Nuclear Interactions and Many-Body Perturbation Theory

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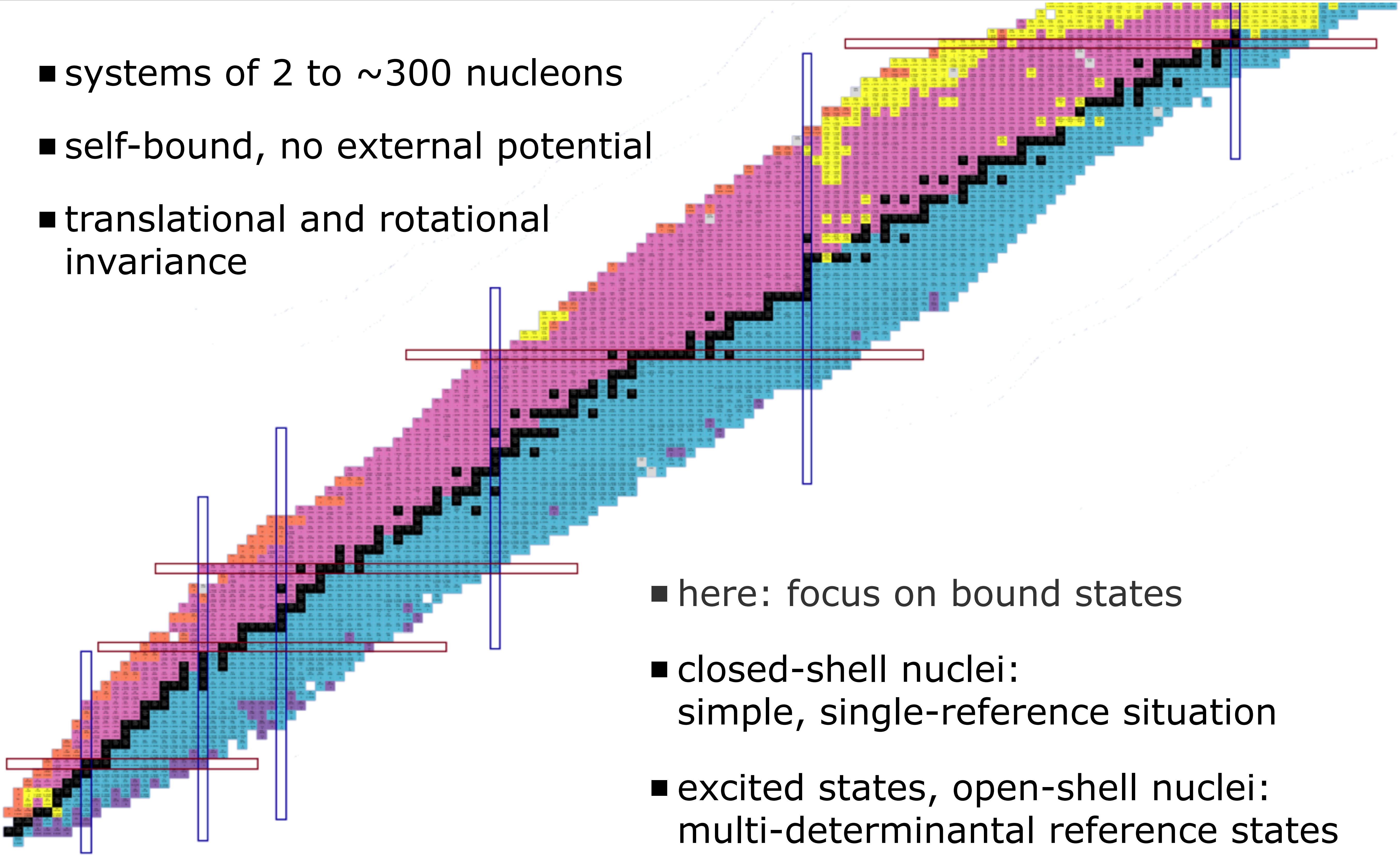
The Problem

- systems of 2 to ~300 nucleons
- self-bound, no external potential
- translational and rotational invariance



- here: focus on bound states
- closed-shell nuclei: simple, single-reference situation
- excited states, open-shell nuclei: multi-determinantal reference states

The Problem

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

Hamiltonian
Chiral Eff. Field Theory

Pre-Conditioning
Similarity Renorm. Group

Many-Body Solution
CI, CC, IM-SRG, MBPT...

- bridge to underlying theory of the strong interaction
- systematic and improvable input for all ab initio calculations
- large selection of chiral NN+3N interactions available

The Problem

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

Hamiltonian
Chiral Eff. Field Theory

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Many-Body Solution
CI, CC, IM-SRG, MBPT...

- unitary transformation of all operators as preparatory step
- drastically improves convergence of many-body calculation
- induces many-body interactions that can be sizeable

The Problem

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

Hamiltonian
Chiral Eff. Field Theory

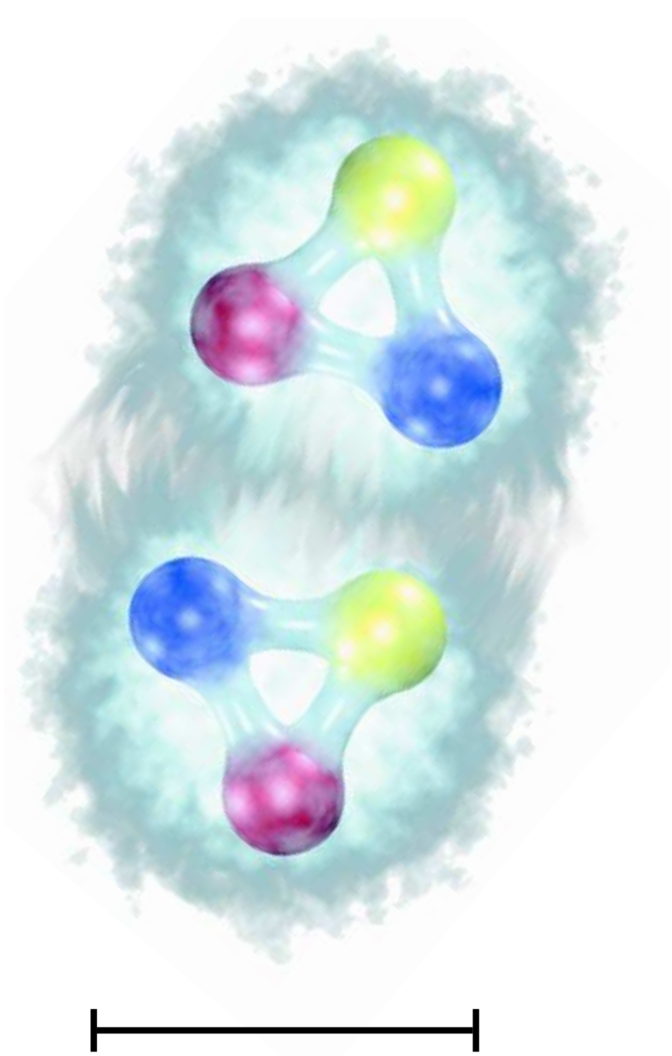
Pre-Conditioning
Similarity Renorm. Group

Many-Body Solution
CI, CC, IM-SRG, MBPT...

- different many-body methods for different mass regions and different observables
- established: light nuclei and closed-shell isotopes
- frontiers: continuum and open-shell medium-mass nuclei

Nuclear Hamiltonian

Nature of the Nuclear Interaction



$\sim 1.6\text{fm}$

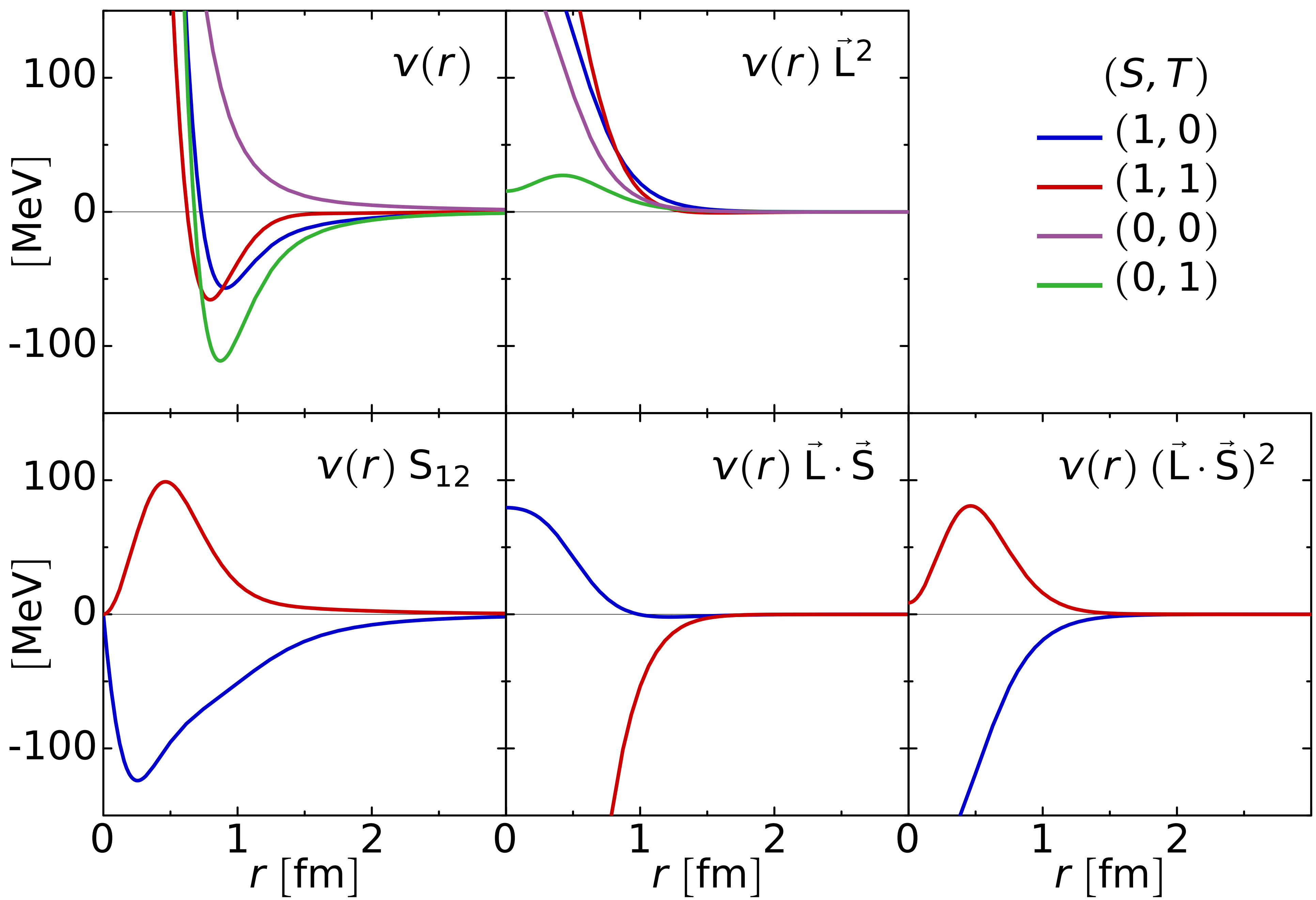
$\rho_0^{-1/3} = 1.8\text{fm}$

- 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

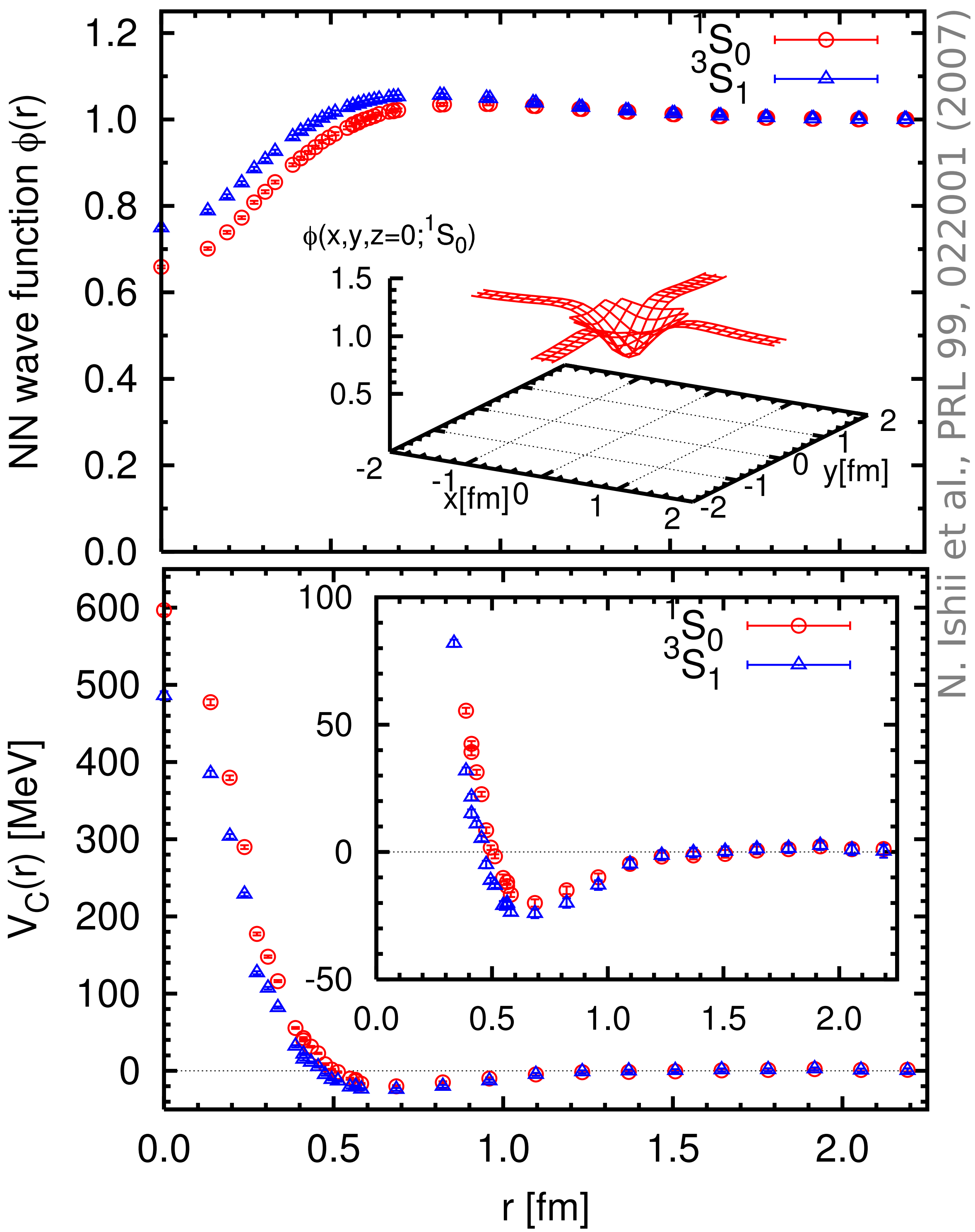
Wiringa, Machleidt,...

- until 2005: high-precision **phenomenological NN interactions** were state-of-the-art in ab initio nuclear structure theory, e.g., **Argonne V18 potential**



Tomorrow… from Lattice QCD

Hatsuda, Aoki, Ishii, Beane, Savage, Bedaque,…

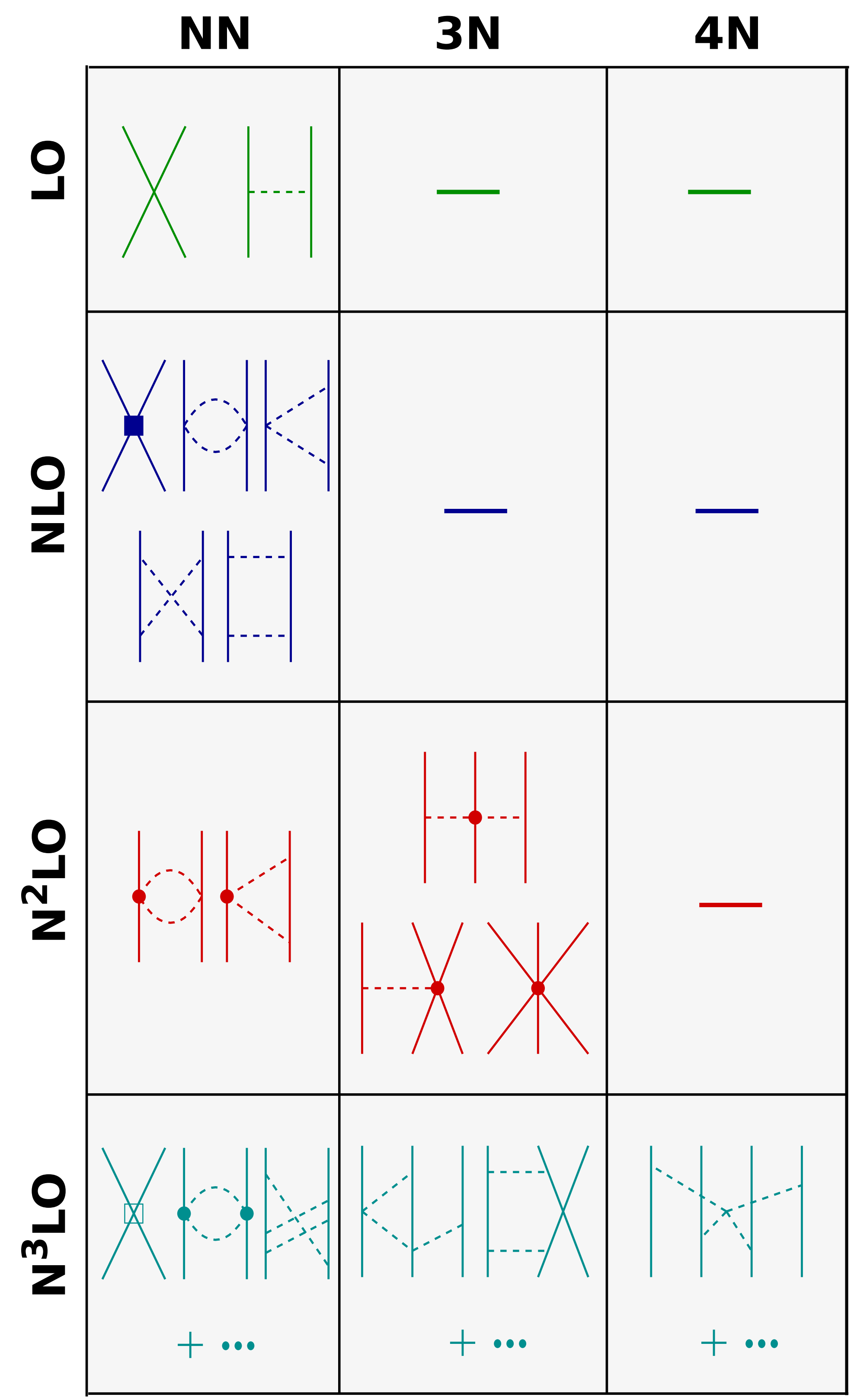


- first attempts towards construction of nuclear interactions directly from **lattice QCD simulations**
- compute relative **two-nucleon wave function** on the lattice
- **invert Schrödinger equation** to extract effective two-nucleon potential
- only **schematic results** so far (unphysical masses and 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

systematic order-by-order uncertainty analysis

...

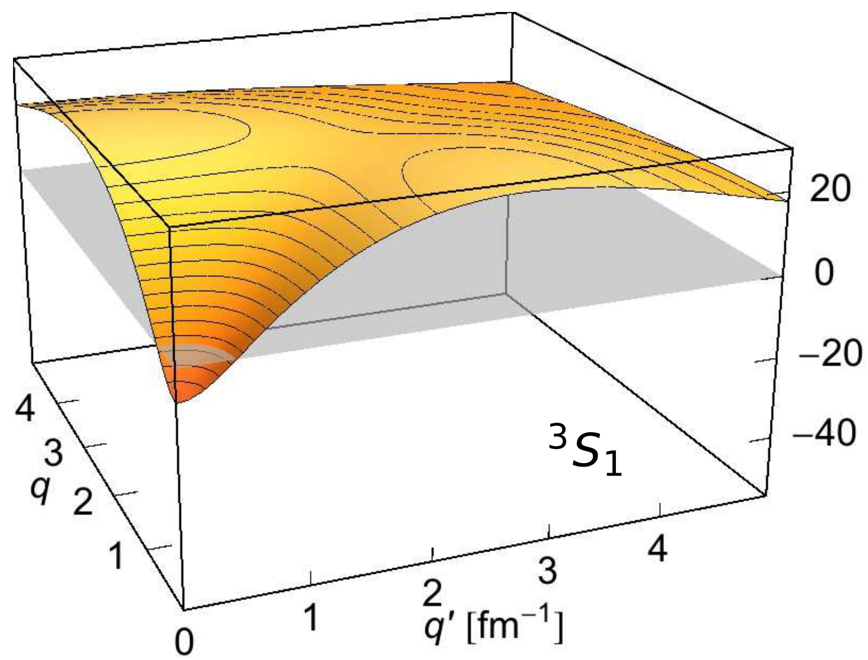
Momentum-Space Matrix Elements

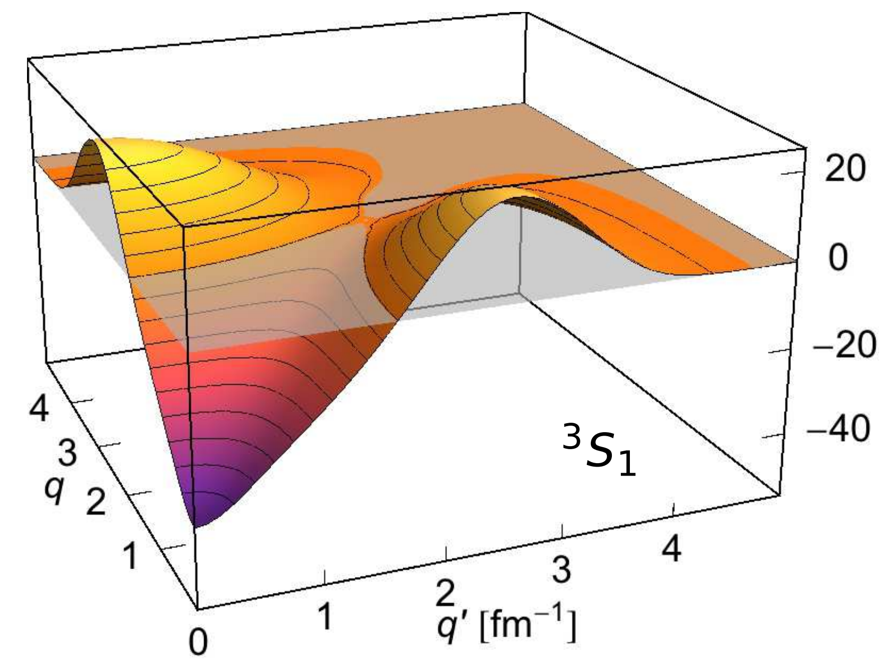
$$\langle q(LS)JM;TM_T|\,\mathrm{v}_{NN}\,|q'(L'S)JM;TM_T\rangle$$

Argonne V18

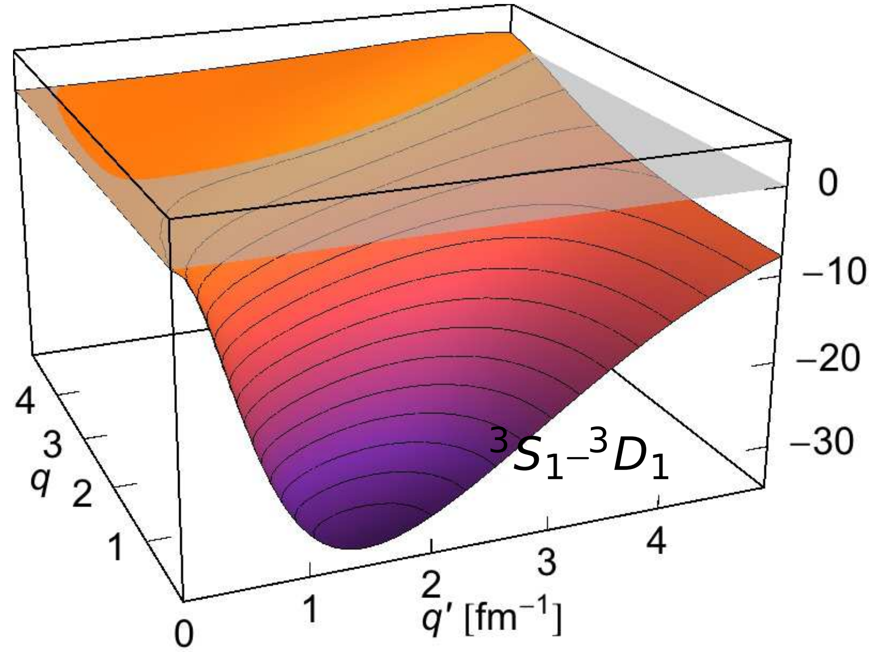
chiral NN
(N3LO, E&M, 500 MeV)

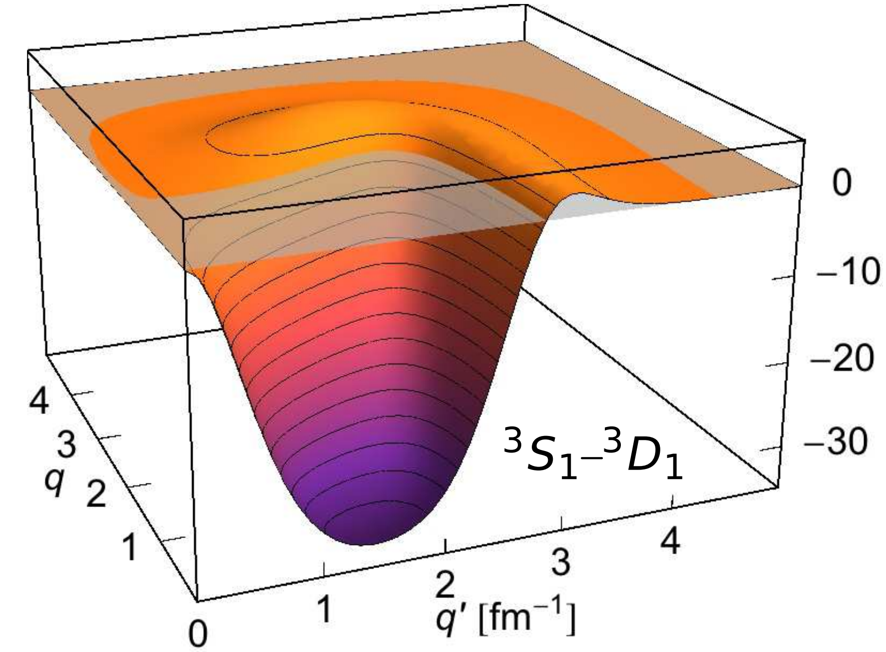
J=1
L=0
L'=0
S=1
T=0





J=1
L=0
L'=2
S=1
T=0





Similarity Renormalization Group

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

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

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

- **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-diagonalization" or "decoupling" 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 fix 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 fix 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 $|Ei J^{\pi} T\rangle$

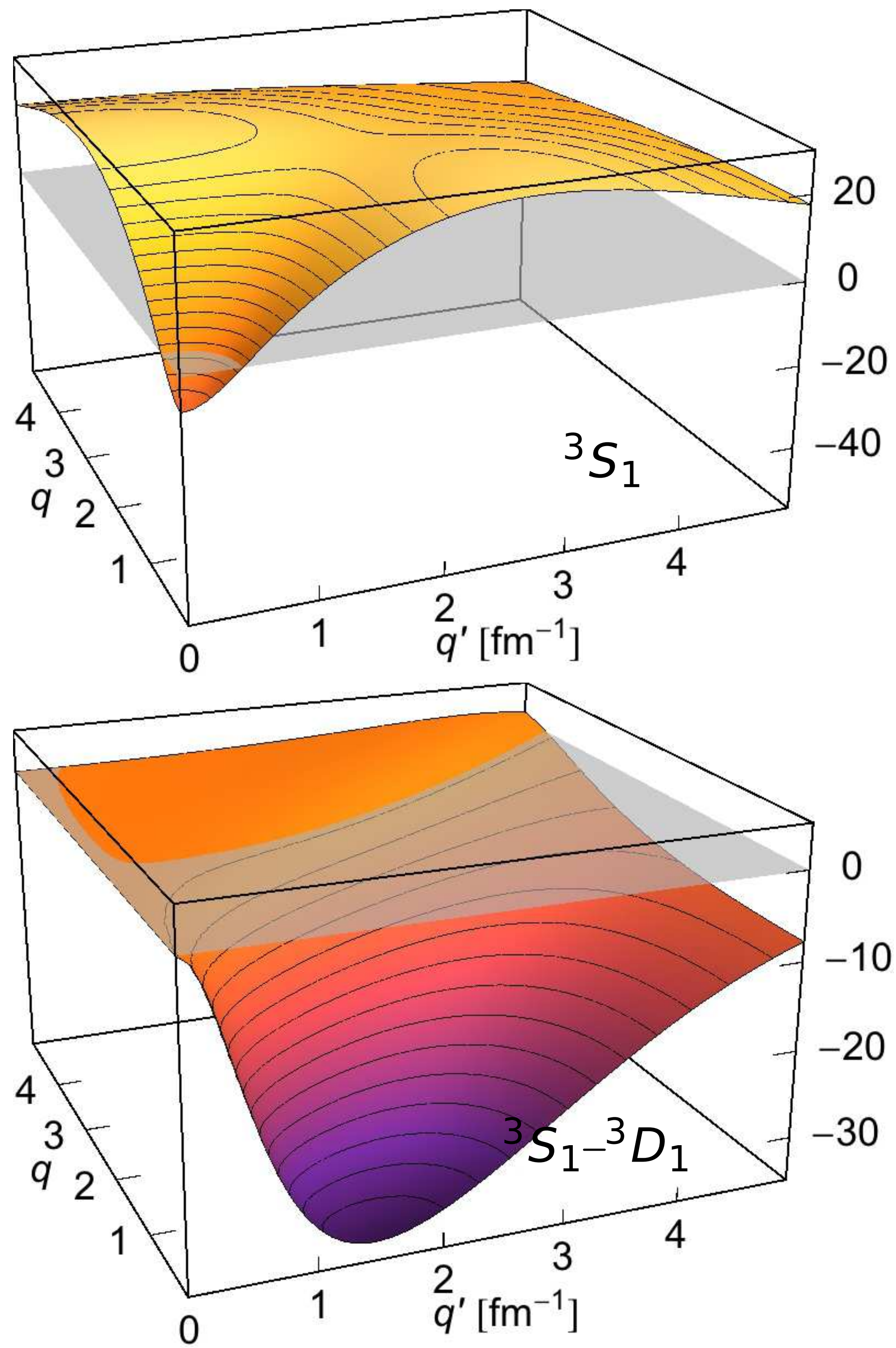
- matrix-evolution equations for n=3 with antisym. three-body Jacobi HO states:

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

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

SRG Evolution in Two-Body Space

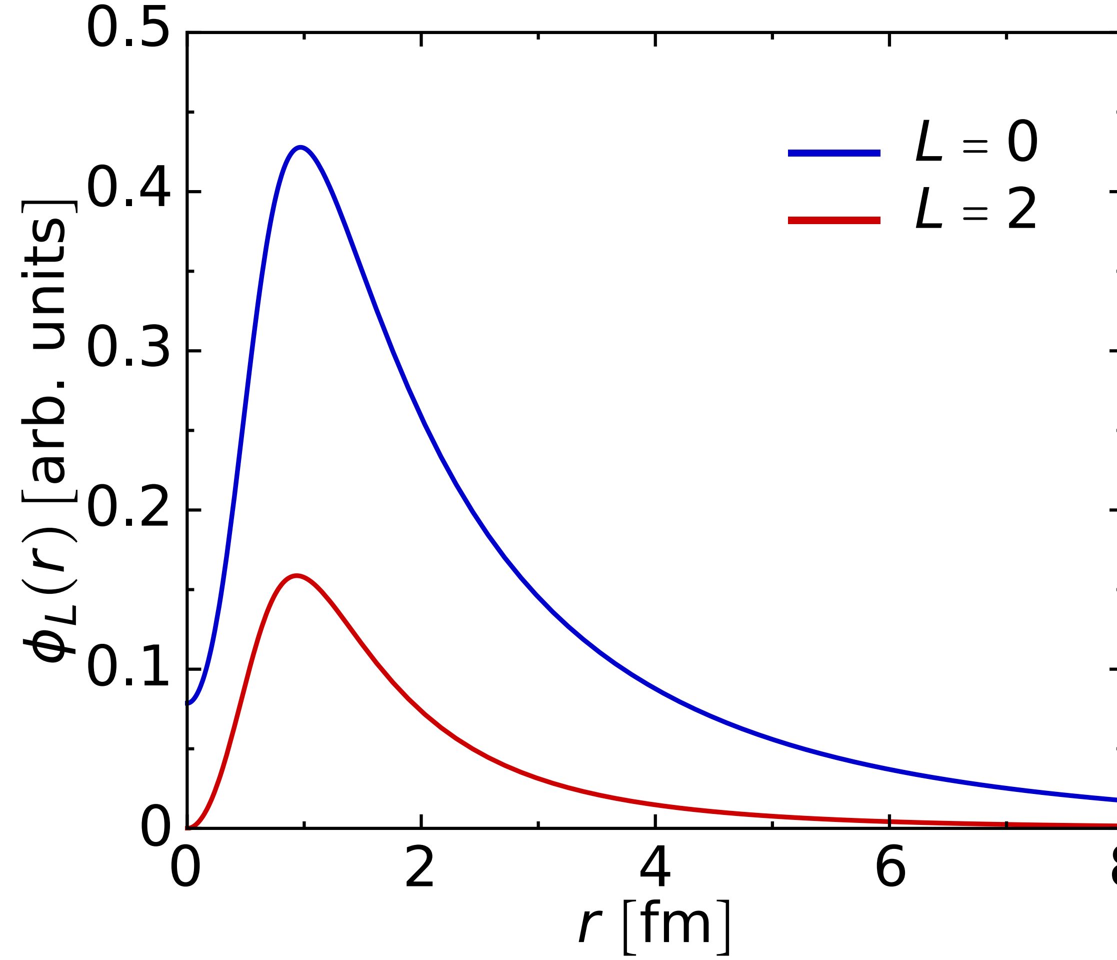
momentum-space matrix elements



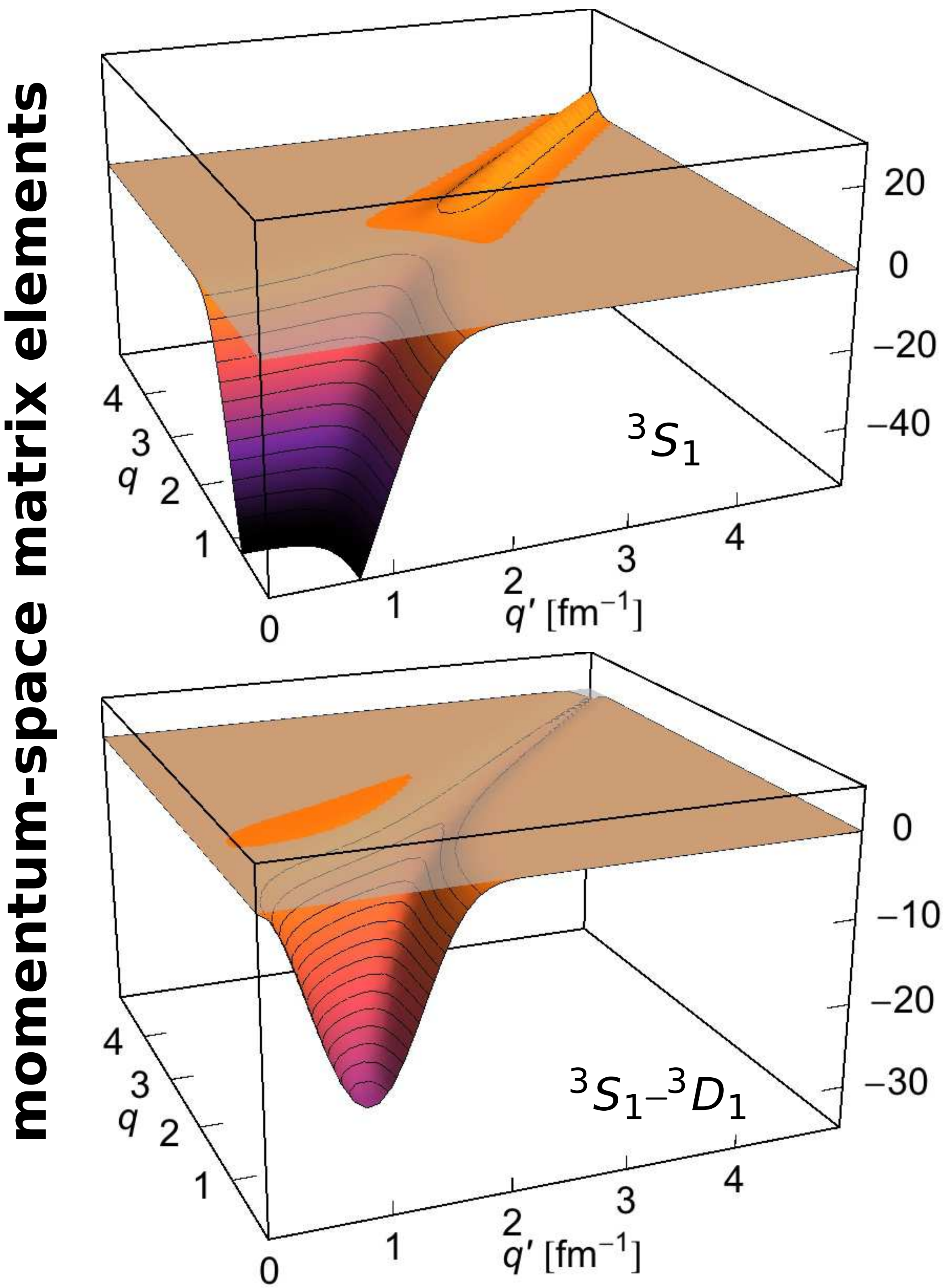
Argonne V18

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

deuteron wave-function



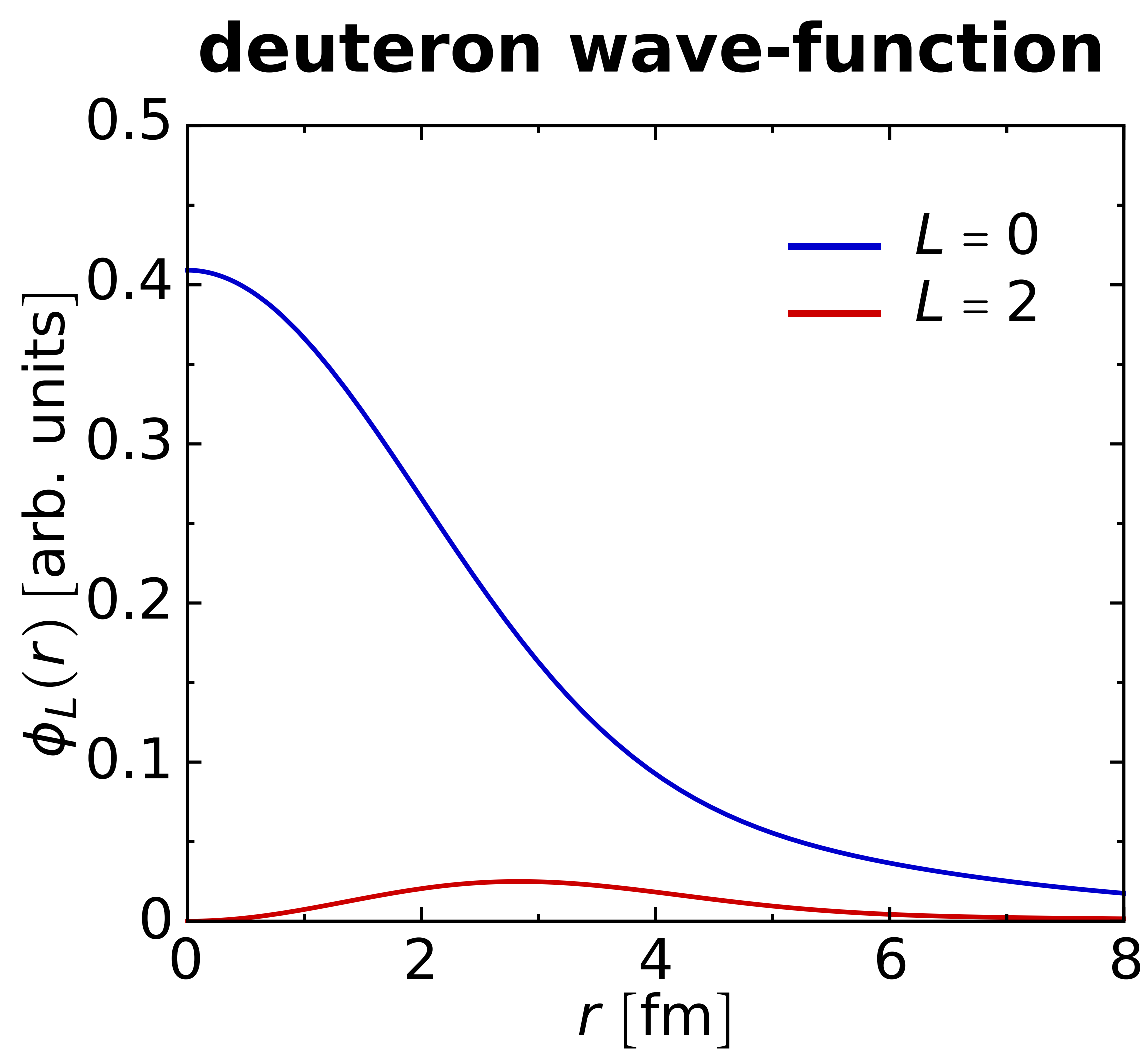
SRG Evolution in Two-Body Space



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

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

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



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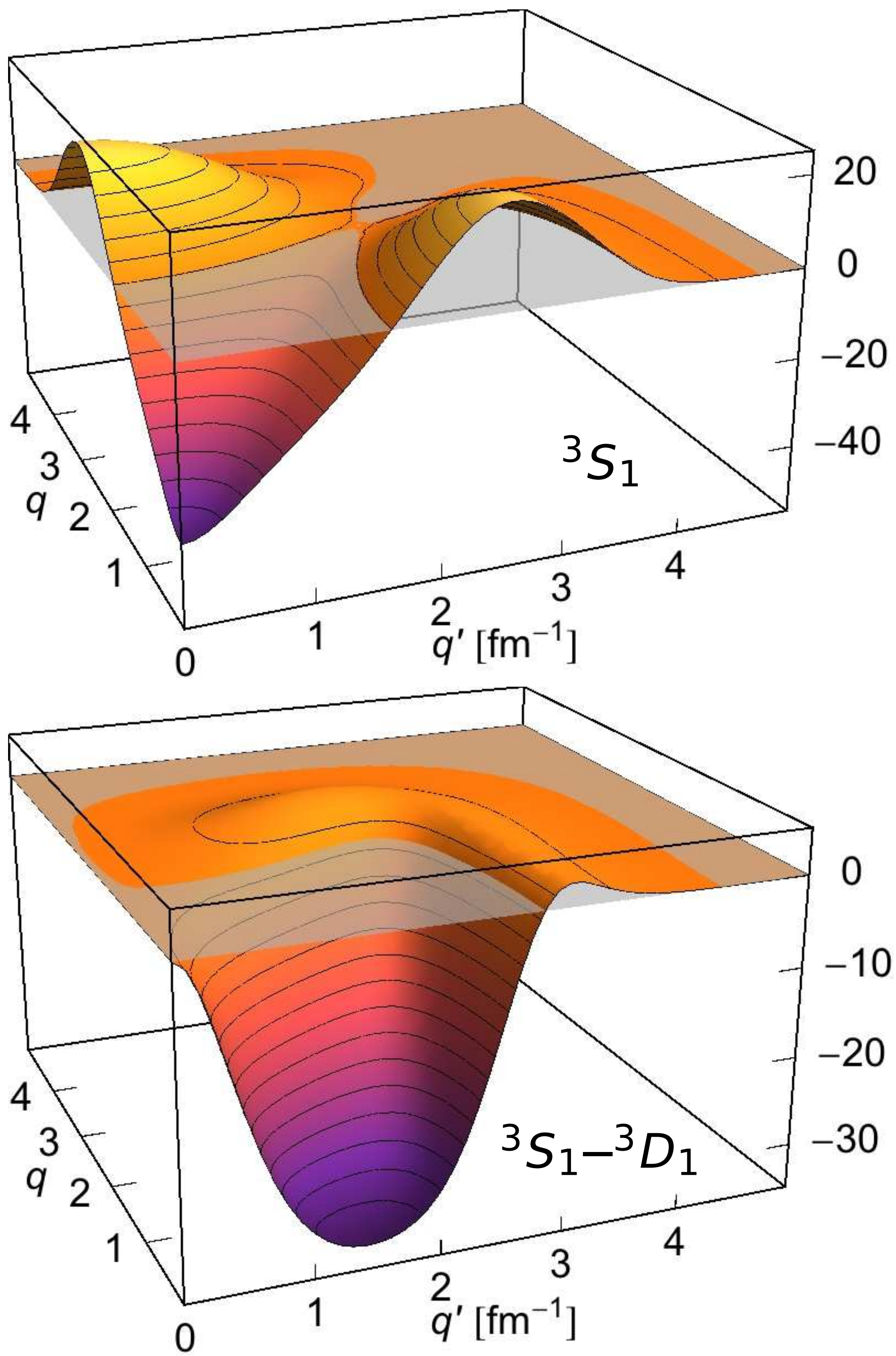
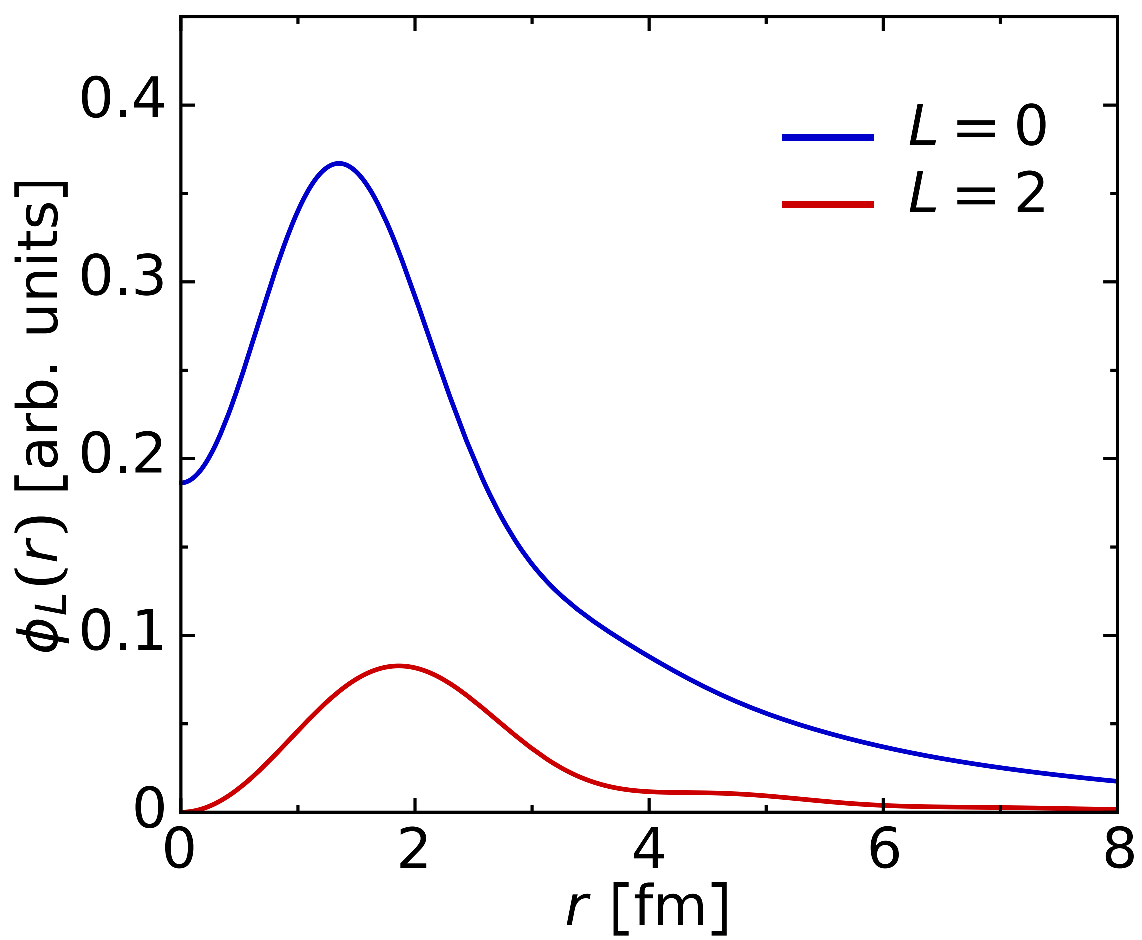


chiral NN

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

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

deuteron wave-function



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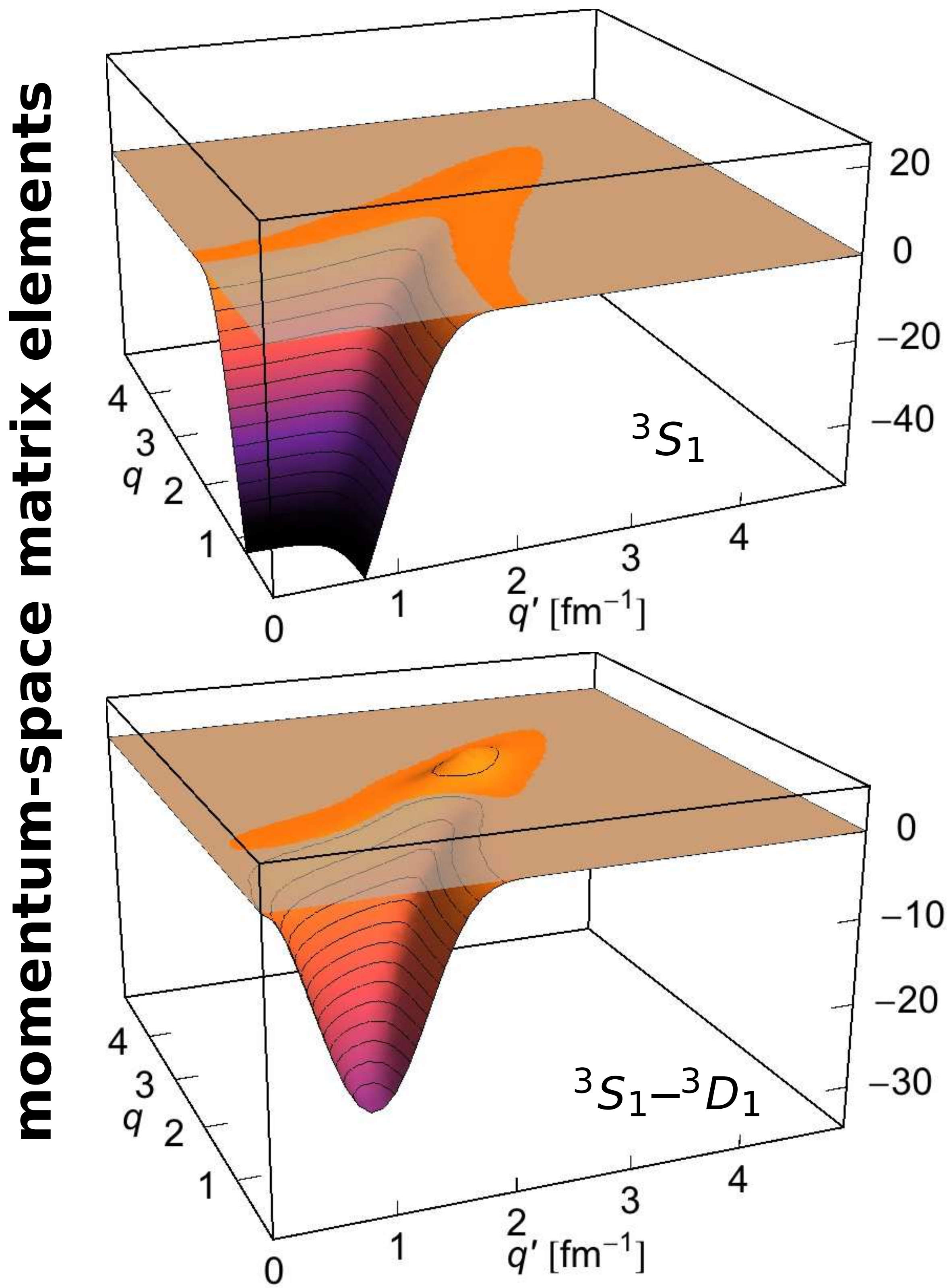

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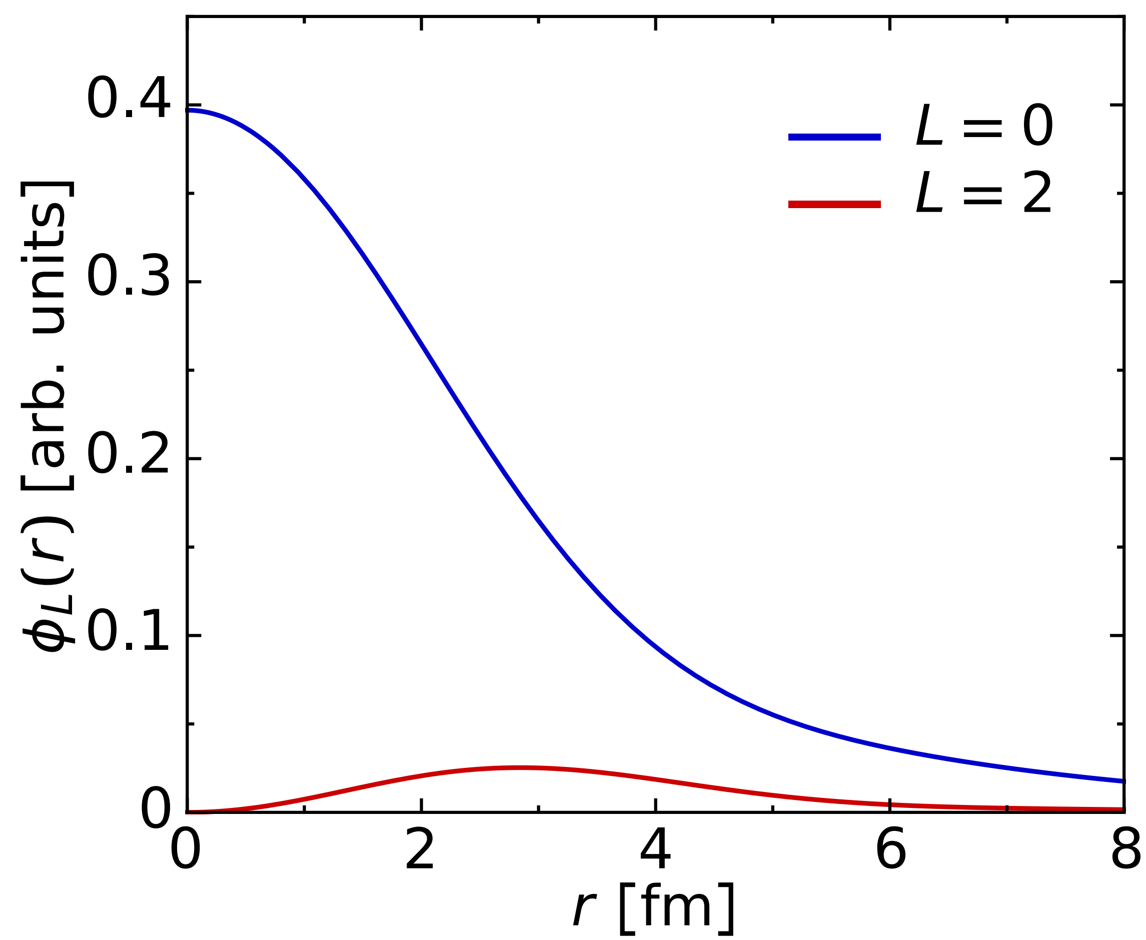
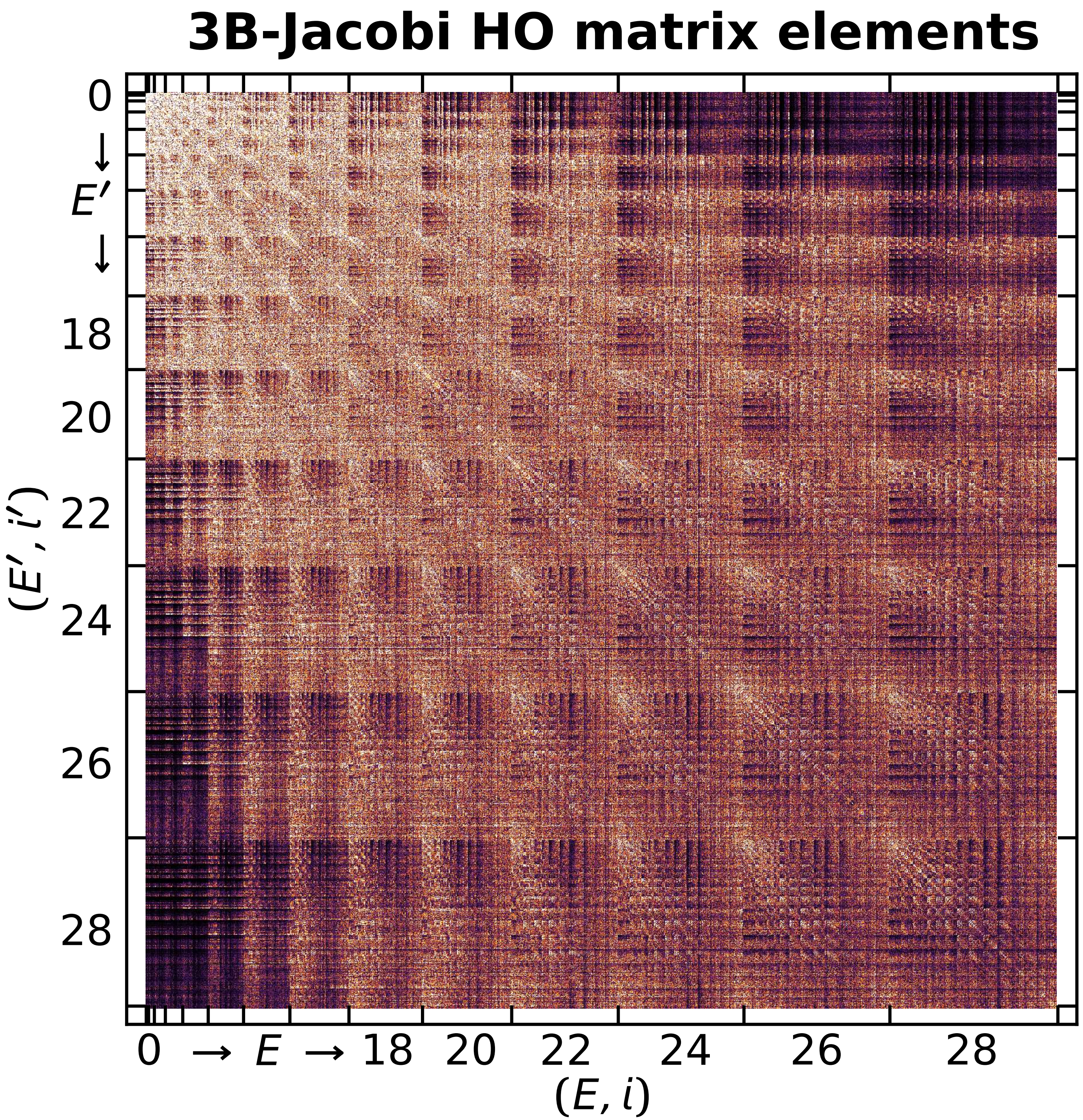


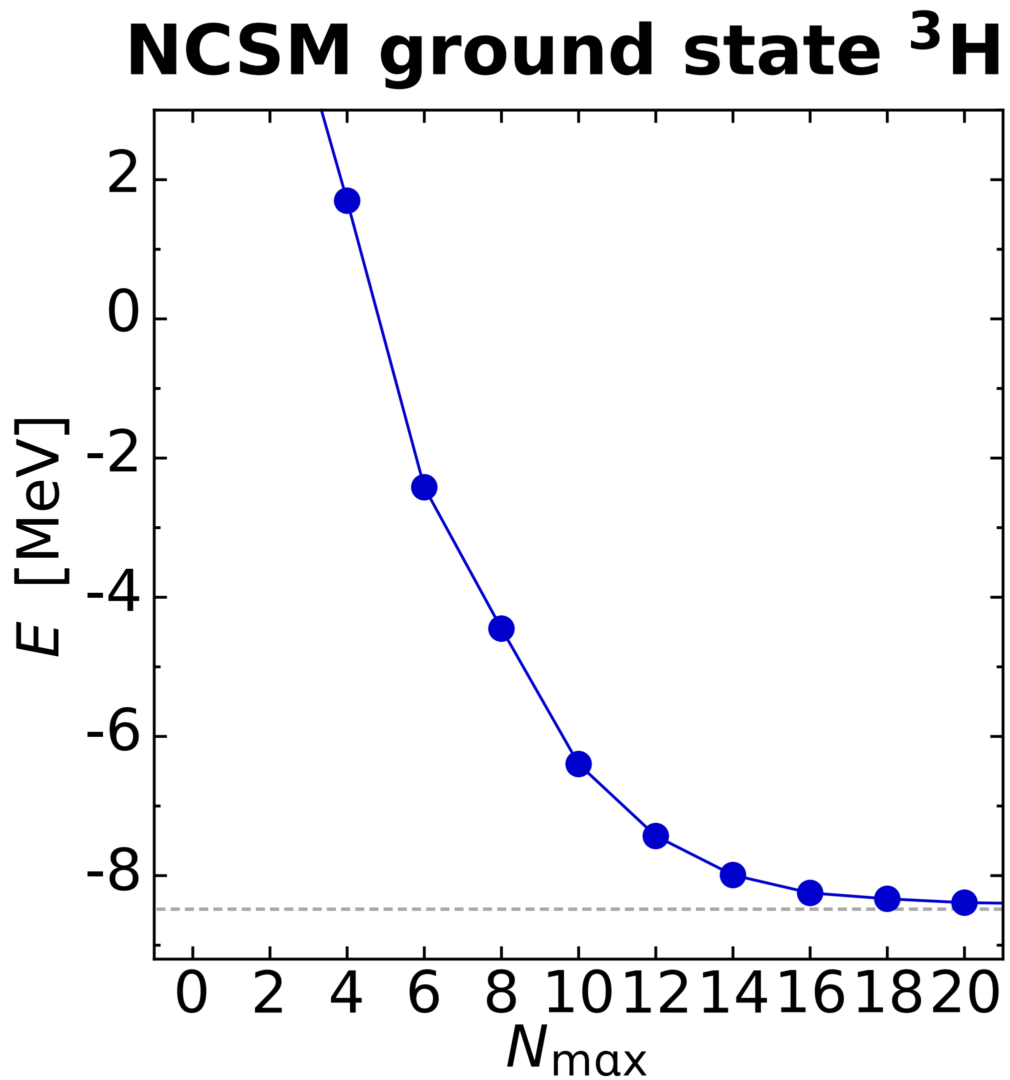
SRG Evolution in Three-Body Space



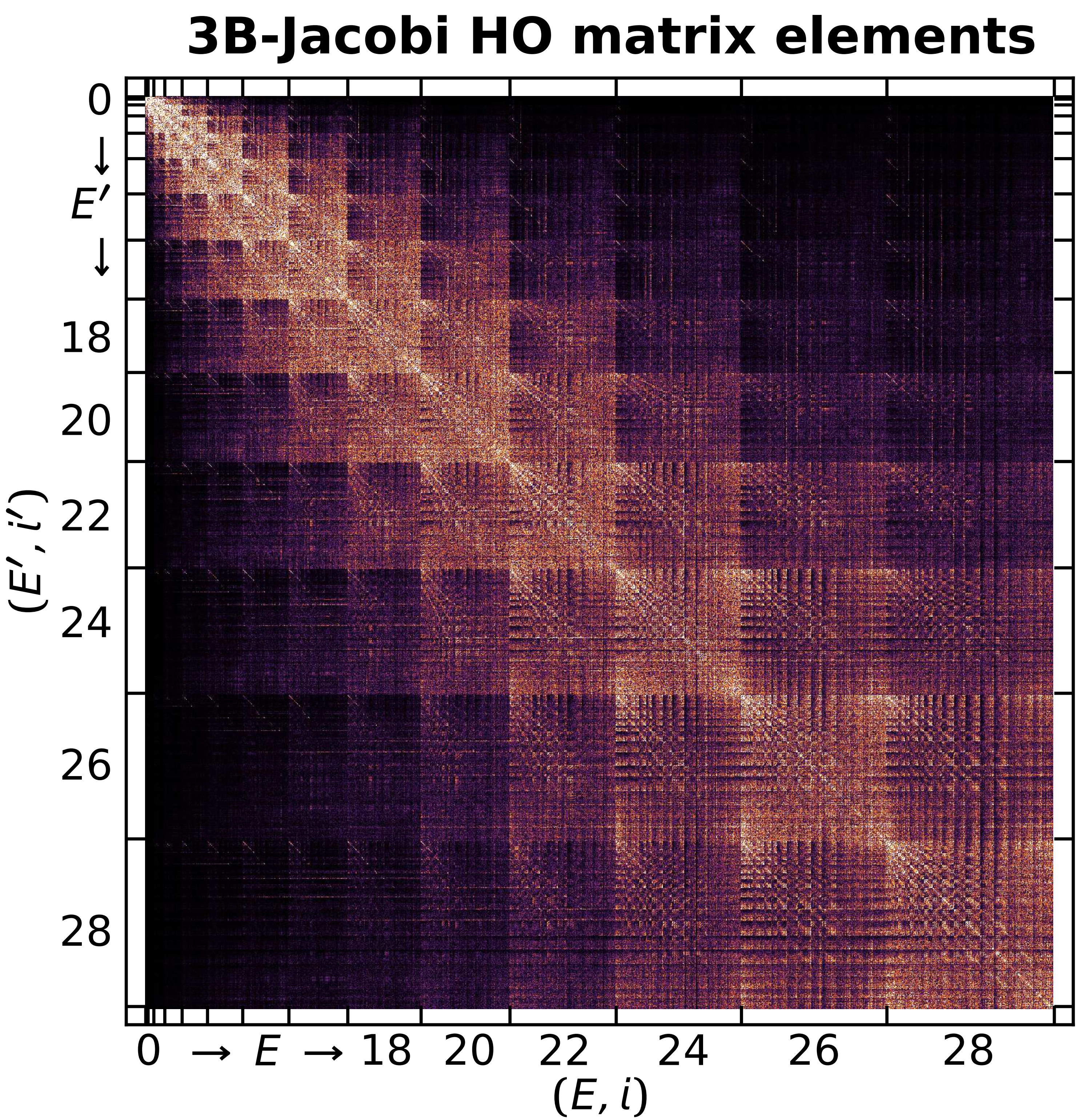
chiral NN+3N

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

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



SRG Evolution in Three-Body Space



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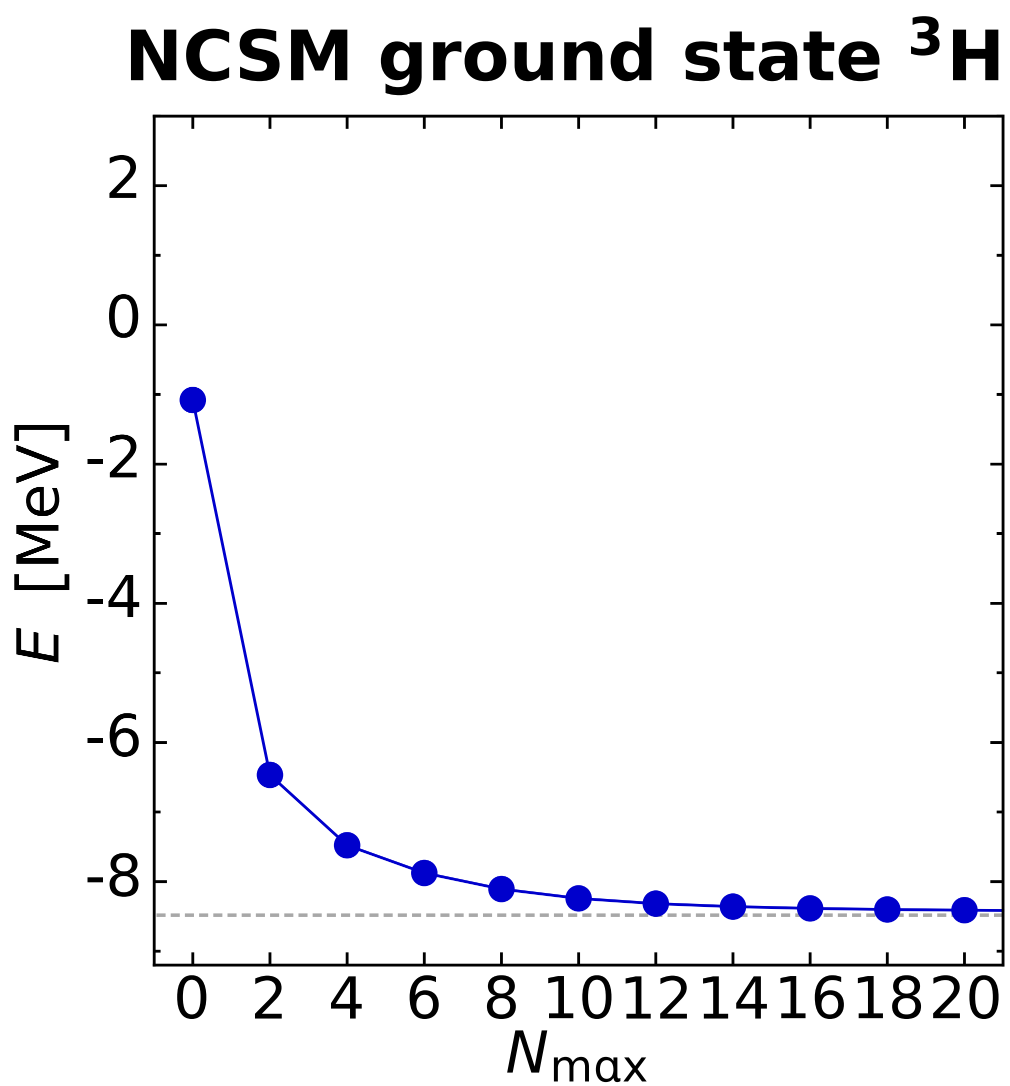


SRG Evolution in A-Body Space

- 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

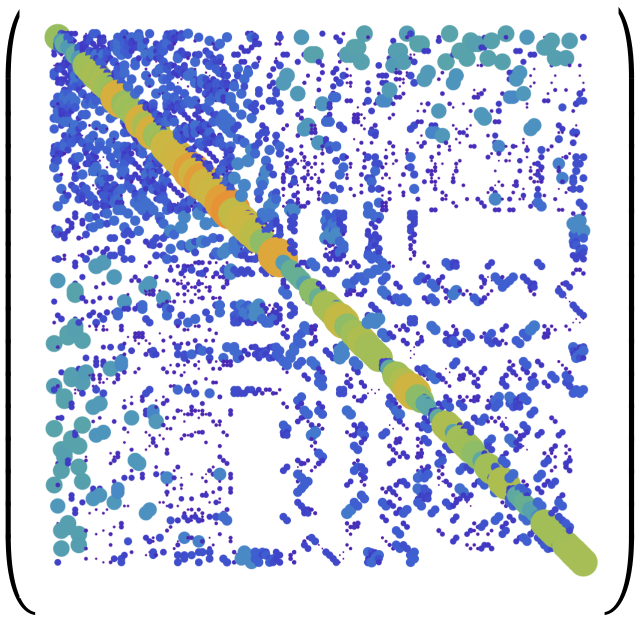
$NN+3N_{ind}$: use initial NN, keep evolved NN+3N

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

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

Many-Body Problem

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

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

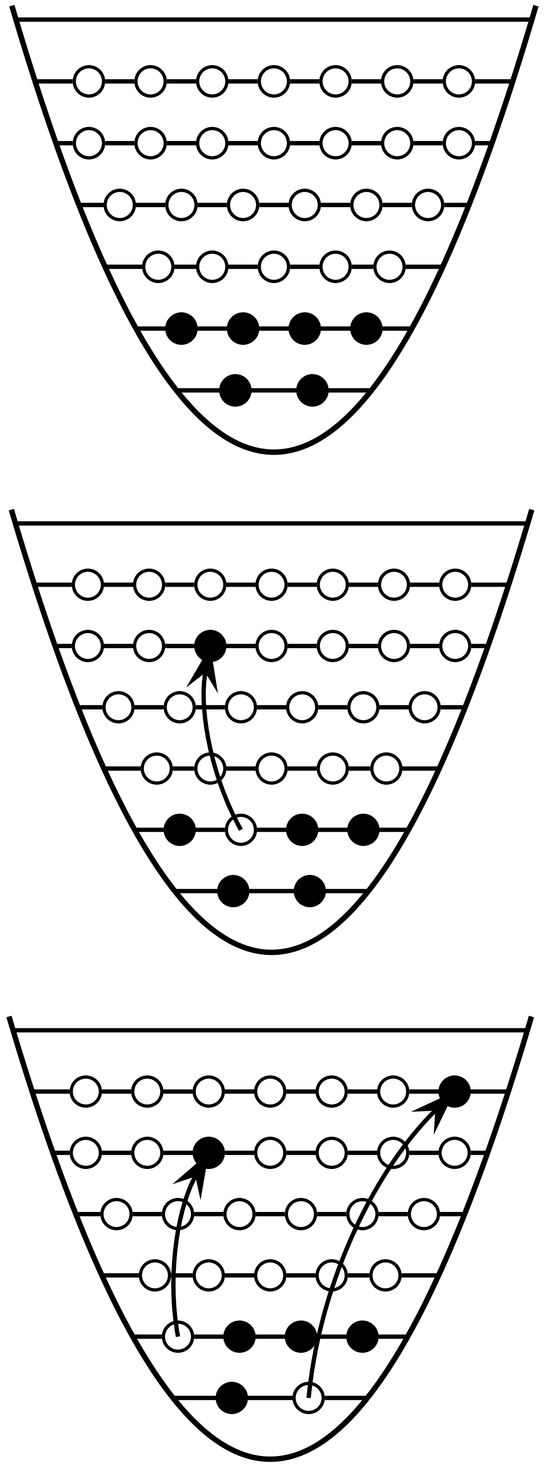
- convert eigenvalue problem of the Hamiltonian into a **matrix eigenvalue problem** in the Slater determinant representation

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

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

No-Core Shell Model (NCSM)

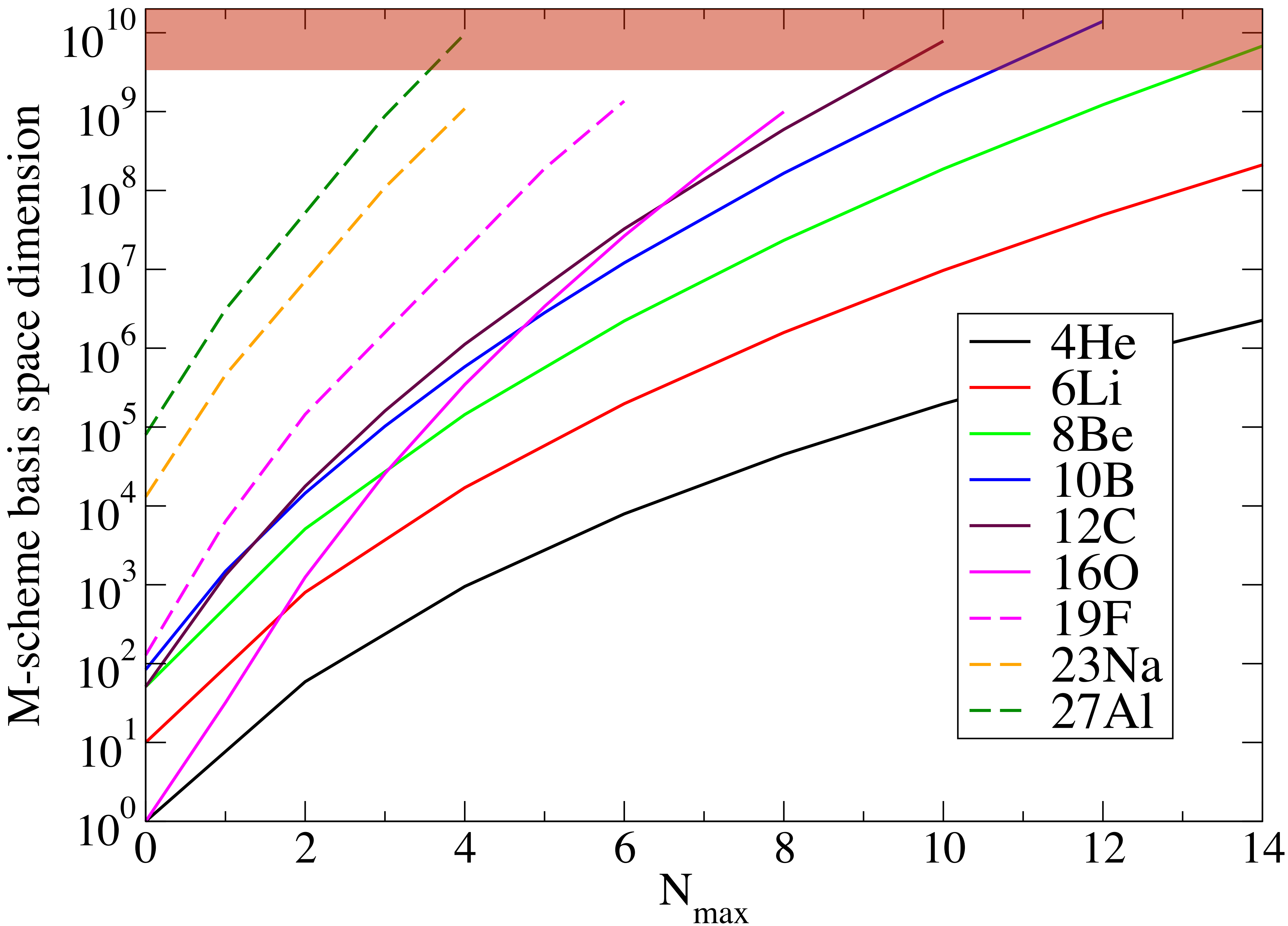
- NCSM is a special case of a CI approach:
  - single-particle basis is a **spherical HO basis**
  - truncation in terms of the total **number of HO excitation quanta $N_{\max}$** in the many-body states



- **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 $N_{\max}$

NCSM Basis Dimension

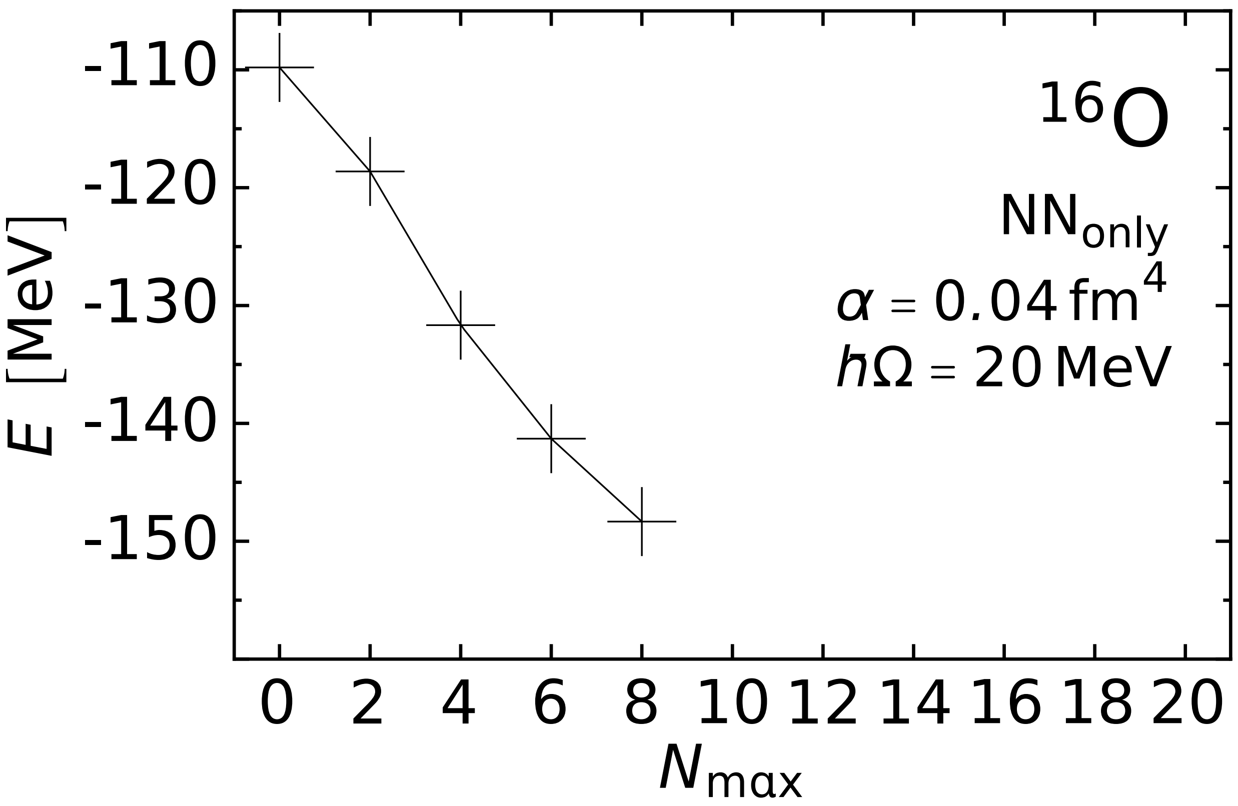
Vary et al.; J. Phys.: Conf. Series 180, 012083 (2009)



Importance Truncated NCSM

Roth, PRC 79, 064324 (2009)

- **converged NCSM** calculations limited to lower & mid p-shell nuclei
- example: full N_{max}=10 calculation for ^{16}O would be very difficult, basis dimension $D > 10^{10}$



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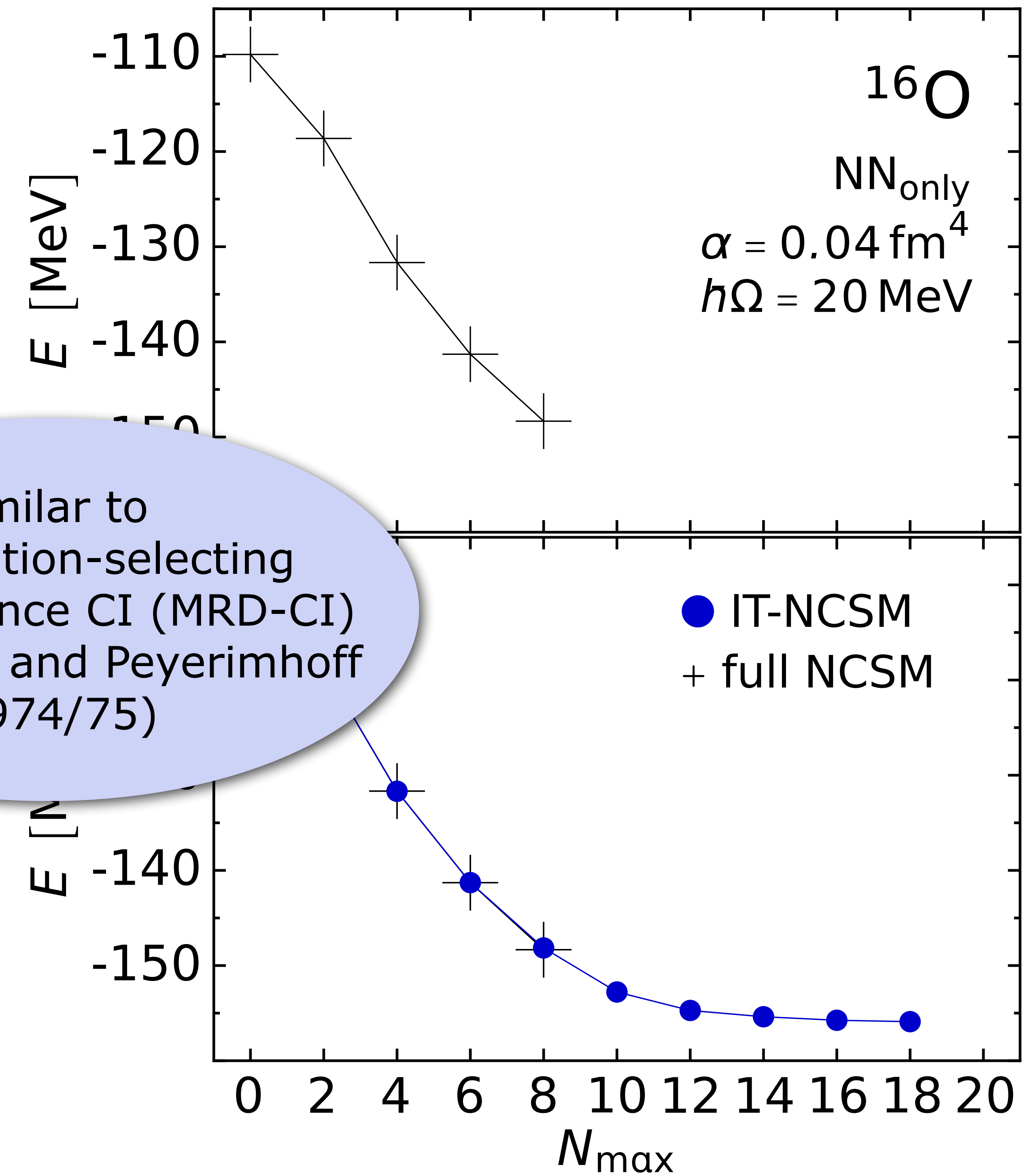


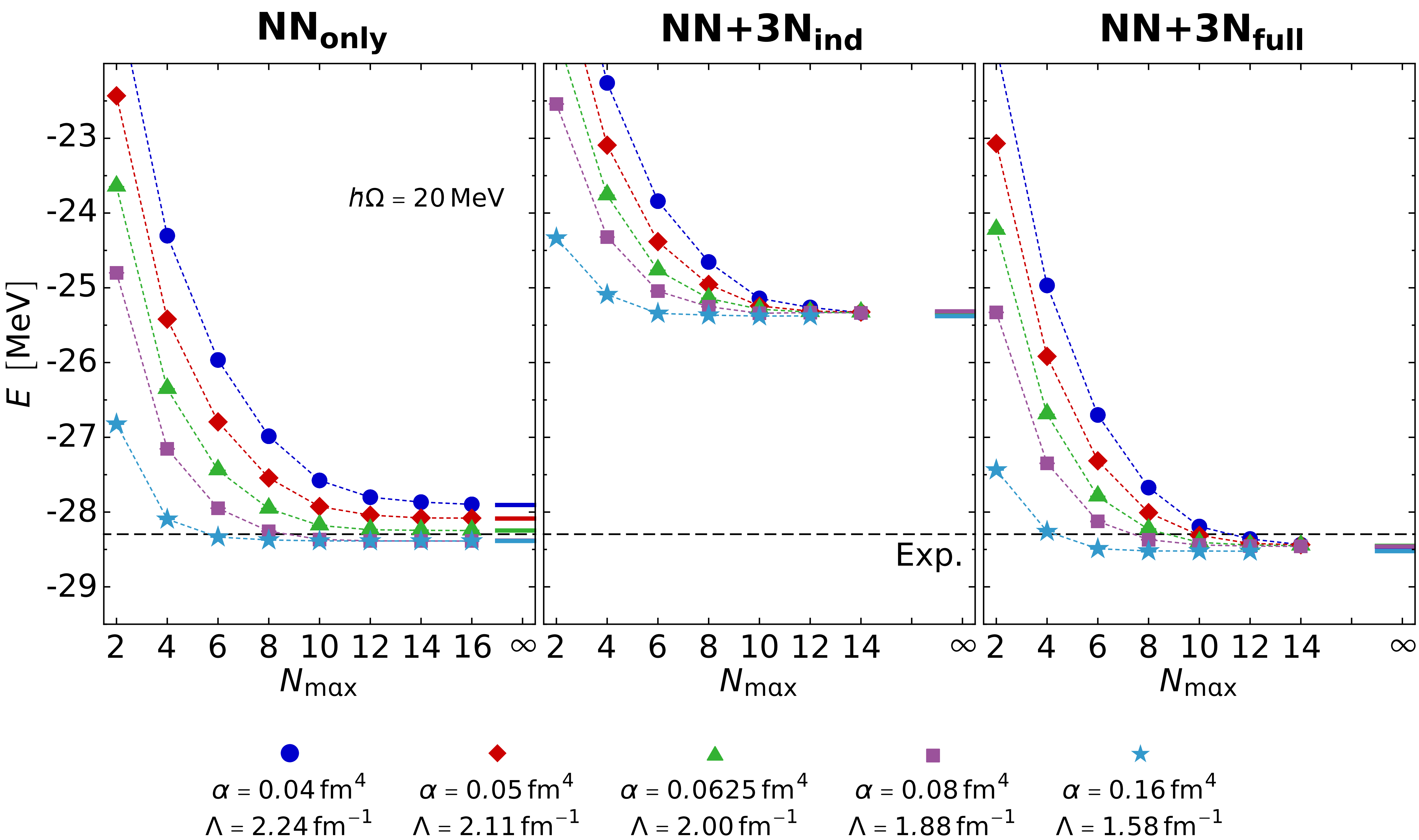
similar to configuration-selecting multi-reference CI (MRD-CI) by Buenker and Peyerimhoff (1974/75)

Importance Truncation

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

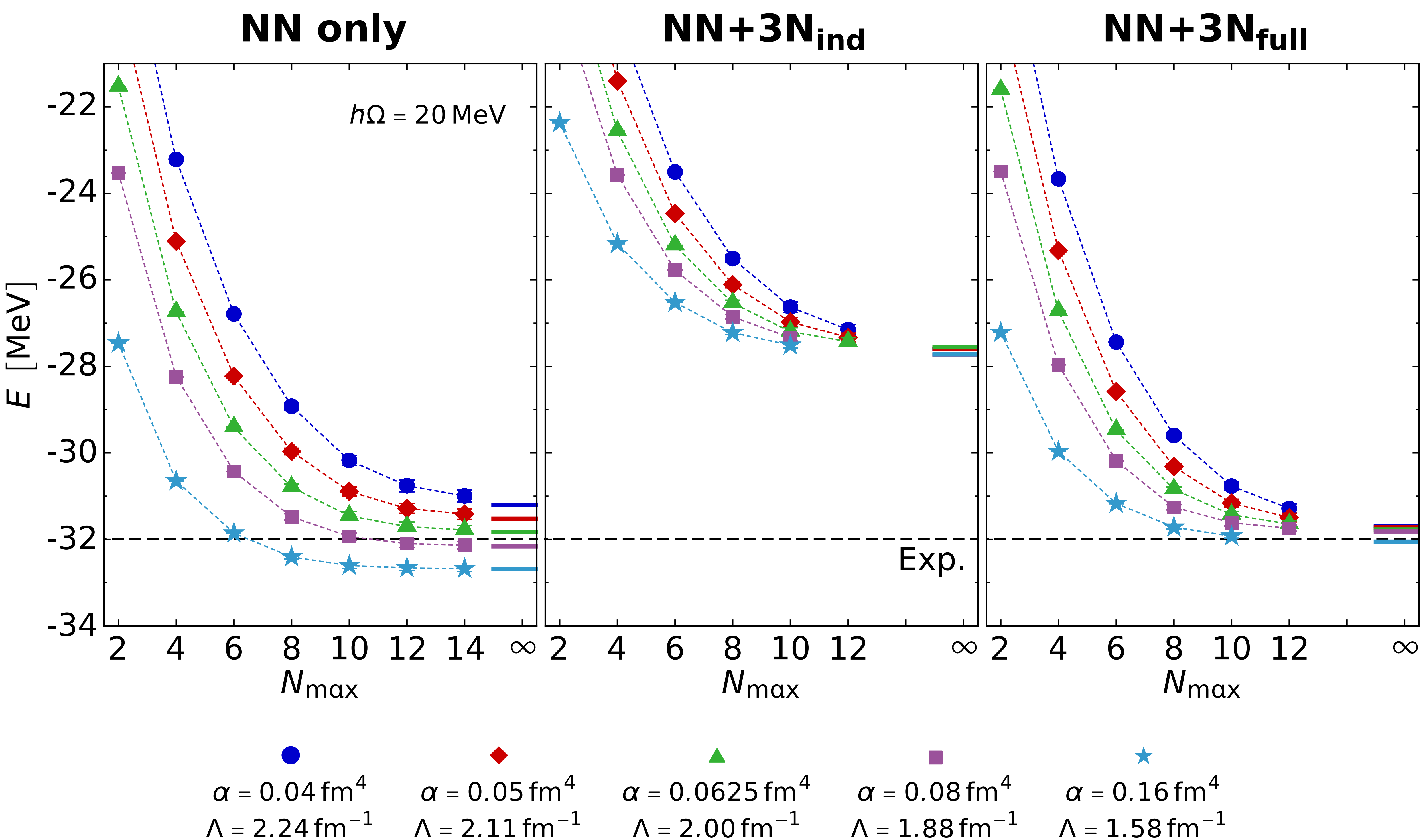
^{4}He: Ground-State Energy

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



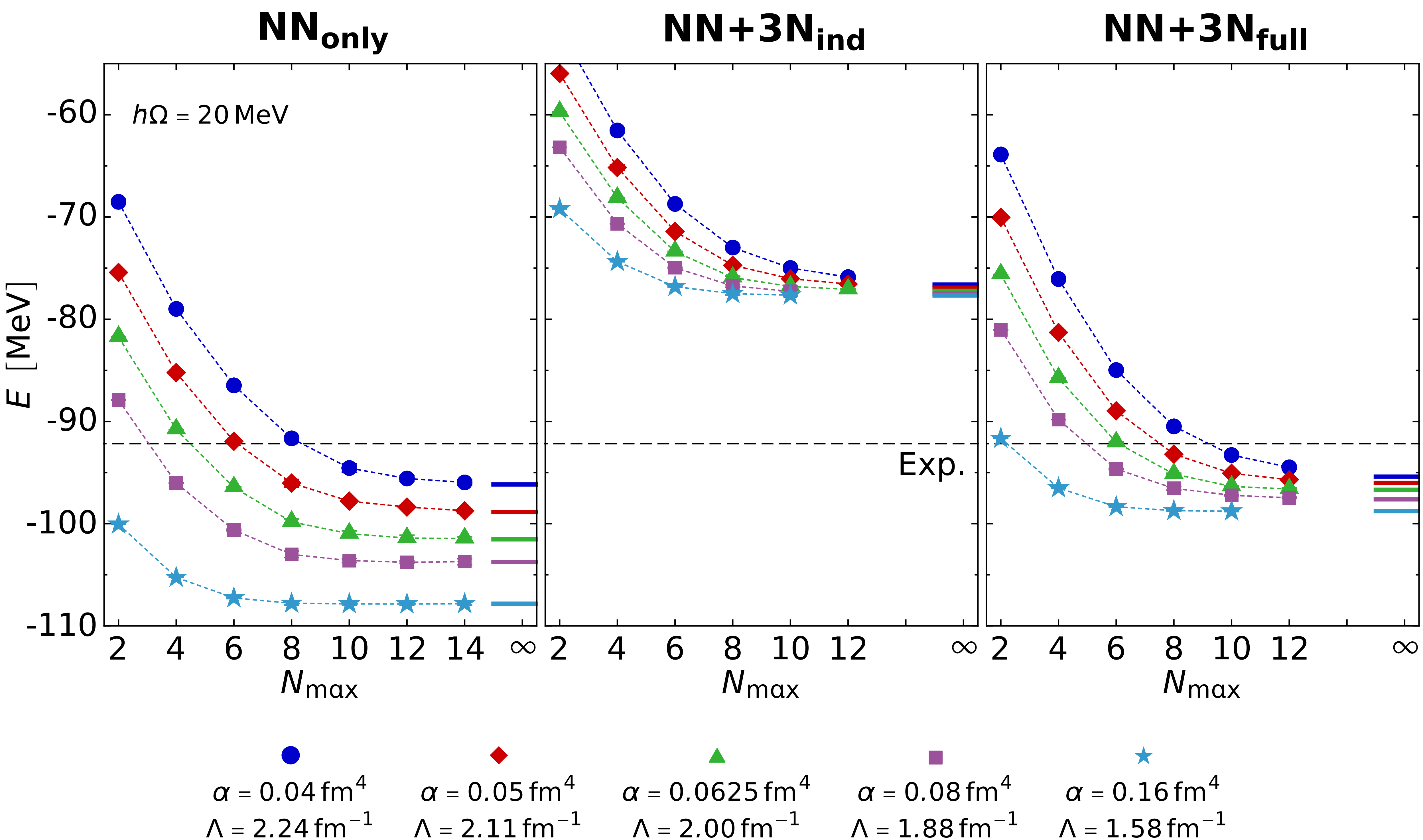
^{7}Li: Ground-State Energy

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



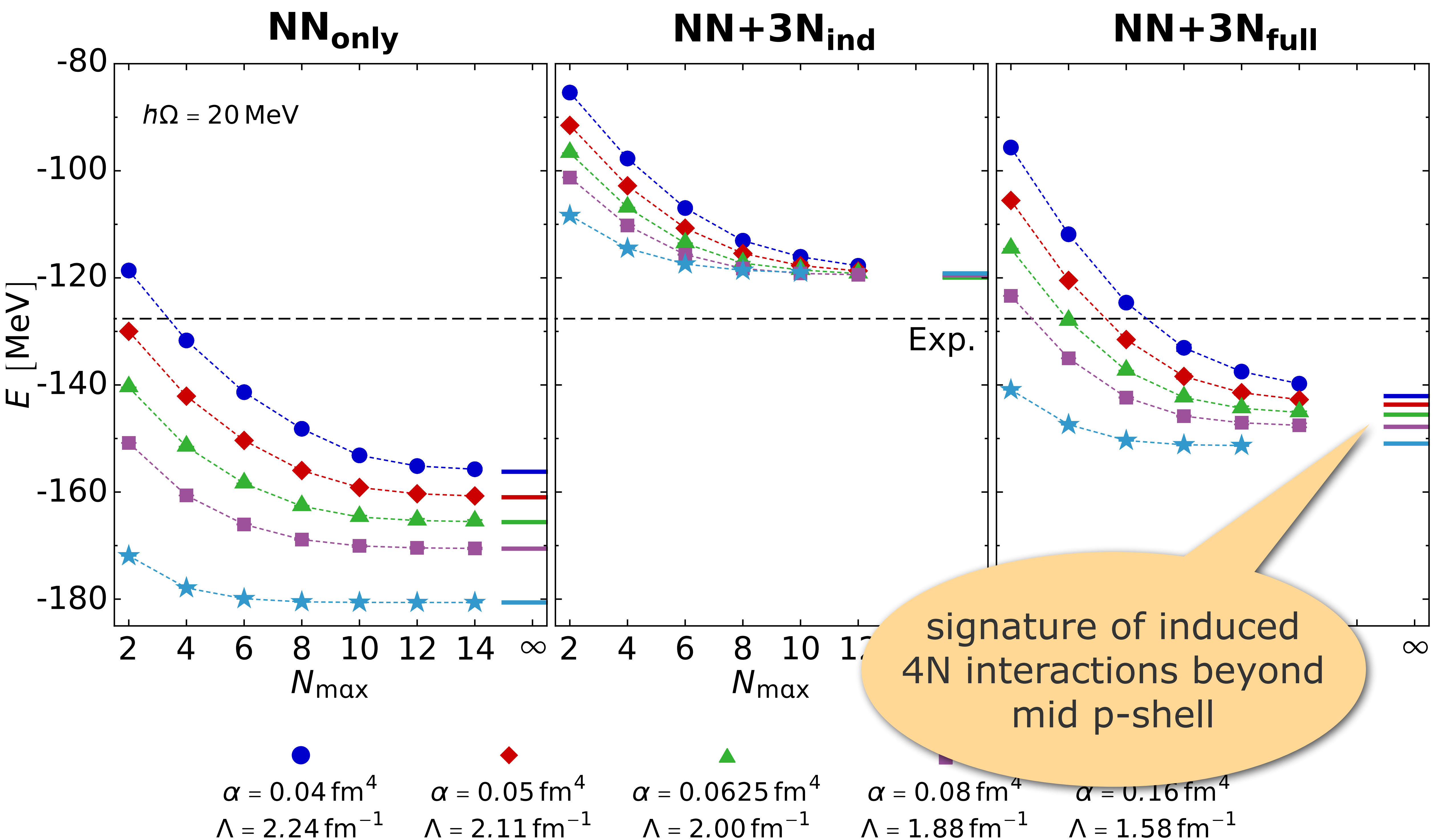
^{12}C: Ground-State Energy

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)



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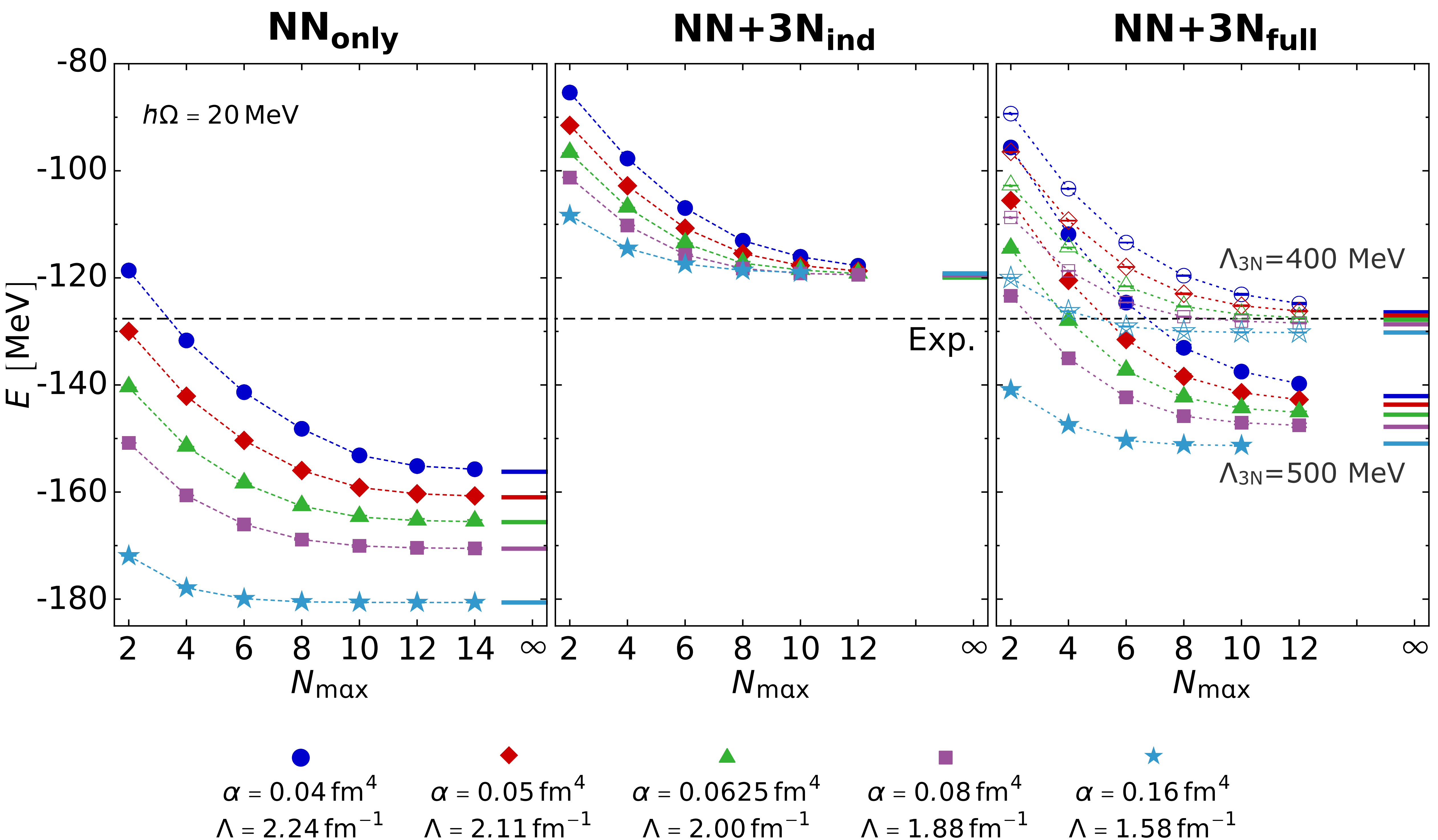
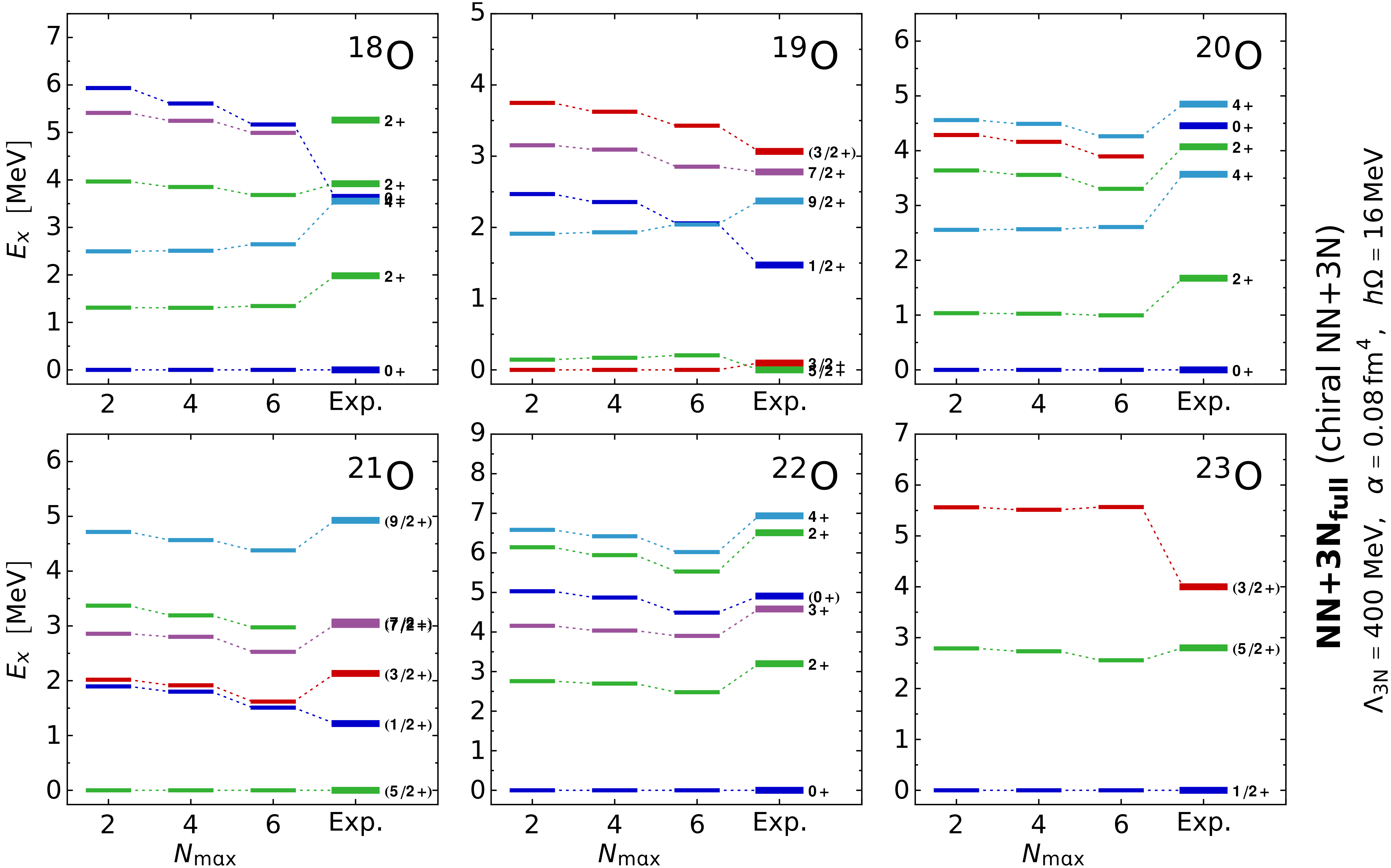


Spectra of Oxygen Isotopes

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



Role of the Single-Particle Basis

Single-Particle Basis

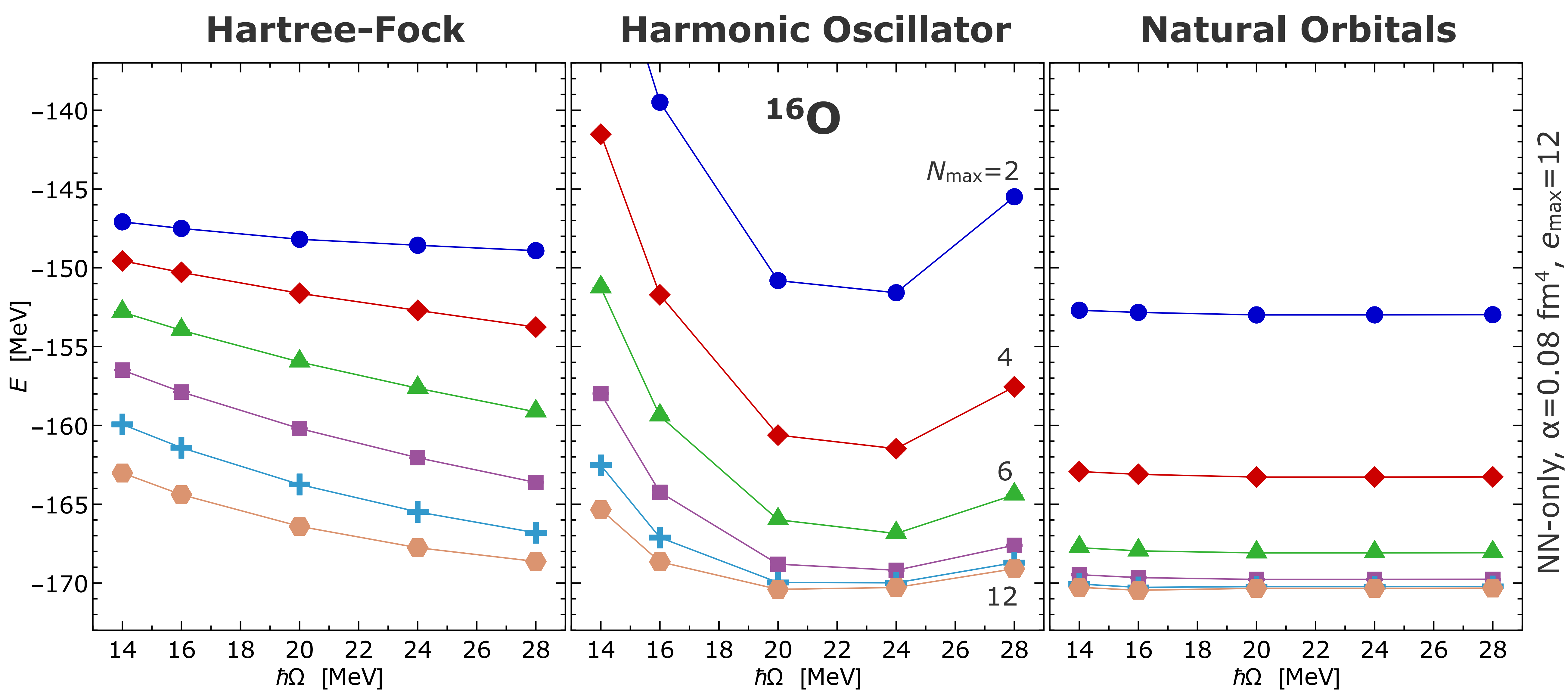
- **Harmonic-Oscillator Basis**
  - essential for computation of matrix elements, always first step
  - separation of center of mass and intrinsic states, translational invariance
  - wrong asymptotic behavior, slow convergence of long-range observables

- **Hartree-Fock Basis**
  - spherical Hartree-Fock calculation to optimize single-particle basis
  - adapt basis to typical size of nuclear ground state
  - only for soft interactions, pathological asymptotics for unbound states

- **Natural-Orbital Basis**
  - one-body density matrix obtained from second-order MBPT calculation
  - natural orbital basis adapted to size of correlated ground state
  - correct asymptotic behavior, independence of underlying basis

NCSM Convergence: Energies

J. Müller, A. Tichai, K. Vobig, R. Roth, in prep.



- MBPT natural-orbital basis **eliminates frequency dependence** and **accelerates convergence** of NCSM

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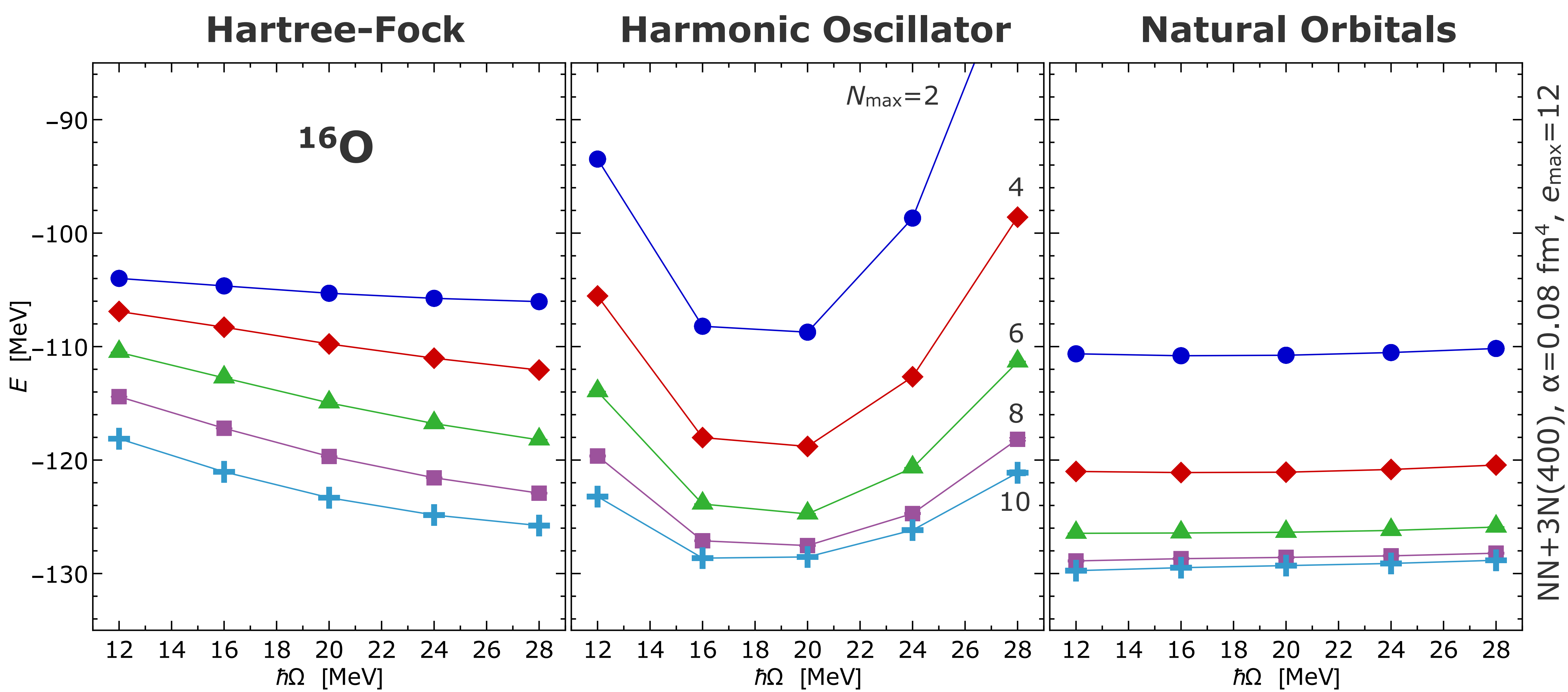

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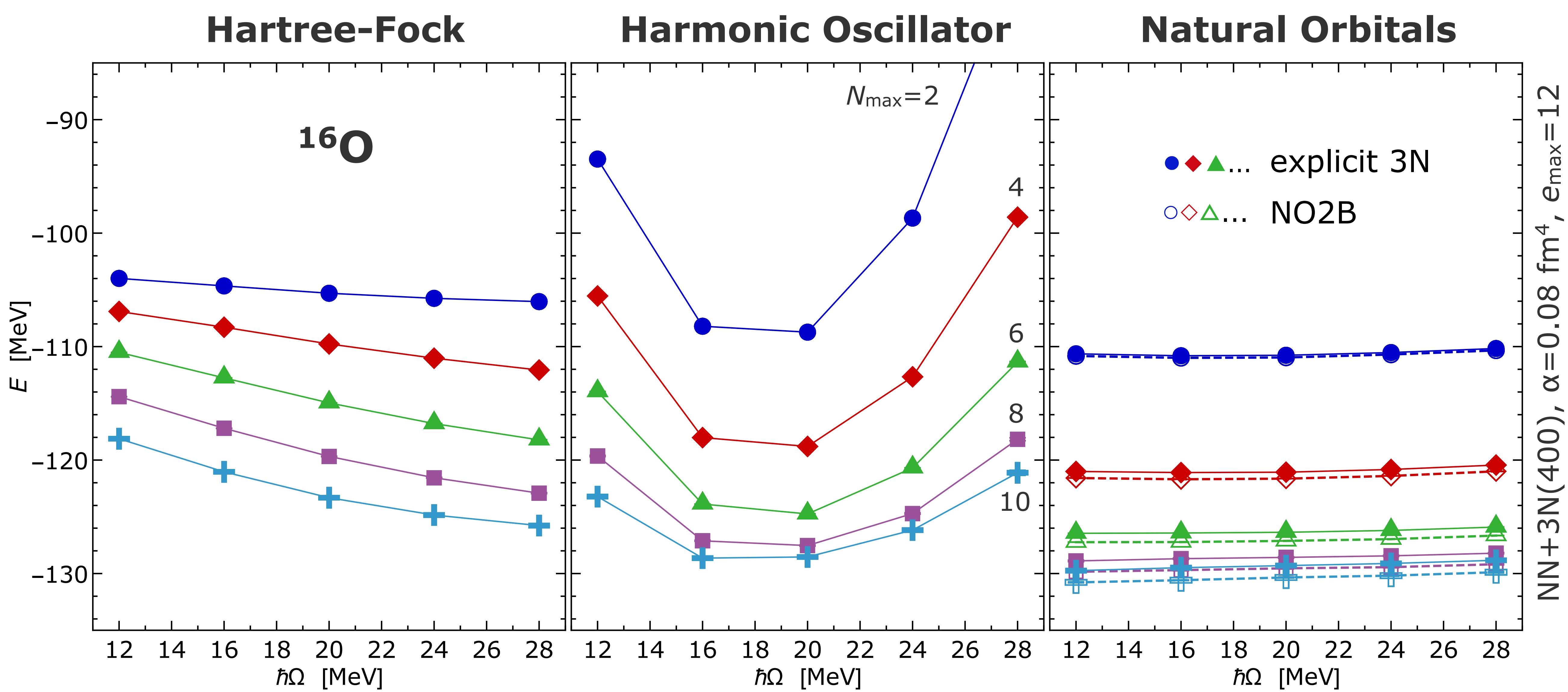

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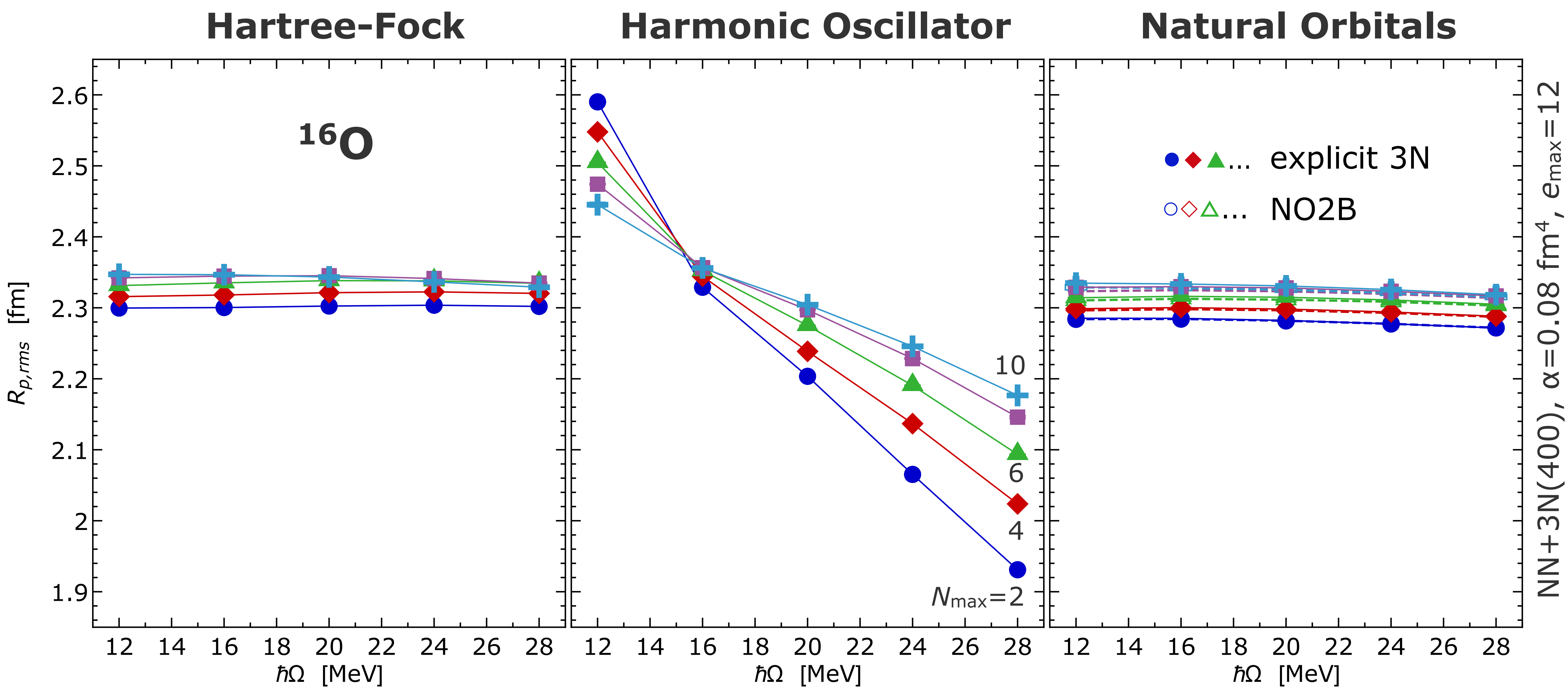
NCSM Convergence: Radii

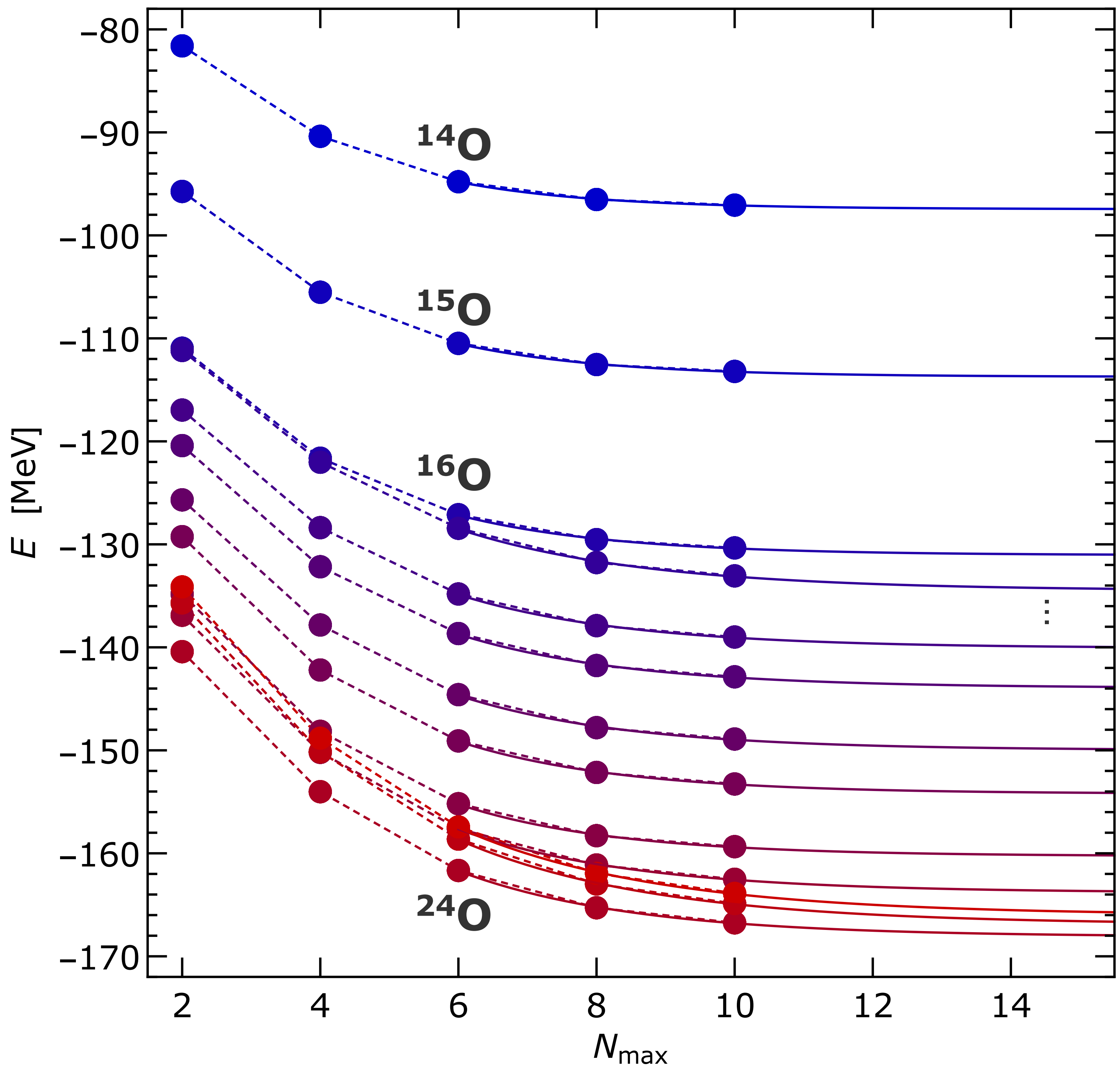
J. Müller, A. Tichai, K. Vobig, R. Roth, in prep.



- MBPT natural-orbital basis **eliminates frequency dependence** and **accelerates convergence** of NCSM

Oxygen Isotopes

J. Müller, A. Tichai, K. Vobig, R. Roth, in prep.



- excellent convergence with natural-orbital basis for all oxygen isotopes

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

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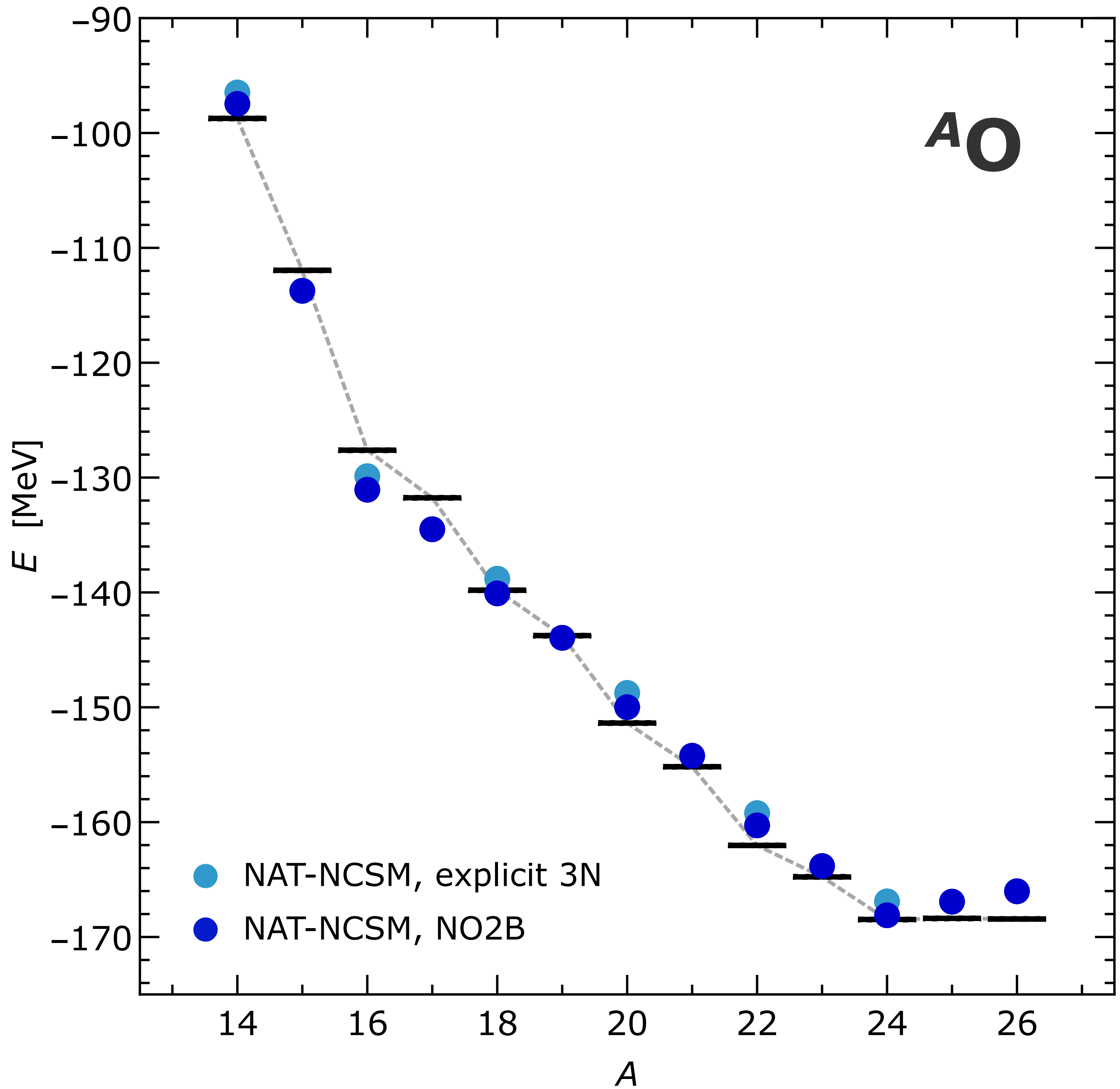


- excellent convergence with natural-orbital basis for all oxygen isotopes
- very good agreement with experimental systematics and dripline
- NO2B instead of explicit 3N causes ~1% overbinding

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

Many-Body Perturbation Theory

The Many Lives of MBPT

- MBPT has **turbulent history** in nuclear structure physics

- **key tool in the 1970’s…**
  - valence-space shell-model interactions from MBPT
  - G-matrix, Brueckner-Hartree-Fock method

- **great depression in the 1980’s…**
  - no convergence with interactions of the time (core, tensor part)
  - intruder states and multi-reference character

- **today** MBPT is coming back as…
  - auxiliary method (cf. importance truncation, natural orbital basis)
  - stand-alone many-body approach (cf. this workshop)

Single-Reference
Many-Body Perturbation Theory

Textbook MBPT

- **Rayleigh-Schrödinger perturbation theory** with partitioning defined though choice single-particle basis

$$\mathrm{H}_\lambda = \mathrm{H}_0 + \lambda \mathrm{W} \qquad\qquad \mathrm{H}_0 |\Phi_n\rangle = \epsilon_n |\Phi_n\rangle$$

- power series for energy eigenvalues and eigenstates and expansion of state corrections in unperturbed basis

$$E_n = \epsilon_n + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \ldots$$
$$|\Psi_n\rangle = |\Phi_n\rangle + \lambda |\Psi_n^{(1)}\rangle + \lambda^2 |\Psi_n^{(2)}\rangle + \ldots$$

$$|\Psi_n^{(p)}\rangle = \sum_\nu C_{n,\nu}^{(p)} |\Phi_\nu\rangle$$

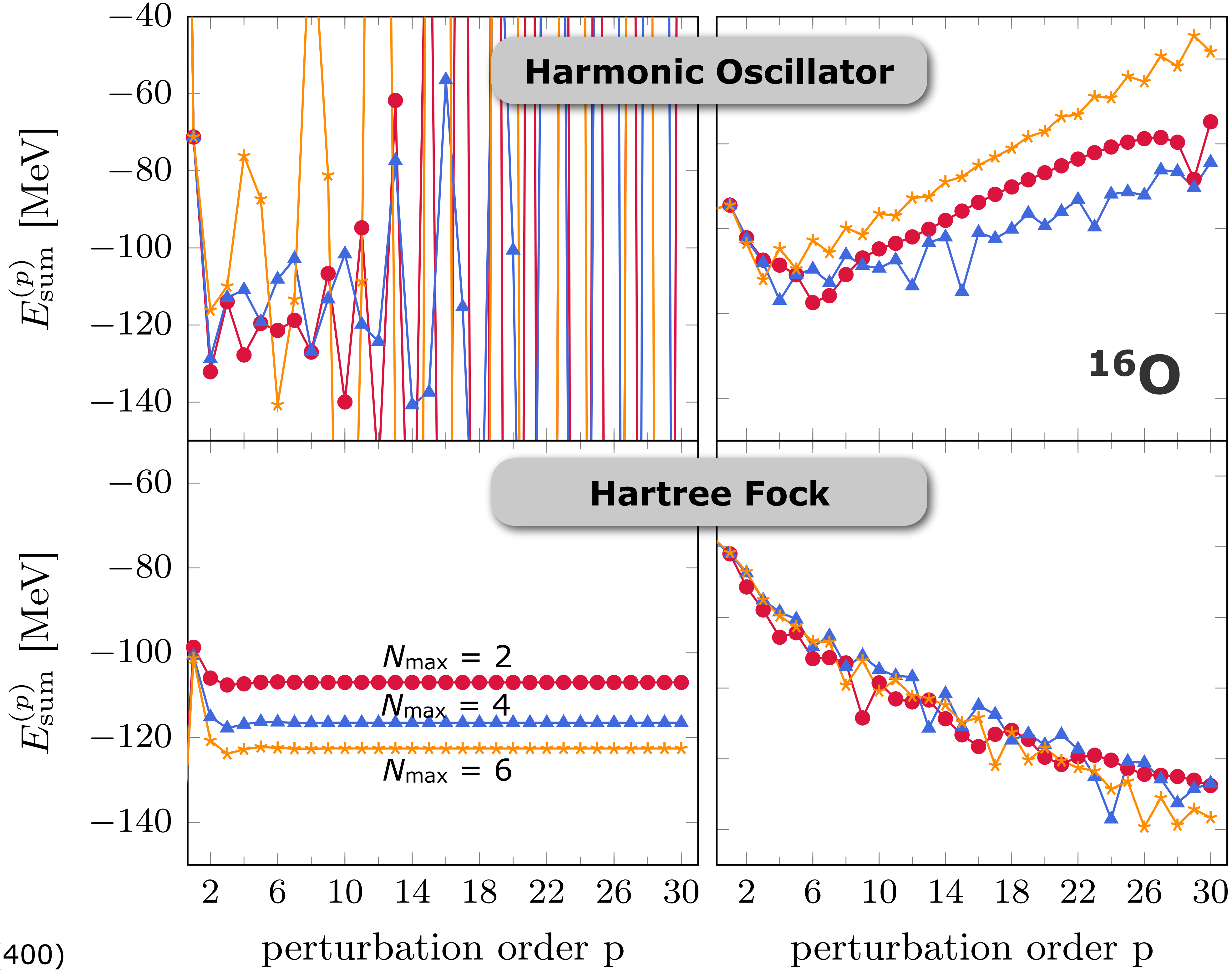
- **recursive relations for energy and state corrections** depending only on matrix elements of W in unperturbed basis

$$E_n^{(p)} = \sum_\nu \langle \Phi_n | \mathrm{W} | \Phi_\nu \rangle C_{n,\nu}^{(p-1)}$$
$$C_{n,\nu}^{(p)} = \frac{1}{\epsilon_n - \epsilon_\nu} \Big(\sum_{\nu'} \langle \Phi_\nu | \mathrm{W} | \Phi_{\nu'} \rangle C_{n,\nu'}^{(p-1)} - \sum_{j=1}^{p} E_n^{(j)} C_{n,\nu}^{(p-j)} \Big)$$

- evaluated at the level of many-body matrix elements **using NCSM technology**

Convergence: Single-Particle Basis

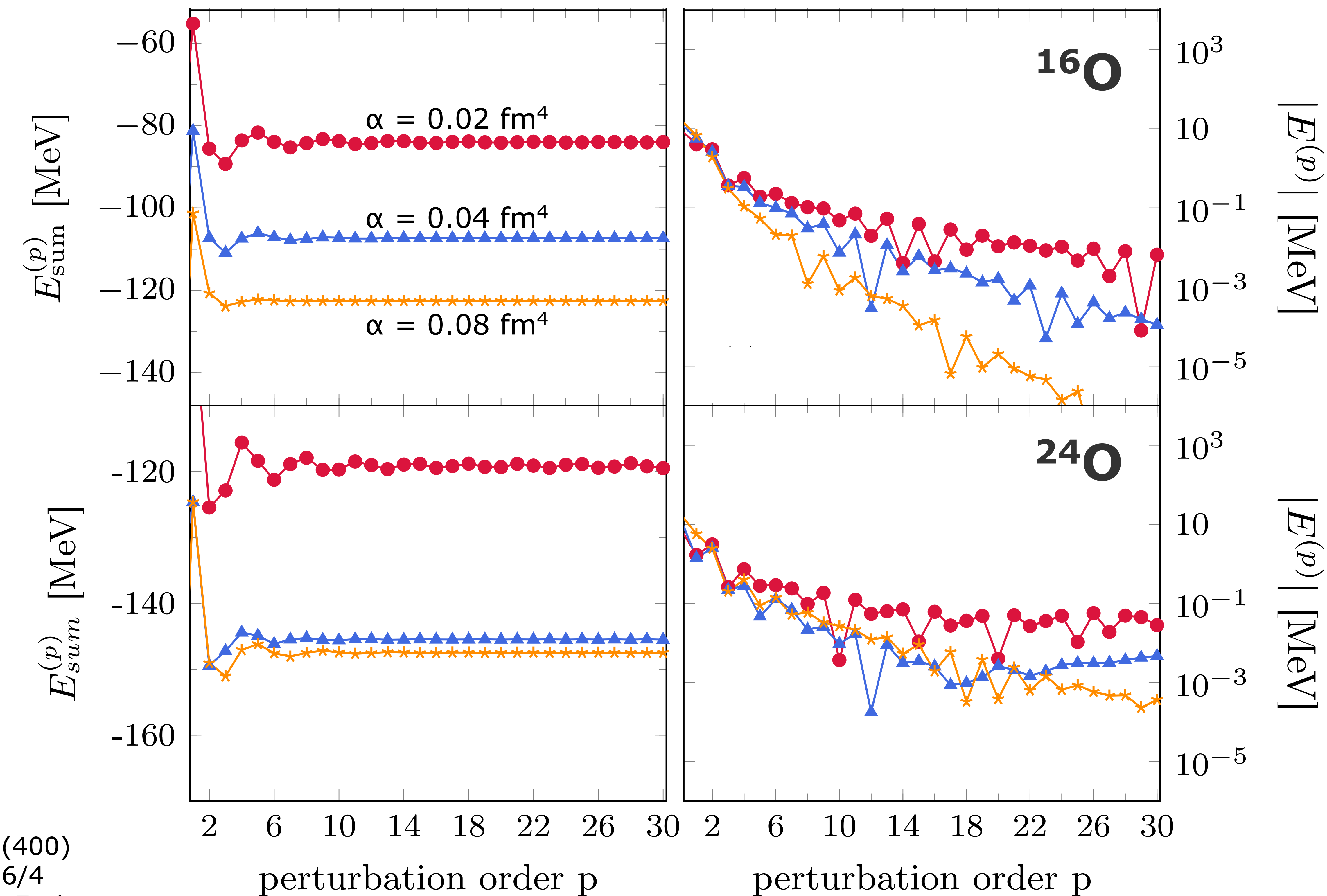
Tichai et al., PLB 756, 283 (2016)



NN+3N(400)
α = 0.08 fm^4

Convergence: SRG Evolution

Tichai et al., PLB 756, 283 (2016)



NN+3N(400)

N_{max} = 6/4

Hartree-Fock

Low-Order MBPT

- switch to **explicit expressions** for low-order energy corrections involving summations over m-scheme single-particle states, e.g.,

$$E^{(2)} = \frac{1}{4} \sum_{a,b}^{<\epsilon_F} \sum_{m,n}^{>\epsilon_F} \frac{|\langle ab| \mathrm{W} |mn\rangle|^2}{\epsilon_a + \epsilon_b - \epsilon_m - \epsilon_n}$$

➡ **large model spaces**, truncated wrt. single-particle energy $e_{\max}$ are easily accessible

- make use of **angular-momentum** coupling for closed-shell nuclei, reducing summations to orbital indices

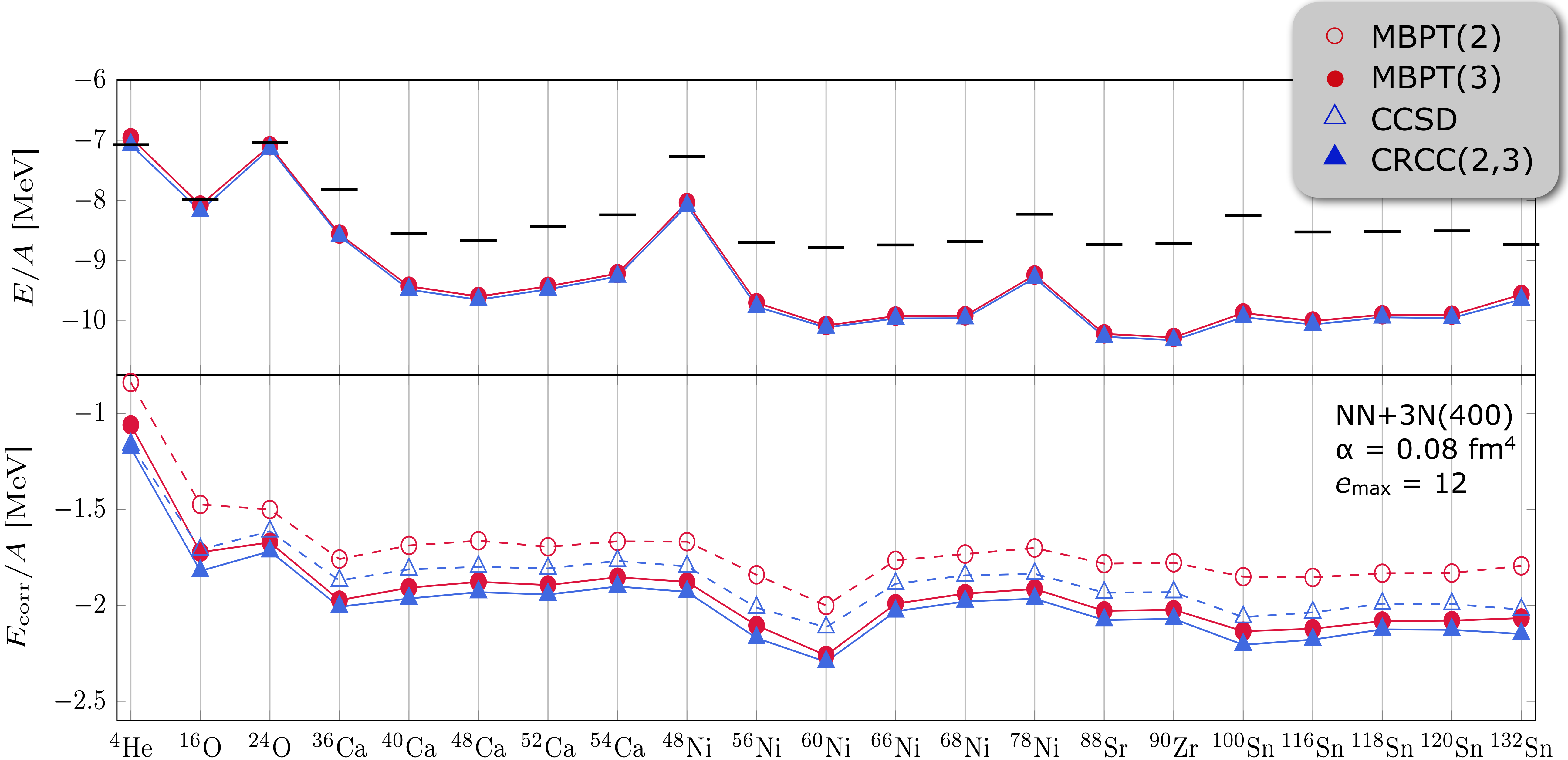
$$E^{(2)} = \frac{1}{4} \sum_{\bar{a},\bar{b}}^{<\epsilon_F} \sum_{\bar{m},\bar{n}}^{>\epsilon_F} \sum_{J} (2J+1) \frac{|\langle \bar{a}\bar{b}; J| \mathrm{W} |\bar{m}\bar{n}; J\rangle|^2}{\epsilon_{\bar{a}} + \epsilon_{\bar{b}} - \epsilon_{\bar{m}} - \epsilon_{\bar{n}}}$$

➡ makes evaluation of sums **much more efficient** since coupled matrix elements are directly available

- quickly gets tedious when going to higher orders…

Low-Order MBPT

Tichai et al., PLB 756, 283 (2016)



- **good agreement** of MBPT(3) ground-state energies with **advanced coupled-cluster calculations** throughout the complete mass range

Multi-Configurational Many-Body Perturbation Theory

JOURNAL OF CHEMICAL PHYSICS VOLUME 119, NUMBER 4 22 JULY 2003

On the perturbation of multiconfiguration wave functions

Zoltán Rolik, Ágnes Szabados, and Péter R. Surján
Department of Theoretical Chemistry, Eötvös University, H-1518 Budapest 112, POB 32, Hungary

(Received 22 January 2003; accepted 29 April 2003)

A simple variant of perturbation theory is used to correct reference states of a general multiconfigurational character. The full solution of an active space is not required, and no iterative procedure is applied to construct the resolvent operator. The perturbed wave function is expanded in a complete set of determinants from which the reference function is projected out, and the overlap between projected determinants is handled by an explicit, analytic inversion of the overlap matrix.
 [DOI: 10.1063/1.1584424]

I. INTRODUCTION

Perturbation theory (PT) has been an important tool to account for fine interactions and correlation effects in many-electron systems. Its simplest variant, the single-reference PT that starts from a single determinantal zero order state, has a limited field of application due to the well known problems of the inadequacy of a single determinant in describing several chemically important situations. This motivated an extensive research for developing multireference perturbation theories (MRPT). Various formulations emerged,[1–20] which

II. MULTICONFIGURATIONAL PERTURBATION THEORY

A. Basic notions

Consider a normalized, multiconfigurational reference state denoted by $|0\rangle$, and the associated projector

$$\hat{O}=|0\rangle\langle 0|.$$

The projector to the orthogonal complement space is $\hat{P}=1-\hat{O}$. Next, we consider a set of determinants, denoted by $|k\rangle$.

Multi-Configurational Perturbation Theory

Tichai, Gebrerufael, Vobig, Roth; arXiv:1703.05664

- select **NCSM reference space** $\mathcal{M}_{\text{ref}}$ and solve full eigenvalue problem

$$|\Psi_n^{\text{ref}}\rangle = \sum_{\mu \in \mathcal{M}_{\text{ref}}} B_{n,\mu}^{\text{ref}} \, |\Phi_\mu\rangle$$

- define **unperturbed Hamiltonian** with reference-space eigenstates

$$\mathrm{H}_0 = \sum_{\mu \in \mathcal{M}_{\text{ref}}} \epsilon_\mu^{\text{ref}} \, |\Psi_\mu^{\text{ref}}\rangle\langle\Psi_\mu^{\text{ref}}| + \sum_{\nu \notin \mathcal{M}_{\text{ref}}} \epsilon_\nu \, |\Phi_\nu\rangle\langle\Phi_\nu|$$

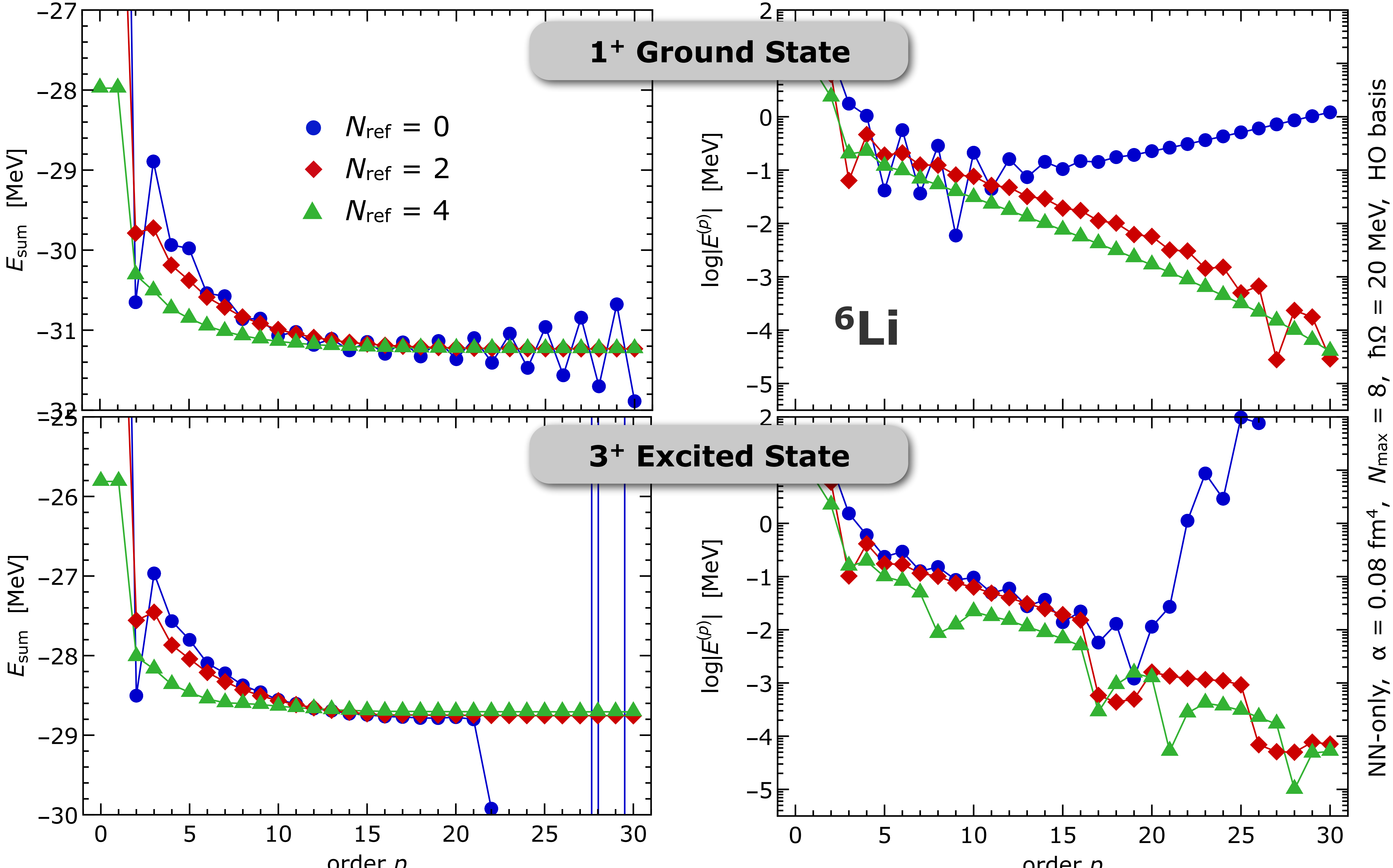
- usual MBPT derivation yields **recursive relations** for energy and state corrections

$$E_n^{(p)} = \sum_{\nu \notin \mathcal{M}_{\text{ref}}} \langle\Psi_n^{\text{ref}}|\mathrm{W}|\Phi_\nu\rangle \, C_{n,\nu}^{(p-1)} \qquad |\Psi_n^{(p)}\rangle = \sum_{\mu \in \mathcal{M}_{\text{ref}}} D_{n,\mu}^{(p)} \, |\Psi_\mu^{\text{ref}}\rangle + \sum_{\nu \notin \mathcal{M}_{\text{ref}}} C_{n,\nu}^{(p)} \, |\Phi_\nu\rangle$$

$$C_{n,\nu}^{(p)} = \frac{1}{\epsilon_n - \epsilon_\nu}\left(\sum_{\nu' \notin \mathcal{M}_{\text{ref}}} \langle\Phi_\nu|\mathrm{W}|\Phi_{\nu'}\rangle \, C_{n,\nu'}^{(p-1)} + \sum_{\mu \in \mathcal{M}_{\text{ref}}} \langle\Phi_\nu|\mathrm{W}|\Psi_\mu^{\text{ref}}\rangle \, D_{n,\mu}^{(p-1)} - \sum_{j=1}^{p} E_n^{(j)} C_{n,\nu}^{(p-j)} \right)$$

$$D_{n,\mu}^{(p)} = \frac{1}{\epsilon_n - \epsilon_\mu}\left(\langle\Psi_\mu^{\text{ref}}|\mathrm{W}|\psi_n^{(p-1)}\rangle - \sum_{j=1}^{p} E_n^{(j)} D_{n,\mu}^{(p-j)} \right)$$

Convergence: Reference Space



Perturbatively Improved NCSM

Tichai, Gebrerufael, Vobig, Roth; arXiv:1703.05664

NCSM
many-body solution

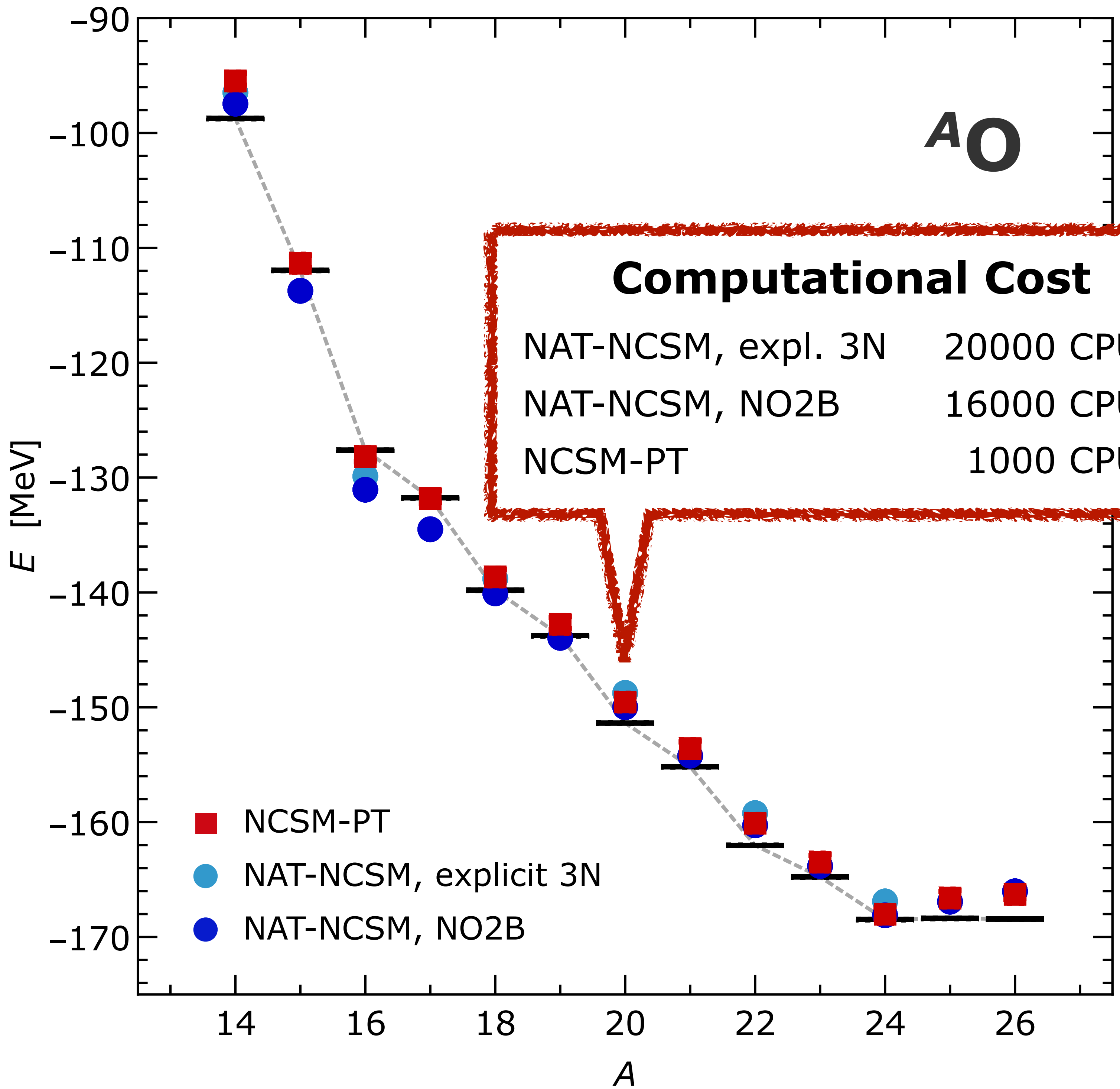
MBPT
convergence booster

- eigenstates from NCSM at small N_{max} as unperturbed states
- access to all open-shell nuclei and systematically improvable

- multi-configurational MBPT at second order for individual unperturbed states
- capture couplings in huge model-space through perturbative corrections

Oxygen Isotopes

Tichai, Gebrerufael, Vobig, Roth; arXiv:1703.05664



Computational Cost

NAT-NCSM, expl. 3N	20000 CPU-h
NAT-NCSM, NO2B	16000 CPU-h
NCSM-PT	1000 CPU-h

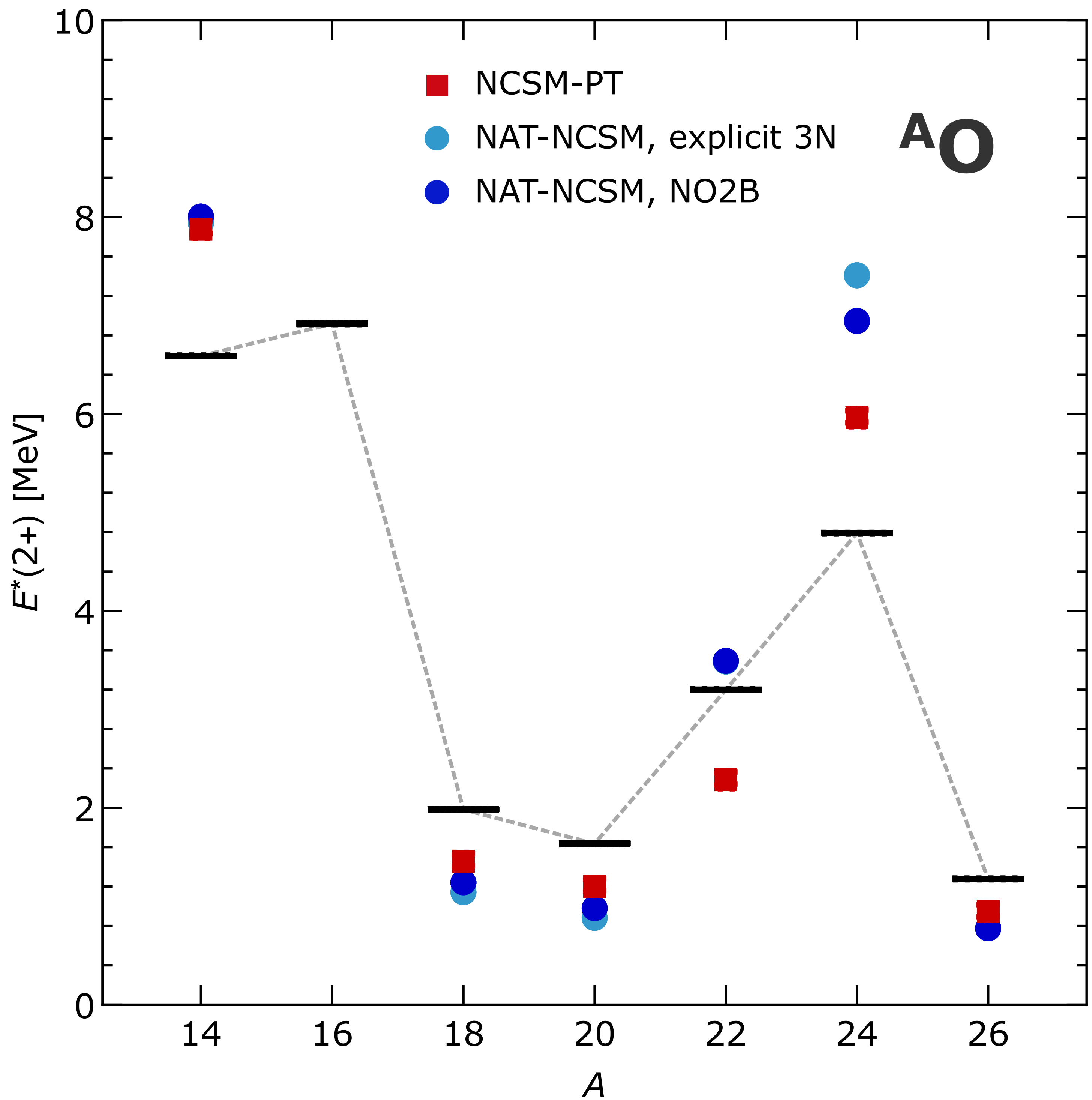
- excellent agreement with direct NCSM
- all isotopes are accessible due to simple m-scheme implementation

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

HF basis
N_{max}=2 reference

Oxygen Isotopes: Excited 2^+ States

Tichai, et al.; in prep.



- can address excited states natively
- example: first 2^+ states in even oxygen isotopes
- excellent agreement among methods except for closed (sub-)shells ^{22}O, ^{24}O…

chiral NN+3N
Λ_{3N}=400 MeV
α=0.08 fm^4
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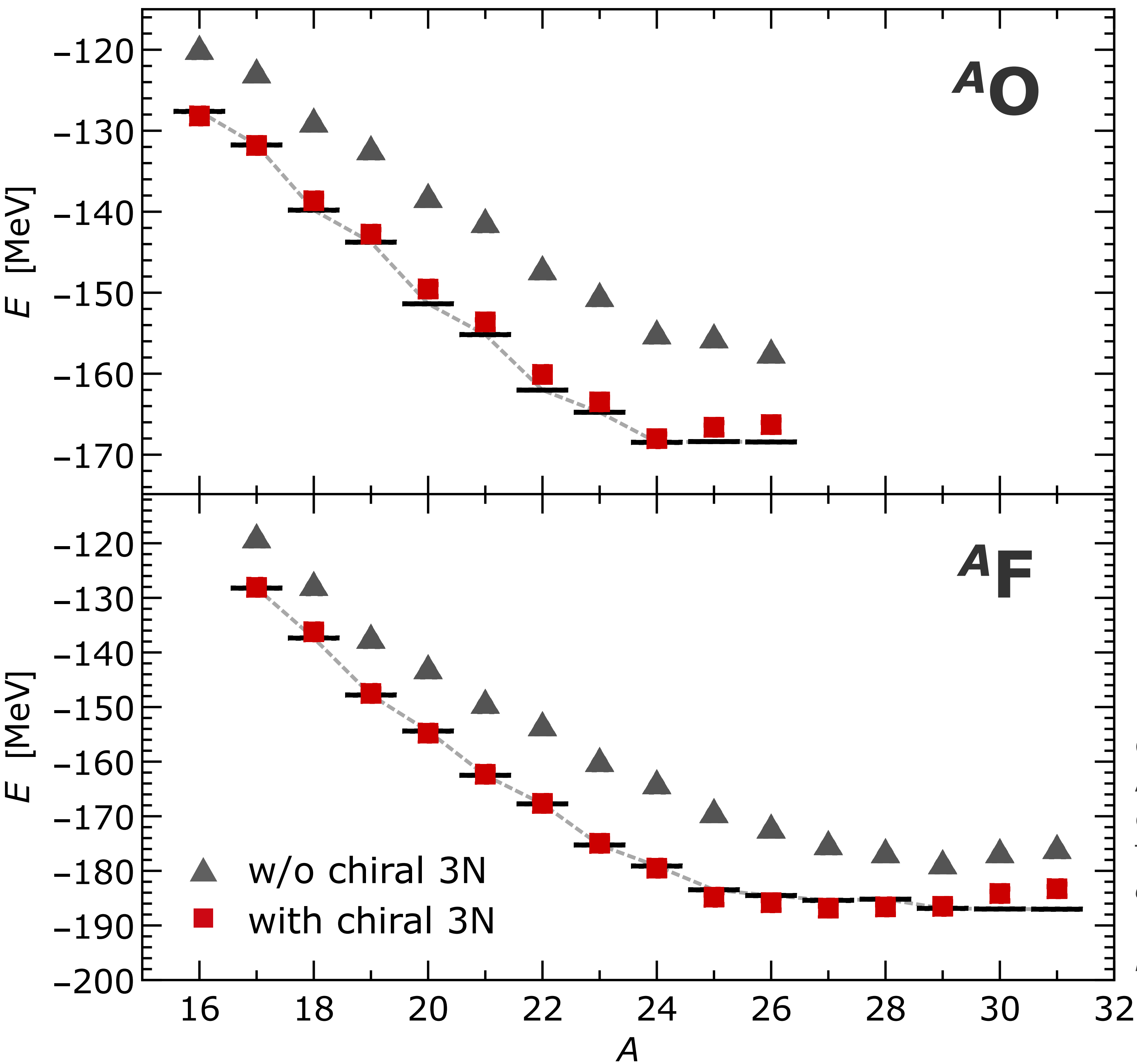
HF basis
N_{max}=2 reference

Exploring sd-Shell Phenomena

Tichai, Gebrerufael, Vobig, Roth; arXiv:1703.05664



- exploring various sd-shell phenomena, e.g., oxygen anomaly
- low computational cost enables surveys with different interactions

NCSM-PT

chiral NN+3N

Λ_{3N}=400 MeV

α=0.08 fm^4

$\hbar\Omega$=20 MeV

e_{max}=12

HF basis

N_{max}=2 reference

In-Medium NCSM

In-Medium NCSM

NCSM
reference state

IM-SRG
decoupling

NCSM
many-body solution

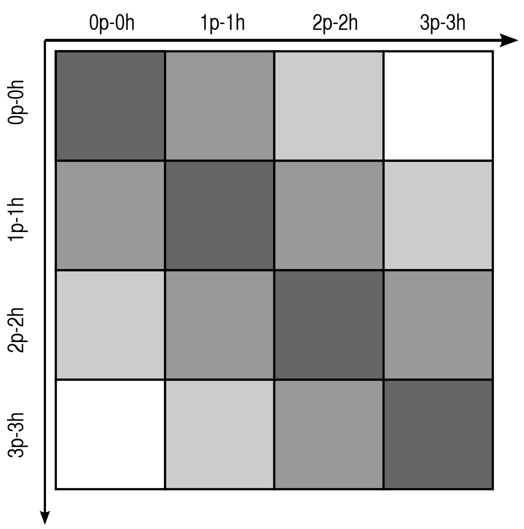
- ground-state from NCSM at small N_{max} as reference state for multi-reference IM-SRG
- access to all open-shell nuclei and systematically improvable

- IM-SRG evolution of multi-reference normal-ordered Hamiltonian (and other operators)
- decoupling of particle-hole excitations, i.e., pre-diagonalization in many-body space

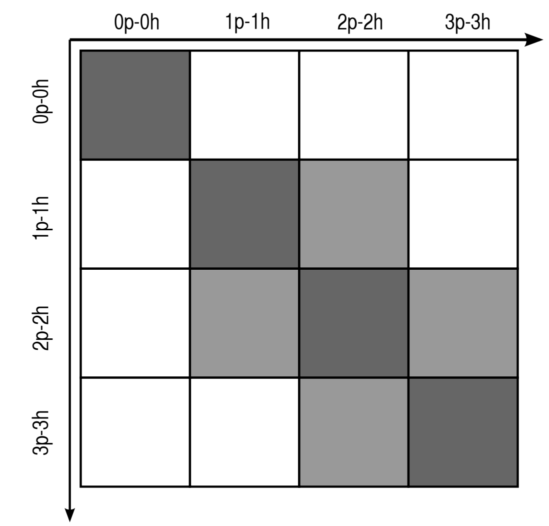
- use in-medium evolved Hamiltonian for a subsequent NCSM calculation
- access to ground and excited states and full suite of observables

In-Medium SRG

Tsukiyama, Bogner, Schwenk, Hergert,…



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



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

- Hamiltonian and generator in normal order with respect to single or multi-determinant reference state, omit residual three-body piece

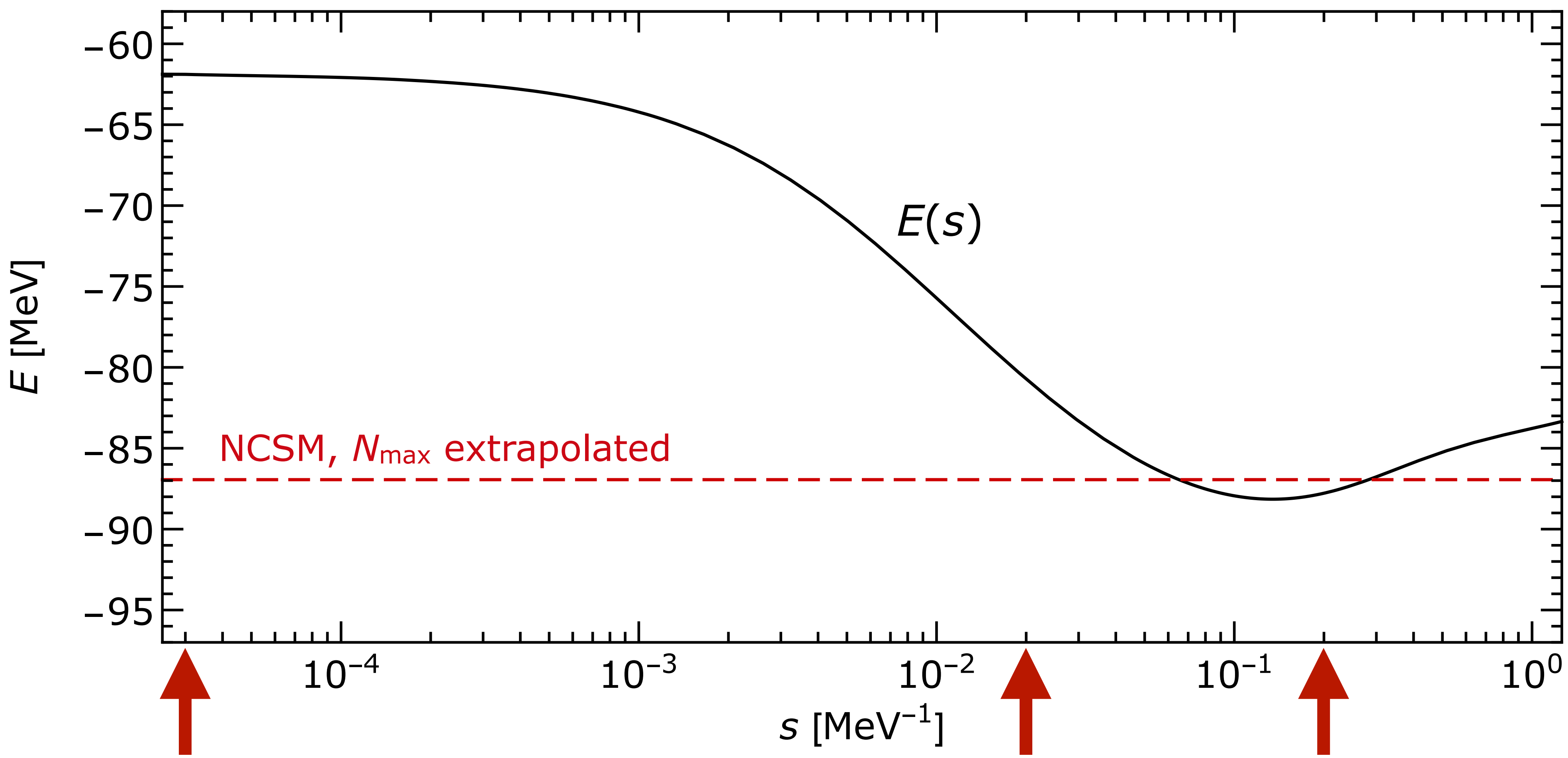
$$H(s) = E(s) + \sum_{ij} f^i_j(s)\, \tilde{A}^i_j + \frac{1}{4}\sum_{ijkl} \Gamma^{ij}_{kl}(s)\, \tilde{A}^{ij}_{kl} + \cancel{\frac{1}{36}\sum_{ijklmn} W^{ijk}_{lmn}(s)\, \tilde{A}^{ijk}_{lmn}}$$

- define generator to suppress off-diagonal contributions that couple reference state to ph excitations

$$\eta(s) = \left[H(s), H^{\mathrm{d}}(s)\right] = \left[H^{\mathrm{od}}(s), H^{\mathrm{d}}(s)\right]$$

In-Medium SRG: Multi Reference

Gebrerufael, Vobig, Hergert, Roth; PRL 118, 152503 (2017)



^{12}C

chiral NN+3N

Λ_{3N}=400 MeV

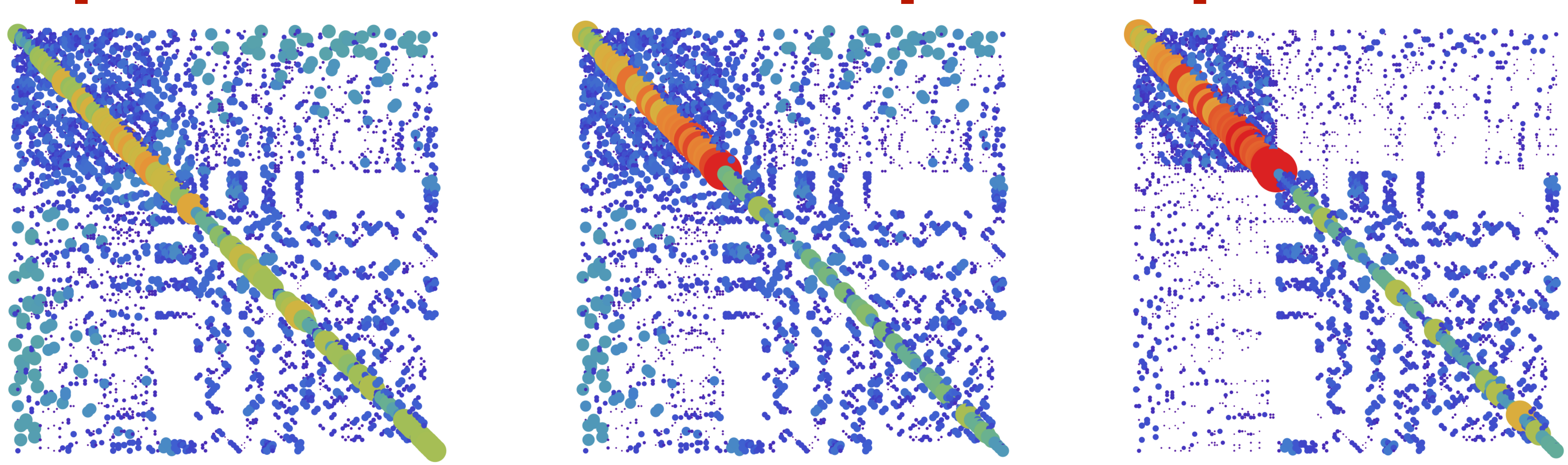
α=0.08 fm^4

$\hbar\Omega$=20 MeV

e_{max}=12

N_{max}=0 reference

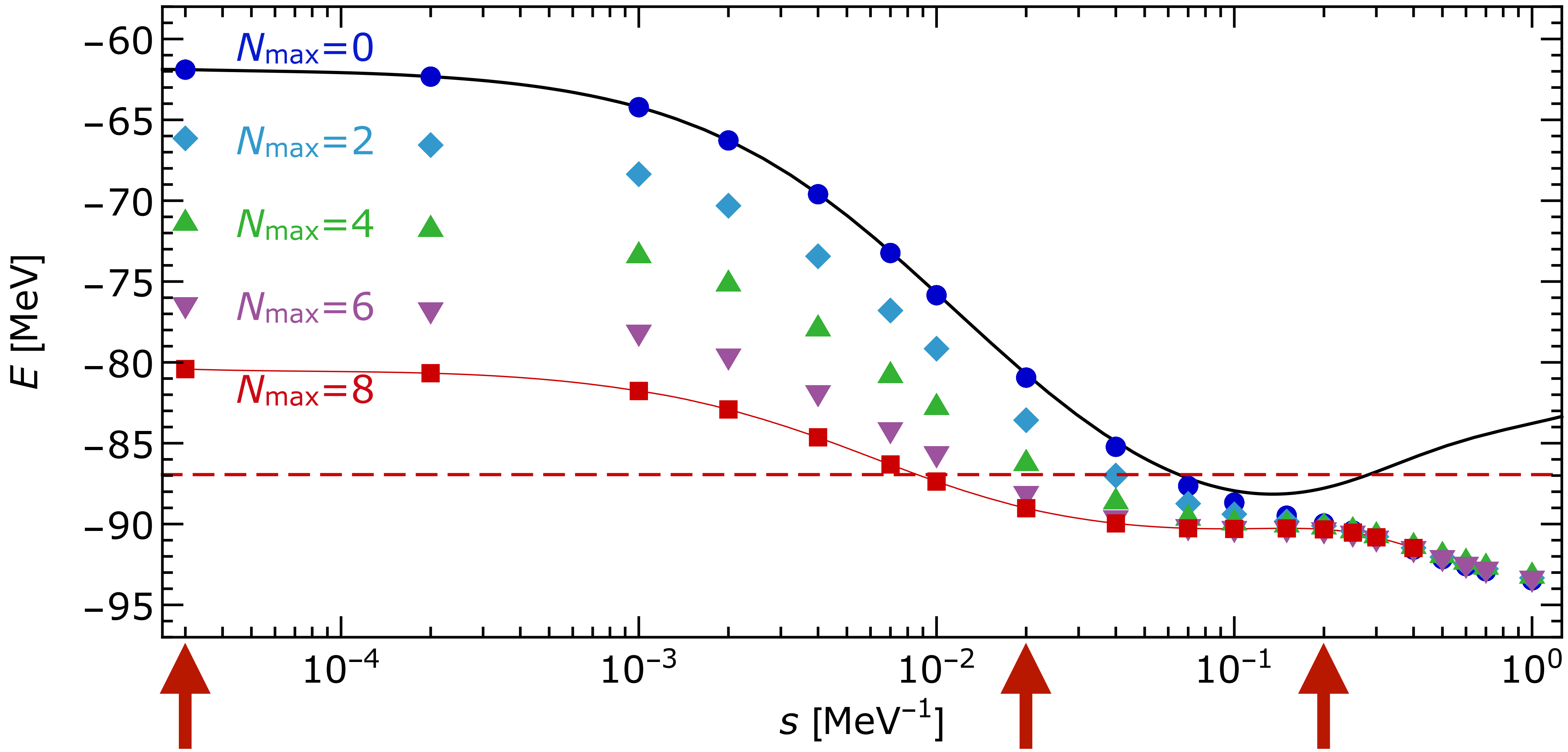
HF basis



Hamilton matrix in N_{max}=2 space

In-Medium SRG: Multi Reference

Gebrerufael, Vobig, Hergert, Roth; PRL 118, 152503 (2017)



^{12}C

chiral NN+3N

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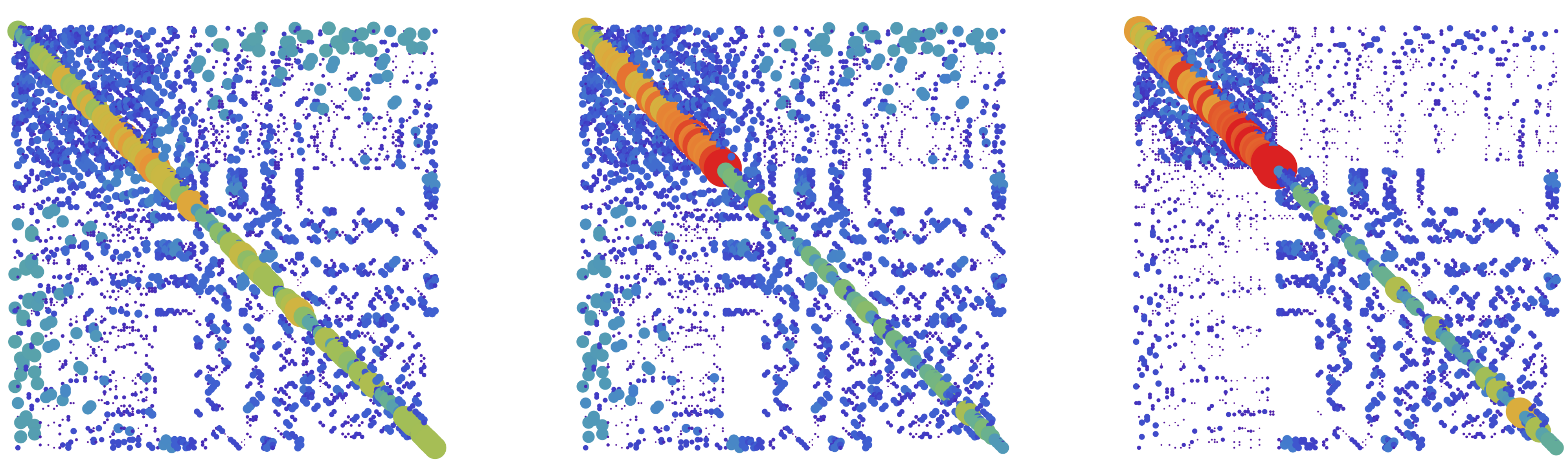
α=0.08 fm^4

$\hbar\Omega$=20 MeV

e_{max}=12

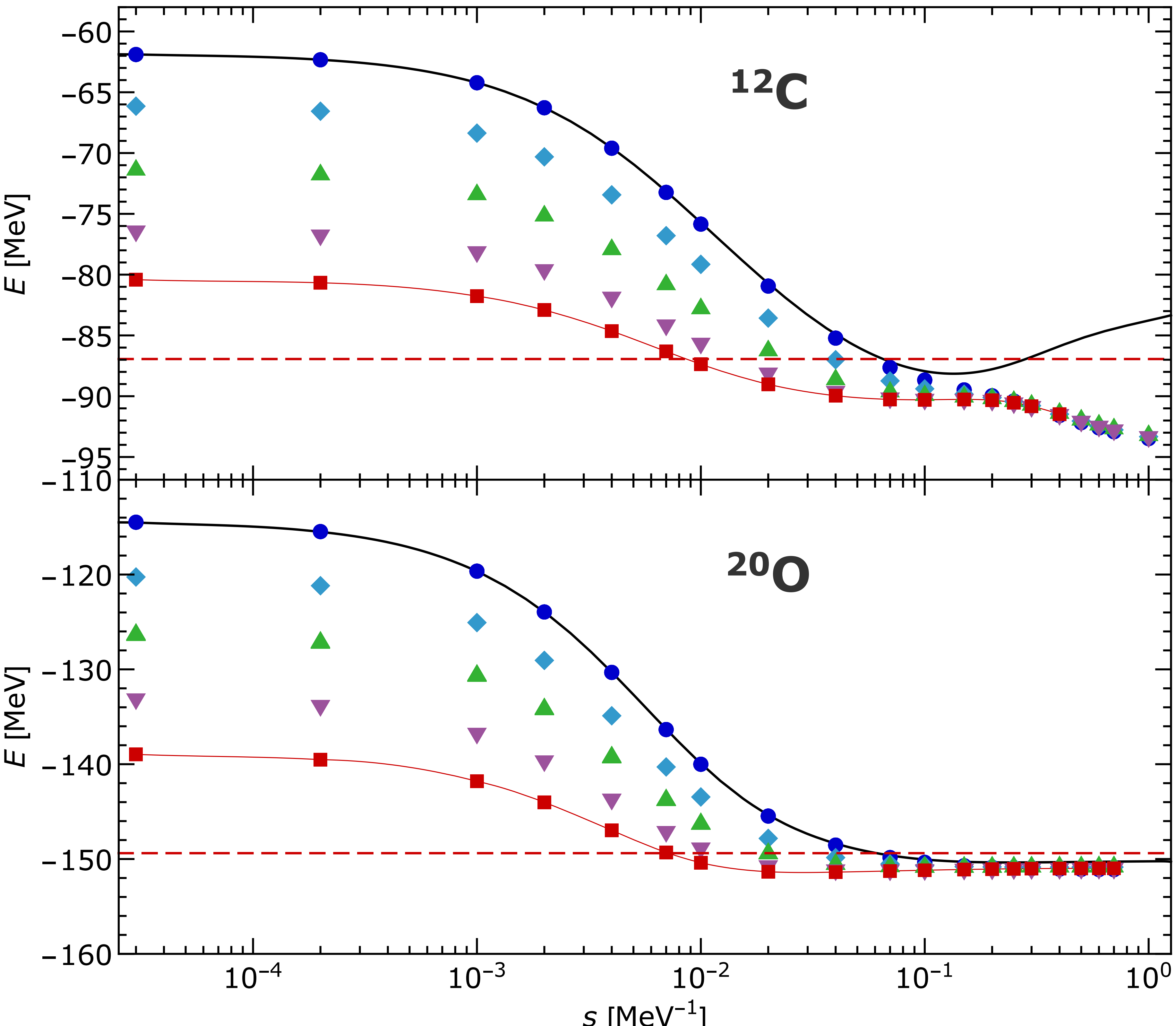
N_{max}=0 reference HF basis



Hamilton matrix in N_{max}=2 space

Flow: Ground-State Energy

Gebrerufael, Vobig, Hergert, Roth; PRL 118, 152503 (2017)



- NCSM convergence is drastically improved
- N_{max}=0 eigenvalues deviated from $E(s)$

chiral NN+3N
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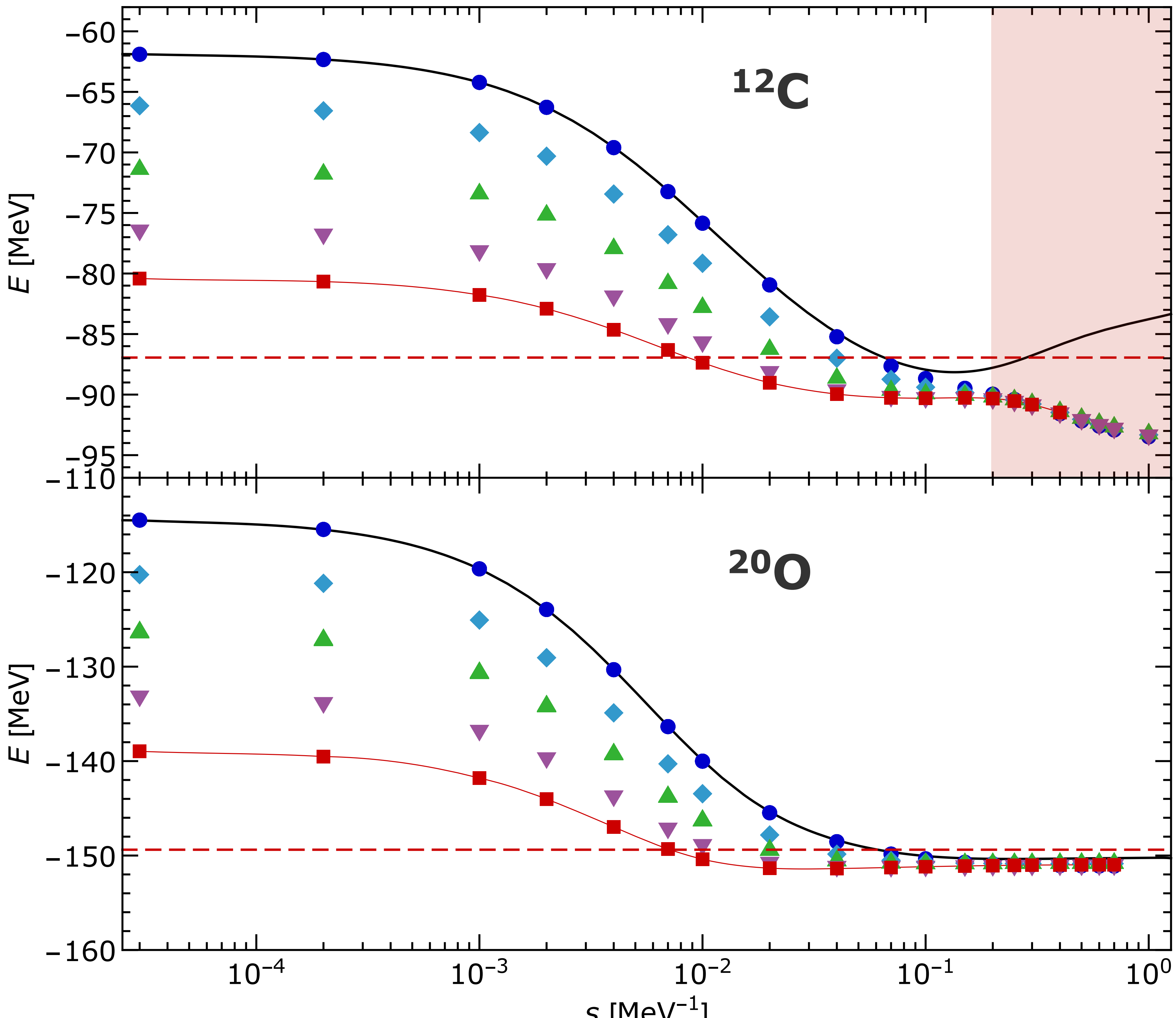
e_{max}=12

HF basis
N_{max}=0 reference state
N_{max}=0,2,4,6,8

Flow: Ground-State Energy

Gebrerufael, Vobig, Hergert, Roth; PRL 118, 152503 (2017)



- NCSM convergence is drastically improved
- N_{max}=0 eigenvalues deviated from $E(s)$
- induced many-body contributions might affect large-s results

chiral NN+3N
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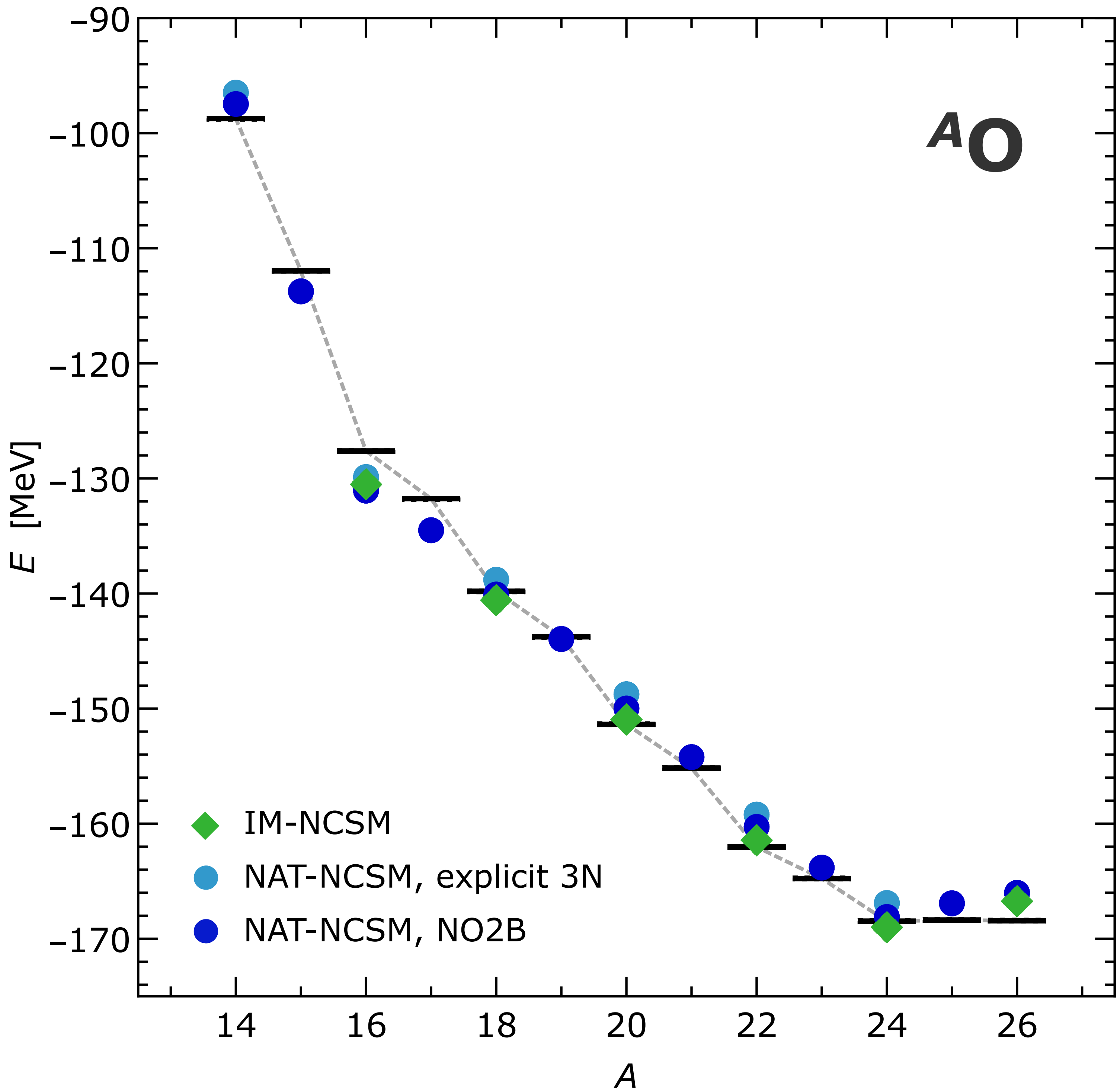
$\hbar\Omega$=20 MeV
e_{max}=12

HF basis
N_{max}=0 reference state
N_{max}=0,2,4,6,8

Oxygen Isotopes

Gebrerufael, Vobig, Hergert, Roth; PRL 118, 152503 (2017)



- excellent agreement with direct NCSM
- IM-SRG evolution limited to J=0 reference states and thus even-mass isotopes
- odd-mass nuclei via simple particle attachment or removal in final NCSM run

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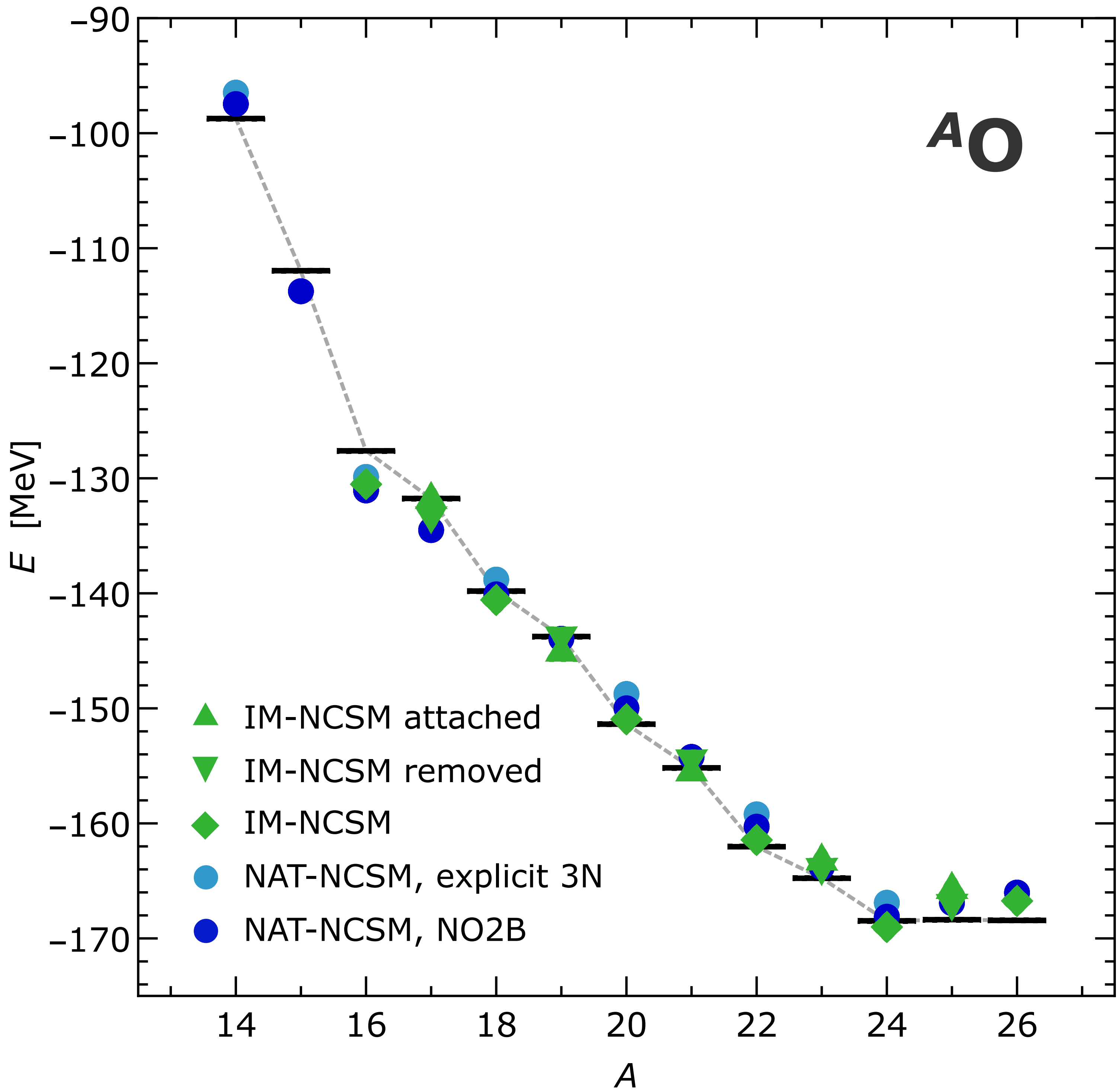
HF basis
N_{max}=0 reference

Oxygen Isotopes

Vobig, Gebrerufael, Roth; in prep.



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HF basis
N_{max}=0 reference

Epilogue

- **thanks to my group and my collaborators**
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  - H. Hergert
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