The
Unitary Correlation Operator Method

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New Horizons in Ab Initio Nuclear Structure Theory

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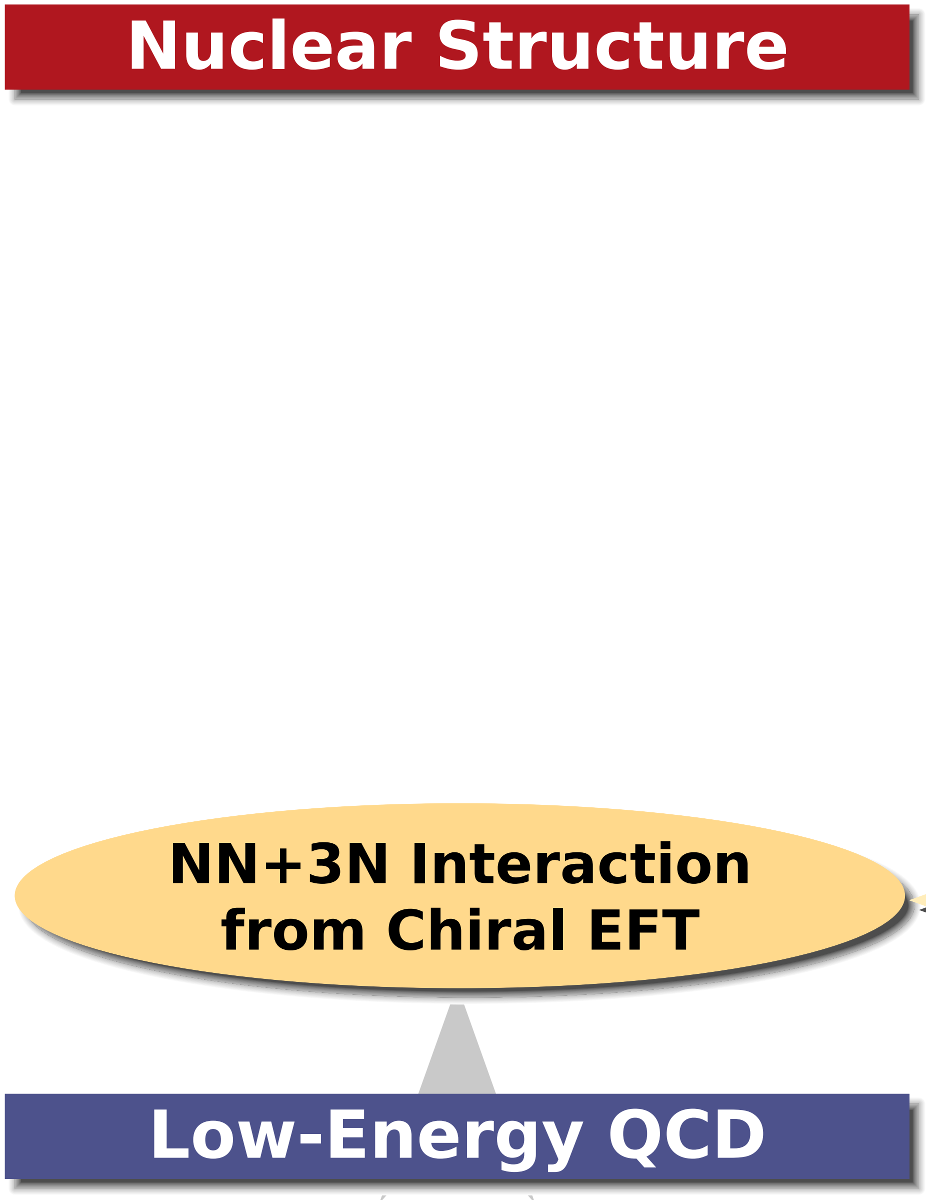
From QCD to Nuclear Structure

Nuclear Structure

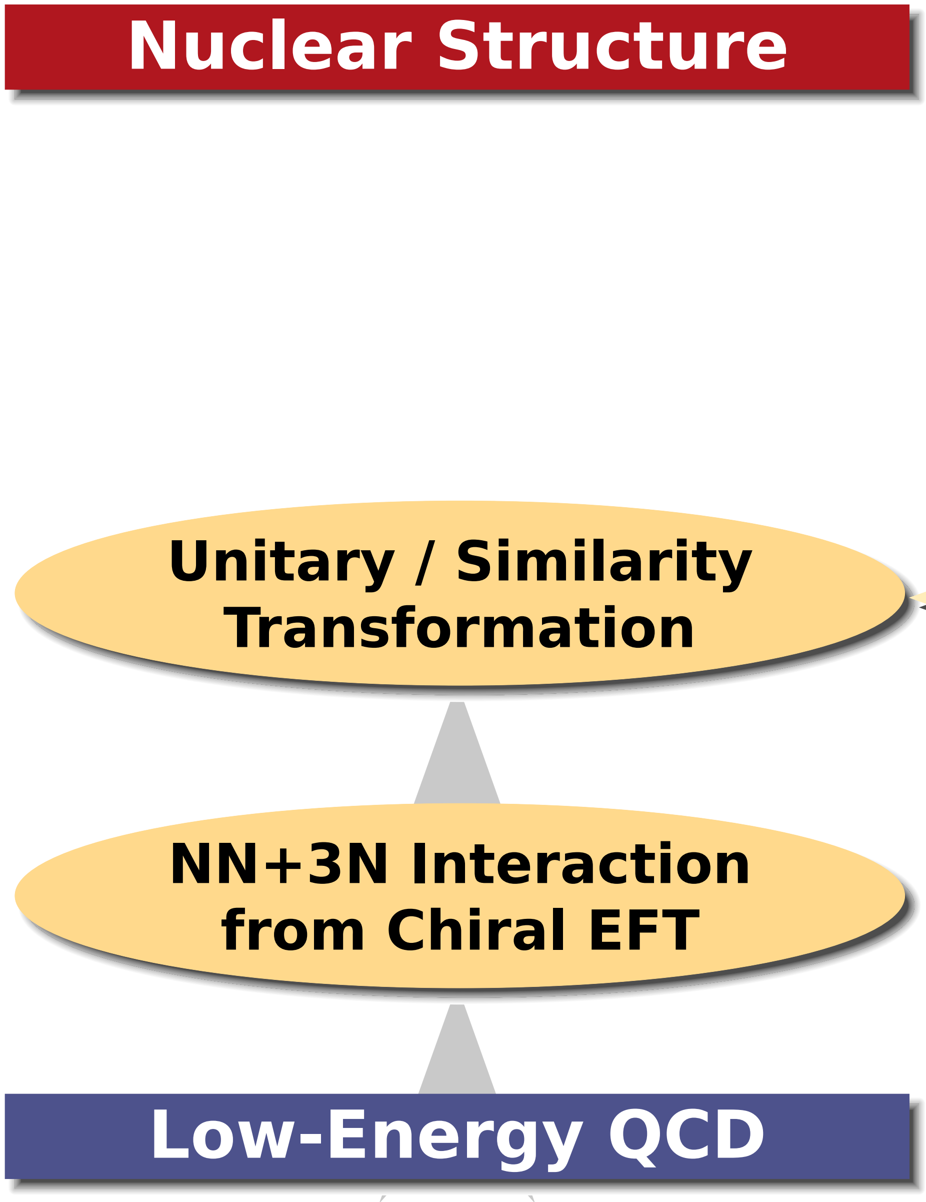
Low-Energy QCD

From QCD to Nuclear Structure



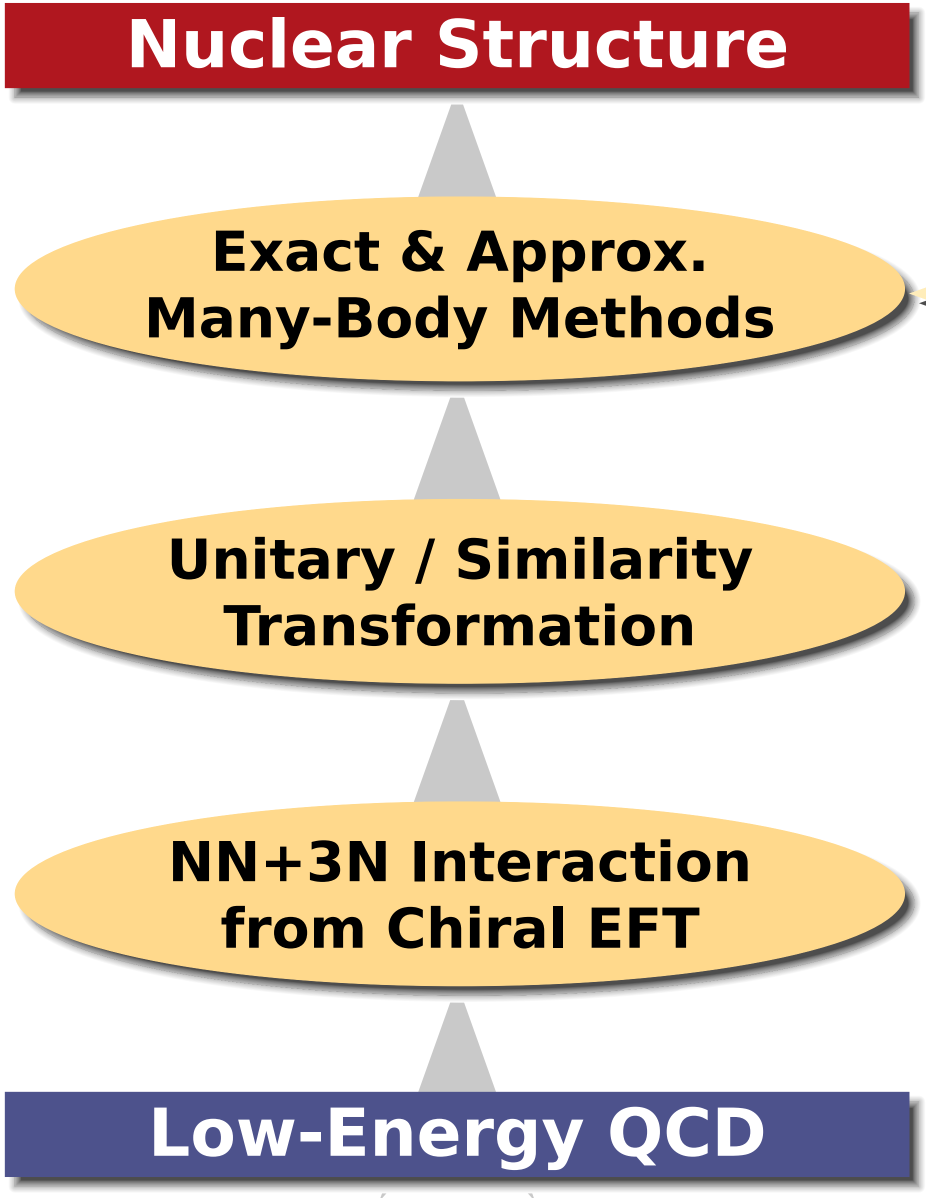
- chiral EFT based on the relevant degrees of freedom & symmetries of QCD
- provides consistent NN, 3N,... interaction plus currents
- initial Hamiltonian:
  - NN at N^3LO
    Entem & Machleidt, 500 MeV cutoff
  - 3N at N^2LO
    Navrátil, A=3 fit, 500 MeV cutoff

From QCD to Nuclear Structure



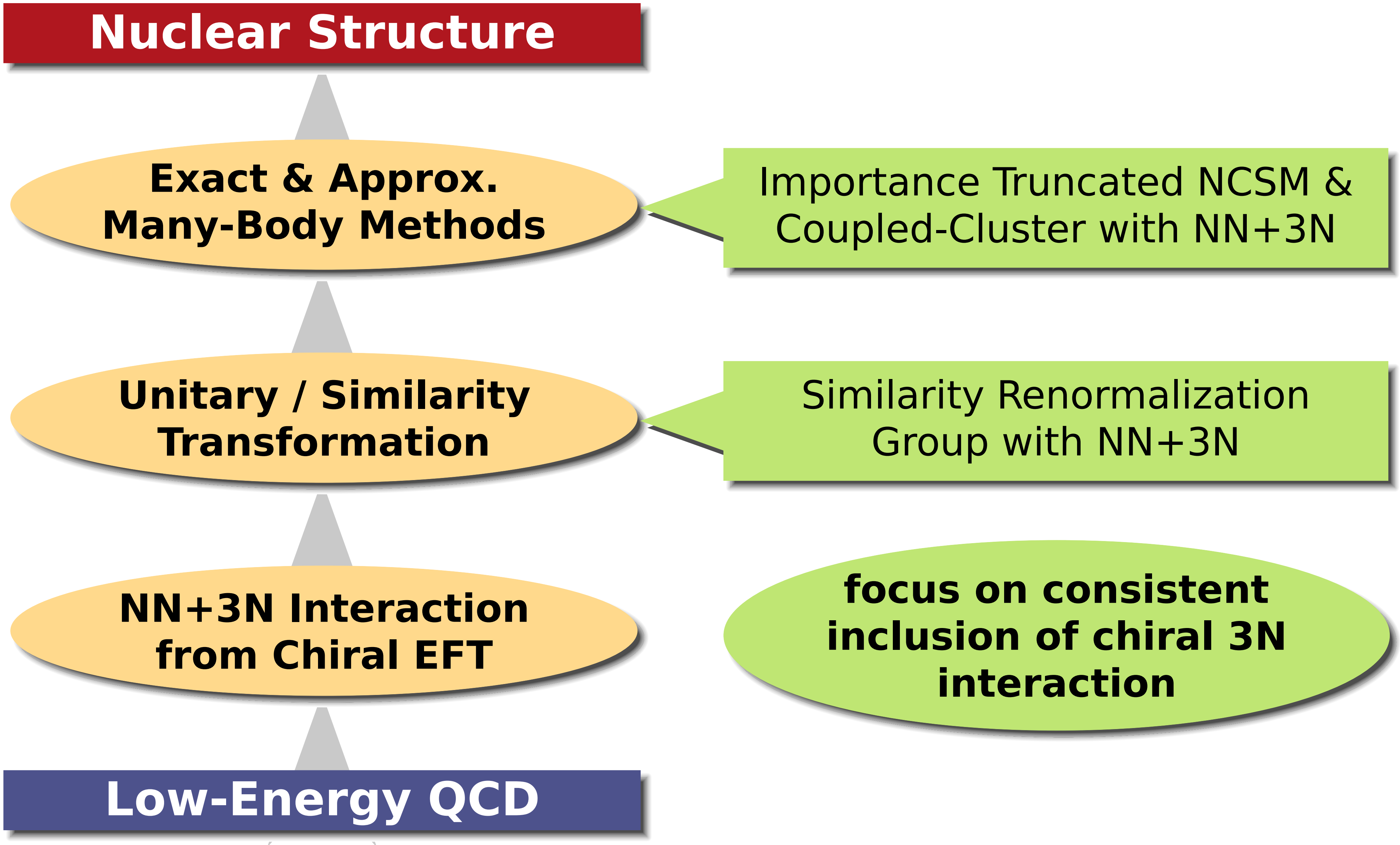
- adapt Hamiltonian to truncated low-energy model space
  - tame short-range correlations
  - improve convergence behavior
- transform Hamiltonian & observables consistently

From QCD to Nuclear Structure



- accurate solution of the many-body problem for light & intermediate masses (NCSM, CC,...)
- controlled approximations for heavier nuclei (MBPT,...)
- all rely on truncated model spaces & benefit from unitary transformation

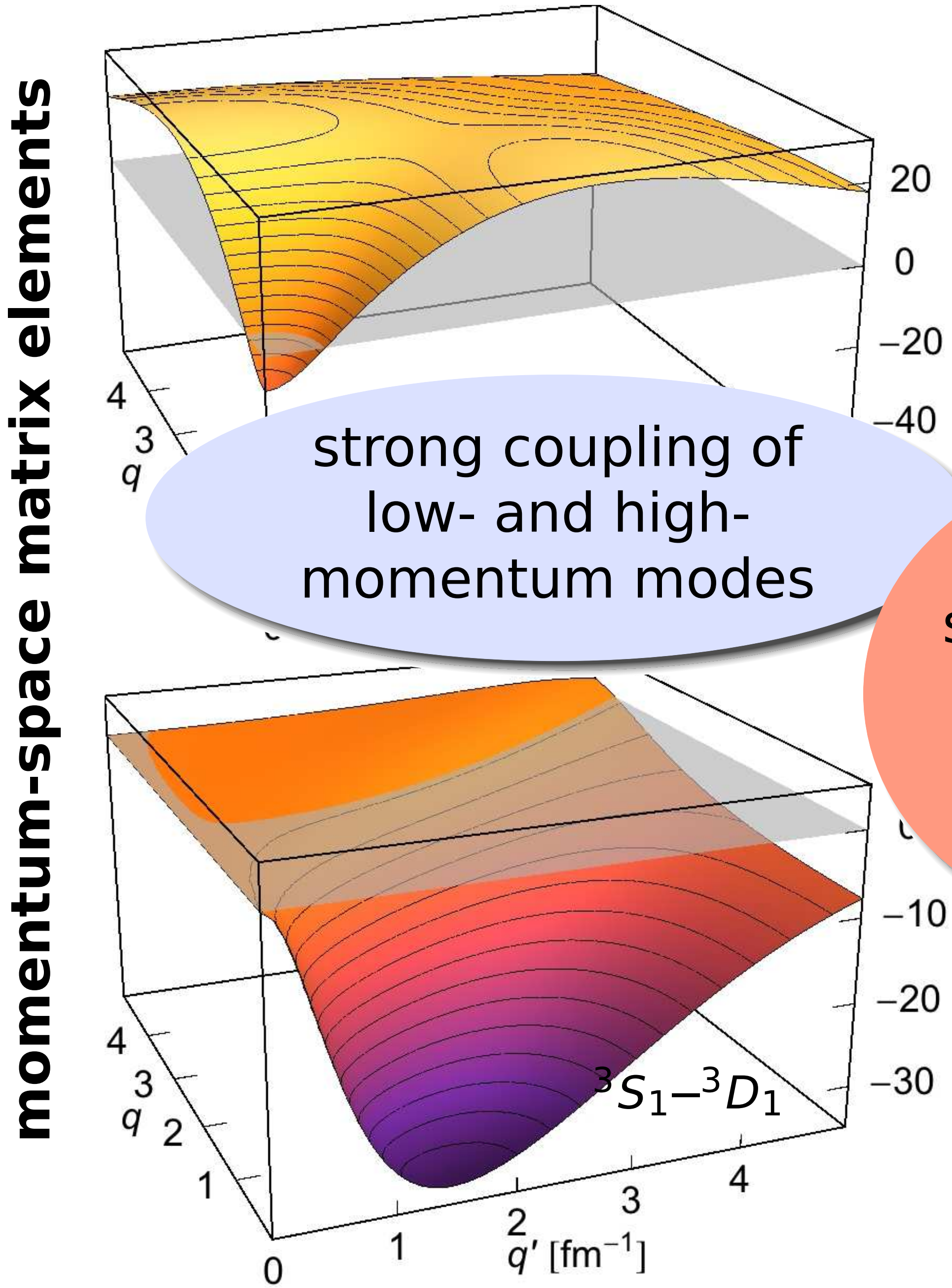
From QCD to Nuclear Structure



Similarity Renormalization Group

Roth, Langhammer, Calci 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)

Why Similarity Transformations?



Argonne V18

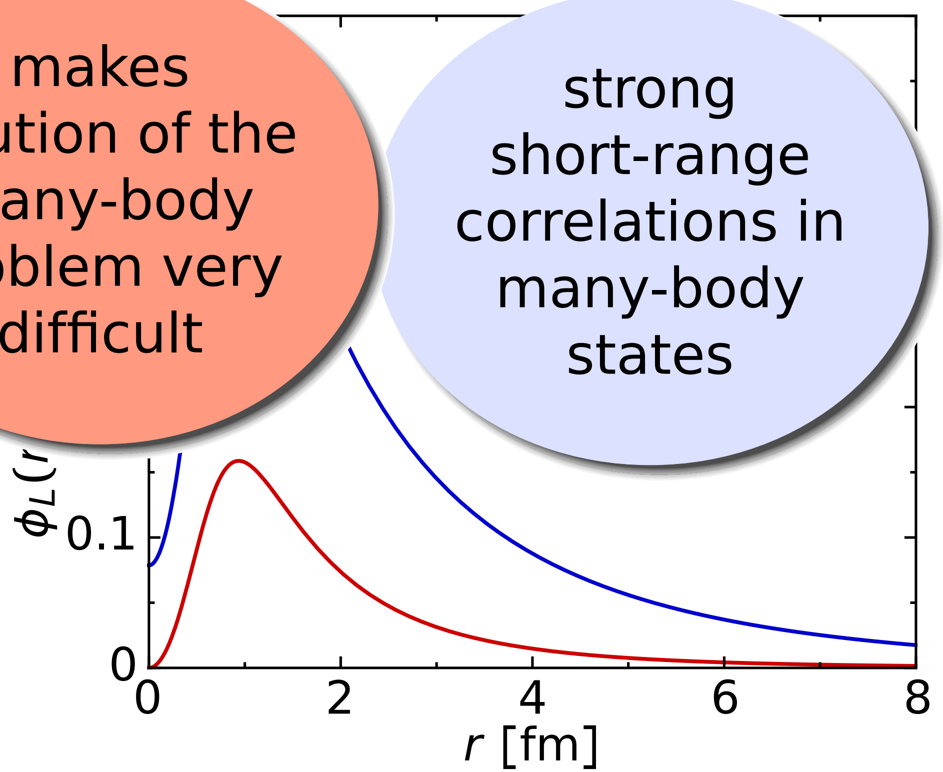
$J^\pi = 1^+, T = 0$

strong coupling of low- and high-momentum modes

makes solution of the many-body problem very difficult

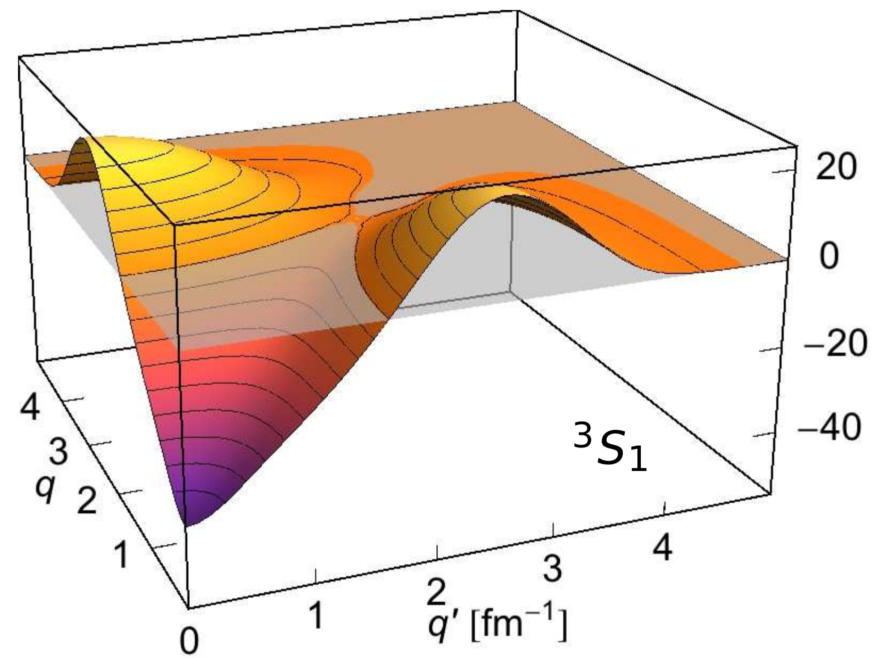
strong short-range correlations in many-body states

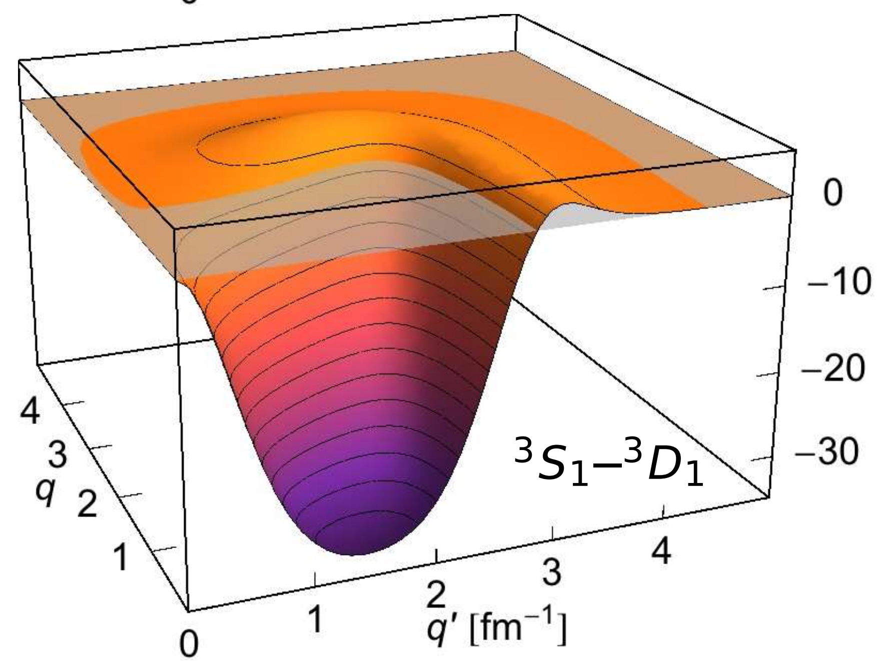
deuteron wave-function



Why Similarity Transformations?

momentum-space matrix elements



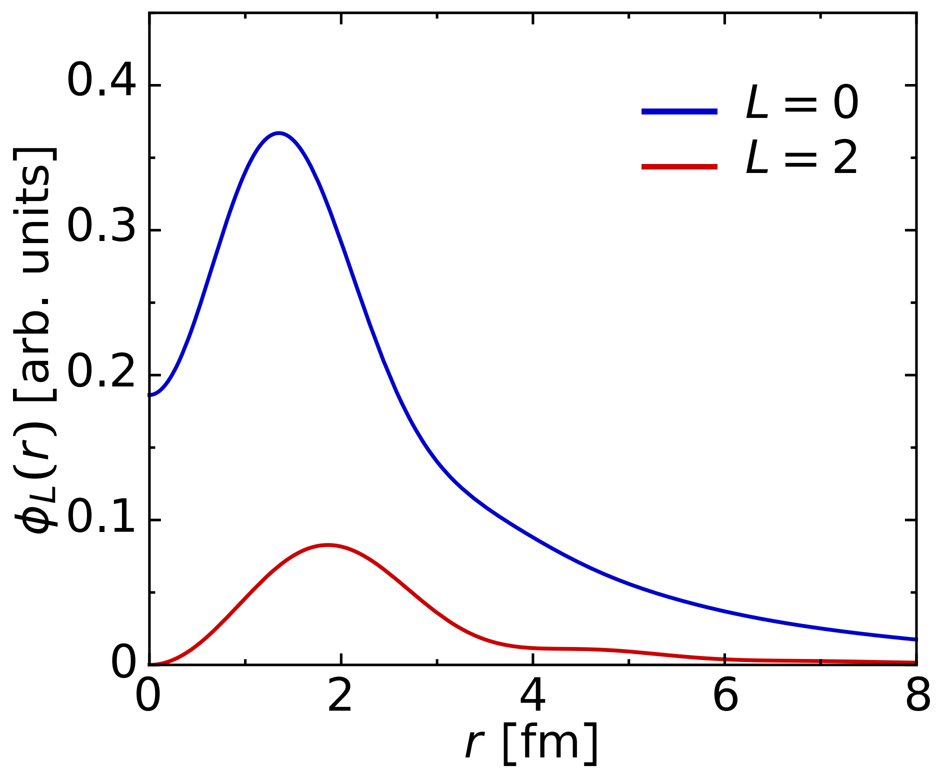


chiral N^3LO

Entem & Machleidt, 500 MeV

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

deuteron wave-function



Unitary Correlation Operator Method

Correlation Operator

define a unitary operator C to describe the effect of short-range correlations

$$C = \exp[-\mathrm{i}\,G] = \exp\Big[-\mathrm{i}\sum_{i<j} g_{ij}\Big]$$

Correlated States

imprint short-range correlations onto uncorrelated many-body states

$$|\tilde{\psi}\rangle = C\,|\psi\rangle$$

Correlated Operators

adapt Hamiltonian to uncorrelated states (pre-diagonalization)

$$\tilde{O} = C^{\dagger}\,O\,C$$

$$\langle\tilde{\psi}|\,O\,|\tilde{\psi}'\rangle = \langle\psi|\,C^{\dagger}\,O\,C\,|\psi'\rangle = \langle\psi|\,\tilde{O}\,|\psi'\rangle$$

Unitary Correlation Operator Method

explicit ansatz for unitary transformation operator **motivated by the physics of short-range correlations**

- **explicit unitary transformation** with correlation operator C

$$C = C_\Omega C_r = \exp\Big(-\mathrm{i}\sum_{i<j} g_{\Omega,ij}\Big)\exp\Big(-\mathrm{i}\sum_{i<j} g_{r,ij}\Big)$$

- **central correlator** C_r: radial distance-dependent shift in the relative coordinate of a nucleon pair

$$g_r = \tfrac{1}{2}\big[s(r)\, q_r + q_r\, s(r)\big] \qquad q_r = \tfrac{1}{2}\big[\tfrac{\vec{r}}{r}\cdot\vec{q} + \vec{q}\cdot\tfrac{\vec{r}}{r}\big]$$

- **tensor correlator** C_Ω: angular shift depending on the orientation of spin and relative coordinate of a nucleon pair

$$g_\Omega = \tfrac{3}{2}\vartheta(r)\big[(\vec{\sigma}_1\cdot\vec{q}_\Omega)(\vec{\sigma}_2\cdot\vec{r}) + (\vec{r}\leftrightarrow\vec{q}_\Omega)\big] \qquad \vec{q}_\Omega = \vec{q} - \tfrac{\vec{r}}{r}\, q_r$$

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

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

solve SRG evolution equations using two- & three-body matrix representation

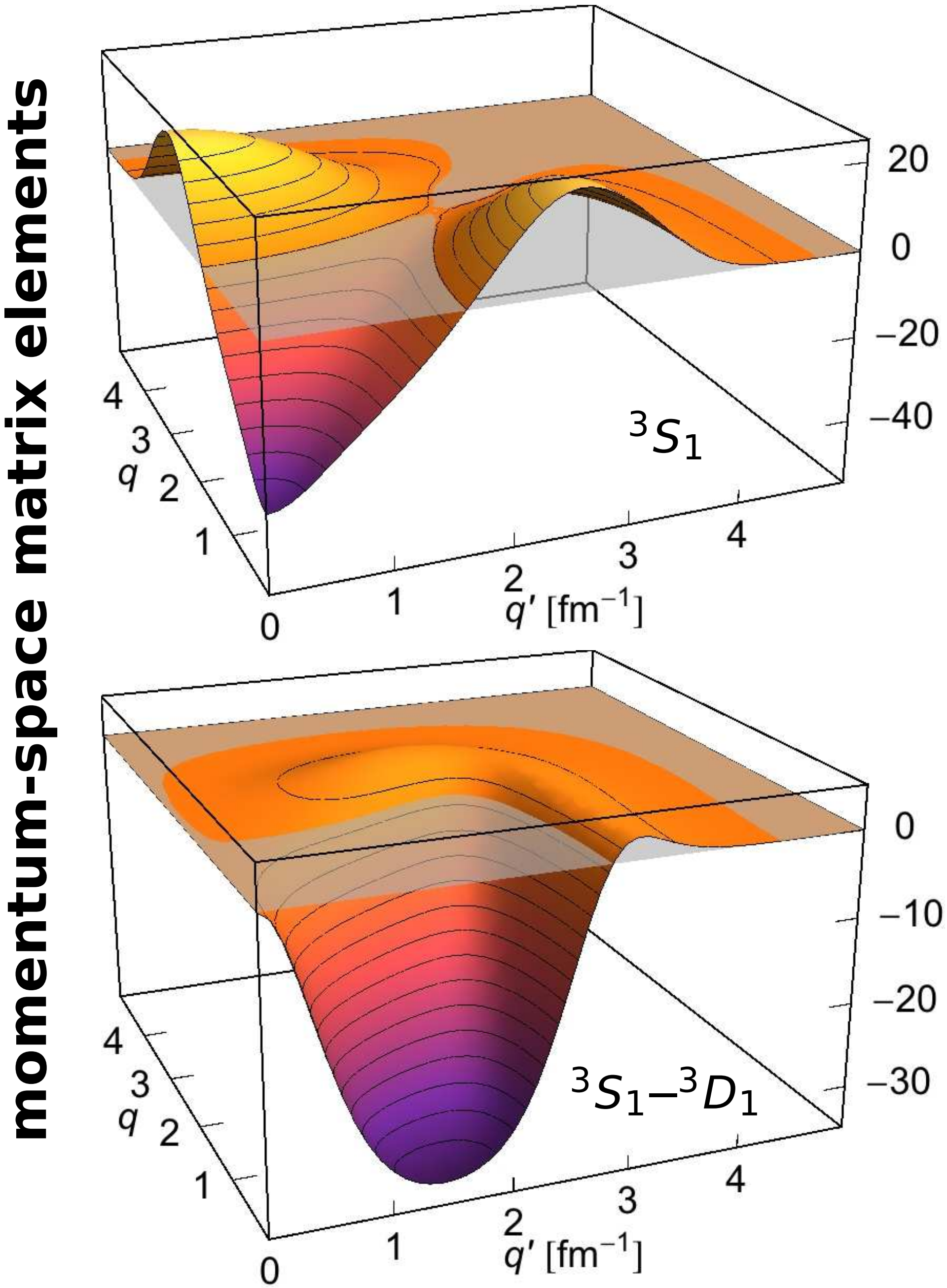
- **evolution equations** for $\widetilde{H}_\alpha$ and U

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

- **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 Two-Body Space

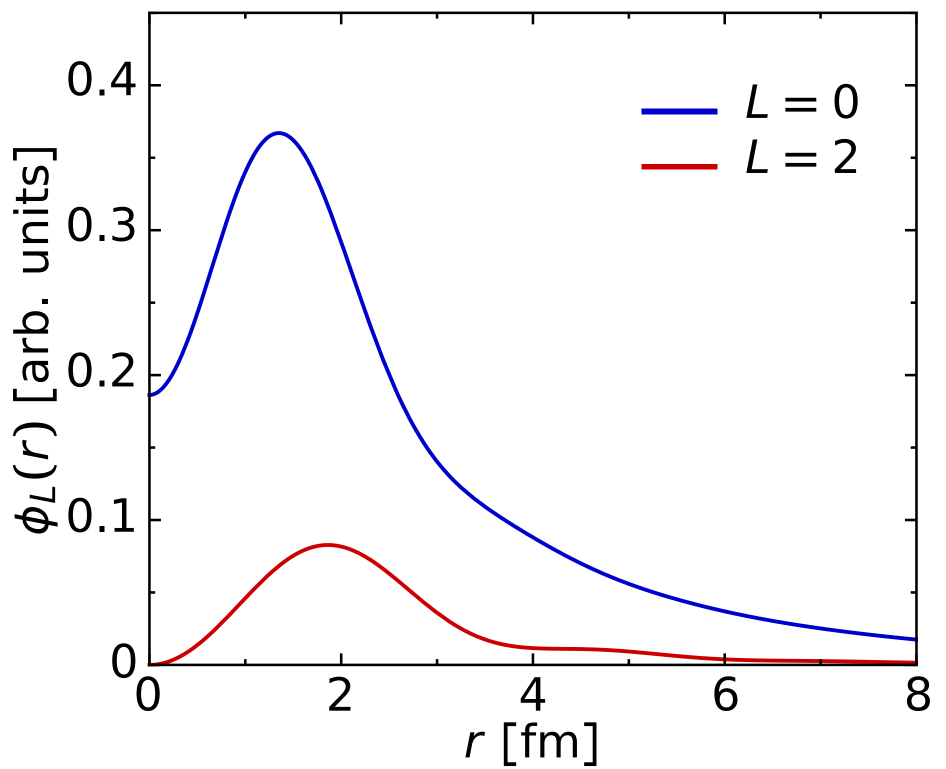


$\alpha = 0.000\,\mathrm{fm}^4$

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

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

deuteron wave-function

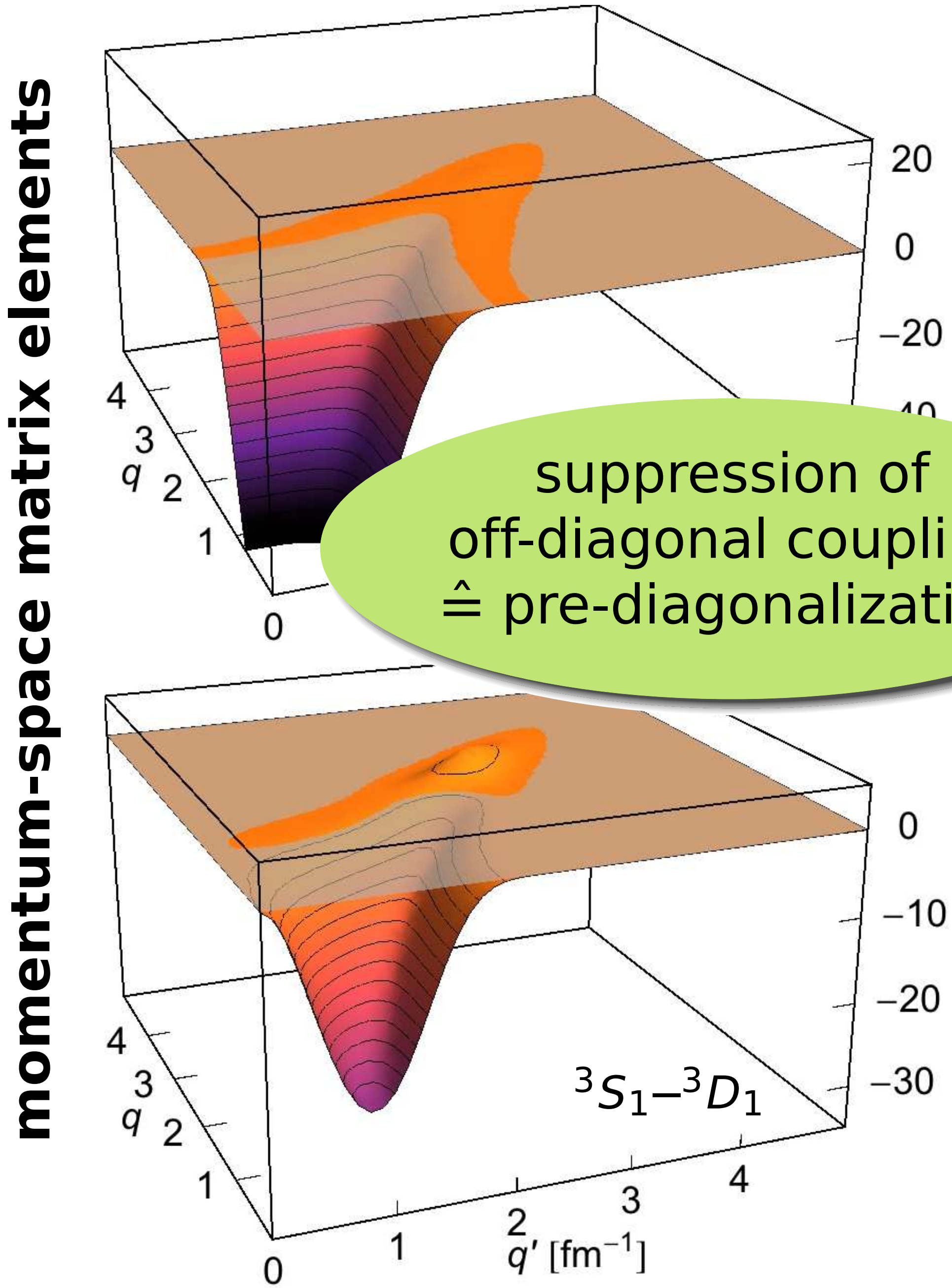


SRG Evolution in Two-Body Space

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

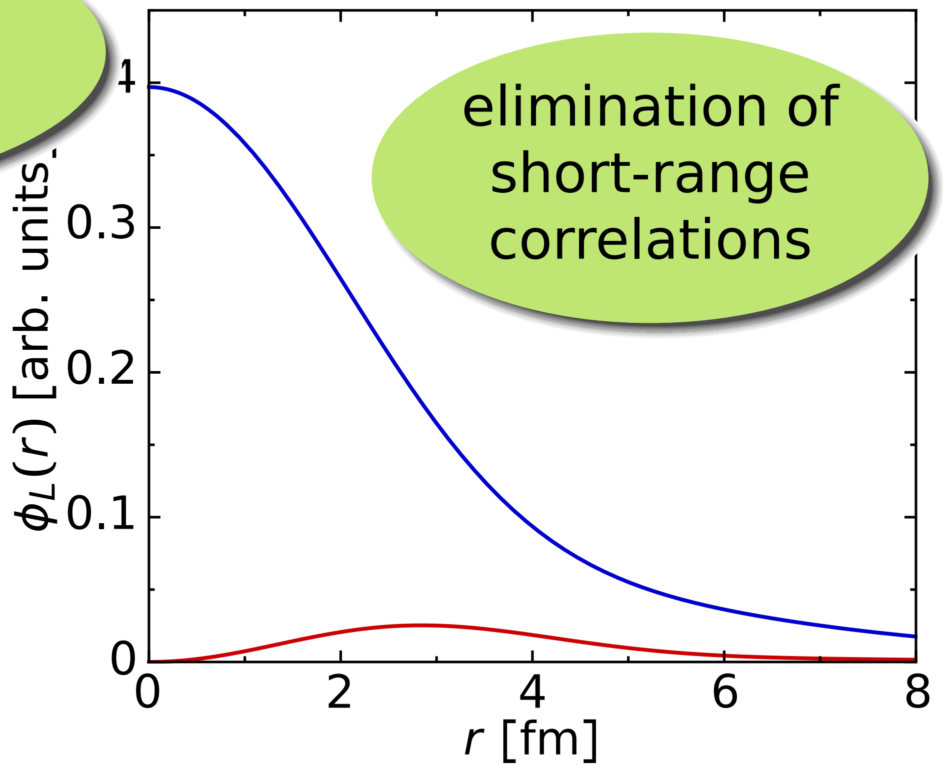
$\Lambda = 1.33\,\mathrm{fm}^{-1}$

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



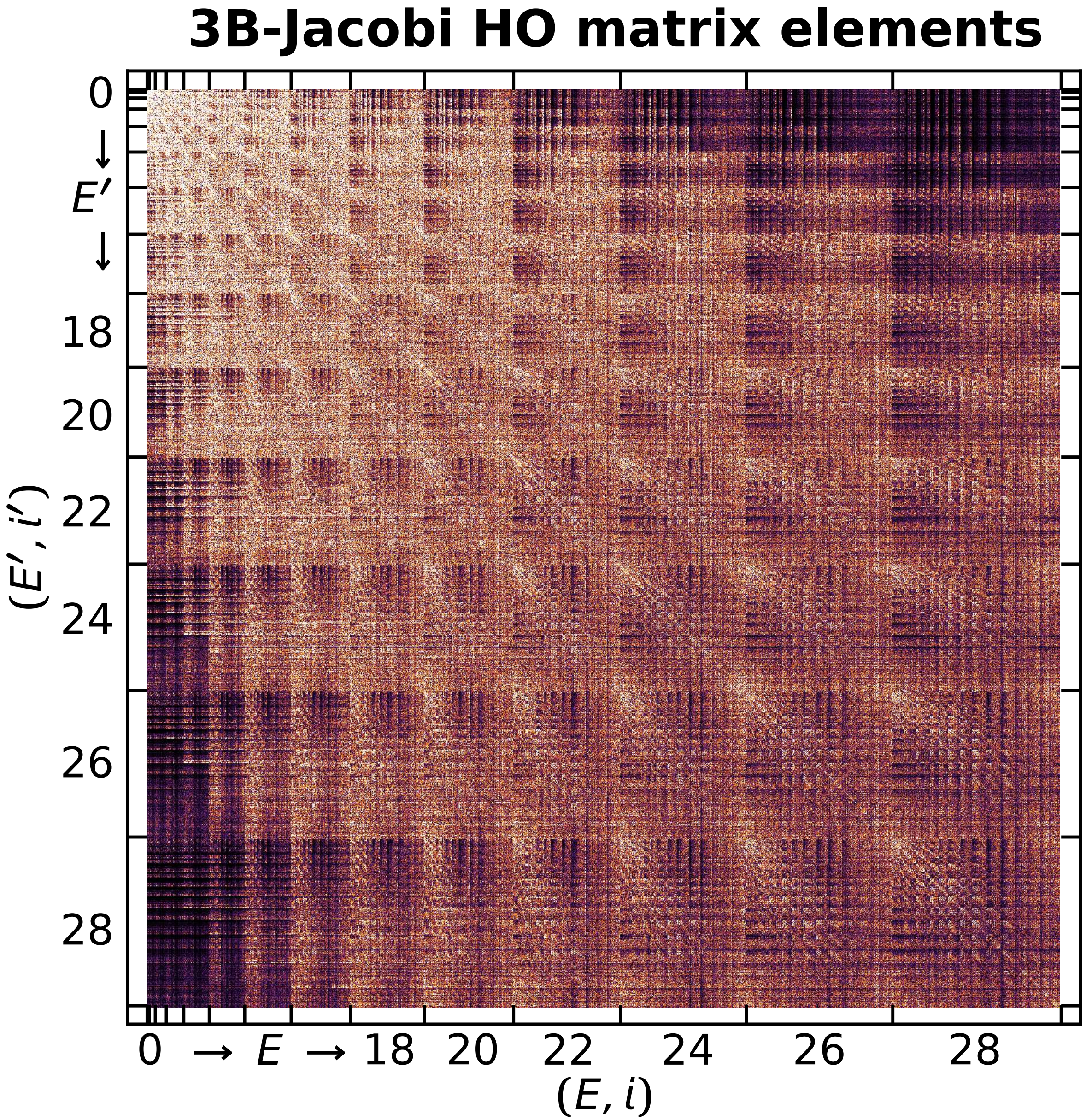
suppression of
off-diagonal coupling
≙ pre-diagonalization

deuteron wave-function



elimination of
short-range
correlations

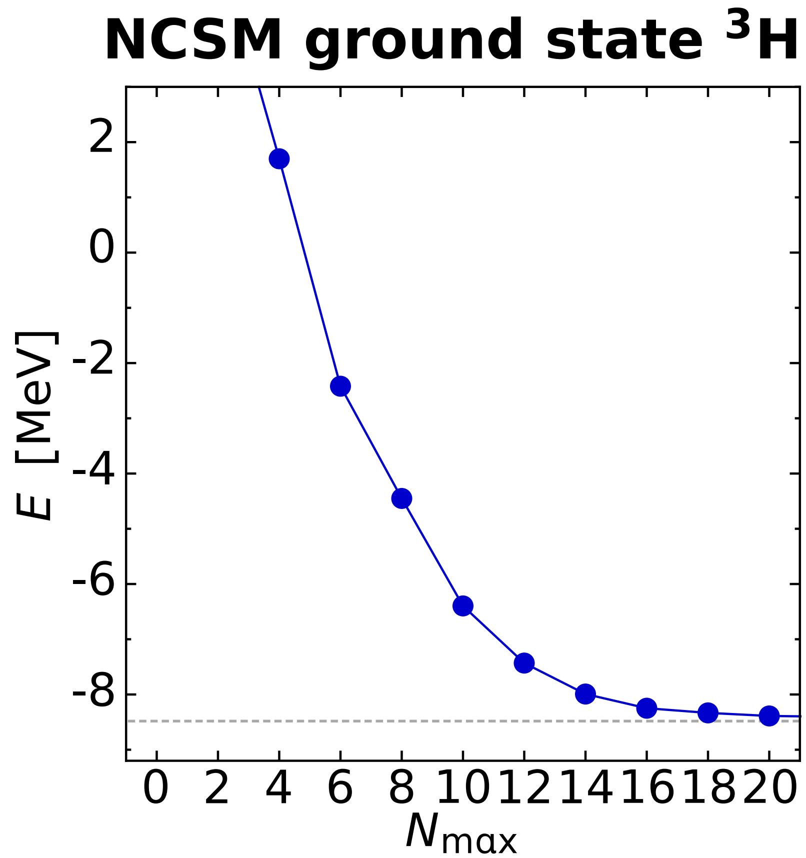
SRG Evolution in Three-Body Space



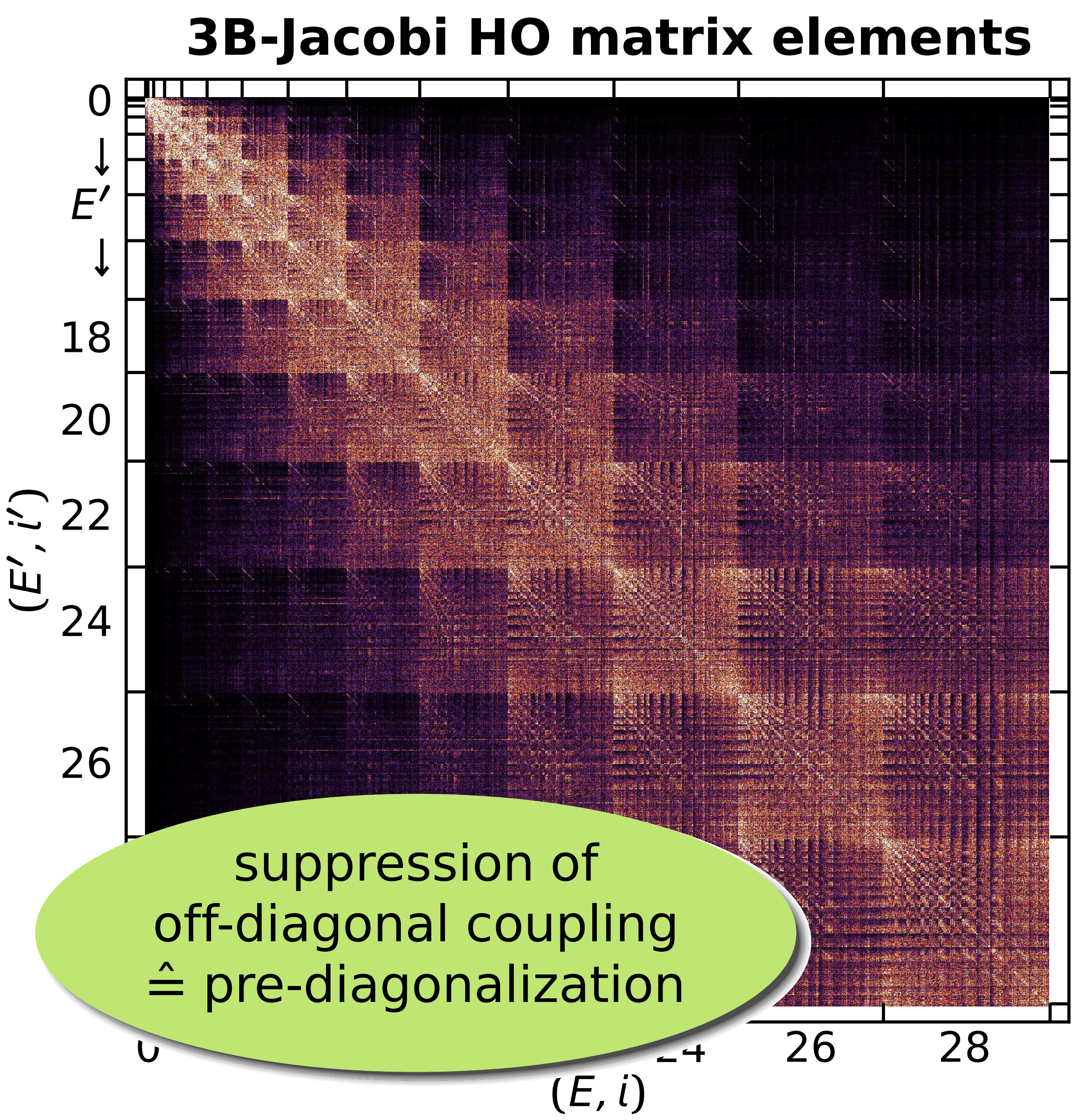
$\alpha = 0.000\,\text{fm}^4$

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

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



SRG Evolution in Three-Body Space



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

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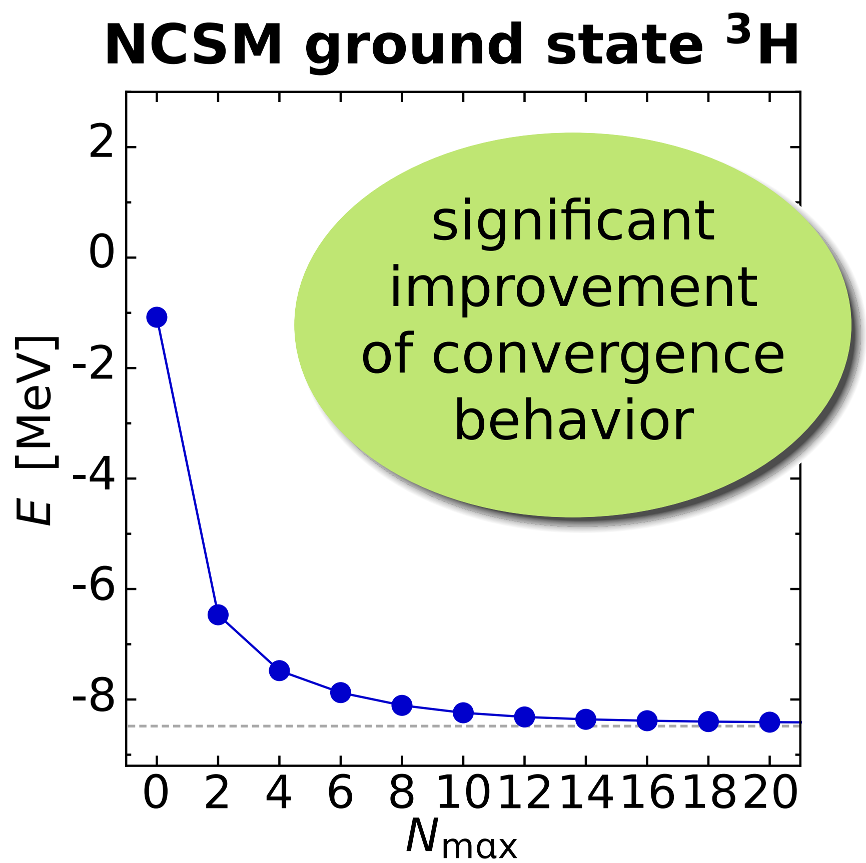
$J^\pi = \frac{1}{2}^+, T = \frac{1}{2}, \hbar\Omega = 28\,\mathrm{MeV}$



Calculations in *A*-Body Space

- evolution **induces *n*-body contributions** $\widetilde{H}_\alpha^{[n]}$ to Hamiltonian

$$\widetilde{H}_\alpha = \widetilde{H}_\alpha^{[1]} + \widetilde{H}_\alpha^{[2]} + \widetilde{H}_\alpha^{[3]} + \widetilde{H}_\alpha^{[4]} + \ldots$$

- truncation of cluster series inevitable — formally destroys unitarity and invariance of energy eigenvalues (independence of α)

Three SRG-Evolved Hamiltonians

- **NN only**: start with NN initial Hamiltonian and keep two-body terms only
- **NN+3N-induced**: start with NN initial Ham… …nd keep two- and induced three-body terms
- **NN+3N-full**: start with NN+3… and all three-body terms

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

Importance Truncated NCSM

Roth, Langhammer, Calci et al. — Phys. Rev. Lett. 107, 072501 (2011)
Navrátil, Roth, Quaglioni — Phys. Rev. C 82, 034609 (2010)
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

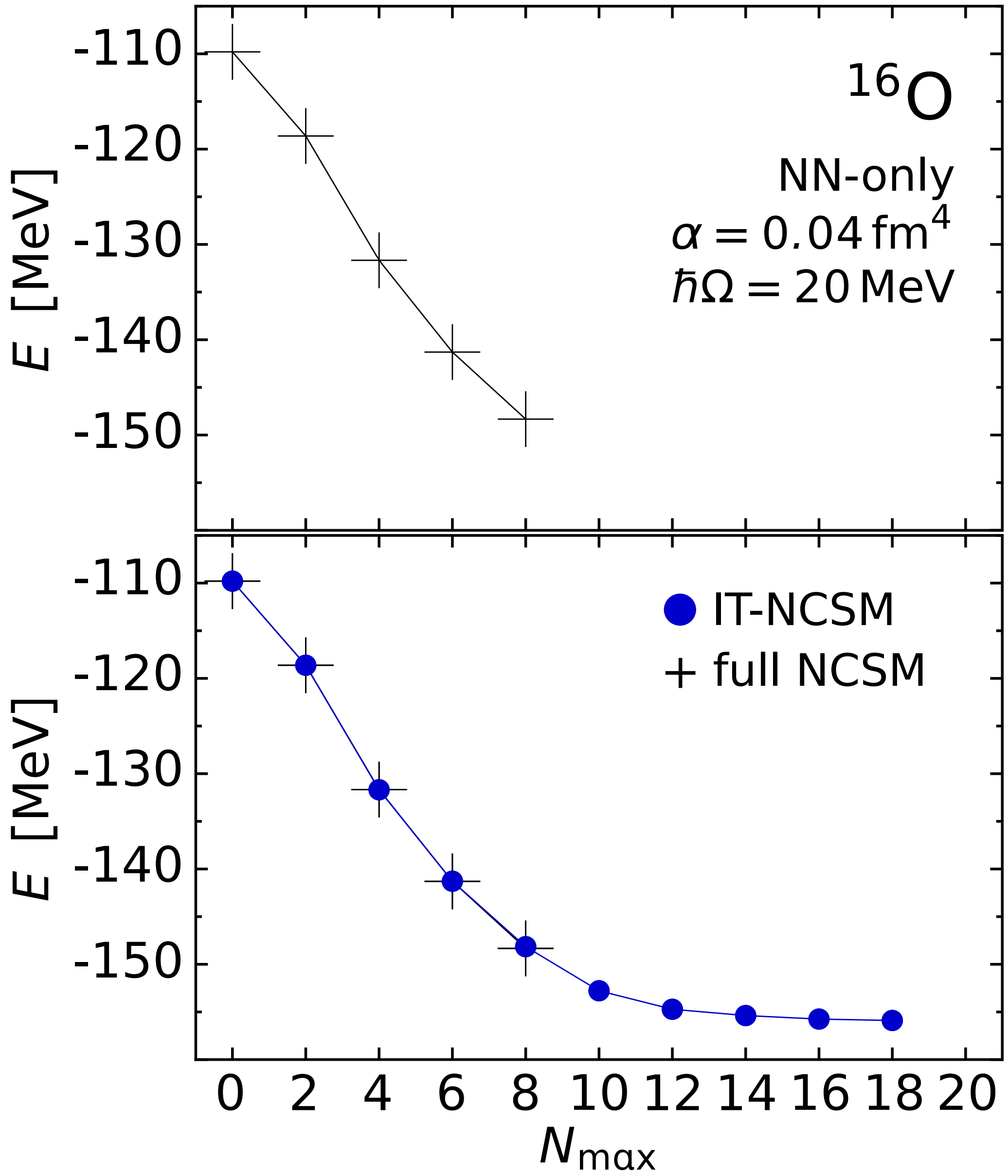
- construct matrix representation of Hamiltonian using a **basis of HO Slater determinants** truncated w.r.t. HO excitation energy $N_{\max}\hbar\Omega$
- solve **large-scale eigenvalue problem** for a few extremal eigenvalues
- **all relevant observables** can be computed from the eigenstates
- range 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

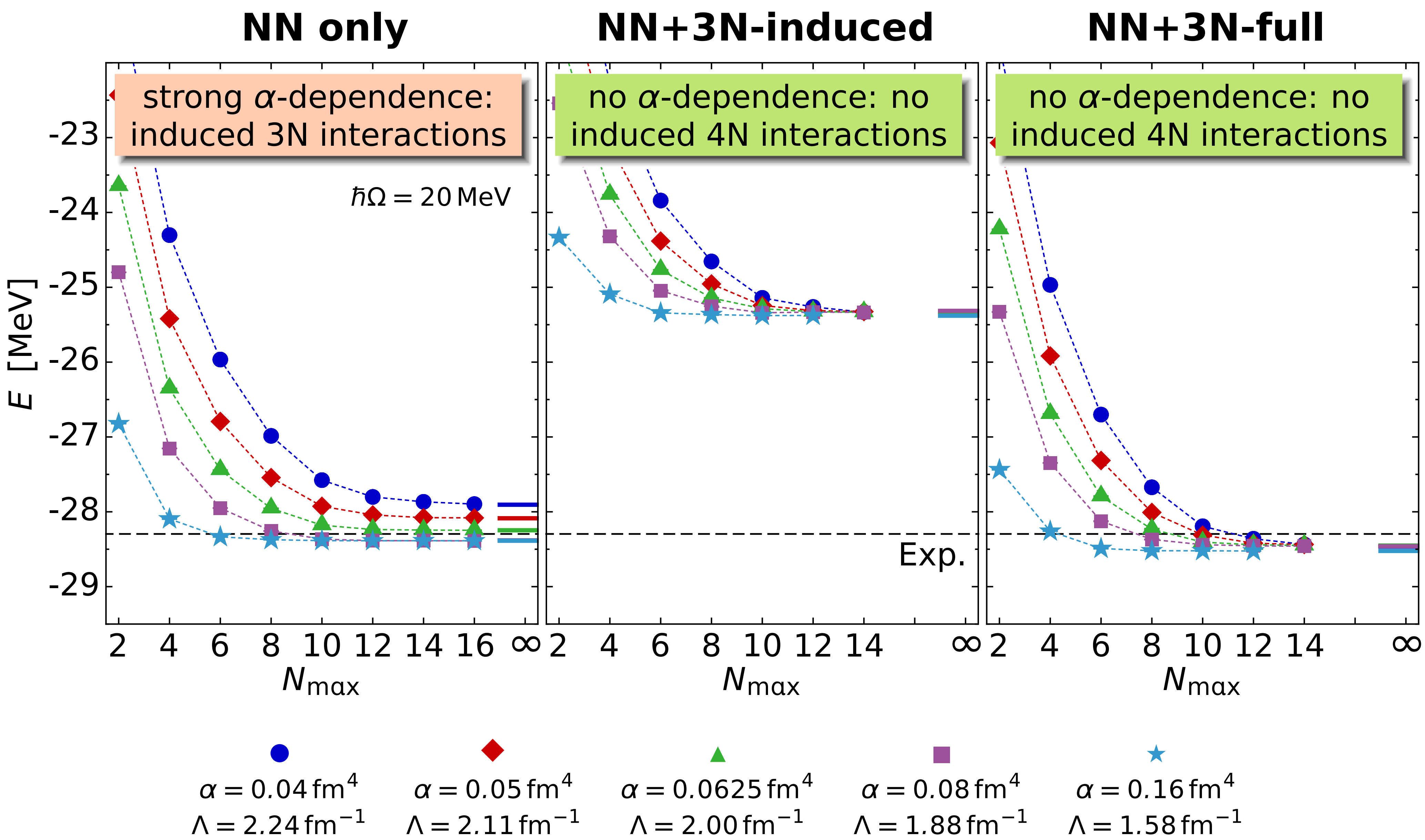
- converged NCSM calculations essentially restricted to lower/mid p-shell
- full $10\hbar\Omega$ calculation for ^{16}O getting very difficult (basis dimension > 10^{10})

Importance Truncation

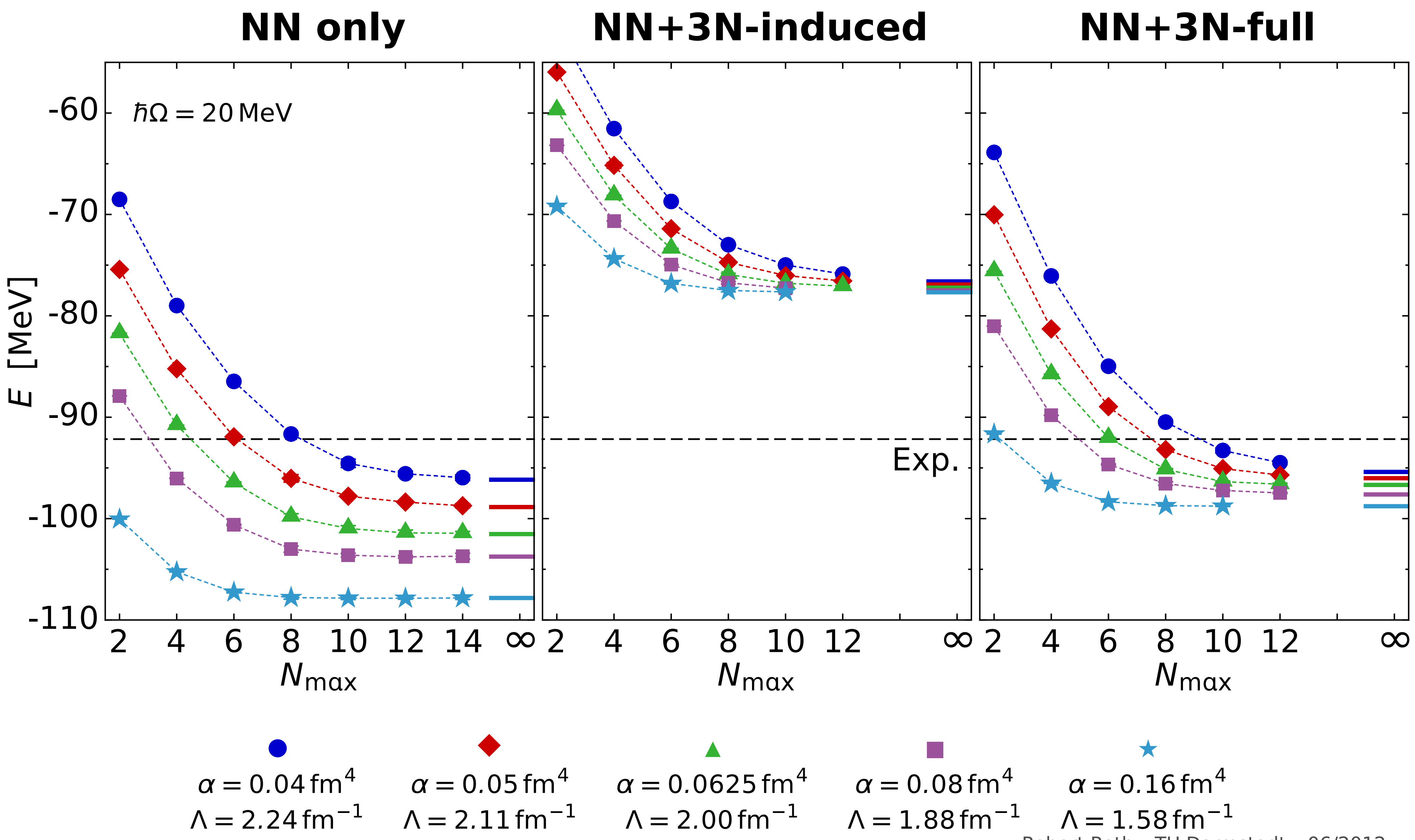
reduce model space to the relevant basis states using an **a priori importance measure** derived from MBPT



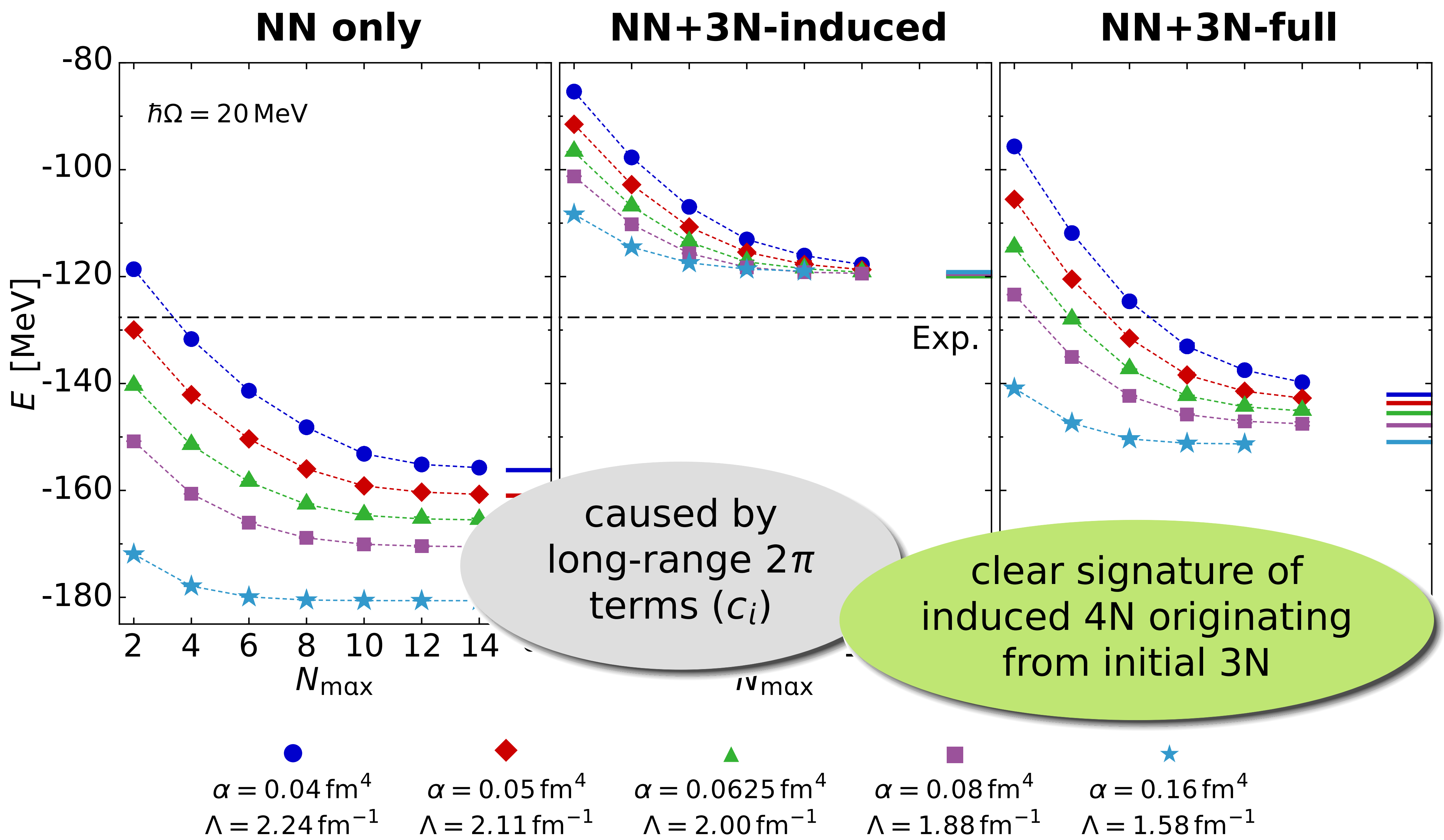
^{4}He: Ground-State Energies



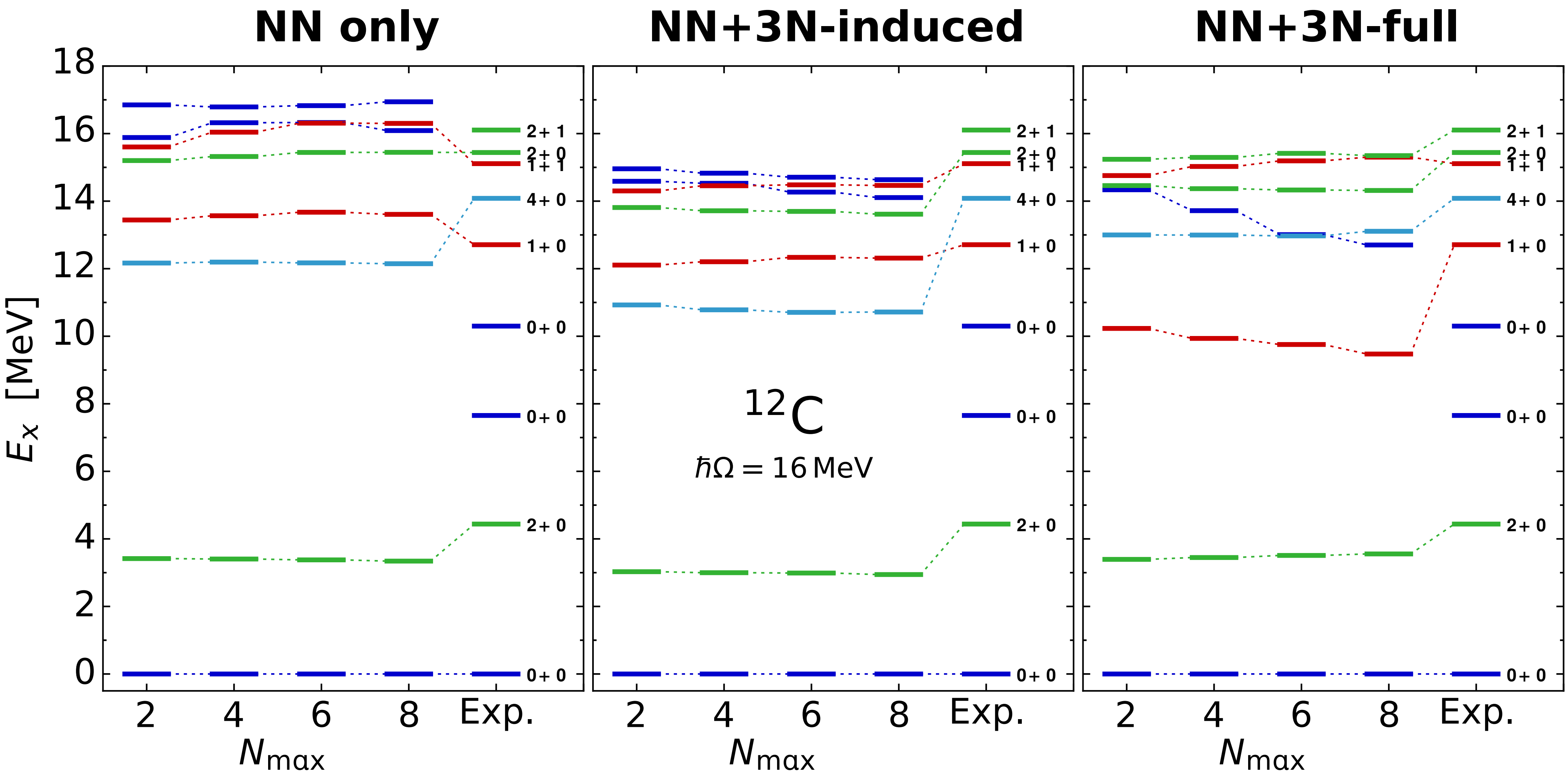
^{12}C: Ground-State Energies



^{16}O: Ground-State Energies



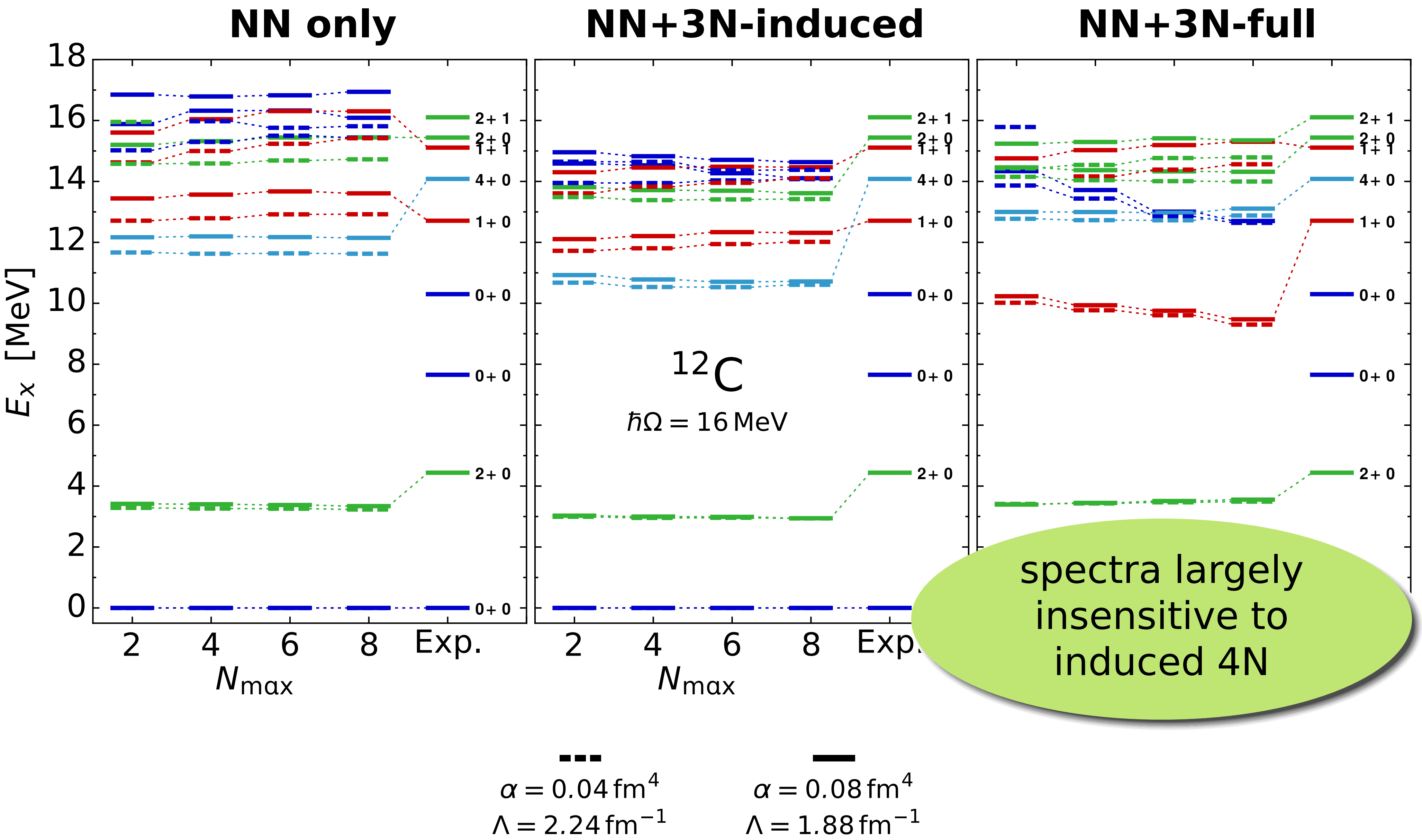
Spectroscopy of ^{12}C



$\alpha = 0.04\,\text{fm}^4$ $\Lambda = 2.24\,\text{fm}^{-1}$

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

Spectroscopy of ^{12}C



spectra largely insensitive to induced 4N

The Bottom Line...

- 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 **good description** of spectra (and ground states)
- **breakthrough** in computation, transformation and management of 3N matrix-elements

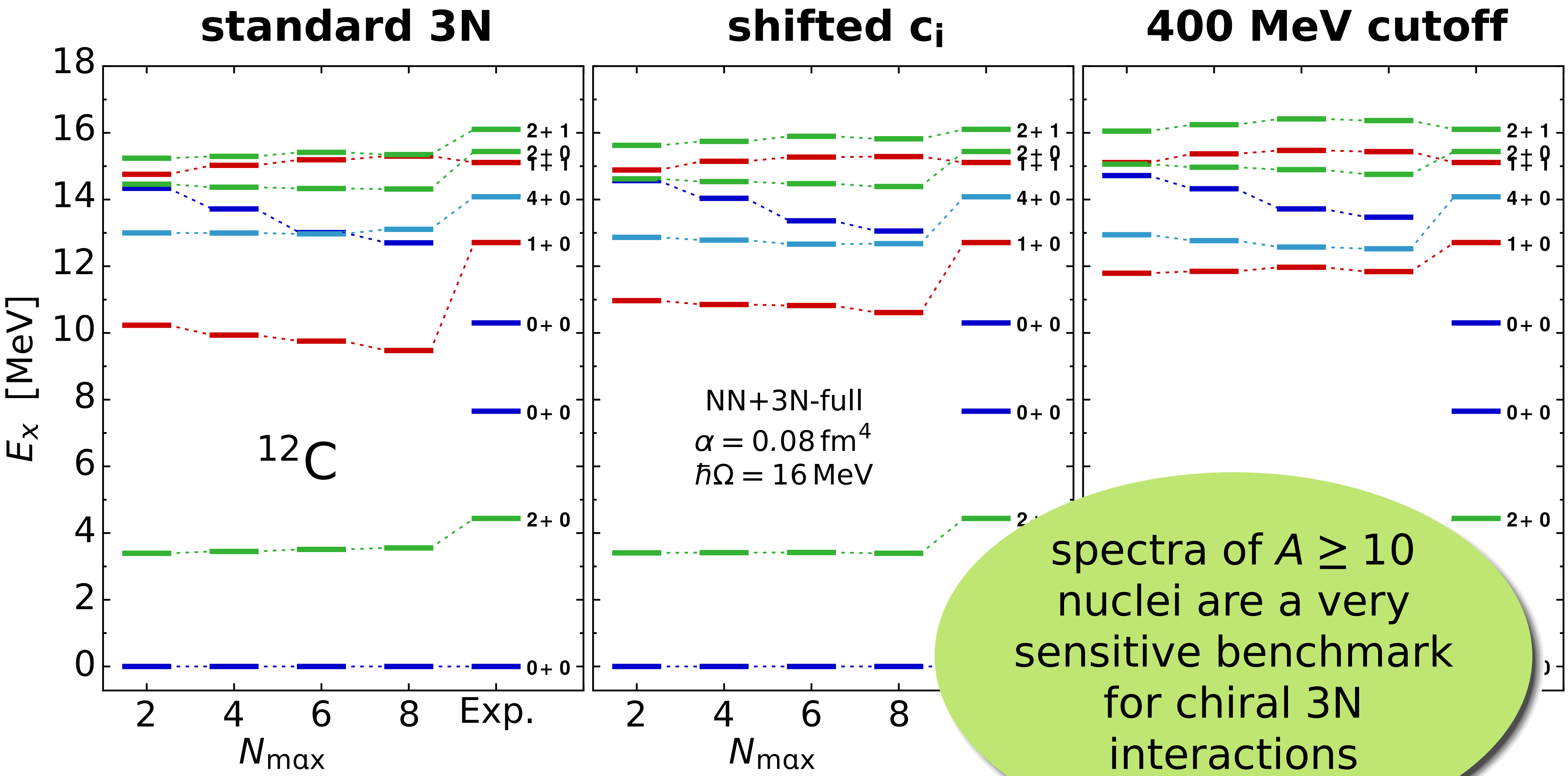
- **next-generation SRG**: can we find new SRG-generators that do not induce as much 4N but still give good convergence?
- **next-generation chiral 3N**: how will N3LO or Δ-full chiral 3N interactions affect the picture?
- **applications**: which experiment-related applications are in reach with the present framework?

Physics Applications

(work in progress... all preliminary)

Outlook: Sensitivity on Initial 3N

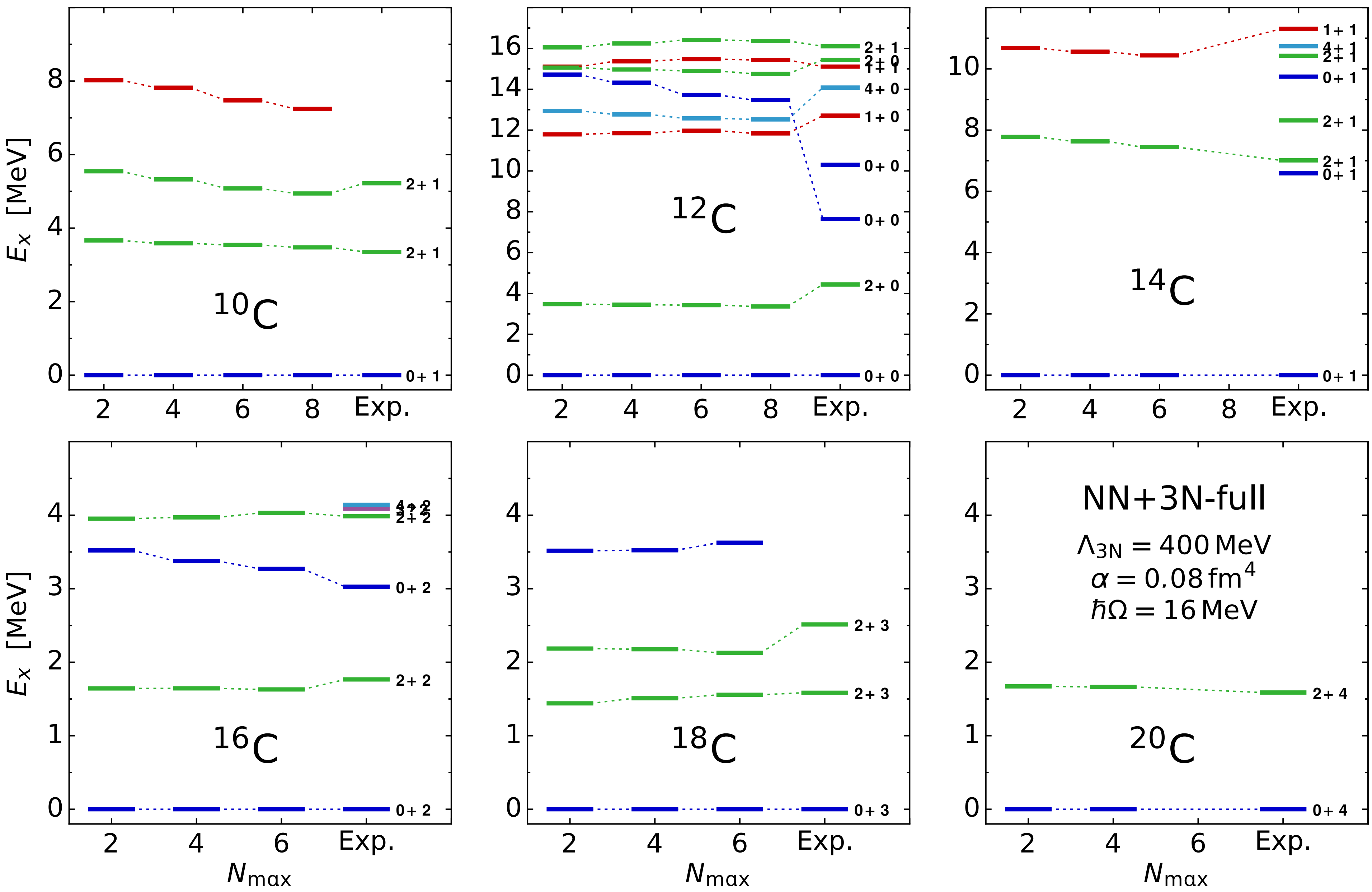
modified 3N interaction* with



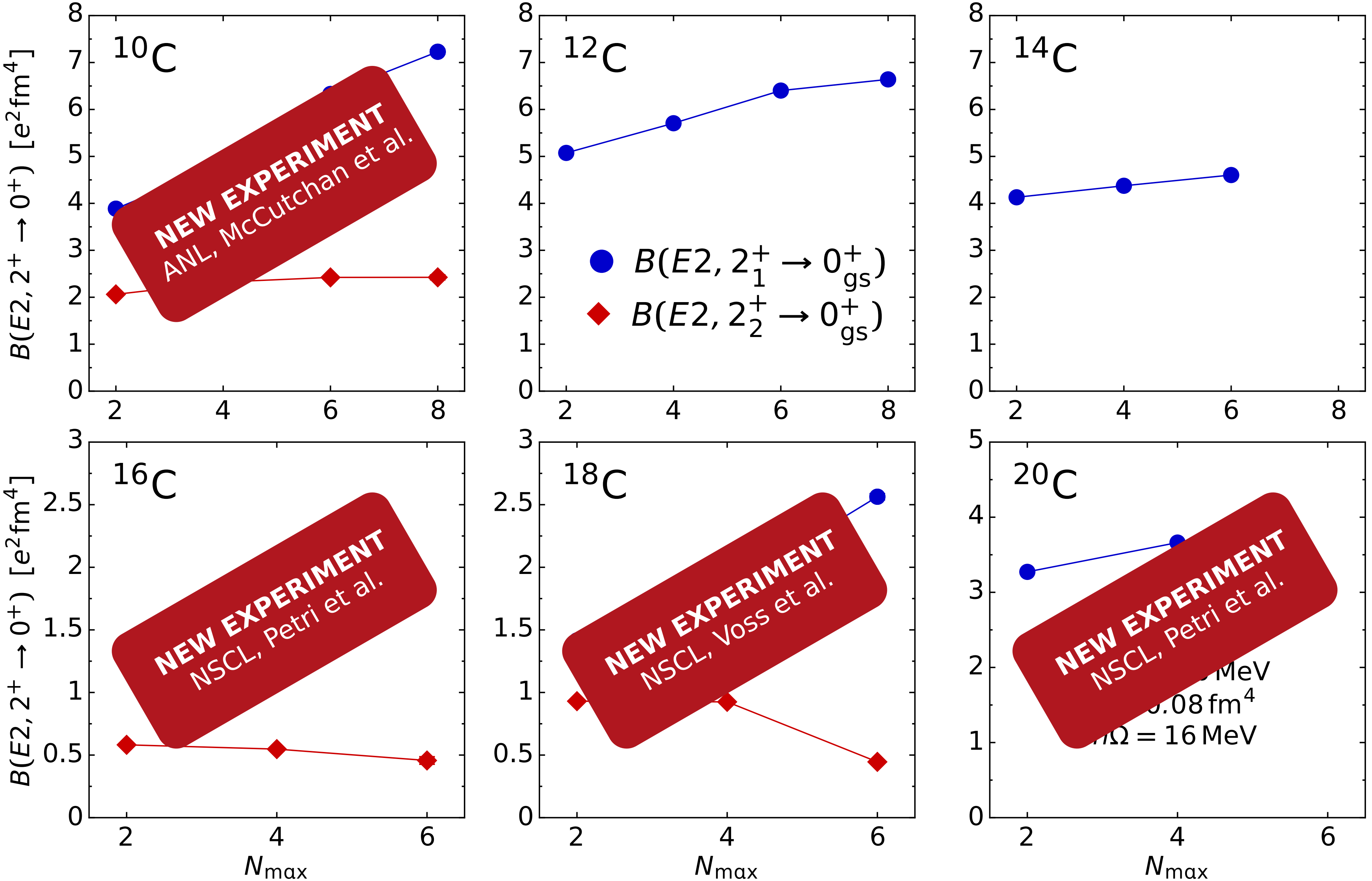
spectra of $A \geq 10$ nuclei are a very sensitive benchmark for chiral 3N interactions

* c_E refit to ^{4}He ground-state energy

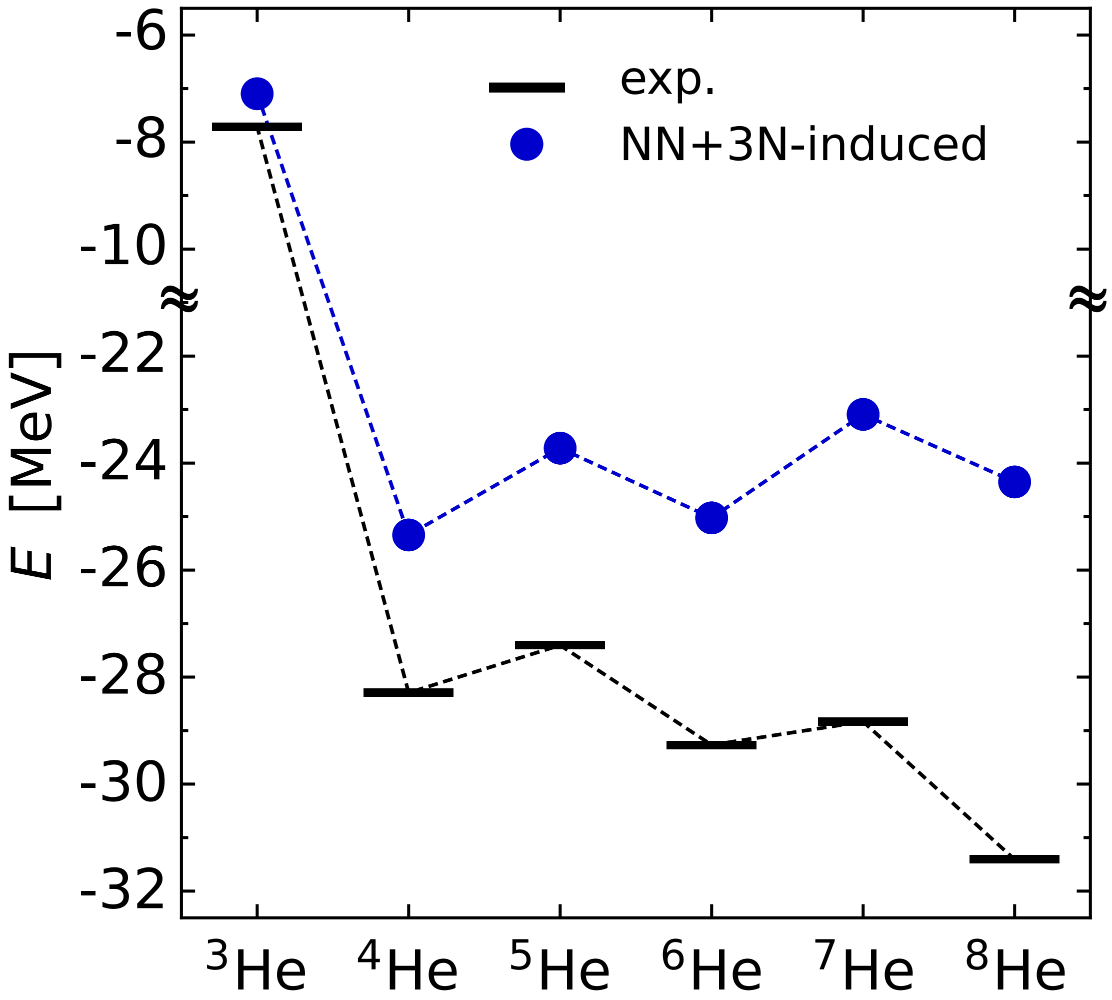
Outlook: Carbon Isotopic Chain



Outlook: Carbon Isotopic Chain



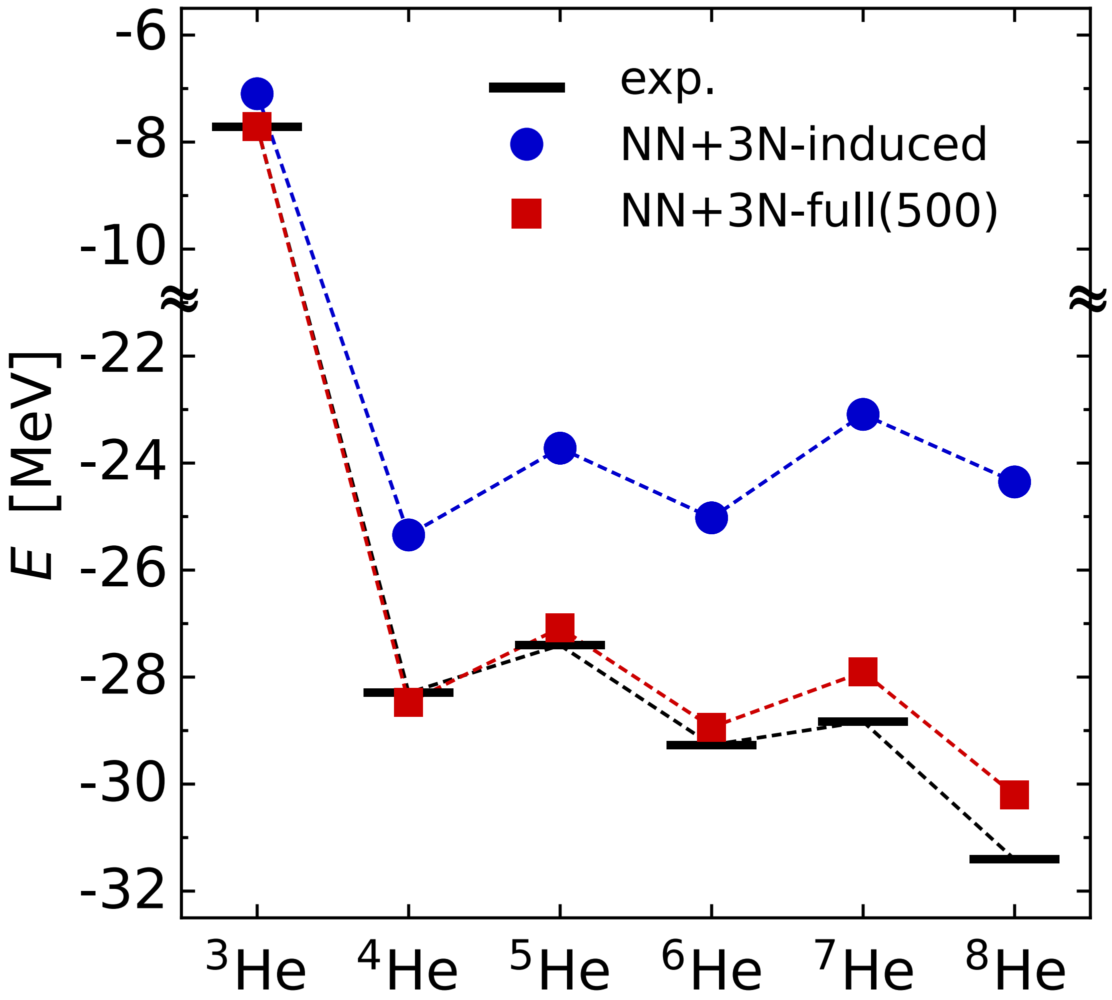
Outlook: Ground-States of Helium Isotopes



$\alpha = 0.08\,\mathrm{fm}^4, \; E_{3\,\mathrm{max}} = 12$

- chiral NN interaction cannot reproduce mass systematics

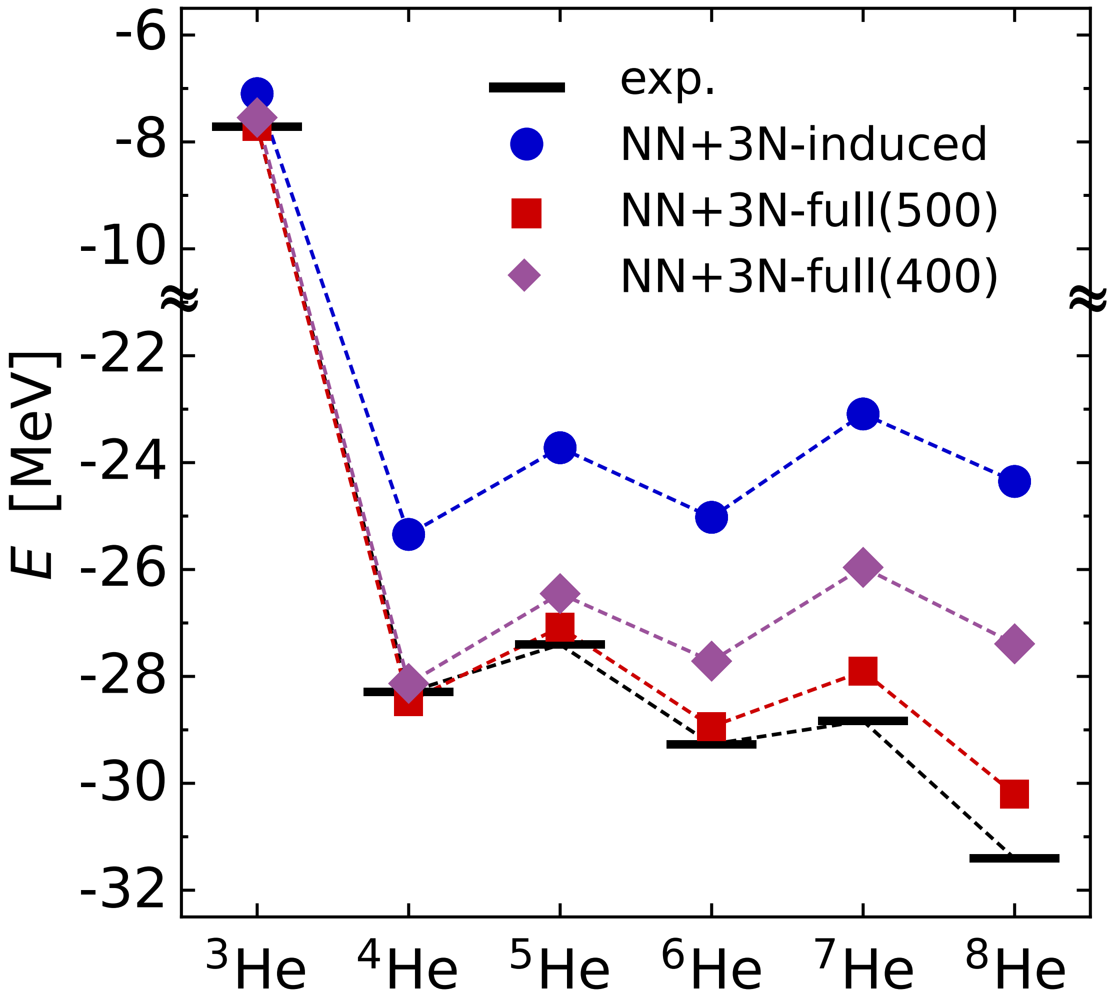
Outlook: Ground-States of Helium Isotopes



$\alpha = 0.08\,\mathrm{fm}^4,\ E_{3\,\mathrm{max}} = 12$

- chiral NN interaction cannot reproduce mass systematics
- inclusion of chiral 3N gives a **very good systematic agreement**

Outlook: Ground-States of Helium Isotopes



$\alpha = 0.08\,\text{fm}^4, \;\; E_{3\,\text{max}} = 12$

- chiral NN interaction cannot reproduce mass systematics
- inclusion of chiral 3N gives a **very good systematic agreement**
- sensitive to details of the initial 3N interaction, e.g. the cutoff
- next: **consistent coupling to continuum** within NCSMC

Normal-Ordered 3N Interaction & Coupled-Cluster Method

Roth, Binder, Vobig et al. — Phys. Rev. Lett. (2012) in print

Heavy Nuclei with 3N Interactions

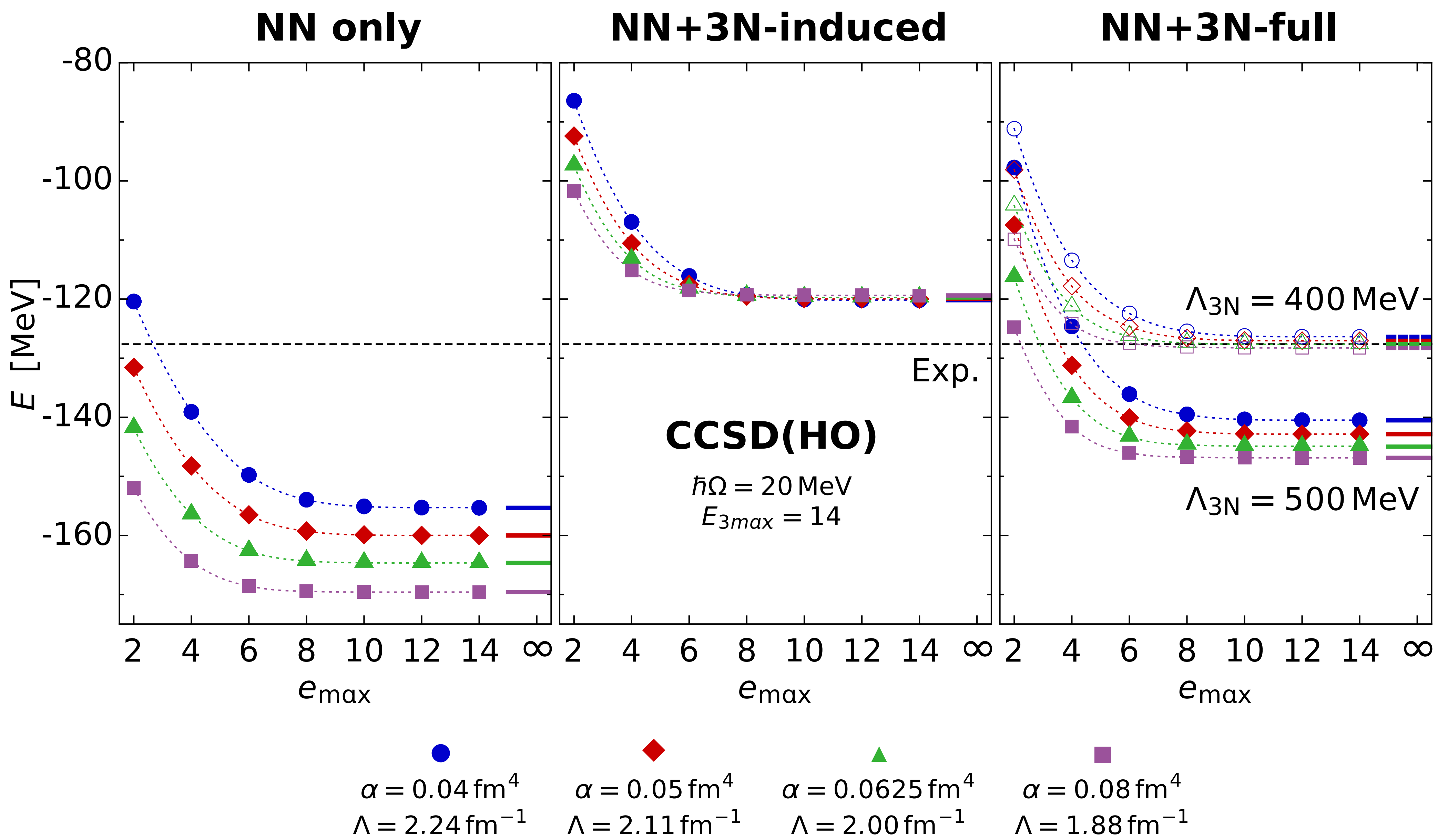
'ab initio' calculations for heavier nuclei require alternative many-body tools and approximate treatment of 3N interactions

- **coupled-cluster method** for ground states of closed-shell nuclei
  - exponential ansatz for many-body states using singles and doubles excitations (CCSD)

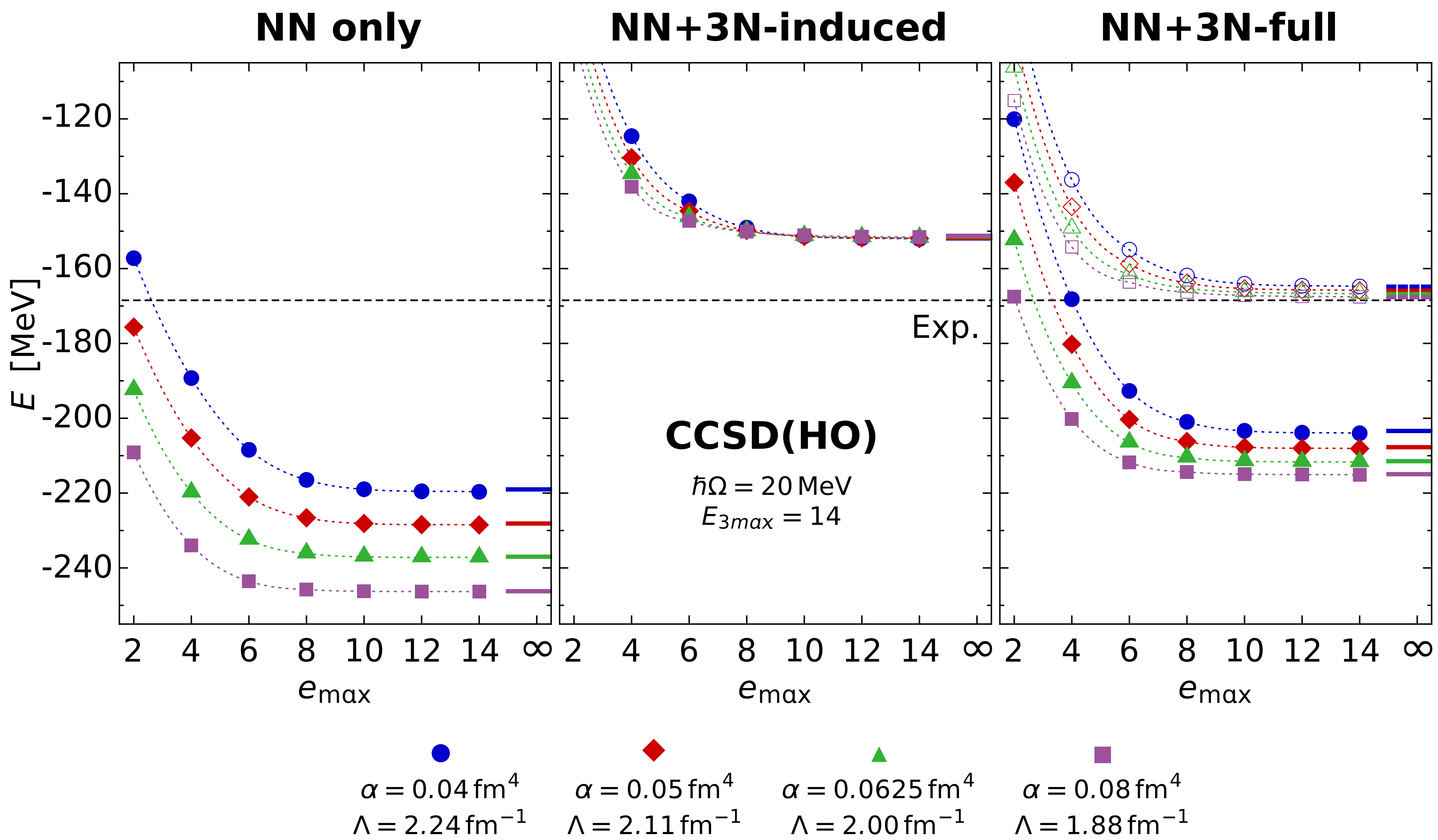
- **normal-ordering approximation** of the 3N interaction truncated at the two-body level
  - summation over reference state converts part of 3N interaction to zero-, one- and two-body terms

- both approximations are controlled and systematically improvable

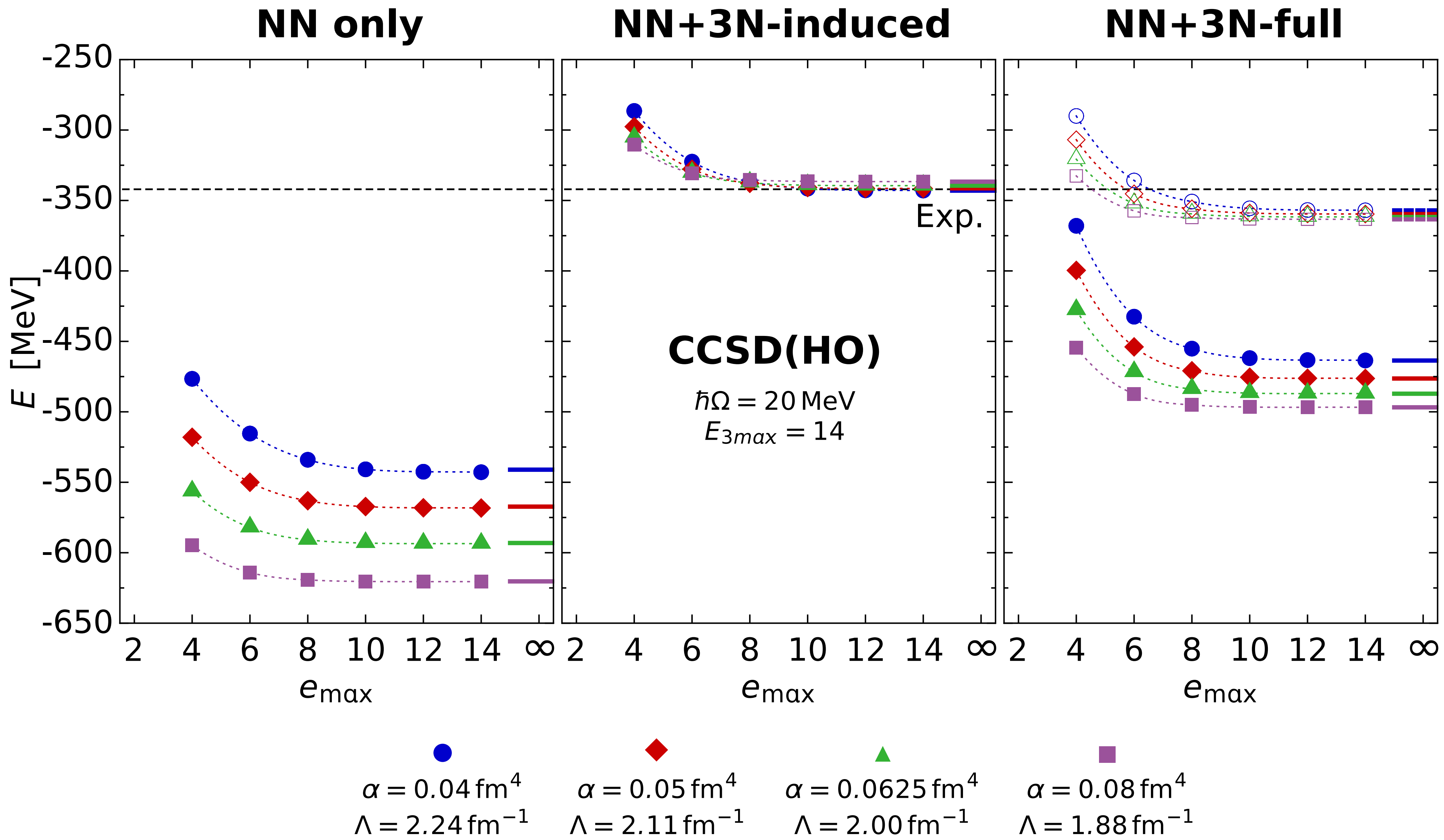
^{16}O: Coupled-Cluster with $3N_{NO2B}$



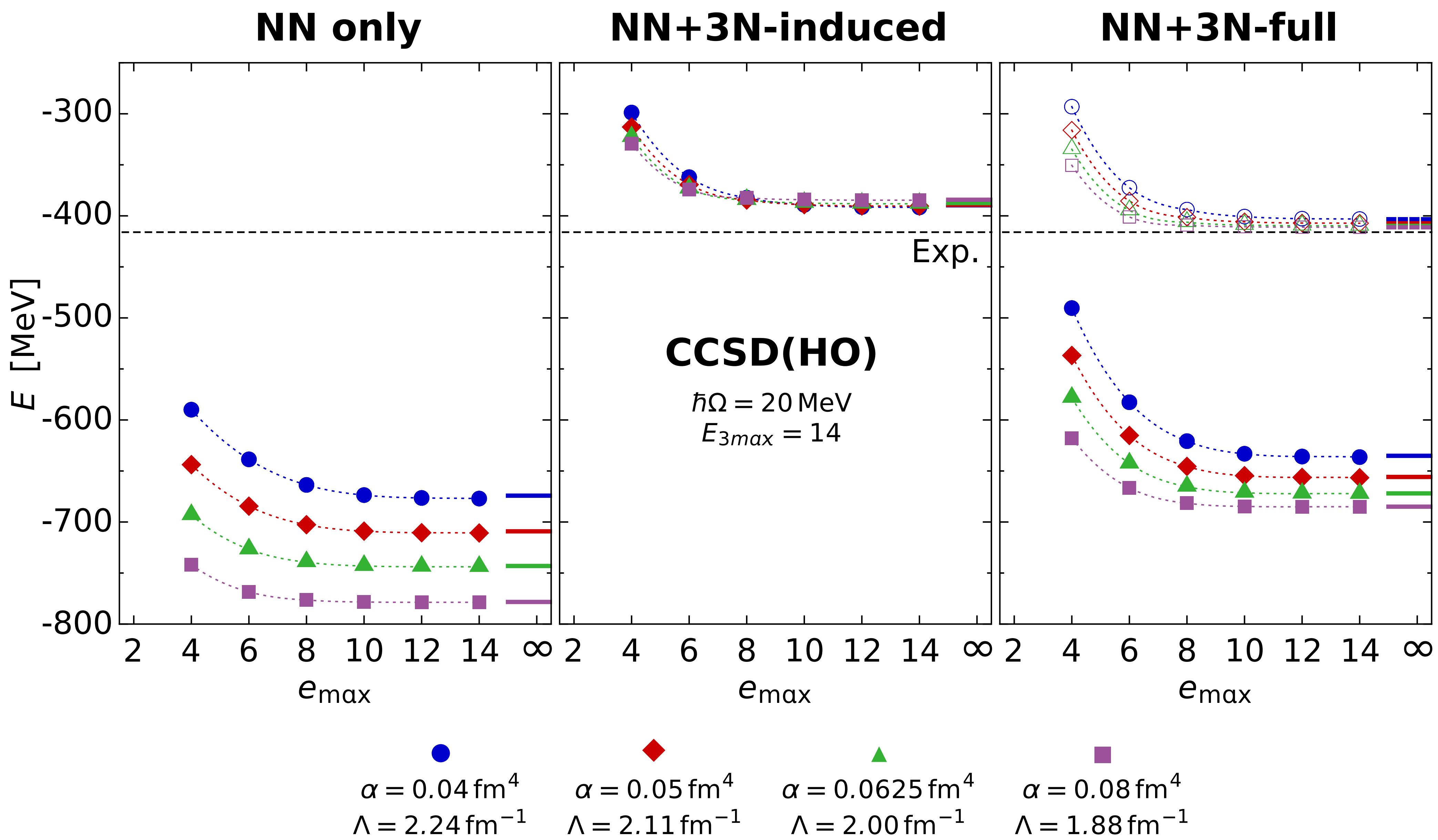
^{24}O: Coupled-Cluster with $3N_{NO2B}$



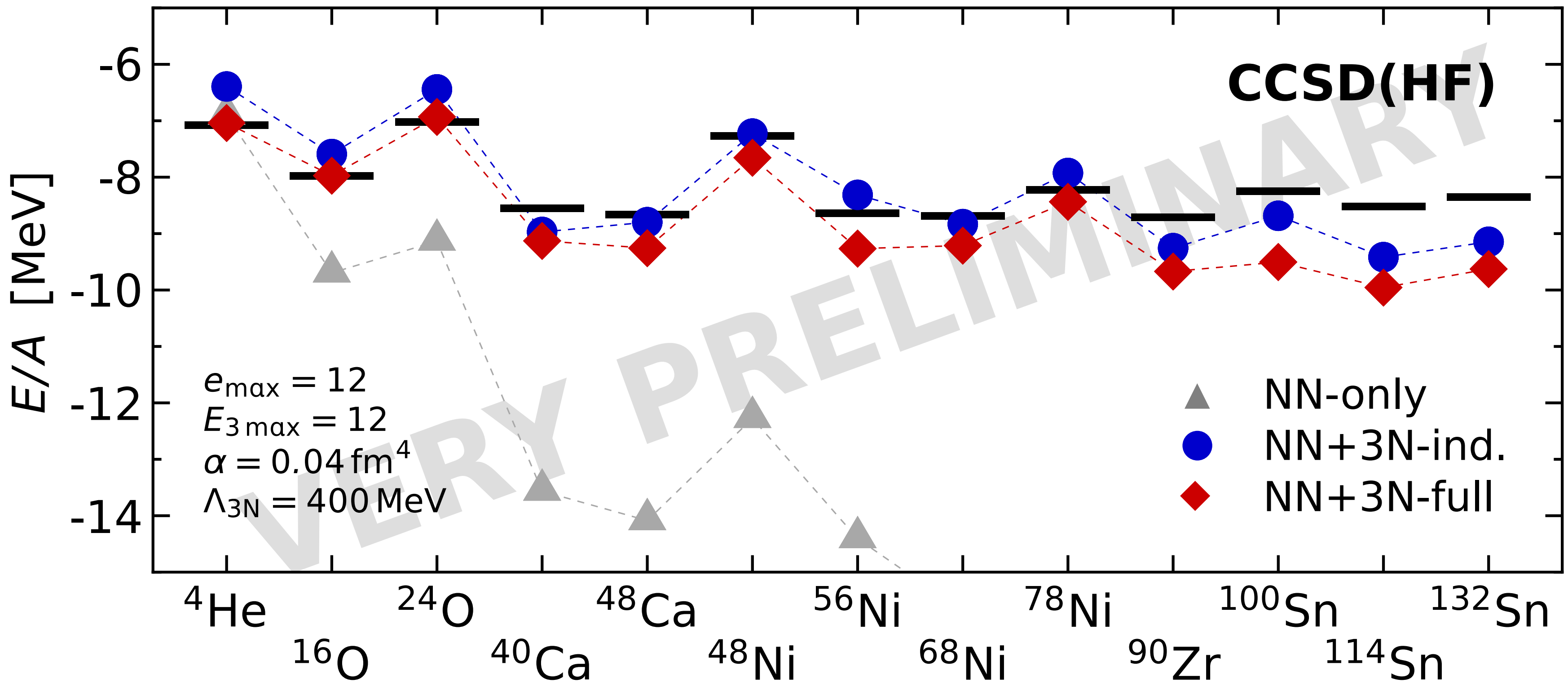
^{40}Ca: Coupled-Cluster with $3N_{NO2B}$



^{48}Ca: Coupled-Cluster with $3N_{NO2B}$



Outlook: Chiral 3N for Heavy Nuclei



- first ab initio calculations with **chiral NN+3N Hamiltonians for heavy nuclei**
- **realistic mass systematics** without phenomenological adjustments — α-dependence might hold surprises...

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, E. Gebrerufael, A. Günther, H. Krutsch, **J. Langhammer**, S. Reinhardt, C. Stumpf, R. Trippel, K. Vobig, R. Wirth
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    Chalmers University, Sweden
  - H. Feldmeier, T. Neff
    GSI Helmholtzzentrum

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HIC for FAIR
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LOEWE – Landes-Offensive zur Entwicklung Wissenschaftlich-ökonomischer Exzellenz

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