Ab Initio Approaches to Light Nuclei

Lecture 1: Fundamentals

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Overview

- **Lecture 1: Fundamentals**

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

- **Lecture 2: Correlations**

  Two-Body Problem • Similarity Transformations • Similarity Renormalization Group

- **Lecture 3: Light Nuclei**

  Many-Body Problem • Conf. Interaction • No-Core Shell Model • Importance Truncation

- **Lecture 4: Beyond Light Nuclei**

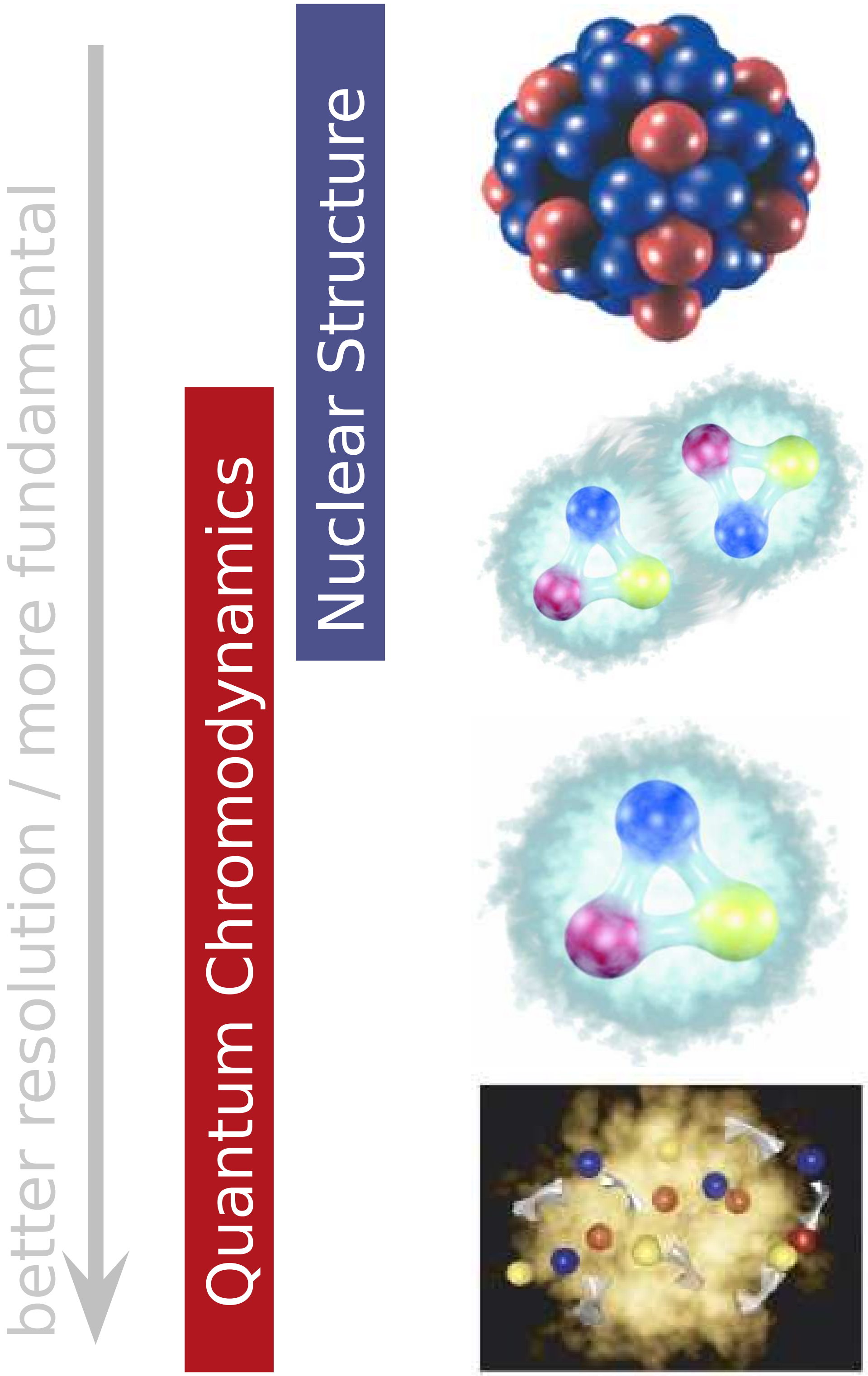
  Hartree-Fock • Many-Body Perturbation Theory • Coupled Cluster Theory

- **Lecture 5: Perspectives**

  In-Medium Similarity Renormalization Group • Multi-Reference • Configuration Interaction

Prelude

Theoretical Context



- finite nuclei
- few-nucleon systems
- nuclear interaction
- hadron structure
- quarks & gluons
- deconfinement

New Era of Ab Initio Theory

- **QCD at low energies**

  improved understanding through lattice simulations & effective field theories

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  increase of computational resources and developments of algorithms

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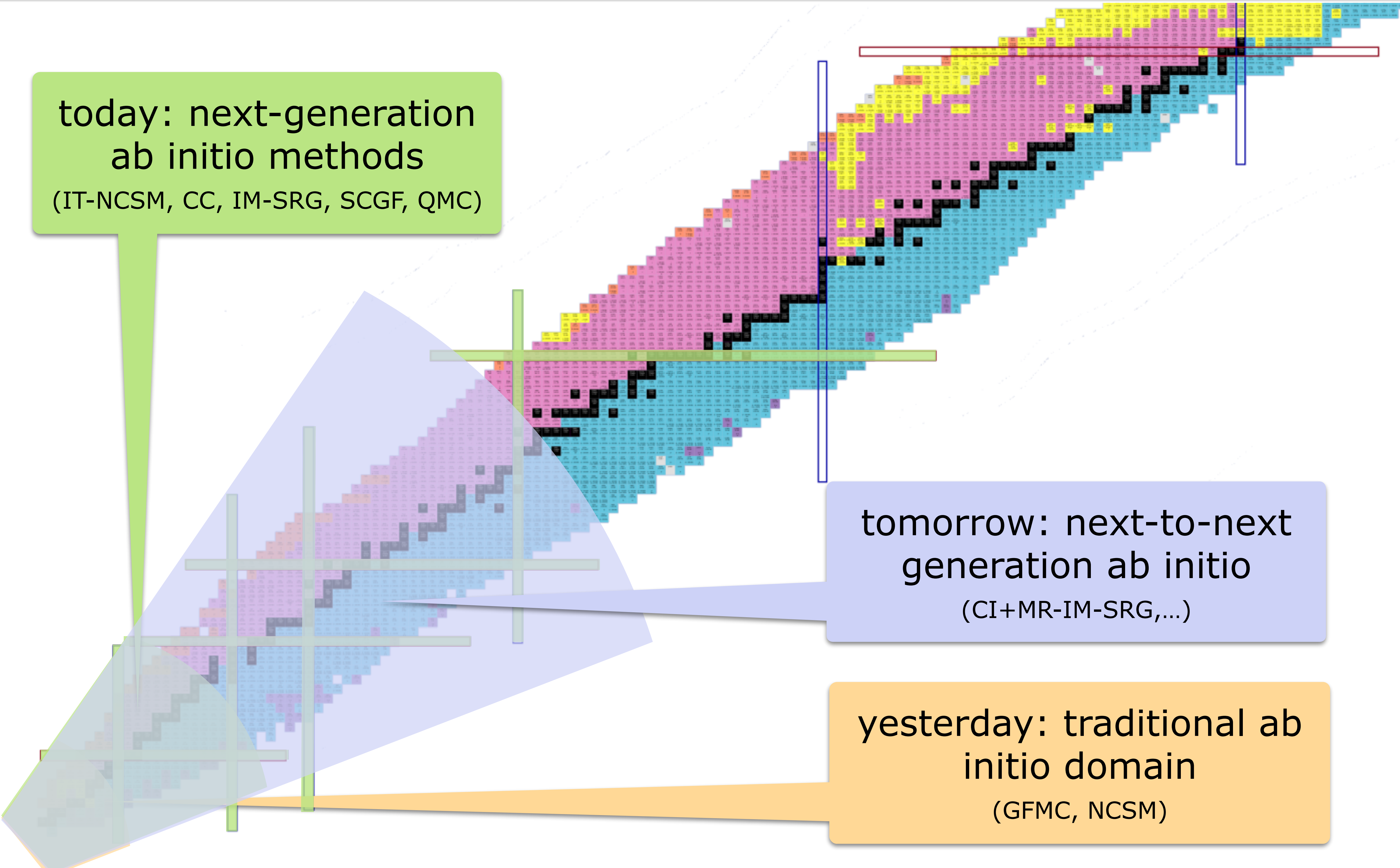
- **computing and algorithms**

  increase of computational resources and developments of algorithms

- **experimental facilities**

  amazing perspectives for the exploration of nuclei far-off stability

Ab Initio Landscape



The Problem

$$H\ |\Psi_n\rangle = E_n\,|\Psi_n\rangle$$

What is this many-body Hamiltonian?

nuclear forces, chiral effective field theory, three-body interactions, consistency, convergence,…

What about these many-body states?

many-body quantum mechanics, antisymmetry, second quantisation, many-body basis, truncations,…

How to solve this equation?

ab initio methods, correlations, similarity transformations, large-scale diagonalization, coupled-cluster theory,…

Many-Body Quantum Mechanics

... a very quick reminder

Single-Particle Basis

- effective constituents are nucleons characterized by **position, spin and isospin** degrees of freedom

$$|\alpha\rangle = |\text{position}\rangle \otimes |\text{spin}\rangle \otimes |\text{isospin}\rangle$$

- typical **basis choice** for configuration-type bound-state methods

$|\text{position}\rangle = |nlm_l\rangle$	spherical harmonic oscillator or other spherical single-particle potential
$|\text{spin}\rangle = |s=\frac{1}{2}, m_s\rangle$	eigenstates of s^2 and s_z with s=1/2
$|\text{isospin}\rangle = |t=\frac{1}{2}, m_t\rangle$	eigenstates of t^2 and t_3 with t=1/2

- use **spin-orbit coupling** at the single-particle level

$$|n(l\tfrac{1}{2})jm;\tfrac{1}{2}m_t\rangle = \sum_{m_l,m_s} c\begin{pmatrix} l & 1/2 & j \\ m_l & m_s & m \end{pmatrix} |nlm_l\rangle \otimes |\tfrac{1}{2}m_s\rangle \otimes |\tfrac{1}{2}m_t\rangle$$

Identical Particles & Spin-Statistics Theorem

- **systems of identical particles**: many-body states have to be eigenstates of the transposition operator for any particle pair with eigenvalues ±1

$$T_{ij} \,|\, \Psi \rangle = +1 \,|\, \Psi \rangle$$
states symmetric under transposition of any pair of particle indices

$$T_{ij} \,|\, \Psi \rangle = -1 \,|\, \Psi \rangle$$
states antisymmetric under transposition of any pair of particles

- simple **product states** are not suitable for systems of identical particles

$$|\, \Phi \rangle = |\, \alpha_1 \rangle \otimes |\, \alpha_2 \rangle \otimes \cdots \otimes |\, \alpha_A \rangle$$

- **spin-statistics theorem** connects transposition symmetry to particle spin:
  - bosons = integer spin = symmetric states
  - fermions = half-integer spin = antisymmetric states

- focus on fermions, i.e., **antisymmetric states in the following**

Slater Determinants

- antisymmetric states can be constructed via the **antisymmetrization operator**

$$\mathcal{A} = \frac{1}{A!} \sum_{\pi} \text{sgn}(\pi)\, \text{P}_{\pi}$$

sum over all permutations — signum of permutation — permutation operator

- technically it is **projection operator** onto the antisymmetric A-body Hilbert space and has the same structure as a **general determinant**

- **Slater determinants**: antisymmetrized product states

$$\begin{aligned} |\alpha_1\alpha_2\dots\alpha_A\rangle &= \sqrt{A!}\, \mathcal{A}\, (\,|\alpha_1\rangle \otimes |\alpha_2\rangle \otimes \cdots \otimes |\alpha_A\rangle) \\ &= \frac{1}{\sqrt{A!}} \sum_{\pi} \text{sgn}(\pi)\, \text{P}_{\pi}\, (\,|\alpha_1\rangle \otimes |\alpha_2\rangle \otimes \cdots \otimes |\alpha_A\rangle) \end{aligned}$$

- **Pauli principle is a consequence of antisymmetry**: you cannot antisymmetrize a product state that contains two identical single-particle states

Slater Determinants as Basis

- given a complete single-particle basis $\{|\alpha\rangle\}$ then the set of Slater determinants formed by all possible combinations of A different single-particle states is a **complete basis of the antisymmetric A-body Hilbert space**

- resolution of the **identity operator**

$$1 = \sum_{\alpha_1<\alpha_2<\ldots<\alpha_A} |\alpha_1\alpha_2\ldots\alpha_A\rangle\langle\alpha_1\alpha_2\ldots\alpha_A| = \frac{1}{A!}\sum_{\alpha_1,\alpha_2,\ldots,\alpha_A} |\alpha_1\alpha_2\ldots\alpha_A\rangle\langle\alpha_1\alpha_2\ldots\alpha_A|$$

- careful with **double counting**: Slater determinants that differ only by the order of the single-particle states are identical up to a sign...

- **expansion of general antisymmetric state** in Slater determinant basis

$$|\Psi\rangle = \sum_{\alpha_1<\alpha_2<\ldots<\alpha_A} C_{\alpha_1\alpha_2\ldots\alpha_A}\ |\alpha_1\alpha_2\ldots\alpha_A\rangle = \sum_i C_i\ |\{\alpha_1\alpha_2\ldots\alpha_A\}_i\rangle$$

Second Quantization: Basics

- define **Fock-space** as direct sum of A-particle Hilbert spaces

$$\mathcal{F} = \mathcal{H}_0 \oplus \mathcal{H}_1 \oplus \mathcal{H}_2 \oplus \cdots \oplus \mathcal{H}_A \oplus \cdots$$

- **vacuum state**: the only state in the zero-particle Hilbert space

$$|0\rangle \in \mathcal{H}_0 \qquad \langle 0|0\rangle = 1 \qquad |0\rangle \neq 0$$

- **creation operators**: add a particle in single-particle state $|\alpha\rangle$ to an A-body Slater determinant yielding an (A+1)-body Slater determinant

$$a^\dagger_\alpha |0\rangle = |\alpha\rangle$$

$$a^\dagger_\alpha |\alpha_1 \alpha_2 ... \alpha_A\rangle = \begin{cases} |\alpha \alpha_1 \alpha_2 ... \alpha_A\rangle & ; \quad \alpha \notin \{\alpha_1 \alpha_2 ... \alpha_A\} \\ 0 & ; \quad \text{otherwise} \end{cases}$$

- resulting states are automatically normalized and antisymmetrized
- new single-particle state is added in the first slot, can be moved elsewhere through transpositions

Second Quantization: Basics

- **annihilation operators**: remove a particle with single-particle state $|\alpha\rangle$ from an A-body Slater determinant yielding an (A-1)-body Slater determinant

$$a_\alpha |0\rangle = 0$$

$$a_\alpha |\alpha_1 \alpha_2 \ldots \alpha_A\rangle = \begin{cases} (-1)^{i-1} |\alpha_1 \alpha_2 \ldots \alpha_{i-1} \alpha_{i+1} \ldots \alpha_A\rangle & ; \quad \alpha = \alpha_i \\ 0 & ; \quad \text{otherwise} \end{cases}$$

- annihilation operator acts on first slot, need transpositions to get correct single-particle state there

- based on these definitions one can easily show that creation and annihilations operators satisfy **anticommutation relations**

$$\{a_\alpha , a_{\alpha'}\} = 0 \qquad \{a^\dagger_\alpha , a^\dagger_{\alpha'}\} = 0 \qquad \{a_\alpha , a^\dagger_{\alpha'}\} = \delta_{\alpha\alpha'}$$

- complication of handling permutations in "first quantization" are translated to the commutation behaviour of strings of operators

Second Quantization: States

- Slater determinants can be written as **string of creation operators** acting on vacuum state

$$|\alpha_1\alpha_2\ldots\alpha_A\rangle = a^{\dagger}_{\alpha_1} a^{\dagger}_{\alpha_2} \cdots a^{\dagger}_{\alpha_A} |0\rangle$$

- alternatively one can define an A-body **reference Slater determinant**

$$|\Phi\rangle = |\alpha_1\alpha_2\ldots\alpha_A\rangle = a^{\dagger}_{\alpha_1} a^{\dagger}_{\alpha_2} \cdots a^{\dagger}_{\alpha_A} |0\rangle$$

and construct arbitrary Slater determinants through **particle-hole excitations** on top of the reference state

$$|\Phi^{p}_{a}\rangle = a^{\dagger}_{\alpha_p} a_{\alpha_a} |\Phi\rangle$$
$$|\Phi^{pq}_{ab}\rangle = a^{\dagger}_{\alpha_p} a^{\dagger}_{\alpha_q} a_{\alpha_b} a_{\alpha_a} |\Phi\rangle$$
$$\vdots$$

index convention: $a,b,c,\ldots$: hole states, occupied in reference state
$p,q,r,\ldots$: particle state, unoccupied in reference states

Second Quantization: Operators

- **operators** can be expressed in terms of creation and annihilation operators as well, e.g., for one-body kinetic energy and two-body interactions:

'first quantization'

$$\mathrm{T} = \sum_{i=1}^{A} \mathrm{t}_i$$

$$\mathrm{V} = \sum_{i<j=1}^{A} \mathrm{v}_{ij}$$

second quantization

$$\mathrm{T} = \sum_{\alpha\alpha'} \langle\alpha|\,\mathrm{t}\,|\alpha'\rangle\, \mathrm{a}^\dagger_\alpha \mathrm{a}_{\alpha'}$$

$$\mathrm{V} = \frac{1}{4} \sum_{\alpha_1\alpha_2\alpha'_1\alpha'_2} \langle\alpha_1\alpha_2|\,\mathrm{v}\,|\alpha'_1\alpha'_2\rangle\, \mathrm{a}^\dagger_{\alpha_1} \mathrm{a}^\dagger_{\alpha_2}\, \mathrm{a}_{\alpha'_2} \mathrm{a}_{\alpha'_1}$$

- **set of one or two-body matrix elements** fully defines the one or two-body operator in Fock space

- second quantization is extremely convenient to **compute matrix elements** of operators with Slater determinants

➜ **problem session today**

Nuclear Hamiltonian

Nuclear Hamiltonian

- general form of **many-body Hamiltonian** can be split into a center-of-mass and an intrinsic part

$$\begin{aligned} \mathrm{H} &= \mathrm{T} + \mathrm{V}_{NN} + \mathrm{V}_{3N} + \cdots = \mathrm{T}_{\text{cm}} + \mathrm{T}_{\text{int}} + \mathrm{V}_{NN} + \mathrm{V}_{3N} + \cdots \\ &= \mathrm{T}_{\text{cm}} + \mathrm{H}_{\text{int}} \end{aligned}$$

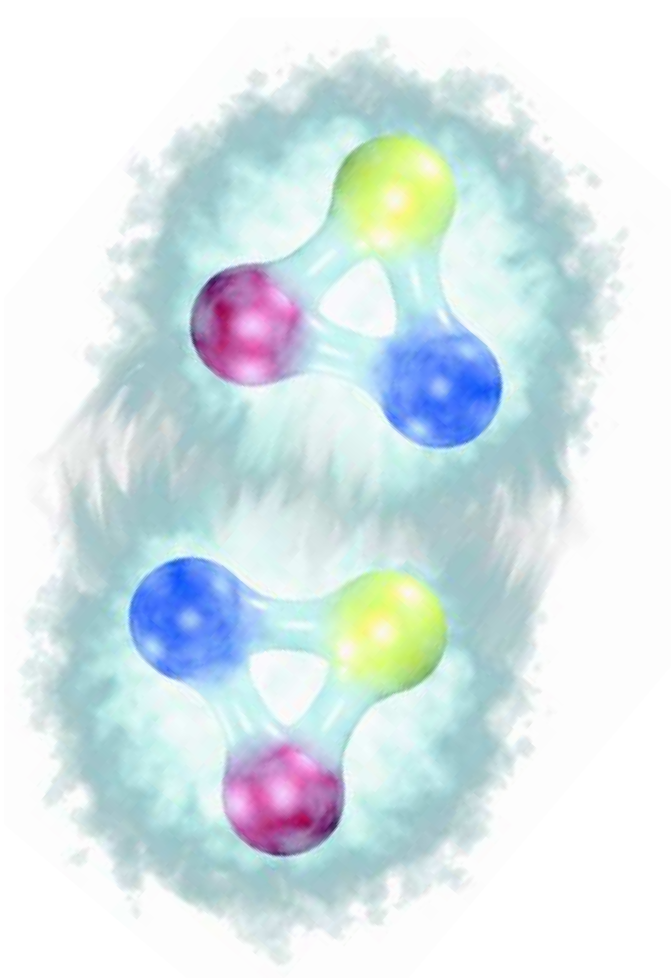
- **intrinsic Hamiltonian** is invariant under translation, rotation, Galilei boost, parity, time evolution, time reversal,...

$$\begin{aligned} \mathrm{H}_{\text{int}} &= \mathrm{T}_{\text{int}} + \mathrm{V}_{NN} + \mathrm{V}_{3N} + \cdots \\ &= \sum_{i<j}^{A} \frac{1}{2mA} (\vec{\mathrm{p}}_i - \vec{\mathrm{p}}_j)^2 + \sum_{i<j}^{A} \mathrm{v}_{NN,ij} + \sum_{i<j<k}^{A} \mathrm{v}_{3N,ijk} + \cdots \end{aligned}$$

- these symmetries constrain the possible operator structures that can appear in the interaction terms...

... but how can we really **determine the nuclear interactions** ?

Nature of the Nuclear Interaction



$\sim 1.6\text{fm}$

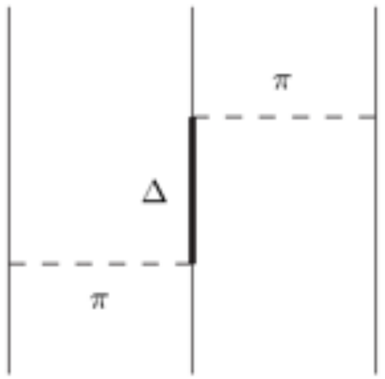
$\rho_0^{-1/3} = 1.8\text{fm}$

- nuclear interaction is **not fundamental**
- residual force analogous to **van der Waals interaction** between neutral atoms
- based on QCD and induced via **polarization** of quark and gluon distributions of nucleons
- **encapsulates all the complications** of the QCD dynamics and the structure of nucleons
- acts only if the nucleons overlap, i.e. at **short ranges**
- irreducible **three-nucleon interactions** are important

Yesterday... from Phenomenology

Wiringa, Machleidt,...

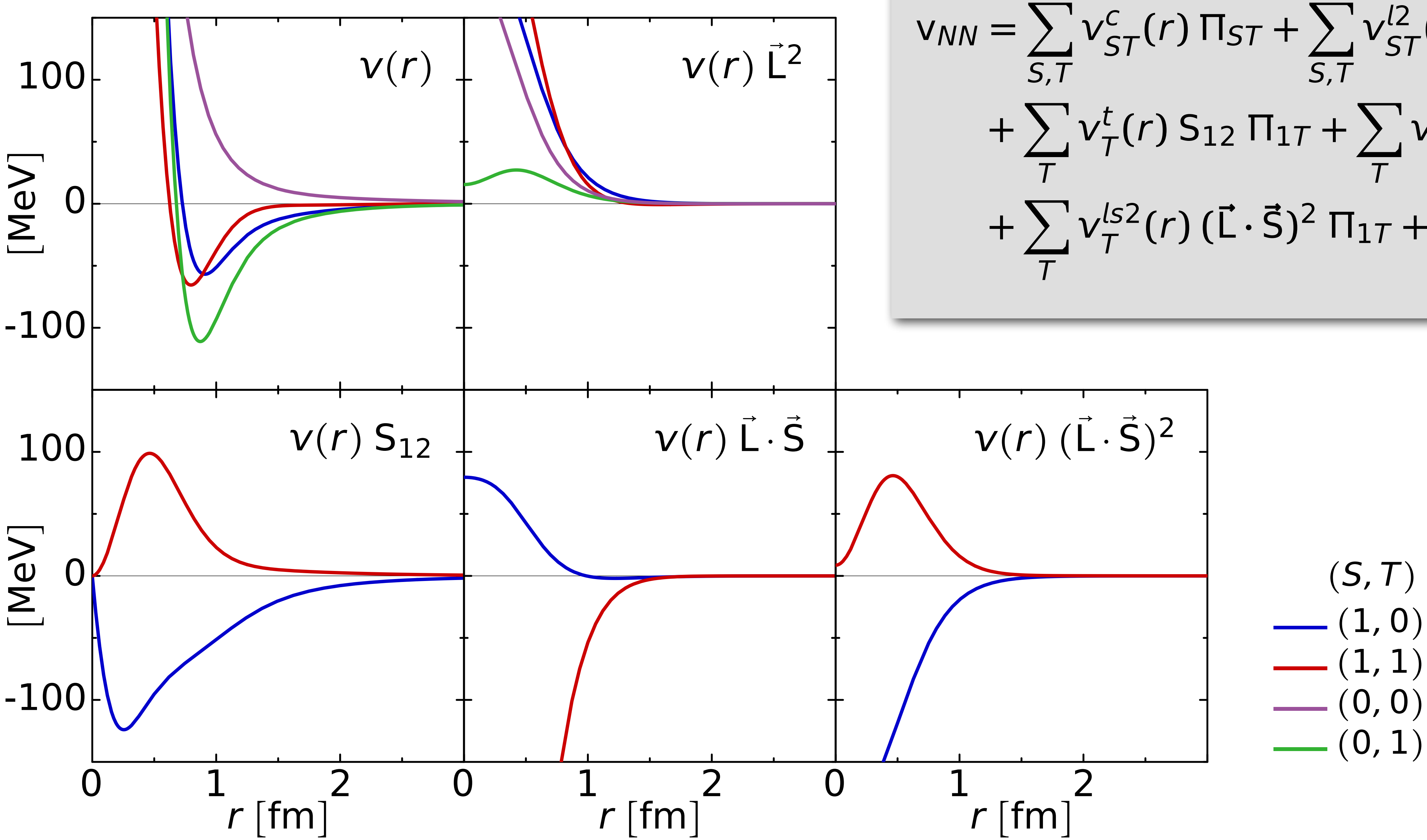
- until 2005: **high-precision phenomenological NN interactions** were state-of-the-art in ab initio nuclear structure theory
  - **Argonne V18**: long-range one-pion exchange plus phenomenological parametrization of medium- and short-range terms, local operator form
  - **CD Bonn 2000**: more systematic one meson-exchange parametrization including pseudo-scalar, scalar and vector mesons, inherently nonlocal
- parameters of the NN potential (~40) **fit to NN phase shifts** up to ~300 MeV and reproduce them with high accuracy
- supplemented by **phenomenological 3N interactions** consisting of a Fujita-Miyazawa-type term plus various hand-picked contributions



- **fit to ground states and spectra of light nuclei**, sometimes up to A≤8

Argonne V18 Potential

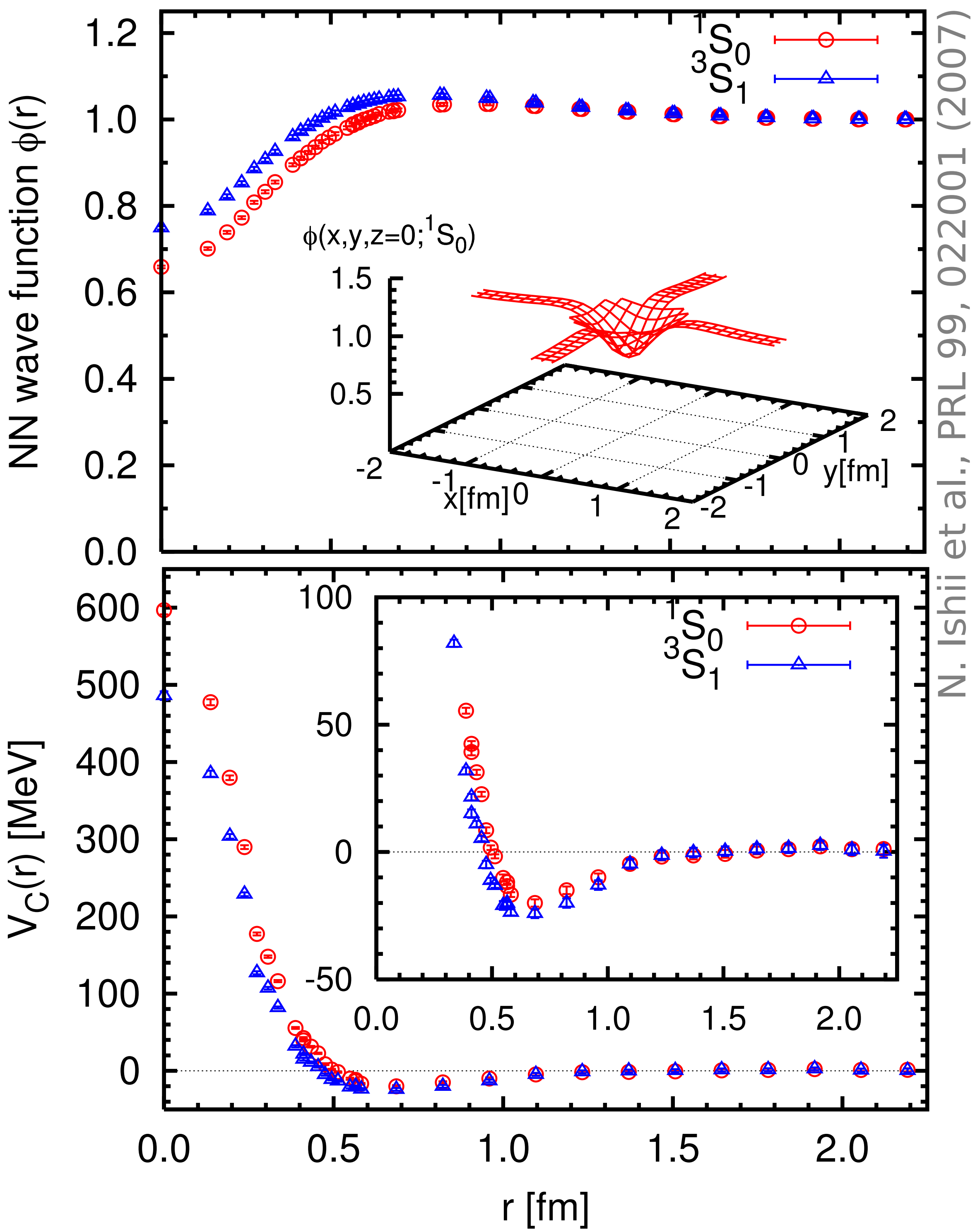
Wiringa, et al., PRC 51, 38 (1995)



$$
\begin{aligned}
v_{NN} = &\sum_{S,T} v^{c}_{ST}(r)\,\Pi_{ST} + \sum_{S,T} v^{l2}_{ST}(r)\,\vec{L}^2\,\Pi_{ST} \\
&+ \sum_{T} v^{t}_{T}(r)\,S_{12}\,\Pi_{1T} + \sum_{T} v^{ls}_{T}(r)\,(\vec{L}\cdot\vec{S})\,\Pi_{1T} \\
&+ \sum_{T} v^{ls2}_{T}(r)\,(\vec{L}\cdot\vec{S})^2\,\Pi_{1T} + \dots
\end{aligned}
$$

Tomorrow... from Lattice QCD

Hatsuda, Aoki, Ishii, Beane, Savage, Bedaque,...

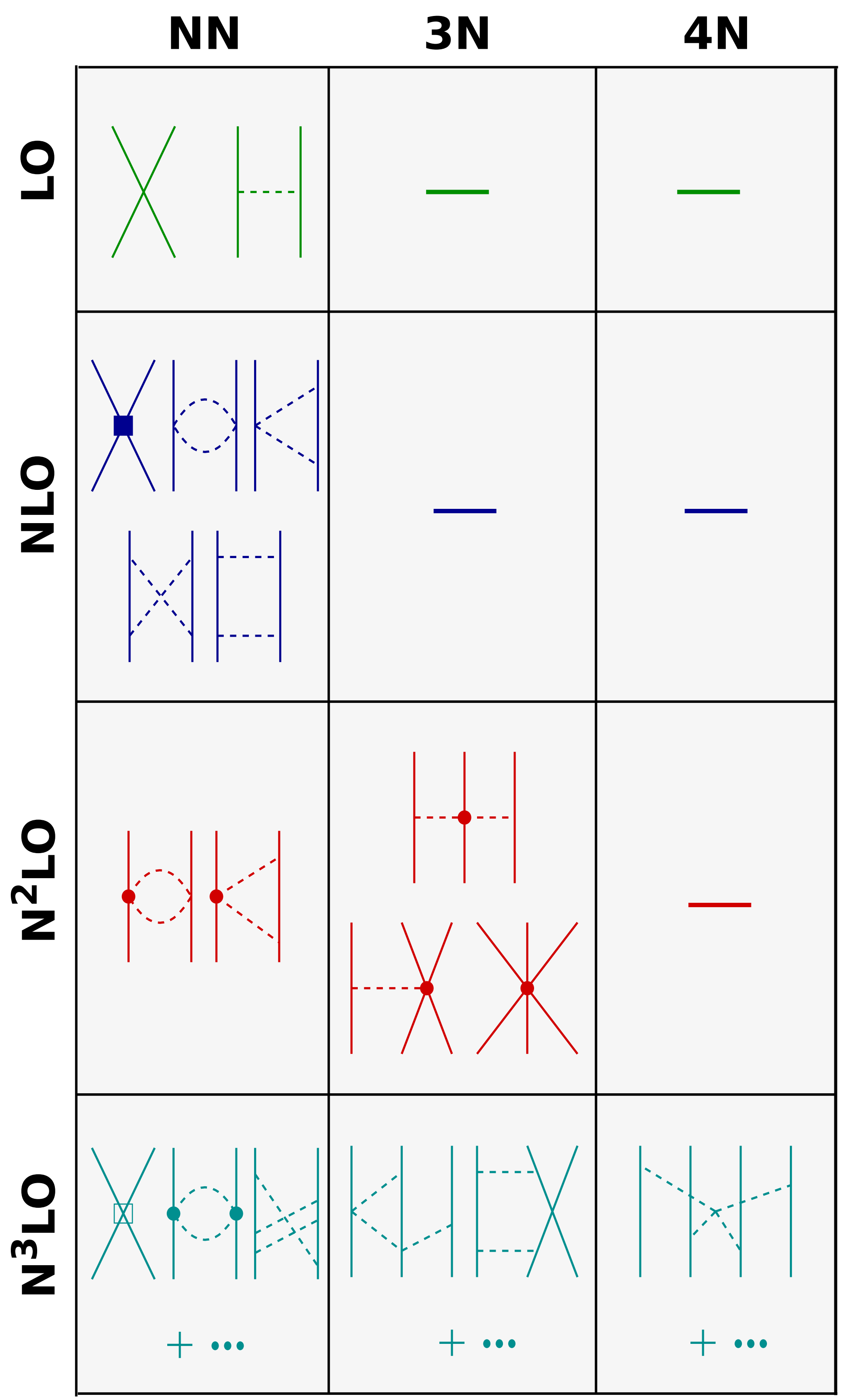


- first attempts towards construction of nuclear interactions directly from **lattice QCD simulations**
- compute relative **two-nucleon wave function** on the lattice
- **invert Schrödinger equation** to extract effective two-nucleon potential
- only **schematic results** so far (unphysical masses and mass dependence, model dependence,...)
- **alternatives**: phase-shifts or low-energy constants from lattice QCD

Today... from Chiral EFT

Weinberg, van Kolck, Machleidt, Entem, Meißner, Epelbaum, Krebs, Bernard,...

- low-energy **effective field theory** for relevant degrees of freedom (π,N) based on symmetries of QCD
- explicit long-range **pion dynamics**
- unresolved short-range physics absorbed in **contact terms**, low-energy constants fit to experiment
- systematic expansion in a small parameter with power counting enable **controlled improvements** and **error quantification**
- hierarchy of **consistent NN, 3N, 4N,...** interactions
- consistent **electromagnetic and weak operators** can be constructed in the same framework



Many Options

- **standard chiral NN+3N**
  - NN: N3LO, Entem&Machleidt, nonlocal, cutoff 500 MeV
  - 3N: N2LO, Navratil, local, cutoff 500 (400) MeV

first generation, most widely used up to now

- **nonlocal LO…N3LO**
  - NN: LO…N3LO, Epelbaum, nonlocal, cutoff 450…600 MeV
  - 3N: N2LO, Nogga, nonlocal, cutoff 450…600 MeV

also first generation, but scarcely used

- **N2LO-opt, N2LO-sat, …**
  - NN: N2LO, Ekström et al., nonlocal, cutoff 500 MeV
  - 3N: N2LO, Ekström et al., nonlocal, cutoff 500 MeV

improved fitting, also many-body inputs

- **local N2LO**
  - NN: N2LO, Gezerlis et al., local, cutoff 1.0…1.2 fm
  - 3N: N2LO, Gezerlis et al., local, cutoff 1.0…1.2 fm

designed specifically for QMC applications

- **semilocal LO…N4LO**
  - NN: LO…N4LO, Epelbaum, semilocal, cutoff 0.8…1.2 fm
  - 3N: N2LO…N3LO, LENPIC, semilocal, cutoff 0.8…1.2 fm

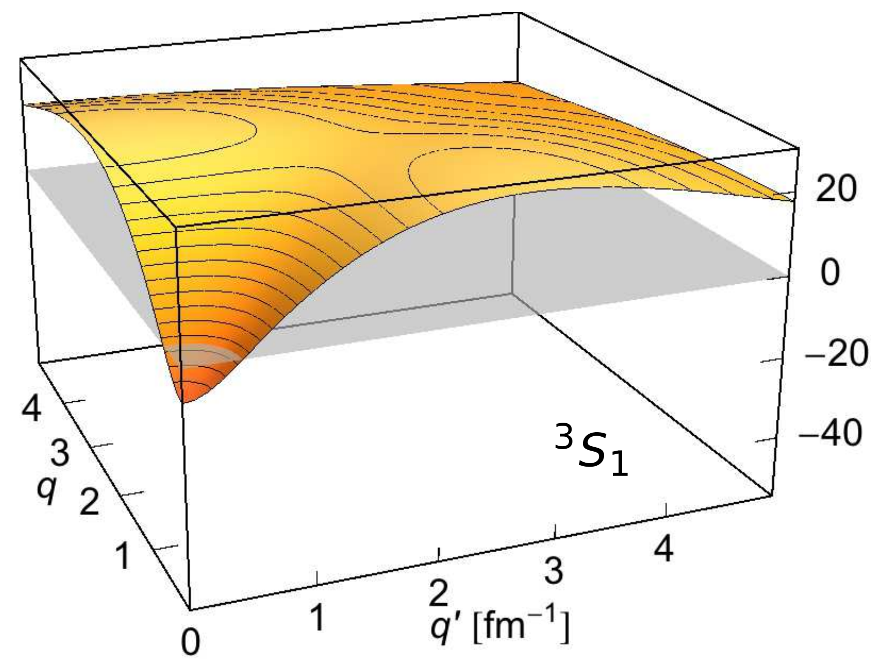
the future…

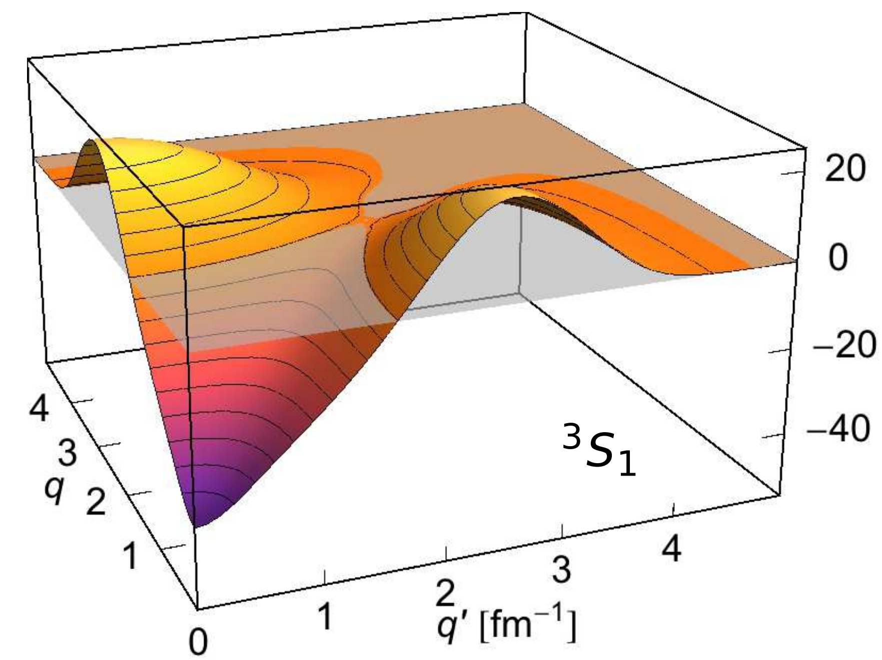
Momentum-Space Matrix Elements

$$\langle q(LS)JM;TM_T|\,v_{NN}\,|q'(L'S)JM;TM_T\rangle$$

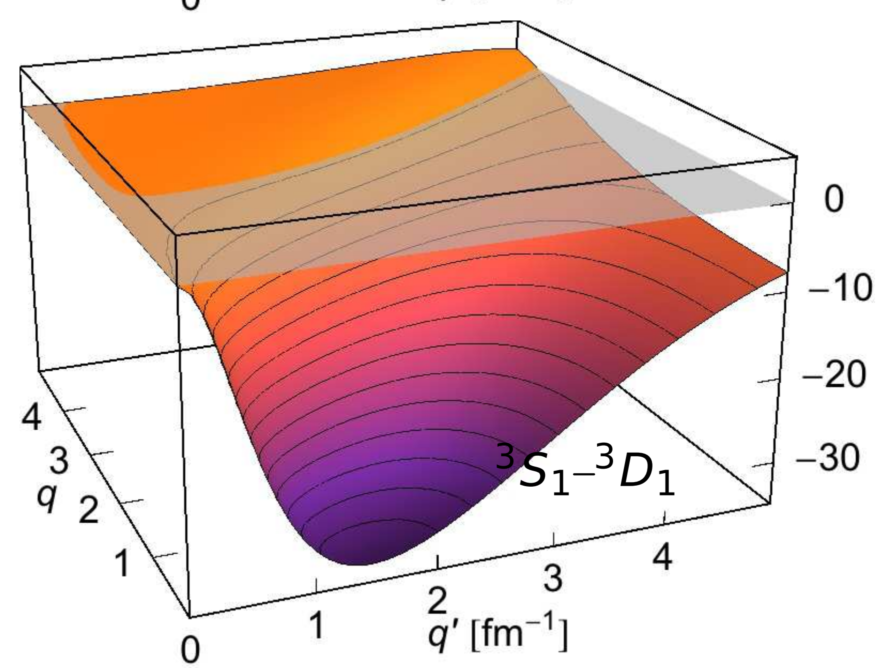
Argonne V18 | **chiral NN** (N3LO, E&M, 500 MeV)

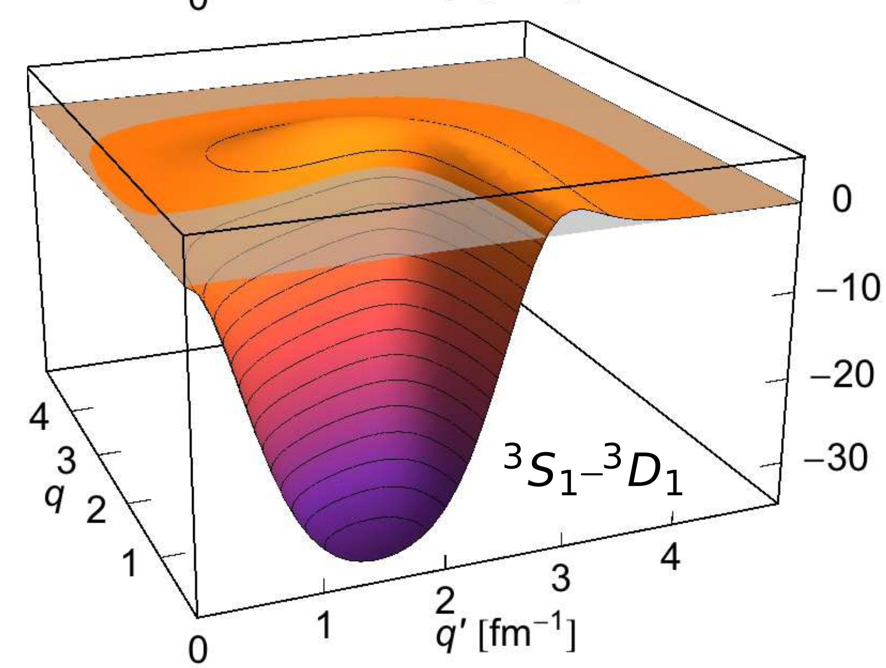
J=1
L=0
L′=0
S=1
T=0





J=1
L=0
L′=2
S=1
T=0





Matrix Elements

Partial-Wave Matrix Elements

- relative **partial-wave matrix elements** of NN and 3N interaction are **universal input** for many-body calculations

- selection of **relevant partial-wave bases** in two and three-body space with all *M* quantum numbers suppressed:

two-body relative momentum: $|q\,(LS)\,JT\rangle$

two-body relative HO: $|N\,(LS)\,JT\rangle$

three-body Jacobi momentum: $|\pi_1\pi_2;\,[(L_1S_1)\,J_1,(L_2\tfrac{1}{2})\,J_2]\,J_{12};(T_1\tfrac{1}{2})\,T_{12}\rangle$

three-body Jacobi HO: $|N_1N_2;\,[(L_1S_1)\,J_1,(L_2\tfrac{1}{2})\,J_2]\,J_{12};(T_1\tfrac{1}{2})\,T_{12}\rangle$

antisym. three-body Jacobi HO: $|E_{12}\,i\,J_{12}^{\pi}\,T_{12}\rangle$

- lots of **transformations** between the different bases are needed in practice

- **exceptions**: MBPT studies of homogeneous systems can use cartesian momentum space directly, QMC studies prefer local operator forms

Symmetries and Matrix Elements

- relative partial-wave matrix elements make **maximum use of the symmetries** of the nuclear interaction
- consider, e.g., the relative two-body matrix elements in HO basis

$$\langle N\,(LS)\,JM;TM_T|\,\mathrm{v}_{NN}\,|N'\,(L'S')\,J'M';T'M'_T\rangle$$

- the matrix elements of the NN interaction

  … do not connect different J

  … do not connect different M and are independent of M

  … do not connect different parities

  … do not connect different S

  … do not connect different T

  … do not connect different M_T

$$\Rightarrow \quad \langle N\,(LS)\,J;TM_T|\,\mathrm{v}_{NN}\,|N'\,(L'S)\,J;TM_T\rangle$$

- relative matrix elements are **efficient and simple to compute**

Transformation to Single-Particle Basis

- most many-body calculations need **matrix elements with single-particle quantum numbers** (cf. second quantization)

$$\langle \alpha_1 \alpha_2 | \mathrm{v}_{NN} | \alpha_1' \alpha_2' \rangle =$$
$$= \langle n_1 l_1 j_1 m_1 m_{t1}, n_2 l_2 j_2 m_2 m_{t2} | \mathrm{v}_{NN} | n_1' l_1' j_1' m_1' m_{t1}', n_2' l_2' j_2' m_2' m_{t2}' \rangle$$

- obtained from relative HO matrix elements via **Talmi transformation**

$$\langle n_1 l_1 j_1, n_2 l_2 j_2; JT | \mathrm{v}_{NN} | n_1' l_1' j_1', n_2' l_2' j_2'; JT \rangle =$$
$$= \sqrt{(2j_1+1)(2j_2+1)(2j_1'+1)(2j_2'+1)} \sum \sum\sum \ldots \sum$$
$$\times \begin{Bmatrix} l_1 & l_2 & L \\ \ldots \end{Bmatrix} \ldots$$
$$\times \ldots \langle\langle N\Lambda, \nu'\lambda' | n_1' l_1', n_2' l_2'; L' \rangle\rangle$$
$$\times (2j+1)(2S+1)(2L+1)(2L'+1)\,(-1)^{L+L'}\,\{1-(-1)^{\lambda+S+T}\}$$
$$\times \langle \nu(\lambda S)jT | \mathrm{v}_{NN} | \nu'(\lambda' S)jT \rangle$$

> **this analytic transformation from relative to single-particle matrix elements only exists for the harmonic oscillator basis**

Matrix Element Machinery

- beneath any ab initio many-body method there is a **machinery for computing, transforming and storing matrix elements** of all operators entering the calculation

compute and store relative two-body HO matrix elements of NN interaction

compute and store Jacobi three-body HO matrix elements of 3N interaction

perform unitary transformations of the two- and three-body relative matrix elements (see Lecture 2)

transform to single-particle JT-coupled two-body HO matrix elements and store

transform to single-particle JT-coupled three-body HO matrix elements and store

• • •

same for 4N with four-body matrix elements

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Lecture 2: Correlations

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Two-Body Problem

Solving the Two-Body Problem

- **simplest ab initio problem**: the only two-nucleon bound state, the deuteron

- start from **Hamiltonian in two-body space**, change to center of mass and intrinsic coordinates

$$\begin{aligned} \mathrm{H} &= \mathrm{H}_{\mathrm{cm}} + \mathrm{H}_{\mathrm{int}} = \mathrm{T}_{\mathrm{cm}} + \mathrm{T}_{\mathrm{int}} + \mathrm{V}_{\mathrm{NN}} \\ &= \frac{1}{2M}\vec{\mathrm{P}}^2_{\mathrm{cm}} + \frac{1}{2\mu}\vec{\mathrm{q}}^2 + \mathrm{V}_{\mathrm{NN}} \end{aligned}$$

- **separate** two-body state into center of mass and intrinsic part

$$|\psi\rangle = |\Phi_{\mathrm{cm}}\rangle \otimes |\phi_{\mathrm{int}}\rangle$$

- solve **eigenvalue problem for intrinsic part** (effective one-body problem)

$$\mathrm{H}_{\mathrm{int}}\,|\phi_{\mathrm{int}}\rangle = E\,|\phi_{\mathrm{int}}\rangle$$

Solving the Two-Body Problem

- expand eigenstates in a **relative partial-wave HO basis**

$$|\phi_{\text{int}}\rangle = \sum_{NLSJMTM_T} C_{NLSJMTM_T} \, |N(LS)JM;TM_T\rangle$$

$$|N(LS)JM;TM_T\rangle = \sum_{M_L M_S} c\left(\begin{smallmatrix} L & S \\ M_L & M_S \end{smallmatrix} \middle| \begin{smallmatrix} J \\ M \end{smallmatrix} \right) \, |NLM_L\rangle \otimes |SM_S\rangle \otimes |TM_T\rangle$$

- **symmetries** simplify the problem dramatically:
  - H_{int} does not connect/mix different J, M, S, T, M_T and parity π
  - angular mom. coupling only allows $J=L+1$, L, $L-1$ for $S=1$ or $J=L$ for $S=0$
  - total antisymmetry requires $L+S+T$=odd

- for given J^π at most two sets of angular-spin-isospin quantum numbers contribute to the expansion

Deuteron Problem

- assume $J^\pi = 1^+$ for the **deuteron ground state**, then the basis expansion reduces to

$$|\phi_{\text{int}}, J^\pi = 1^+\rangle = \sum_N C_N^{(0)} \, |N(01)\,1M;00\rangle + \sum_N C_N^{(2)} \, |N(21)\,1M;00\rangle$$

- inserting into Schrödinger equation and multiplying with basis bra leads to **matrix eigenvalue problem**

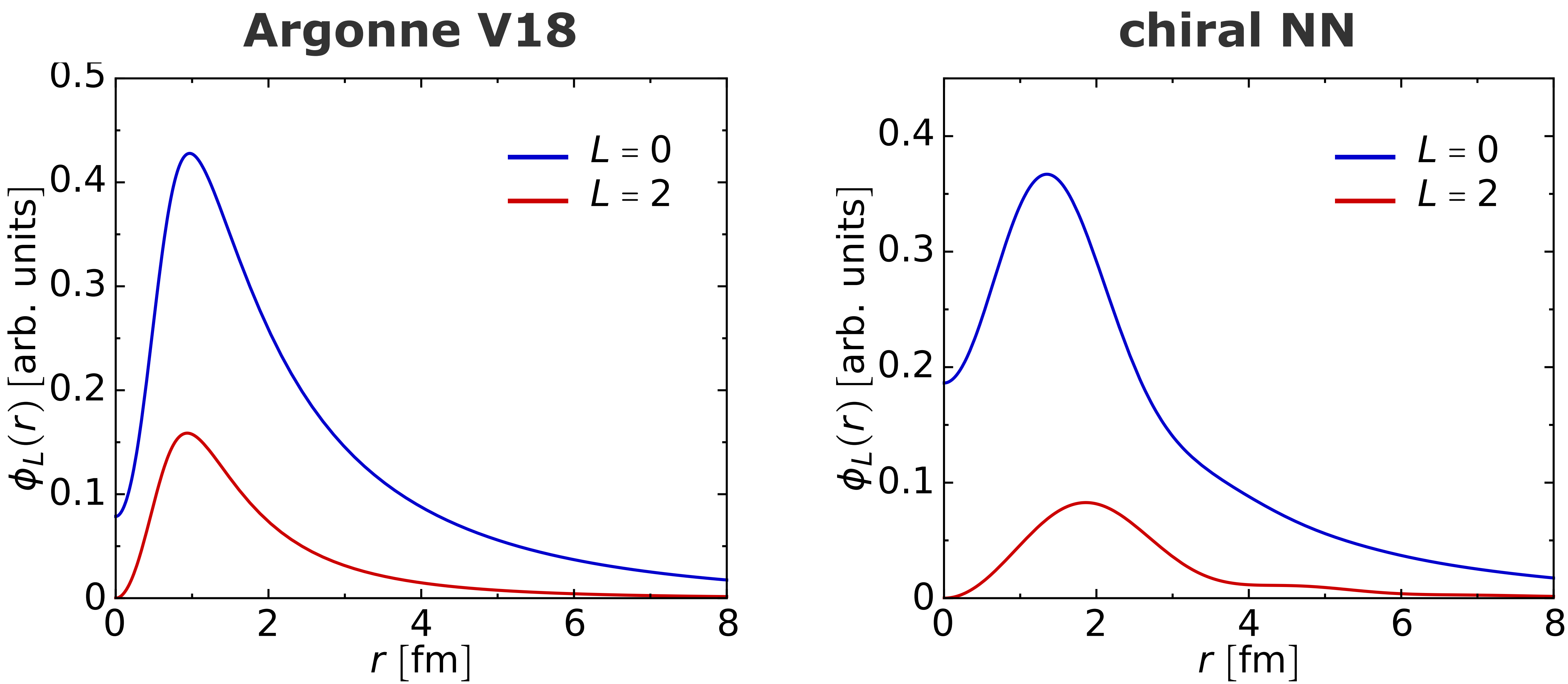
$$\left(\begin{array}{c|c} \langle N'(01)...|\,\mathrm{H}_{\text{int}}\,|N(01)...\rangle & \langle N'(01)...|\,\mathrm{H}_{\text{int}}\,|N(21)...\rangle \\ \hline \langle N'(21)...|\,\mathrm{H}_{\text{int}}\,|N(01)...\rangle & \langle N'(21) \end{array}\right) \left(\begin{array}{c} C_N^{(0)} \\ \hline C_N \end{array}\right) \quad \left(\begin{array}{c} C_{N'}^{(0)} \\ \hline C_{N'}^{(2)} \end{array}\right)$$

simplest possible Jacobi-NCSM calculation

- eigenvectors ... ficients and eigenvalues the energies

- **truncate ... ces to $N \leq N_{\text{max}}$** and choose N_{max} large enough so that observables are converged, i.e., do not depend on N_{max} anymore

Deuteron Solution



- deuteron wave function show two characteristics that are **signatures of correlations** in the two-body system:
  - suppression at small distances due to short-range repulsion
  - L=2 admixture generated by tensor part of the NN interaction

Correlations

correlations:
everything beyond the independent particle picture

- many-body eigenstates of independent-particle models described by one-body Hamiltonians are **Slater determinants**
- thus, a single Slater determinant **does not describe correlations**
- but Slater determinants are a basis of the antisym. A-body Hilbert space, so any state can be expanded in Slater determinants
- to describe **short-range correlations**, a superposition of many Slater determinants is necessary

Unitary Transformations

Why Unitary Transformations ?

realistic nuclear interactions generate strong short-range correlations in many-body states

Unitary Transformations

- adapt Hamiltonian to truncated low-energy model space
- improve convergence of many-body calculations
- preserve the physics of the initial Hamiltonian and all observables

many-body methods rely on truncated Hilbert spaces not capable of describing these correlations

Unitary Transformations

- unitary transformations **conserve the spectrum** of the Hamiltonian, with a unitary operator U we get

$$\begin{aligned} \mathrm{H}\,|\psi\rangle &= E\,|\psi\rangle \\ \mathrm{U}^\dagger \mathrm{H} \mathrm{U}\,\mathrm{U}^\dagger\,|\psi\rangle &= E\,\mathrm{U}^\dagger\,|\psi\rangle \\ \tilde{\mathrm{H}}\,|\tilde{\psi}\rangle &= E\,|\tilde{\psi}\rangle \end{aligned} \qquad \text{with} \qquad \begin{aligned} 1 &= \mathrm{U}^\dagger \mathrm{U} = \mathrm{U}\mathrm{U}^\dagger \\ \tilde{\mathrm{H}} &= \mathrm{U}^\dagger \mathrm{H} \mathrm{U} \\ |\tilde{\psi}\rangle &= \mathrm{U}^\dagger\,|\psi\rangle \end{aligned}$$

- for **other observables** defined via matrix elements of an operator A with the eigenstates we obtain

$$\langle\psi|\,\mathrm{A}\,|\psi'\rangle = \langle\psi|\,\mathrm{U}\,\mathrm{U}^\dagger \mathrm{A} \mathrm{U}\,\mathrm{U}^\dagger\,|\psi'\rangle = \langle\tilde{\psi}|\,\tilde{\mathrm{A}}\,|\tilde{\psi}'\rangle$$

unitary transformations conserve all observables as long as the Hamiltonian and all other operators are transformed consistently

Similarity Renormalization Group

Similarity Renormalization Group

continuous unitary transformation to pre-diagonalize the Hamiltonian with respect to a given basis

- start with an **explicit unitary transformation** of the Hamiltonian with a unitary operator U_α with continuous **flow parameter α**

$$H_\alpha = U_\alpha{}^\dagger H \, U_\alpha$$

- **differentiate both sides** with respect to flow parameter

$$\begin{aligned}
\frac{d}{d\alpha} H_\alpha &= \left(\frac{d}{d\alpha} U_\alpha{}^\dagger\right) H \, U_\alpha + U_\alpha{}^\dagger H \left(\frac{d}{d\alpha} U_\alpha\right) \\
&= \left(\frac{d}{d\alpha} U_\alpha{}^\dagger\right) U_\alpha U_\alpha{}^\dagger H \, U_\alpha + U_\alpha{}^\dagger H \, U_\alpha U_\alpha{}^\dagger \left(\frac{d}{d\alpha} U_\alpha\right) \\
&= \left(\frac{d}{d\alpha} U_\alpha{}^\dagger\right) U_\alpha H_\alpha + H_\alpha U_\alpha{}^\dagger \left(\frac{d}{d\alpha} U_\alpha\right)
\end{aligned}$$

Similarity Renormalization Group

- define the **antihermitian generator** of the unitary transformation via

$$\eta_\alpha = -\mathrm{U}_\alpha{}^\dagger \left(\frac{d}{d\alpha} \mathrm{U}_\alpha \right) = \left(\frac{d}{d\alpha} \mathrm{U}_\alpha{}^\dagger \right) \mathrm{U}_\alpha = -\eta_\alpha{}^\dagger$$

  where the antihermiticity follows explicitly from differentiating the unitarity condition $1 = \mathrm{U}_\alpha{}^\dagger \mathrm{U}_\alpha$

- we thus obtain for the derivative of the transformed Hamiltonian

$$\begin{aligned} \frac{d}{d\alpha} \mathrm{H}_\alpha &= \eta_\alpha \mathrm{H}_\alpha - \mathrm{H}_\alpha \eta_\alpha \\ &= \left[\eta_\alpha, \mathrm{H}_\alpha \right] \end{aligned}$$

  thus, that change of the Hamiltonian as function of the flow parameter is governed by the **commutator of the generator with the Hamiltonian**

- this is the **SRG flow equation**, which has a close resemblance to the Heisenberg equation of motion

Similarity Renormalization Group

Glazek, Wilson, Wegner, Perry, Bogner, Furnstahl, Hergert, Roth,...

continuous unitary transformation to pre-diagonalize the Hamiltonian with respect to a given basis

- **consistent unitary transformation** of Hamiltonian and observables

$$H_\alpha = U_\alpha^\dagger H \, U_\alpha \qquad O_\alpha = U_\alpha^\dagger O \, U_\alpha$$

- **flow equations** for H_α and U_α with continuous **flow parameter α**

$$\frac{d}{d\alpha} H_\alpha = [\eta_\alpha, H_\alpha] \qquad \frac{d}{d\alpha} O_\alpha = [\eta_\alpha, O_\alpha] \qquad \frac{d}{d\alpha} U_\alpha = -U_\alpha \eta_\alpha$$

- the physics of the transformation is governed by the **dynamic generator η_α** and we choose an ansatz depending on the type of "pre-diaognalization" we want to achieve

SRG Generator & Fixed Points

- **standard choice** for antihermitian generator: commutator of intrinsic kinetic energy and the Hamiltonian

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

- this **generator vanishes** if
  - kinetic energy and Hamiltonian commute
  - kinetic energy and Hamiltonian have a simultaneous eigenbasis
  - the Hamiltonian is diagonal in the eigenbasis of the kinetic energy, i.e., in a momentum eigenbasis

- a vanishing generator implies a **trivial fixed point** of the SRG flow equation — the r.h.s. of the flow equation vanishes and the Hamiltonian is stationary

- SRG flow **drives the Hamiltonian towards the fixed point**, i.e., towards the diagonal in momentum representation

Solving the SRG Flow Equation

- convert operator equations into a basis representation to obtain **coupled evolution equations for *n*-body matrix elements** of the Hamiltonian

  n=2: two-body relative momentum $|q\,(LS)\,JT\rangle$

  n=3: antisym. three-body Jacobi HO $|Ei J^{\pi} T\rangle$

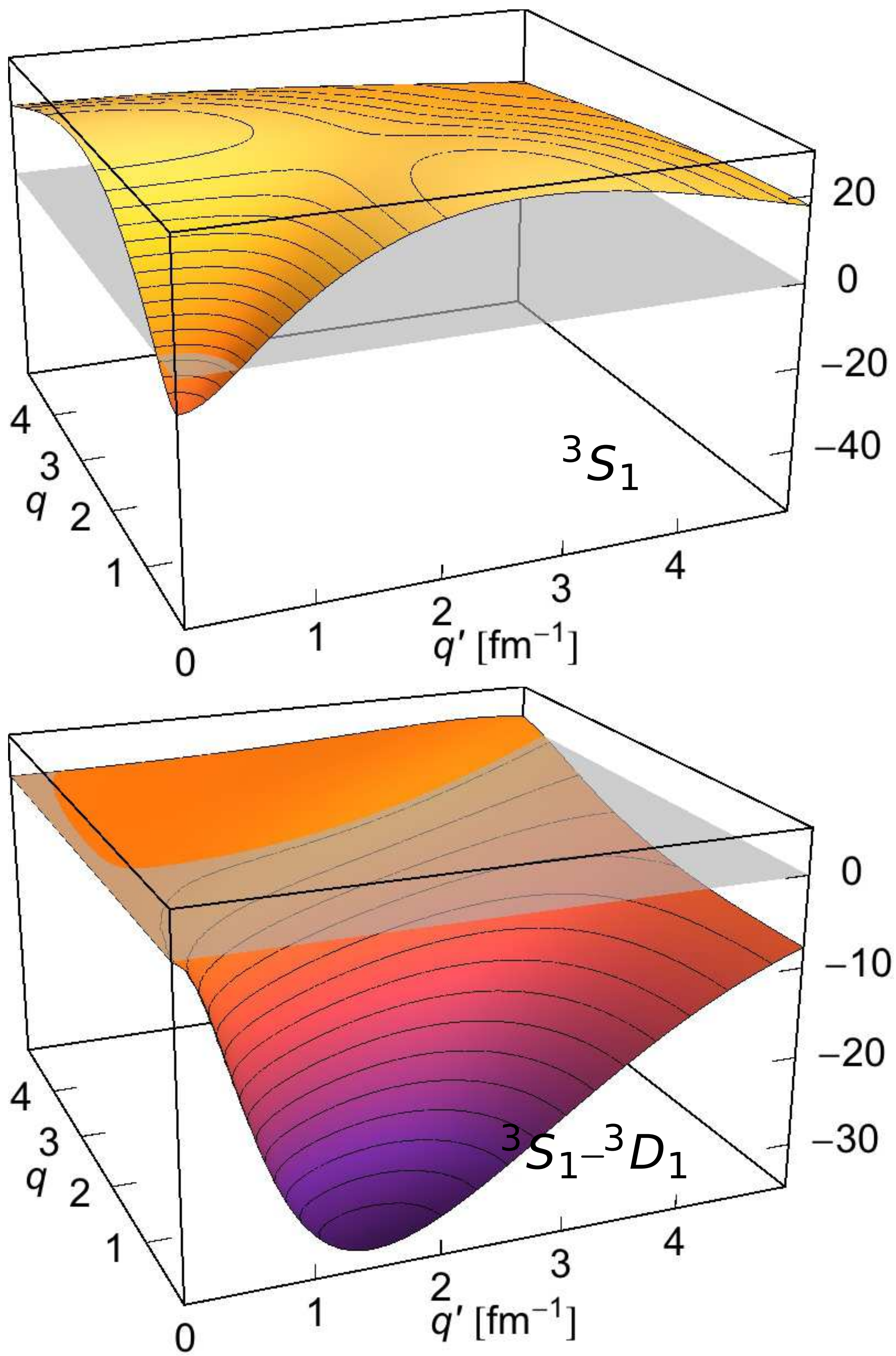
- matrix-evolution equations for n=3 with antisym. three-body Jacobi HO states:

$$\frac{\mathrm{d}}{\mathrm{d}\alpha}\langle Ei J^{\pi} T|\,\mathrm{H}_{\alpha}\,|E' i' J^{\pi} T\rangle = (2\mu)^2 \sum_{E'',i''}^{E_{\mathrm{SRG}}} \sum_{E''',i'''}^{E_{\mathrm{SRG}}} \Big[\langle Ei\ldots|\,\mathrm{T}_{\mathrm{int}}\,|E''i''\ldots\rangle\,\langle E''i''\ldots|\,\mathrm{H}_{\alpha}\,|E'''i'''\ldots\rangle\,\langle E'''i'''\ldots|\,\mathrm{H}_{\alpha}\,|E'i'\ldots\rangle$$
$$-2\langle Ei\ldots|\,\mathrm{H}_{\alpha}\,|E''i''\ldots\rangle\,\langle E''i''\ldots|\,\mathrm{T}_{\mathrm{int}}\,|E'''i'''\ldots\rangle\,\langle E'''i'''\ldots|\,\mathrm{H}_{\alpha}\,|E'i'\ldots\rangle$$
$$+\langle Ei\ldots|\,\mathrm{H}_{\alpha}\,|E''i''\ldots\rangle\,\langle E''i''\ldots|\,\mathrm{H}_{\alpha}\,|E'''i'''\ldots\rangle\,\langle E'''i'''\ldots|\,\mathrm{T}_{\mathrm{int}}\,|E'i'\ldots\rangle \Big]$$

- **note**: when using n-body matrix elements, components of the evolved Hamiltonian with particle-rank > n are discarded

SRG Evolution in Two-Body Space

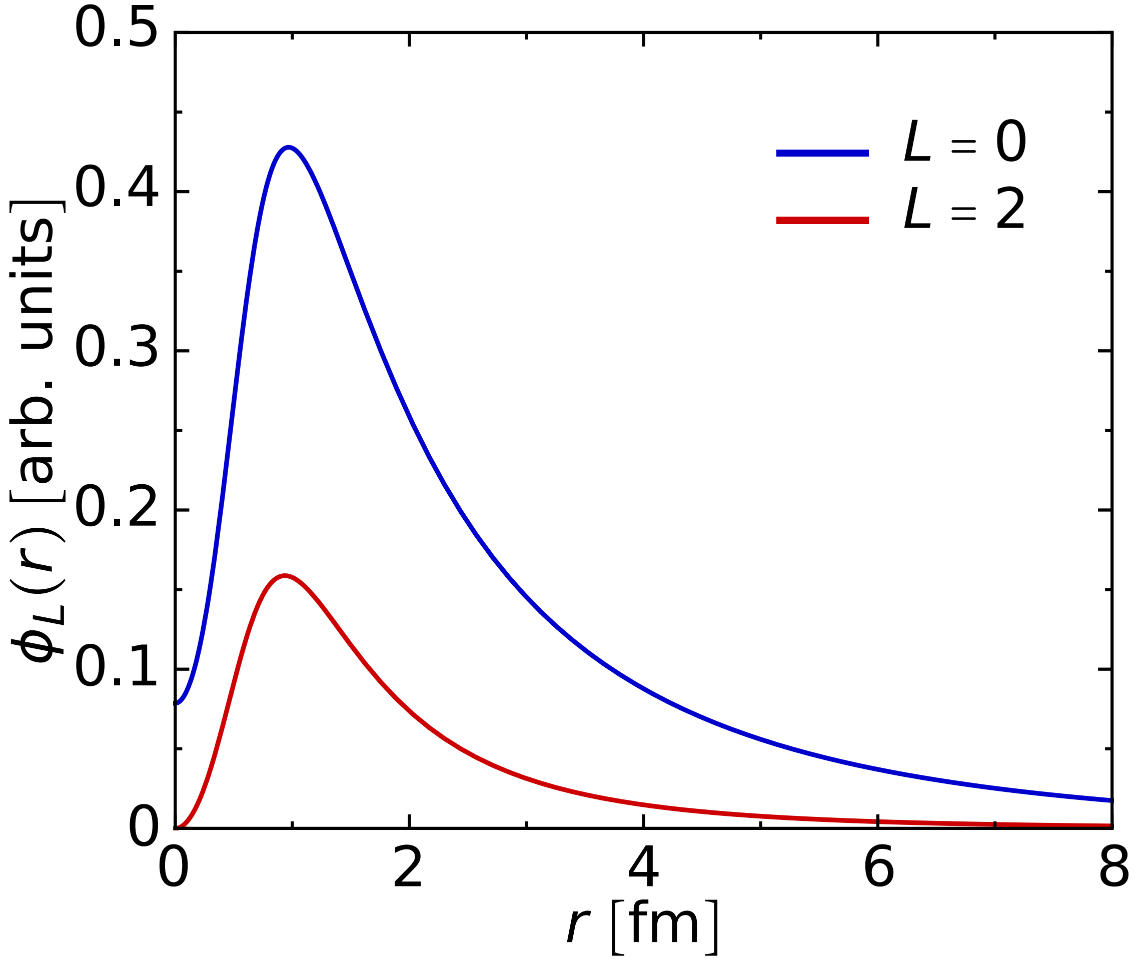
momentum-space matrix elements



Argonne V18

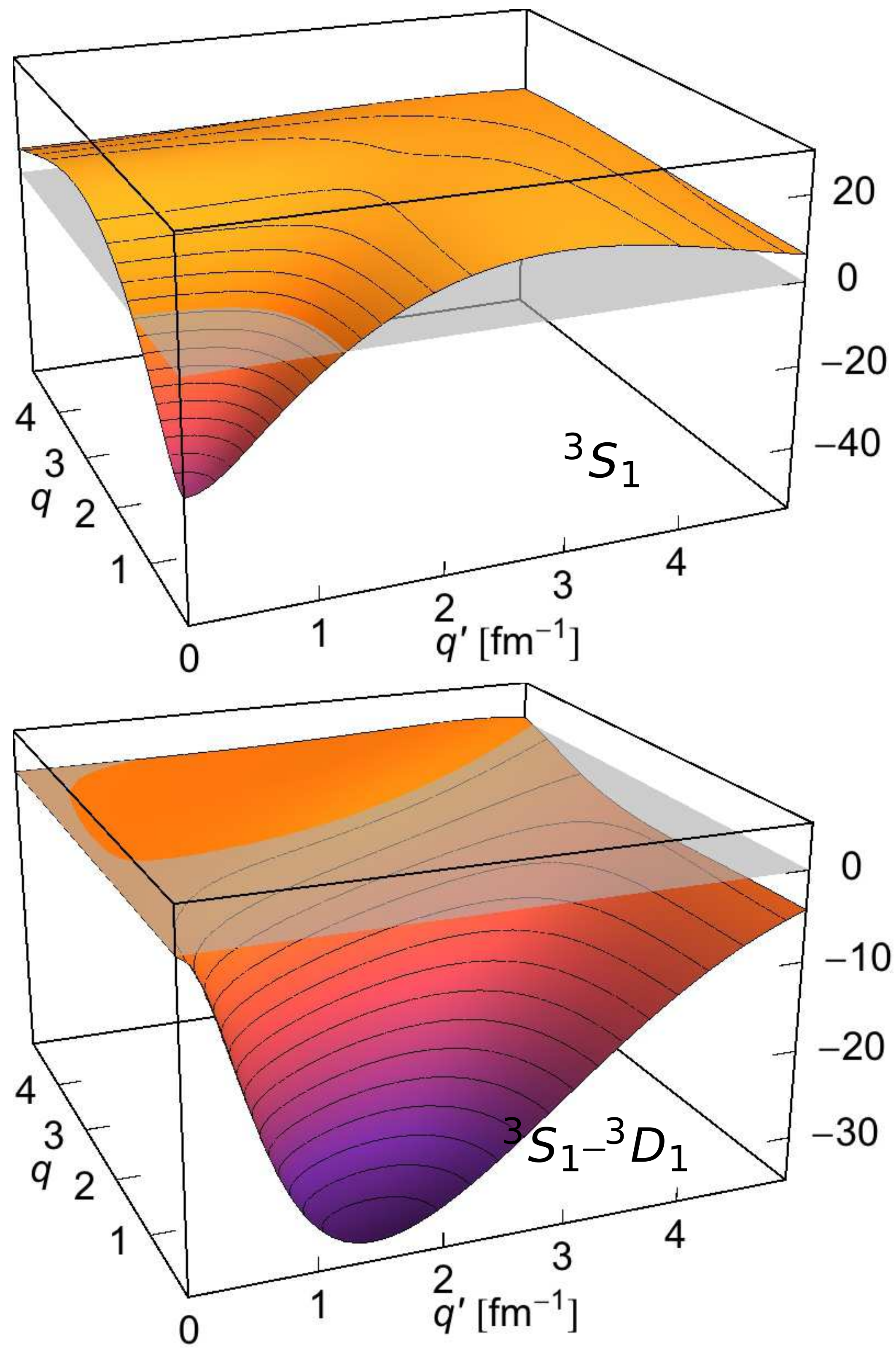
$J^\pi = 1^+, T = 0$

deuteron wave-function



SRG Evolution in Two-Body Space

momentum-space matrix elements

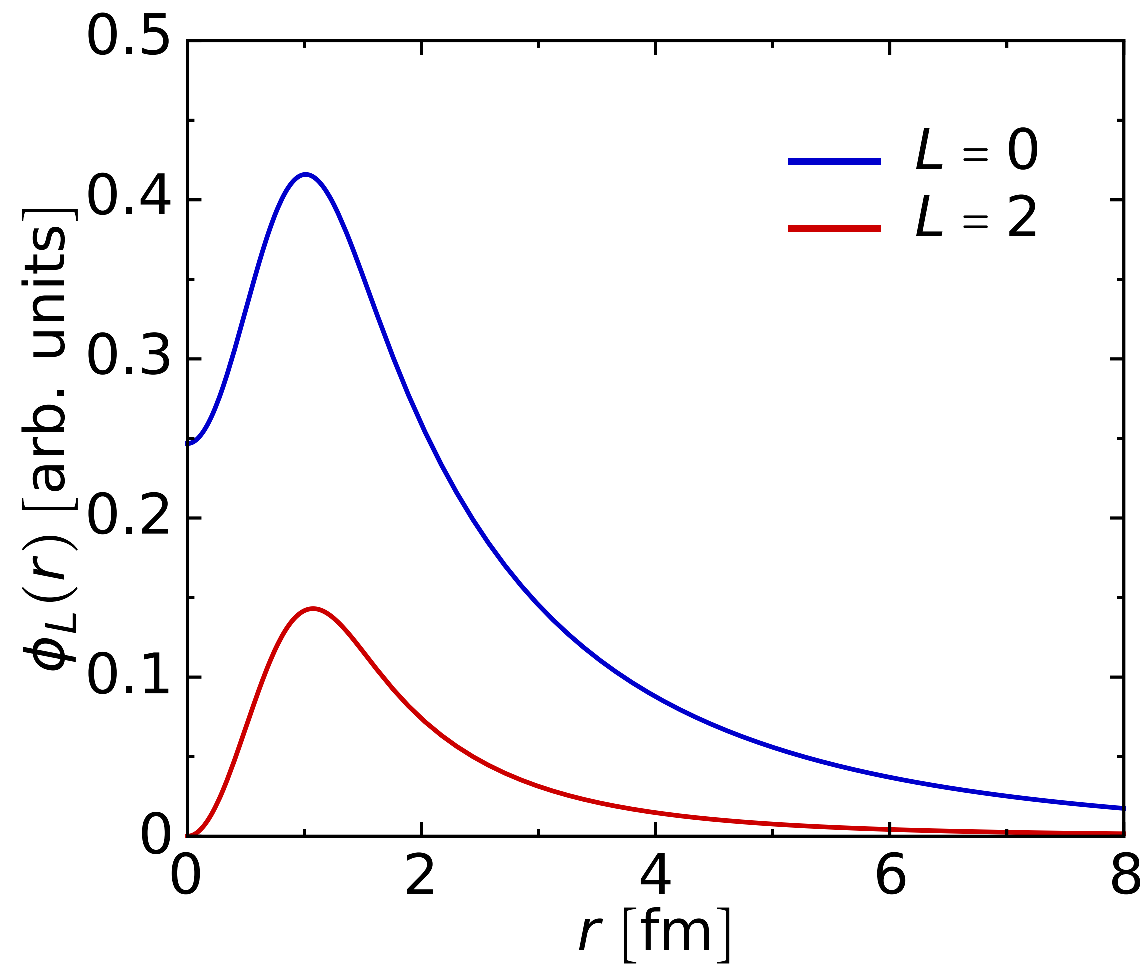


$\alpha = 0.001\,\text{fm}^4$

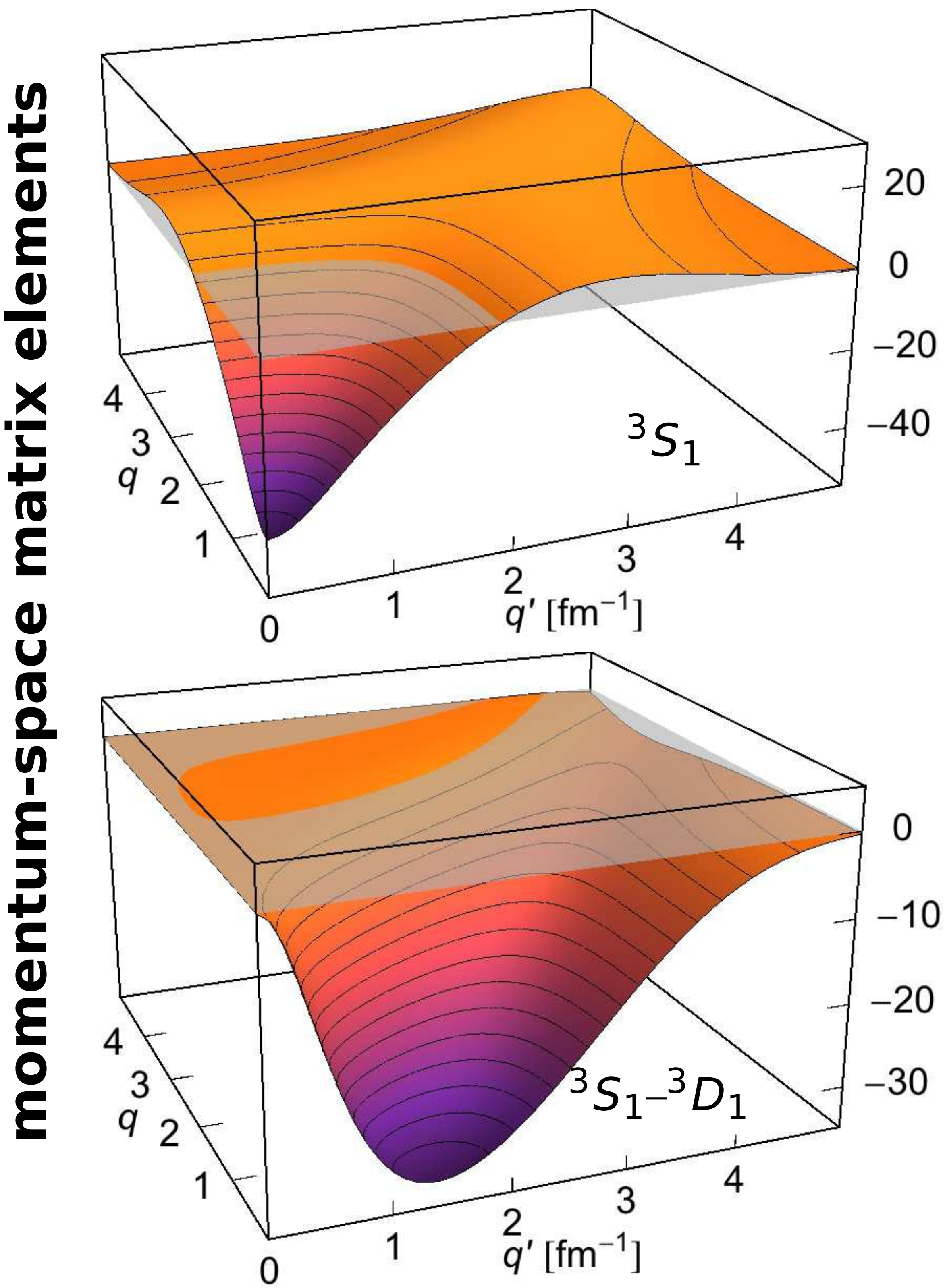
$\Lambda = 5.62\,\text{fm}^{-1}$

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

deuteron wave-function



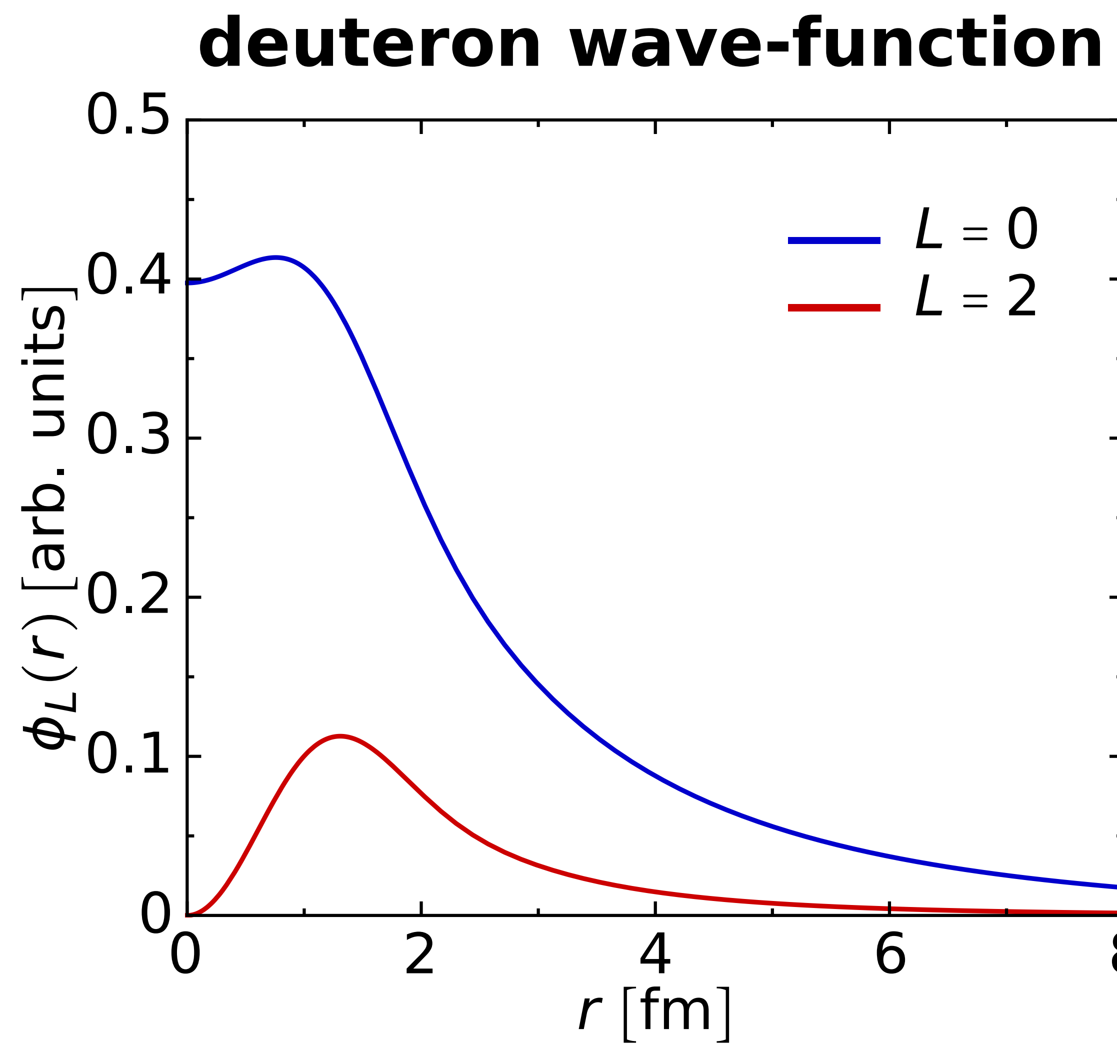
SRG Evolution in Two-Body Space



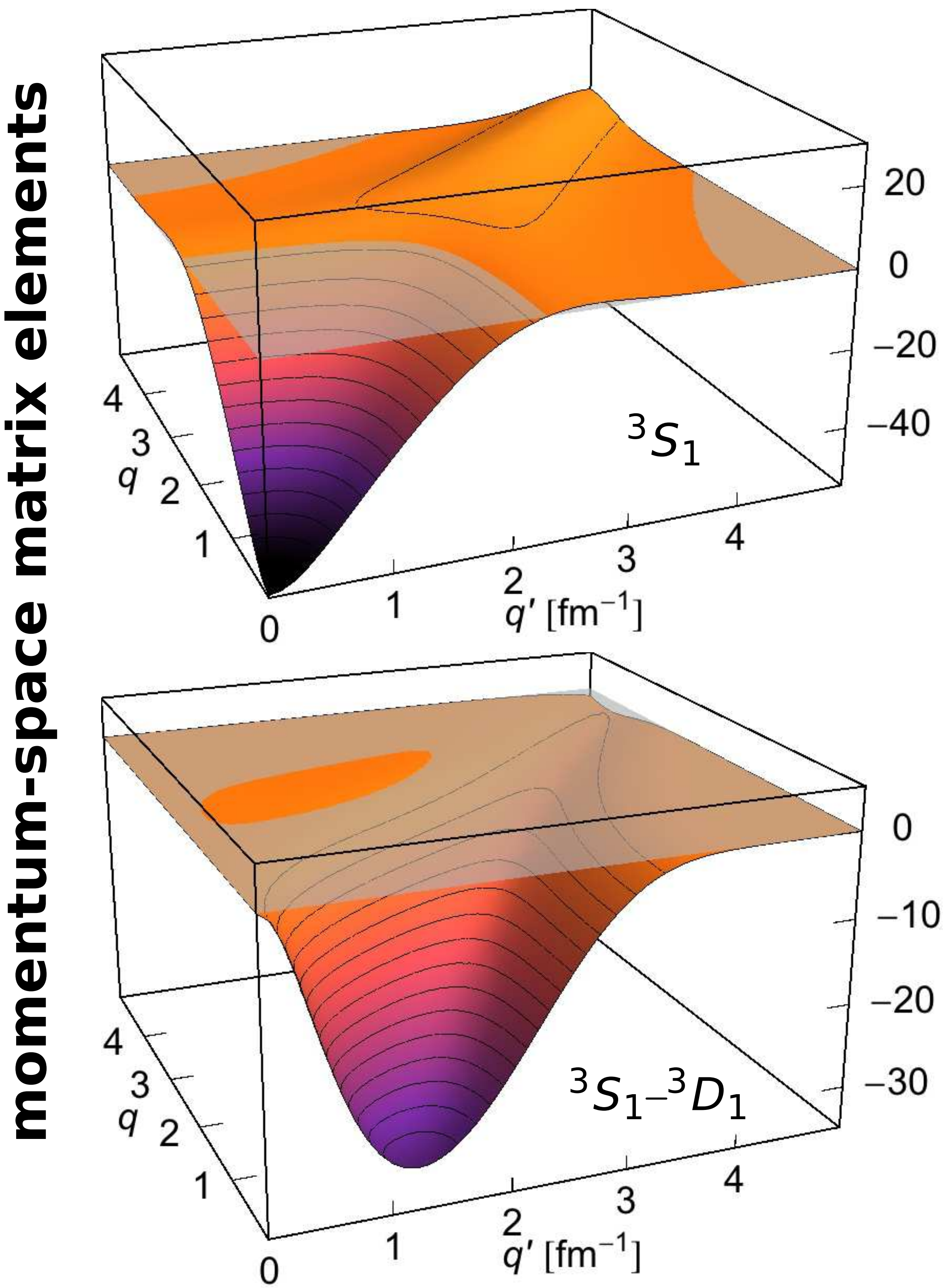
$\alpha = 0.005\,\text{fm}^4$

$\Lambda = 3.76\,\text{fm}^{-1}$

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



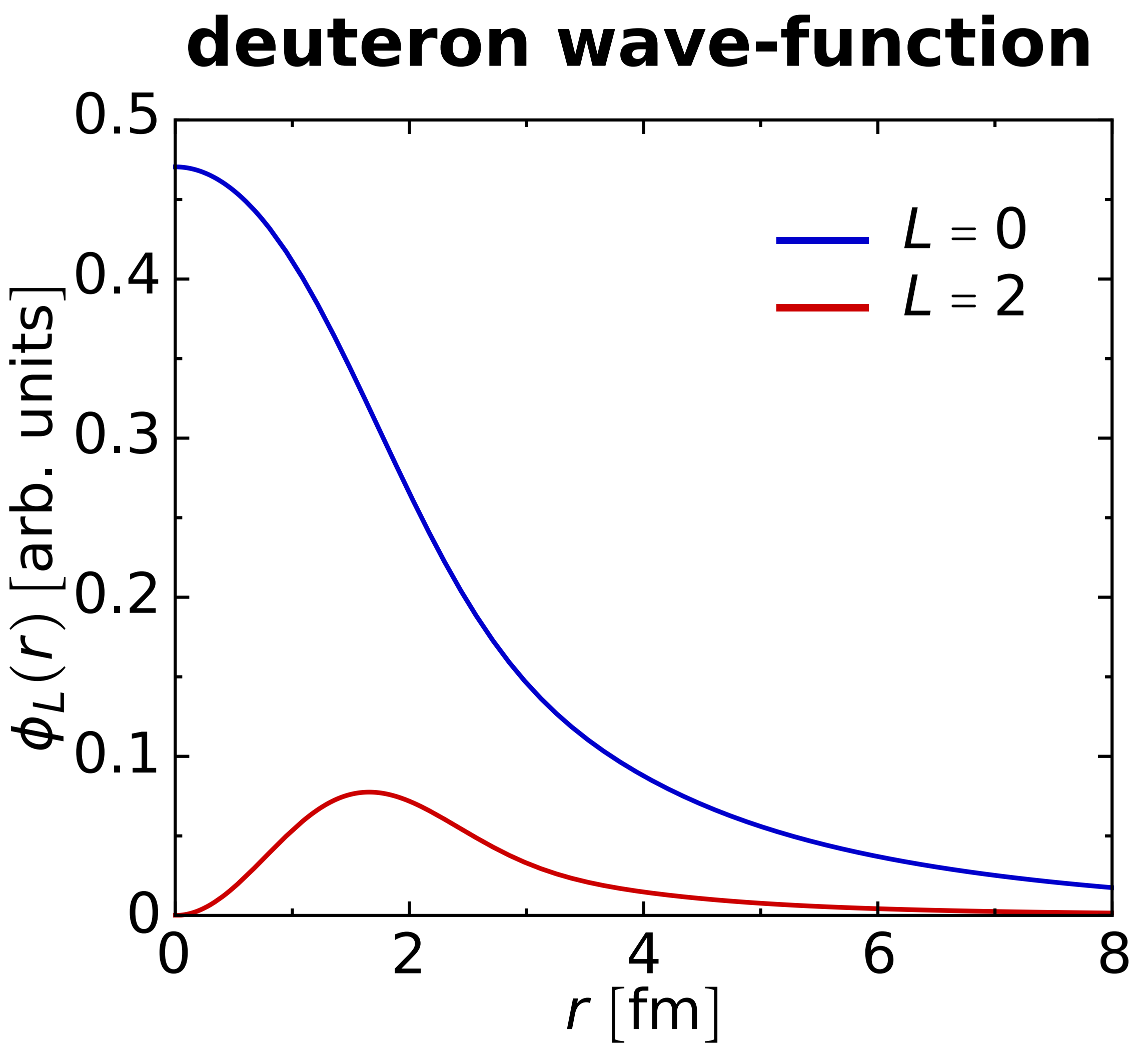
SRG Evolution in Two-Body Space



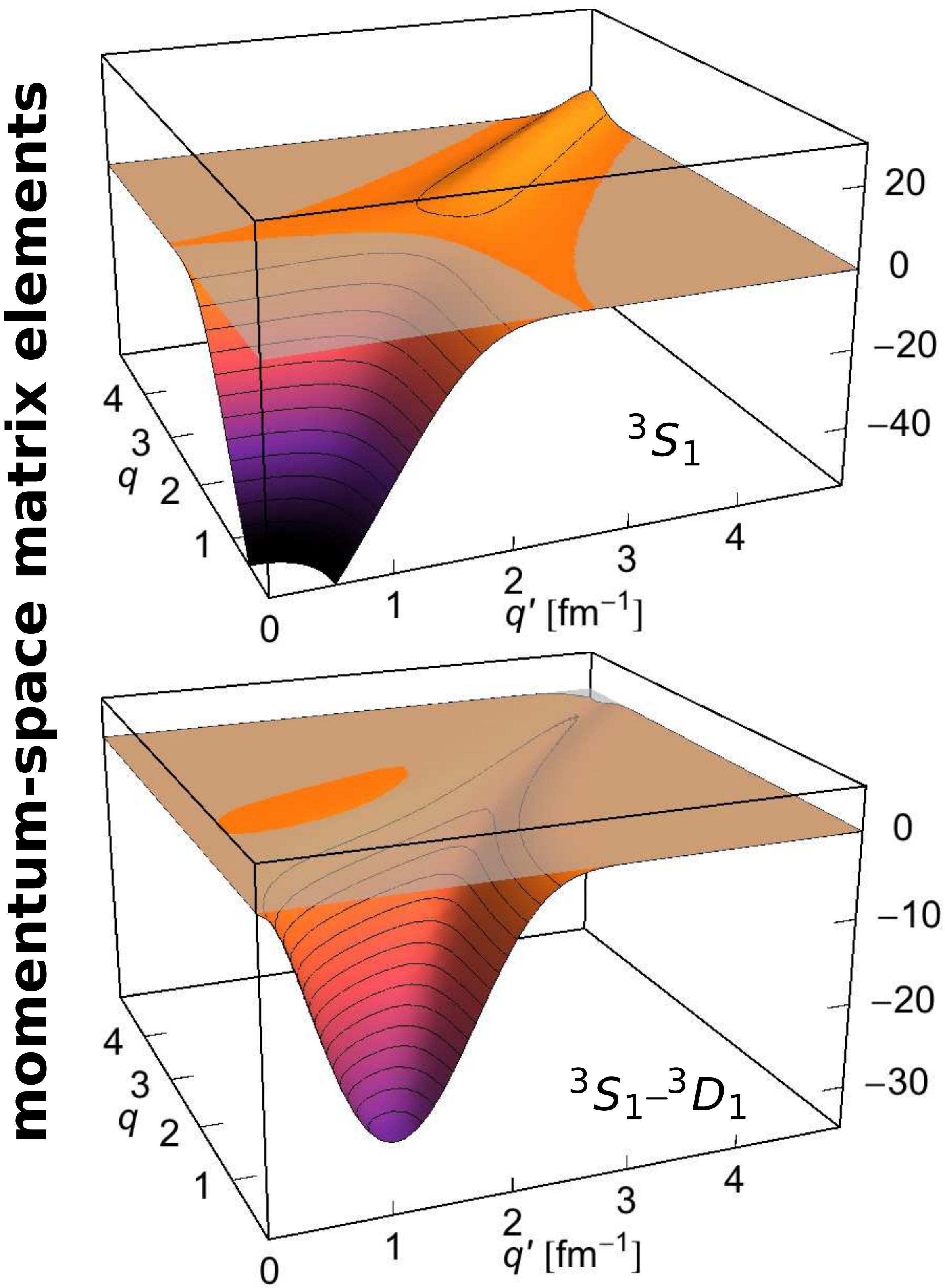
$\alpha = 0.020\,\mathrm{fm}^4$

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

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



SRG Evolution in Two-Body Space

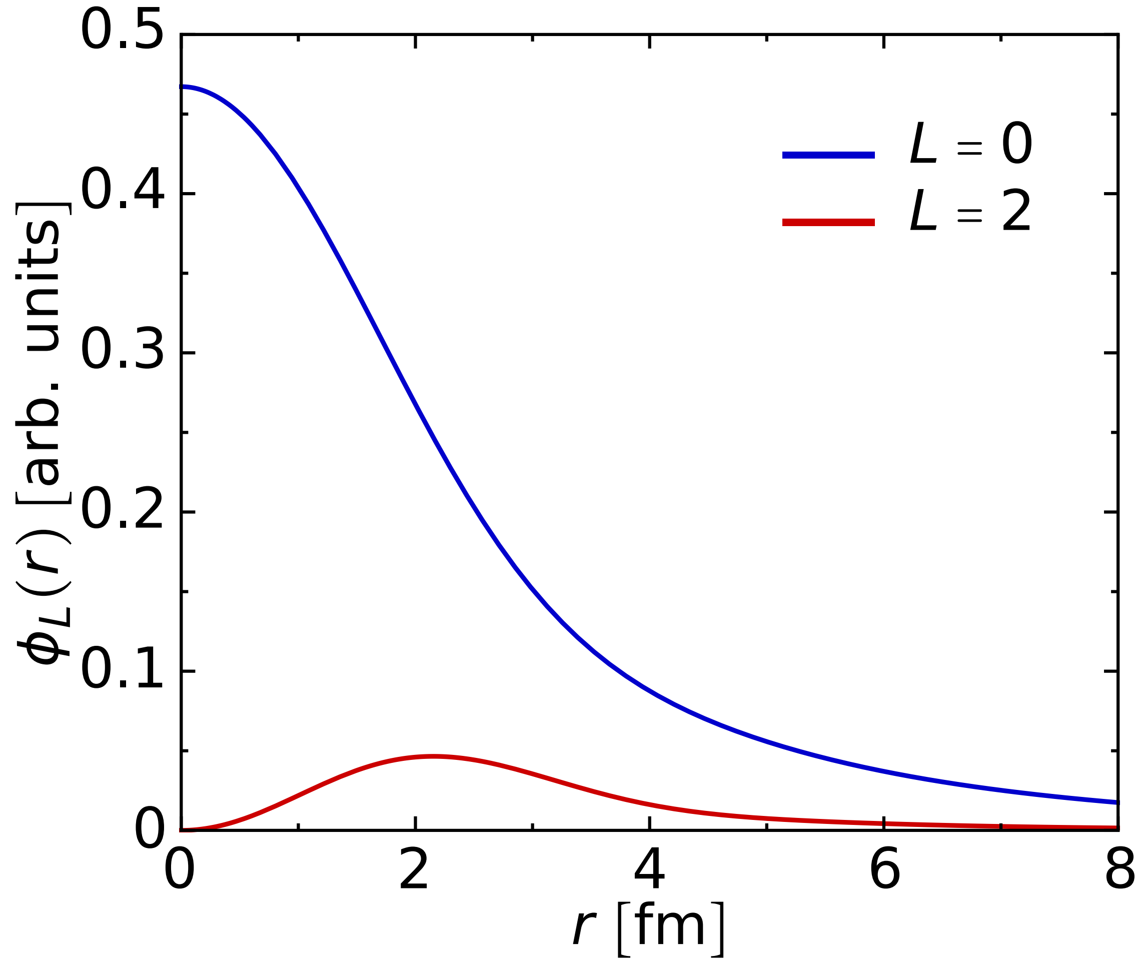


$\alpha = 0.080\,\mathrm{fm}^4$

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

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

deuteron wave-function



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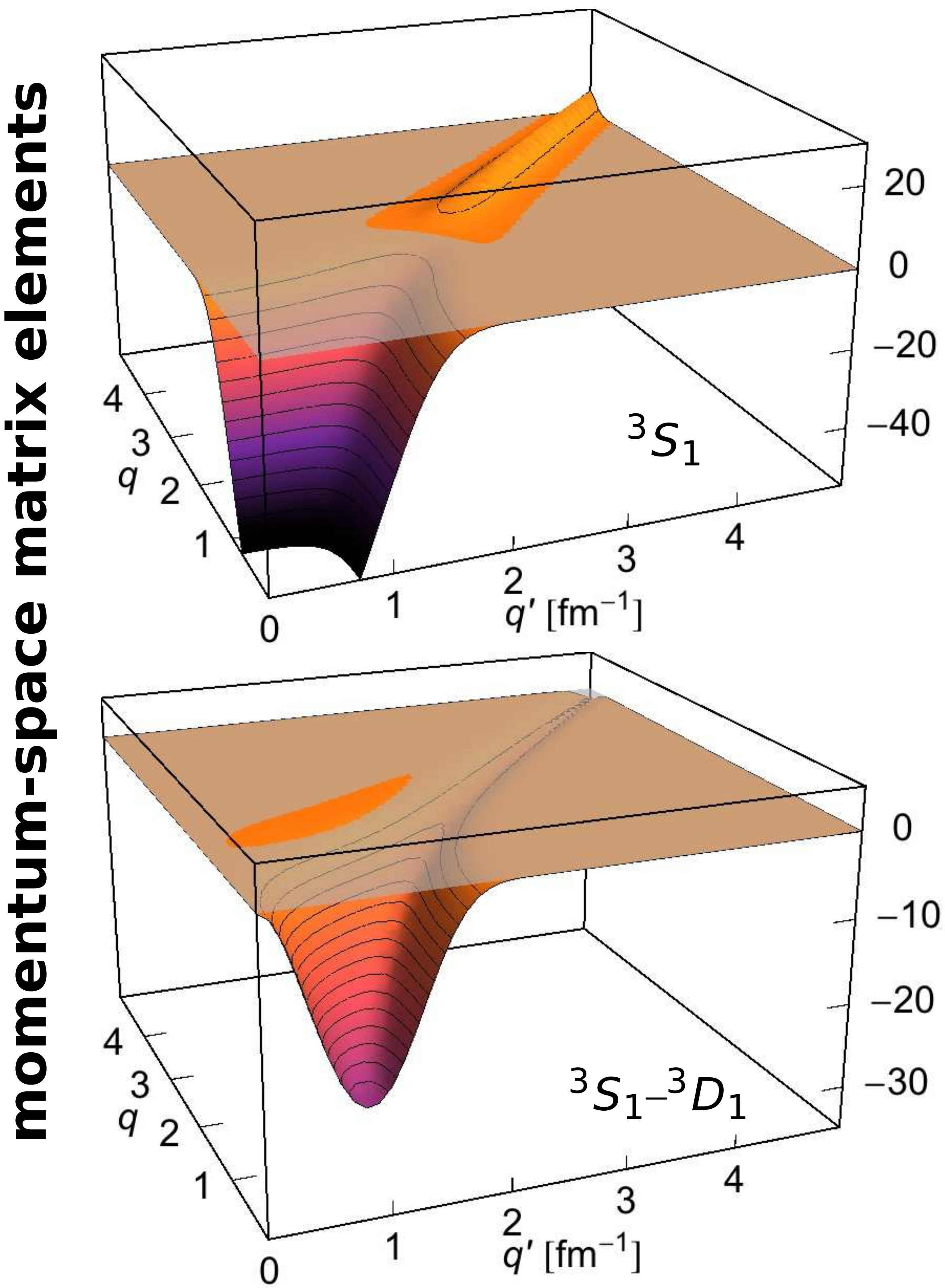
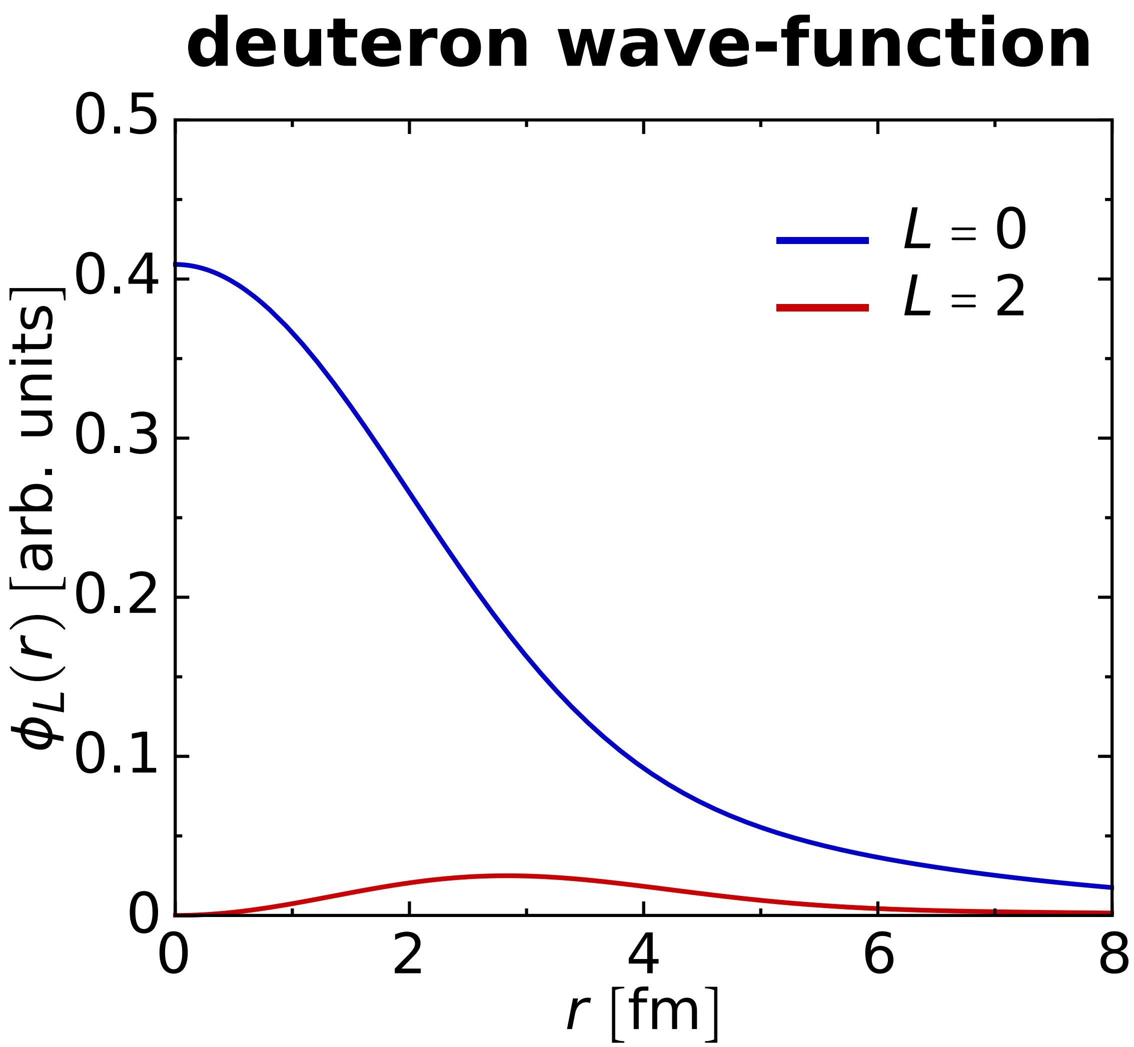


$\alpha = 0.320\,\mathrm{fm}^4$

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

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



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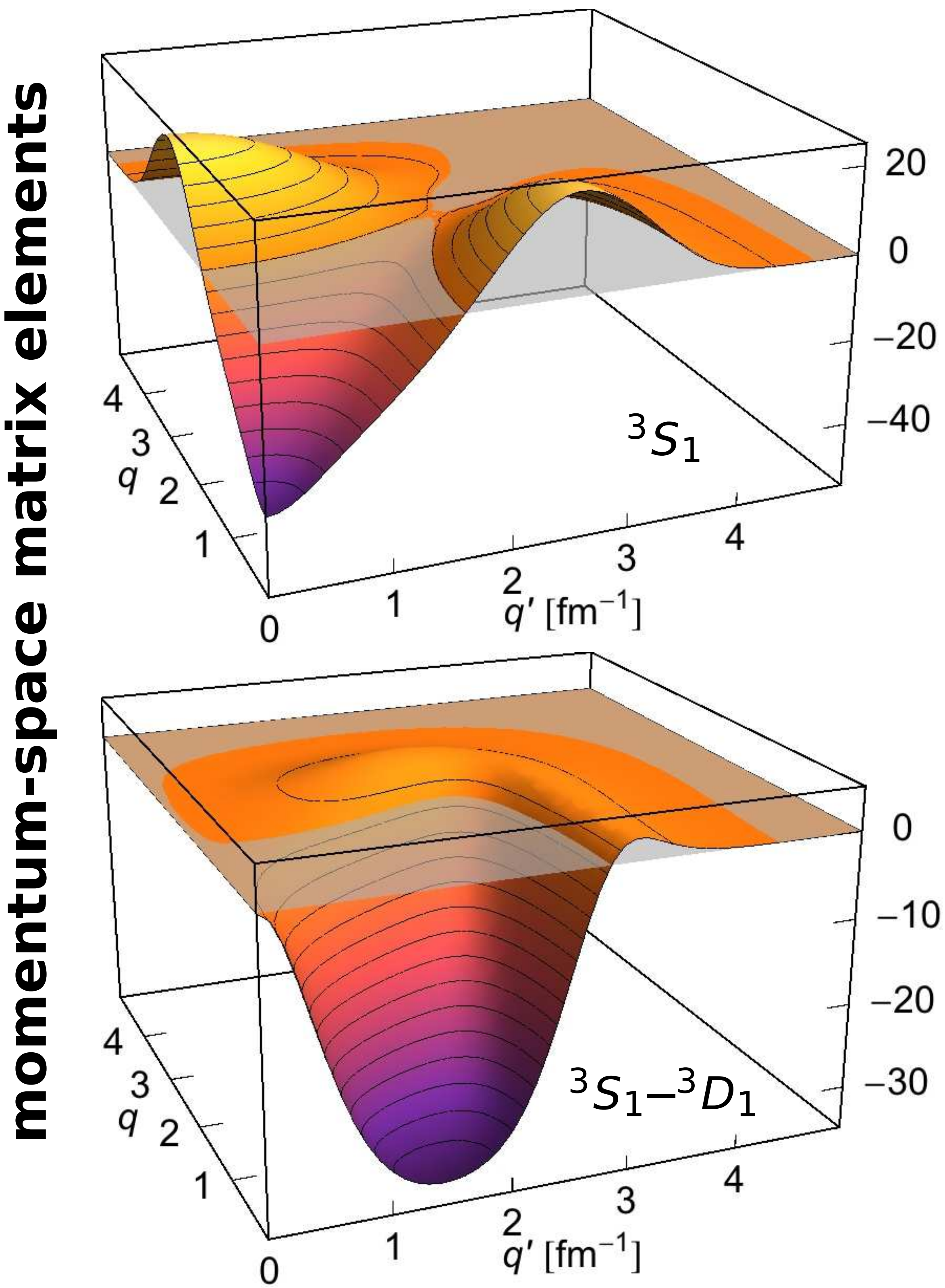
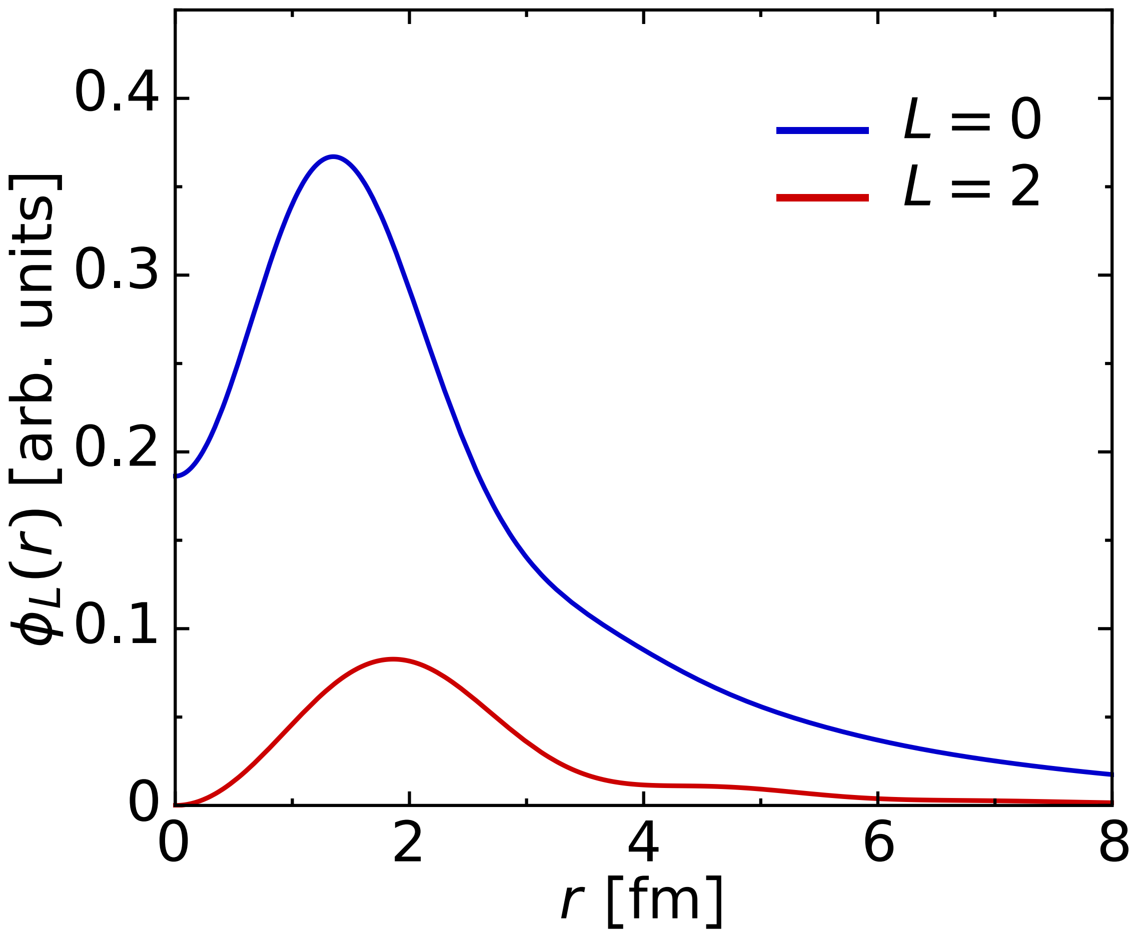


chiral NN

Entem & Machleidt. N^{3}LO, 500 MeV

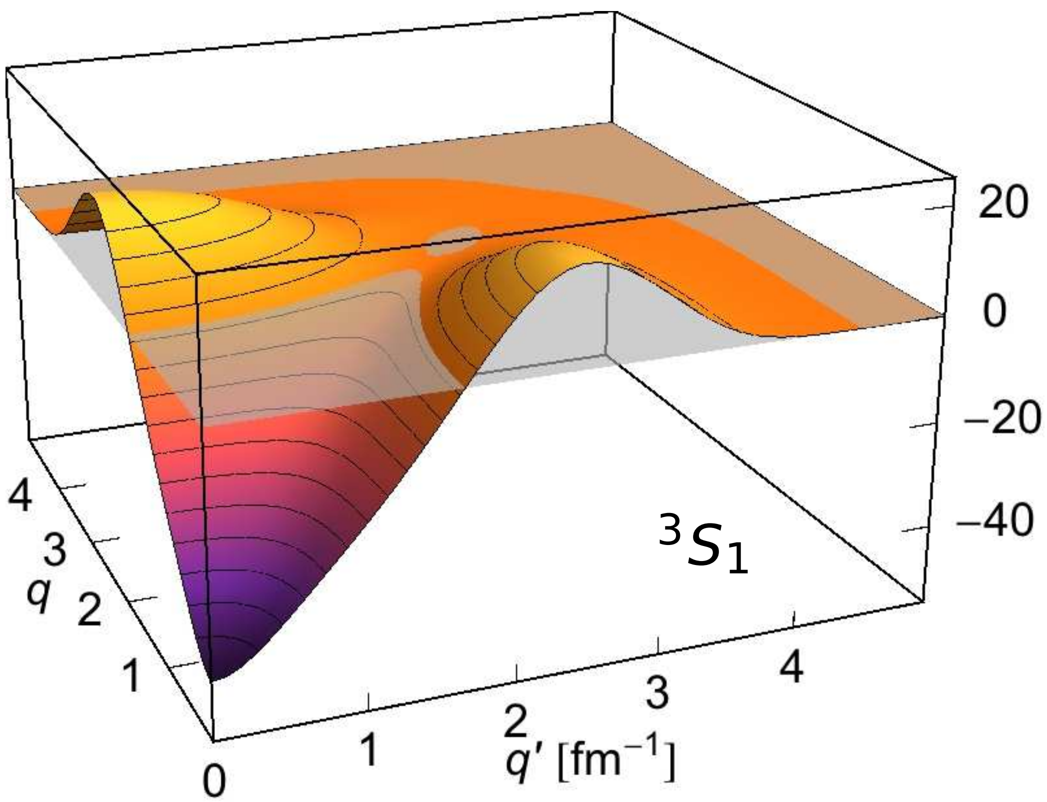
$J^\pi = 1^+, T = 0$

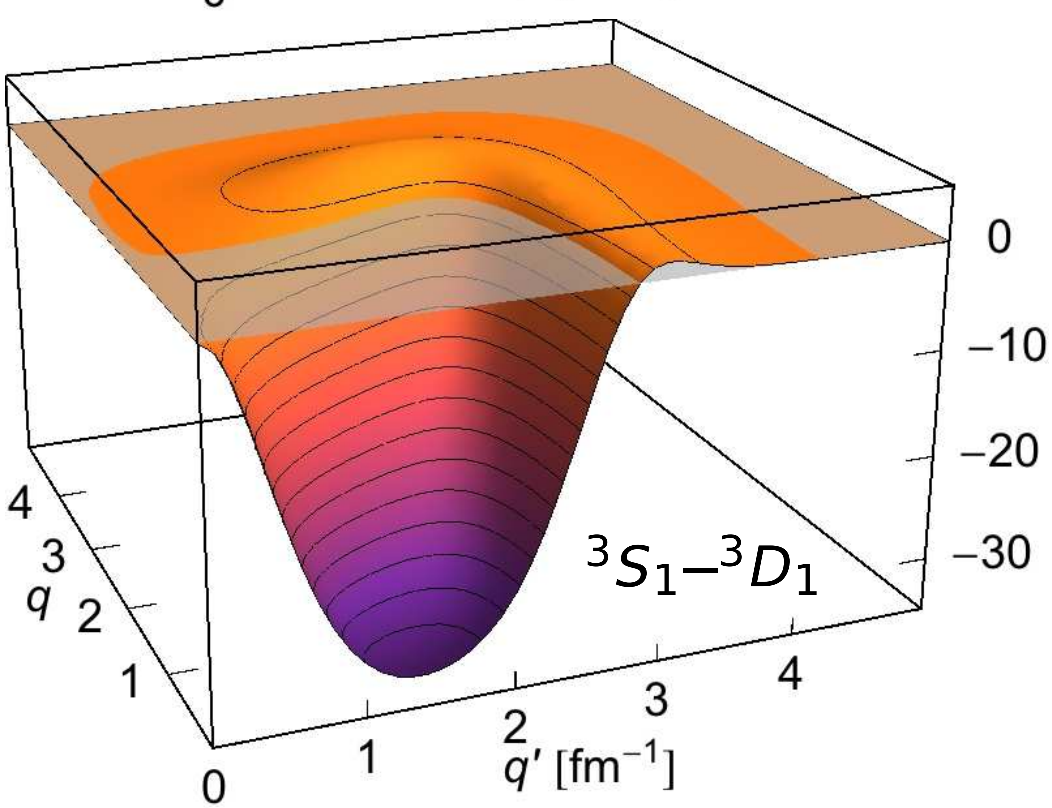
deuteron wave-function



SRG Evolution in Two-Body Space

momentum-space matrix elements





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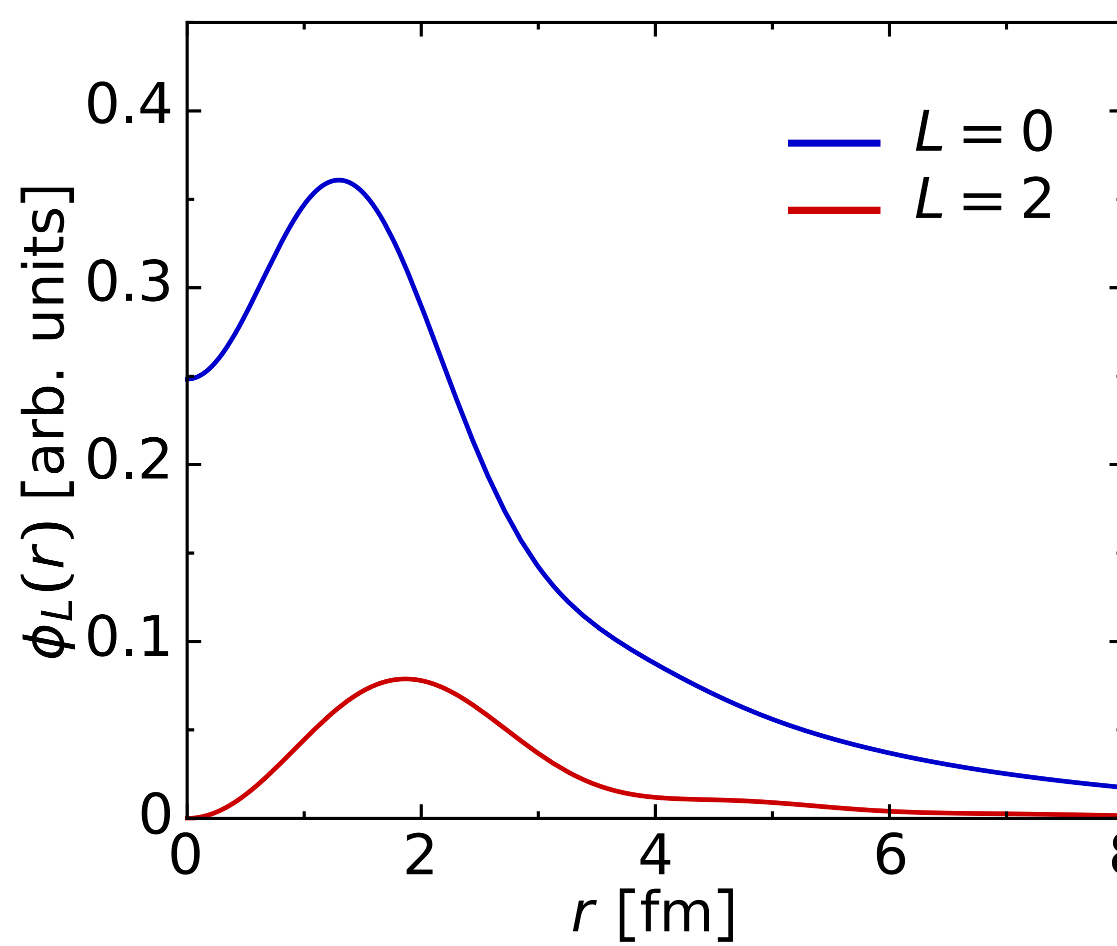
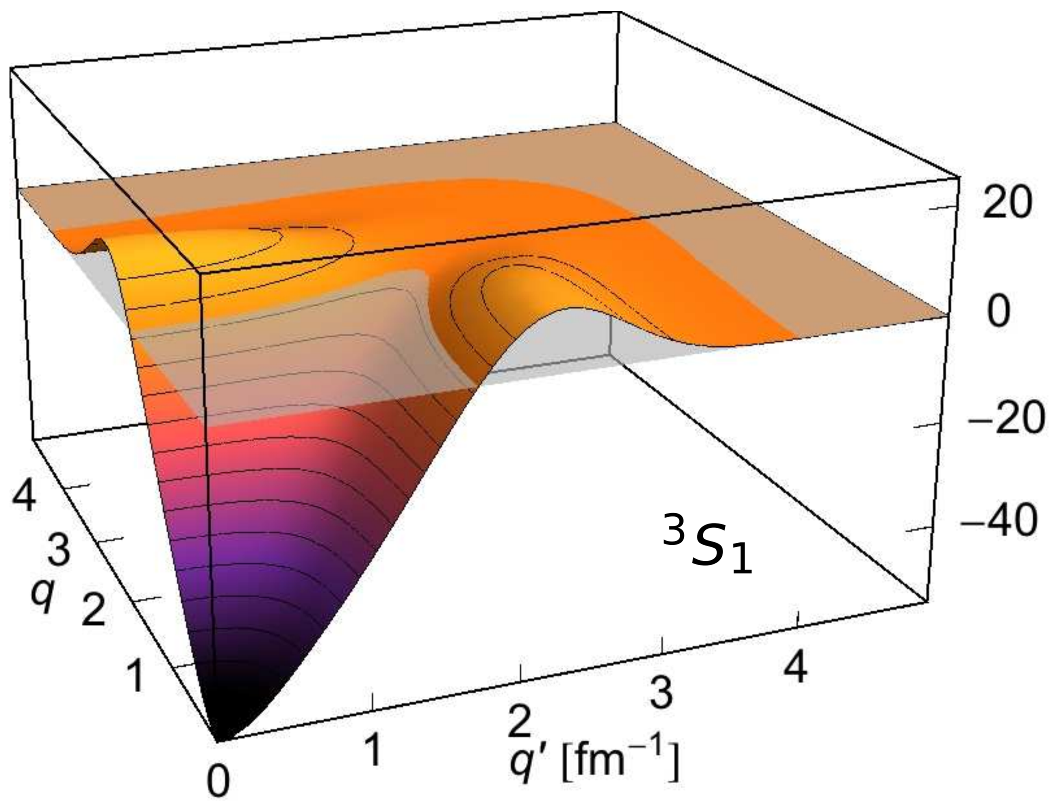
$J^\pi = 1^+, T = 0$

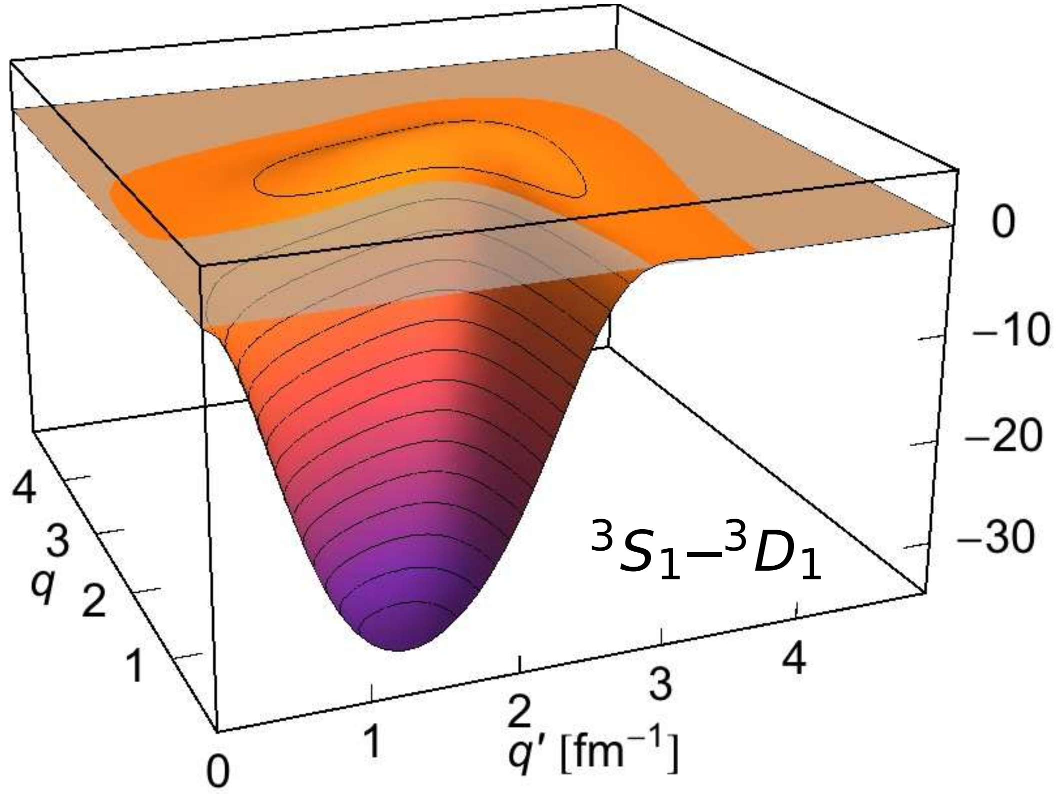
deuteron wave-function



SRG Evolution in Two-Body Space

momentum-space matrix elements



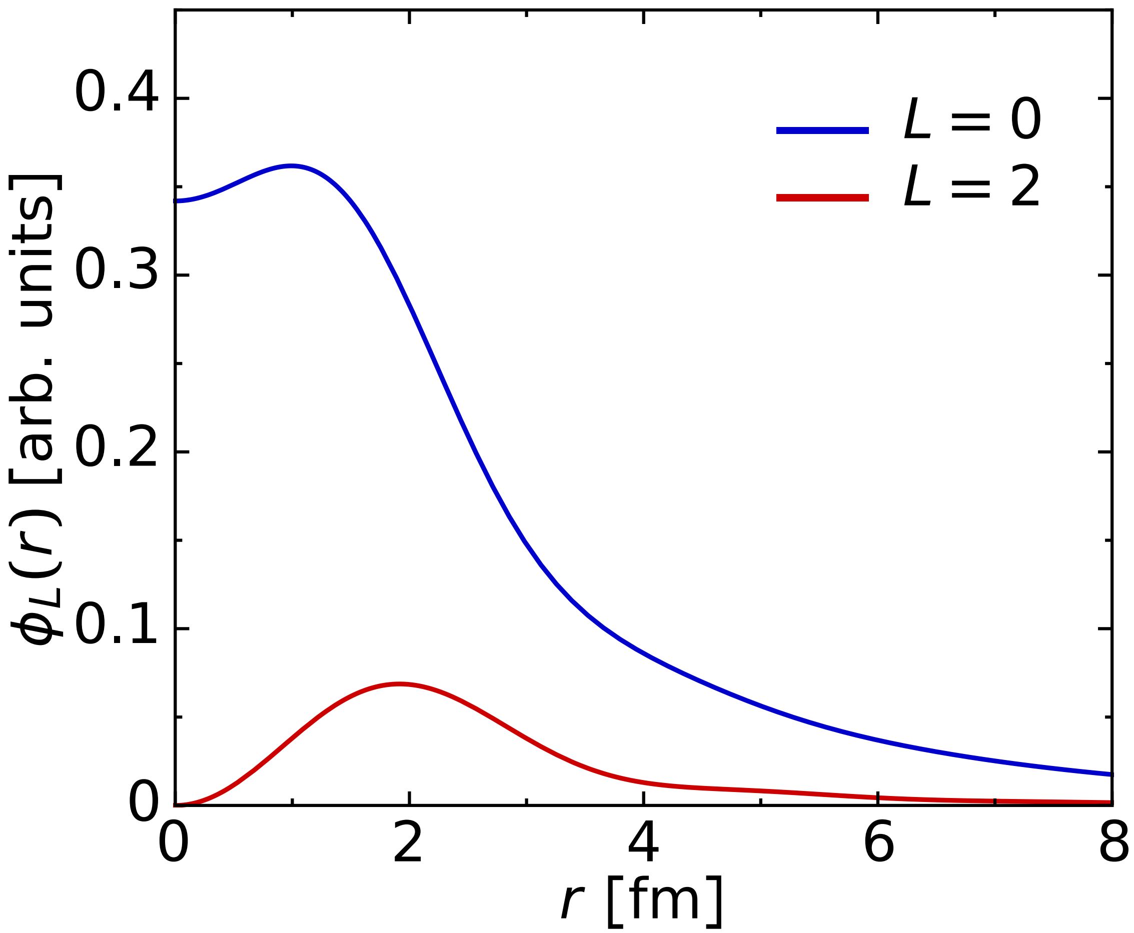


$\alpha = 0.020\,\text{fm}^4$

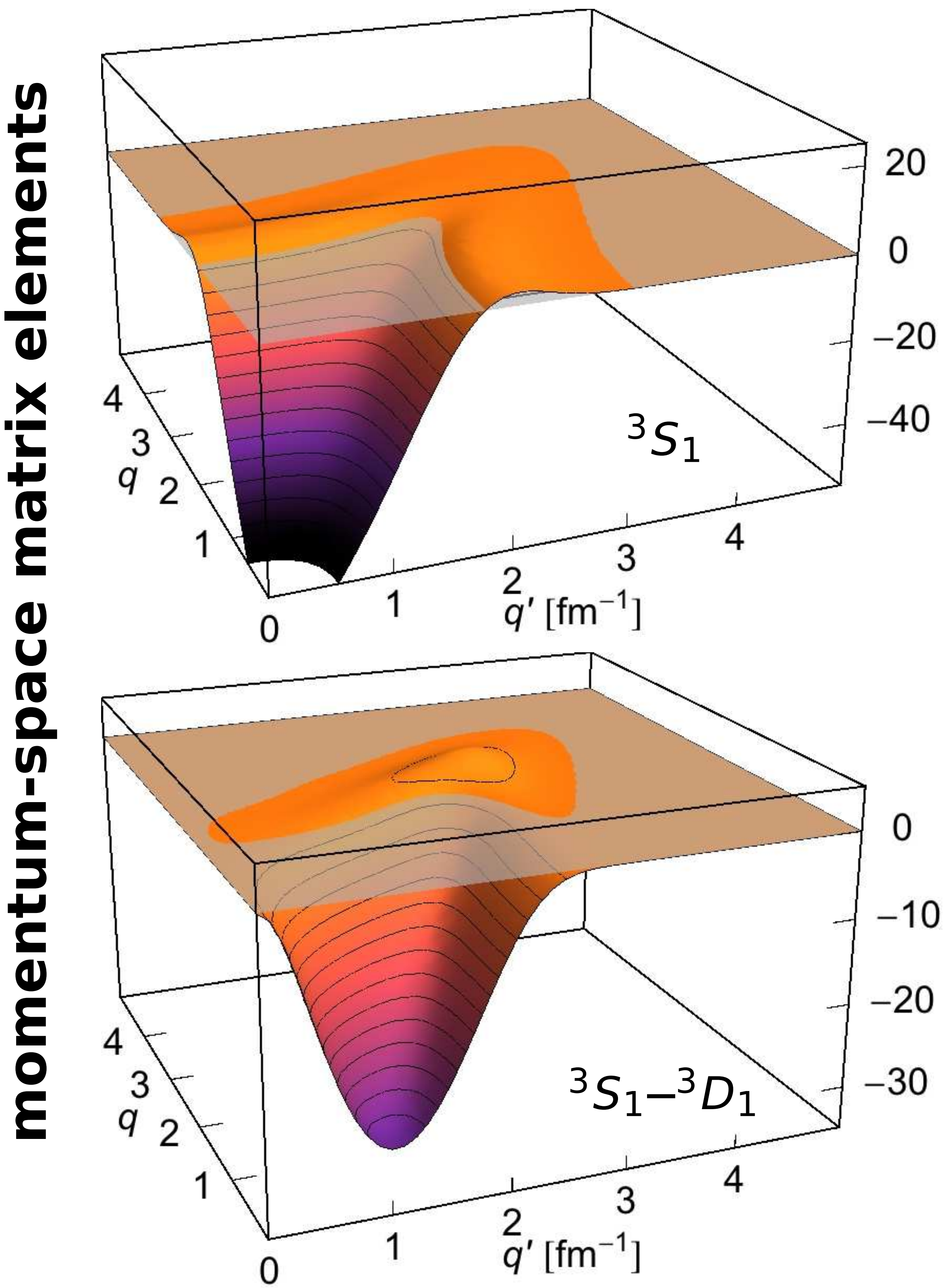
$\Lambda = 2.66\,\text{fm}^{-1}$

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

deuteron wave-function



SRG Evolution in Two-Body Space

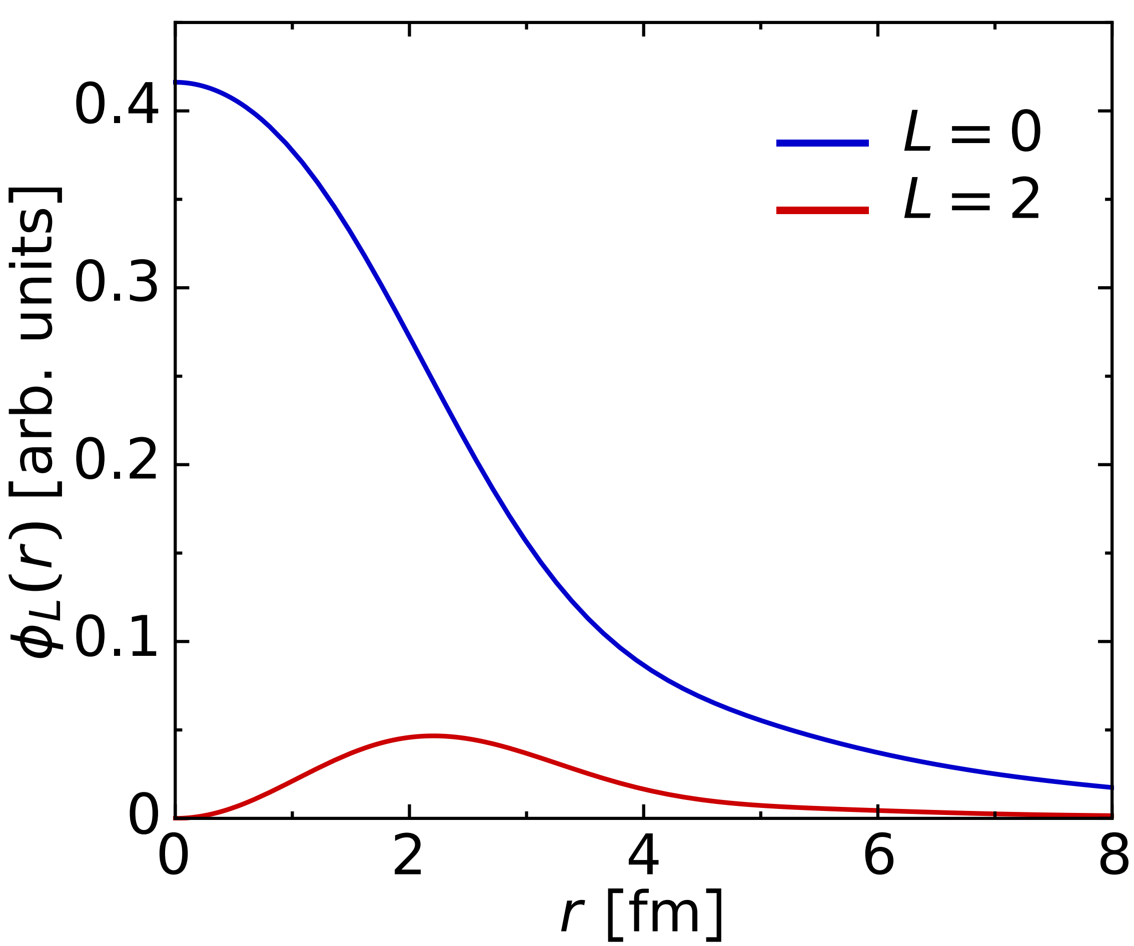


$\alpha = 0.080\,\mathrm{fm}^4$

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

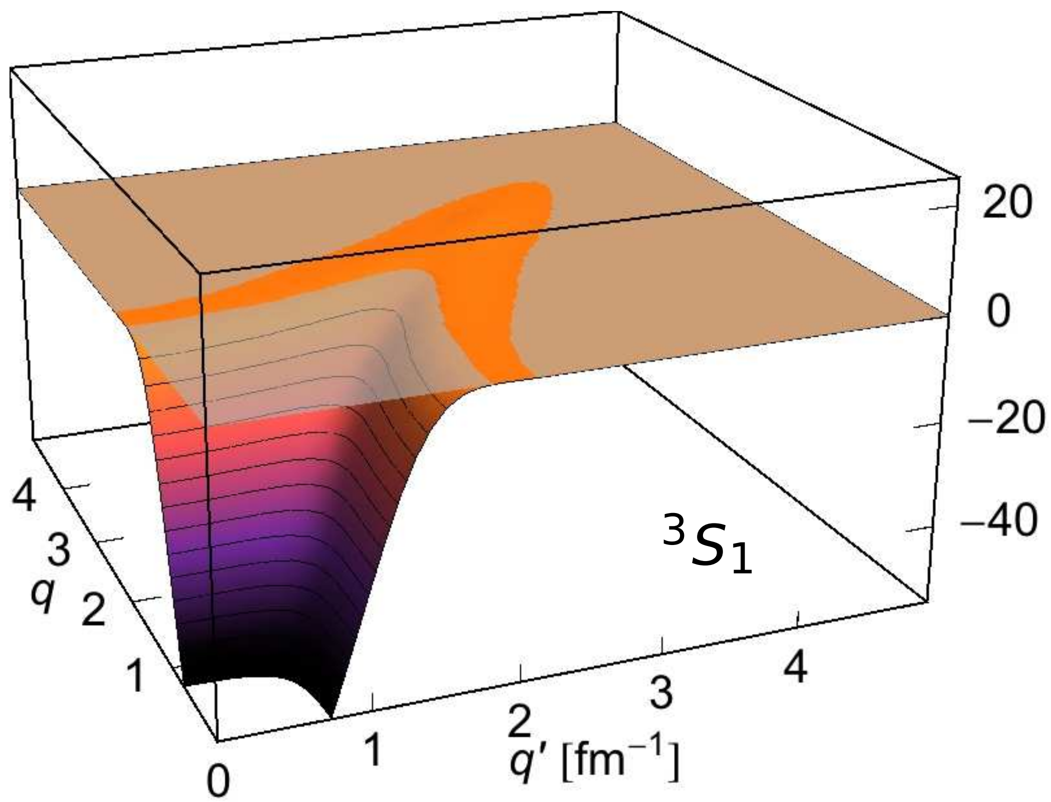
$J^\pi = 1^+, T = 0$

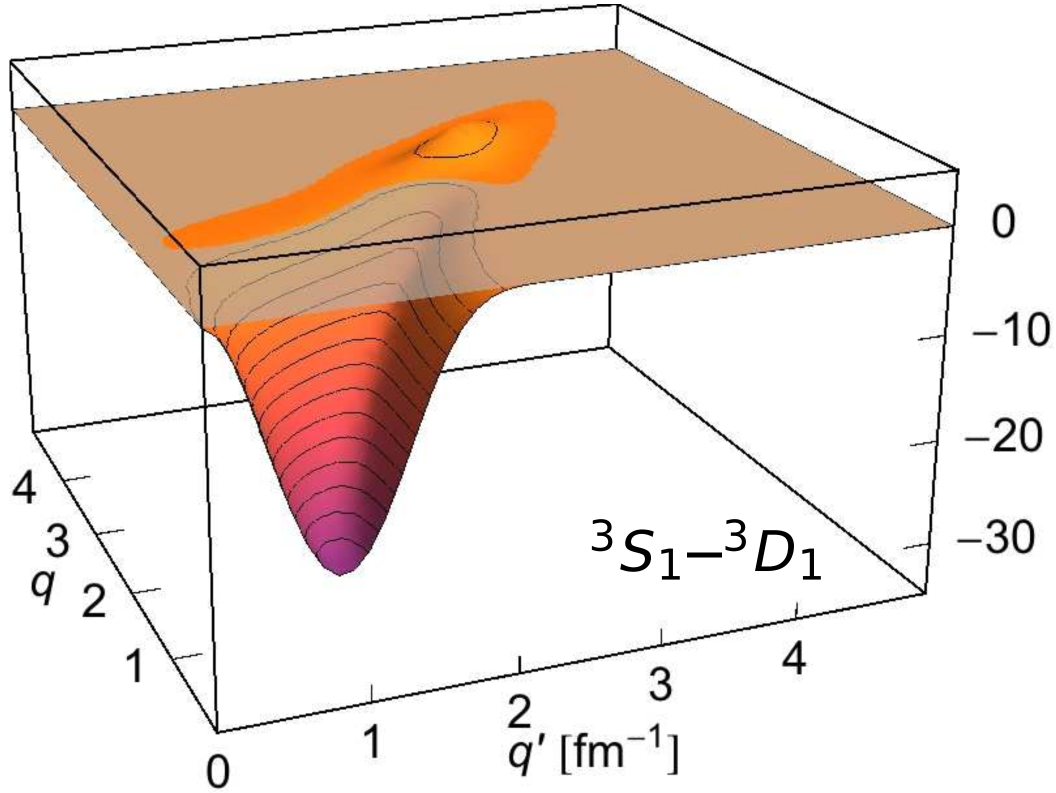
deuteron wave-function



SRG Evolution in Two-Body Space

momentum-space matrix elements





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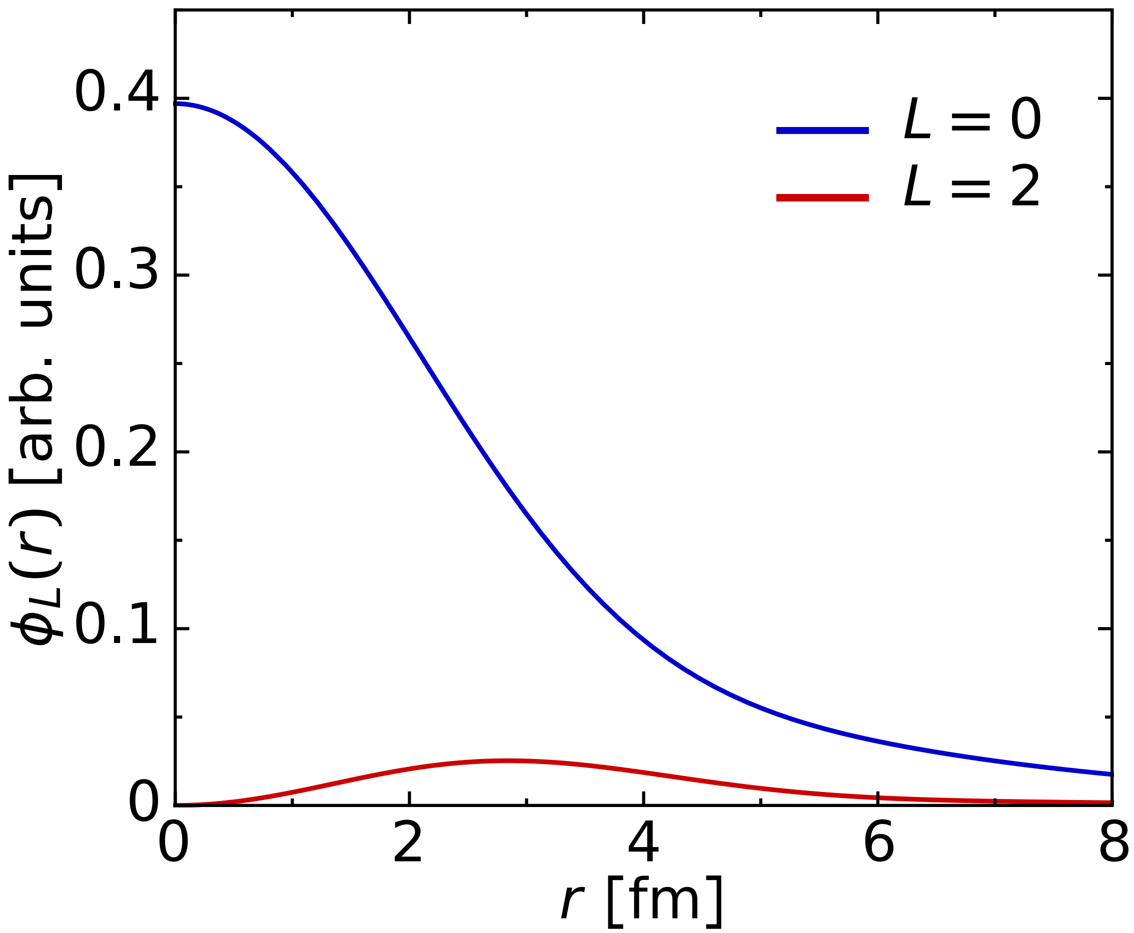
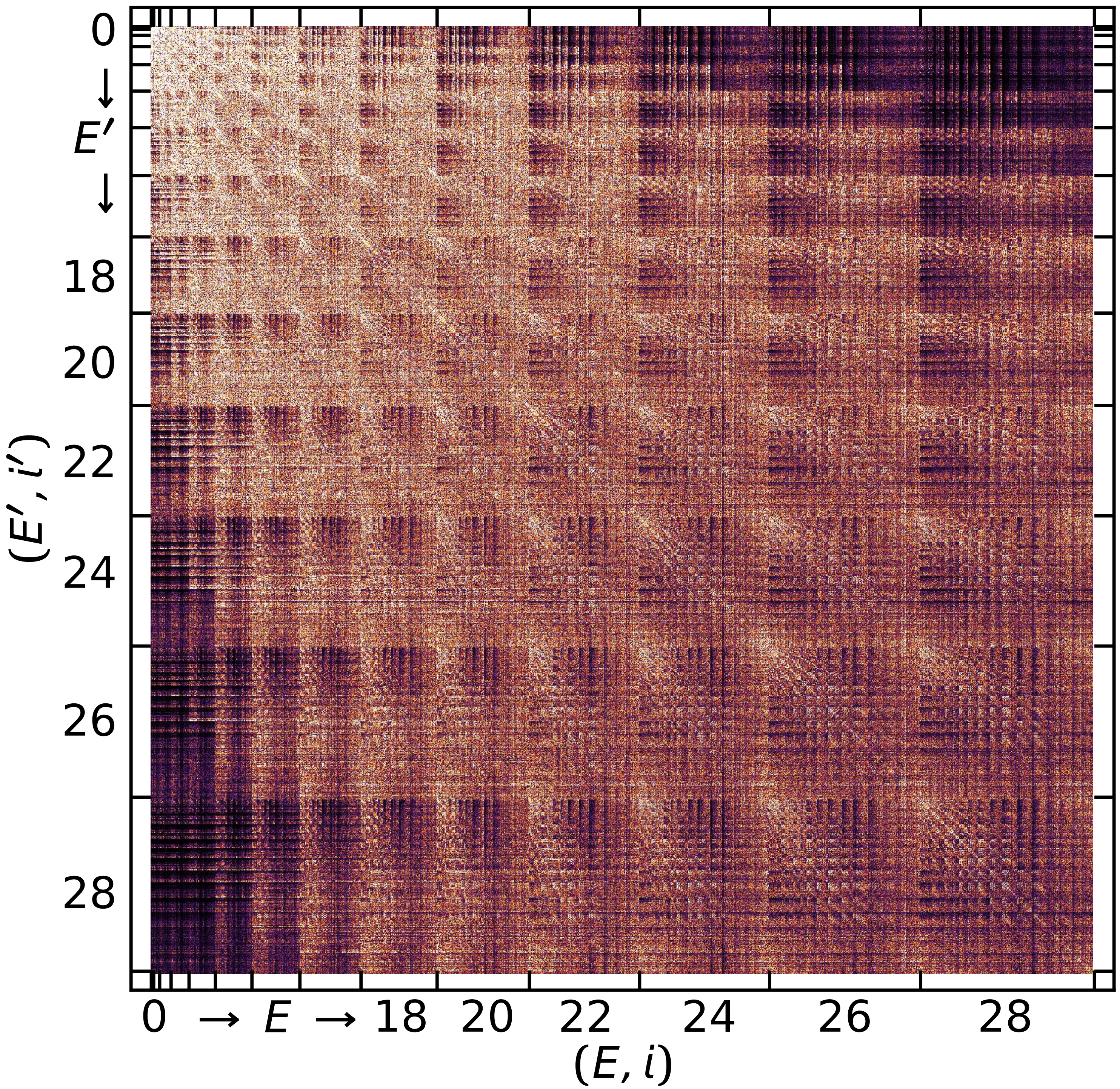


SRG Evolution in Three-Body Space

3B-Jacobi HO matrix elements

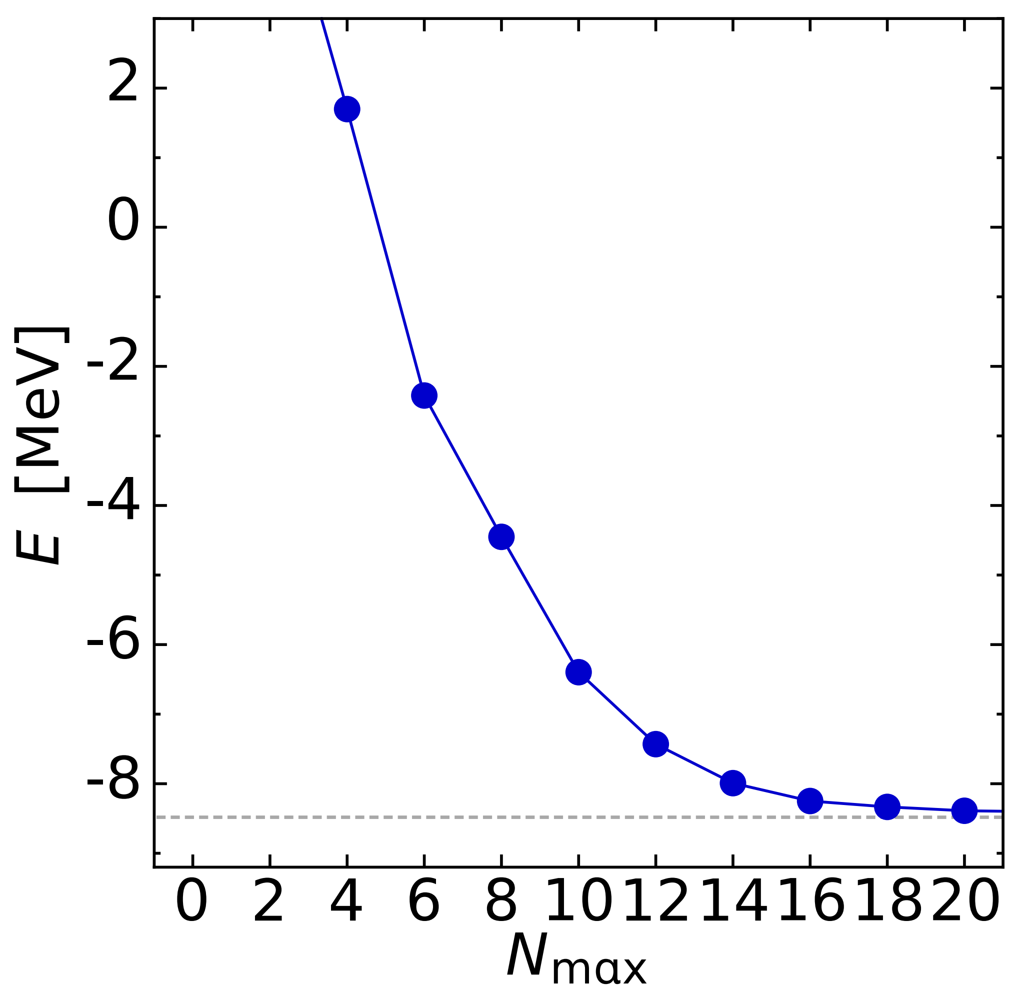


chiral NN+3N

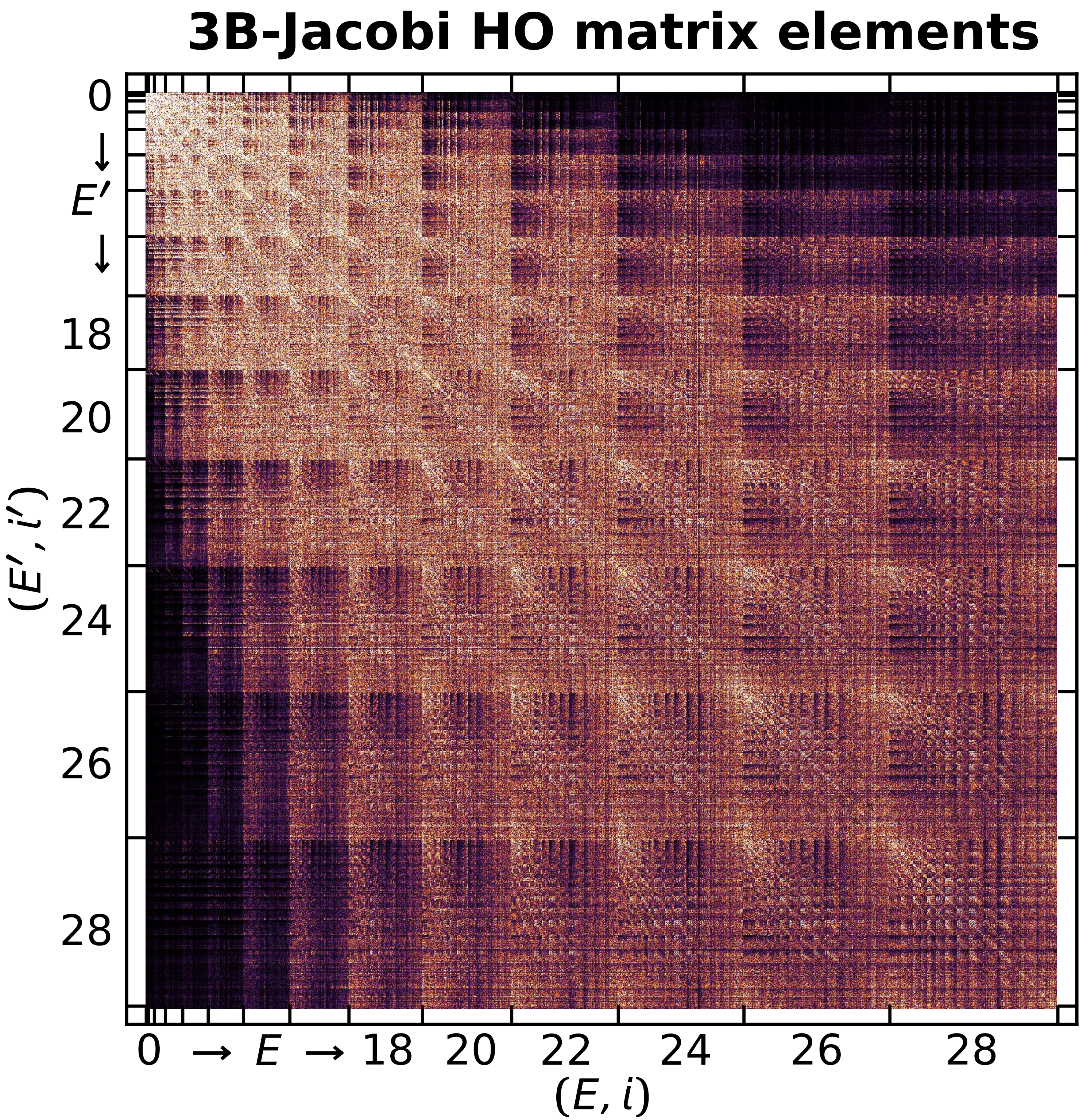
$N^3LO + N^2LO$, triton-fit, 500 MeV

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

NCSM ground state ^3H



SRG Evolution in Three-Body Space



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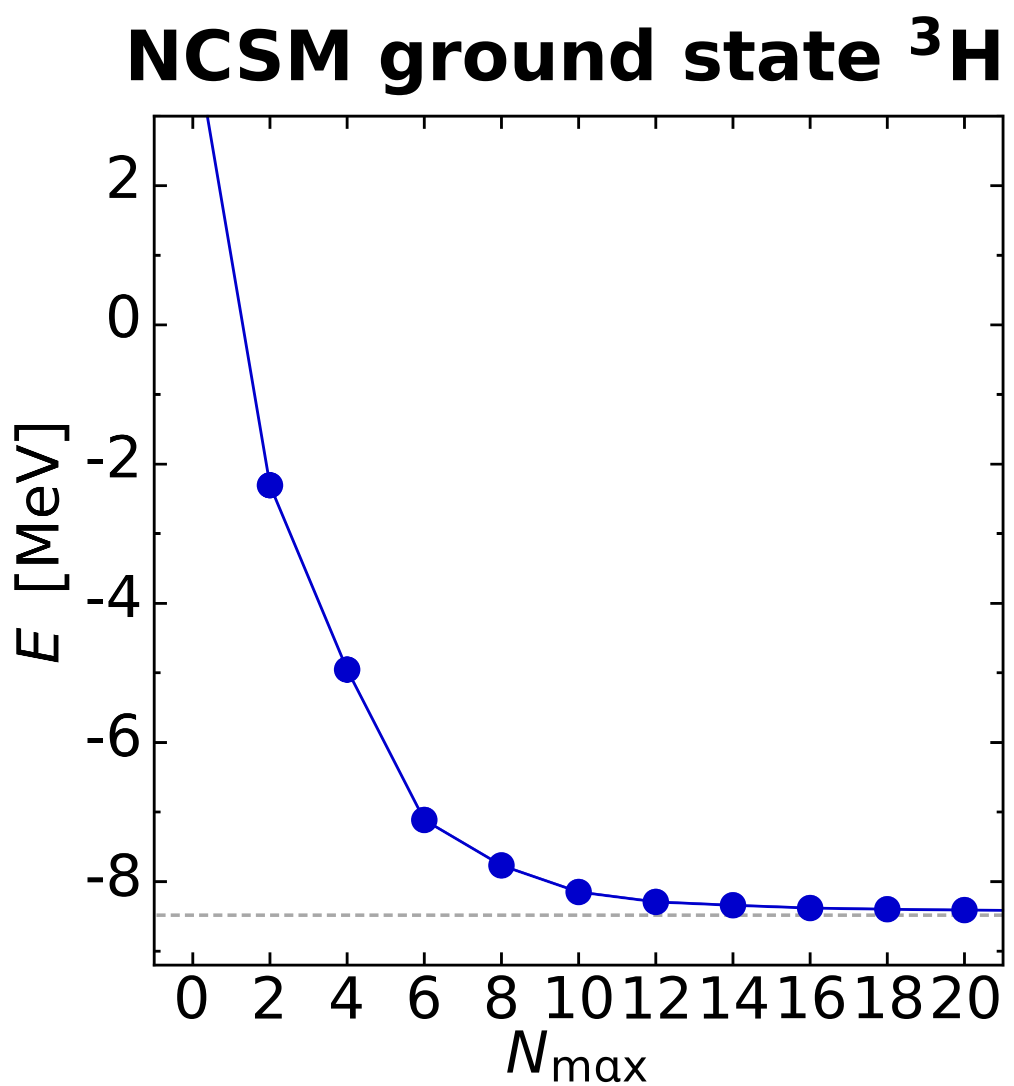
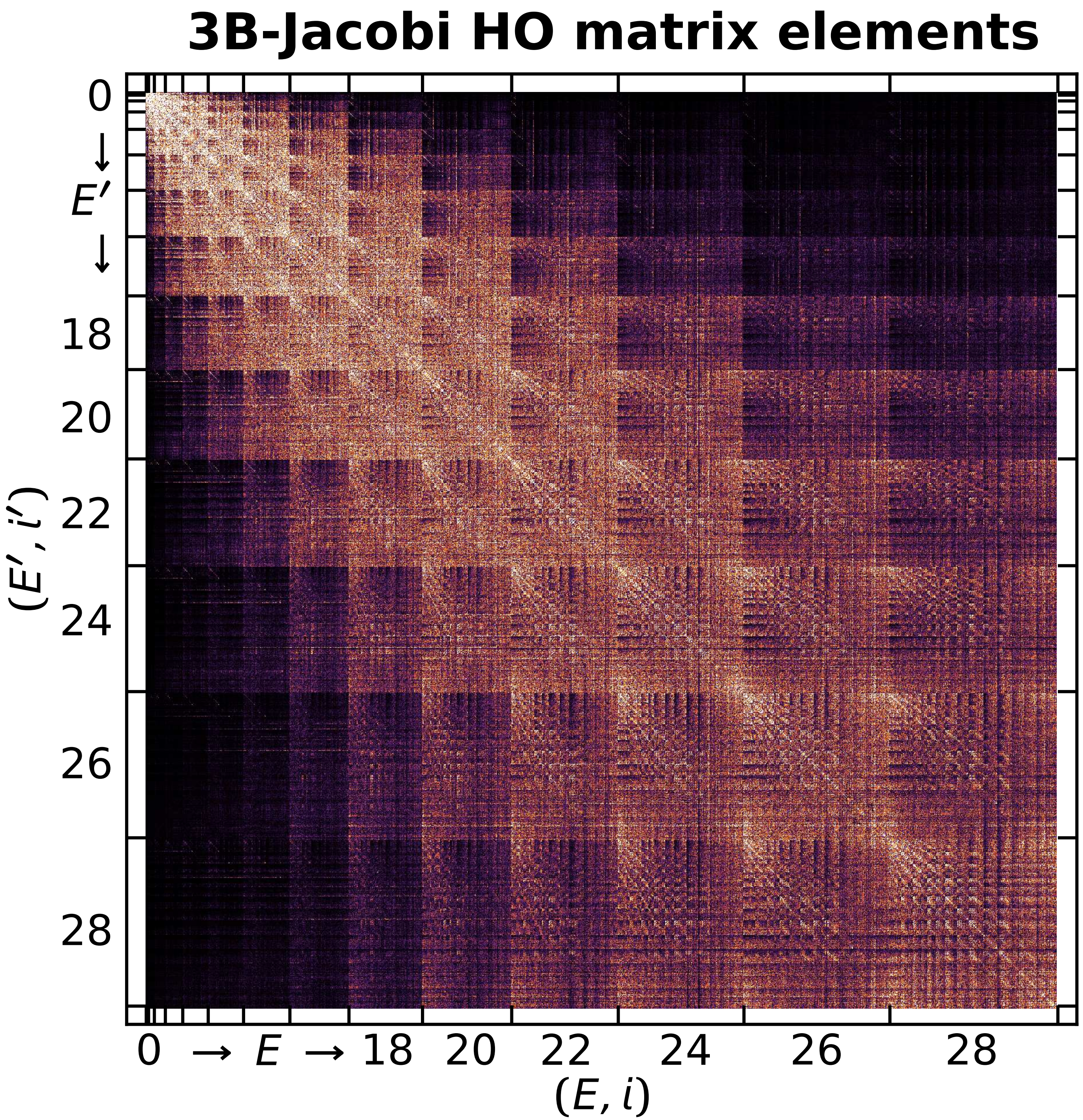
$J^\pi = \frac{1}{2}^+, T = \frac{1}{2}, \hbar\Omega = 28\,\text{MeV}$



SRG Evolution in Three-Body Space



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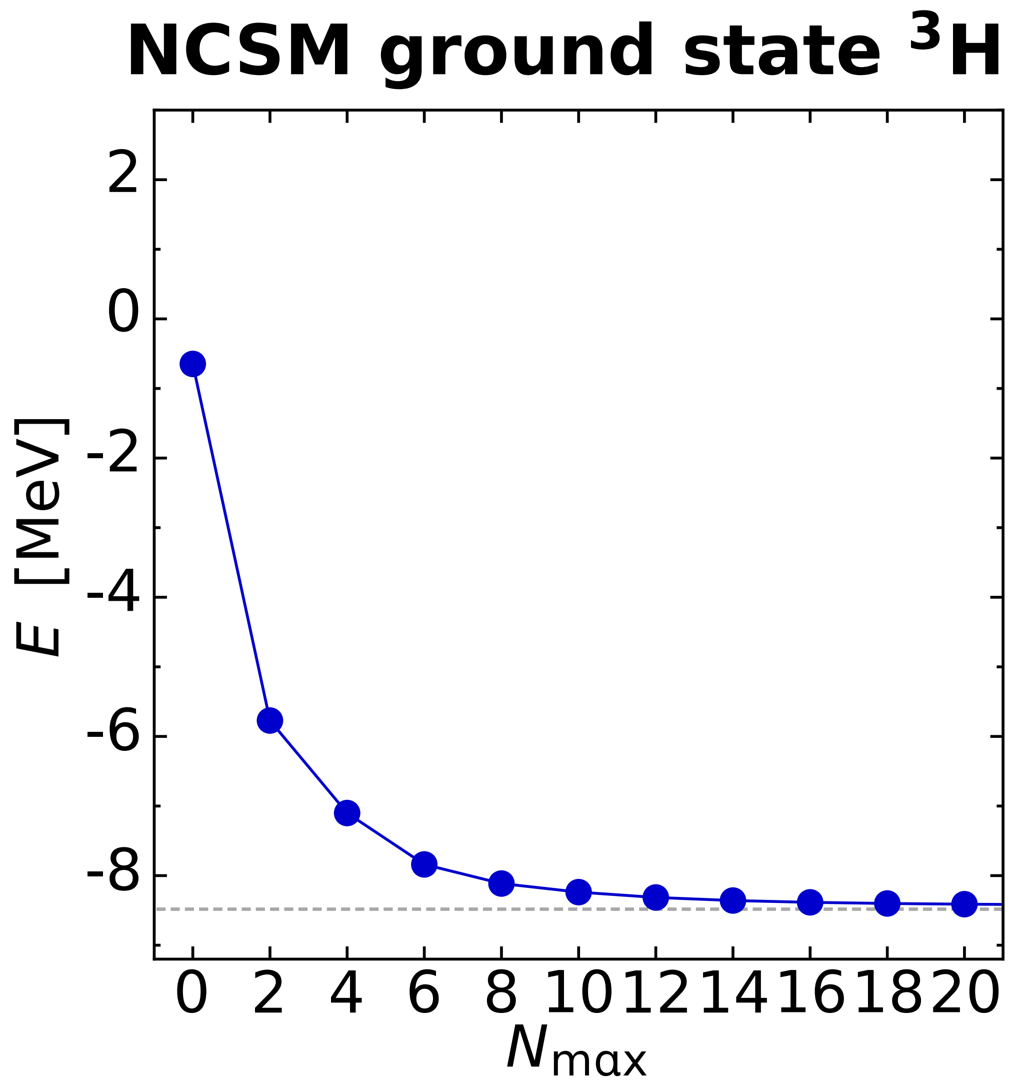
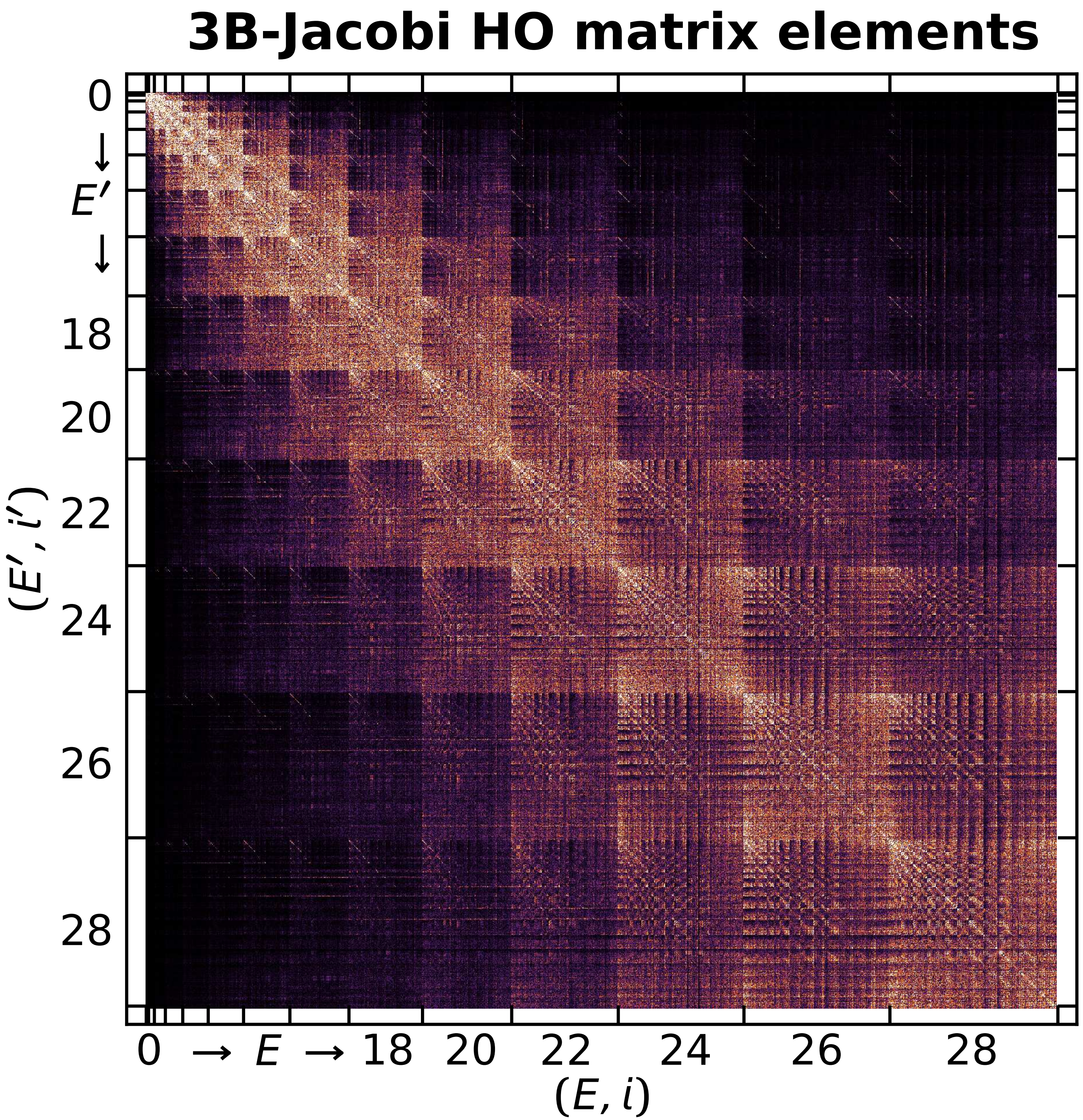


SRG Evolution in Three-Body Space



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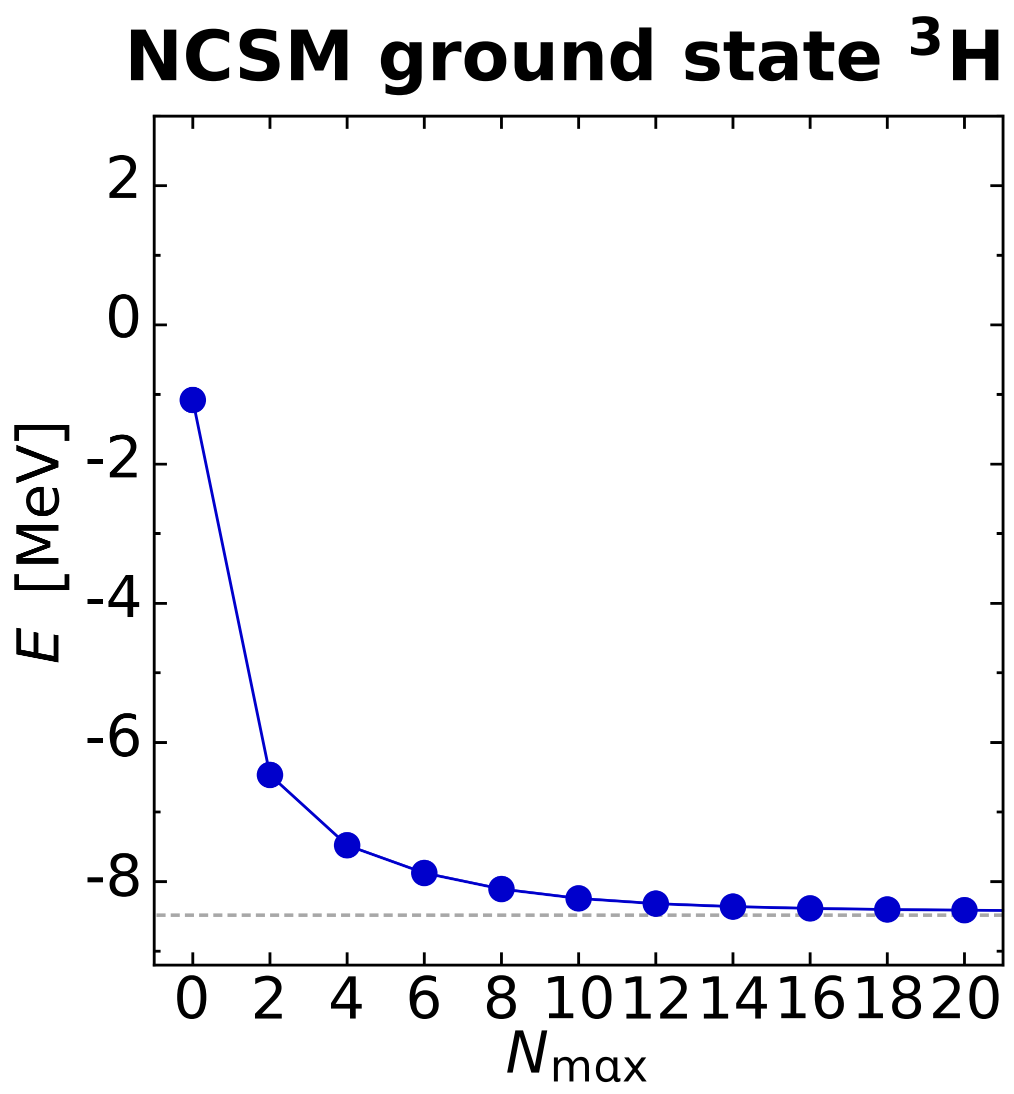


SRG Evolution in A-Body Space

- assume initial Hamiltonian and intrinsic kinetic energy are two-body operators written in second quantization

$$H_0 = \sum \dots a^\dagger a^\dagger a a\,, \qquad T_{int} = T - T_{cm} = \sum \dots a^\dagger a^\dagger a a$$

- perform **single evolution step** $\Delta\alpha$ in Fock-space operator form

$$\begin{aligned} H_{\Delta\alpha} &= H_0 + \Delta\alpha \left[[T_{int}, H_0], H_0 \right] \\ &= \sum \dots a^\dagger a^\dagger a a + \Delta\alpha \sum \dots \left[[a^\dagger a^\dagger a a, a^\dagger a^\dagger a a], a^\dagger a^\dagger a a \right] \\ &= \sum \dots a^\dagger a^\dagger a a + \Delta\alpha \sum \dots a^\dagger a^\dagger a^\dagger a^\dagger a a a a + \Delta\alpha \sum \dots a^\dagger a^\dagger a^\dagger a a a + \dots \end{aligned}$$

- SRG evolution **induces many-body contributions** in the Hamiltonian

- induced many-body contributions are the price to pay for the pre-diagonalization of the Hamiltonian

SRG Evolution in A-Body Space

- decompose evolved Hamiltonian into irreducible ***n*-body contributions $H_\alpha^{[n]}$**

$$H_\alpha = H_\alpha^{[1]} + H_\alpha^{[2]} + H_\alpha^{[3]} + H_\alpha^{[4]} + \cdots$$

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

- flow-parameter variation provides **diagnostic tool** to assess neglected contributions of higher particle ranks

SRG-Evolved Hamiltonians

NN_{only} : use initial NN, keep evolved NN

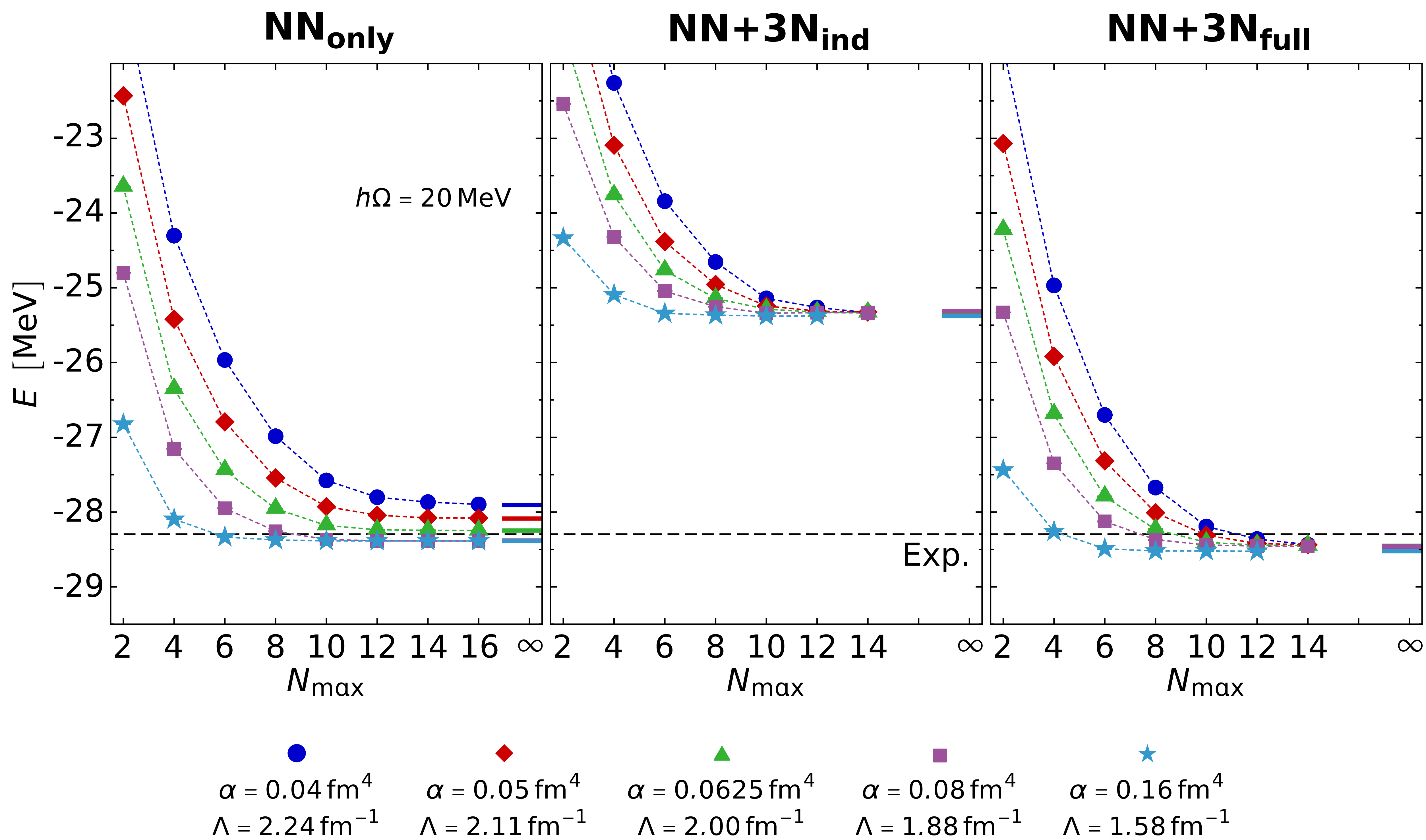
$NN+3N_{ind}$: use initial NN, keep evolved NN+3N

$NN+3N_{full}$: use initial NN+3N, keep evolved NN+3N

$NN+3N_{full}+4N_{ind}$: use initial NN+3N, keep evolved NN+3N+4N

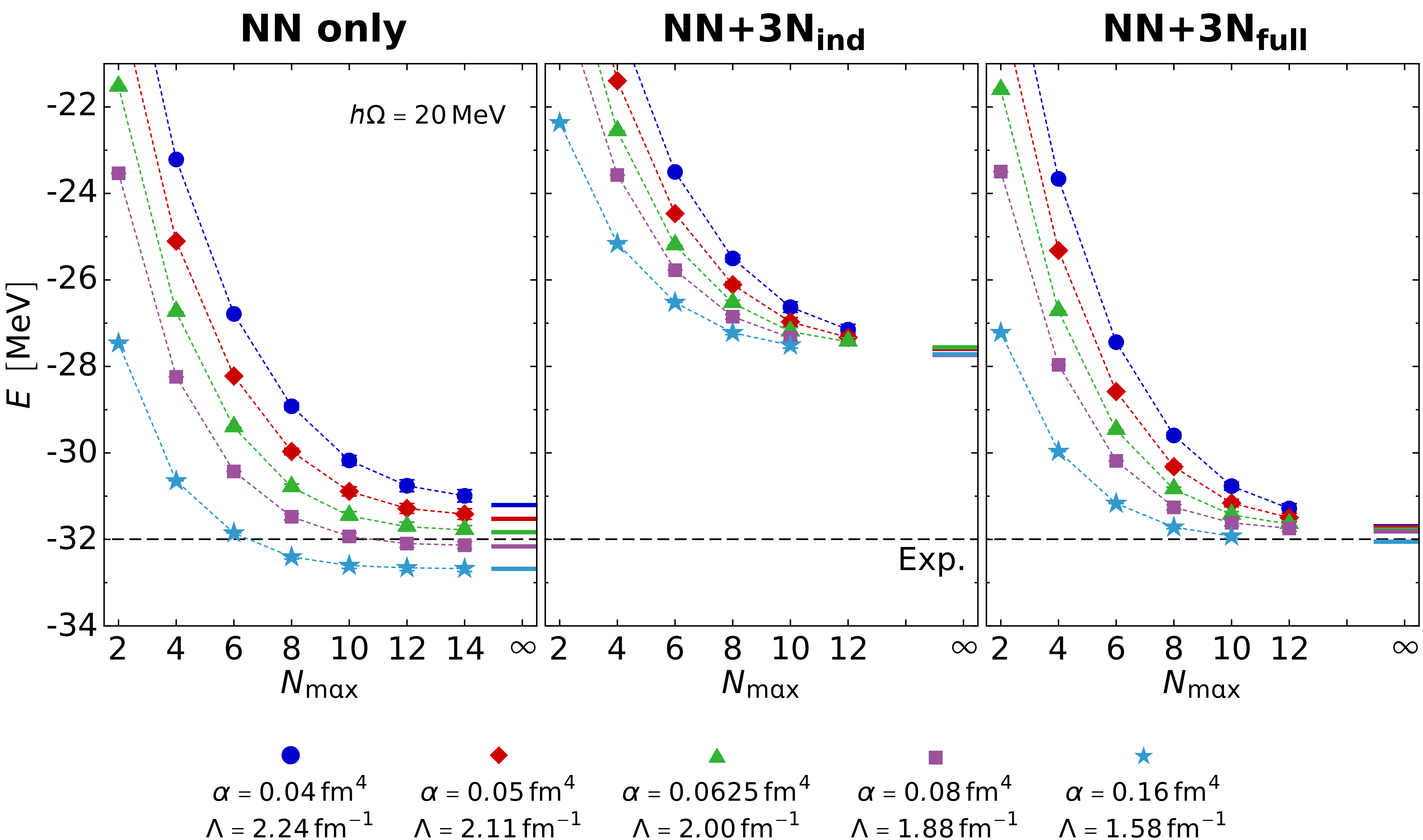
^{4}He: Ground-State Energy

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



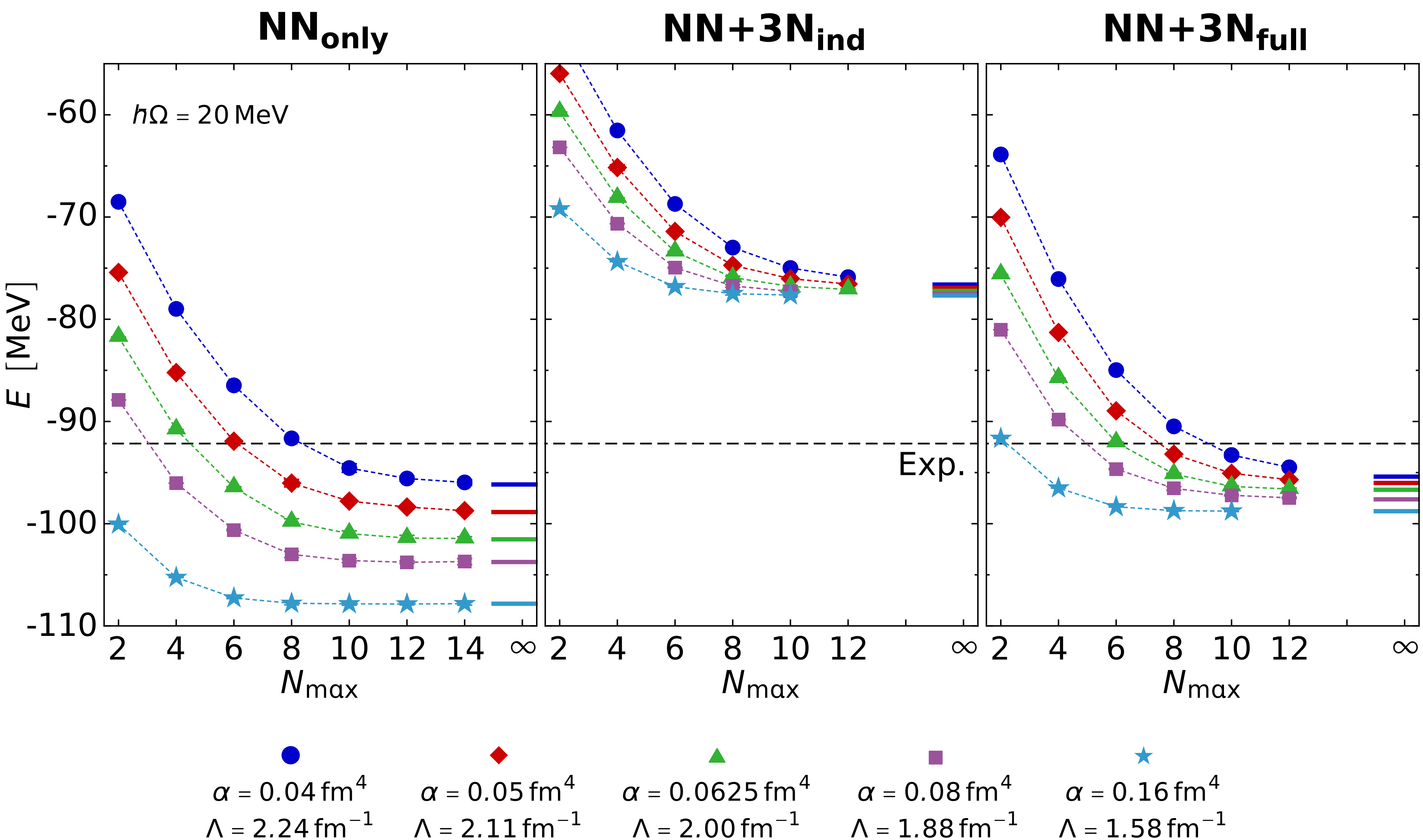
^{7}Li: Ground-State Energy

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



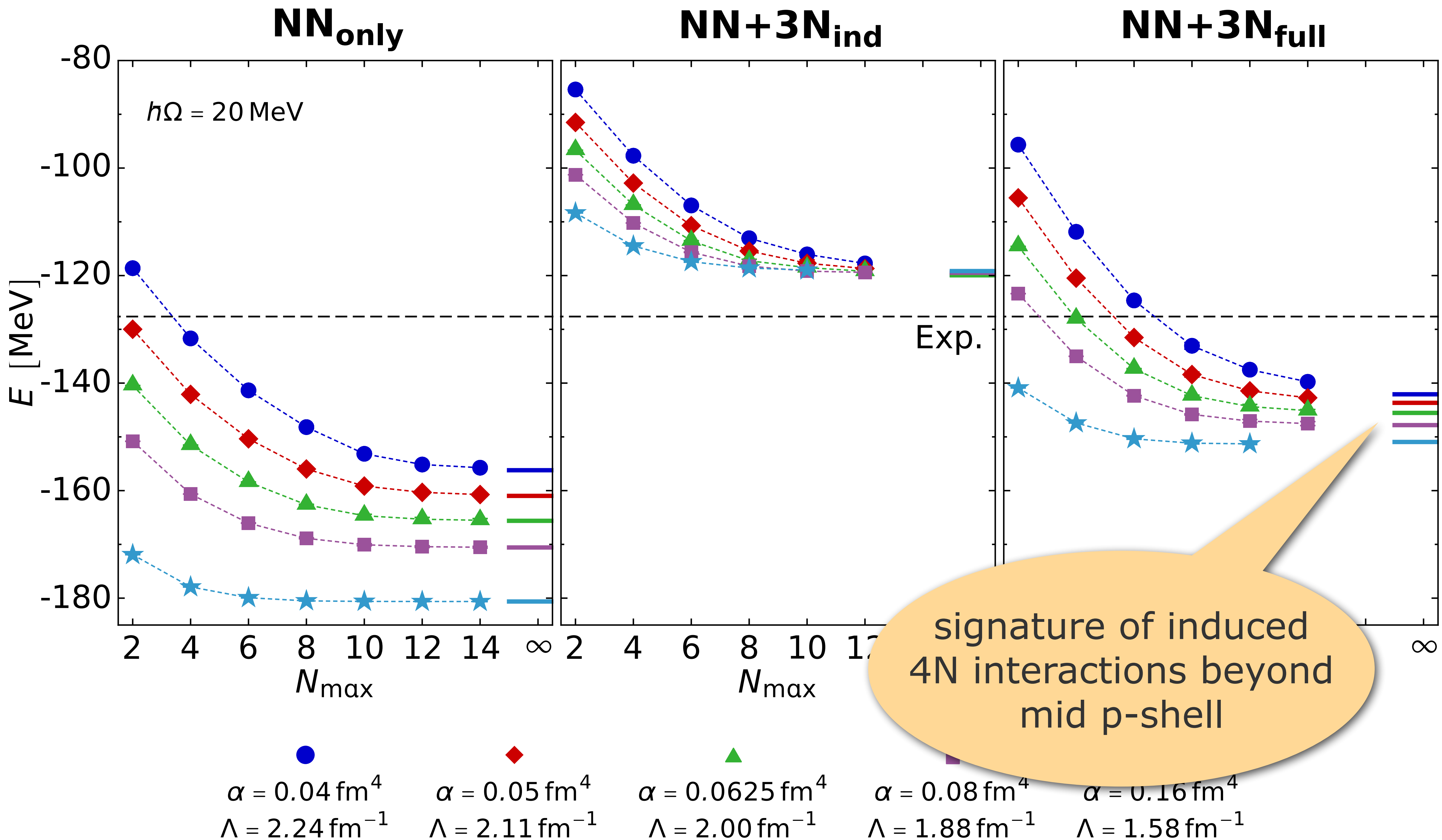
^{12}C: Ground-State Energy

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

Ab Initio Approaches to Light Nuclei

Lecture 3: Light Nuclei

Robert Roth

TECHNISCHE UNIVERSITÄT DARMSTADT

Overview

- **Lecture 1: Fundamentals**

  Prelude • Many-Body Quantum Mechanics

- **Lecture 1’: Nuclear Hamiltonian**

  Nuclear Interactions • Matrix Elements

- **Lecture 2: Correlations**

  Two-Body Problem • Unitary Transformations • Similarity Renormalization Group

- **Lecture 3: Light Nuclei**

  Configuration Interaction • No-Core Shell Model • Importance Truncation

- **Lecture 4: Beyond Light Nuclei**

  Coupled-Cluster Theory • In-Medium Similarity Renormalization Group

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

- smooth transition from approximation to ab initio calculation…

Configuration Interaction Approaches

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

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

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

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

➜ **problem session yesterday**

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

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

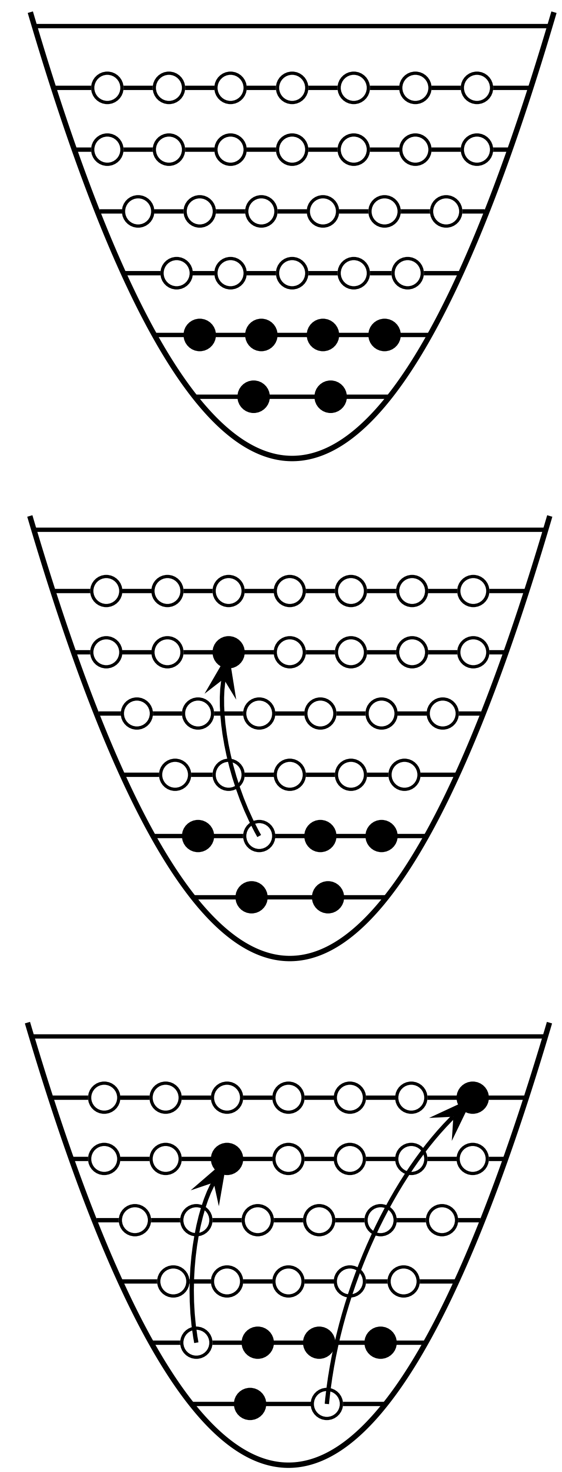
- **Hylleraas-Undheim theorem**: all states of the spectrum have a monotonously decreasing energy with increasing model space dimension

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

No-Core Shell Model

No-Core Shell Model (NCSM)

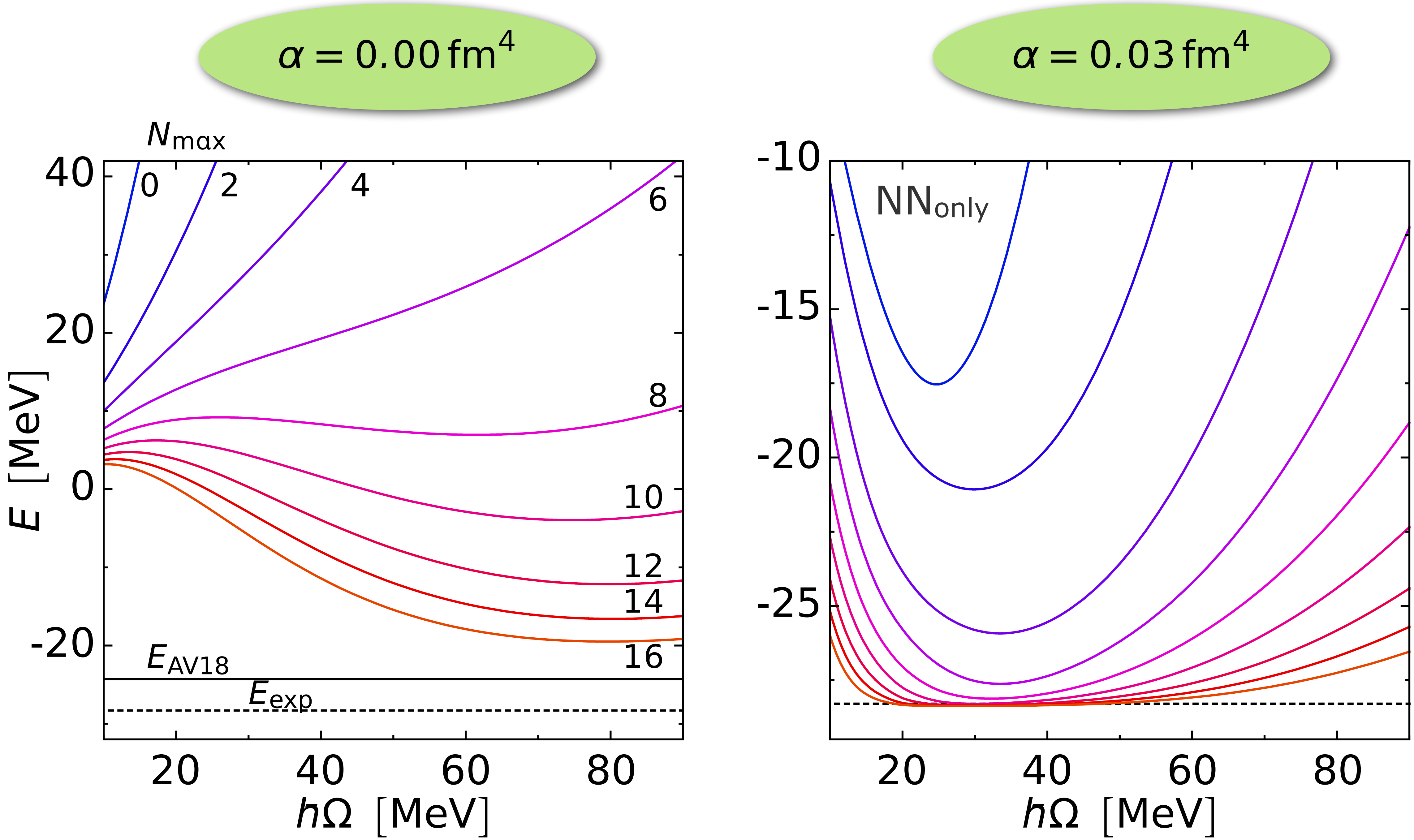
- NCSM is a special case of a CI approach:
  - single-particle basis is a **spherical HO basis**
  - truncation in terms of the total **number of HO excitation quanta N_{max}** in the many-body states



- **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}

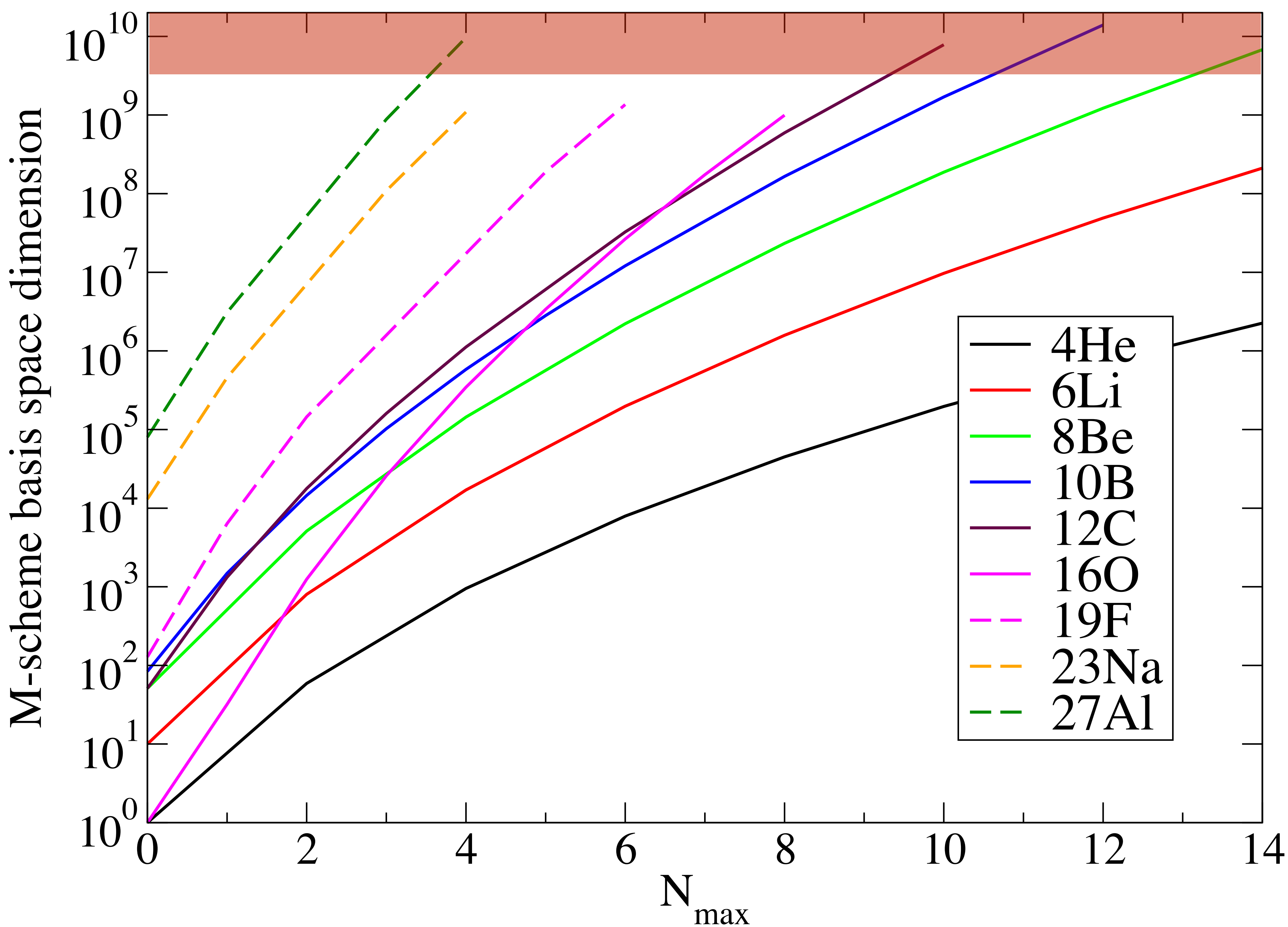
^{4}He: NCSM Convergence

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



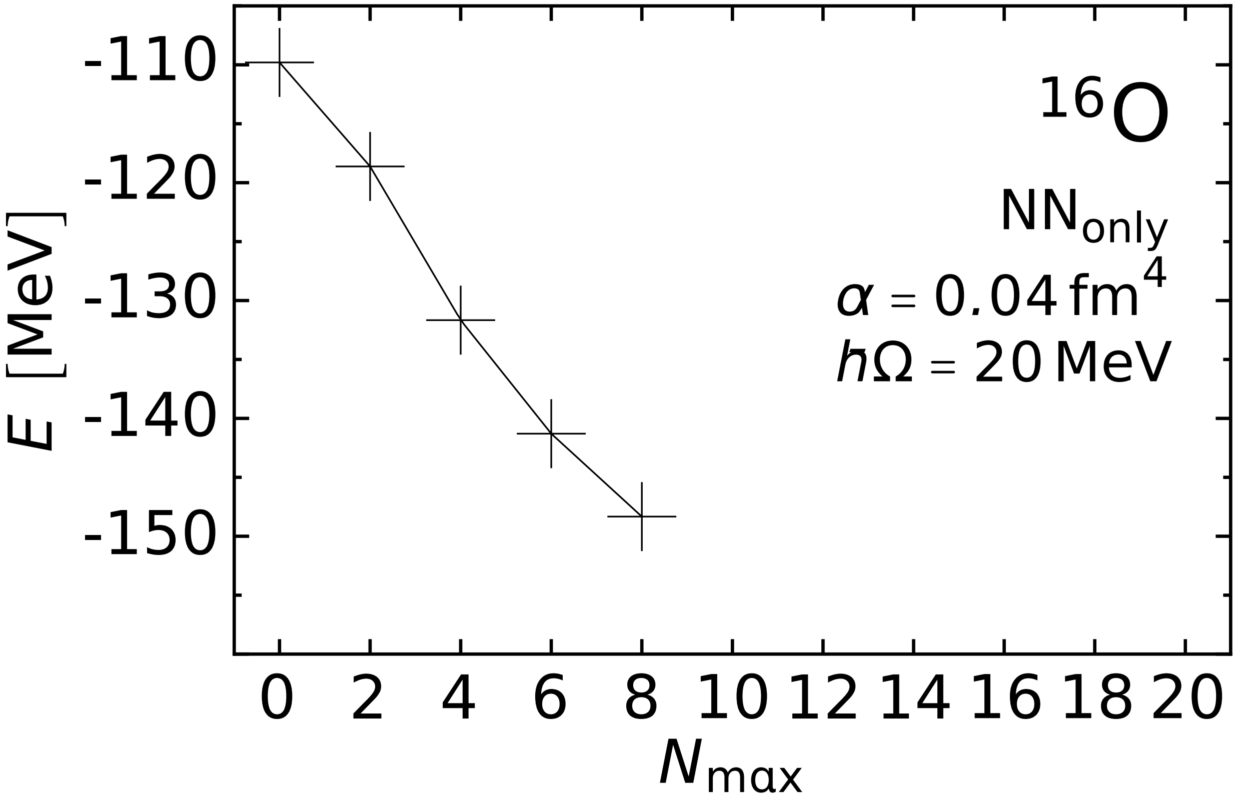
NCSM Basis Dimension

P. Maris



Importance Truncation

- **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 $D > 10^{10}$

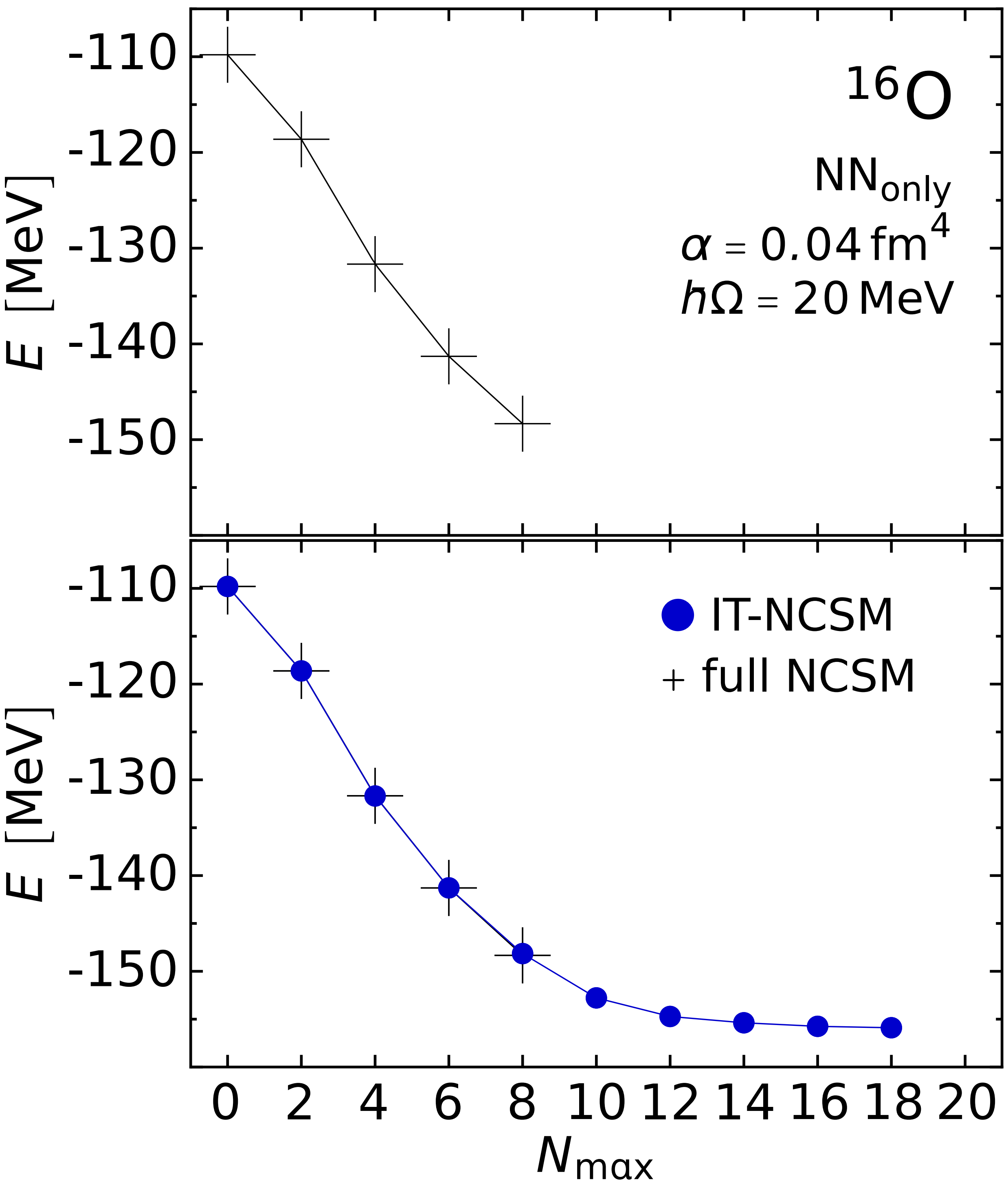


Importance Truncation

- **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 $D > 10^{10}$

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 $\mathcal{M}_{\text{ref}}$

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

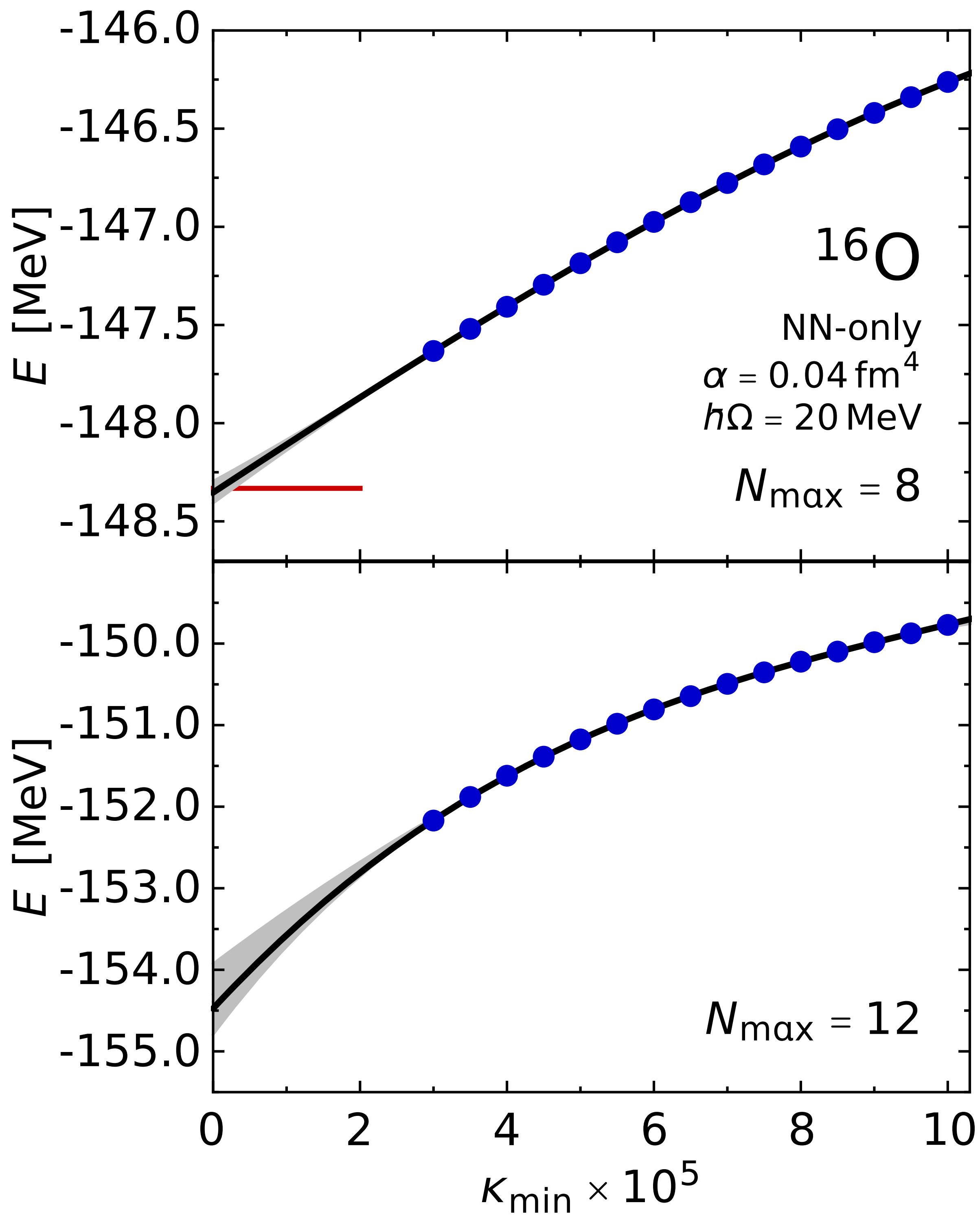
- **measure the importance** of individual basis state $|\Phi_{\nu}\rangle \notin \mathcal{M}_{\text{ref}}$ via first-order multiconfigurational perturbation theory

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

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

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

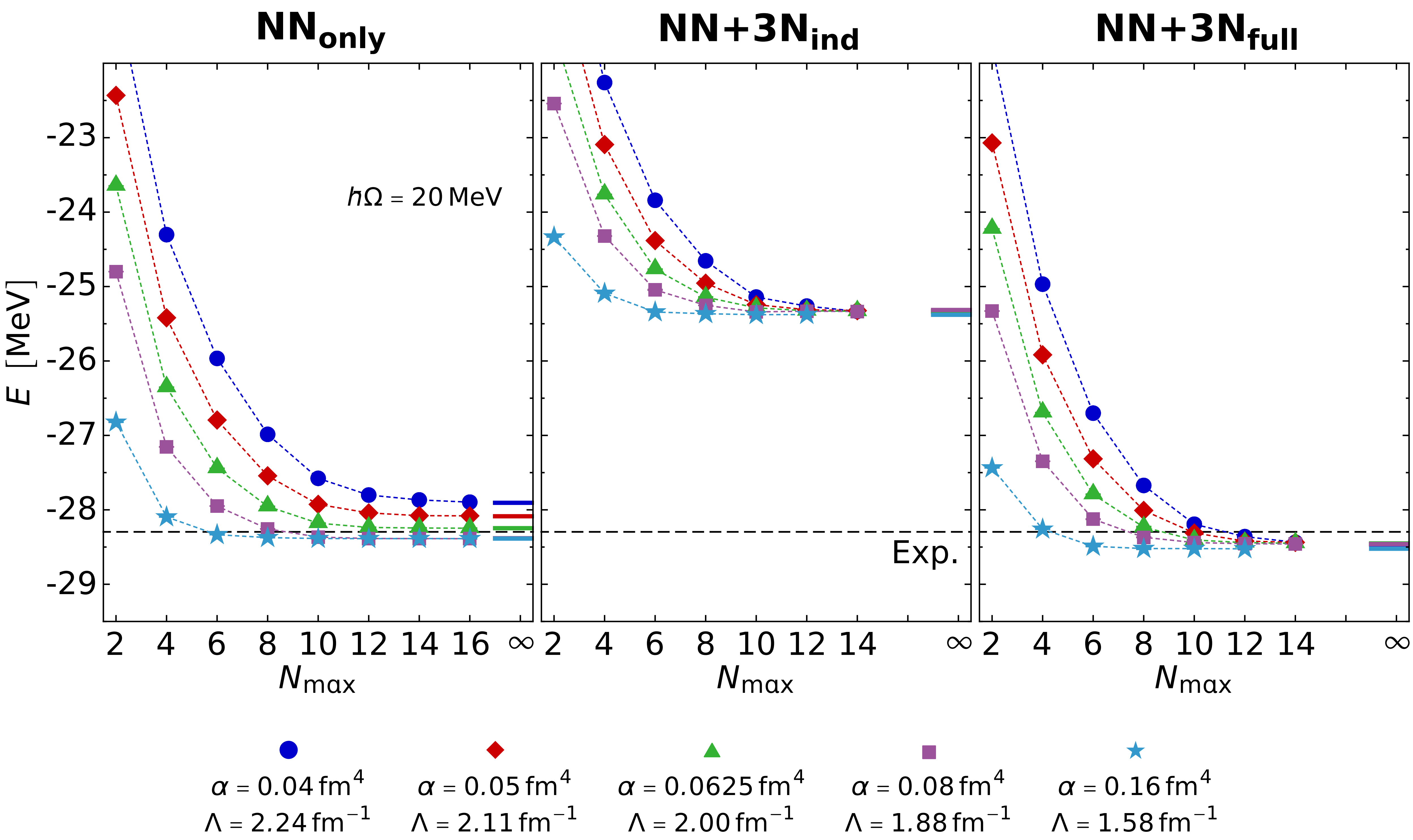
Threshold Extrapolation



- repeat calculations for a **sequence of importance thresholds** κ_{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

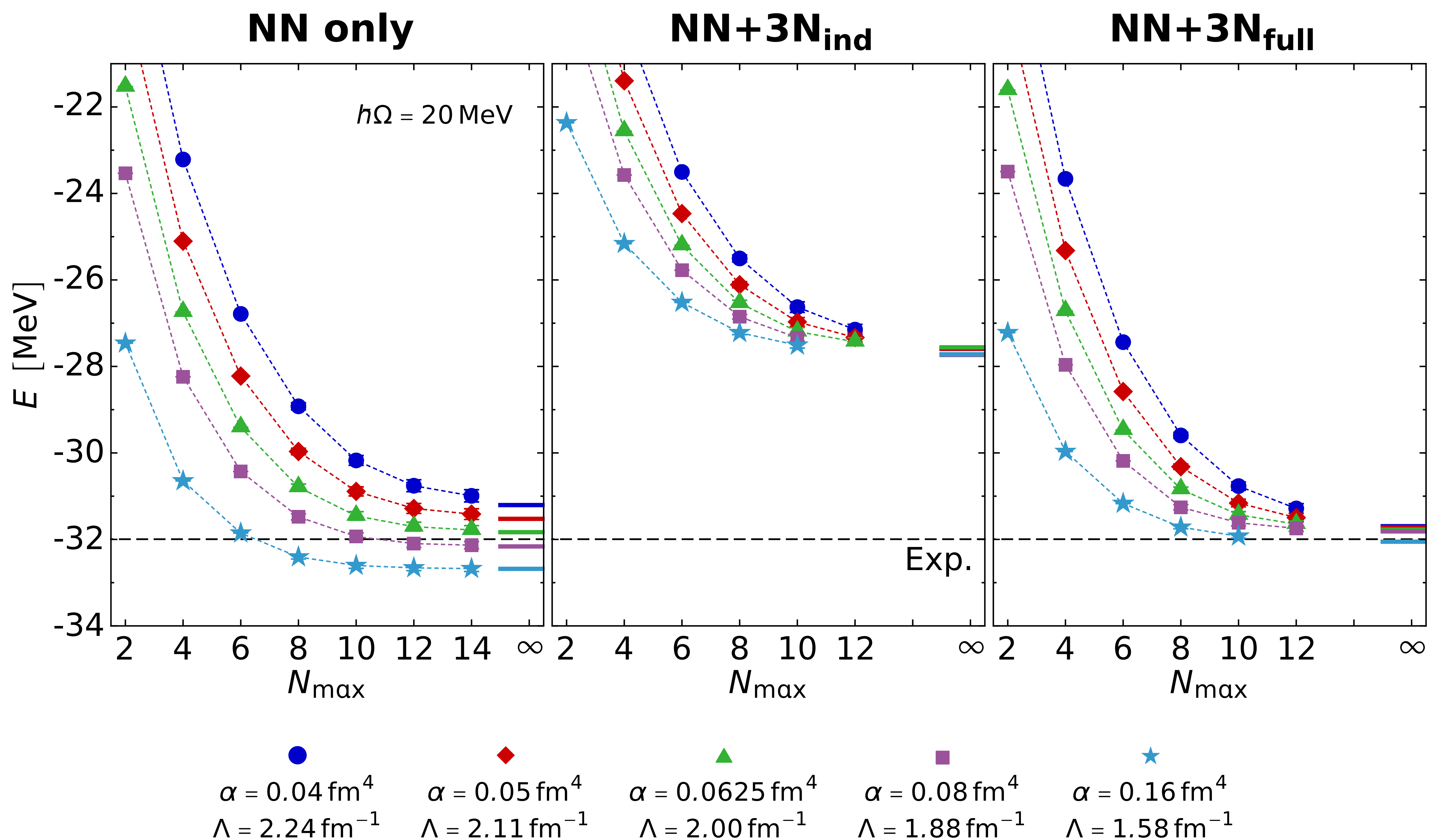
^{4}He: Ground-State Energy

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



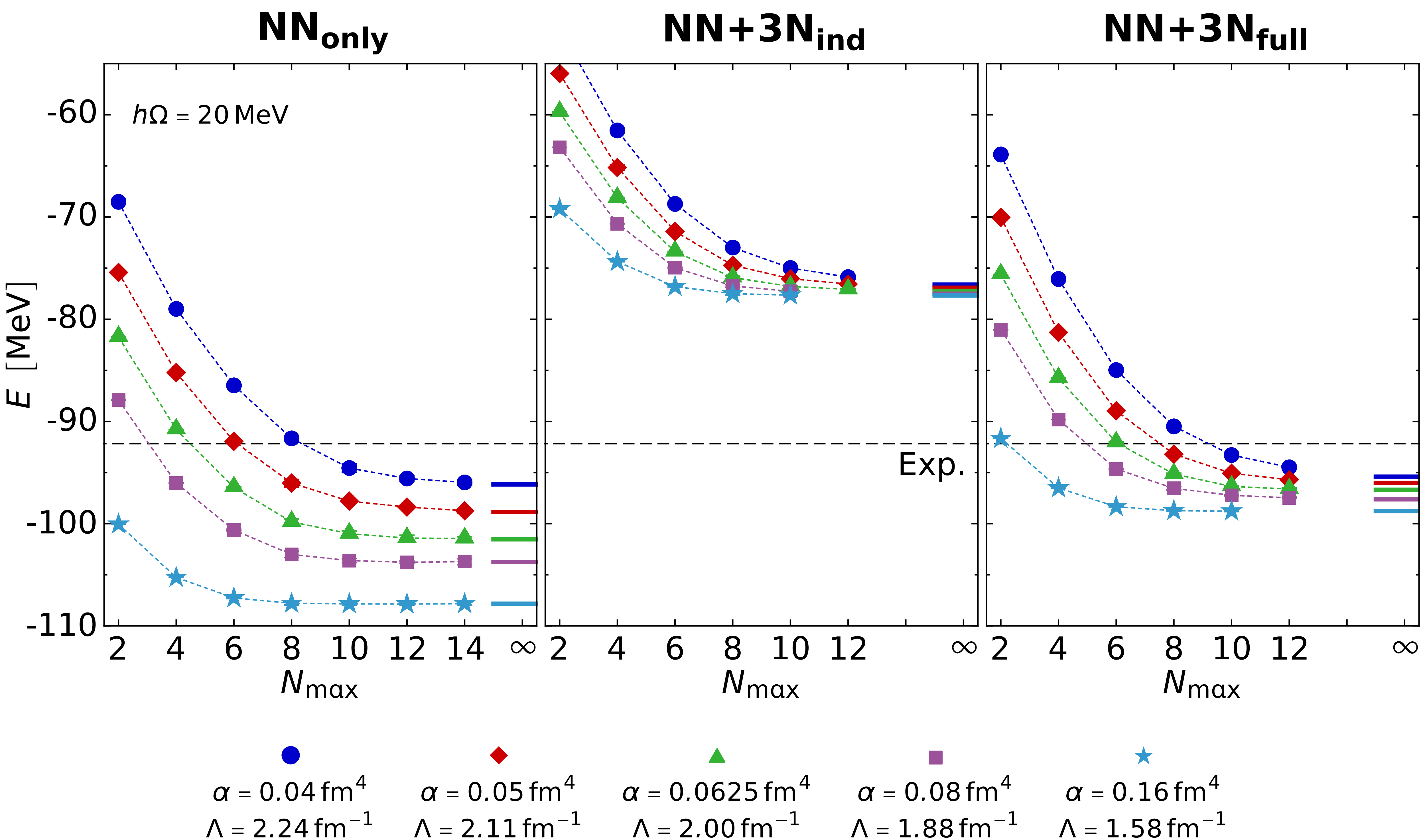
^{7}Li: Ground-State Energy

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



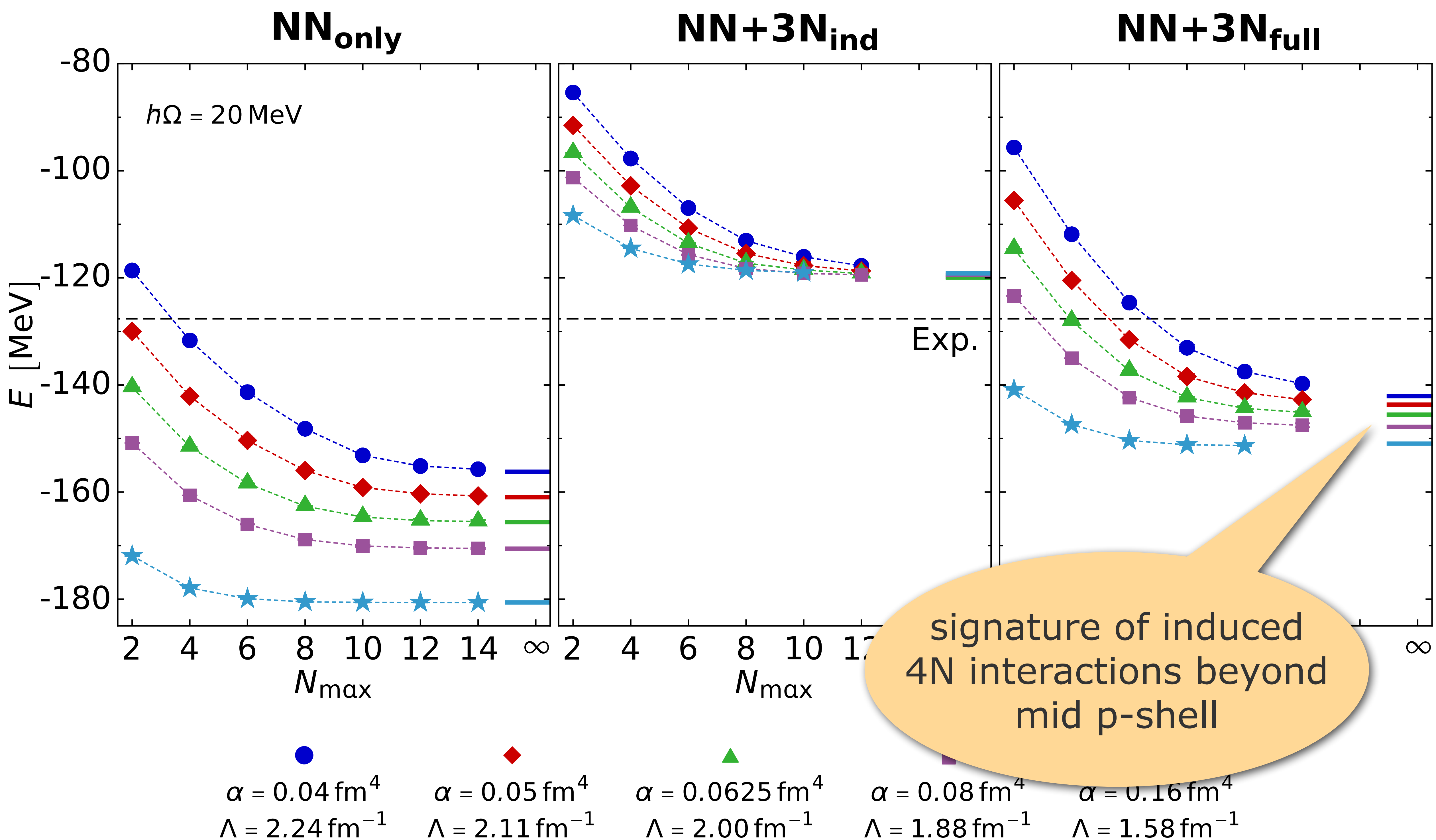
^{12}C: Ground-State Energy

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



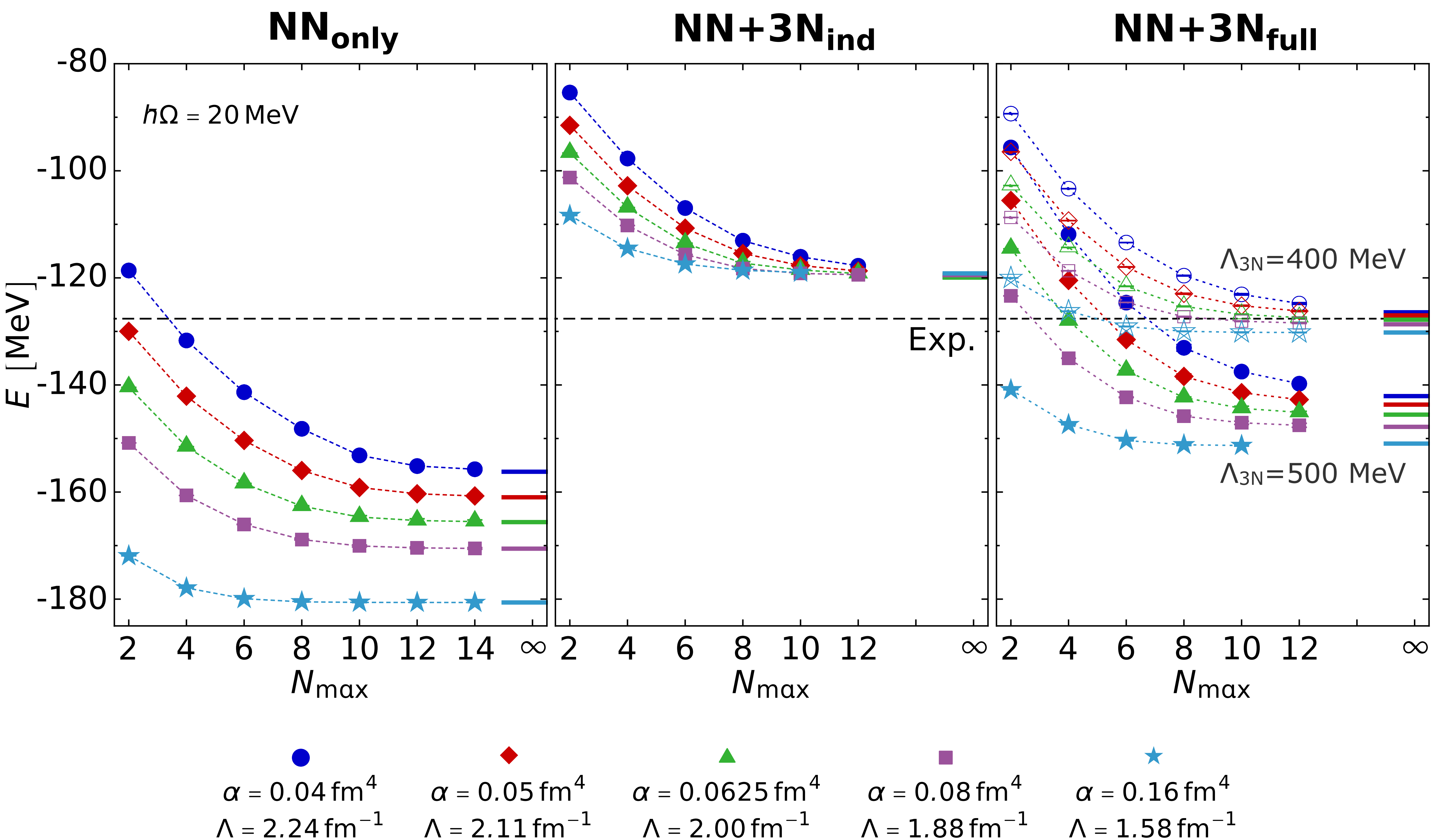
^{16}O: Ground-State Energy

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

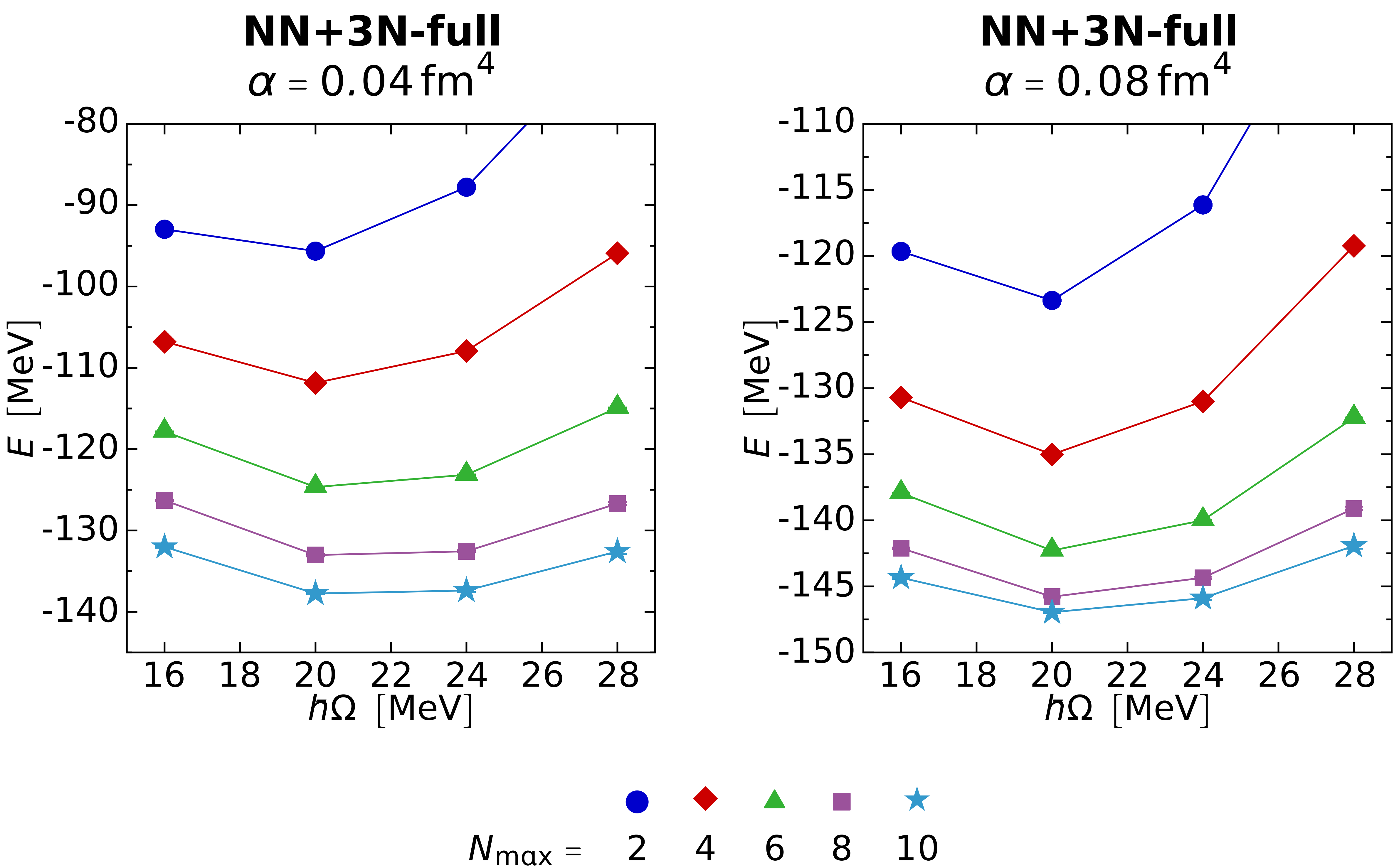


^{16}O: Ground-State Energy

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

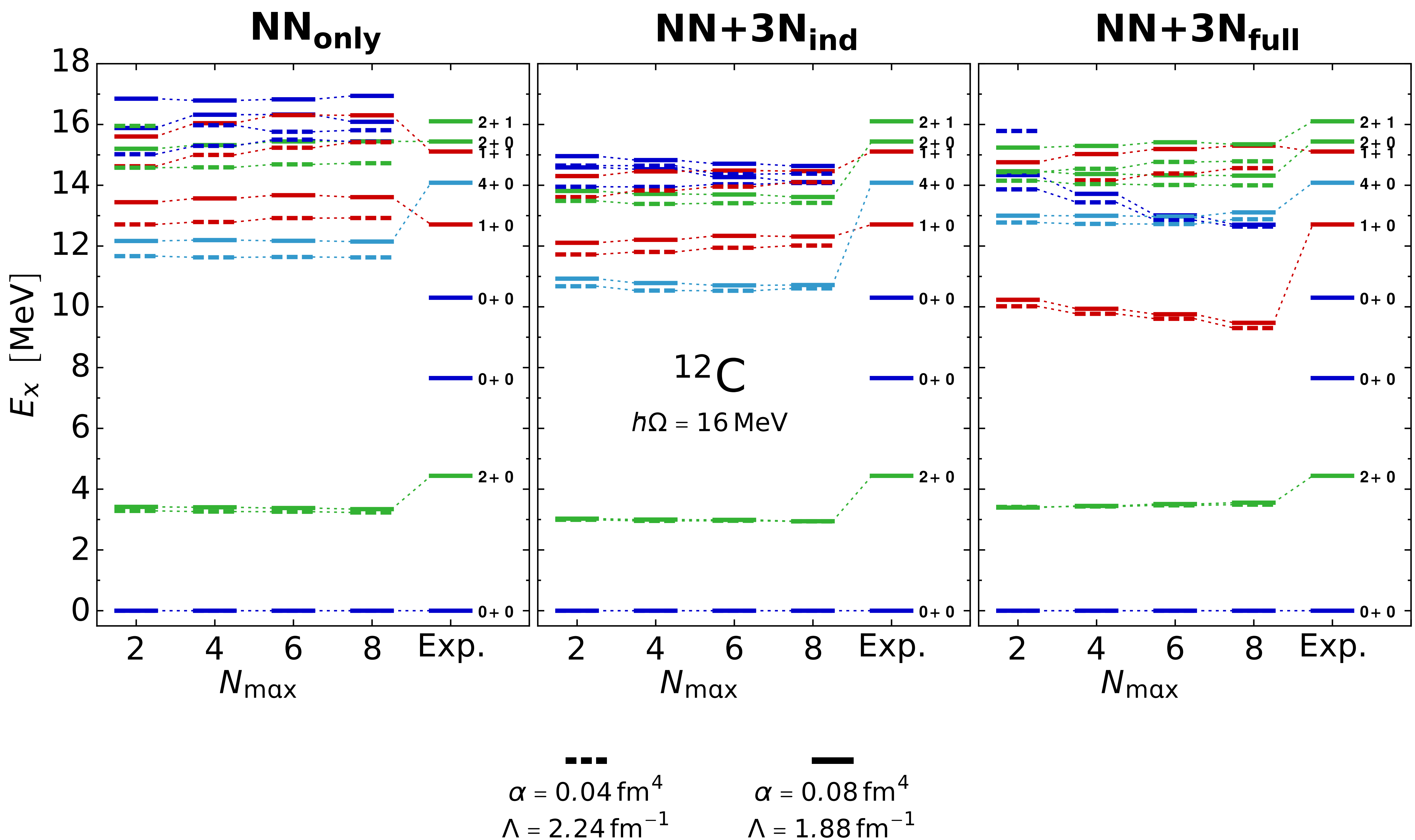


^{16}O: Frequency Dependence



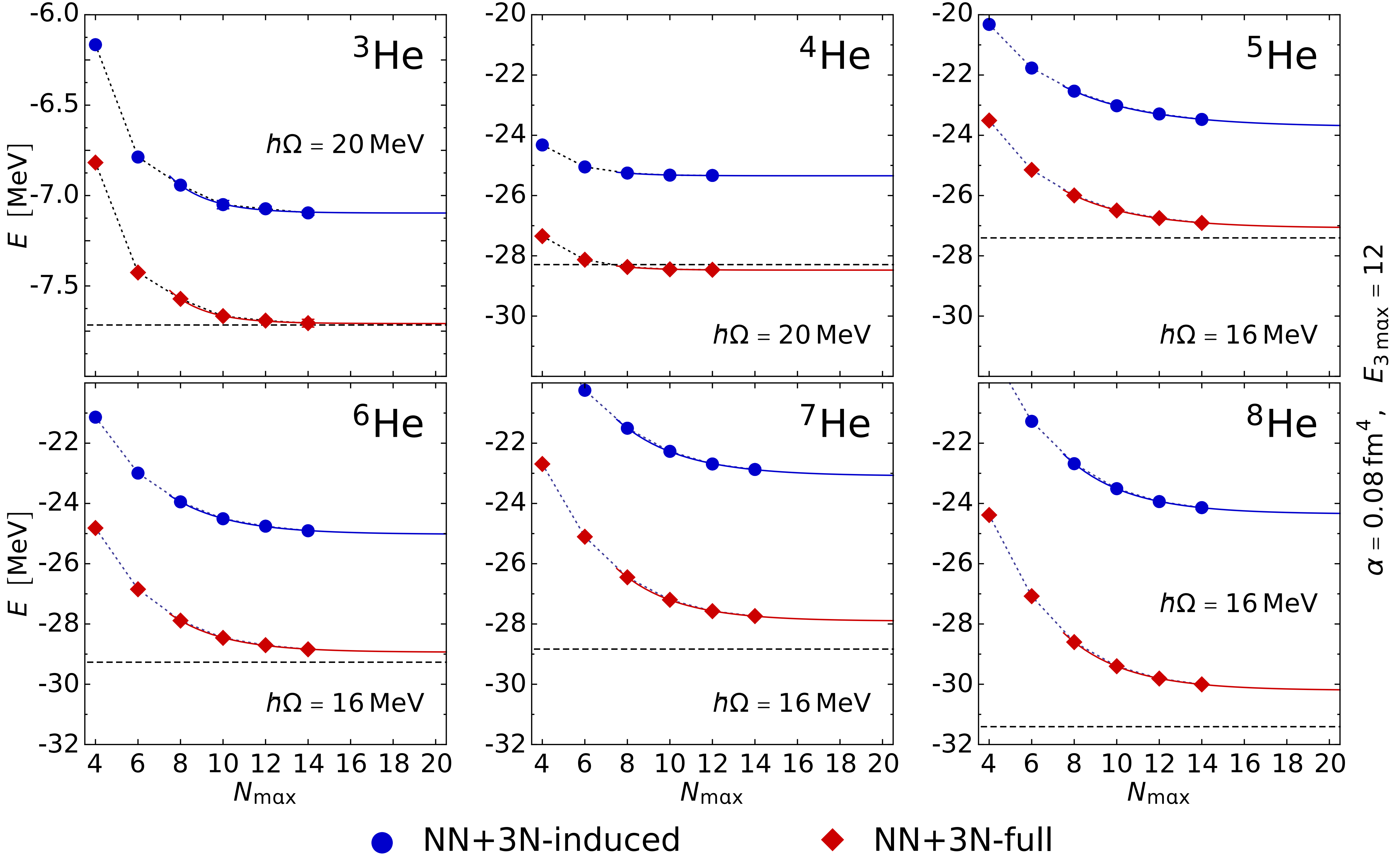
^{12}O: Excitation Spectrum

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

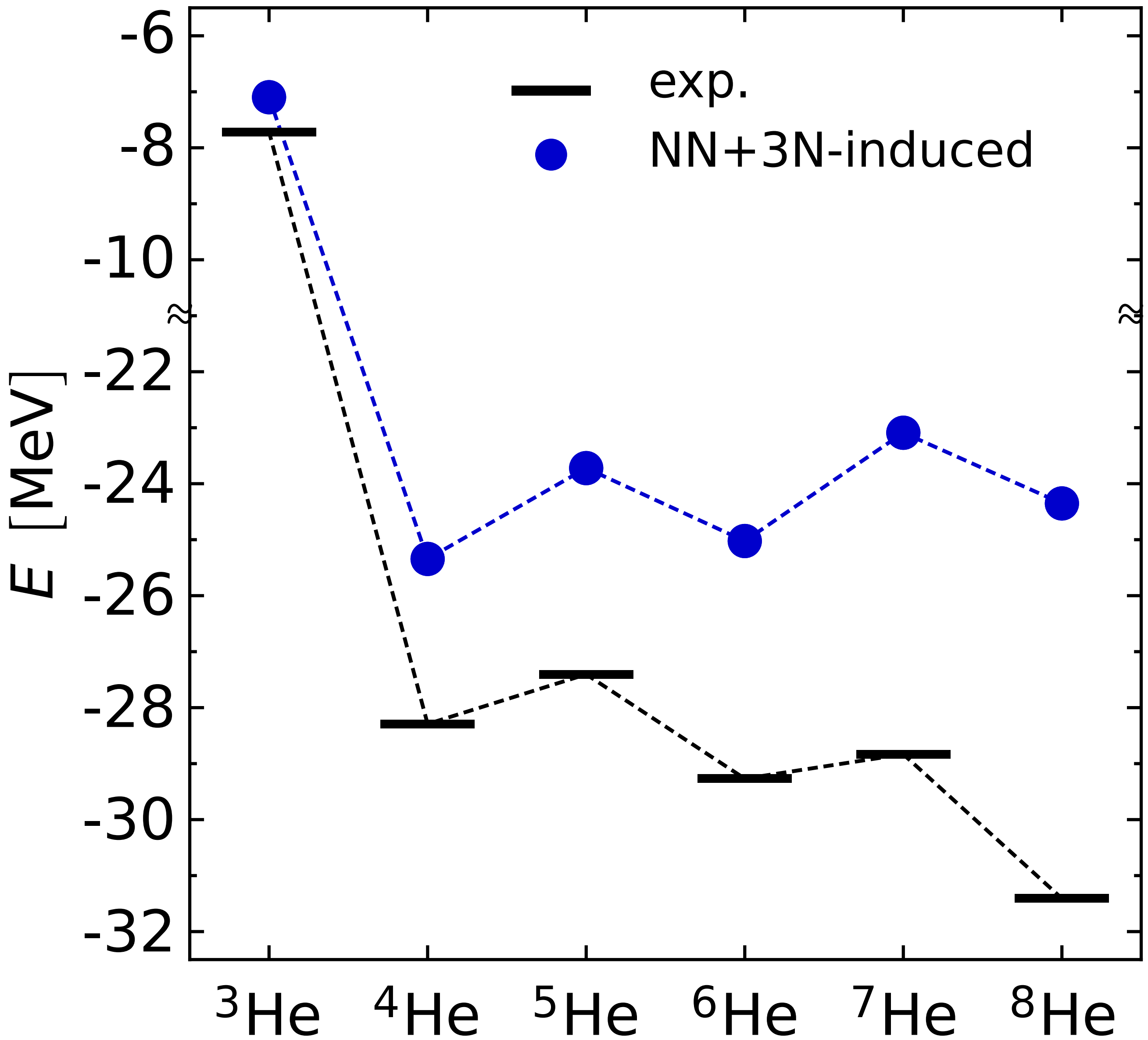


From Dripline to Dripline

Ground States of Helium Isotopes



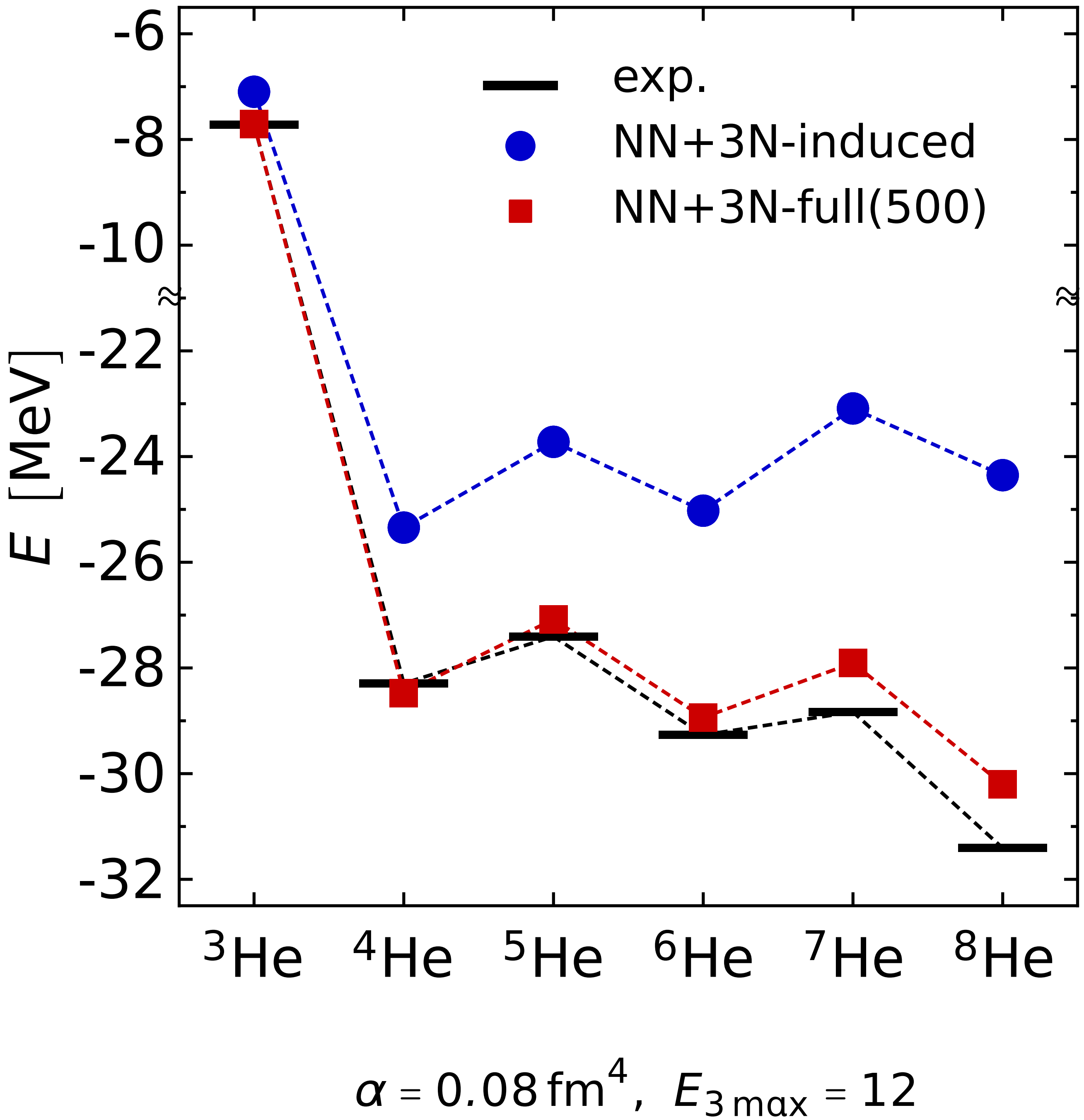
Ground States of Helium Isotopes



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

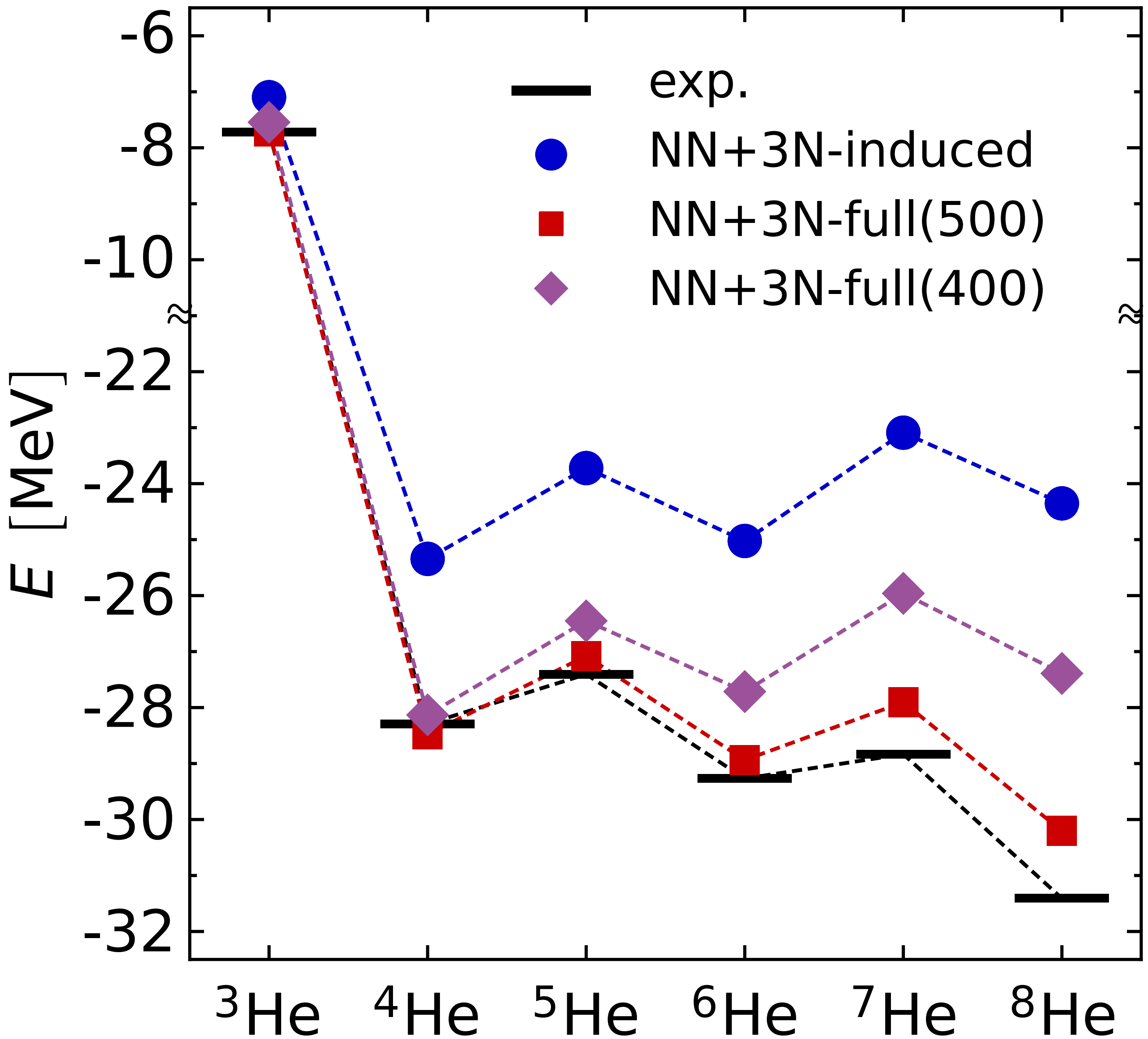
- **chiral NN interaction** cannot reproduce ground-state systematics

Ground States of Helium Isotopes



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

Ground States of Helium Isotopes



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

- **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)

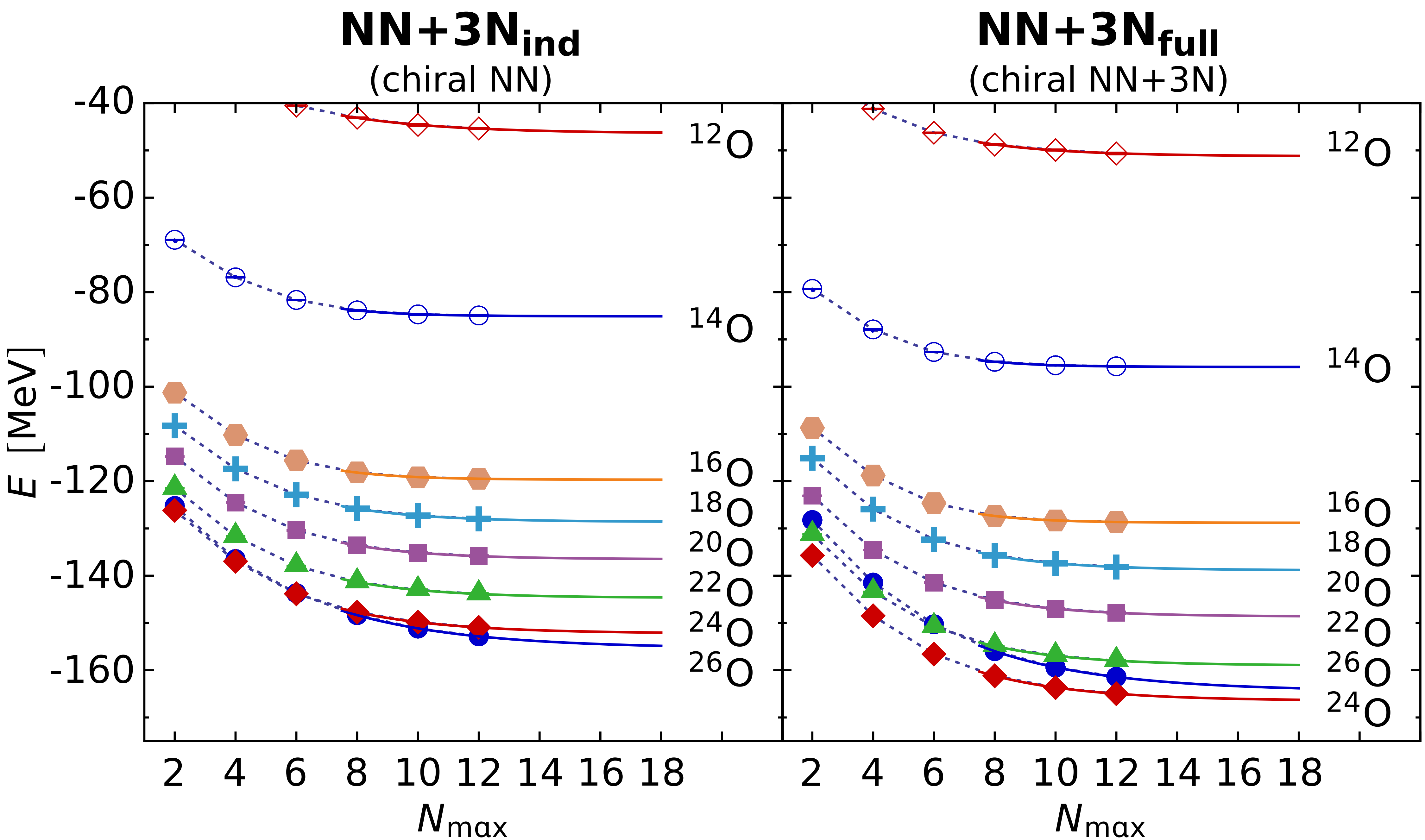
- 2013: **ab initio IT-NCSM** with explicit chiral 3N interactions and first **multi-reference in-medium SRG** calculations...

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

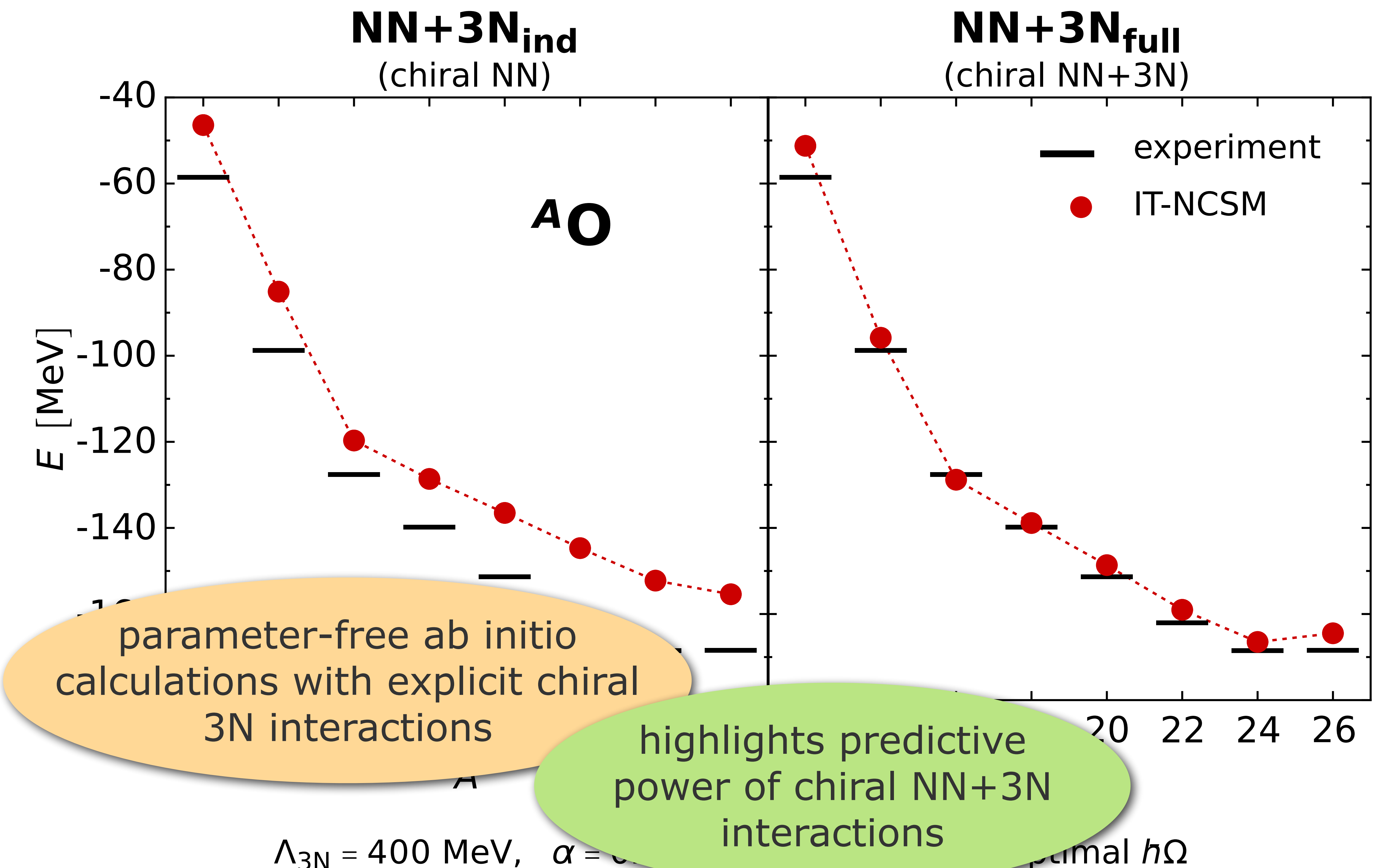
Hergert et al., PRL 110, 242501 (2013)



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

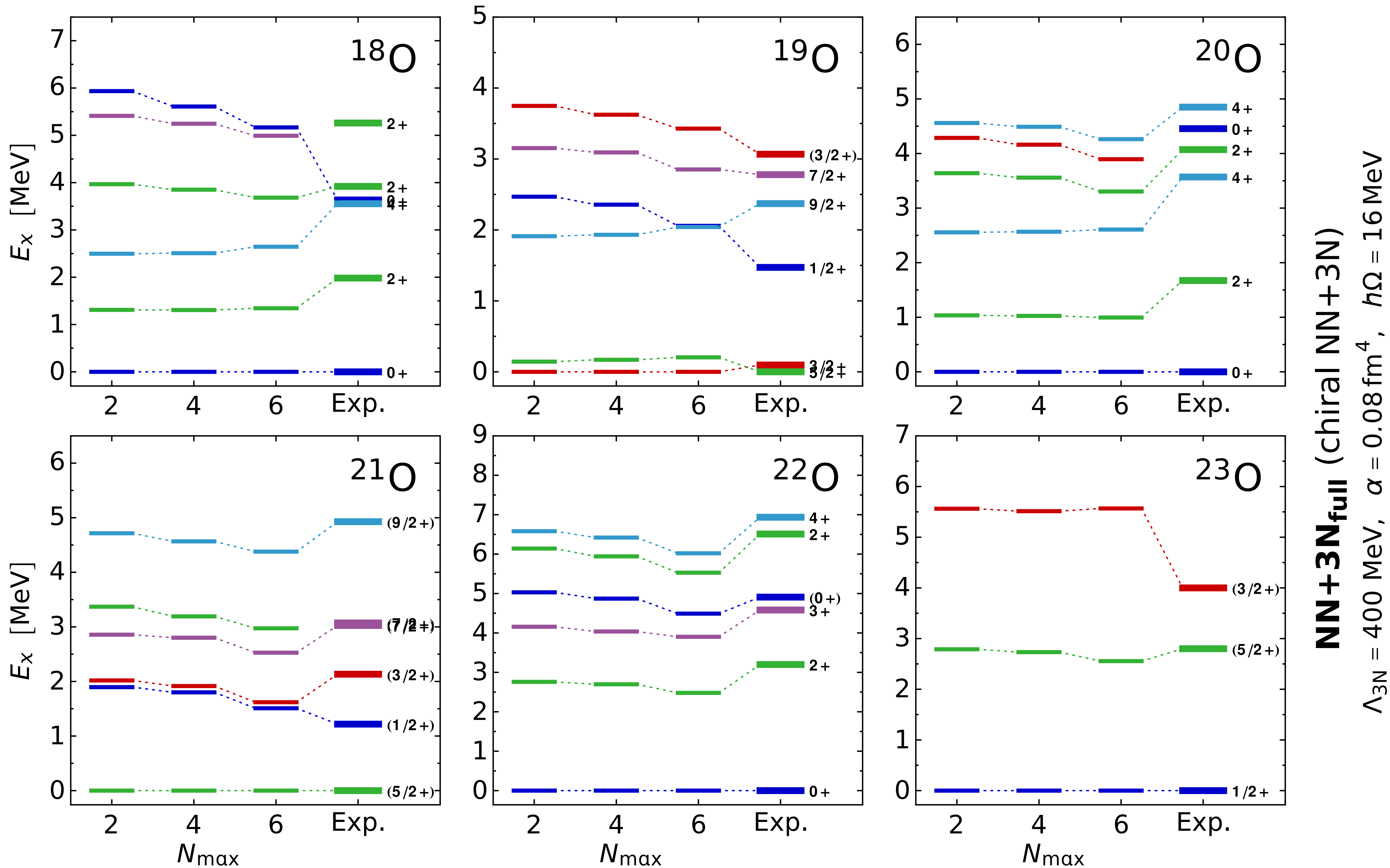
Ground States of Oxygen Isotopes

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

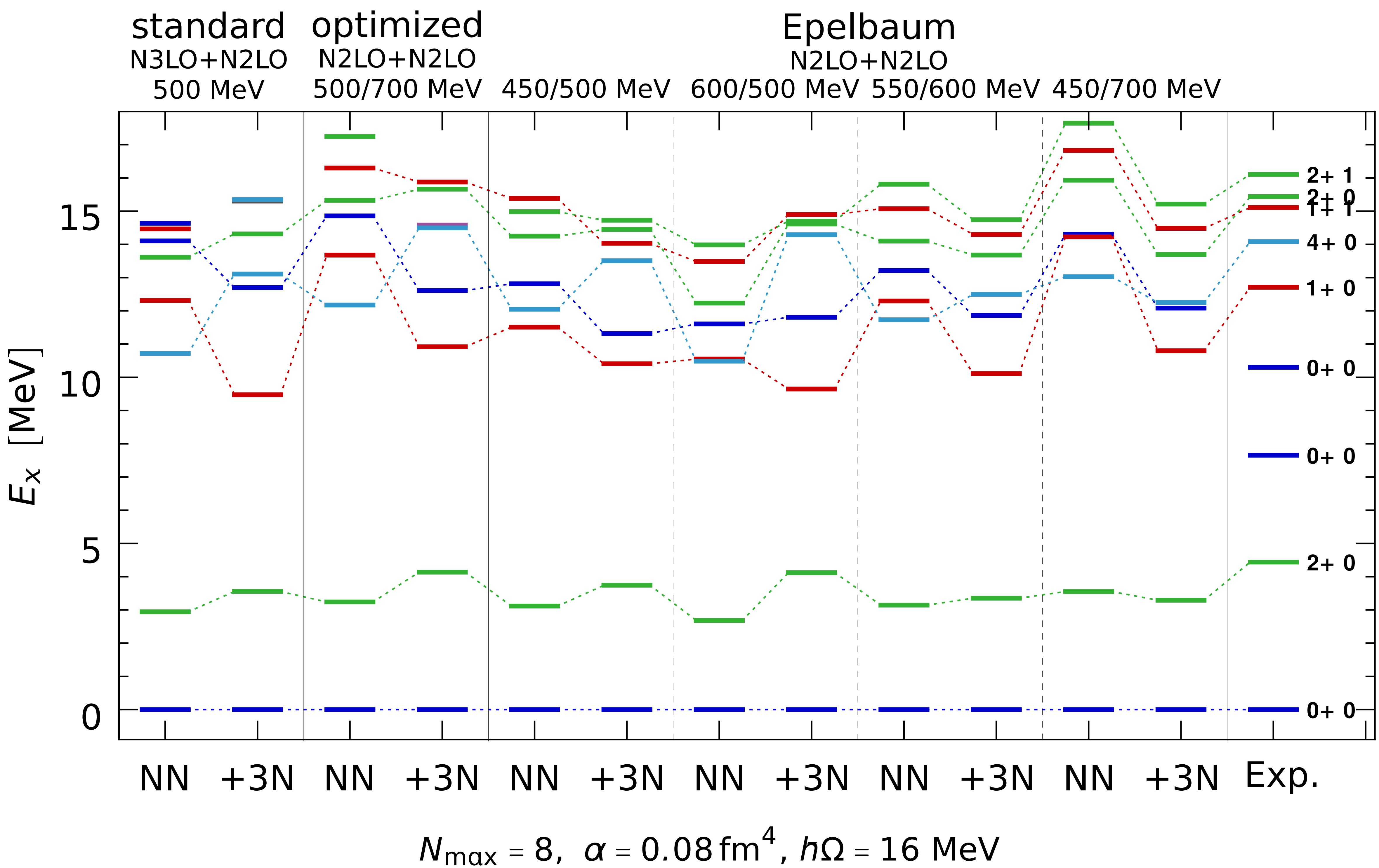


Spectra of Oxygen Isotopes

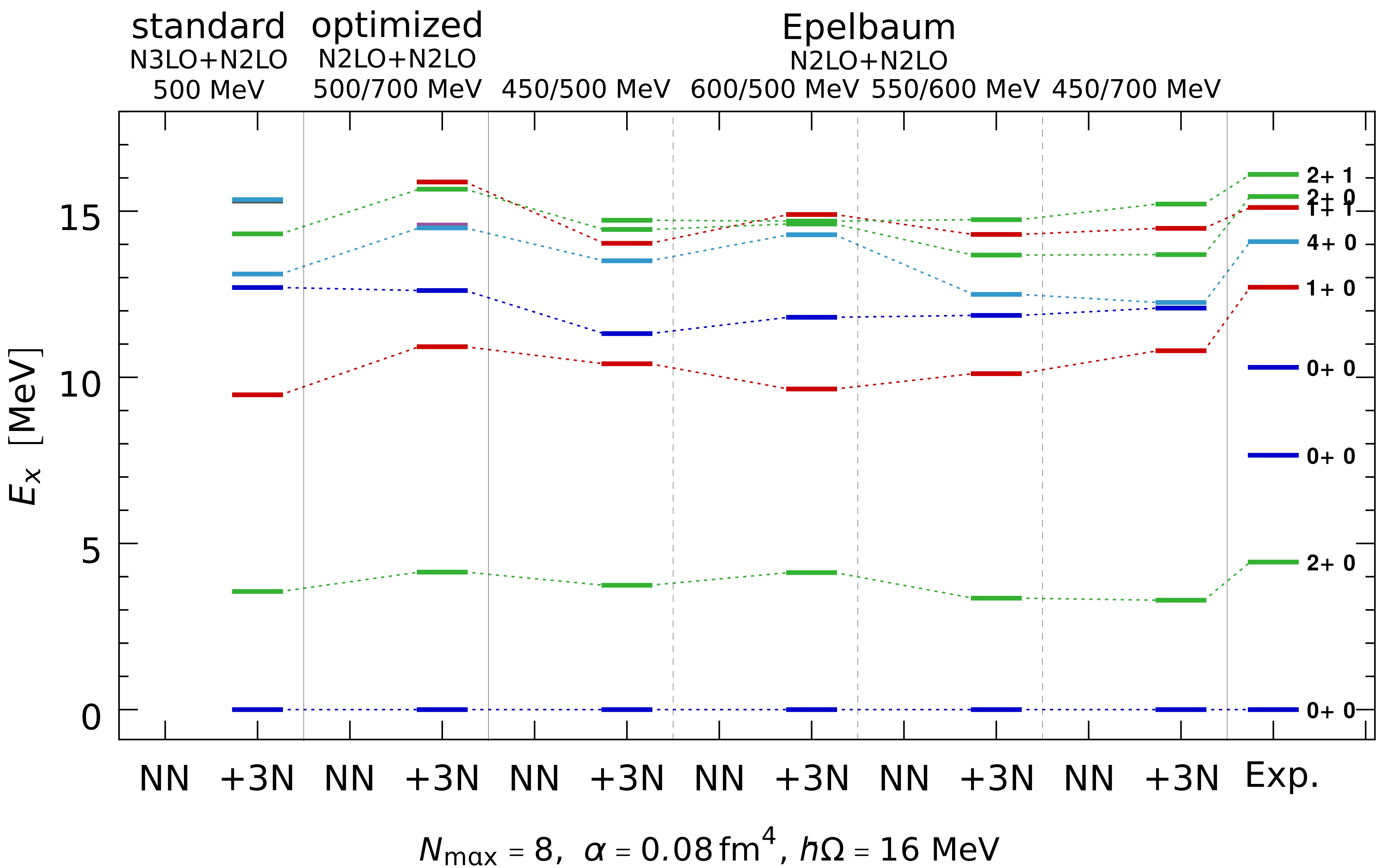
Hergert et al., PRL 110, 242501 (2013) & in prep.



^{12}C: Testing Chiral Hamiltonians



^{12}C: Testing Chiral Hamiltonians



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
- **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

Ab Initio Approaches to Light Nuclei

Lecture 4: Beyond Light Nuclei

Robert Roth

TECHNISCHE UNIVERSITÄT DARMSTADT

Overview

- **Lecture 1: Fundamentals**

  Prelude ● Many-Body Quantum Mechanics

- **Lecture 1’: Nuclear Hamiltonian**

  Nuclear Interactions ● Matrix Elements

- **Lecture 2: Correlations**

  Two-Body Problem ● Unitary Transformations ● Similarity Renormalization Group

- **Lecture 3: Light Nuclei**

  Configuration Interaction ● No-Core Shell Model ● Importance Truncation

- **Lecture 4: Beyond Light Nuclei**

  Coupled-Cluster Theory ● In-Medium Similarity Renormalization Group

Ab Initio Beyond Light Nuclei

advent of novel ab initio many-body approaches
gives access to the medium-mass regime

Hagen, Papenbrock, Dean, Piecuch, Binder,...

- **coupled-cluster theory**: ground-state parametrized by expon...ial wave operator applied to single-determinant reference st...
  - truncation at doubles level (CCSD) plus triples co...
  - equations of motion for excited states an...

...sukiyama, Schwenk, Hergert,...

- **in-medium SRG**: com... ...hole excitations from many-body refe... ...olution
  - nor... ...amiltonian truncated at two-body level
  - ... ...ell ground states; excitations via EOM or SM

Barbieri, Soma, Duguet,...

- self-c...sistent Green's function approaches and others...

controlling and quantifying the uncertainties due to various inherent truncations is a major task

Normal Ordering

Particle-Hole Excitations

- short-hand notation for creation and annihilation operators

$$a_i = a_{\alpha_i} \qquad\qquad a_i^\dagger = a_{\alpha_i}^\dagger$$

- define an A-body **reference Slater determinant**

$$|\Phi\rangle = |\alpha_1 \alpha_2 \ldots \alpha_A\rangle = a_1^\dagger a_2^\dagger \cdots a_A^\dagger |0\rangle$$

and construct arbitrary Slater determinants through **particle-hole excitations** on top of the reference state

$$|\Phi_a^p\rangle = a_p^\dagger a_a |\Phi\rangle$$
$$|\Phi_{ab}^{pq}\rangle = a_p^\dagger a_q^\dagger a_b a_a |\Phi\rangle$$
$$\vdots$$

index convention: $a,b,c,\ldots$: hole states, occupied in reference state
$p,q,r,\ldots$: particle states, unoccupied in reference states
$i,j,k,\ldots$: all states

Normal Ordering

- a string of creation and annihilation operators is in **normal order** with respect to a specific reference state, if all
  - creation operators are on the left
  - annihilation operators are on the right

- standard particle-hole operators are normal ordered with respect to the vacuum state as reference state

$$a_i^\dagger a_j \,, \qquad a_i^\dagger a_j^\dagger a_l a_k \,, \qquad a_i^\dagger a_j^\dagger a_k^\dagger a_n a_m a_l \,, \ldots$$

- **normal-ordered product** of string of operators

$$\{a_n a_i^\dagger \cdots a_m a_j^\dagger\} = \mathrm{sgn}(\pi)\, a_i^\dagger a_j^\dagger \cdots a_n a_m$$

- defining property of a normal-ordered product: **expectation value with the reference state always vanishes**

$$\langle\Phi|\, \{\ldots\}\, |\Phi\rangle = 0$$

Normal Ordering with A-Body Reference

- in particle-hole formulation with respect to an ***A*-body reference Slater determinant** things are more complicated

	particle states	hole states
creation operators	$a^\dagger_p, a^\dagger_q, \ldots$	$a_a, a_b, \ldots$
annihilation operators	$a_p, a_q, \ldots$	$a^\dagger_a, a^\dagger_b, \ldots$

- redefinition of creation and annihilation operators necessary to guarantee vanishing reference expectation value

$$\langle \Phi | \{ \ldots \} | \Phi \rangle = 0$$

- starting from an operator string in vacuum normal order one has to **reorder to arrive at reference normal order**
  - "brute force" using the anticommutation relations for fermionic creation and annihilation operators
  - "elegantly" using Wick's theorem and contractions...

Normal-Ordered Hamiltonian

- **second quantized Hamiltonian** in vacuum normal order

$$H = \frac{1}{4} \sum_{ijkl} \langle ij | T_{int} + V_{NN} | kl \rangle \, a_i^\dagger a_j^\dagger a_l a_k + \ldots$$

normal-ordered two-body approximation: discard residual normal-ordered three-body part

- **normal-ordered Hamiltonian** with respect to reference sta

$$H = E + \sum_{ij} f_j^i \, \{a_i^\dagger a_j\} + \frac{1}{4} \sum_{ijkl} \Gamma_{kl}^{ij} \, \{a_i^\dagger a_j^\dagger a_l a_k\} + \frac{1}{36} \sum_{ijklmn} W_{lmn}^{ijk} \, \{a_i^\dagger a_j^\dagger a_k^\dagger a_n a_m a_l\}$$

$$E = \frac{1}{2} \sum_{ab} \langle ab | T_{int} + V_{NN} | ab \rangle + \frac{1}{6} \sum_{abc} \langle abc | V_{3N} | abc \rangle$$

$$f_j^i = \sum_{a} \langle ai | T_{int} + V_{NN} | aj \rangle + \frac{1}{2} \sum_{ab} \langle abi | V_{3N} | abj \rangle$$

$$\Gamma_{kl}^{ij} = \langle ij | T_{int} + V_{NN} | kl \rangle + \sum_{a} \langle aij | V_{3N} | akl \rangle$$

$$W_{lmn}^{ijk} = \langle ijk | V_{3N} | lmn \rangle$$

Coupled-Cluster Theory

Coupled-Cluster Ansatz

- coupled-cluster ground state parametrized by **exponential of particle-hole excitation operators** acting on reference state

$$|\Psi_{CC}\rangle = \exp(T)\,|\Phi\rangle = \exp(T_1 + T_2 + \cdots T_A)\,|\Phi\rangle$$

- with the **n-particle-n-hole excitation operators** with unknown amplitudes

$$T_1 = \sum_{a,p} t_a^p\ \{a_p^\dagger a_a\}$$

$$T_2 = \sum_{ab,pq} t_{ab}^{pq}\ \{a_p^\dagger a_q^\dagger a_b a_a\}$$

$$\vdots$$

- need to **truncate the excitation operator** at some small particle-hole order, defining different levels of coupled-cluster approximations

T_1	CCS
$T_1 + T_2$	CCSD
$T_1 + T_2 + T_3$	CCSDT

Coupled-Cluster Equations

- insert the coupled-cluster ansatz into the **A-body Schrödinger equation** and manipulate

$$H_{\text{int}} |\Psi_{\text{CC}}\rangle = E |\Psi_{\text{CC}}\rangle \quad \Rightarrow \quad \exp(-T)\, H_{\text{int}} \exp(T)\ |\Phi\rangle = E |\Phi\rangle$$

  to obtain Schrödinger-like equation for a **similarity-transformed Hamiltonian**

$$\mathcal{H}\ |\Phi\rangle = E |\Phi\rangle \quad \text{with} \quad \mathcal{H} = \exp(-T)\, H_{\text{int}} \exp(T)$$

- note: this is **not a unitary transformation** and therefore the transformed Hamiltonian is non-hermitian
  - as a result approximations will be non-variational
- similarity transformation of the Hamiltonian can be expanded in a **Baker–Campbell–Hausdorff series**, which **terminates at finite order**
  - CCSD with a two-body Hamiltonian terminates after order T^4

CCSD Equations

- project the Schrödinger-like equation onto the reference state, 1p1h states, and 2p2h states to obtain **CCSD energy and amplitude equations**

$$\langle \Phi | \mathcal{H} | \Phi \rangle = E_{\mathrm{CCSD}}$$
$$\langle \Phi_a^p | \mathcal{H} | \Phi \rangle = 0$$
$$\langle \Phi_{ab}^{pq} | \mathcal{H} | \Phi \rangle = 0$$

- after BCH-expansion these are **coupled non-linear algebraic equations** for the amplitudes t_a^p, t_{ab}^{pq} and the CCSD energy

- for large-scale calculations use **spherical formulation**, where particle-hole operators are coupled to J=0

- full CCSDT is too expensive, various **non-iterative triples corrections** are being used to include triples contributions

- coupled-cluster with **explicit 3N interactions** can be done and was used to test the NO2B approximation

Coupled Cluster: Pros & Cons

PRO

- much more efficient than ph-truncated CI
- can deal with explicit 3N interaction
- size extensive
- very mild scaling with A

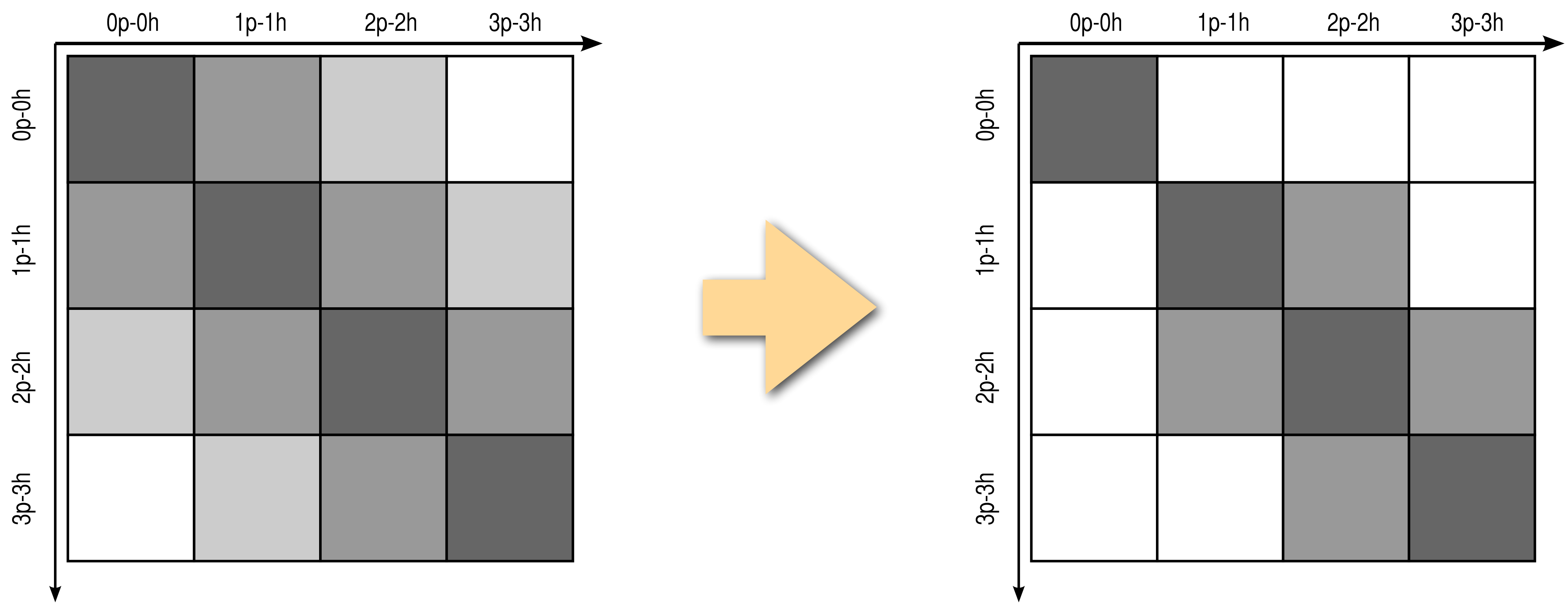
CON

- not variational
- only for closed shell nuclei *
- other observables difficult
- only for ground states *
- non-hermititan Hamiltonian

* equations of motion methods give access to near-closed-shell isotopes and excited states

In-Medium SRG

Decoupling in A-Body Space

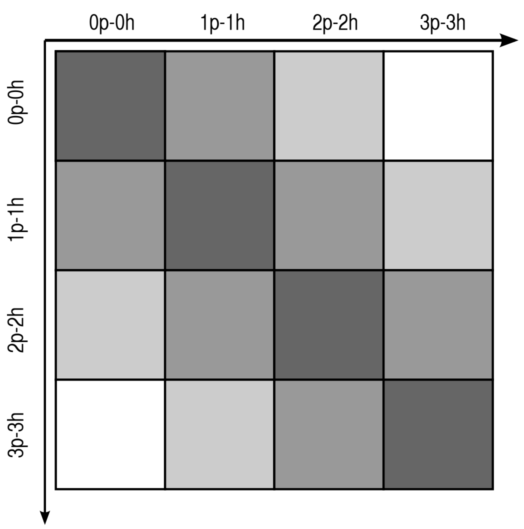


decouple reference state from all particle-hole excited states

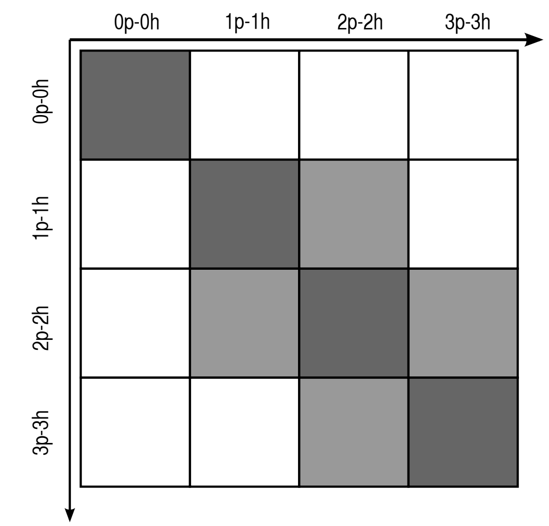
expectation value in reference state represents ground-state energy

In-Medium SRG

Tsukiyama, Bogner, Schwenk, Hergert,...



use SRG flow equations for normal-ordered Hamiltonian to decouple many-body reference state from excitations



- **flow equation** for Hamiltonian

$$\frac{d}{ds}H(s) = [\eta(s), H(s)]$$

- Hamiltonian in single-reference or multi-reference **normal order**, omitting normal-ordered 3B term

$$\mathrm{H}(s) = E(s) + \sum_{ij} f^i_j(s)\, \{a^\dagger_i a_j\} + \frac{1}{4}\sum_{ijkl} \Gamma^{ij}_{kl}(s)\, \{a^\dagger_i a^\dagger_j a_l a_k\}$$

In-Medium SRG Generators

- **Wegner**: simple, intuitive, inefficient

$$\eta = \left[H_\text{d}, H\right] = \left[H_\text{d}, H_\text{od}\right]$$

- **White**: efficient, problems with near degeneracies

$$\eta^1_2 = (\Delta^1_2)^{-1}\, n_1 \bar{n}_2\, f^1_2 - [1 \longleftrightarrow 2]$$

$$\eta^{12}_{34} = (\Delta^{12}_{34})^{-1}\, n_1 n_2 \bar{n}_3 \bar{n}_4\, \Gamma^{12}_{34} - [12 \longleftrightarrow 34]$$

- **Imaginary Time**: good work horse *[Morris, Bogner]*

$$\eta^1_2 = \text{sgn}(\Delta^1_2)\, n_1 \bar{n}_2\, f^1_2 - [1 \longleftrightarrow 2]$$

$$\eta^{12}_{34} = \text{sgn}(\Delta^{12}_{34})\, n_1 n_2 \bar{n}_3 \bar{n}_4\, \Gamma^{12}_{34} - [12 \longleftrightarrow 34]$$

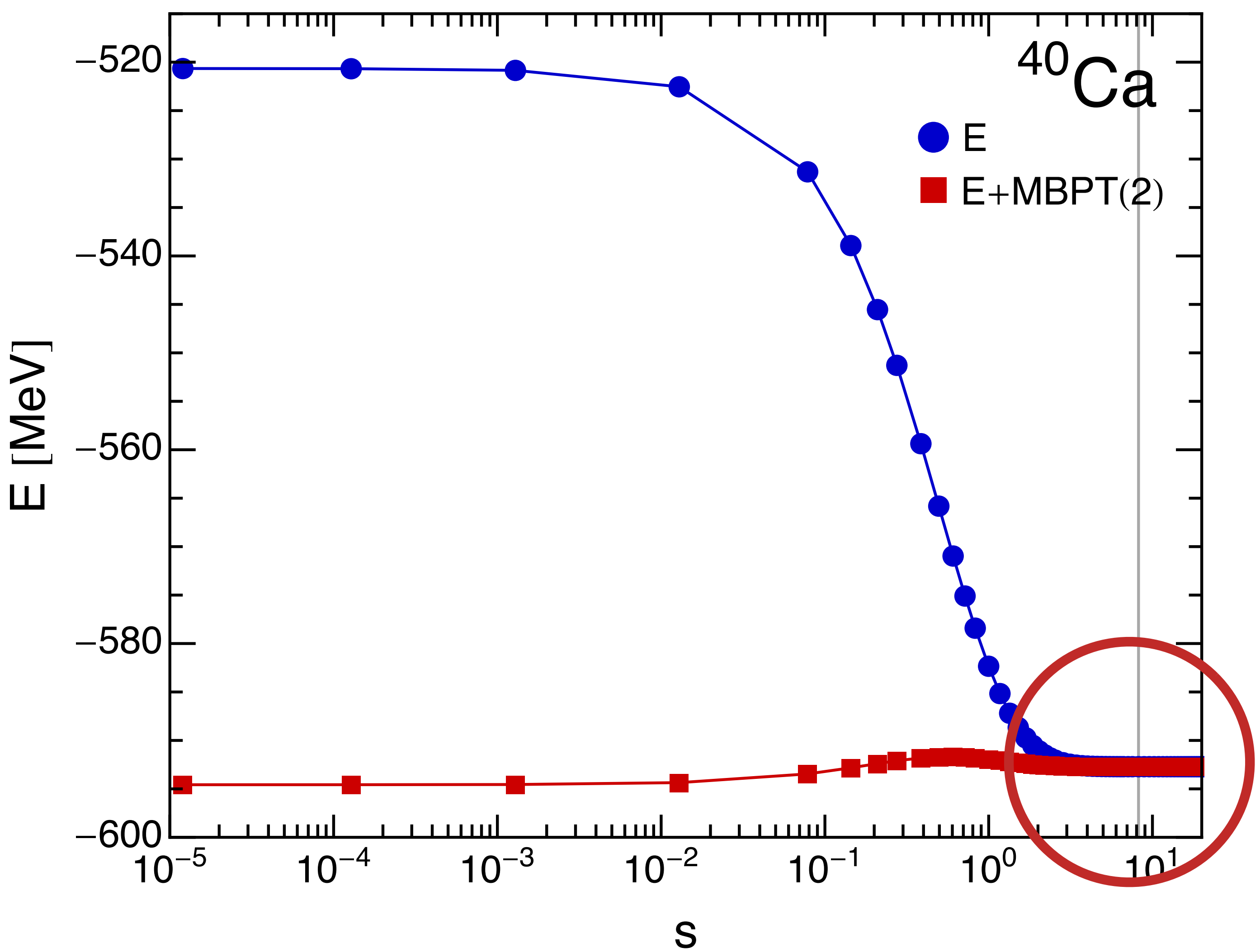
- **Brillouin**: potentially better work horse *[Hergert]*

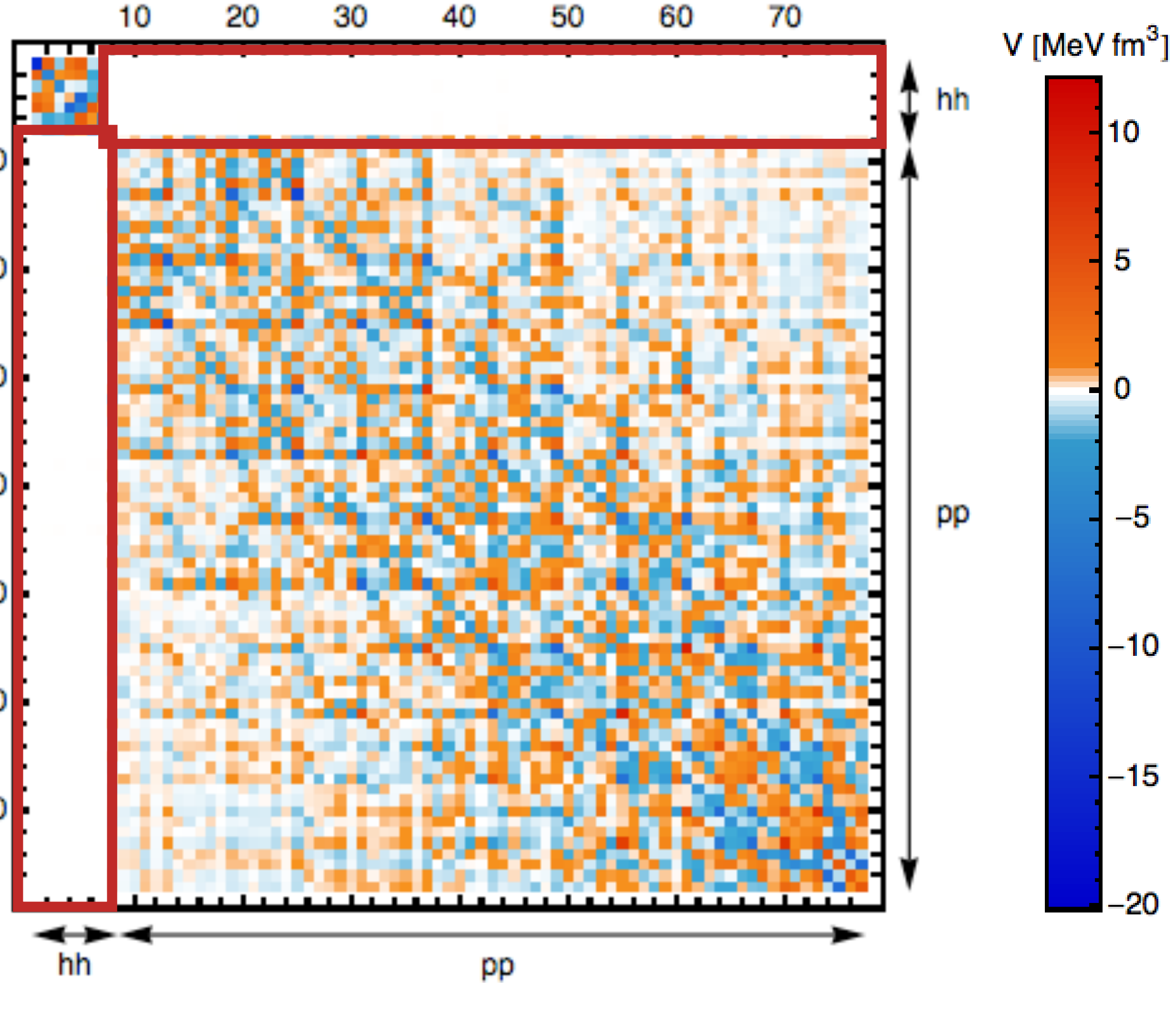
$$\eta^1_2 = \langle\Phi|\, [H, \{a^\dagger_1 a_2\}]\, |\Phi\rangle$$

$$\eta^{12}_{34} = \langle\Phi|\, [H, \{a^\dagger_1 a^\dagger_2 a_4 a_3\}]\, |\Phi\rangle$$

In-Medium SRG Evolution

H. Hergert





In-Medium SRG: Pros & Cons

PRO

- flexibility of generators
- much more efficient than ph-truncated CI
- straight-forward extension to open-shell nuclei
- size extensive
- very mild scaling with A
- hermitian Hamiltonian
- easy access to other observables
- bridge to shell model

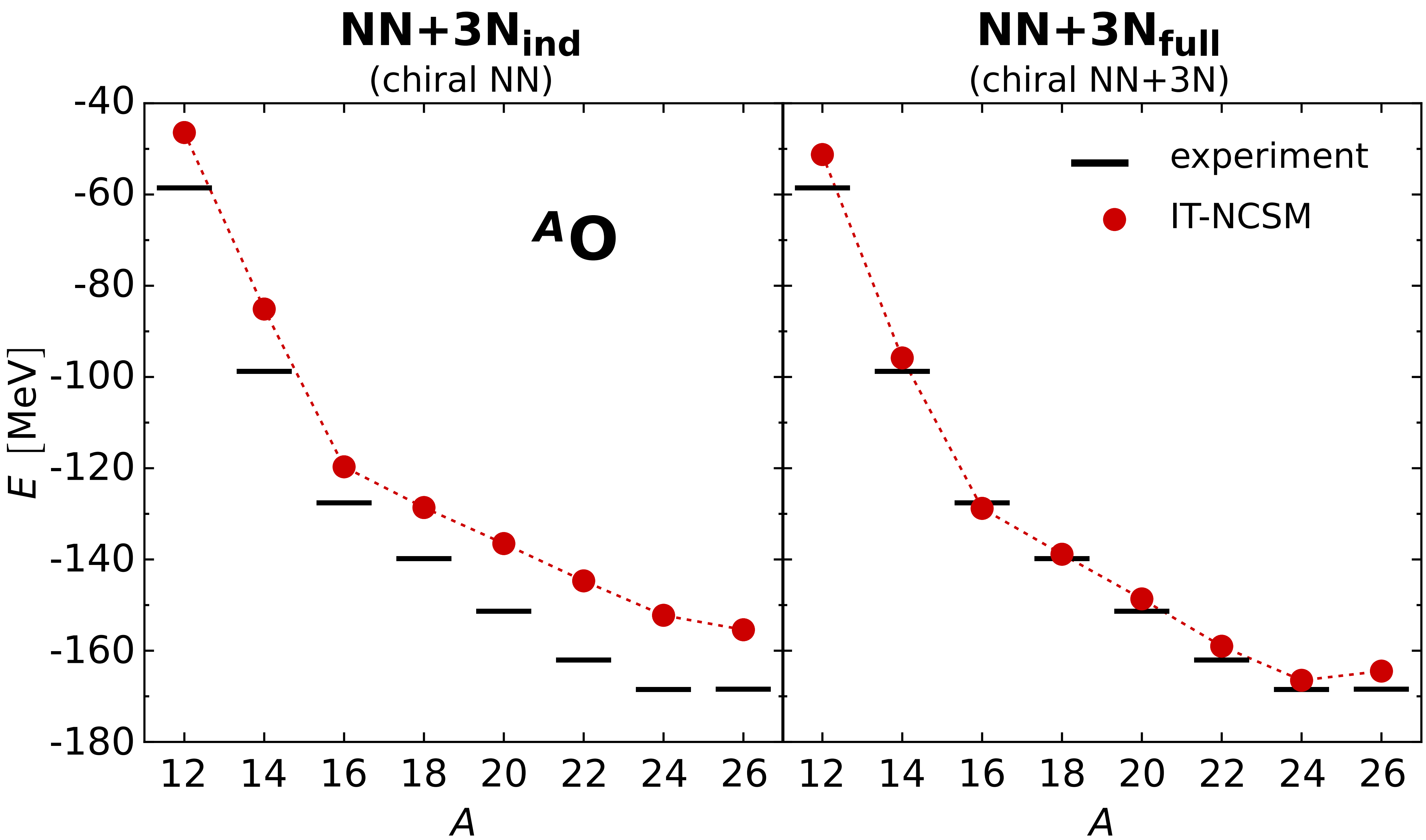
CON

- not variational
- NO3B needs some work

Applications for Medium-Mass Nuclei

Ground States of Oxygen Isotopes

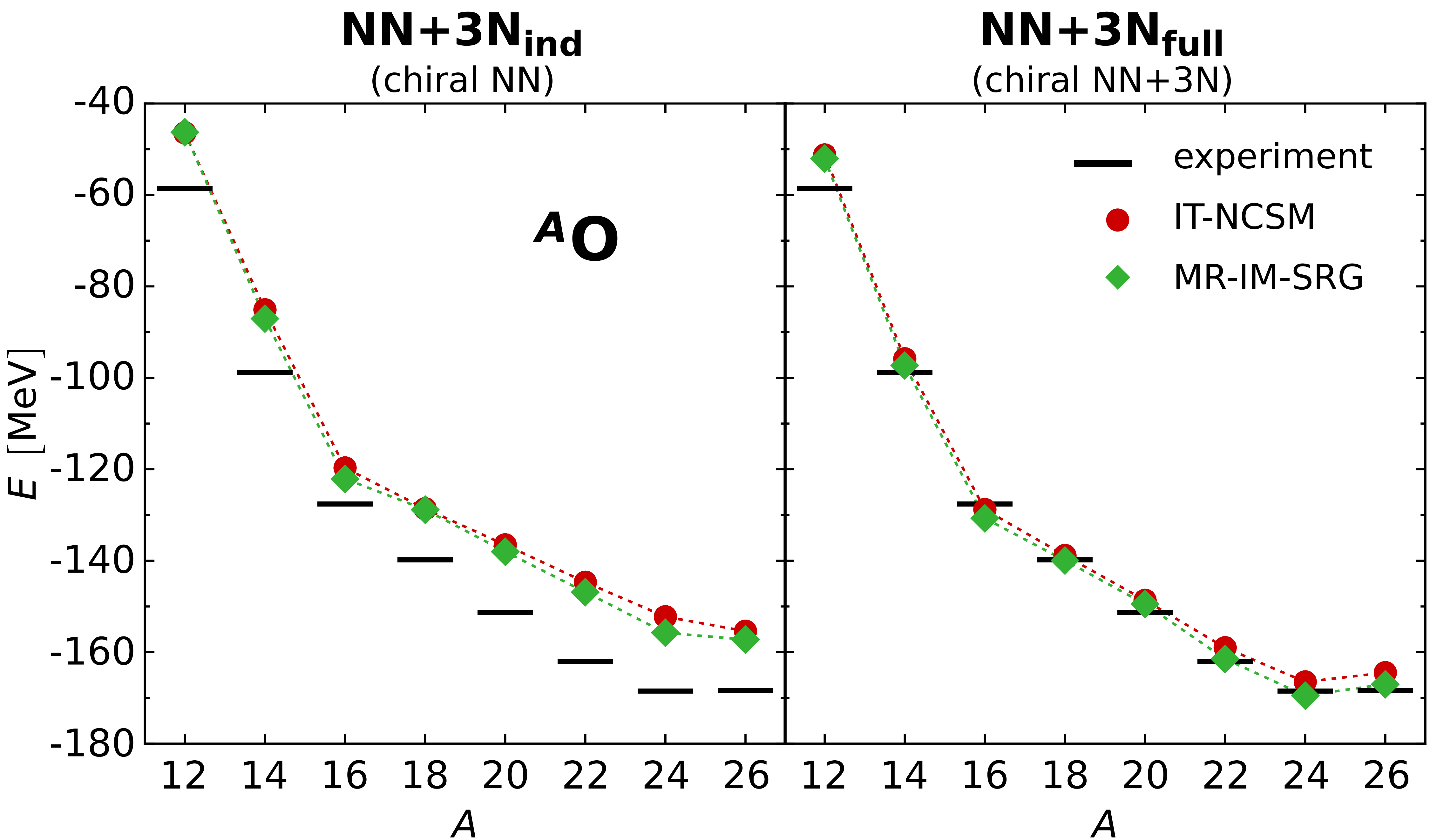
Hergert et al., PRL 110, 242501 (2013)



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

Ground States of Oxygen Isotopes

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



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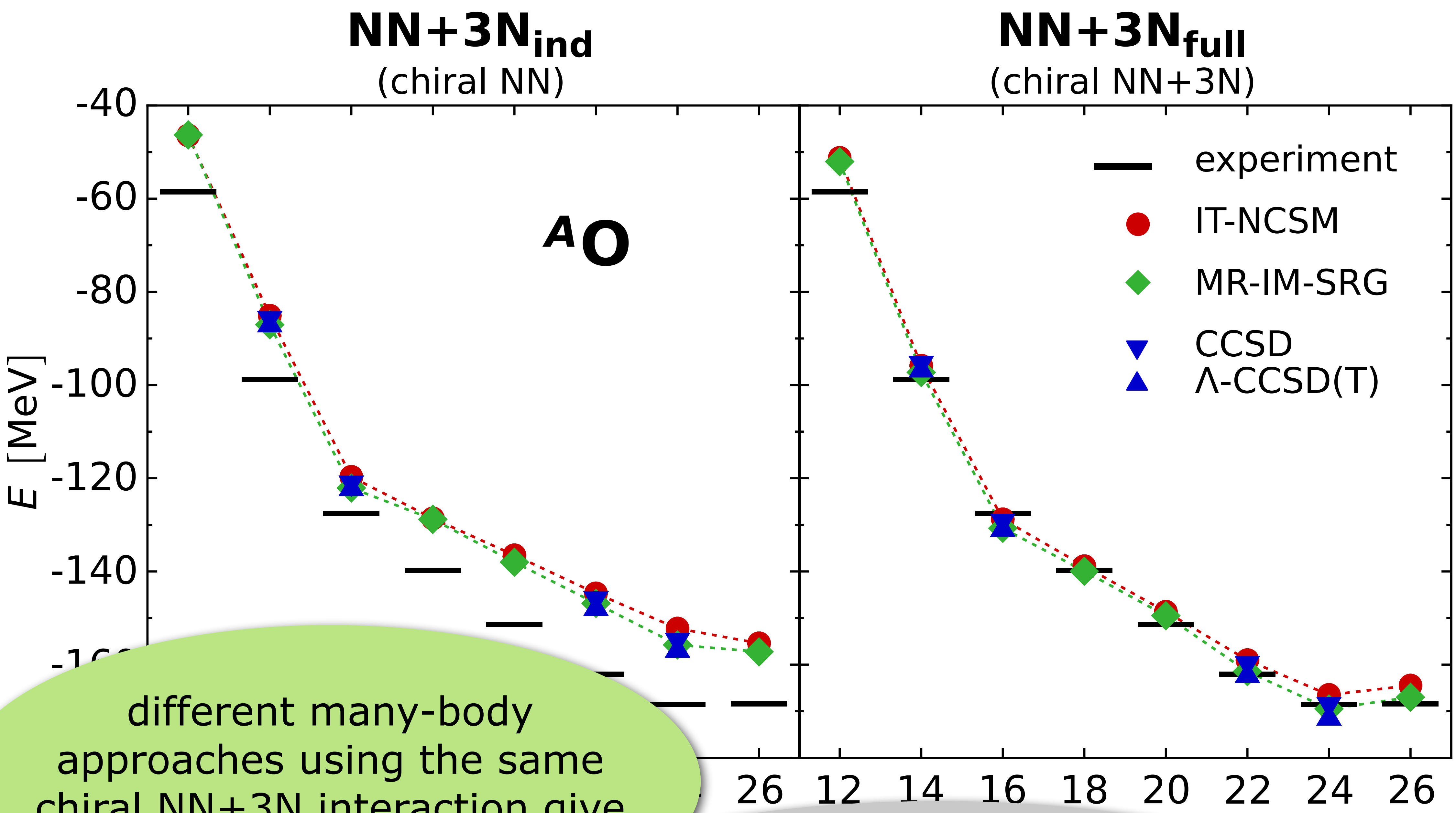
Ground States of Oxygen Isotopes

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

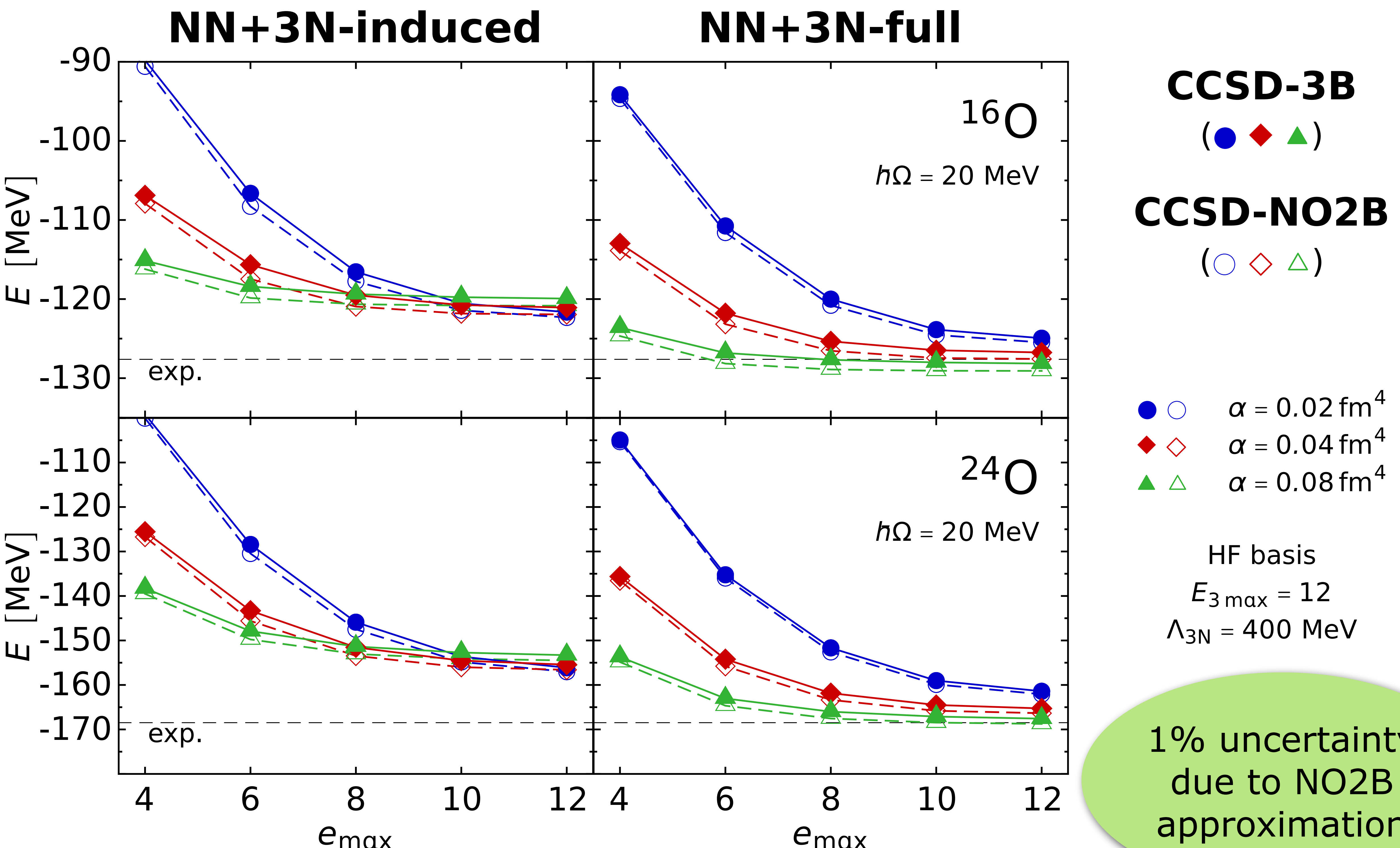


different many-body approaches using the same chiral NN+3N interaction give consistent results

minor differences are understood in terms of uncertainties due to truncations

Benchmark of NO2B Approximation

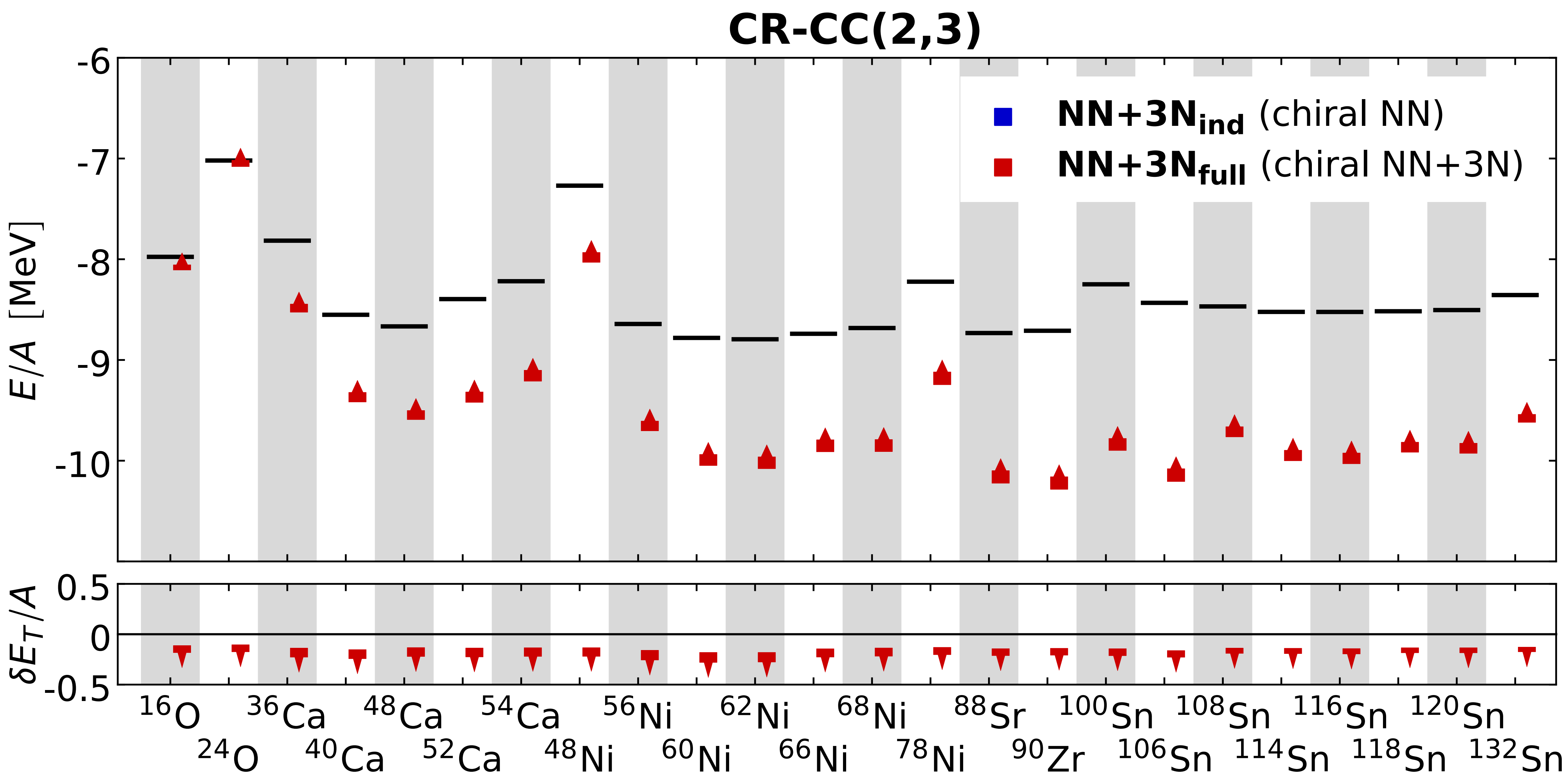
Roth, et al., PRL 109, 052501 (2012); Binder et al., PRC 87, 021303(R) (2013)



1% uncertainty due to NO2B approximation

Towards Heavy Nuclei - Ab Initio

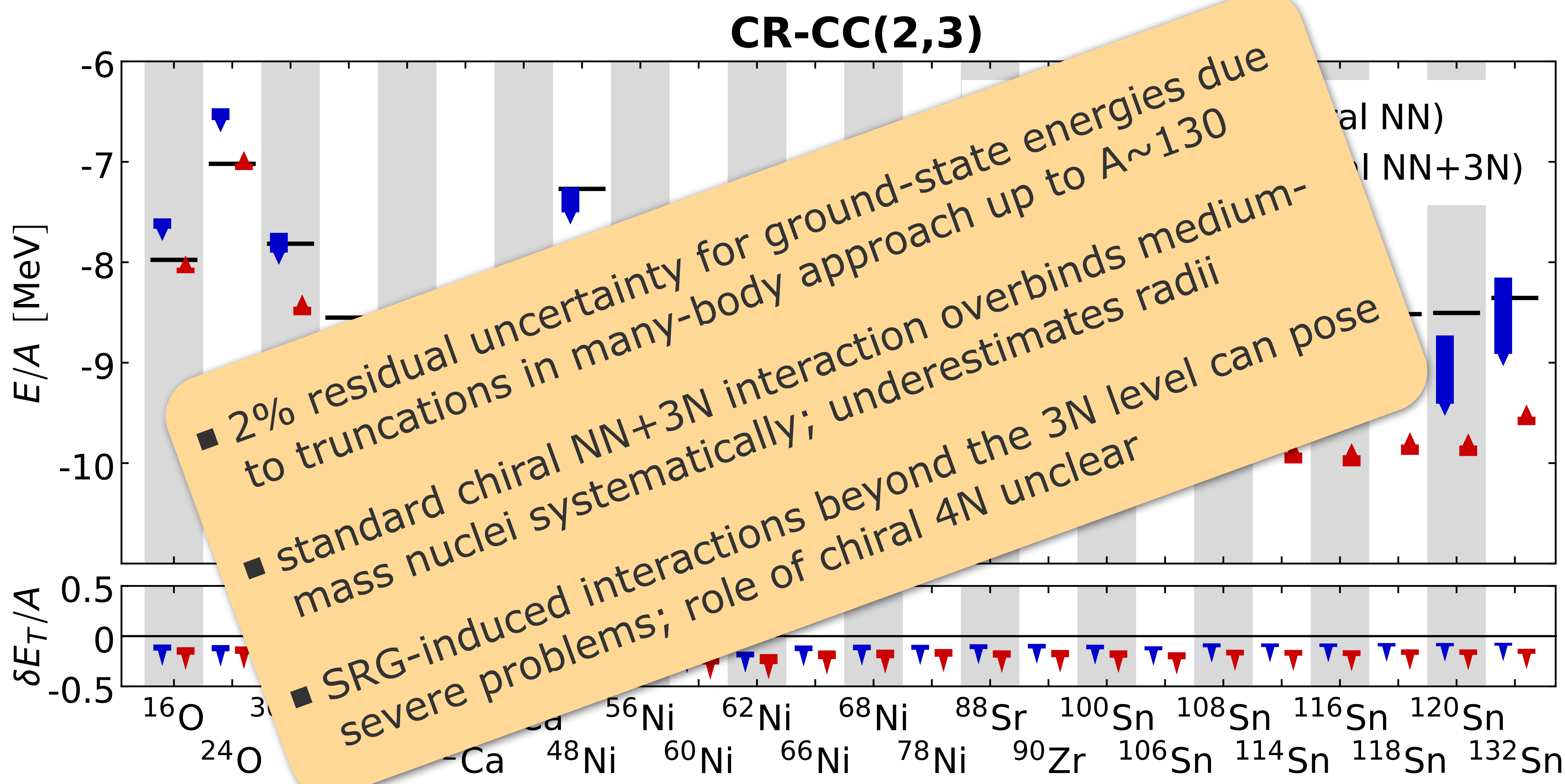
Binder et al., PLB 736, 119 (2014)



$\Lambda_{3N} = 400$ MeV, $\alpha = 0.08 \rightarrow 0.04\,\text{fm}^4$, $E_{3\,max} = 18$, optimal $\hbar\Omega$

Towards Heavy Nuclei - Ab Initio

Binder et al., PLB 736, 119 (2014)

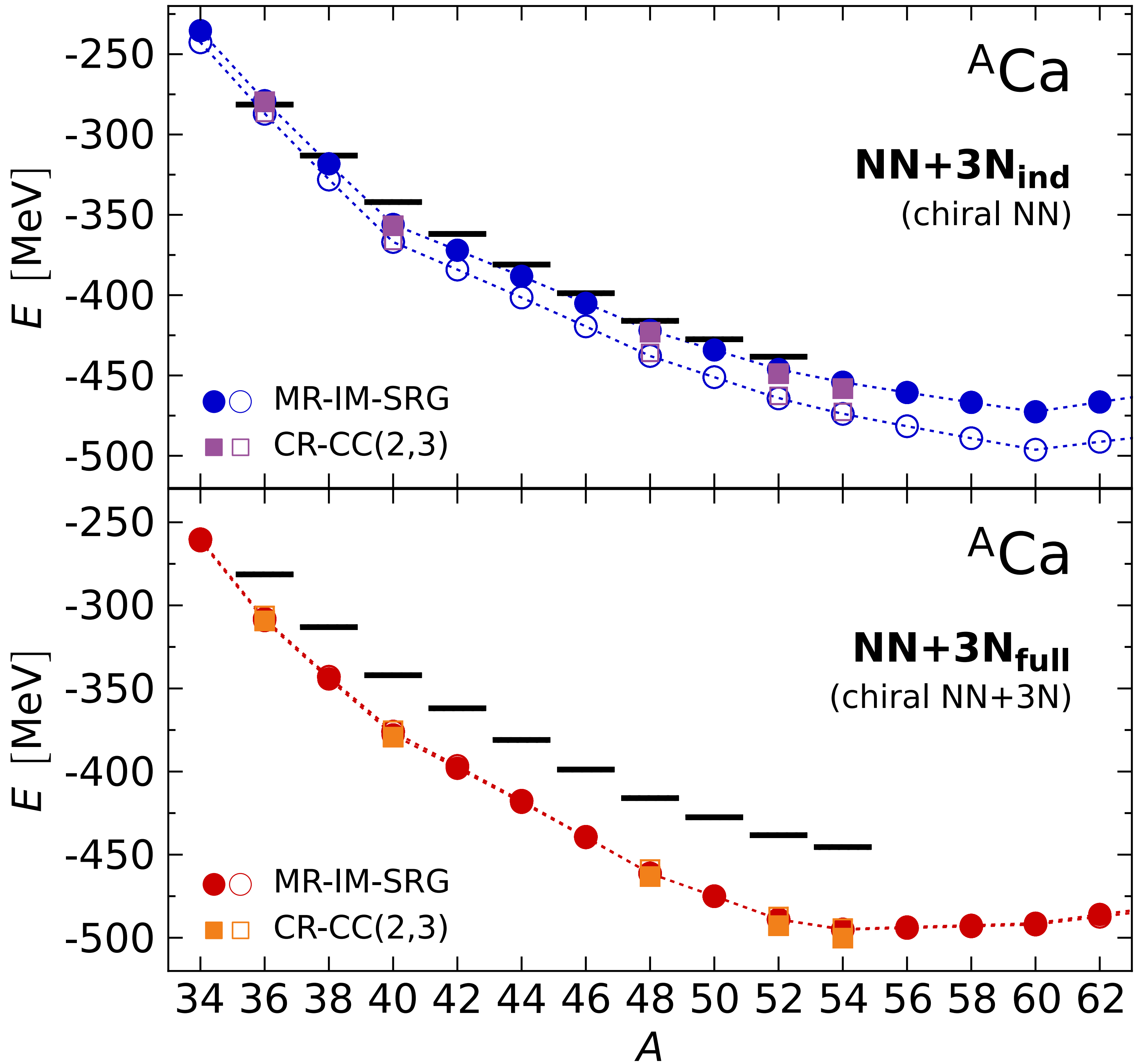


- 2% residual uncertainty for ground-state energies due to truncations in many-body approach up to A~130
- standard chiral NN+3N interaction overbinds medium-mass nuclei systematically; underestimates radii
- SRG-induced interactions beyond the 3N level can pose severe problems; role of chiral 4N unclear

$\Lambda_{3N} = 400$ MeV, $\alpha = 0.08 \rightarrow 0.04\,\mathrm{fm}^4$, $E_{3\,max} = 18$, optimal $\hbar\Omega$

Open-Shell Medium-Mass Nuclei

Hergert et al., PRC 90, 041302(R) (2014)

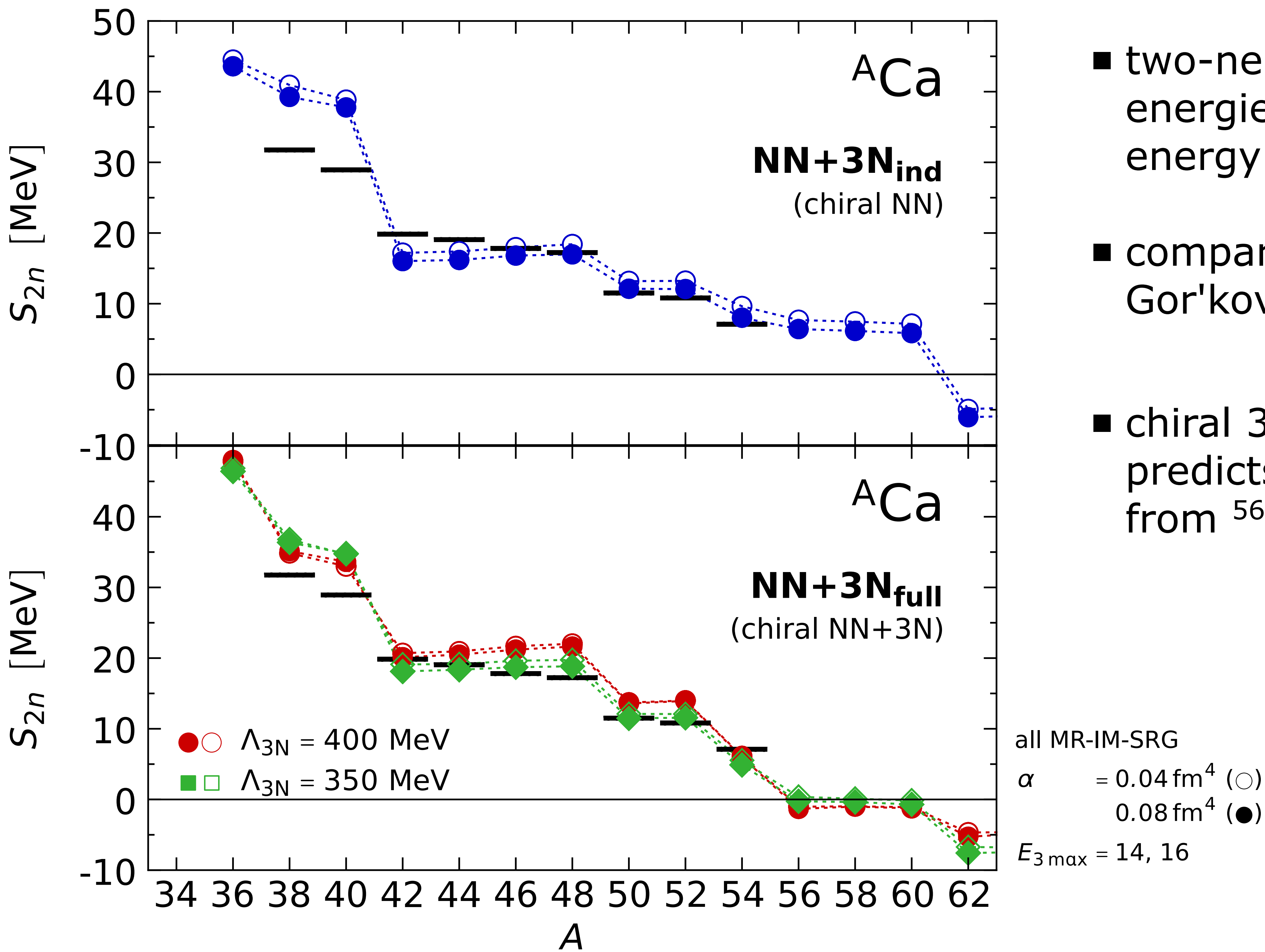


- systematic MR-IM-SRG study of even Ca and Ni isotopes
- excellent agreement with best available coupled-cluster results
- chiral 3N interaction changes behavior at and beyond ^{54}Ca

Λ_{3N} = 400 MeV
α = 0.04 fm^4 (○)
0.08 fm^4 (●)
$E_{3\,max}$ = 14, 16

Open-Shell Medium-Mass Nuclei

Hergert et al., PRC 90, 041302(R) (2014)



- two-neutron separation energies hide overall energy shift
- compares well to updated Gor'kov-GF results *[priv. comm. V. Soma]*
- chiral 3N interaction predicts flat "drip-region" from ^{56}Ca to ^{60}Ca

Conclusions

Ab Initio Frontiers

- **ab initio theory is entering new territory...**
  - **QCD frontier**
    nuclear structure connected systematically to QCD via chiral EFT
  - **precision frontier**
    precision spectroscopy of light nuclei, including current contributions
  - **mass frontier**
    ab initio calculations up to heavy nuclei with quantified uncertainties
  - **open-shell frontier**
    extend to medium-mass open-shell nuclei and their excitation spectrum
  - **continuum frontier**
    include continuum effects and scattering observables consistently
  - **strangeness frontier**
    ab initio predictions for hyper-nuclear structure & spectroscopy

...providing a coherent theoretical framework for nuclear structure & reaction calculations

Epilogue

- **thanks to my group and my collaborators**
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JUROPA — JÜLICH FORSCHUNGSZENTRUM

LOEWE-CSC — CSC Center for Scientific Computing Frankfurt

EDISON — NERSC

COMPUTING TIME

SFB 634

Deutsche Forschungsgemeinschaft DFG

HIC for FAIR Helmholtz International Center

LOEWE Exzellente Forschung für Hessens Zukunft

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