Ab Initio Calculations of Medium-Mass Nuclei and Normal-Ordered Chiral NN+3N Interactions

Sven Binder
INSTITUT FÜR KERNPHYSIK

TECHNISCHE UNIVERSITÄT DARMSTADT

From QCD to Nuclear Structure

Nuclear Structure

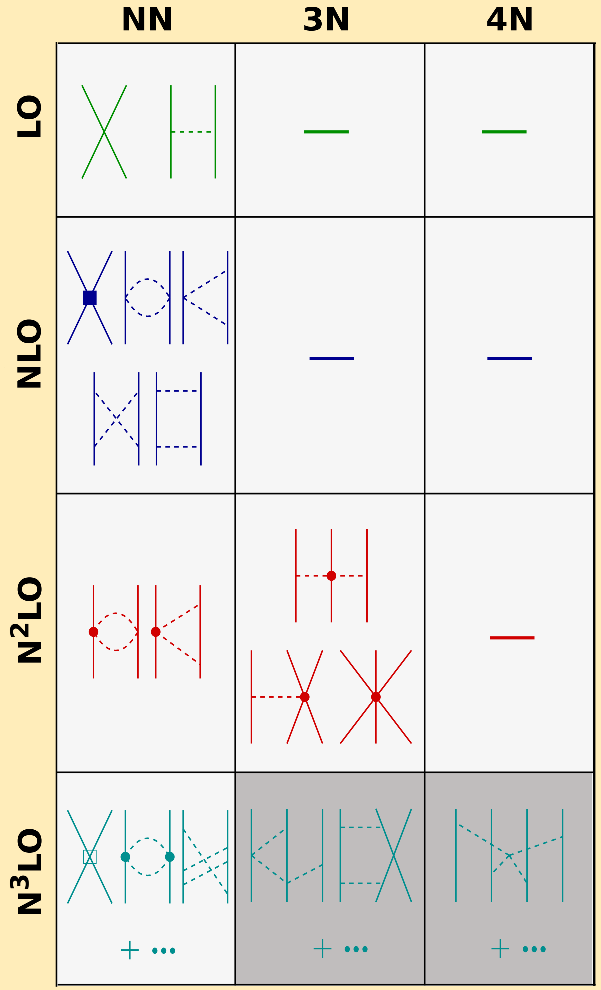
Low-Energy QCD

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

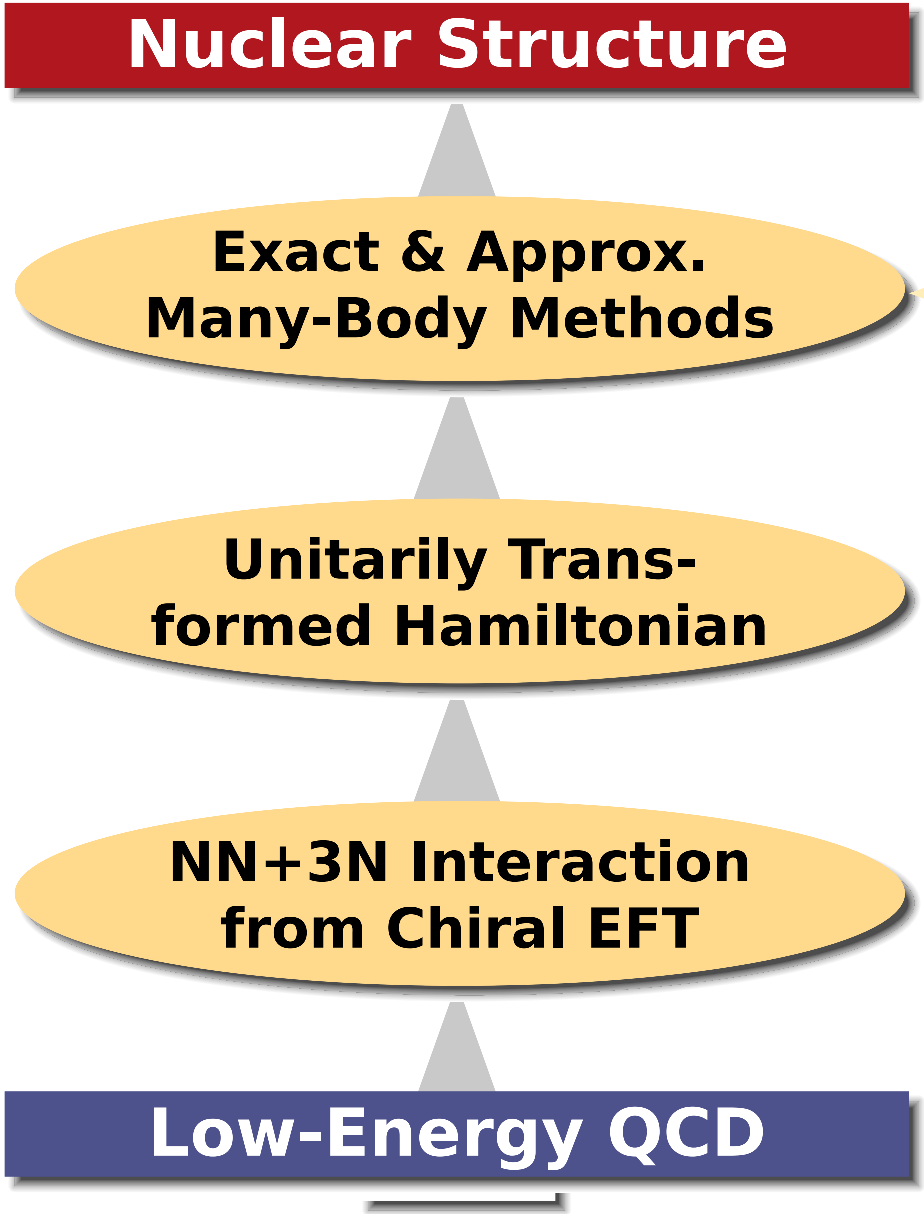
Unitarily Transformed Hamiltonian

- adapt Hamiltonian to truncated low-energy model space

NN+3N Interaction from Chiral EFT

Low-Energy QCD

From QCD to Nuclear Structure



- 'exact' 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

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

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

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

Similarity Renormalization Group

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

- **unitary transformation** of Hamil

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

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

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

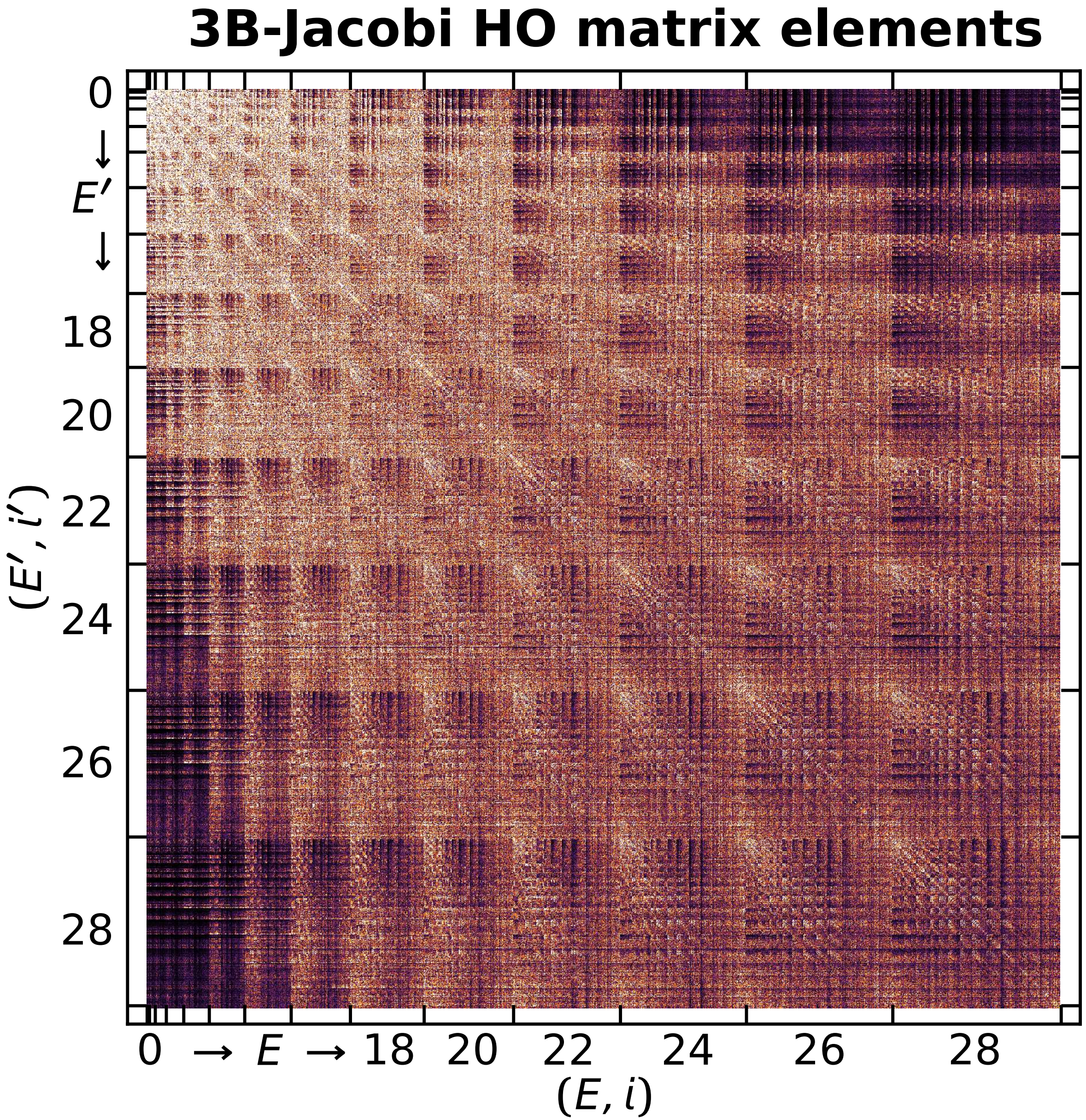
- **dynamic generator**: commutator with the operator in whose eigenbasis H shall be diagonalized

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

simplicity and flexibility
are great advantages of
the SRG approach

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

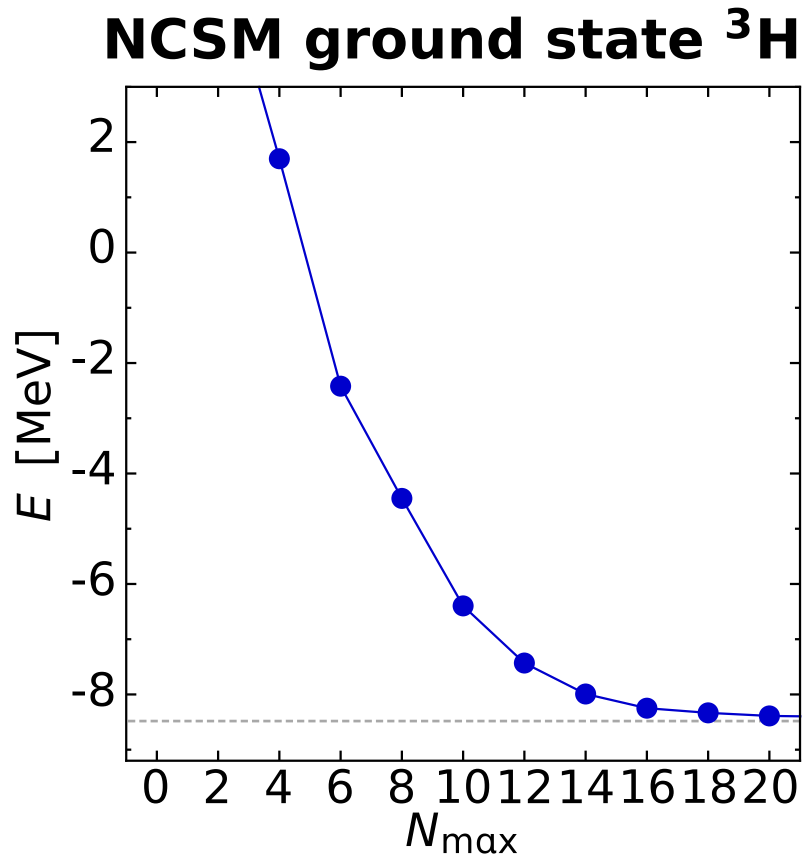
SRG Evolution in Three-Body Space



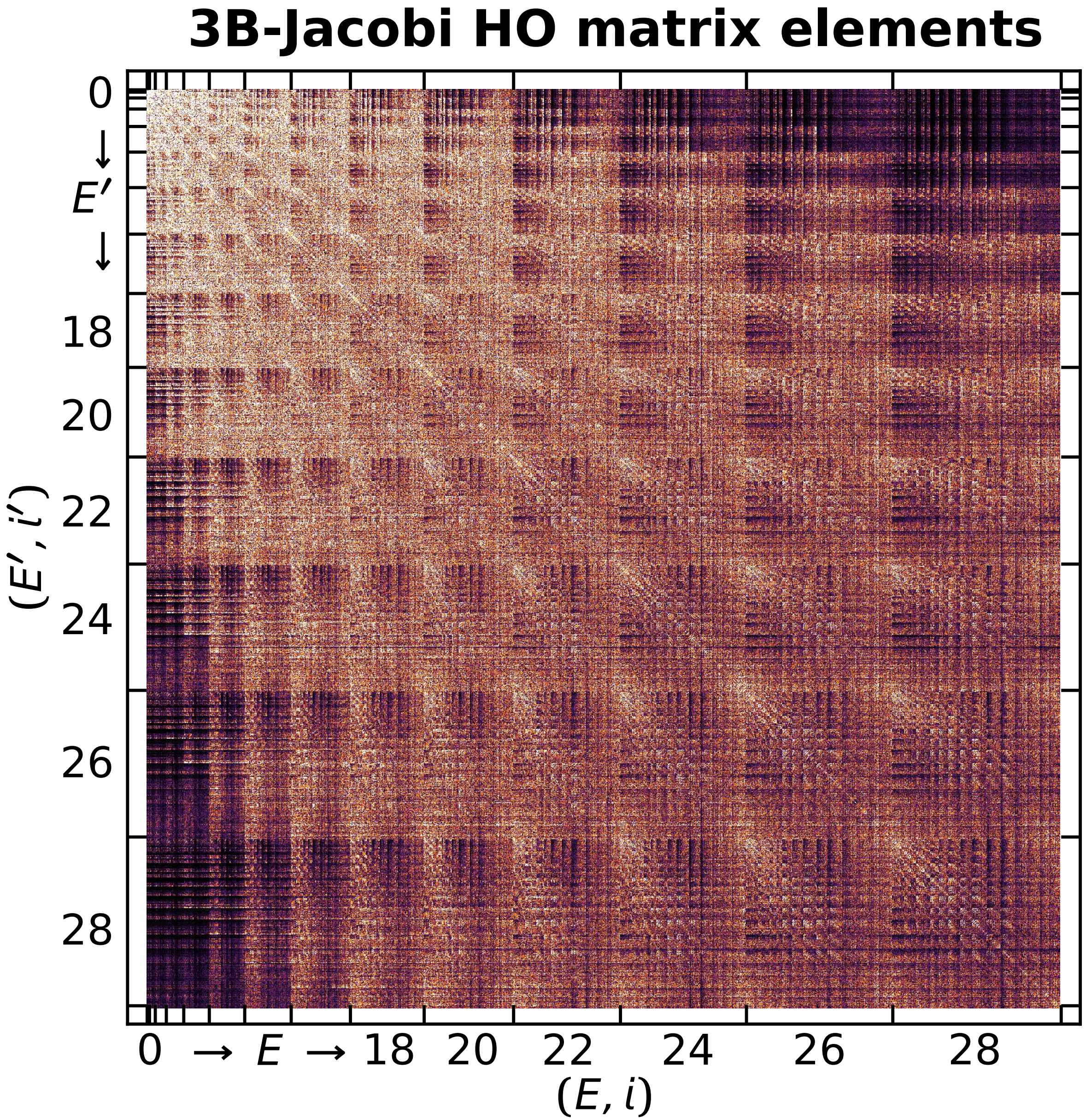
chiral NN+3N

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

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



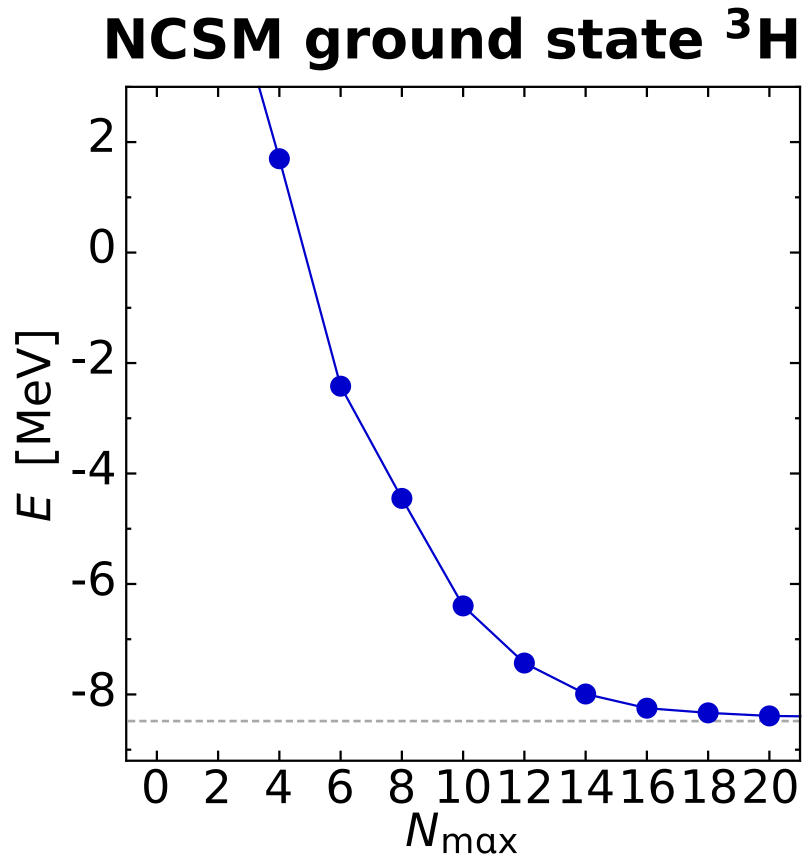
SRG Evolution in Three-Body Space



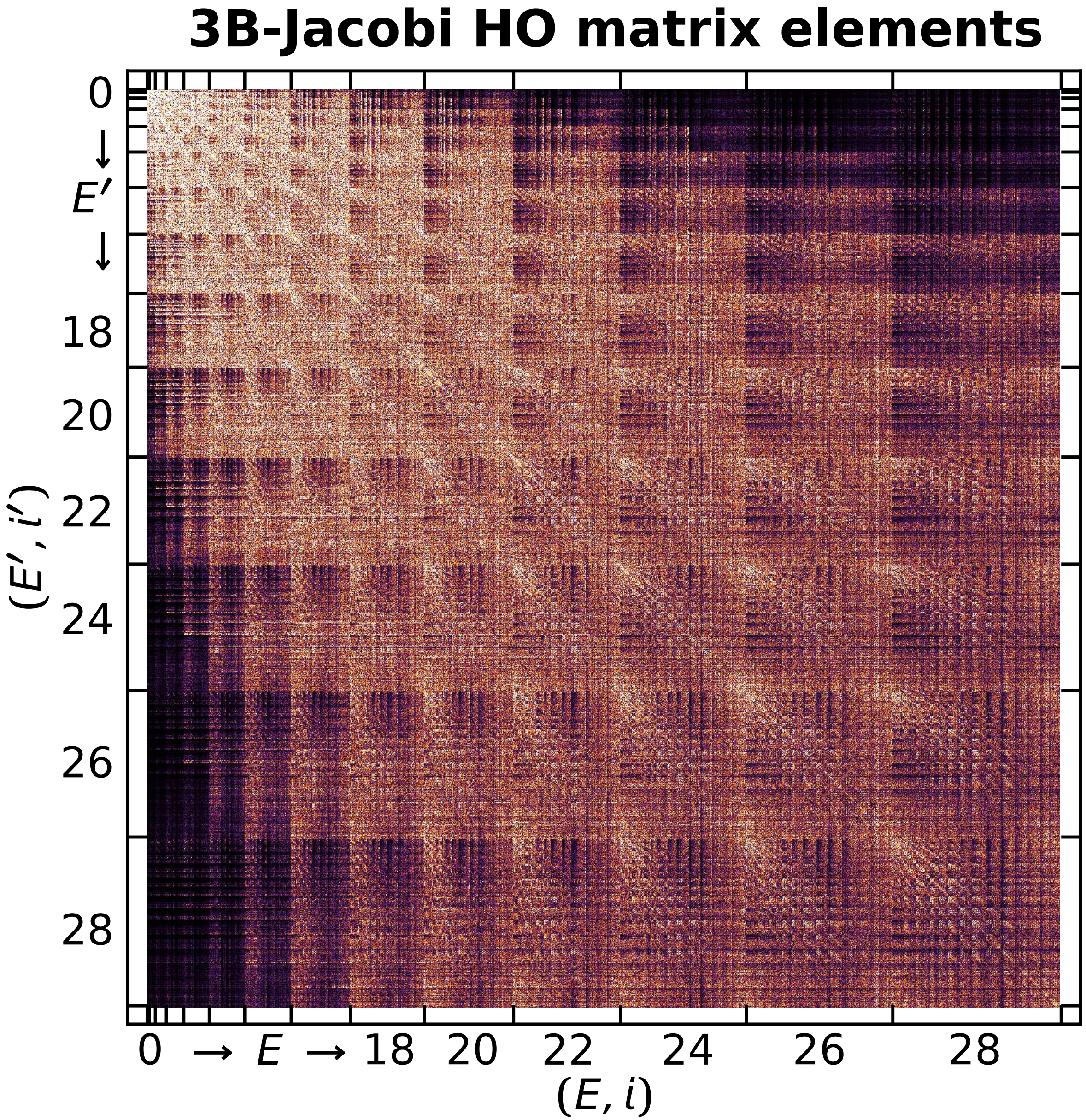
$\alpha = 0.000\,\mathrm{fm}^4$

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

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



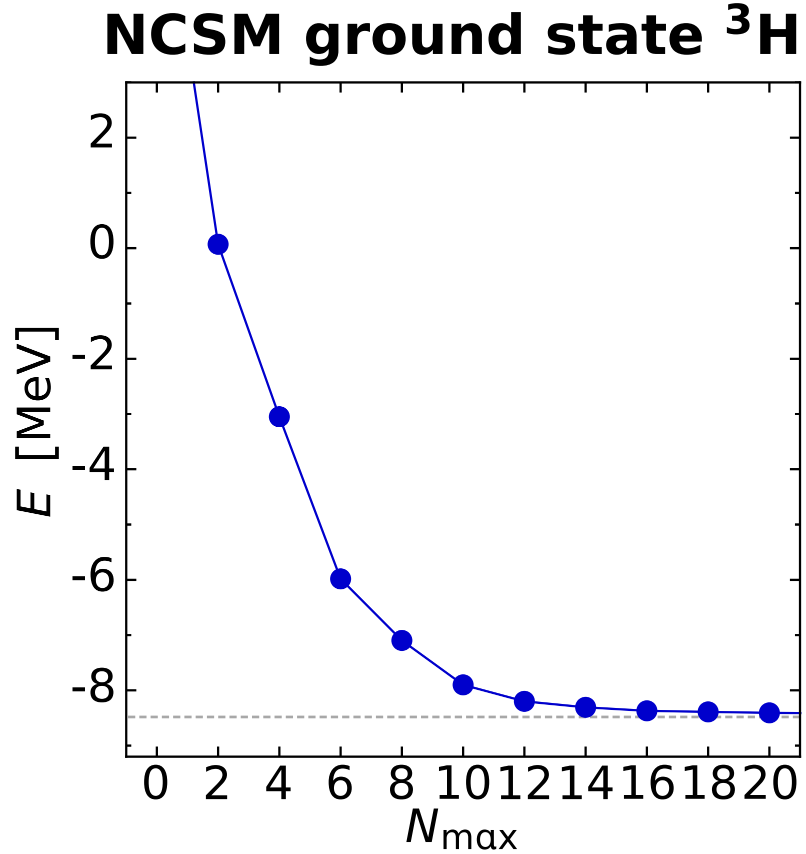
SRG Evolution in Three-Body Space



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

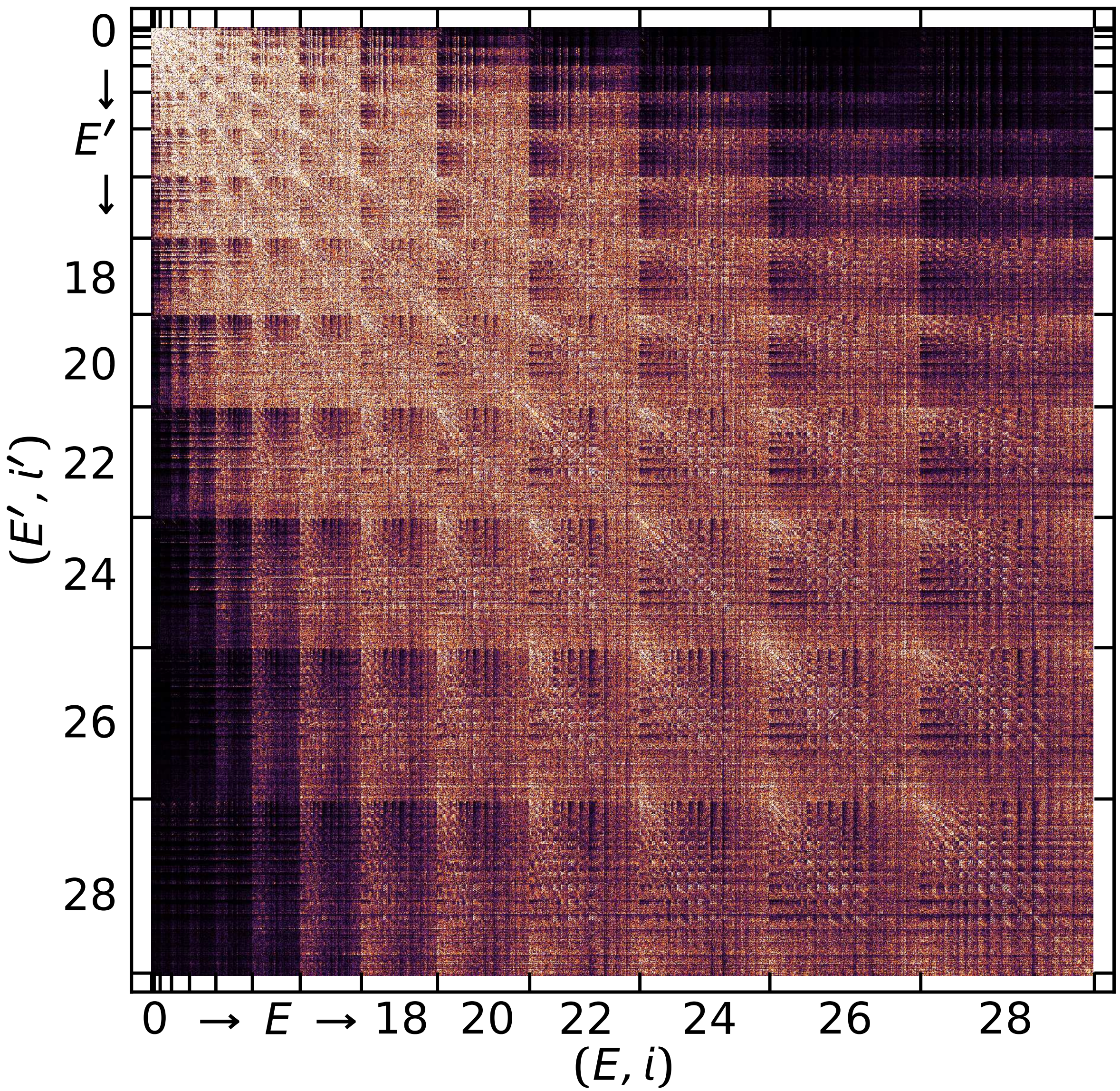
$\Lambda = 3.16\,\text{fm}^{-1}$

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



SRG Evolution in Three-Body Space

3B-Jacobi HO matrix elements

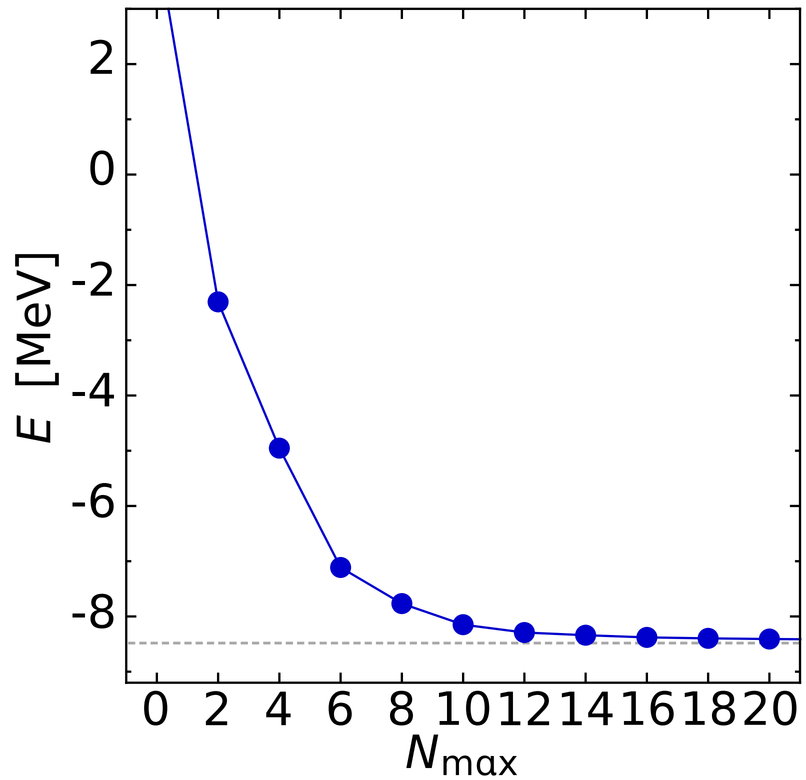


$$\alpha = 0.020\,\mathrm{fm}^4$$

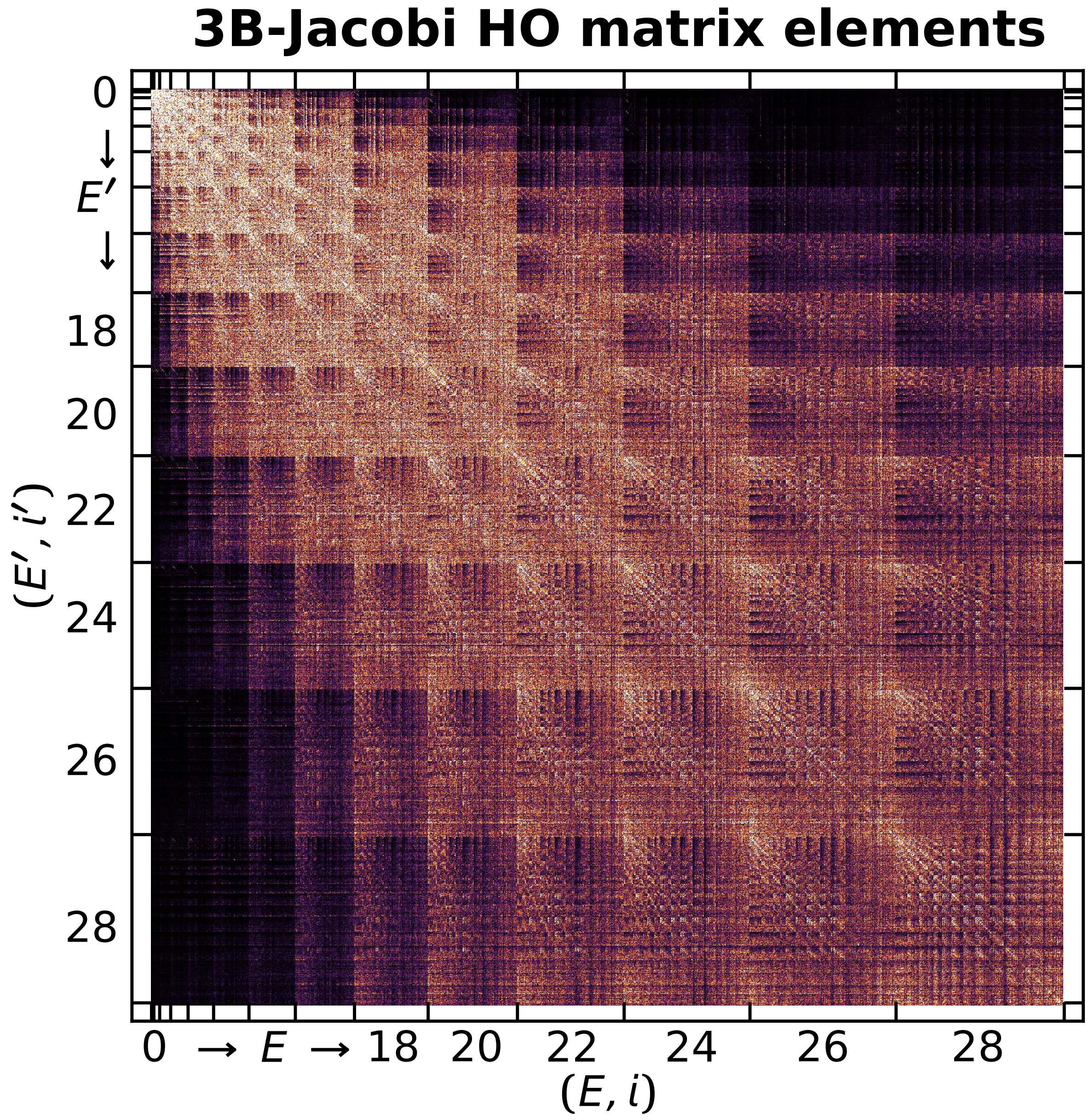
$\Lambda = 2.66\,\mathrm{fm}^{-1}$

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

NCSM ground state ^{3}H



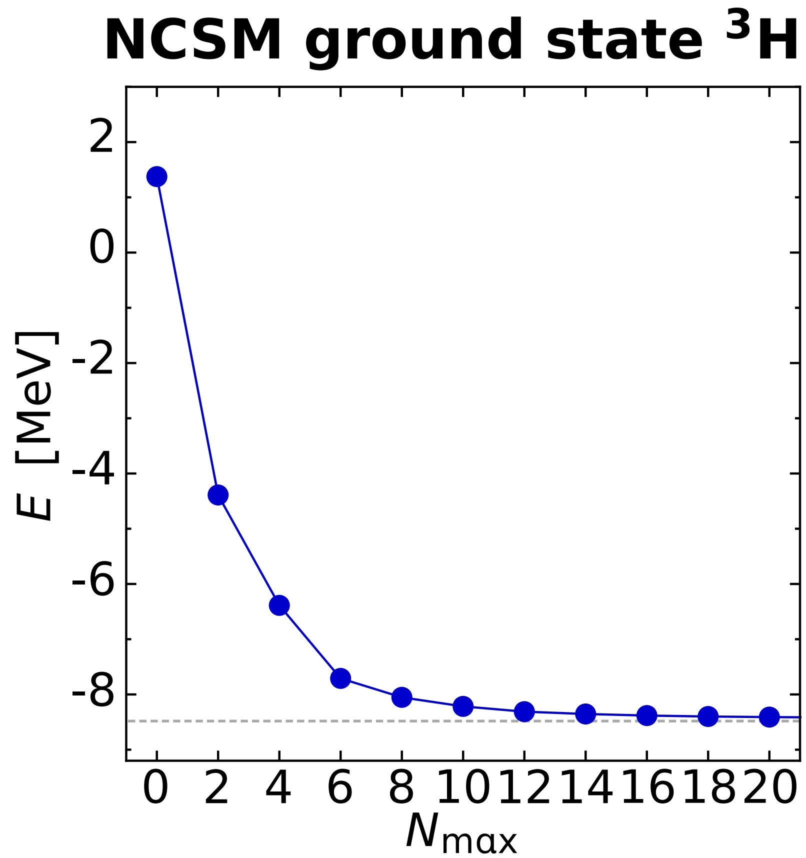
SRG Evolution in Three-Body Space



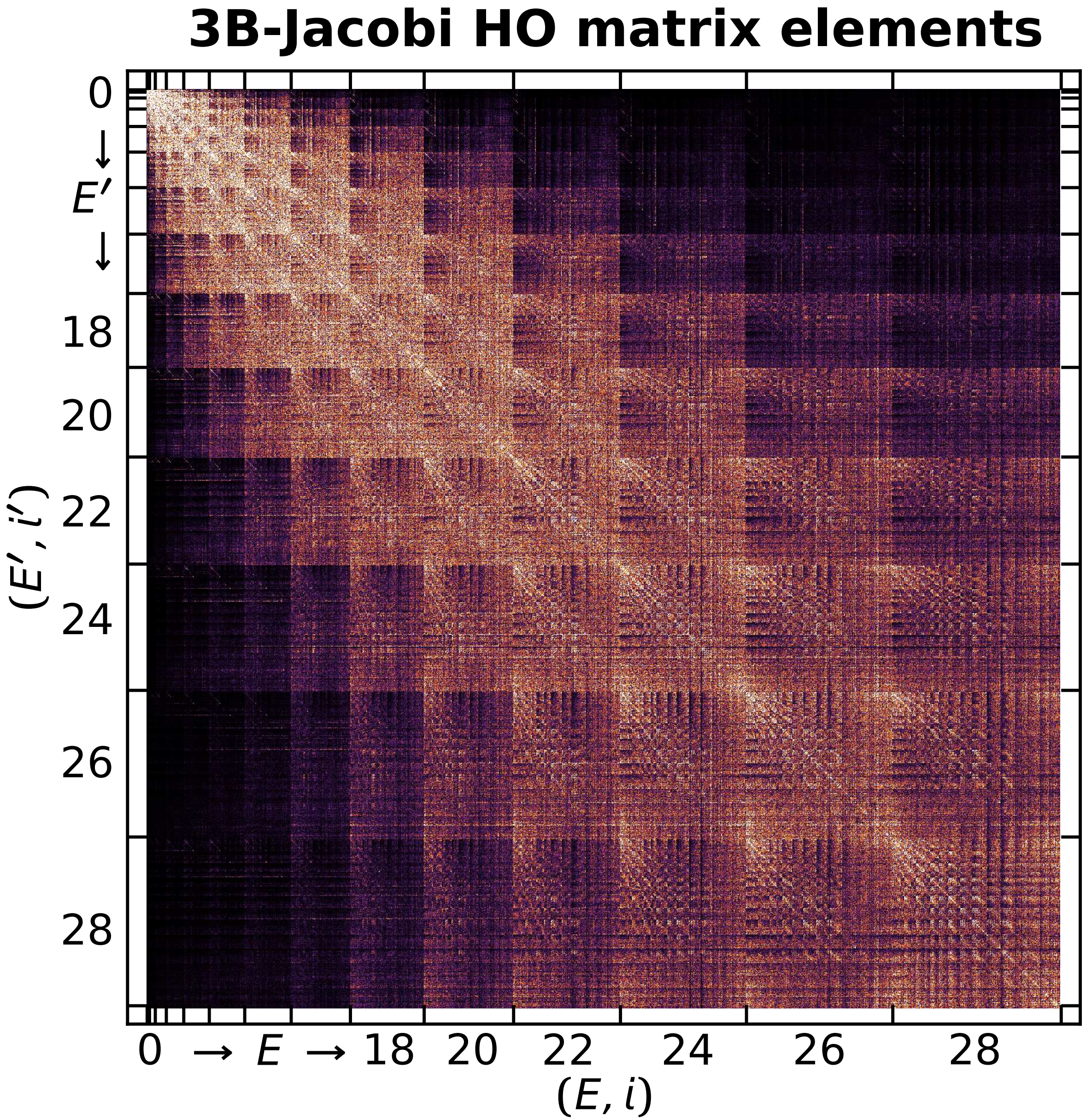
$\alpha = 0.040\,\text{fm}^4$

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

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



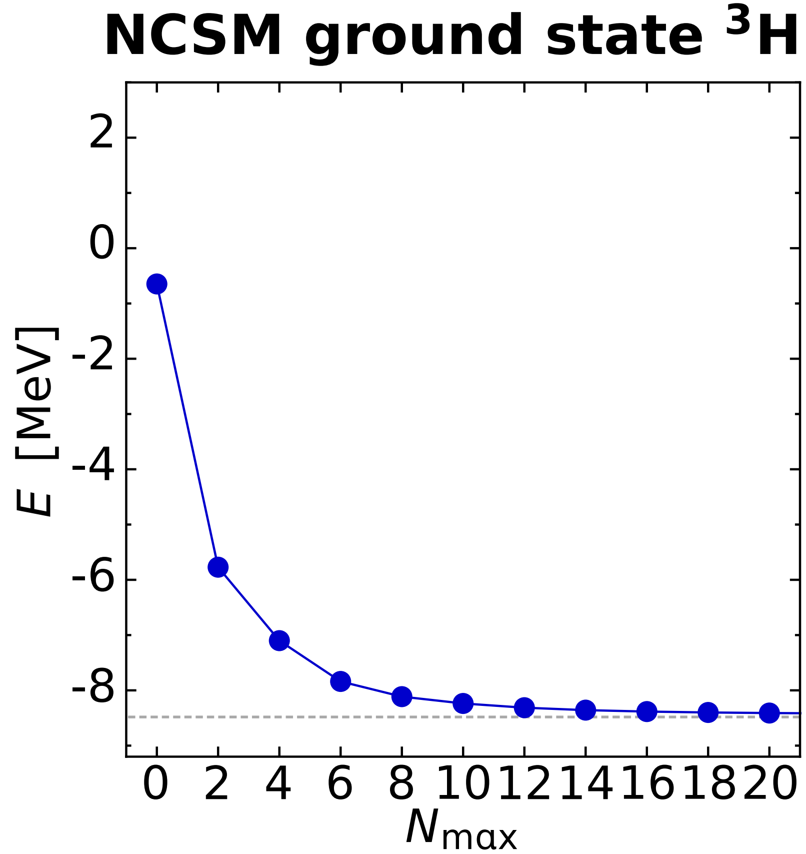
SRG Evolution in Three-Body Space



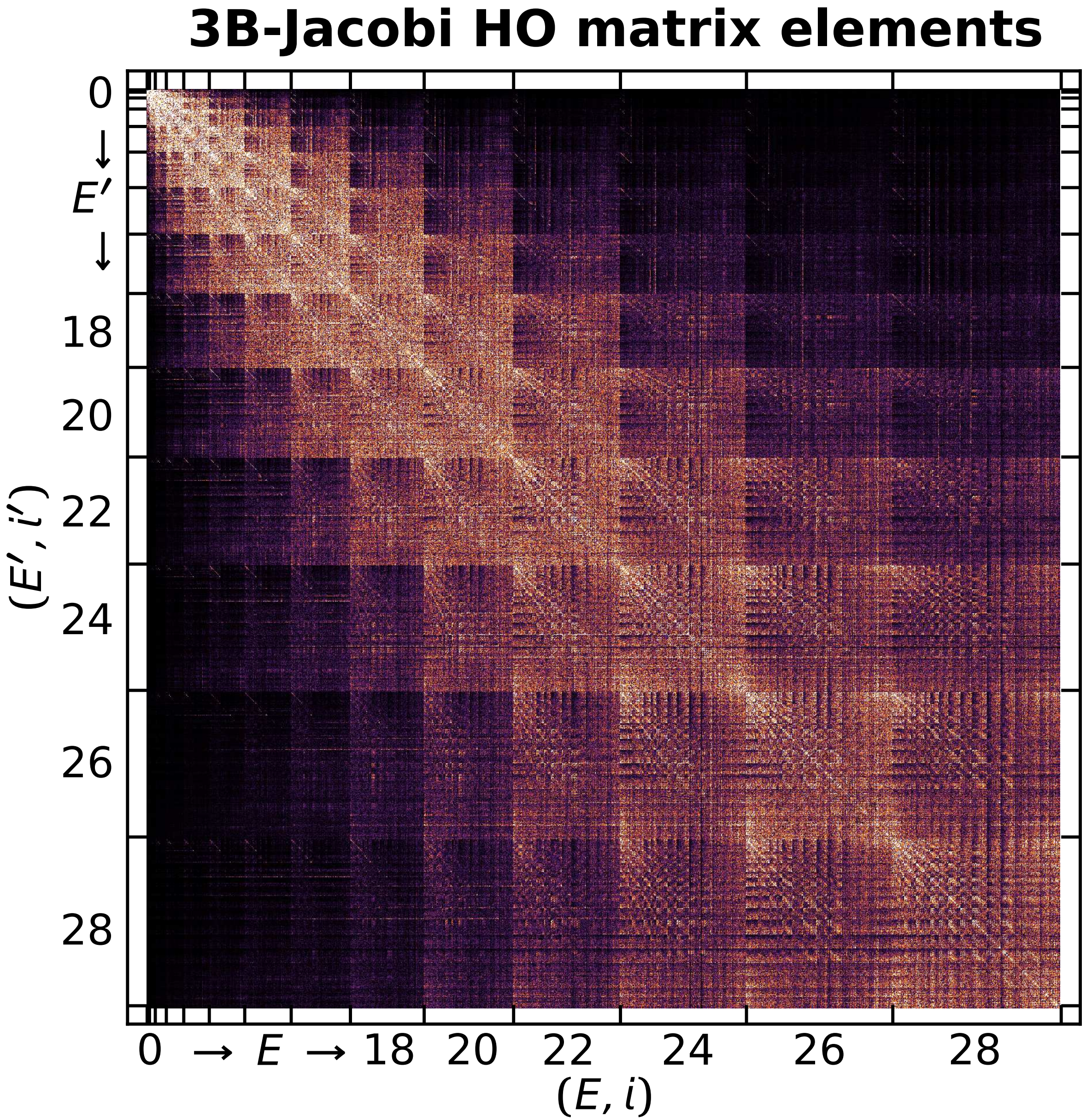
$\alpha = 0.080\,\mathrm{fm}^4$

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

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



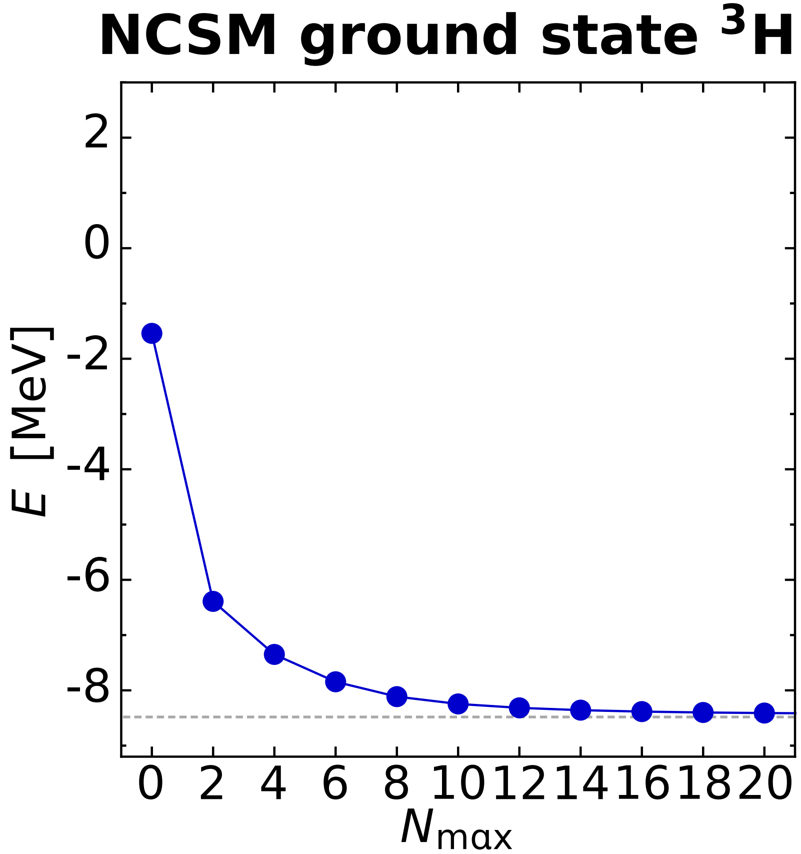
SRG Evolution in Three-Body Space



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

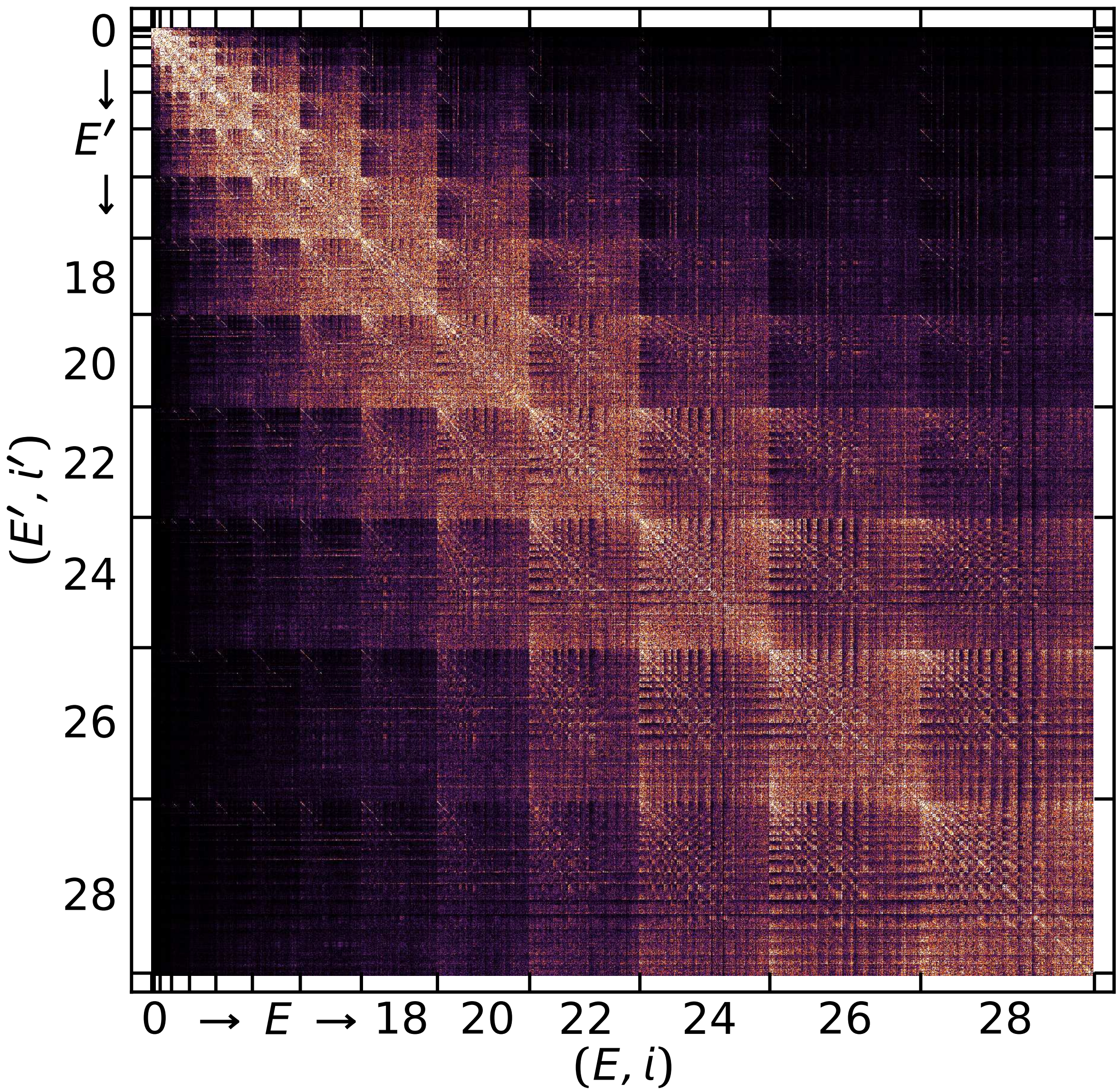
$\Lambda = 1.58\,\mathrm{fm}^{-1}$

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



SRG Evolution in Three-Body Space

3B-Jacobi HO matrix elements

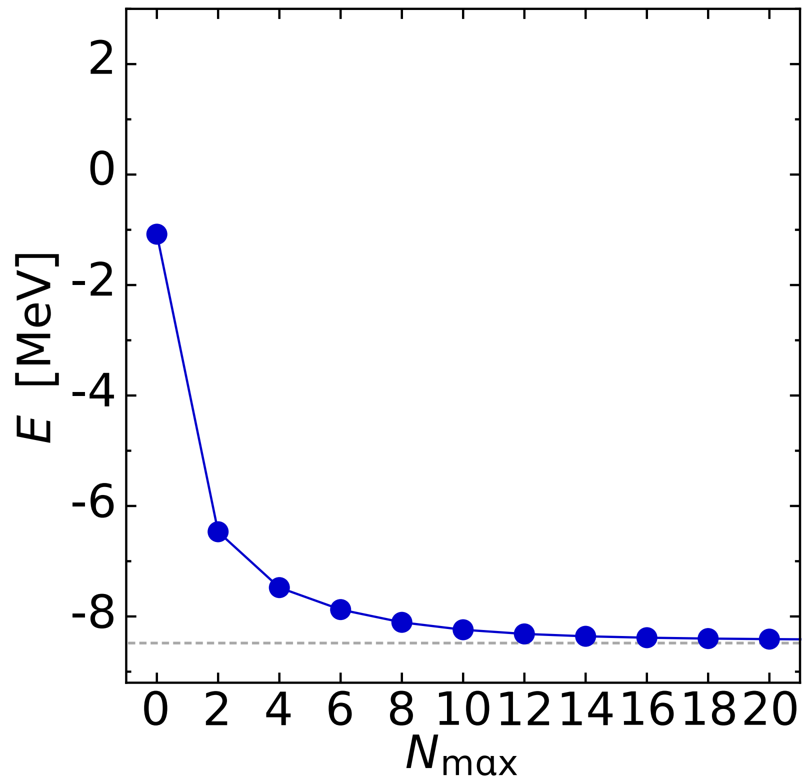


$$\alpha = 0.320\,\mathrm{fm}^4$$

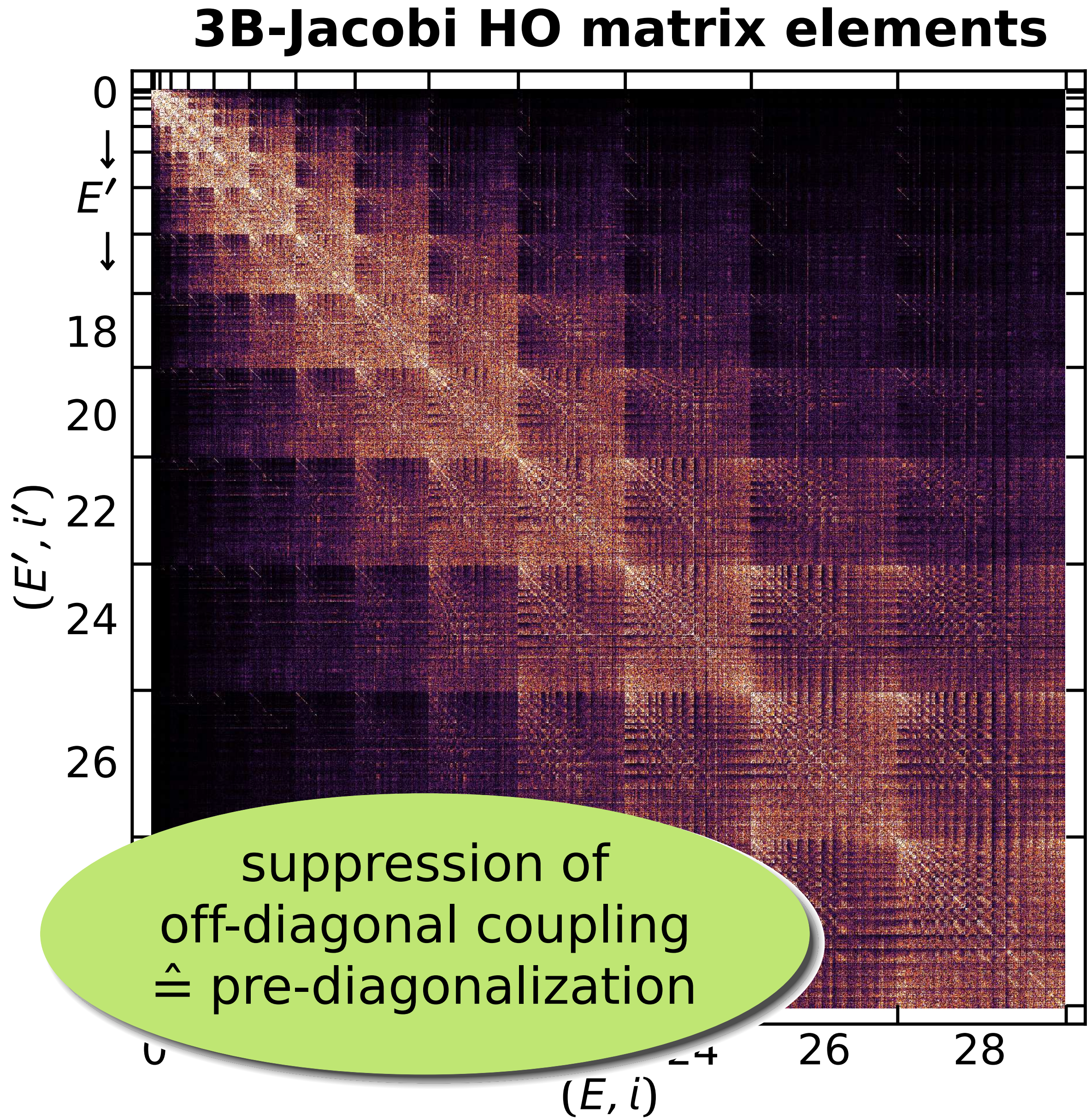
$\Lambda = 1.33\,\mathrm{fm}^{-1}$

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

NCSM ground state ^{3}H



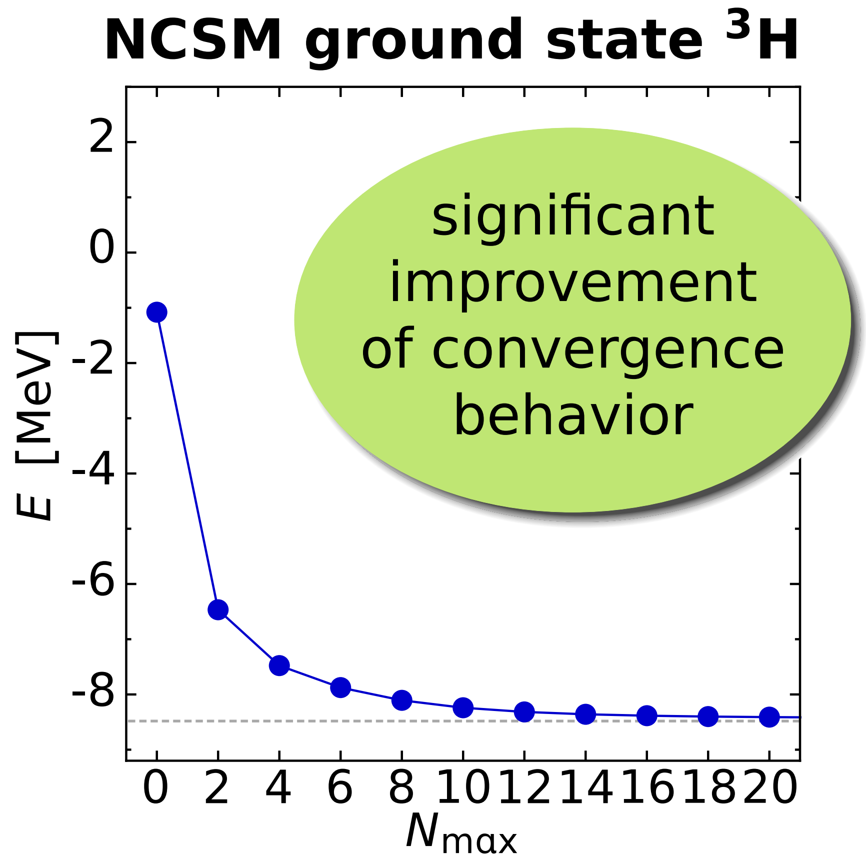
SRG Evolution in Three-Body Space



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

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

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



Calculations in *A*-Body Space

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

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

- 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

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

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

- 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

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

Importance-Truncated No-Core Shell Model

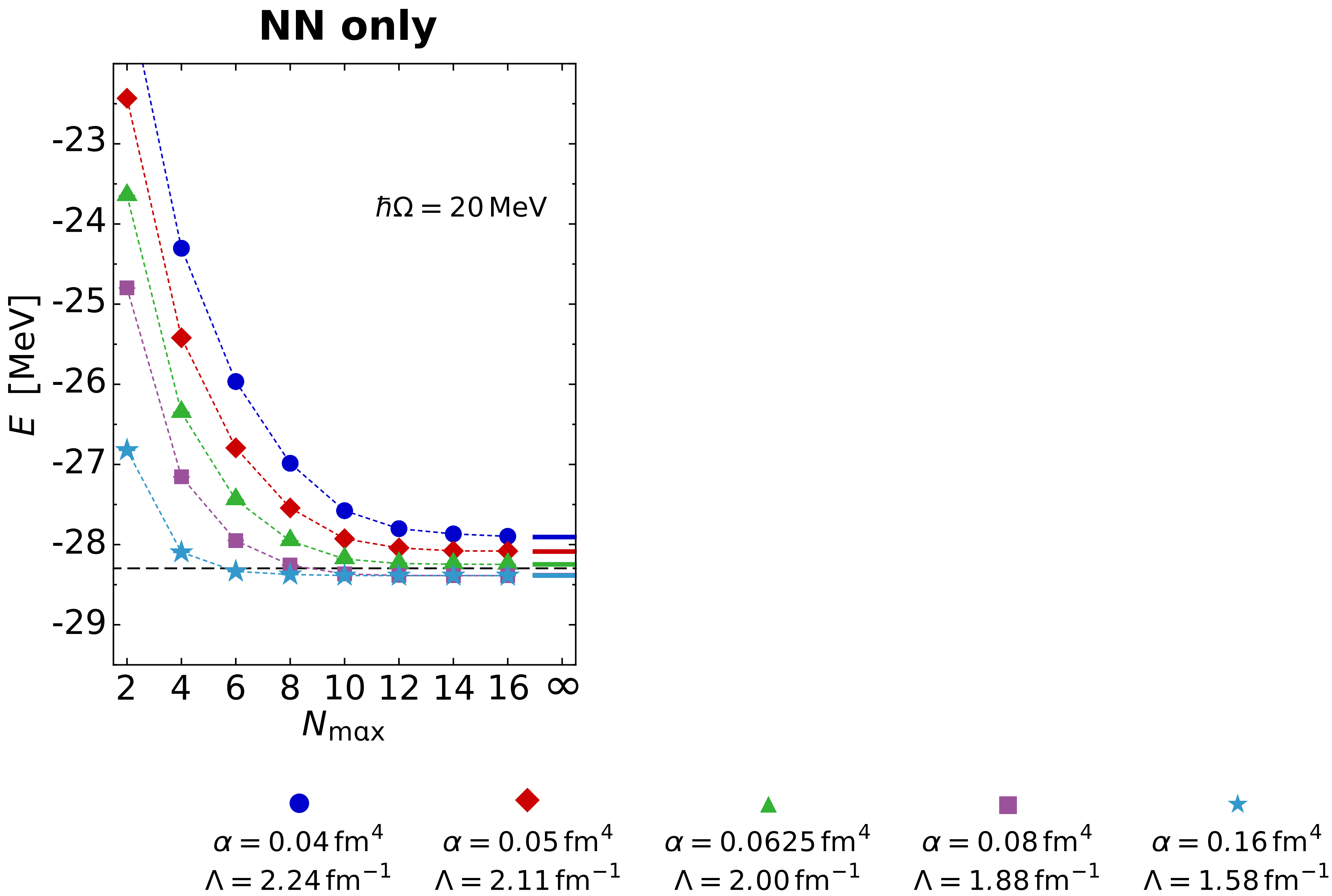
Roth, Langhammer, Calci et al. — Phys. Rev. Lett. 107, 072501 (2011)
Navrátil et al. — Phys. Rev. C 82, 034609 (2010)
Roth — Phys. Rev. C 79, 064324 (2009)

Importance Truncated NCSM

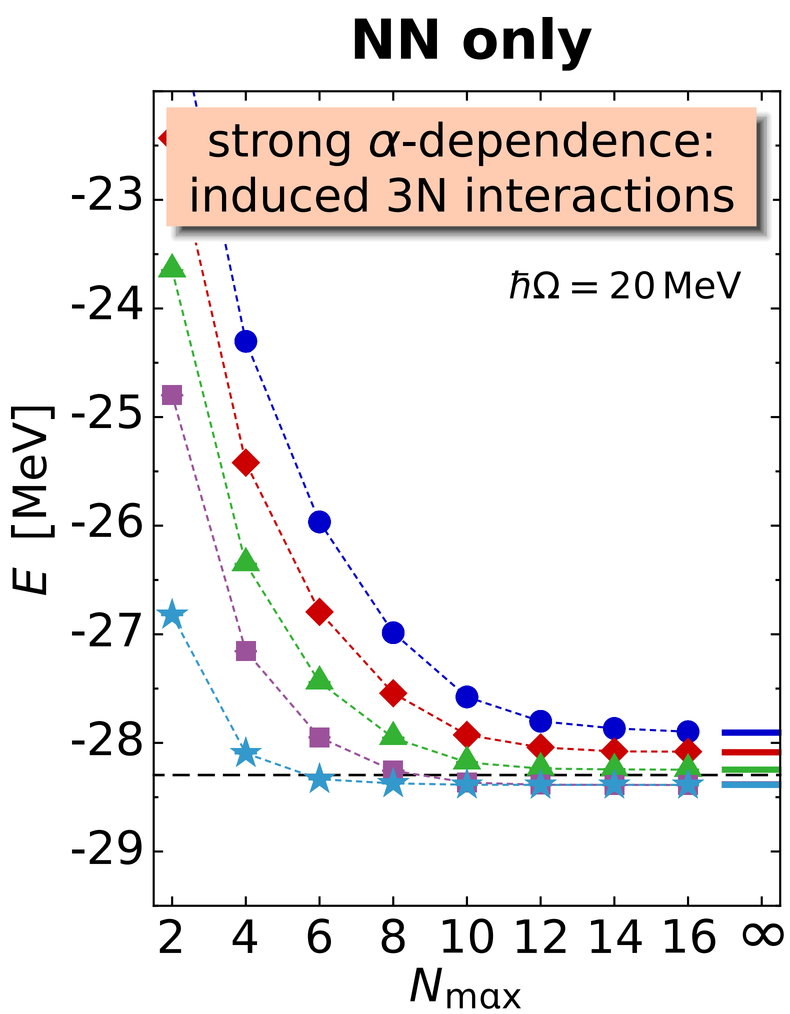
NCSM is one of the most powerful and universal exact ab-initio methods

- 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 $E_{3\max} = 16$

^{4}He: Ground-State Energies

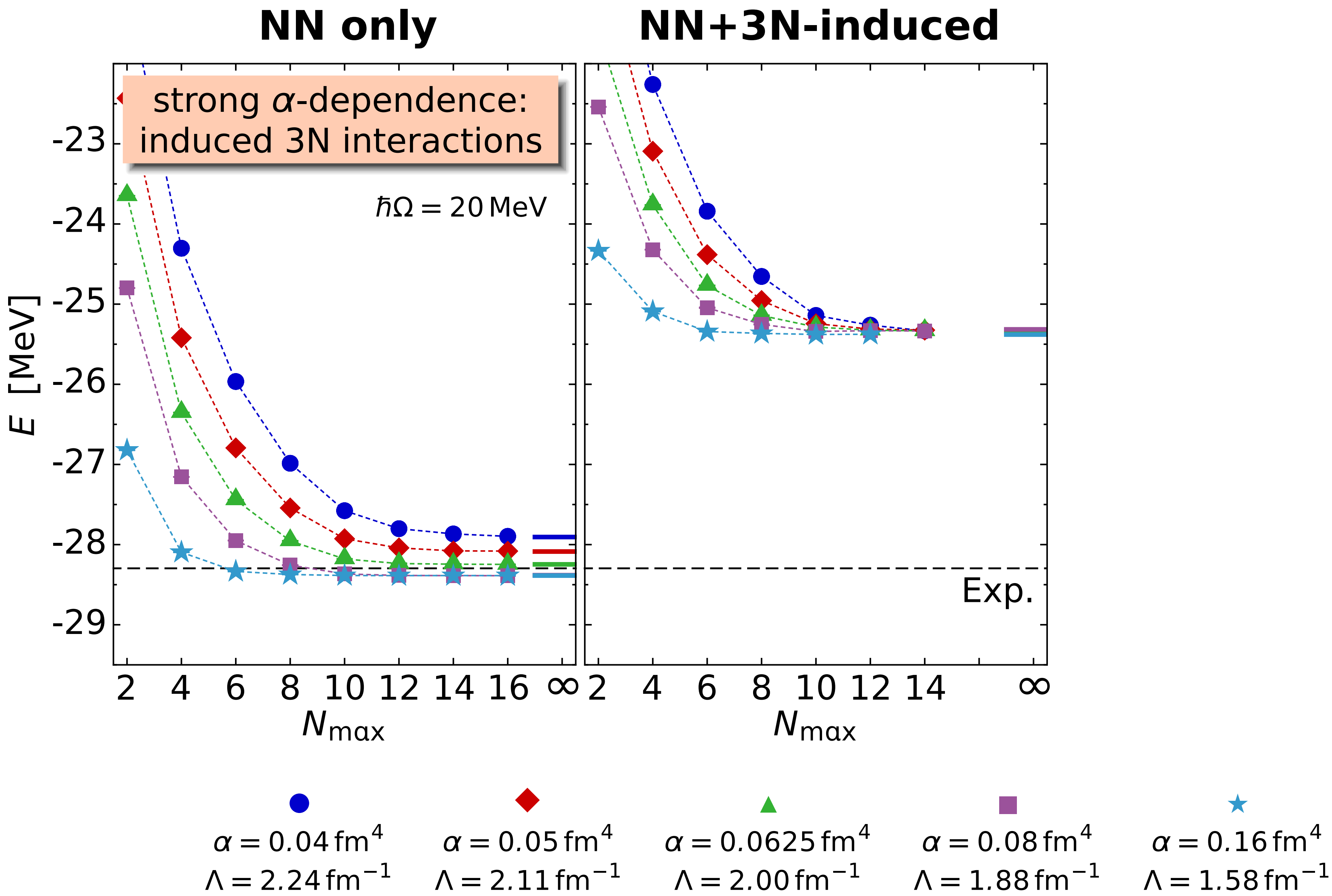


^{4}He: Ground-State Energies

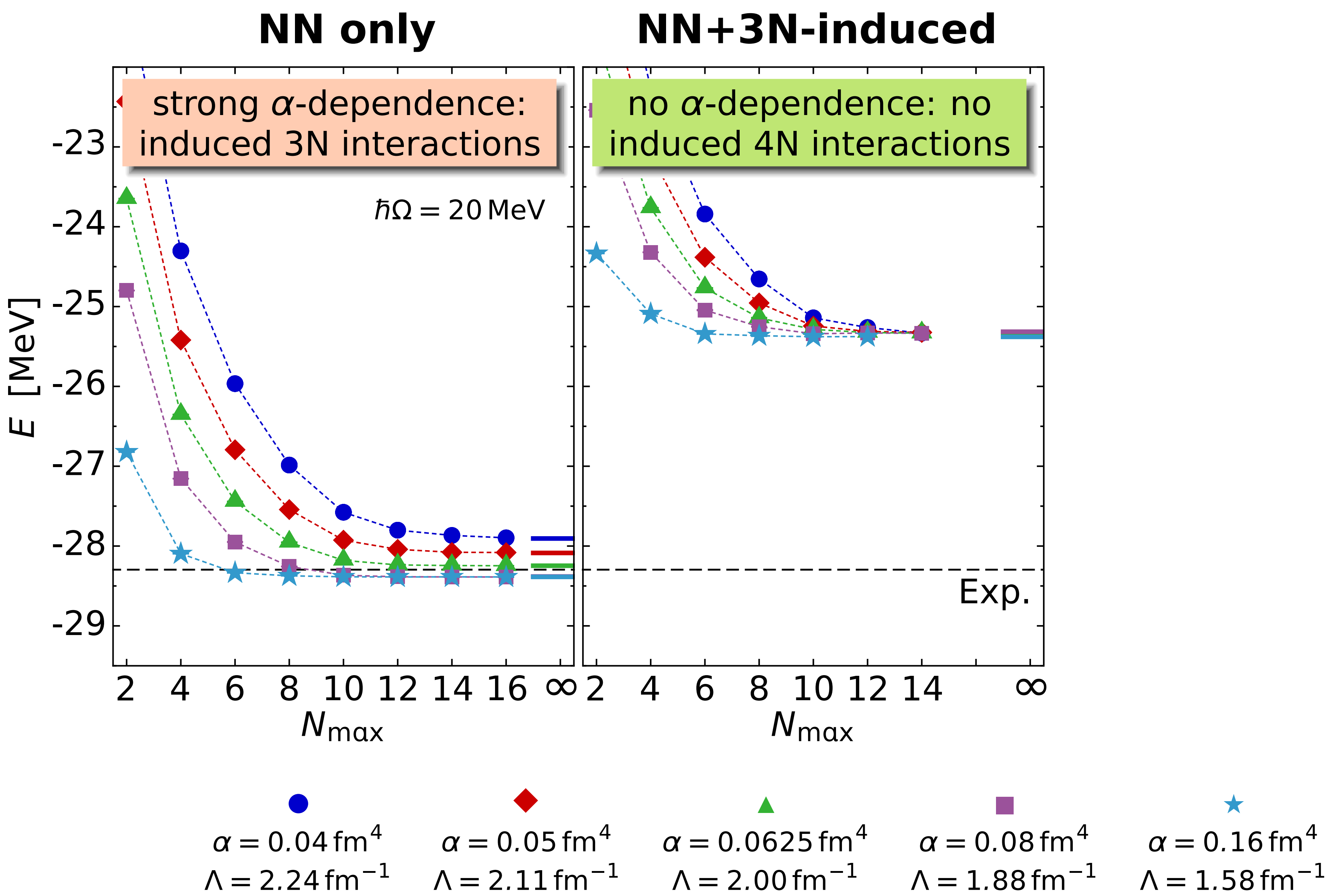


$\alpha = 0.04\,\mathrm{fm}^4$, $\Lambda = 2.24\,\mathrm{fm}^{-1}$ | $\alpha = 0.05\,\mathrm{fm}^4$, $\Lambda = 2.11\,\mathrm{fm}^{-1}$ | $\alpha = 0.0625\,\mathrm{fm}^4$, $\Lambda = 2.00\,\mathrm{fm}^{-1}$ | $\alpha = 0.08\,\mathrm{fm}^4$, $\Lambda = 1.88\,\mathrm{fm}^{-1}$ | $\alpha = 0.16\,\mathrm{fm}^4$, $\Lambda = 1.58\,\mathrm{fm}^{-1}$

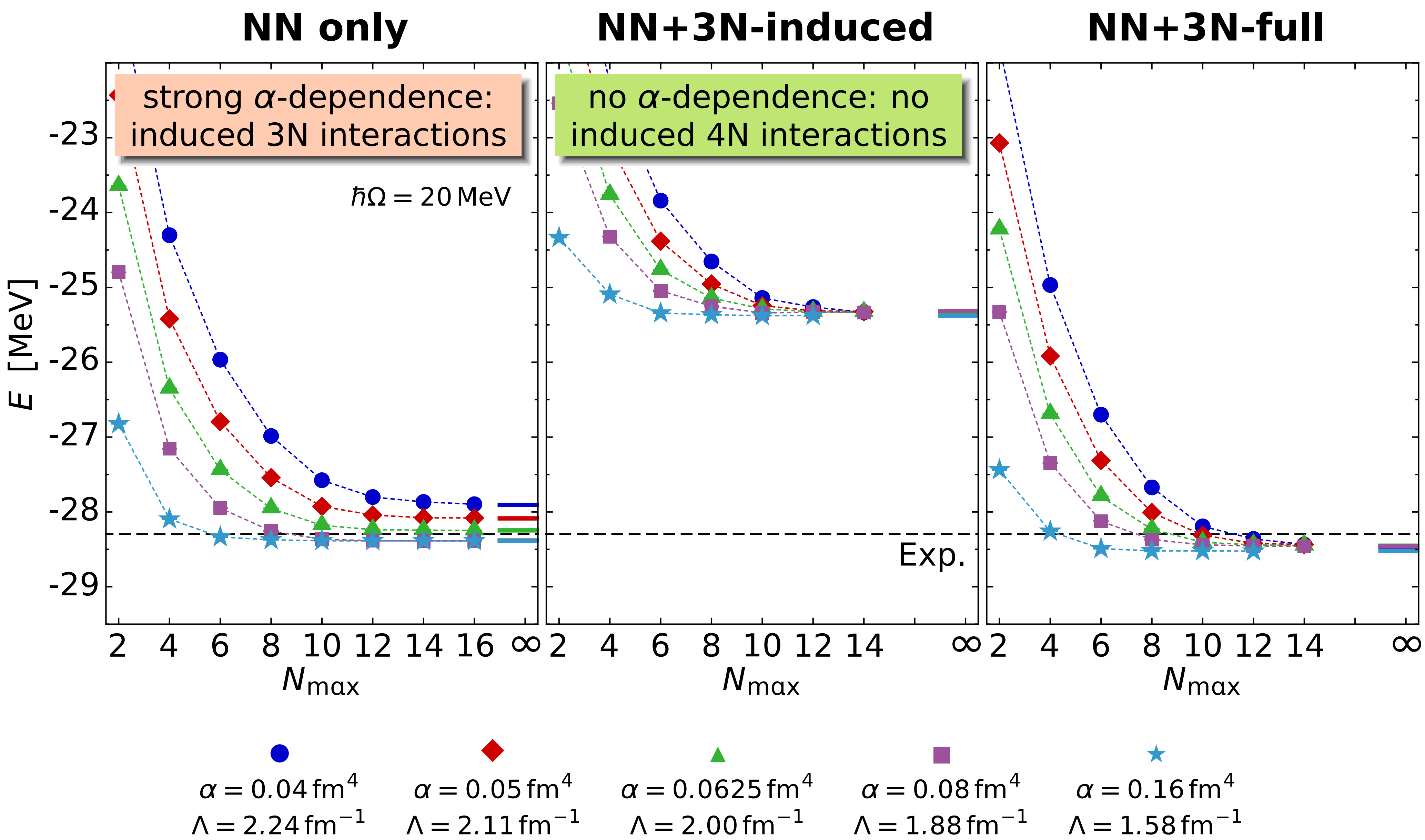
^{4}He: Ground-State Energies



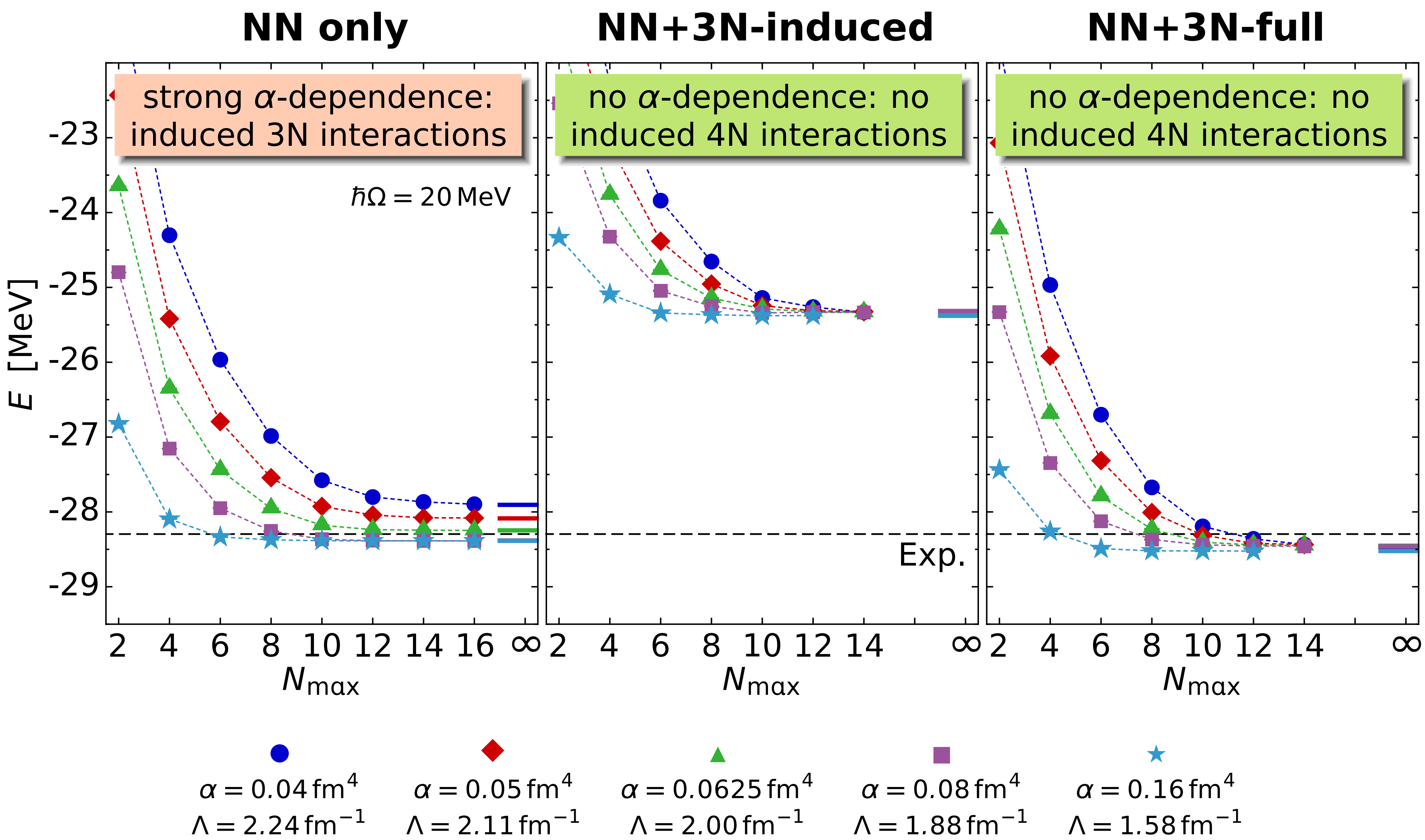
^{4}He: Ground-State Energies



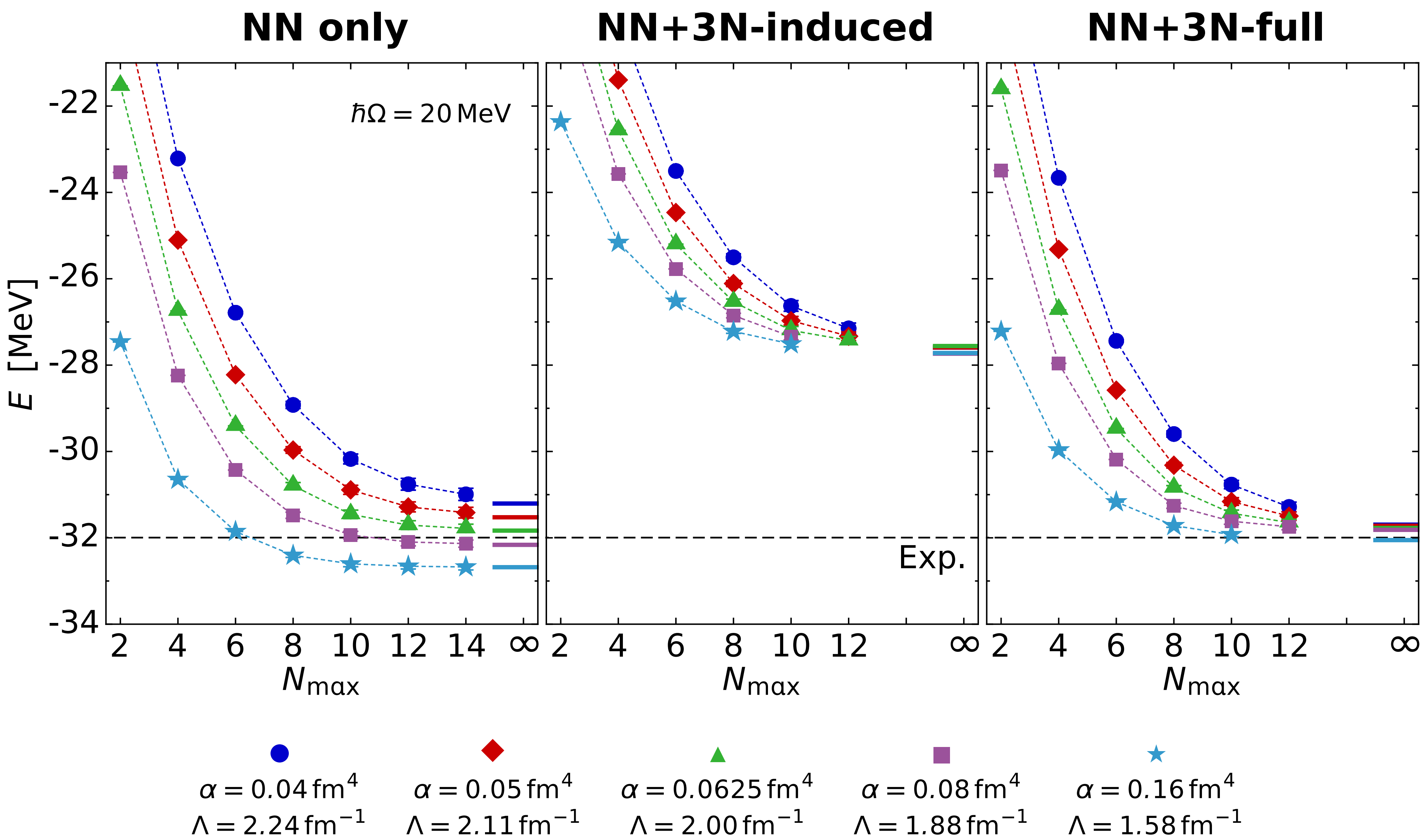
^{4}He: Ground-State Energies



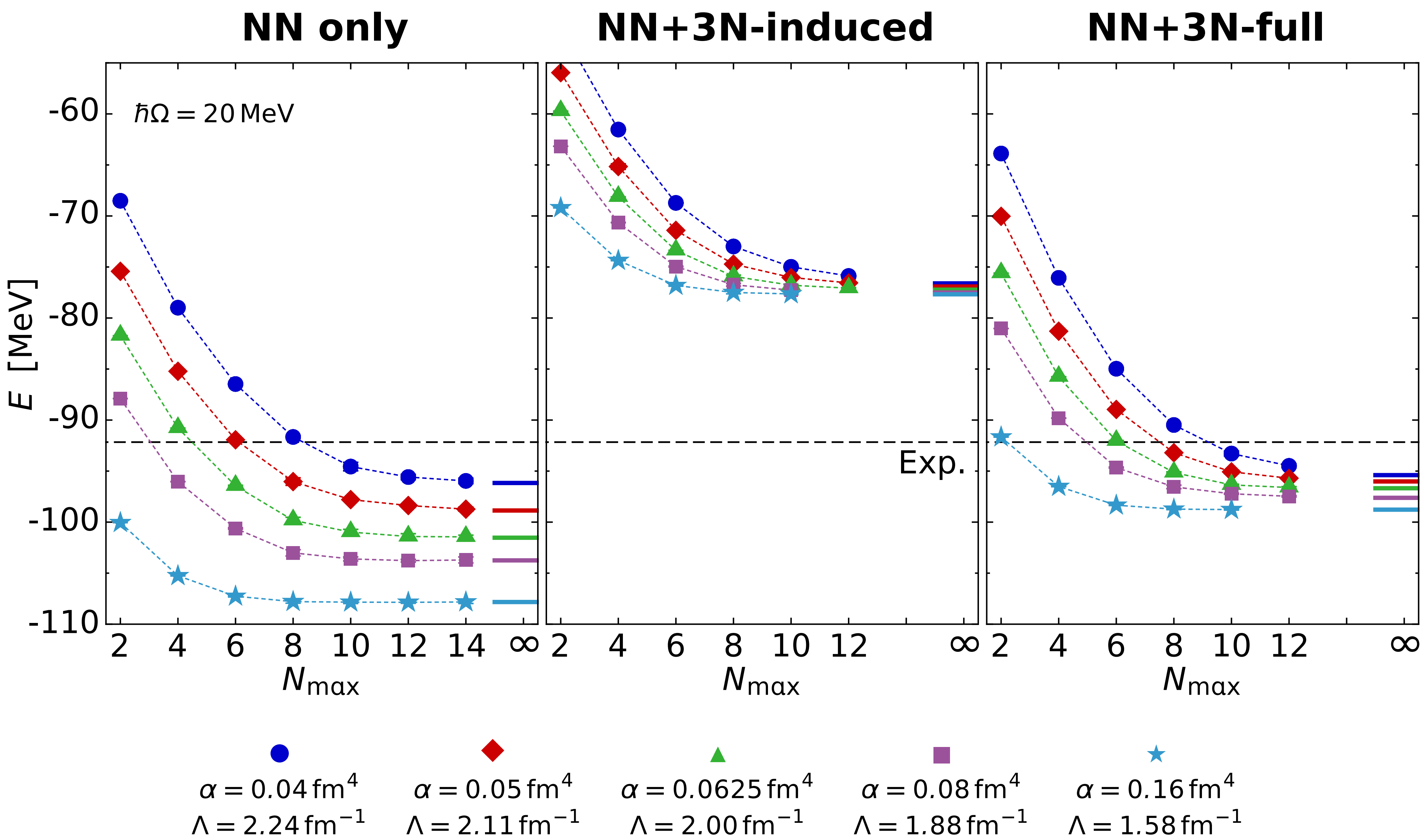
^{4}He: Ground-State Energies



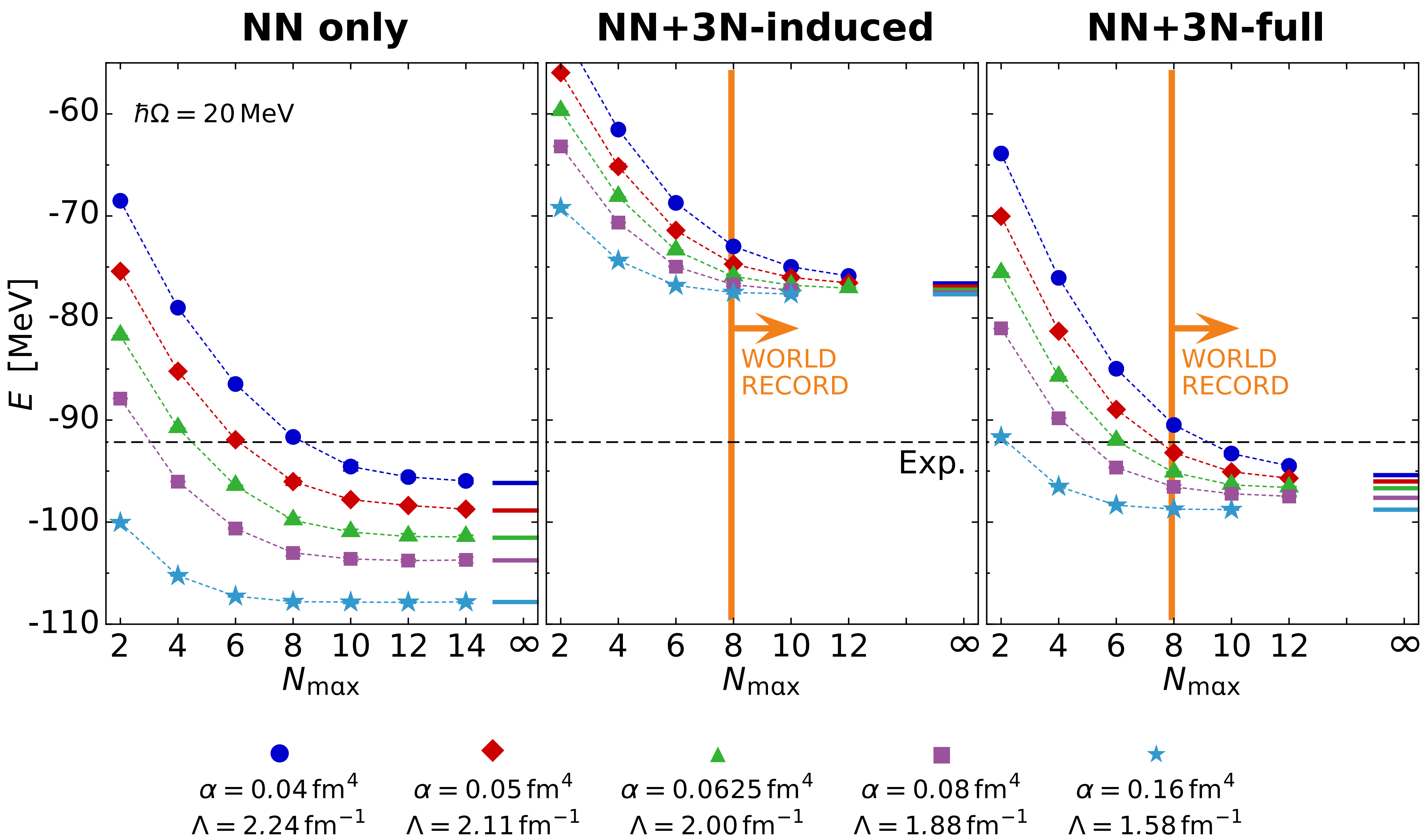
^{6}Li: Ground-State Energies



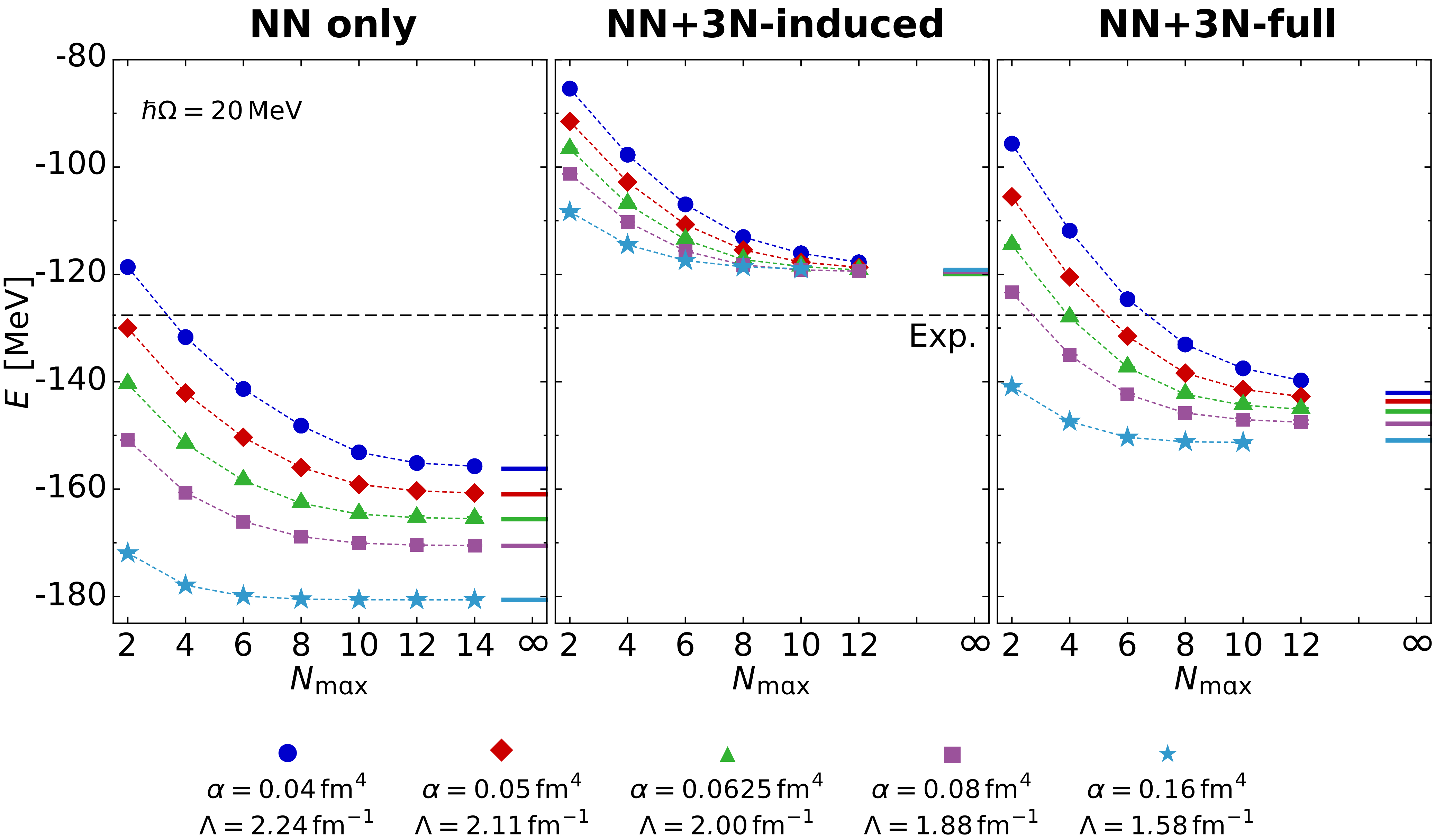
^{12}C: Ground-State Energies



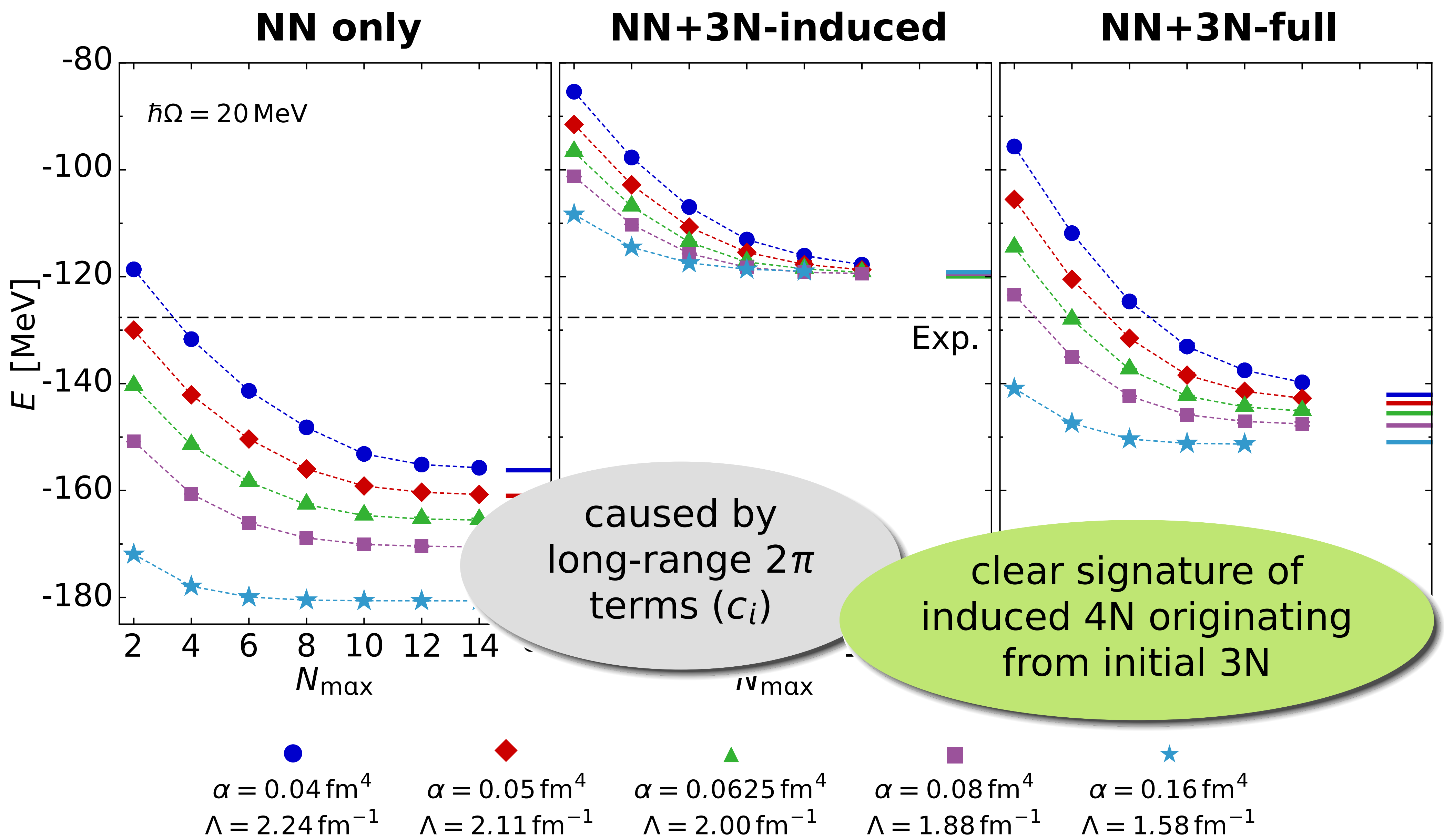
^{12}C: Ground-State Energies



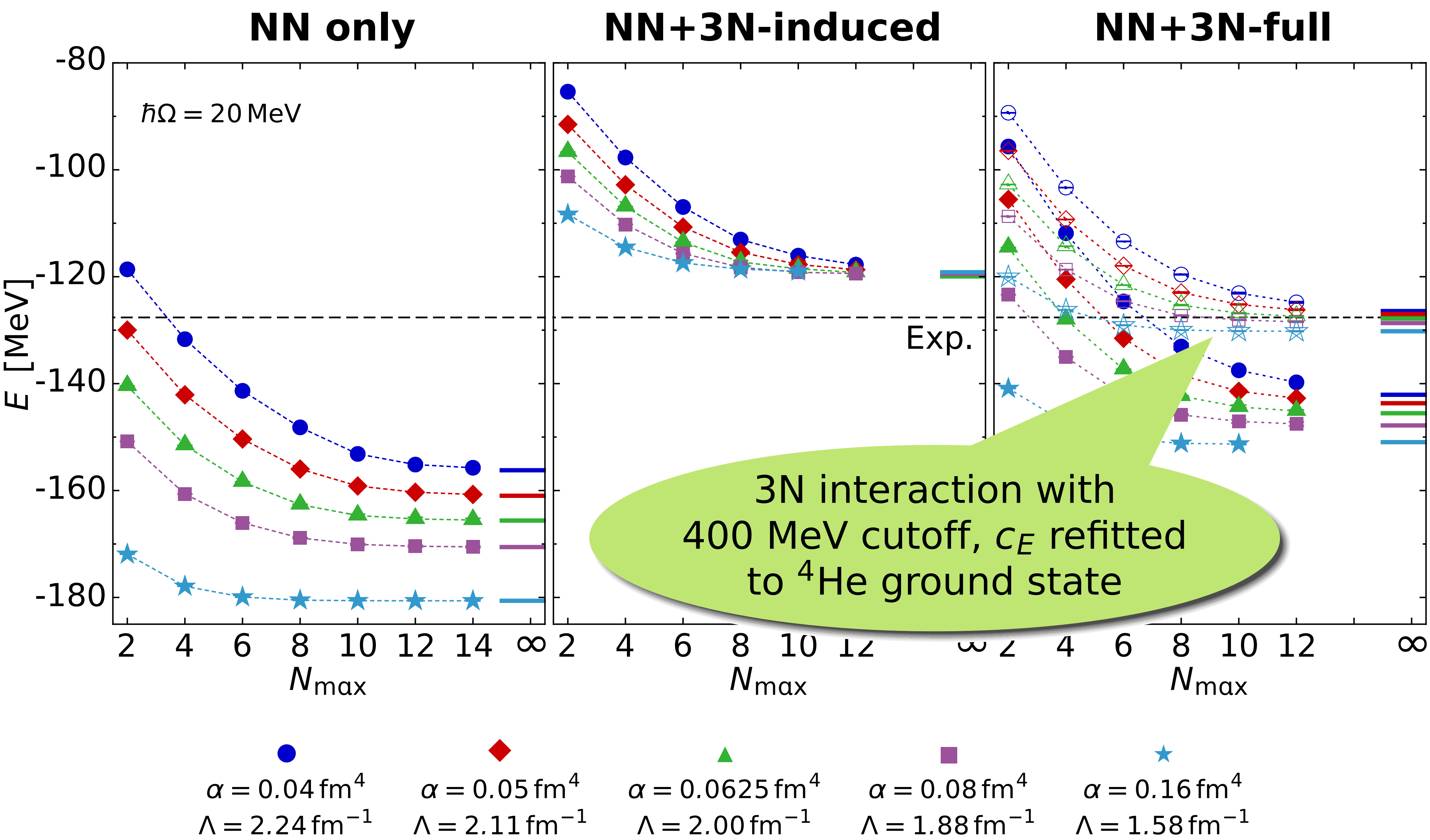
^{16}O: Ground-State Energies



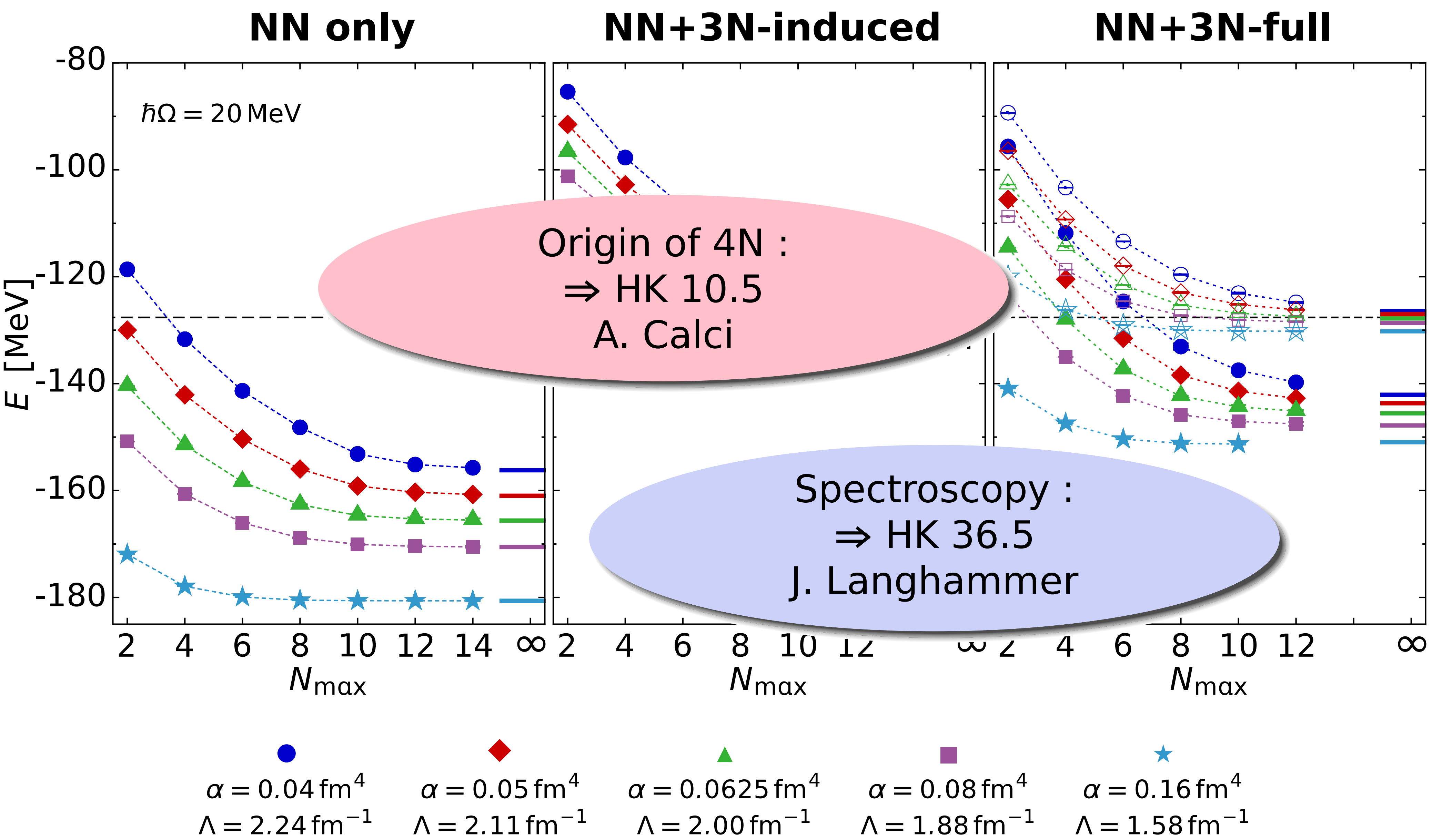
^{16}O: Ground-State Energies



^{16}O: Ground-State Energies



^{16}O: Ground-State Energies



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

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

Coupled Cluster Approach

- **exponential Ansatz** for wave operator

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

- $\hat{T}_n$: ***n*p*n*h excitation** ("cluster") operators

$$\hat{T}_n = \frac{1}{(n!)^2} \sum_{\substack{ijk\ldots \\ abc\ldots}} t_{ijk\ldots}^{abc\ldots} \{\hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_c^\dagger \ldots \hat{a}_k \hat{a}_j \hat{a}_i\}$$

Coupled Cluster Approach

- **exponential Ansatz** for wave operator

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

- $\hat{T}_n$: ***n*p*n*h excitation** ("cluster") operators

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

- **similarity transformed** Schrödinger Eq.

$$\hat{\mathcal{H}}|\Phi_0\rangle = \Delta E|\Phi_0\rangle \ , \quad \hat{\mathcal{H}} \equiv e^{-\hat{T}} \hat{H}_N e^{\hat{T}}$$

Coupled Cluster Approach

- **exponential Ansatz** for wave operator

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

- $\hat{T}_n$: ***n*p*n*h excitation** ("cluster") operators

$$\hat{T}_n = \frac{1}{(n!)^2} \sum_{\substack{ijk\ldots\\abc\ldots}} t_{ijk\ldots}^{abc\ldots} \{\hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_c^\dagger \ldots \hat{a}_k \hat{a}_j \hat{a}_i\}$$

- **similarity transformed** Schrödinger Eq.

$$\hat{\mathcal{H}}|\Phi_0\rangle = \Delta E|\Phi_0\rangle \ , \quad \hat{\mathcal{H}} \equiv e^{-\hat{T}}\hat{H}_N e^{\hat{T}}$$

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

Coupled Cluster - Equations

Coupled Cluster - Equations

- **CCSD** : truncate $\hat{T}$ at **2p2h** level, $\hat{T} = \hat{T}_1 + \hat{T}_2$

Coupled Cluster - Equations

- **CCSD** : truncate $\hat{T}$ at **2p2h** level, $\hat{T} = \hat{T}_1 + \hat{T}_2$
- projection of $\hat{\mathcal{H}}|\Phi_0\rangle = \Delta E|\Phi_0\rangle$ onto

$$\left\{ \; |\Phi_0\rangle, \quad |\Phi_i^a\rangle \equiv \hat{a}_a^\dagger \hat{a}_i |\Phi_0\rangle, \quad |\Phi_{ij}^{ab}\rangle \equiv \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i |\Phi_0\rangle \; \right\}$$

leads to **CCSD equations**

Coupled Cluster - Equations

- **CCSD** : truncate $\hat{T}$ at **2p2h** level, $\hat{T} = \hat{T}_1 + \hat{T}_2$

- projection of $\hat{\mathcal{H}}|\Phi_0\rangle = \Delta E|\Phi_0\rangle$ onto

  $$\left\{ |\Phi_0\rangle, \quad |\Phi_i^a\rangle \equiv \hat{a}_a^\dagger \hat{a}_i |\Phi_0\rangle, \quad |\Phi_{ij}^{ab}\rangle \equiv \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i |\Phi_0\rangle \right\}$$

  leads to **CCSD equations**

  - $\Delta E = \langle\Phi_0|\hat{\mathcal{H}}|\Phi_0\rangle$

Coupled Cluster - Equations

- **CCSD** : truncate $\hat{T}$ at **2p2h** level, $\hat{T} = \hat{T}_1 + \hat{T}_2$

- projection of $\hat{\mathcal{H}}|\Phi_0\rangle = \Delta E|\Phi_0\rangle$ onto

  $$\left\{ |\Phi_0\rangle, \quad |\Phi_i^a\rangle \equiv \hat{a}_a^\dagger \hat{a}_i|\Phi_0\rangle, \quad |\Phi_{ij}^{ab}\rangle \equiv \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i|\Phi_0\rangle \right\}$$

  leads to **CCSD equations**

  - $\Delta E = \langle\Phi_0|\hat{\mathcal{H}}|\Phi_0\rangle$

  - $0 = \langle\Phi_i^a|\hat{\mathcal{H}}|\Phi_0\rangle$

Coupled Cluster - Equations

- **CCSD** : truncate $\hat{T}$ at **2p2h** level, $\hat{T} = \hat{T}_1 + \hat{T}_2$
- projection of $\hat{\mathcal{H}}|\Phi_0\rangle = \Delta E|\Phi_0\rangle$ onto

$$\left\{ |\Phi_0\rangle, \quad |\Phi_i^a\rangle \equiv \hat{a}_a^\dagger \hat{a}_i|\Phi_0\rangle, \quad |\Phi_{ij}^{ab}\rangle \equiv \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i|\Phi_0\rangle \right\}$$

leads to **CCSD equations**

- $\Delta E = \langle\Phi_0|\hat{\mathcal{H}}|\Phi_0\rangle$
- $0 = \langle\Phi_i^a|\hat{\mathcal{H}}|\Phi_0\rangle$
- $0 = \langle\Phi_{ij}^{ab}|\hat{\mathcal{H}}|\Phi_0\rangle$

Coupled Cluster - Equations

- **CCSD** : truncate $\hat{T}$ at **2p2h** level, $\hat{T} = \hat{T}_1 + \hat{T}_2$
- projection of $\hat{\mathcal{H}}|\Phi_0\rangle = \Delta E|\Phi_0\rangle$ onto

$$\left\{ |\Phi_0\rangle, \quad |\Phi_i^a\rangle \equiv \hat{a}_a^\dagger \hat{a}_i |\Phi_0\rangle, \quad |\Phi_{ij}^{ab}\rangle \equiv \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i |\Phi_0\rangle \right\}$$

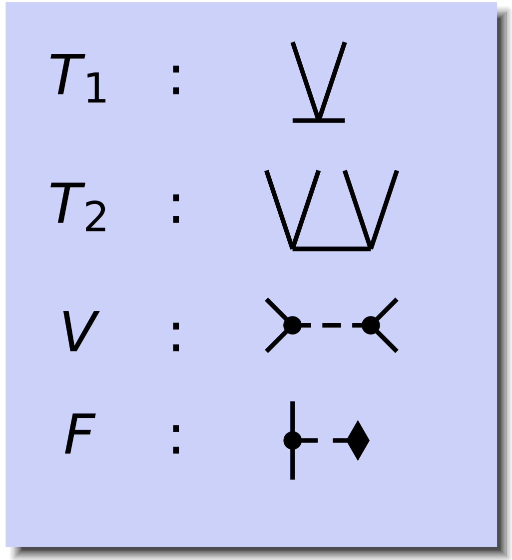
leads to **CCSD equations**

- $\Delta E = \langle\Phi_0|\hat{\mathcal{H}}|\Phi_0\rangle = \langle\Phi_0|\hat{H}_N(\hat{T}_2 + \hat{T}_1 + \frac{1}{2}\hat{T}_1^2)|\Phi_0\rangle_C$
- $0 = \langle\Phi_i^a|\hat{\mathcal{H}}|\Phi_0\rangle = \langle\Phi_0|\hat{H}_N(1 + \hat{T}_2 + \hat{T}_1 + \hat{T}_1\hat{T}_2 + \frac{1}{2}\hat{T}_1^2 + \frac{1}{3!}\hat{T}_1^3)|\Phi_0\rangle_C$
- $0 = \langle\Phi_{ij}^{ab}|\hat{\mathcal{H}}|\Phi_0\rangle = \langle\Phi_0|\hat{H}_N(1 + \hat{T}_2 + \frac{1}{2}\hat{T}_2^2 + \hat{T}_1 + \hat{T}_1\hat{T}_2$

$$+\frac{1}{2}\hat{T}_1^2 + \frac{1}{2}\hat{T}_1^2\hat{T}_2 + \frac{1}{3!}\hat{T}_1^3 + \frac{1}{4!}\hat{T}_1^4)|\Phi_0\rangle_C$$

Coupled Cluster - Equations

- **CCSD** : truncate $\hat{T}$ at **2p2h** level, $\hat{T} = \hat{T}_1 + \hat{T}_2$

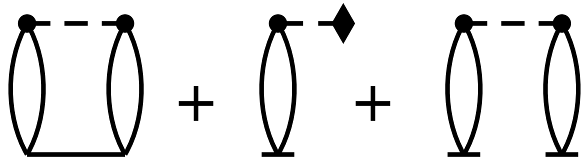


- projection of $\hat{\mathcal{H}}|\Phi_0\rangle = \Delta E|\Phi_0\rangle$ onto

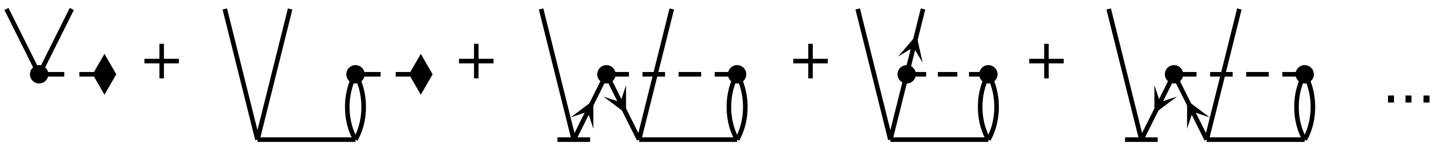
$$\left\{ |\Phi_0\rangle, \quad |\Phi_i^a\rangle \equiv \hat{a}_a^\dagger \hat{a}_i|\Phi_0\rangle, \quad |\Phi_{ij}^{ab}\rangle \equiv \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i|\Phi_0\rangle \right\}$$

leads to **CCSD equations**

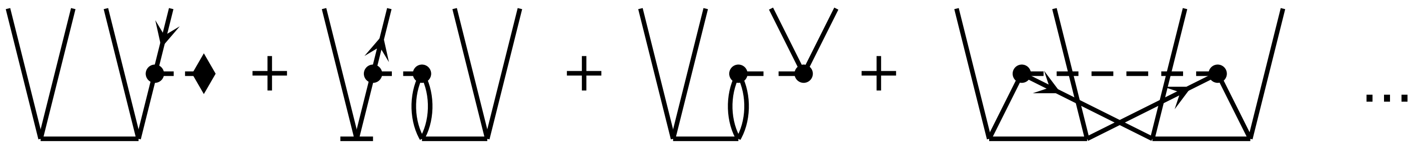
- $\Delta E = \langle\Phi_0|\hat{\mathcal{H}}|\Phi_0\rangle =$



- $0 = \langle\Phi_i^a|\hat{\mathcal{H}}|\Phi_0\rangle =$



- $0 = \langle\Phi_{ij}^{ab}|\hat{\mathcal{H}}|\Phi_0\rangle =$



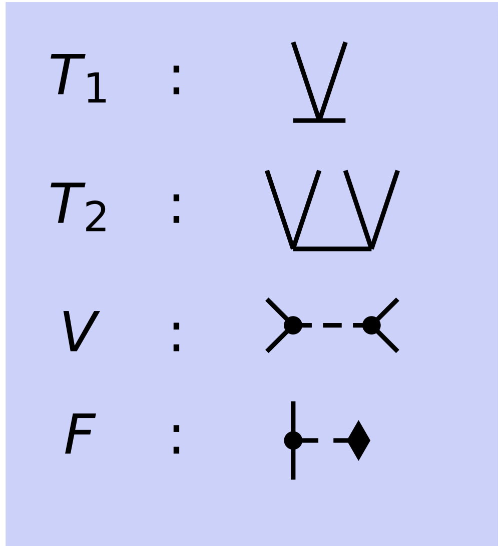
Coupled Cluster - Equations

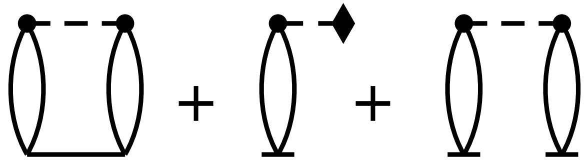
- **CCSD** : truncate $\hat{T}$ at **2p2h** level, $\hat{T} = \hat{T}_1 + \hat{T}_2$

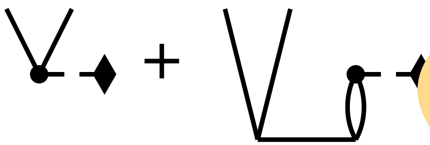
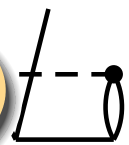
- projection of $\hat{\mathcal{H}}|\Phi_0\rangle = \Delta E|\Phi_0\rangle$ onto

$$\left\{ |\Phi_0\rangle, \quad |\Phi_i^a\rangle \equiv \hat{a}_a^\dagger \hat{a}_i|\Phi_0\rangle, \quad |\Phi_{ij}^{ab}\rangle \equiv \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i|\Phi_0\rangle \right\}$$

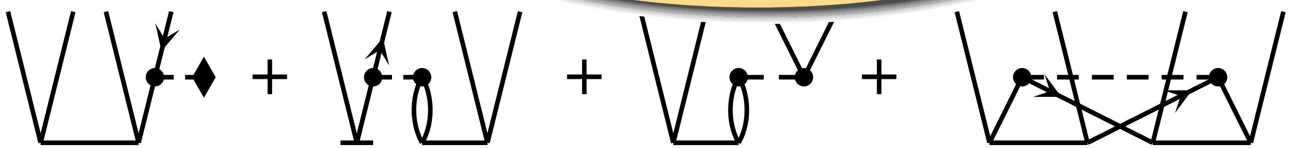
  leads to **CCSD equations**



- $\Delta E = \langle\Phi_0|\hat{\mathcal{H}}|\Phi_0\rangle =$ 

- $0 = \langle\Phi_i^a|\hat{\mathcal{H}}|\Phi_0\rangle =$   ...

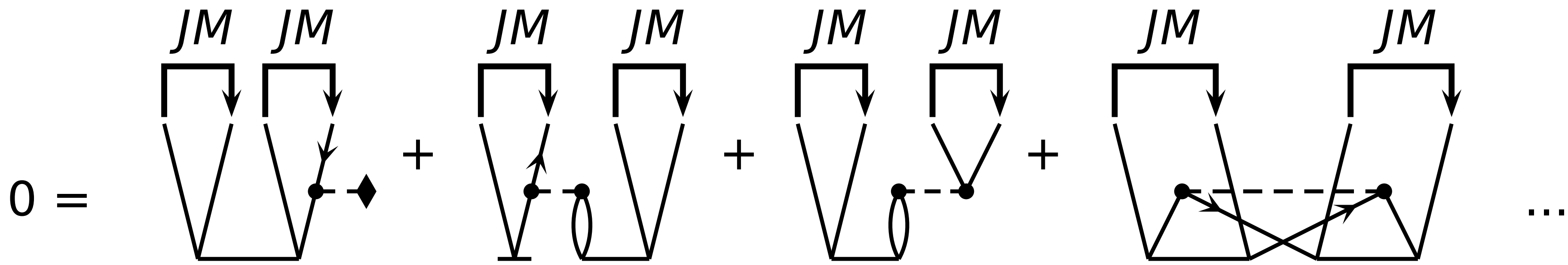
linked diagrams only
⇒ size extensive

- $0 = \langle\Phi_{ij}^{ab}|\hat{\mathcal{H}}|\Phi_0\rangle =$  ...

Coupled Cluster - Spherical Scheme

Coupled Cluster - Spherical Scheme

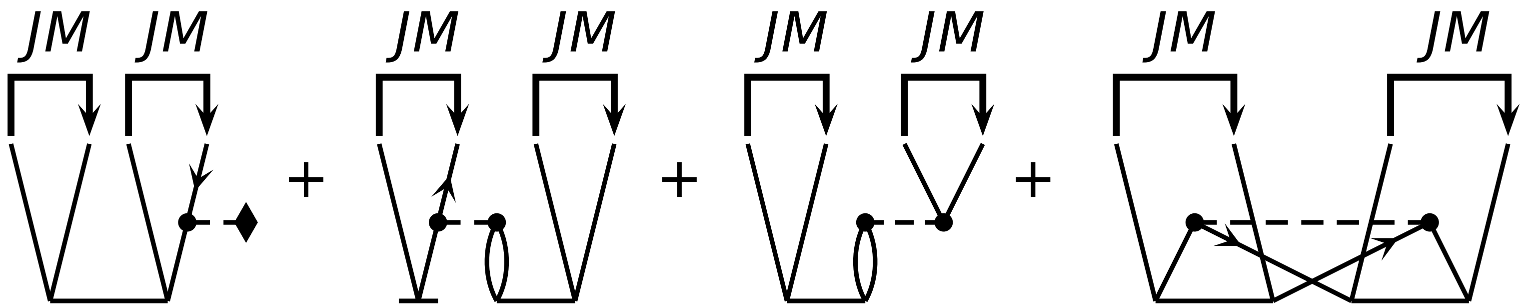
- **coupling of external lines** to good J



etc.

Coupled Cluster - Spherical Scheme

- **coupling of external lines** to good *J*

0 =


...

etc.

- express CCSD equations in terms of

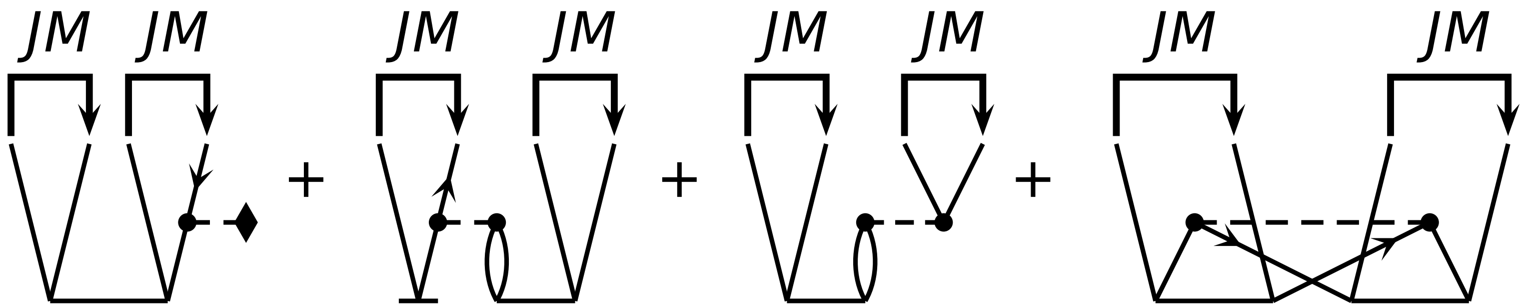
$J0 \quad J0 \qquad J0 \quad J0 \qquad 00$

$$\langle p \; q \| r \; s \rangle, \; \langle a \; b | t | i \; j \rangle, \; \langle \tilde{a} | t | i \rangle, \; etc.$$

Coupled Cluster - Spherical Scheme

- **coupling of external lines** to good J

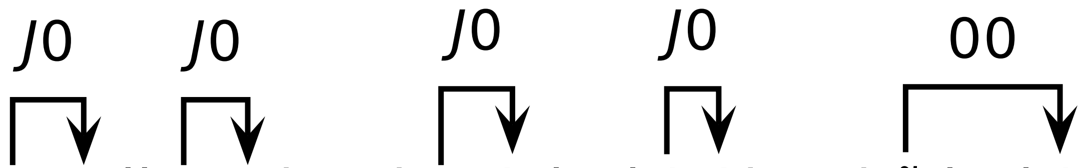
$0 =$



$\ldots$

etc.

- express CCSD equations in terms of

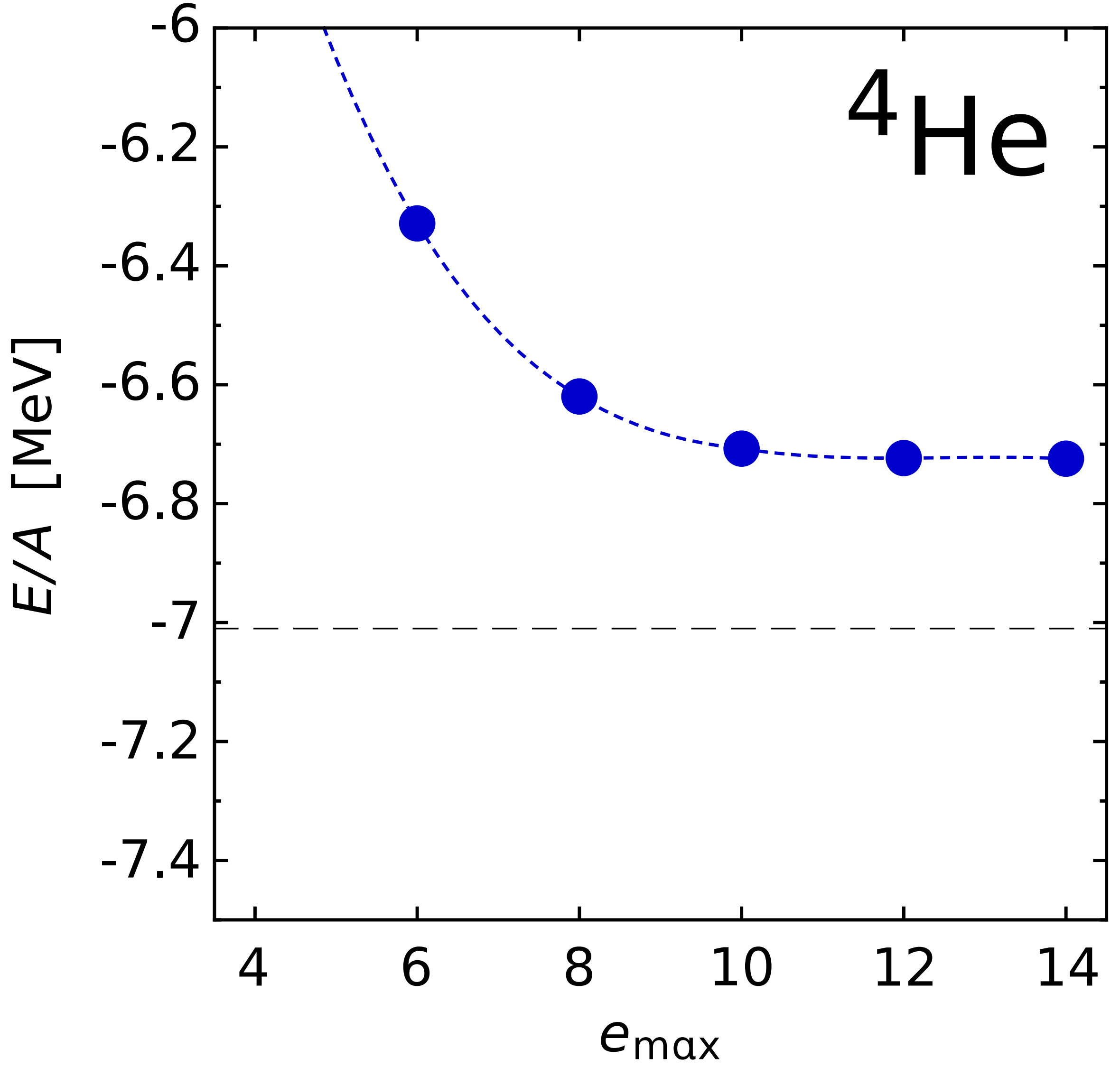


$\langle p \;\; q \,||\, r \;\; s \rangle, \;\; \langle a \;\; b \,|\, t \,|\, i \;\; j \rangle, \;\; \langle \tilde{a} \,|\, t \,|\, i \rangle, \;\; etc.$

- $\Rightarrow$ **drastic reduction** of number of amplitudes

Coupled Cluster - Convergence Rate

Coupled Cluster - Convergence Rate



CCSD(HO)

NN only
$\hbar\Omega = 20\,\mathrm{MeV}$

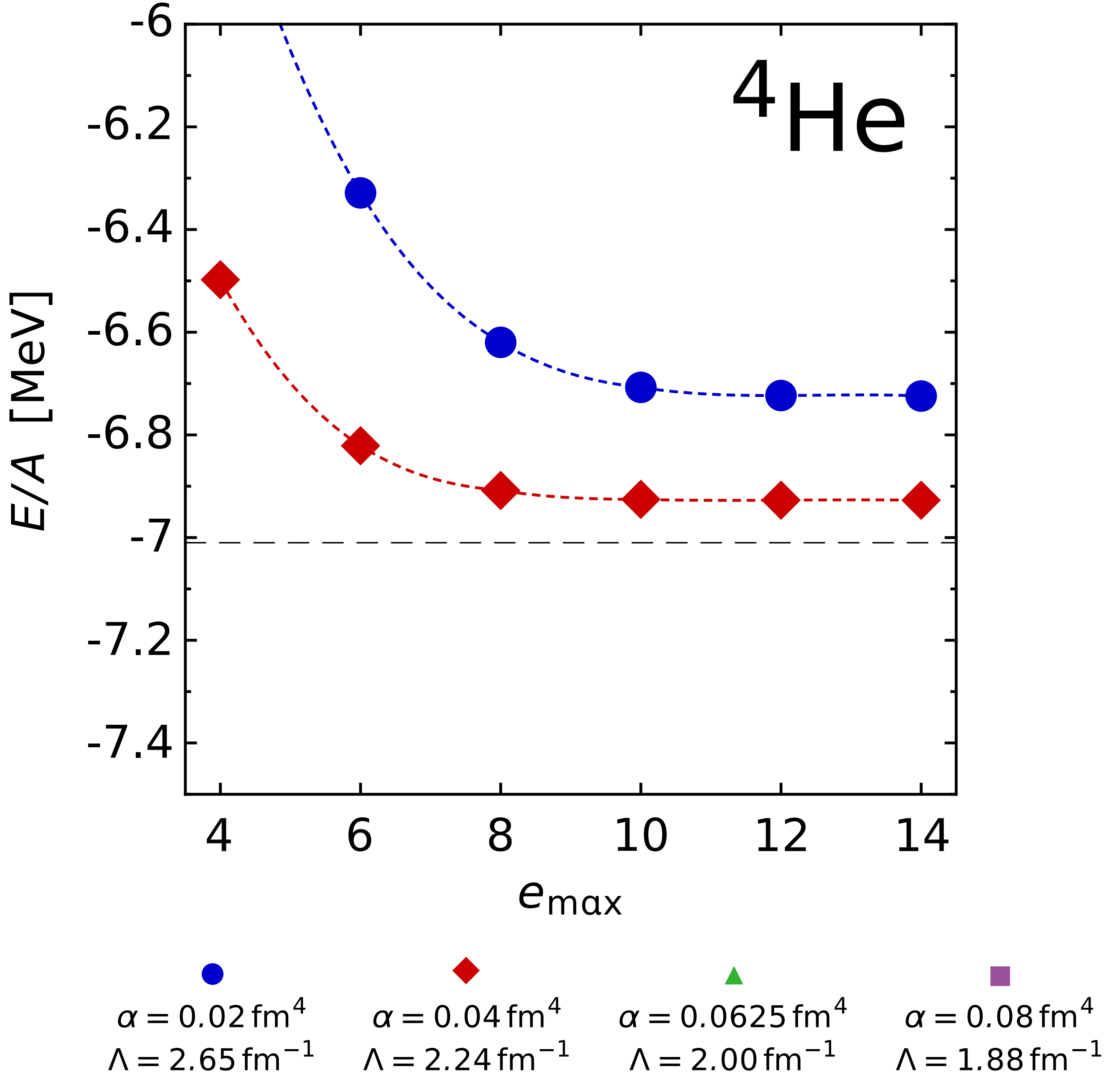
$\alpha = 0.02\,\mathrm{fm}^4$
$\Lambda = 2.65\,\mathrm{fm}^{-1}$

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

$\alpha = 0.0625\,\mathrm{fm}^4$
$\Lambda = 2.00\,\mathrm{fm}^{-1}$

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

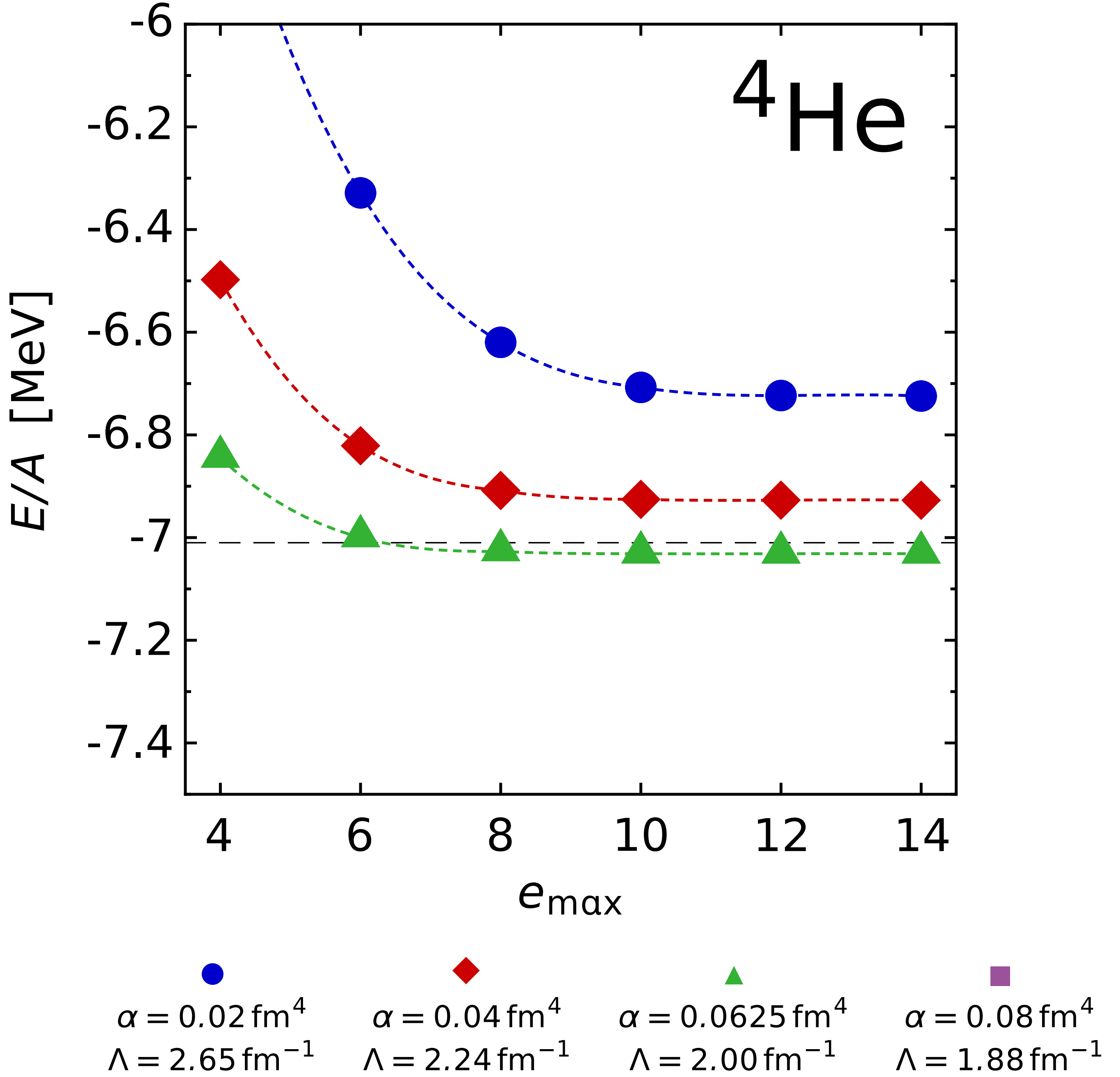
Coupled Cluster - Convergence Rate



CCSD(HO)

NN only
$\hbar\Omega = 20\,\mathrm{MeV}$

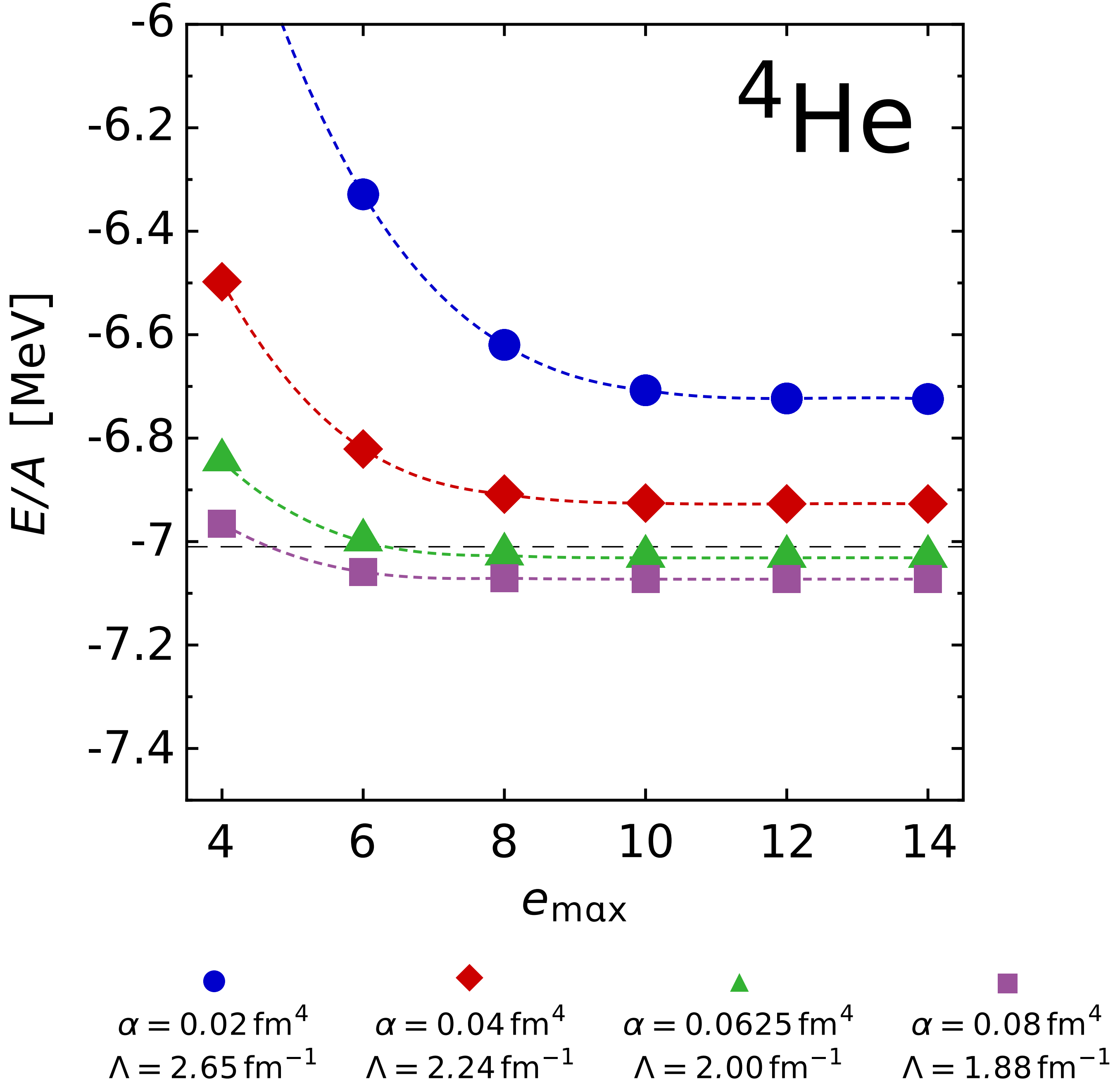
Coupled Cluster - Convergence Rate



CCSD(HO)

NN only
$\hbar\Omega = 20\,\mathrm{MeV}$

Coupled Cluster - Convergence Rate

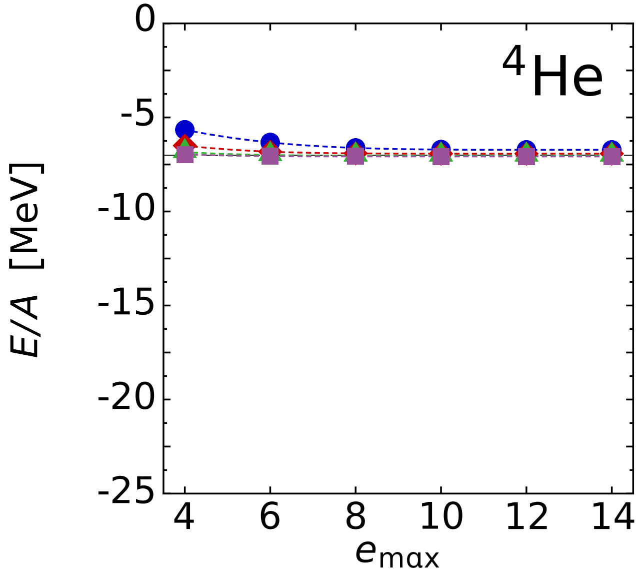


CCSD(HO)

NN only

$\hbar\Omega = 20\,MeV$

Coupled Cluster - Convergence Rate

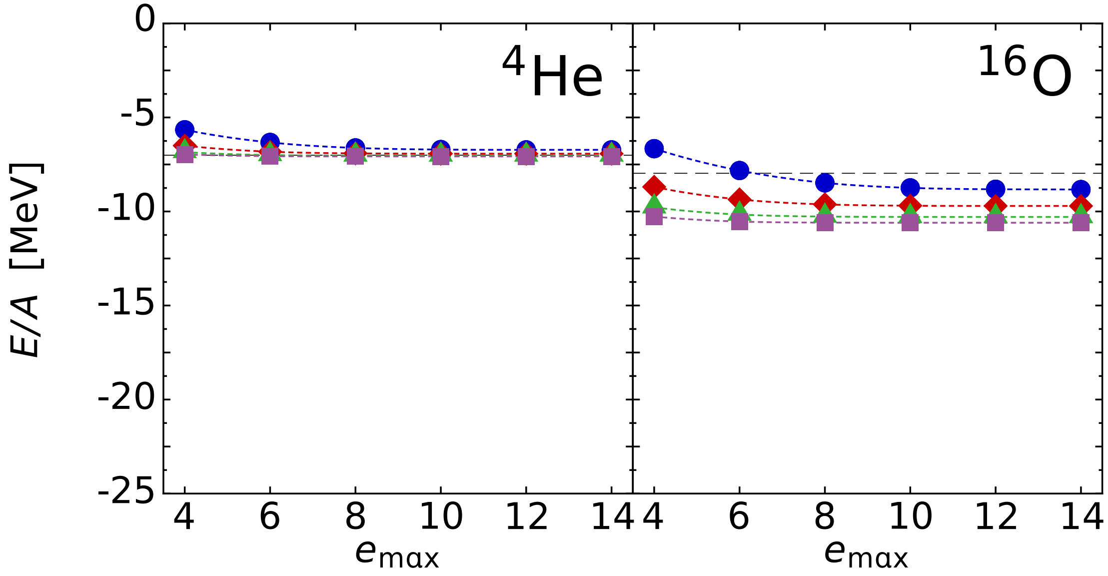


CCSD(HO)

NN only
$\hbar\Omega = 20\,\mathrm{MeV}$

$\alpha = 0.02\,\mathrm{fm}^4$	$\alpha = 0.04\,\mathrm{fm}^4$	$\alpha = 0.0625\,\mathrm{fm}^4$	$\alpha = 0.08\,\mathrm{fm}^4$
$\Lambda = 2.65\,\mathrm{fm}^{-1}$	$\Lambda = 2.24\,\mathrm{fm}^{-1}$	$\Lambda = 2.00\,\mathrm{fm}^{-1}$	$\Lambda = 1.88\,\mathrm{fm}^{-1}$

Coupled Cluster - Convergence Rate



CCSD(HO)

NN only

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

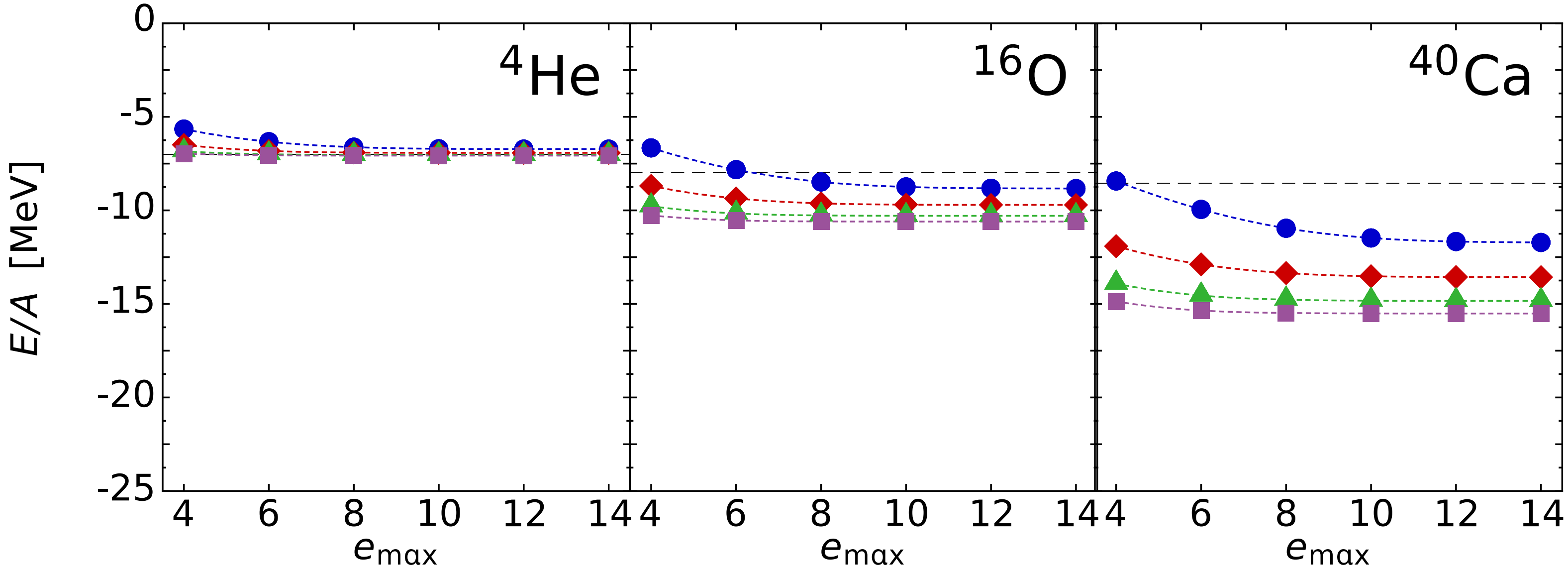
$\alpha = 0.02\,\text{fm}^4$ $\Lambda = 2.65\,\text{fm}^{-1}$

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

$\alpha = 0.0625\,\text{fm}^4$ $\Lambda = 2.00\,\text{fm}^{-1}$

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

Coupled Cluster - Convergence Rate

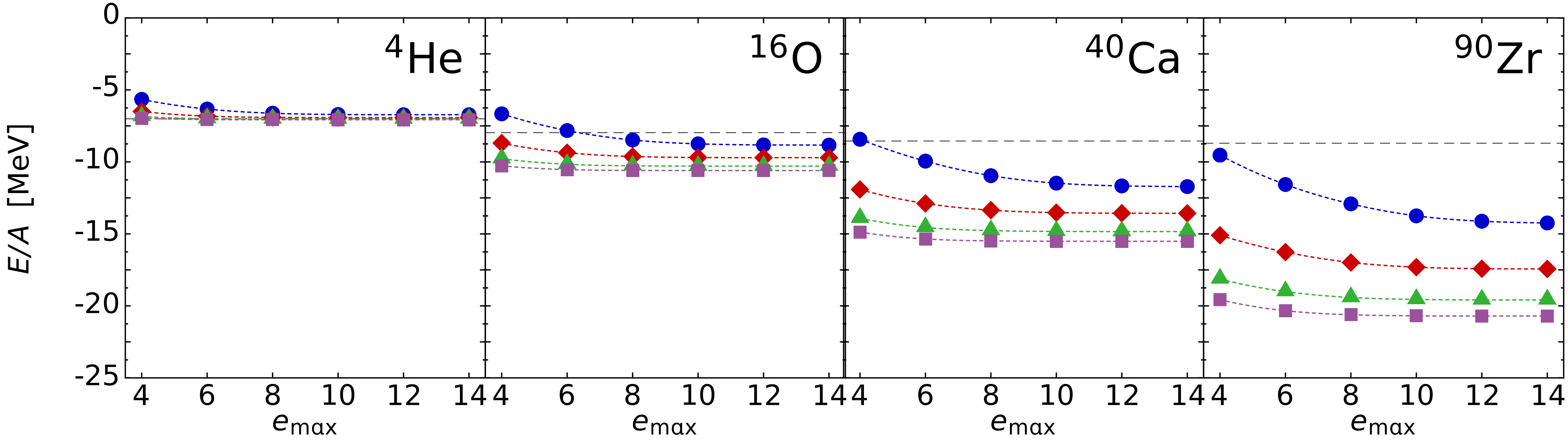


CCSD(HO)

NN only
$\hbar\Omega = 20\,\text{MeV}$

$\alpha = 0.02\,\text{fm}^4$	$\alpha = 0.04\,\text{fm}^4$	$\alpha = 0.0625\,\text{fm}^4$	$\alpha = 0.08\,\text{fm}^4$
$\Lambda = 2.65\,\text{fm}^{-1}$	$\Lambda = 2.24\,\text{fm}^{-1}$	$\Lambda = 2.00\,\text{fm}^{-1}$	$\Lambda = 1.88\,\text{fm}^{-1}$

Coupled Cluster - Convergence Rate



CCSD(HO)

NN only
$\hbar\Omega = 20\,\mathrm{MeV}$

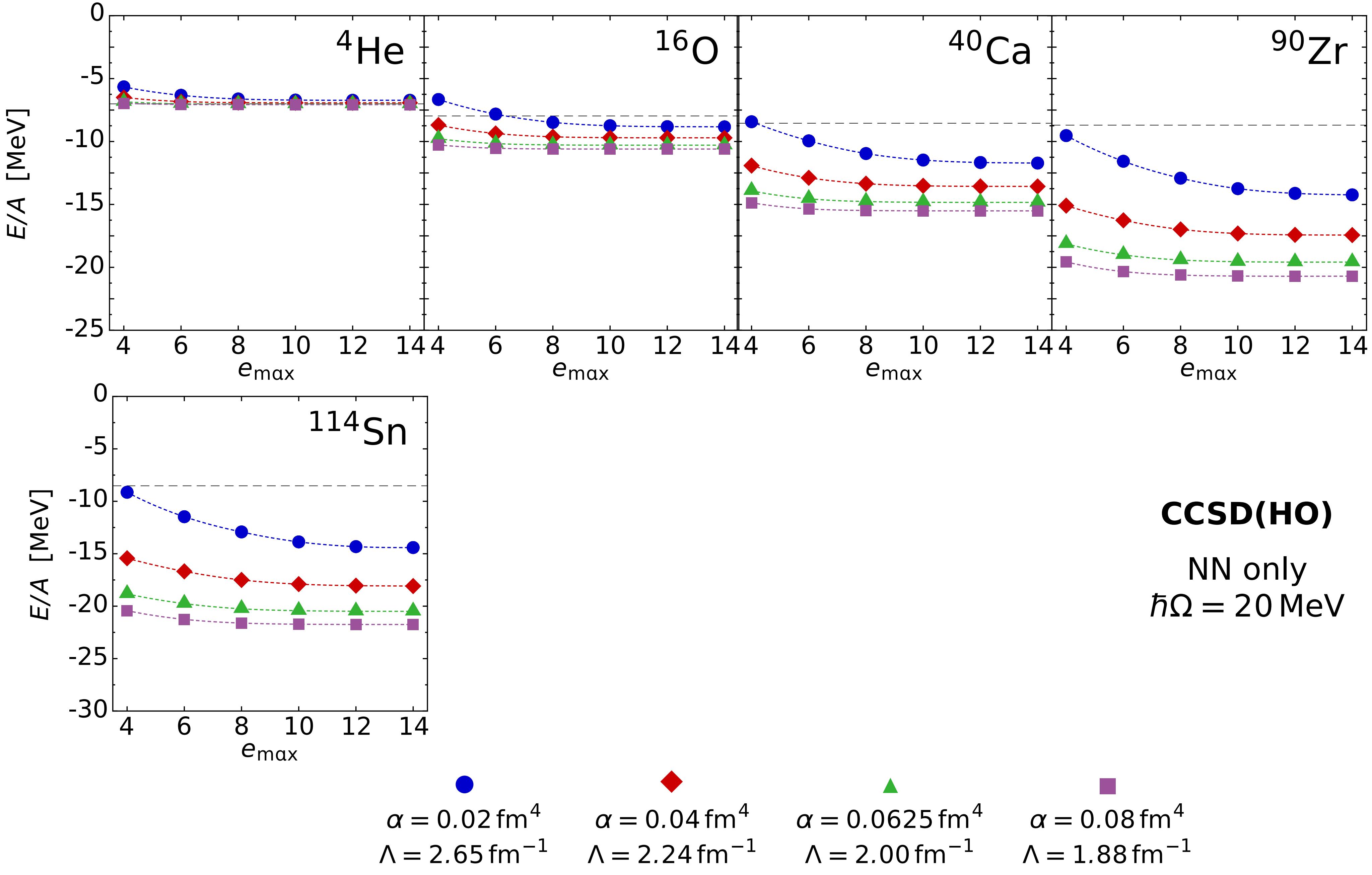
$\alpha = 0.02\,\mathrm{fm}^4$ $\Lambda = 2.65\,\mathrm{fm}^{-1}$

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

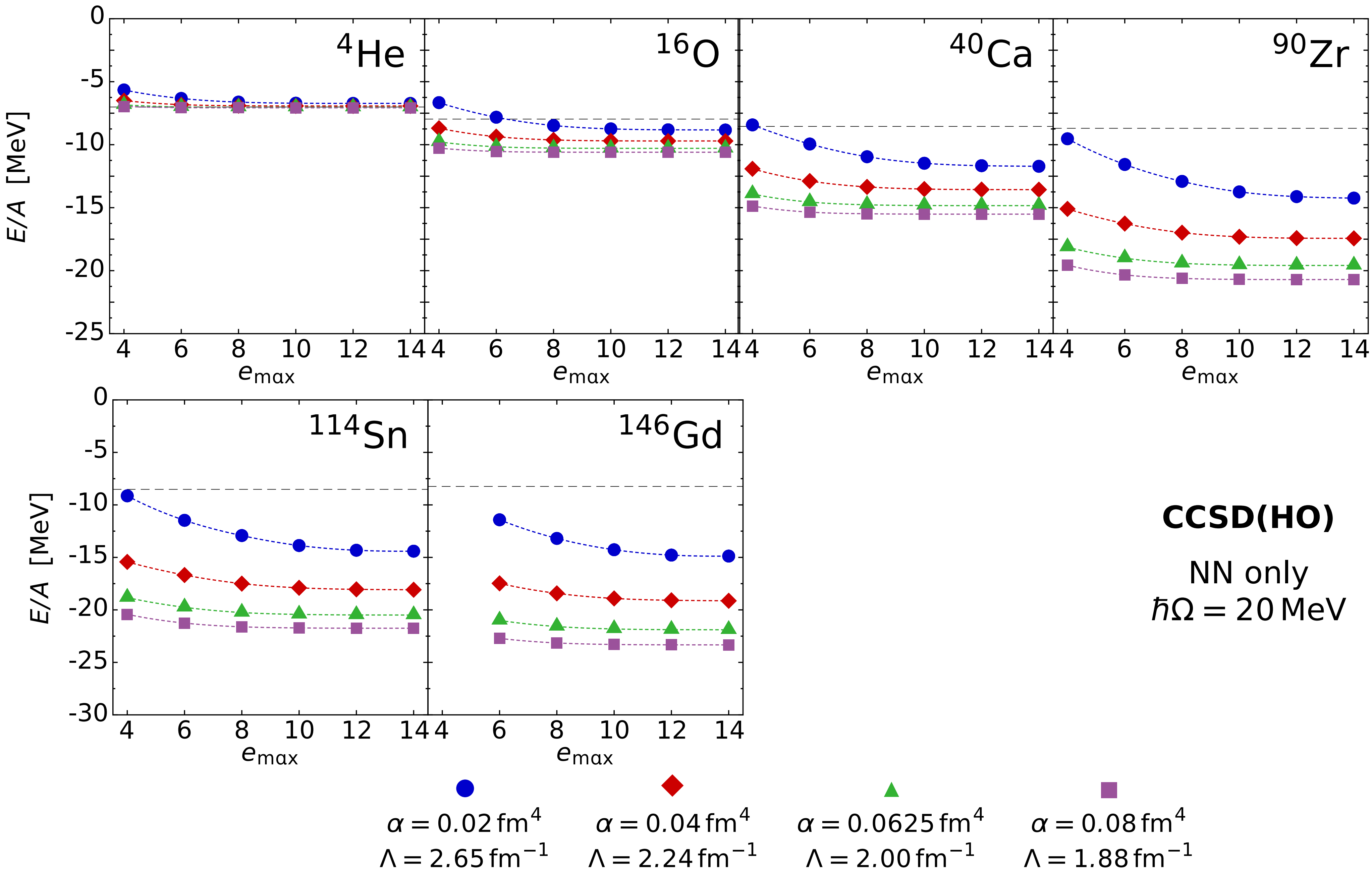
$\alpha = 0.0625\,\mathrm{fm}^4$ $\Lambda = 2.00\,\mathrm{fm}^{-1}$

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

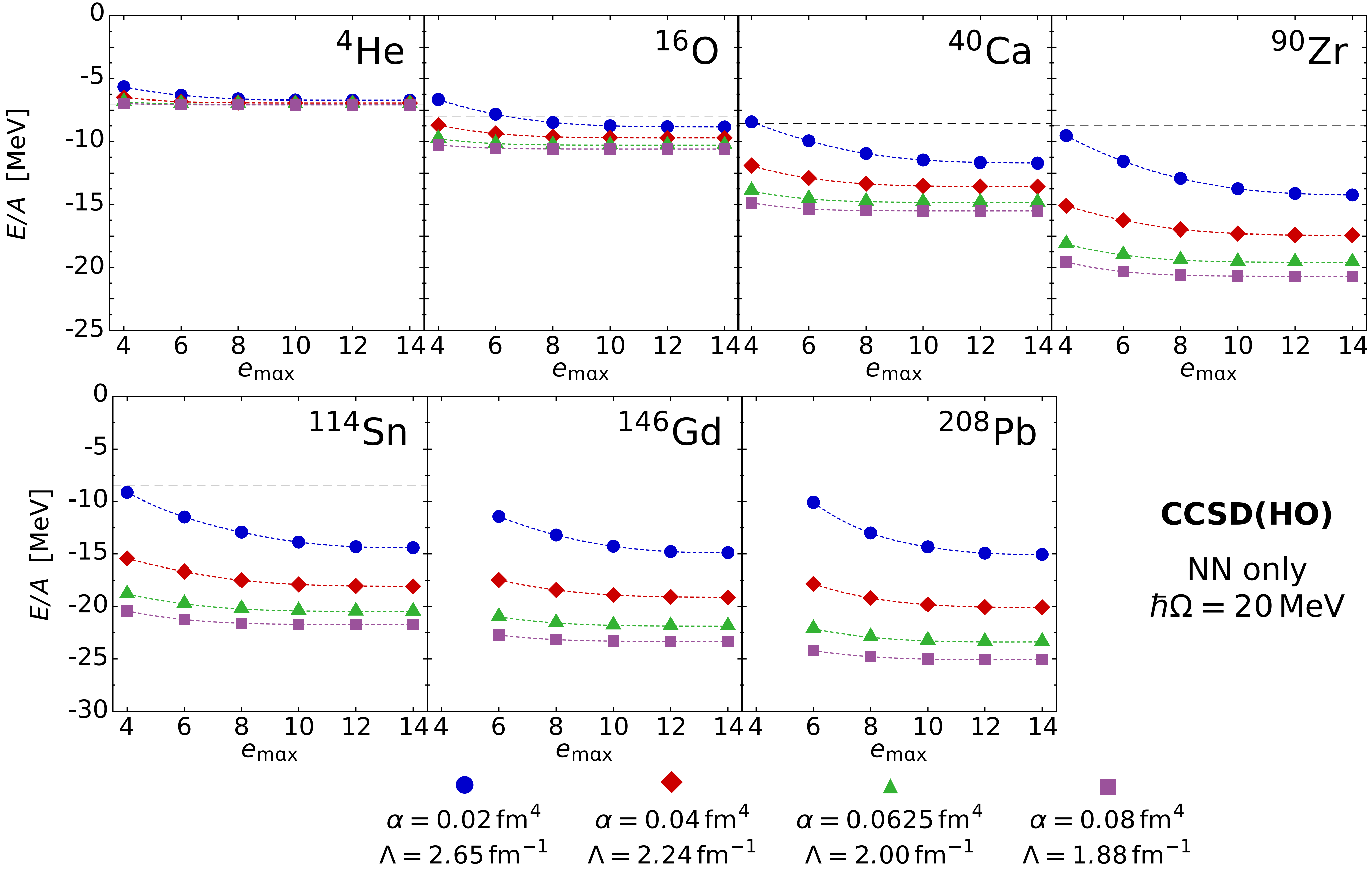
Coupled Cluster - Convergence Rate



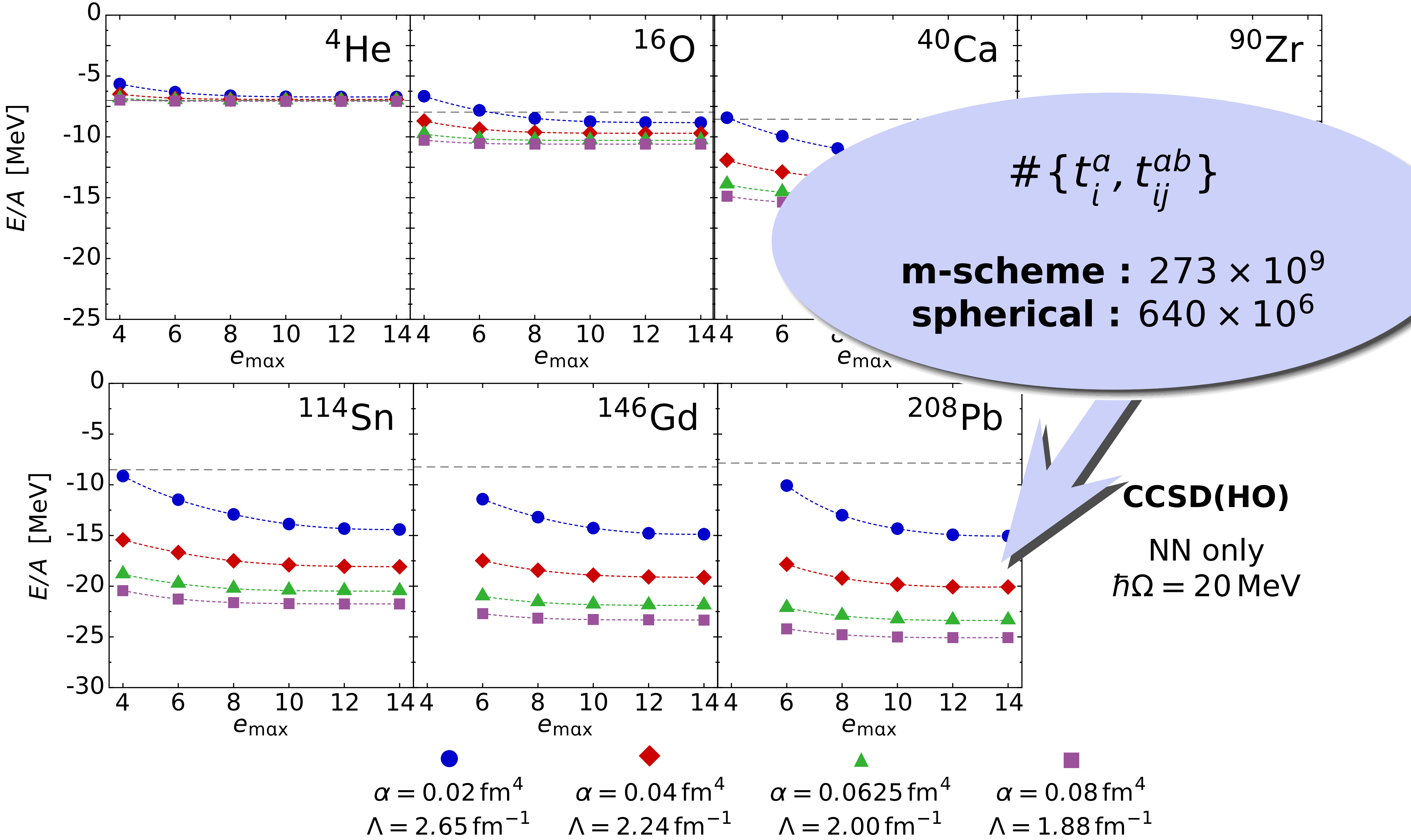
Coupled Cluster - Convergence Rate



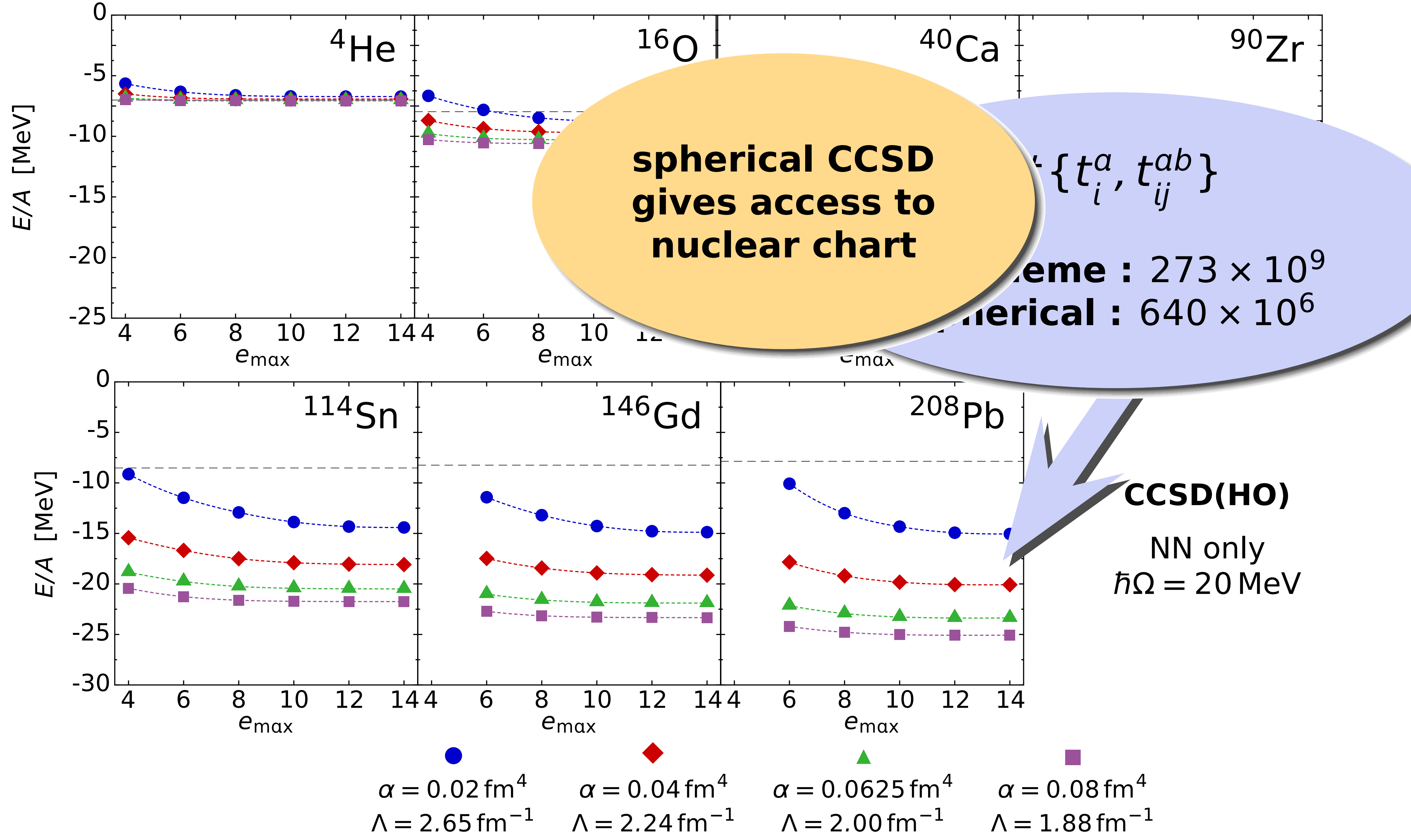
Coupled Cluster - Convergence Rate



Coupled Cluster - Convergence Rate



Coupled Cluster - Convergence Rate



Normal-Ordered 3N Interaction

Roth, Binder, Vobig et al. — arXiv: 1112.0287 (2011)

Normal-Ordered 3N Interaction

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

Normal-Ordered 3N Interaction

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

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

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

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

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

Normal-Ordered 3N Interaction

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

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

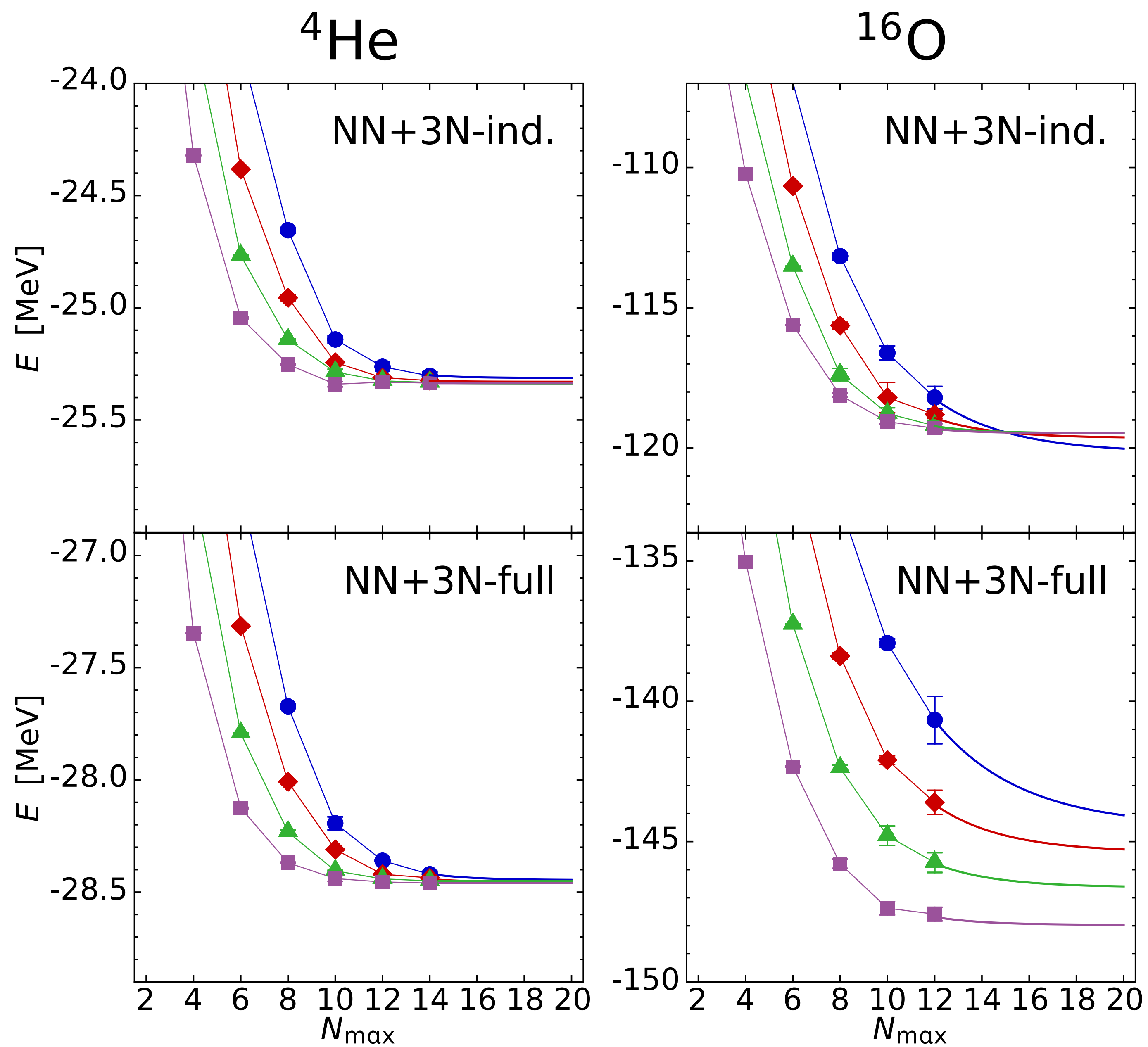
$$\hat{V}_{3N} = \sum V^{3N}_{\circ\circ\circ\circ\circ\circ} \hat{a}^\dagger_\circ \hat{a}^\dagger_\circ \hat{a}^\dagger_\circ \hat{a}_\circ \hat{a}_\circ \hat{a}_\circ$$

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

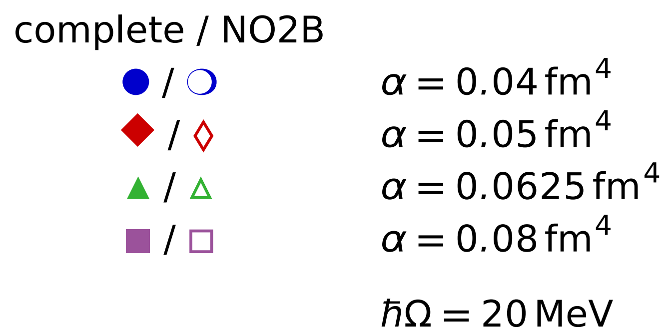
$$+ \sum W^{3B}_{\circ\circ\circ\circ\circ\circ} \{\hat{a}^\dagger_\circ \hat{a}^\dagger_\circ \hat{a}^\dagger_\circ \hat{a}_\circ \hat{a}_\circ \hat{a}_\circ\}$$

- **question**: if we neglect the normal-ordered 3B term, how well does this approximation work ?

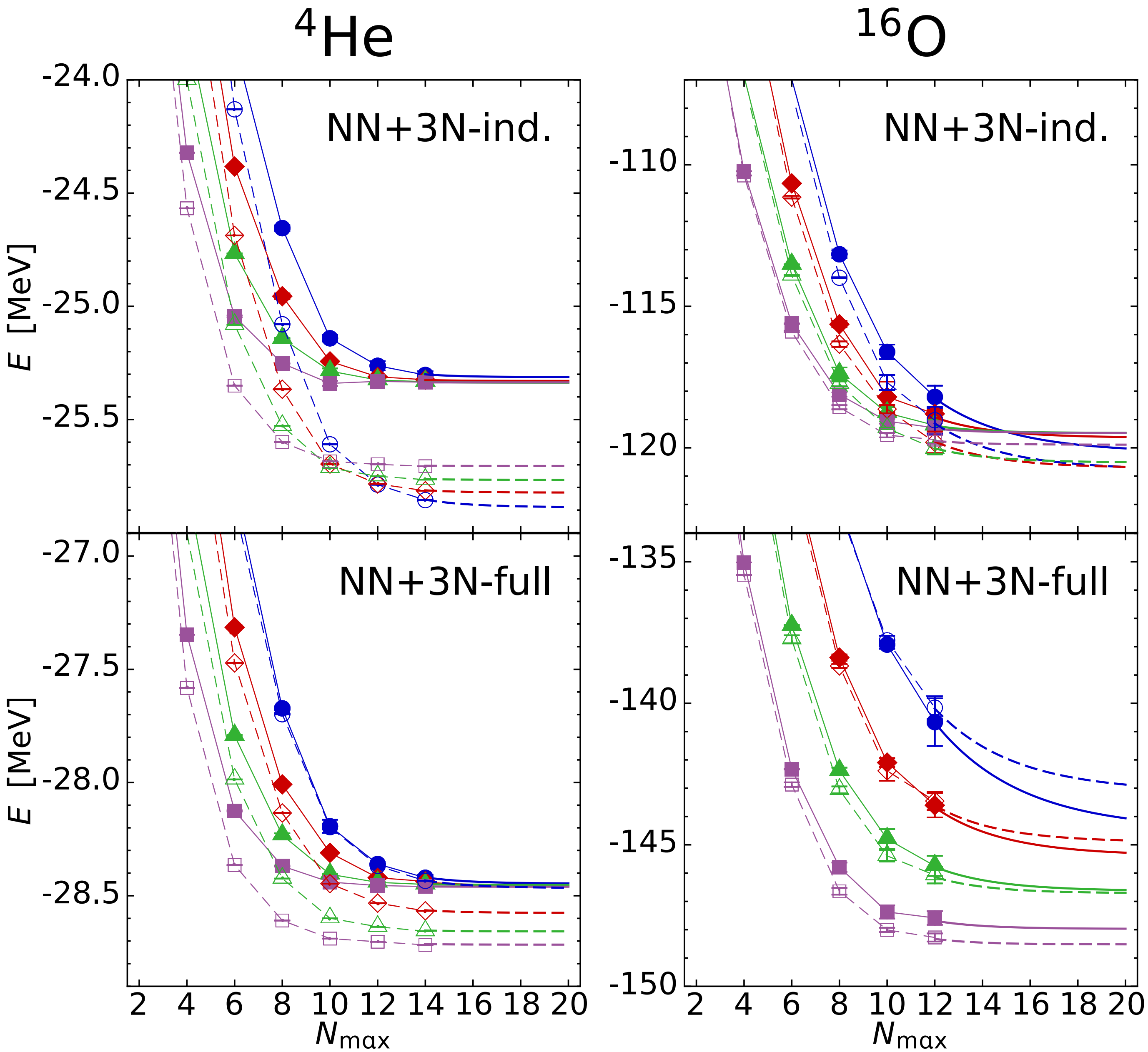
Benchmark of Normal-Ordered 3N



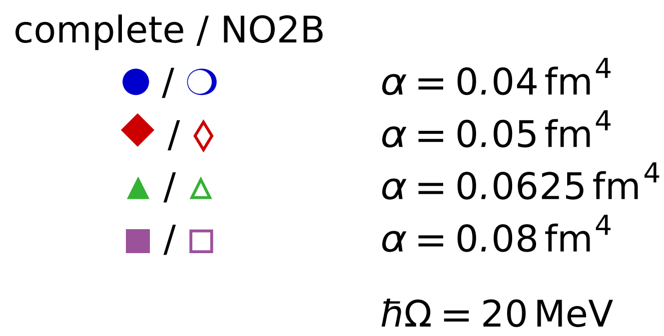
- compare IT-NCSM results with complete 3N to normal-ord. 3N truncated at the 2B level



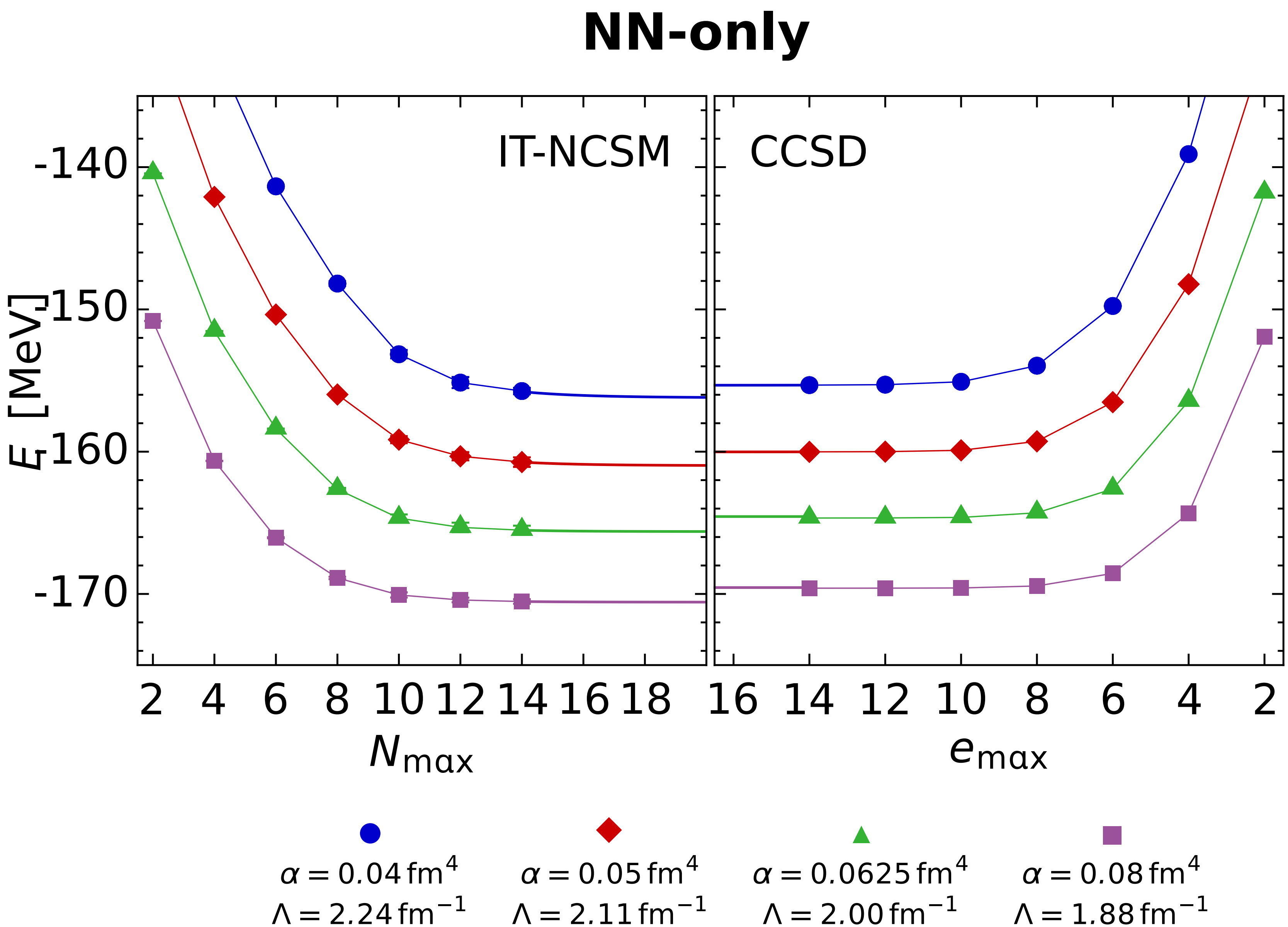
Benchmark of Normal-Ordered 3N



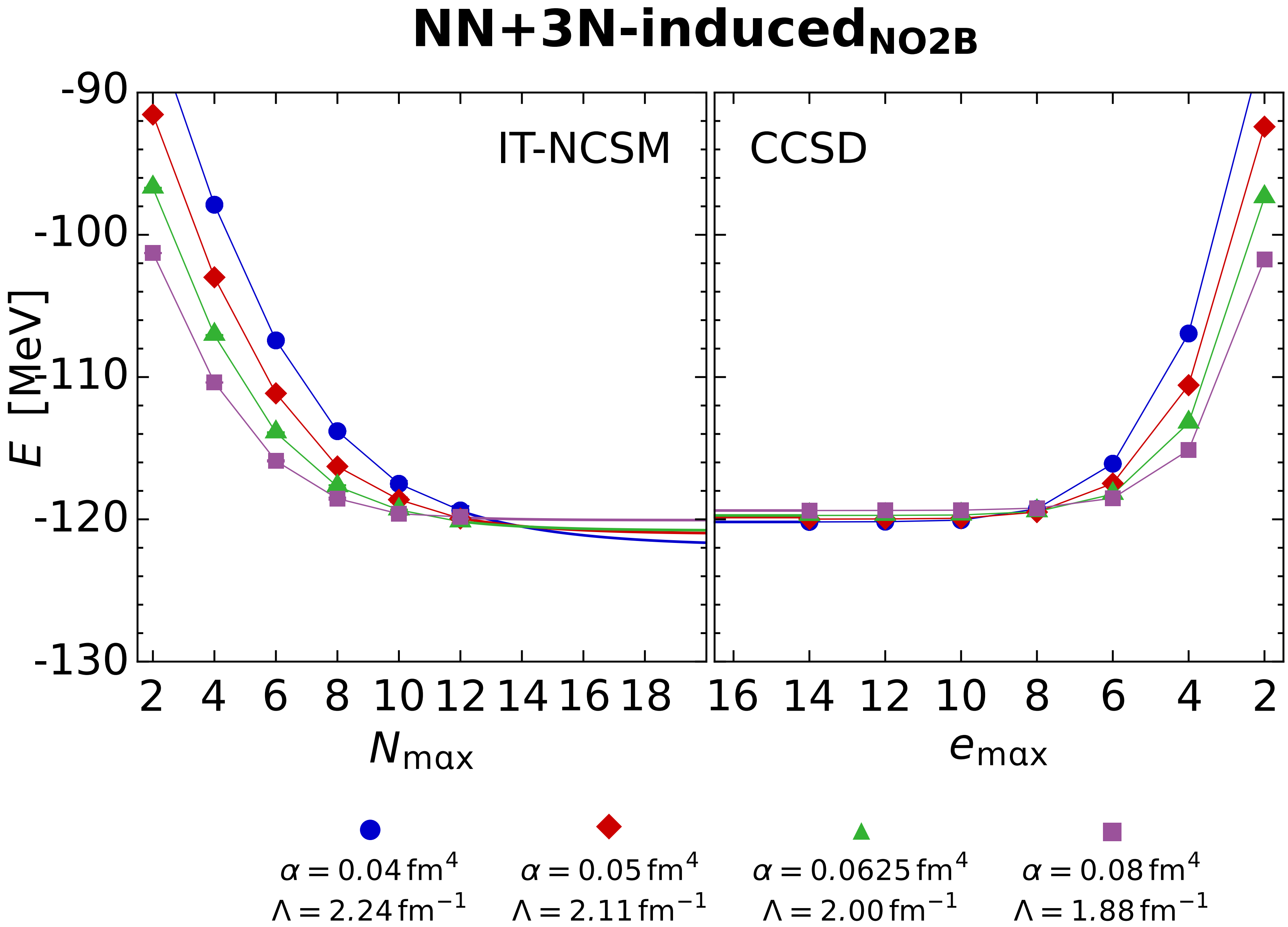
- compare IT-NCSM results with complete 3N to normal-ord. 3N truncated at the 2B level
- typical deviations up to 2% for ^{4}He and 1% for ^{16}O



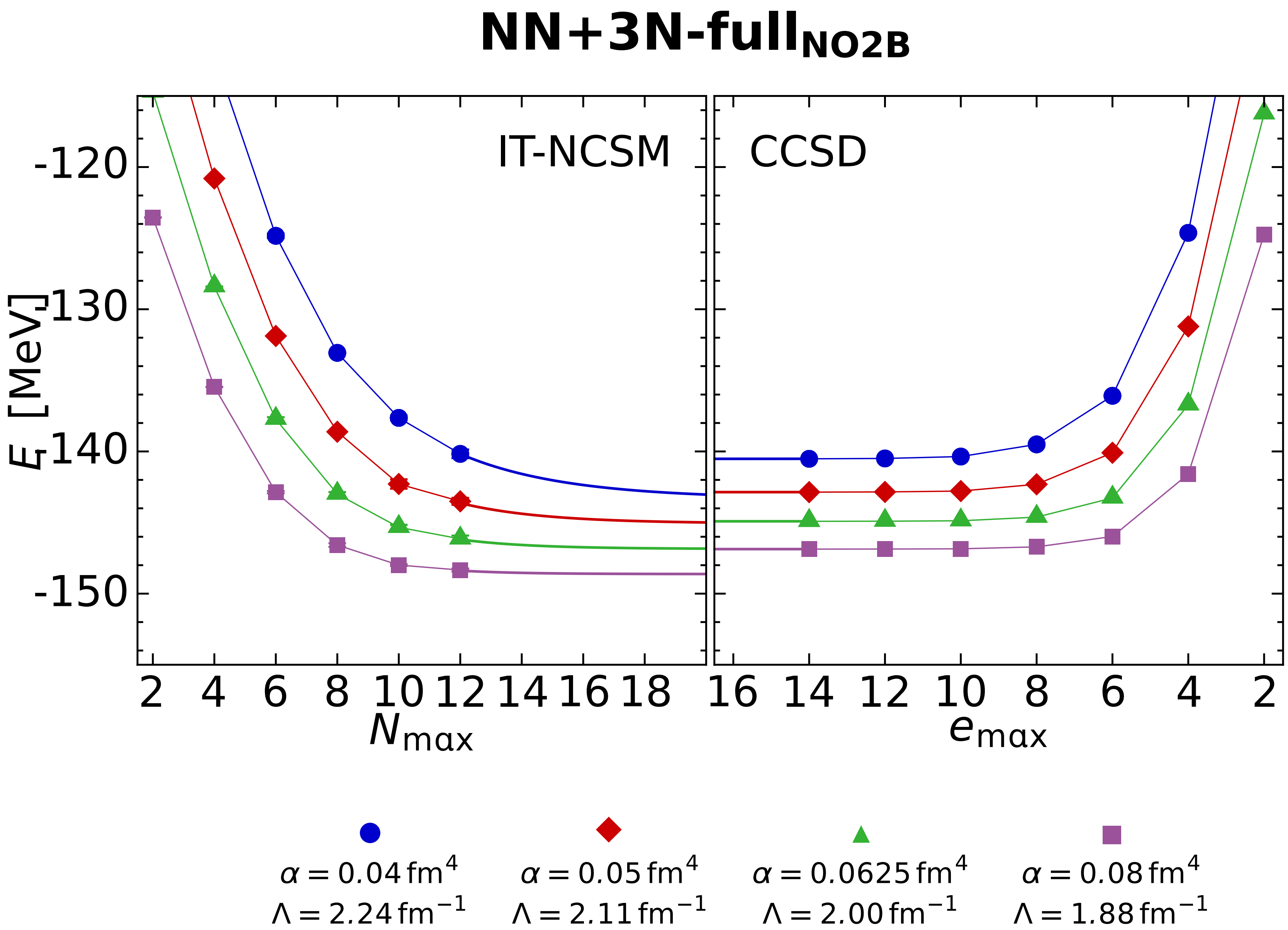
^{16}O: IT-NCSM vs. Coupled-Cluster



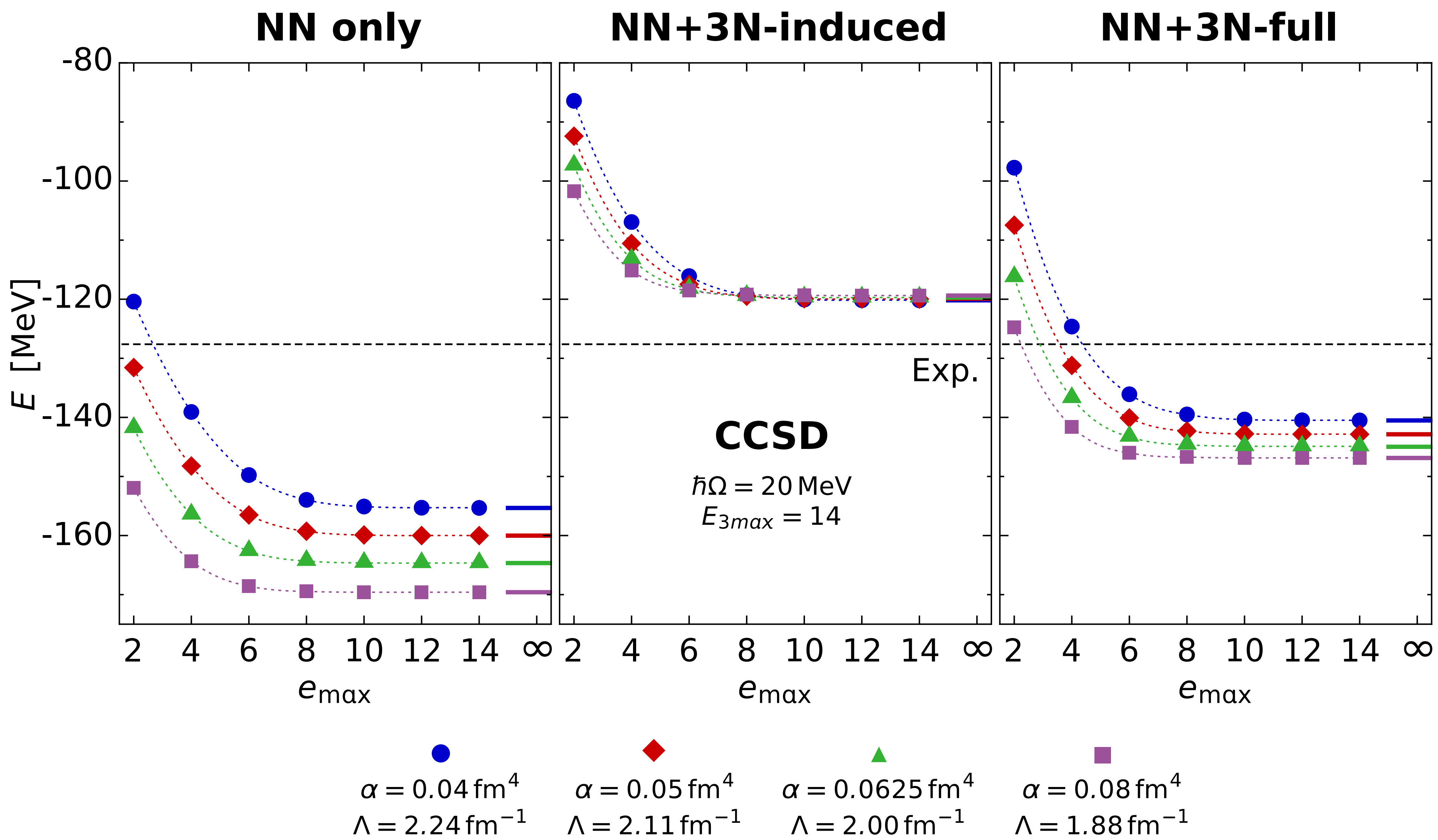
^{16}O: IT-NCSM vs. Coupled-Cluster



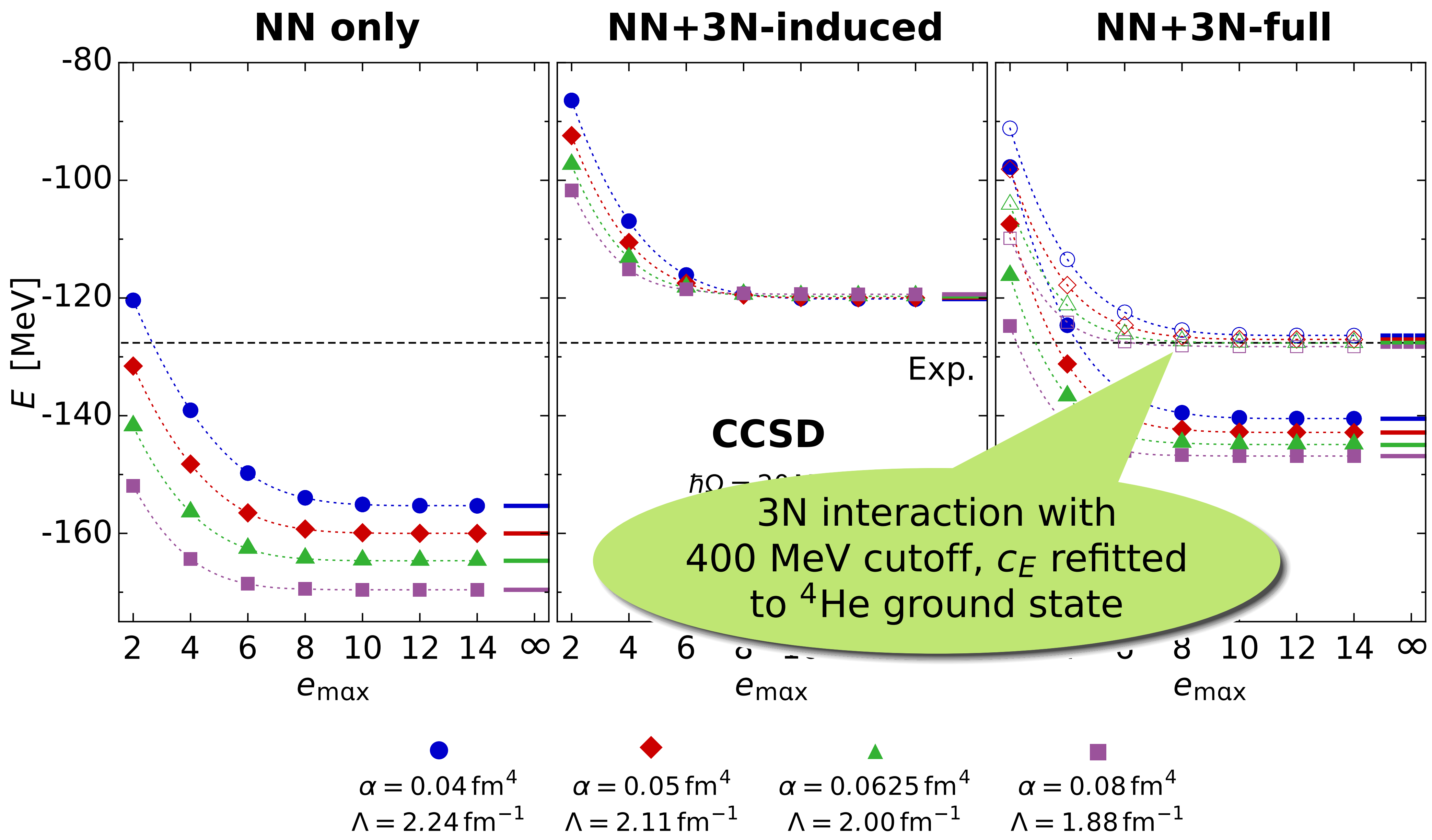
^{16}O: IT-NCSM vs. Coupled-Cluster



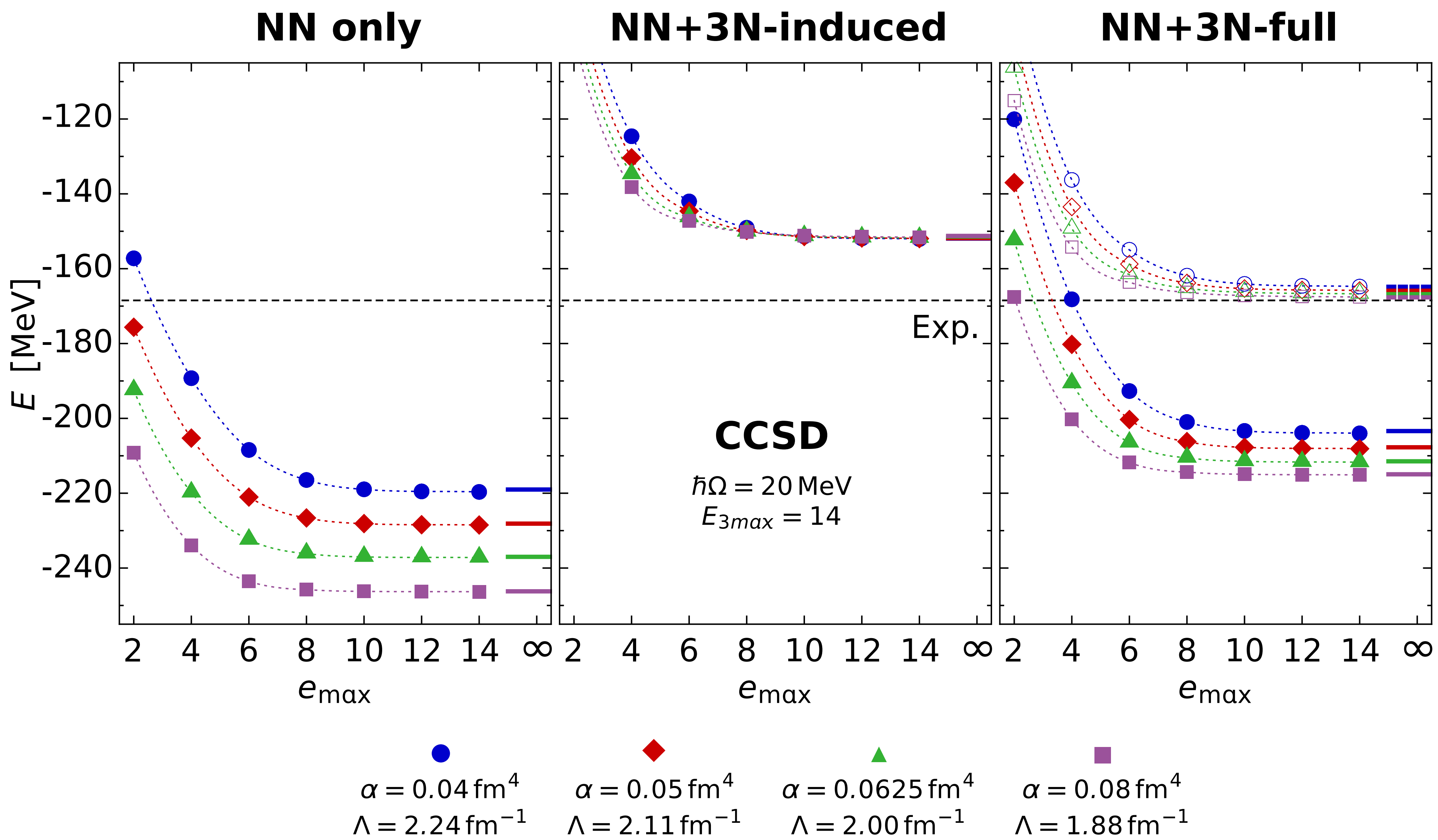
^{16}O: Coupled-Cluster with $3N_{NO2B}$



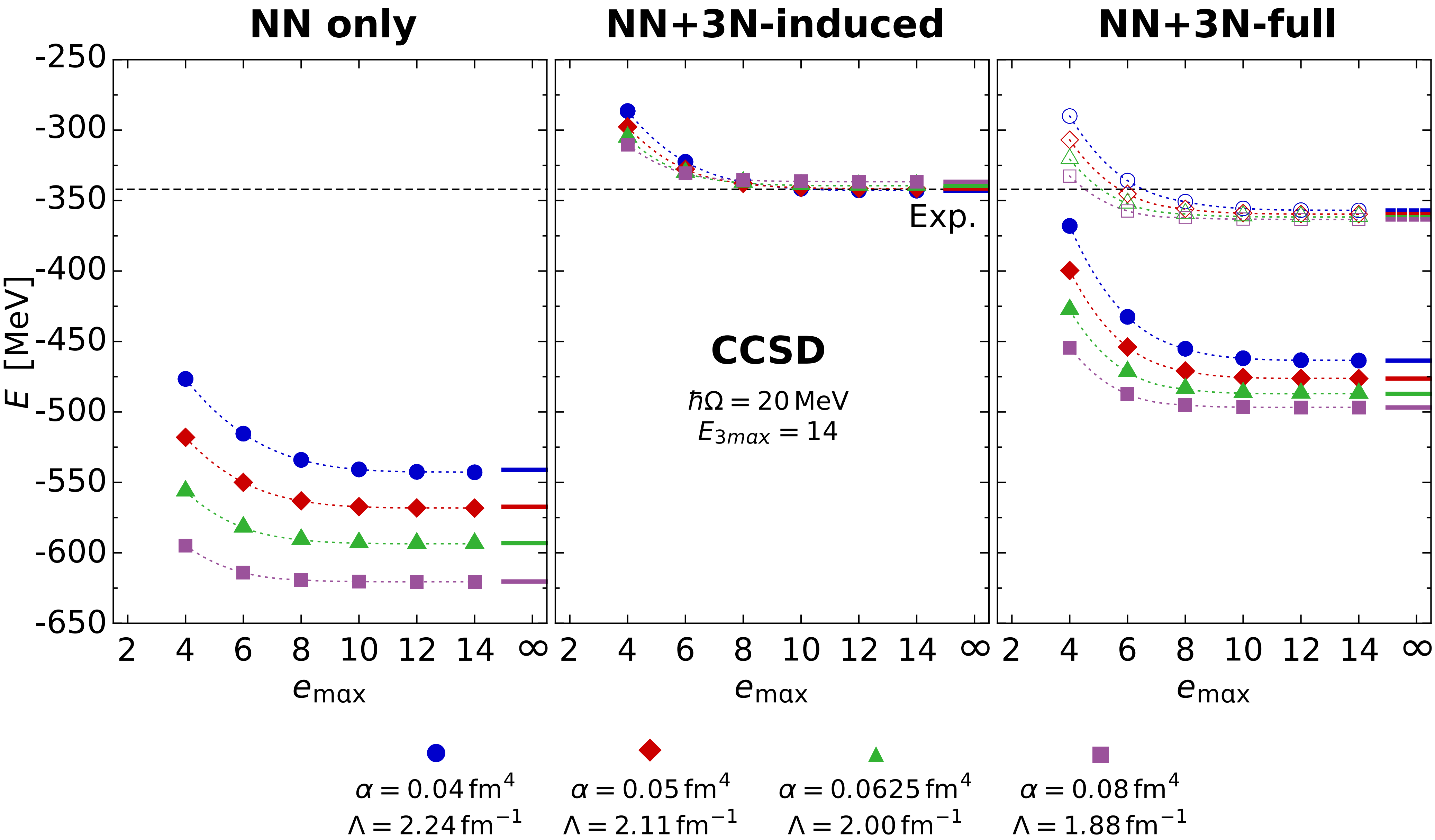
^{16}O: Coupled-Cluster with 3N$_{NO2B}$



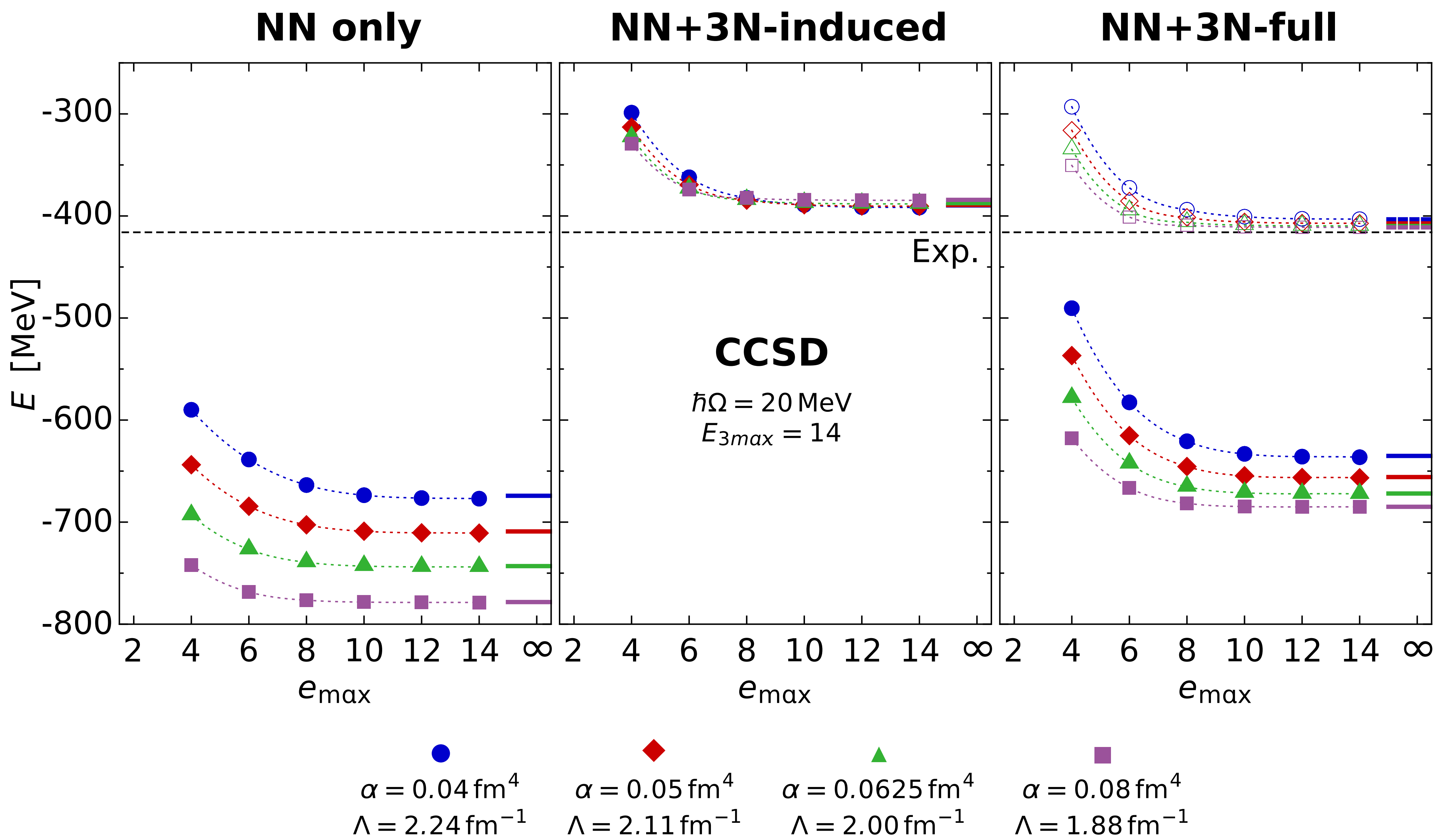
^{24}O: Coupled-Cluster with $3N_{NO2B}$



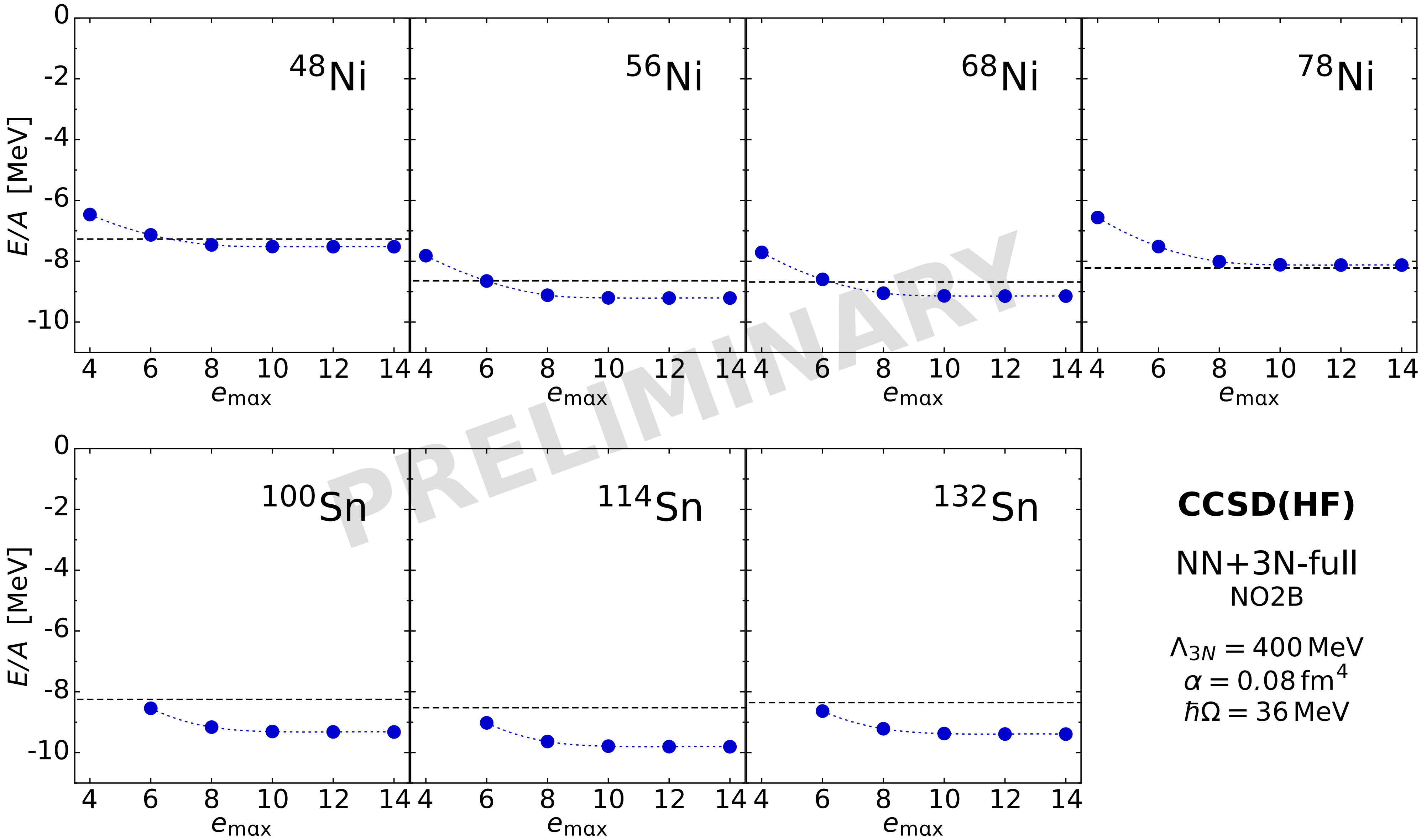
^{40}Ca: Coupled-Cluster with $3N_{NO2B}$



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



Chiral 3N for Heavy Nuclei



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
    Institut für Kernphysik, TU Darmstadt
  - **P. Navrátil**
    TRIUMF Vancouver, Canada
  - J. Vary, P. Maris
    Iowa State University, USA
  - 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

JUROPA — JÜLICH FORSCHUNGSZENTRUM
LOEWE-CSC — CSC Center for Scientific Computing Frankfurt
HOPPER — NERSC

COMPUTING TIME

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