Ab Initio Nuclear Structure Theory

Lecture 3: Light Nuclei

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Overview

- **Lecture 1: Hamiltonian**

  Prelude • Many-Body Quantum Mechanics • Nuclear Hamiltonian • Matrix Elements

- **Lecture 2: Correlations**

  Two-Body Problem • Correlations & Unitary Transformations • Similarity Renormalization Group

- **Lecture 3: Light Nuclei**

  Many-Body Problem • Configuration Interaction • No-Core Shell Model • Applications

- **Lecture 4: Beyond Light Nuclei**

  Normal Ordering • Coupled-Cluster Theory • In-Medium Similarity Renormalization Group

Many-Body Problem

Definition: Ab Initio

solve nuclear many-body problem based on realistic interactions using controlled and improvable truncations with quantified theoretical uncertainties

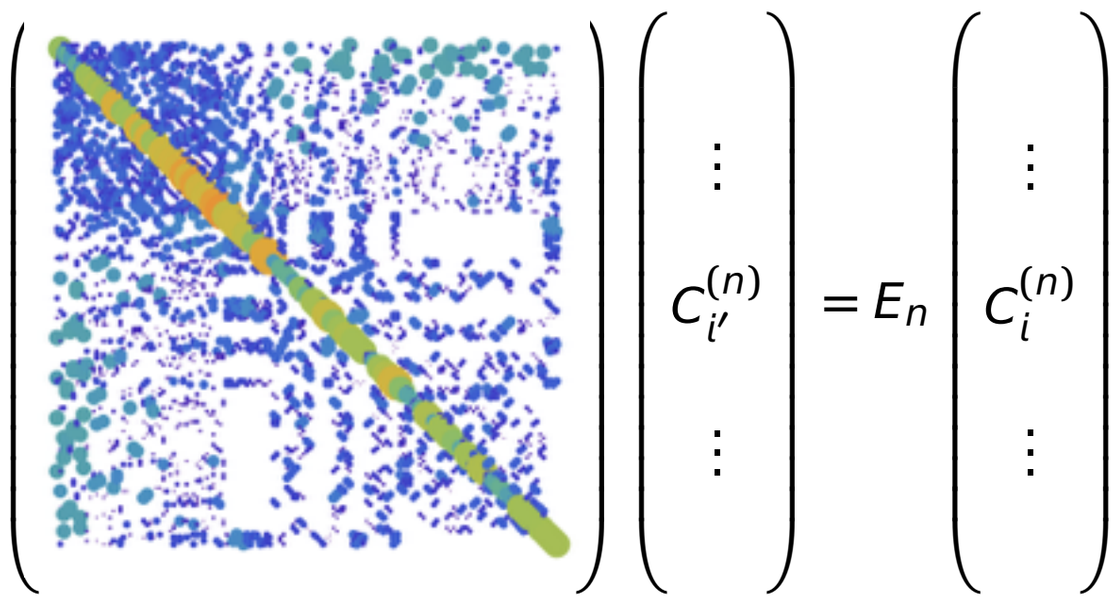
- numerical treatment with some **truncations or approximations** is inevitable for any nontrivial nuclear structure application

- **challenges for ab initio calculations** are to
  - control the truncation effects
  - quantify the resulting uncertainties
  - reduce them to an acceptable level

- **convergence** with respect to truncations is important: demonstrate that observables become independent of truncations

- continuous transition from approximation to ab initio calculation…

Configuration Interaction Approaches



$$\begin{pmatrix} & \\ & \\ & \end{pmatrix} \begin{pmatrix} \vdots \\ C_{i'}^{(n)} \\ \vdots \end{pmatrix} = E_n \begin{pmatrix} \vdots \\ C_i^{(n)} \\ \vdots \end{pmatrix}$$

Configuration Interaction (CI)

- select a convenient **single-particle basis**

$$|\alpha\rangle = |n\, l\, j m\, t m_t\rangle$$

- construct **A-body basis** of Slater determinants from all possible combinations of A different single-particle states

$$|\Phi_i\rangle = |\{\alpha_1 \alpha_2 \ldots \alpha_A\}_i\rangle$$

- convert eigenvalue problem of the Hamiltonian into a **matrix eigenvalue problem** in the Slater determinant representation

$$\mathrm{H}_{\mathrm{int}}\,|\Psi_n\rangle = E_n\,|\Psi_n\rangle \qquad |\Psi_n\rangle = \sum_i C_i^{(n)}\,|\Phi_i\rangle$$

$$\begin{pmatrix} & \vdots & \\ \ldots & \langle\Phi_i|\,\mathrm{H}_{\mathrm{int}}\,|\Phi_{i'}\rangle & \ldots \\ & \vdots & \end{pmatrix} \begin{pmatrix} \vdots \\ C_{i'}^{(n)} \\ \vdots \end{pmatrix} = E_n \begin{pmatrix} \vdots \\ C_i^{(n)} \\ \vdots \end{pmatrix}$$

Model Space Truncations

- have to **introduce truncations** of the single/many-body basis to make the Hamilton matrix **finite and numerically tractable**

  - **full CI**:
    truncate the single-particle basis, e.g., at a maximum single-particle energy

  - **particle-hole truncated CI**:
    truncate single-particle basis and truncate the many-body basis at a maximum n-particle-n-hole excitation level

  - **interacting shell model**:
    truncate single-particle basis and freeze low-lying single-particle states (core)

- in order to qualify as ab initio one has to **demonstrate convergence** with respect to all those truncations

- there is freedom to **optimize the single-particle basis**, instead of HO states one can use single-particle states from a Hartree-Fock calculation

Variational Perspective

- solving the eigenvalue problem in a finite model space is **equivalent to a variational calculation** with a trial state

$$|\Psi_n(D)\rangle = \sum_{i=1}^{D} C_i^{(n)} |\Phi_i\rangle$$

- formally, the stationarity condition for the energy expectation value directly leads to the matrix eigenvalue problem in the truncated model space

- **Ritz variational principle**: the ground-state energy in a D-dimensional model space is an upper bound for the exact ground-state energy

$$E_0(D) \geq E_0(\text{exact})$$

- **Hylleraas-Undheim theorem**: all states of the spectrum have a monotonously decreasing energy with increasing model space dimension

$$E_n(D) \geq E_n(D+1)$$

Theory Uncertainties

- model-space truncation is the **sole source of uncertainties** in the solution of the many-body problem

- absolute energies are **protected by the variational principle**, i.e., smooth and monotonic dependence on model-space size (not so for other observables)

convergence with respect to model-space size is the only thing we have to worry about

- **efficient truncations**: closer to convergence with smaller model-space dimension, i.e., physics-informed truncation scheme

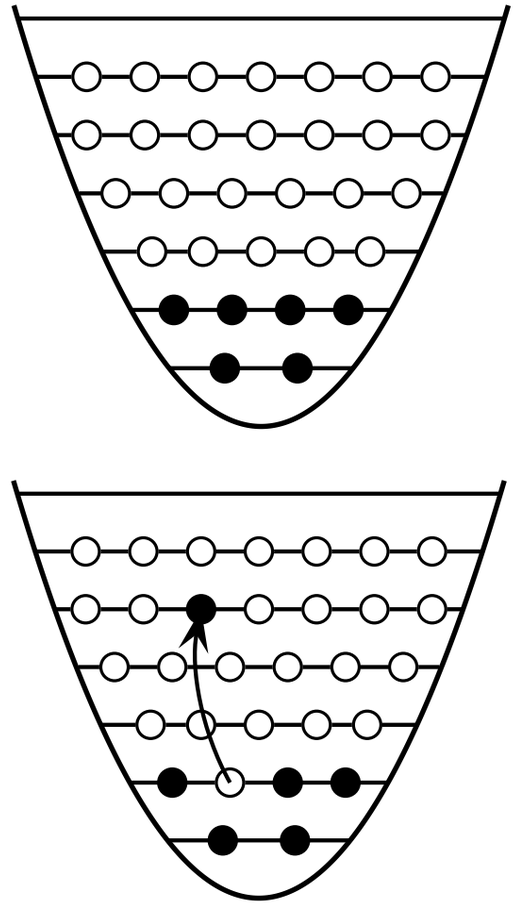
- **extrapolations**: extrapolate observables to infinite model-space from sequence of finite-space calculations

- **uncertainty quantification**: extract many-body uncertainty from residual model-space dependence or extrapolation

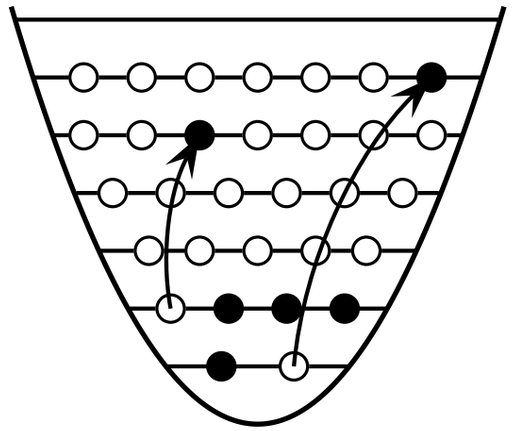
No-Core Shell Model

No-Core Shell Model (NCSM)

- NCSM is a special case of a CI approach:
  - single-particle basis is a **spherical HO basis**
  - truncation in terms of the total **number of HO excitation quanta N_{max}** in the many-body states



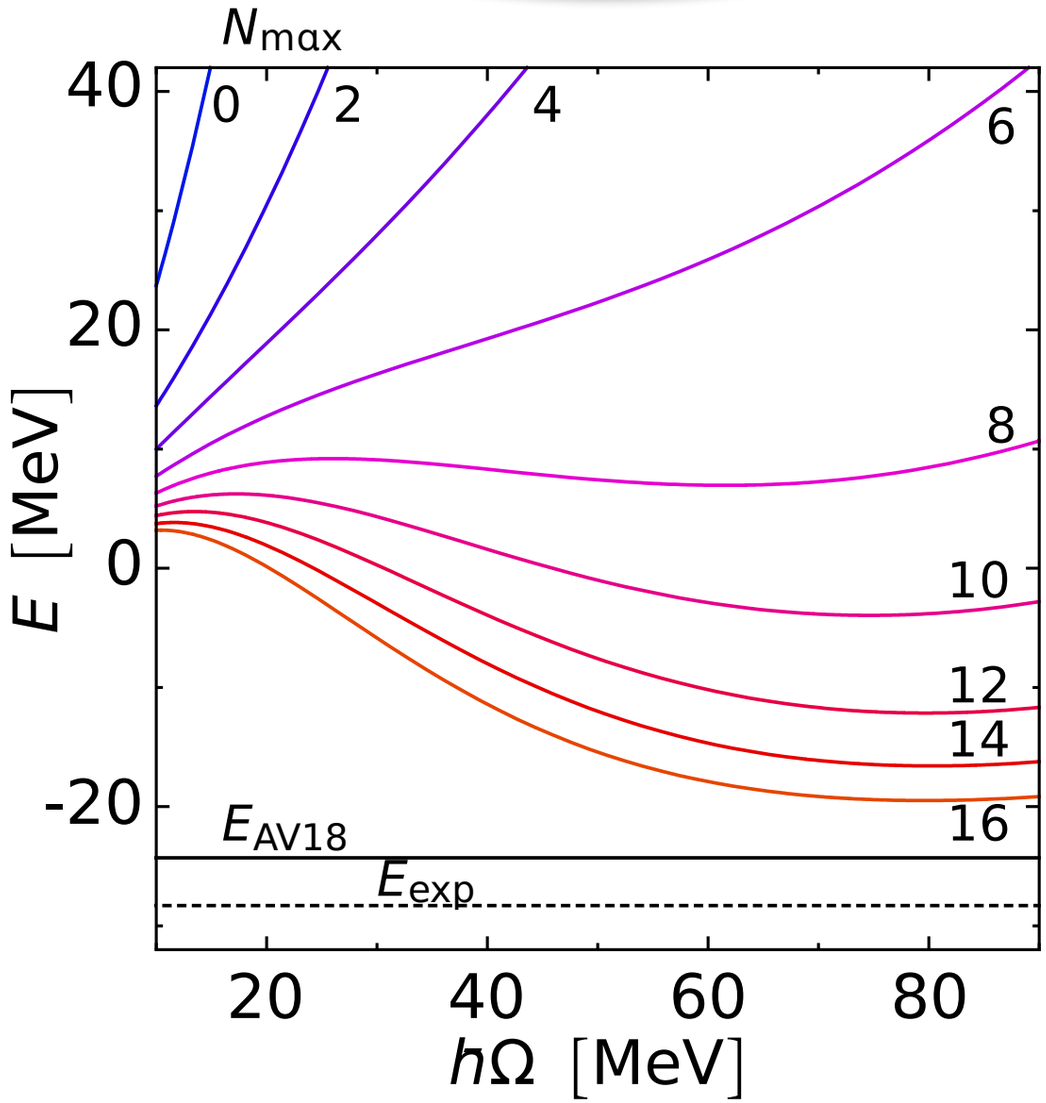
- **specific advantages** of the NCSM:
  - many-body energy truncation (N_{max}) truncation is much **more efficient** than single-particle energy truncation (e_{max})
  - equivalent NCSM formulation in relative Jacobi coordinates for each N_{max} — **Jacobi-NCSM**
  - **explicit separation** of center of mass and intrinsic states possible for each N_{max}



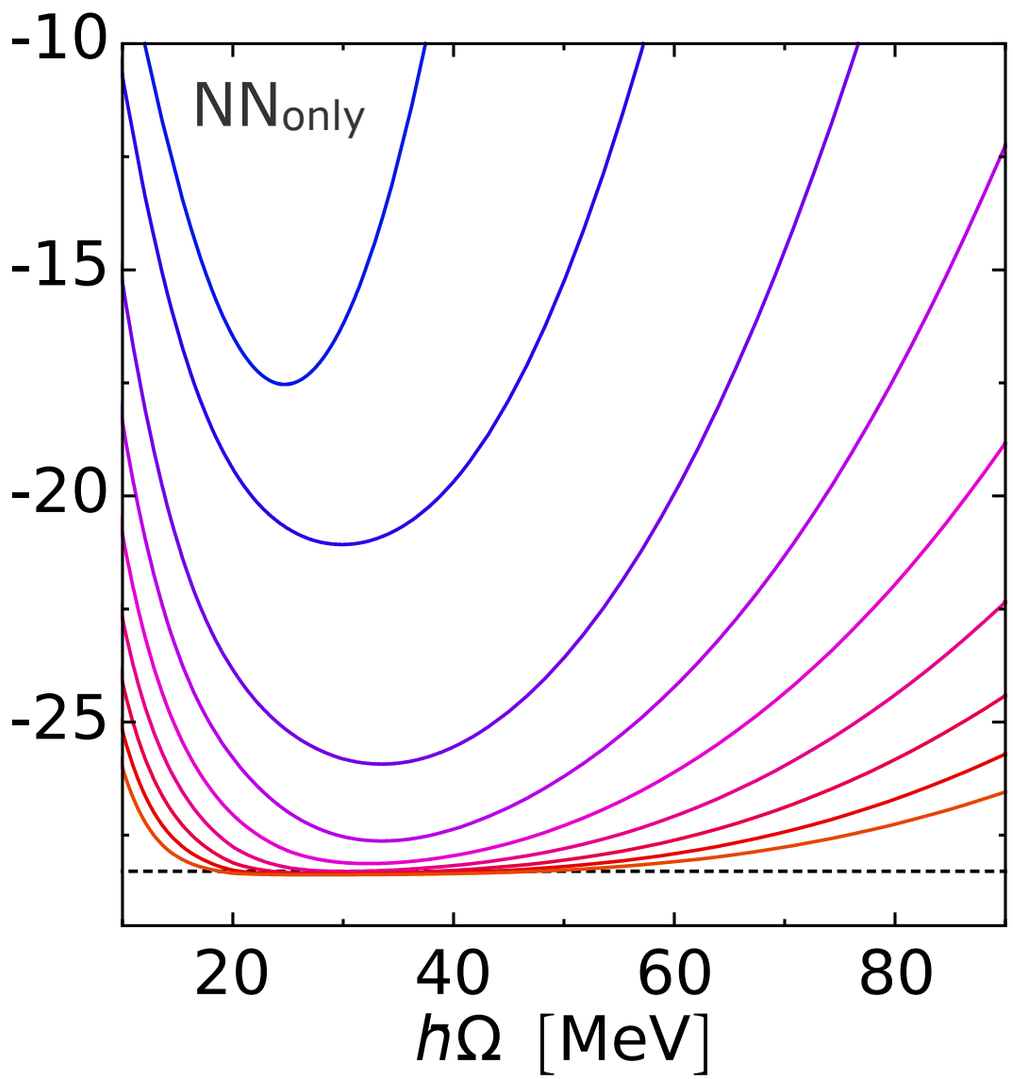
^{4}He: NCSM Convergence

- worst case scenario for NCSM convergence: **Argonne V18 potential**

$\alpha = 0.00\,\mathrm{fm}^4$

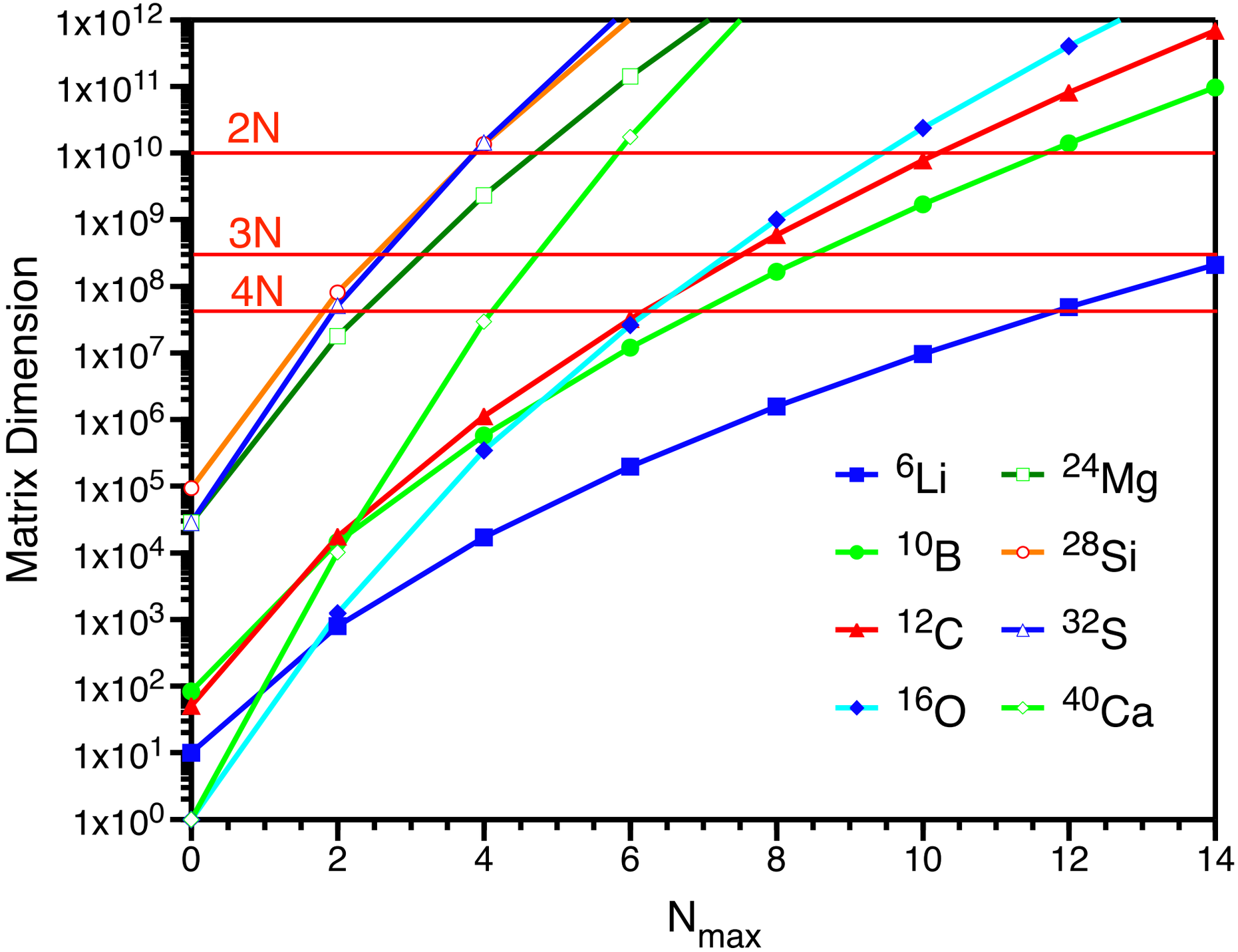


$\alpha = 0.03\,\mathrm{fm}^4$

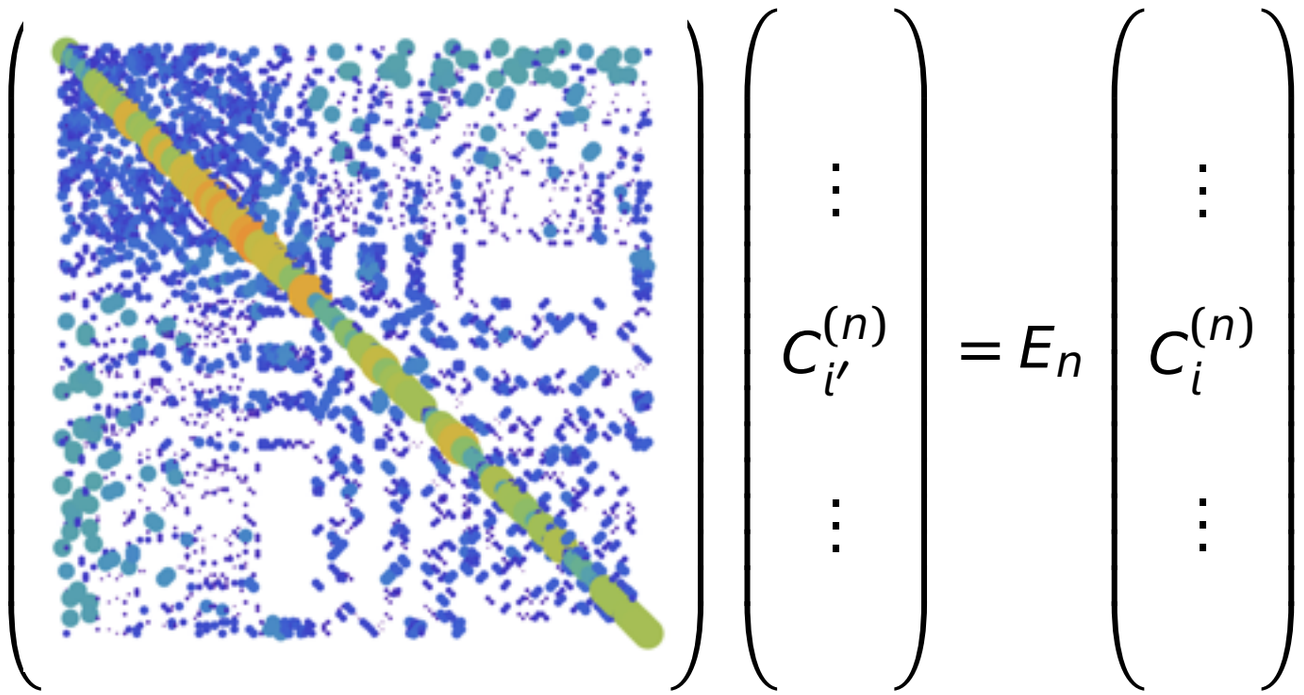


NCSM Basis Dimension

Vary et al.; J. Phys.: Conf. Series 180, 012083 (2009)



Computational Strategy



- **key properties** of the computational problem:
  - only interested in a **few low-lying eigenstates**
  - Hamilton matrix is **very sparse** (typically <0.01% non-zeros)
- **Laczos-type algorithms** for an iterative solution of the eigenvalue problem
- amount of **fast storage** for non-zero matrix elements & a few eigenvectors sets the limits and drives parallelization strategies

Lanczos Algorithm

- **Lanczos Algorithm**: convert the eigenvalue problem of a huge matrix $\boldsymbol{H}$ in an iterative process to an eigenvalue problem of small matrices $\boldsymbol{T_m}$ which converge to the same extremal eigenvalues

$$\boldsymbol{H} = \begin{pmatrix} & & \\ & 10^{10} \times 10^{10} & \\ & & \end{pmatrix}$$

$\vec{v}_0 := \vec{0}$
$\vec{v}_1 :=$ any norm. vector
$\beta_1 := 0$

for $i = 1, m$ **do**

$\vec{w} := \boldsymbol{H} \cdot \vec{v}_i - \beta_i \vec{v}_{i-1}$
$\alpha_i := \vec{w} \cdot \vec{v}_i$
$\vec{w} := \vec{w} - \alpha_i \vec{v}_i$
$\beta_{i+1} := \|\vec{w}\|$
$\vec{v}_{i+1} := \vec{w} / \beta_{i+1}$

end for

$$\boldsymbol{T}_m = \begin{pmatrix} \alpha_1 & \beta_2 & & & \\ \beta_2 & \alpha_2 & \beta_3 & & \\ & \beta_3 & \alpha_3 & \ddots & \\ & & \ddots & \ddots & \beta_m \\ & & & \beta_m & \alpha_m \end{pmatrix}$$

Lanczos Algorithm

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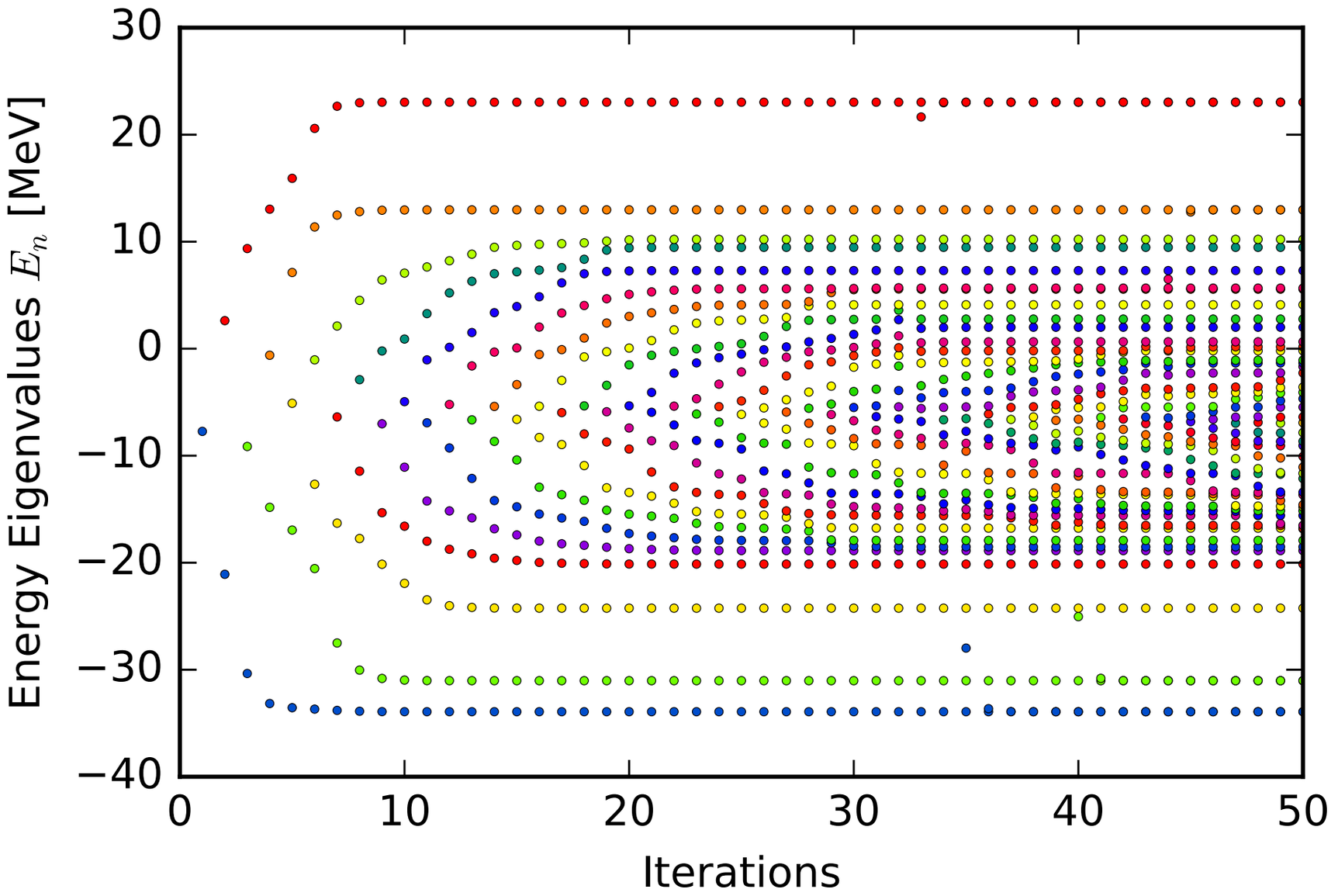

Importance Truncation

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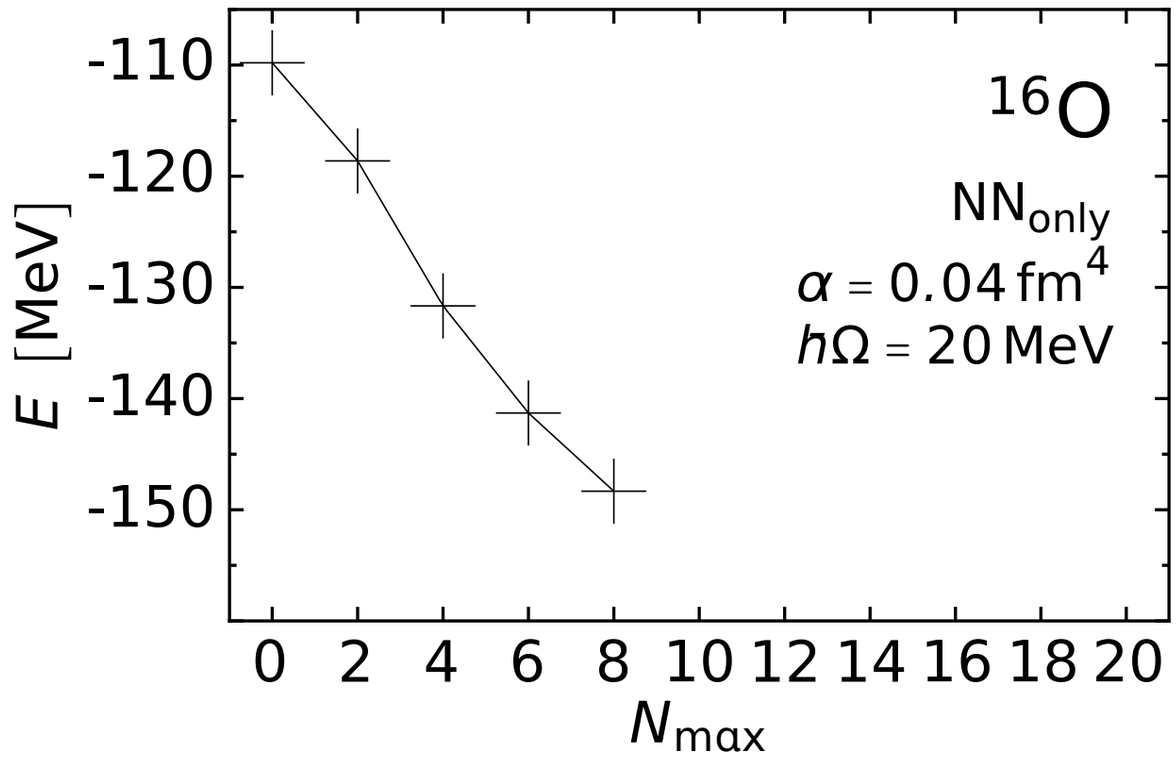
- **converged NCSM** calculations limited to lower & mid p-shell nuclei

- example: full N_{max}=10 calculation for ^{16}O would be very difficult, basis dimension $D > 10^{10}$



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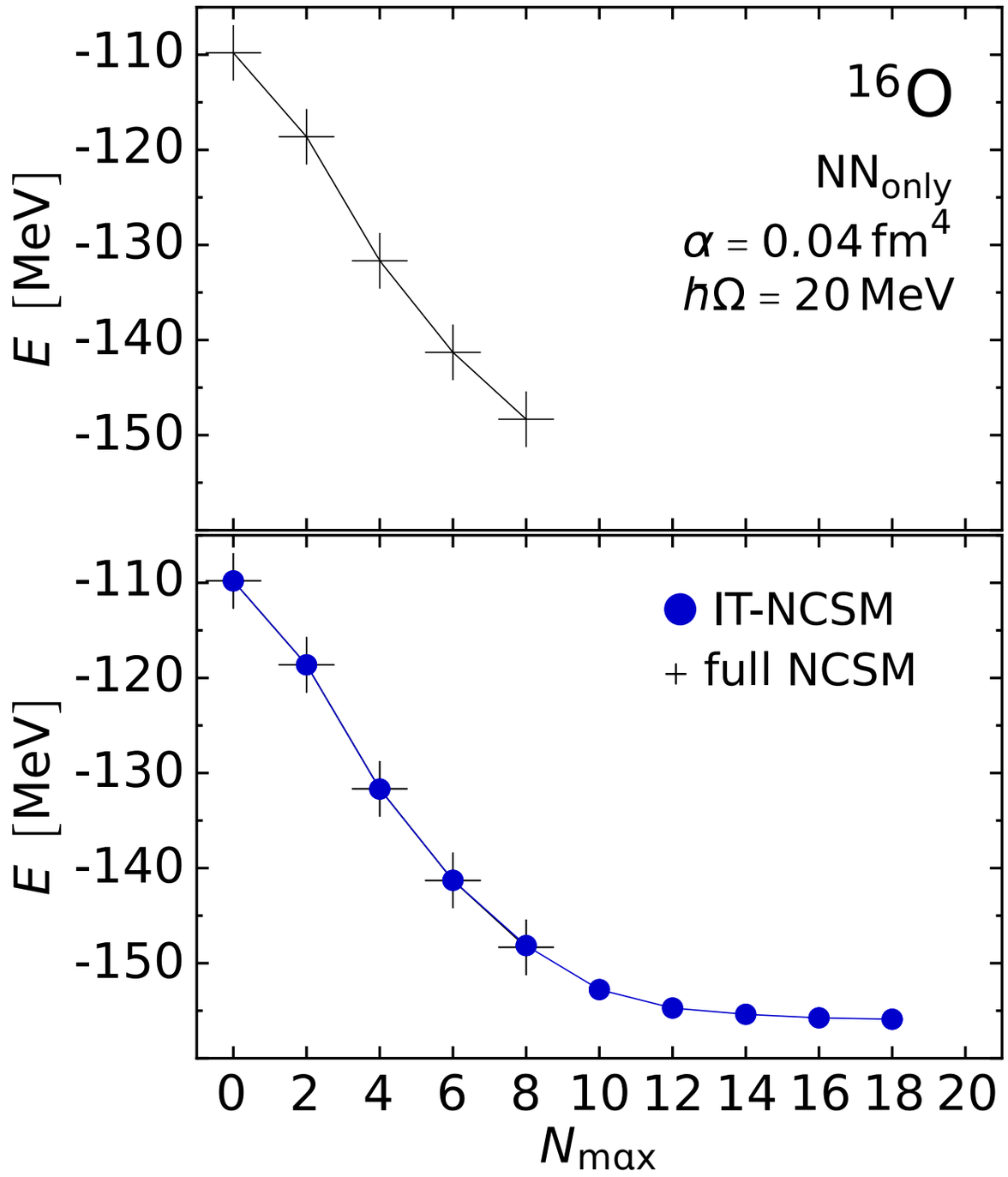
Importance Truncation

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



Importance Truncation

- **starting point**: approximation $|\Psi_{\text{ref}}\rangle$ for the **target state** within a limited reference space $\mathcal{M}_{\text{ref}}$

$$|\Psi_{\text{ref}}\rangle = \sum_{\nu \in \mathcal{M}_{\text{ref}}} C_\nu^{(\text{ref})} |\Phi_\nu\rangle$$

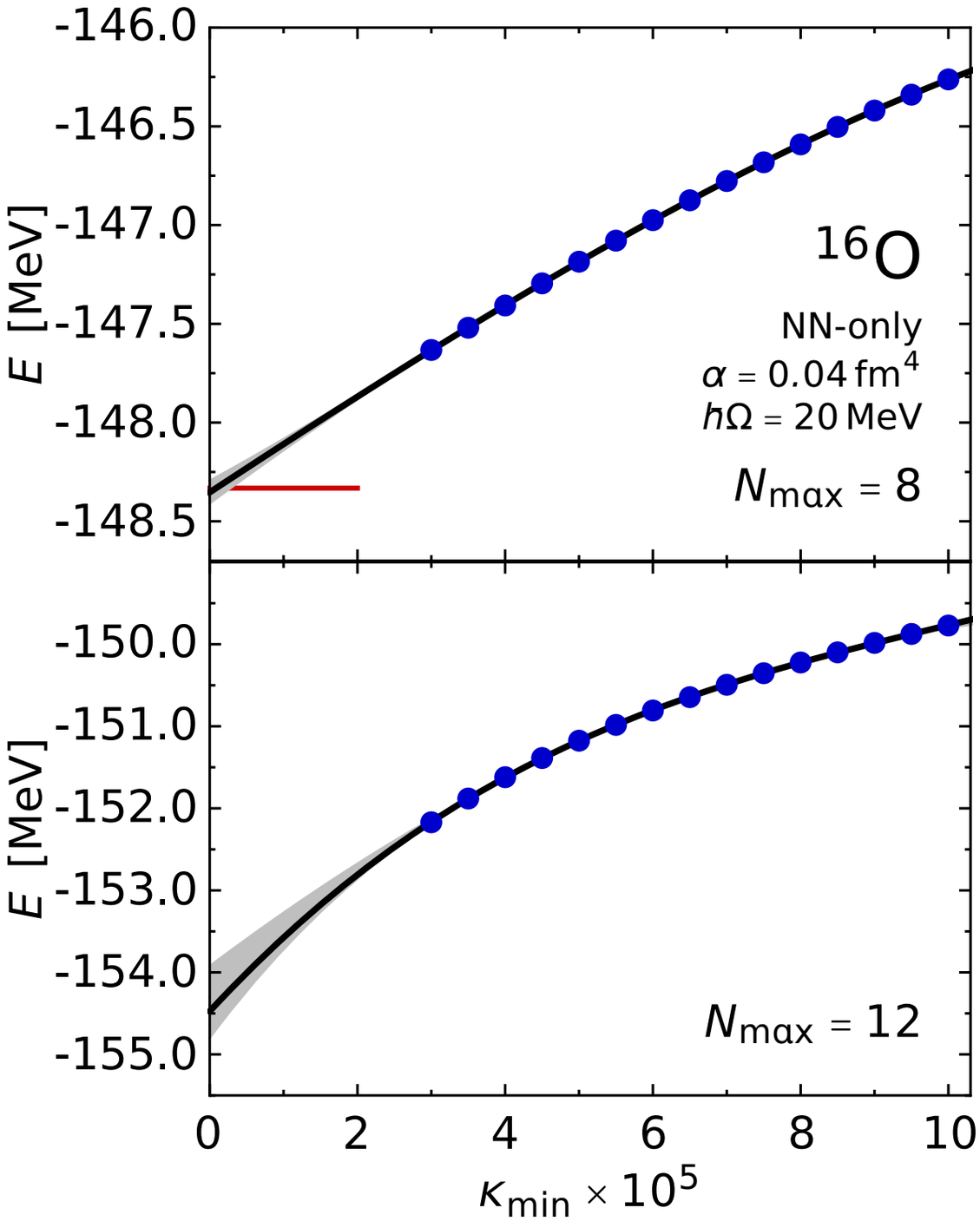
- **measure the importance** of individual basis state $|\Phi_\nu\rangle \notin \mathcal{M}_{\text{ref}}$ via first-order multiconfigurational perturbation theory

$$\kappa_\nu = -\frac{\langle \Phi_\nu | H | \Psi_{\text{ref}} \rangle}{\Delta\epsilon_\nu}$$

- construct **importance-truncated space** $\mathcal{M}(\kappa_{\text{min}})$ from all basis states with $|\kappa_\nu| \geq \kappa_{\text{min}}$

- **solve eigenvalue problem** in importance truncated space $\mathcal{M}_{\text{IT}}(\kappa_{\text{min}})$ and obtain improved approximation of target state

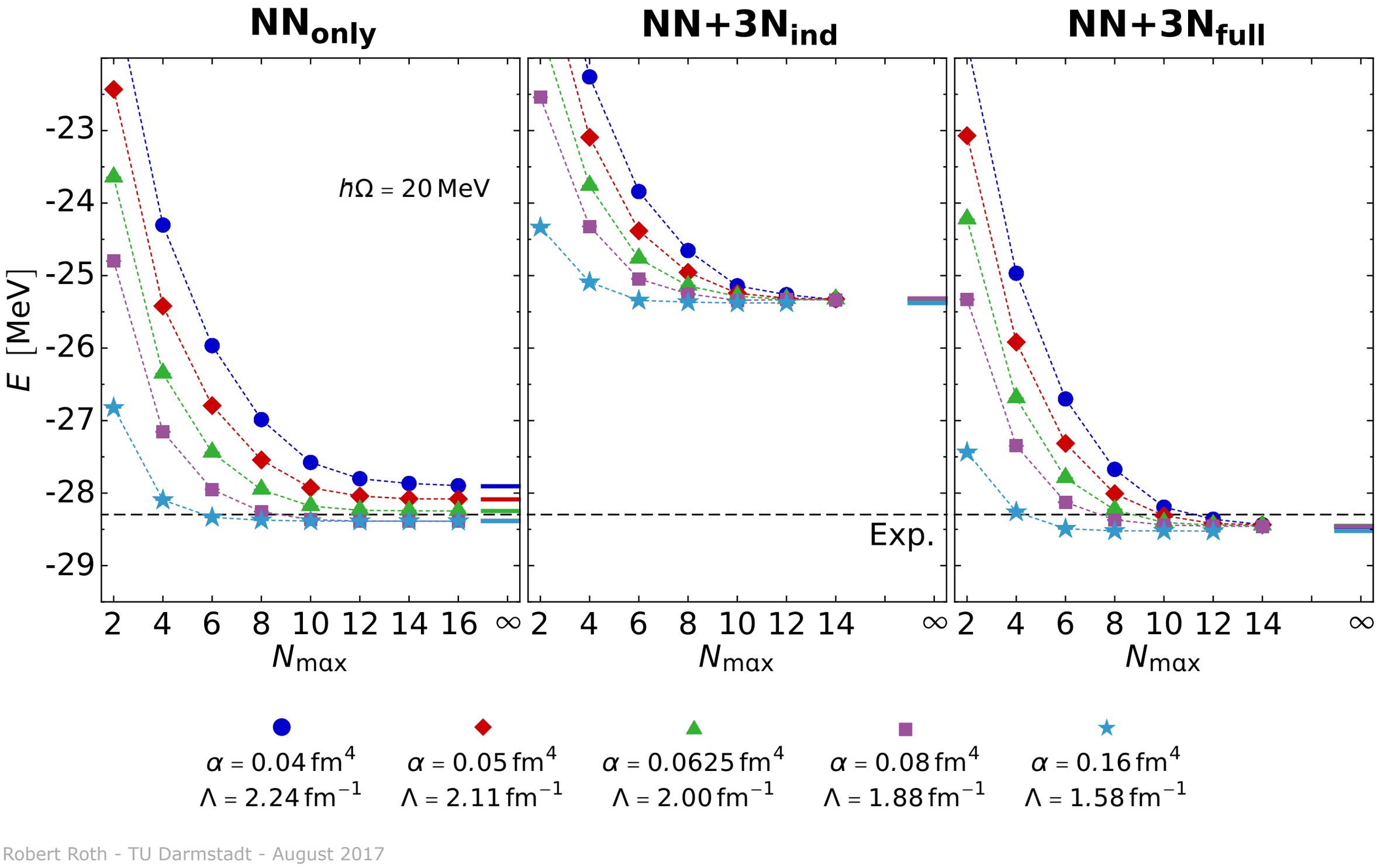
Threshold Extrapolation



- repeat calculations for a **sequence of importance thresholds** $\kappa_{\min}$
- observables show **smooth threshold dependence** and systematically approach the full NCSM limit
- use **a posteriori extrapolation** $\kappa_{\min} \to 0$ of observables to account for effect of excluded configurations
- **uncertainty quantification** via set of extrapolations

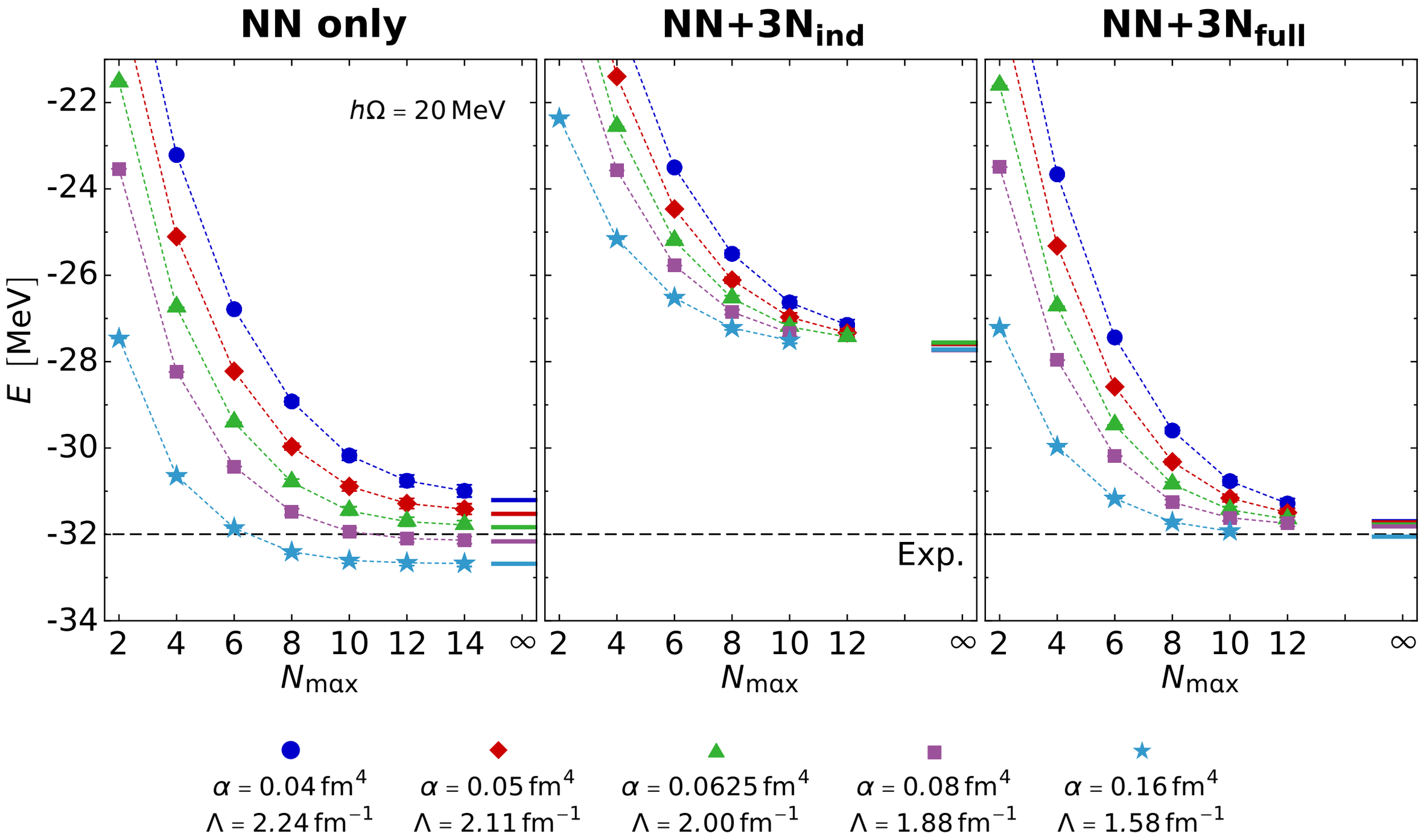
^{4}He: Ground-State Energy

Roth, et al; PRL 107, 072501 (2011); PRL 109, 052501 (2012)



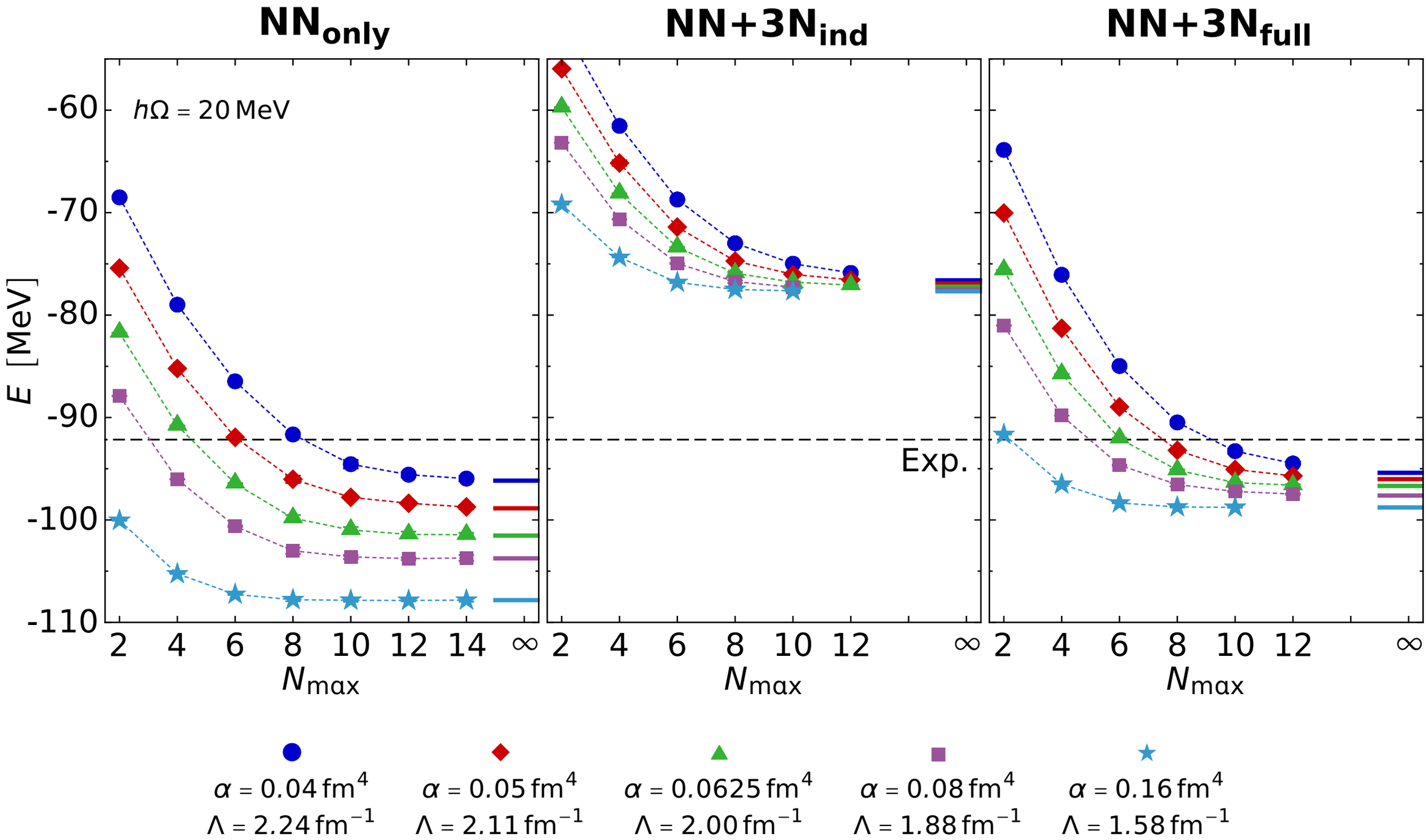
^{7}Li: Ground-State Energy

Roth, et al; PRL 107, 072501 (2011); PRL 109, 052501 (2012)



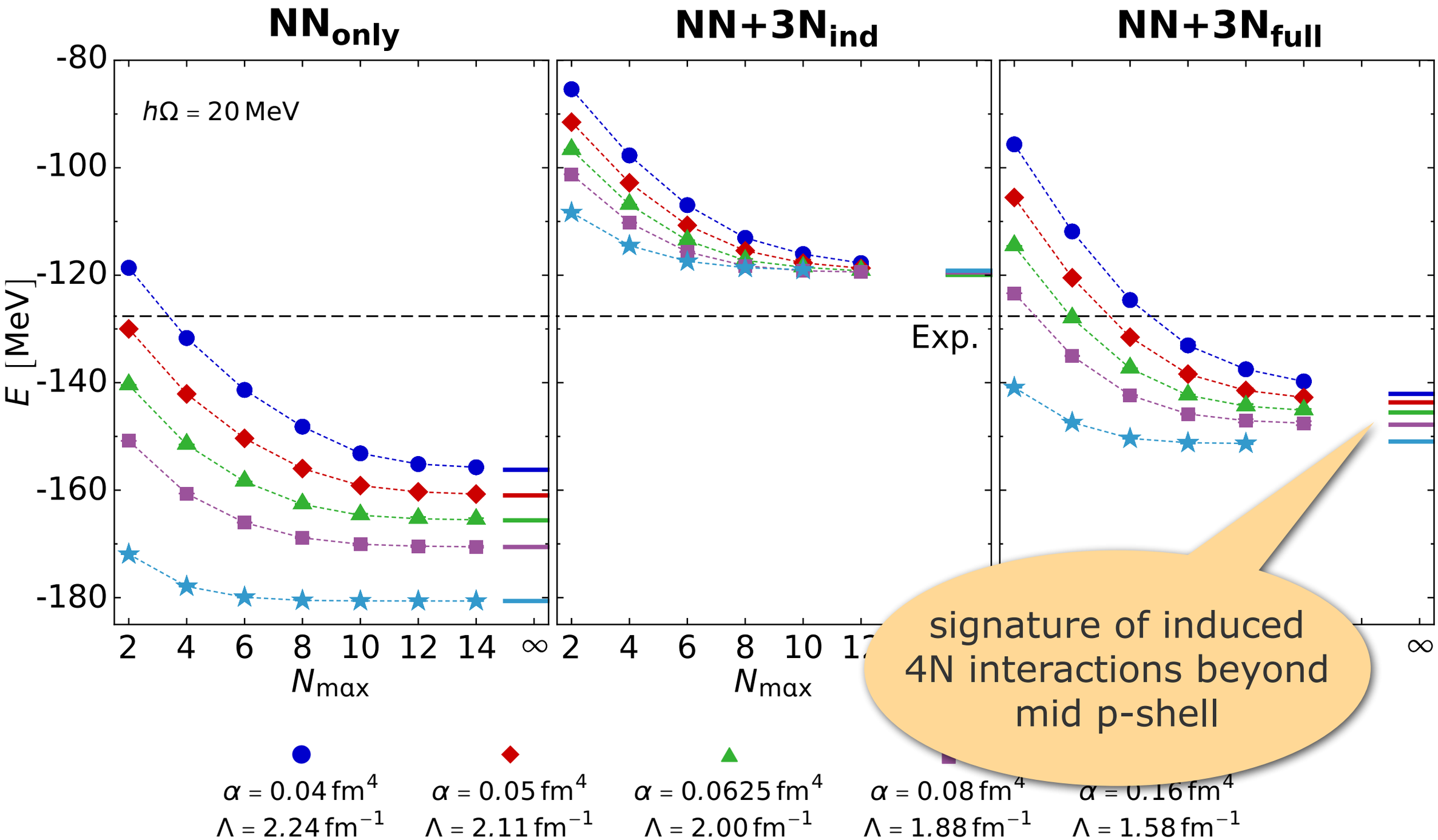
^{12}C: Ground-State Energy

Roth, et al; PRL 107, 072501 (2011); PRL 109, 052501 (2012)



^{16}O: Ground-State Energy

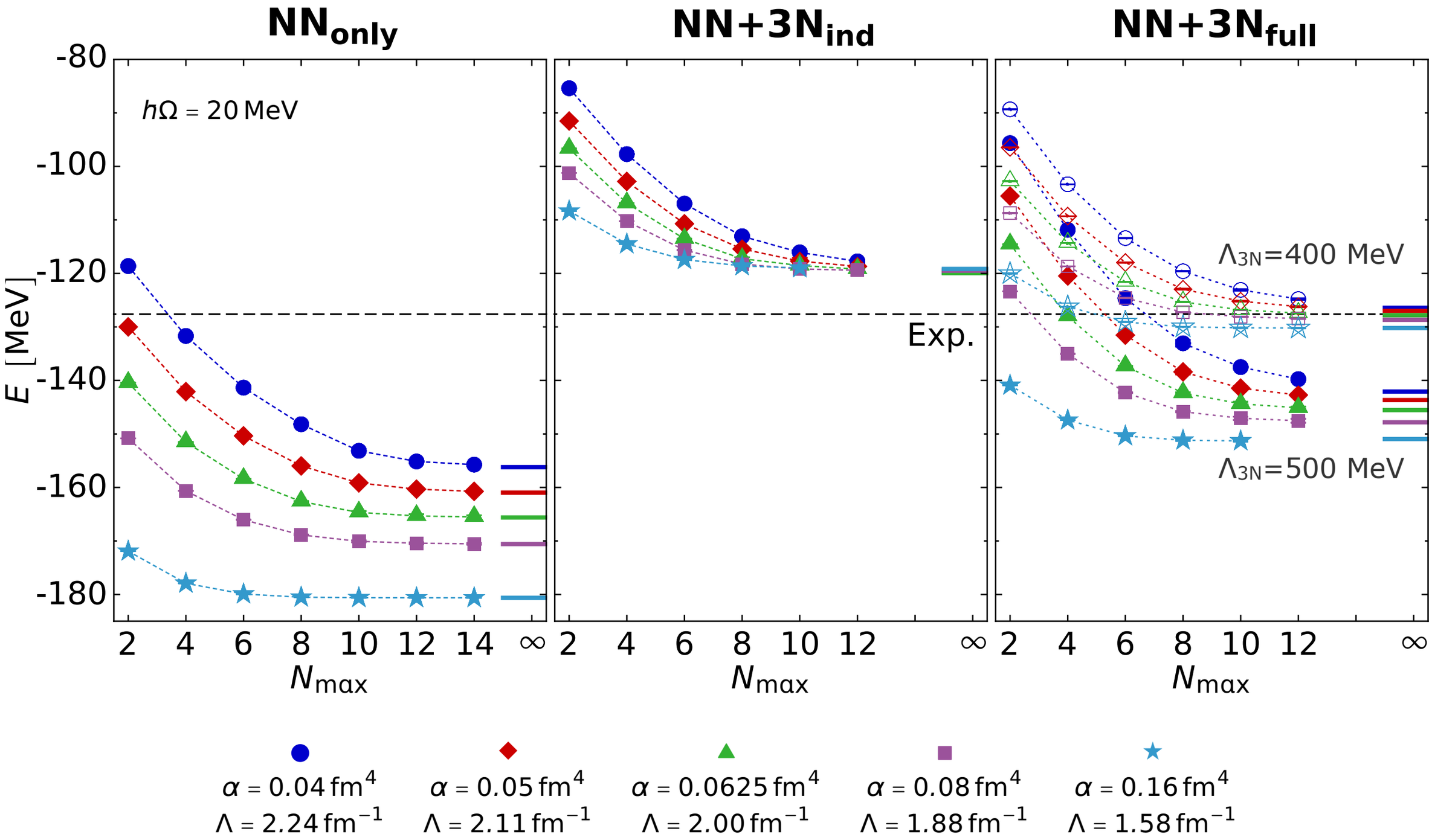
Roth, et al; PRL 107, 072501 (2011); PRL 109, 052501 (2012)



signature of induced 4N interactions beyond mid p-shell

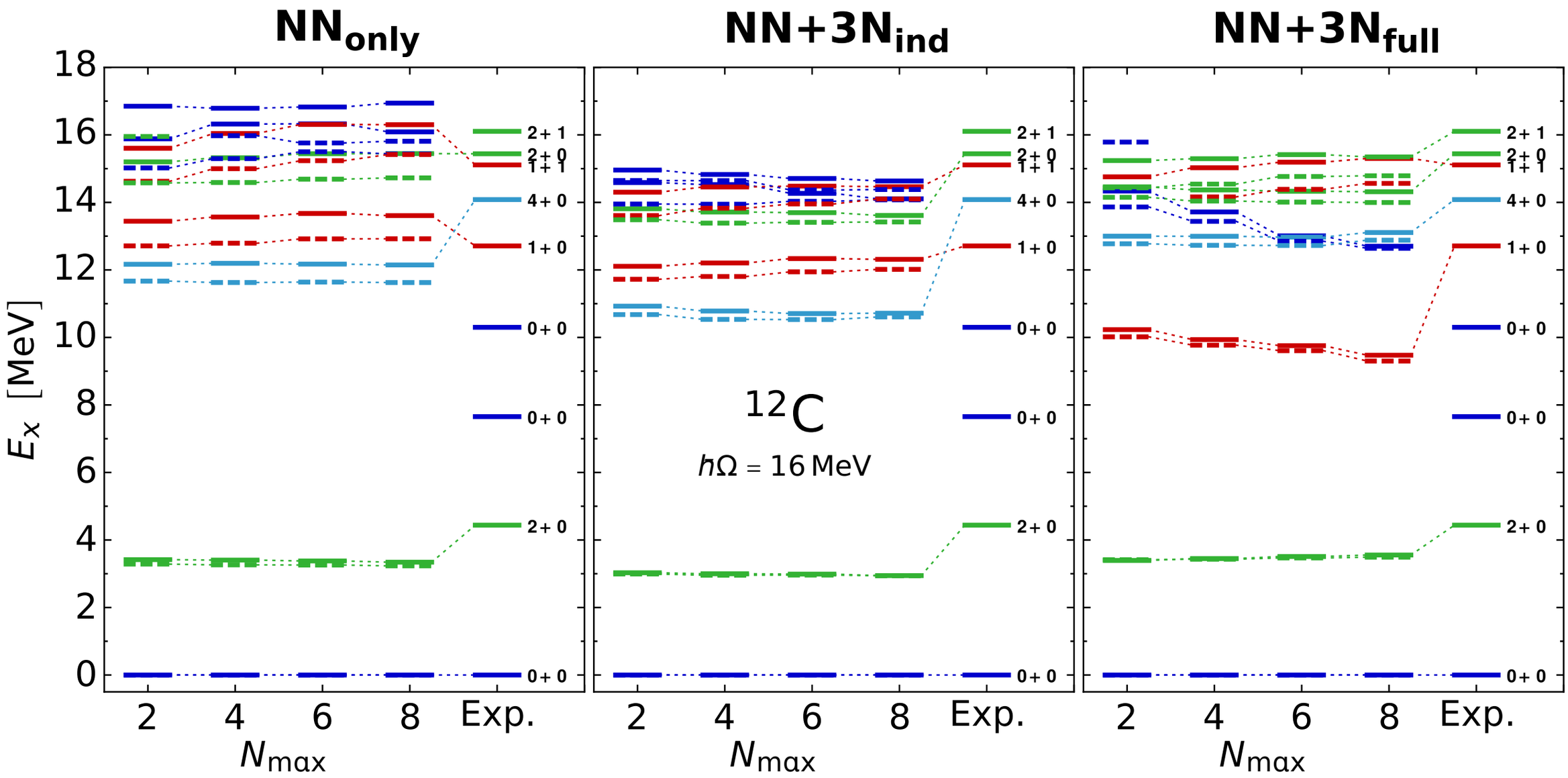
^{16}O: Ground-State Energy

Roth, et al; PRL 107, 072501 (2011); PRL 109, 052501 (2012)



^{12}C: Excitation Spectrum

Roth, et al; PRL 107, 072501 (2011); PRL 109, 052501 (2012)

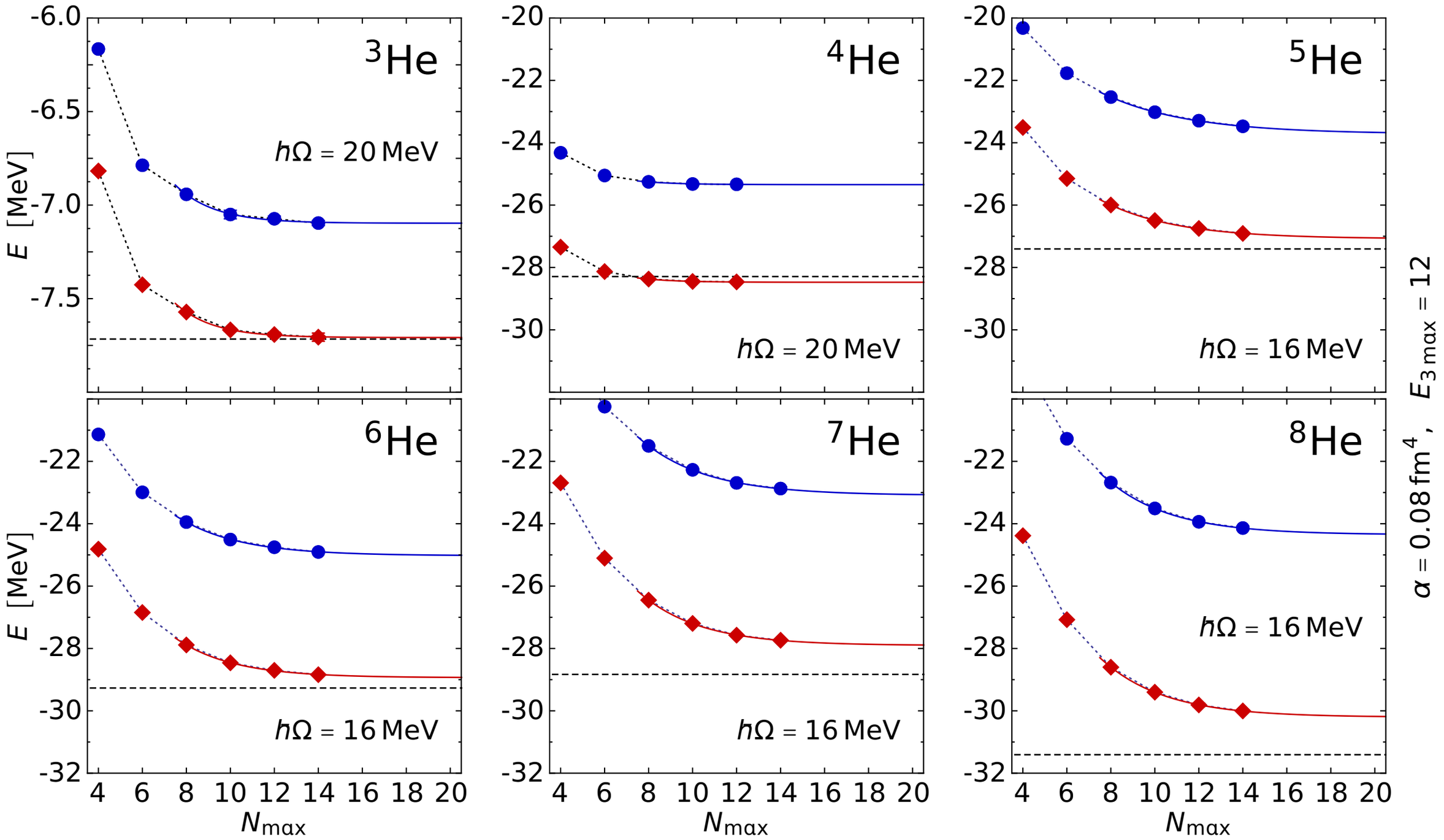


$\alpha = 0.04\,\mathrm{fm}^4$ $\Lambda = 2.24\,\mathrm{fm}^{-1}$

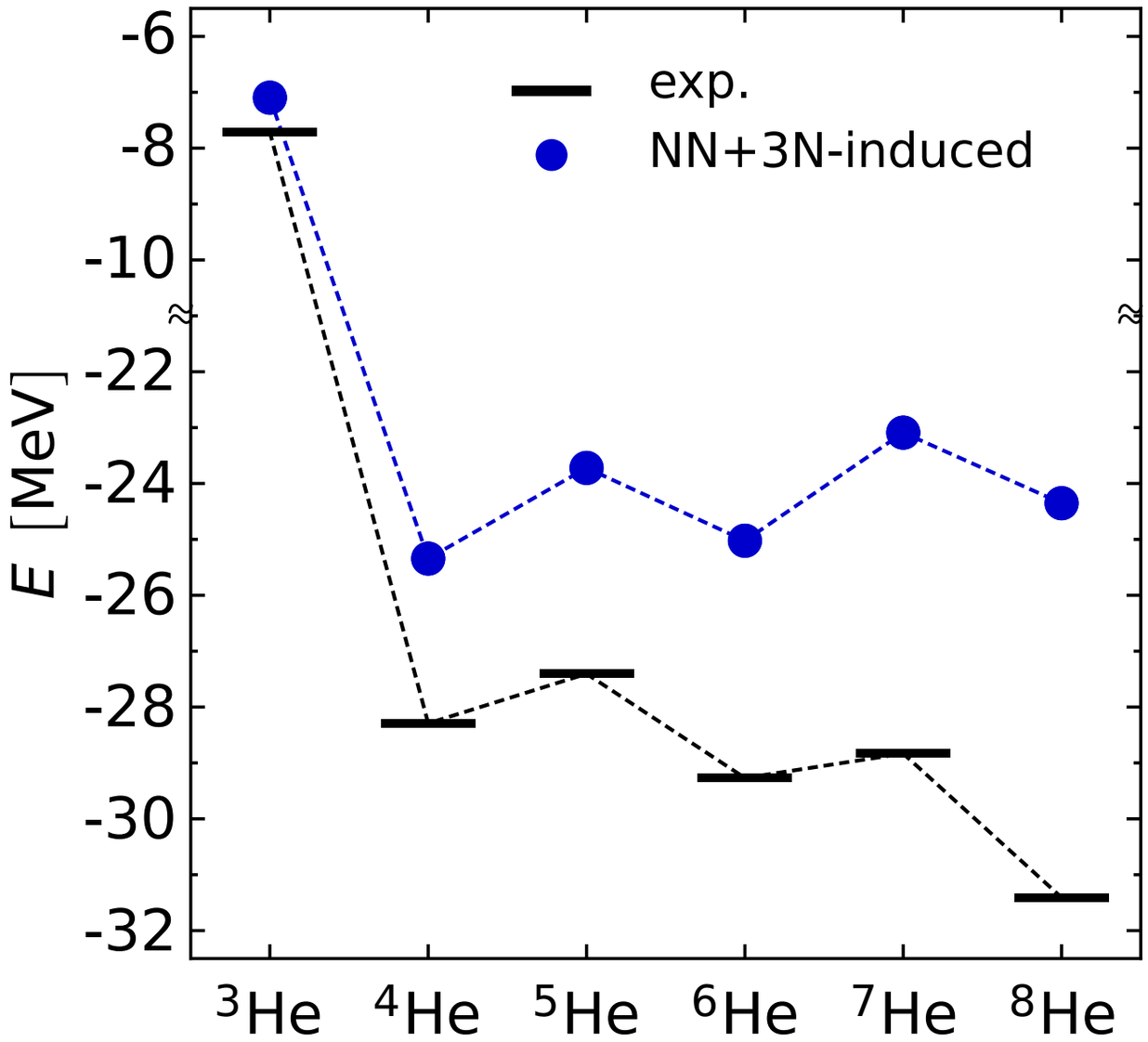
$\alpha = 0.08\,\mathrm{fm}^4$ $\Lambda = 1.88\,\mathrm{fm}^{-1}$

From Dripline to Dripline

Ground States of Helium Isotopes



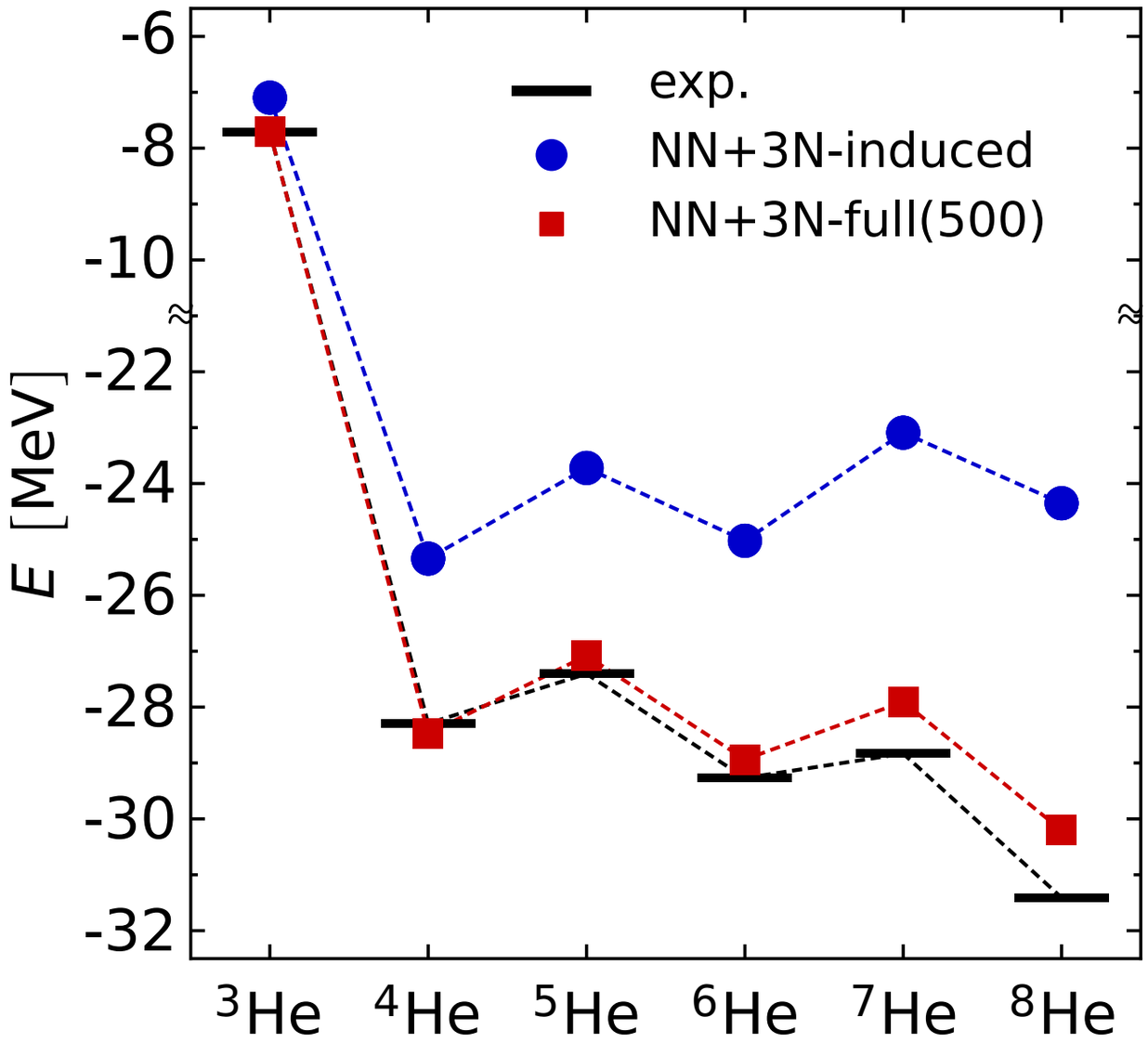
Ground States of Helium Isotopes



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

- **chiral NN interaction** cannot reproduce ground-state systematics

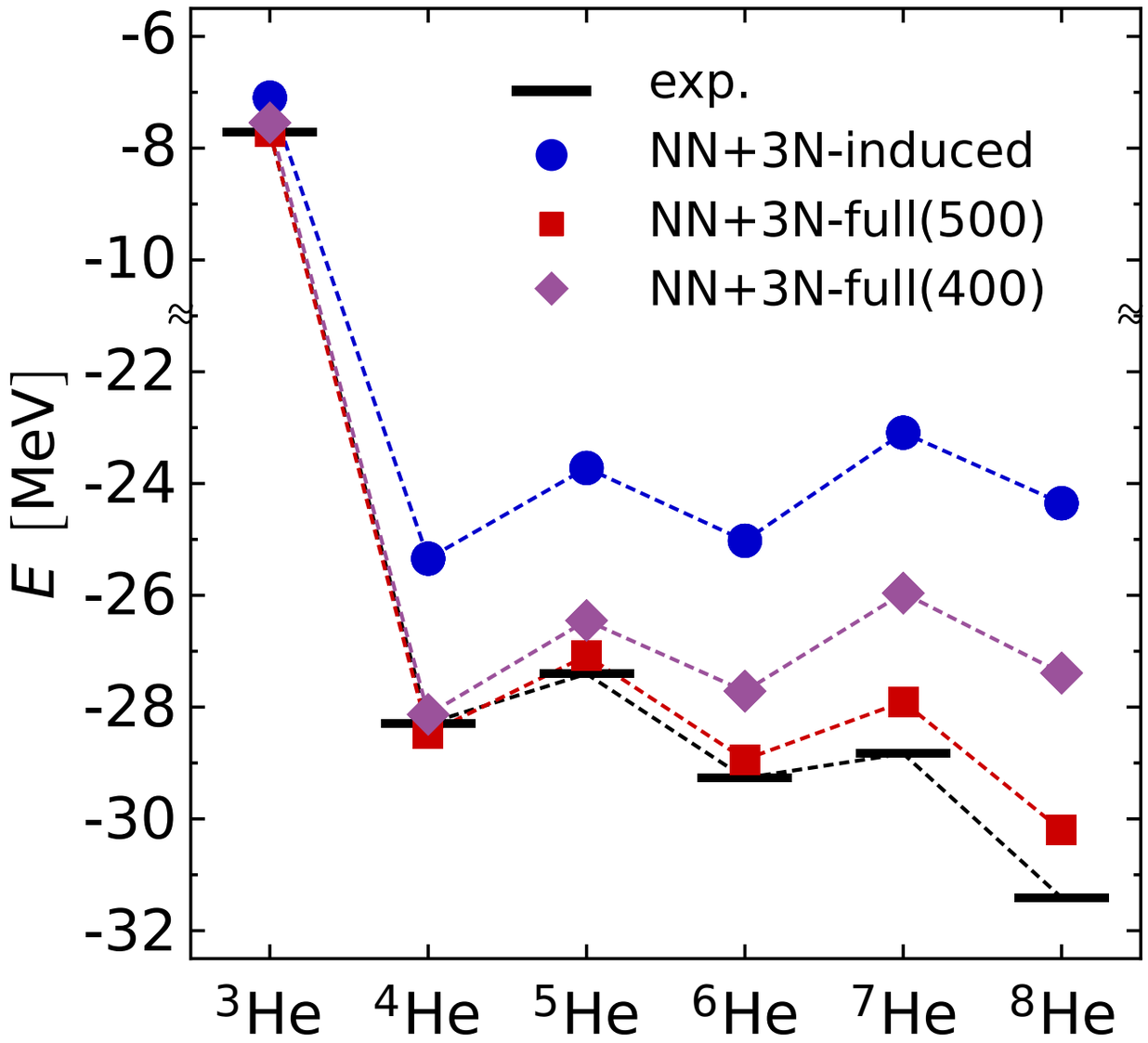
Ground States of Helium Isotopes



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

- **chiral NN interaction** cannot reproduce ground-state systematics
- **inclusion of chiral 3N** interaction improves trend significantly

Ground States of Helium Isotopes



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

- **chiral NN interaction** cannot reproduce ground-state systematics
- **inclusion of chiral 3N** interaction improves trend significantly
- systematics is **sensitive to details of the 3N interaction**, test for new chiral Hamiltonians
- continuum needs to be included: **NCSM with Continuum**

Oxygen Isotopes

- **oxygen isotopic chain** has received significant attention and documents the **rapid progress** over the past years

Otsuka, Suzuki, Holt, Schwenk, Akaishi, PRL 105, 032501 (2010)

- 2010: **shell-model calculations** with 3N effects highlighting the role of 3N interaction for drip line physics

Hagen, Hjorth-Jensen, Jansen, Machleidt, Papenbrock, PRL 108, 242501 (2012)

- 2012: **coupled-cluster calculations** with phenomenological two-body correction simulating chiral 3N forces

Hergert, Binder, Calci, Langhammer, Roth, PRL 110, 242501 (2013)

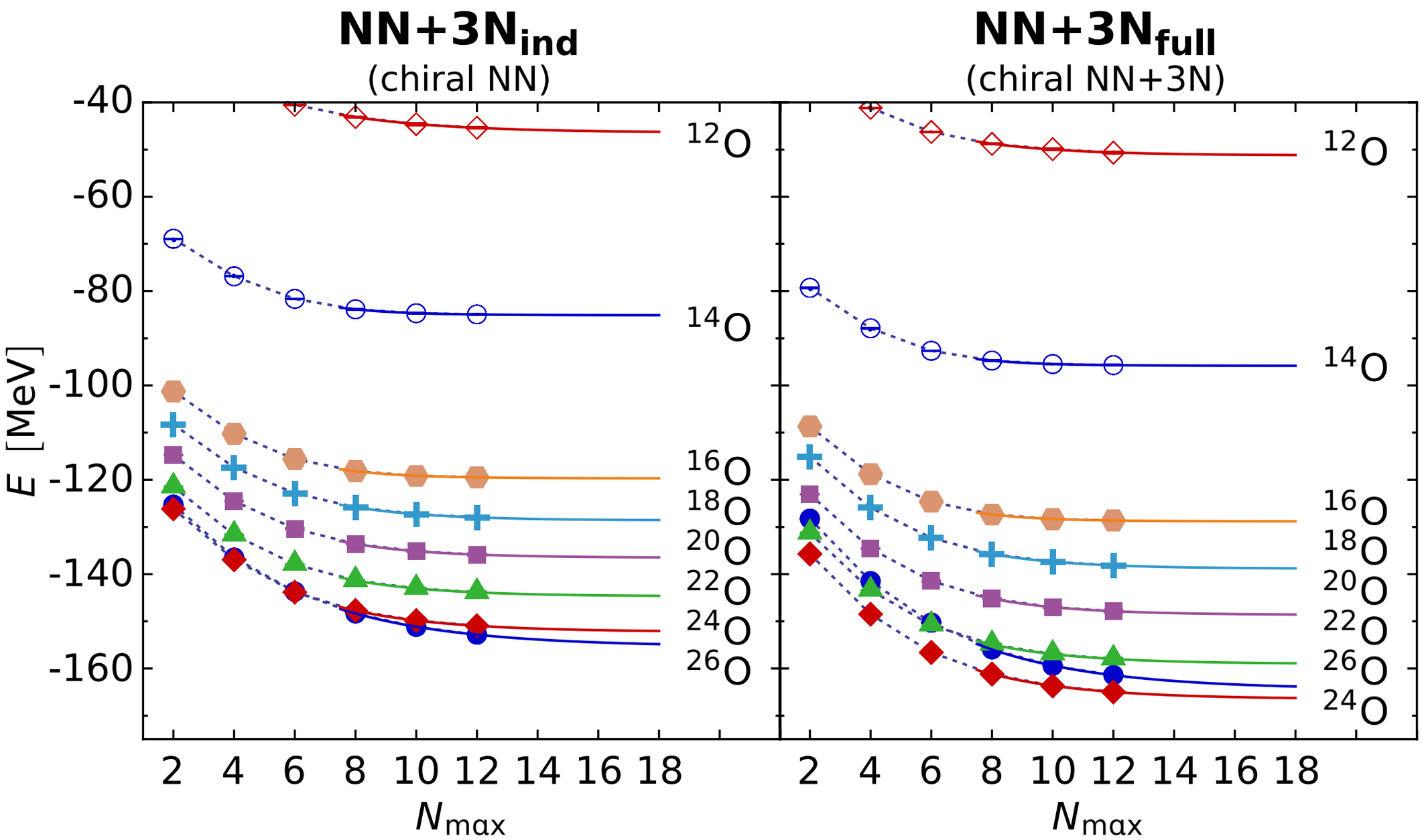
- 2013: **ab initio IT-NCSM** with explicit chiral 3N interactions and first **multi-reference in-medium SRG** calculations...

Cipollone, Barbieri, Navrátil, PRL 111, 062501 (2013)
Bogner, Hergert, Holt, Schwenk, Binder, Calci, Langhammer, Roth, PRL 113, 142501 (2014)
Jansen, Engel, Hagen, Navratil, Signoracci, PRL 113, 142502 (2014)

- since: self-consistent Green's function, shell model with valence-space interactions from in-medium SRG or Lee-Suzuki,...

Ground States of Oxygen Isotopes

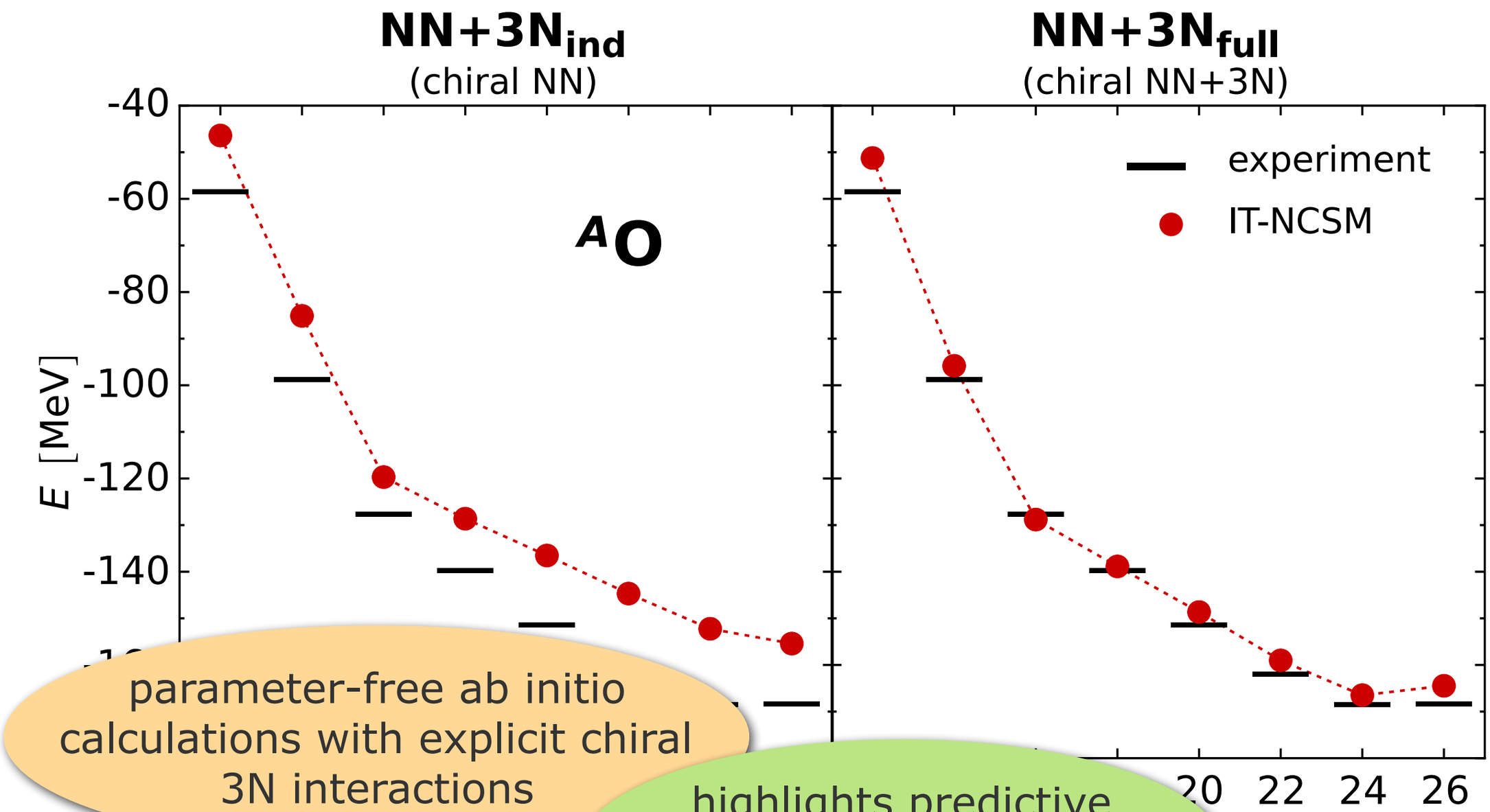
Hergert et al., PRL 110, 242501 (2013)



$\Lambda_{3N} = 400$ MeV, $\alpha = 0.08\,\mathrm{fm}^4$, $E_{3\,max} = 14$, optimal $\hbar\Omega$

Ground States of Oxygen Isotopes

Hergert et al., PRL 110, 242501 (2013)



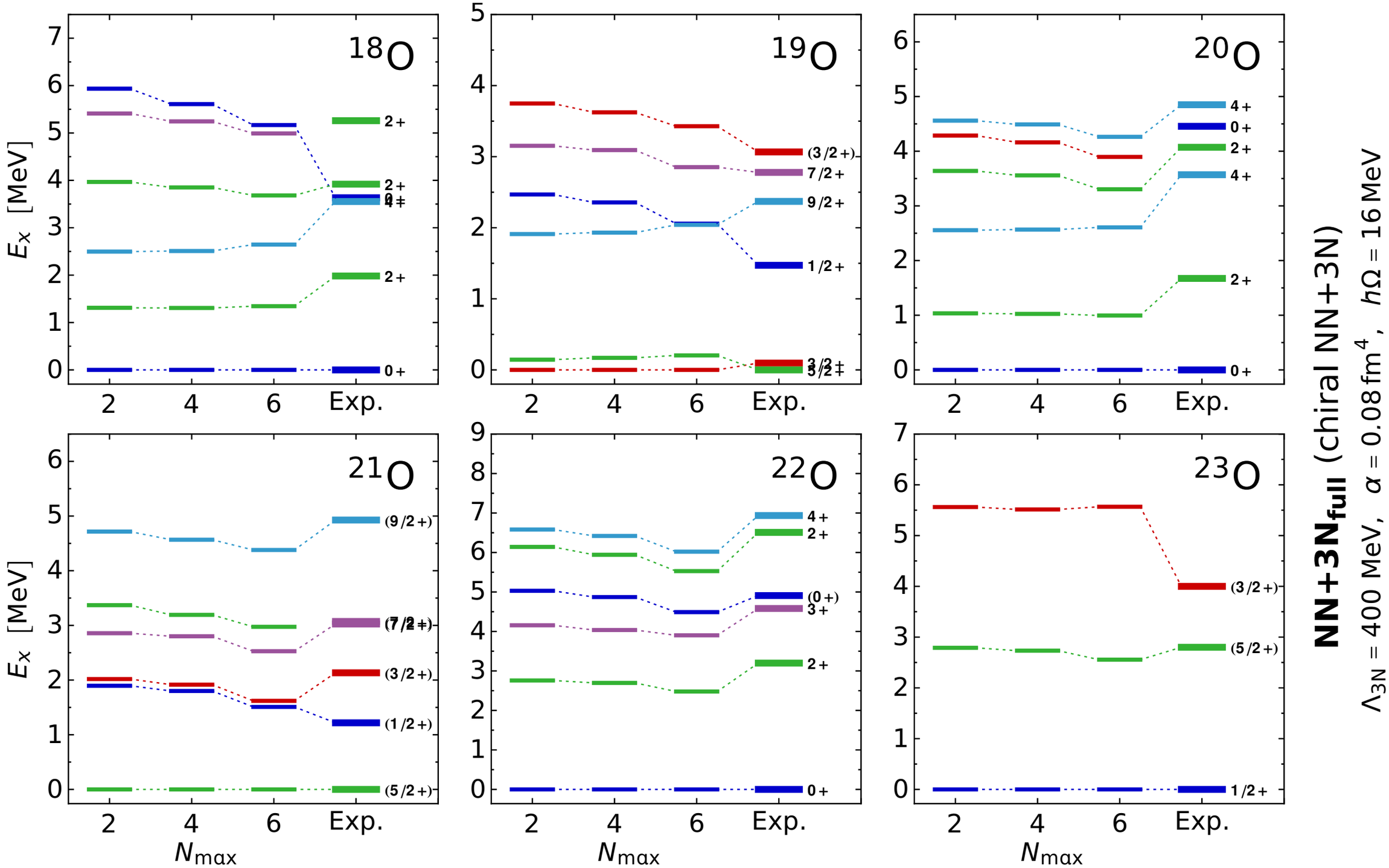
parameter-free ab initio calculations with explicit chiral 3N interactions

highlights predictive power of chiral NN+3N interactions

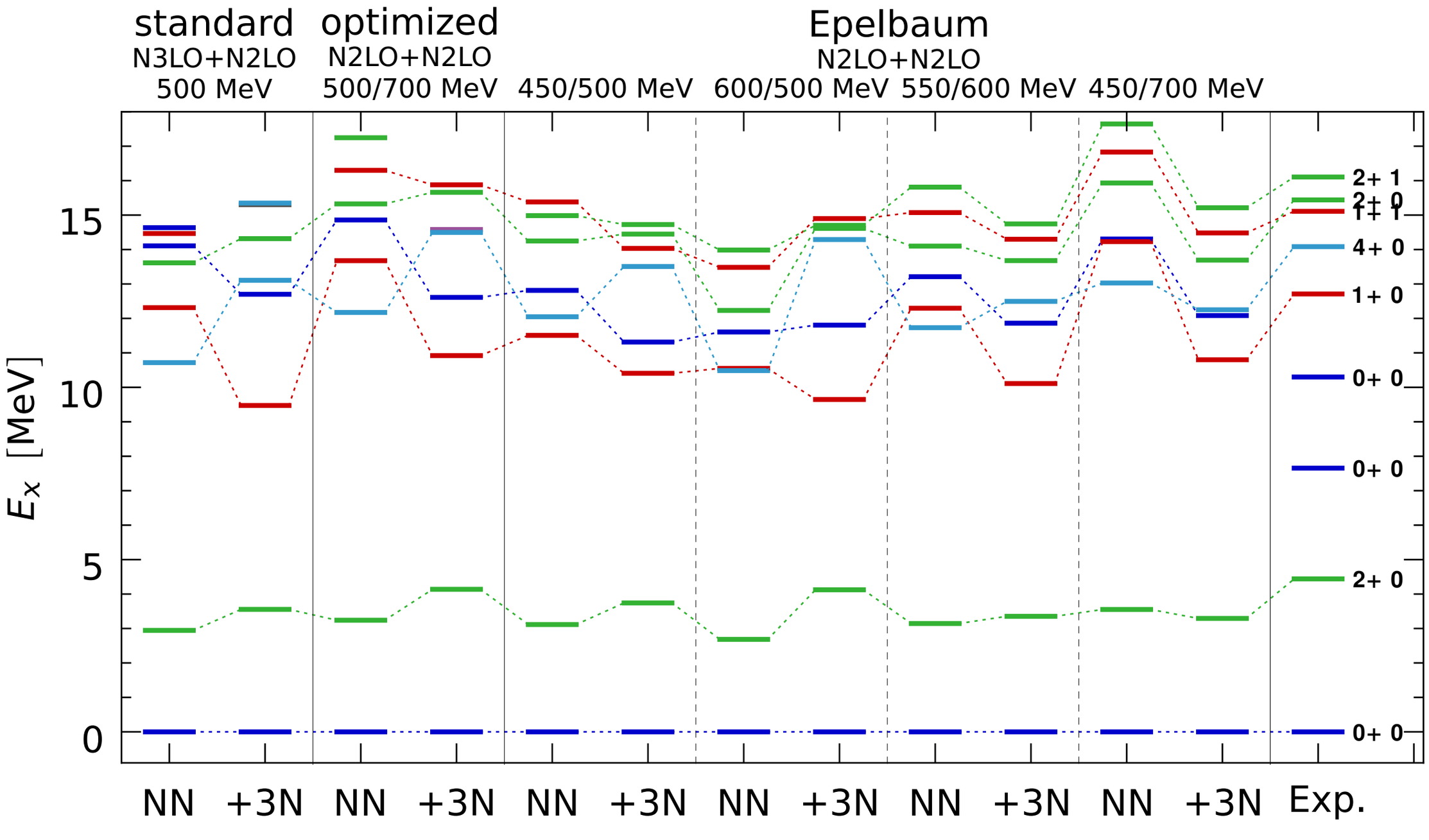
Λ_{3N} = 400 MeV, α = … optimal $\hbar\Omega$

Spectra of Oxygen Isotopes

Hergert et al., PRL 110, 242501 (2013) & in prep.

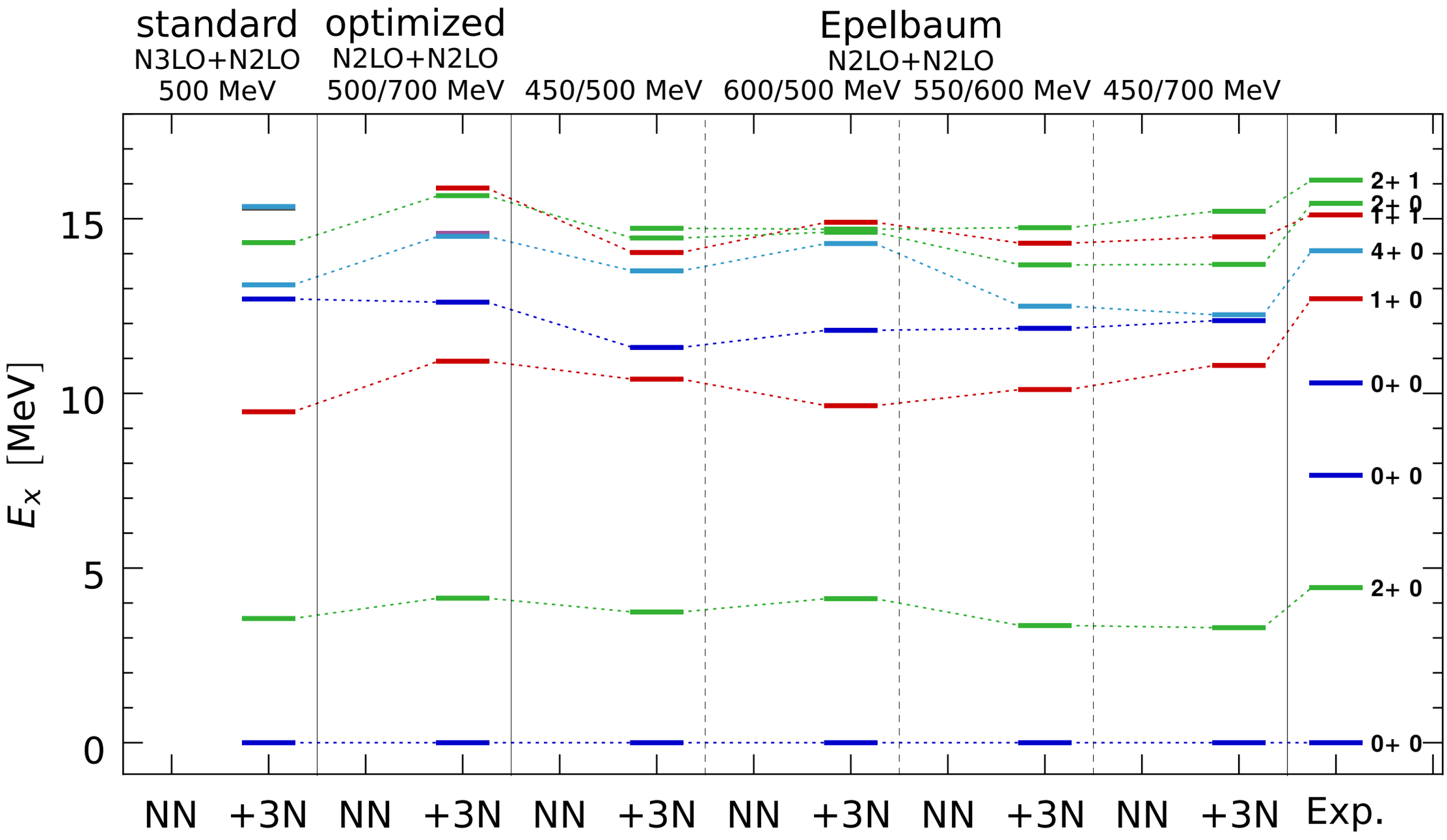


^{12}C: Testing Chiral Hamiltonians



$N_{max} = 8,\ \alpha = 0.08\,\mathrm{fm}^4,\ \hbar\Omega = 16$ MeV

^{12}C: Testing Chiral Hamiltonians



$N_{max} = 8,\ \alpha = 0.08\,\mathrm{fm}^4,\ \hbar\Omega = 16$ MeV

The NCSM Family

- **NCSM**
  HO Slater determinant basis with N_{max} truncation

- **Jacobi NCSM**
  relative-coordinate Jacobi HO basis with N_{max} truncation

- **Importance Truncated NCSM**
  HO Slater determinant basis with N_{max} and importance truncation

- **Monte Carlo NCSM**
  Monte Carlo sampling to select important basis states

- **Symmetry Adapted NCSM**
  group-theoretical basis with SU(3) deformation quantum numbers & truncations

- **Gamow NCSM/CI**
  Slater determinant basis including Gamow single-particle resonance states

- **NCSM with Continuum**
  NCSM for sub-clusters with explicit RGM treatment of relative motion