Ab Initio Nuclear Structure for Light and Medium-Mass Nuclei

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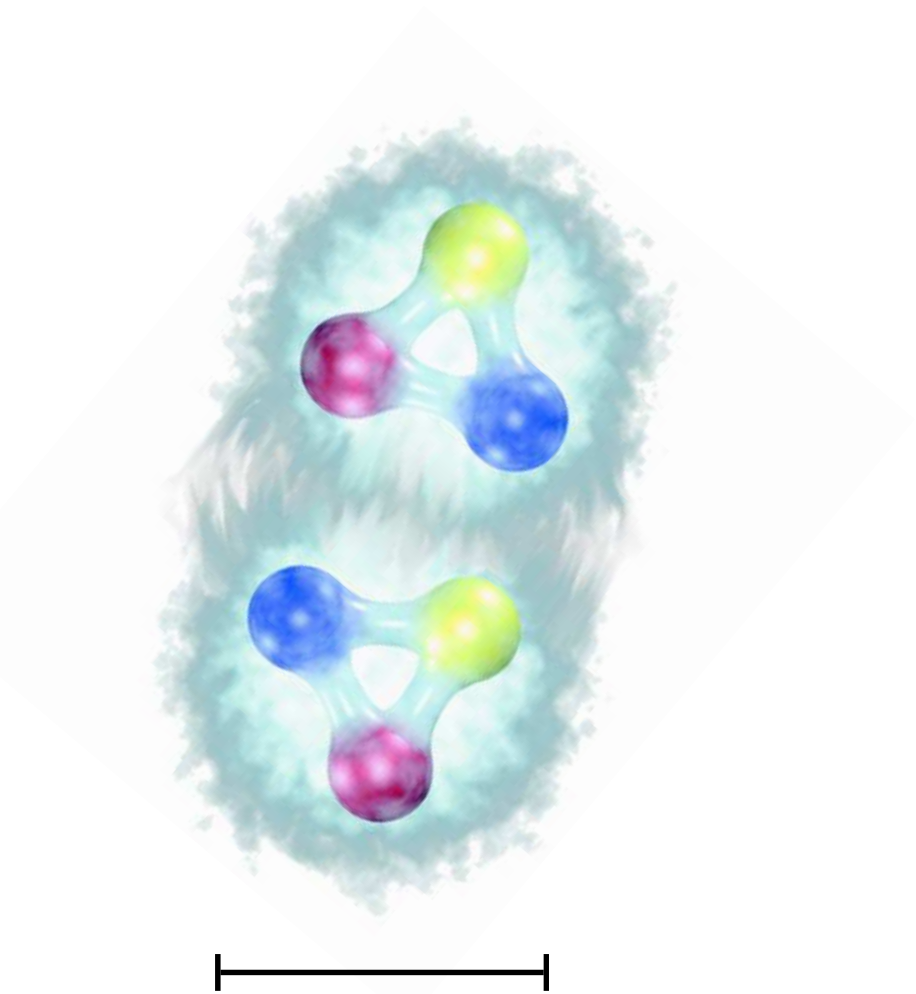
Nature of the Nuclear Interaction



$\sim 1.6\text{fm}$

$\rho_0^{-1/3} = 1.8\text{fm}$

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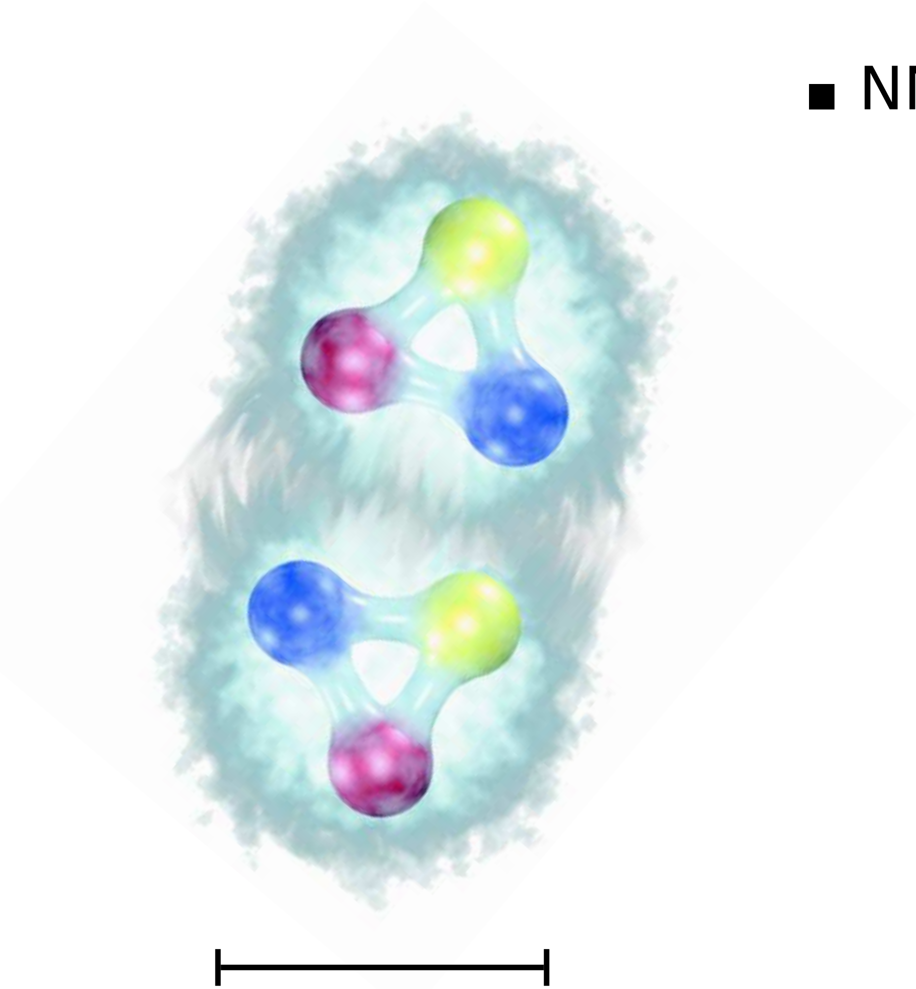

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- NN-interaction is **not fundamental**

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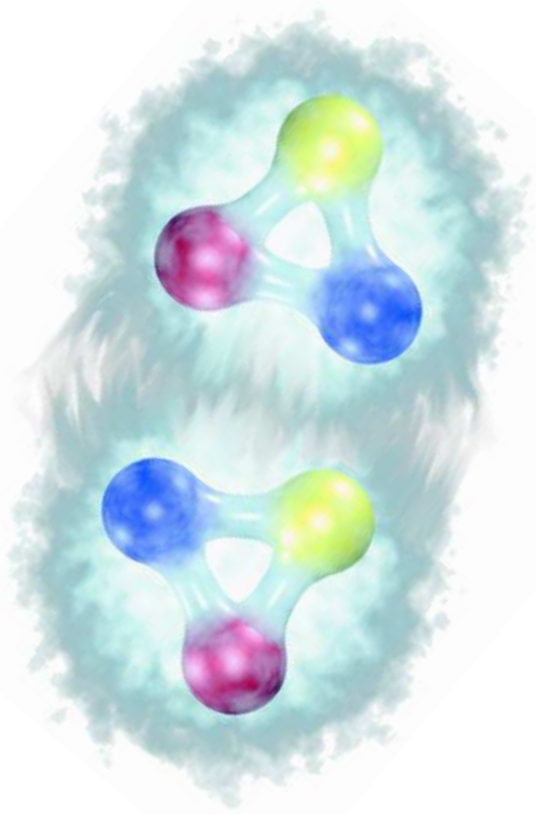

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- analogous to **van der Waals** interaction between neutral atoms

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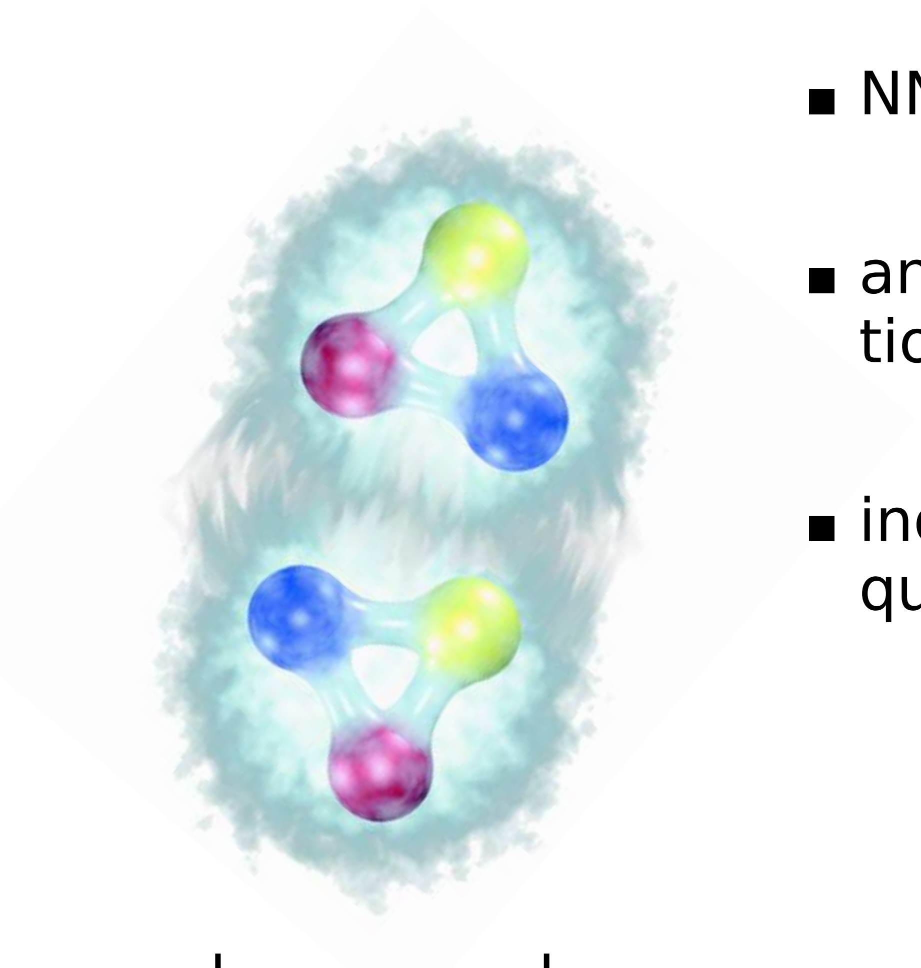

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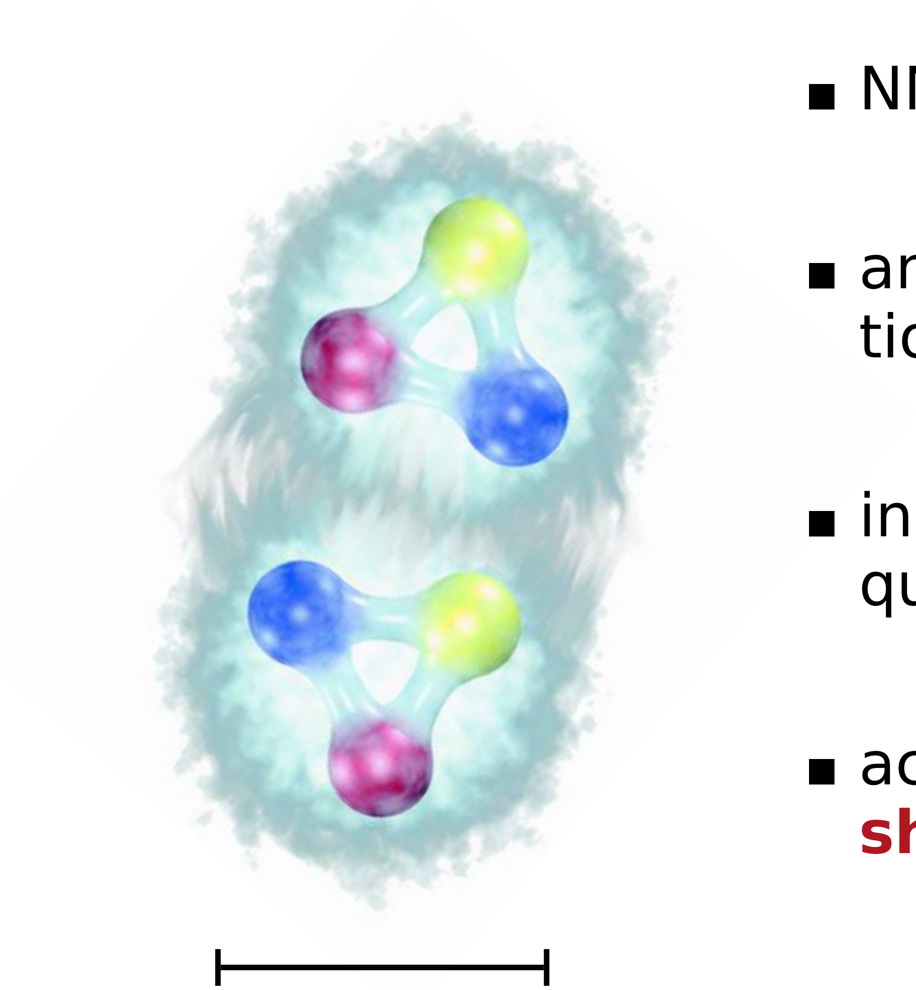

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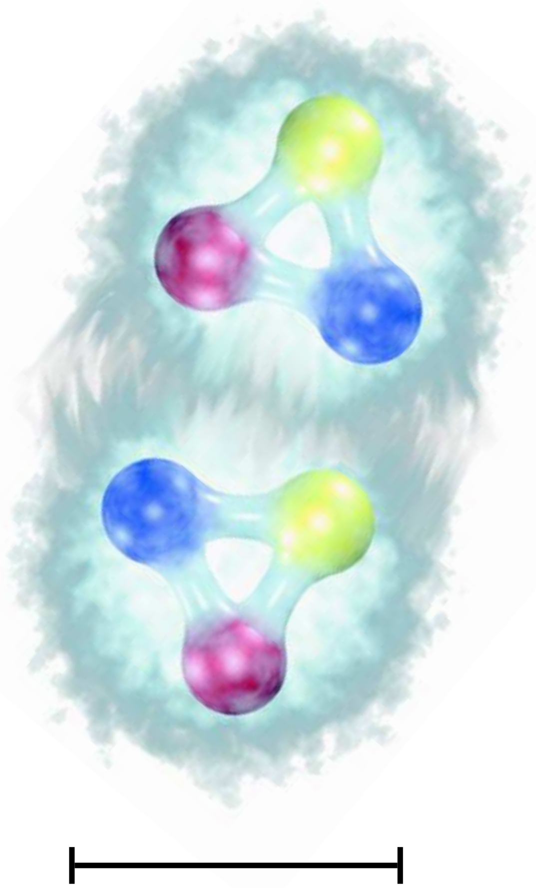

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- acts only if the nucleons overlap, i.e. at **short ranges**
- genuine **3N-interaction** is important

Nuclear Interactions from Chiral EFT

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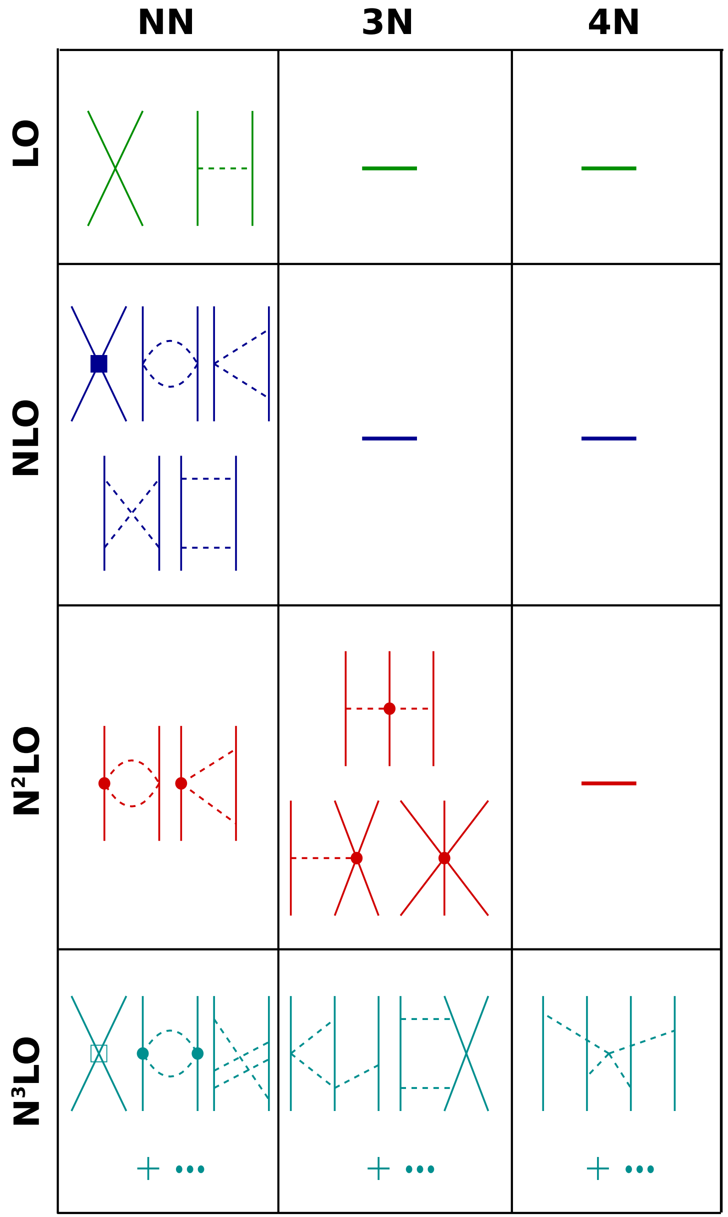

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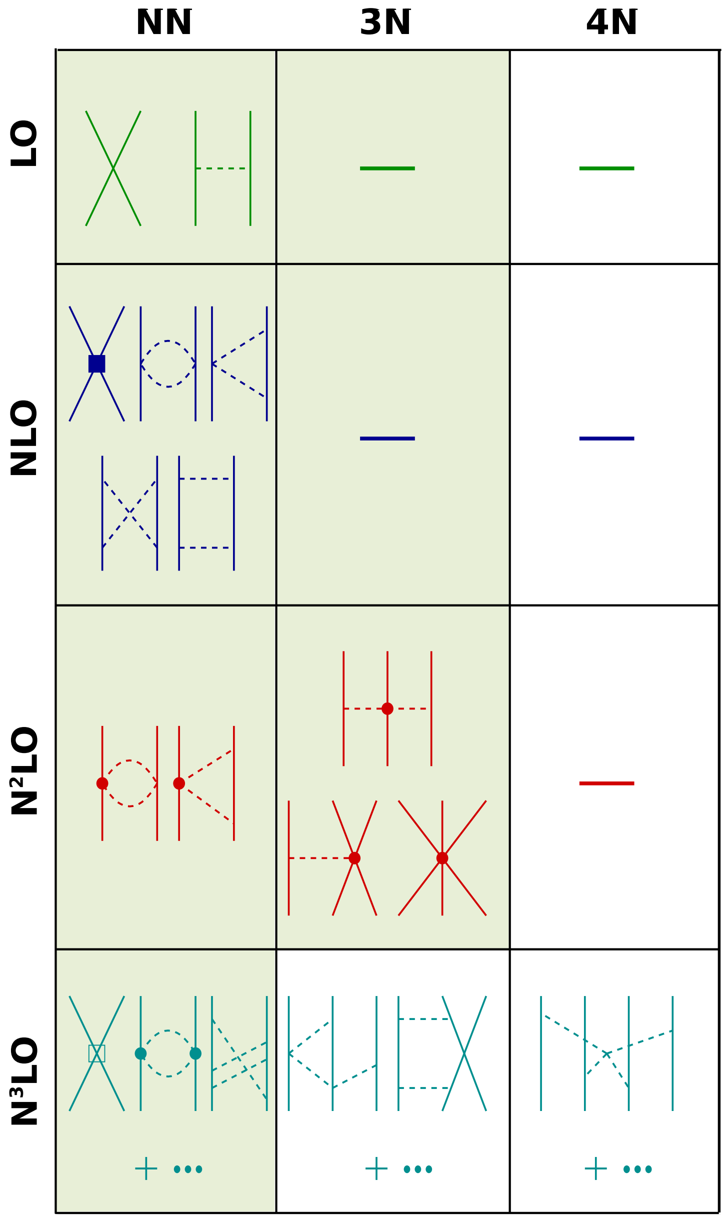
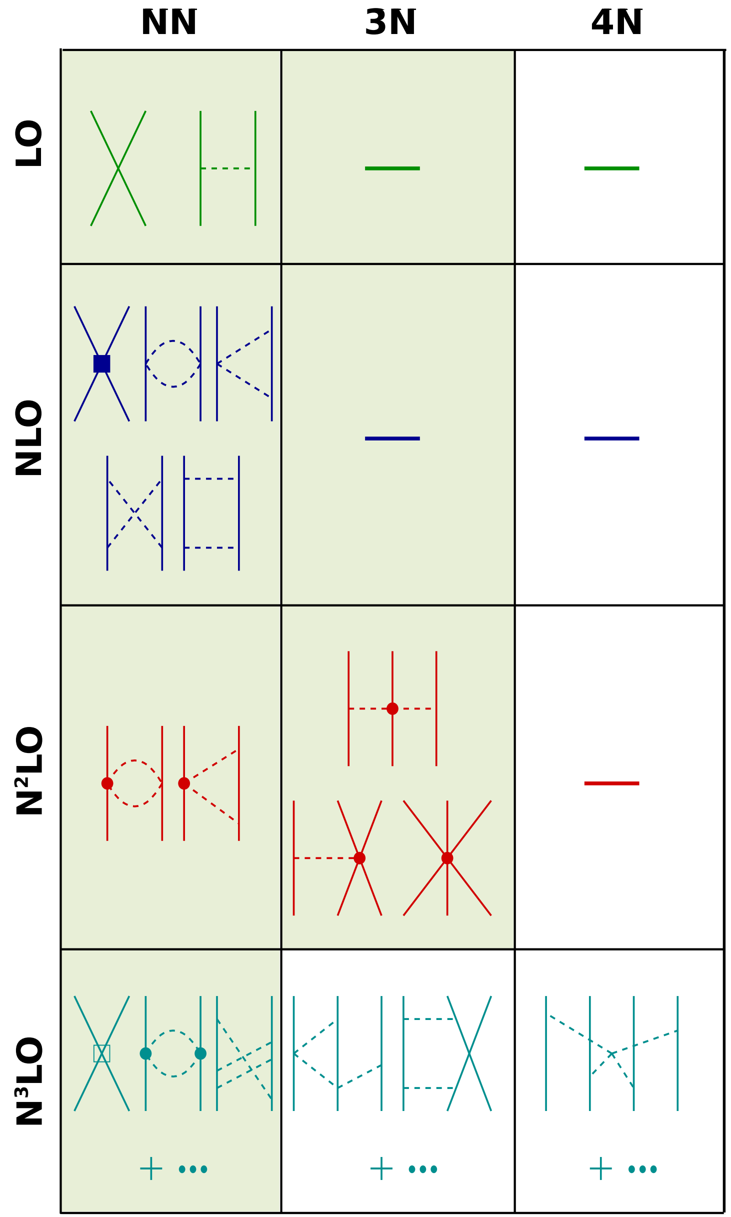


Nuclear Interactions from Chiral EFT

- low-energy **effective field theory** for relevant degrees of freedom (π,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, πN,...)
- hierarchy of **consistent NN, 3N,... interactions** (plus currents)
- many **ongoing developments**
  - 3N interaction at N^3LO
  - explicit inclusion of Δ-resonance



From QCD to Nuclear Structure

Nuclear Structure

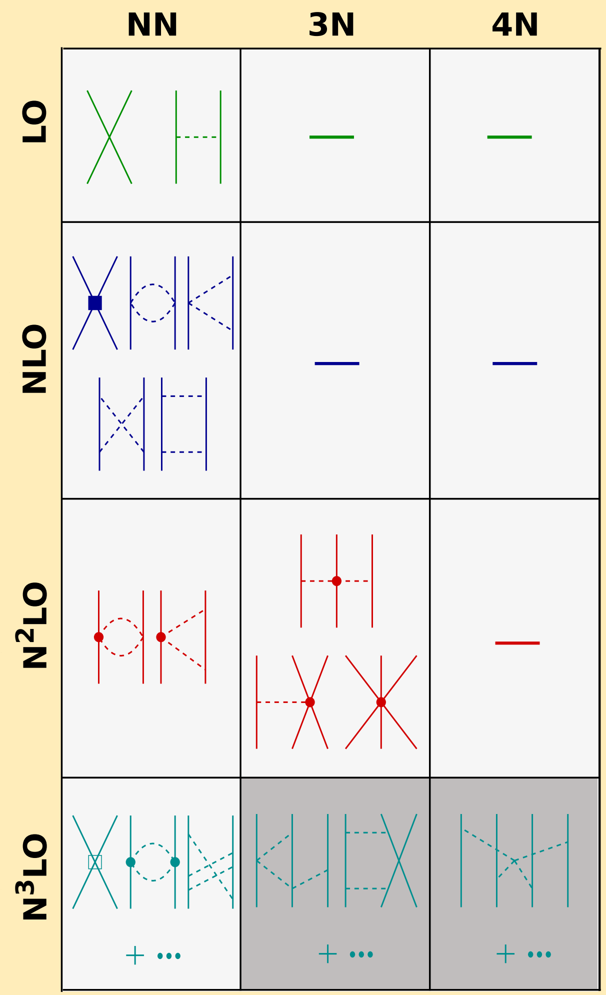
Low-Energy QCD

From QCD to Nuclear Structure

Nuclear Structure

NN+3N Interaction from Chiral EFT

Low-Energy QCD



- derive consistent 2N & 3N forces from chiral EFT with nucleons and pions as DOF

From QCD to Nuclear Structure

Nuclear Structure

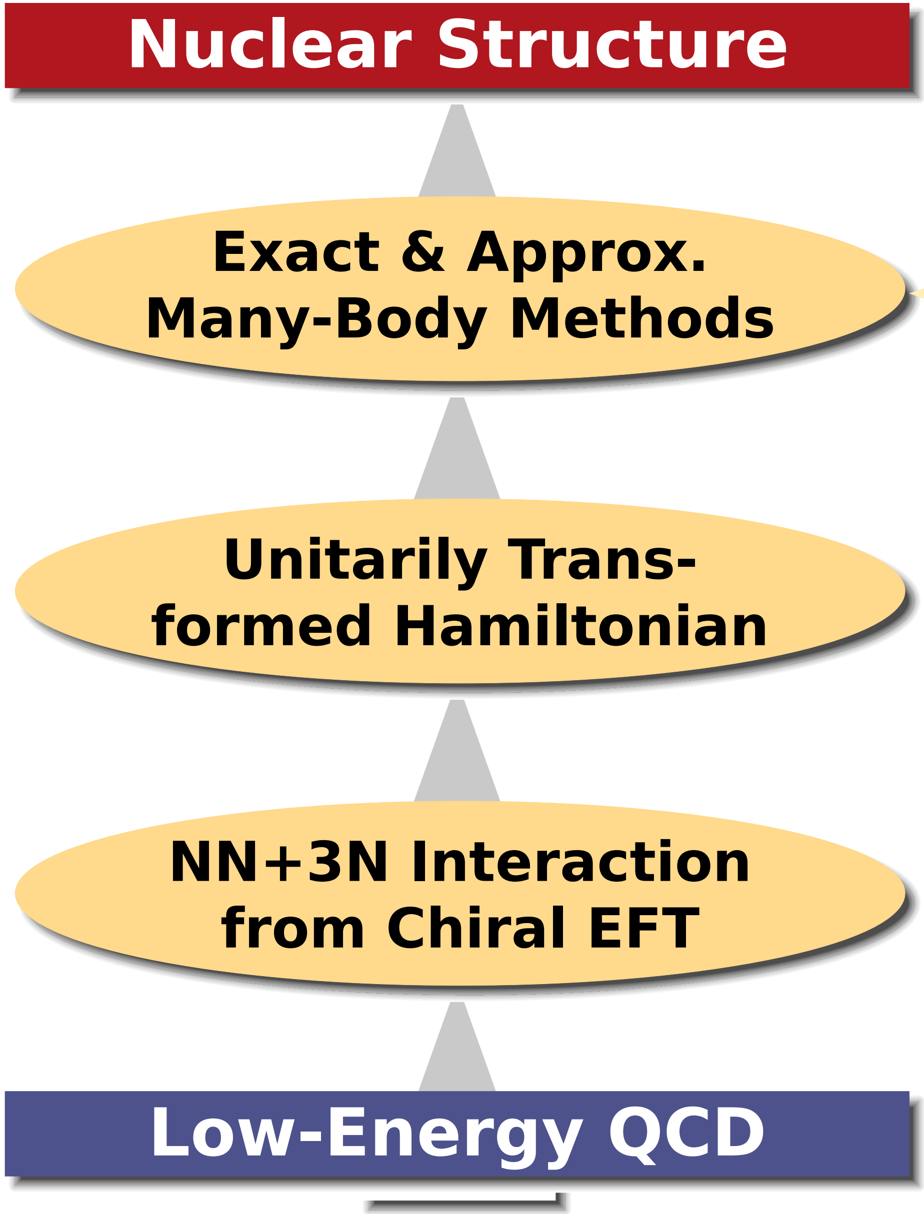
Unitarily Transformed Hamiltonian

- adapt Hamiltonian to truncated low-energy model space

NN+3N Interaction from Chiral EFT

Low-Energy QCD

From QCD to Nuclear Structure



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

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

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

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

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

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

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

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

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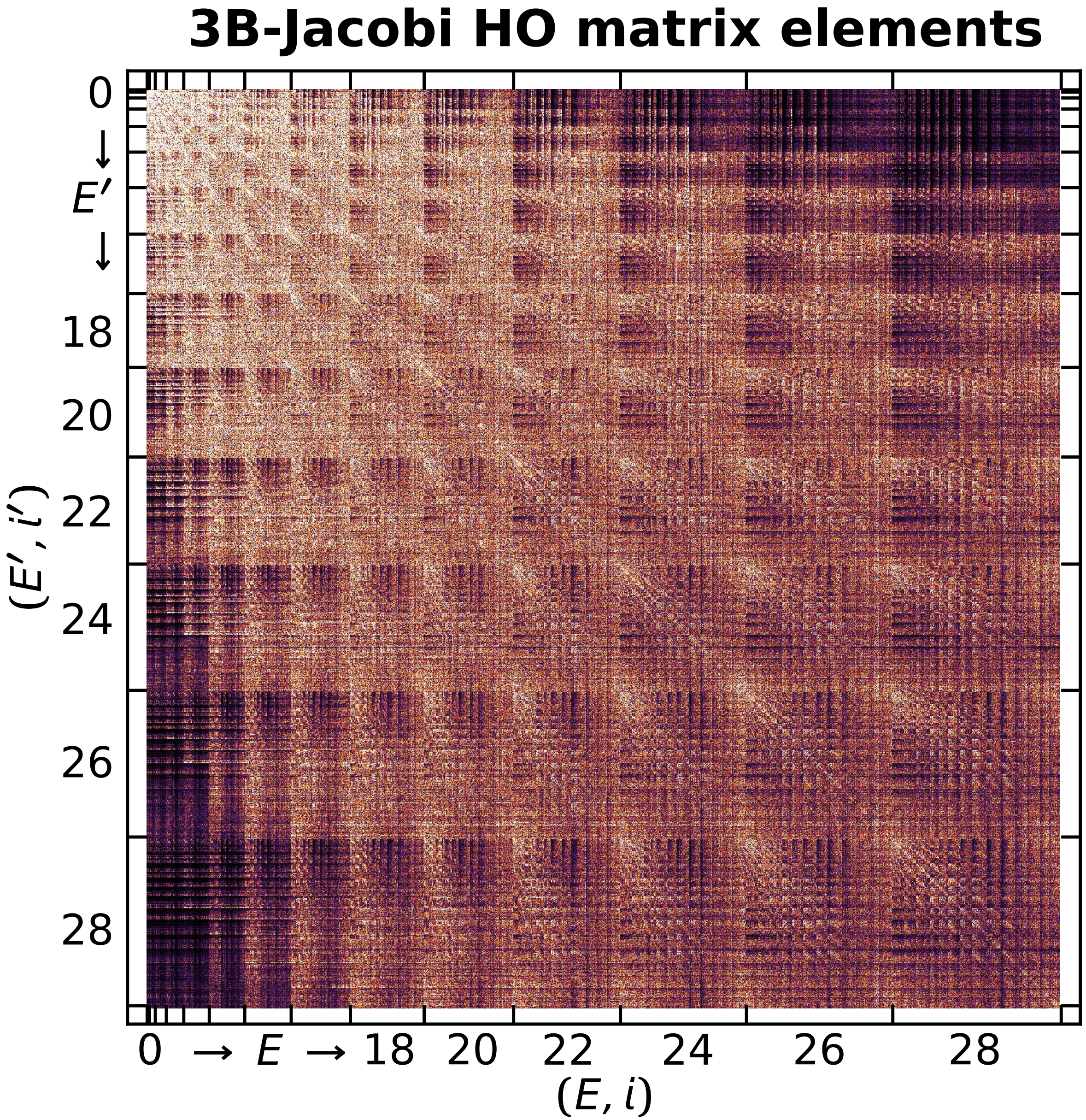
$$\eta_\alpha = (2\mu)^2 [T_{int}, \widetilde{H}_\alpha]$$

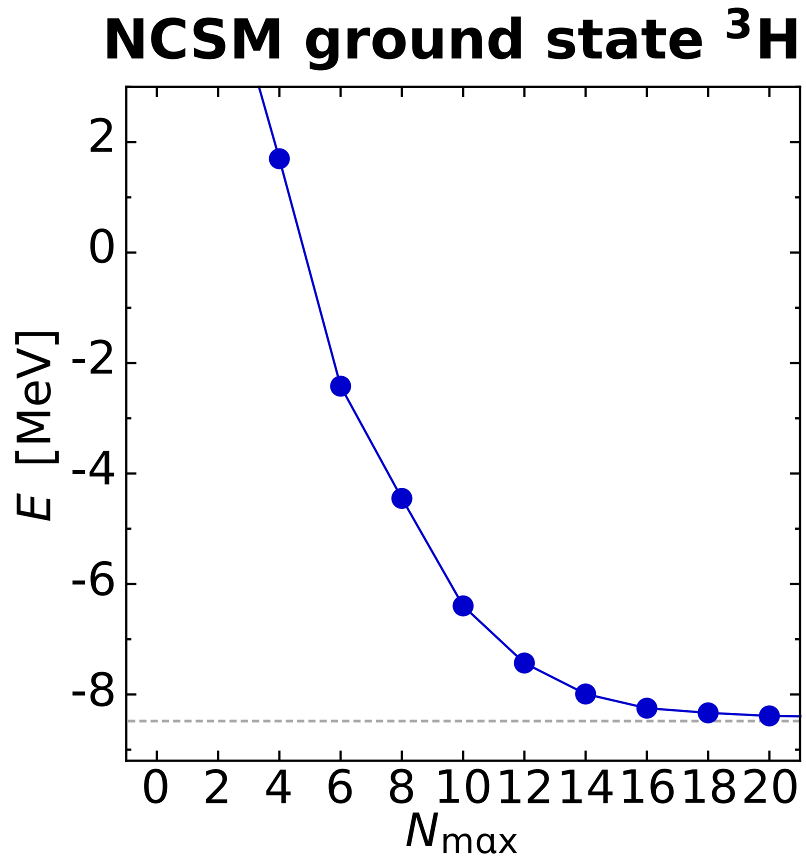
SRG Evolution in Three-Body Space



chiral NN+3N

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

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



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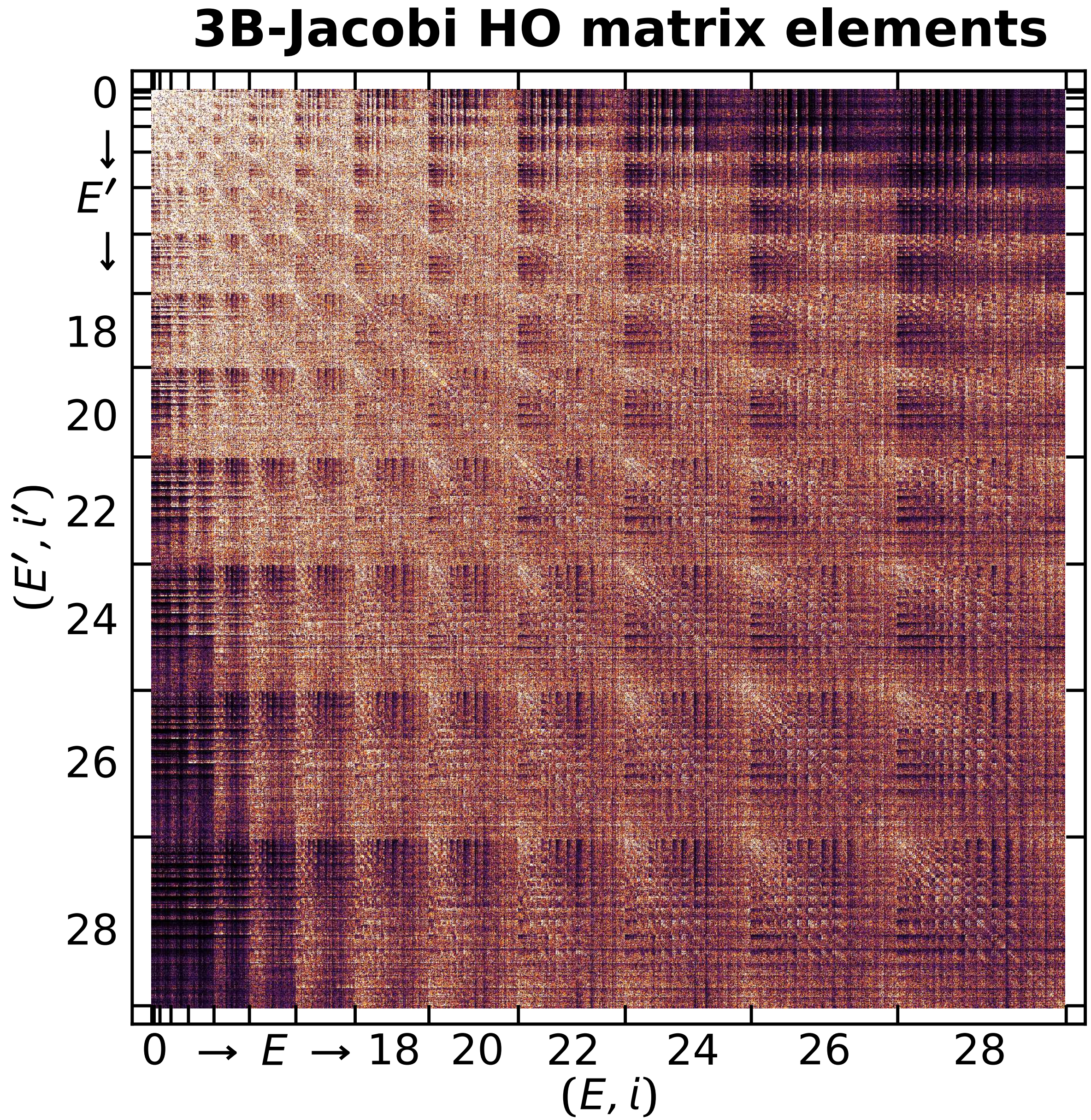
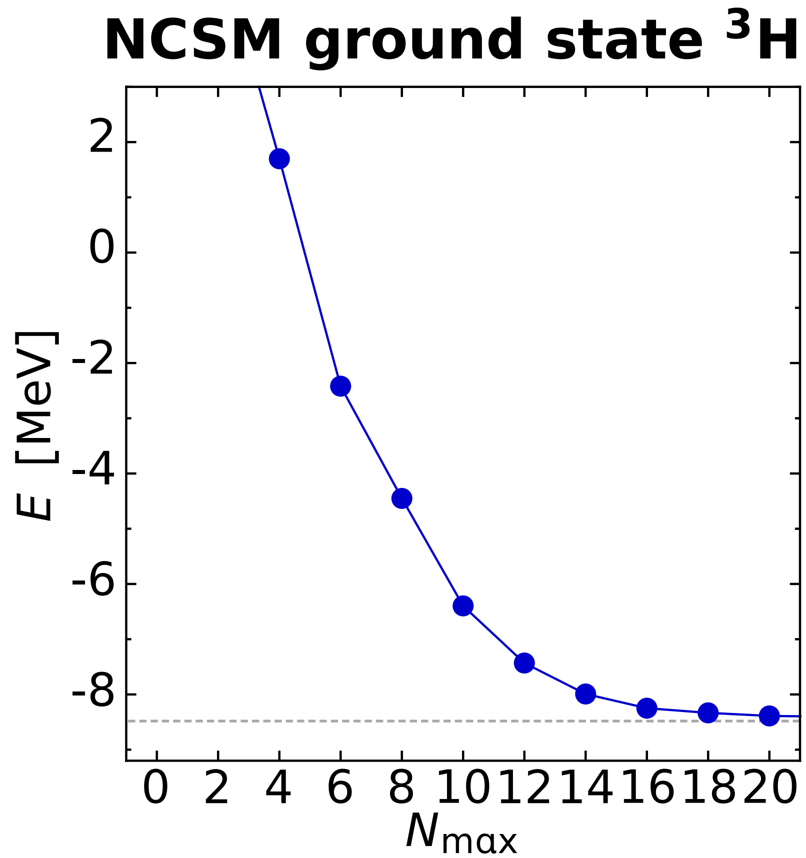


$\alpha = 0.000\,\mathrm{fm}^4$

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

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



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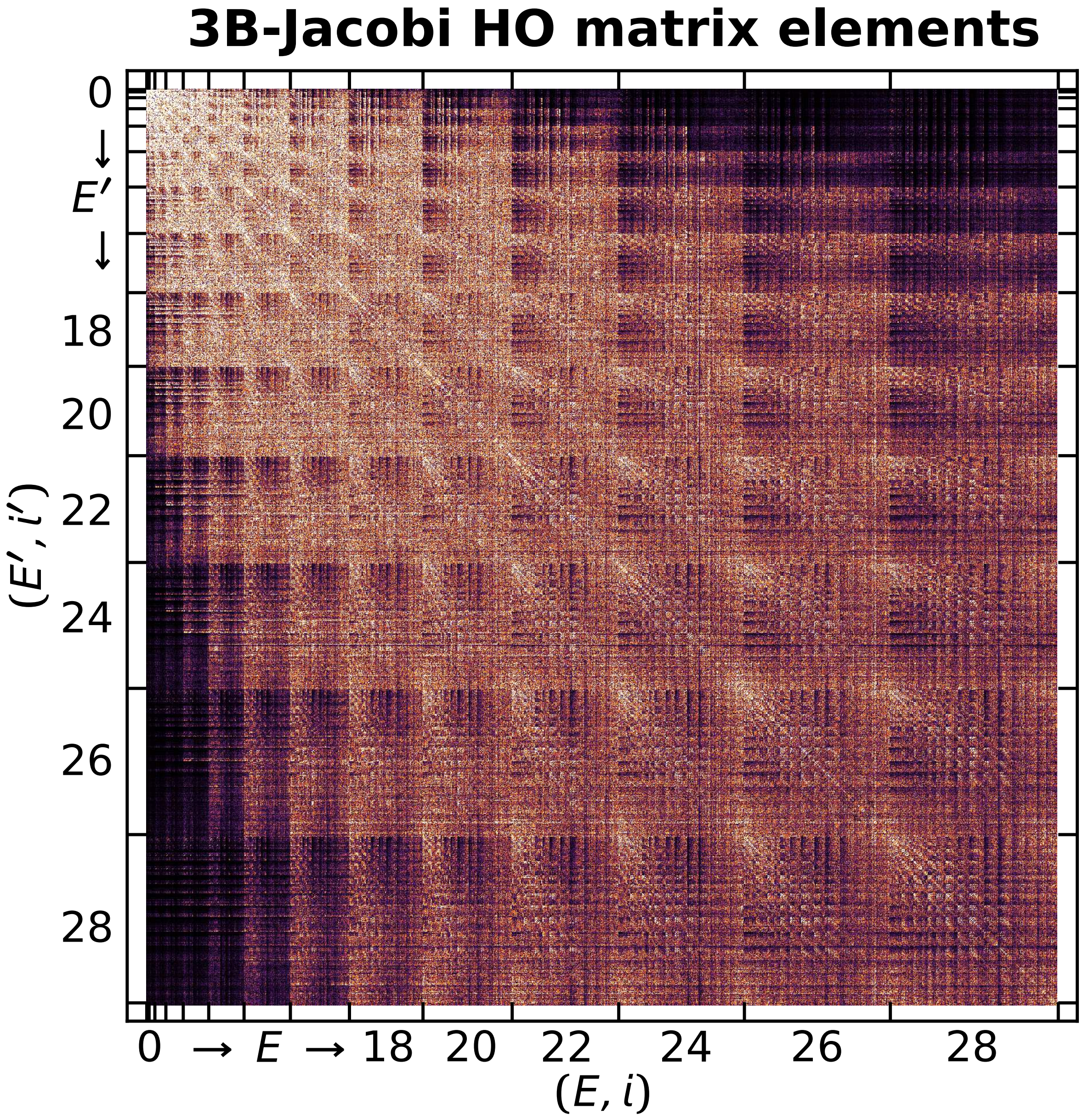
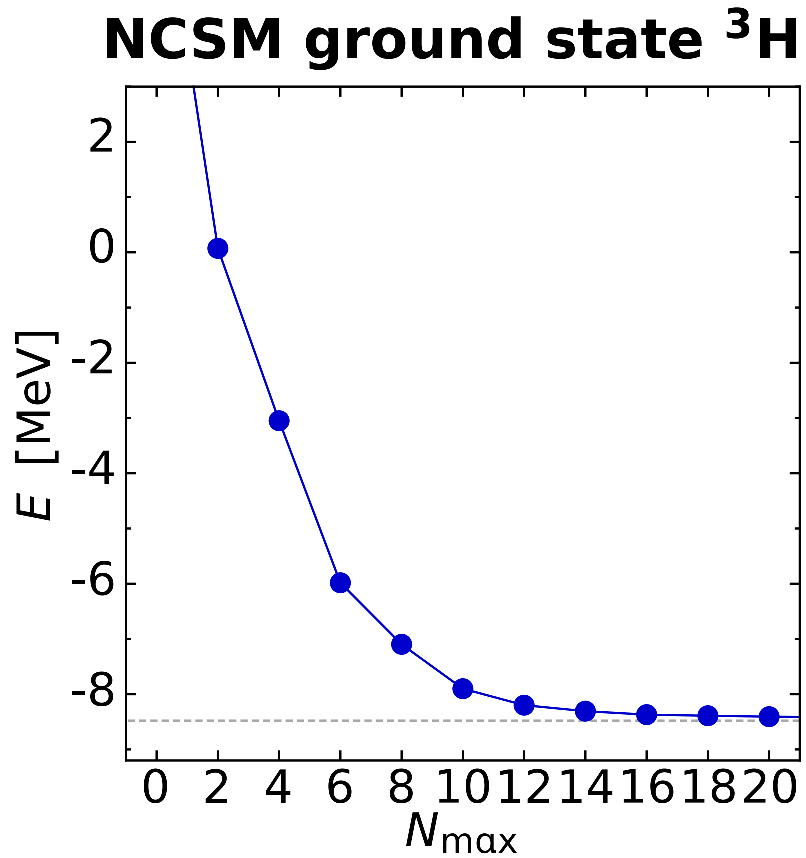


$\alpha = 0.010\,\mathrm{fm}^4$

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

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



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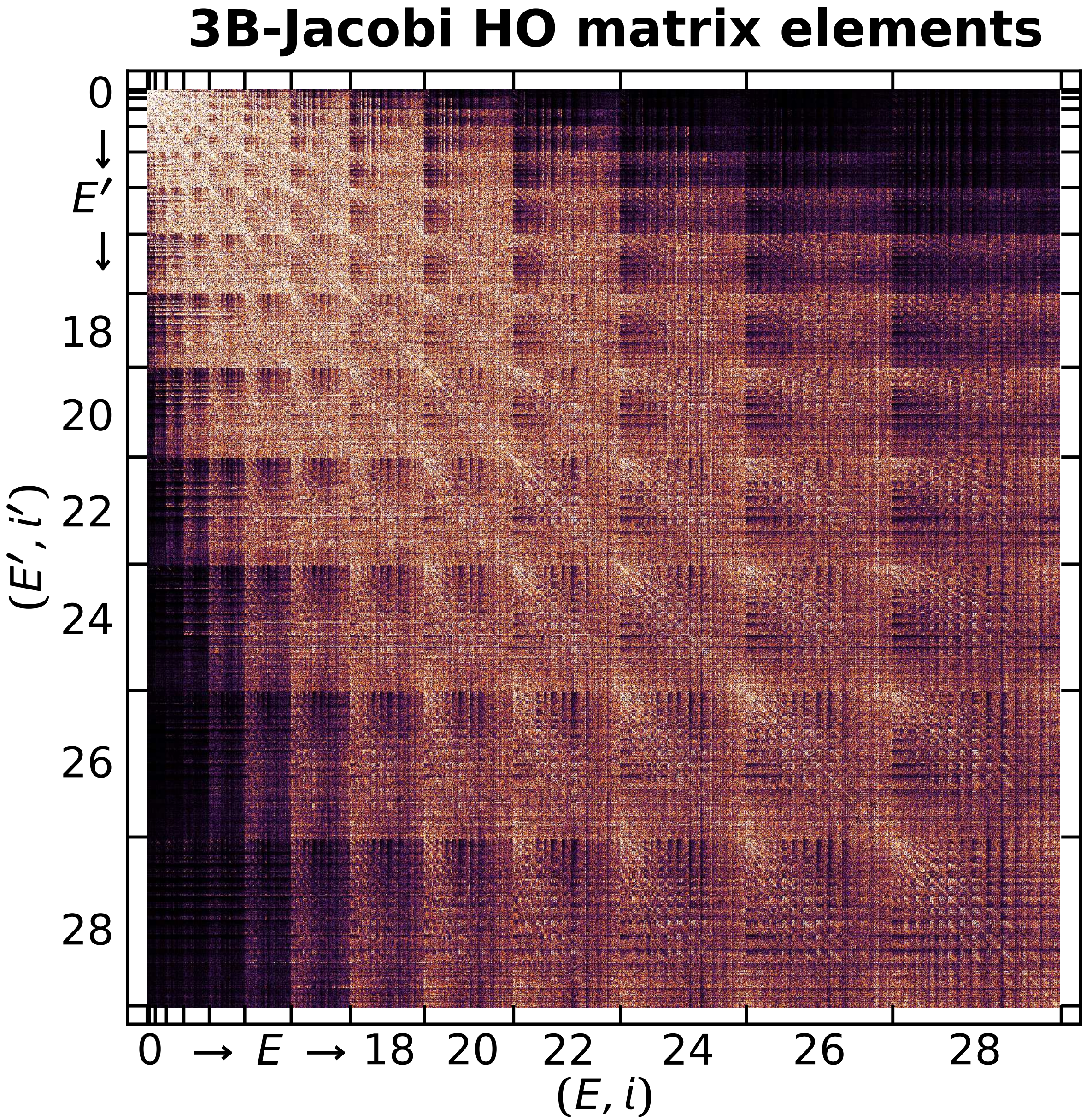
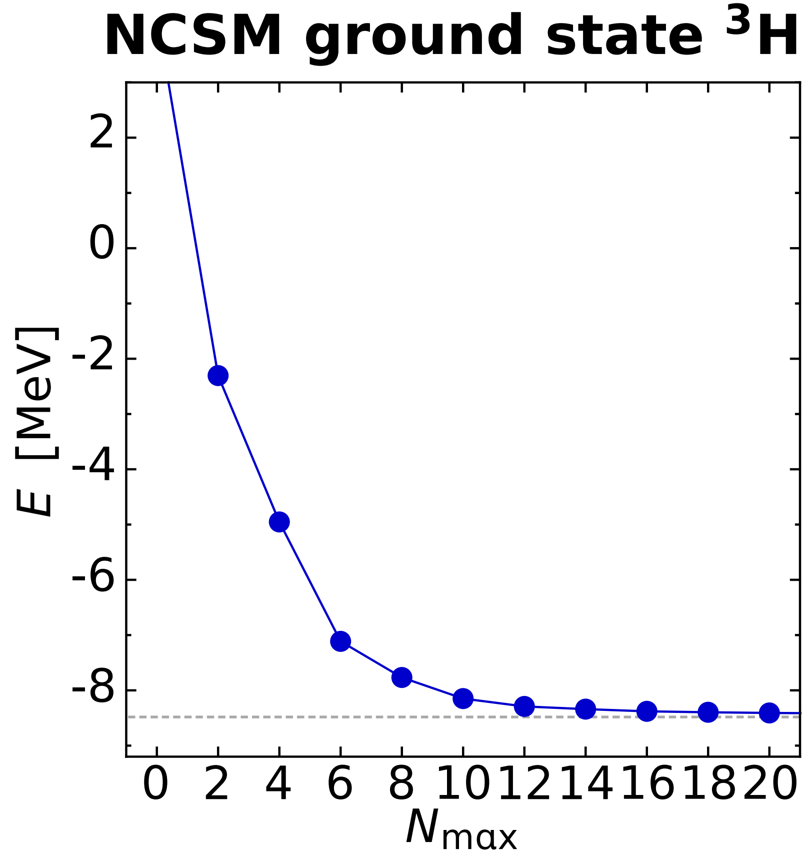


$\alpha = 0.020\,\mathrm{fm}^4$

$\Lambda = 2.66\,\mathrm{fm}^{-1}$

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



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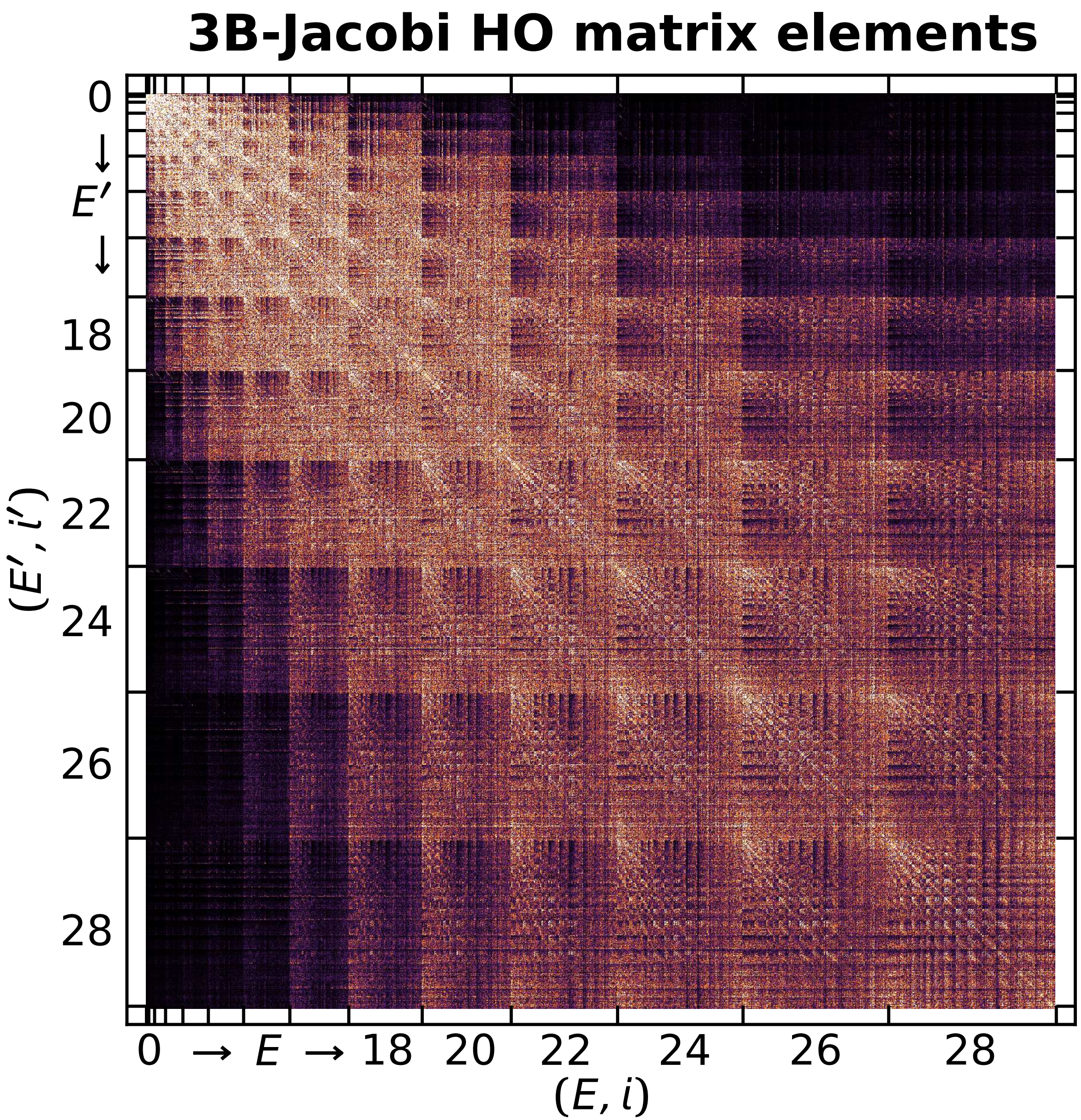
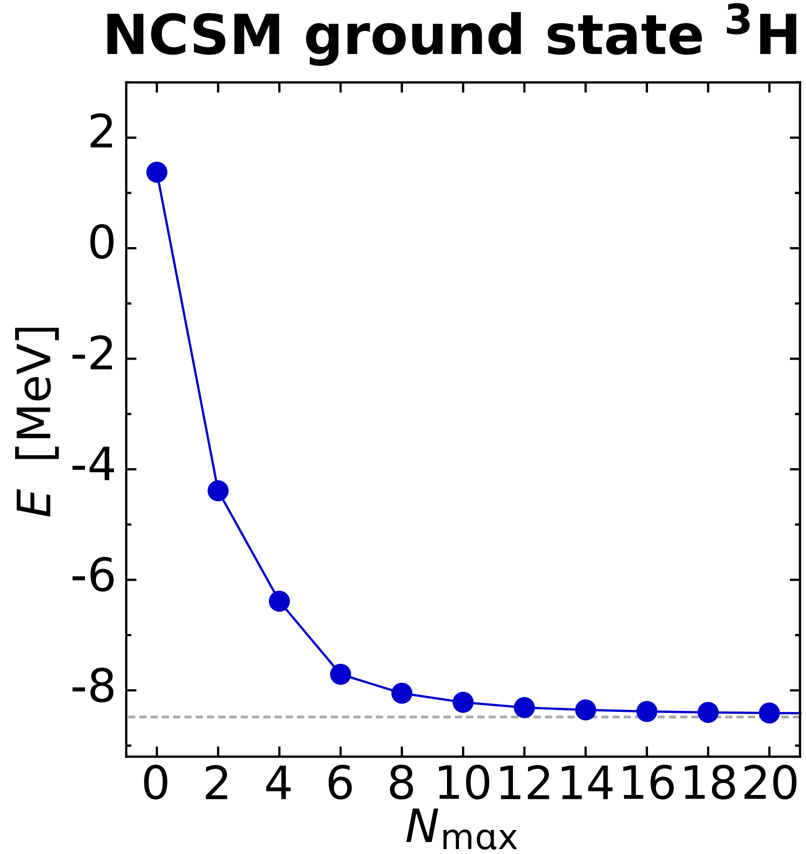


$\alpha = 0.040\,\mathrm{fm}^4$

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

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



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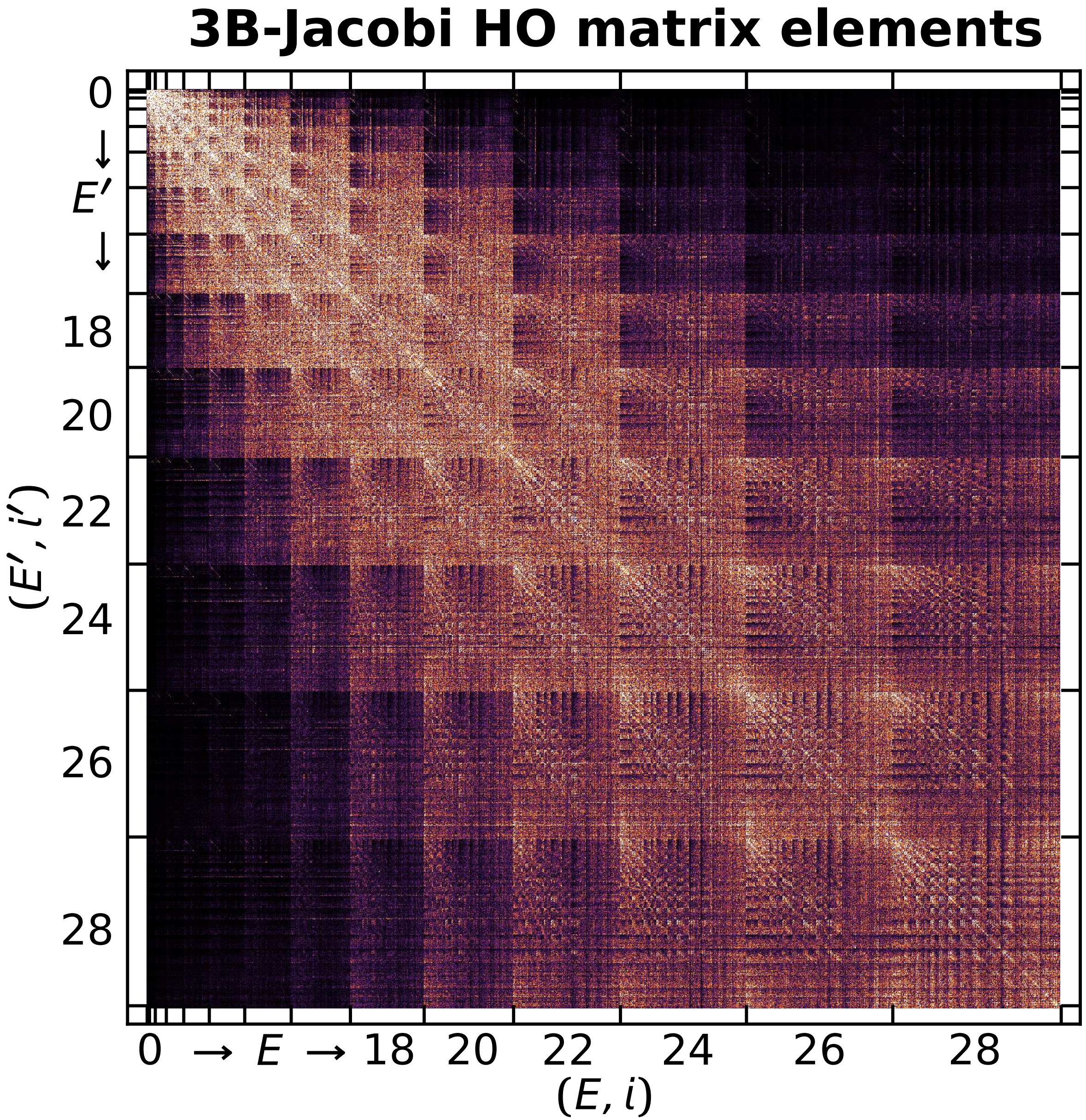
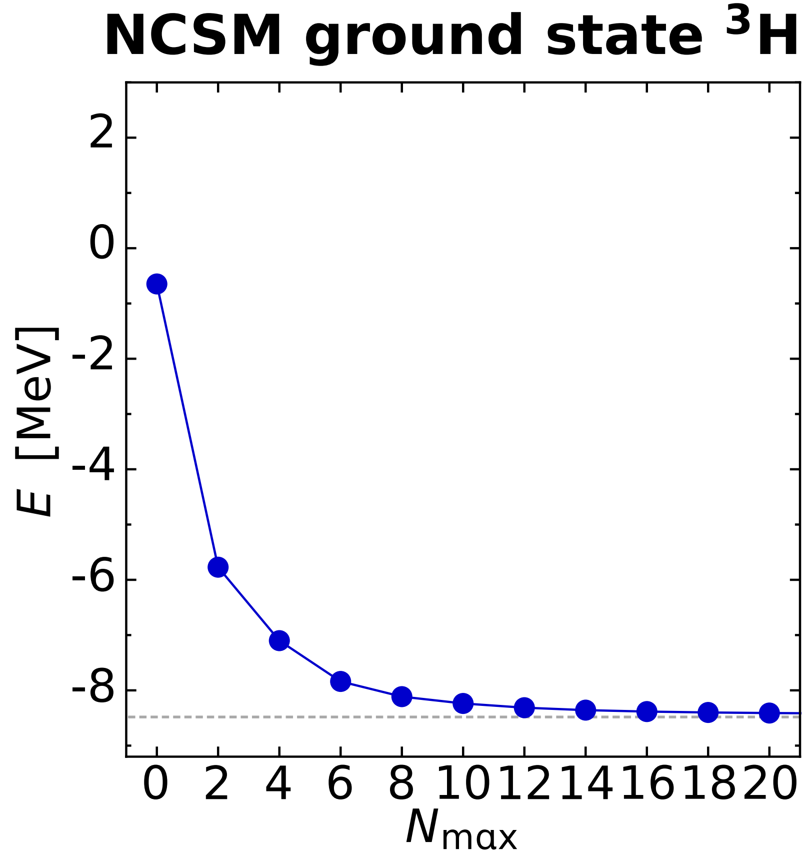


$\alpha = 0.080\,\mathrm{fm}^4$

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

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



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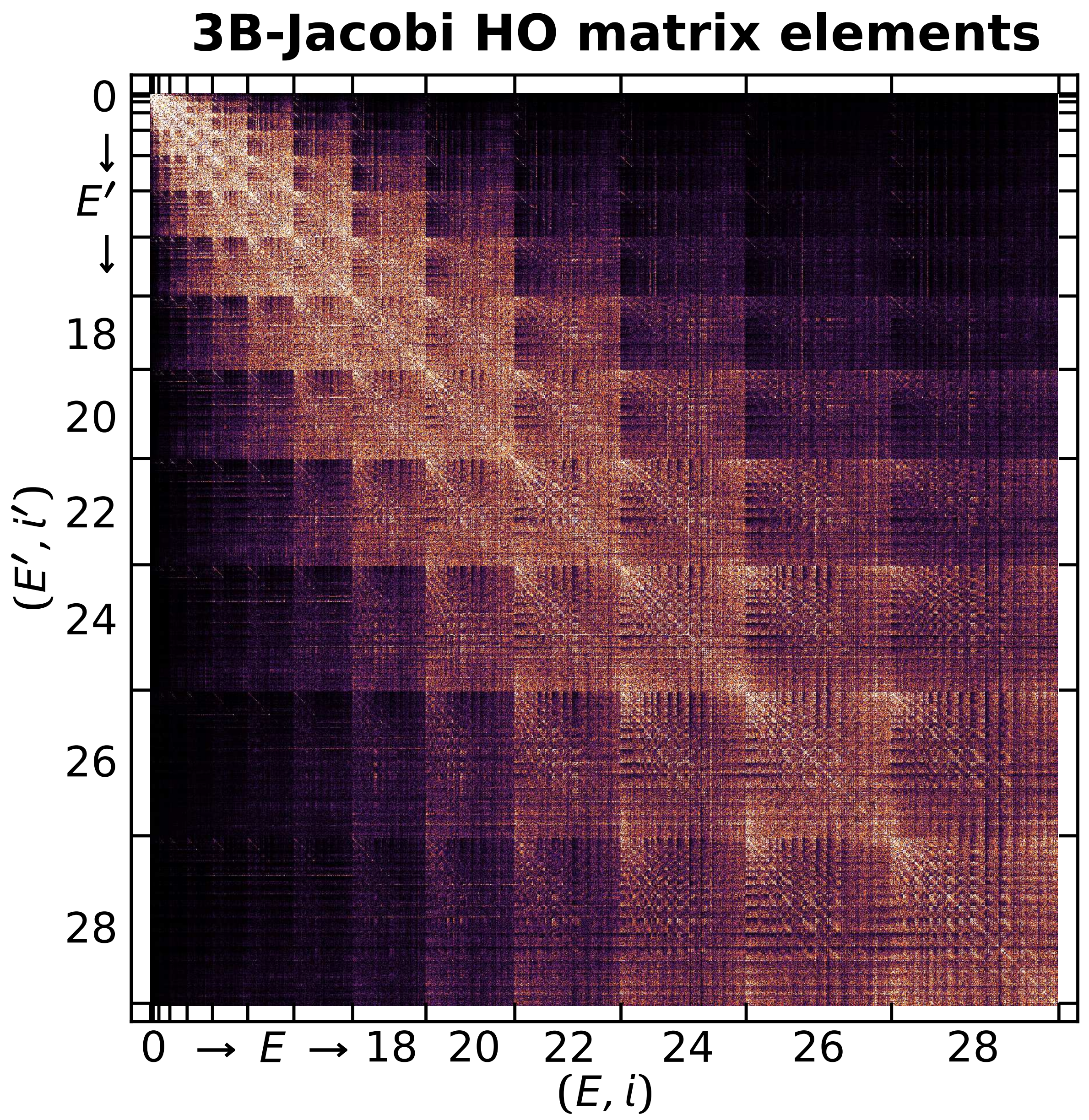
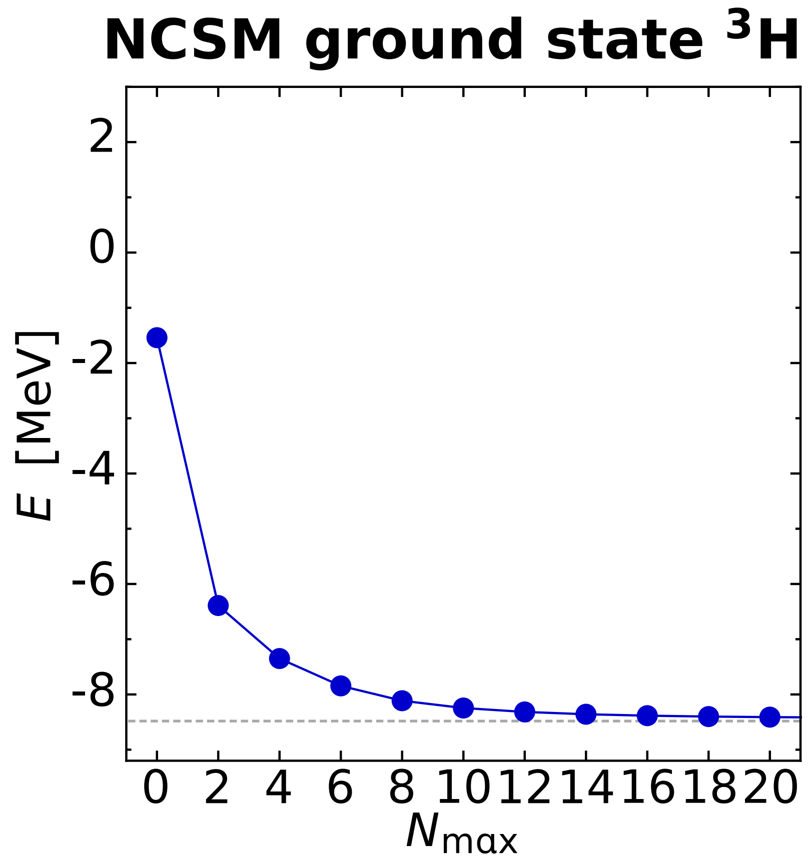


$\alpha = 0.160\,\mathrm{fm}^4$

$\Lambda = 1.58\,\mathrm{fm}^{-1}$

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



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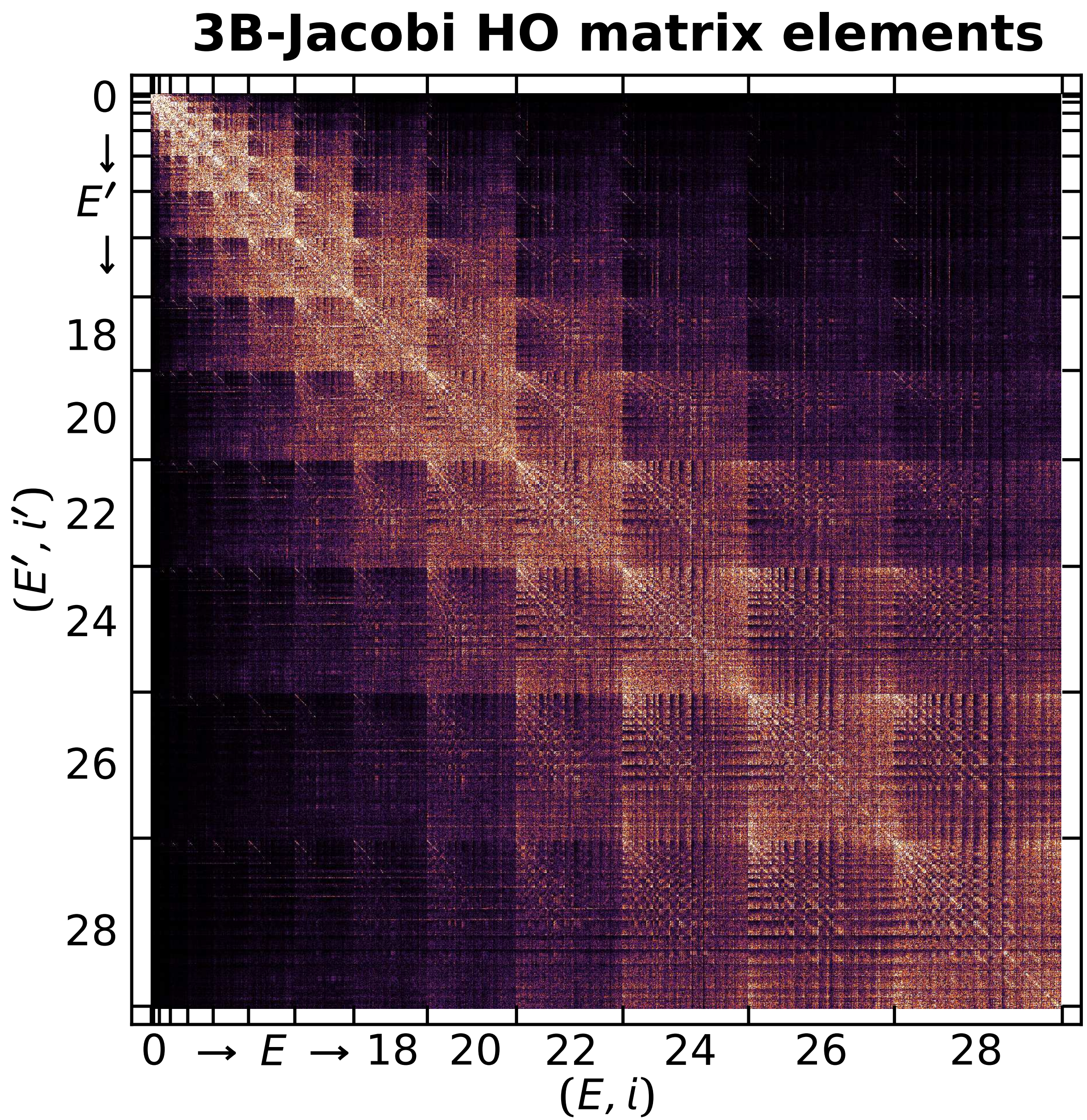
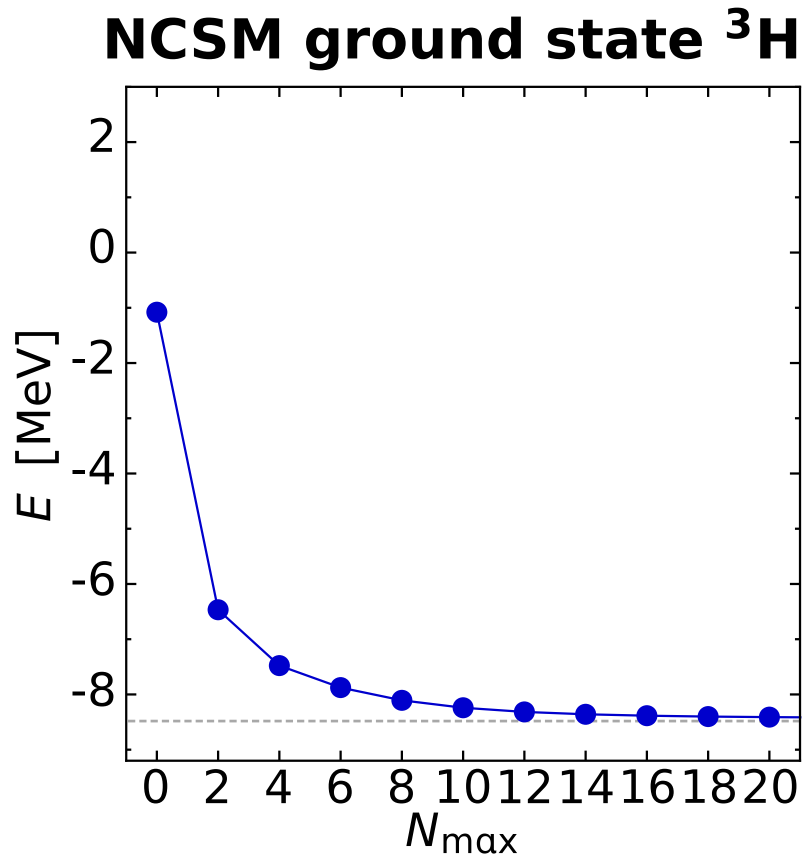


$\alpha = 0.320\,\text{fm}^4$

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

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



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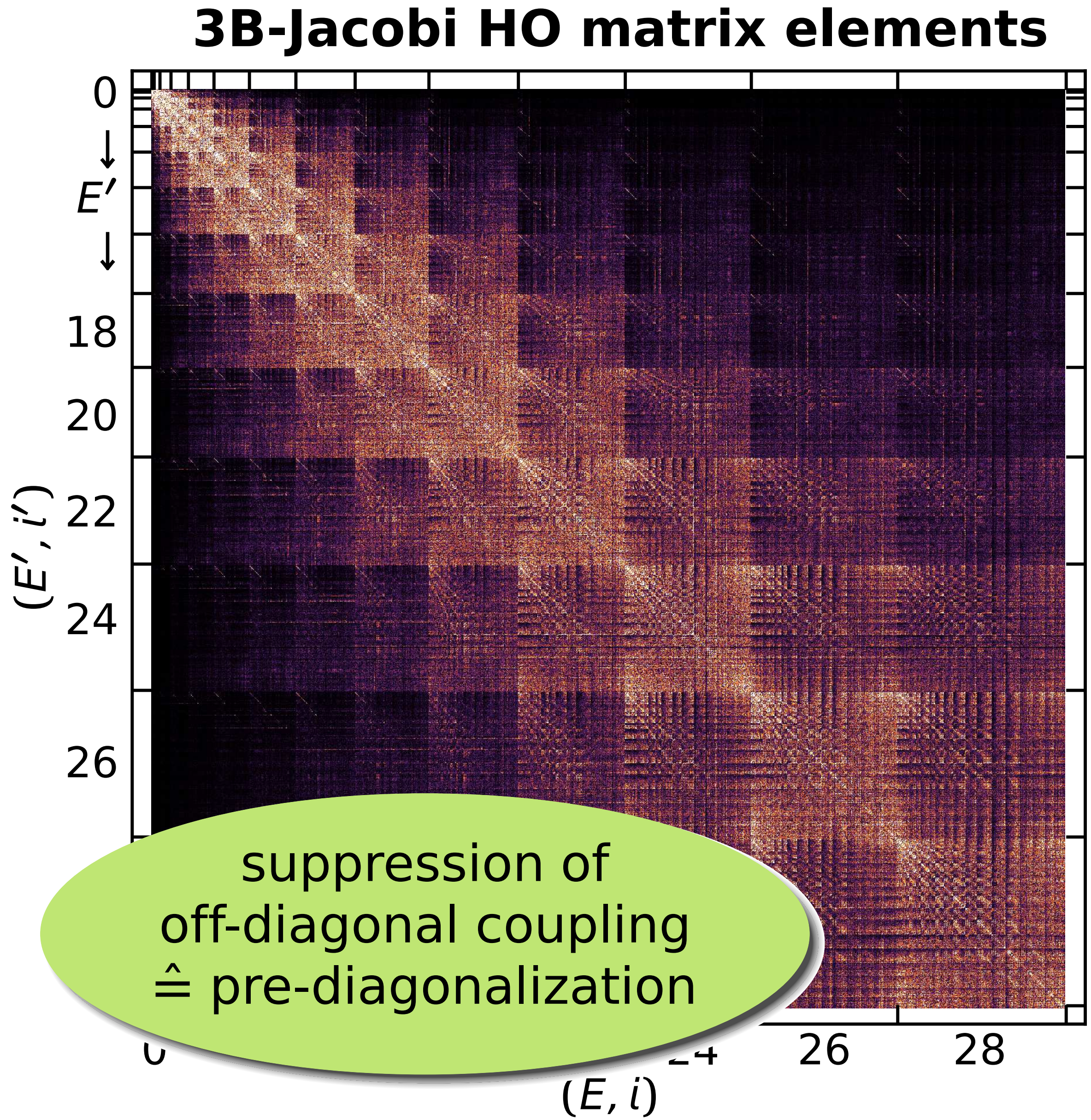

suppression of
off-diagonal coupling
≙ pre-diagonalization

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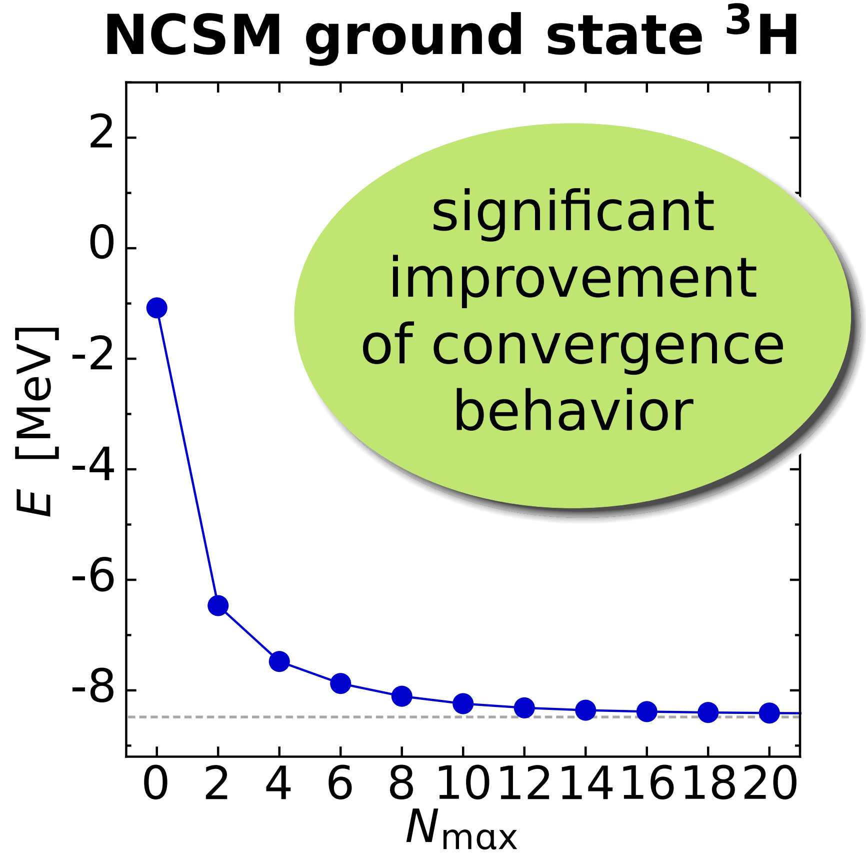
$\Lambda = 1.33\,\mathrm{fm}^{-1}$

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



significant
improvement
of convergence
behavior

Calculations in A-Body Space

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

Calculations in *A*-Body Space

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- truncation of cluster series inevitable
  and invariance of energy eigenvalues

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

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Importance-Truncated No-Core Shell Model

Roth, Langhammer, Calci et al. — Phys. Rev. Lett. 107, 072501 (2011)
Navrátil et al. — Phys. Rev. C 82, 034609 (2010)
Roth — Phys. Rev. C 79, 064324 (2009)

No-Core Shell Model — Basics

- **many-body basis**: Slater determinants $|\Phi_\nu\rangle$ composed of harmonic oscillator single-particle states (m-scheme)

$$|\Psi\rangle = \sum_\nu C_\nu |\Phi_\nu\rangle$$

- **model space**: spanned by basis states $|\Phi_\nu\rangle$ with unperturbed excitation energies of up to $N_{\mathrm{max}}\hbar\Omega$

No-Core Shell Model — Basics

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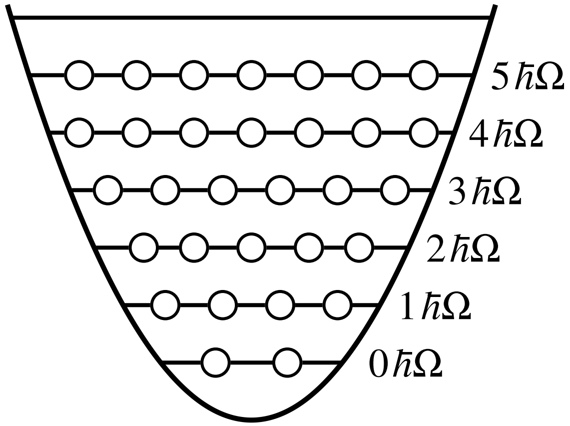
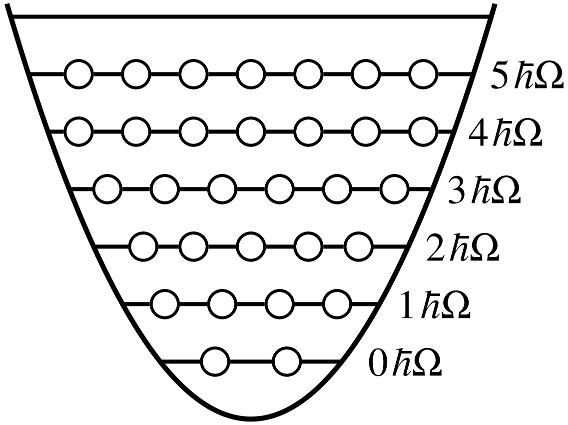


$$\{|i\rangle\}$$

$$e_i = 2n_i + l_i$$

No-Core Shell Model — Basics



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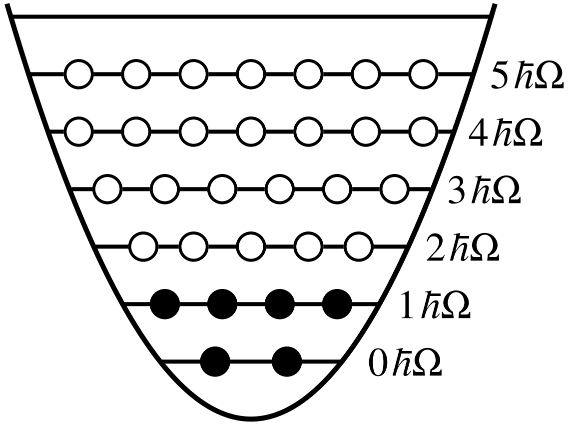

$|\Phi_0\rangle$

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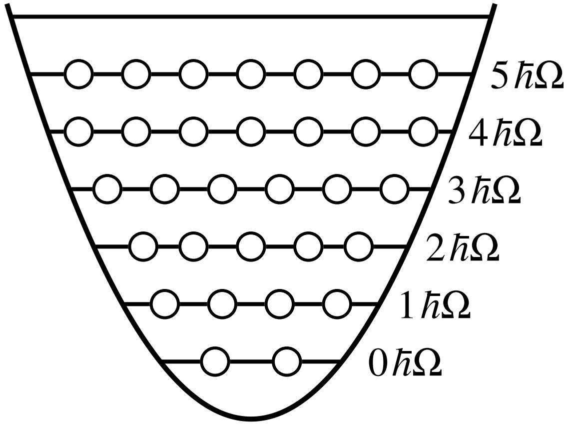

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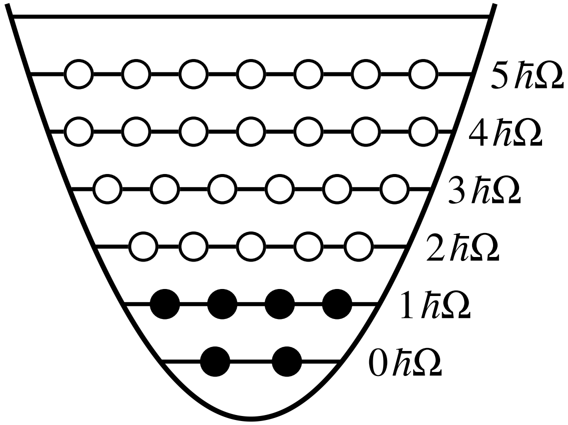

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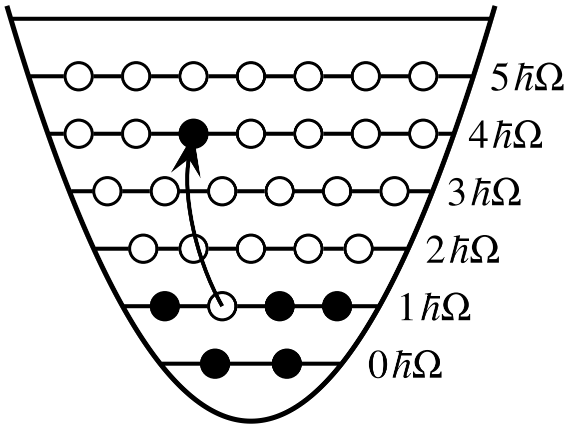
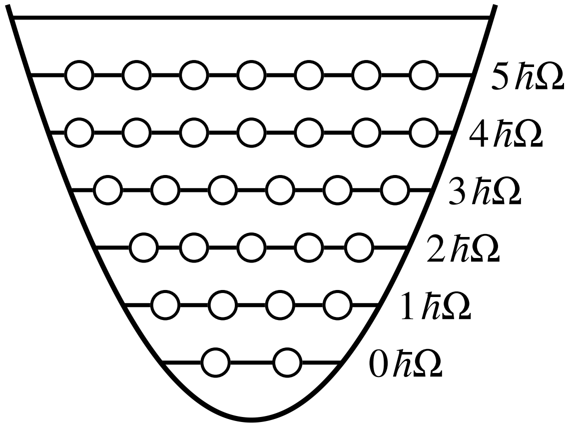


$|\Phi_\nu\rangle$

$X_\nu = 3\hbar\Omega$

No-Core Shell Model — Basics



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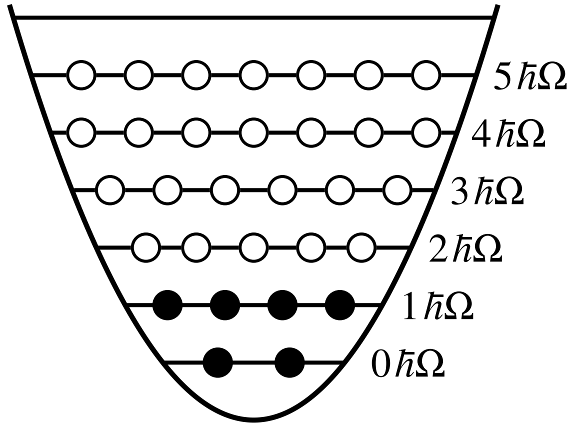
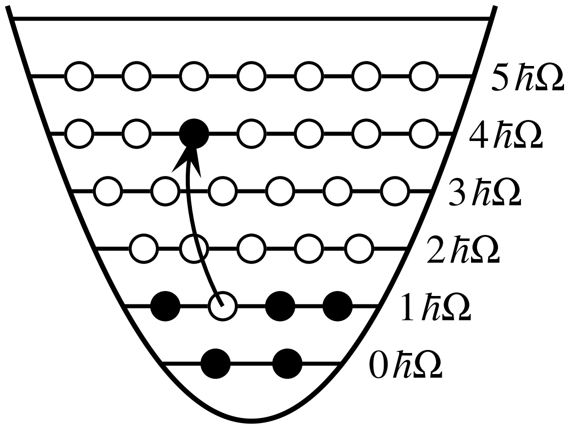
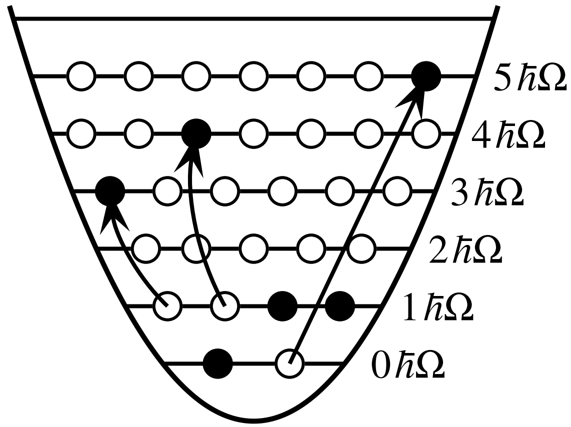


$|\Phi_0\rangle$



$|\Phi_\nu\rangle$

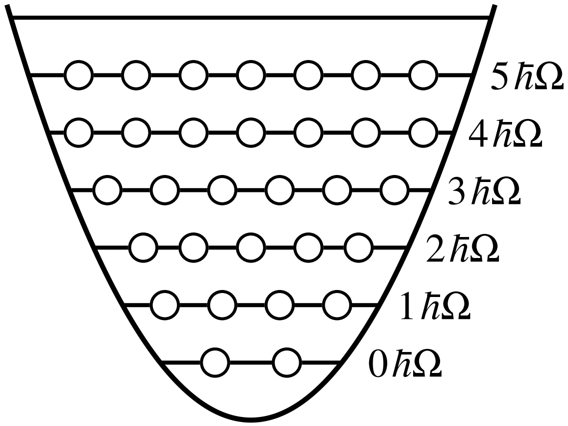
$X_\nu = 3\hbar\Omega$



$|\Phi_\mu\rangle$

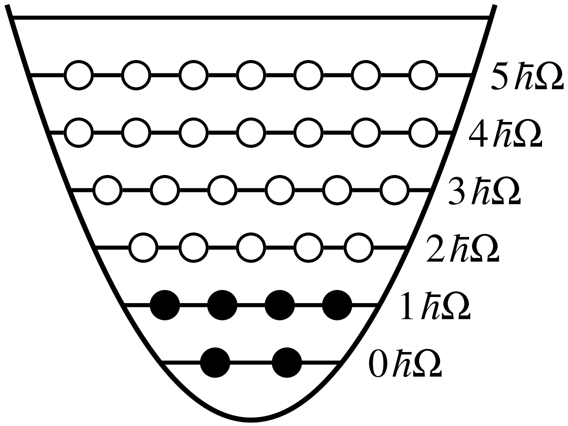
$X_\mu = (2+3+5)\hbar\Omega$

No-Core Shell Model — Basics

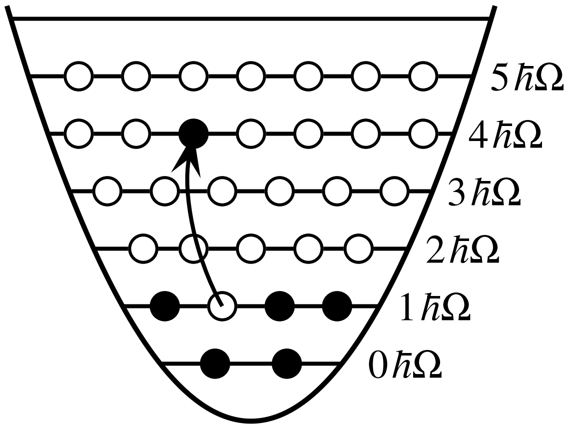


$\{|i\rangle\}$

$e_i = 2n_i + l_i$

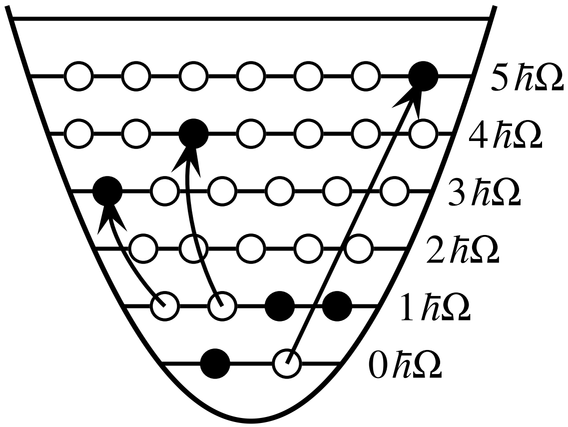


$|\Phi_0\rangle$



$|\Phi_\nu\rangle$

$X_\nu = 3\hbar\Omega$



$|\Phi_\mu\rangle$

$X_\mu = (2+3+5)\hbar\Omega$

- model space :

$$\mathcal{V} = \text{span}\left\{ |\Phi_\nu\rangle : X_\nu \leq N_{\max}\hbar\Omega \right\}$$

- "low-energy part" of the many-body Hilbert space
- allows separation of center-of-mass and intrinsic degrees of freedom

No-Core Shell Model — Basics

- **many-body basis**: Slater determinants $|\Phi_\nu\rangle$ composed of harmonic oscillator single-particle states (m-scheme)

$$|\Psi\rangle = \sum_\nu C_\nu |\Phi_\nu\rangle$$

- **model space**: spanned by basis states $|\Phi_\nu\rangle$ with unperturbed excitation energies of up to $N_{\mathrm{max}}\hbar\Omega$

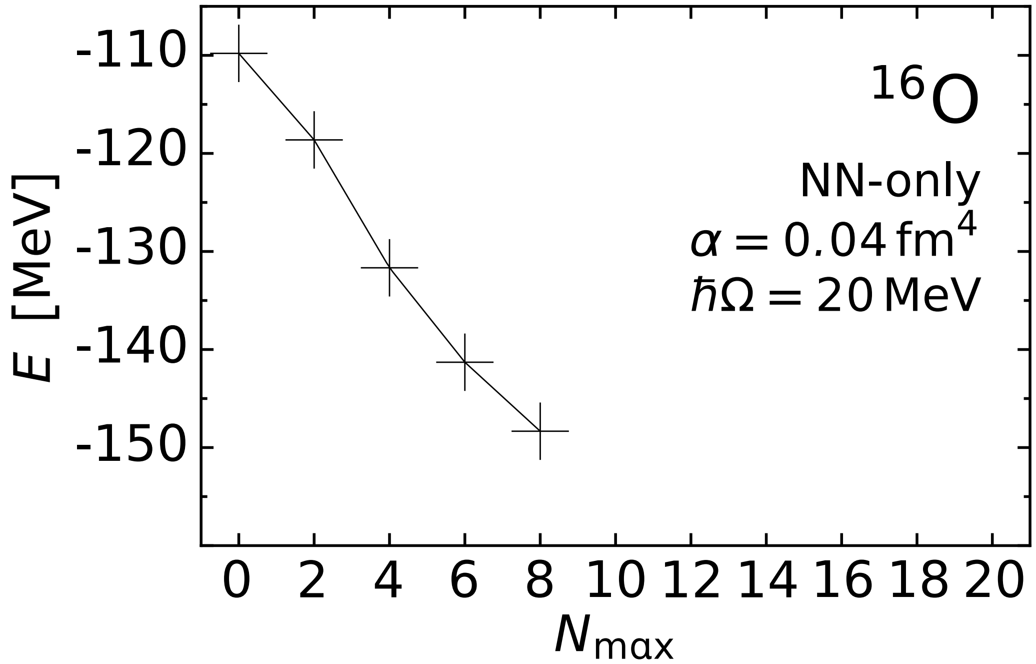
- numerical solution of **matrix eigenvalue problem** for the intrinsic Hamiltonian H within truncated model space

$$\mathrm{H}|\Psi\rangle = E|\Psi\rangle \quad \rightarrow \quad \begin{pmatrix} & \vdots & \\ \dots & \langle\Phi_\nu|\mathrm{H}|\Phi_\mu\rangle & \dots \\ & \vdots & \end{pmatrix} \begin{pmatrix} \vdots \\ C_\mu \\ \vdots \end{pmatrix} = E \begin{pmatrix} \vdots \\ C_\nu \\ \vdots \end{pmatrix}$$

- model spaces of **up to 10^9 basis states** are used routinely

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})



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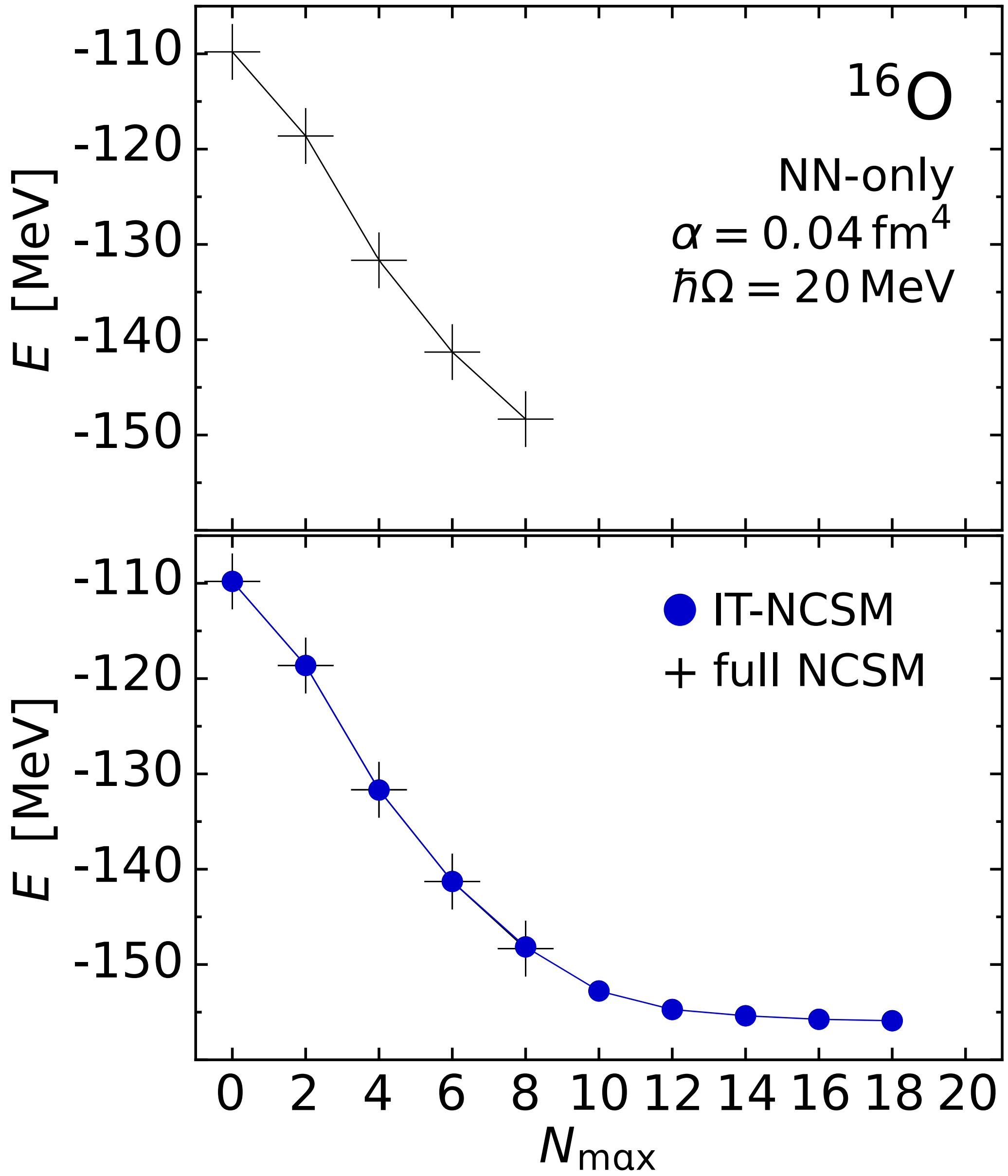
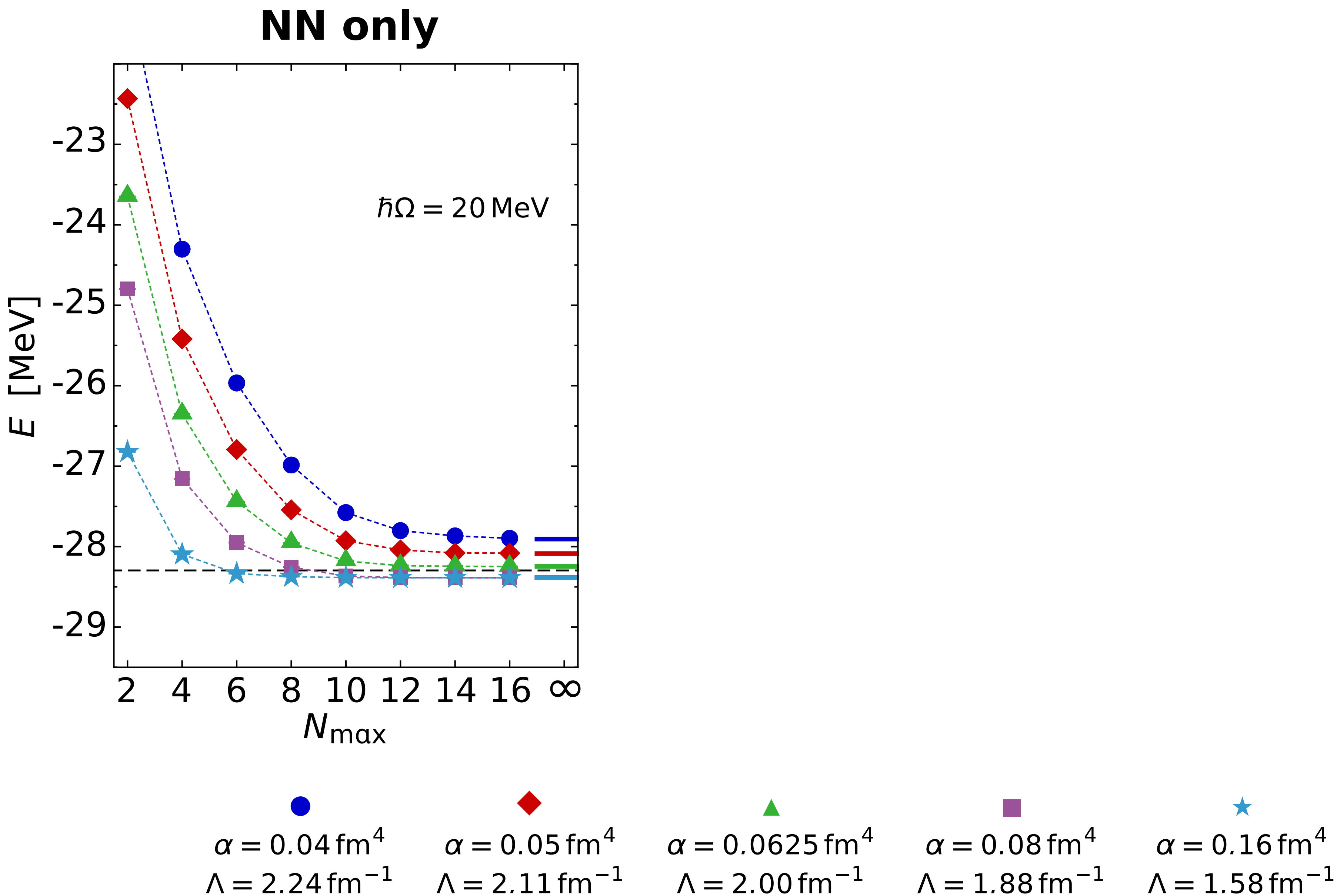
- converged NCSM calculations essentially restricted to lower/mid p-shell
- full $10\hbar\Omega$ calculation for ^{16}O getting very difficult (basis dimension > 10^{10})

Importance Truncation

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



^{4}He: Ground-State Energies



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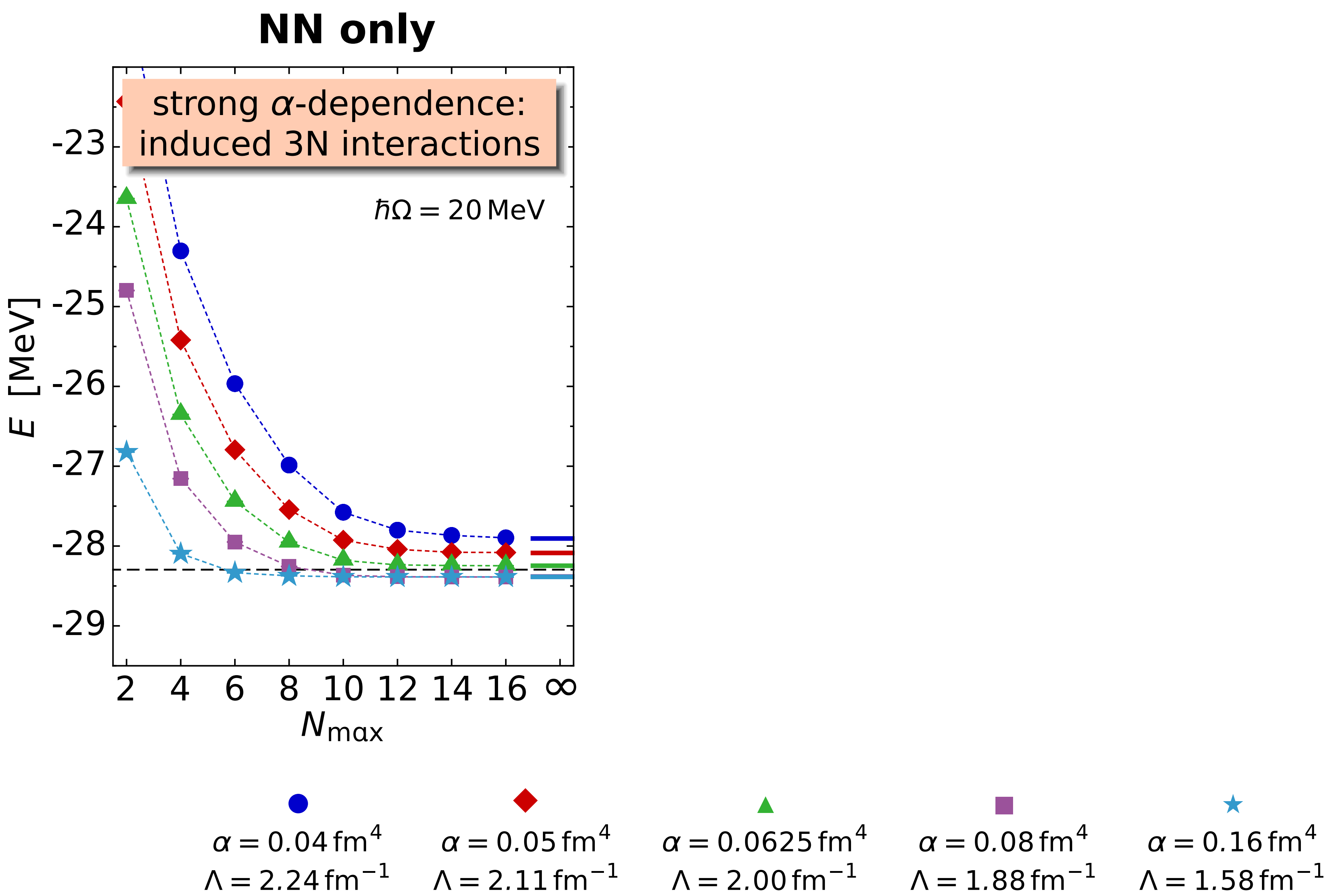

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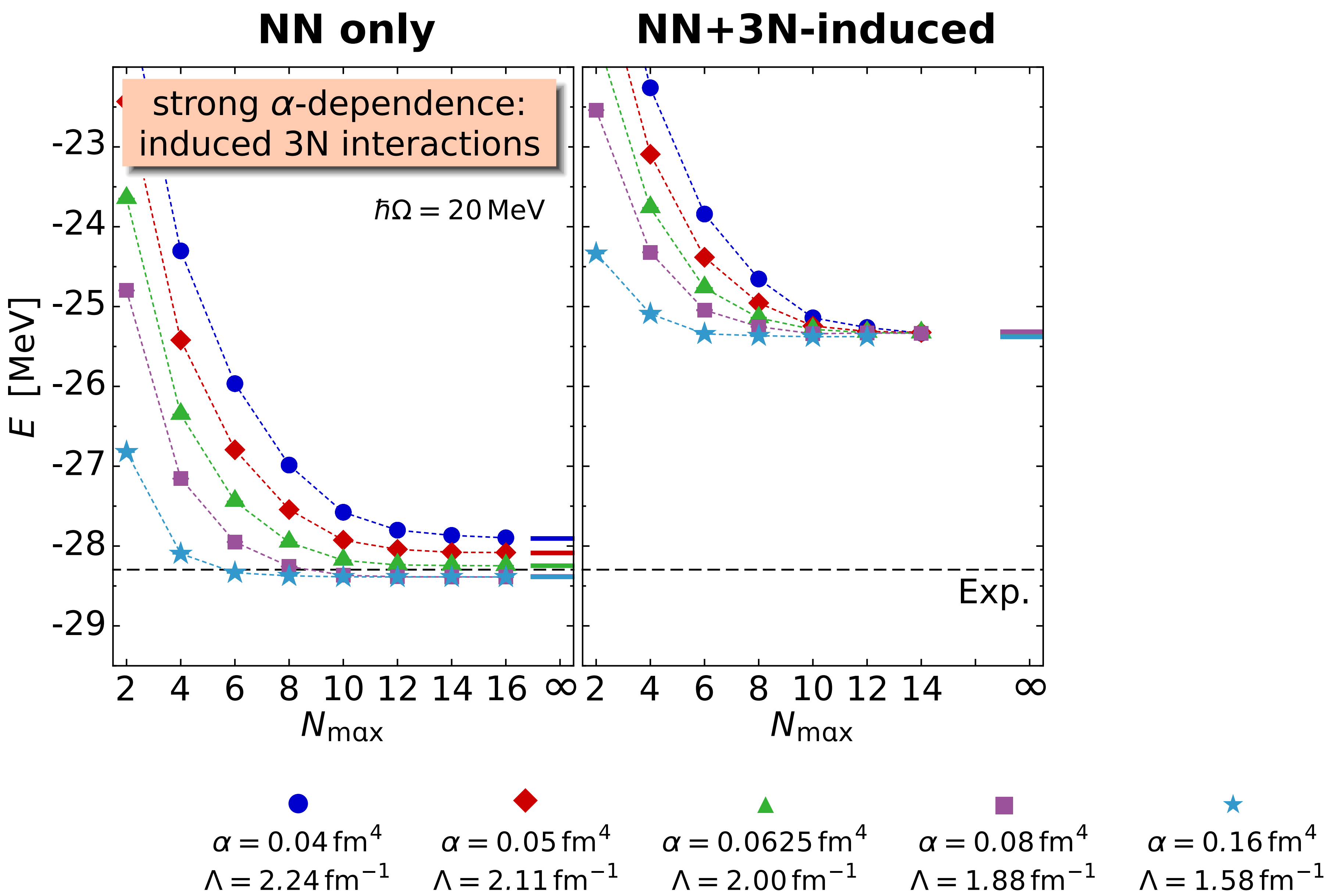

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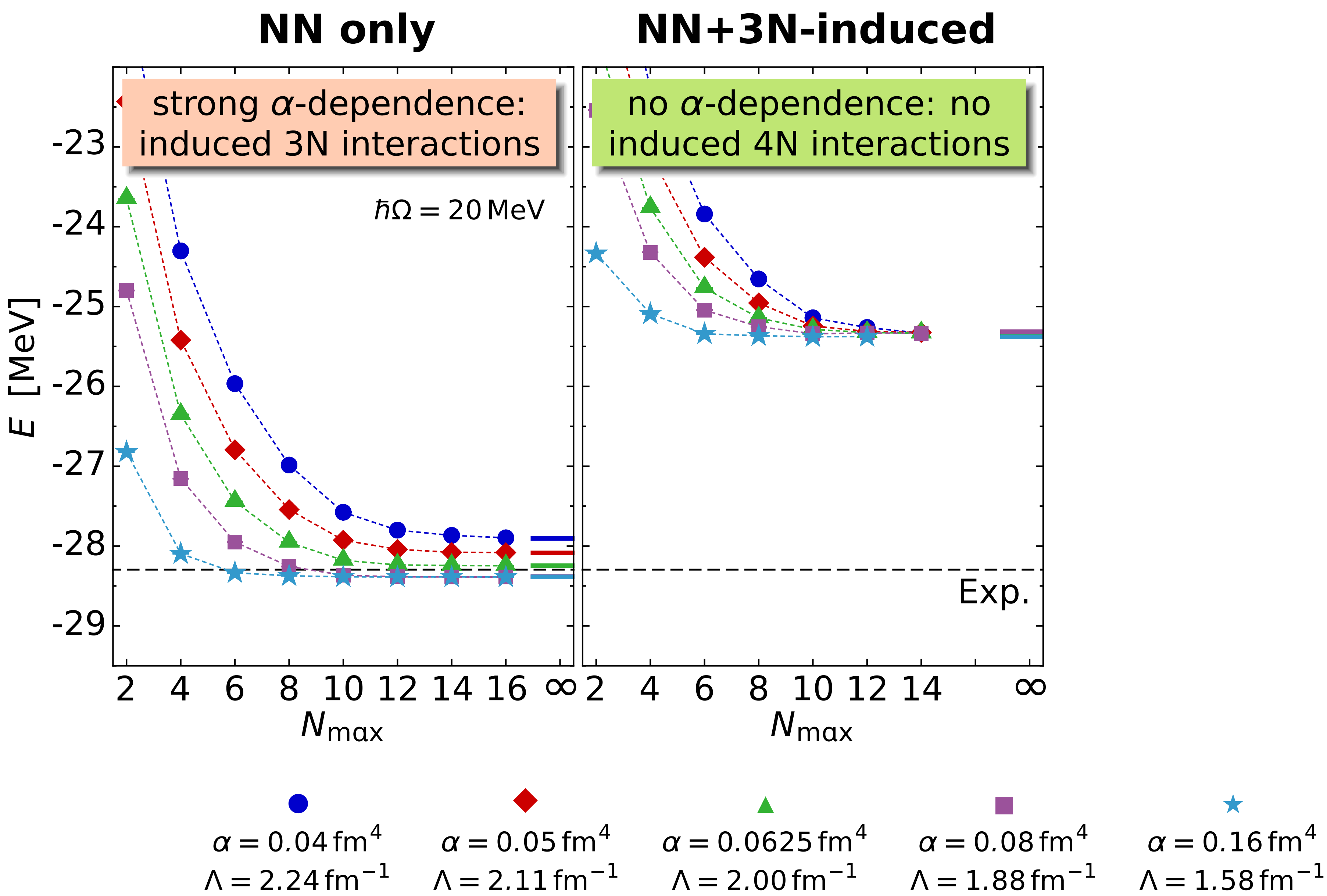

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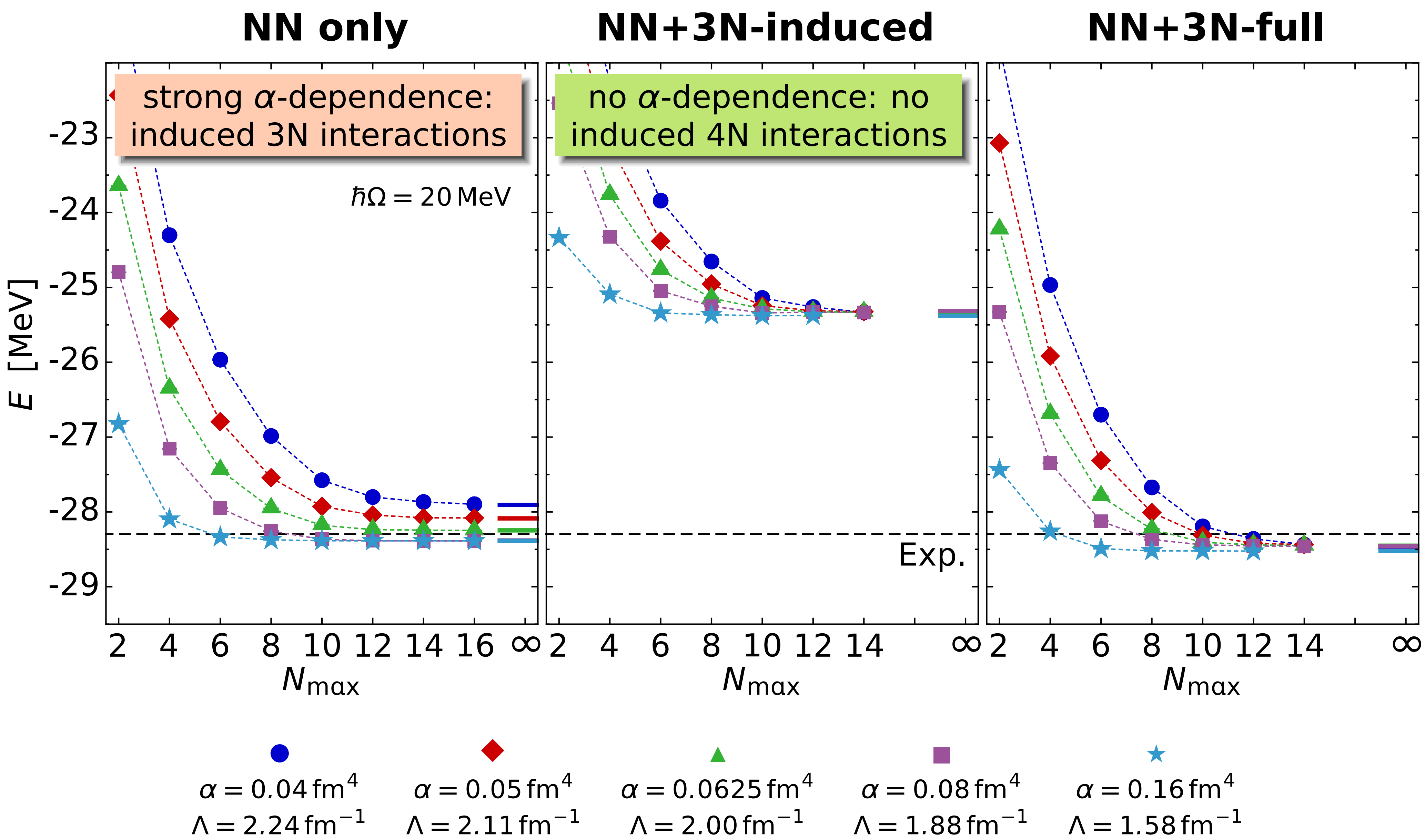

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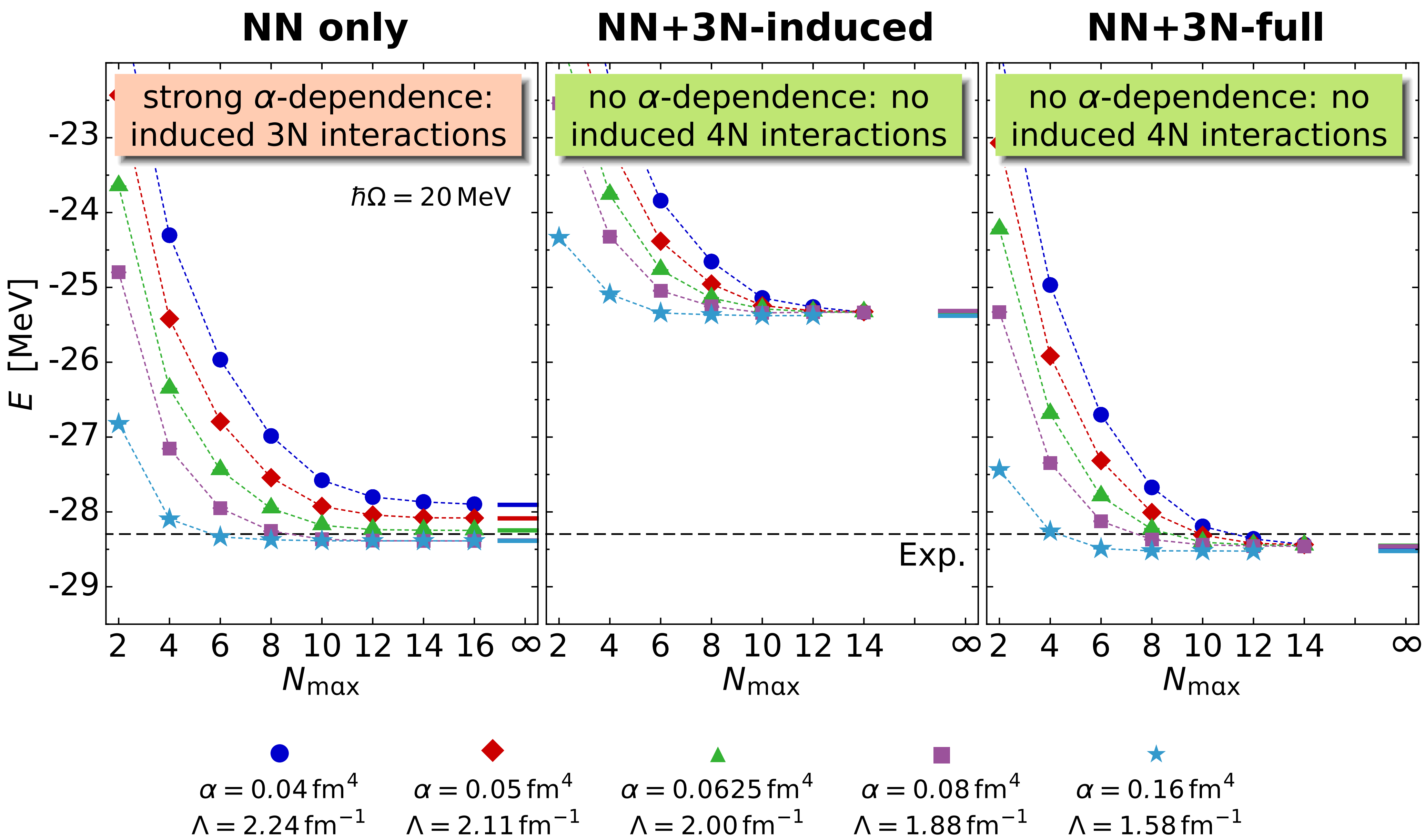
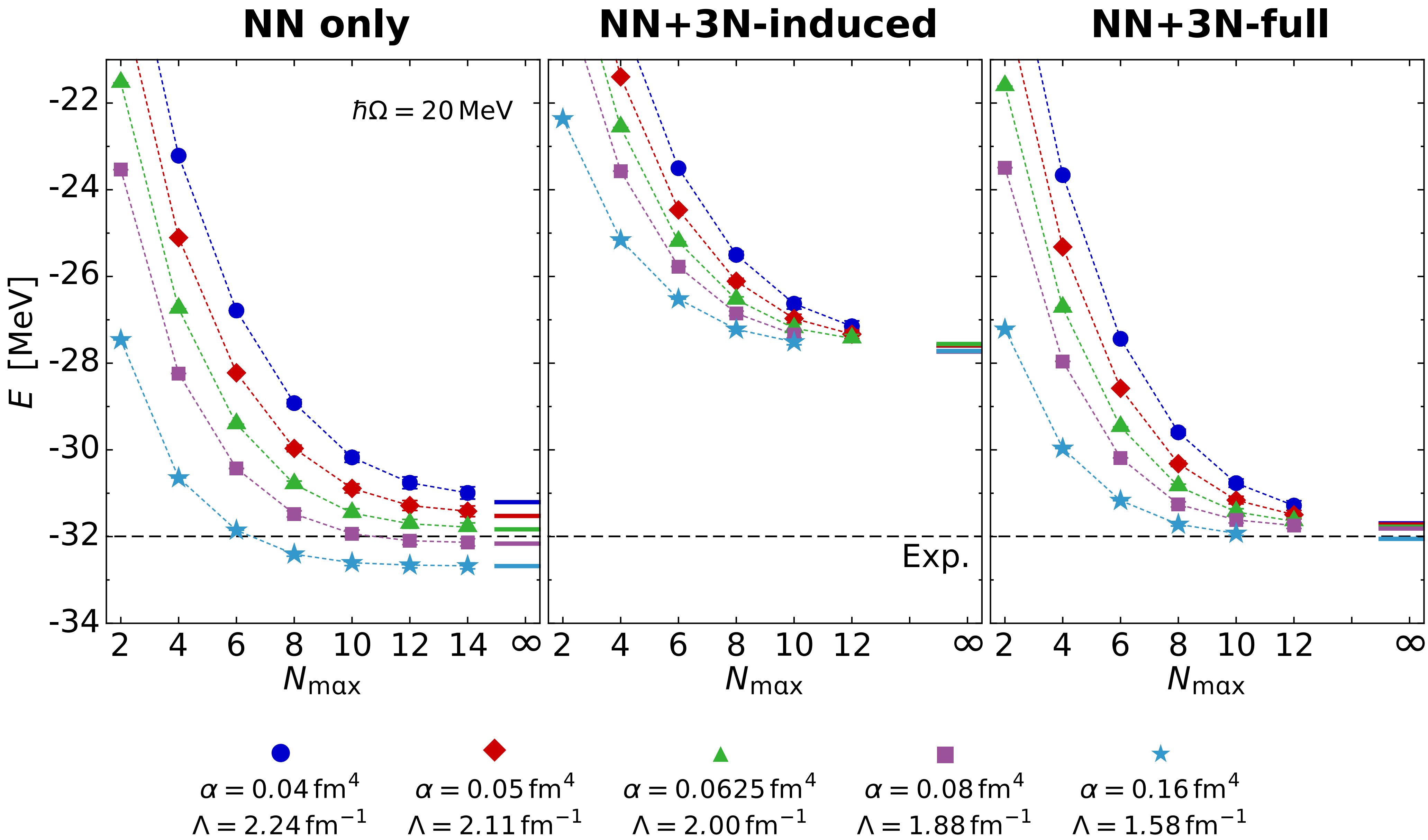
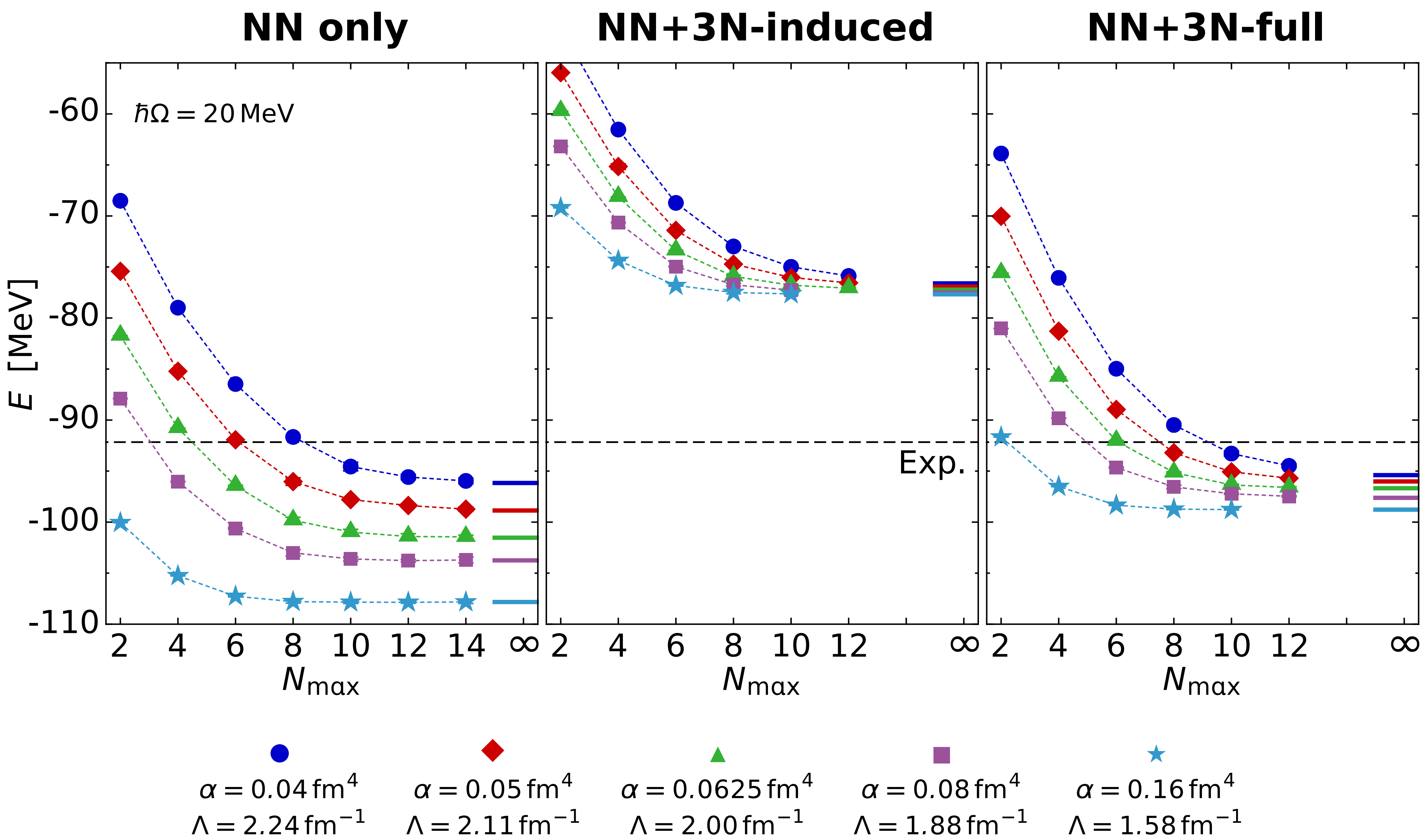


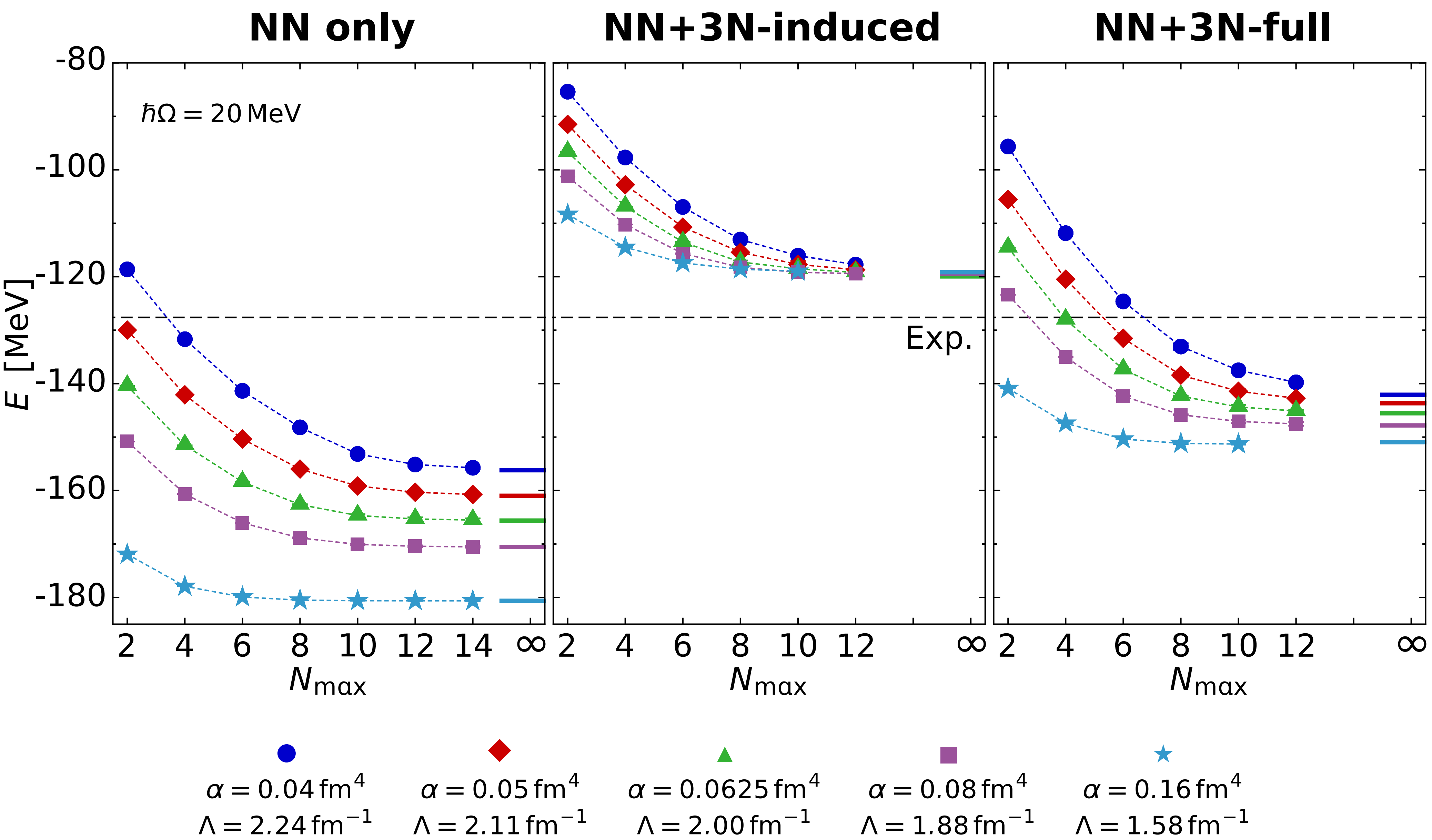
^{6}Li: Ground-State Energies



^{12}C: Ground-State Energies



^{16}O: Ground-State Energies



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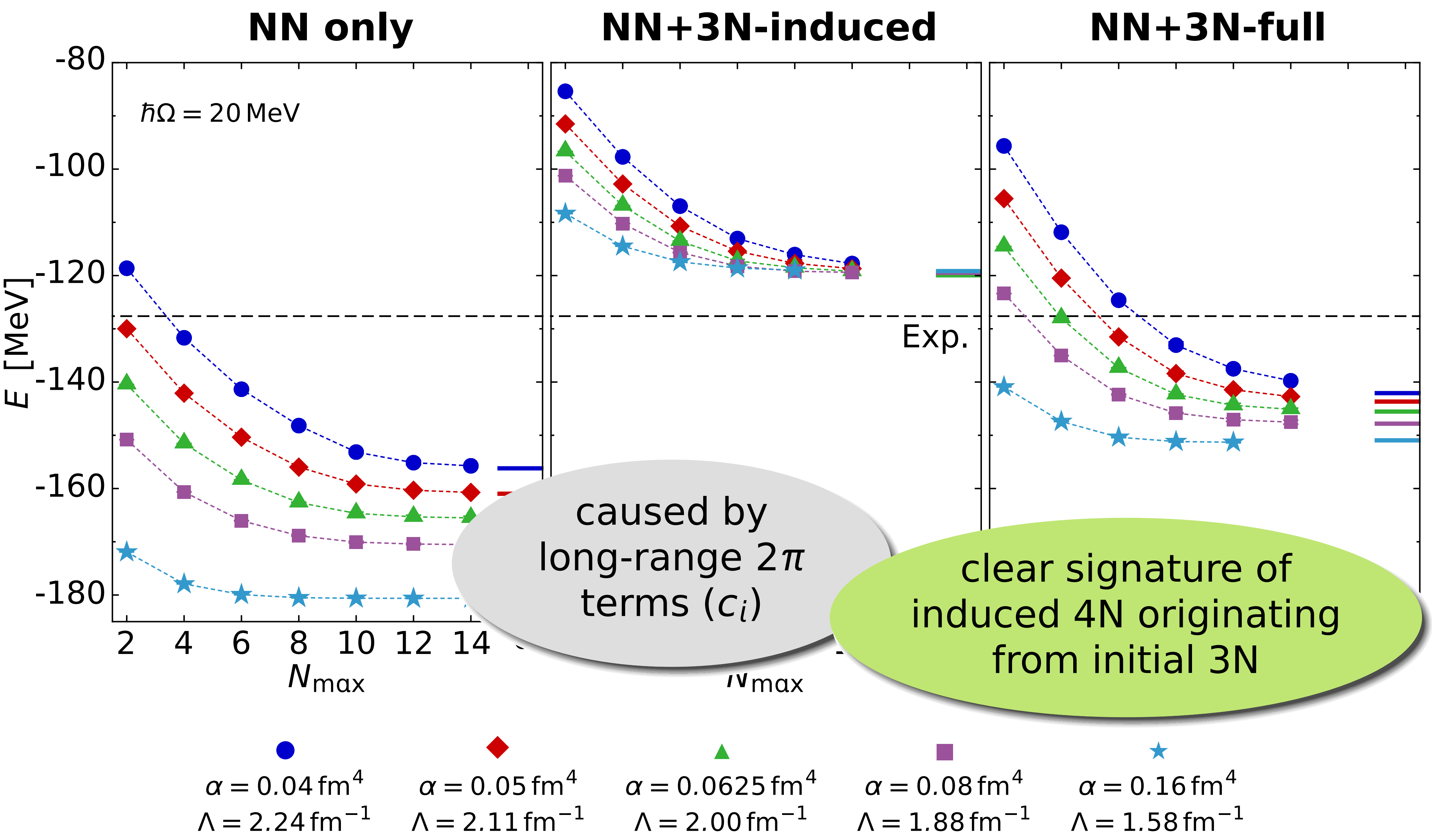

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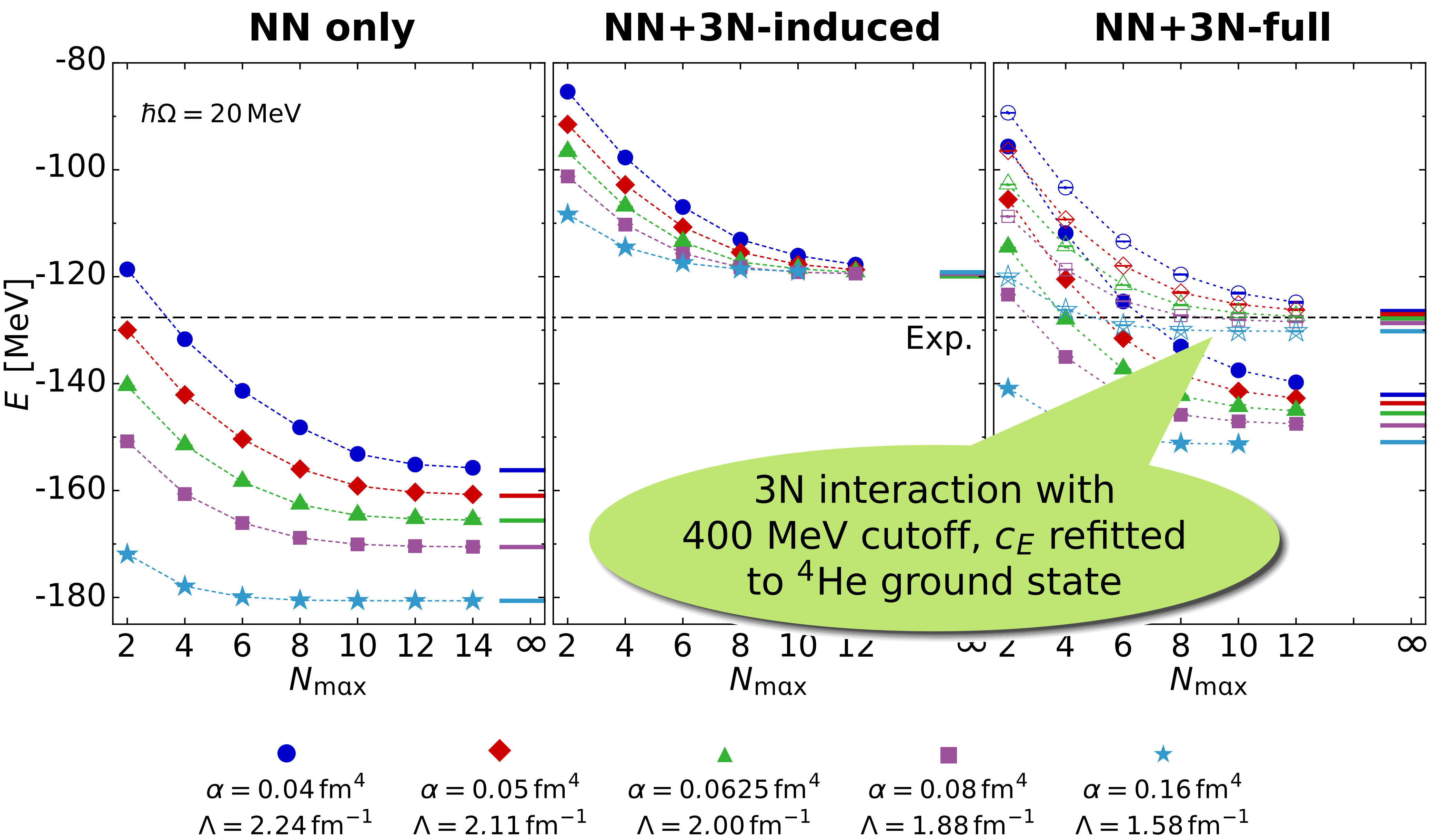
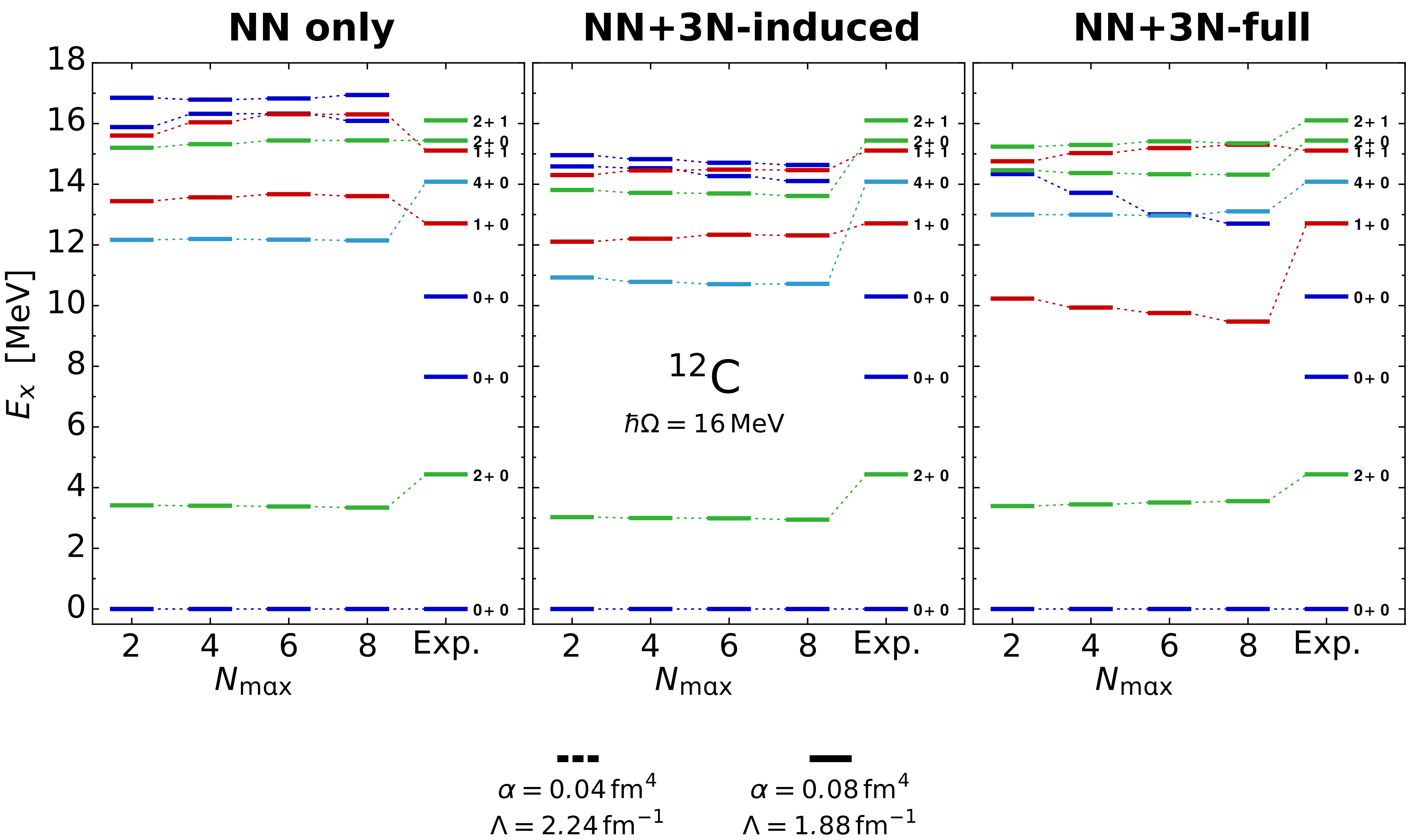


Spectroscopy of ^{12}C



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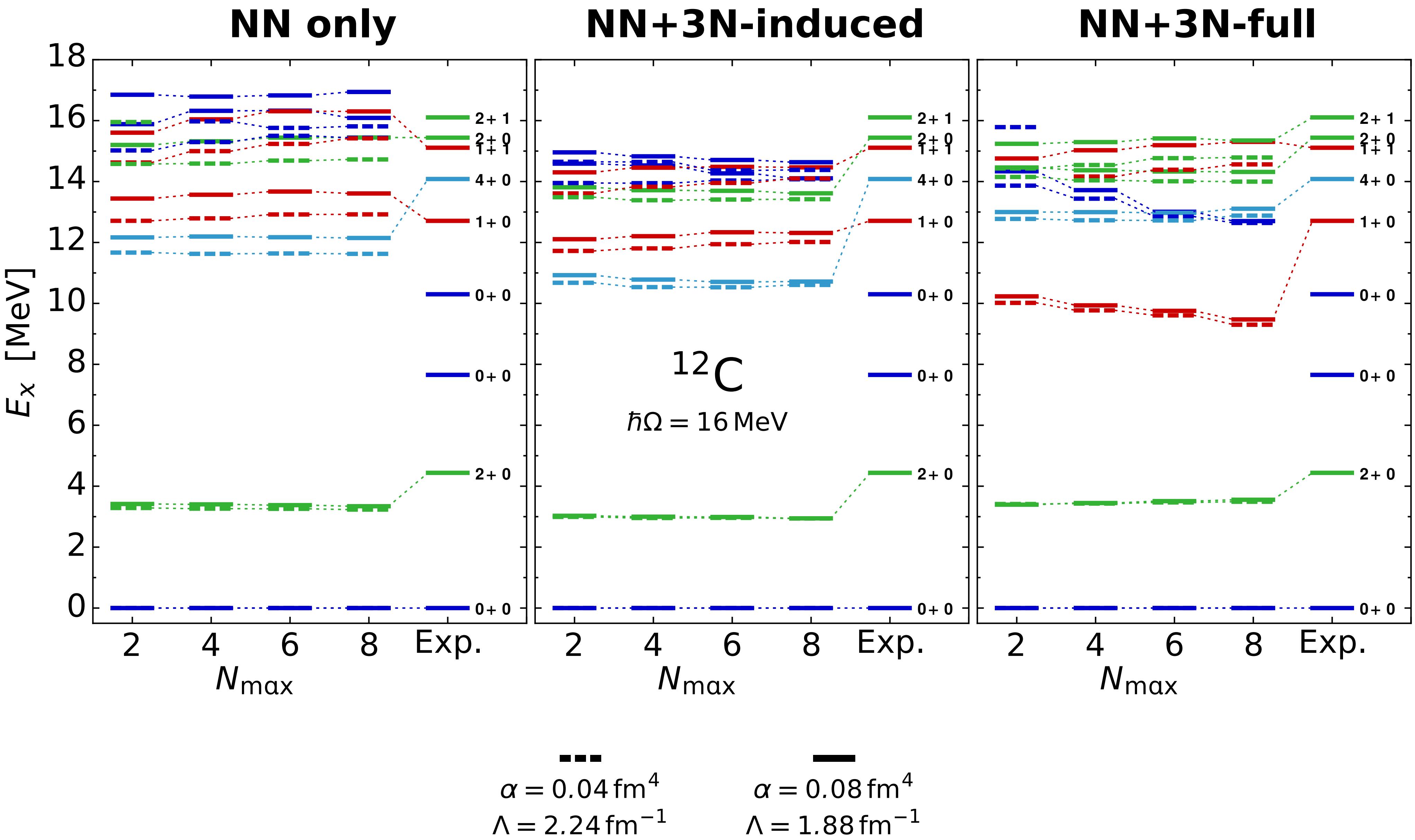

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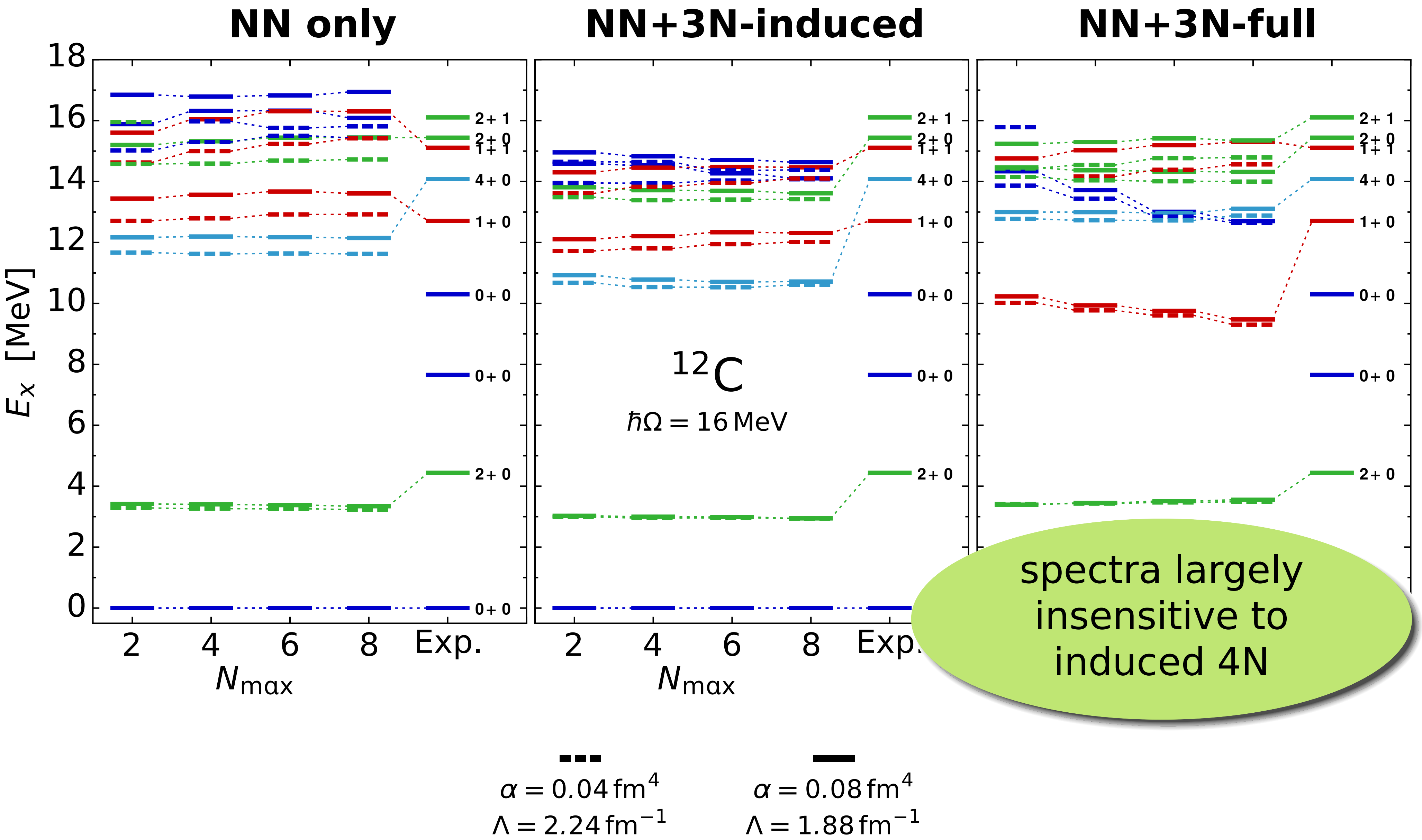

spectra largely insensitive to induced 4N

Normal-Ordered 3N Interaction

Hagen, Papenbrock, Dean et al. — Phys. Rev. C 76, 034302 (2007)
Roth, Binder, Vobig et al. — Phys. Rev. Lett 109, 052501 (2012)
Binder, Langhammer, Calci et al. — arXiv: 1211.4748 (2013)

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avoid technical challenge of including explicit 3N interactions in many-body calculation

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- **idea**: write 3N interaction in normal-ordered form with respect to an *A*-body reference Slater-determinant ($0\hbar\Omega$ state)

$$\hat{V}_{3N} = \sum V^{3N}_{\circ\circ\circ\circ\circ\circ}\, \hat{a}^\dagger_\circ \hat{a}^\dagger_\circ \hat{a}^\dagger_\circ\, \hat{a}_\circ \hat{a}_\circ \hat{a}_\circ$$

$$= W^{0B} + \sum W^{1B}_{\circ\circ}\, \{\hat{a}^\dagger_\circ\, \hat{a}_\circ\} + \sum W^{2B}_{\circ\circ\circ\circ}\, \{\hat{a}^\dagger_\circ \hat{a}^\dagger_\circ\, \hat{a}_\circ \hat{a}_\circ\}$$

$$+ \sum W^{3B}_{\circ\circ\circ\circ\circ\circ}\, \{\hat{a}^\dagger_\circ \hat{a}^\dagger_\circ \hat{a}^\dagger_\circ\, \hat{a}_\circ \hat{a}_\circ \hat{a}_\circ\}$$

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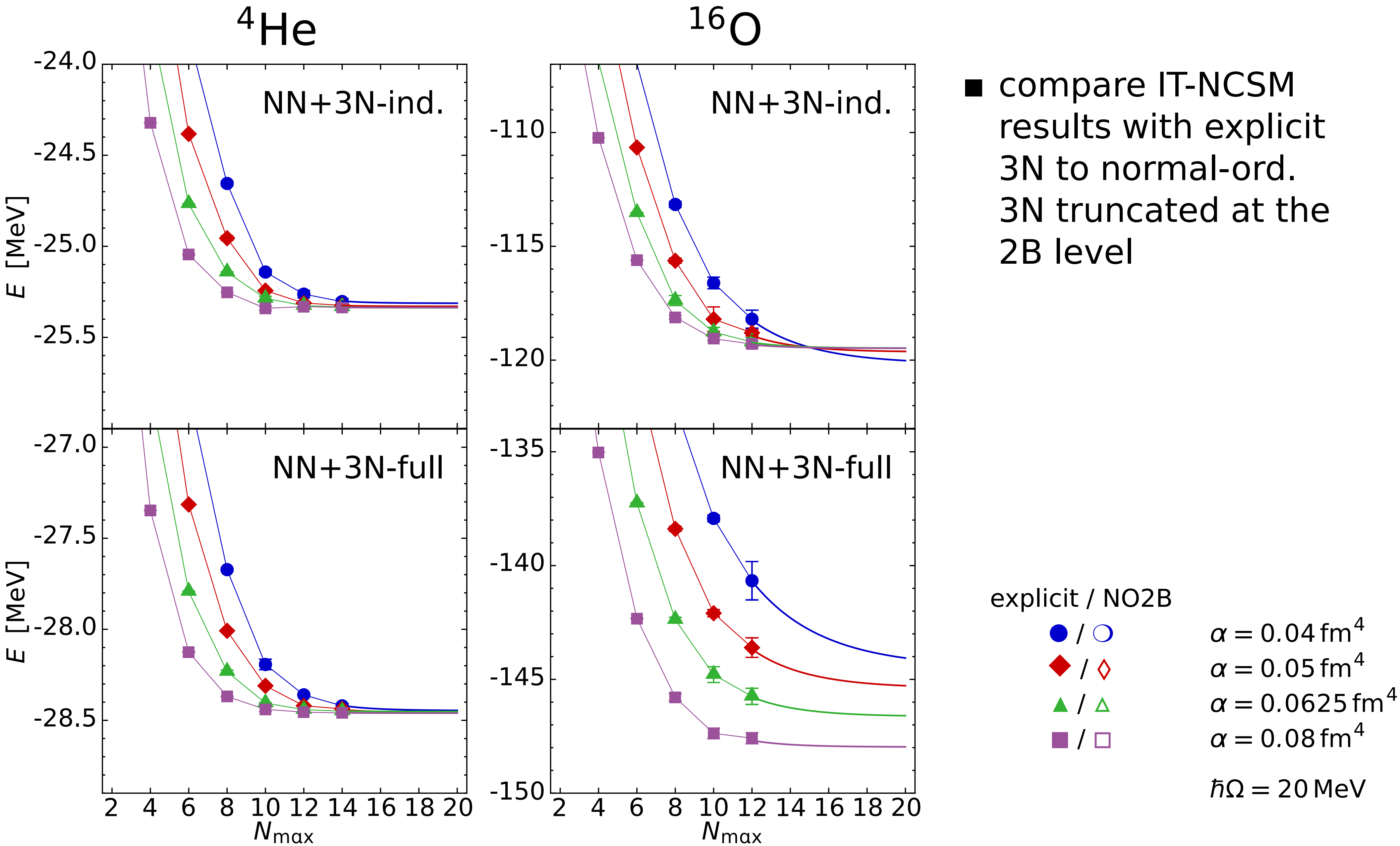
- **Normal-Ordering Approximation** (NO2B): discard residual 3B part W^{3B}

Benchmark of Normal-Ordered 3N



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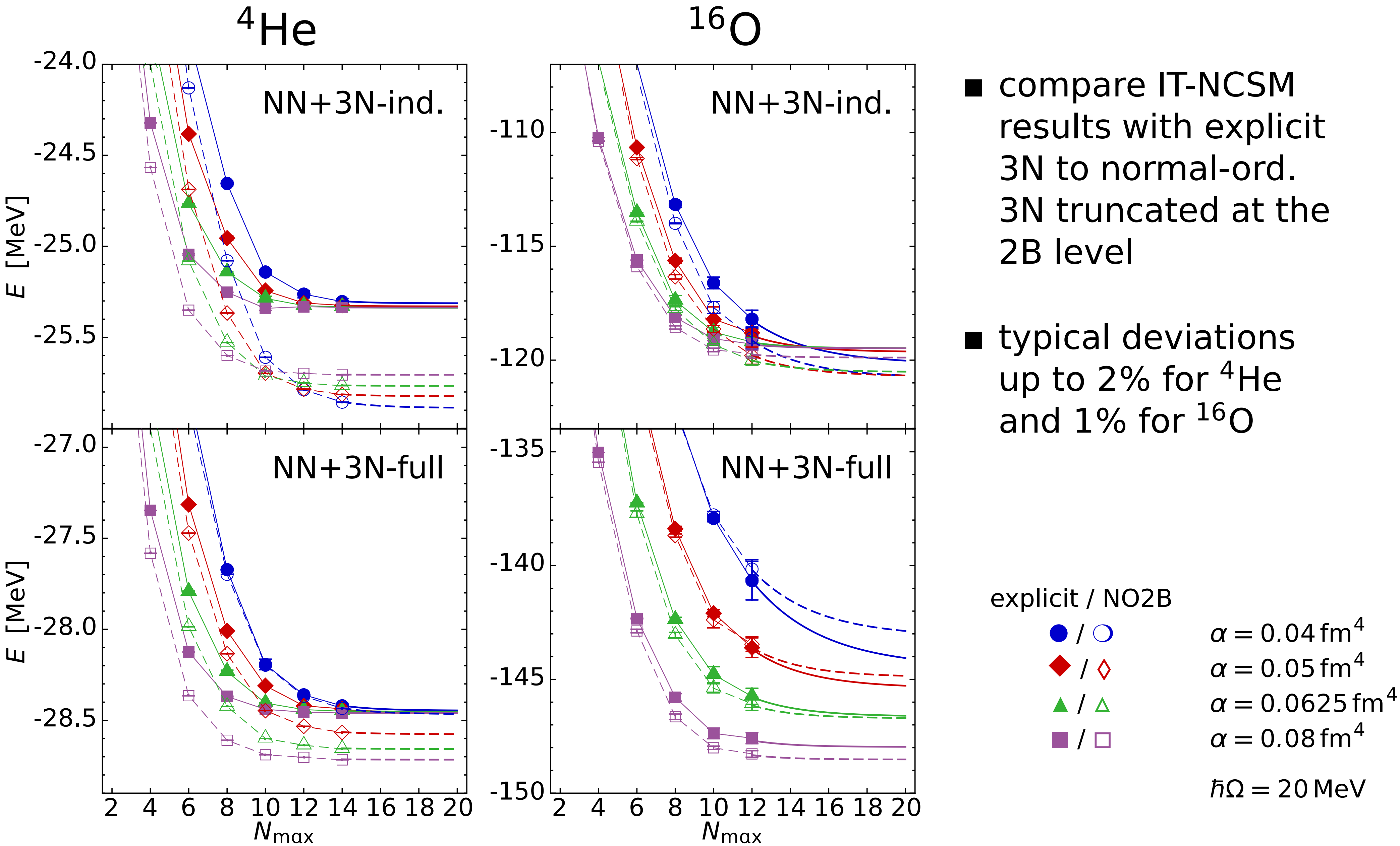

- compare IT-NCSM results with explicit 3N to normal-ord. 3N truncated at the 2B level
- typical deviations up to 2% for ^{4}He and 1% for ^{16}O

Coupled Cluster Method

G. Hagen, T. Papenbrock, D.J. Dean, and M. Hjorth-Jensen — Phys. Rev. C 82, 034330 (2010)

Coupled Cluster Approach

Coupled Cluster Approach

- **exponential Ansatz** for wave operator

$$|\Psi\rangle = \hat{\Omega}|\Phi_0\rangle = e^{\hat{T}_1+\hat{T}_2+\hat{T}_3+\cdots+\hat{T}_A}|\Phi_0\rangle$$

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$$\hat{T}_n = \frac{1}{(n!)^2} \sum_{\substack{ijk...\\abc...}} t^{abc...}_{ijk...} \{\hat{a}^\dagger_a \hat{a}^\dagger_b \hat{a}^\dagger_c \ldots \hat{a}_k \hat{a}_j \hat{a}_i\}$$

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- **similarity transformed** Schrödinger Eq.

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- $\hat{\mathcal{H}}$: non-Hermitian **effective Hamiltonian**

Coupled Cluster Approach

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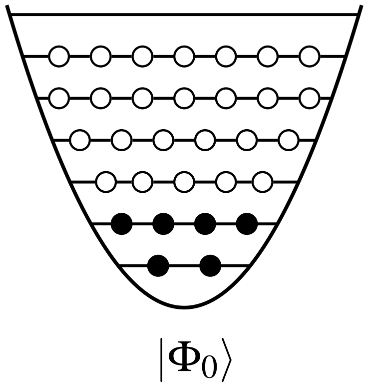

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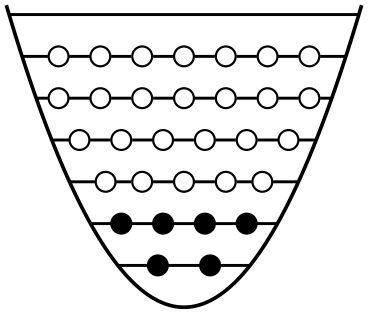
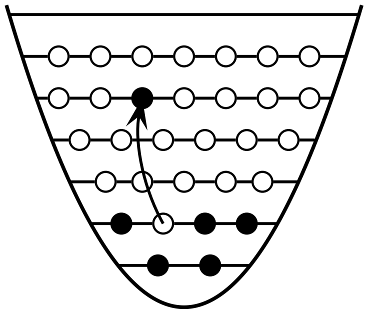


$|\Phi_0\rangle$



$\hat{T}_1 \, |\Phi_0\rangle$

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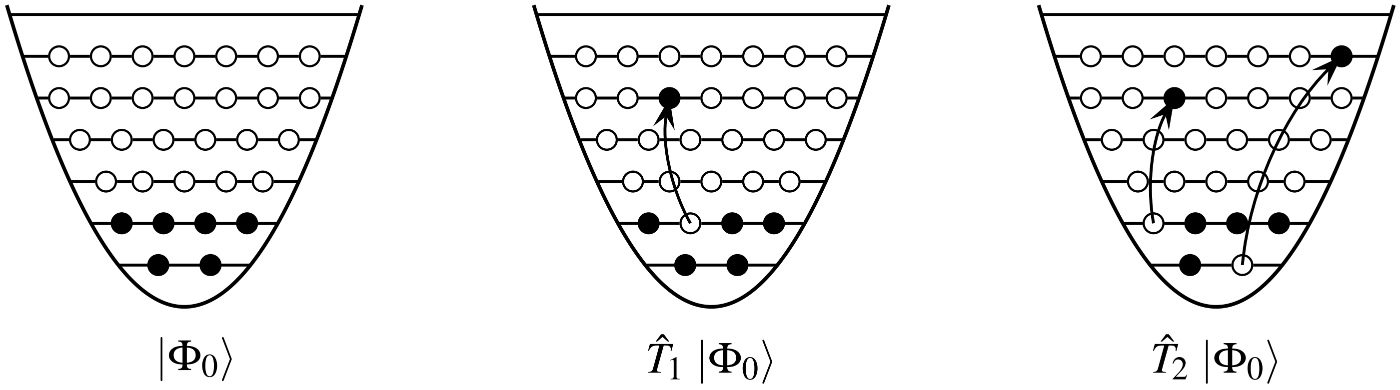

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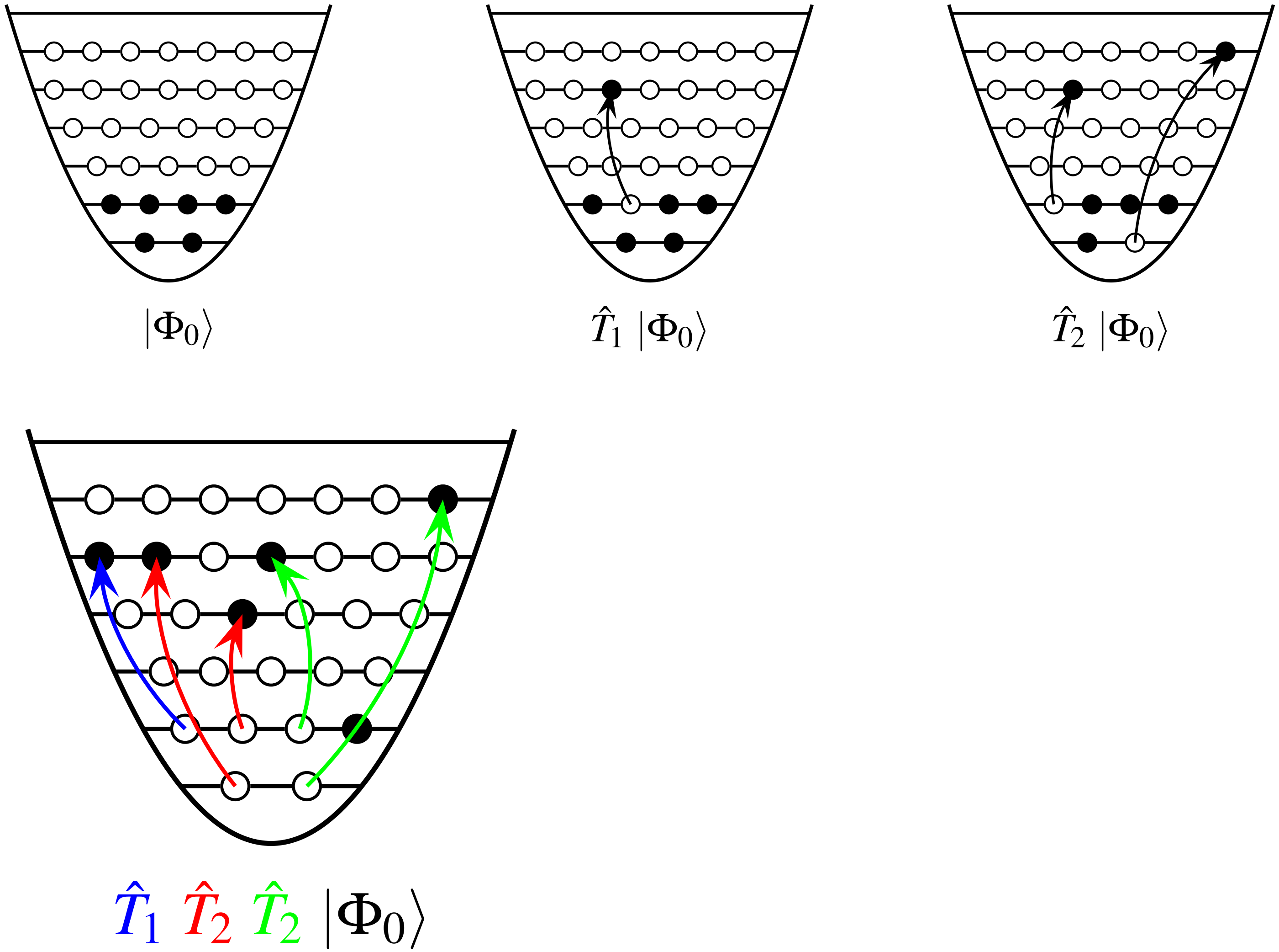

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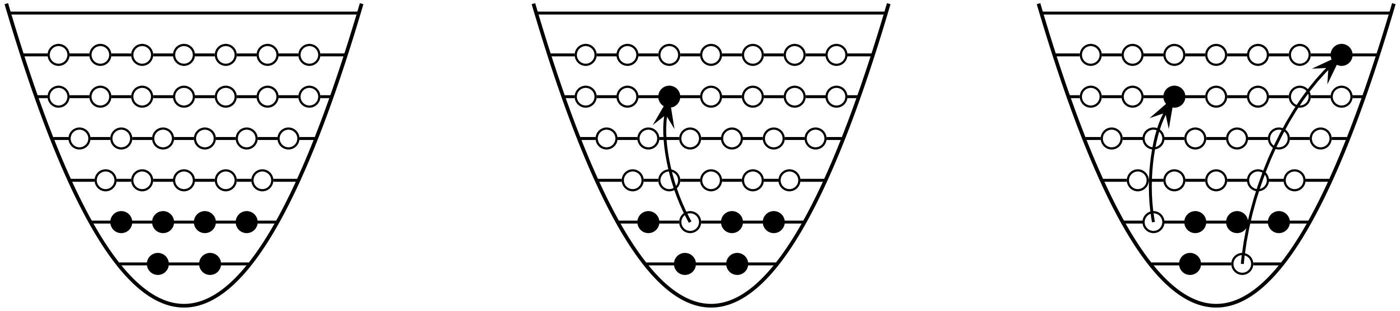
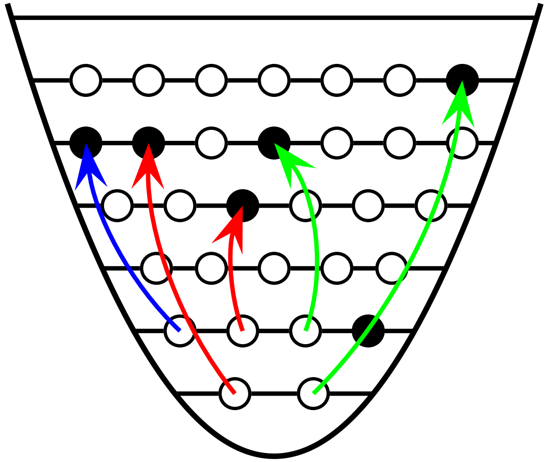


$|\Phi_0\rangle$ $\hat{T}_1\,|\Phi_0\rangle$ $\hat{T}_2\,|\Phi_0\rangle$



$\hat{T}_1\,\hat{T}_2\,\hat{T}_2\,|\Phi_0\rangle$

- higher excitations from products of lower-excitation operators

Coupled Cluster Approach

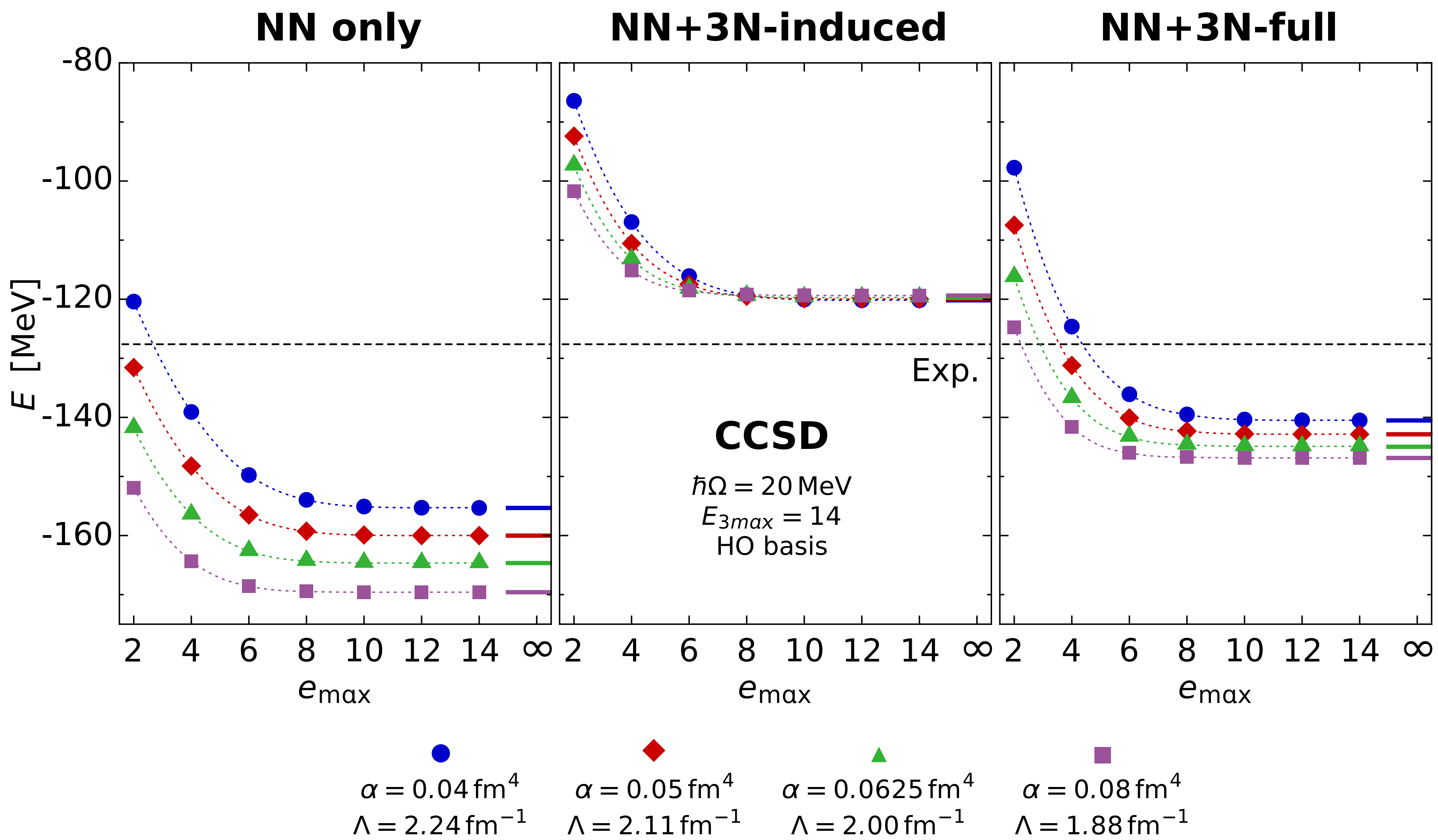
- $|\Psi\rangle$ is parametrized by cluster operator amplitudes t_i^a, t_{ij}^{ab}
- avoid explicit expansion in **many-body basis** (particle number information carried by $|\Phi_0\rangle$)
- **polynomial**, rather than factorial, scaling with mass number A
- exploit **symmetries** (esp. spherical symmetry for closed-shell nuclei)

$$\hat{T}_1 = \sum_{ai} t_i^a \left\{\hat{a}_a^\dagger \otimes \hat{\tilde{a}}_i\right\}_0^{(0)}$$

$$\hat{T}_2 = \sum_{abij}\sum_{J} t_{ij}^{ab}(J) \left\{\left\{\hat{a}_a^\dagger \otimes \hat{a}_b^\dagger\right\}^{(J)} \otimes \left\{\hat{\tilde{a}}_j \otimes \hat{\tilde{a}}_i\right\}^{(J)}\right\}_0^{(0)}$$

- CC suited for **medium-mass** and **heavy regime**

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



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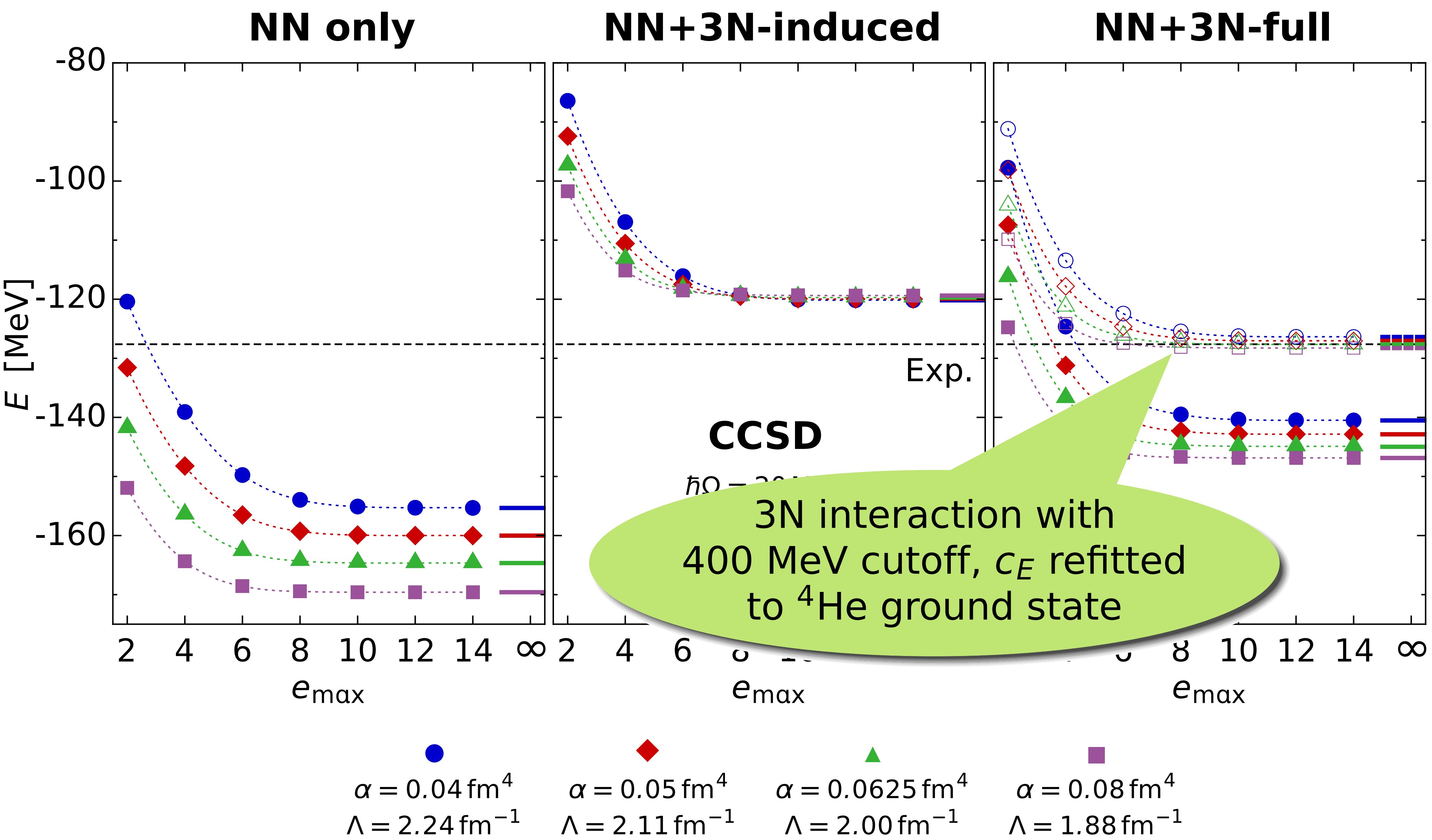
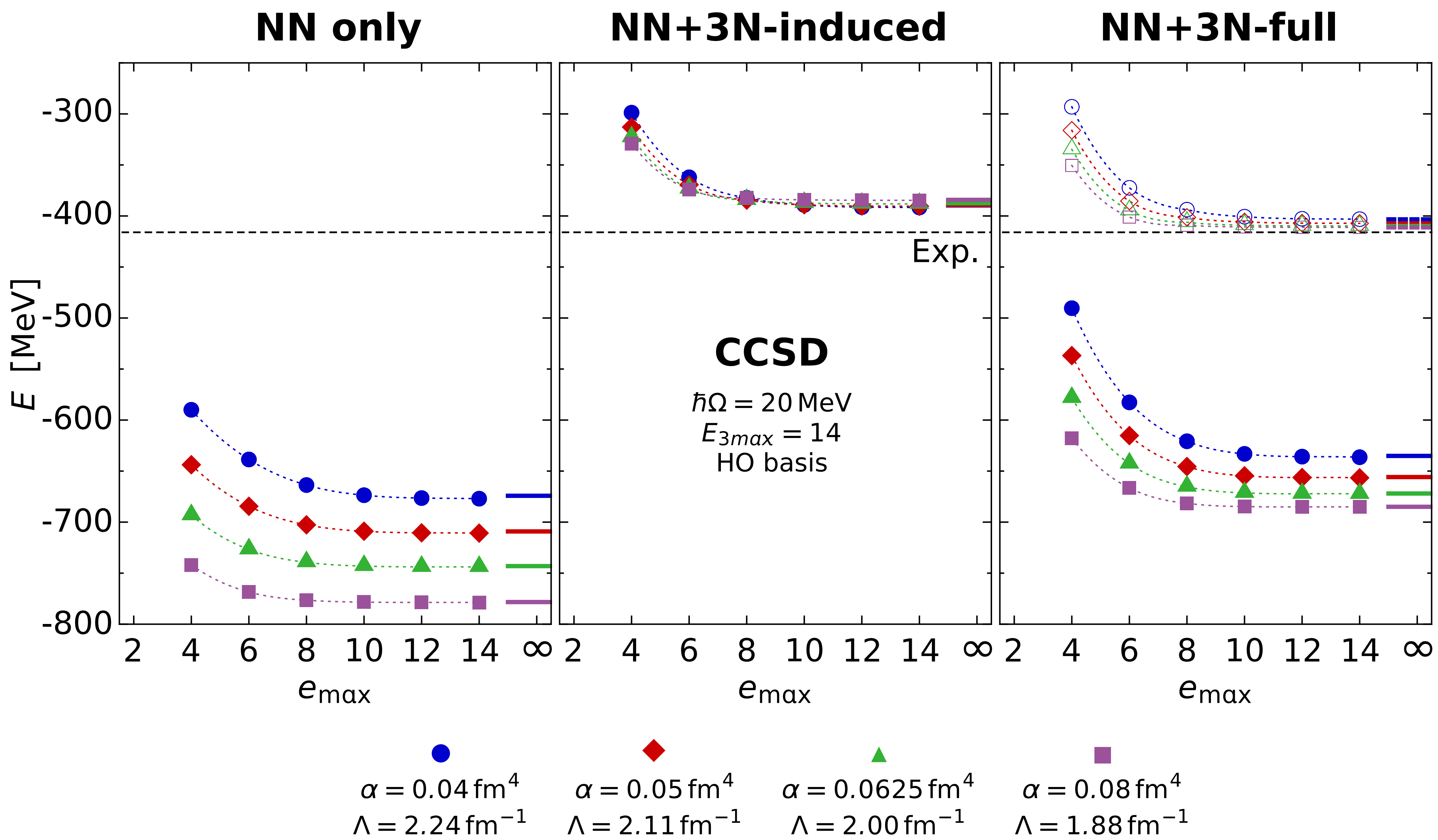


^{48}Ca: Coupled-Cluster with $3N_{NO2B}$



Coupled Cluster Method with Explicit 3N Interactions

Hagen, Papenbrock, Dean et al. — Phys. Rev. C 76, 034302 (2007)
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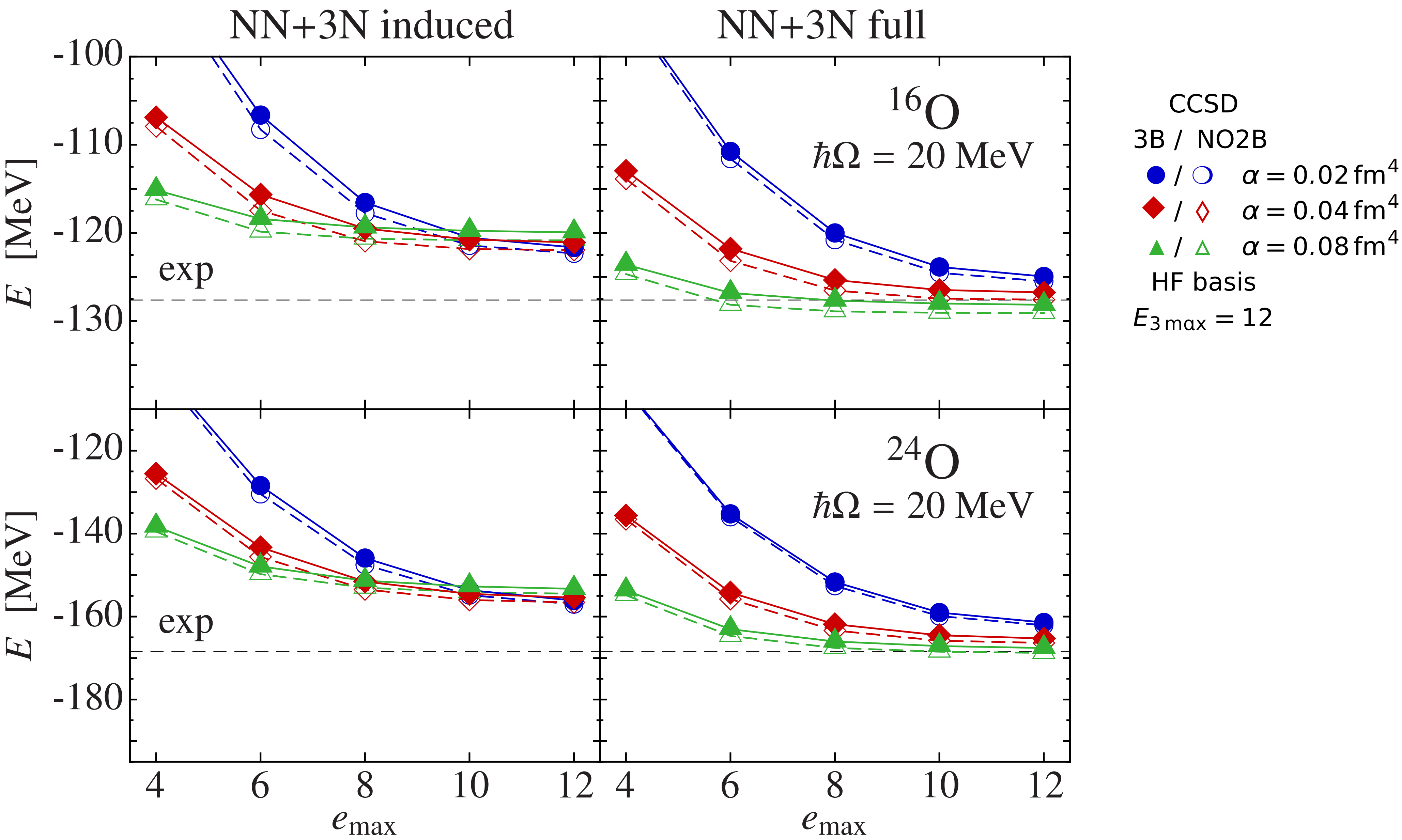
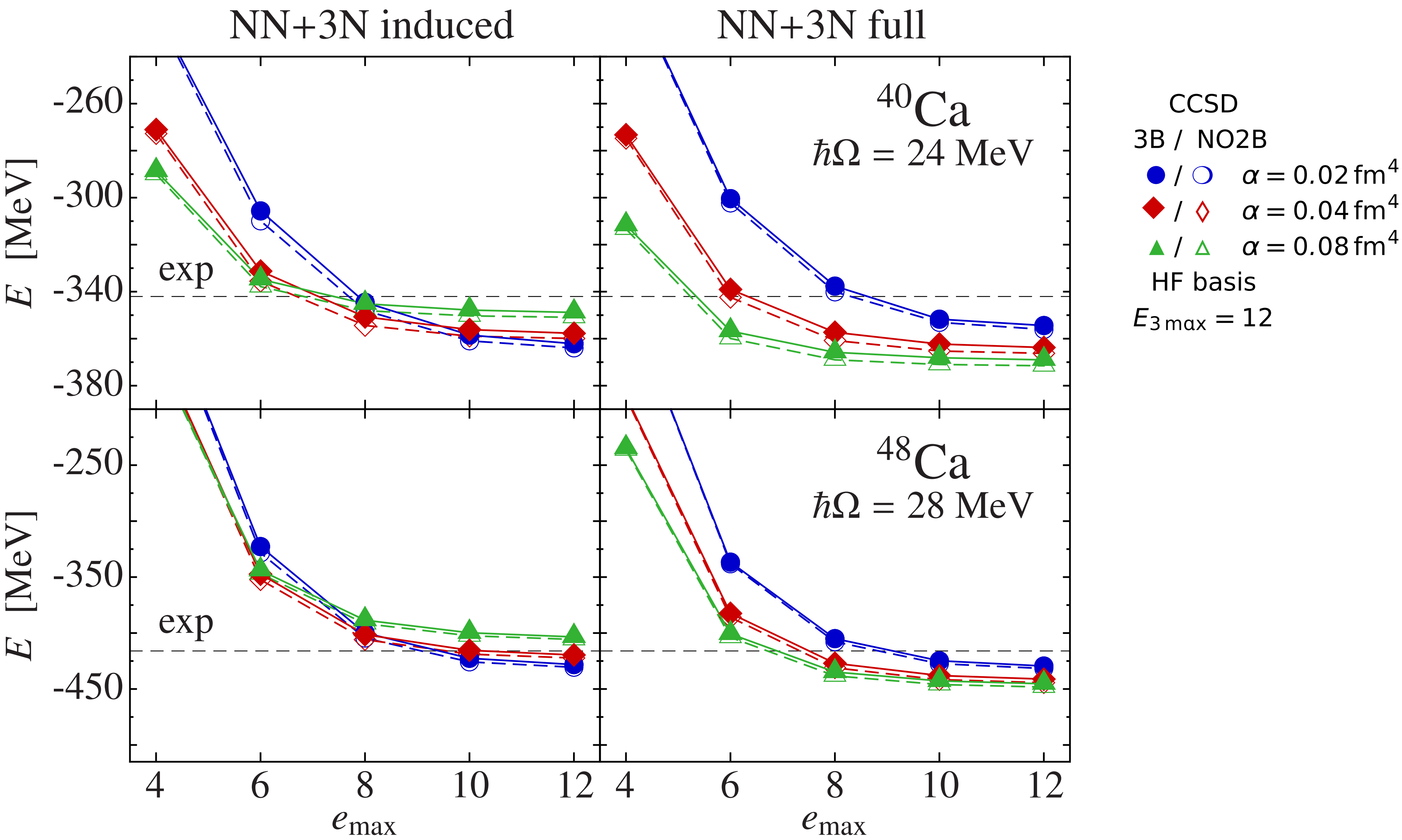


CCSD with Explicit 3N Interaction



$E_{3\text{max}}$ truncation

- full $\hat{V}_{3B}$ matrix **too large** to handle

- ***$E_{\mathbf{3max}}$* truncation** : use $\hat{V}_{3B}$ matrix elements $\langle pqr|\hat{V}_{3B}|stu\rangle$ with

$$e_p + e_q + e_r \ \leq E_{3\text{max}} \ \vee \ e_s + e_t + e_u \ \leq E_{3\text{max}}$$

$$e_p = 2n_p + l_p$$

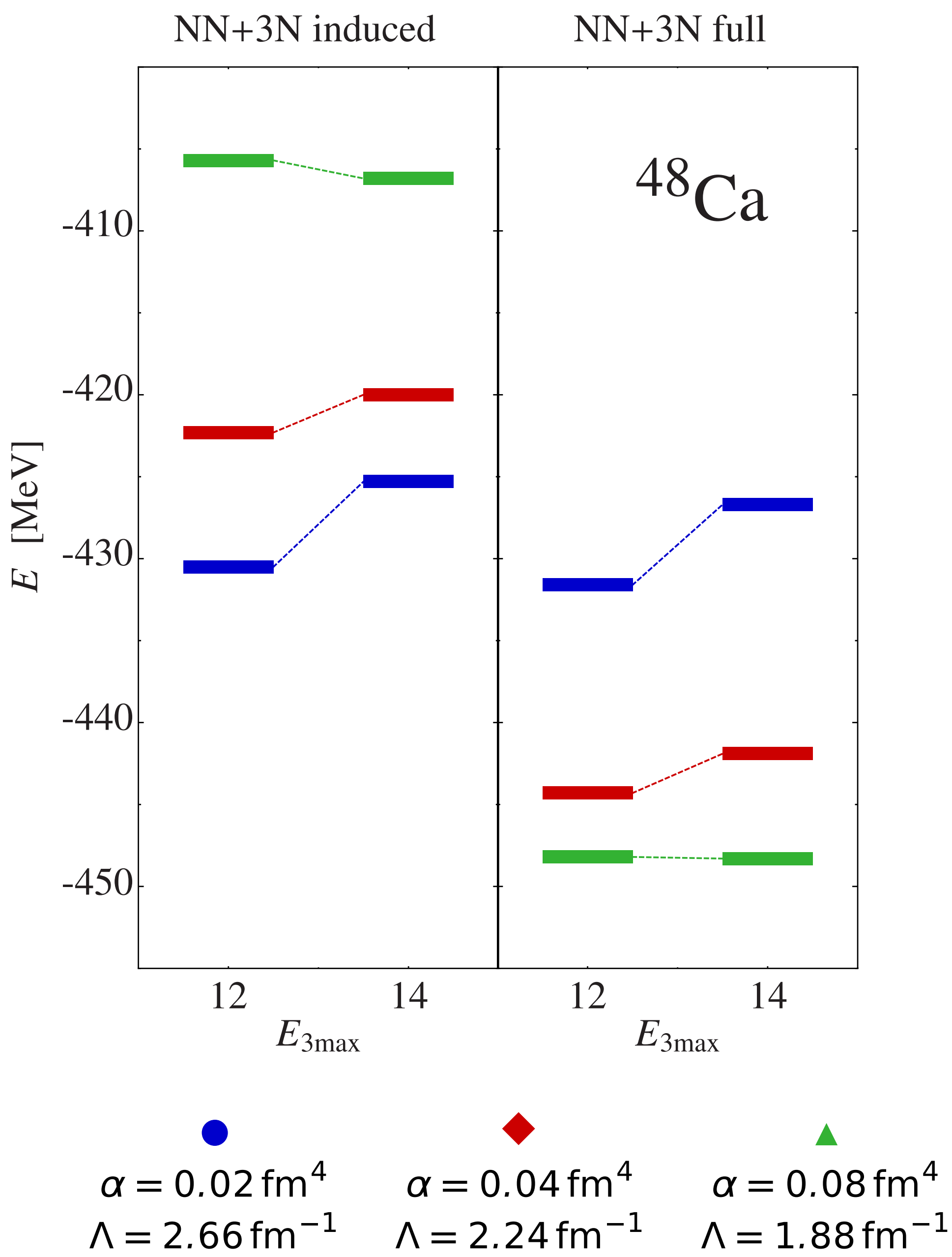
- **current limits**:

$$E_{3\text{max}} \leq \begin{cases} 12 & : \quad \text{CC,} \qquad \text{explicit 3N} \\ 14, \ldots & : \quad \text{NCSM,} \qquad \text{explicit 3N} \\ 14, \ldots & : \quad \text{CC,NCSM} \quad \text{NO2B} \end{cases}$$

storage

availability

E_{3max} Dependence ($CCSD_{NO2B}$)



- E_{3max} not significant for **soft interactions**
- **harder interactions** : up to 2% change in g.s. energies for $E_{3max} = 12 \rightarrow 14$
- α-dependence for **NN+3N induced reduced** for larger E_{3max}
- α-dependence for **NN+3N full enhanced** for larger E_{3max}

ΛCCSD(T) - Improving upon CCSD

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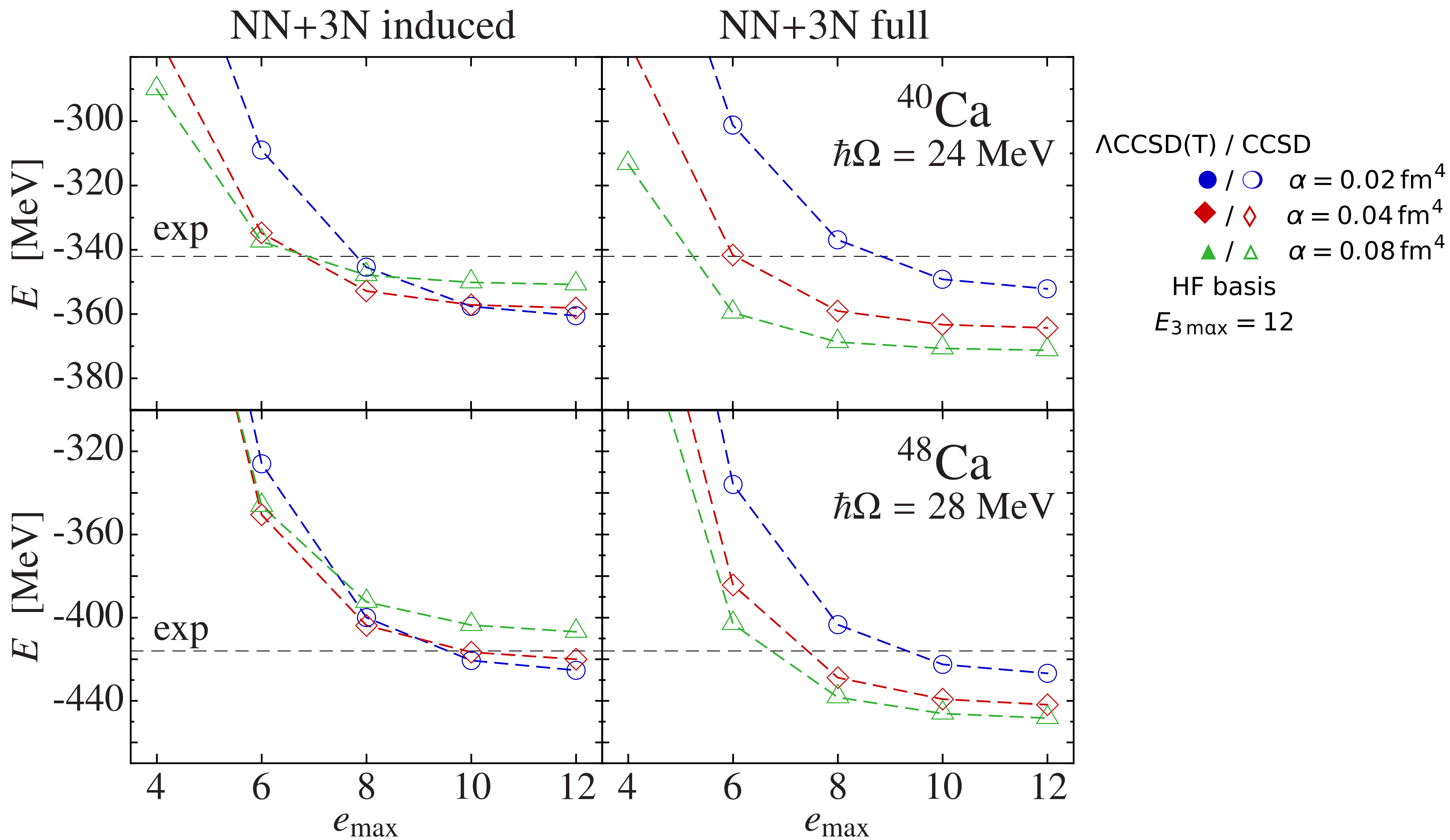
- solution of the Coupled Cluster Λ equations give **a posteriori** fourth order correction to CC energy functional

$$\mathcal{E} = \langle \Phi_0 | (1 + \Lambda) \hat{\mathcal{H}} | \Phi_o \rangle_C$$

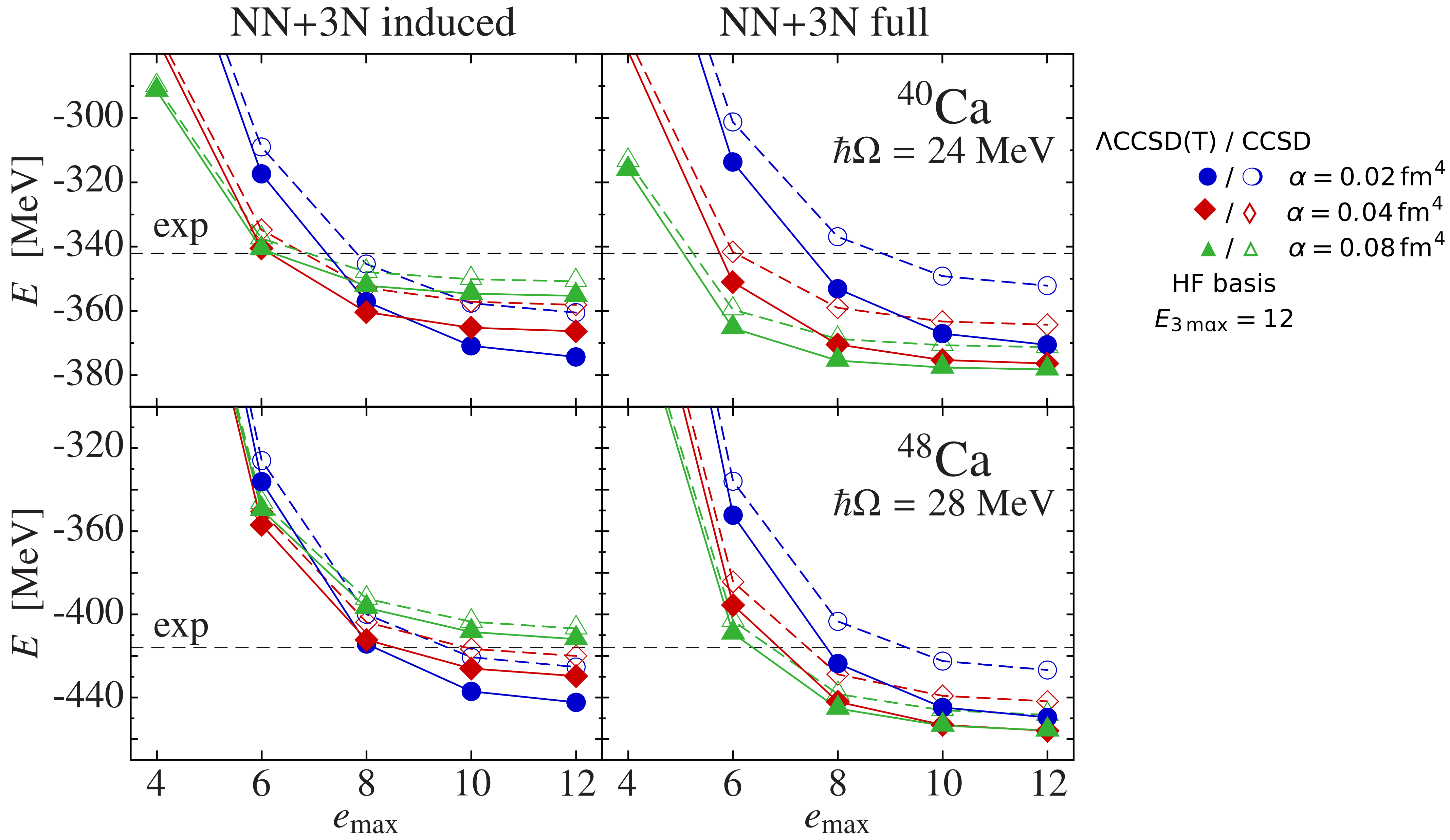
due to triples excitations

$$\delta E_{\Lambda\mathrm{CCSD(T)}} = \frac{1}{(3!)^2} \sum_{\substack{abc \\ ijk}} \tilde{\lambda}^{ijk}_{abc} \frac{1}{\epsilon^{abc}_{ijk}} \tilde{t}^{abc}_{ijk}$$

ΛCCSD(T)$_{NO2B}$


NN+3N induced
NN+3N full
^{40}Ca
ħΩ = 24 MeV
^{48}Ca
ħΩ = 28 MeV
exp
E [MeV]
e_{max}
ΛCCSD(T) / CCSD
α = 0.02 fm^4
α = 0.04 fm^4
α = 0.08 fm^4
HF basis
E_{3max} = 12

ΛCCSD(T)$_{NO2B}$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exp
exp
E [MeV]
E [MeV]
-300
-320
-340
-360
-380
-320
-360
-400
-440
4
6
8
10
12
4
6
8
10
12
e_{max}
e_{max}
ΛCCSD(T) / CCSD
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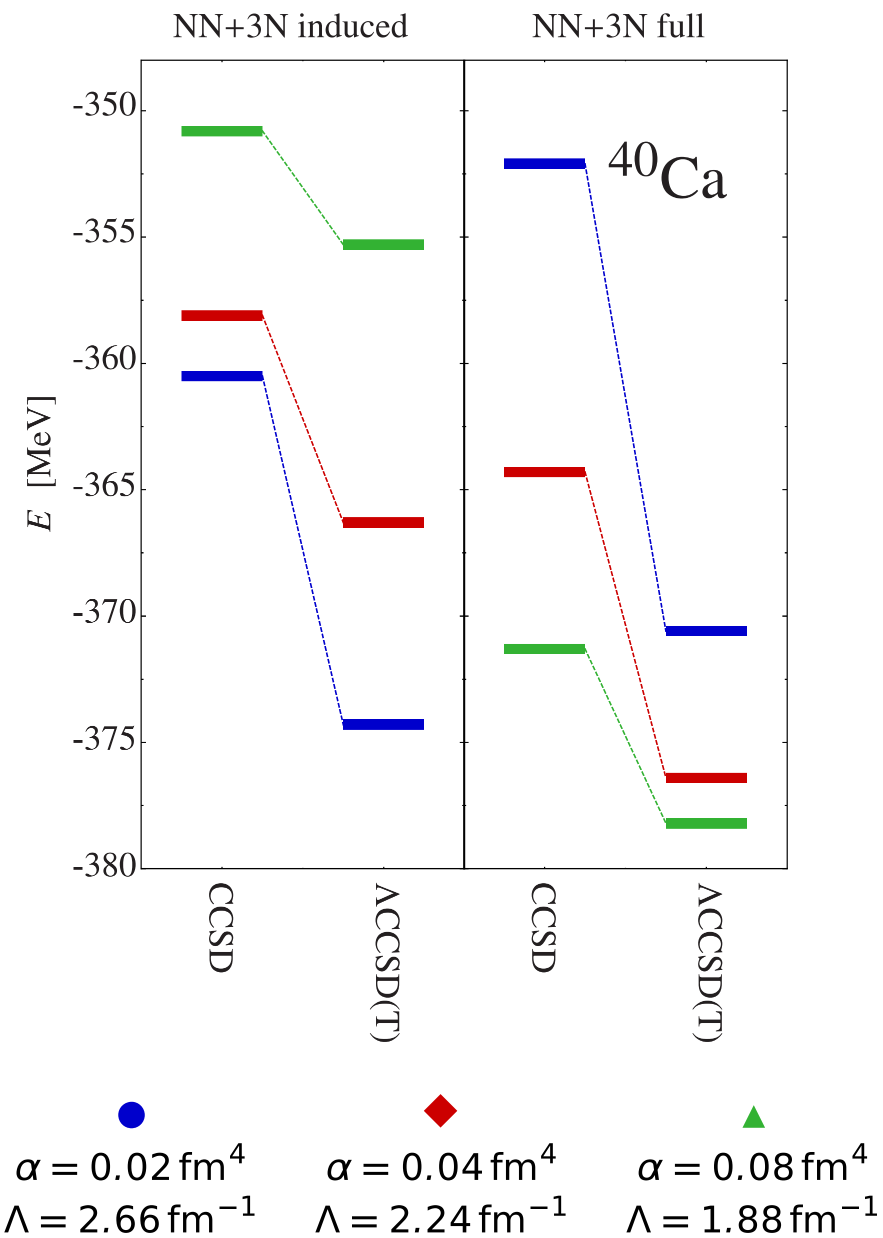
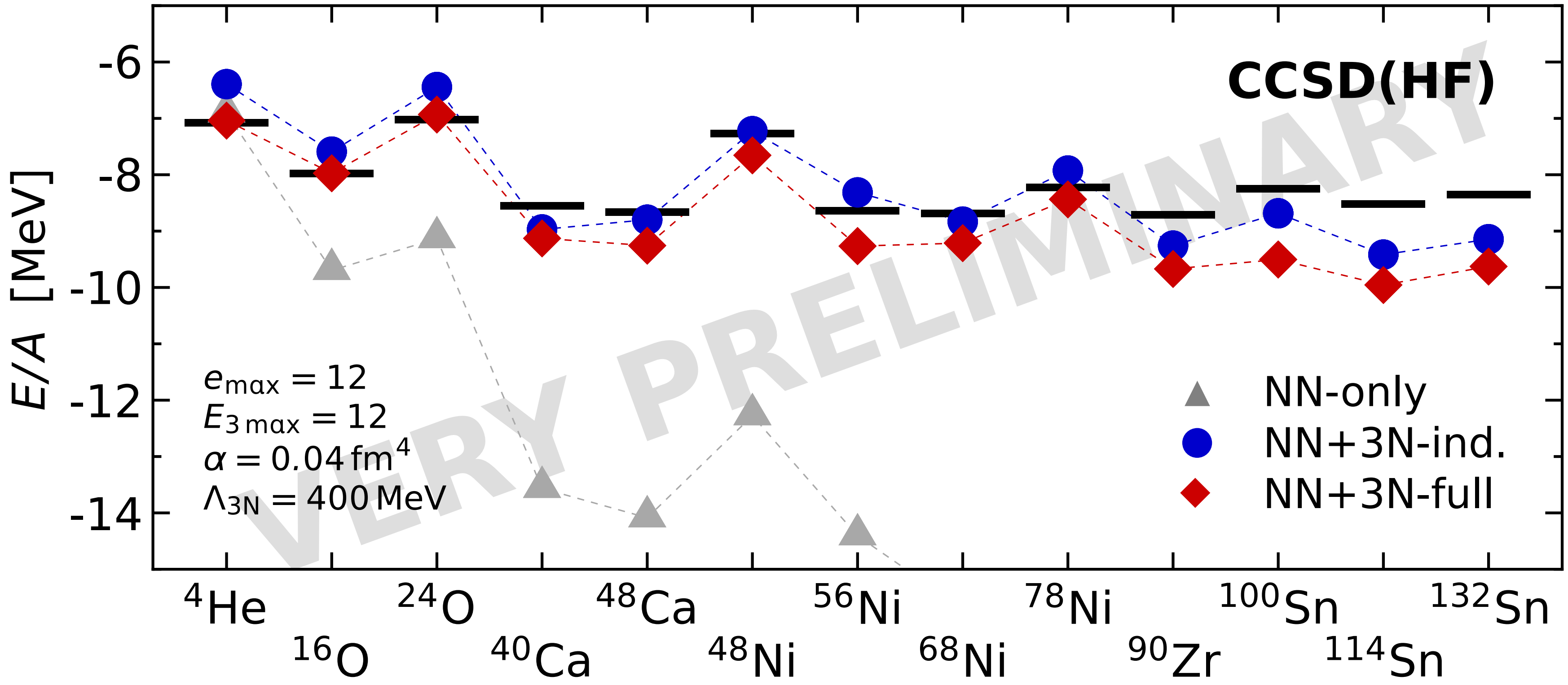
CCSD$_{NO2B}$ vs. ΛCCSD(T)$_{NO2B}$



- inclusion of **triples excitations mandatory** (up to 6 % more binding for heavier nuclei)
- cluster truncation works better for **softer interactions**
- $\alpha = 0.02\ \text{fm}^4$ results not necessarily closer to **exact result** than $\alpha = 0.08\ \text{fm}^4$
- ⇒ calculations with **bare** 3N interaction suffer from cluster truncation and $E_{3\text{max}}$ cut

Goal: Heavy Nuclei



- current $E_{3\,max}$ limits **do not allow for reasonable calculations** beyond $A \geq 60$

Conclusions

- new era of **ab-initio nuclear structure theory** connected to QCD via chiral EFT
- consistent **inclusion of 3N interactions** in similarity transformations & many-body calculations
- normal-ordering approximation as **efficient and accurate way** to include 3N interactions
- many-body calculations extended to the **medium-mass** regime

Epilogue

- **thanks to my group & my collaborators**
  - **A. Calci**, B. Erler, E. Gebrerufael, A. Günther, H. Krutsch, **J. Langhammer**, S. Reinhardt, **R. Roth**, C. Stumpf, R. Trippel, K. Vobig, R. Wirth
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  - S. Quaglioni
    LLNL Livermore, USA
  - P. Piecuch
    Michigan State University, USA
  - H. Hergert
    Ohio State University, USA
  - P. Papakonstantinou
    IPN Orsay, F
  - C. Forssén
    Chalmers University, Sweden
  - H. Feldmeier, T. Neff
    GSI Helmholtzzentrum

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Deutsche Forschungsgemeinschaft DFG

HIC for FAIR Helmholtz International Center

LOEWE – Landes-Offensive zur Entwicklung Wissenschaftlich-ökonomischer Exzellenz

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