Nuclei as Bound States

Lecture 1: Hamiltonian

Robert Roth

TECHNISCHE
UNIVERSITÄT
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Overview

- **Lecture 1: Hamiltonian**

  Prelude • Nuclear Hamiltonian • Matrix Elements • Two-Body Problem • Correlations & Unitary Transformations

- **Lecture 2: Light Nuclei**

  Similarity Renormalization Group • Many-Body Problem • Configuration Interaction • No-Core Shell Model • Hypernuclei

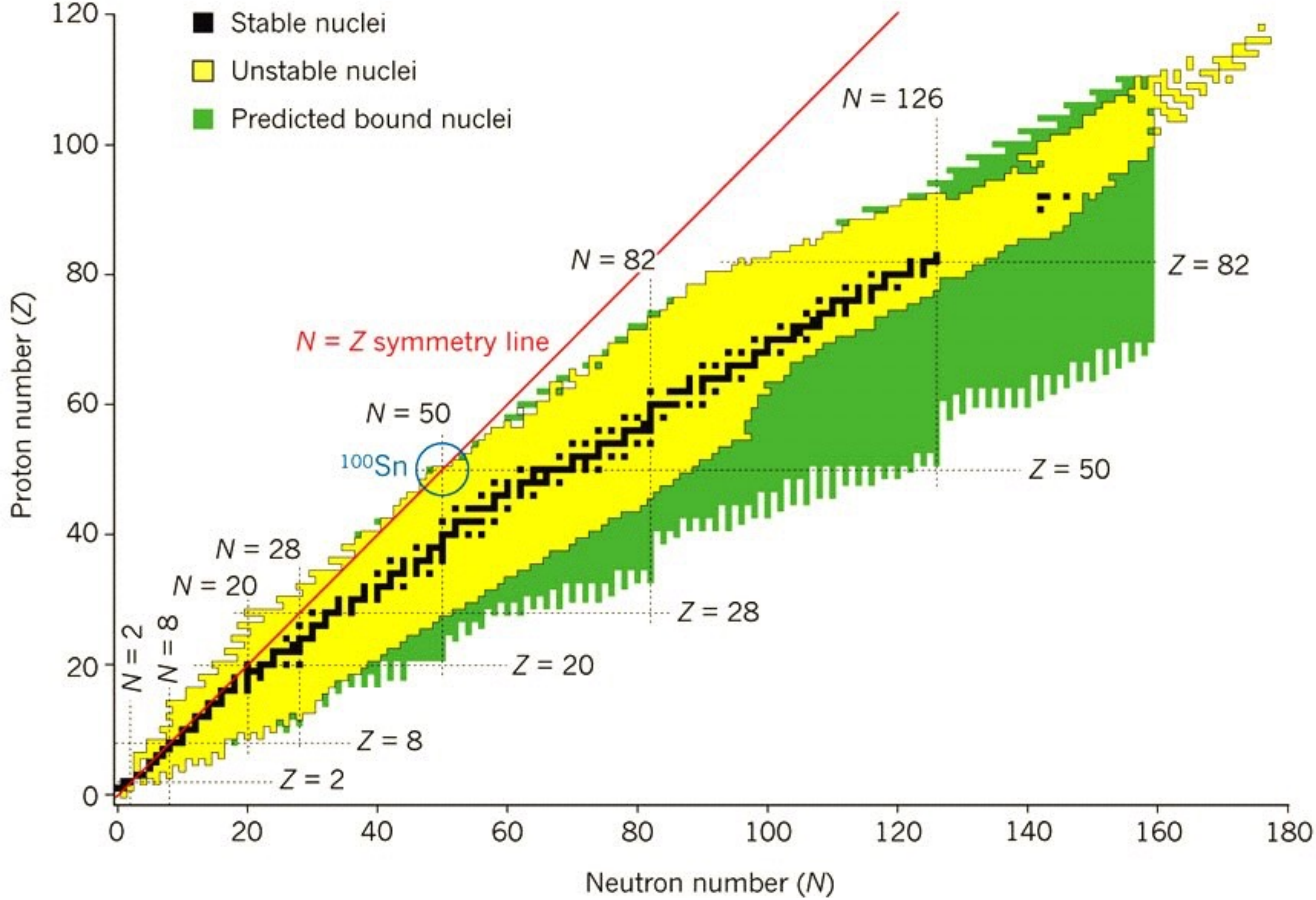
- **Lecture 3: Beyond Light Nuclei**

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

Prelude

Playground

Bazin, Nature 486, 330 (2012)



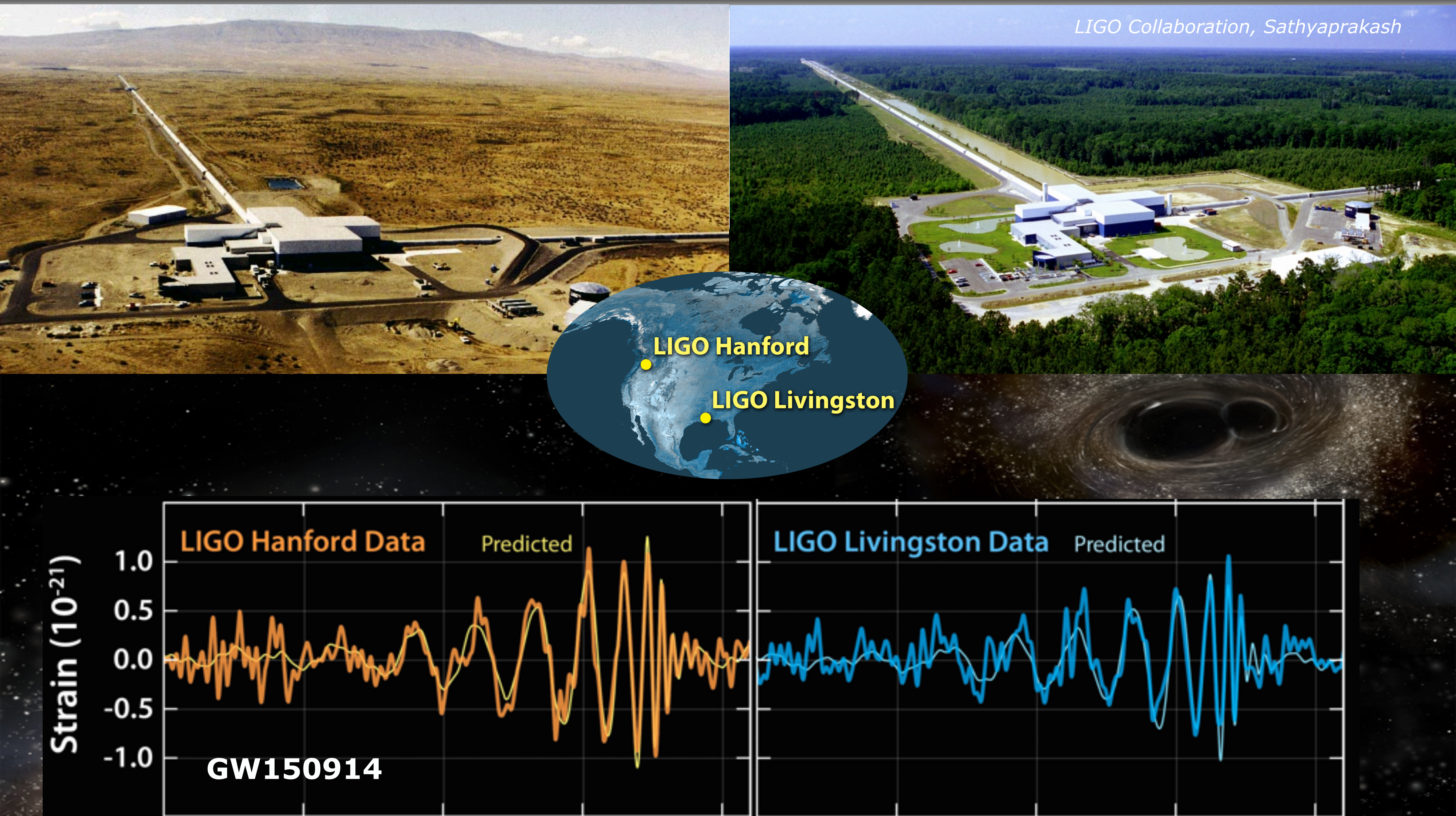
Why Should We Care?

properties of stable and exotic nuclei impact the world at large

nuclear structure meets astrophysics

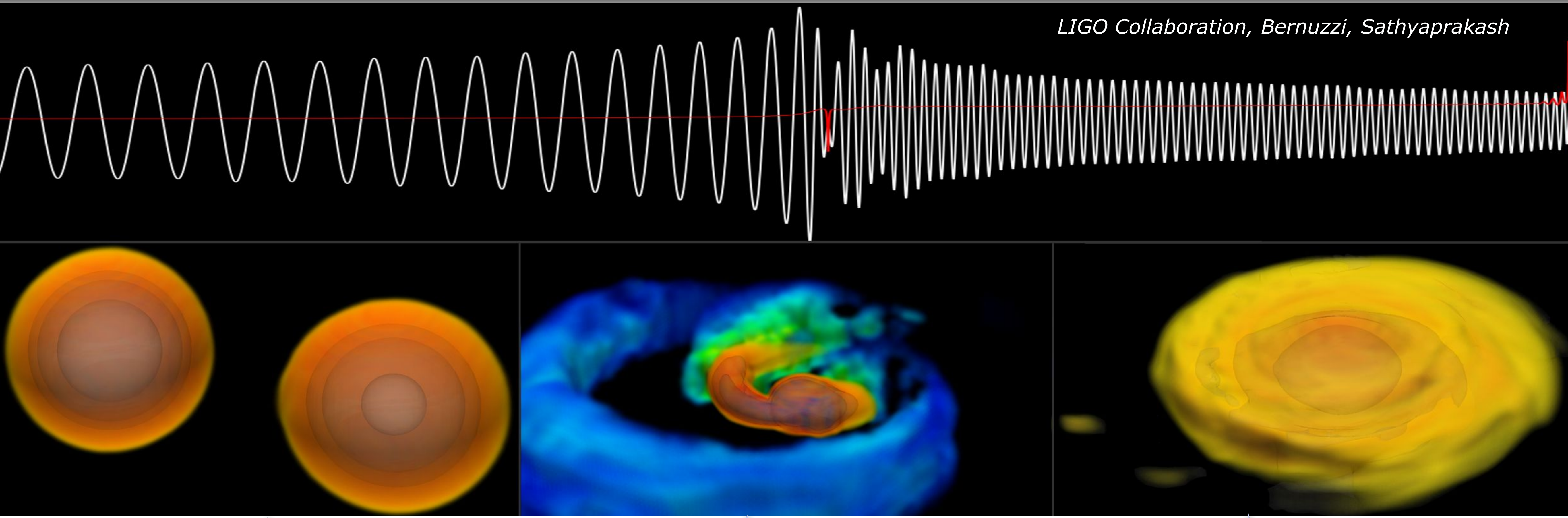
- life and burning cycles of stars
- death of stars: supernova explosions
- nucleosynthesis
- mass, size and structure of neutron stars
- transients: kilo-novae, gamma-ray bursts,…

LIGO: Gravitational Waves



Abbott et al., PRL 116, 061102 (2016)

Neutron Star Mergers



Inspiral Phas

maximum mass and s
neutron stars determir
the equation of stat
neutron-rich matt

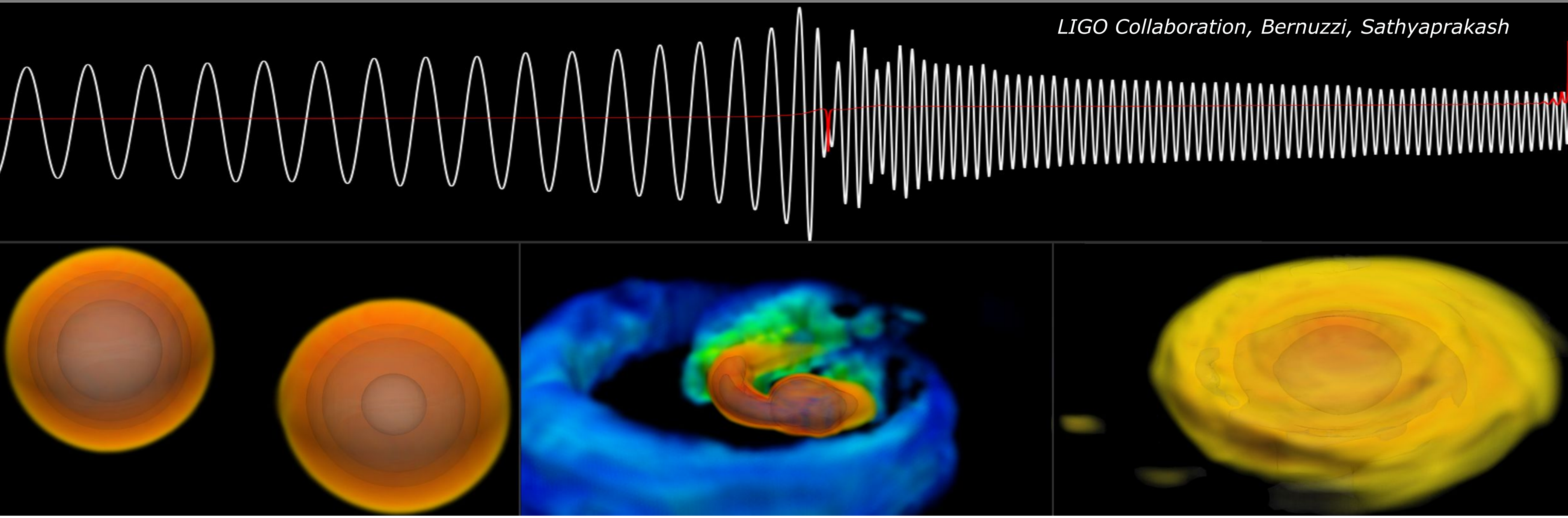
Merger Phase

neutron-rich material is
ejected; rapid neutron-captu
process; synthesis of heavy
elements

Ringdown Phase

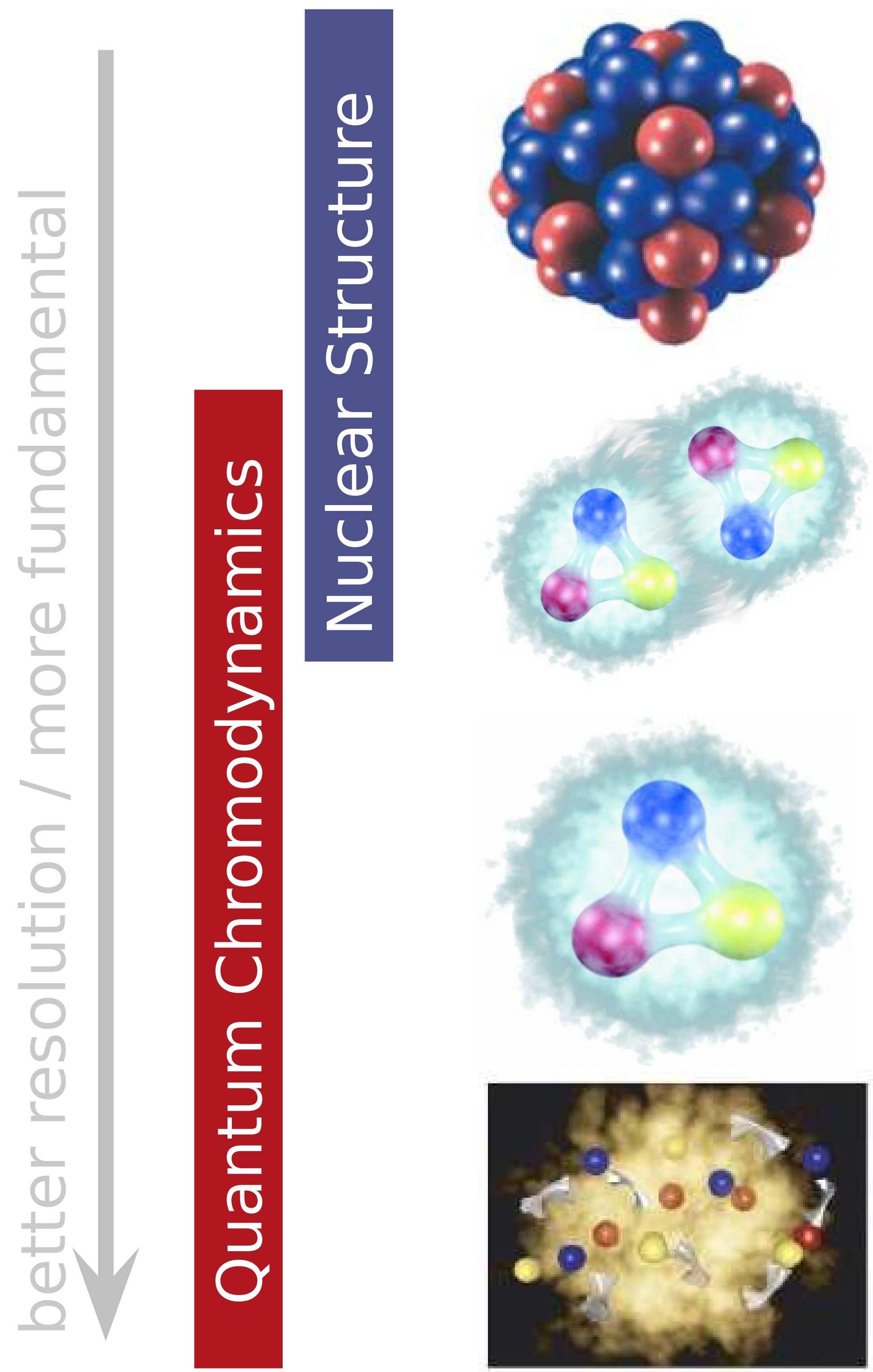
equation of state of
neutron-rich matter
determines ringdown
dynamics

Neutron Star Mergers



structure of nuclei and nuclear matter at the extremes, often beyond the reach of laboratory experiments

Theoretical Context



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

New Era of Nuclear Structure Theory

- **QCD at low energies**

  improved understanding through lattice simulations & effective field theories

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  advances in ab initio treatment of the nuclear many-body problem

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- **computing and algorithms**

  increase of computational resources and developments of algorithms

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  advances in ab initio treatment of the nuclear many-body problem

- **computing and algorithms**

  increase of computational resources and developments of algorithms

- **experimental facilities**

  amazing perspectives for the exploration of nuclei far-off stability

The Problem

$$\mathrm{H}\;|\Psi_n\rangle = E_n\,|\Psi_n\rangle$$

Assumptions

- use nucleons as effective degrees of freedom
- use non-relativistic framework, relativistic corrections are absorbed in Hamiltonian
- use Hamiltonian formulation, i.e., conventional many-body quantum mechanics
- focus on bound states, though continuum aspects are very interesting

The Problem

$$\mathrm{H}\,|\Psi_n\rangle = E_n\,|\Psi_n\rangle$$

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,…

Nuclear Hamiltonian

Nuclear Hamiltonian

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

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

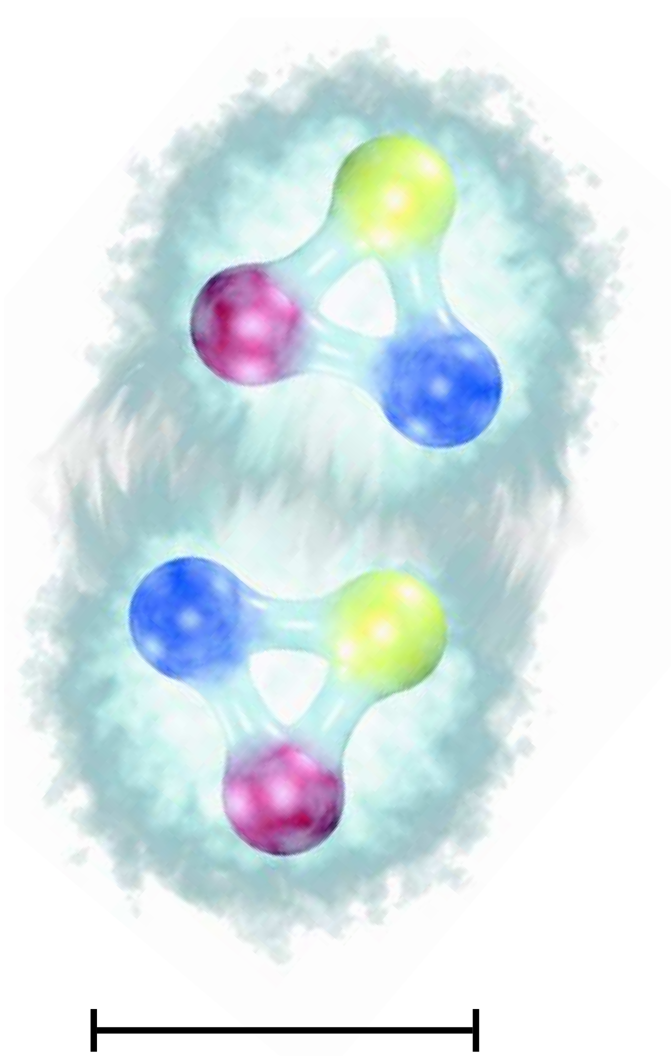
- **intrinsic Hamiltonian** is invariant under translation, rotation, Galilei boost, parity, time evolution, time reversal,...

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

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

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

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

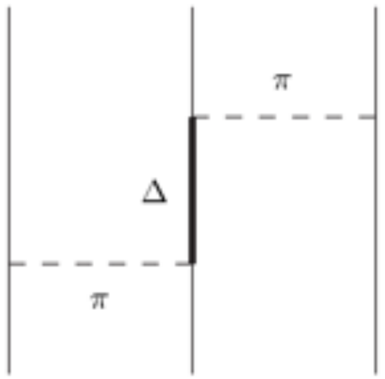
Yesterday... from Phenomenology

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-ran... ...erms, local operator form
  - **CD Bonn 2000**: more systematic ... ...hange parametrization including pseudo-scalar, scalar ... ... inherently nonlocal

no consistency
no systematics
no connection to QCD

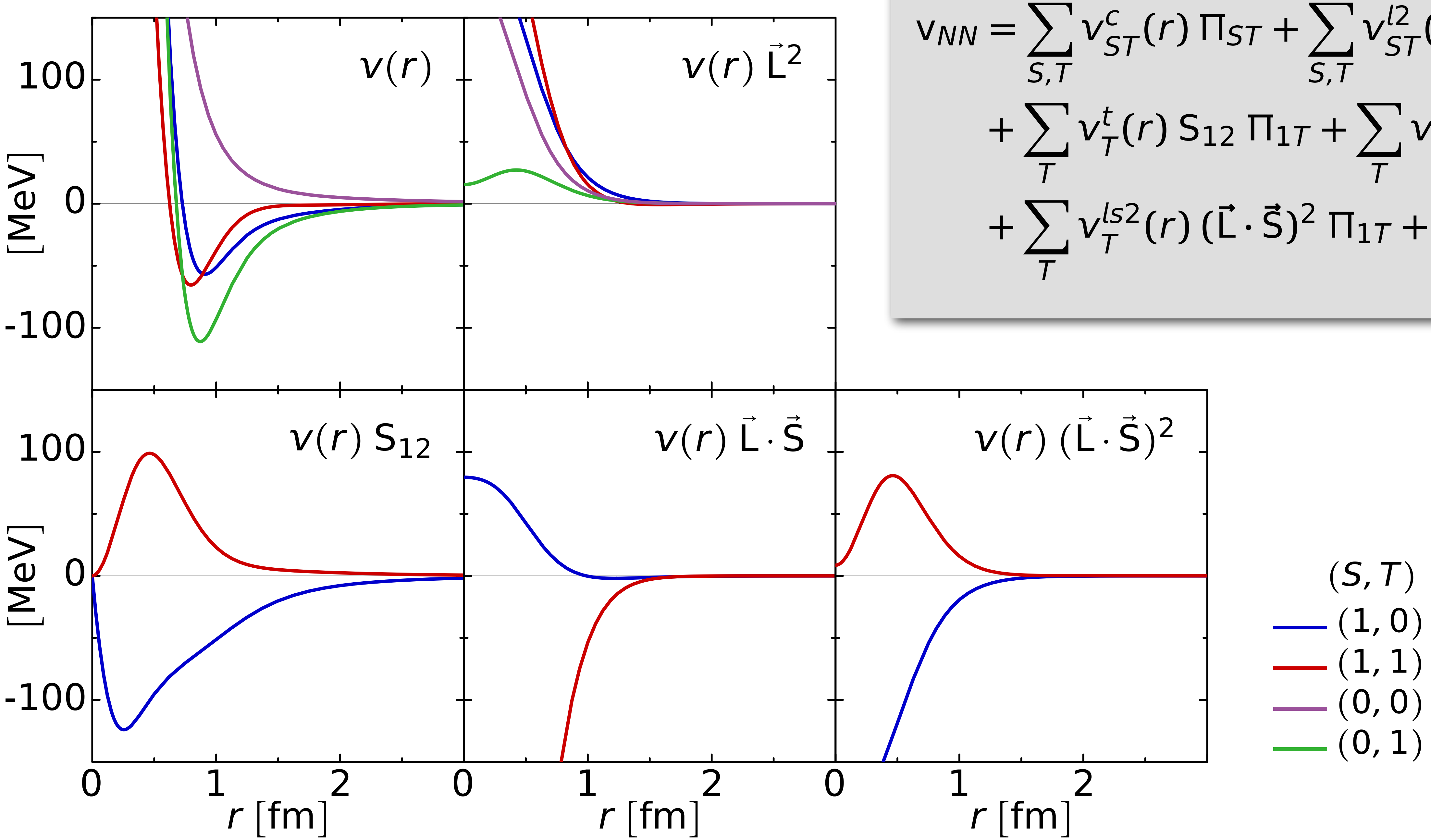
- parameters of the NN ... ...N **phase shifts** up to ~300 MeV and reproduce the ...
- supplemented by **phe... ...ological 3N interactions** consisting of a Fujita-M...zawa-type term plus various hand-picked contributions



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

Argonne V18 Potential

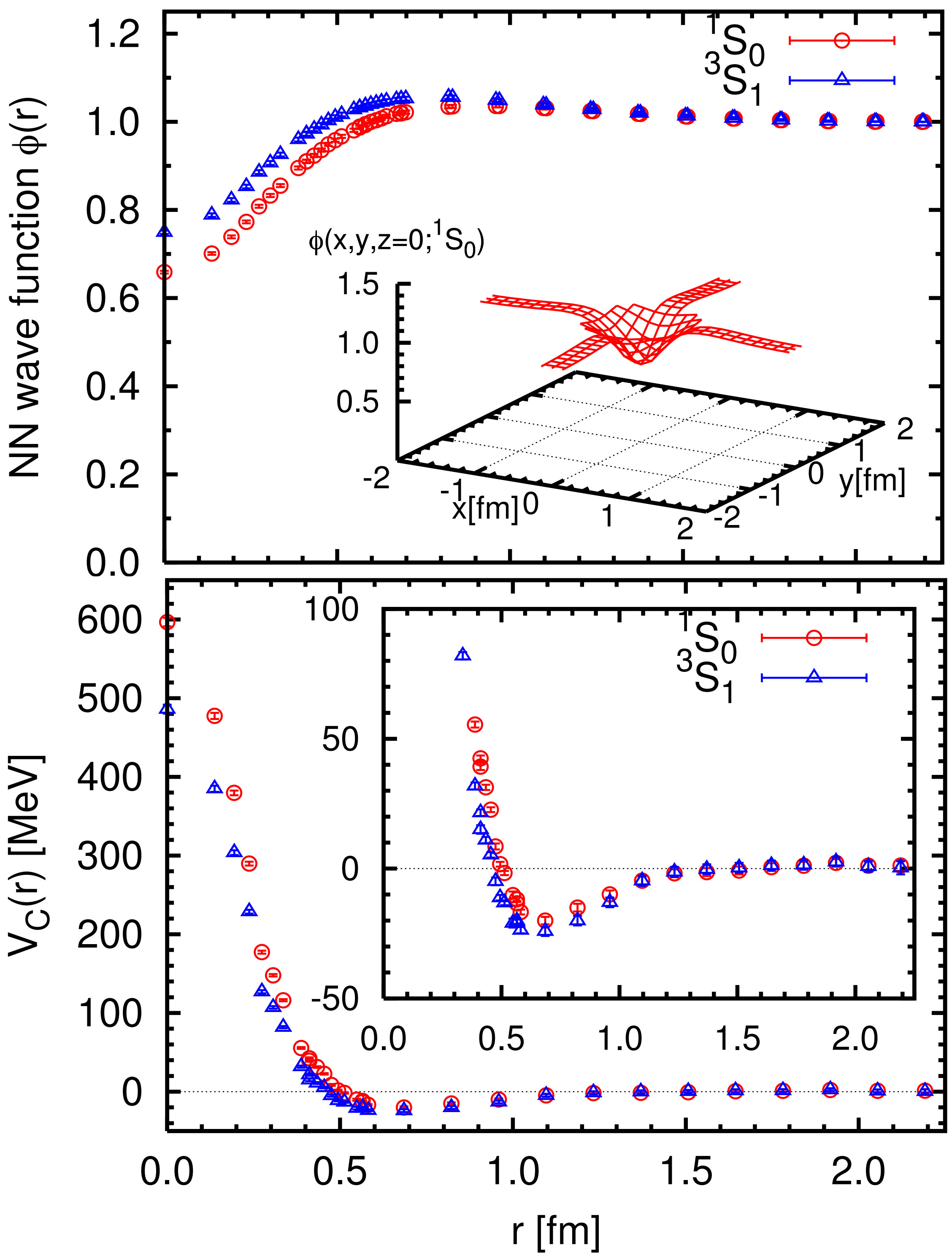
Wiringa, et al., PRC 51, 38 (1995)



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

Tomorrow... from Lattice QCD

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



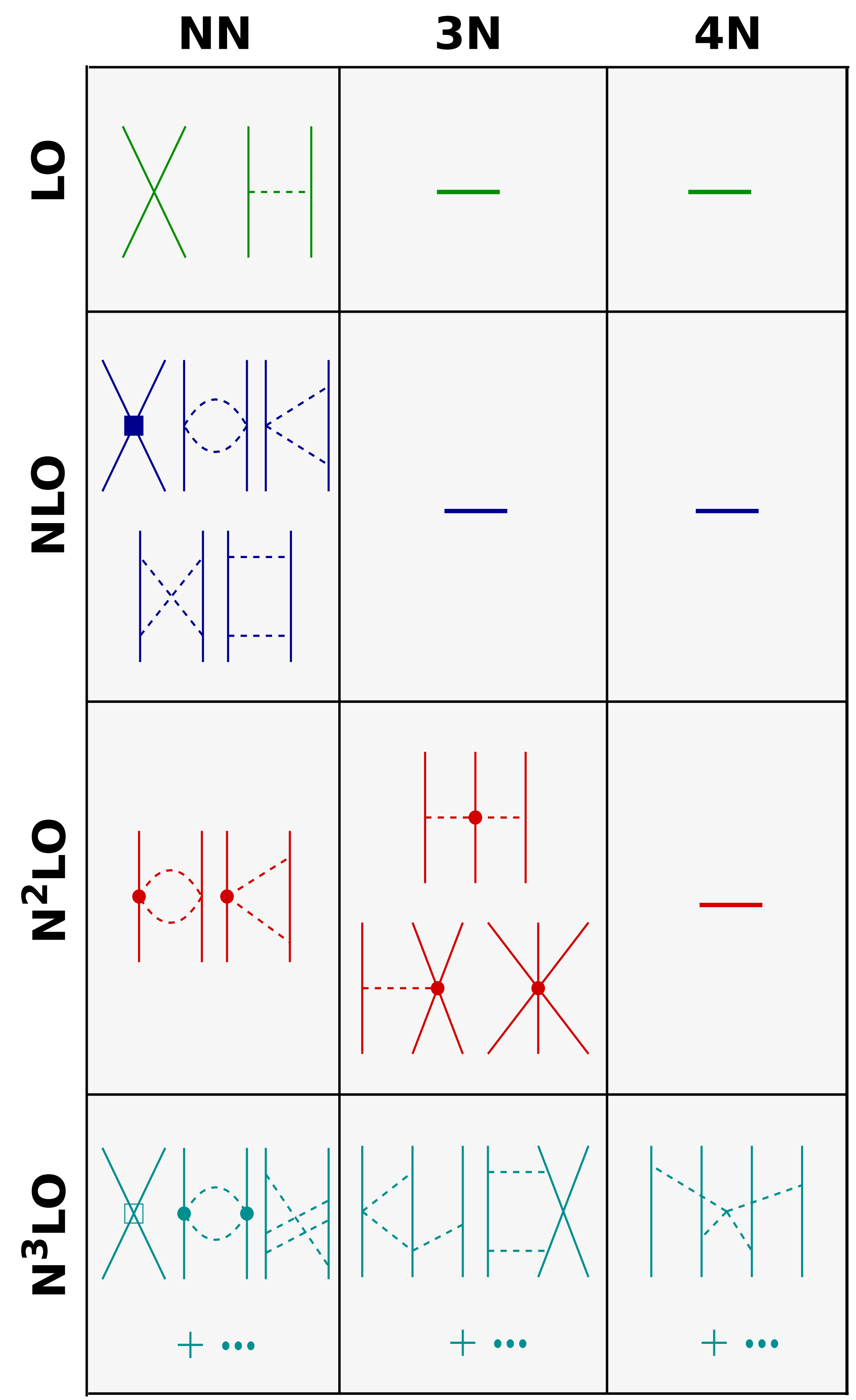
N. Ishii et al., PRL 99, 022001 (2007)

- 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…

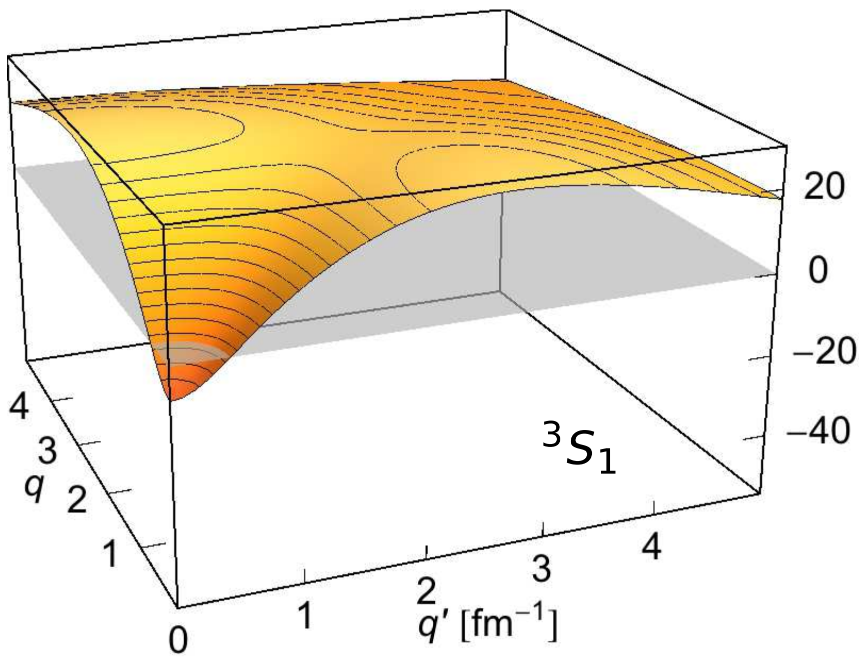
Momentum-Space Matrix Elements

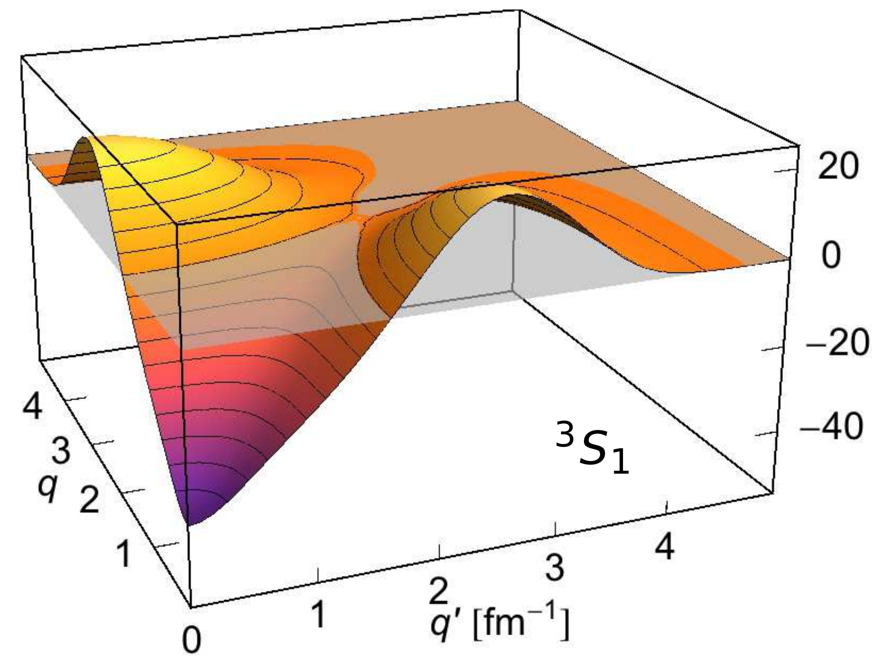
$$\langle q(LS)JM;TM_T|\,\mathrm{v}_{NN}\,|q'(L'S)JM;TM_T\rangle$$

Argonne V18

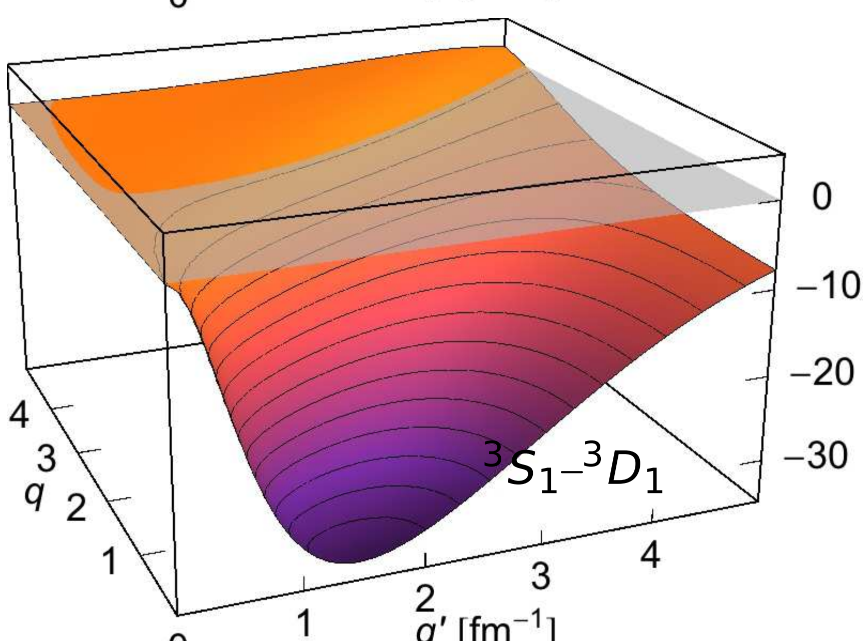
chiral NN
(N3LO, E&M, 500 MeV)

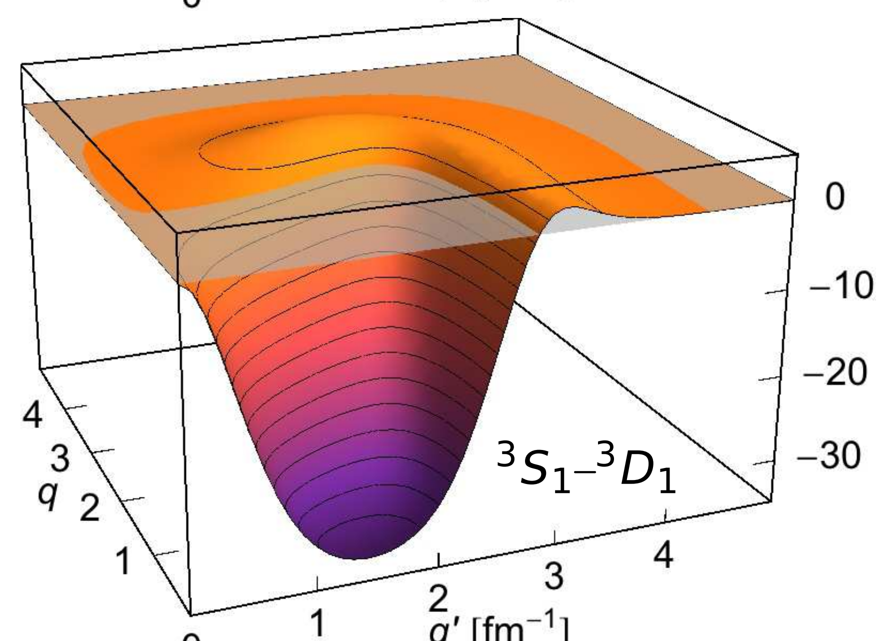
J=1
L=0
L′=0
S=1
T=0





J=1
L=0
L′=2
S=1
T=0





Matrix Elements

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
$\|\text{spin}\rangle = \|s = \tfrac{1}{2}, m_s\rangle$	eigenstates of s^2 and s_z with s=1/2
$\|\text{isospin}\rangle = \|t = \tfrac{1}{2}, m_t\rangle$	eigenstates of t^2 and t_3 with t=1/2

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

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

Many-Body Basis

- **Slater determinants**: antisymmetrized A-body product states

$$|\alpha_1\alpha_2\ldots\alpha_A\rangle = \frac{1}{\sqrt{A!}}\sum_{\pi}\text{sgn}(\pi)\,\mathrm{P}_{\pi}\left(|\alpha_1\rangle\otimes|\alpha_2\rangle\otimes\cdots\otimes|\alpha_A\rangle\right)$$

- convenient to work with **second quantization**: string of creation operators acting on vacuum state

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

- 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**

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

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

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:	$\vert q\,(LS)\,JT\rangle$
two-body relative HO:	$\vert N\,(LS)\,JT\rangle$
three-body Jacobi momentum:	$\vert \pi_1\pi_2;\,[(L_1S_1)\,J_1,(L_2\tfrac{1}{2})\,J_2]\,J_{12};(T_1\tfrac{1}{2})\,T_{12}\rangle$
three-body Jacobi HO:	$\vert N_1N_2;\,[(L_1S_1)\,J_1,(L_2\tfrac{1}{2})\,J_2]\,J_{12};(T_1\tfrac{1}{2})\,T_{12}\rangle$
antisym. three-body Jacobi HO:	$\vert E_{12}\,i\,J_{12}^{\pi}\,T_{12}\rangle$

- lots of **transformations** between the different bases are needed in practice
- **exception**: Quantum Monte-Carlo methods working in coordinate representation need local operator form

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

$$\langle N\,(LS)\,JM;TM_T|\,v_{NN}\,|N'\,(L'S')\,J'M';T'M_T'\rangle$$

- 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

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

- 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 **Moshinsky-transformation**

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

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 (e.g. Similarity Renormalization Group)

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

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**

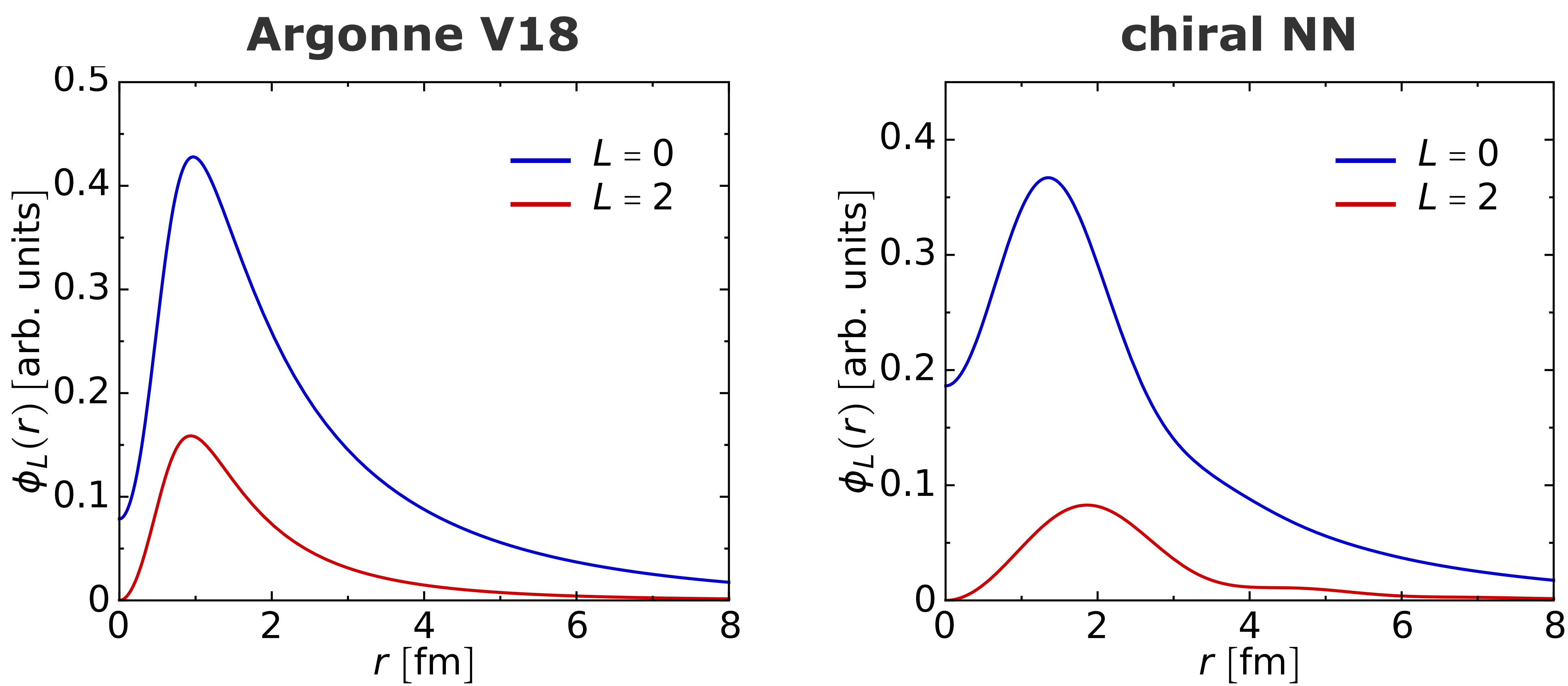
$$\left(\begin{array}{c|c} \langle N'(01)\ldots|\,\text{H}_{\text{int}}\,|N(01)\ldots\rangle & \langle N'(01)\ldots|\,\text{H}_{\text{int}}\,|N(21)\ldots\rangle \\ \hline \langle N'(21)\ldots|\,\text{H}_{\text{int}}\,|N(01)\ldots\rangle & \langle N'(21) \ldots \end{array}\right) \left(\begin{array}{c}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

simplest possible Jacobi-NCSM calculation

- eigenvectors [illegible] coefficients and eigenvalues the energies

- **truncate** [illegible] **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 &
Unitary Transformations

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

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

$$\mathrm{H}\,|\psi\rangle = E\,|\psi\rangle \qquad\qquad 1 = \mathrm{U}^\dagger\mathrm{U} = \mathrm{U}\mathrm{U}^\dagger$$

$$\mathrm{U}^\dagger\mathrm{H}\mathrm{U}\,\mathrm{U}^\dagger\,|\psi\rangle = E\,\mathrm{U}^\dagger\,|\psi\rangle \qquad \text{with} \qquad \tilde{\mathrm{H}} = \mathrm{U}^\dagger\mathrm{H}\mathrm{U}$$

$$\tilde{\mathrm{H}}\,|\tilde{\psi}\rangle = E\,|\tilde{\psi}\rangle \qquad\qquad |\tilde{\psi}\rangle = \mathrm{U}^\dagger\,|\psi\rangle$$

- 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

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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

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

  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

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

- 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 $|Ei J^\pi T\rangle$

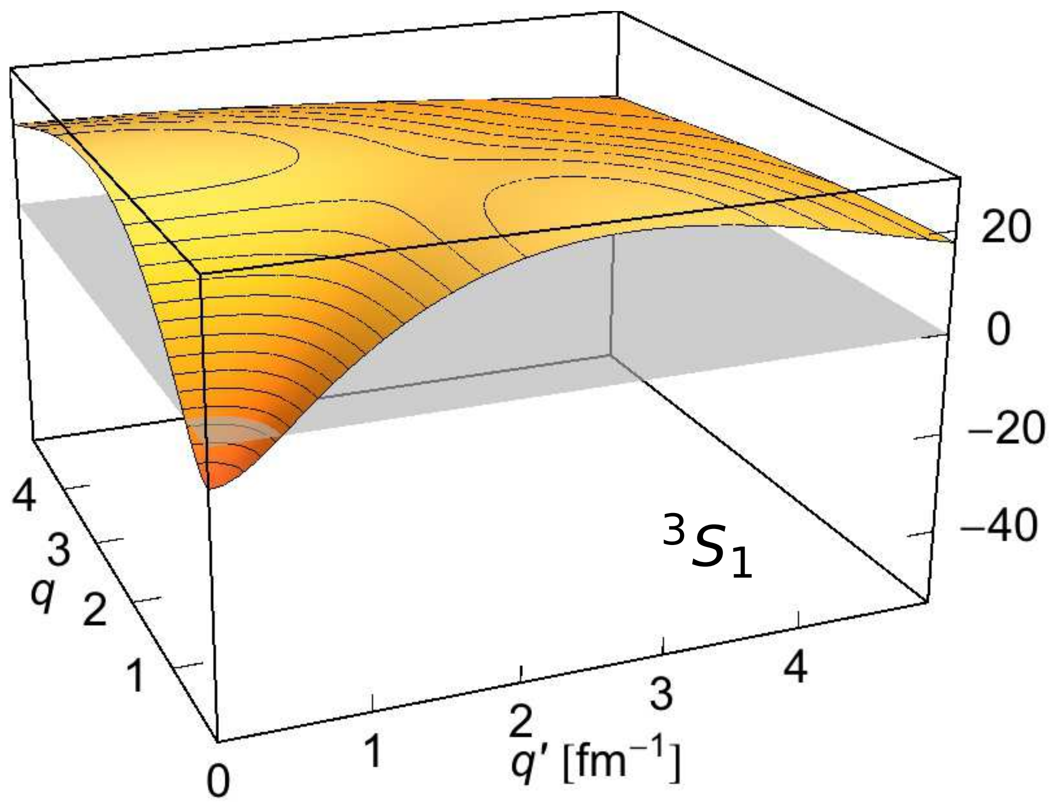
- matrix-evolution equations for n=3 with antisym. three-body Jacobi HO states:

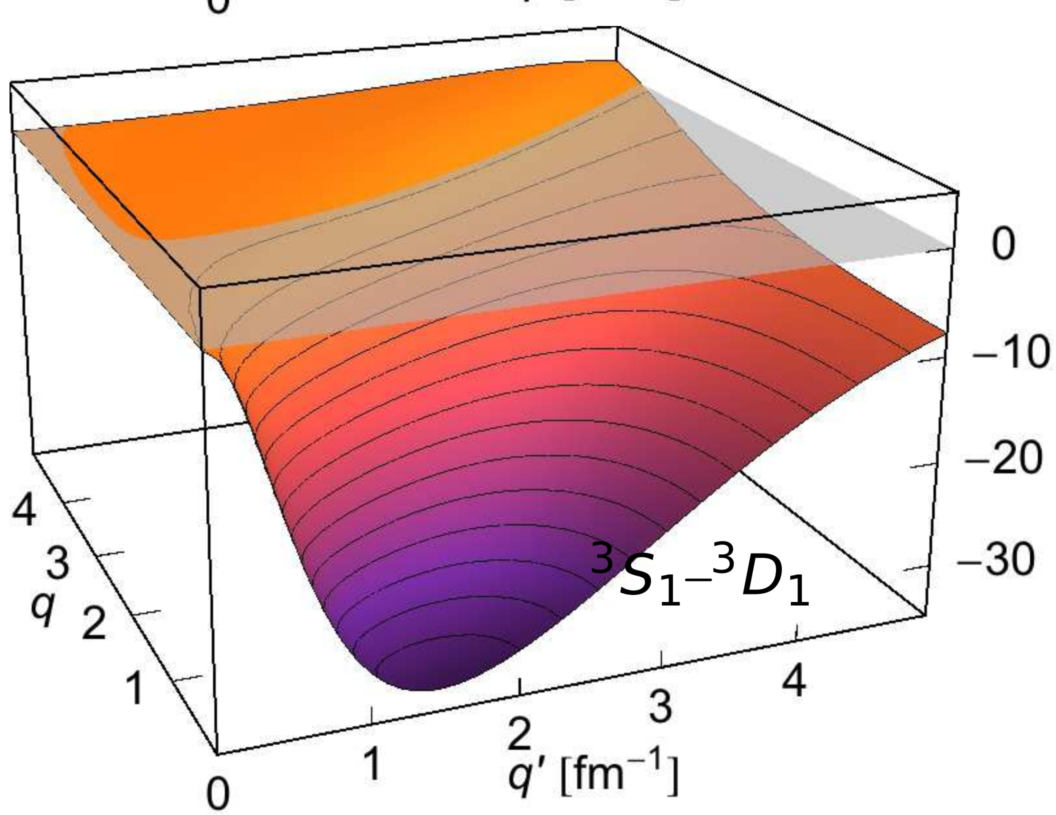
$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}\alpha}\langle E i J^\pi T|\,\mathrm{H}_\alpha\,|E' i' J^\pi T\rangle = (2\mu)^2 \sum_{E'',i''}^{E_{\mathrm{SRG}}}\sum_{E''',i'''}^{E_{\mathrm{SRG}}} \Big[& \langle E i \ldots|\,\mathrm{T}_{\mathrm{int}}\,|E'' i'' \ldots\rangle\,\langle E'' i'' \ldots|\,\mathrm{H}_\alpha\,|E'''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

- **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

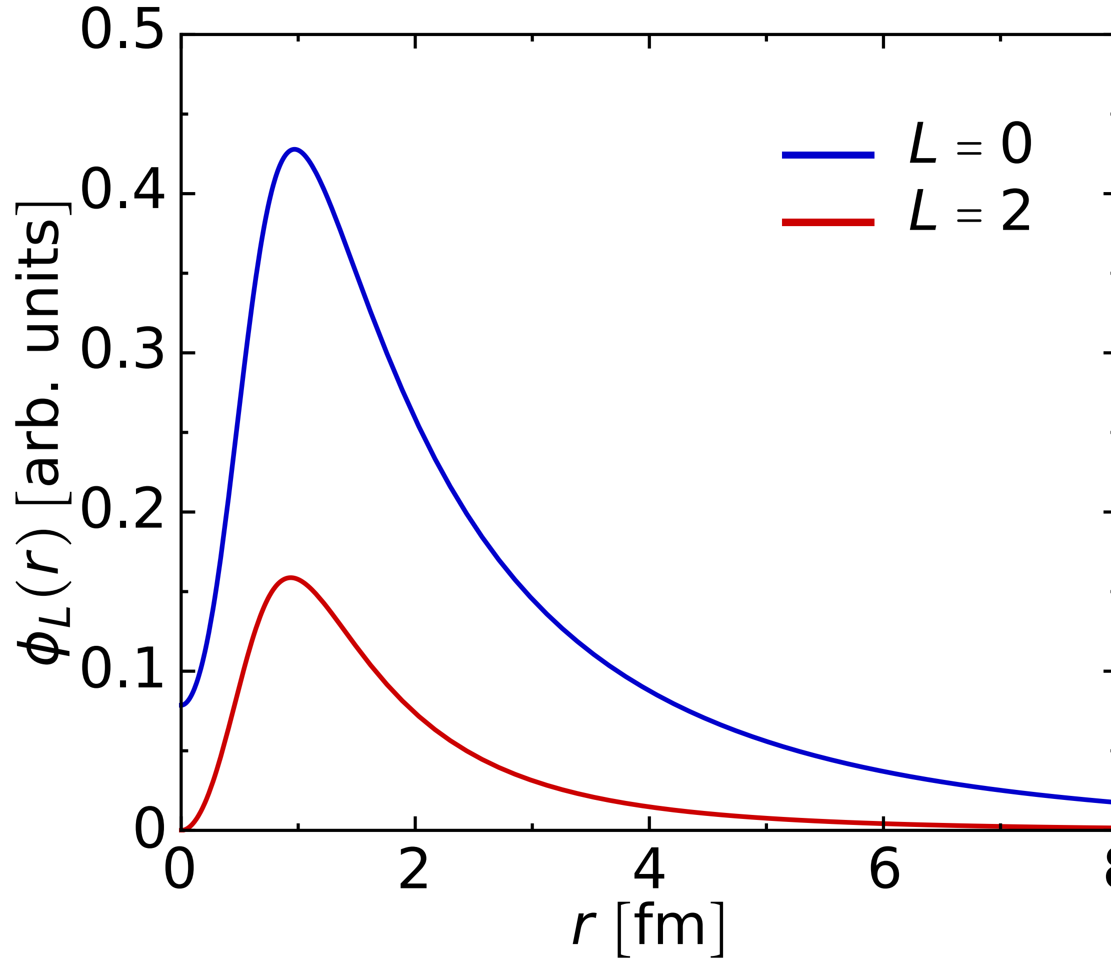




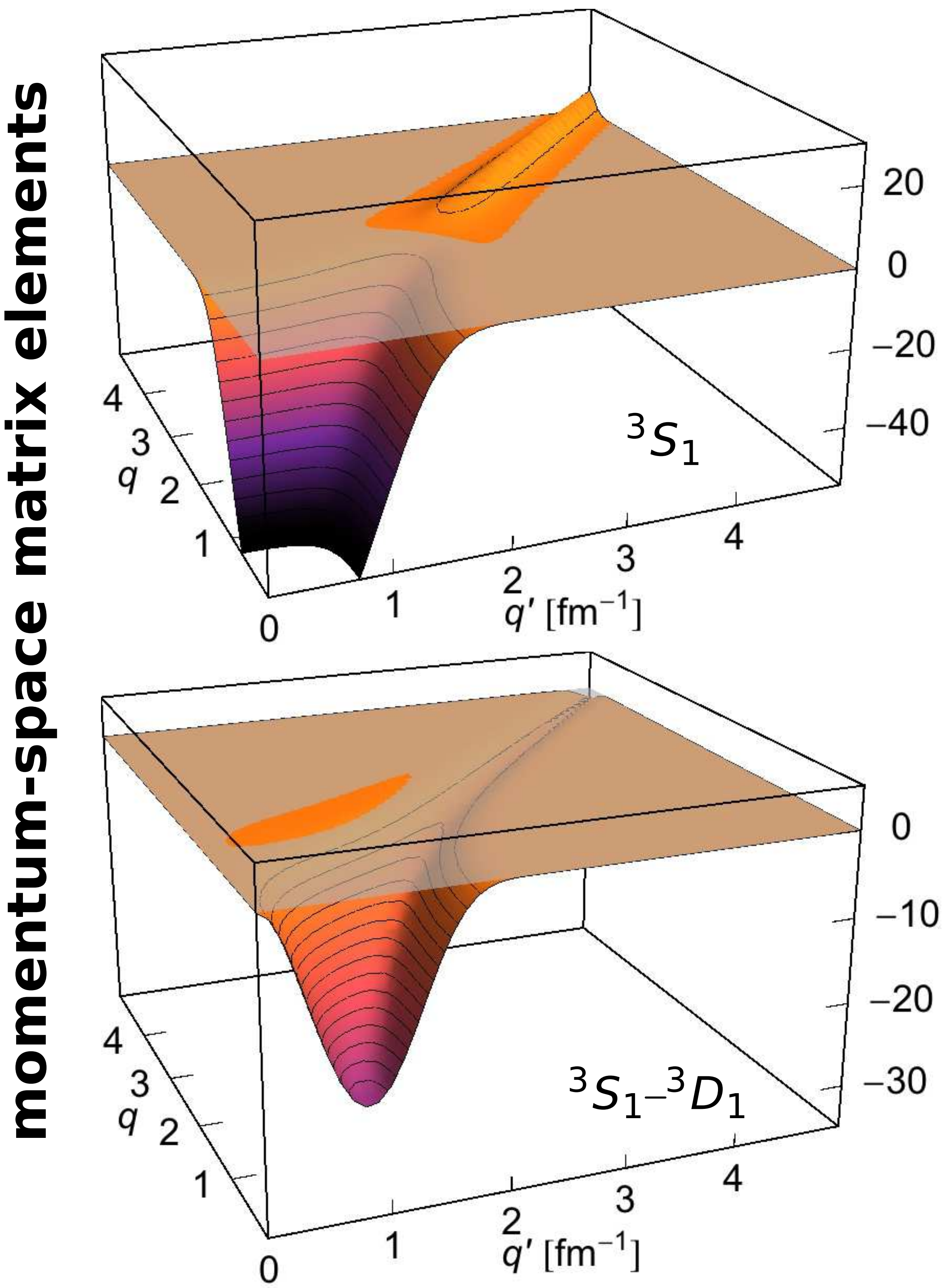
Argonne V18

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

deuteron wave-function



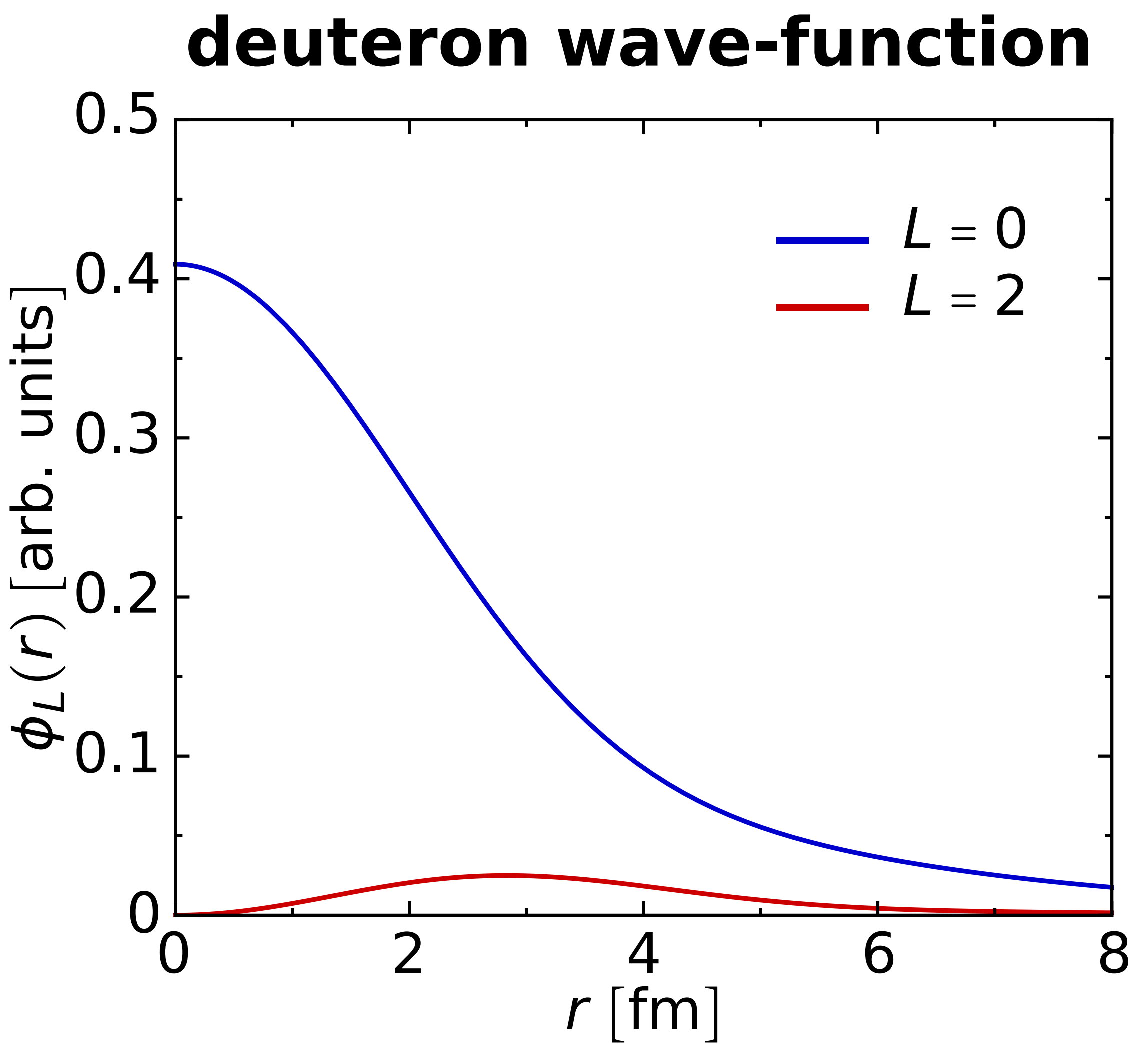
SRG Evolution in Two-Body Space



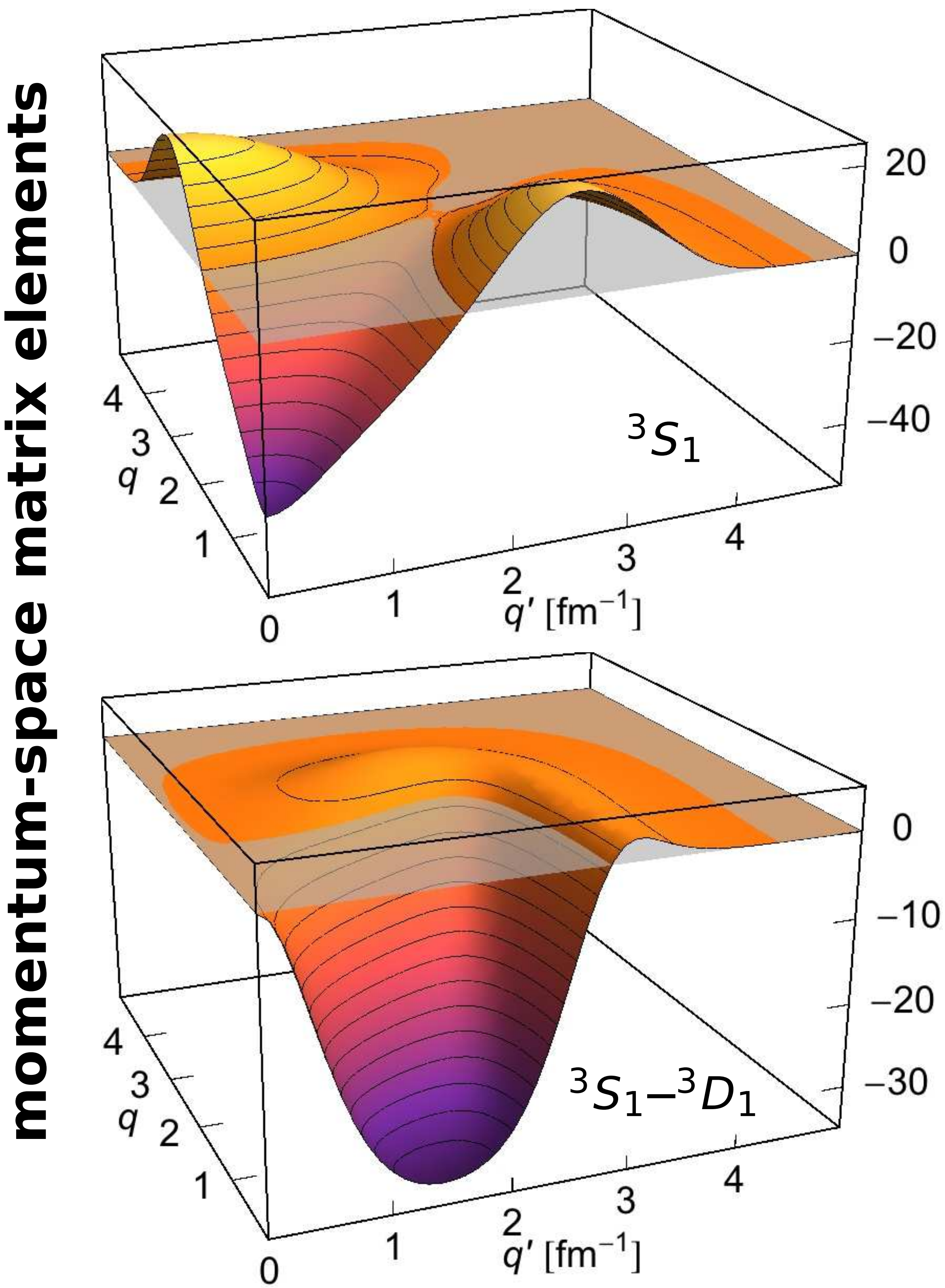
$\alpha = 0.320\,\mathrm{fm}^4$

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

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



SRG Evolution in Two-Body Space

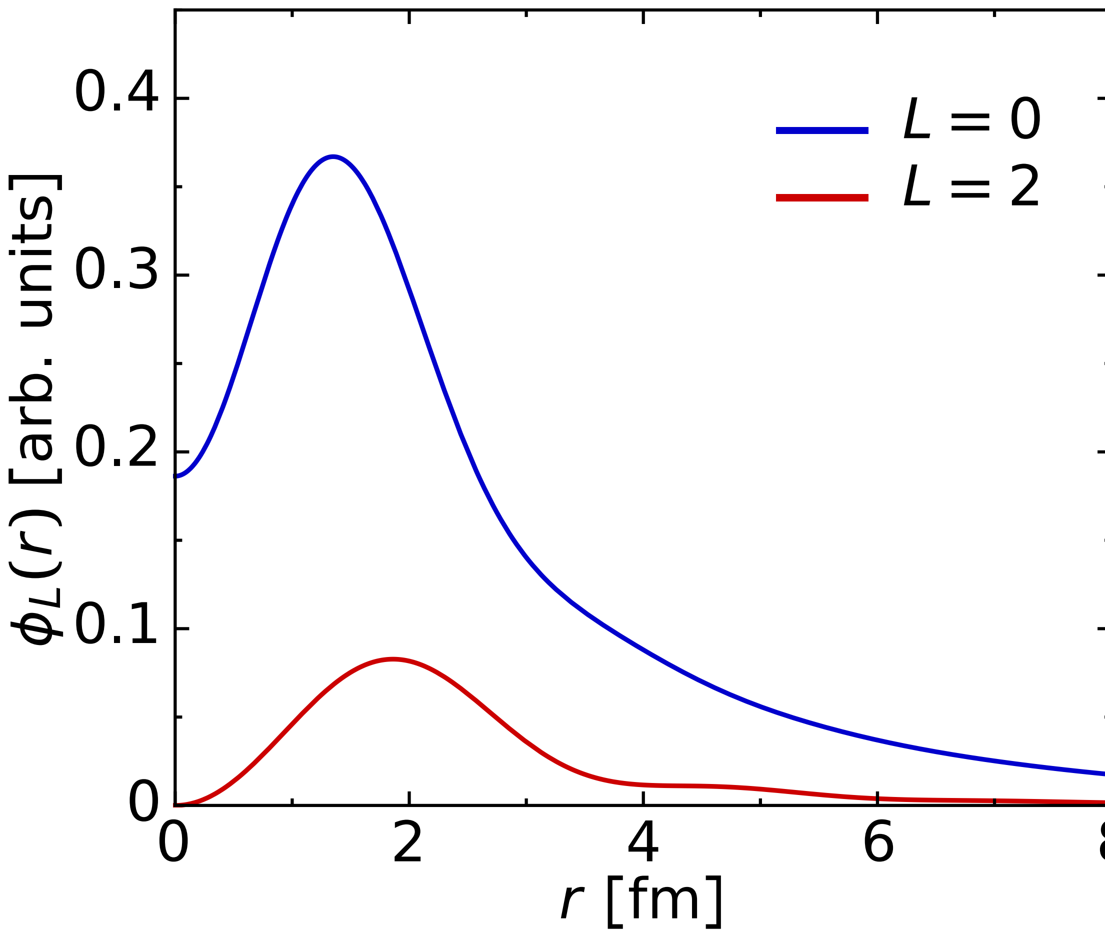


chiral NN

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

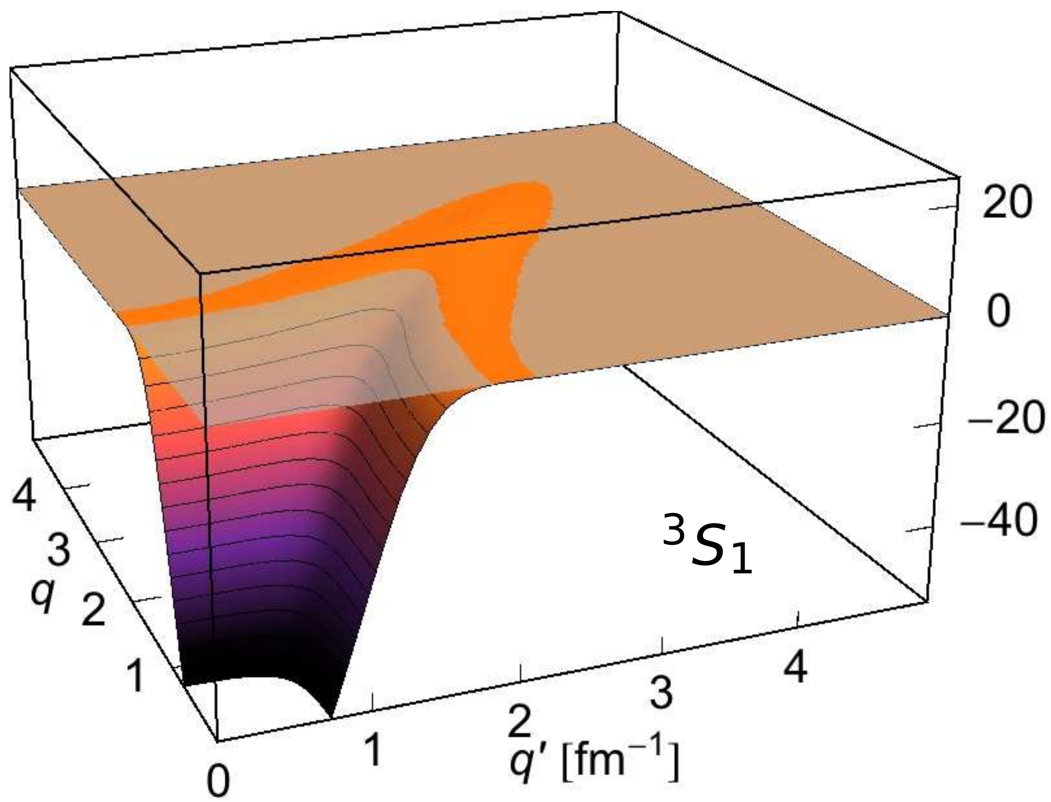
$J^\pi = 1^+, T = 0$

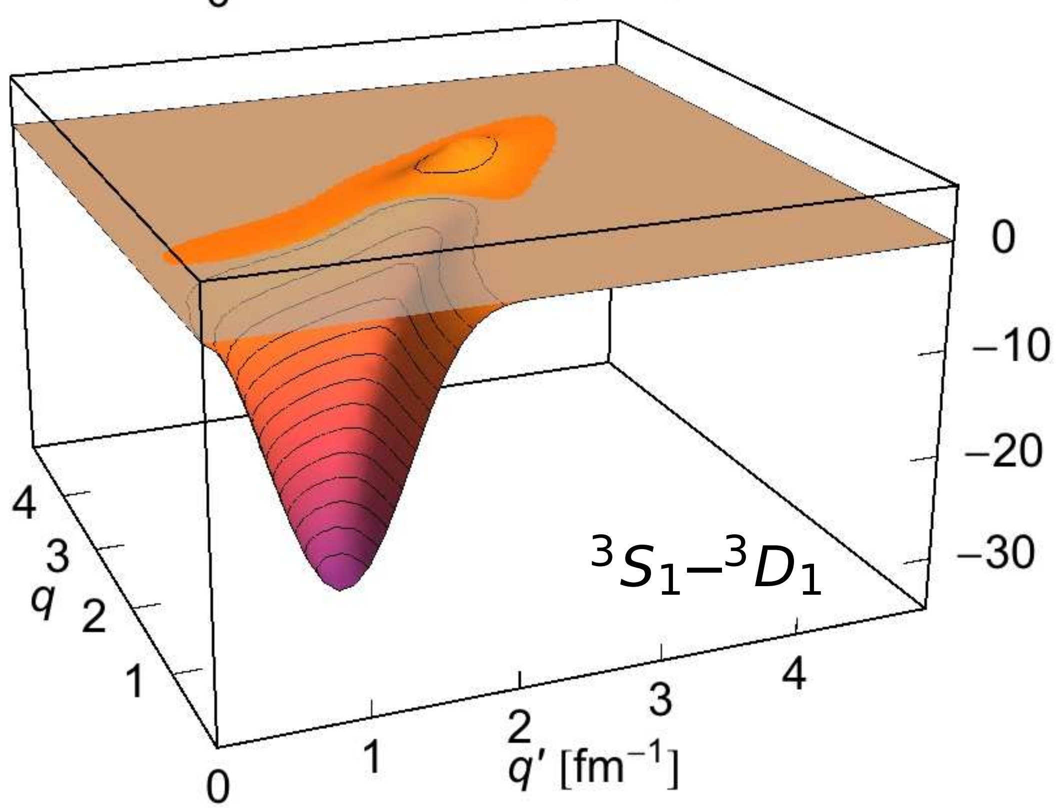
deuteron wave-function



SRG Evolution in Two-Body Space

momentum-space matrix elements





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

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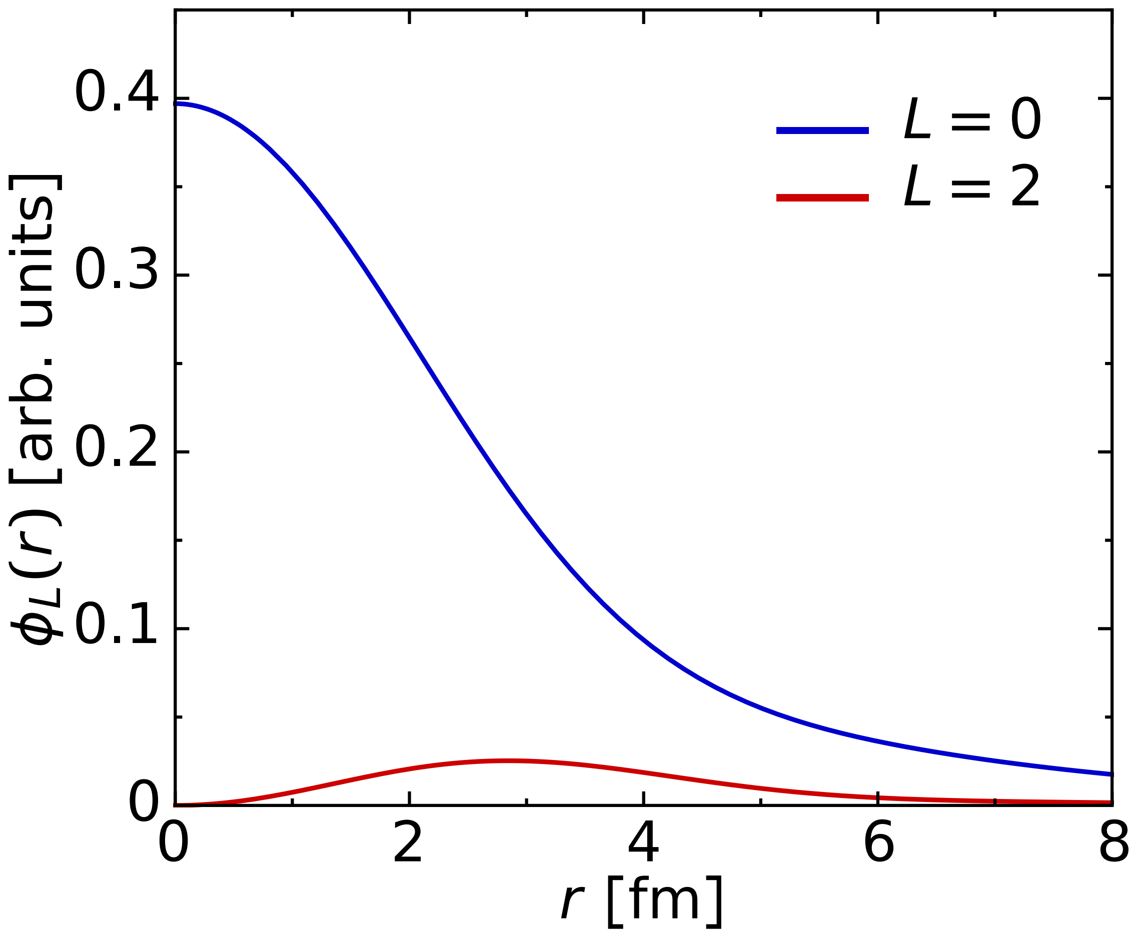
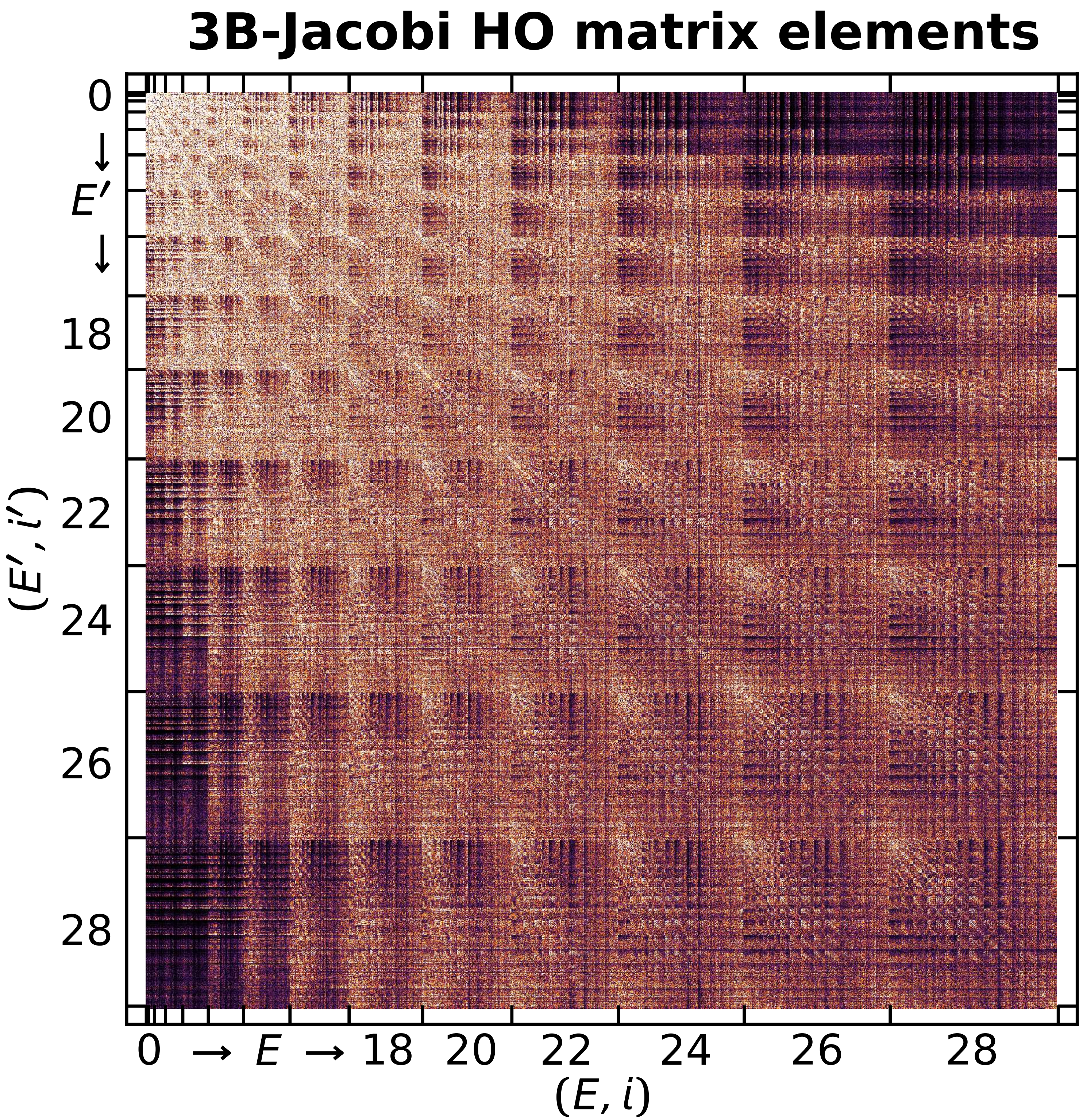
$J^\pi = 1^+, T = 0$

deuteron wave-function



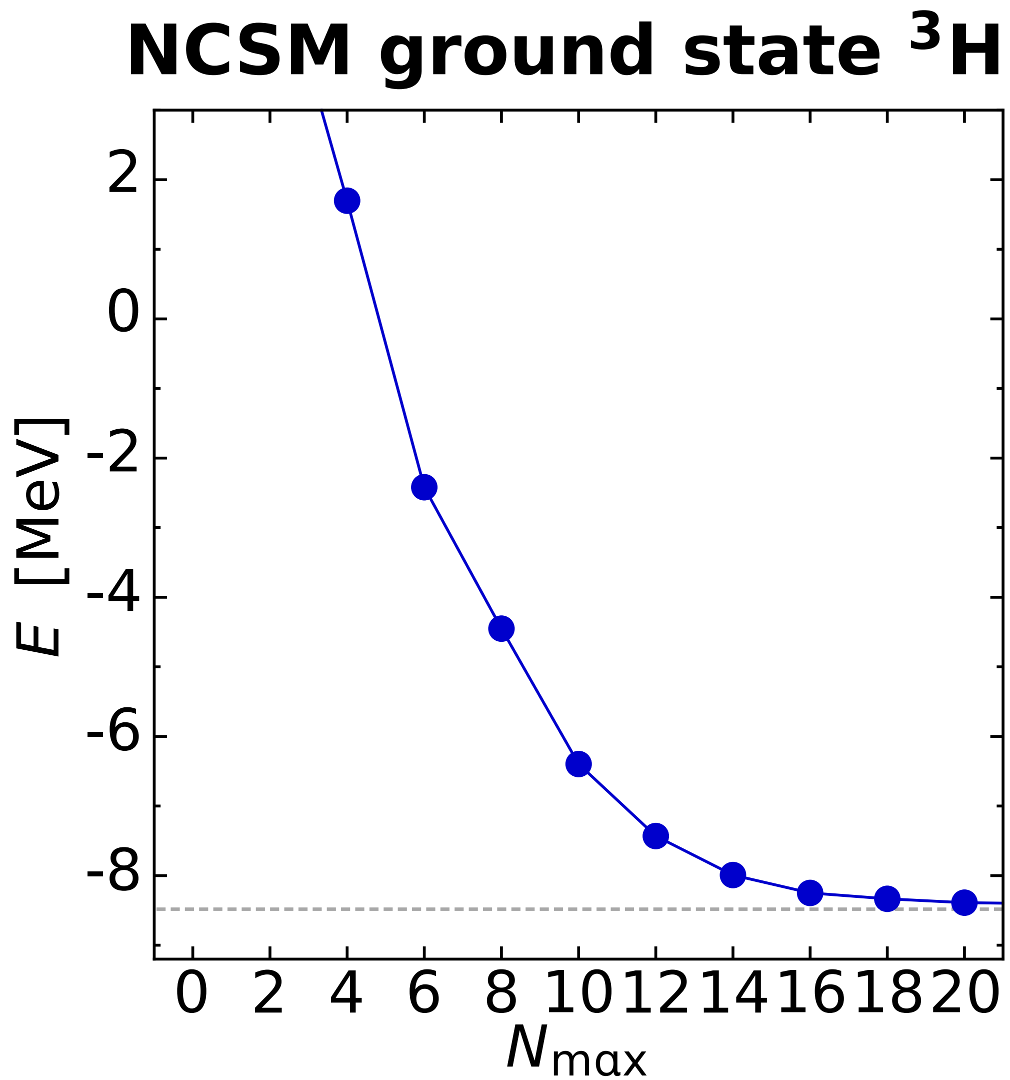
SRG Evolution in Three-Body Space



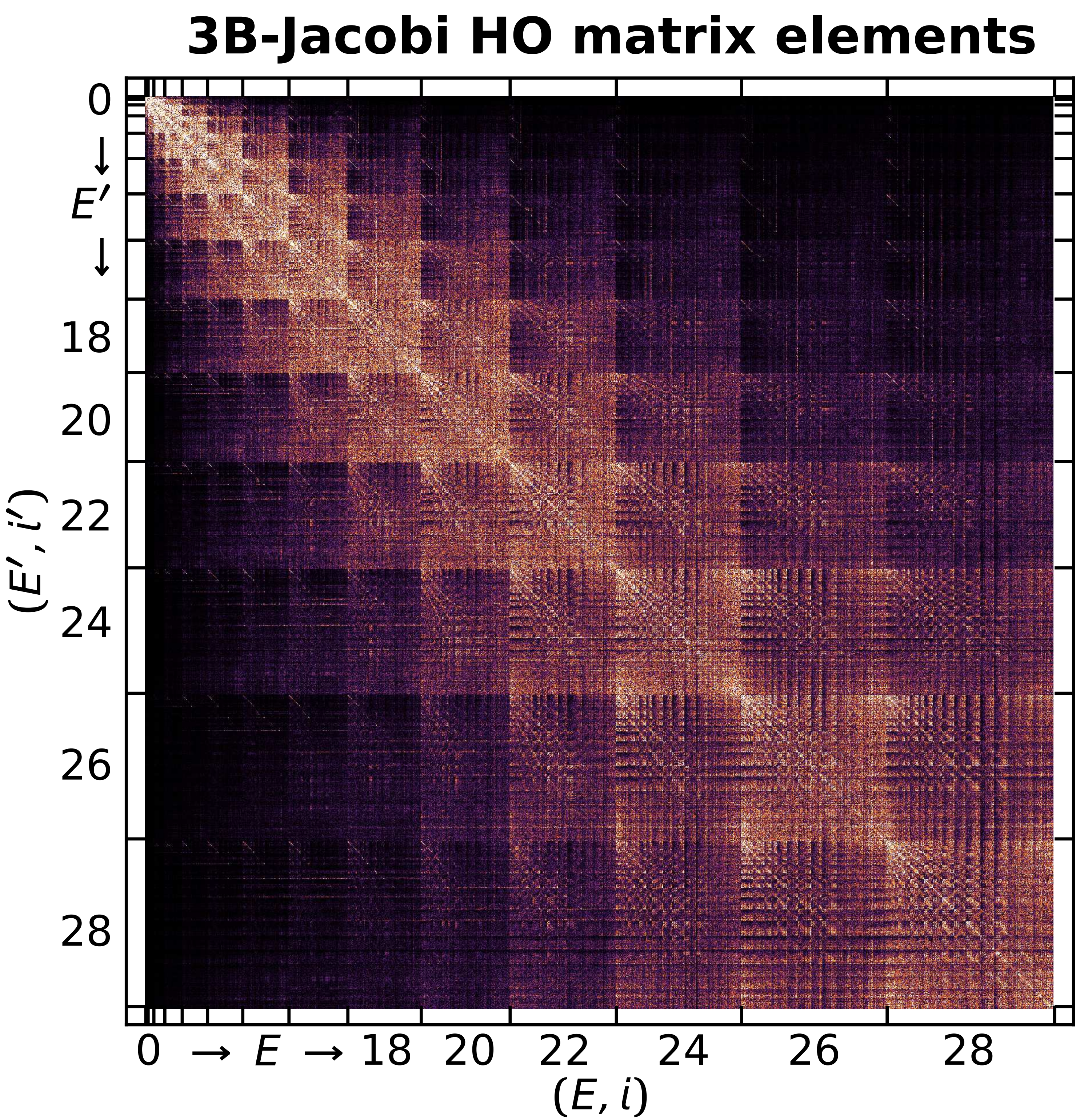
chiral NN+3N

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

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



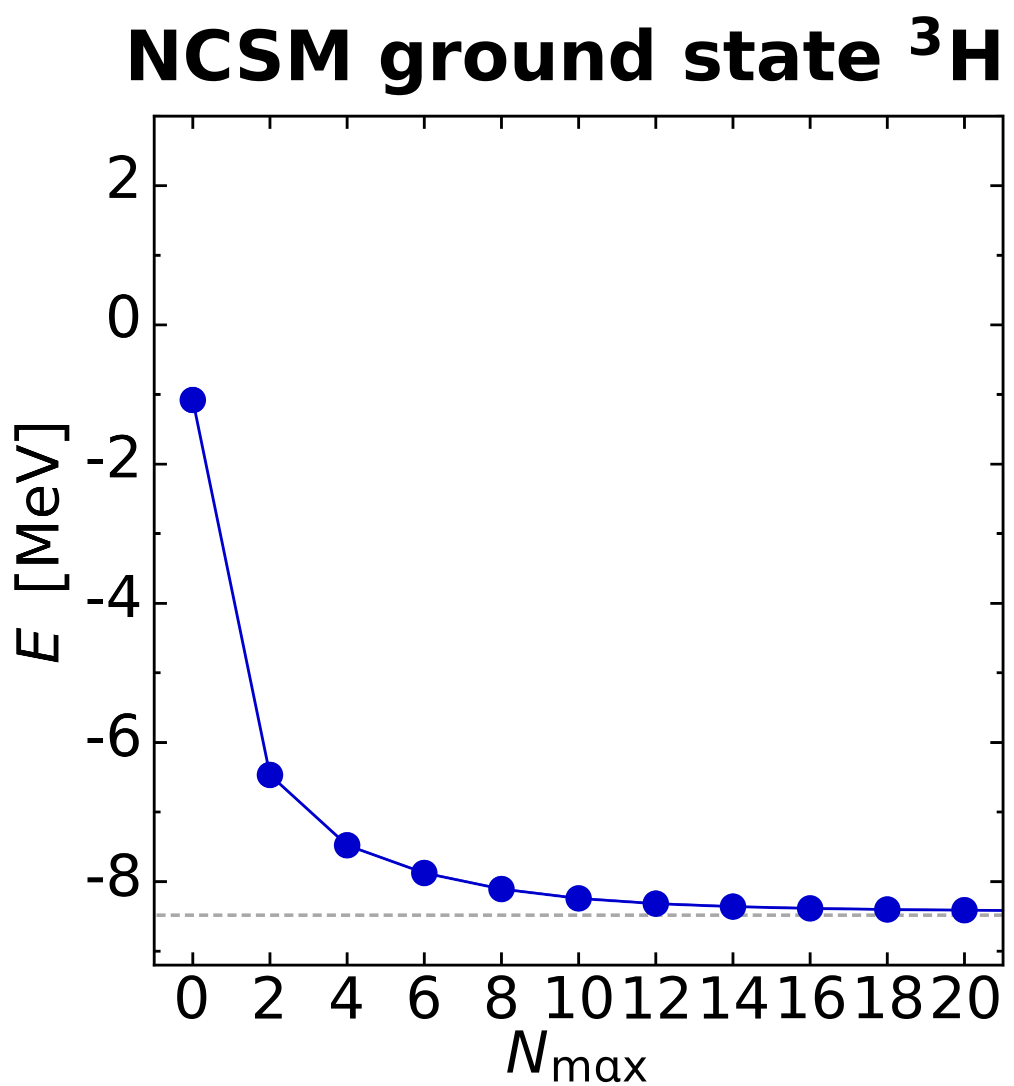
SRG Evolution in Three-Body Space



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

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

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



SRG Evolution in A-Body Space

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

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

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

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

- 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

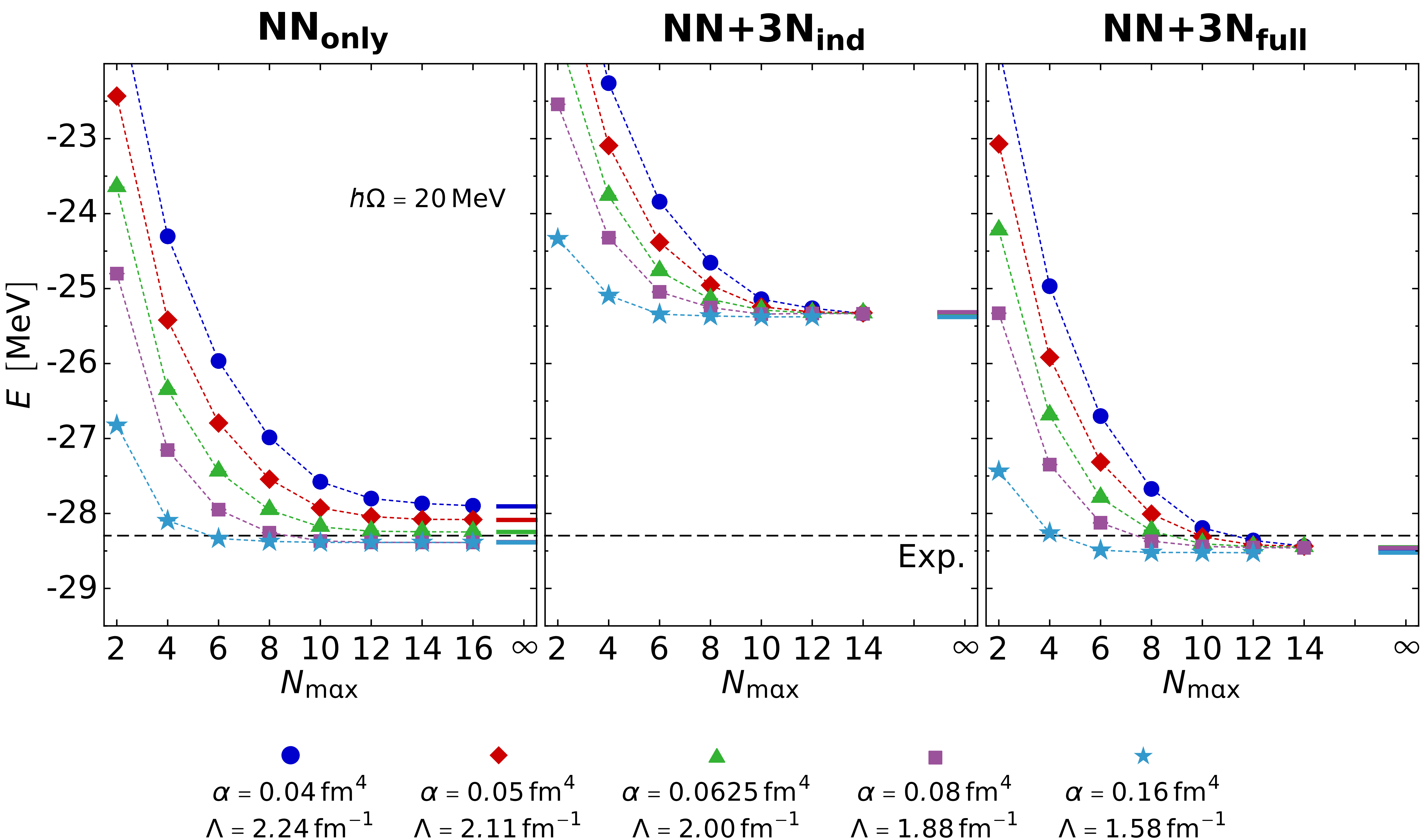
$NN+3N_{ind}$: use initial NN, keep evolved NN+3N

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

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

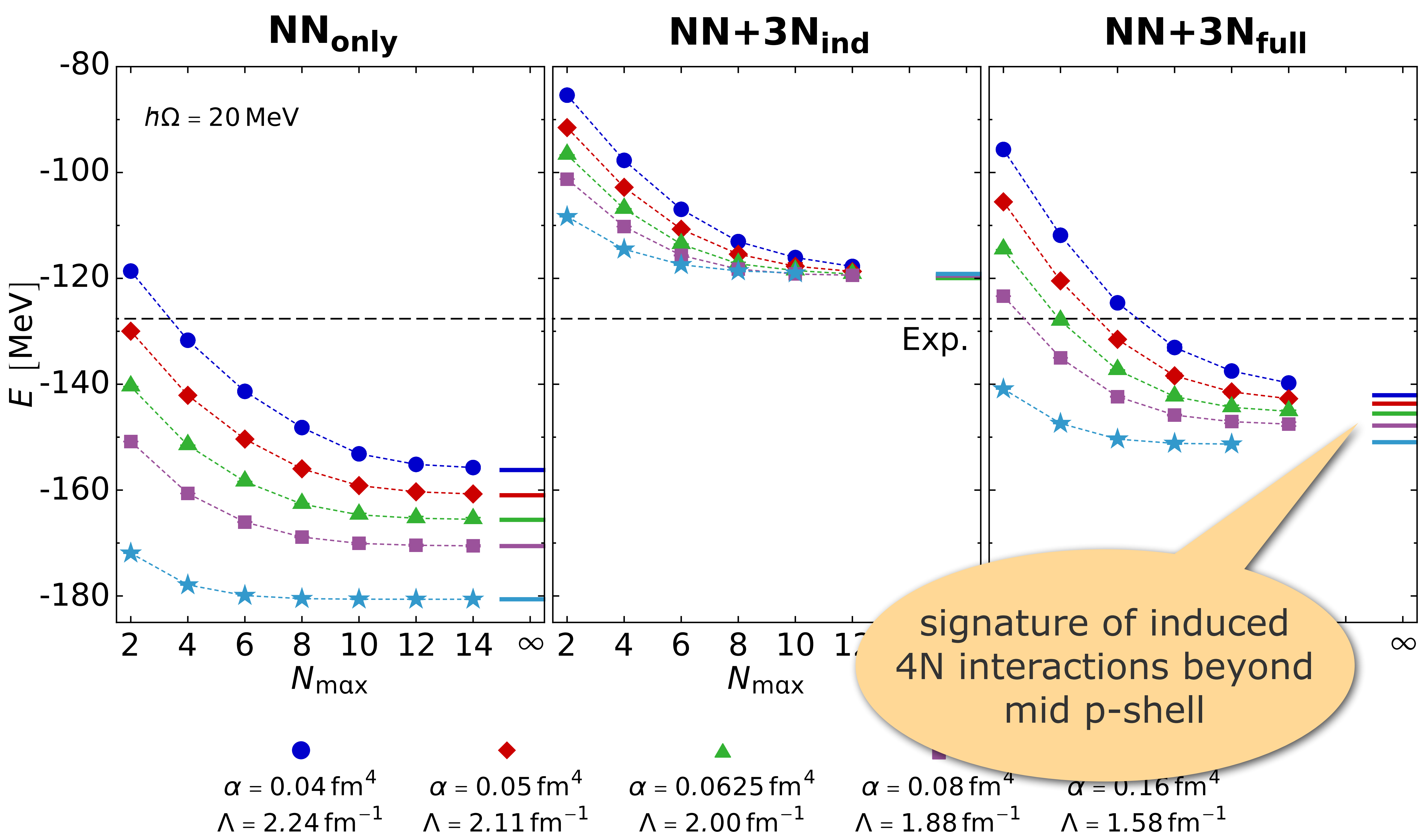
^{4}He: Ground-State Energy

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



^{16}O: Ground-State Energy

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



Many-Body Problem

Definition: Ab Initio

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

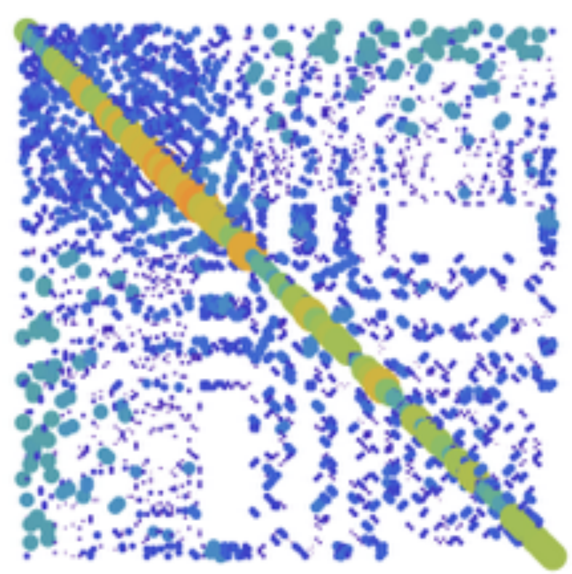
- numerical treatment with some **truncations or approximations** is inevitable for any nontrivial nuclear structure application

- **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



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

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

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

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

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

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

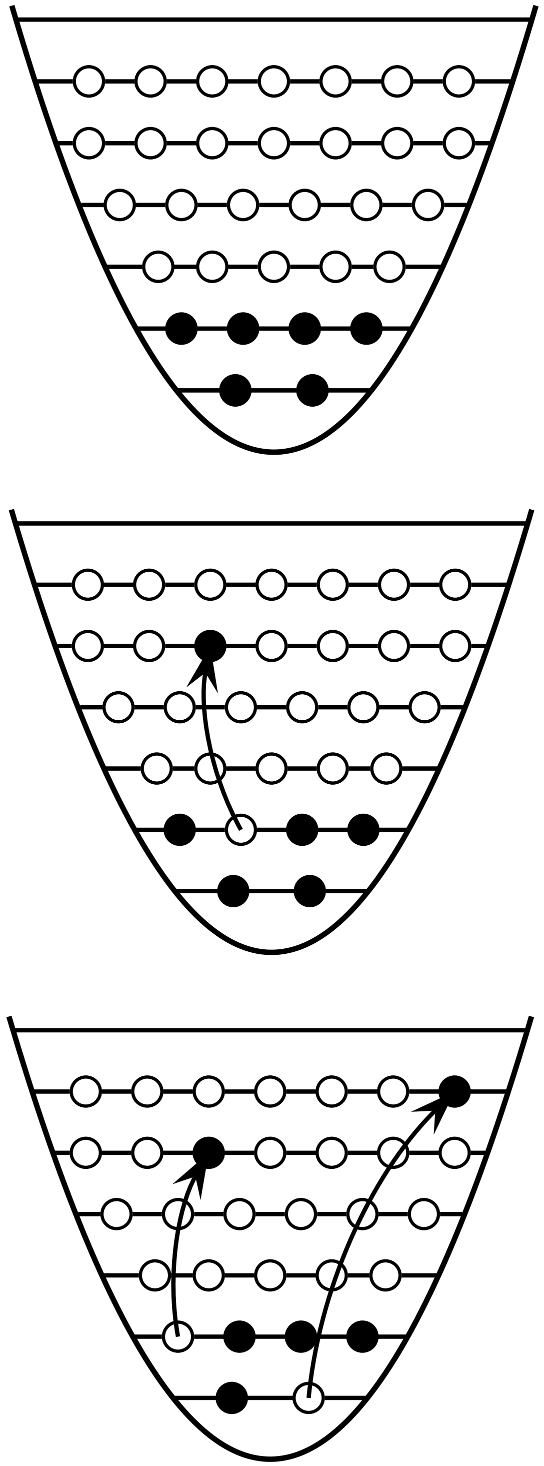
- **Hylleraas-Undheim theorem**: all states of the spectrum have a monotonously decreasing energy with increasing model space dimension

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

No-Core Shell Model

No-Core Shell Model (NCSM)

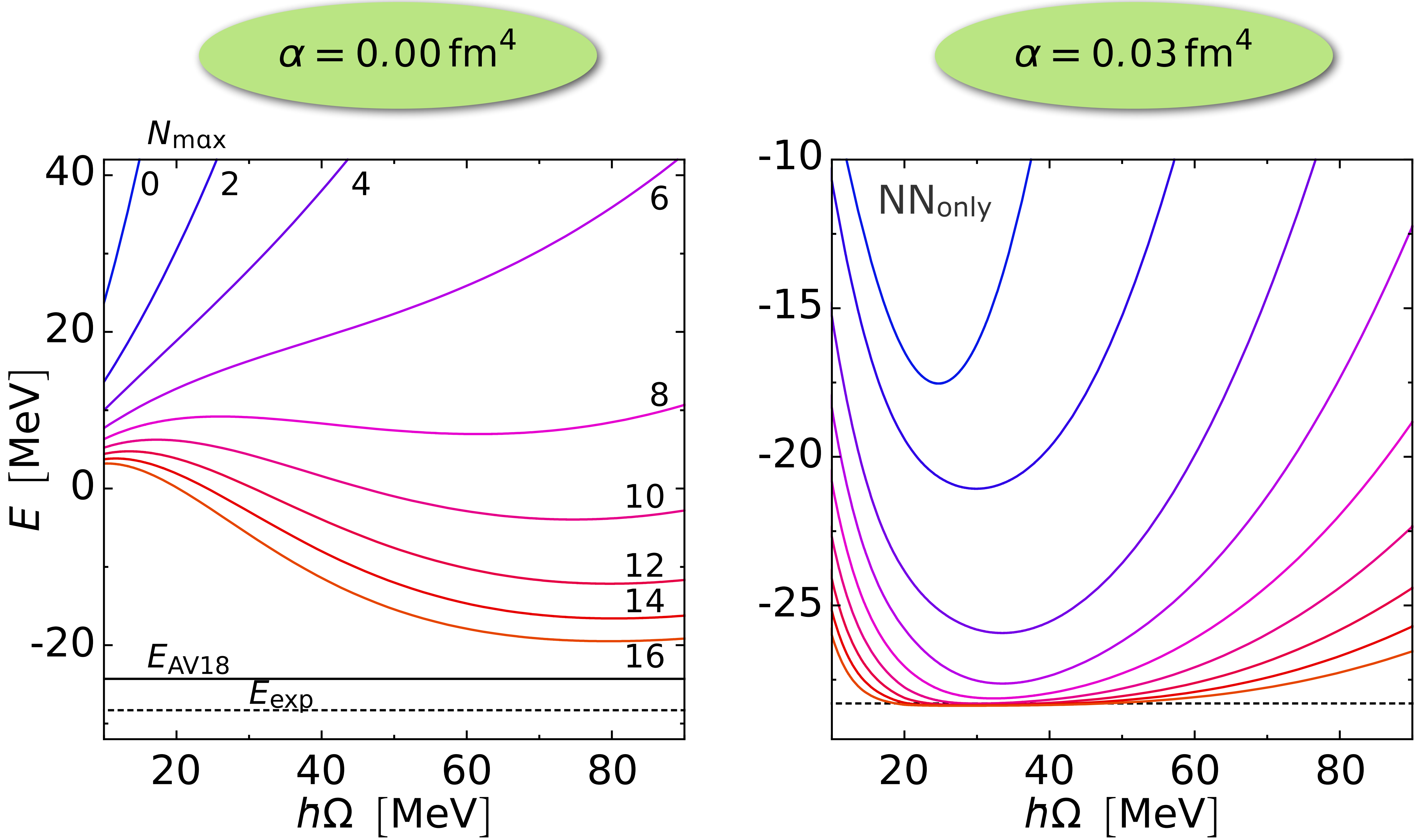
- NCSM is a special case of a CI approach:
  - single-particle basis is a **spherical HO basis**
  - truncation in terms of the total **number of HO excitation quanta $N_{\max}$** in the many-body states



- **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 $N_{\max}$

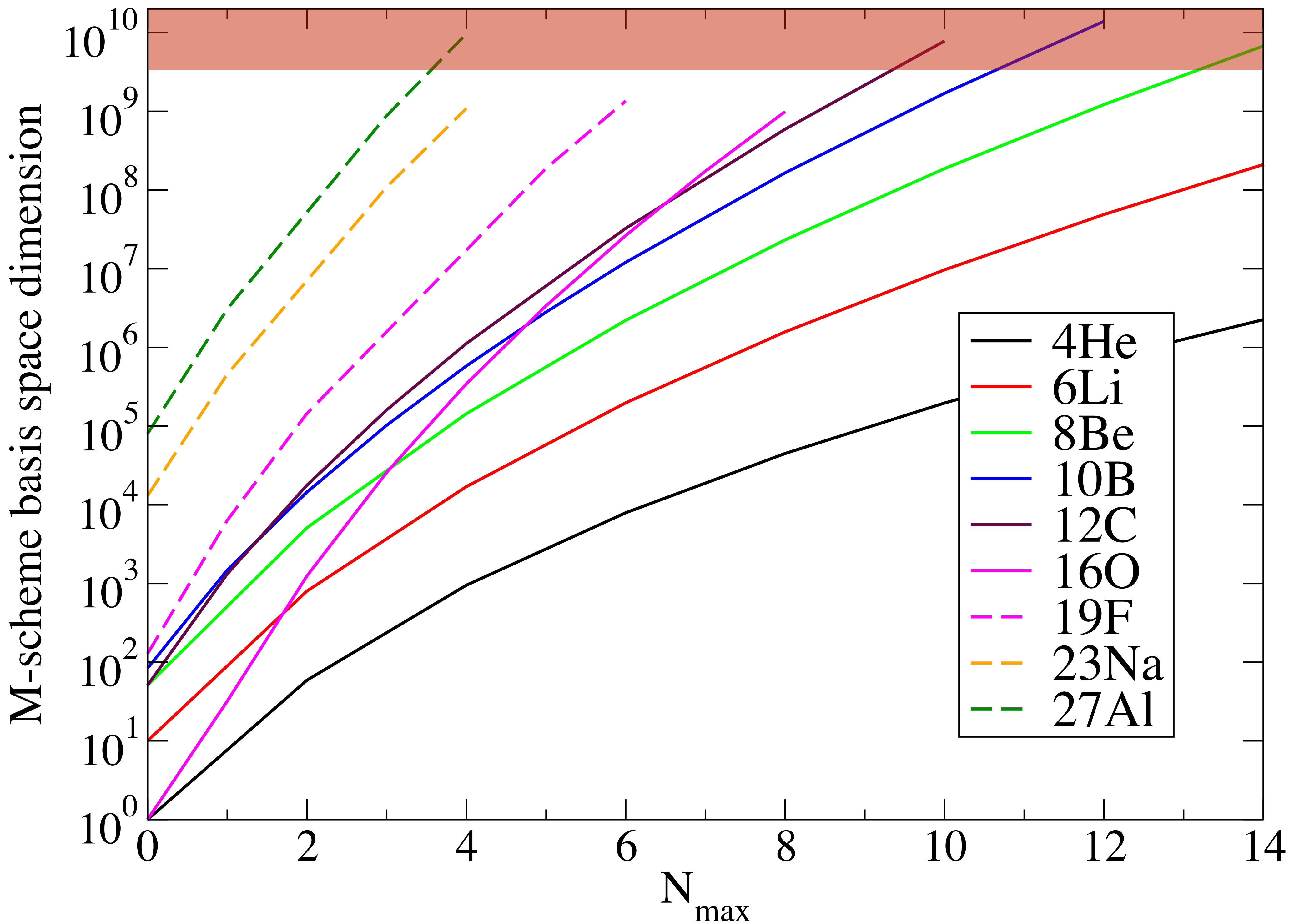
^{4}He: NCSM Convergence

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



NCSM Basis Dimension

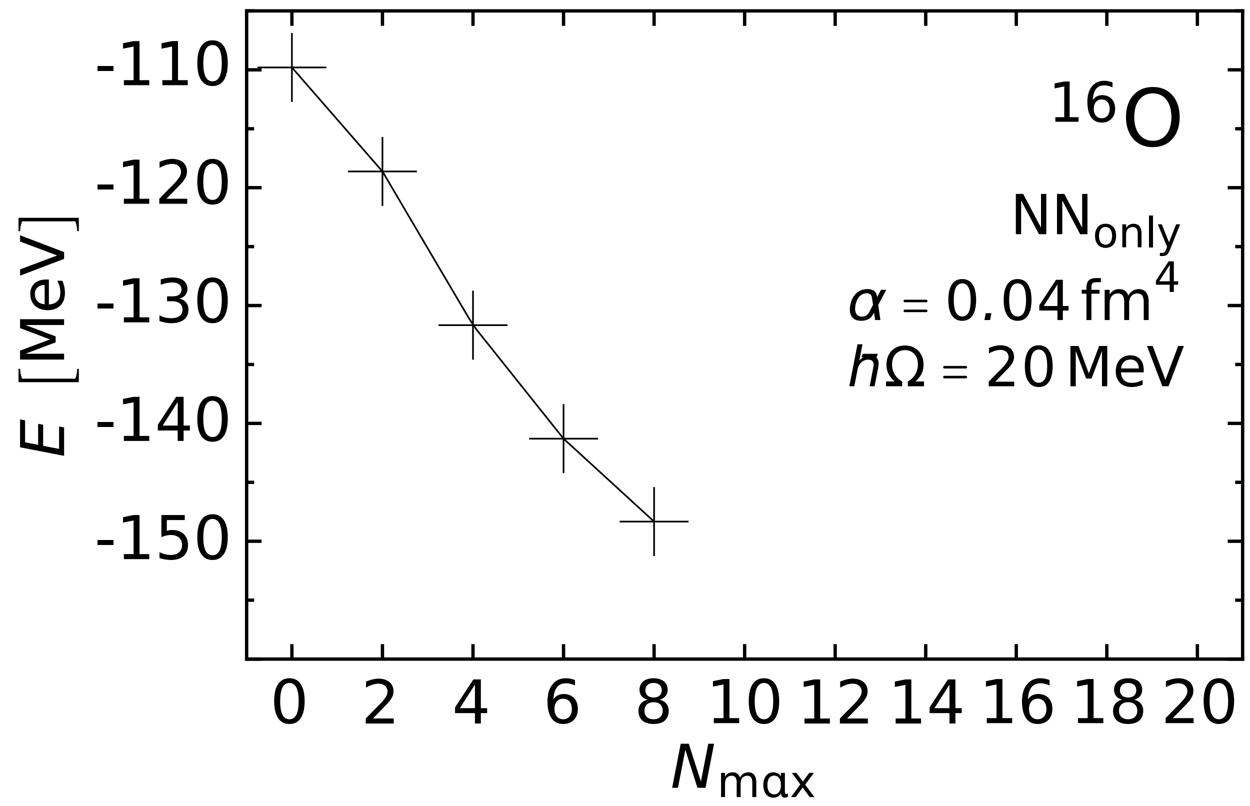
P. Maris



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 $D > 10^{10}$

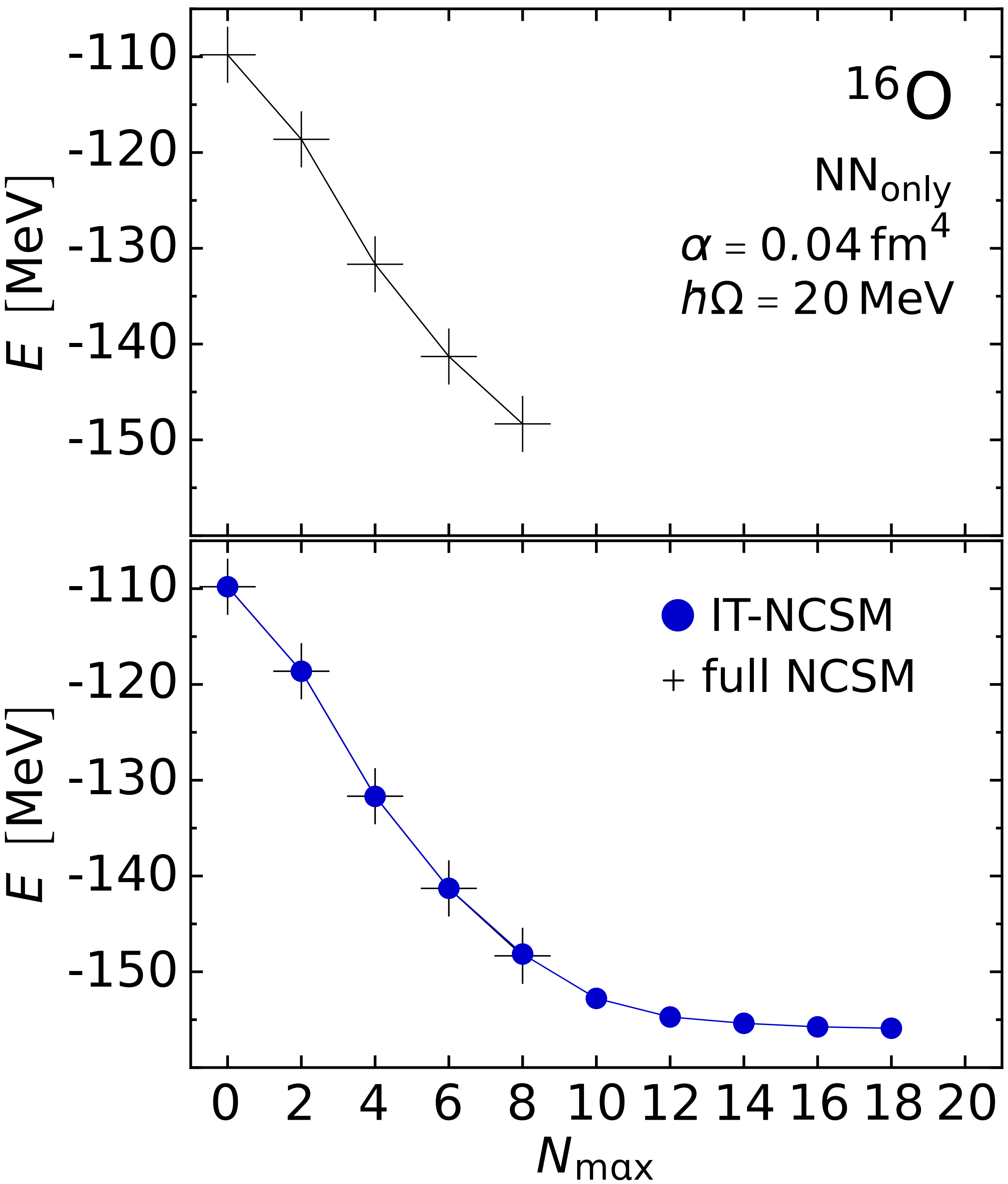


Importance Truncation

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

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

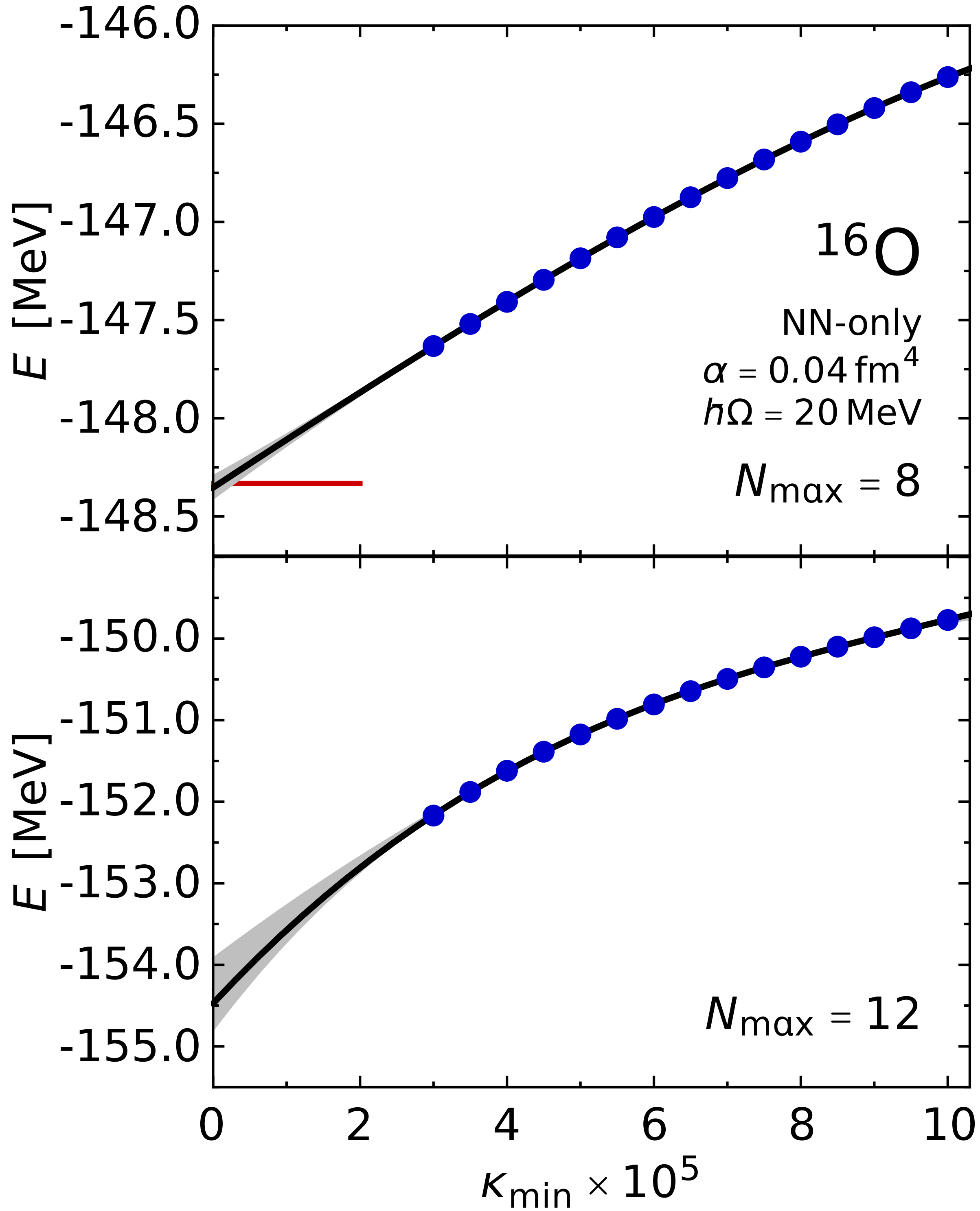
- **measure the importance** of individual basis state $|\Phi_\nu\rangle \notin \mathcal{M}_{\text{ref}}$ via first-order multiconfigurational perturbation theory

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

- 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

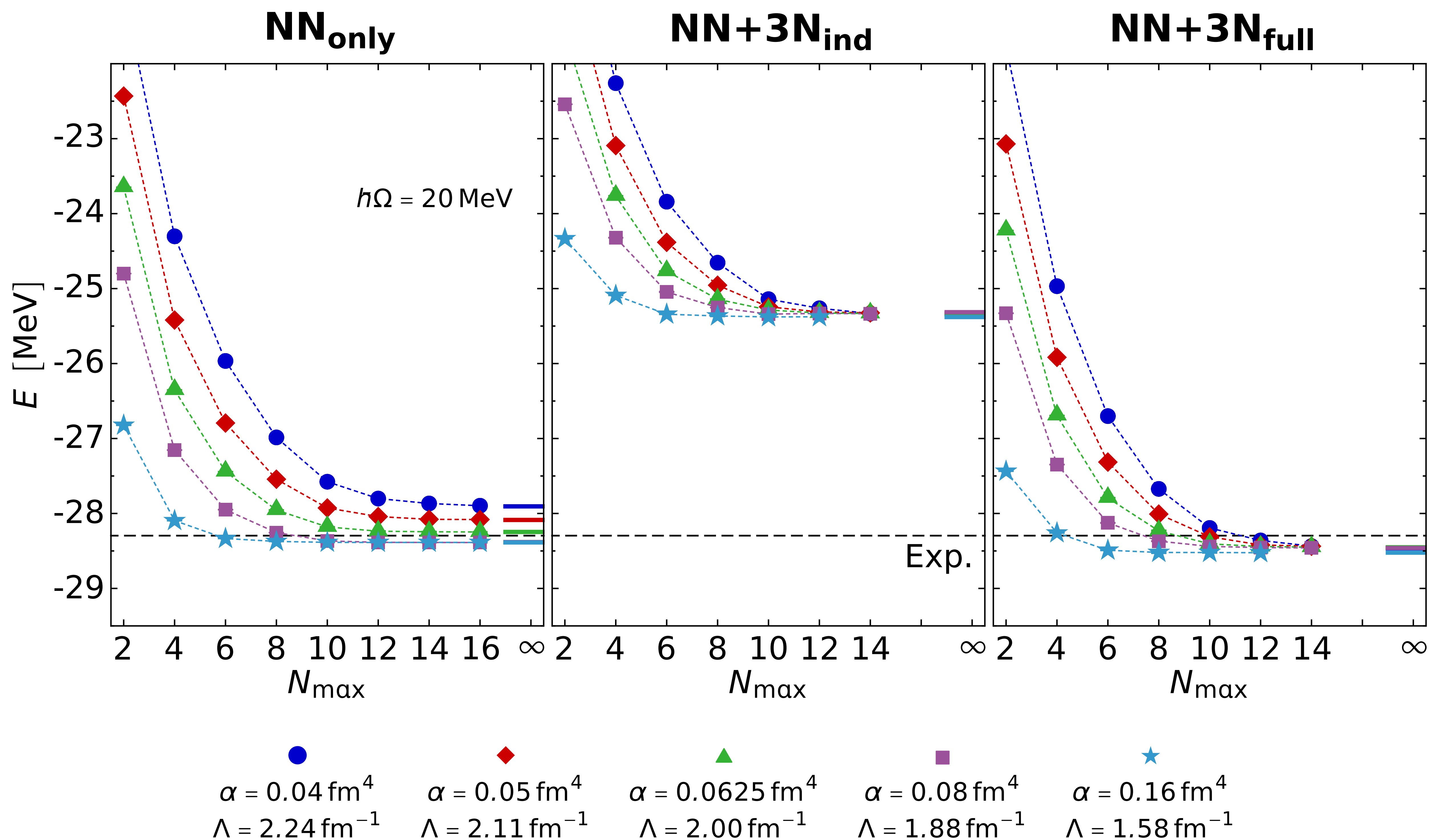
Threshold Extrapolation



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

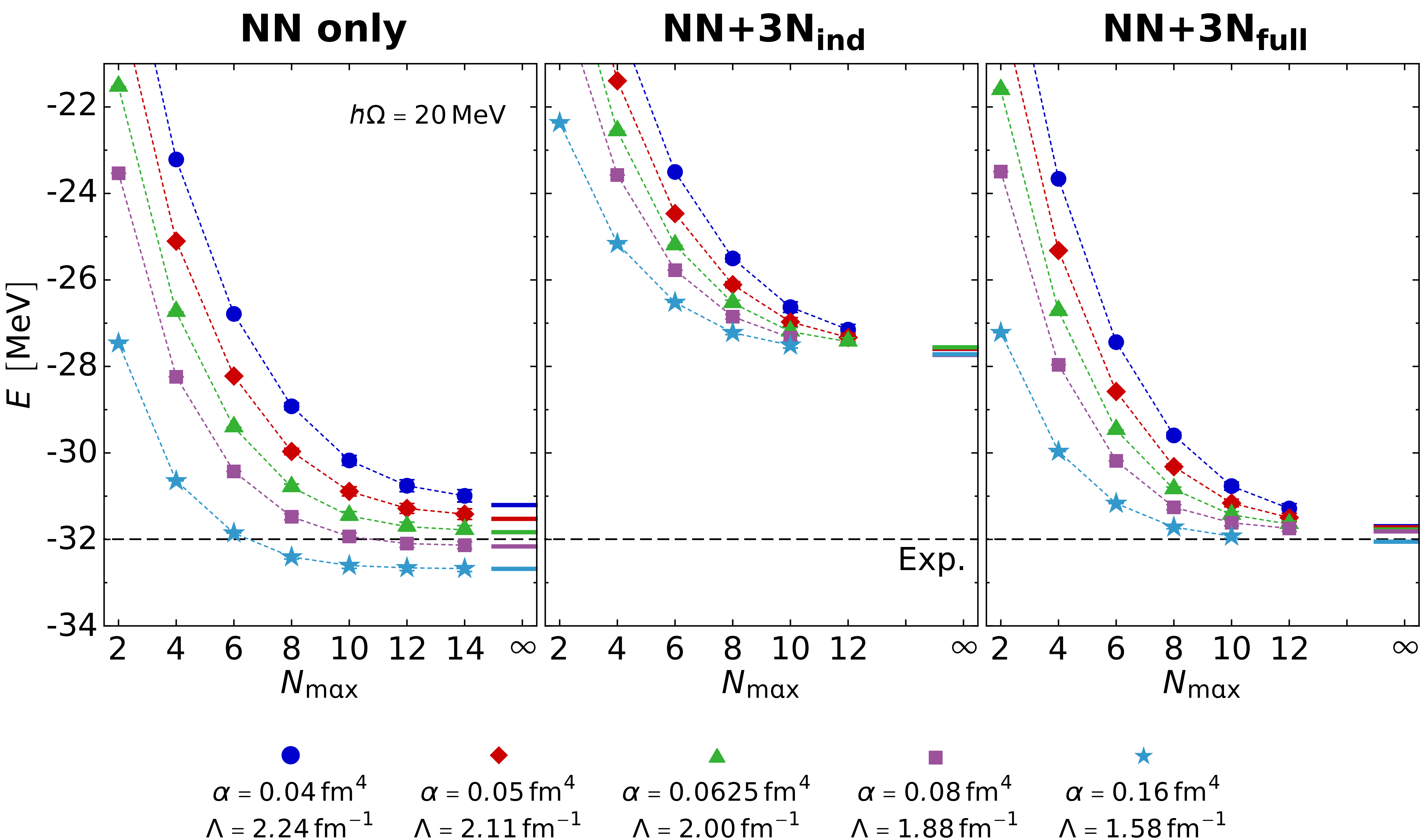
^{4}He: Ground-State Energy

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



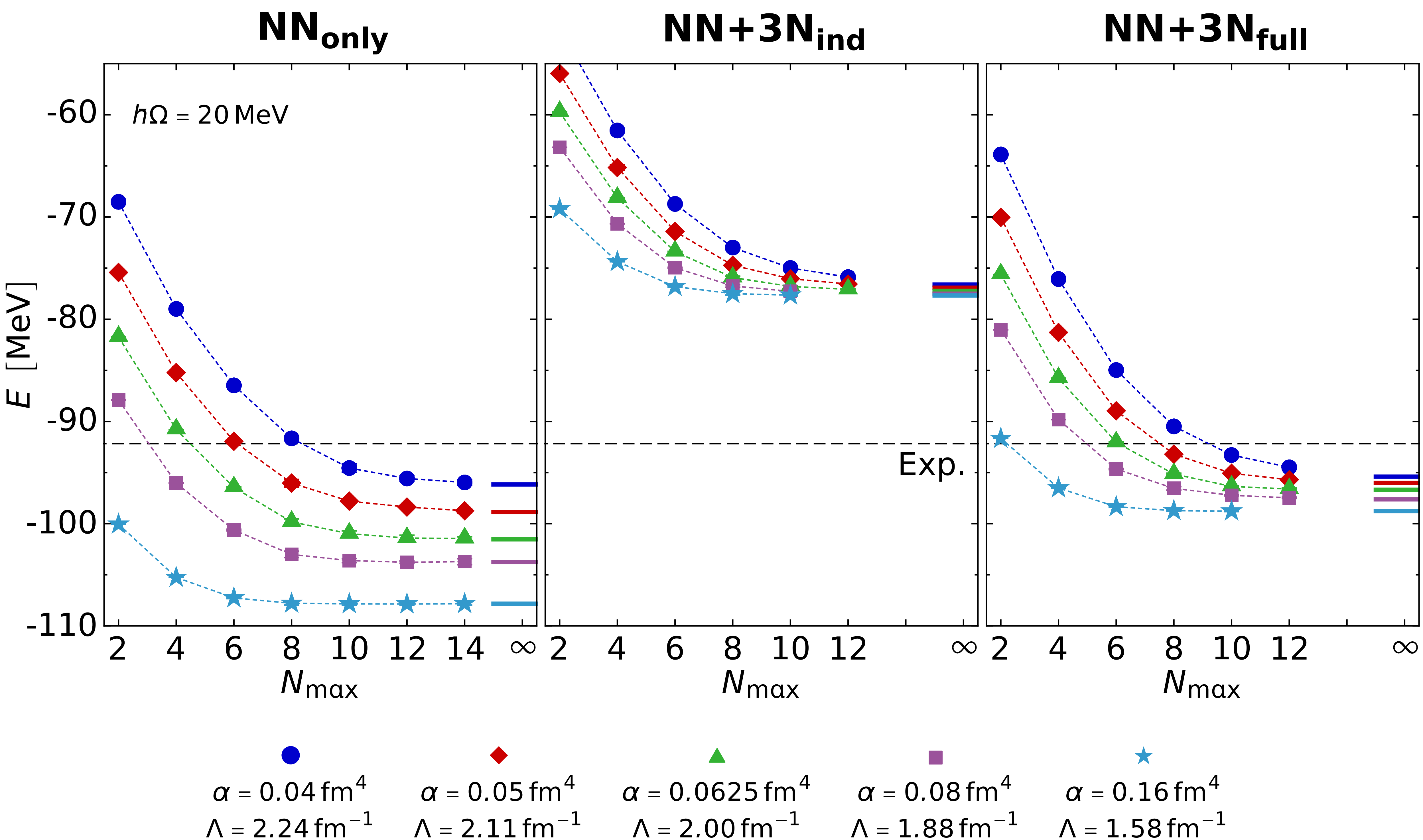
^{7}Li: Ground-State Energy

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



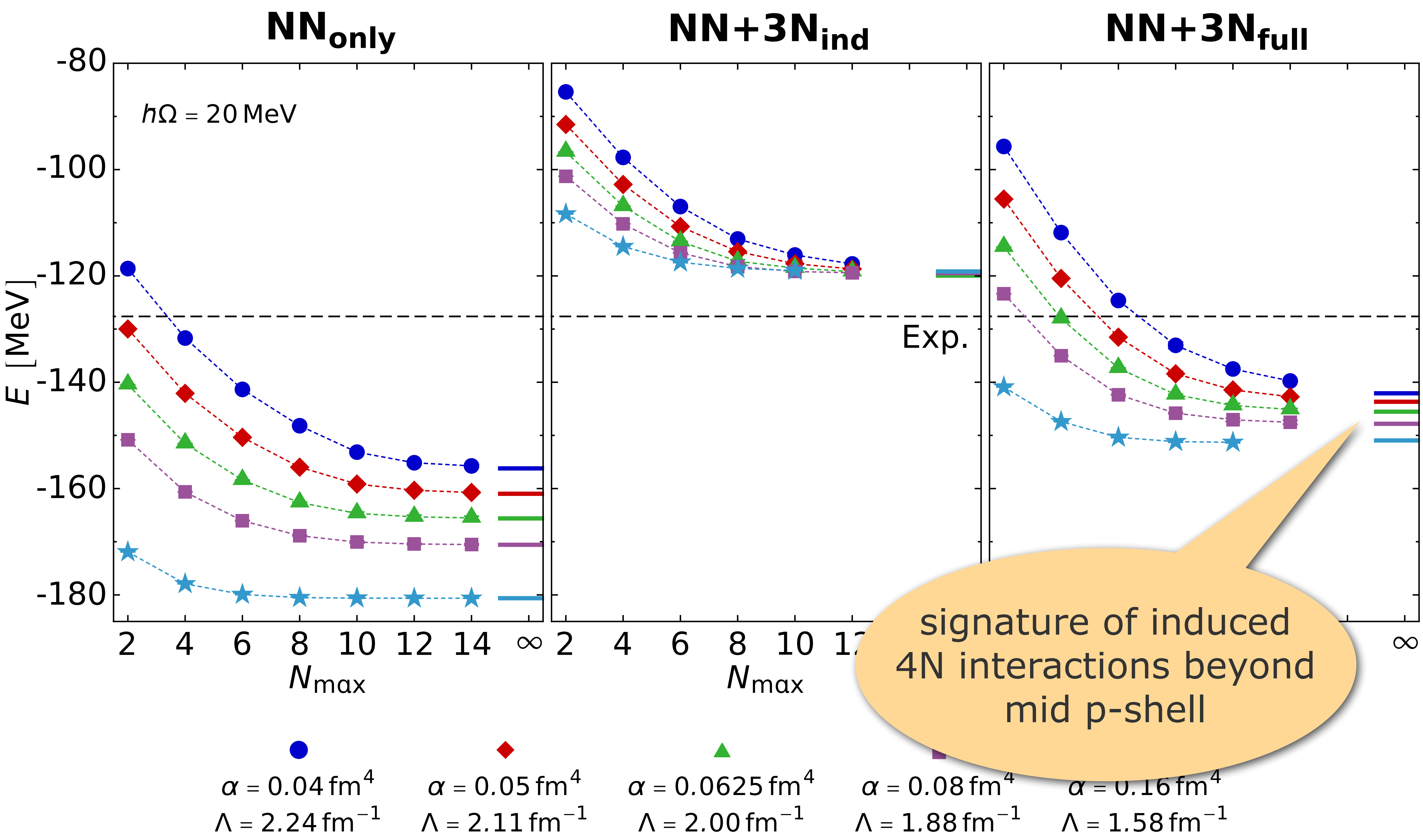
^{12}C: Ground-State Energy

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



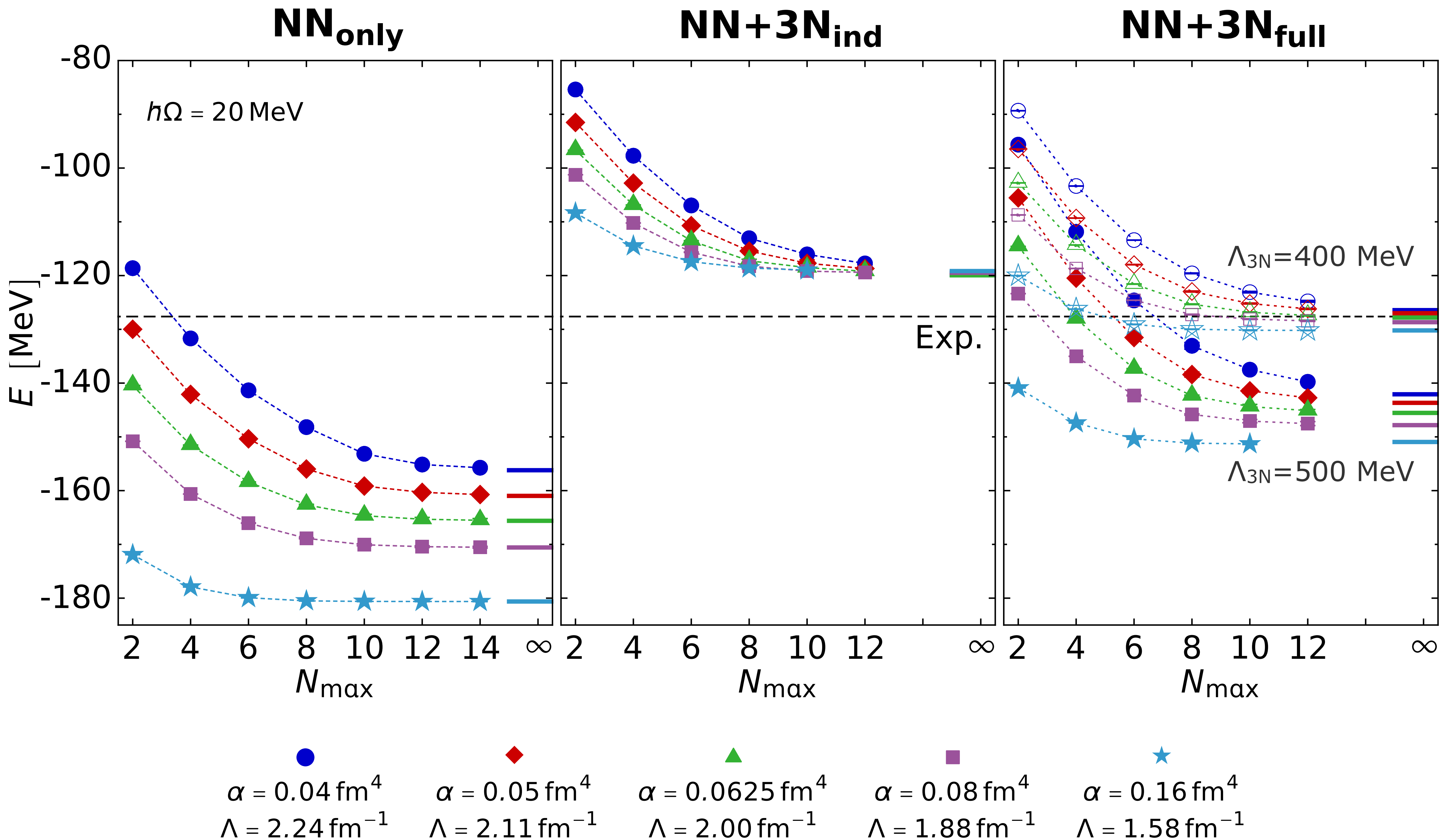
^{16}O: Ground-State Energy

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



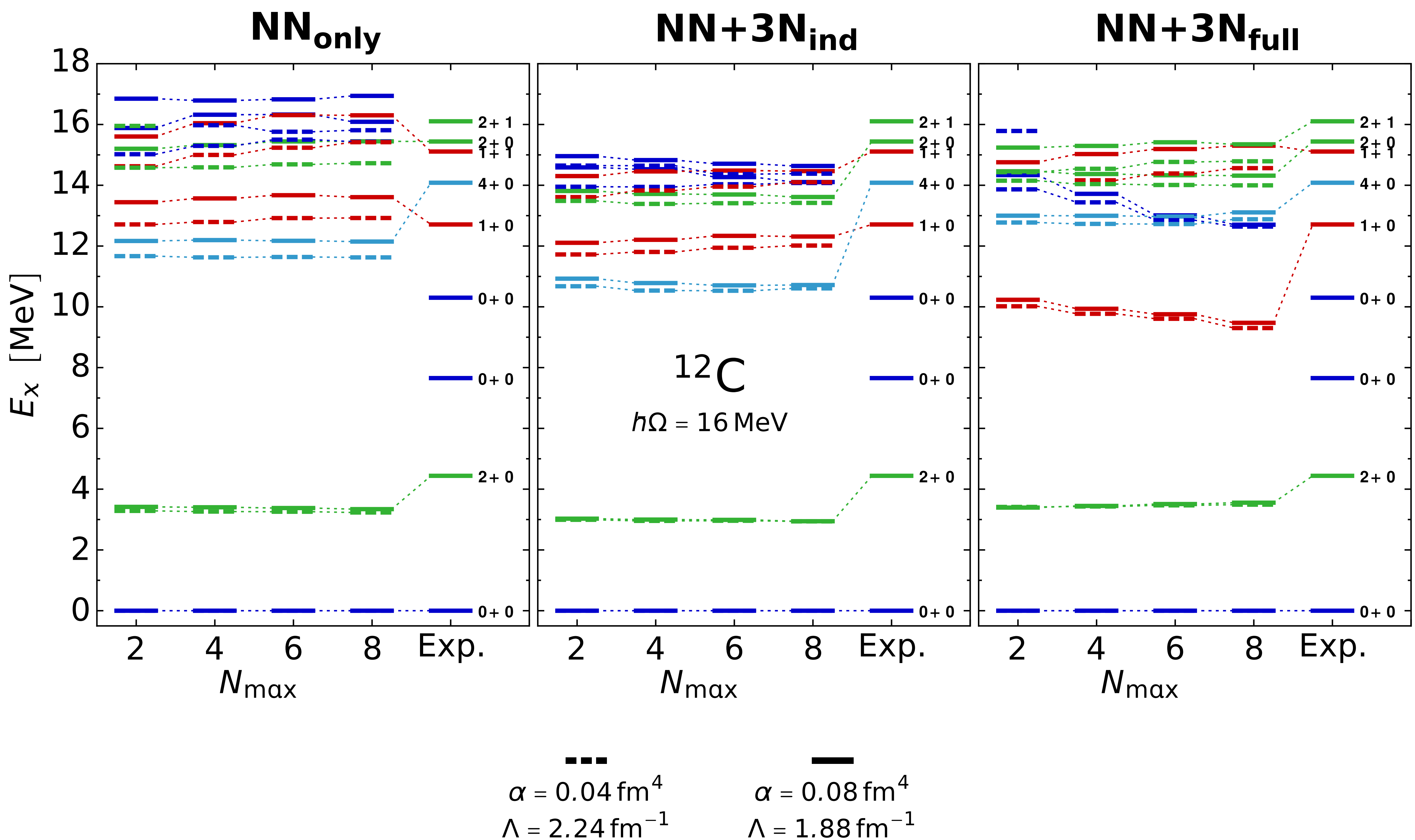
^{16}O: Ground-State Energy

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



^{12}C: Excitation Spectrum

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



From Dripline to Dripline

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)

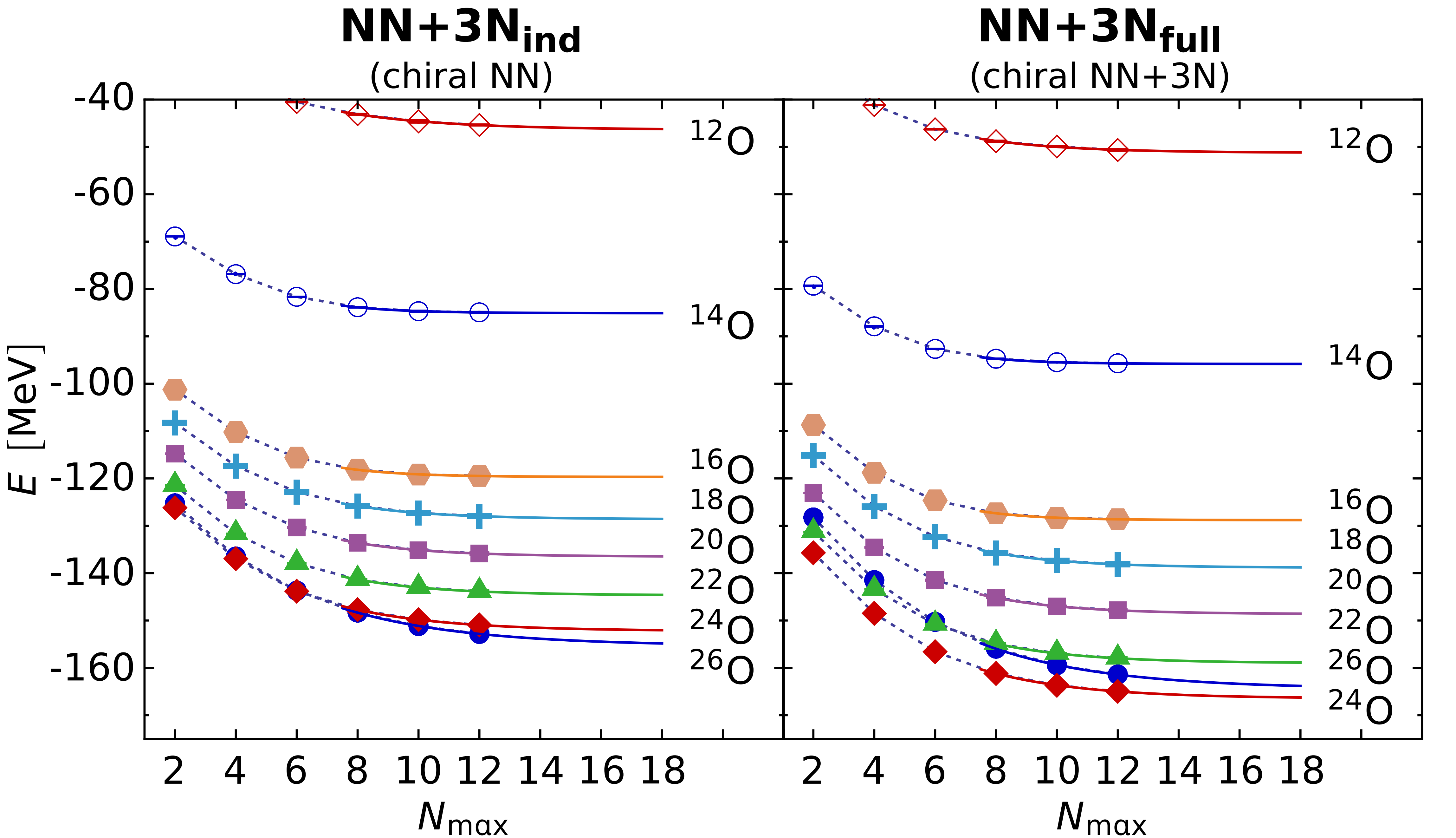
- 2013: **ab initio IT-NCSM** with explicit chiral 3N interactions and first **multi-reference in-medium SRG** calculations...

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

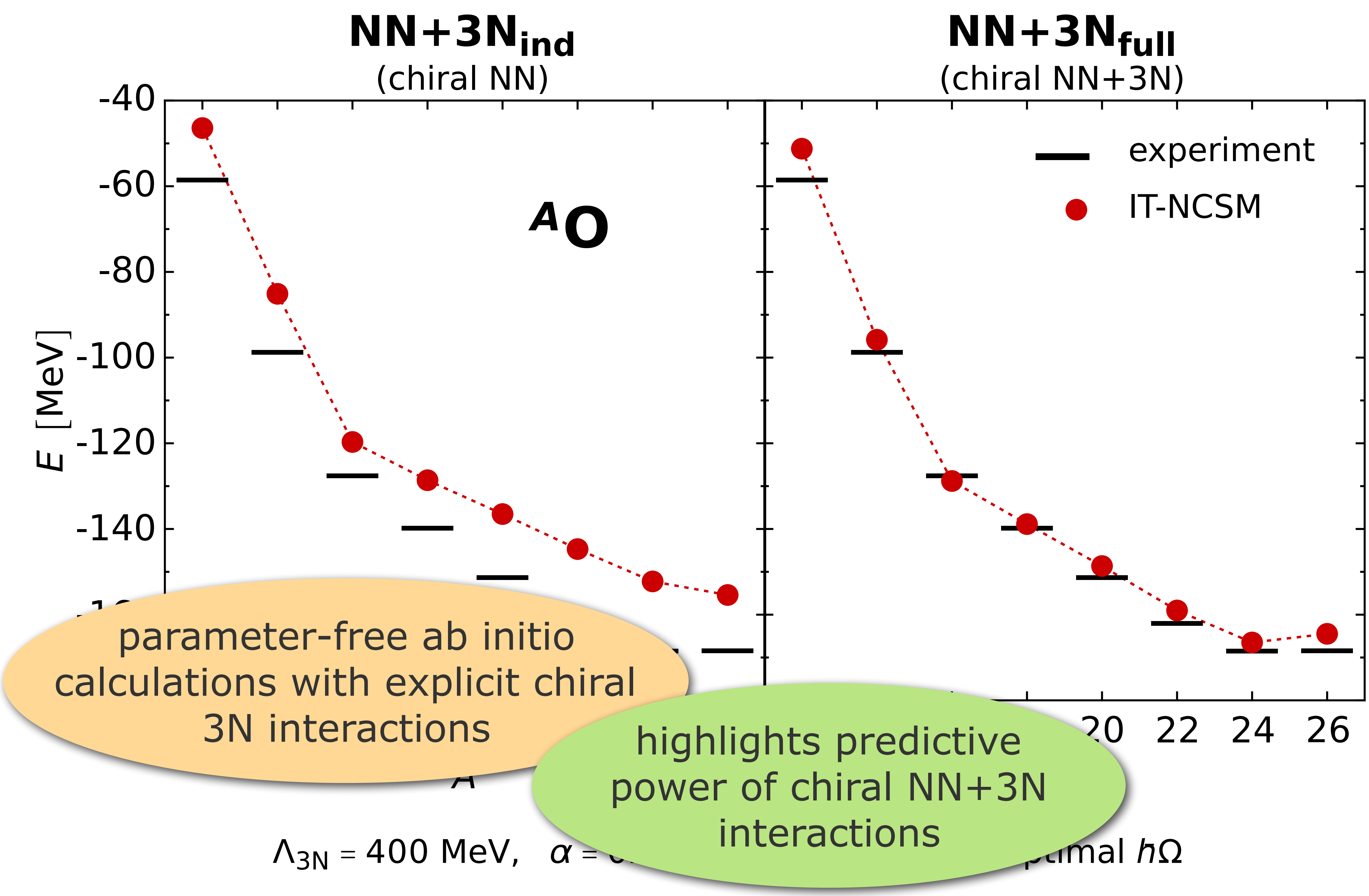
Hergert et al., PRL 110, 242501 (2013)



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

Ground States of Oxygen Isotopes

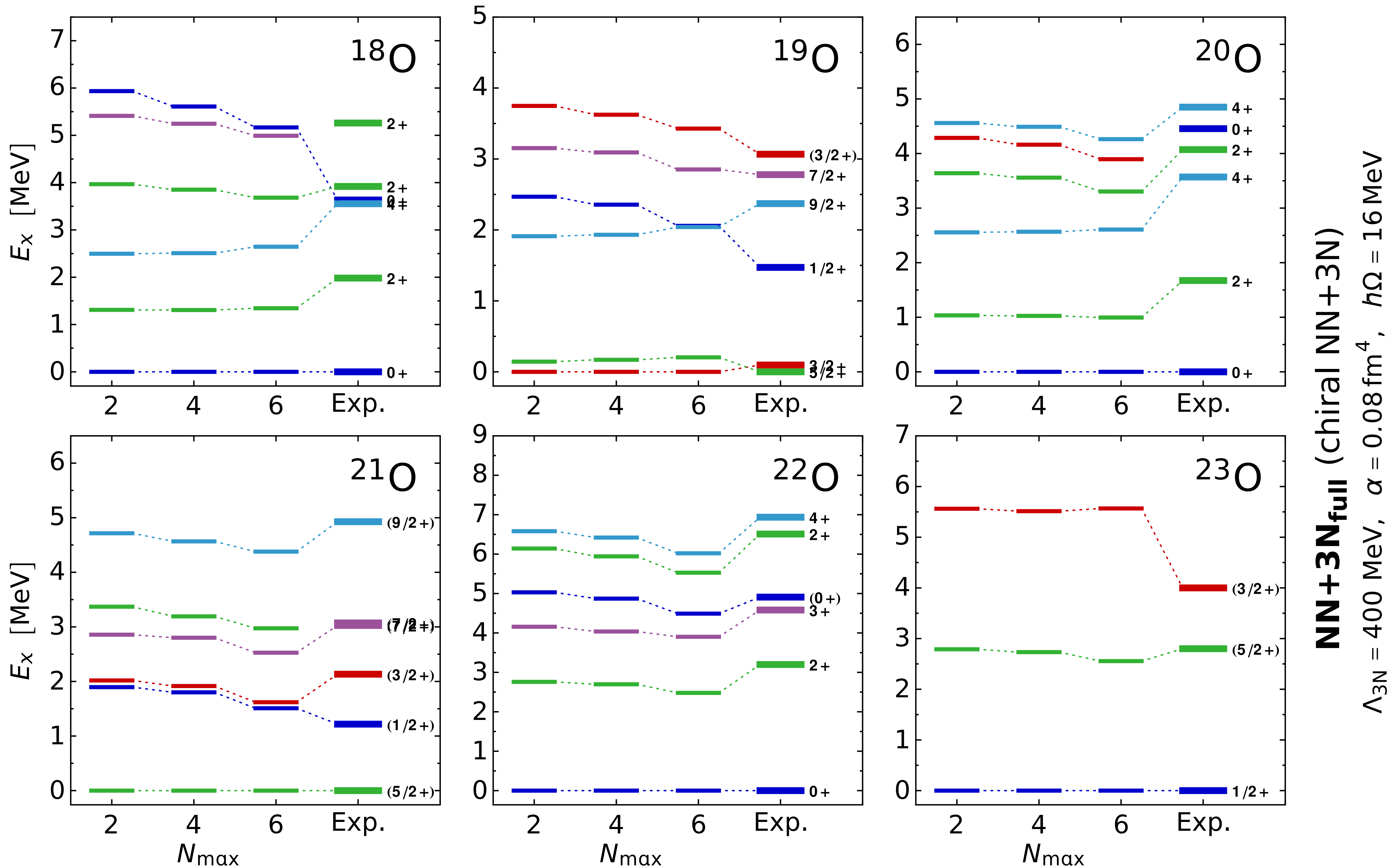
Hergert et al., PRL 110, 242501 (2013)



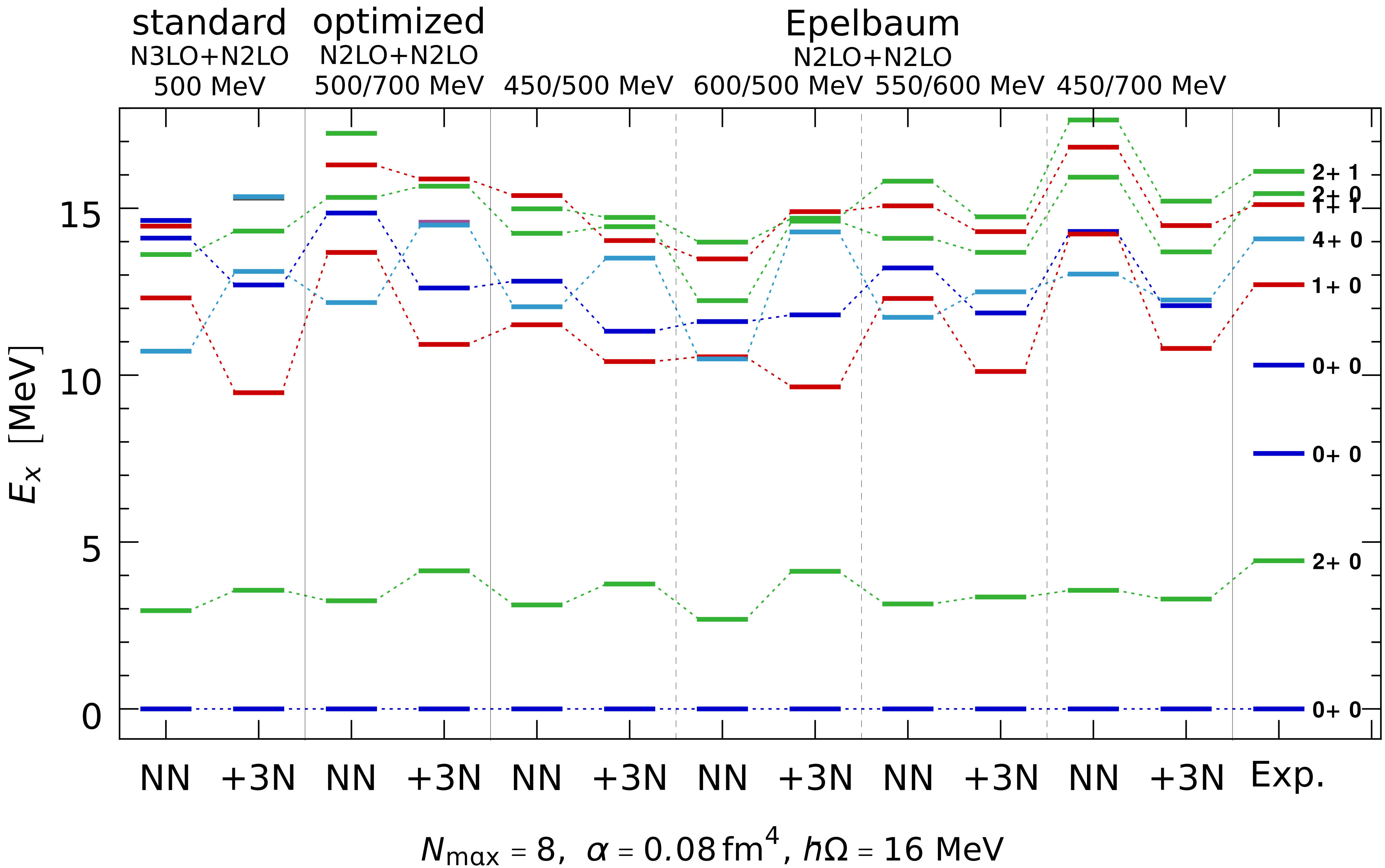
Λ_{3N} = 400 MeV, α = ... optimal $\hbar\Omega$

Spectra of Oxygen Isotopes

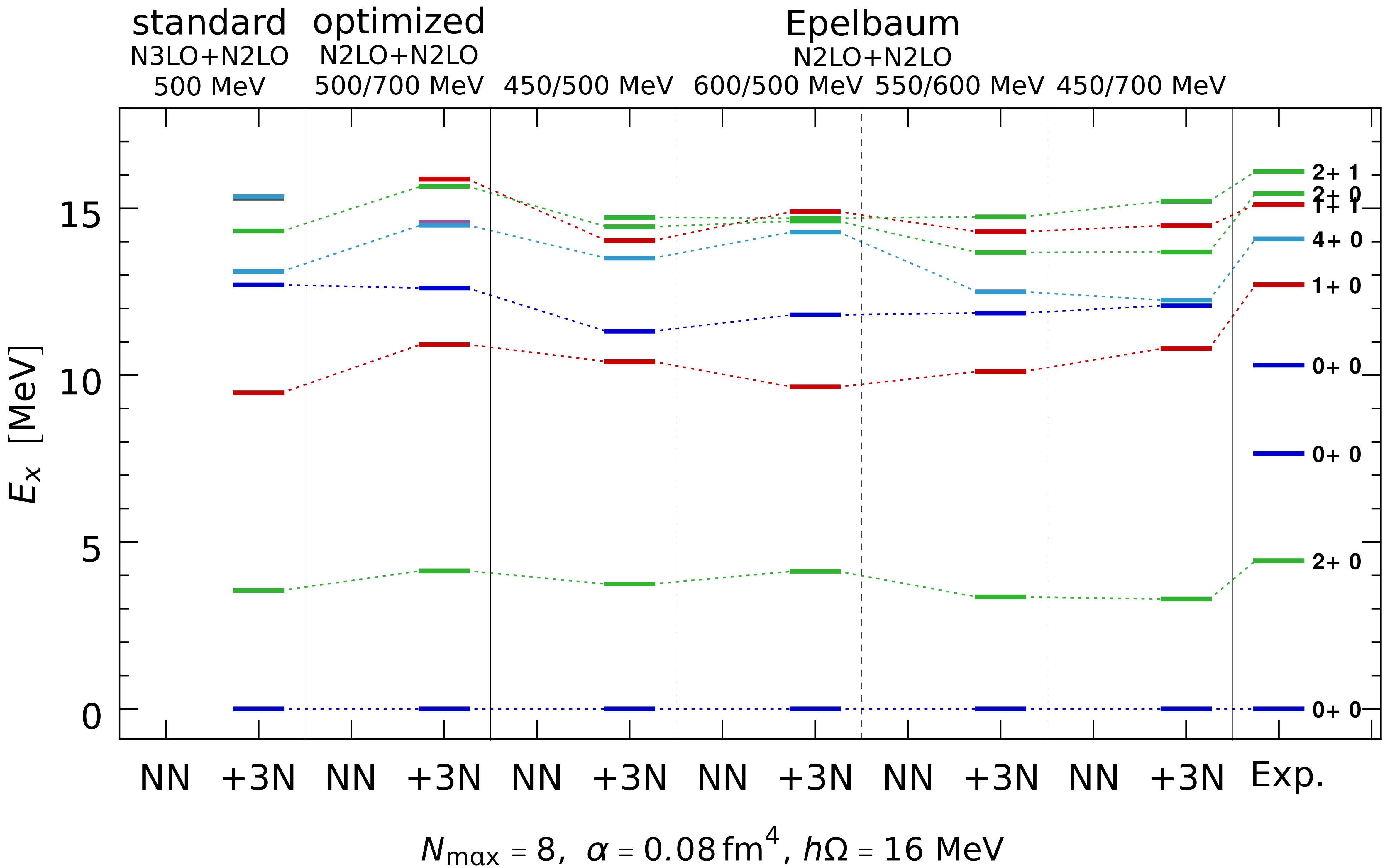
Hergert et al., PRL 110, 242501 (2013) & in prep.



^{12}C: Testing Chiral Hamiltonians



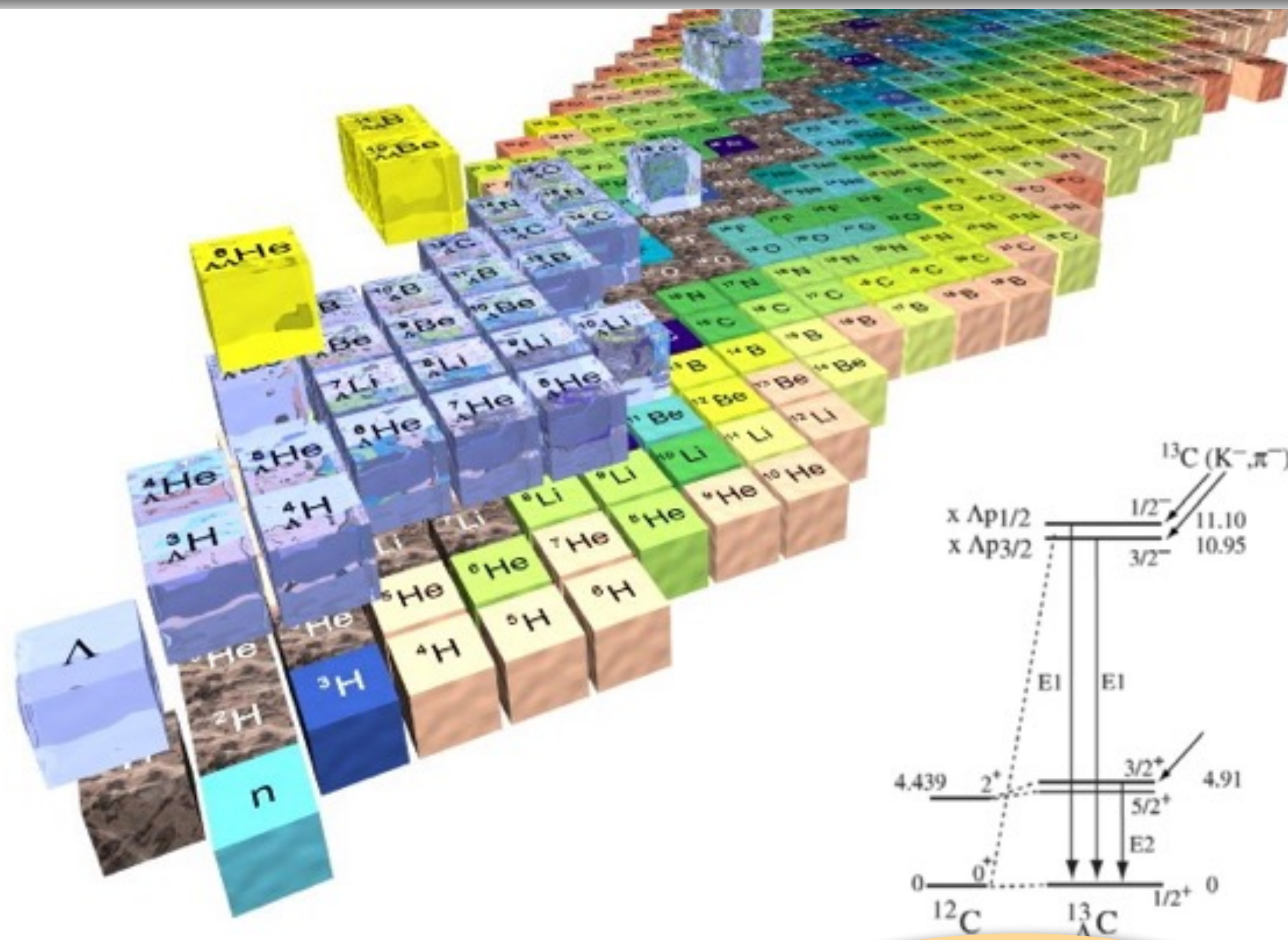
^{12}C: Testing Chiral Hamiltonians

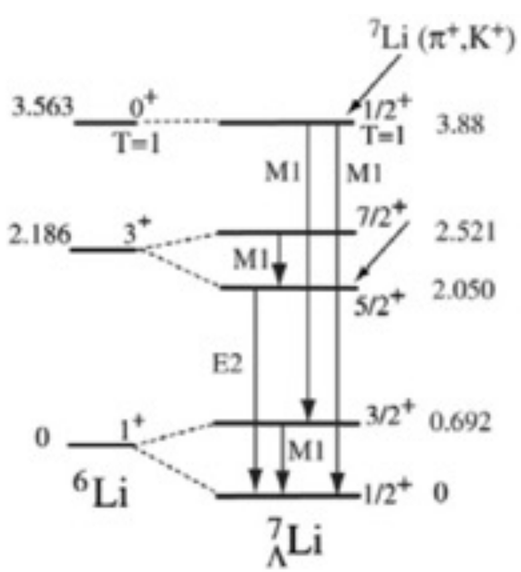


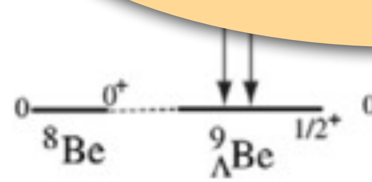
Hypernuclei

$$N_f = 2 \quad \rightarrow \quad N_f = 3$$

Ab Initio Hypernuclear Structure





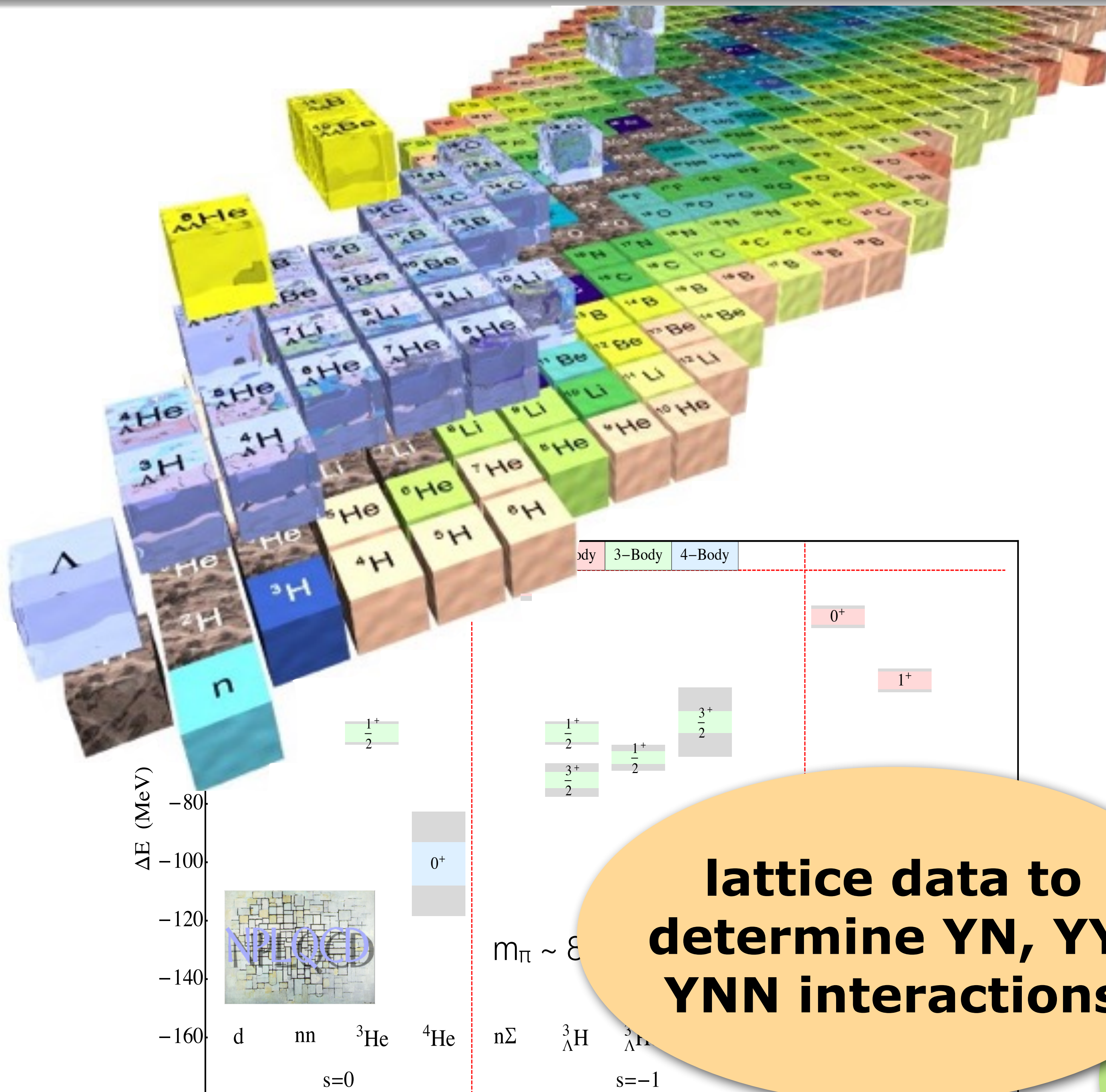


- precise data on ground states & spectroscopy of hypernuclei
- ab initio few-body and phenomenological shell or cluster model calculations done so far
- chiral YN & YY interactions at (N)LO are available

constrain YN interactions with hypernuclear spectroscopy

time to transfer ab initio toolbox to hypernuclei

Ab Initio Hypernuclear Structure



- Lattice QCD can be a game changer in hypernuclear physics
- extract YN & YY phase shifts from Lattice QCD, possibly also YNN
- compute light hypernuclei directly on the lattice

lattice data to determine YN, YY, YNN interactions

structure theory for consistency check and access to heavier hypernuclei

Ab Initio Toolbox for Hypernuclei

Wirth et al., PRL 113, 192502 (2014) & PRL 117, 182501 (2016)

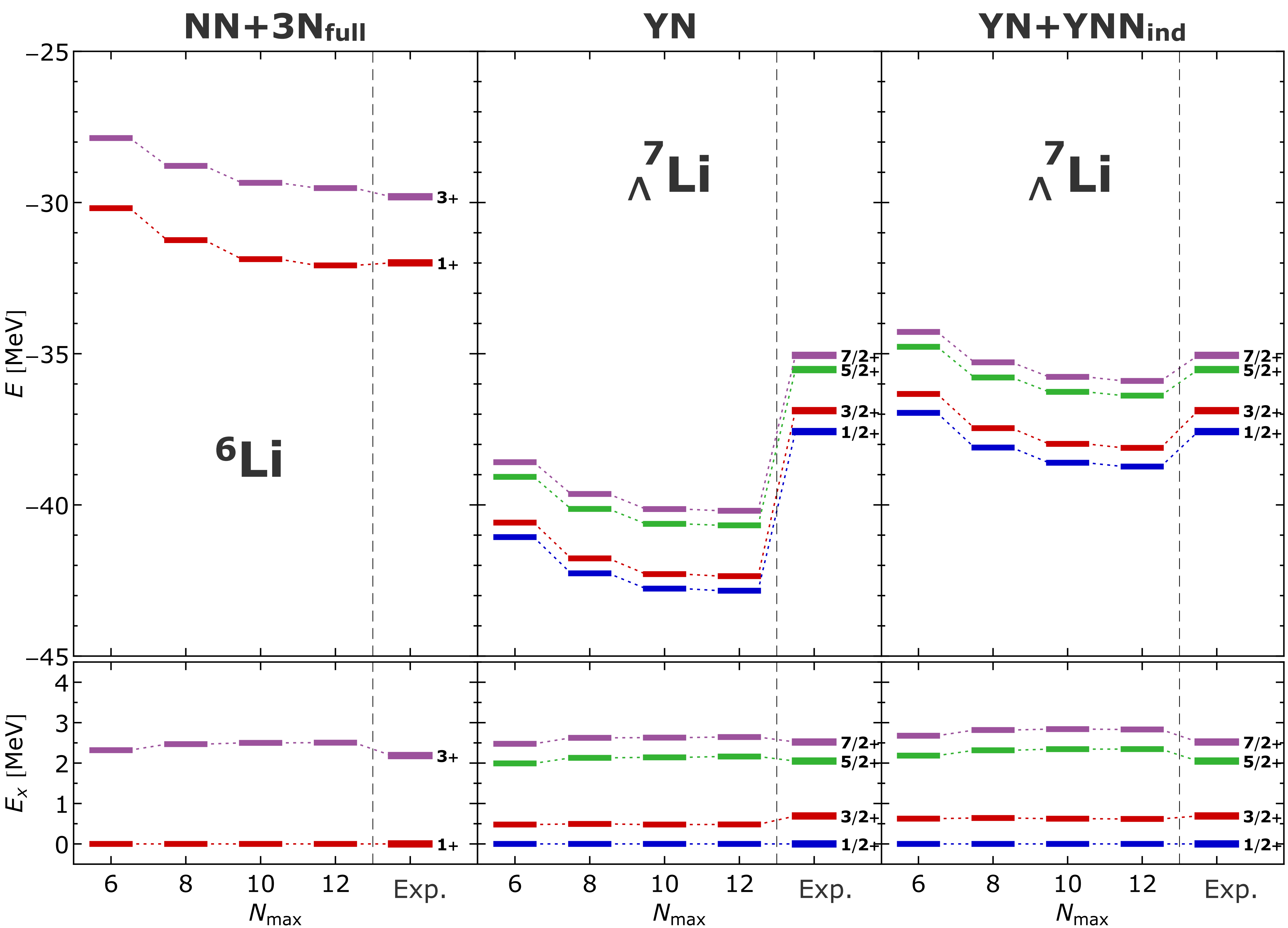
- **Hamiltonian from chiral EFT**
  - NN+3N: standard chiral Hamiltonian (Entem&Machleidt, Navrátil)
  - YN: LO chiral interaction (Haidenbauer et al.), NLO in progress

- **Similarity Renormalization Group**
  - consistent SRG-evolution of NN, 3N, YN interactions
  - using particle basis and including ΛΣ-coupling (larger matrices)
  - Λ-Σ mass difference and $p\Sigma^{\pm}$ Coulomb included consistently

- **Importance Truncated No-Core Shell Model**
  - include explicit $(p, n, \Lambda, \Sigma^{+}, \Sigma^{0}, \Sigma^{-})$ with physical masses
  - larger model spaces easily tractable with importance truncation
  - all p-shell single-Λ hypernuclei are accessible

Application: $^{7}_{\Lambda}$Li

Wirth et al., PRL 117, 182501 (2016)



IT-NCSM

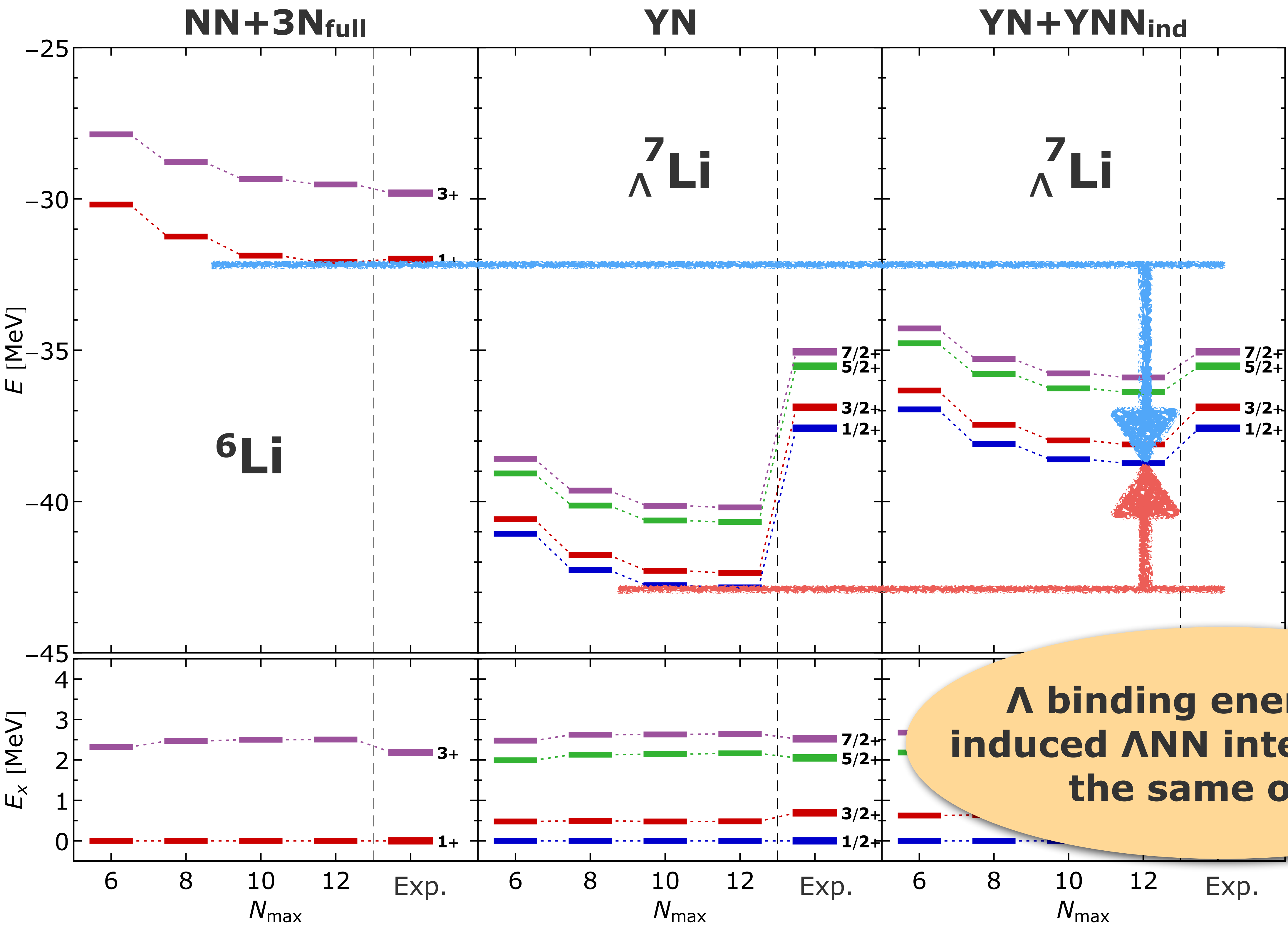
chiral NN+3N
standard
N3LO+N2LO
Λ_{3N}=500 MeV
α=0.08 fm⁴

chiral YN
LO
Λ_{YN}=700 MeV
α=0.08 fm⁴

ħΩ=20 MeV

Application: $^{7}_{\Lambda}$Li

Wirth et al., PRL 117, 182501 (2016)



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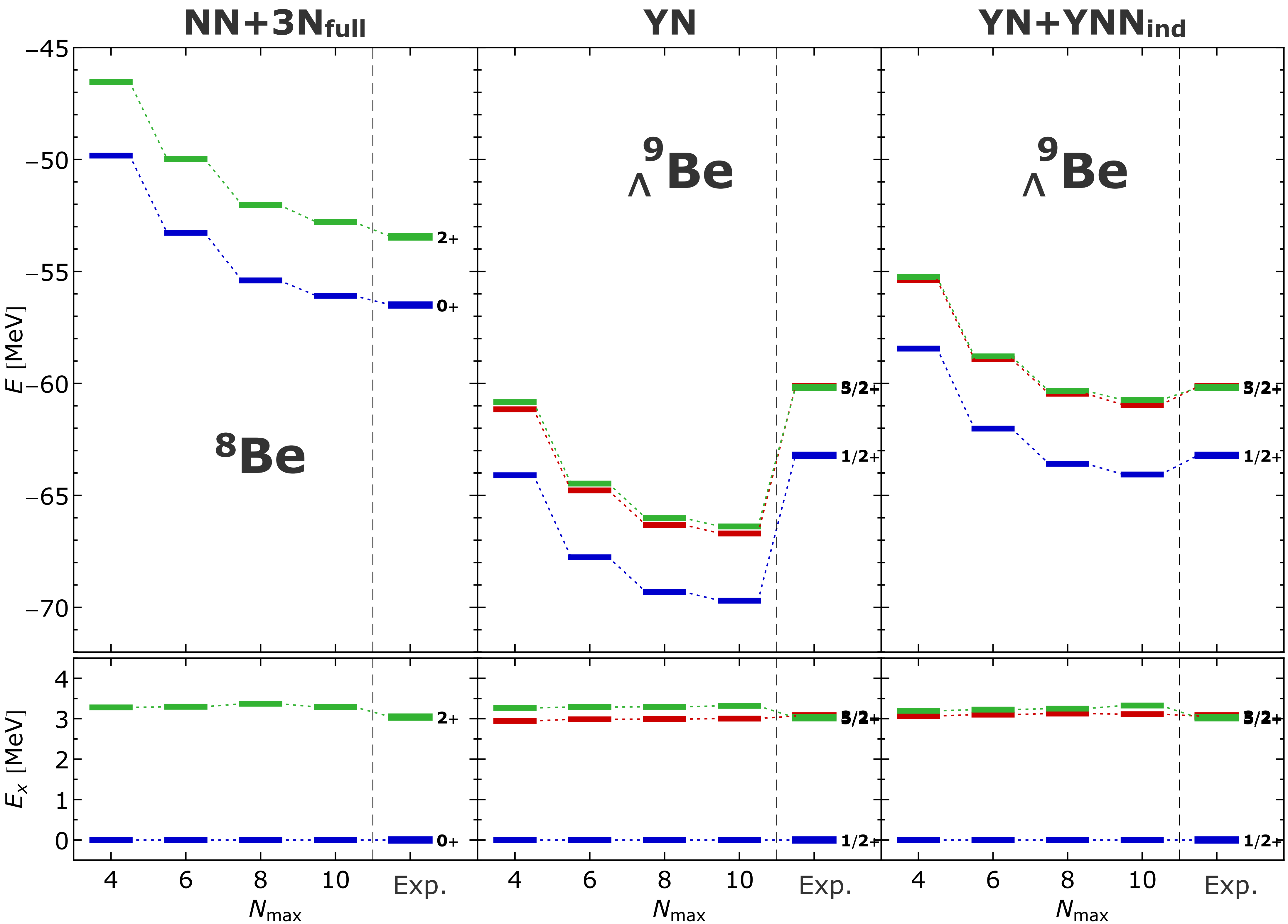
Λ_{YN}=700 MeV
α=0.08 fm^4

Λ binding energy and induced ΛNN interaction of the same order

Application: $^{9}_{\Lambda}$Be

Wirth et al., PRL 117, 182501 (2016)



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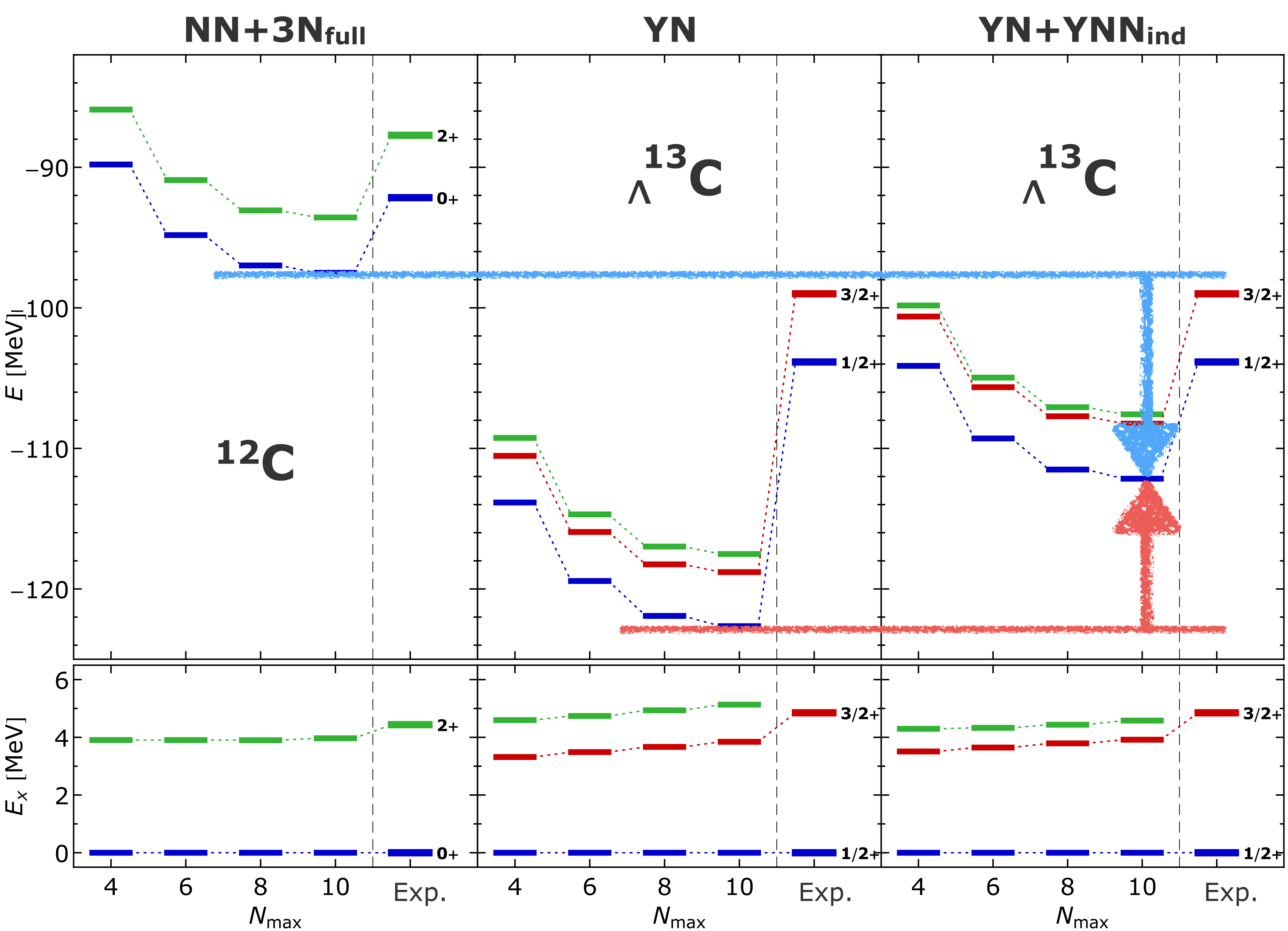
Application: $^{13}_{\Lambda}C$

Wirth et al., PRL 117, 182501 (2016)



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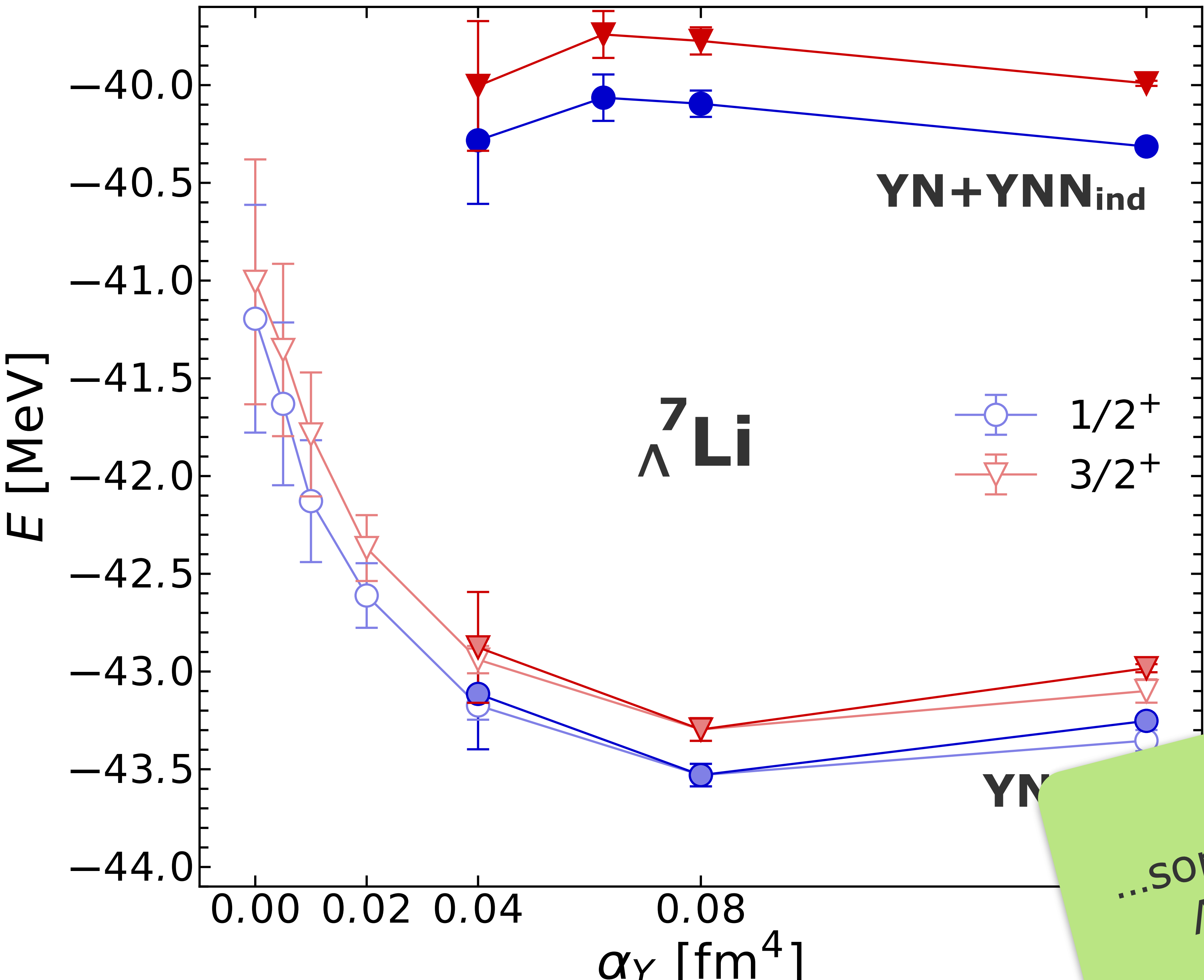
Induced YNN Interactions

Wirth et al., PRL 117, 182501 (2016)



- **induced YNN interactions** are surprisingly large in light hypernuclei

$V_{\mathrm{YNN_{ind}},\alpha} \sim 0.80\ |B_\Lambda|$

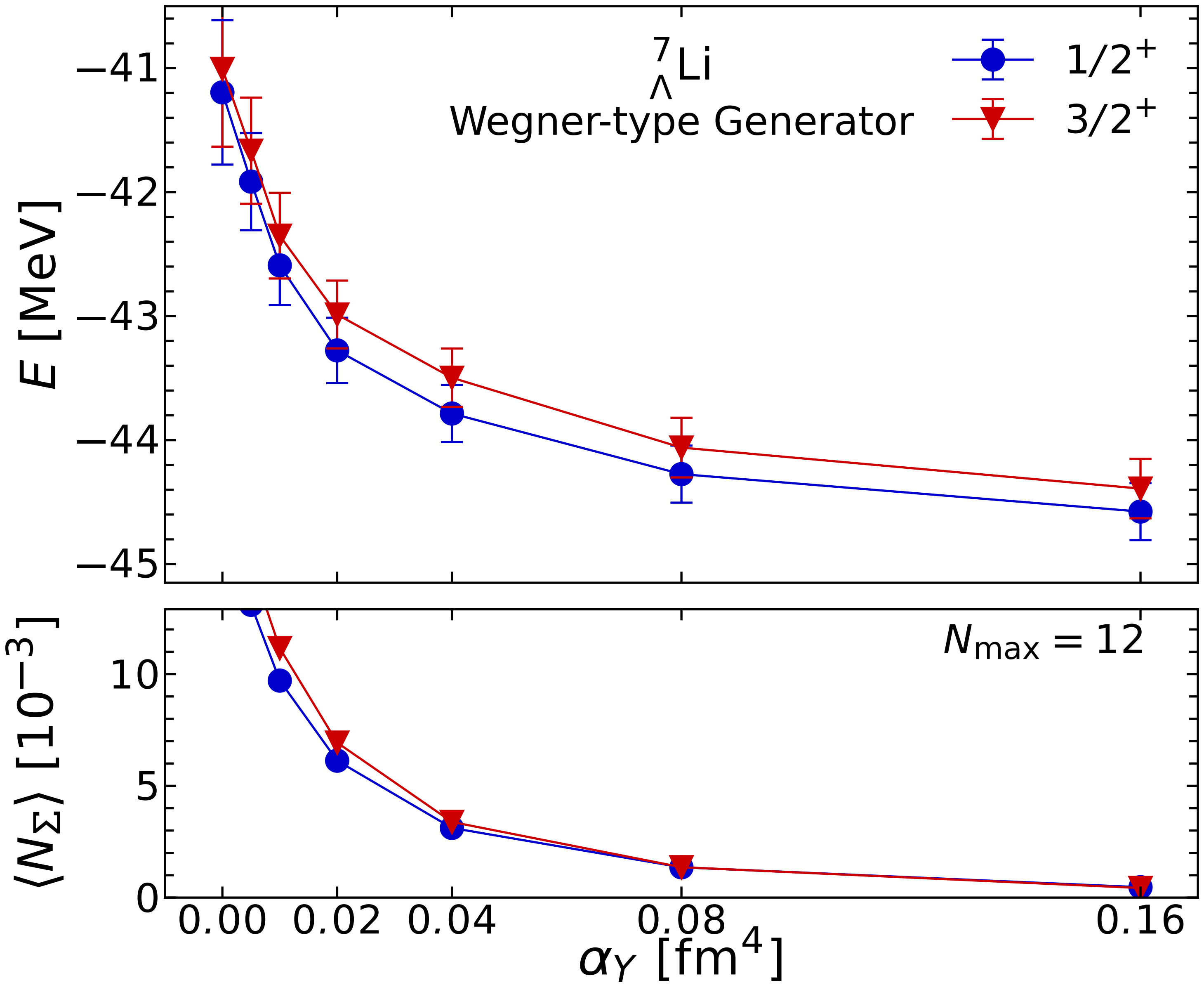
$V_{\mathrm{YNN_{ind}},\alpha} \sim 0.40\ |V_{\mathrm{YN},\alpha}|$

$V_{\mathrm{NNN_{ind}},\alpha} \sim 0.07\ |V_{\mathrm{NN},\alpha}|$

WHY ?
...something to do with Λ-Σ conversion ?

Suppression of Λ-Σ Conversion

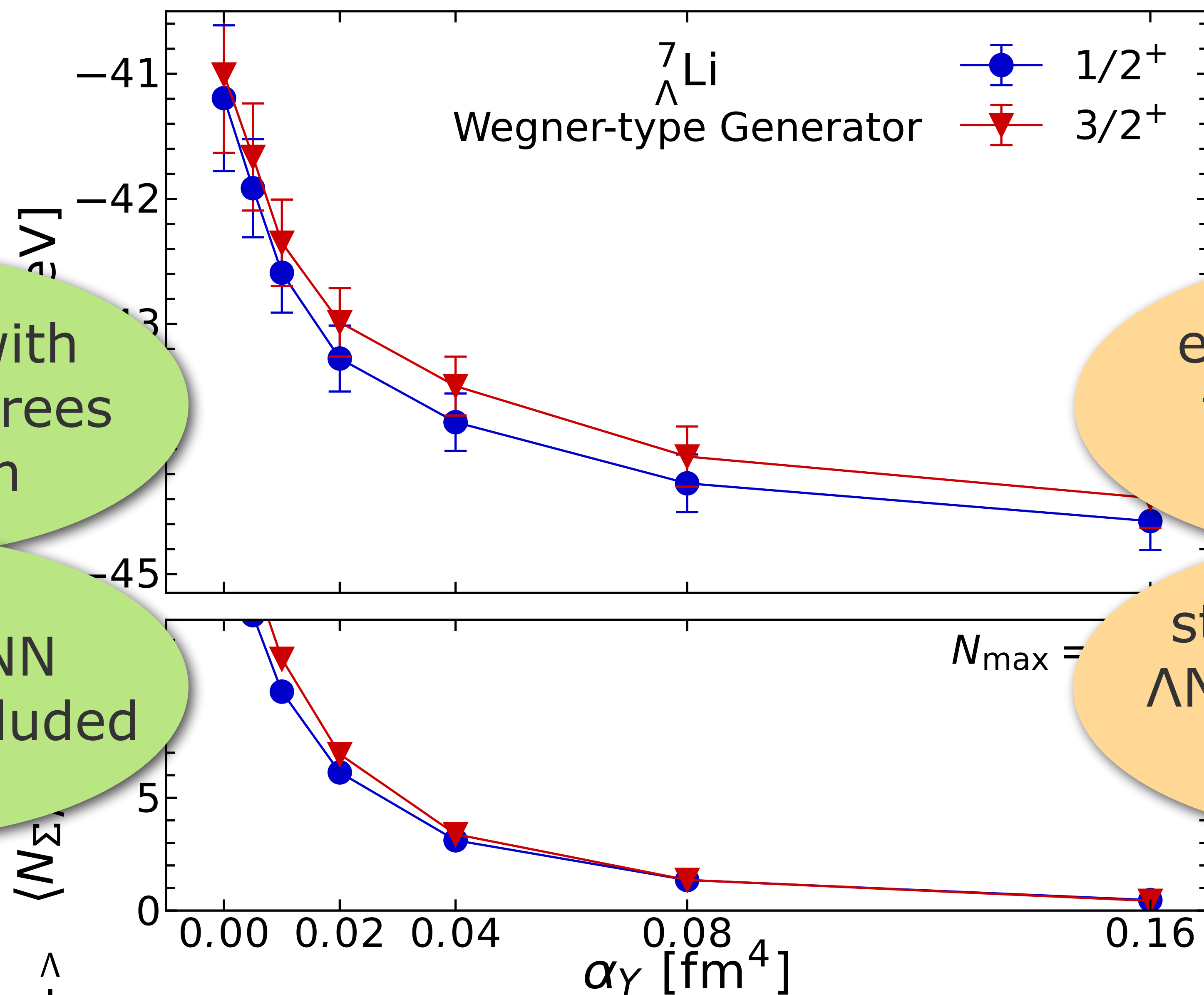
Wirth et al., PRL 117, 182501 (2016)



- design SRG-generator that **suppresses the Λ-Σ conversion** exclusively
- Σ admixture in the wave functions eliminated or "integrated out"
- same large induced YNN interactions as in standard SRG

Suppression of Λ-Σ Conversion

Wirth et al., PRL 117, 182501 (2016)

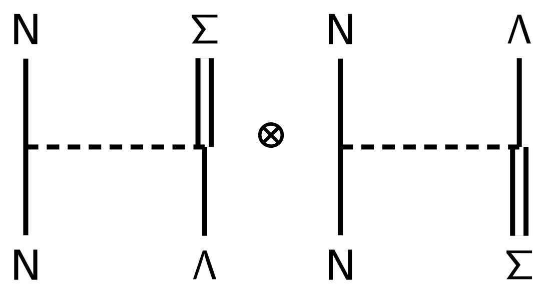


full theory with explicit Σ degrees of freedom

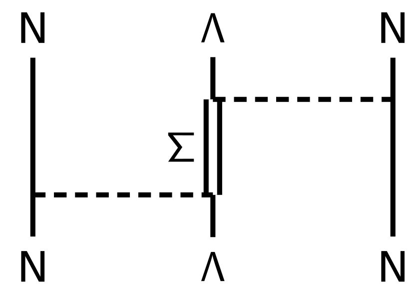
no initial YNN interaction included

effective Λ-only theory, Σ fully decoupled

strong repulsive ΛNN interaction is induced

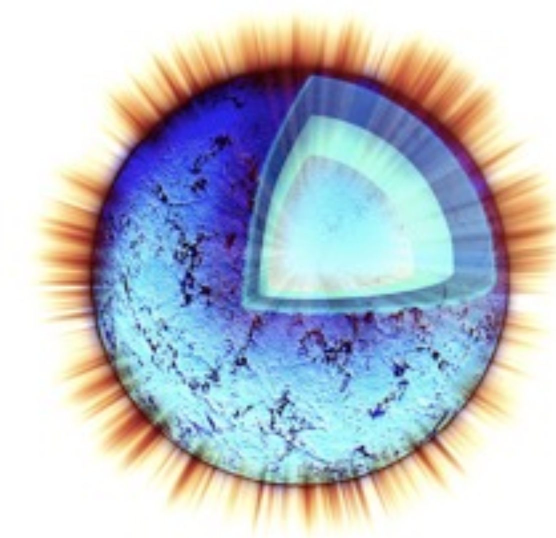


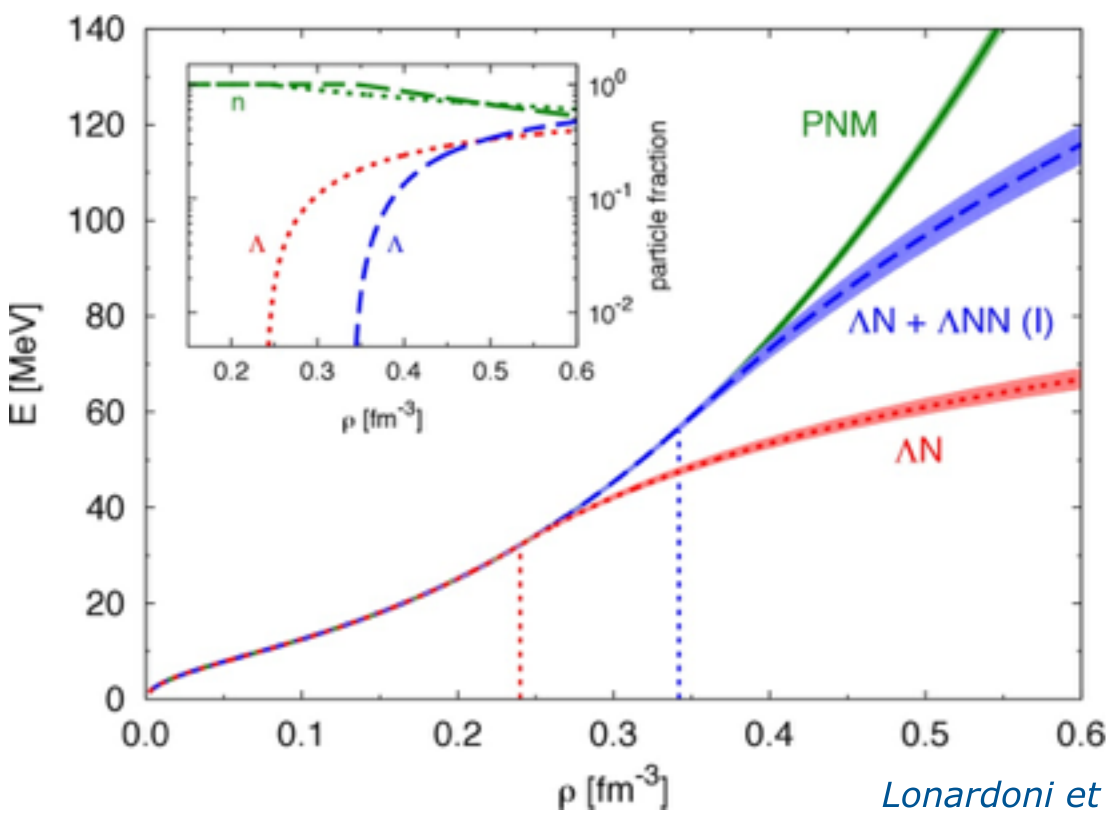
SRG evolves full coupled-channel theory to effective Λ-only theory

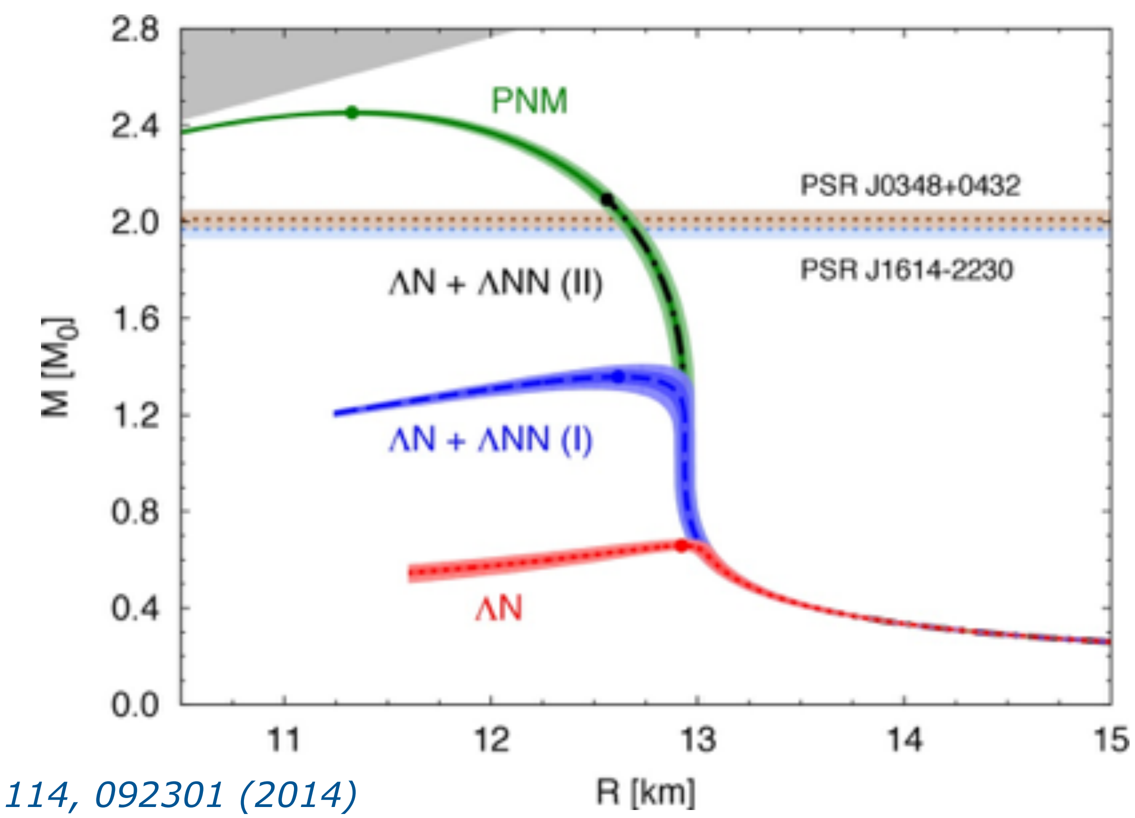


Implications for the Hyperon Puzzle

- neutron stars reach densities, where hyperon production should be energetically favorable
- including explicit Λs with ΛN interaction softens EOS - does not support 2M⊙ neutron star
- possible phenomenological fix: include strongly repulsive ΛNN interaction





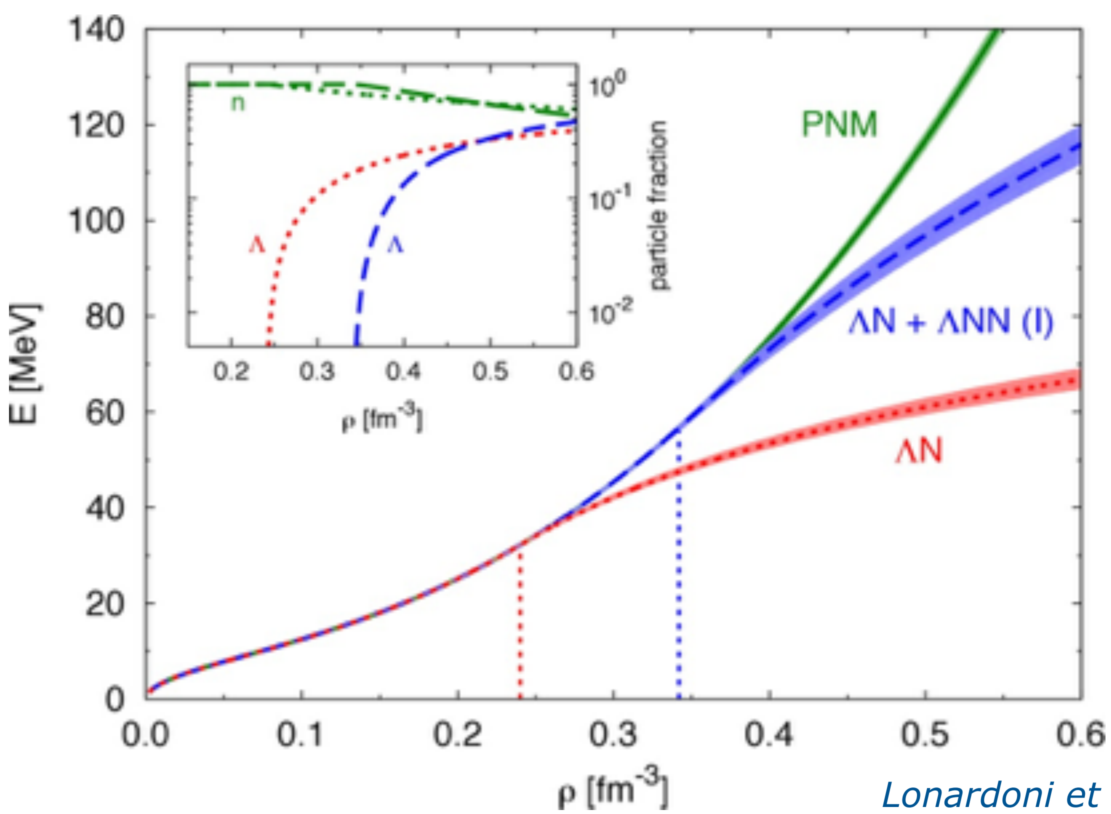


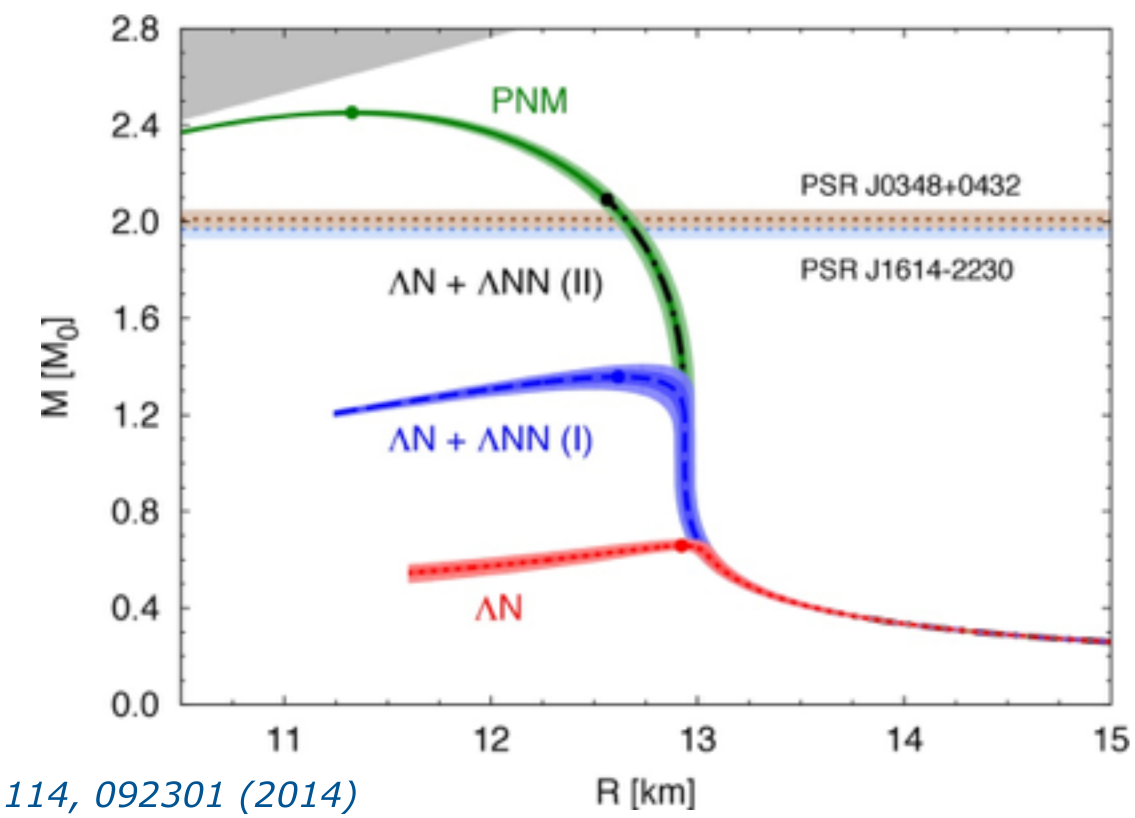
Lonardoni et al.; PRL 114, 092301 (2014)

Recent Example: AFDMC

Lonardoni et al.; PRL 114, 092301 (2014)

- **Auxiliary Field Diffusion Monte Carlo** calculations for hypernuclei and homogeneous matter
- **only include Λ degrees of freedom** explicitly with phenomenological ΛN and ΛNN interactions fitted to hypernuclei
- strongly repulsive ΛNN interaction shifts onset of Λ production to larger densities and **increases maximum neutron-star mass**





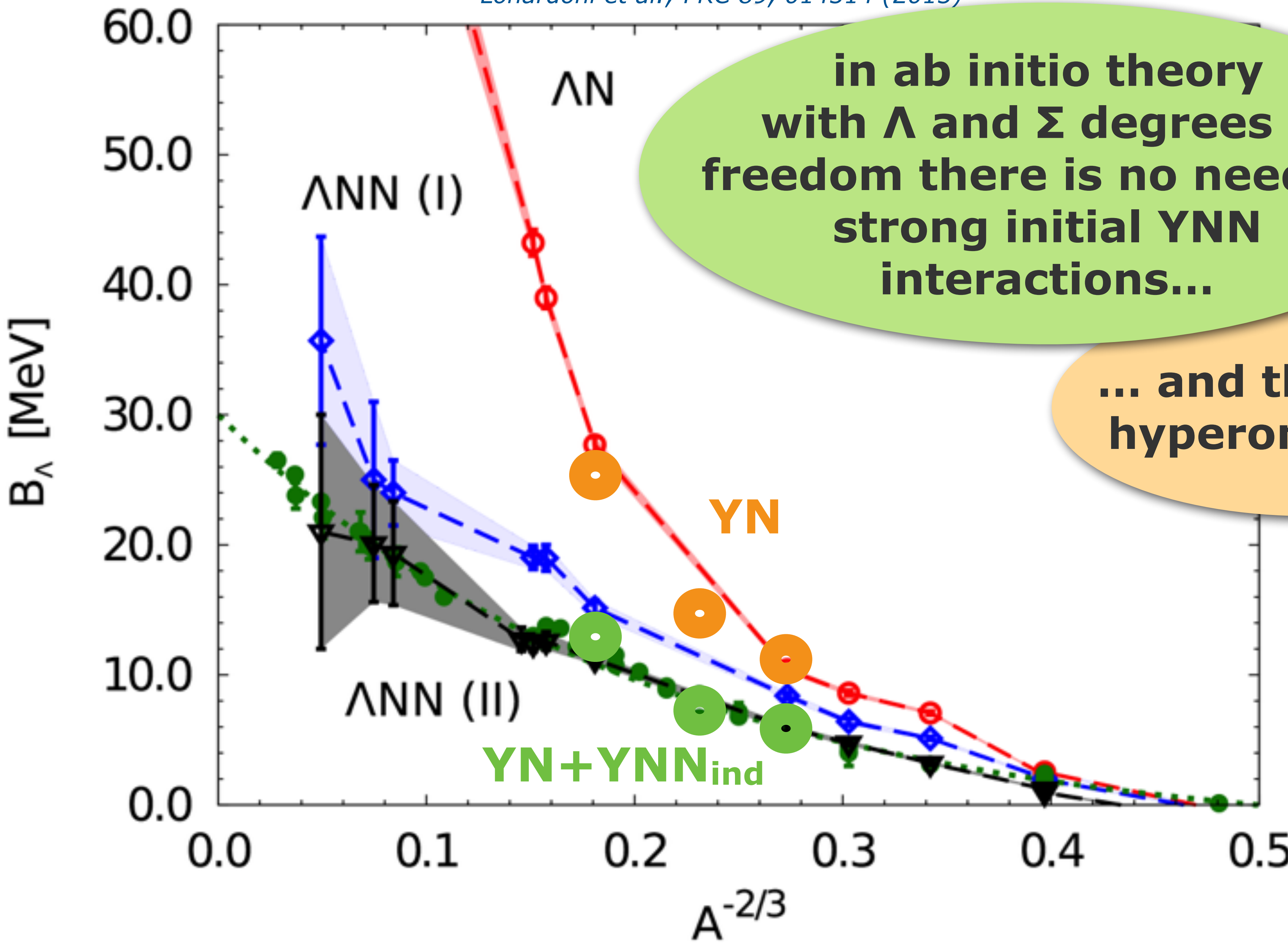
Lonardoni et al.; PRL 114, 092301 (2014)

Comparison to AFDMC

Lonardoni et al.; PRL 114, 092301 (2014); PRC 89, 014314 (2013)

- How do the binding energies of hypernuclei look like with AFDMC ?

Lonardoni et al.; PRC 89, 014314 (2013)



in ab initio theory with Λ and Σ degrees of freedom there is no need for strong initial YNN interactions...

... and there is no hyperon puzzle !

Overview

- **Lecture 1: Hamiltonian**

  Prelude • Nuclear Hamiltonian • Matrix Elements • Two-Body Problem • Correlations & Unitary Transformations

- **Lecture 2: Light Nuclei**

  Similarity Renormalization Group • Many-Body Problem • Configuration Interaction • No-Core Shell Model • Hypernuclei

- **Lecture 3: Beyond Light Nuclei**

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

Nuclei as Bound States

Lecture 3: Beyond Light Nuclei

Robert Roth

TECHNISCHE UNIVERSITÄT DARMSTADT

Overview

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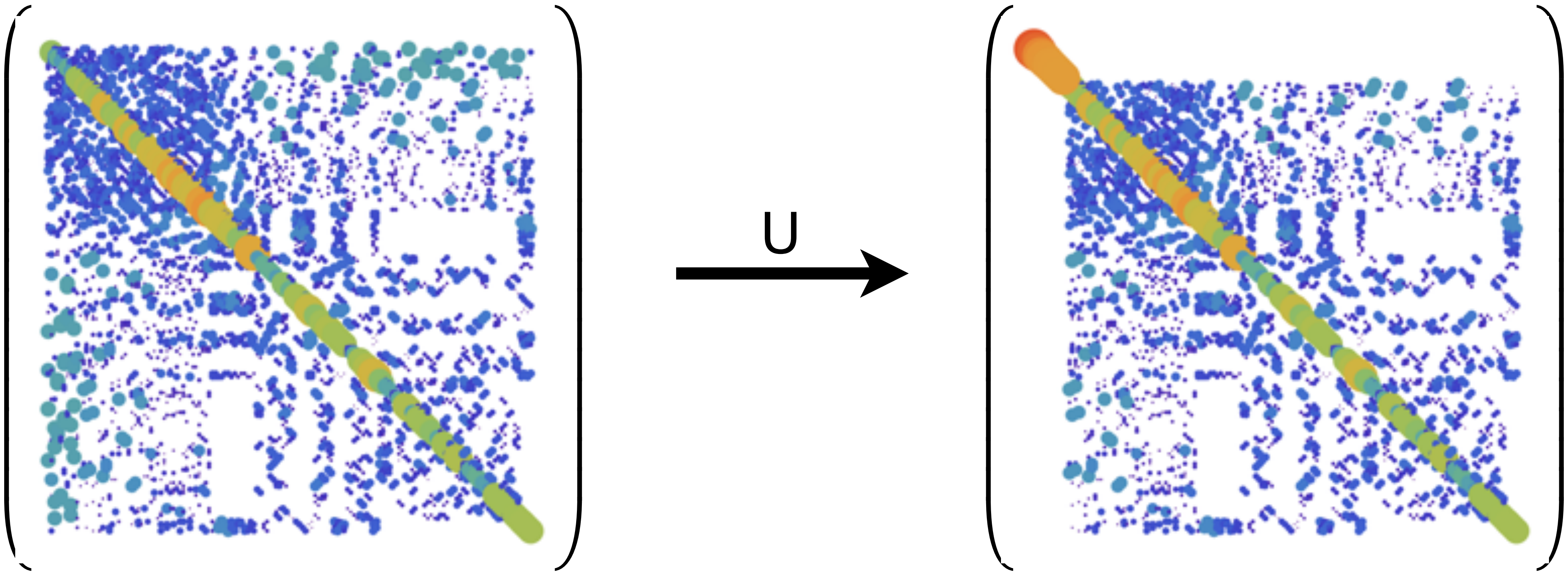
Beyond Light Nuclei

advent of novel ab initio approaches
targeting the ground state of medium-mass nuclei
very efficiently

- **idea**: decouple reference state from particle-hole excitations by a unitary or similarity transformation of Hamiltonian



Beyond Light Nuclei

advent of novel ab initio approaches
targeting the ground state of medium-mass nuclei
very efficiently

- **idea**: decouple reference state from particle-hole excitations by a unitary or similarity transformation of Hamiltonian

Tsukiyama, Bogner, Schwenk, Hergert,...

- **In-Medium Similarity Renormalisation Group**: decouple many-body reference state from particle-hole excitations by SRG transformation
  - normal-ordered A-body Hamiltonian truncated at the two-body level
  - open and closed-shell nuclei can be targeted directly

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

- **Coupled-Cluster Theory**: ground-state is parametrised by exponential wave operator acting on single-determinant reference state
  - truncation at doubles level (CCSD) with corrections for triples contributions
  - directly applicable for closed-shell nuclei, equations-of-motion methods for open-shell

Normal Ordering

Particle-Hole Excitations

- short-hand notation for creation and annihilation operators

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

- 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,...* : hole states, occupied in reference state
p,q,r,... : particle states, unoccupied in reference states
i,j,k,... : 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

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

- **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**

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

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

$$H = \frac{1}{4}\sum_{ijkl} \langle ij|\, T_{\text{int}} + V_{NN}\, |kl\rangle\; a^\dagger_i a^\dagger_j a_l a_k + \cdots$$

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

- **normal-ordered Hamiltonian** with respect to reference sta[te]

$$H = E + \sum_{ij} f^i_j\, \{a^\dagger_i a_j\} + \frac{1}{4}\sum_{ijkl} \Gamma^{ij}_{kl}\, \{a^\dagger_i a^\dagger_j a_l a_k\} + \frac{1}{36}\sum_{ijklmn} W^{ijk}_{lmn}\, \{a^\dagger_i a^\dagger_j a^\dagger_k a_n a_m a_l\}$$

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

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

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

$$W^{ijk}_{lmn} = \langle ijk|\, V_{3N}\, |lmn\rangle$$

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

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

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

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

- 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**

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

- 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

CCSD Equations for Amplitudes

$$\Delta E^{(\mathrm{CCSD})} = \overset{(EA)}{+} \frac{1}{4}\sum_{abij} v^{ij}_{ab}\, t^{ab}_{ij} \overset{(EB)}{+} \sum_{ai} f^{i}_{a}\, t^{a}_{i} \overset{(EC)}{+} \frac{1}{2}\sum_{abij} v^{ij}_{ab}\, t^{a}_{i}\, t^{b}_{j}$$

$$\overset{(SA)}{+} f^{a}_{i} \overset{(SBa)}{+} \sum_{ck} f^{k}_{c}\, t^{ac}_{ik} \overset{(SBb)}{+} \tfrac{1}{2}\sum_{cdk} v^{ak}_{cd}\, t^{cd}_{ik} \overset{(SBc)}{-} \tfrac{1}{2}\sum_{ckl} v^{kl}_{ic}\, t^{ac}_{kl}$$
$$\overset{(SCa)}{+} \sum_{c} f^{a}_{c}\, t^{c}_{i} \overset{(SCb)}{-} \sum_{i} f^{k}_{i}\, t^{a}_{k} \overset{(SCc)}{+} \sum_{ck} v^{ak}_{ic}\, t^{c}_{k} \overset{(SDa)}{-} \tfrac{1}{2}\sum_{cdkl} v^{kl}_{cd}\, t^{ad}_{kl}\, t^{c}_{i}$$
$$\overset{(SDb)}{-} \tfrac{1}{2}\sum_{cdkl} v^{kl}_{cd}\, t^{cd}_{il}\, t^{a}_{k} \overset{(SDc)}{+} \sum_{cdkl} v^{kl}_{cd}\, t^{da}_{li}\, t^{c}_{k} \overset{(SEa)}{-} \sum_{ck} f^{k}_{c}\, t^{c}_{i}\, t^{a}_{k}$$
$$\overset{(SEb)}{+} \sum_{cdk} v^{ak}_{cd}\, t^{c}_{i}\, t^{d}_{k} \overset{(SEc)}{-} \sum_{ckl} v^{kl}_{ic}\, t^{a}_{k}\, t^{c}_{l} \overset{(SF)}{-} \sum_{cdkl} v^{kl}_{cd}\, t^{a}_{k}\, t^{c}_{i}\, t^{d}_{l}$$
$$= 0\,,\ \forall\, a,i$$

$$\overset{(DA)}{+} v^{ab}_{ij} \overset{(DBa)}{+} \hat{P}_{ab} \sum_{c} f^{b}_{c}\, t^{ac}_{ij} \overset{(DBb)}{-} \hat{P}_{ij} \sum_{k} f^{k}_{j}\, t^{ab}_{ik}$$
$$\overset{(DBc)}{+} \tfrac{1}{2}\sum_{cd} v^{ab}_{cd}\, t^{cd}_{ij} \overset{(DBd)}{+} \tfrac{1}{2}\sum_{k} v^{kl}_{ij}\, t^{ab}_{kl} \overset{(DBe)}{+} \hat{P}_{ab}\,\hat{P}_{ij} \sum_{ck} v^{kb}_{cj}\, t^{ac}_{ik}$$
$$\overset{(DCa)}{+} \tfrac{1}{4}\sum_{cdkl} v^{kl}_{cd}\, t^{cd}_{ij}\, t^{ab}_{kl} \overset{(DCb)}{+} \hat{P}_{ij} \sum_{cdkl} v^{kl}_{cd}\, t^{ac}_{ik}\, t^{bd}_{jl}$$
$$\overset{(DCc)}{-} \tfrac{1}{2}\hat{P}_{ij} \sum_{cdkl} v^{kl}_{cd}\, t^{dc}_{ik}\, t^{ab}_{lj} \overset{(DCd)}{-} \tfrac{1}{2}\hat{P}_{ab} \sum_{cdkl} v^{kl}_{cd}\, t^{ac}_{lk}\, t^{db}_{ij}$$
$$\overset{(DDa)}{+} \hat{P}_{ij} \sum_{c} v^{ab}_{cj}\, t^{c}_{i} \overset{(DDb)}{-} \hat{P}_{ab} \sum_{k} v^{kb}_{ij}\, t^{a}_{k} \overset{(DEa)}{-} \hat{P}_{ij} \sum_{ck} f^{k}_{c}\, t^{ab}_{kj}\, t^{c}_{i}$$
$$\overset{(DEb)}{-} \hat{P}_{ab} \sum_{ck} f^{k}_{c}\, t^{cb}_{ij}\, t^{a}_{k} \overset{(DEc)}{+} \hat{P}_{ab}\,\hat{P}_{ij} \sum_{cdk} v^{ak}_{cd}\, t^{db}_{kj}\, t^{c}_{i}$$
$$\overset{(DEd)}{-} \hat{P}_{ab}\,\hat{P}_{ij} \sum_{ckl} v^{kl}_{ic}\, t^{cb}_{lj}\, t^{a}_{k} \overset{(DEe)}{-} \tfrac{1}{2}\hat{P}_{ab} \sum_{cdk} v^{kb}_{cd}\, t^{cd}_{ij}\, t^{a}_{k}$$
$$\overset{(DEf)}{+} \tfrac{1}{2}\hat{P}_{ij} \sum_{ckl} v^{kl}_{cj}\, t^{ab}_{kl}\, t^{c}_{i} \overset{(DEg)}{+} \hat{P}_{ab} \sum_{cdk} v^{ka}_{cd}\, t^{db}_{ij}\, t^{c}_{k}$$
$$\overset{(DEh)}{-} \hat{P}_{ij} \sum_{ckl} v^{kl}_{ci}\, t^{ab}_{lj}\, t^{c}_{k} \overset{(DFa)}{+} \sum_{cd} v^{ab}_{cd}\, t^{c}_{i}\, t^{d}_{j} \overset{(DFb)}{+} \sum_{kl} v^{kl}_{ij}\, t^{a}_{k}\, t^{b}_{l}$$
$$\overset{(DFc)}{-} \hat{P}_{ab}\,\hat{P}_{ij} \sum_{ck} v^{kb}_{cj}\, t^{a}_{k}\, t^{c}_{i} \overset{(DGa)}{+} \tfrac{1}{2}\sum_{cdkl} v^{kl}_{cd}\, t^{ab}_{kl}\, t^{c}_{i}\, t^{d}_{j}$$
$$\overset{(DGb)}{+} \tfrac{1}{2}\sum_{cdkl} v^{kl}_{cd}\, t^{cd}_{ij}\, t^{a}_{k}\, t^{b}_{l} \overset{(DGc)}{-} \hat{P}_{ab}\,\hat{P}_{ij} \sum_{cdkl} v^{kl}_{cd}\, t^{db}_{lj}\, t^{a}_{k}\, t^{c}_{i}$$
$$\overset{(DGd)}{-} \hat{P}_{ij} \sum_{cdkl} v^{kl}_{cd}\, t^{ab}_{lj}\, t^{c}_{k}\, t^{d}_{i} \overset{(DGe)}{-} \hat{P}_{ab} \sum_{cdkl} v^{kl}_{cd}\, t^{db}_{ij}\, t^{a}_{l}\, t^{c}_{k}$$
$$\overset{(DHa)}{-} \hat{P}_{ab} \sum_{cdk} v^{kb}_{cd}\, t^{a}_{k}\, t^{c}_{i}\, t^{d}_{j} \overset{(DHb)}{+} \hat{P}_{ij} \sum_{ckl} v^{kl}_{cj}\, t^{a}_{k}\, t^{b}_{l}\, t^{c}_{i}$$
$$\overset{(DI)}{+} \sum_{cdkl} v^{kl}_{cd}\, t^{a}_{k}\, t^{b}_{l}\, t^{c}_{i}\, t^{d}_{j} = 0\,,\quad \forall\, a,b,i,j$$

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

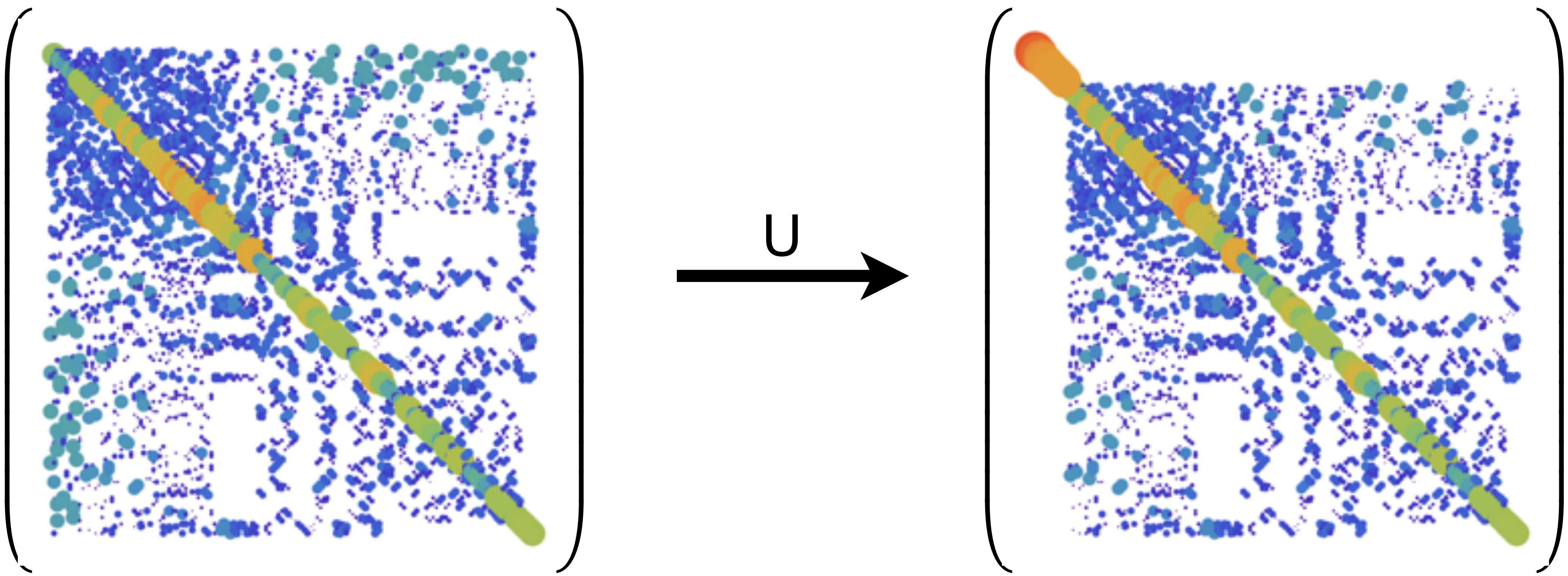
- not variational
- only for closed shell nuclei *
- other observables difficult
- only for ground states *
- non-hermititan Hamiltonian

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

In-Medium SRG

Decoupling in A-Body Space

- partially **diagonalize Hamilton matrix** through a unitary transformation and read-off eigenvalues from the diagonal



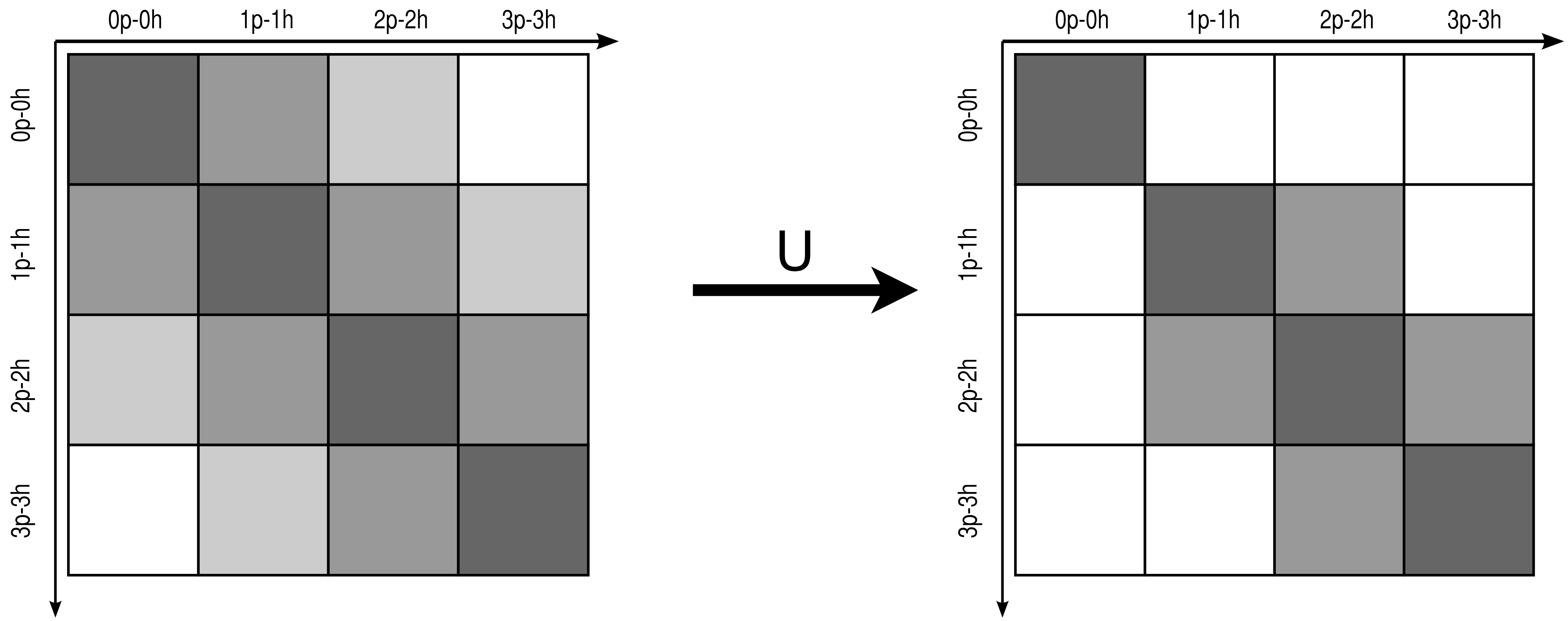
- **continuous unitary transformation** of many-body Hamiltonian

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

morphs the initial Hamilton matrix ($\alpha = 0$) to diagonal form ($\alpha \to \infty$)

Decoupling in A-Body Space

- partially **diagonalize Hamilton matrix** through a unitary transformation and read-off eigenvalues from the diagonal



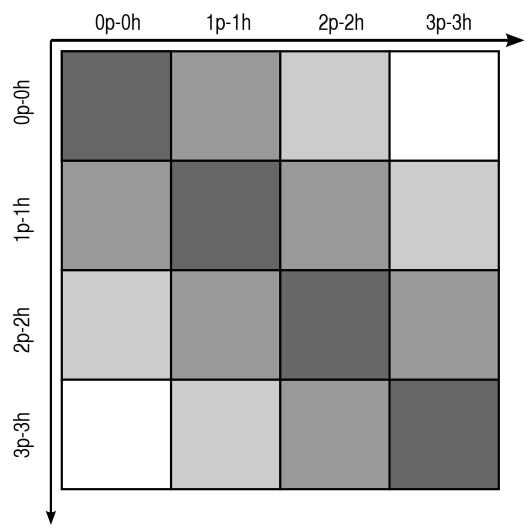
- **continuous unitary transformation** of many-body Hamiltonian

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

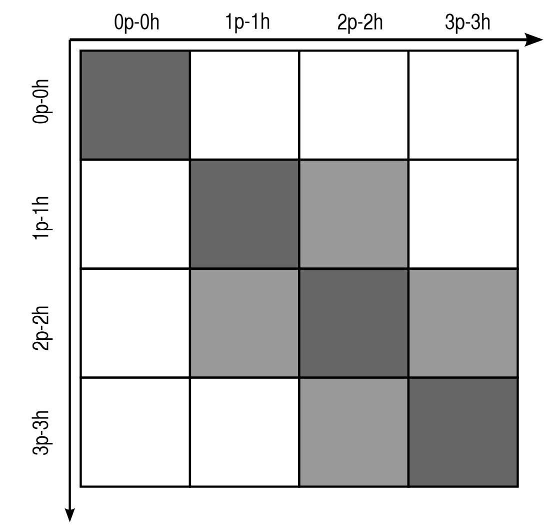
morphs the initial Hamilton matrix ($\alpha = 0$) to diagonal form ($\alpha \to \infty$)

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

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

- **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]*

$$\eta^{1}_{2} = \langle \Phi |\, [H, \{a^{\dagger}_{1} a_2\}]\, | \Phi \rangle$$

$$\eta^{12}_{34} = \langle \Phi |\, [H, \{a^{\dagger}_{1} a^{\dagger}_{2} a_4 a_3\}]\, | \Phi \rangle$$

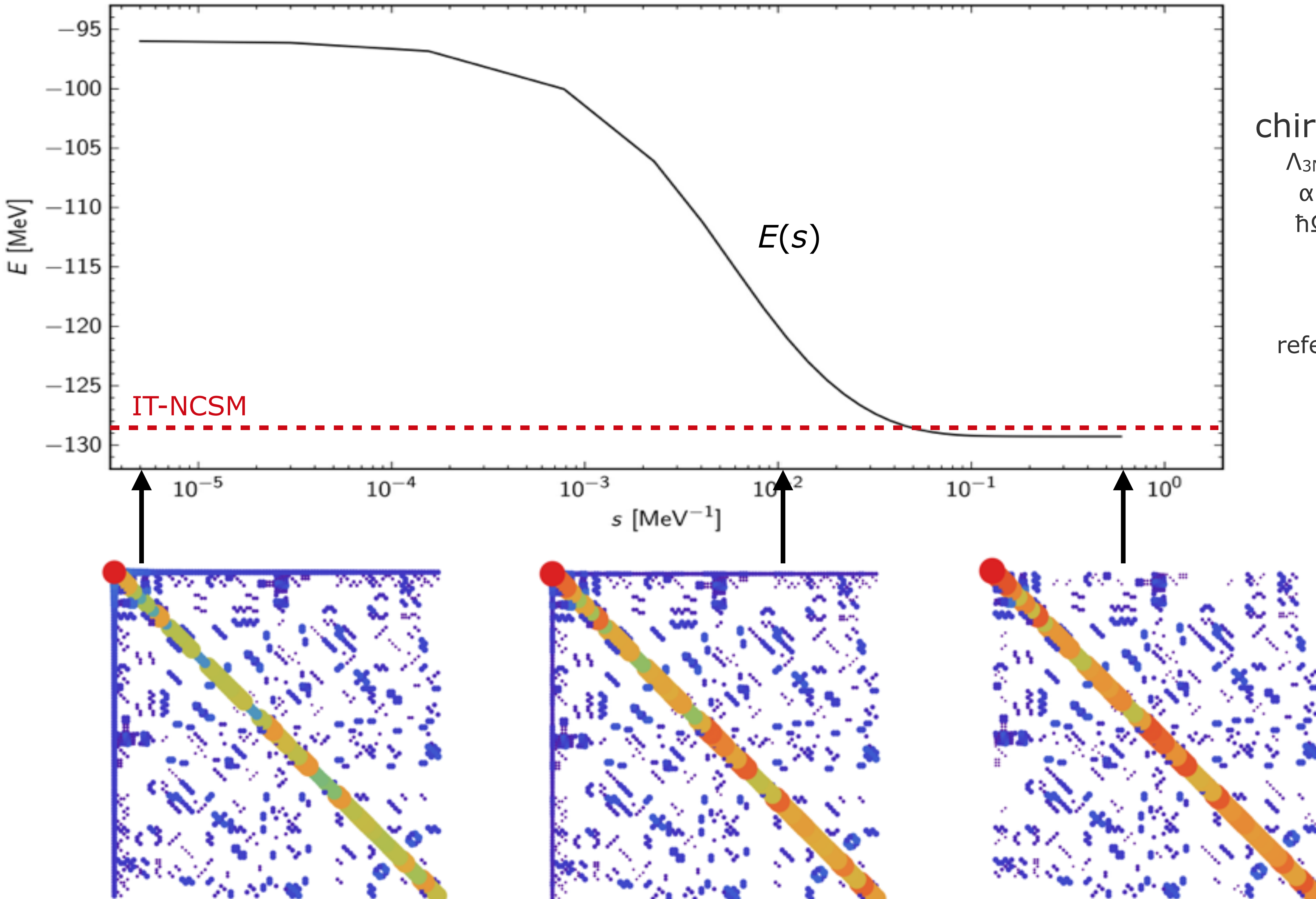
Flow-Equations for Matrix Elements

$$\frac{dE}{ds} = \sum_{ab}(n_a - n_b)\left(\eta^a_b f^b_a - f^a_b \eta^b_a\right) + \frac{1}{4}\sum_{abcd}\left(\eta^{ab}_{cd}\Gamma^{cd}_{ab} - \Gamma^{ab}_{cd}\eta^{cd}_{ab}\right) n_a n_b \bar{n}_c \bar{n}_d$$

$$\frac{d}{ds}f^1_2 = \sum_a \left(\eta^1_a f^a_2 - f^1_a \eta^a_2\right) + \sum_{ab}\left(\eta^a_b \Gamma^{b1}_{a2} - f^a_b \eta^{b1}_{a2}\right)(n_a - n_b)$$
$$+ \frac{1}{2}\sum_{abcdef}\left(\eta^{1a}_{bc}\Gamma^{bc}_{2a} - \Gamma^{1a}_{bc}\eta^{bc}_{2a}\right)(n_a \bar{n}_b \bar{n}_c + \bar{n}_a n_b n_c)$$

$$\frac{d}{ds}\Gamma^{12}_{34} = \sum_a \left(\eta^1_a \Gamma^{a2}_{34} + \eta^2_a \Gamma^{1a}_{34} - \eta^a_3 \Gamma^{12}_{a4} - \eta^a_4 \Gamma^{12}_{3a} - f^1_a \eta^{a2}_{34} - f^2_a \eta^{1a}_{34} + f^a_3 \eta^{12}_{a4} + f^a_4 \eta^{12}_{3a}\right)$$
$$+ \frac{1}{2}\sum_{ab}\left(\eta^{12}_{ab}\Gamma^{ab}_{34} - \Gamma^{12}_{ab}\eta^{ab}_{34}\right)(1 - n_a - n_b)$$
$$+ \sum_{ab}(n_a - n_b)\left(\left(\eta^{1a}_{3b}\Gamma^{2b}_{4a} - \Gamma^{1a}_{3b}\eta^{2b}_{4a}\right) - \left(\eta^{2a}_{3b}\Gamma^{1b}_{4a} - \Gamma^{2a}_{3b}\eta^{1b}_{4a}\right)\right)$$

Flowing Energy



^{16}O

chiral NN+3N

Λ_{3N}=400 MeV

α=0.08 fm^4

ħΩ=20 MeV

e_{max}=12

N_{max}=0 reference state

Hamilton matrix in N_{max}=2 space

Merging NCSM and IM-SRG =: IM-NCSM

- combine CI/NCSM with IM-SRG to get the **best aspects of both methods**

- solve NCSM problem in small N_{max}
- extract reference state

↓

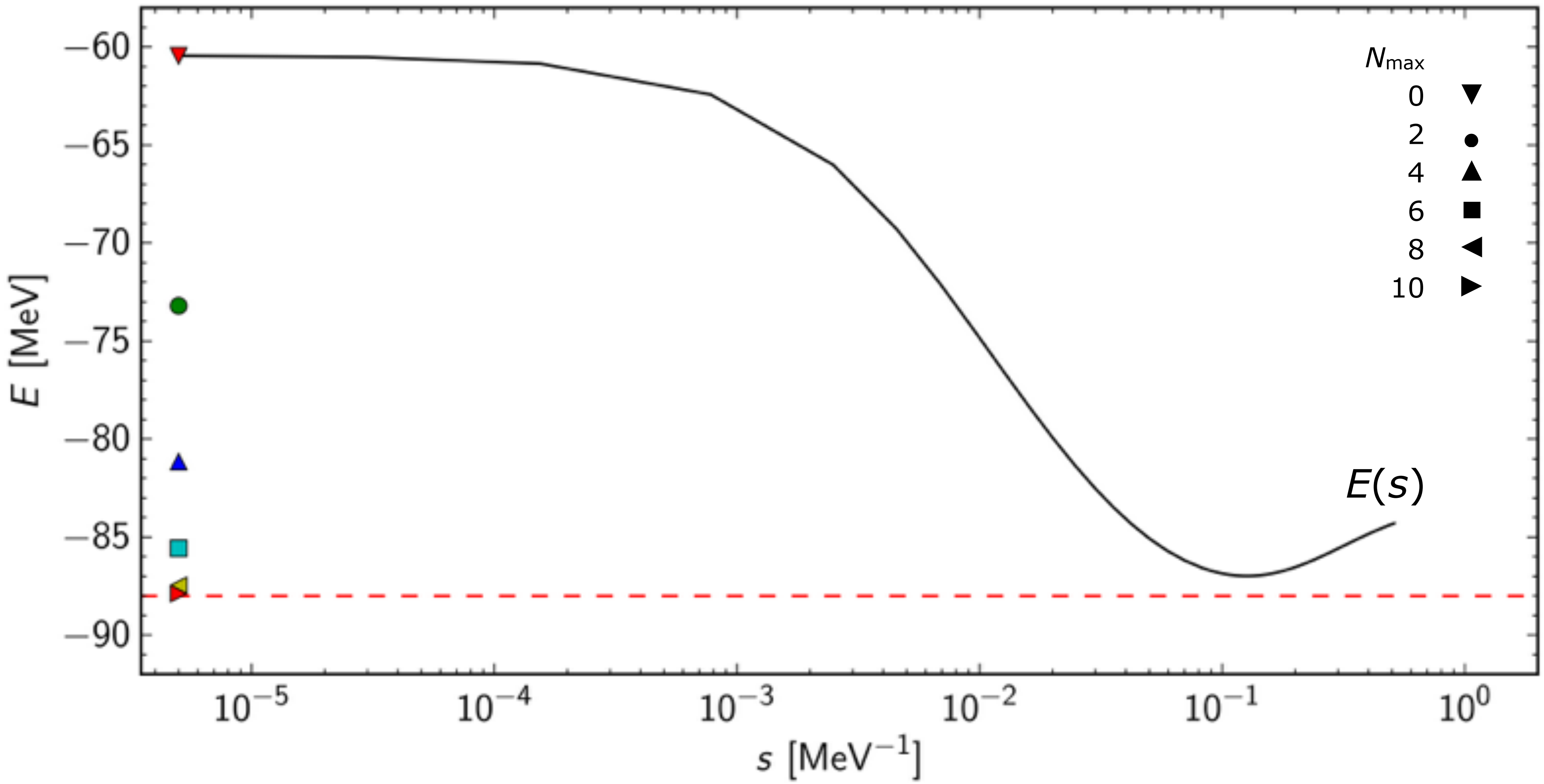
- solve MR-IM-SRG flow equations
- decoupling of particle-hole excitations in many-body space

↓

- solve NCSM problem with IM-SRG evolved Hamiltonian
- extract ground and excitation energies and other observables

IM-NCSM: Ground State

Gebrerufael et al.; arXiv:1610.05254



^{12}C

chiral NN+3N

Λ_{3N}=400 MeV

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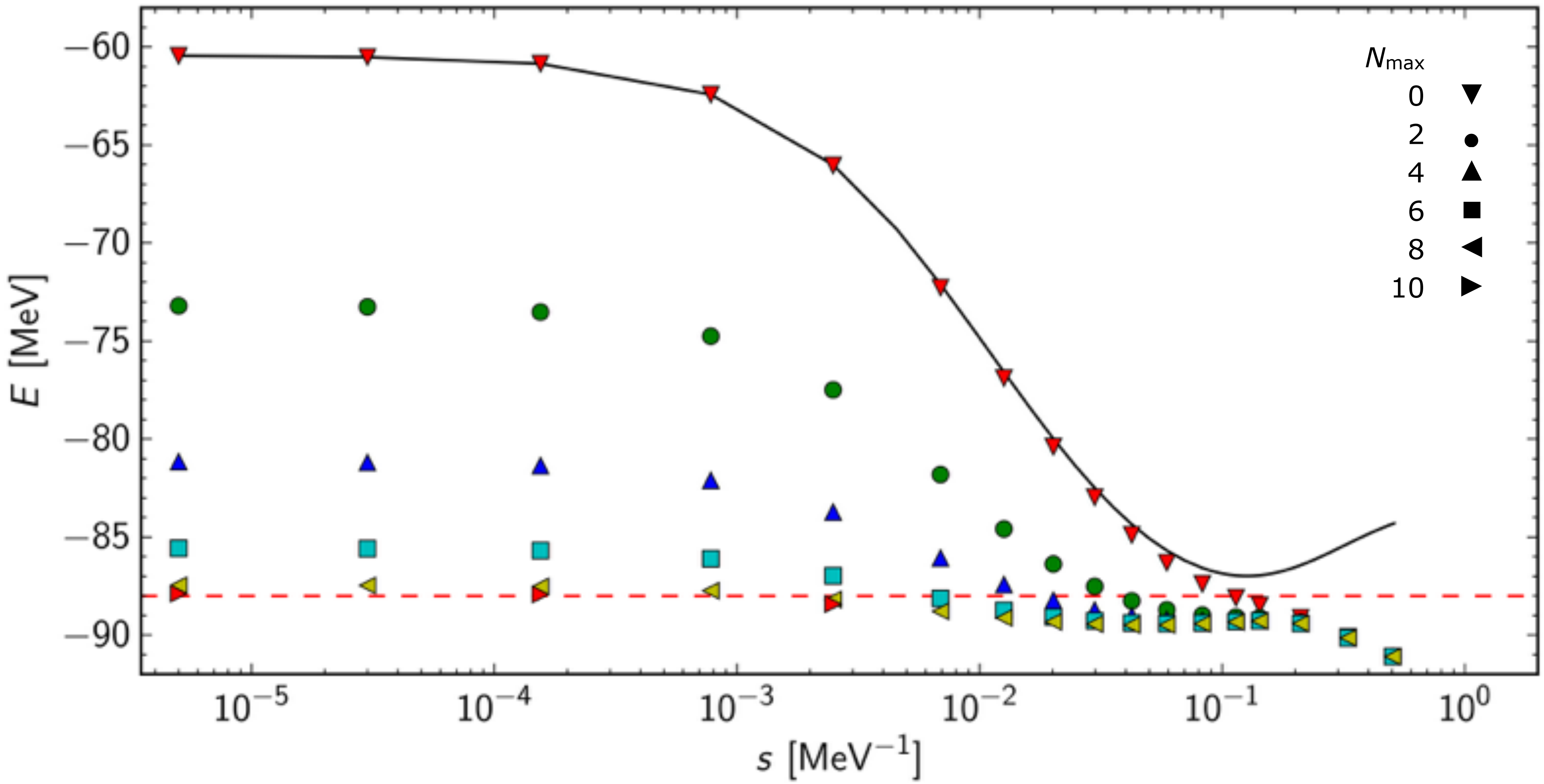
e_{max}=12

N_{max}=0 reference state

- instead of using the zero-body piece of the normal-ordered Hamiltonian, we can use the complete **flowing Hamiltonian in a NCSM calculation**

IM-NCSM: Ground State

Gebrerufael et al.; arXiv:1610.05254



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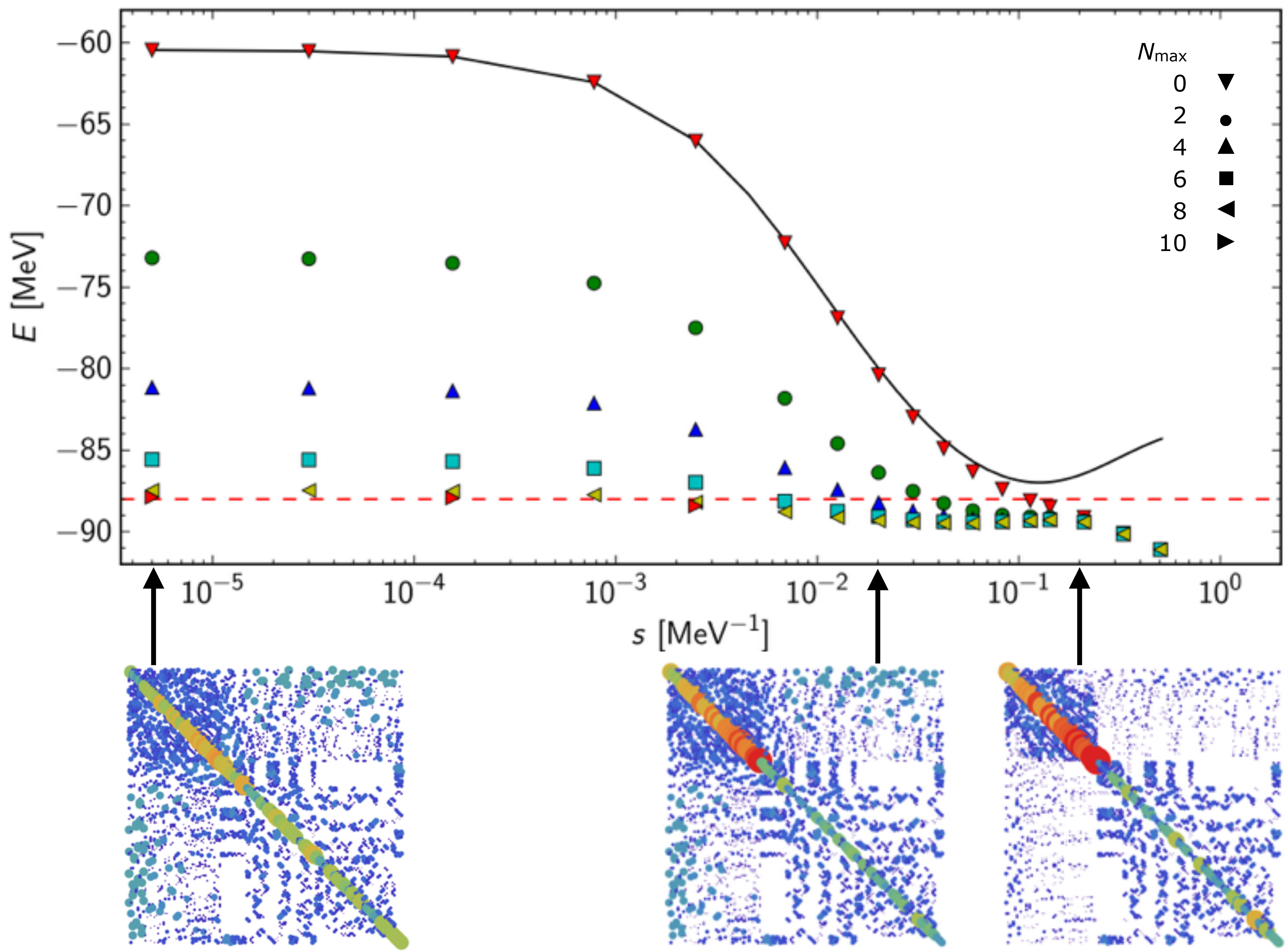
e_{max}=12

N_{max}=0 reference state

- instead of using the zero-body piece of the normal-ordered Hamiltonian, we can use the complete **flowing Hamiltonian in a NCSM calculation**
- decoupling though the IM-SRG transformation causes **ridiculously fast convergence** of NCSM calculation

IM-NCSM: Ground State

Gebrerufael et al.; arXiv:1610.05254



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IM-NCSM: Ground State

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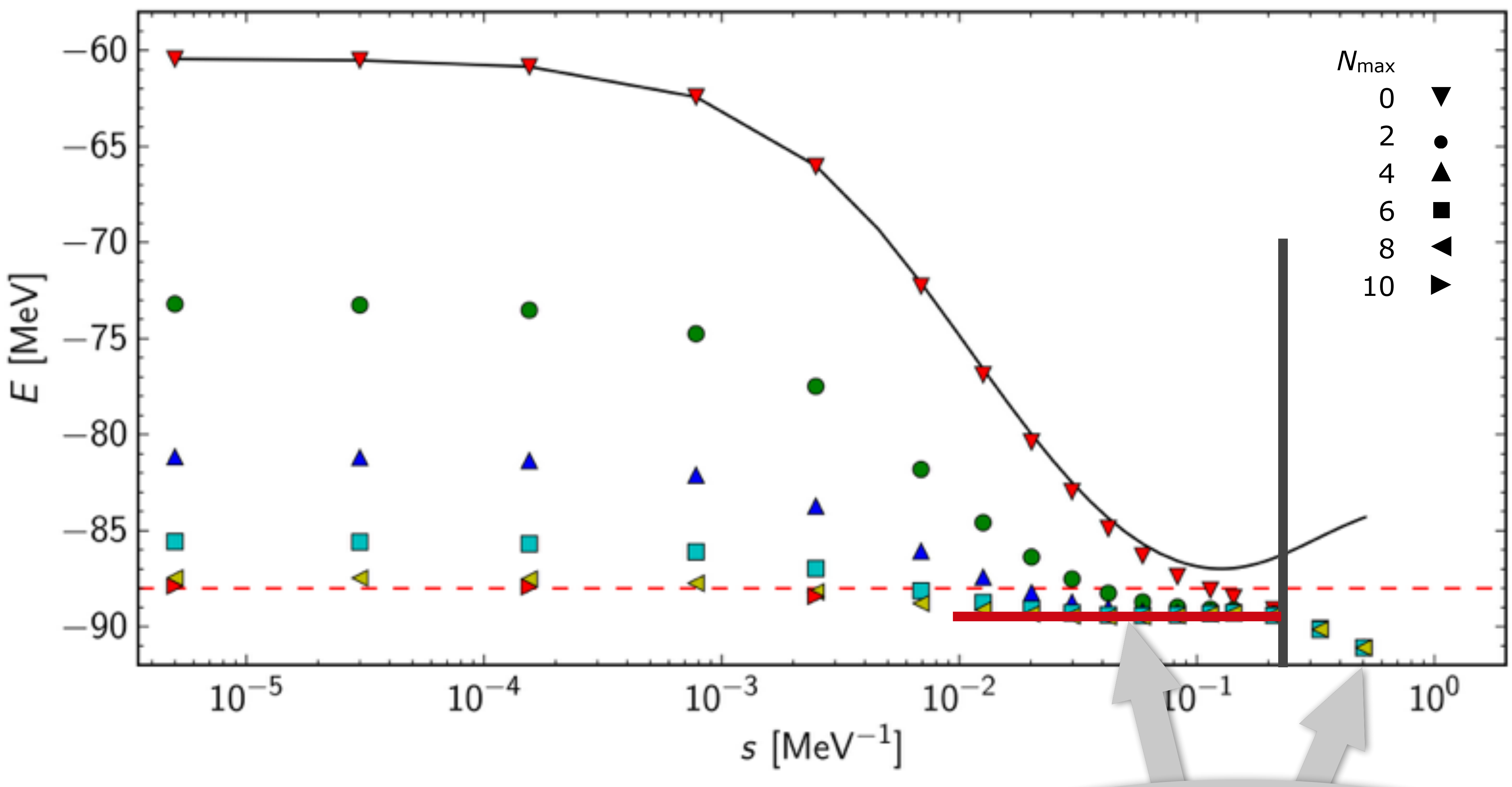

^{12}C

chiral NN+3N

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ħΩ=20 MeV

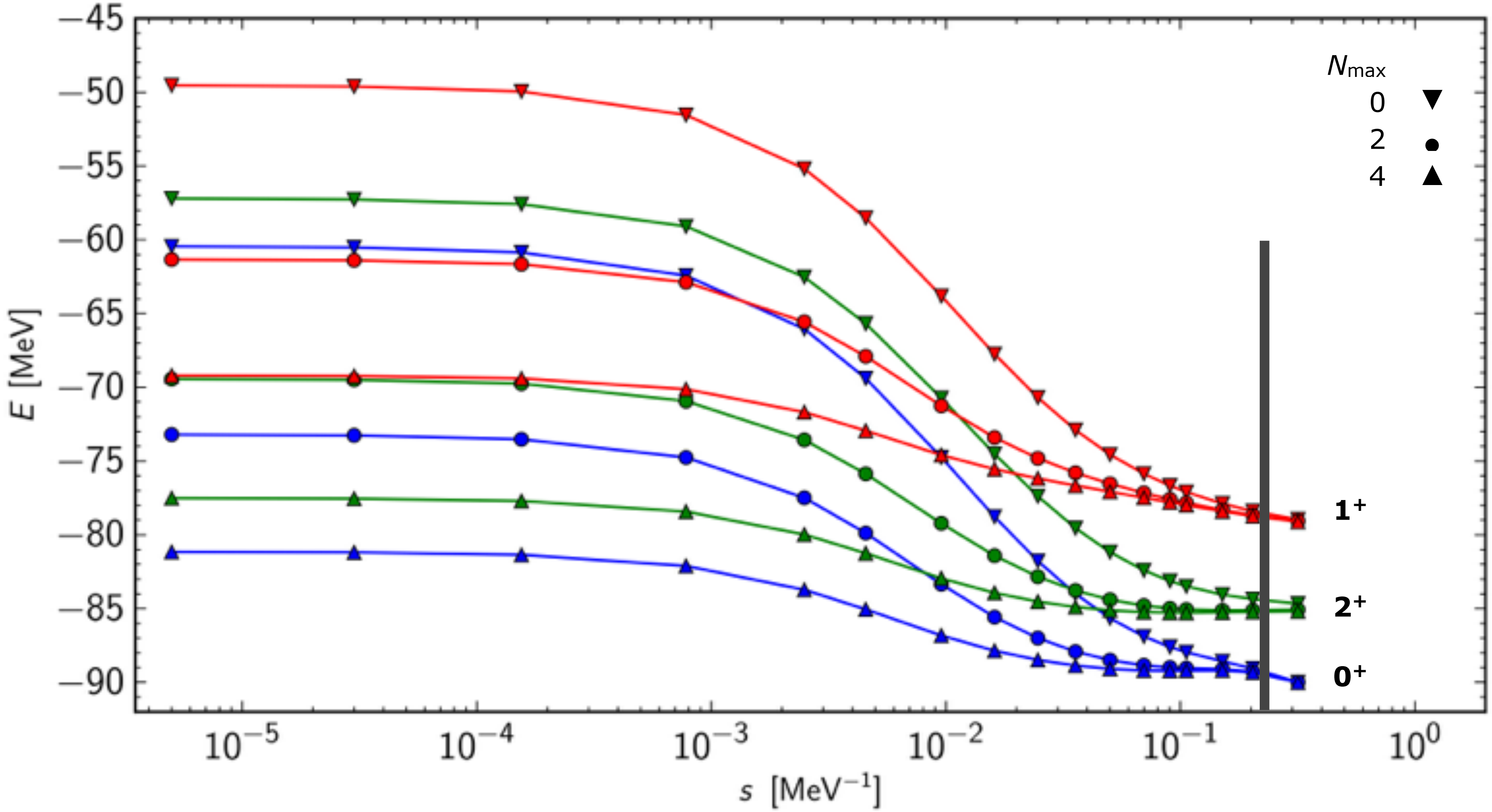
e_{max}=12

N_{max}=0
reference state

effects of IM-SRG truncation at the normal-ordered two-body level

IM-NCSM: Excited States

Gebrerufael et al.; arXiv:1610.05254



^{12}C

chiral NN+3N

Λ_{3N}=400 MeV

α=0.08 fm^4

$\hbar\Omega$=20 MeV

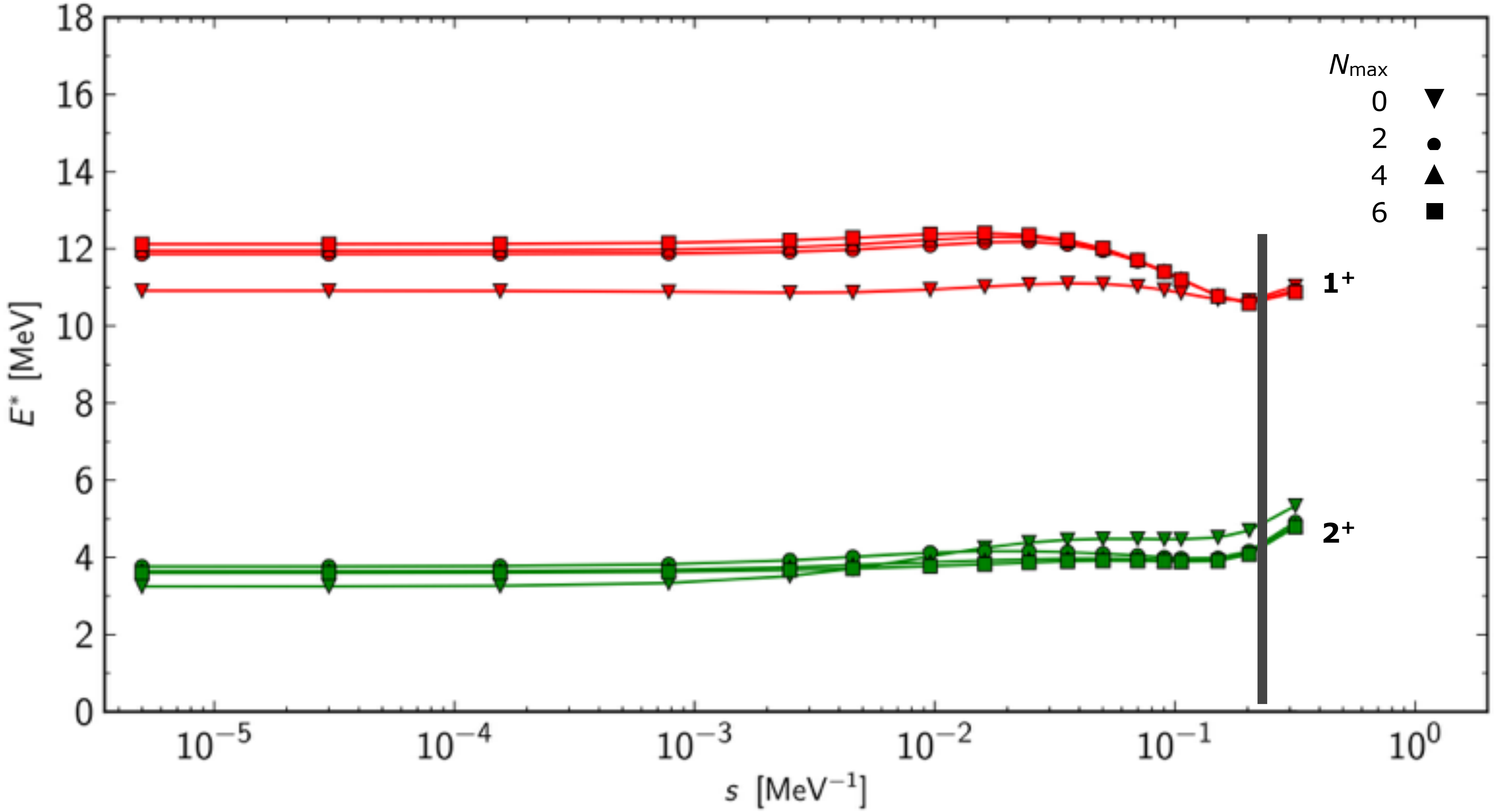
e_{max}=12

N_{max}=0 reference state

- from the same NCSM calculation we get the **excited states**

IM-NCSM: Excited States

Gebrerufael et al.; arXiv:1610.05254



^{12}C

chiral NN+3N

Λ_{3N}=400 MeV

α=0.08 fm^4

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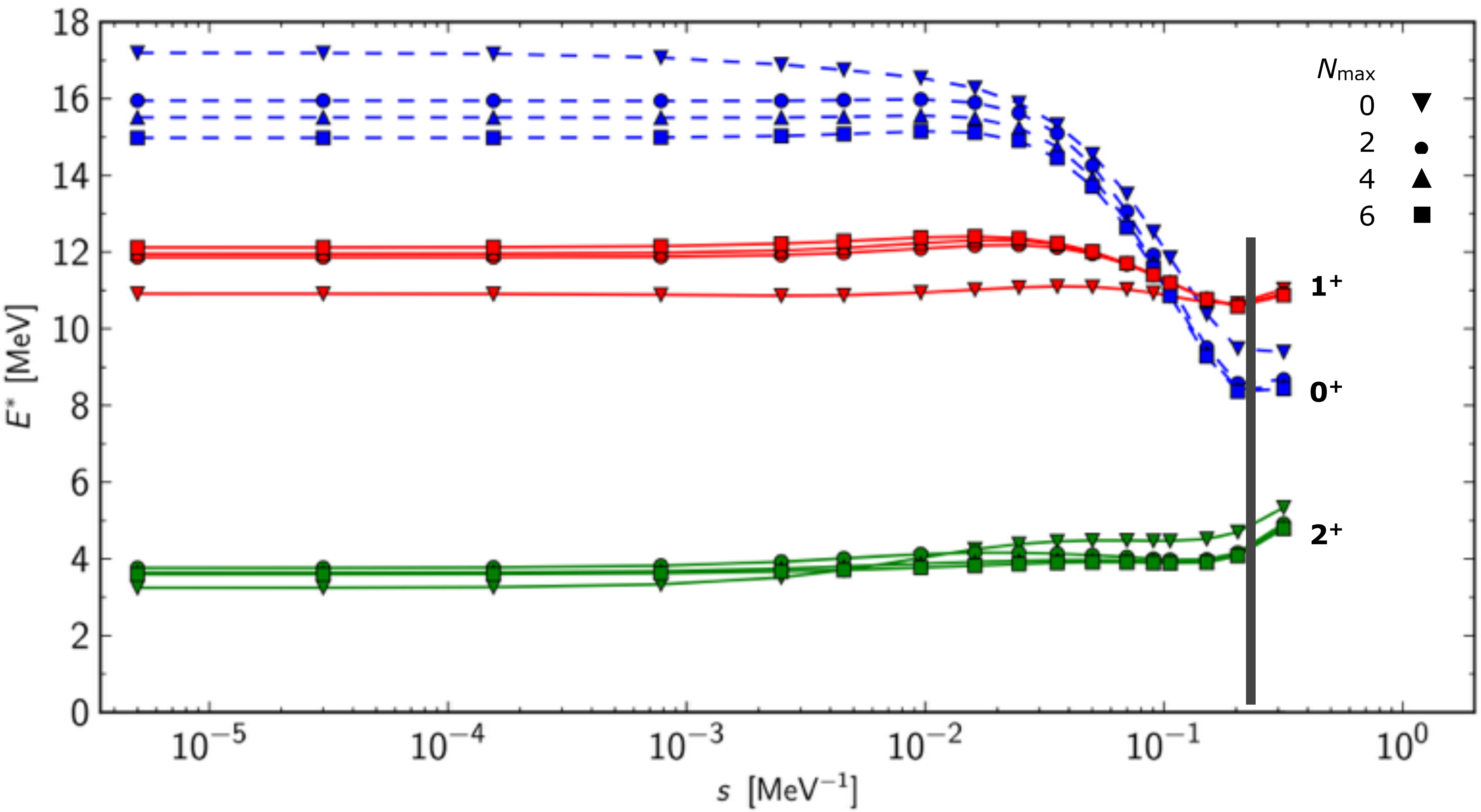
e_{max}=12

N_{max}=0 reference state

- from the same NCSM calculation we get the **excited states**
- excitation energies only show subtle changes with IM-SRG flow…

IM-NCSM: Excited States

Gebrerufael et al.; arXiv:1610.05254



^{12}C

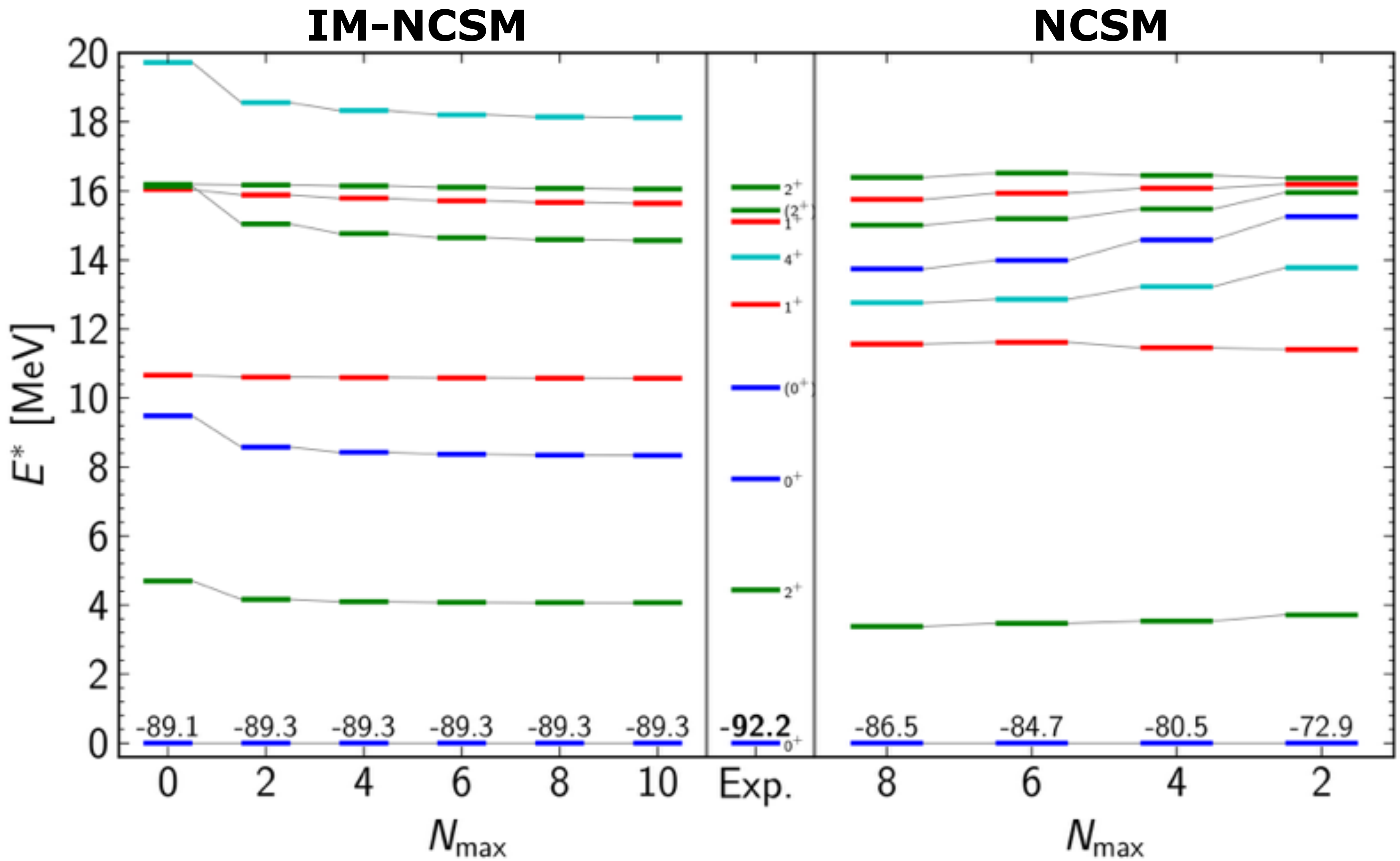
chiral NN+3N
Λ_{3N}=400 MeV
α=0.08 fm^4
$\hbar\Omega$=20 MeV
e_{max}=12

N_{max}=0
reference state

- from the same NCSM calculation we get the **excited states**
- excitation energies only show subtle changes with IM-SRG flow…
  …but there are notable exceptions… **Hoyle state?**

IM-NCSM: Spectrum

Gebrerufael et al.; arXiv:1610.05254



^{12}C

chiral NN+3N

Λ_{3N}=400 MeV

α=0.08 fm^4

ħΩ=20 MeV

e_{max}=12

N_{max}=0 reference state

s=0.2 MeV^{-1}

- **promising starting point** for ab initio studies of arbitrary open-shell nuclei

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

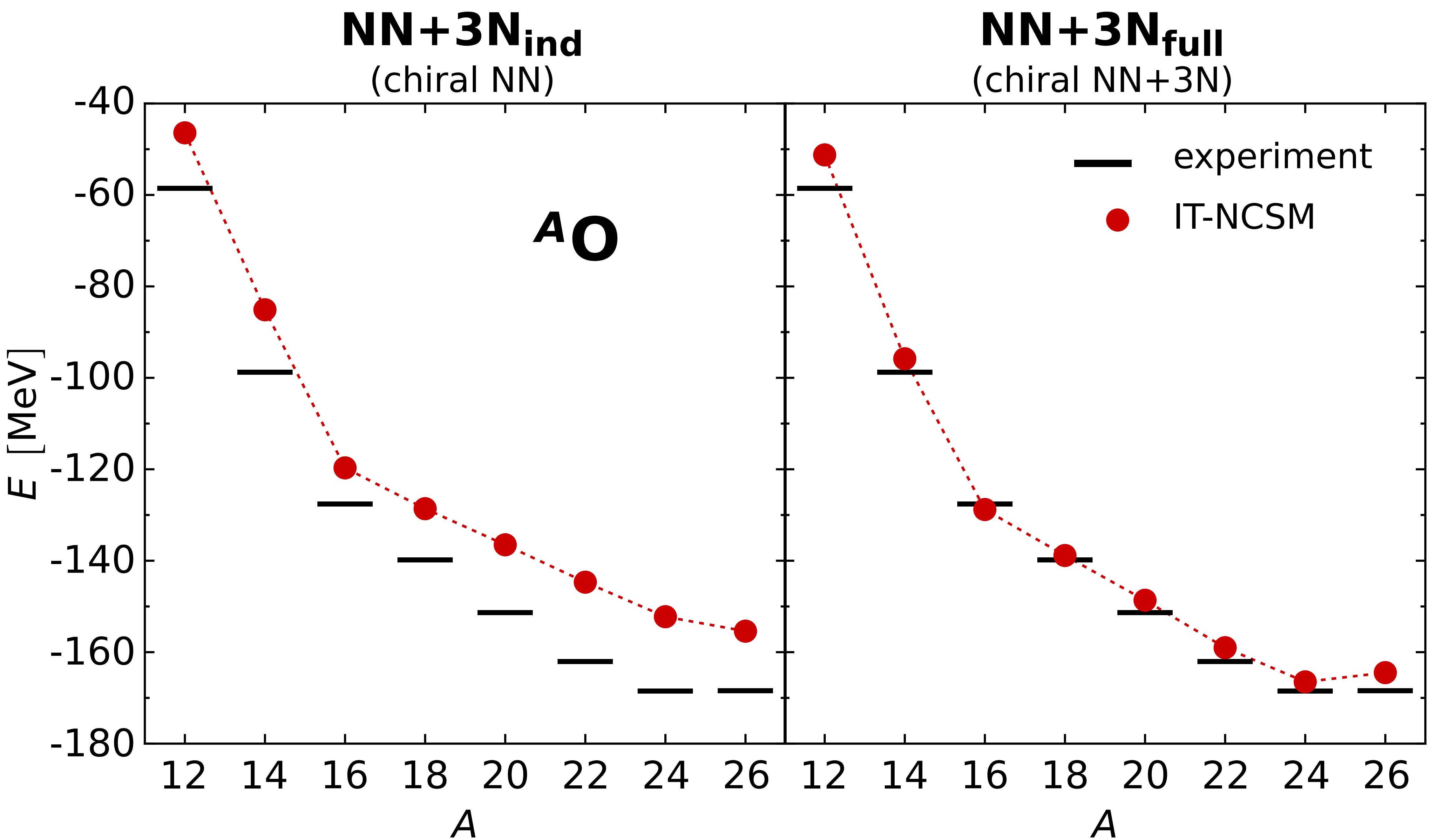
CON

- not variational
- NO3B needs some work

Applications for Medium-Mass Nuclei

Ground States of Oxygen Isotopes

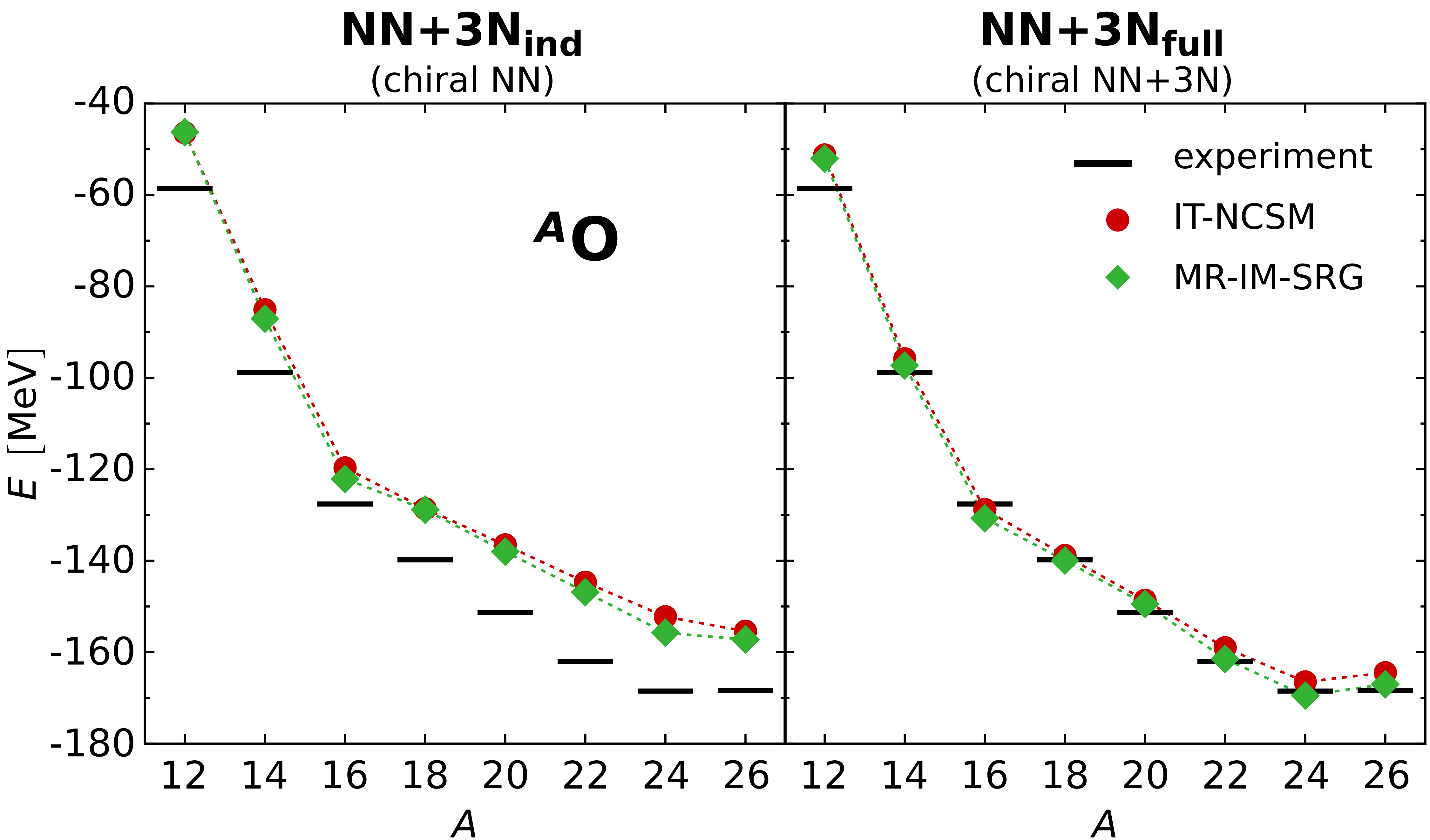
Hergert et al., PRL 110, 242501 (2013)



$\Lambda_{3N} = 400$ 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)



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Ground States of Oxygen Isotopes

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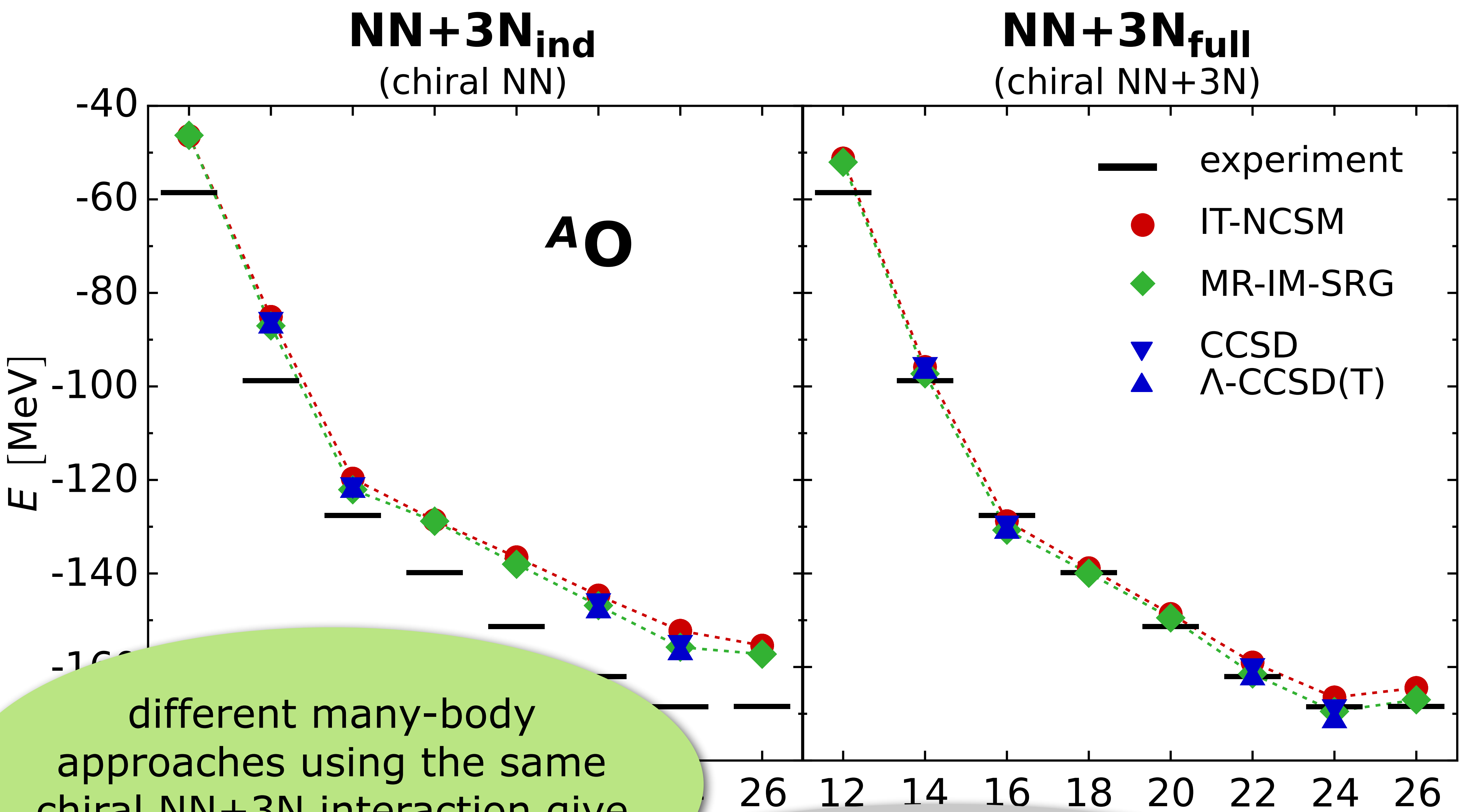
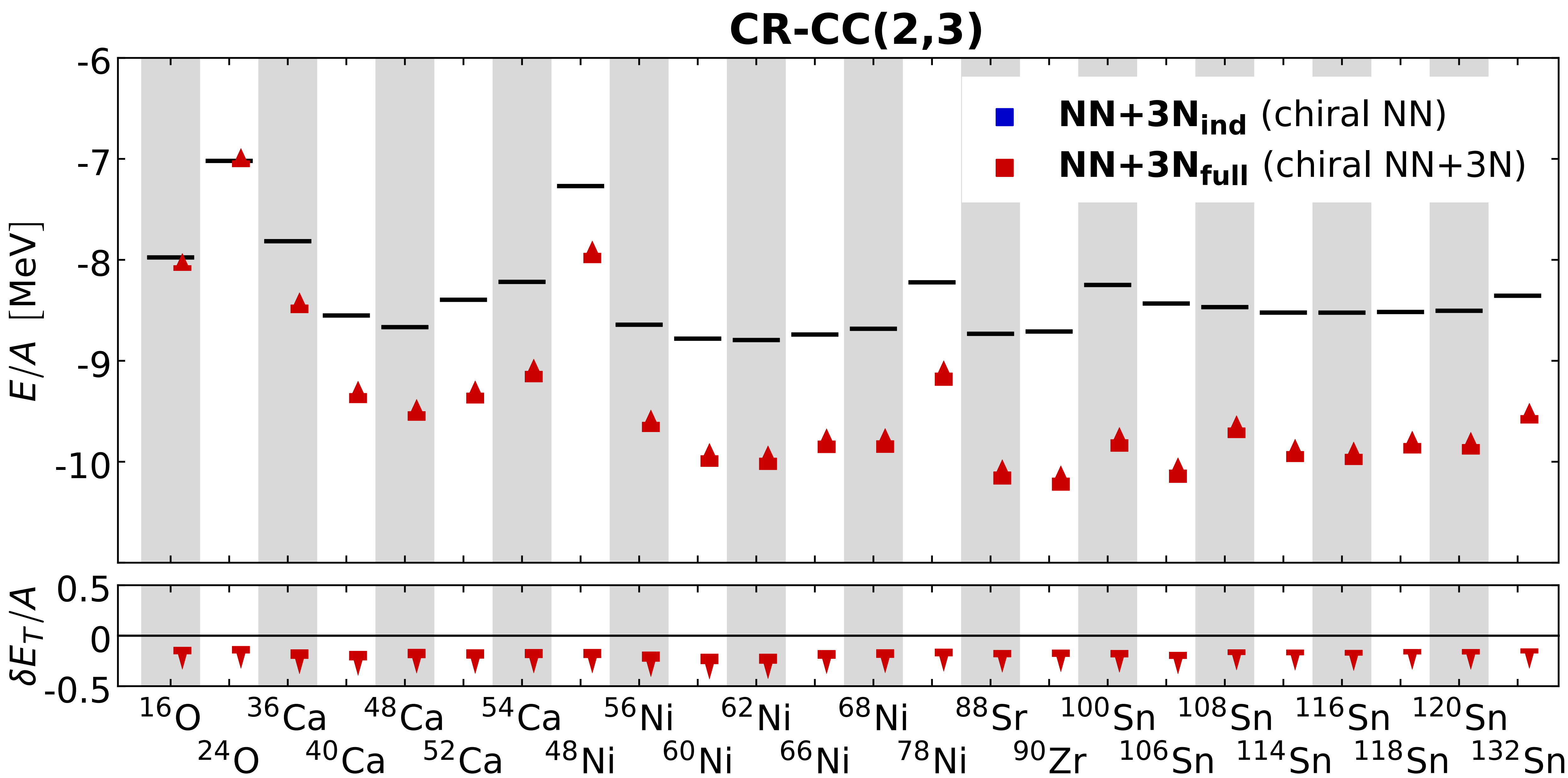


different many-body approaches using the same chiral NN+3N interaction give consistent results

minor differences are understood in terms of uncertainties due to truncations

Towards Heavy Nuclei - Ab Initio

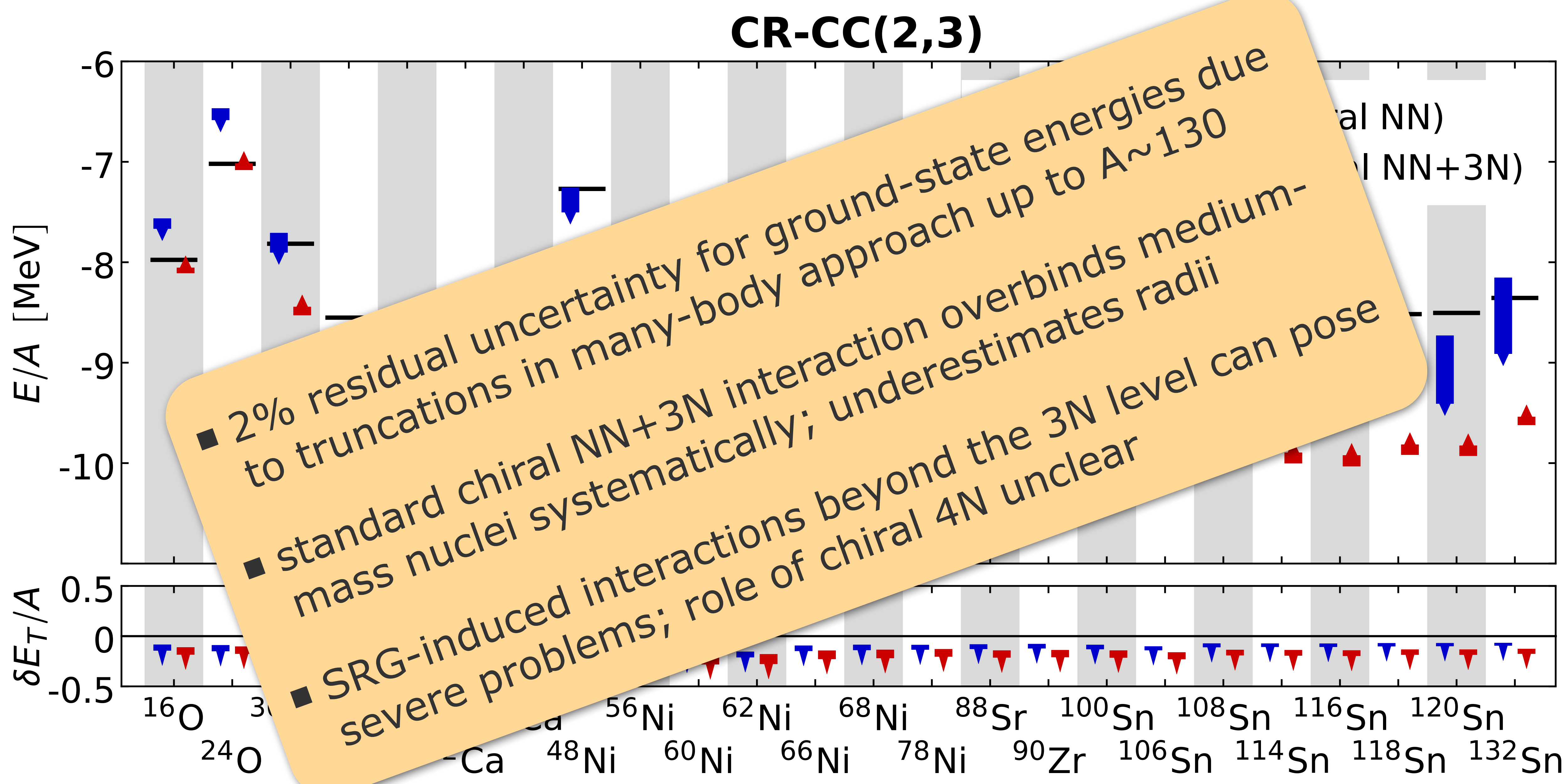
Binder et al., PLB 736, 119 (2014)



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

Towards Heavy Nuclei - Ab Initio

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

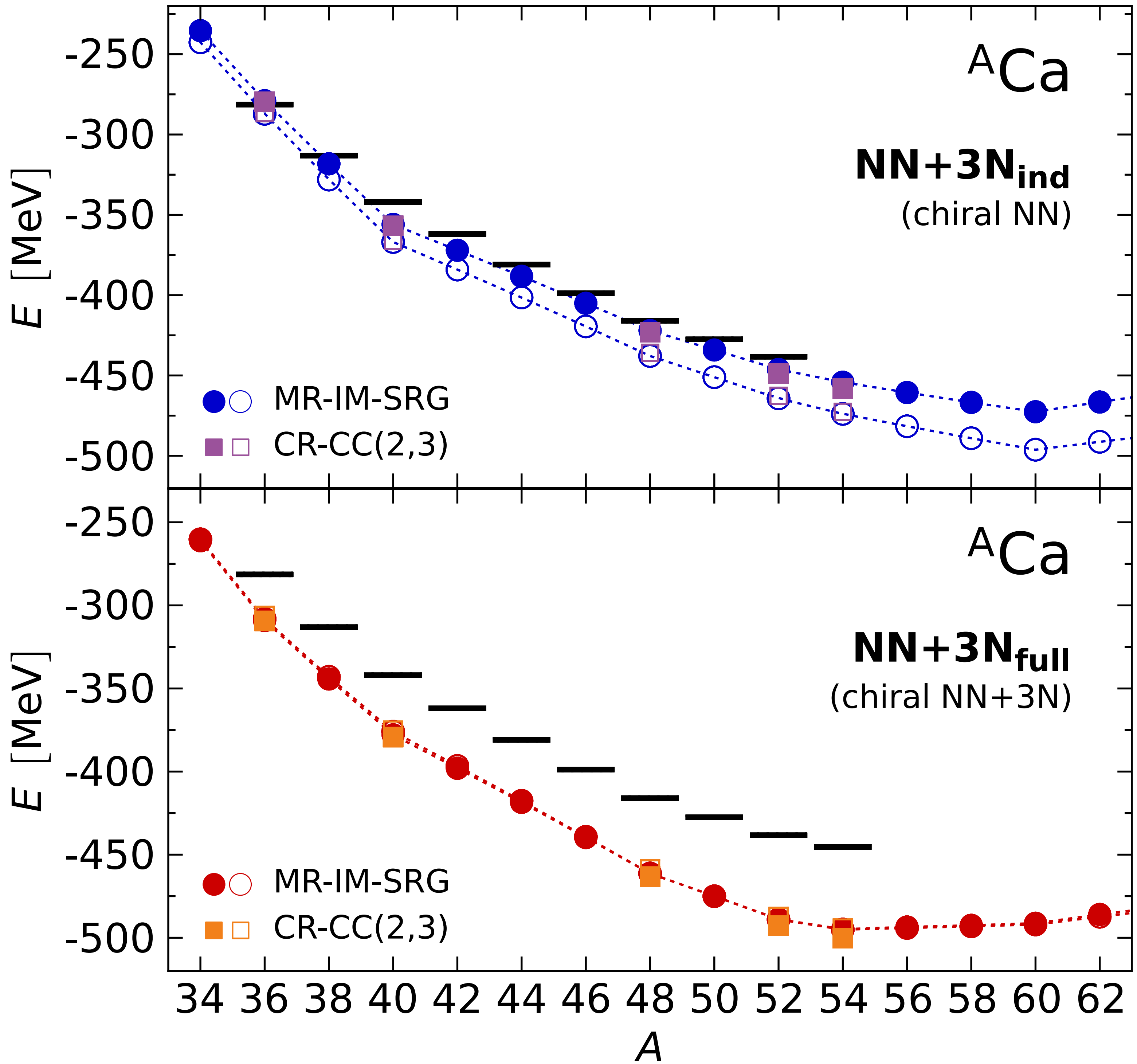


- 2% residual uncertainty for ground-state energies due to truncations in many-body approach up to A~130
- standard chiral NN+3N interaction overbinds medium-mass nuclei systematically; underestimates radii
- SRG-induced interactions beyond the 3N level can pose severe problems; role of chiral 4N unclear

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

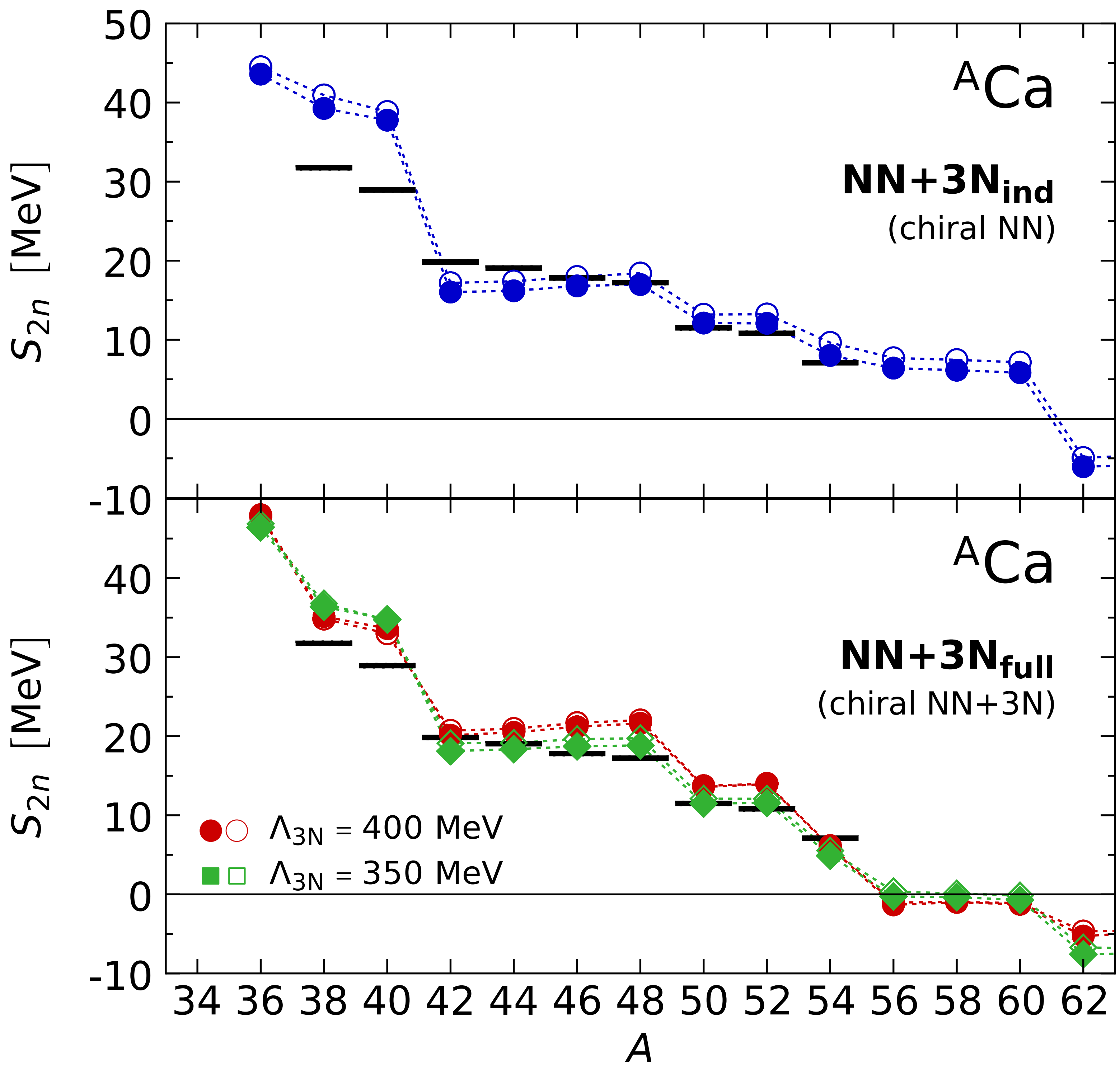
Λ_{3N} = 400 MeV

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

all MR-IM-SRG

α = 0.04 fm^4 (○)
0.08 fm^4 (●)

$E_{3\,max}$ = 14, 16

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**
  - S. Alexa, E. Gebrerufael, T. Hüther, L. Mertes, S. Schulz, H. Spies, C. Stumpf, A. Tichai, R. Trippel, K. Vobig, R. Wirth
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  - P. Navrátil, A. Calci
    TRIUMF, Vancouver
  - S. Binder
    Oak Ridge National Laboratory
  - H. Hergert
    NSCL / Michigan State University
  - J. Vary, P. Maris
    Iowa State University
  - S. Quaglioni
    Lawrence Livermore National Laboratory
  - E. Epelbaum, H. Krebs & the LENPIC Collaboration
    Universität Bochum, …

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