Ab Initio Nuclear Structure with QCD-based 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

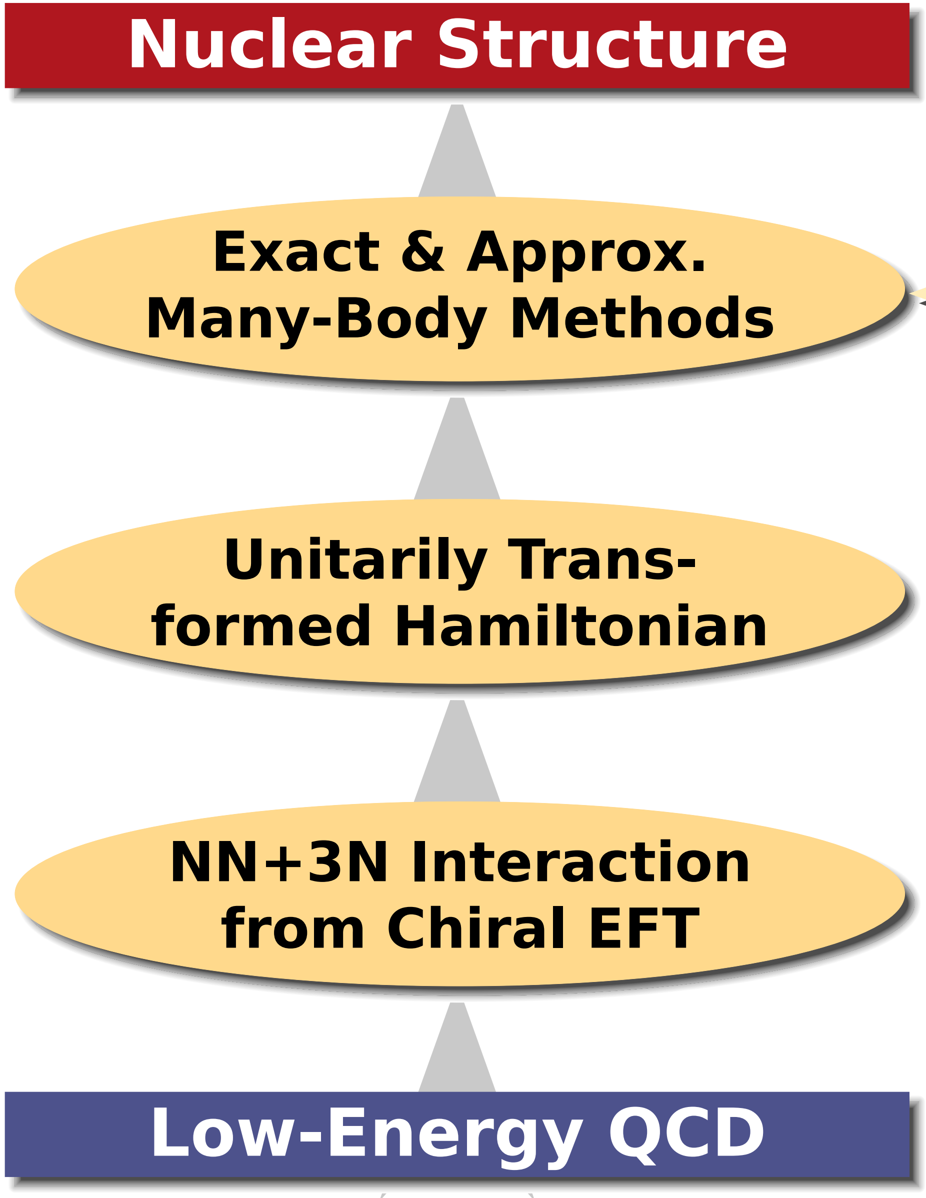
Unitarily Transformed Hamiltonian

- 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

Nuclear Structure

Exact & Approx. Many-Body Methods — Importance Truncated No-Core Shell Model with NN+3N

Unitarily Transformed Hamiltonian — Similarity Renormalization Group with NN+3N

NN+3N Interaction from Chiral EFT

Low-Energy QCD

focus on consistent inclusion of chiral 3N interaction

Unitarily Transformed Hamiltonian

Similarity Renormalization Group

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

simplicity and flexibility are great advantages of the SRG approach

solve SRG evolution equations using two- & three-body Jacobi HO representation

- **unitary transformation** of Hamil

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

- **evolution equations** for $\widetilde{H}_\alpha$ and U

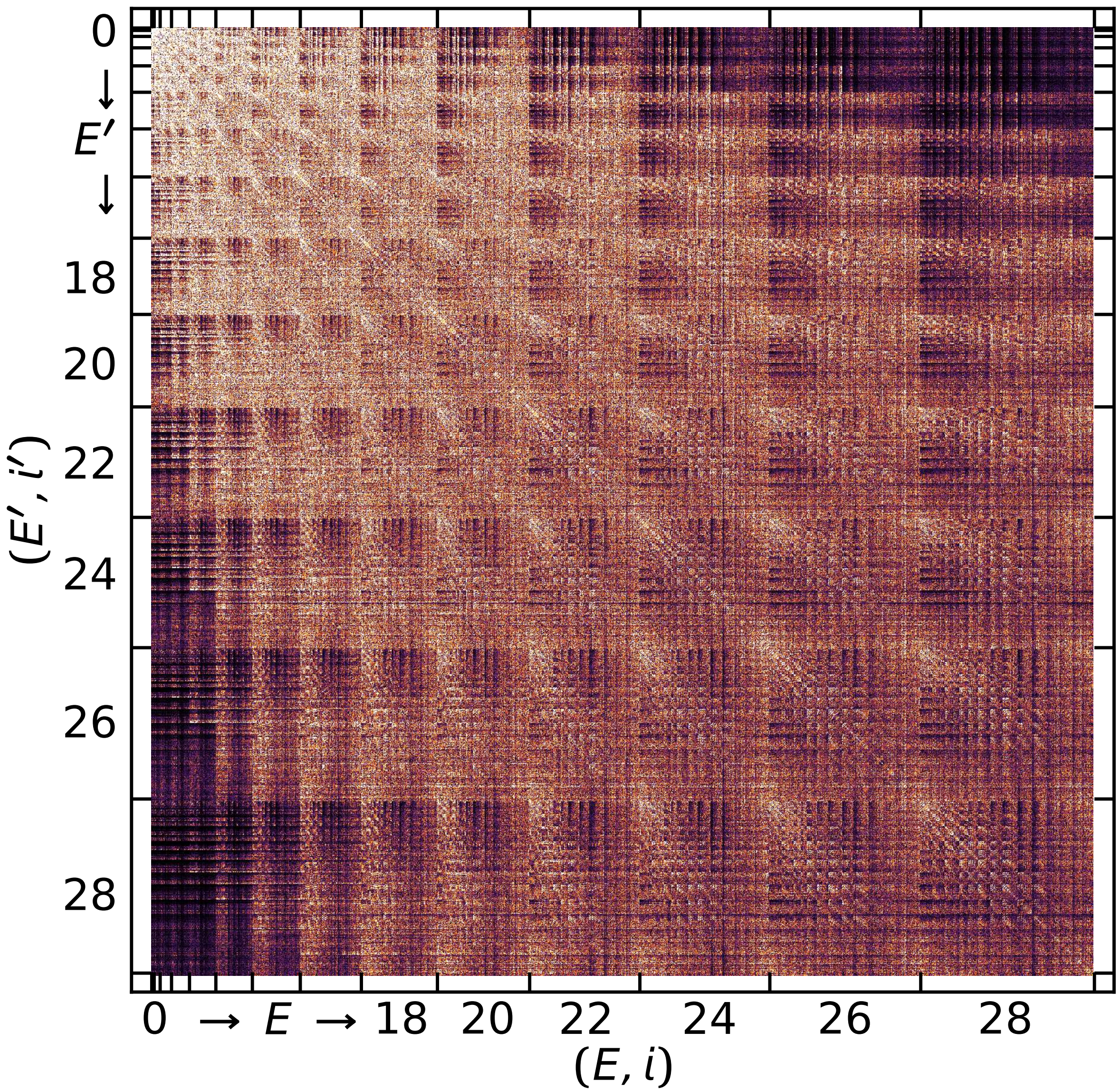
$$\frac{d}{d\alpha}\widetilde{H}_\alpha = [\eta_\alpha, \widetilde{H}_\alpha]$$

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

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

SRG Evolution in Three-Body Space

3B-Jacobi HO matrix elements

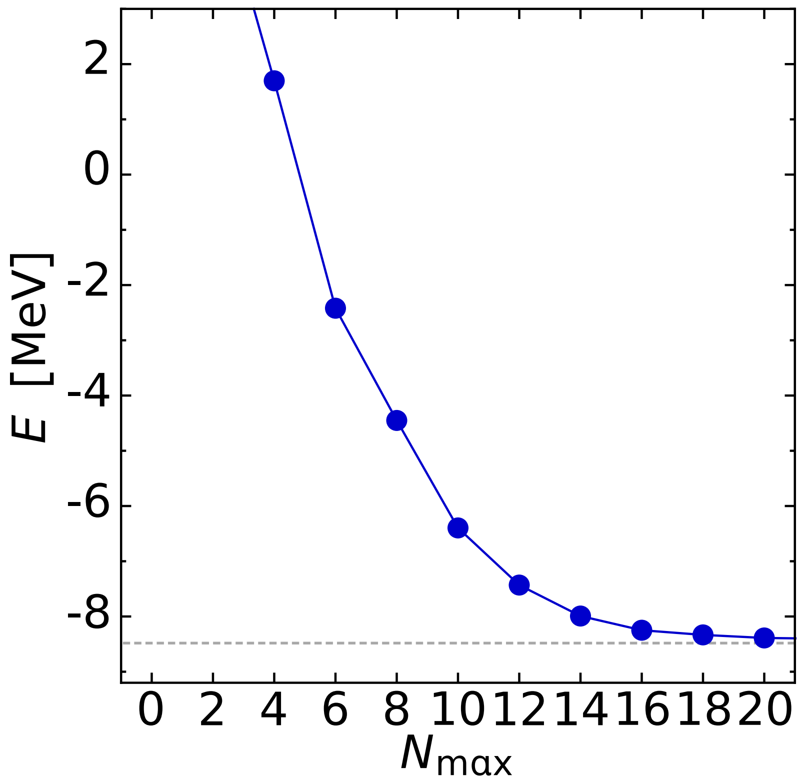


$\alpha = 0.000\,\mathrm{fm}^4$

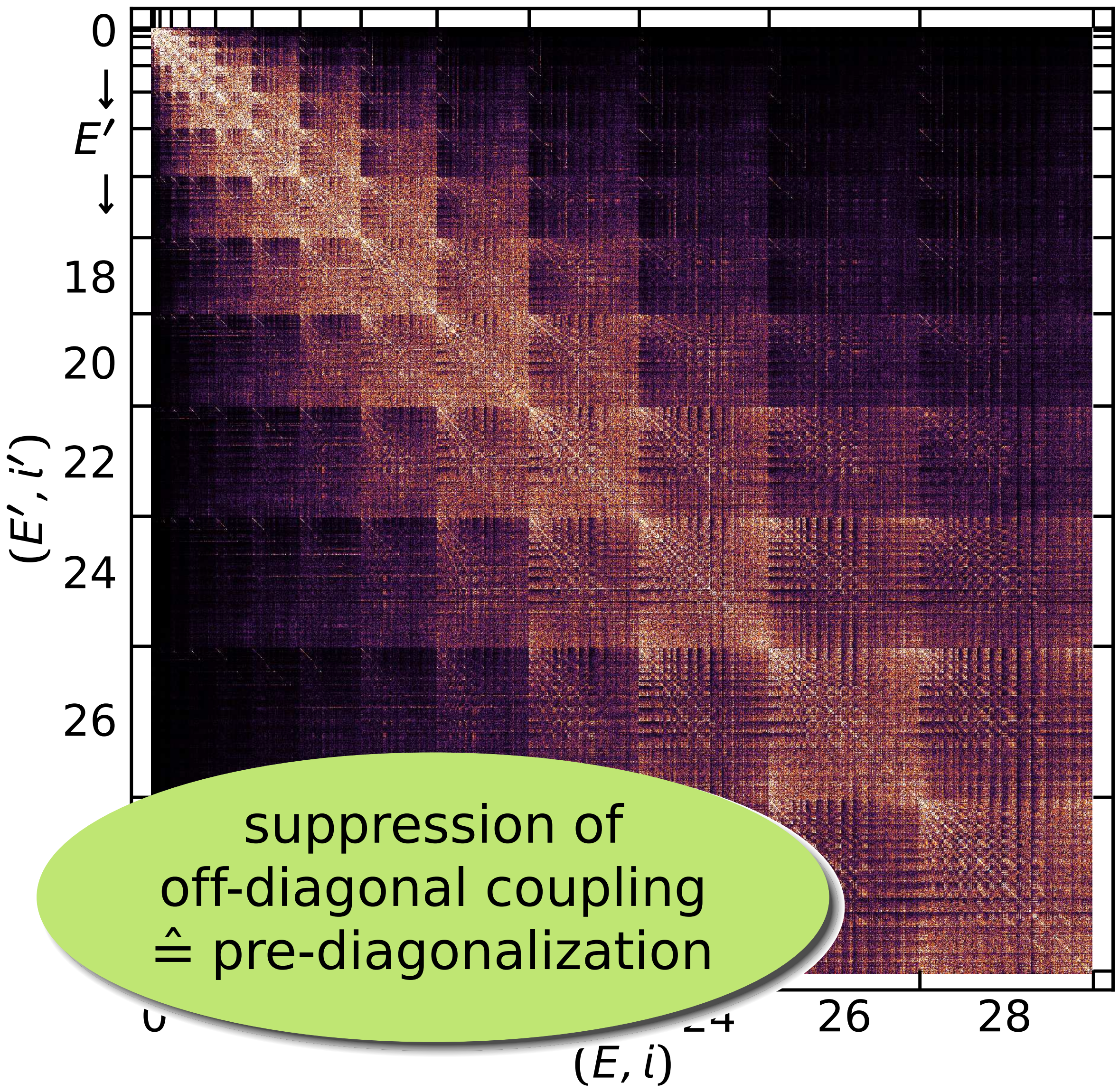
$\Lambda = \infty\,\mathrm{fm}^{-1}$

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

NCSM ground state ^{3}H



SRG Evolution in Three-Body Space

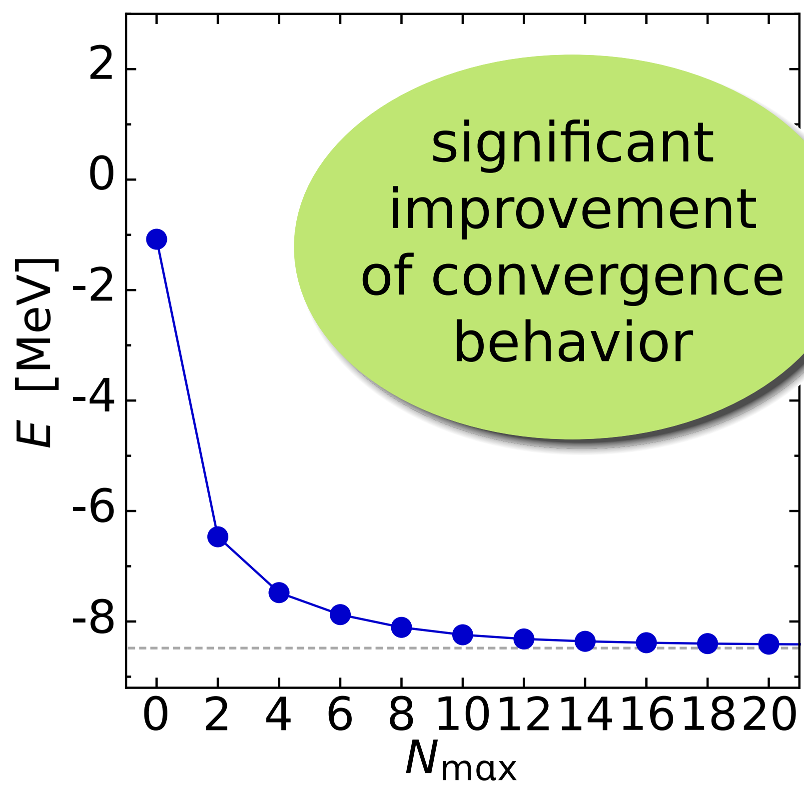


suppression of
off-diagonal coupling
≙ pre-diagonalization

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

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

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



significant
improvement
of convergence
behavior

Calculations in *A*-Body Space

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

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

- **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 ...s

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 $E_{3\,max} = 16$ 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 $E_{3\,max} = 16$ in memory

Exact Many-Body Methods

Importance Truncated NCSM

Roth et al. — Phys. Rev. Lett. 107, 072501 (2011)
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 $E_{3\max} = 16$

A Tale of Three Hamiltonians

Initial Hamiltonian

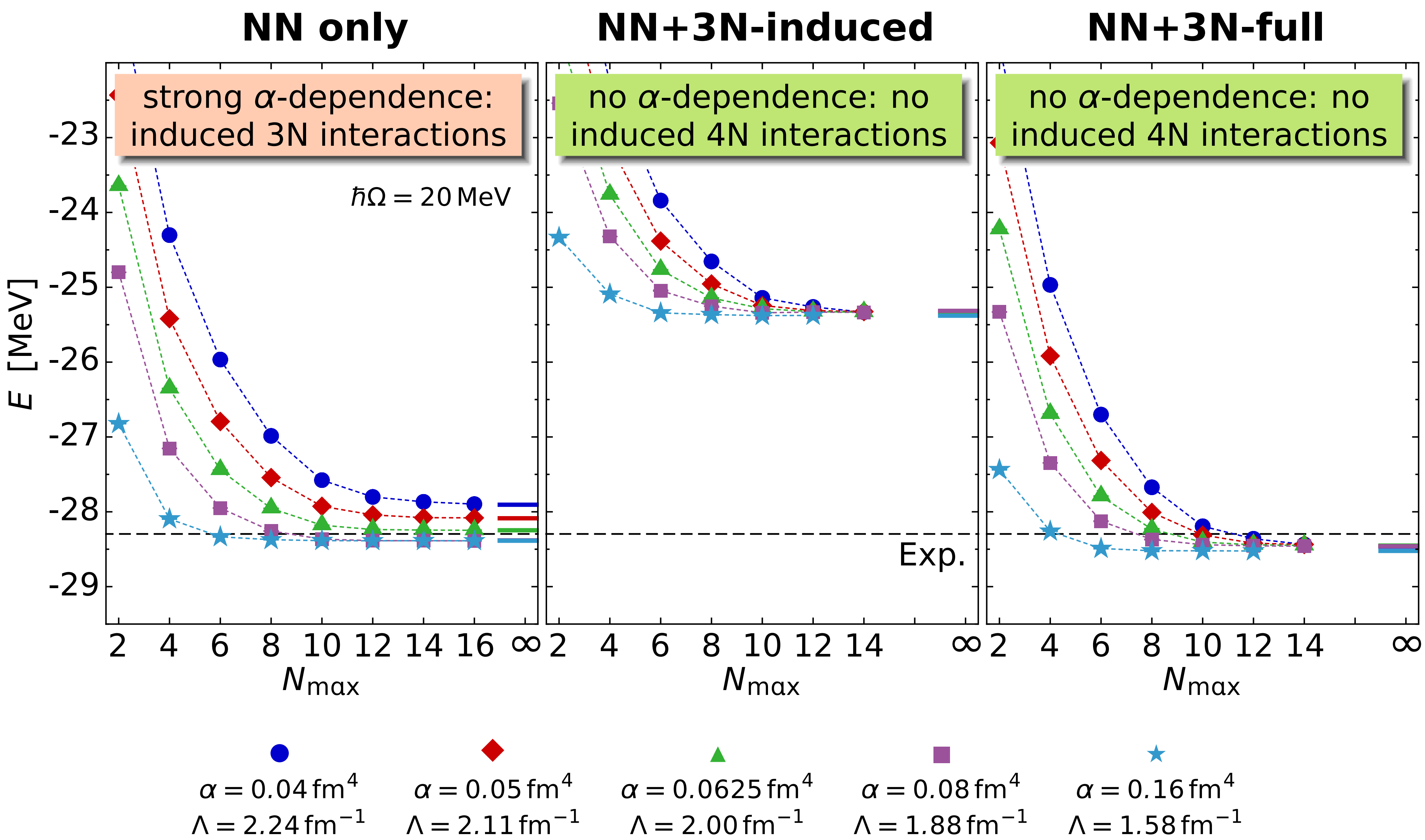
- NN: chiral interaction at N^3LO (Entem & Machleidt, 500 MeV)
- 3N: chiral interaction at N^2LO (c_D, c_E from ^3H binding & half-live)

SRG-Evolved Hamiltonians

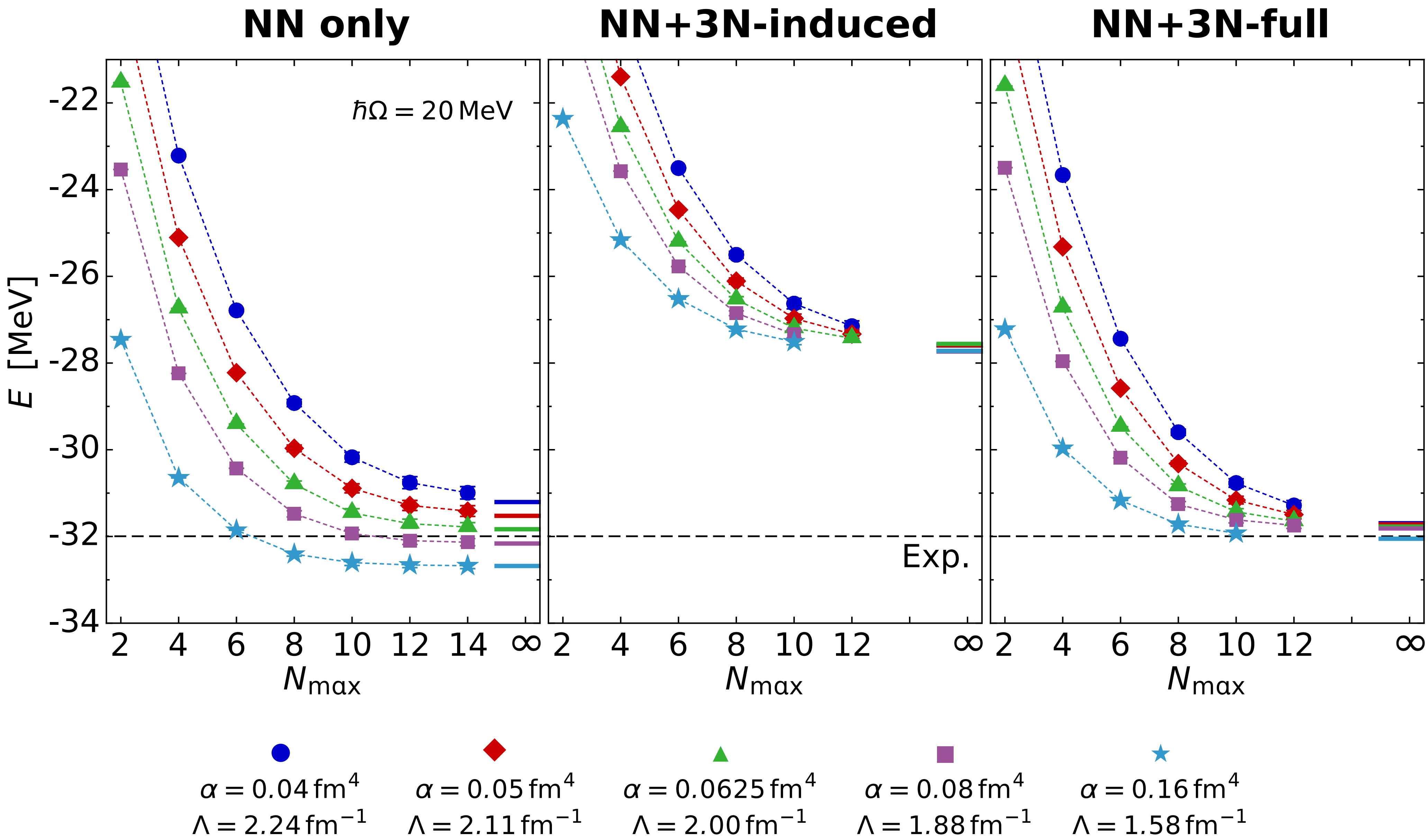
- **NN only**: start with NN initial Hamiltonian and keep two-body terms only
- **NN+3N-induced**: start with NN initial Hamiltonian and keep two- and three-body terms
- **NN+3N-full**: start with NN+3N in[...] two- and three-body terms

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

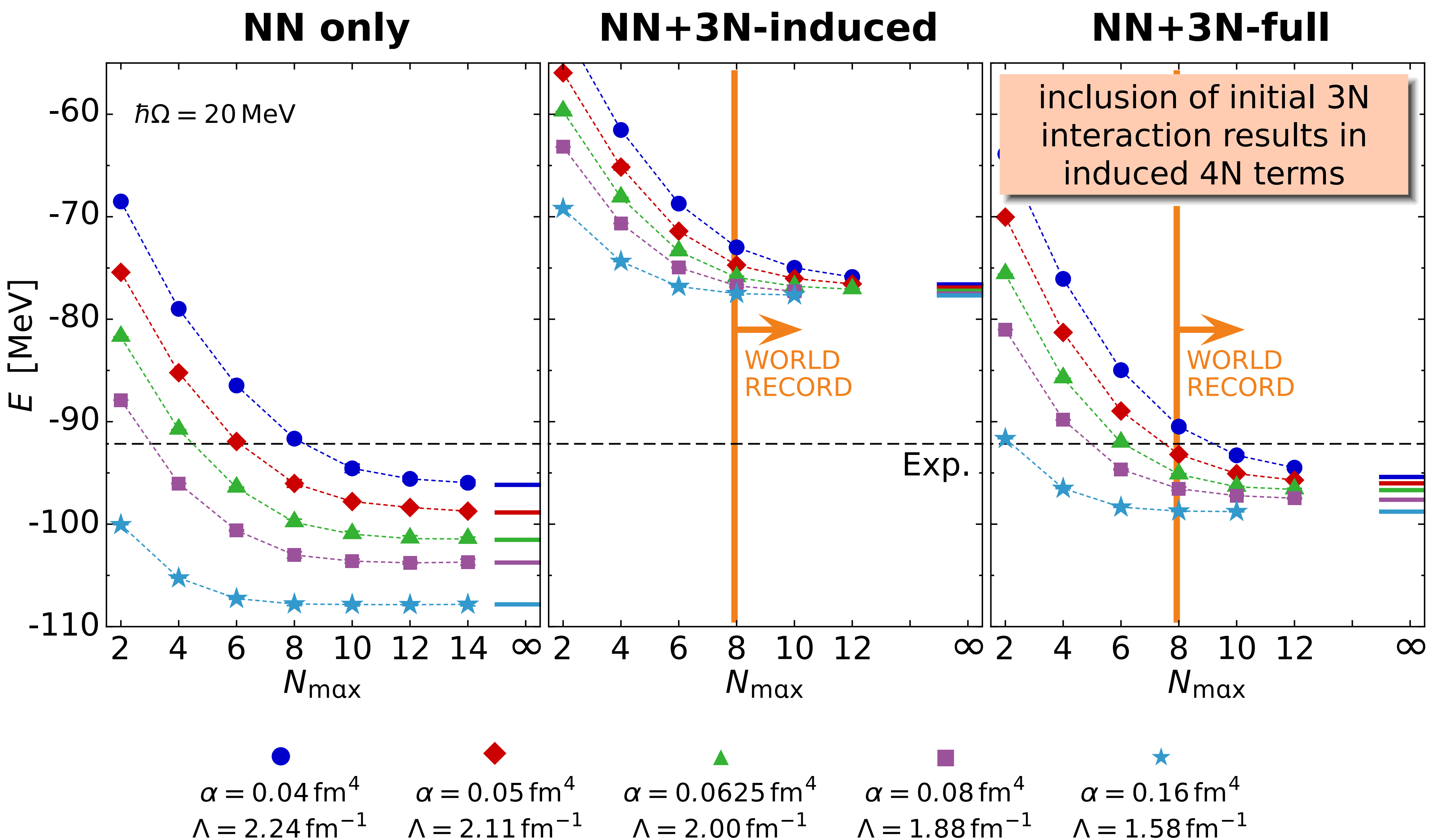
^{4}He: Ground-State Energies



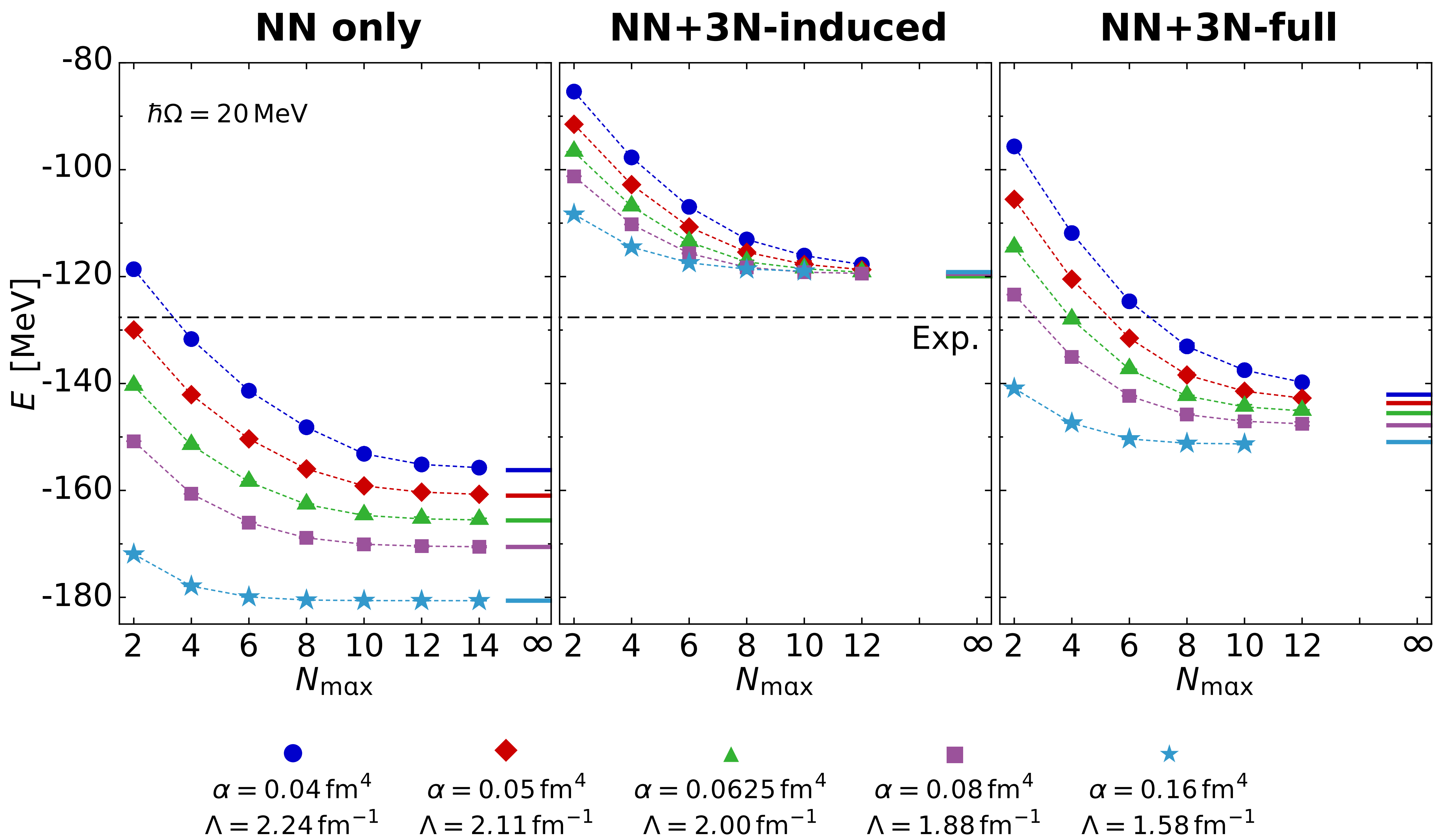
^{6}Li: Ground-State Energies



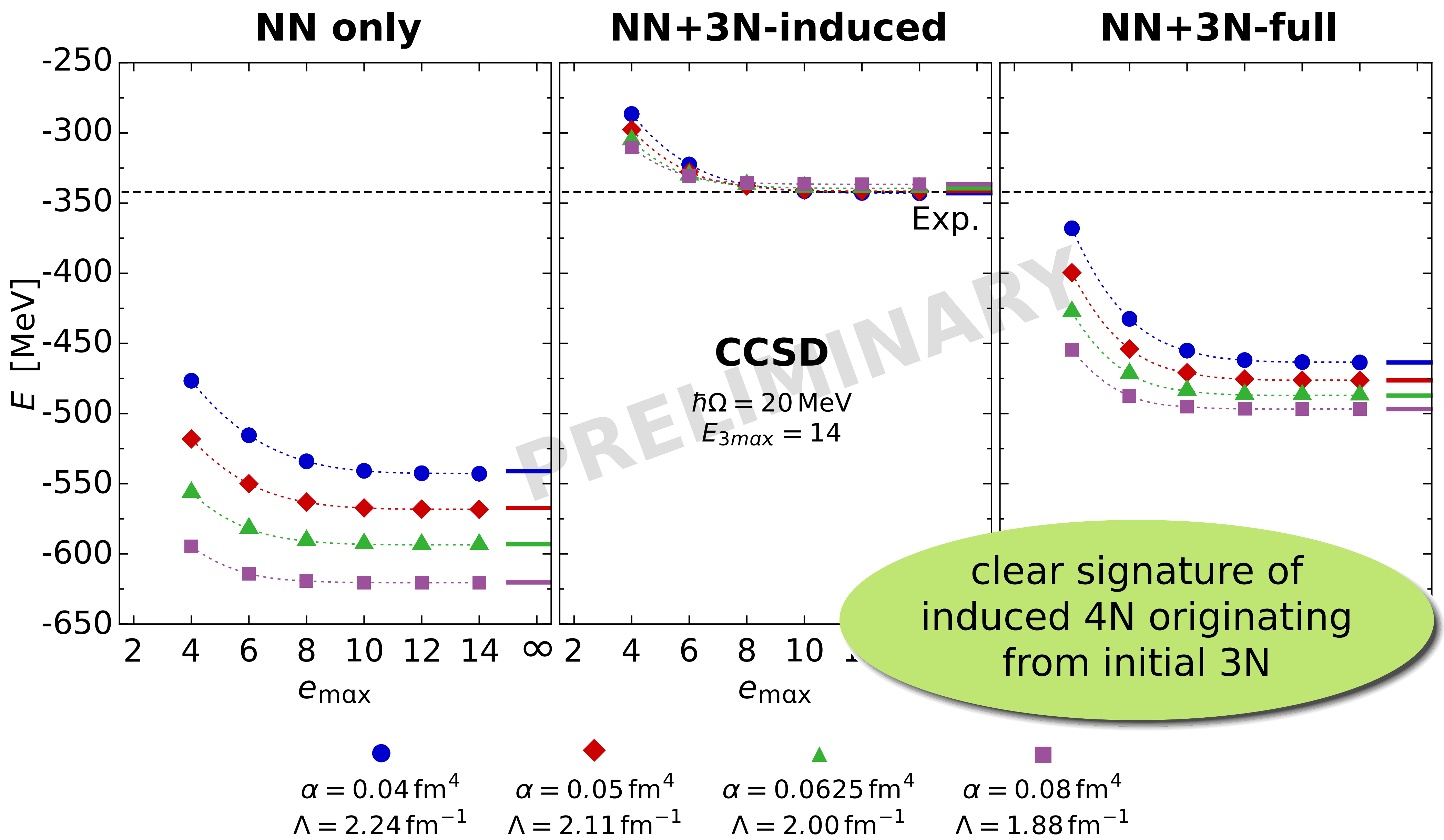
^{12}C: Ground-State Energies



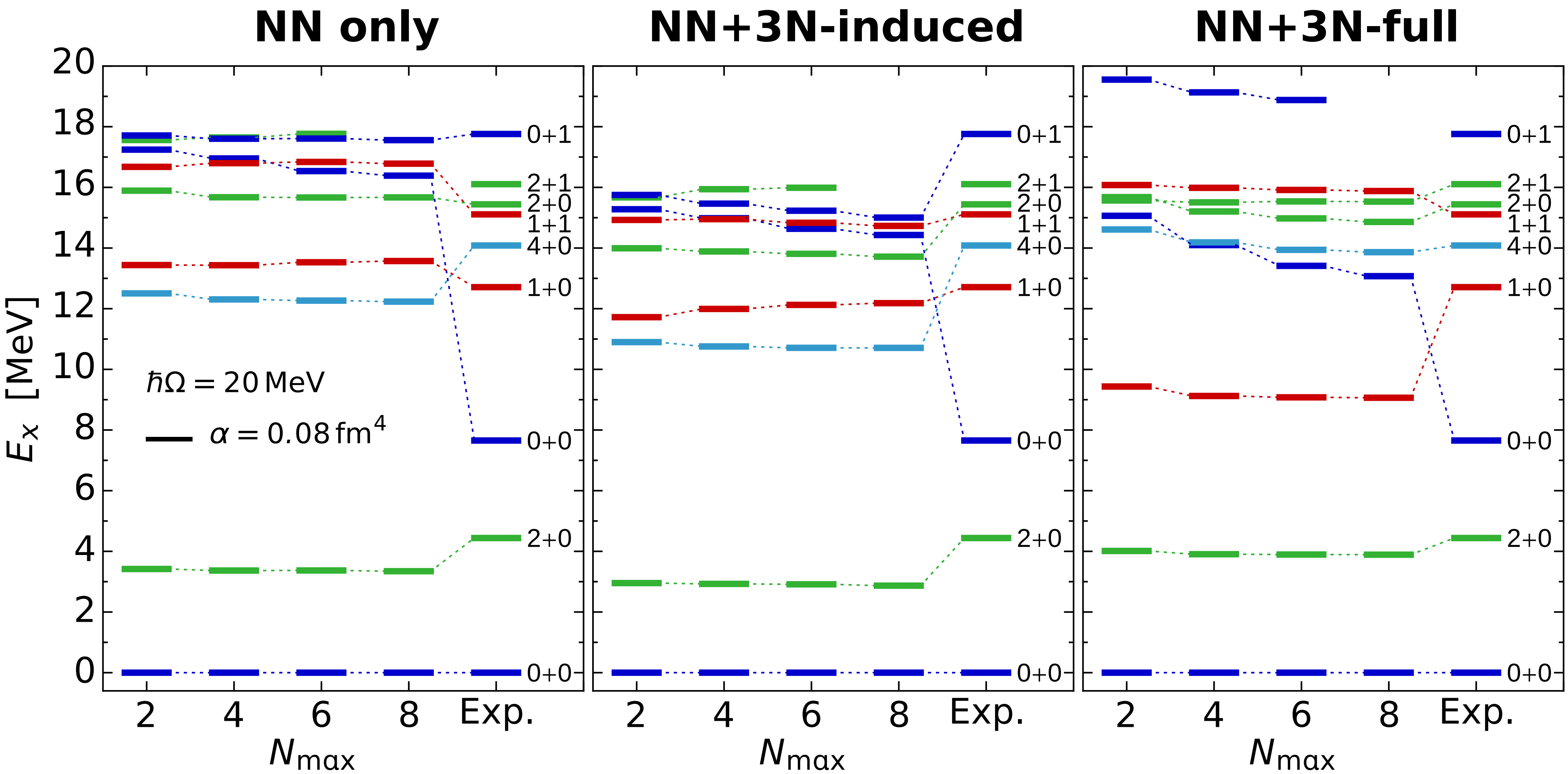
^{16}O: Ground-State Energies



^{40}Ca: First Coupled-Cluster Results

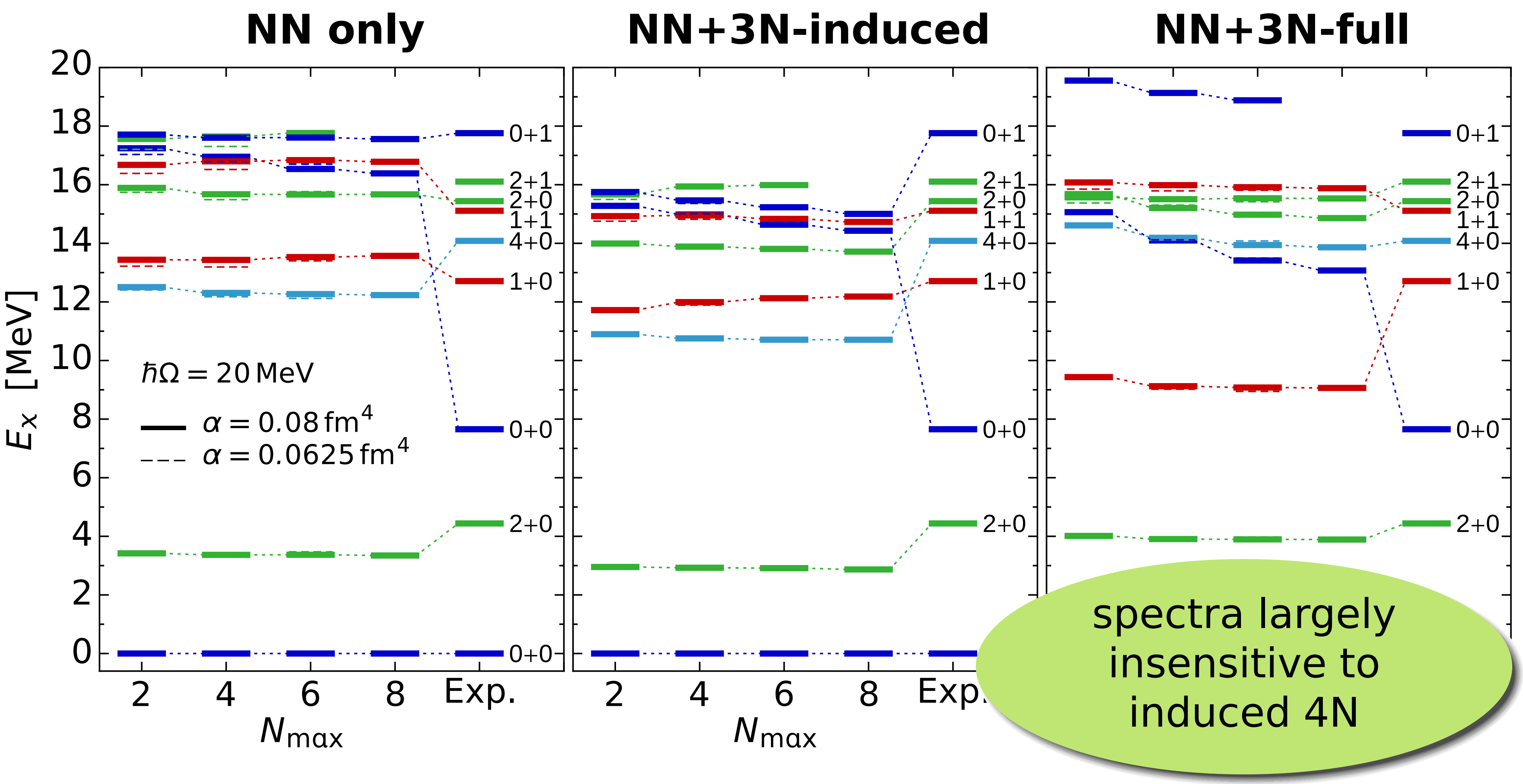


Spectroscopy of ^{12}C



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

Spectroscopy of ^{12}C



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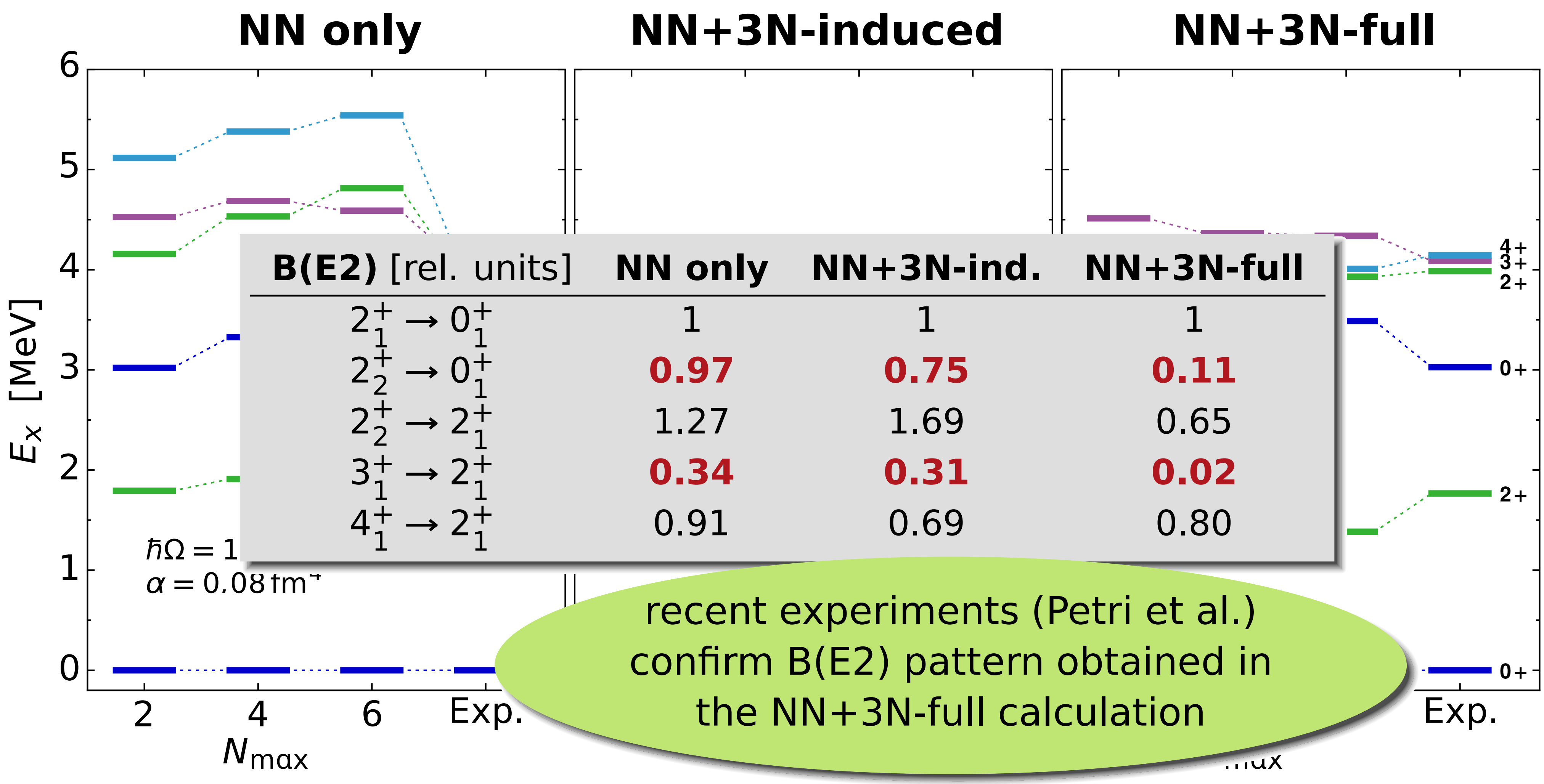
Spectroscopy of ^{16}C



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**
$4^+_1 \rightarrow 2^+_1$	0.91	0.69	0.80

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

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 ?

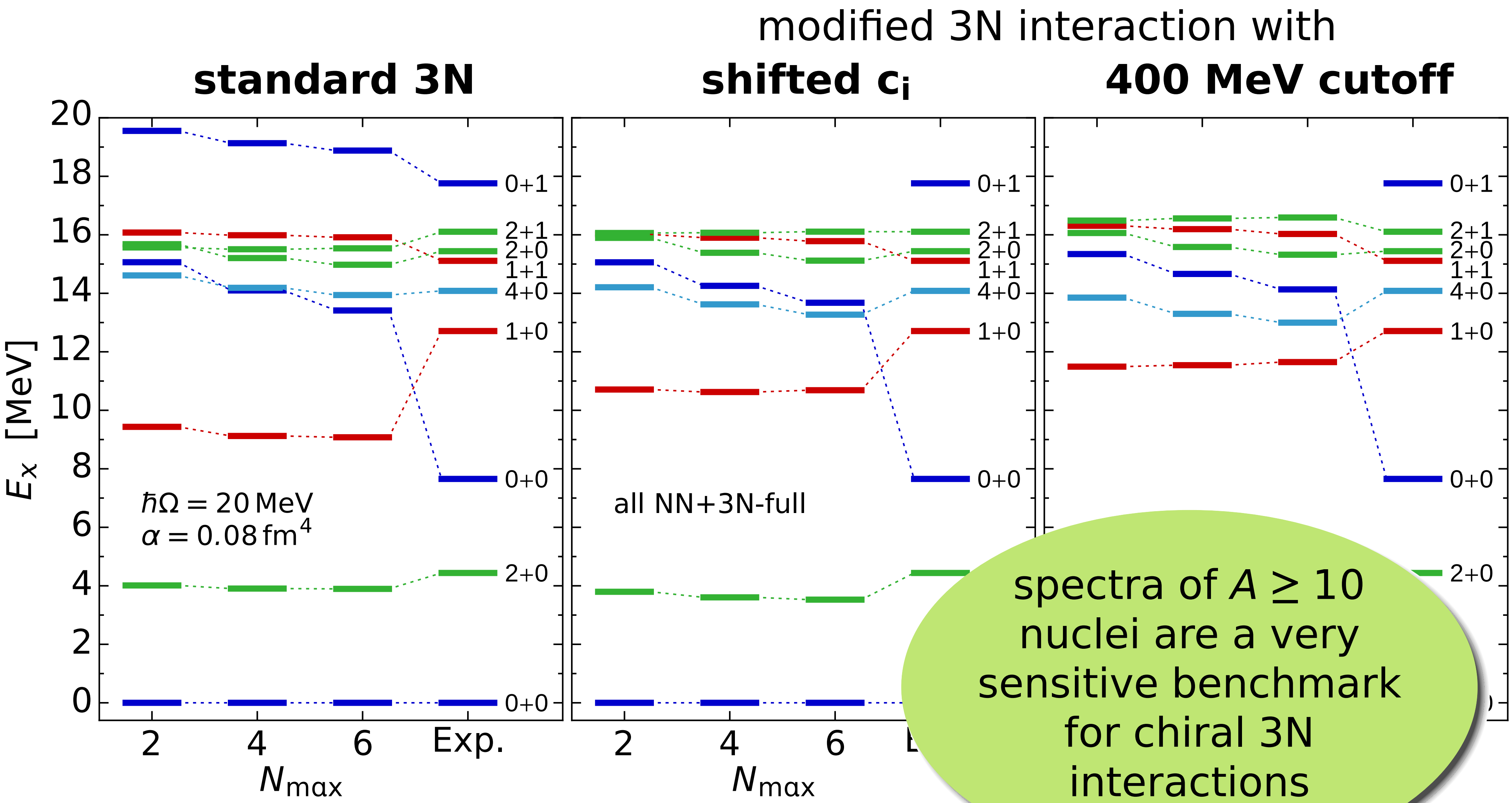
- Can we find alternative SRG generators with suppressed induced 4N ?

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 3N — ^{12}C



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**
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COMPUTING TIME

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