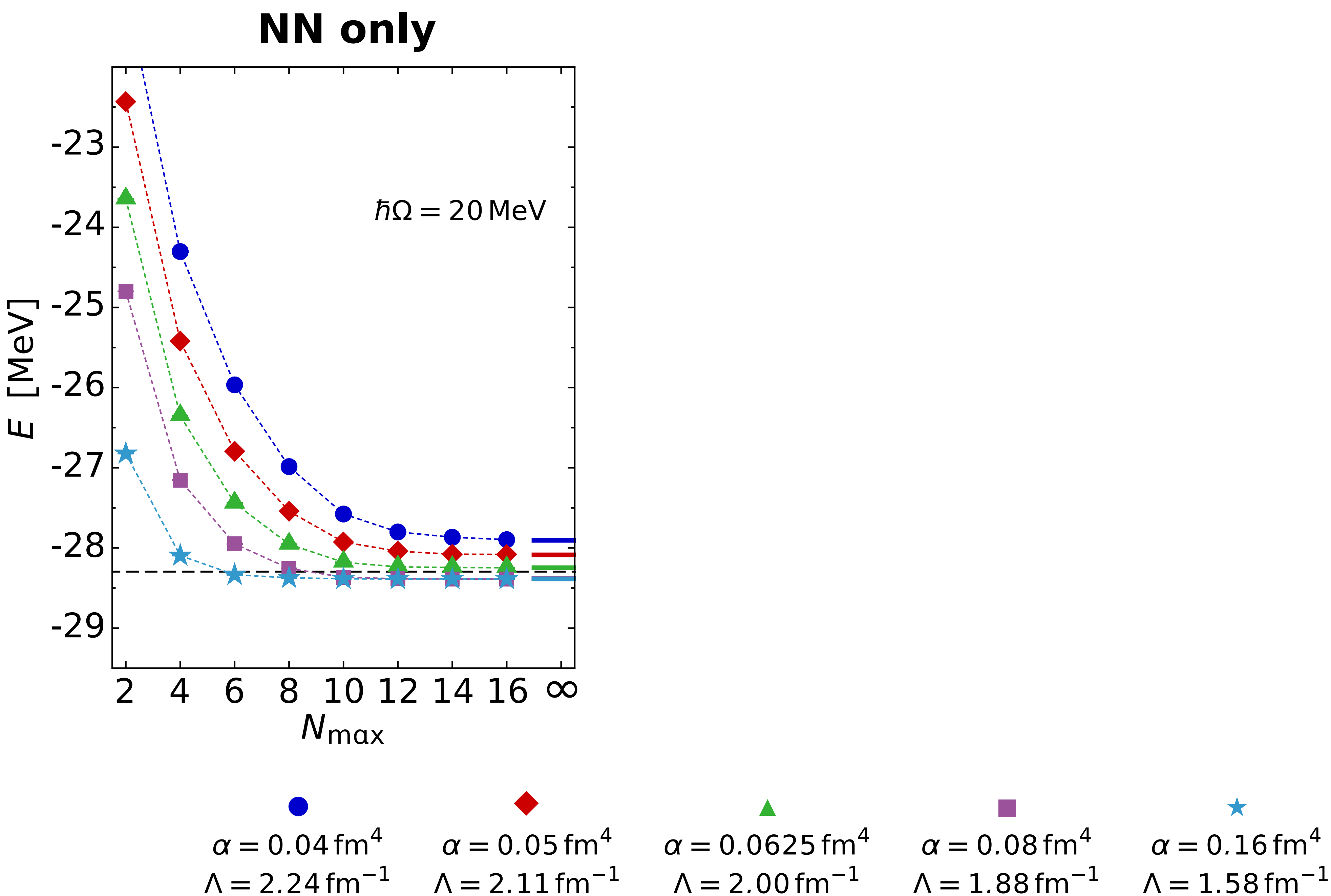
α-variation provides a **diagnostic tool** to assess the contributions of omitted many-body interactions

^{4}He: Ground-State Energies



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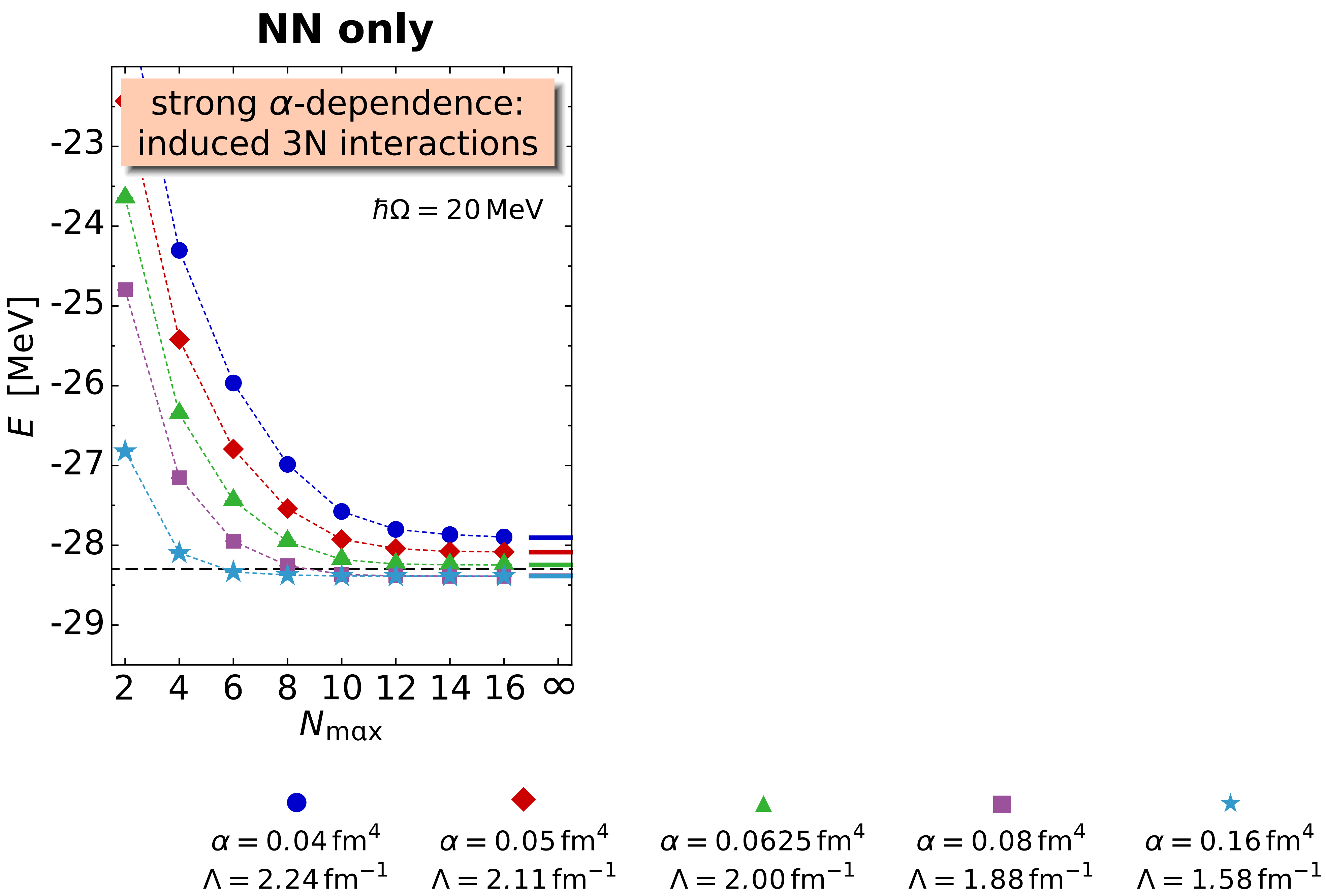

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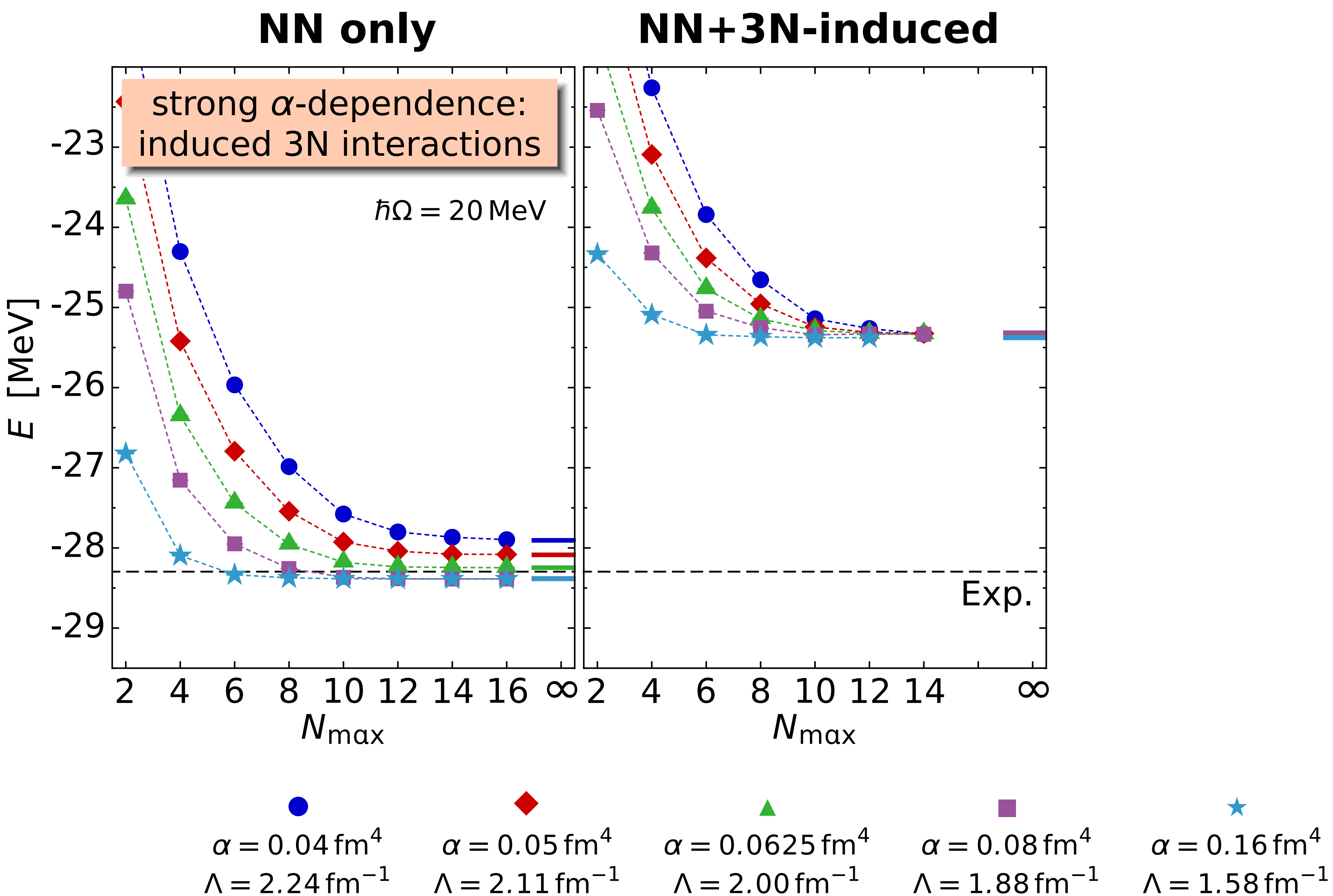

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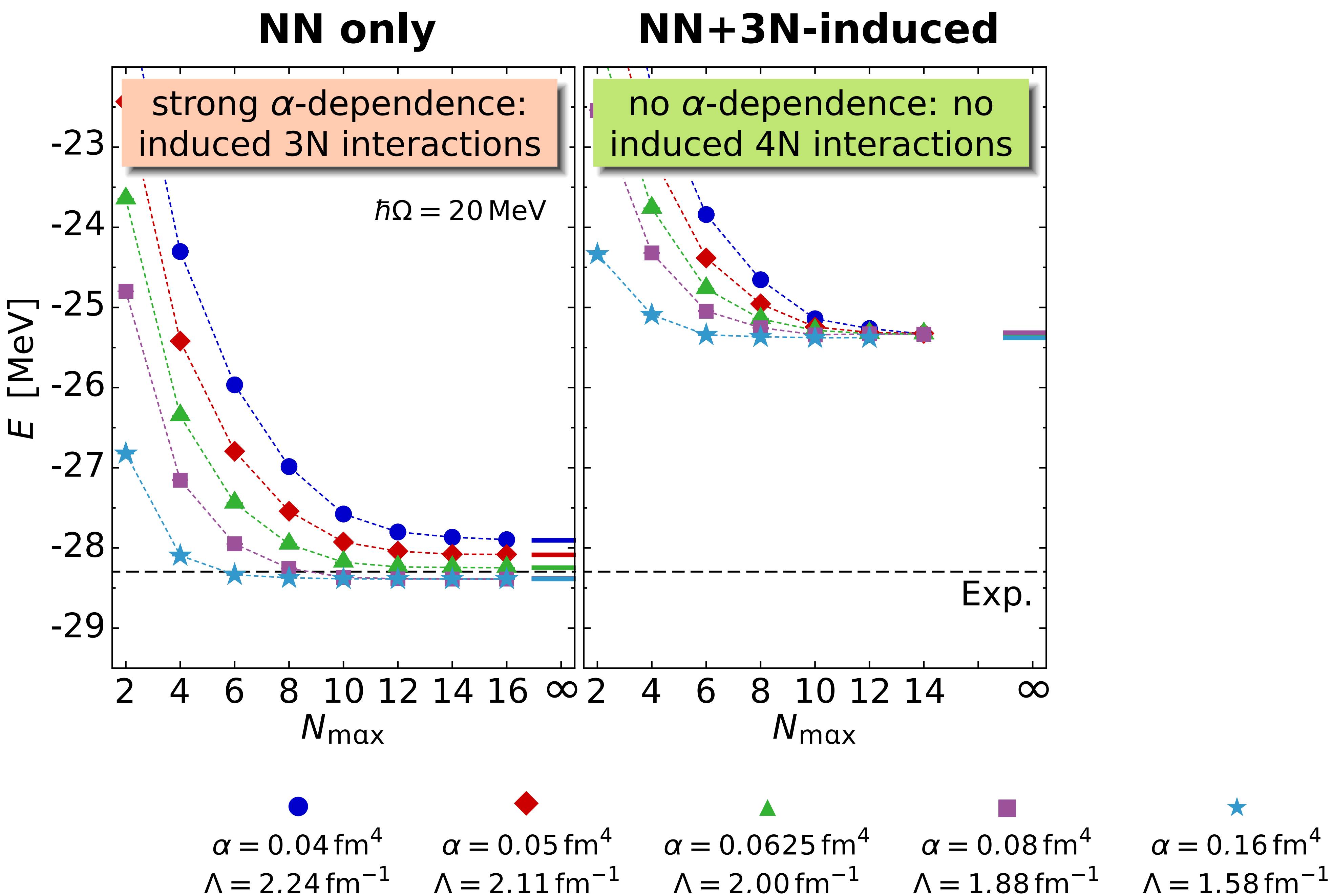

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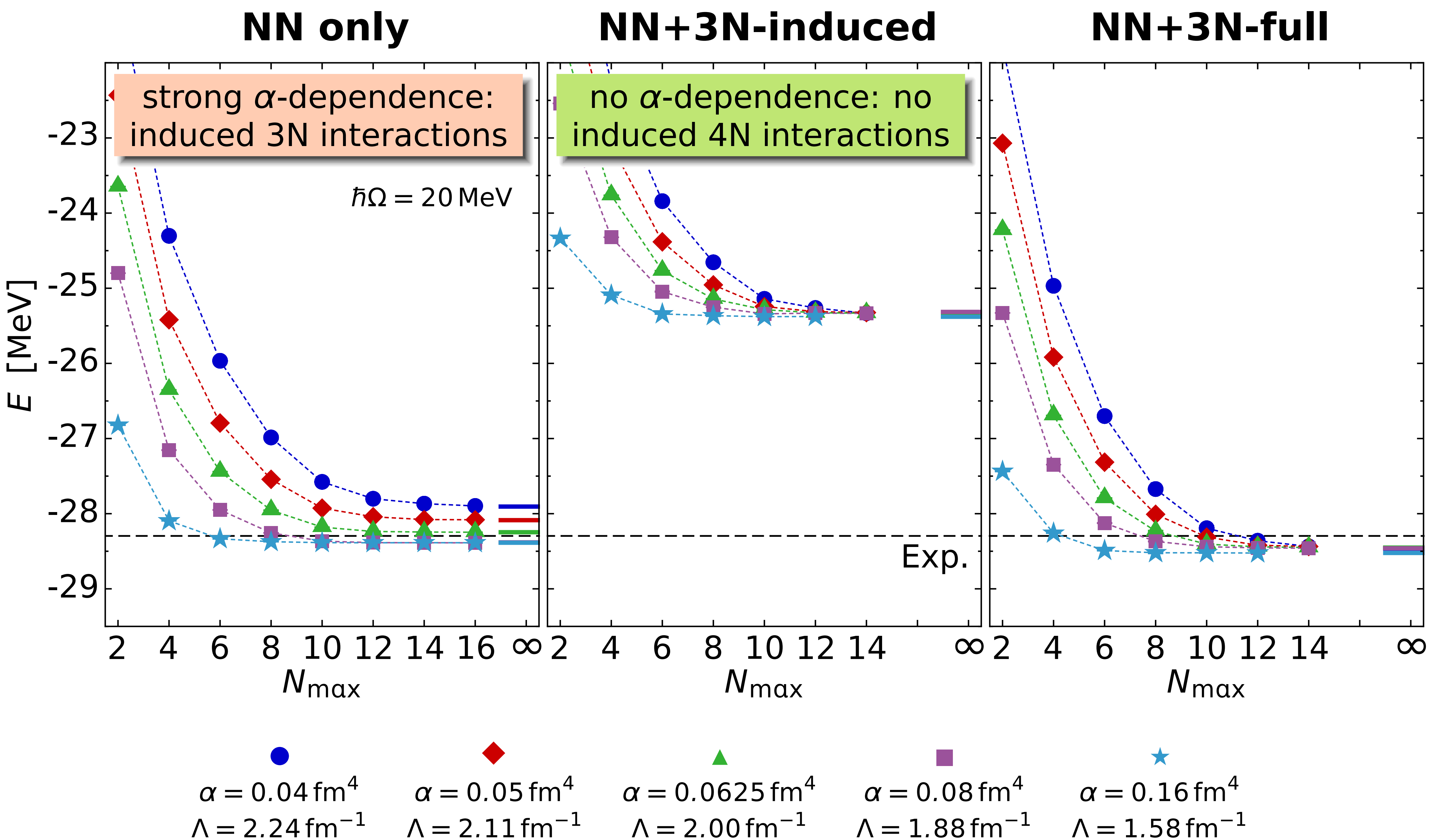

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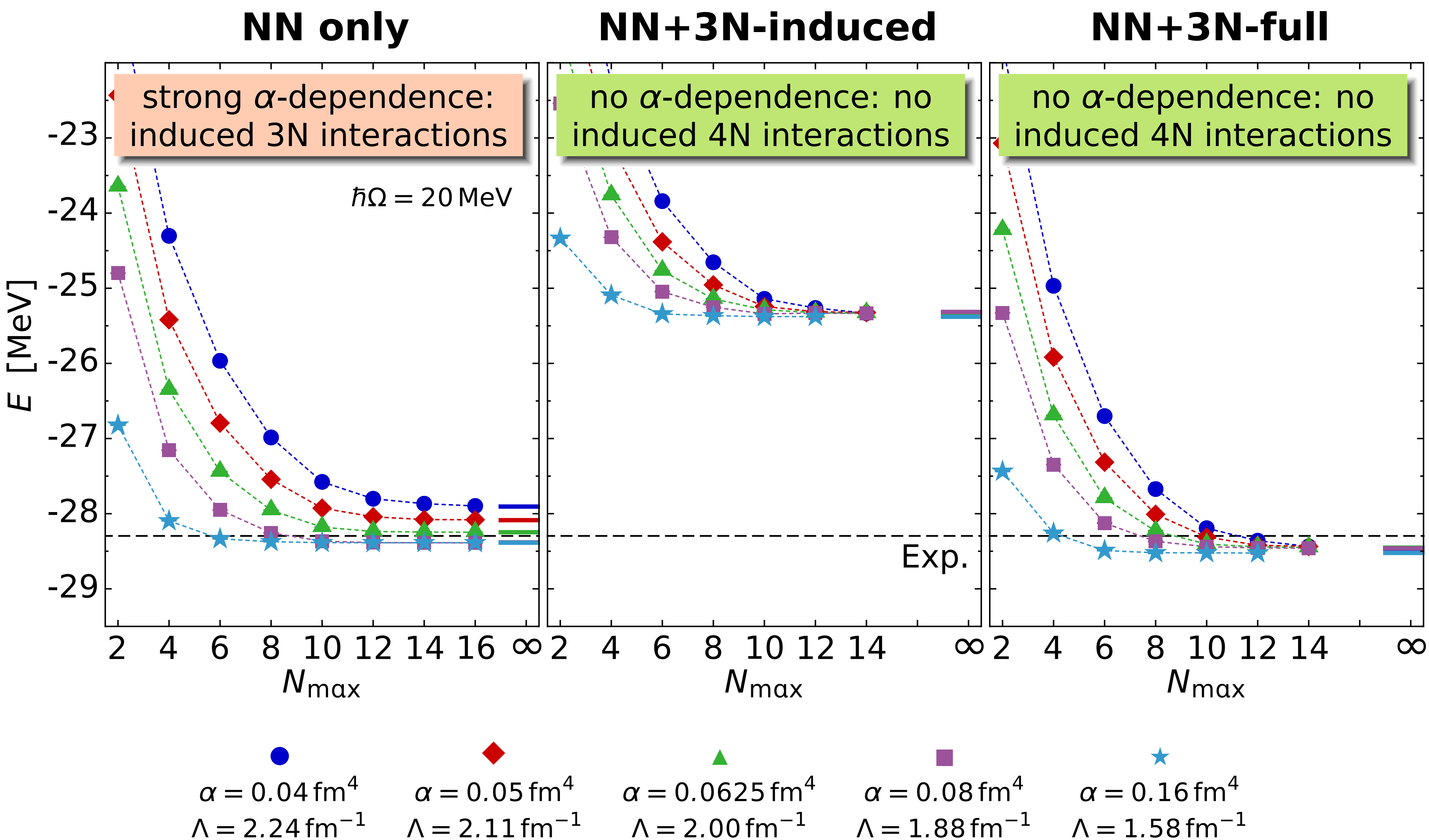
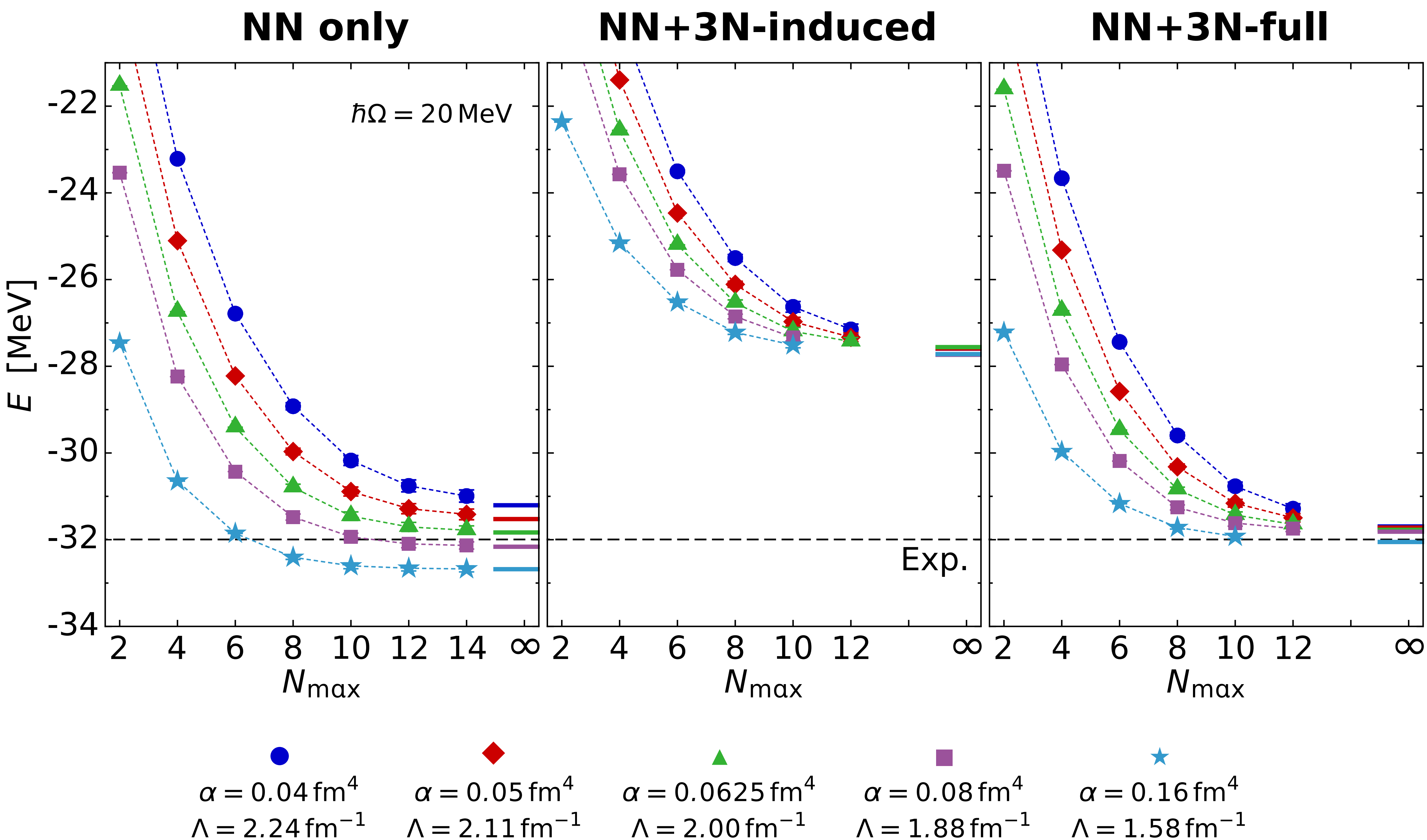
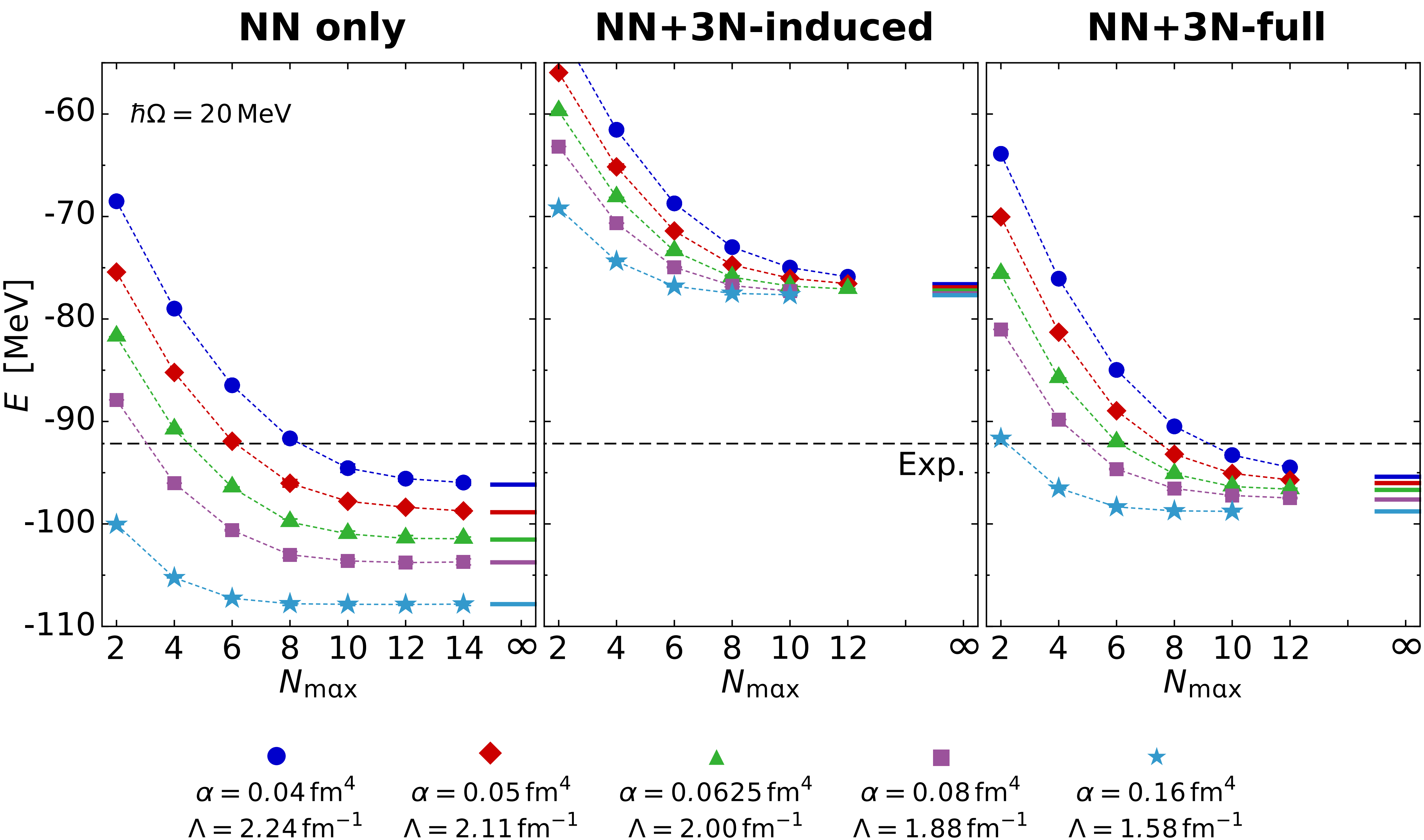


^{6}Li: Ground-State Energies



^{12}C: Ground-State Energies



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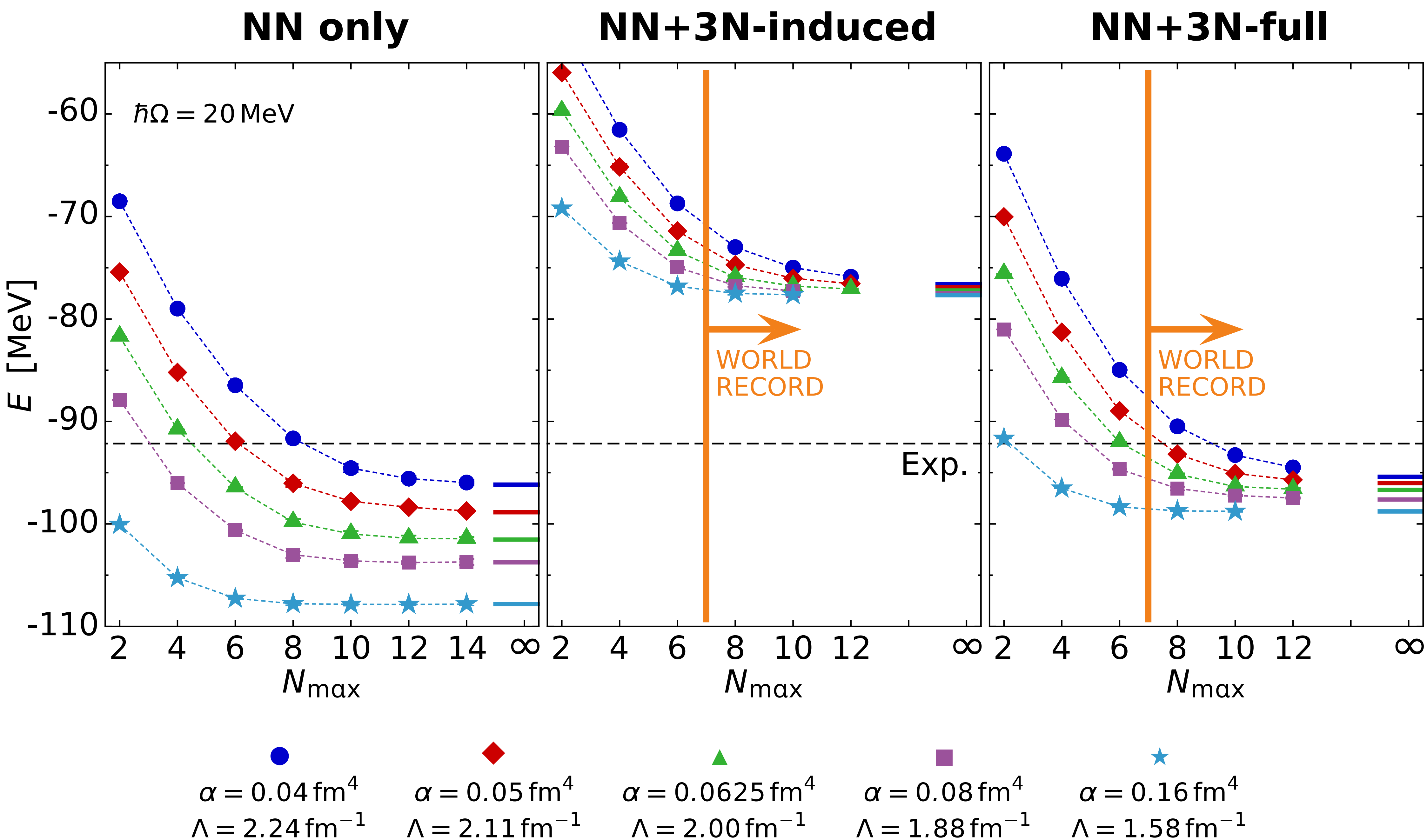

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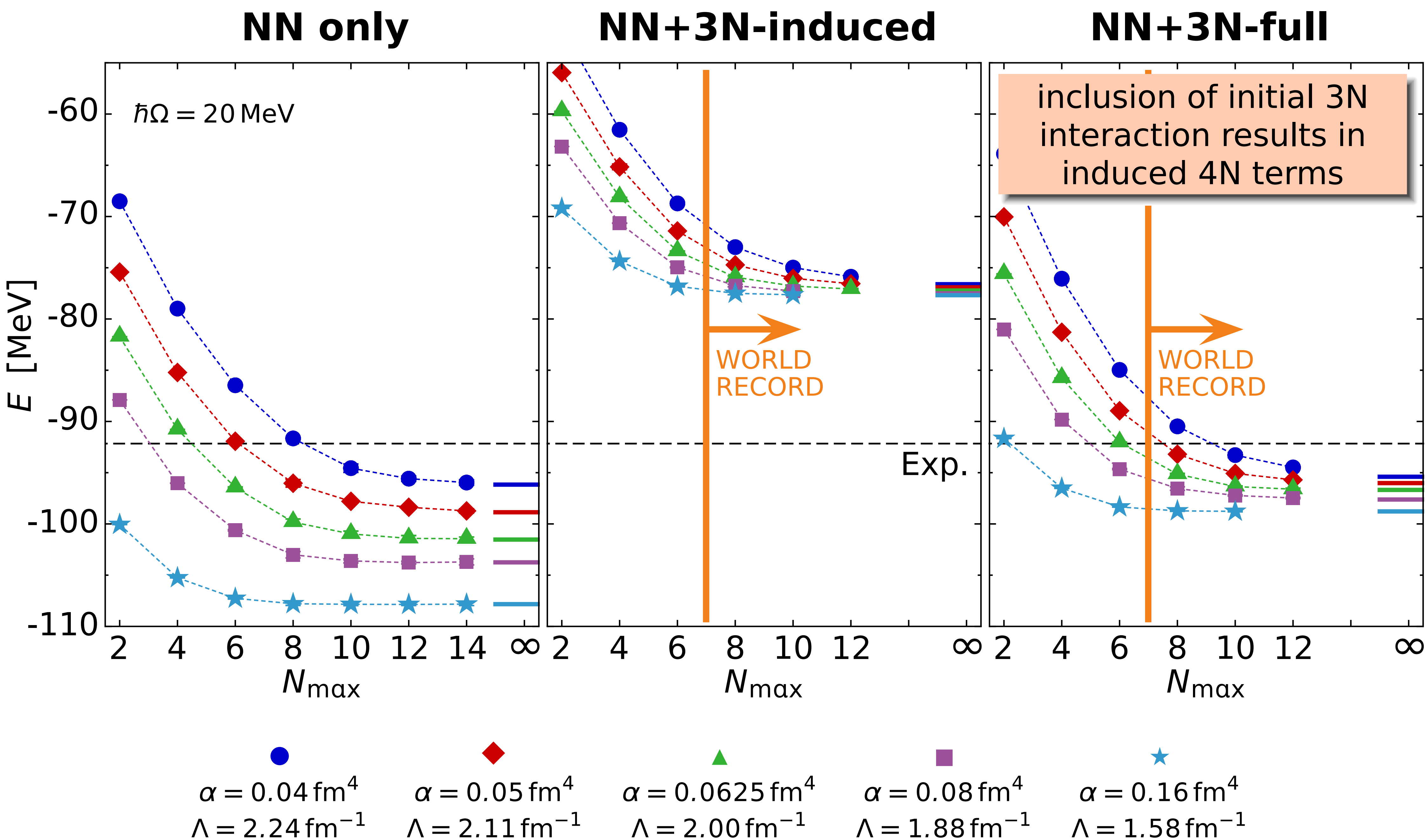
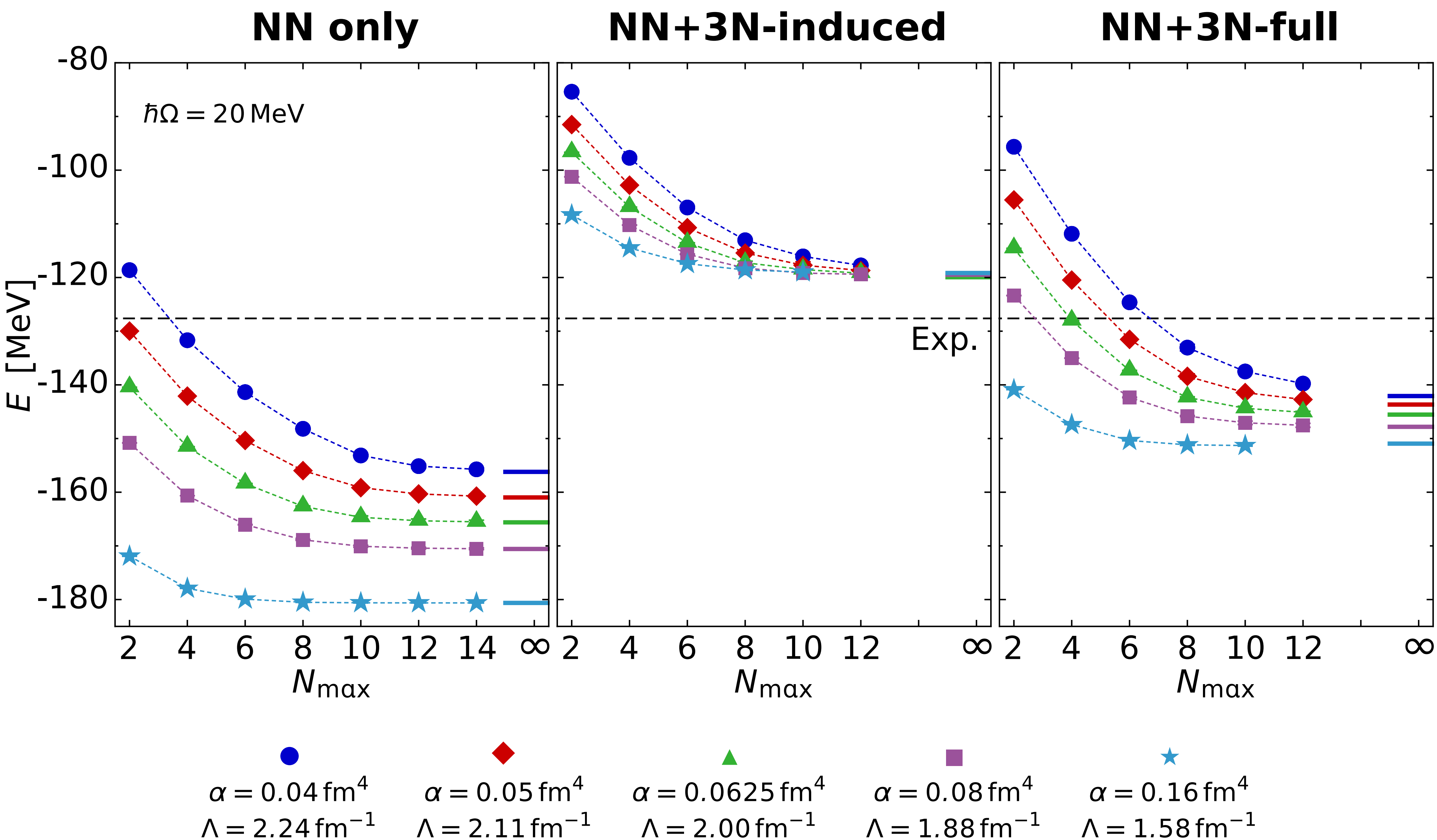


^{16}O: Ground-State Energies



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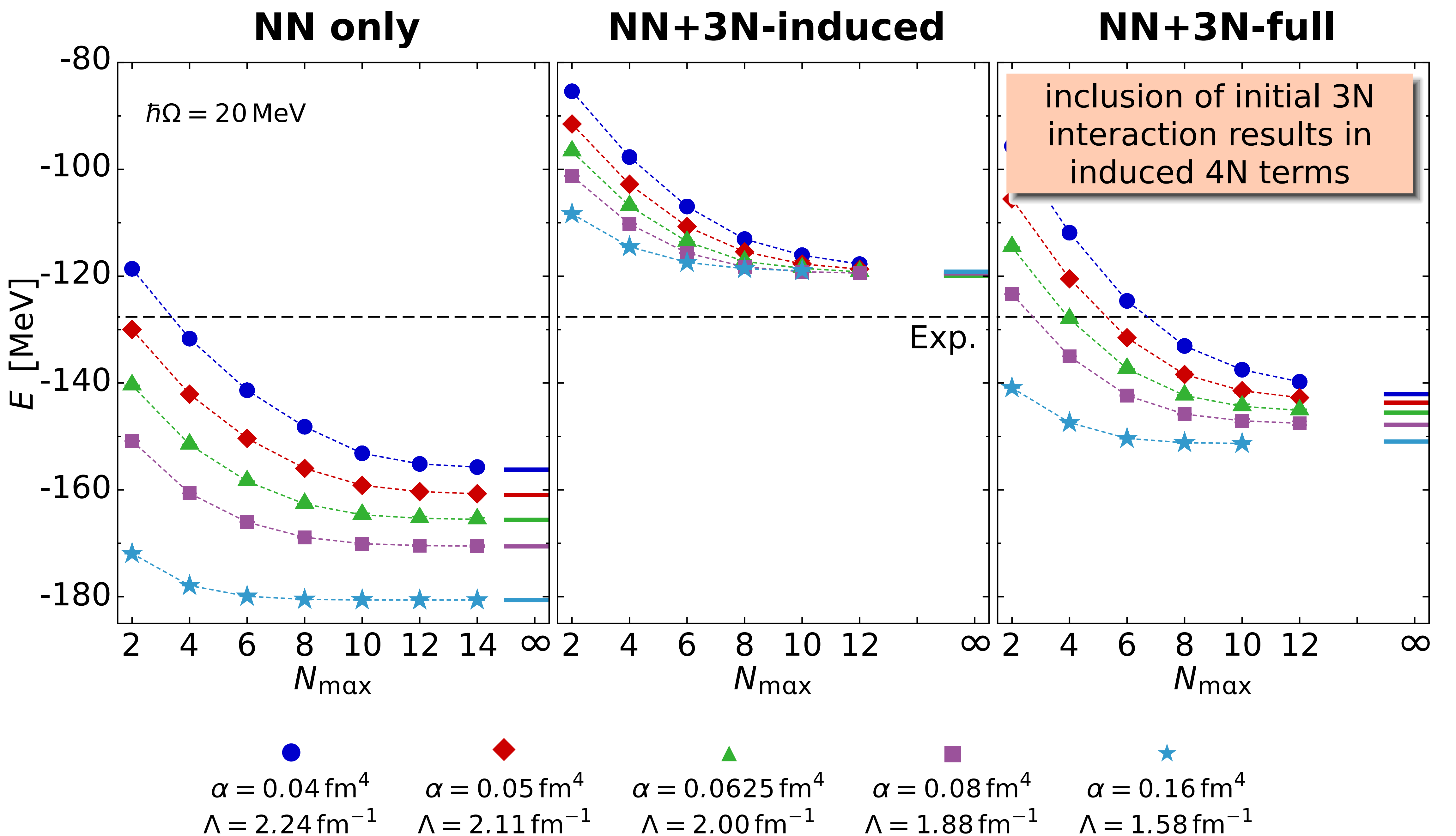
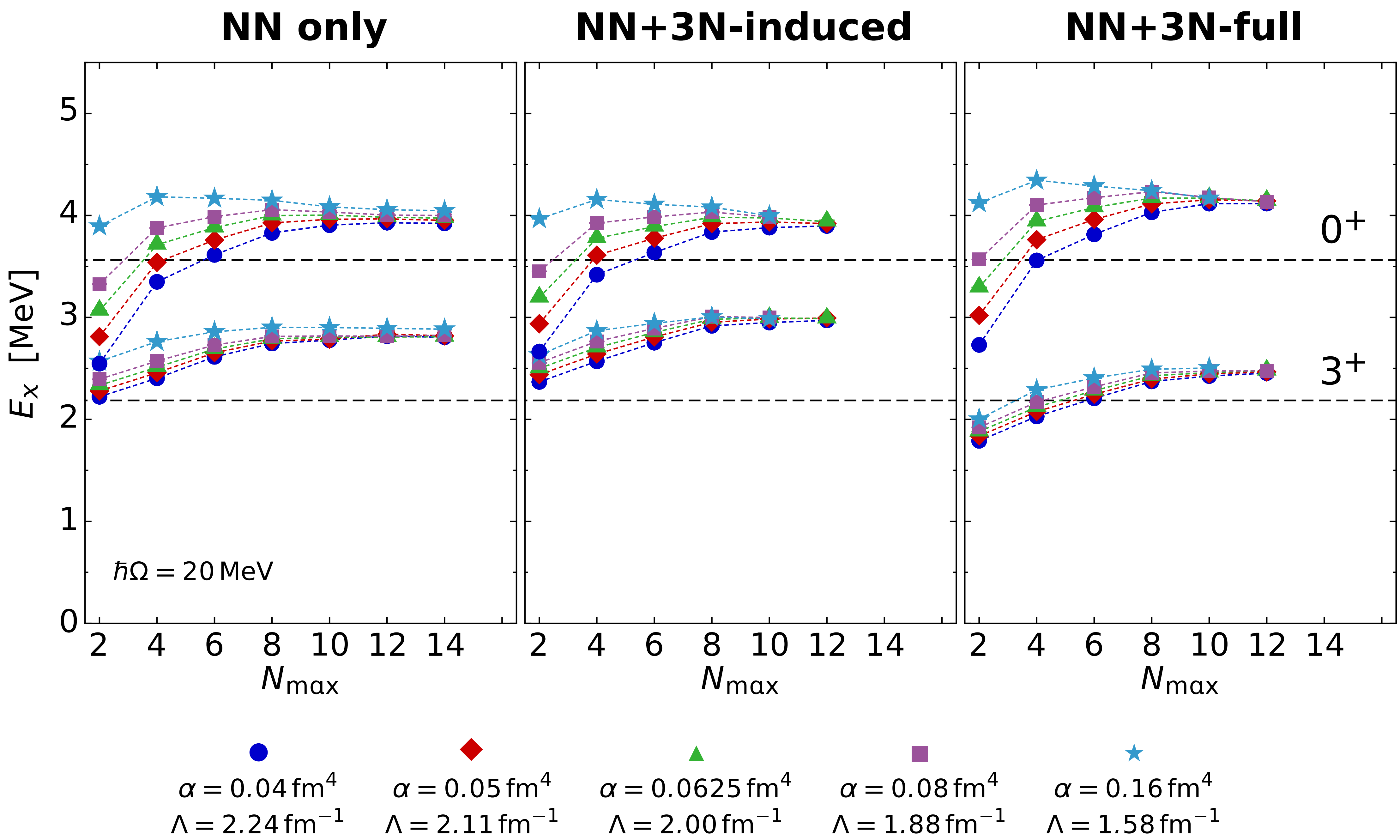
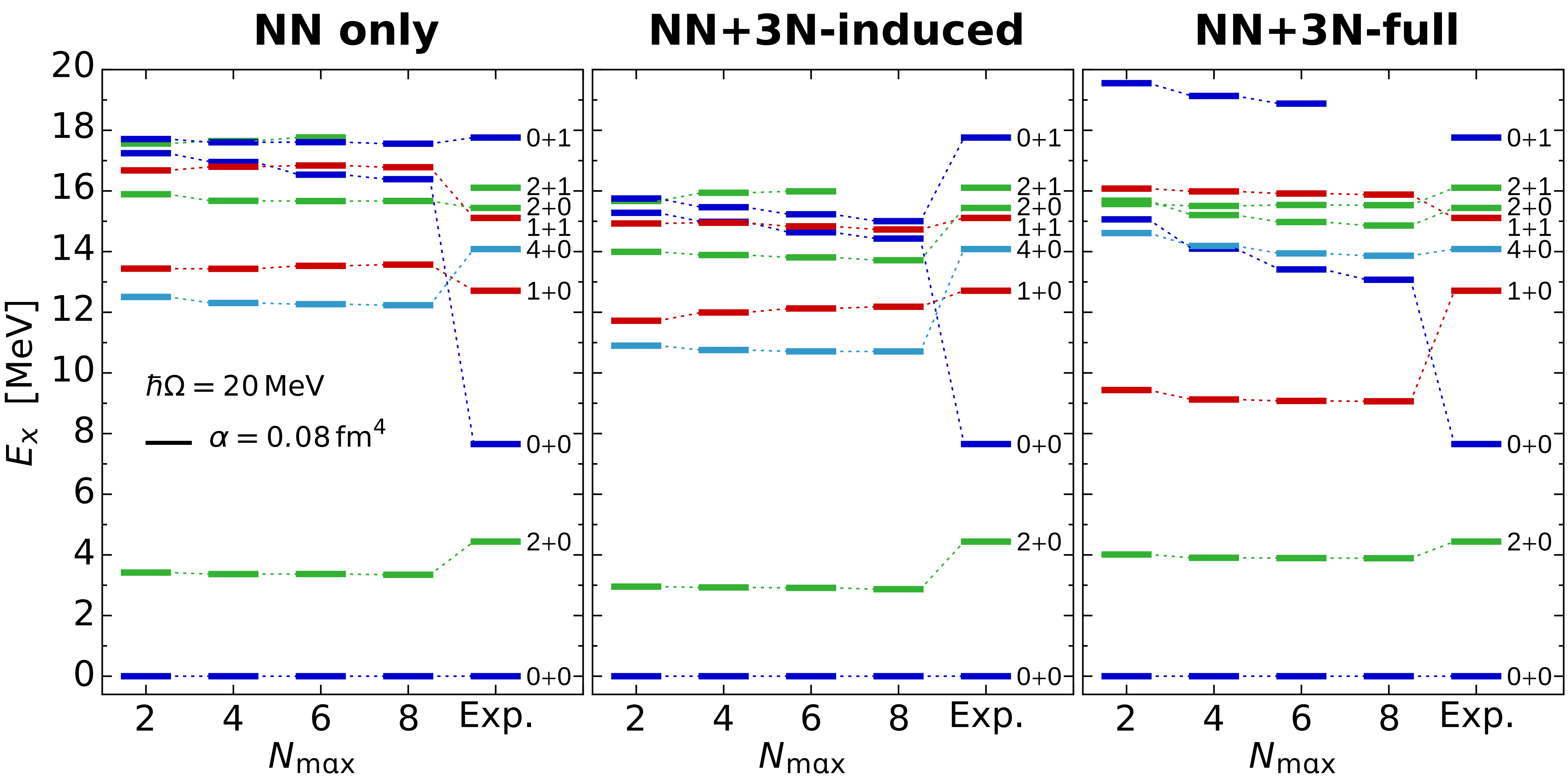


^{6}Li: Excitation Energies



Spectroscopy of ^{12}C



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

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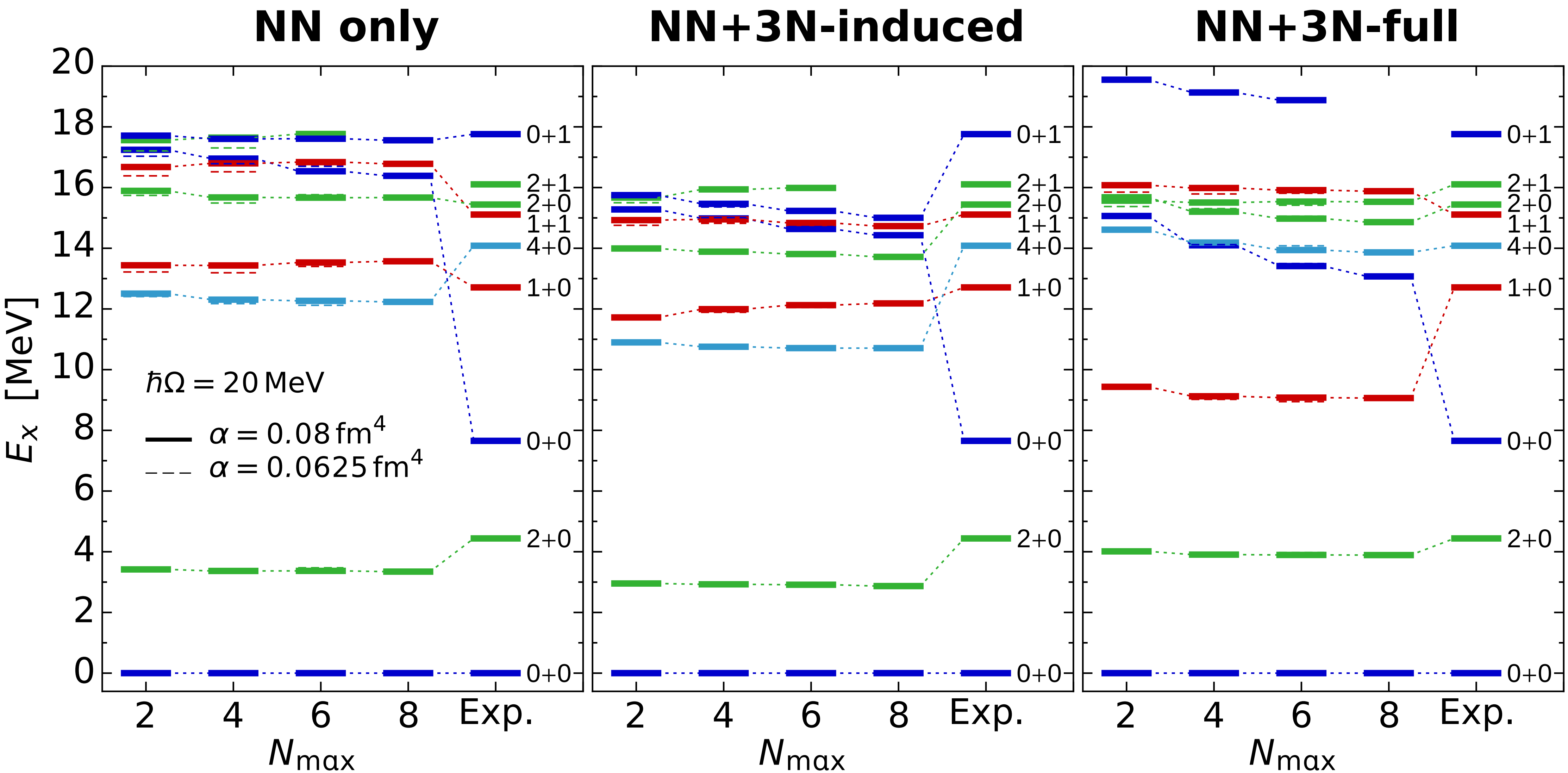

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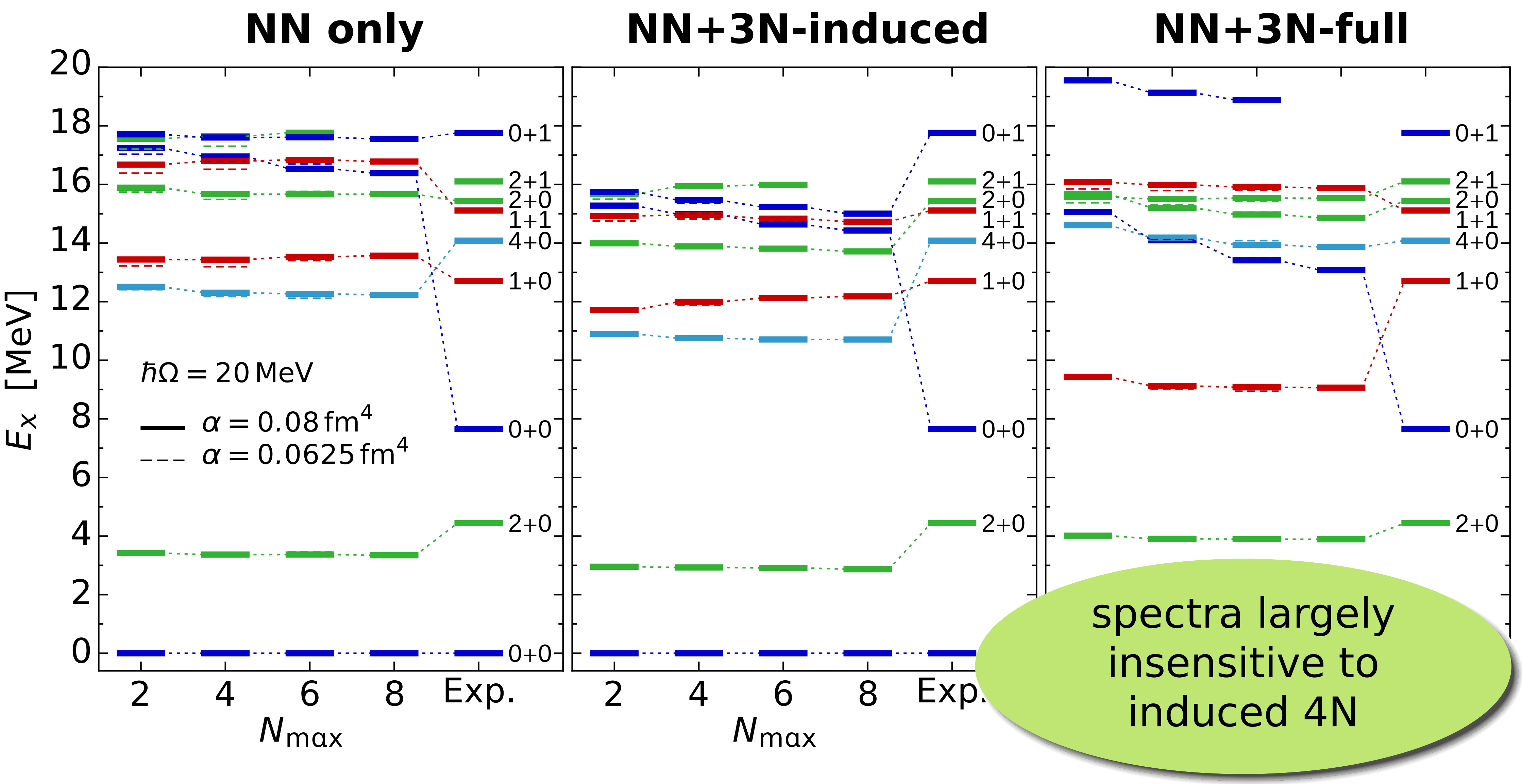

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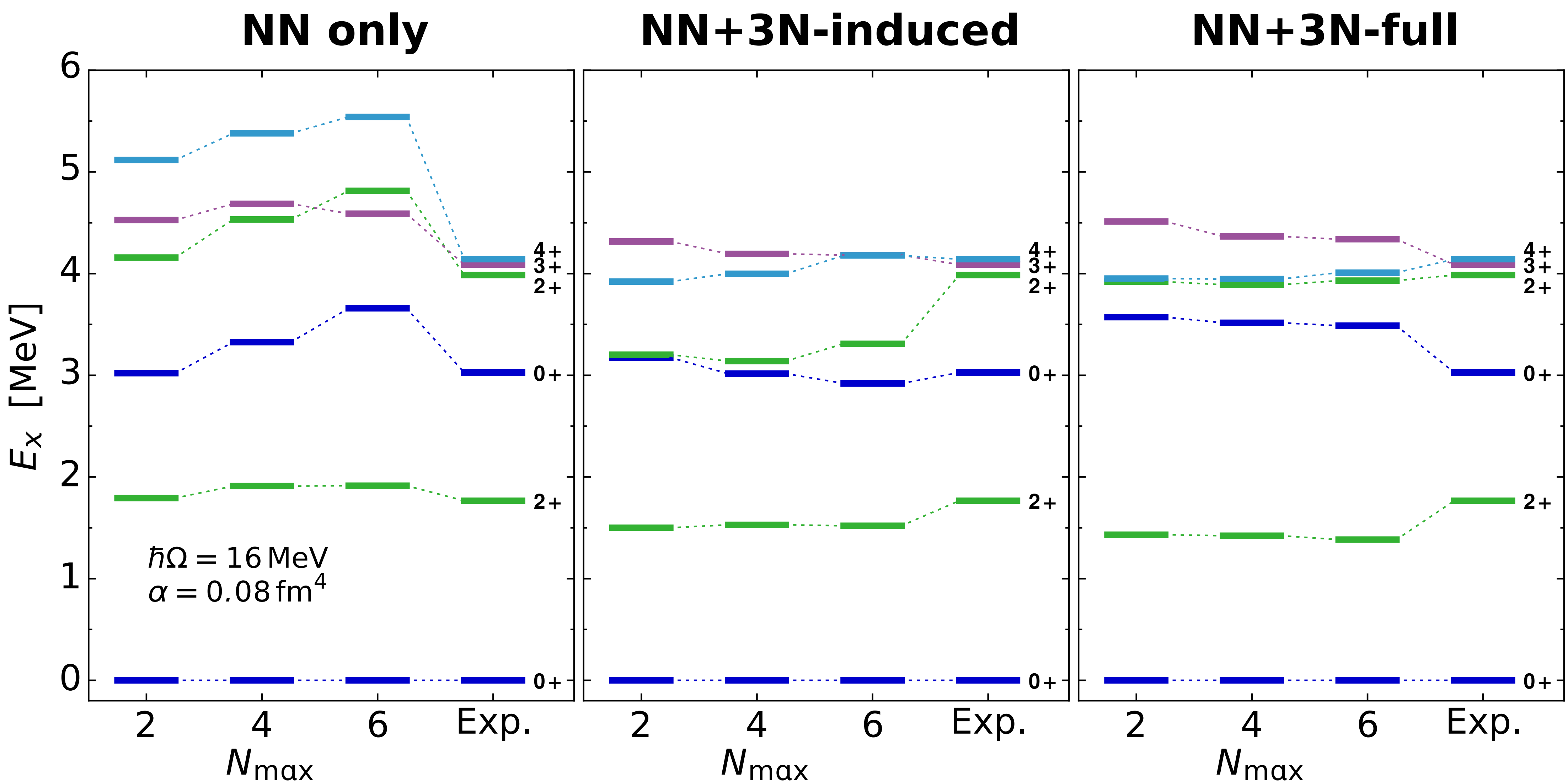
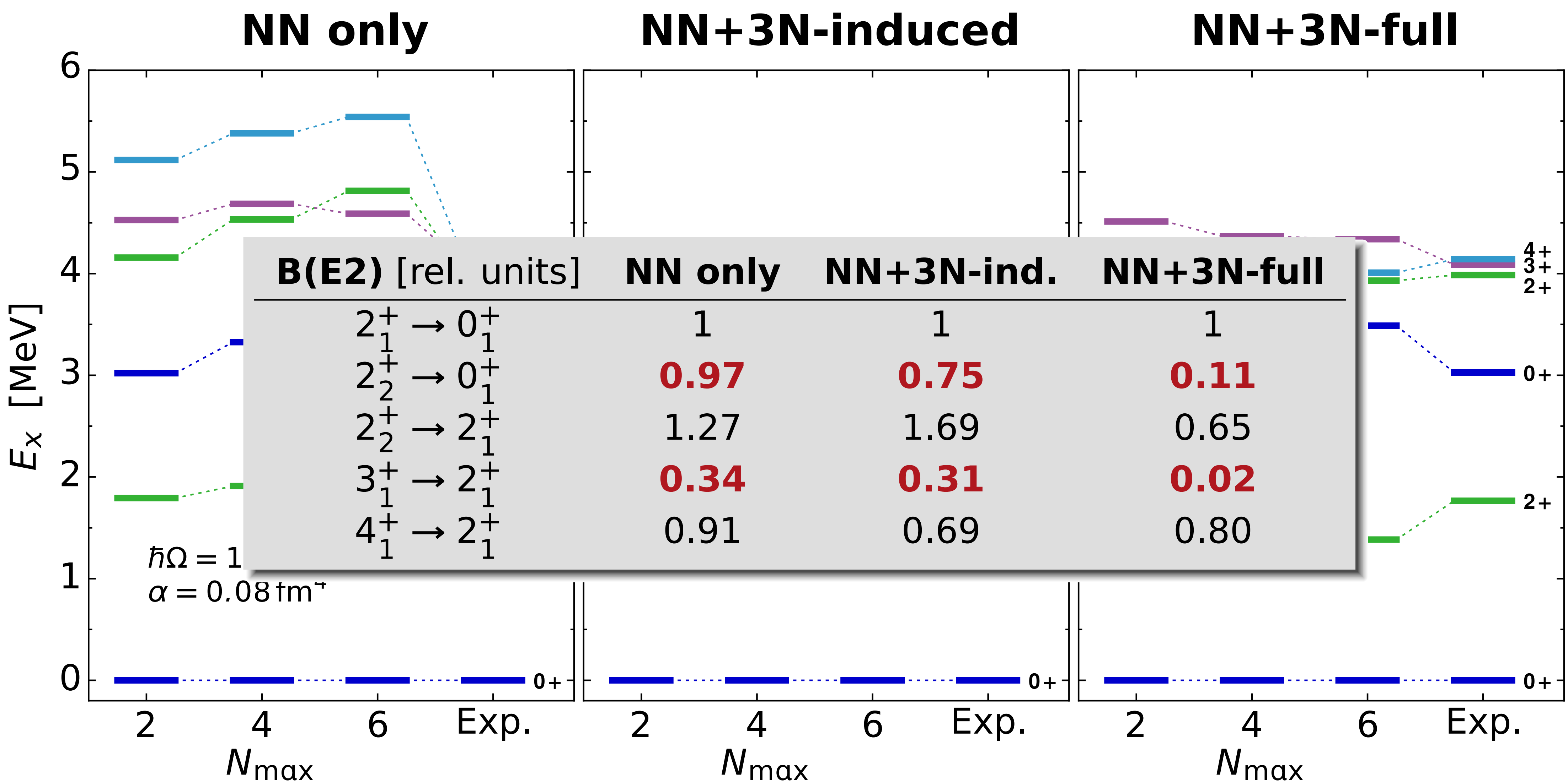


PRELIMINARY

Spectroscopy of ^{16}C



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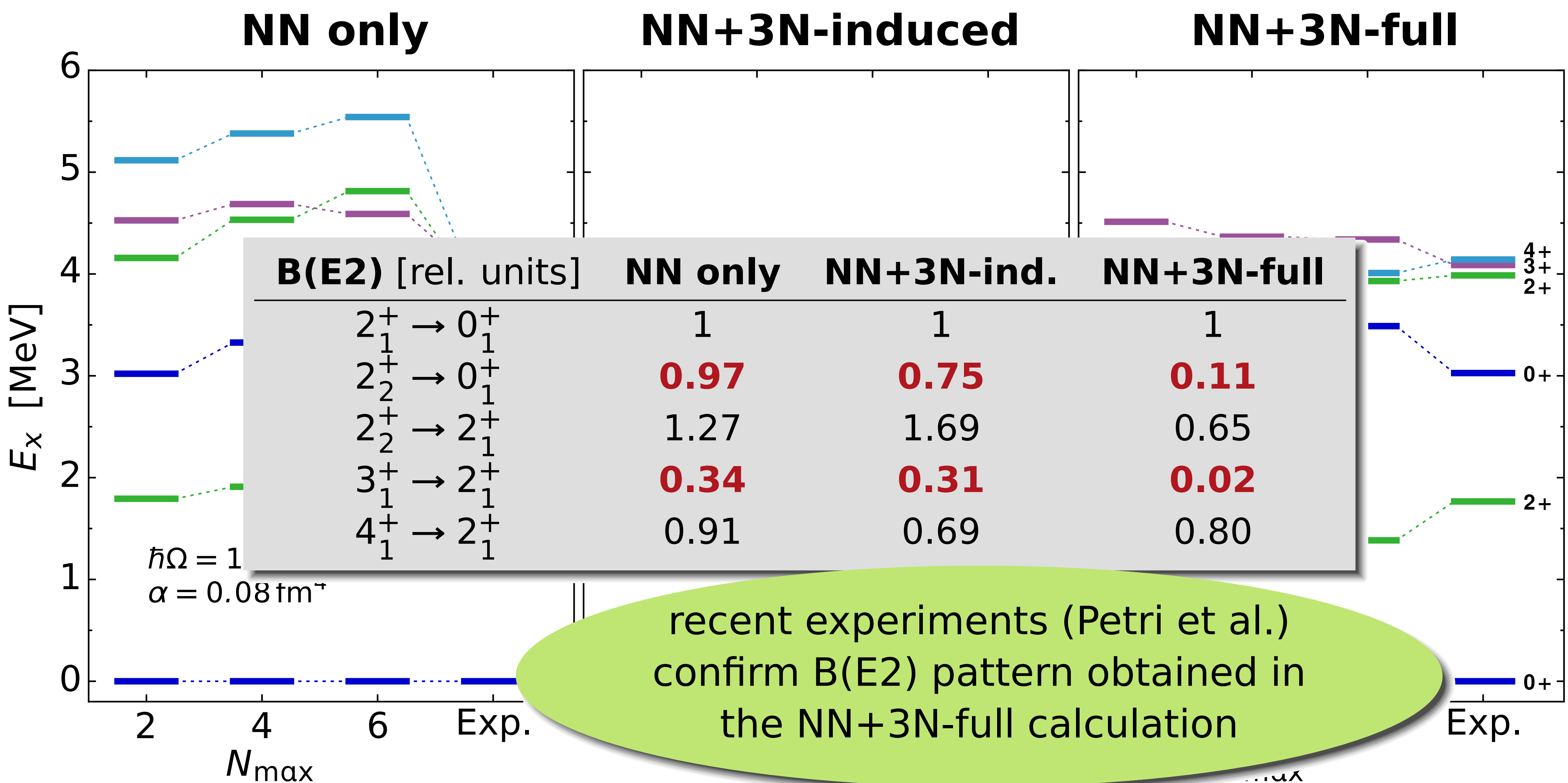

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recent experiments (Petri et al.) confirm B(E2) pattern obtained in the NN+3N-full calculation

PRELIMINARY

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 ?

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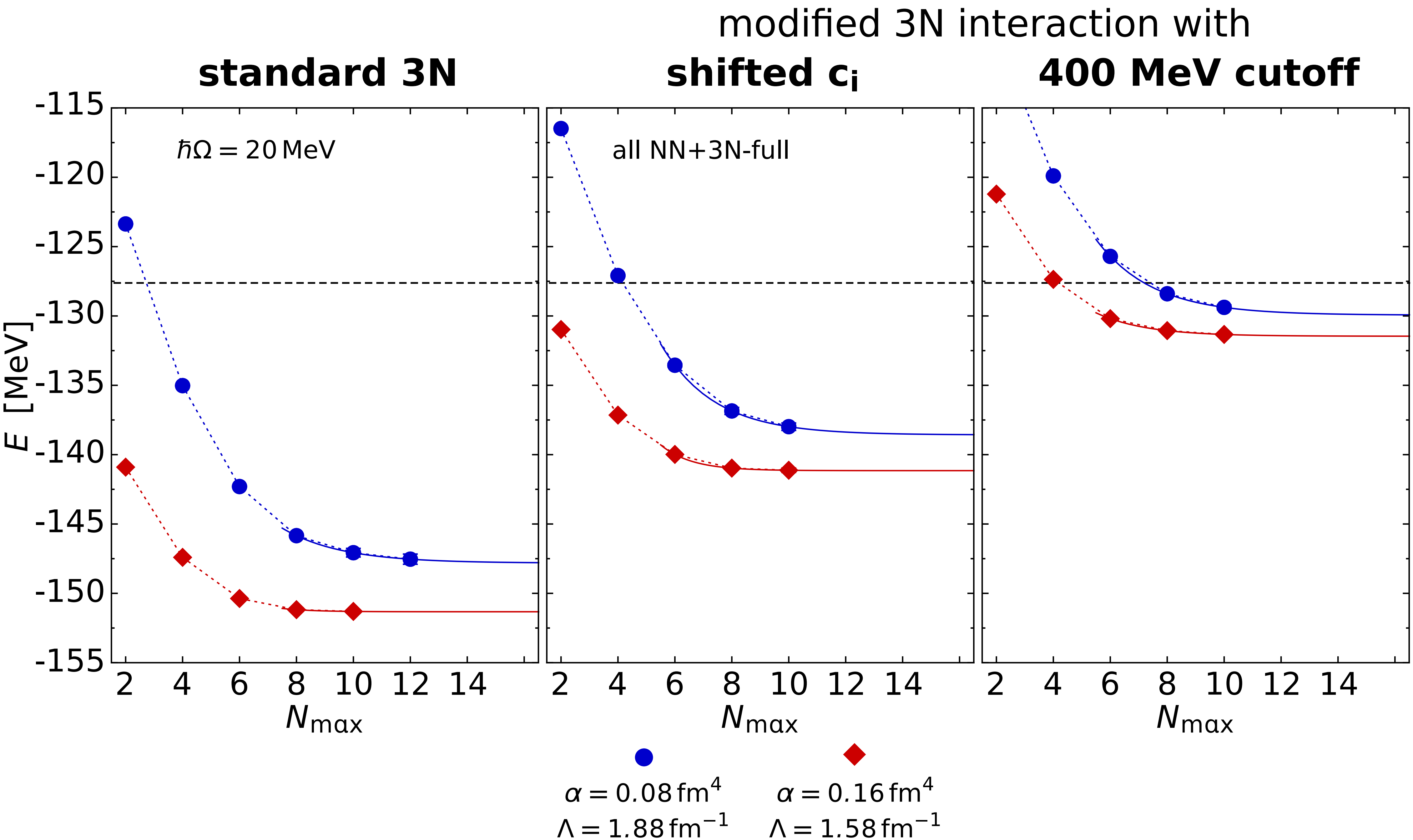
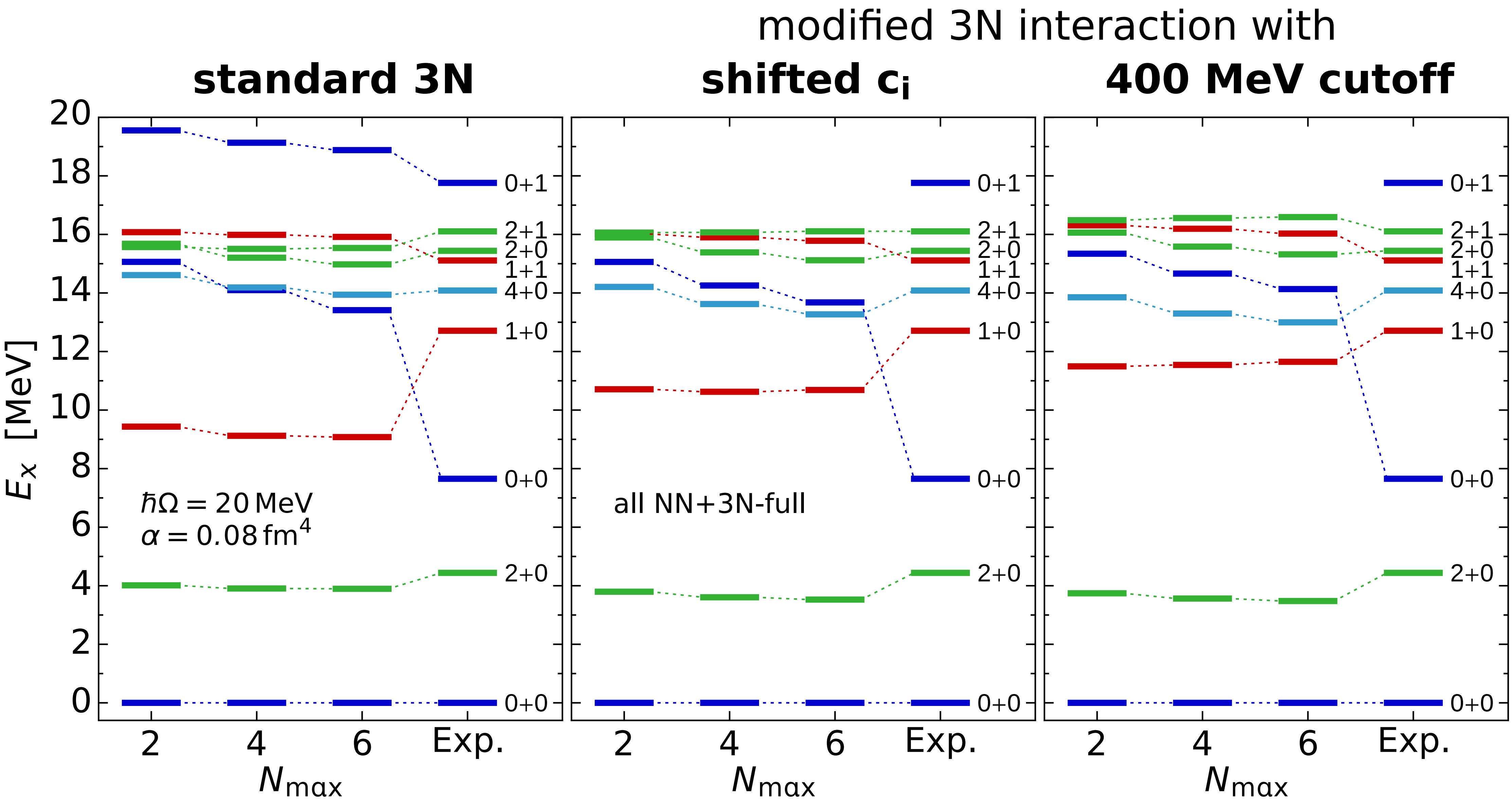
first answers in Joachim Langhammer's talk on Friday...

Sensitivity on Initial 3N — ^{16}O



Sensitivity on Initial 3N — ^{12}C



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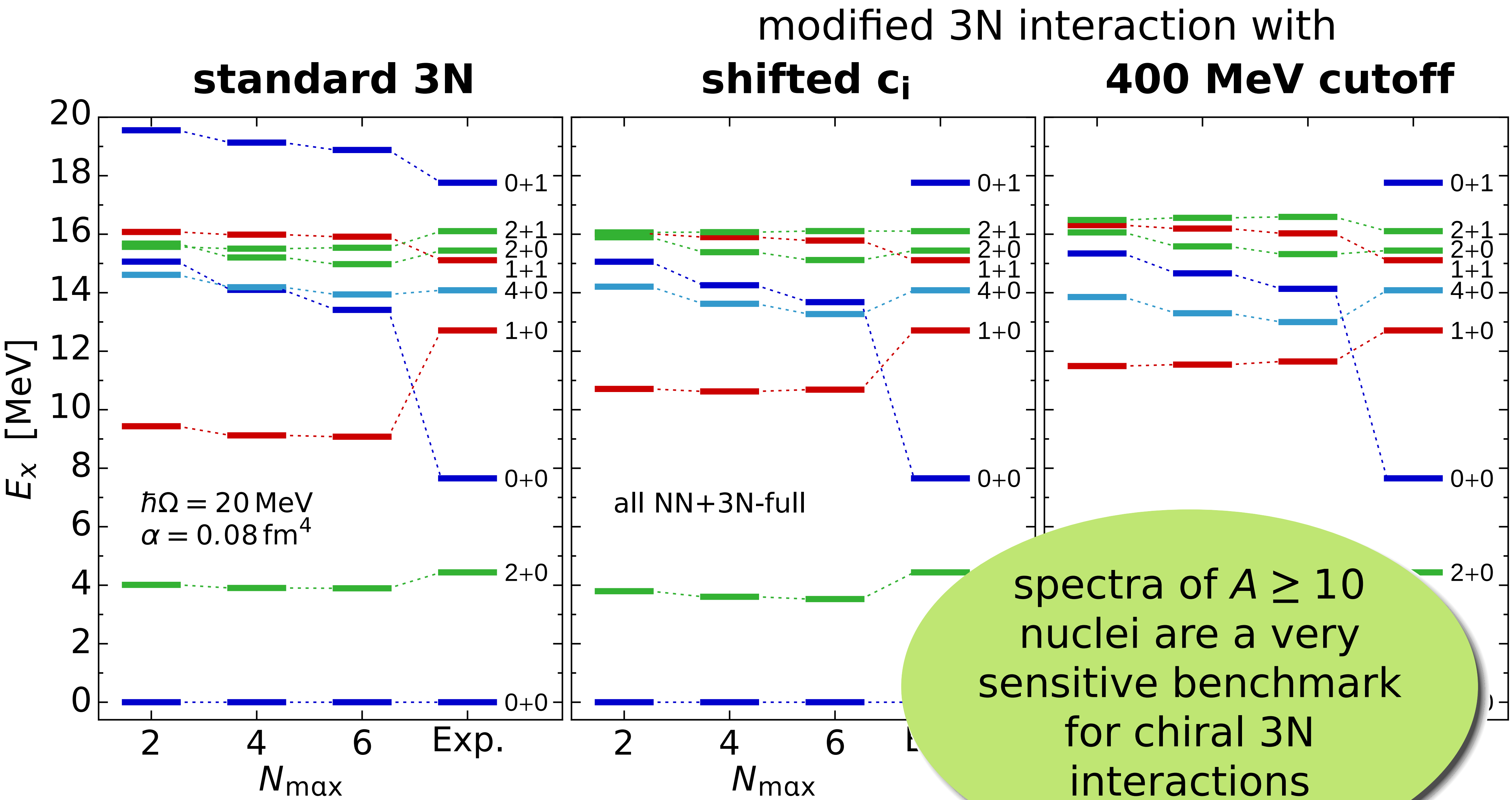

spectra of $A \geq 10$ nuclei are a very sensitive benchmark for chiral 3N interactions

Conclusions

Conclusions

- 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, A. Günther, M. Hild, H. Krutsch, **J. Langhammer**, P. Papakonstantinou, S. Reinhardt, F. Schmitt, C. Stumpf, K. Vobig, R. Wirth
    Institut für Kernphysik, TU Darmstadt
  - **P. Navrátil**
    TRIUMF Vancouver, Canada
  - S. Quaglioni
    LLNL Livermore, USA
  - H. Hergert, P. Piecuch
    Michigan State University, USA
  - C. Forssén
    Chalmers University, Sweden
  - H. Feldmeier, T. Neff,...
    GSI Helmholtzzentrum

COMPUTING TIME

JUROPA

JÜLICH FORSCHUNGSZENTRUM

LOEWE-CSC

Center for Scientific Computing Frankfurt

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

Supplements

Importance Truncation: General Idea

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

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

- construct **importance truncated space** spanned by basis states with $|\kappa_\nu^{(m)}| \geq \kappa_{\text{min}}$ and solve eigenvalue problem
- **sequential scheme**: construct importance truncated space for next N_{max} using previous eigenstates as reference $\left|\Psi_{\text{ref}}^{(m)}\right\rangle$
- a posteriori **threshold extrapolation** and **perturbative correction** used to recover contributions from discarded basis states

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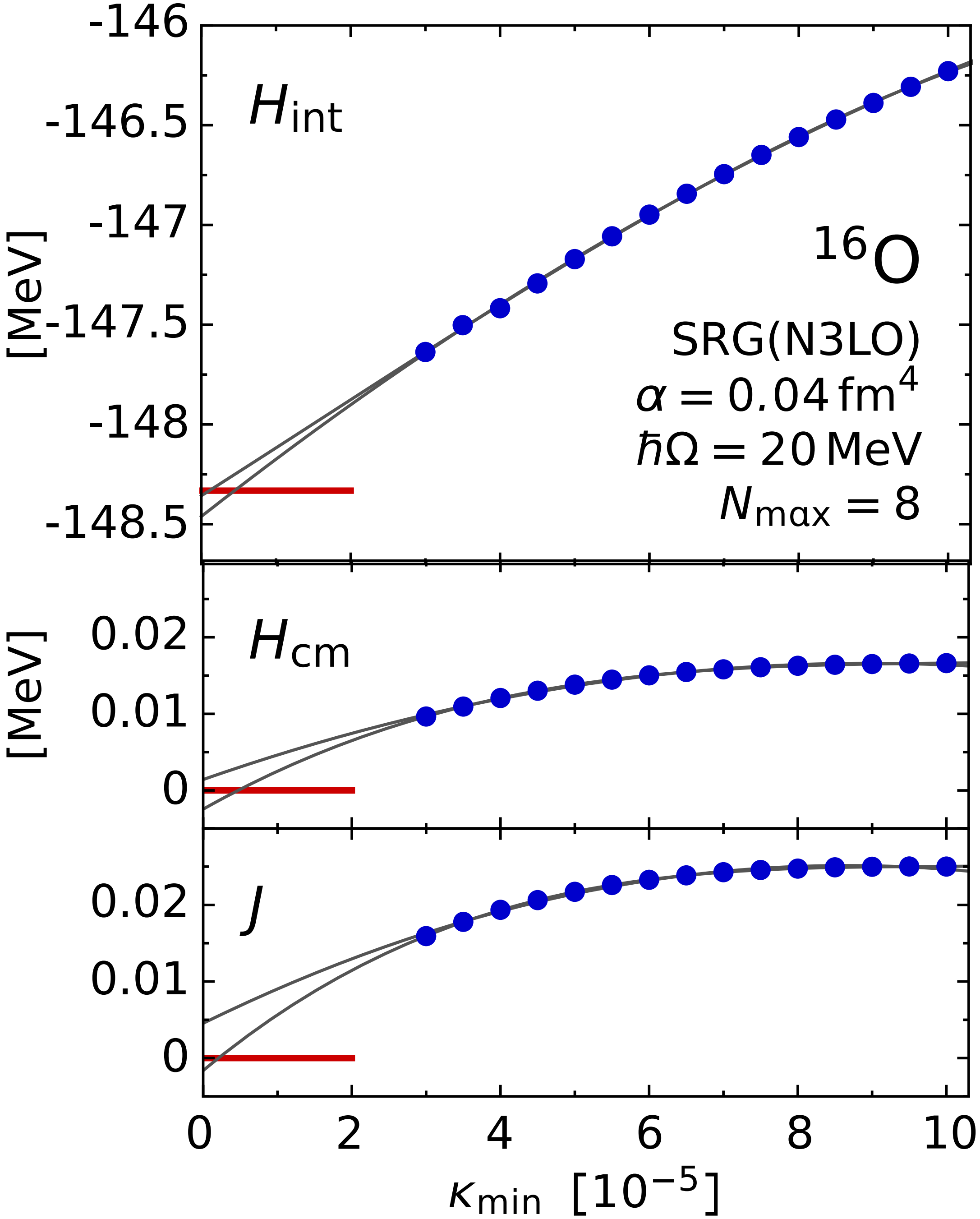
for $\kappa_{\min} \to 0$ the full NCSM model space and thus the **exact solution is recovered**

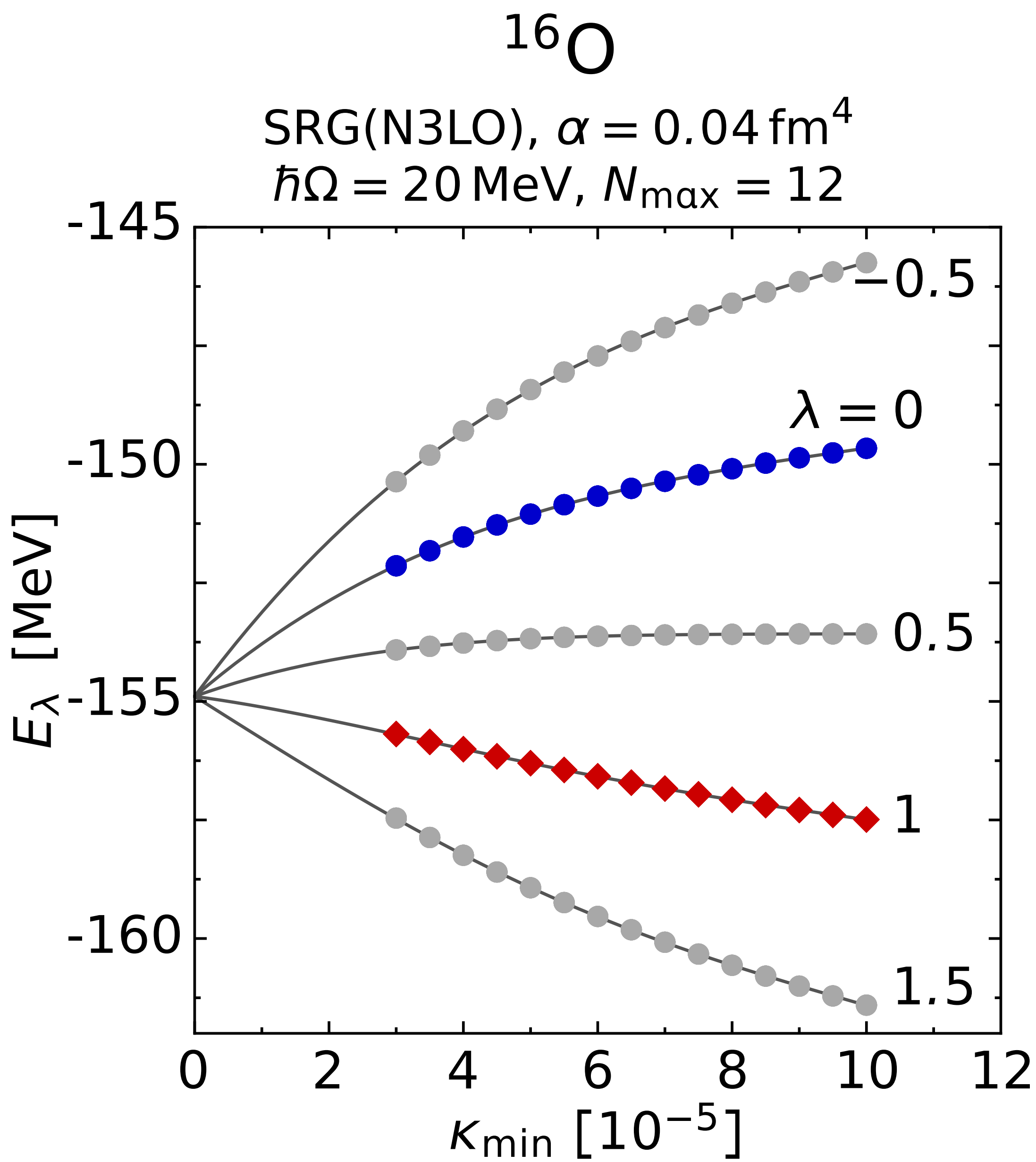
- a posteriori **threshold extrapolation** and **perturbative correction** used to recover contributions from discarded basis states

Threshold Extrapolation



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

Constrained Threshold Extrapolation



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

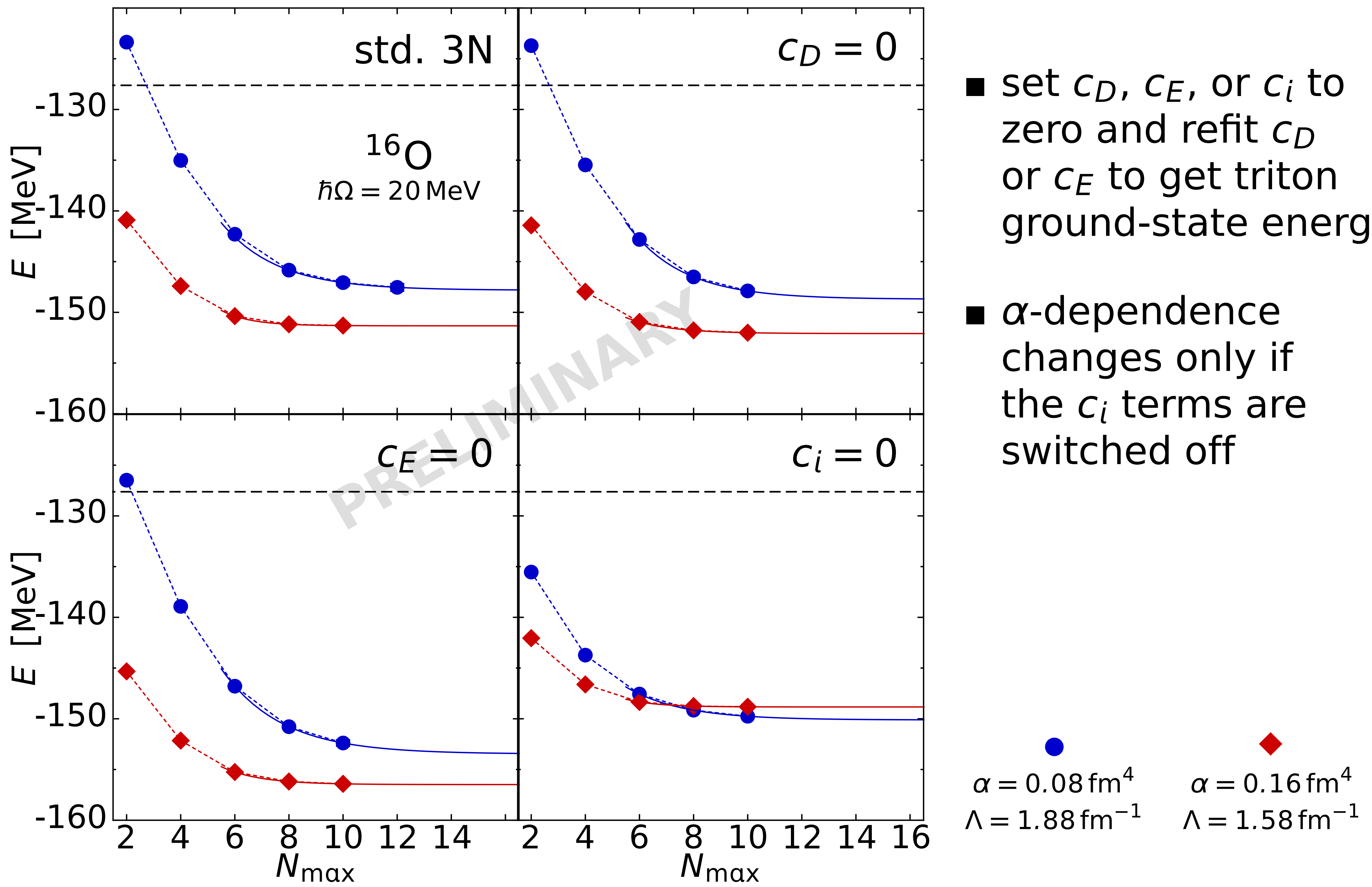
- **simultaneous fit** of combined energy

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

  for set of λ-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



- set c_D, c_E, or c_i to zero and refit c_D or c_E to get triton ground-state energy
- α-dependence changes only if the c_i terms are switched off

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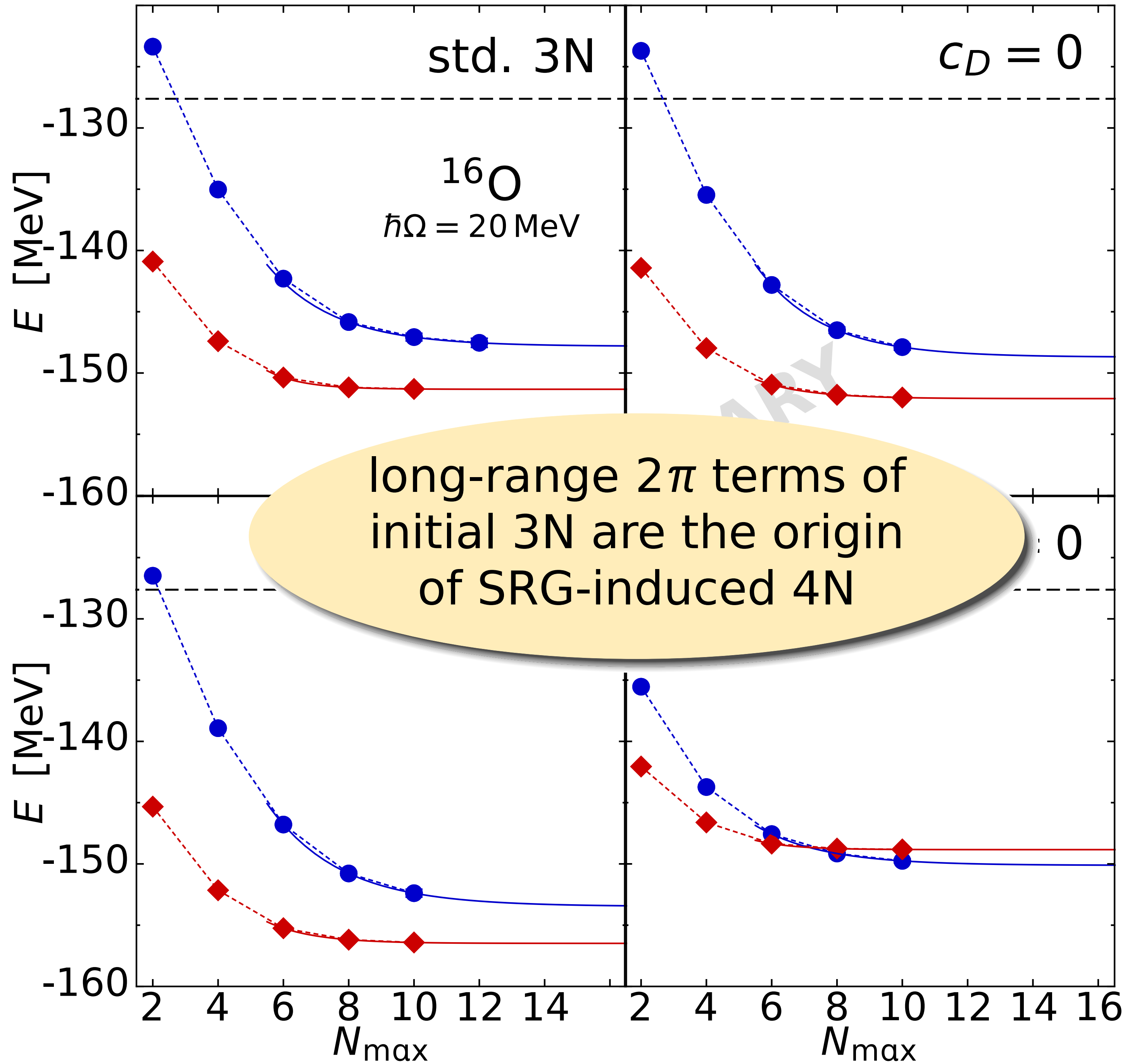

long-range 2π terms of initial 3N are the origin of SRG-induced 4N

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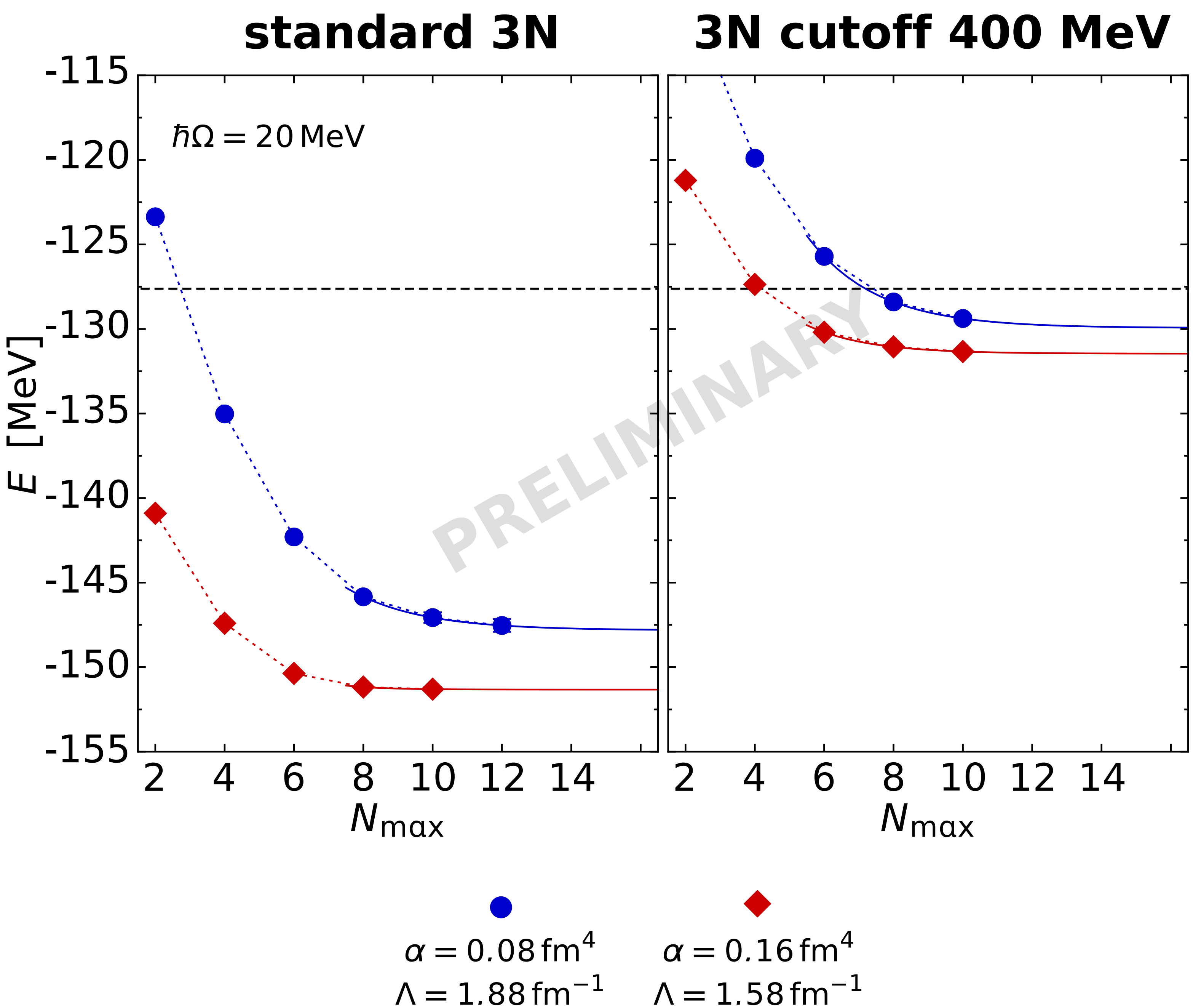
- α-dependence changes only if the c_i terms are switched off

● $\alpha = 0.08\,\text{fm}^4$ $\Lambda = 1.88\,\text{fm}^{-1}$

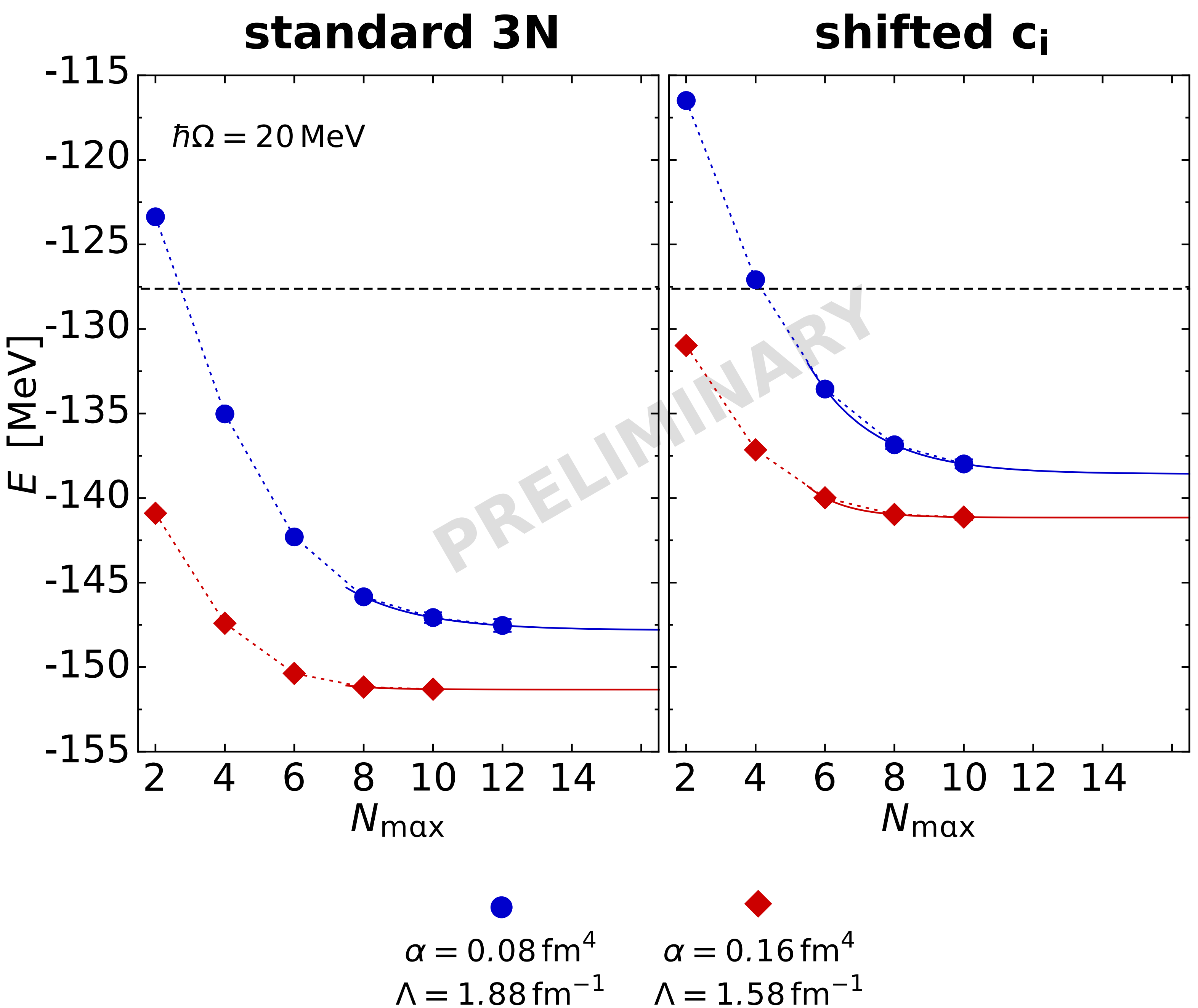
◆ $\alpha = 0.16\,\text{fm}^4$ $\Lambda = 1.58\,\text{fm}^{-1}$

Sensitivity on 3N Cutoff: ^{16}O



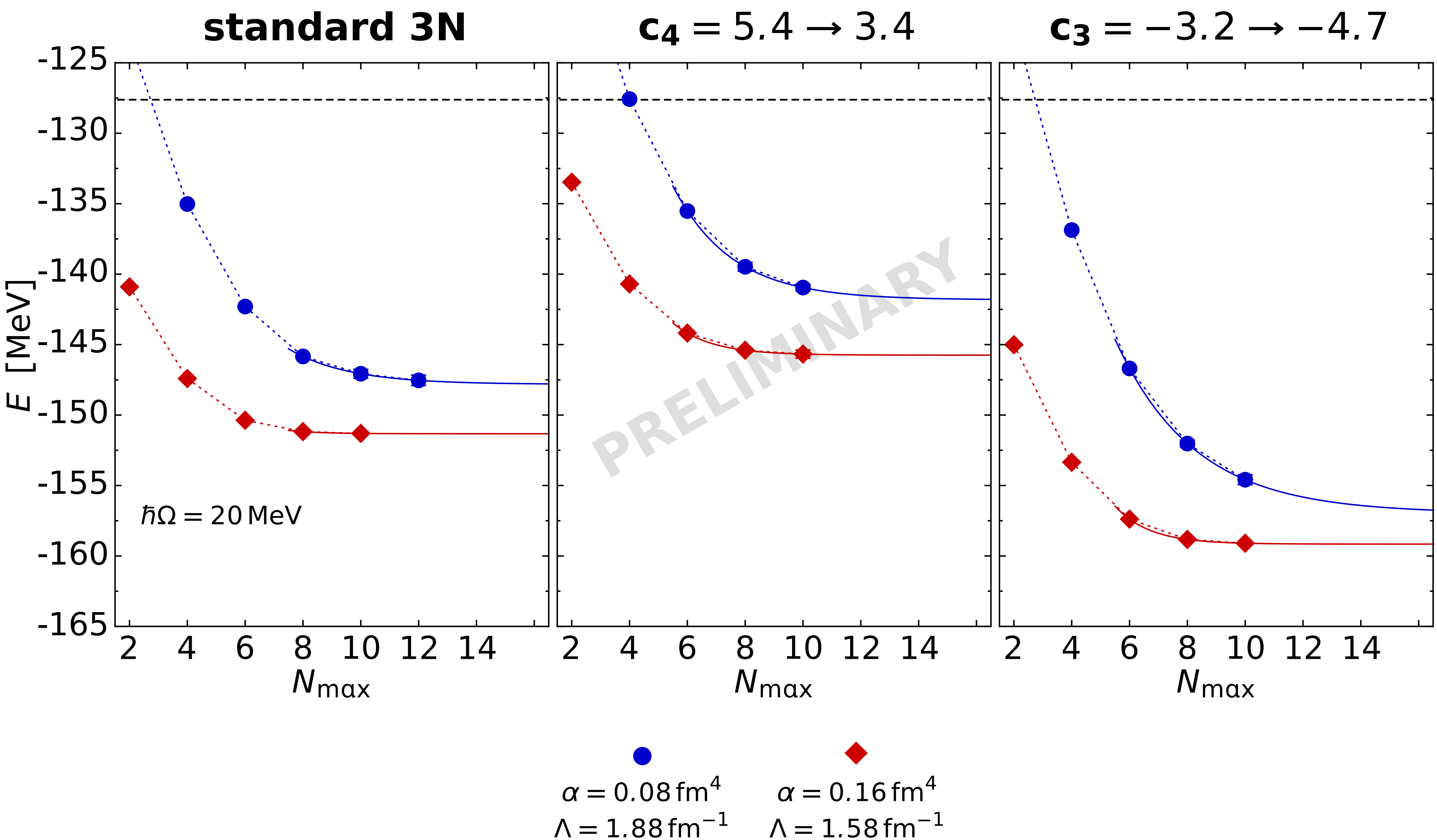
- reduce **3N cut-off to 400 MeV** and refit c_E to reproduce the ^{4}He ground-state energy
- strong impact on α-dependence and absolute ground-state energy

Sensitivity on c_i Shift: ^{16}O

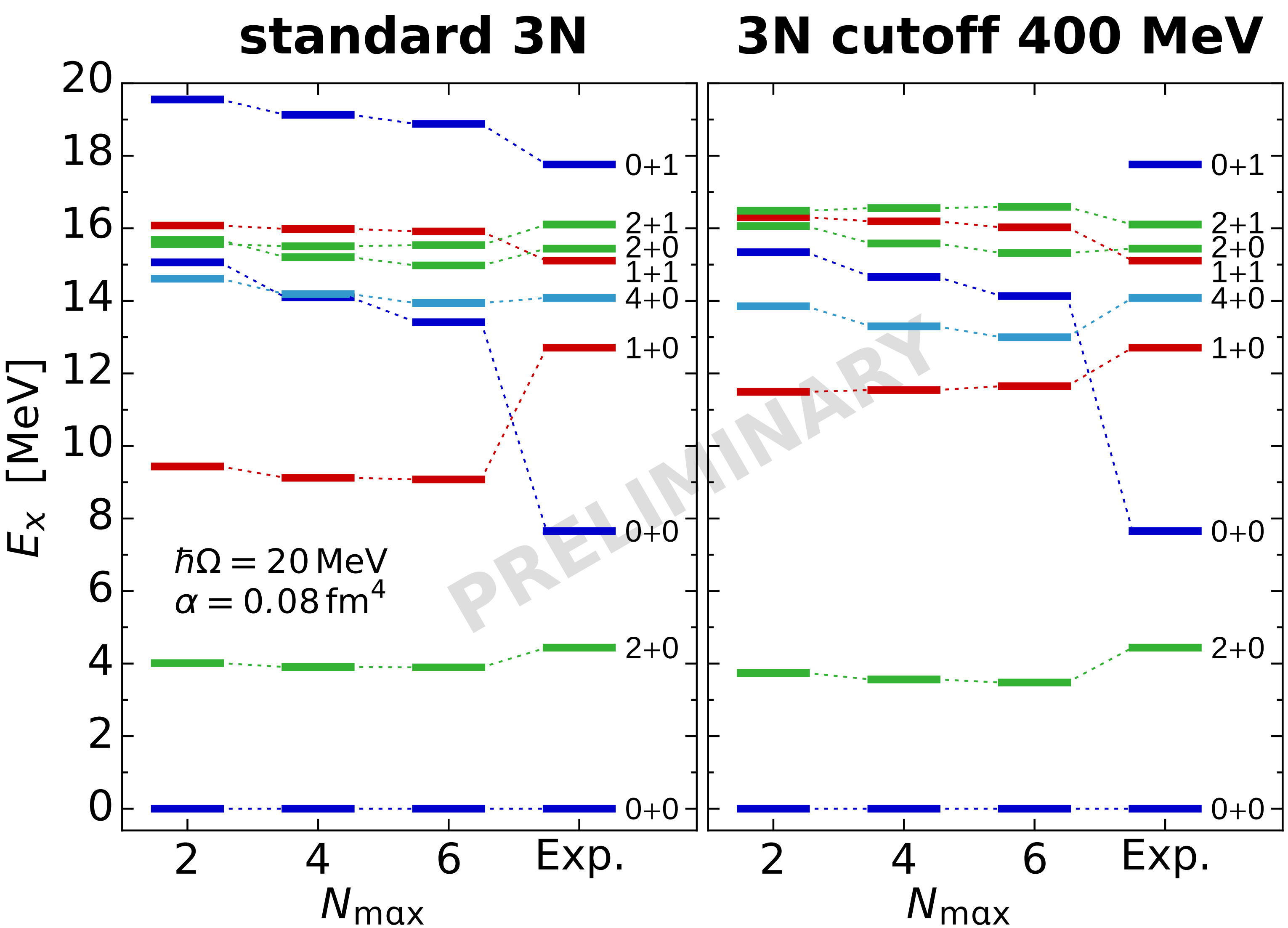


- include **shifts of c_i values from N^3LO** terms and refit c_E to reproduce the ^4He ground-state energy
- sizable impact on α-dependence and absolute ground-state energy

Sensitivity on c_3 & c_4: ^{16}O

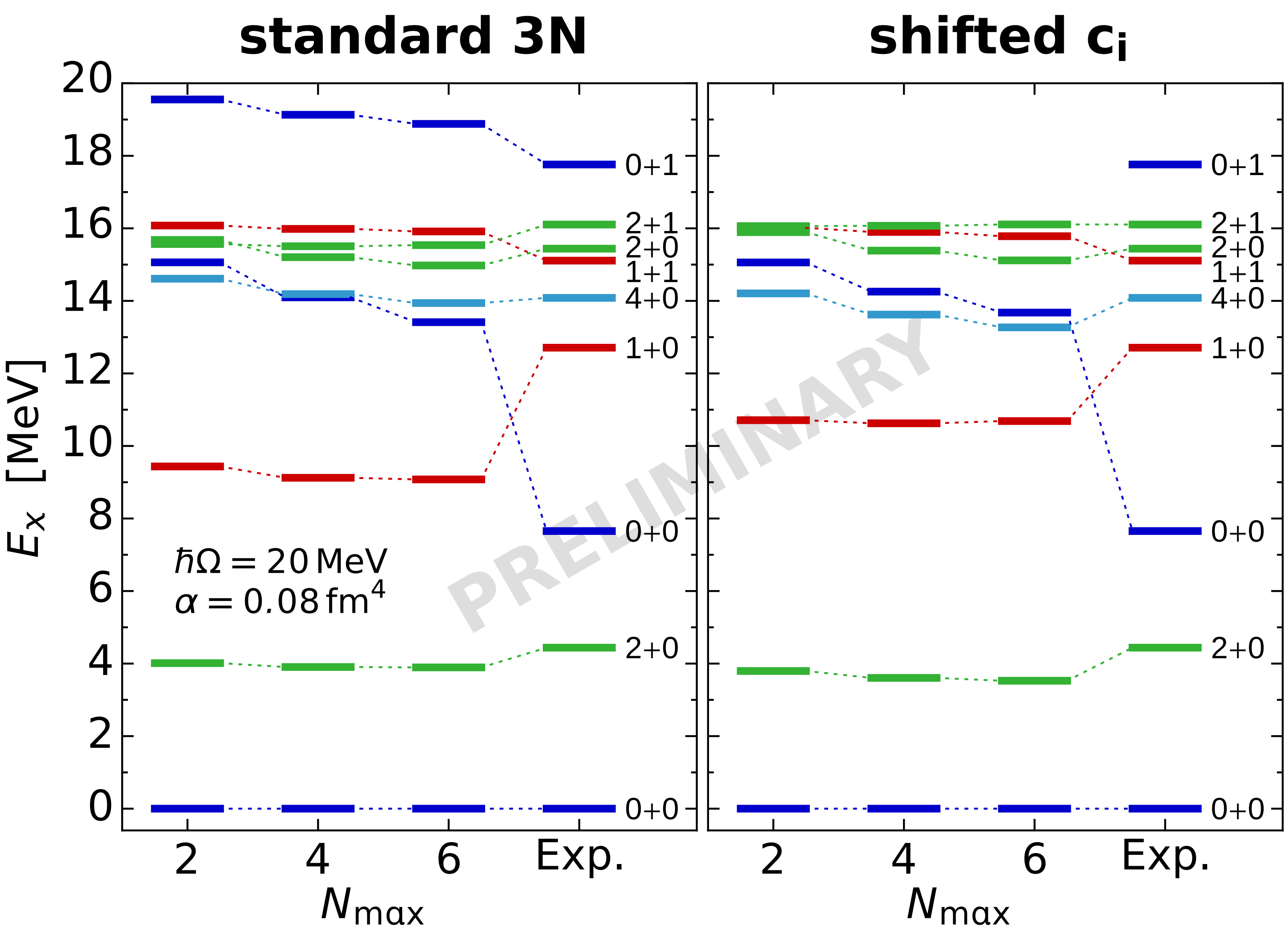


Sensitivity on 3N Cutoff: ^{12}C



- significant improvement of 1^+0 energy and of overall agreement

Sensitivity on c_i Shift: ^{12}C



- slight improvement of 1^+0 energy and of overall agreement

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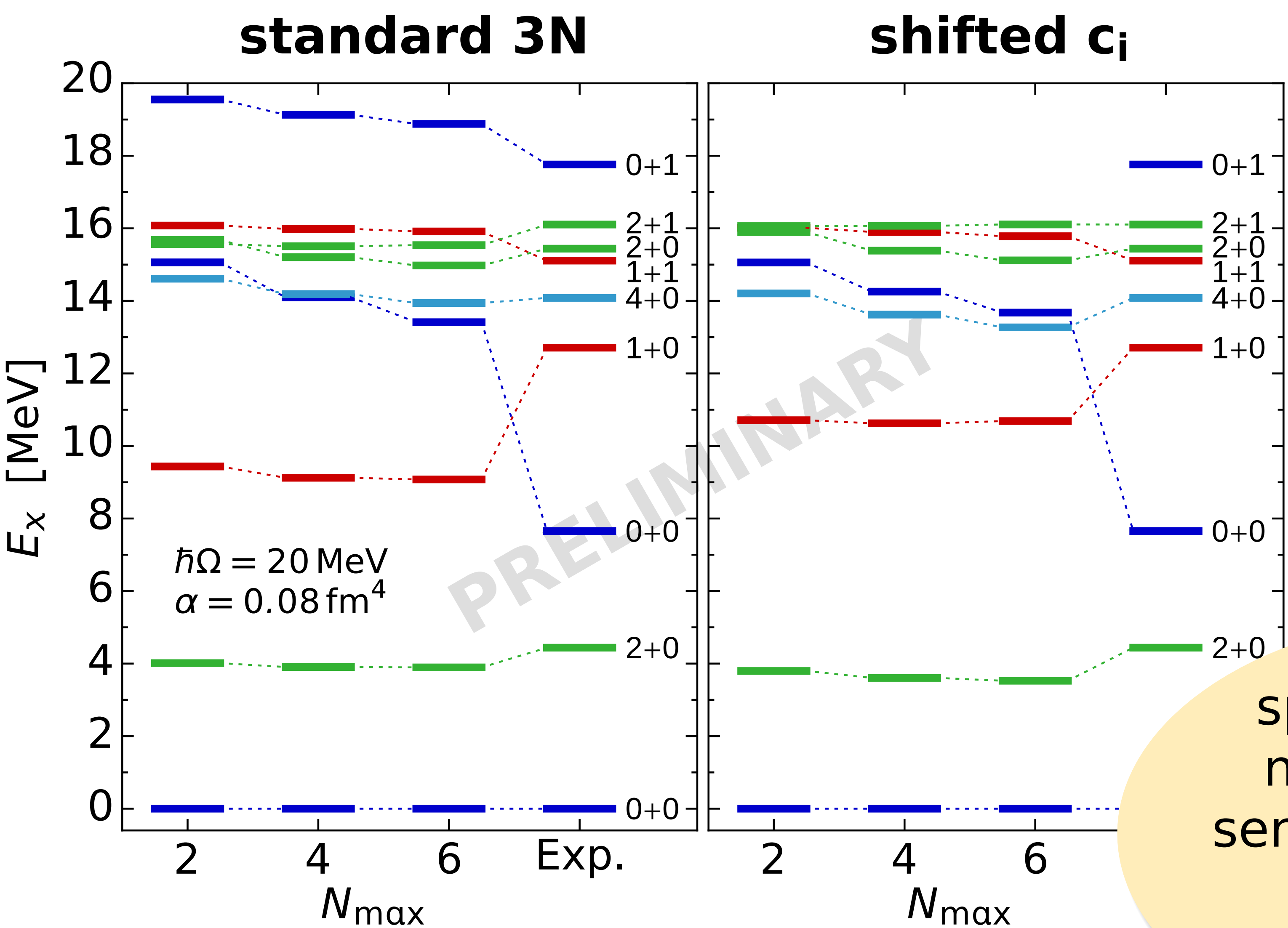

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