Perspectives in Low-Energy Nuclear Physics

Robert Roth

TECHNISCHE UNIVERSITÄT DARMSTADT

A Kind Request...

Dear Robert,

David and I would like to ask you if you are willing to give a colloquium at TRIUMF on February 19th 2016.

This is the week before the Nuclear Theory workshop, during which we will have another colloquium by Thomas Papenbrock on "Recent Advances in Nuclear Theory".

In the light of this, we thought that having a preparatory talk where the big questions in nuclear physics are introduced in a very simple manner would be useful…

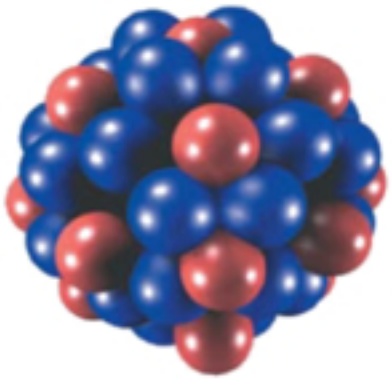
We feel this will help to communicate the importance of nuclear physics and nuclear theory to the general laboratory…

Please let us know if you are interested in this.

Thanks a lot,
Sonia

The Big Picture

Low-Energy Nuclear Physics



...a multi-faceted lab connecting fundamental physics with daily life

Diversity

- structure emerging from microscopic dynamics
- thousands of isotopes, many very special
- zoo of phenomena: shell structure, clustering, deformation, stability, excitations, resonances, transitions, decays, reactions,...

Complexity

- multi-physics: strong, weak and el.mag. interactions
- multi-scale: from keV to GeV
- multi-process: structure, decays and reactions
- multi-observable: energies, el.mag.,...

Impact

- key input for under-standing the evolution of the universe
- tiny things have huge implications: deuteron, Hoyle state,...
- foundation for atomic and molecular physics, chemistry, solid state,...
- direct applications

Low-Energy Nuclear Theory

the most challenging quantum many-body problem...

systems of 2 - 300 nucleons

nucleons are composite themselves

dominated by correlations

self-bound system

translational & rotational symmetry

competition of large energy contributions

interaction inherits complexity of QCD

residual van der Waals interaction

significant three-body forces

bound and continuum states

range of different observables

weak binding and threshold physics

...try a non-relativistic quantum description with nucleons as relevant degrees of freedom

The Problem

$$H\ |\Psi\rangle = E\ |\Psi\rangle$$

We do not know the interaction…

…we need additional models to construct a nuclear interaction to start with

We do not know how to solve the equation…

…we need truncations or approximations to make the problem tractable

Strategy I: Phenomenology

$$H \, |\Psi\rangle = E \, |\Psi\rangle$$

- pick a **simple approximation scheme** for the Schrödinger equation tailored for the observables of interest
- construct a computationally convenient **model for the nuclear interaction** compatible with this approximation
- **fit the parameters** of the interaction model **to observables** within the chosen approximation scheme

Skyrme-Hartree-Fock

approximate many-body state by single Slater determinant and parameterize interaction with contact terms

Valence-Space Shell Model

freeze core nucleons and treat a few valence nucleons in small valence space with fitted interaction matrix elements

Strategy II: Ab Initio

$$H\ |\Psi\rangle = E\ |\Psi\rangle$$

- construct **realistic nuclear interactions** based on as much QCD input as possible and fit to few-nucleon properties in exact calculations
- **solve the Schrödinger equation** using systematic truncations with **controlled uncertainties**

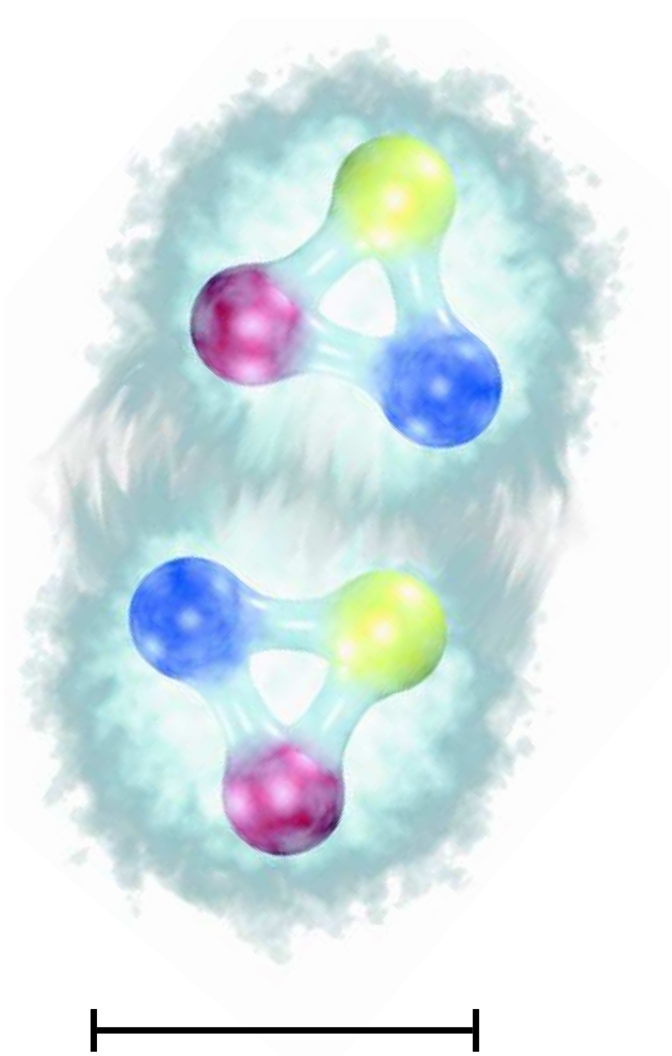
interactions are independent of many-body framework

different many-body methods can employ the same interaction

different interactions can be tested in one many-body approach

Interactions

Nature of the Nuclear Interaction



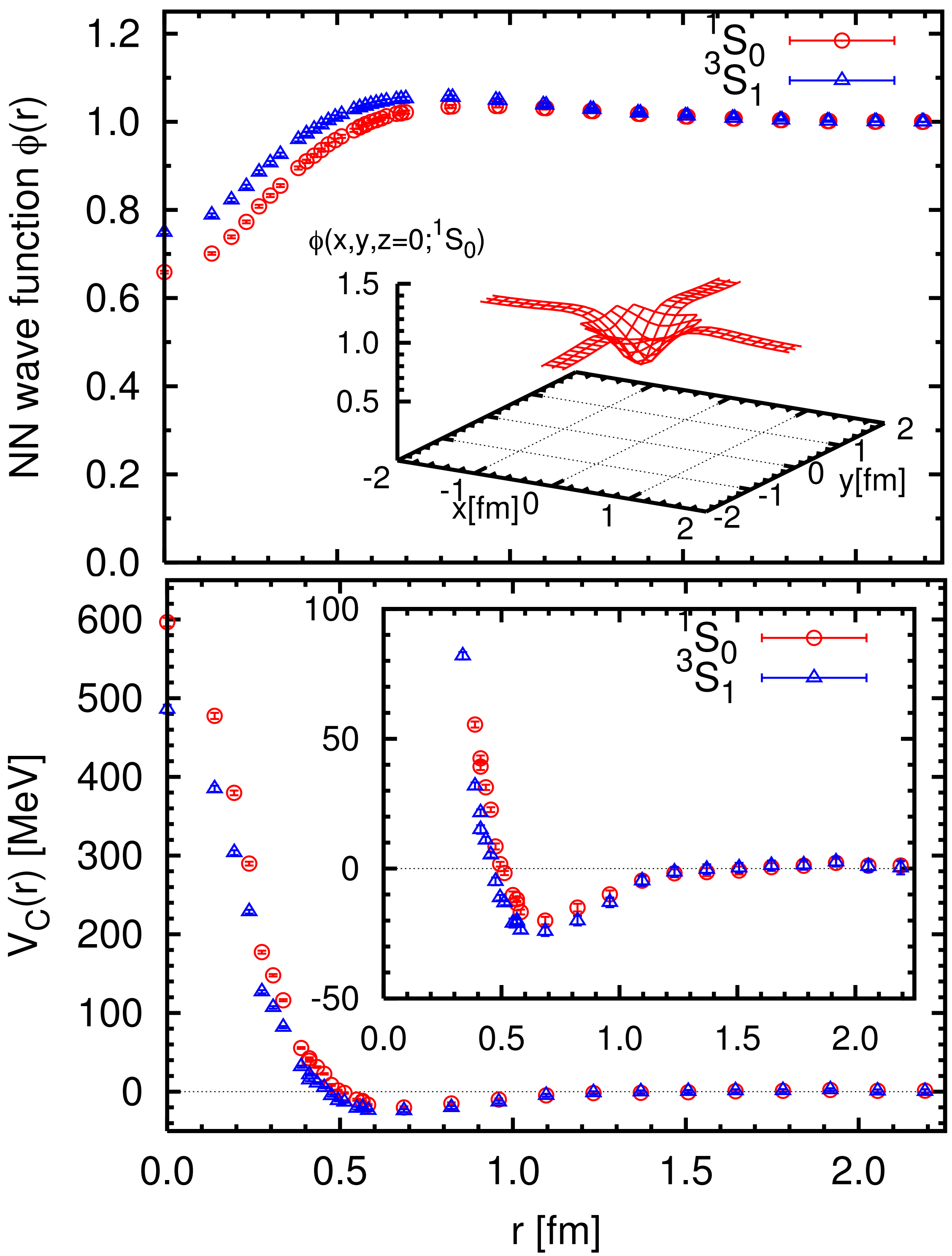
$\sim 1.6\text{fm}$

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

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

Tomorrow... from Lattice QCD

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

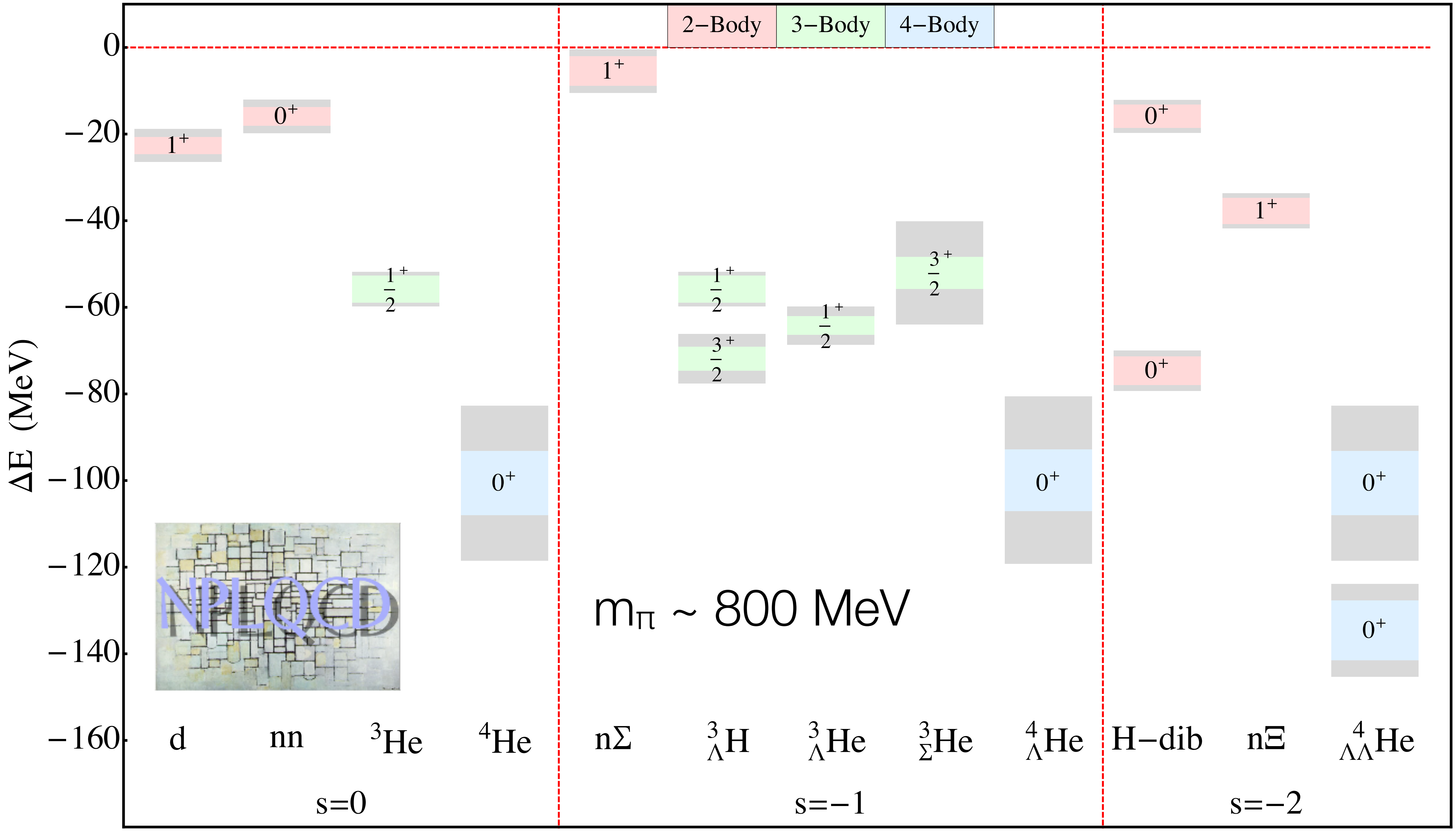


N. Ishii et al., PRL 99, 022001 (2007)

- 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

Tomorrow... from Lattice QCD

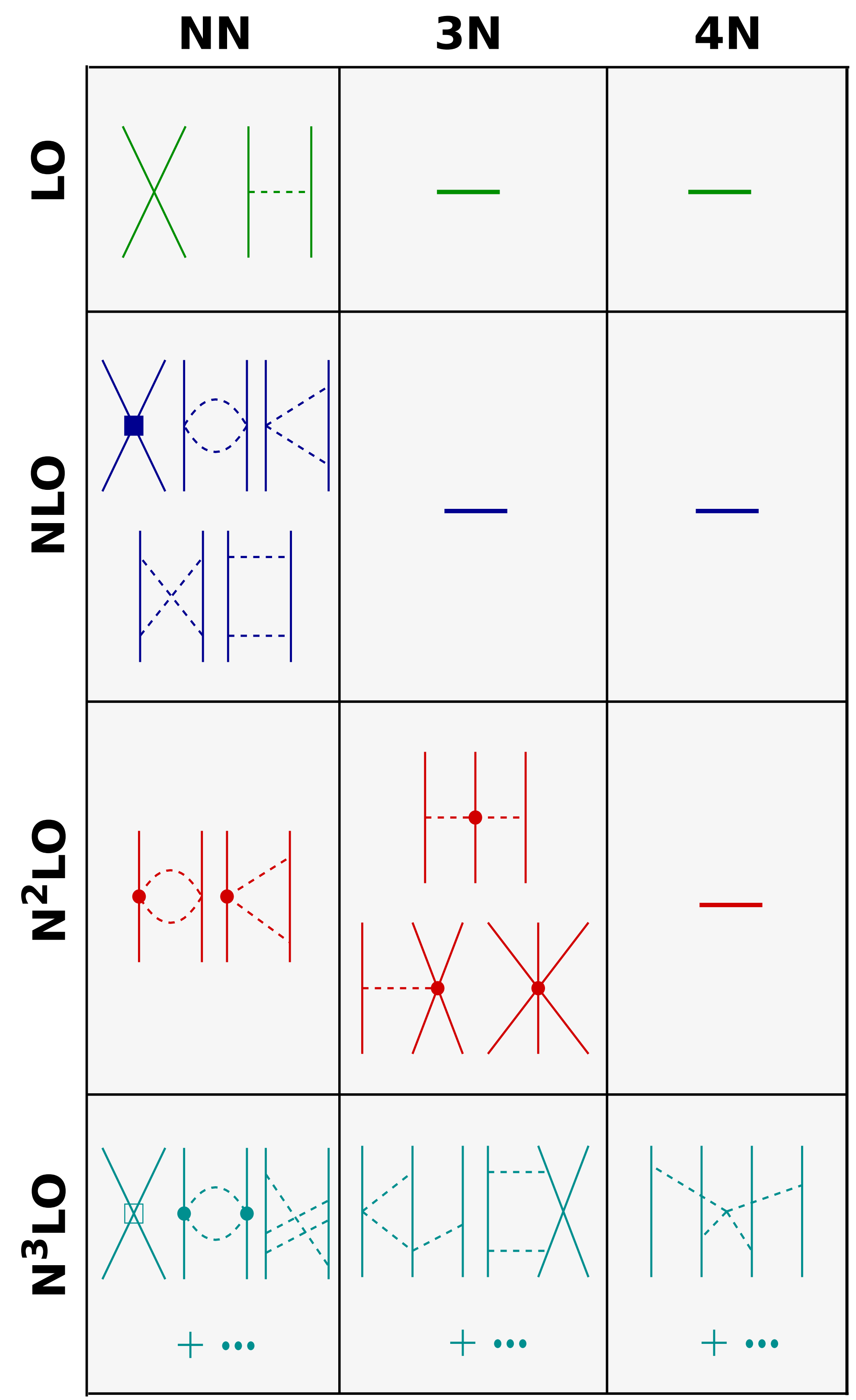
Beane et al., PRD87, 034506 (2013), PRC88, 024003 (2013)



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, cut… MeV

also first generation, but scarcely used

- **N2LO-opt, N…**
  - NN: … MeV
  - 3N: N… cutoff 500 MeV

improved fitting, also many-body inputs

- **local N2…**
  - 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

order-by-order uncertainty estimates

all these interactions are equally valid, use them all to study uncertainties

Many-Body Solution

- Eigenvalue Problem -

Eigenvalue Problem

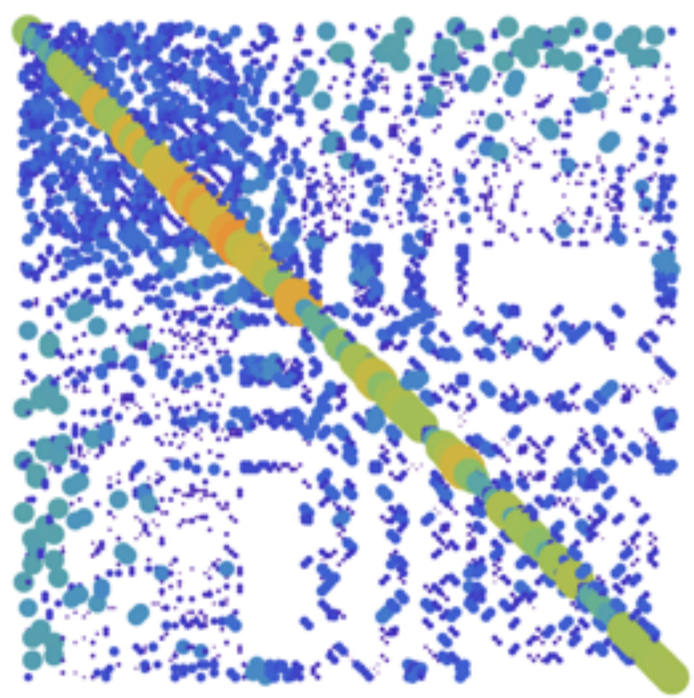
- start from **many-body Schrödinger equation**

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

- define an **many-body basis** and expand eigenstates in this basis

$$|\Psi_n\rangle = \sum_i C_i^{(n)}\,|\Phi_i\rangle$$

- convert Schrödinger equation into a **matrix eigenvalue problem**



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

up to 10^{10} x 10^{10}

numerically solve large-scale matrix eigenvalue problem for few low-lying eigenvalues

Configuration Interaction

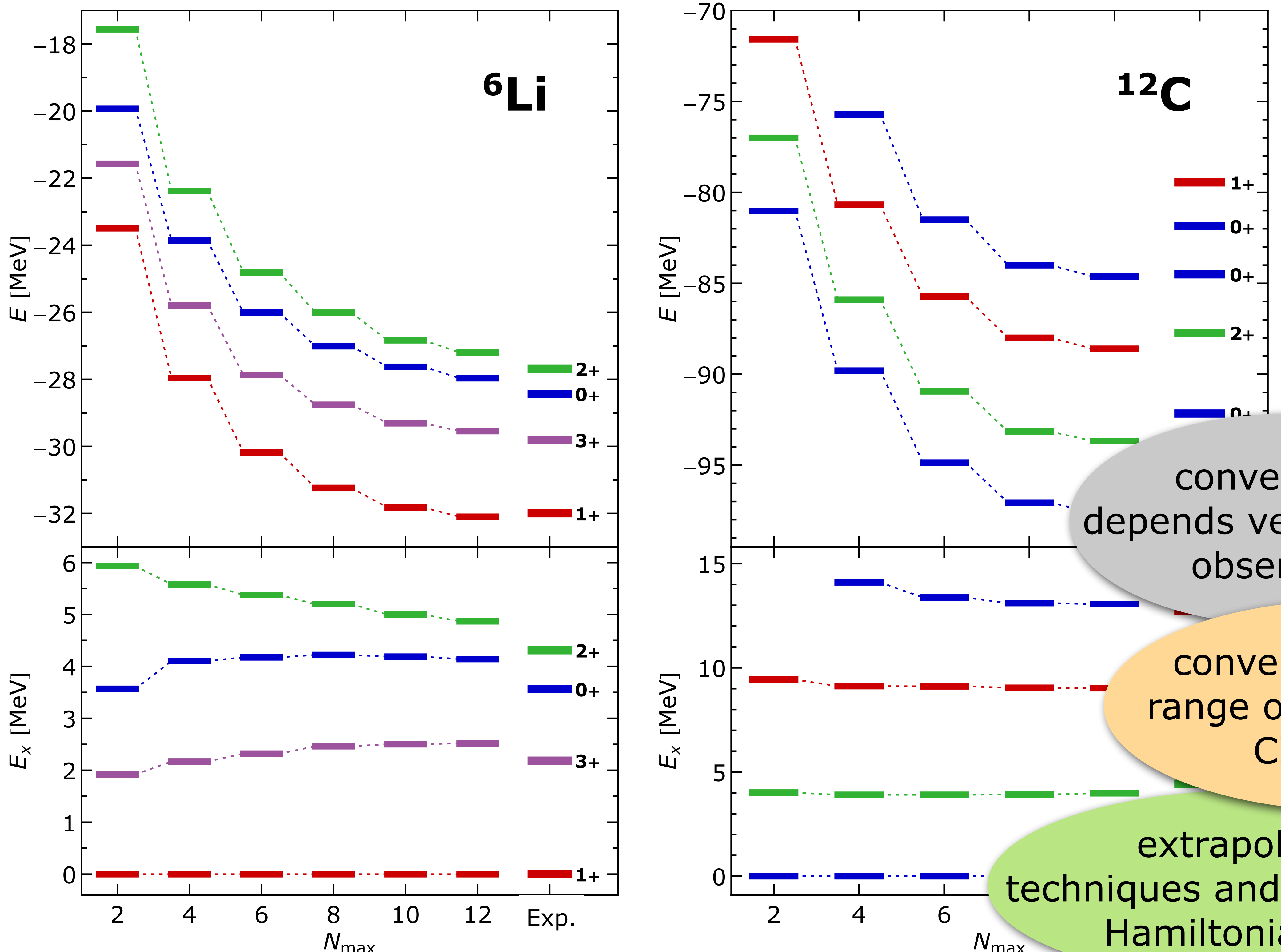
- have to **introduce truncations** of the basis to make the Hamilton matrix finite and numerically tractable
  - **single-particle truncation (full CI)**:
    truncate the underlying single-particle basis, e.g., at a maximum single-particle energy e_{max}, and construct all possible Slater determinants
  - **many-body truncation (NCSM)**:
    truncate the many-body Slater-determinant basis at a maximum number of harmonic-oscillator excitation quanta N_{max}

one has to **demonstrate convergence** with respect to the model-space truncation for accurate results

model space dimension **grows dramatically** with truncation parameter e_{max} or N_{max} and particle number

incomplete convergence as **only source of uncertainties** in the many-body treatment

Convergence



IT-NCSM

chiral NN+3N
EM, 500 MeV

$\alpha = 0.08\ \text{fm}^4$
$\hbar\Omega = 20$ MeV

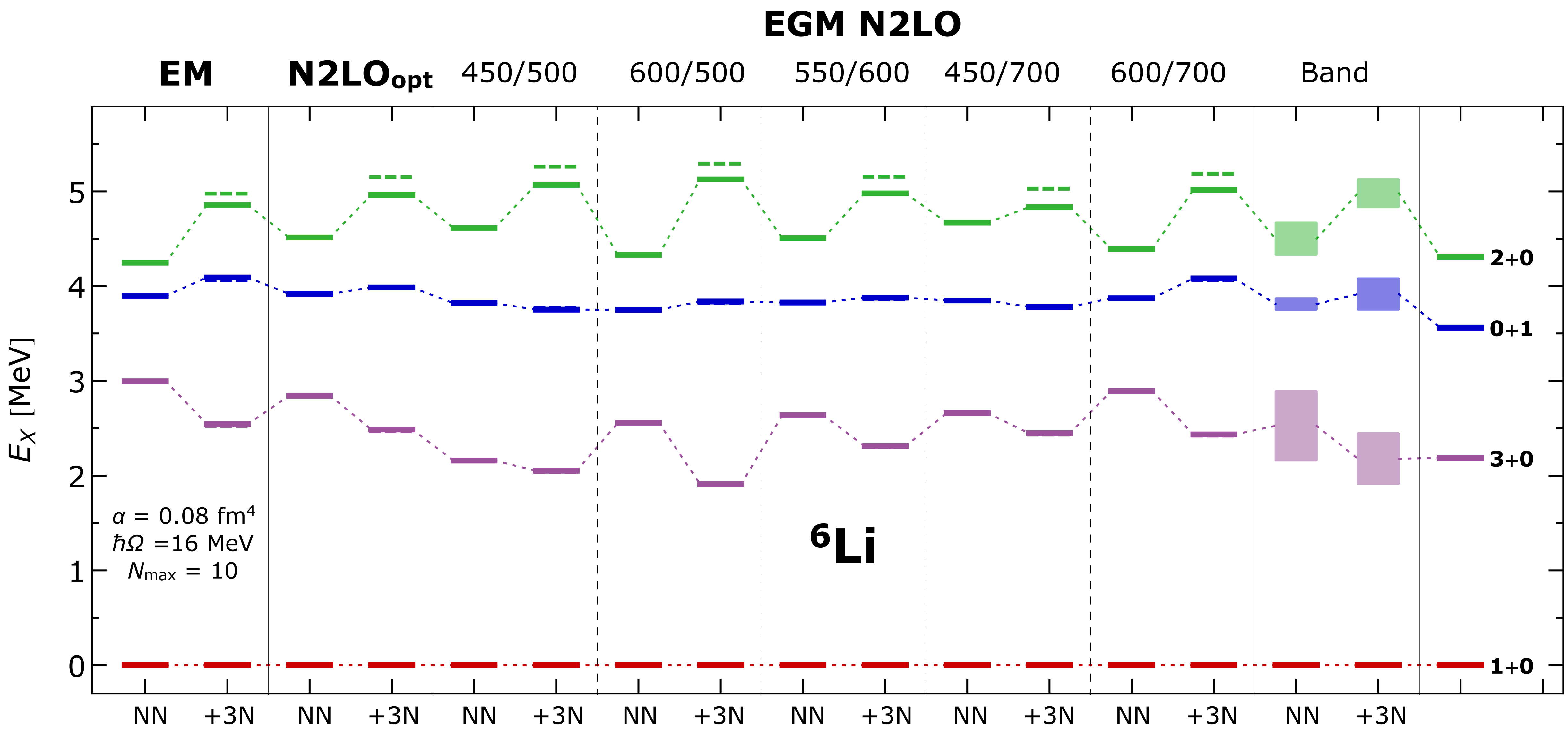
convergence depends very much on observable

convergence defines range of applicability of CI methods

extrapolation techniques and softening of Hamiltonian help

p-Shell Spectroscopy: Sensitivity

Calci, Roth; arXiv:1601.07209



- of course, spectra depend on choice of initial chiral NN+3N interaction, but the dependence is not dramatic
- important contribution to the total theory uncertainty

p-Shell Spectroscopy: Sensitivity

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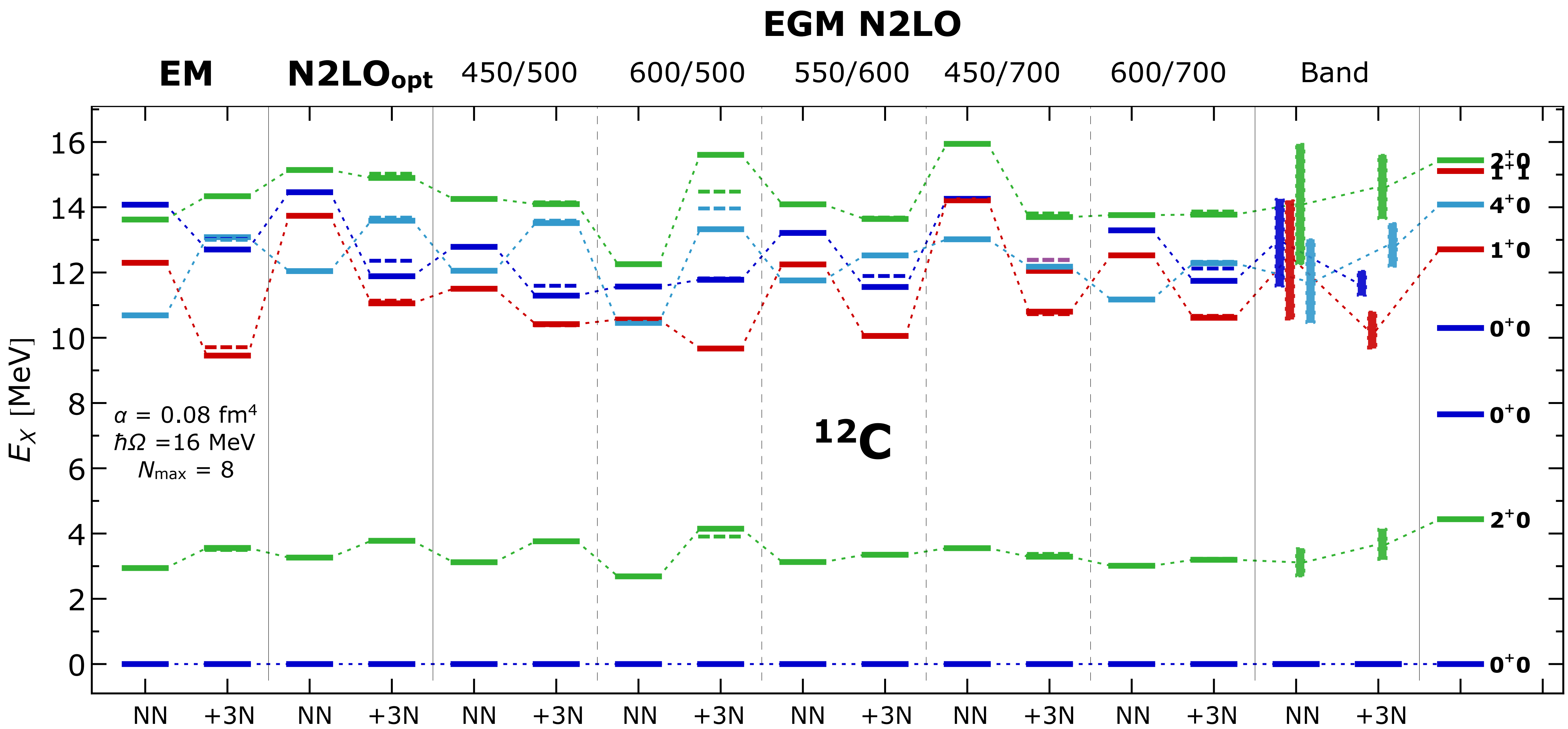
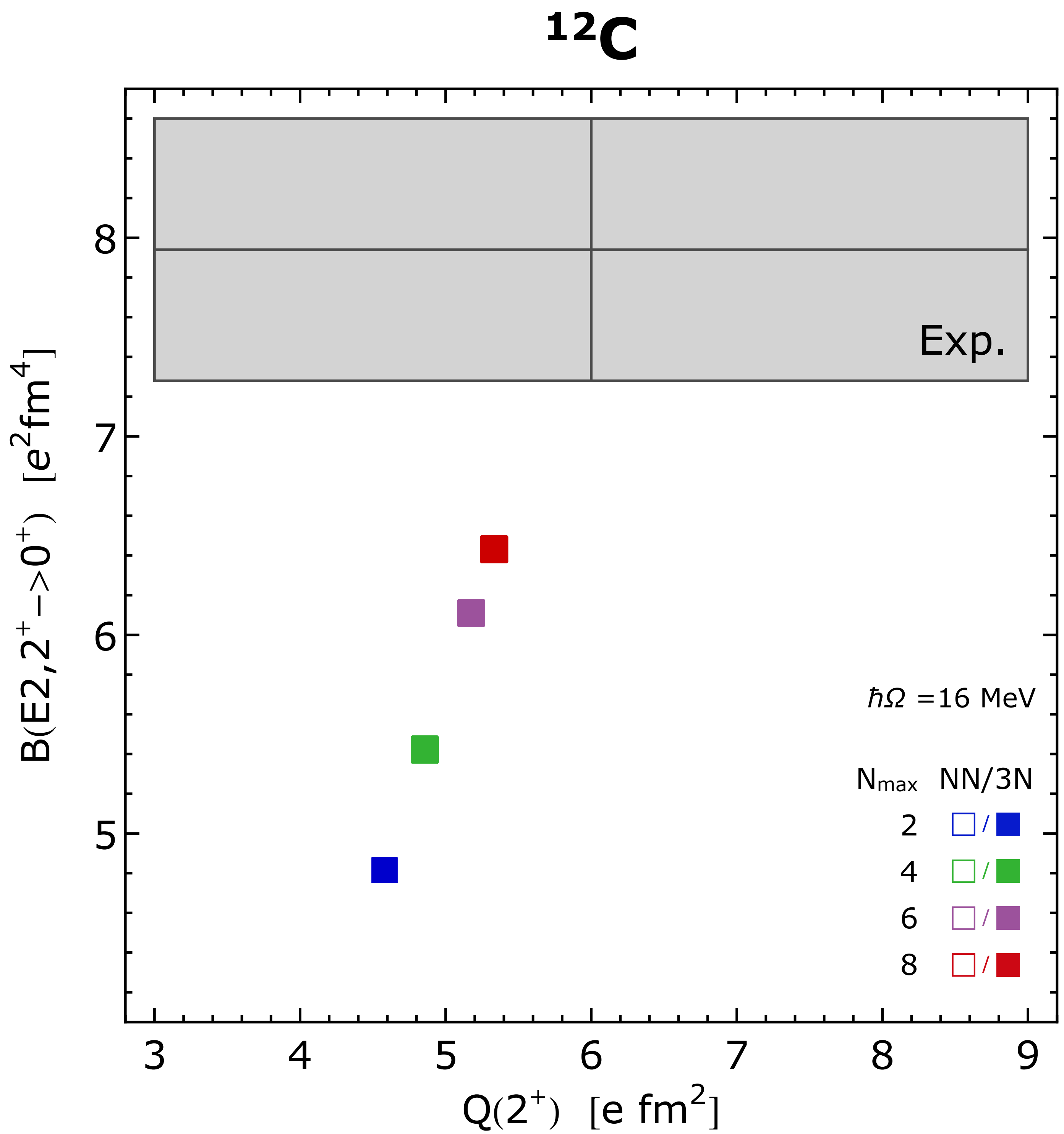


- individual states show systematic disagreement with experiment:
  - second 0^+: Hoyle state, cluster structure not captured in HO basis
  - first 1^+: systematic problem with N2LO-3N interaction ?

p-Shell Spectroscopy: Correlations

Calci, Roth; arXiv:1601.07209



- **electric quadrupole (E2)** observables involving 0^+ ground state & first excited 2^+
- model-space convergence is terrible, E2 operator sensitive to long-range wave functions

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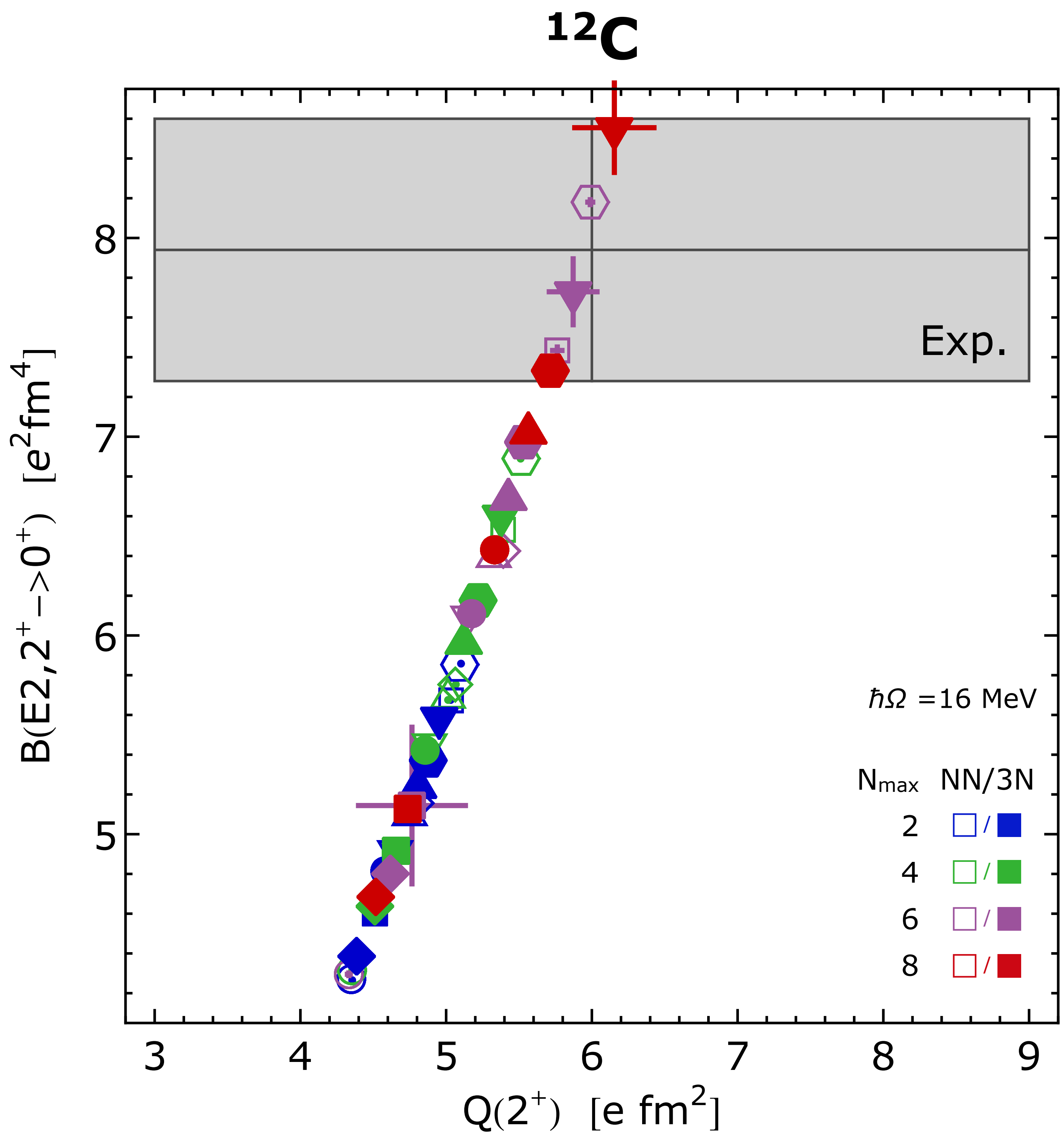

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- **extremely robust correlation** predicted by NCSM for all interactions and model spaces

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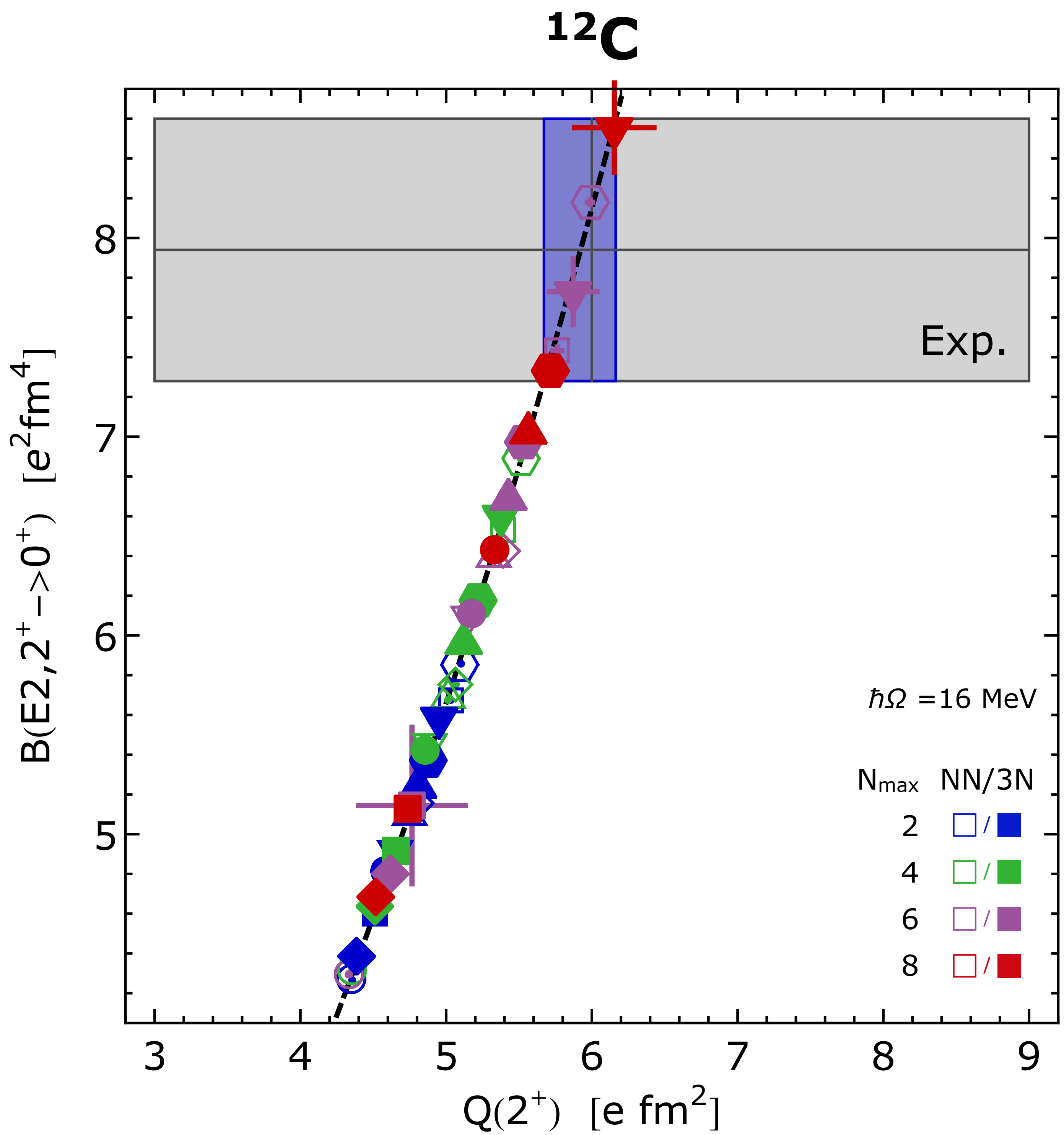
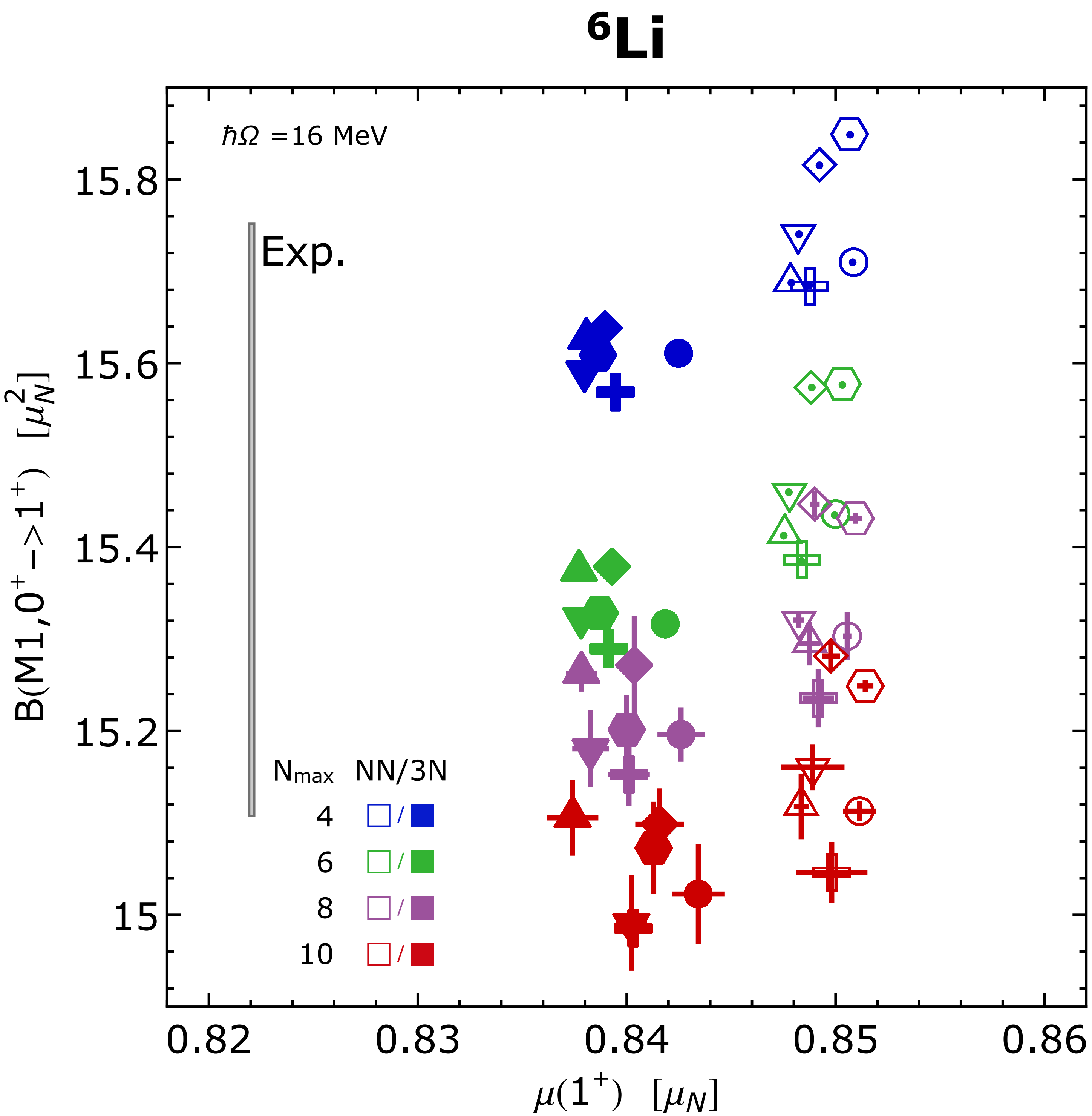


- **electric quadrupole (E2)** observables involving 0^+ ground state & first excited 2^+
- model-space convergence is terrible, E2 operator sensitive to long-range wave functions
- **extremely robust correlation** predicted by NCSM for all interactions and model spaces
- predict Q(2^+) with very high accuracy based on ... al datum for ...

new way to exploit ab initio calculations and to bridge to effective models

p-Shell Spectroscopy: Precision

Calci, Roth; arXiv:1601.07209



- **magnetic dipole (M1)** observables involving 1^+ ground state & 0^+ excited state
- dipole moment and B(M1) are **very robust** (few % changes)
- mild systematic model-space dependence of B(M1)
- dipole moment affected by 3N interaction and in slight disagreement with experiment

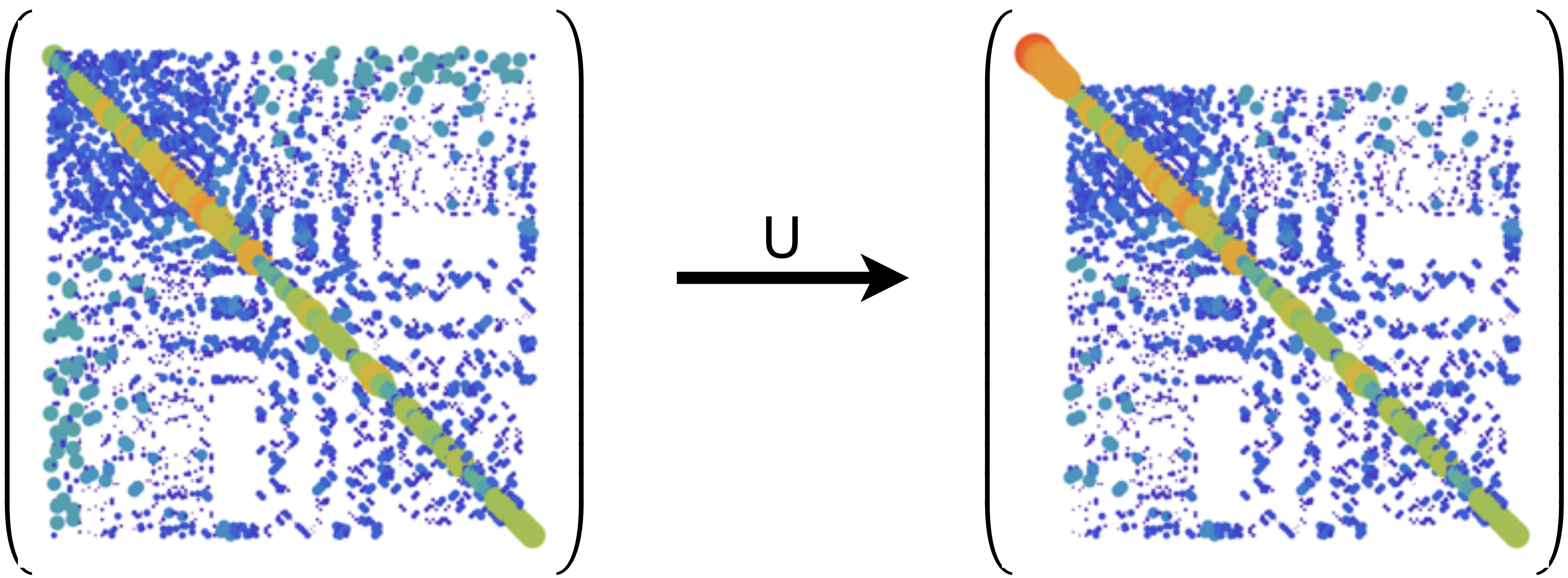
ready for precision studies, e.g., on electromagnetic two-body currents

Many-Body Solution

- Unitary Transformation -

Unitary Transformations

- 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 ($\alpha \to \infty$)

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 contin… …meter α

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

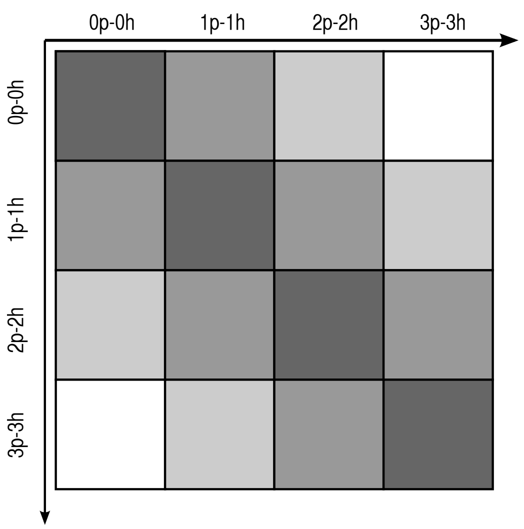
Free-Space SRG

well established for softening the Hamiltonian in two- and three-body space

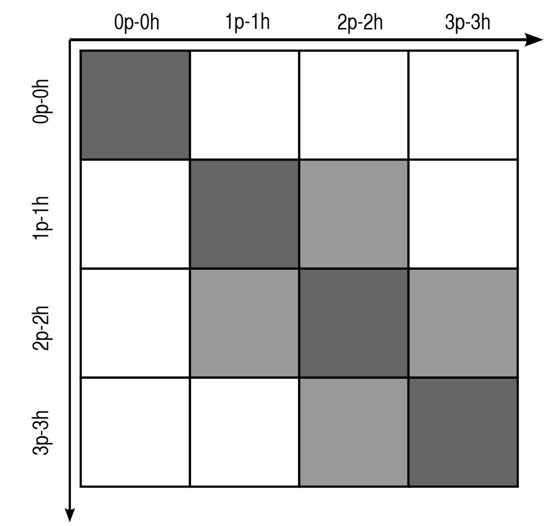
- the physics of the tra… …overned by the **dynamic generator η_α**
- design generator for desired **diagonalization or decoupling pattern**

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 and Wegner-type generator

$$\frac{d}{ds}H(s) = \left[\eta(s), H(s)\right] \qquad \eta(s) = \left[H(s), H^{\text{off-}}\right.$$

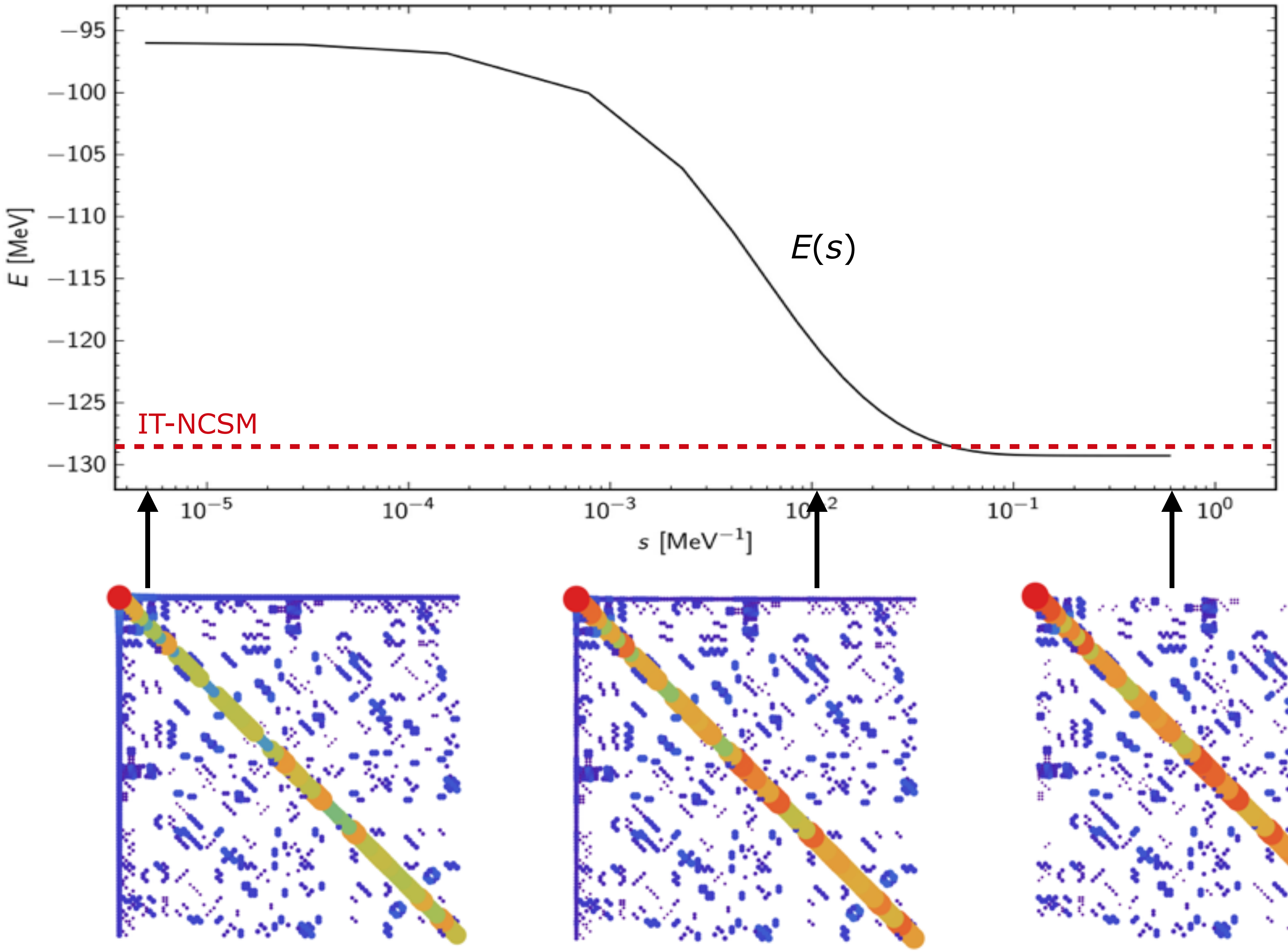
additional truncation that causes uncertainties

- write everything in normal ordered form with respect … ulti-determinantal reference state

discard normal-ordered three-body terms

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

Flowing Energy



^{16}O

chiral NN+3N

Λ_{3N}=400 MeV

α=0.08 fm^4

$\hbar\Omega$=20 MeV

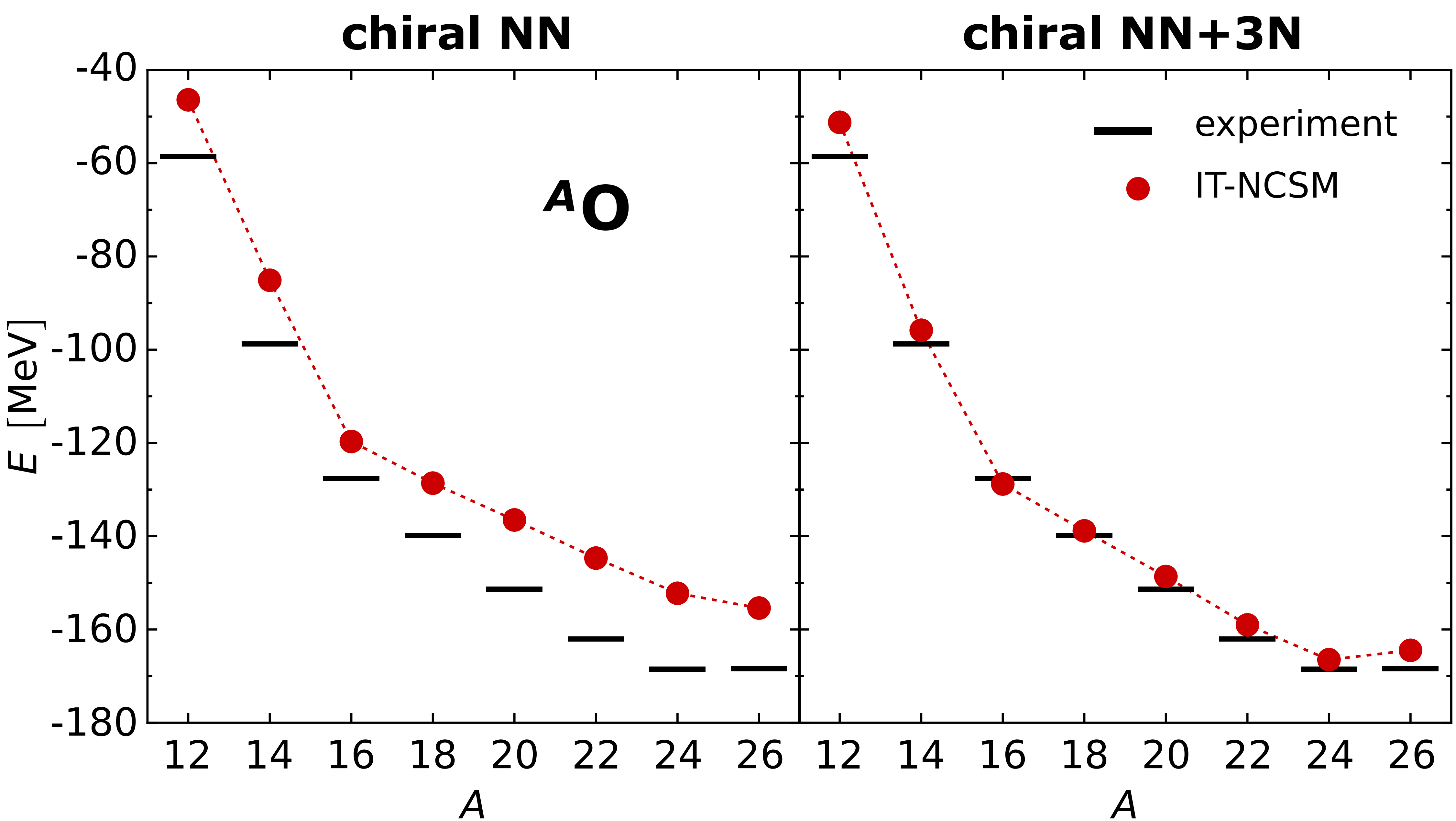
e_{max}=12

N_{max}=0
reference state

Hamilton
matrix in
N_{max}=2
space

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 $\hbar\Omega$

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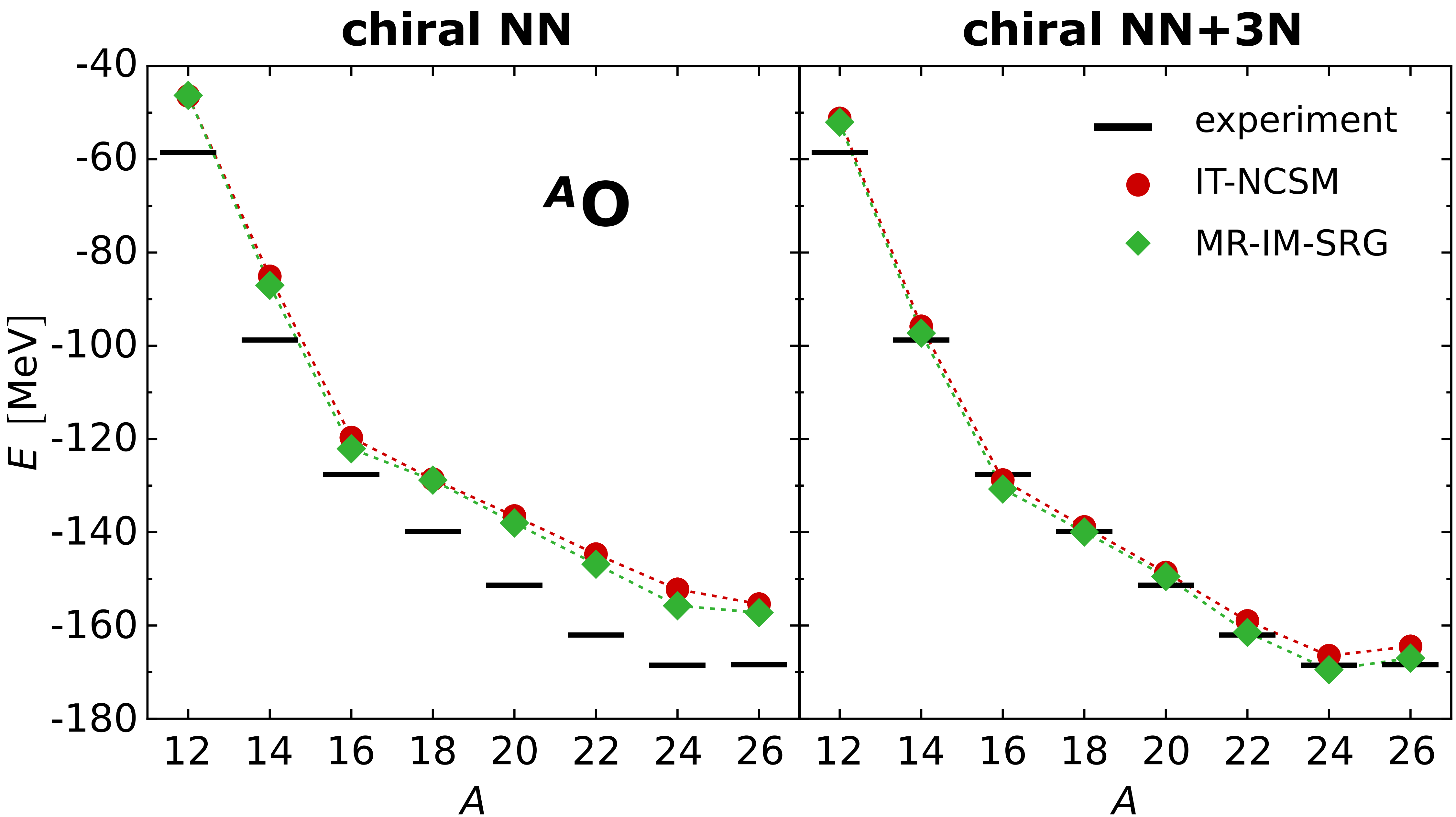

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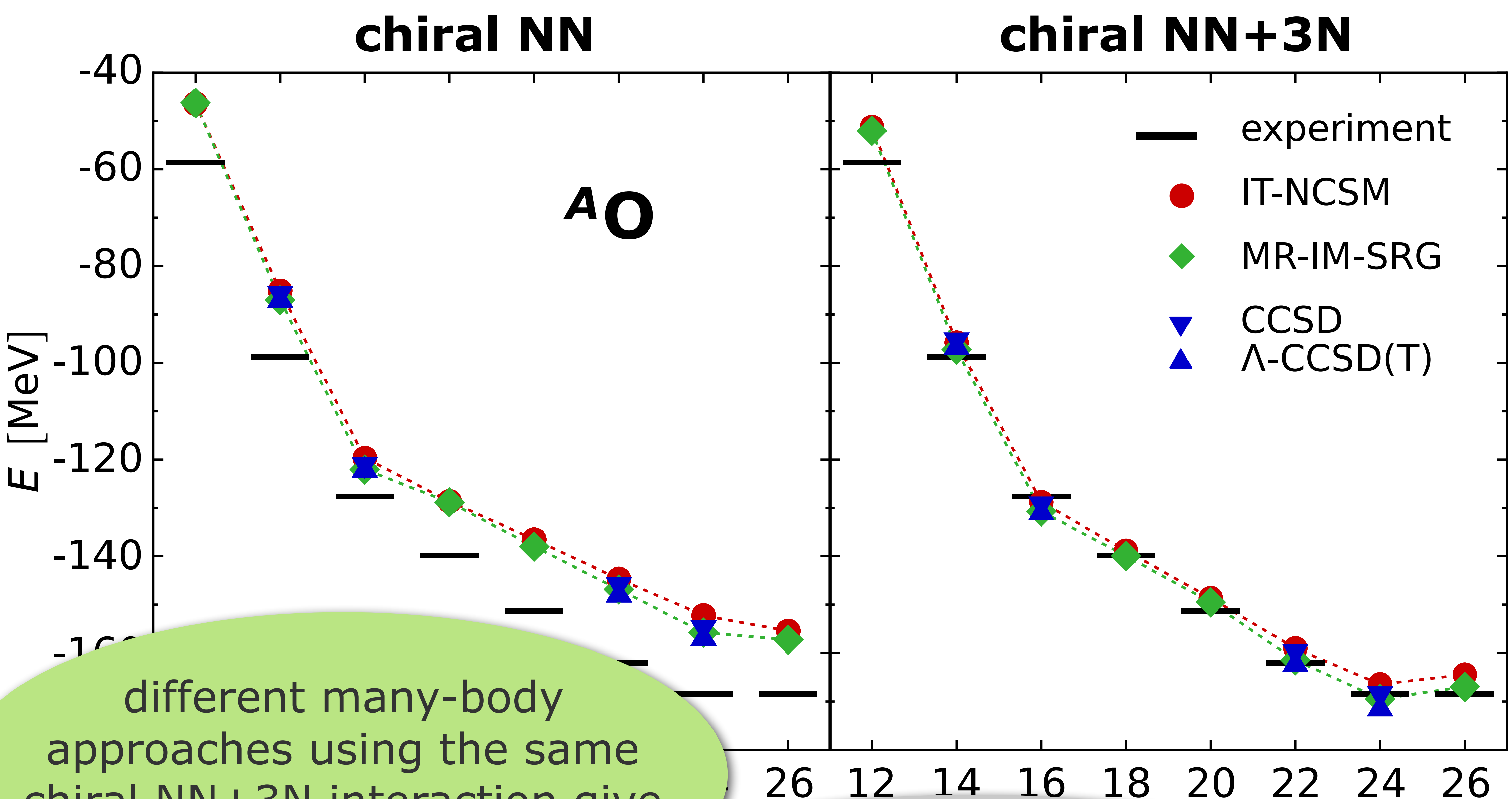


different many-body approaches using the same chiral NN+3N interaction give consistent results

minor differences are understood in terms of uncertainties due to truncations

Merging CI and IM-SRG

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

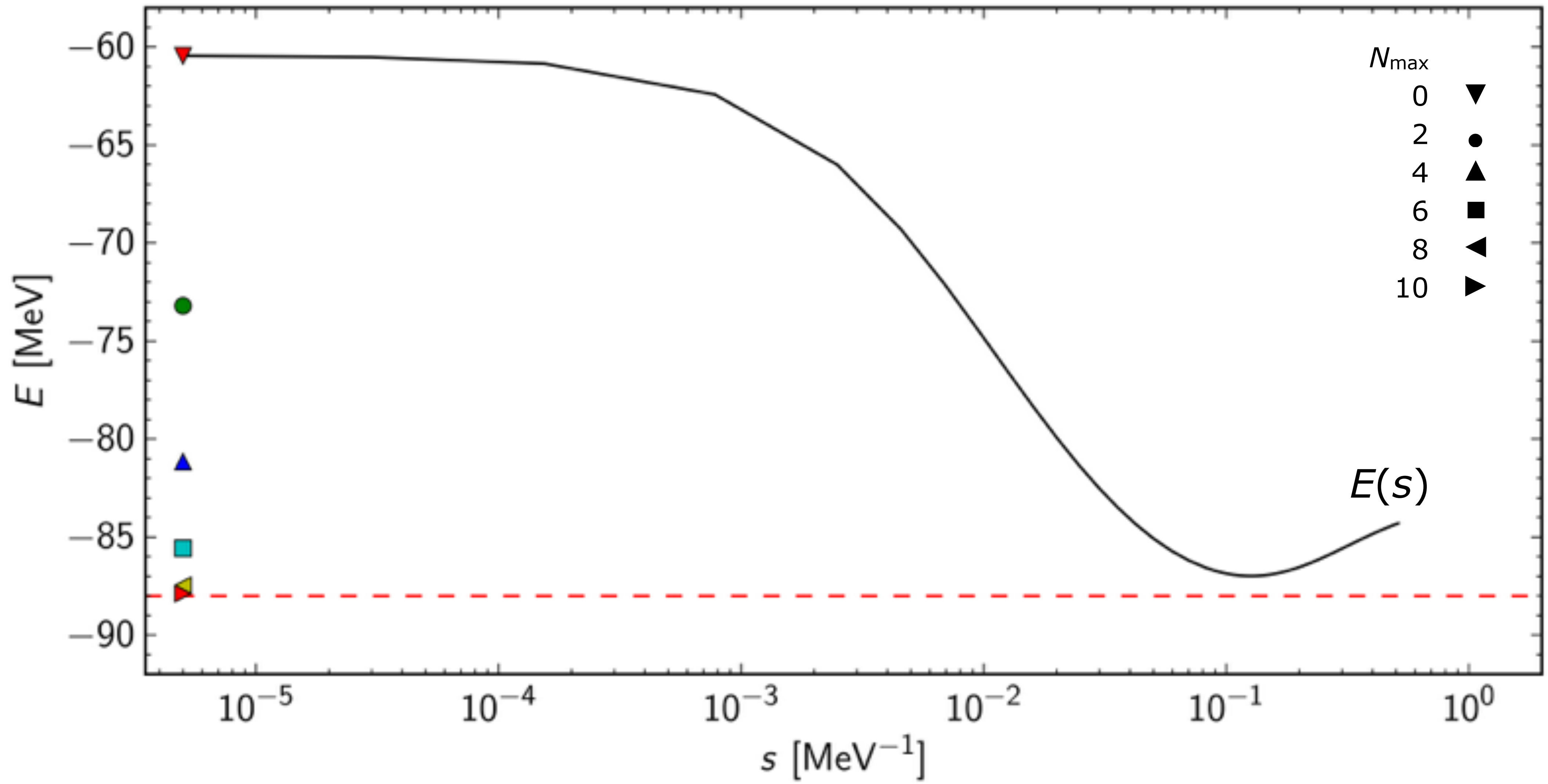
- solve NCSM problem in small N_{max}
- extract reference state

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

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

CI-IM-SRG: Ground State

Gebrerufael et al.; in prep.



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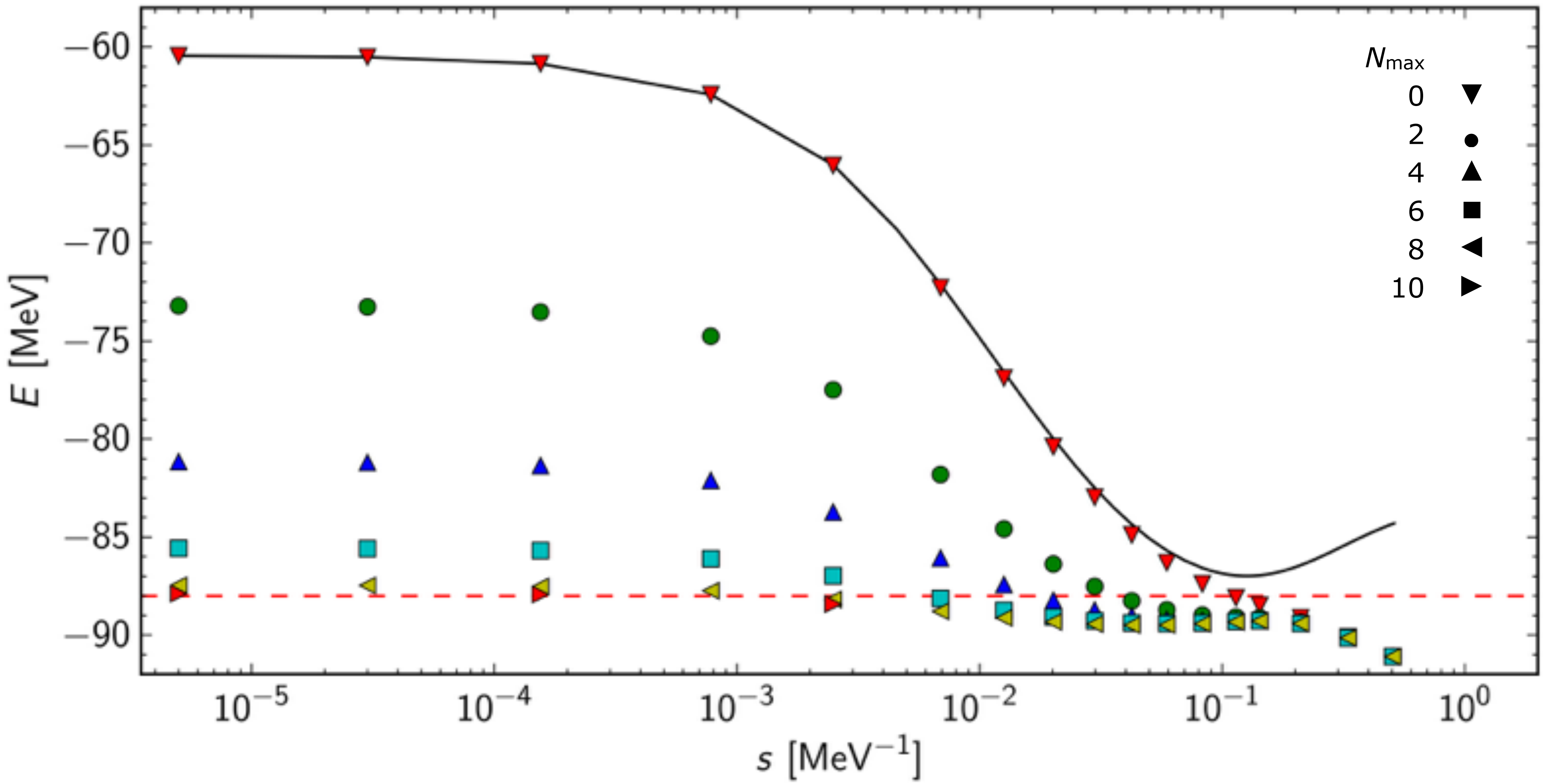

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- instead of using the zero-body piece of the normal-ordered Hamiltonian, we can use the complete **flowing Hamiltonian in a CI calculation**
- decoupling though the IM-SRG transformation causes **ridiculously fast convergence** of CI calculation

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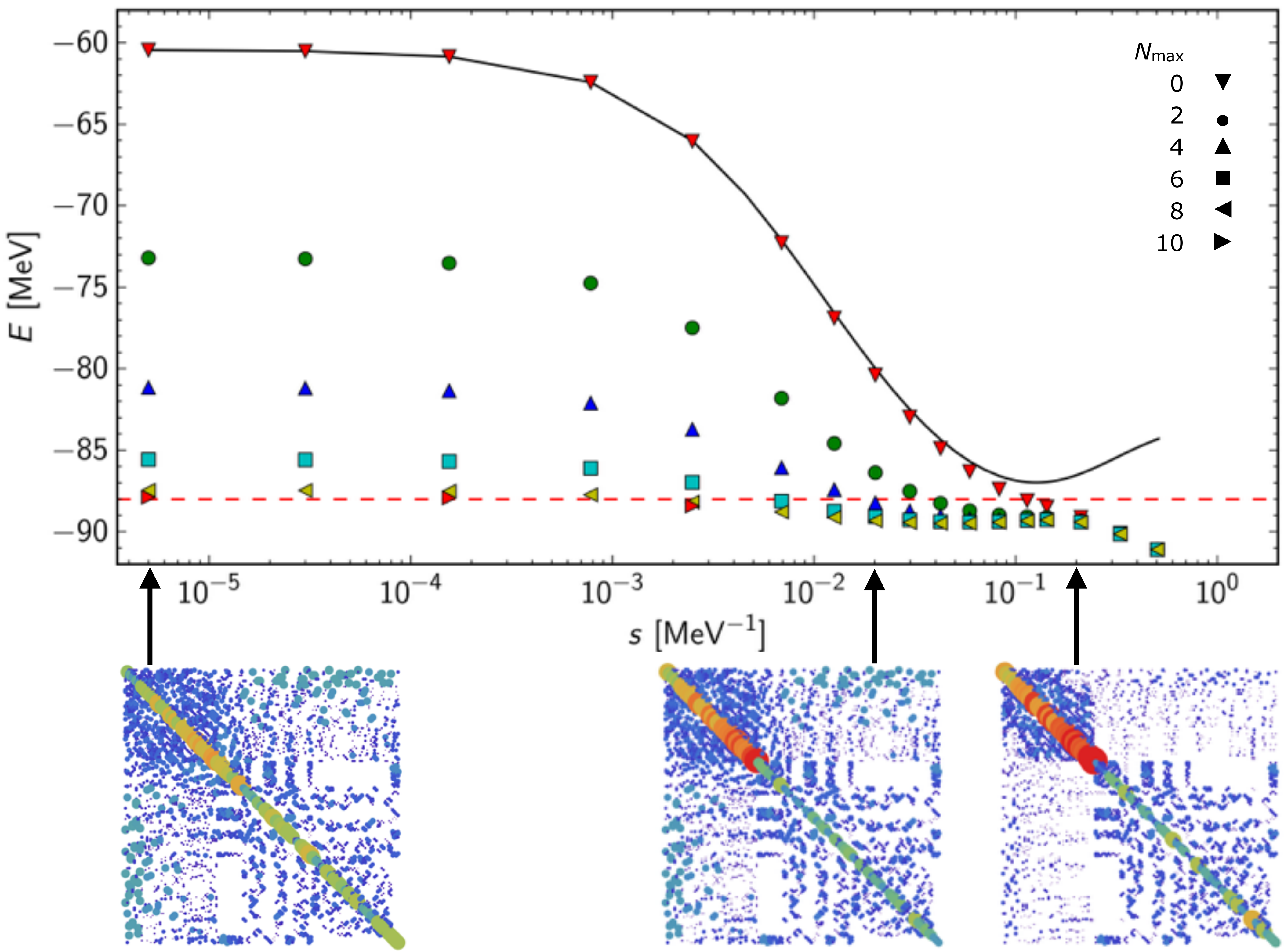

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Hamilton matrix in N_{max}=2 space

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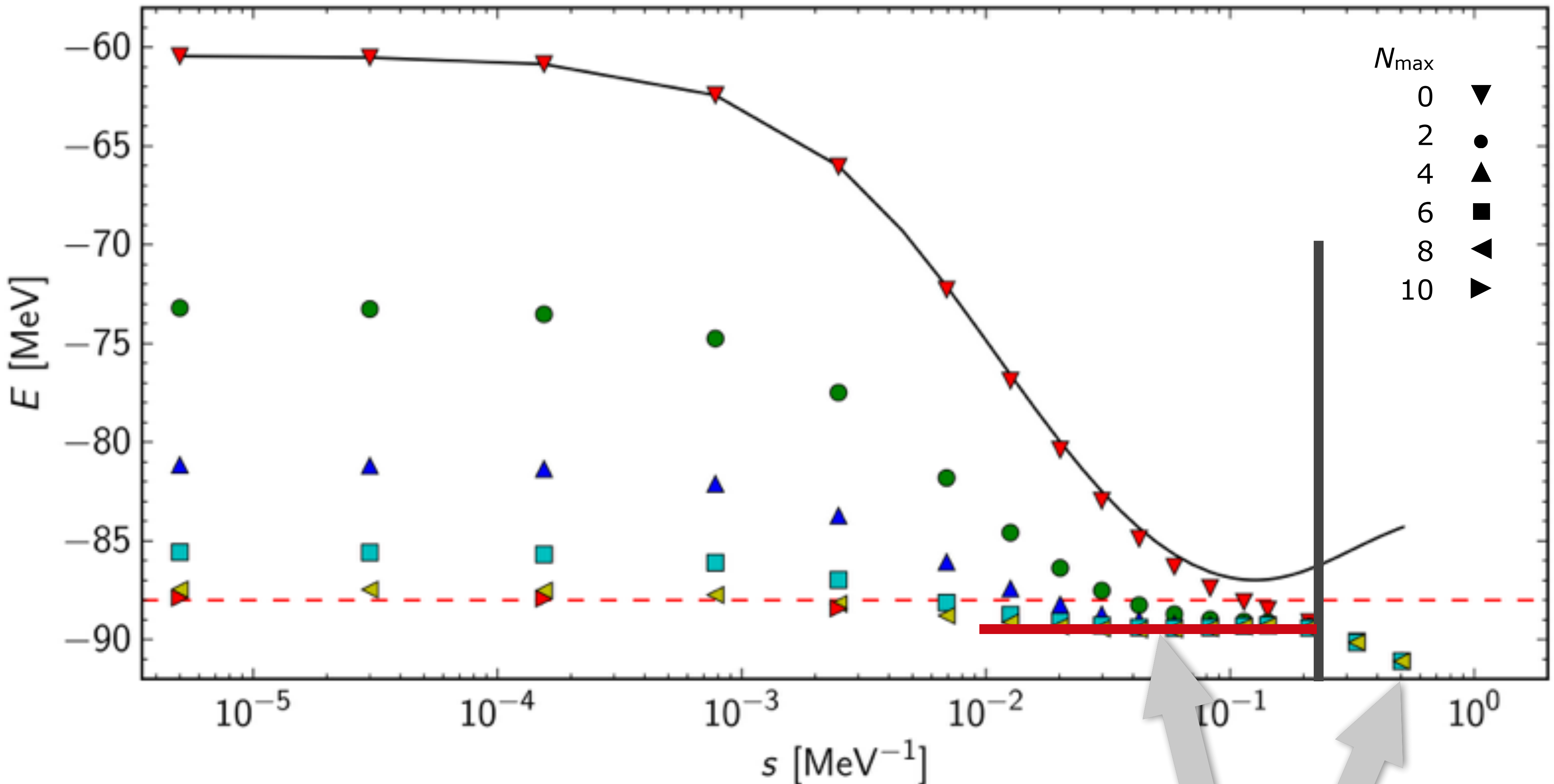

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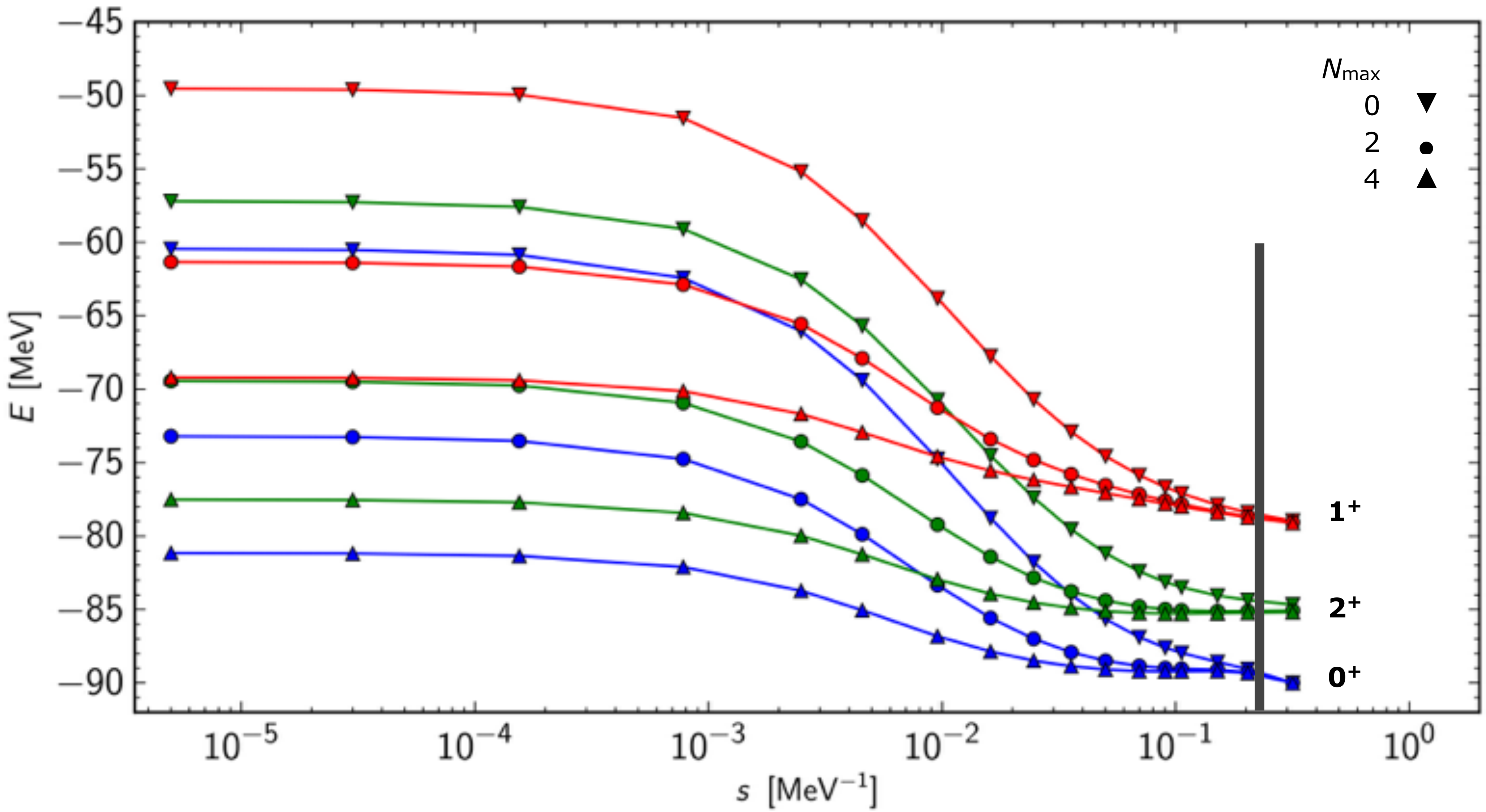
effects of IM-SRG truncation at the normal-ordered two-body level

CI-IM-SRG: Excited States

Gebrerufael et al.; in prep.



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

CI-IM-SRG: Excited States

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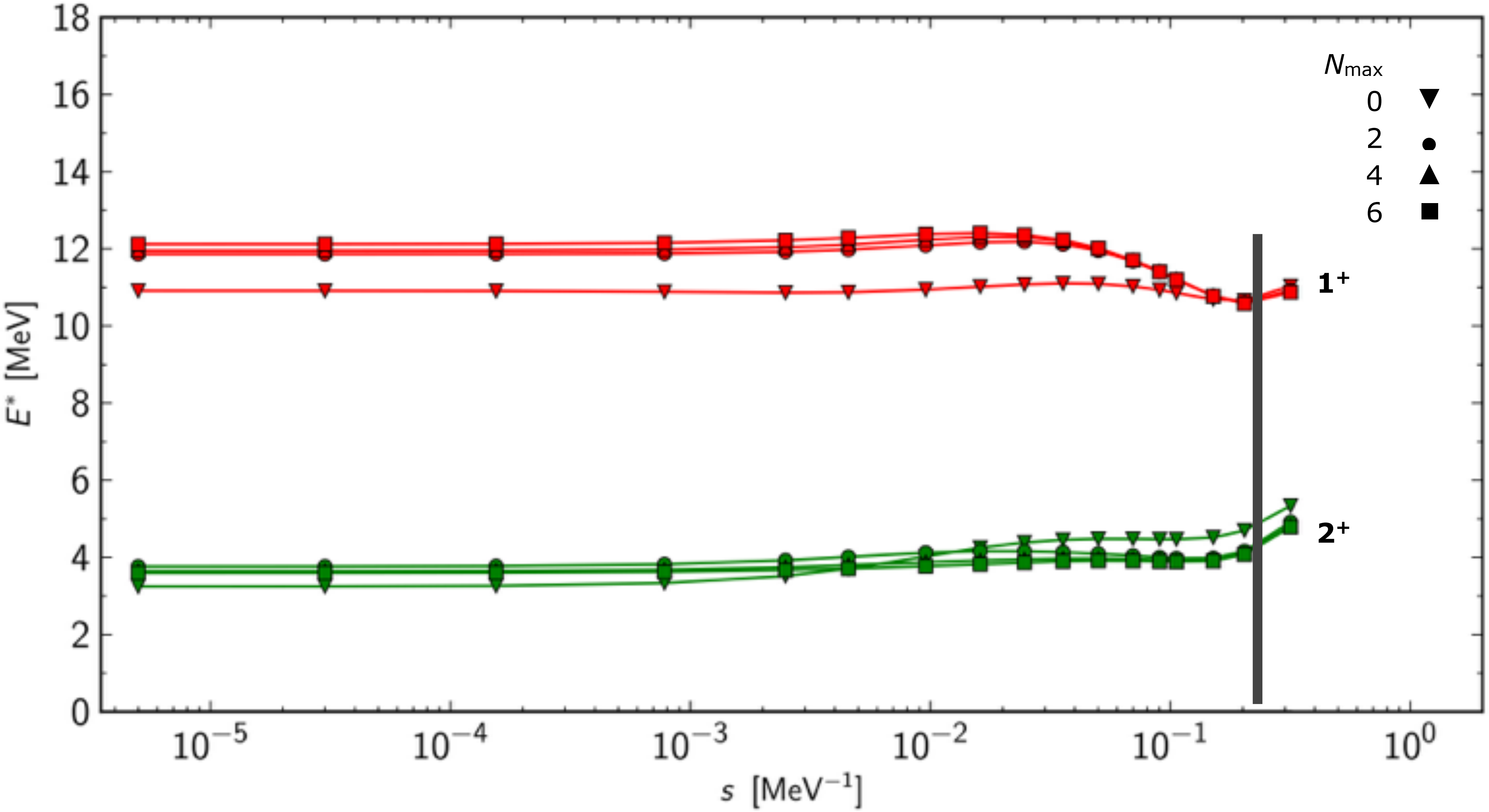

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- from the same CI calculation we get the **excited states**
- excitation energies only show subtle changes with IM-SRG flow…

CI-IM-SRG: Excited States

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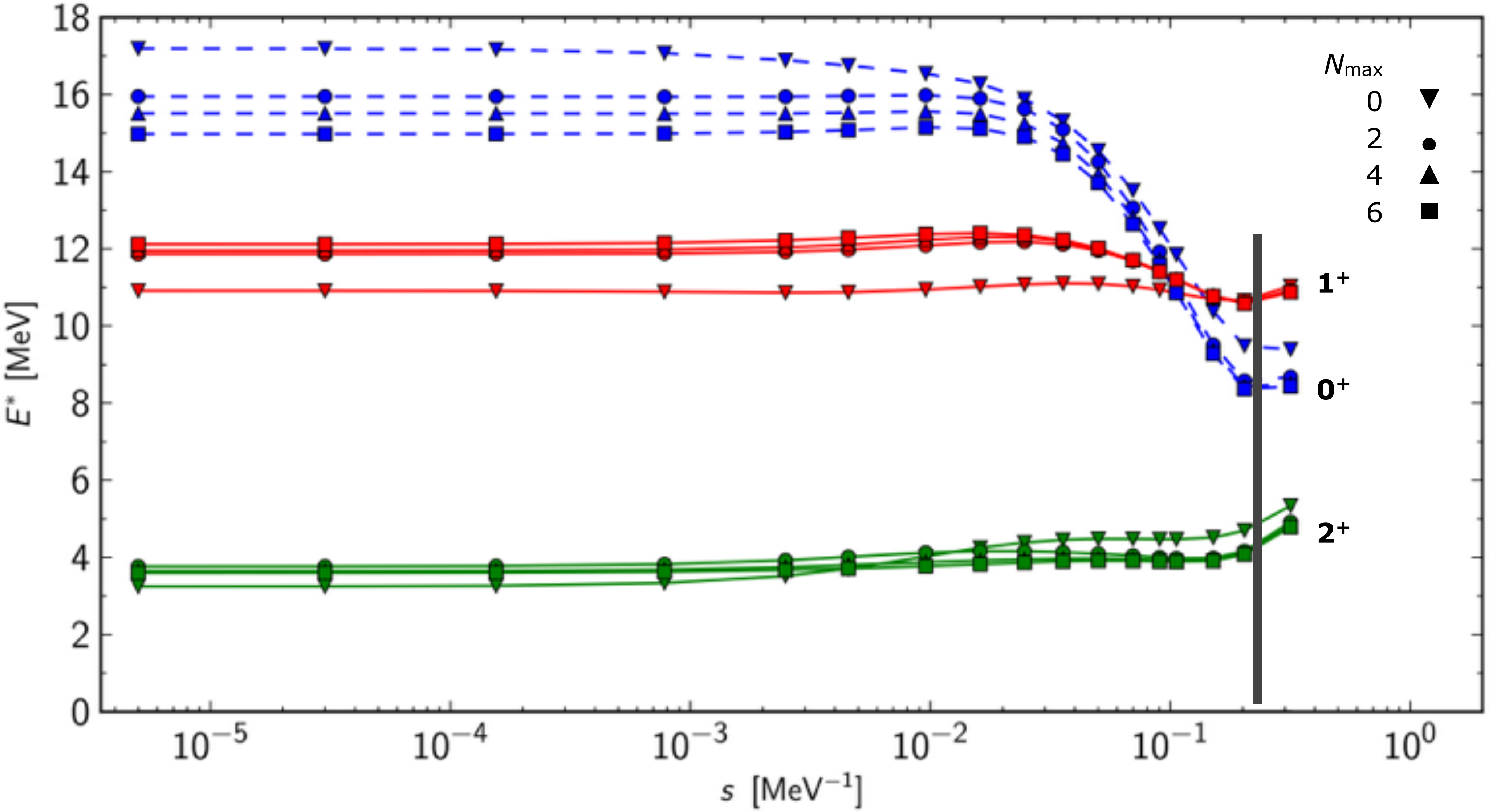

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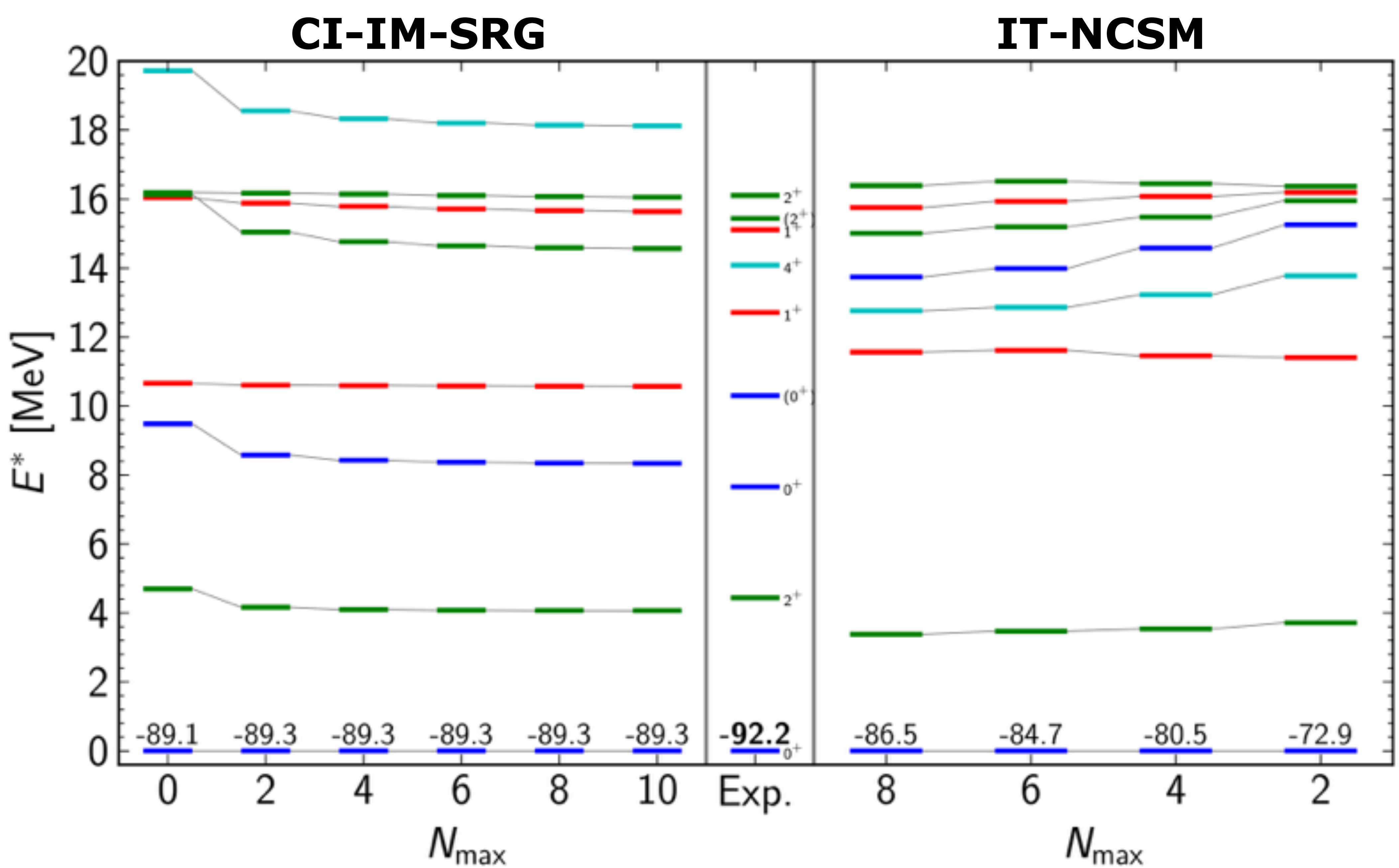
- from the same CI calculation we get the **excited states**
- excitation energies only show subtle changes with IM-SRG flow… …but there are notable exceptions… **Hoyle state?**

CI-IM-SRG: Spectrum

Gebrerufael et al.; in prep.



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chiral NN+3N

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reference state

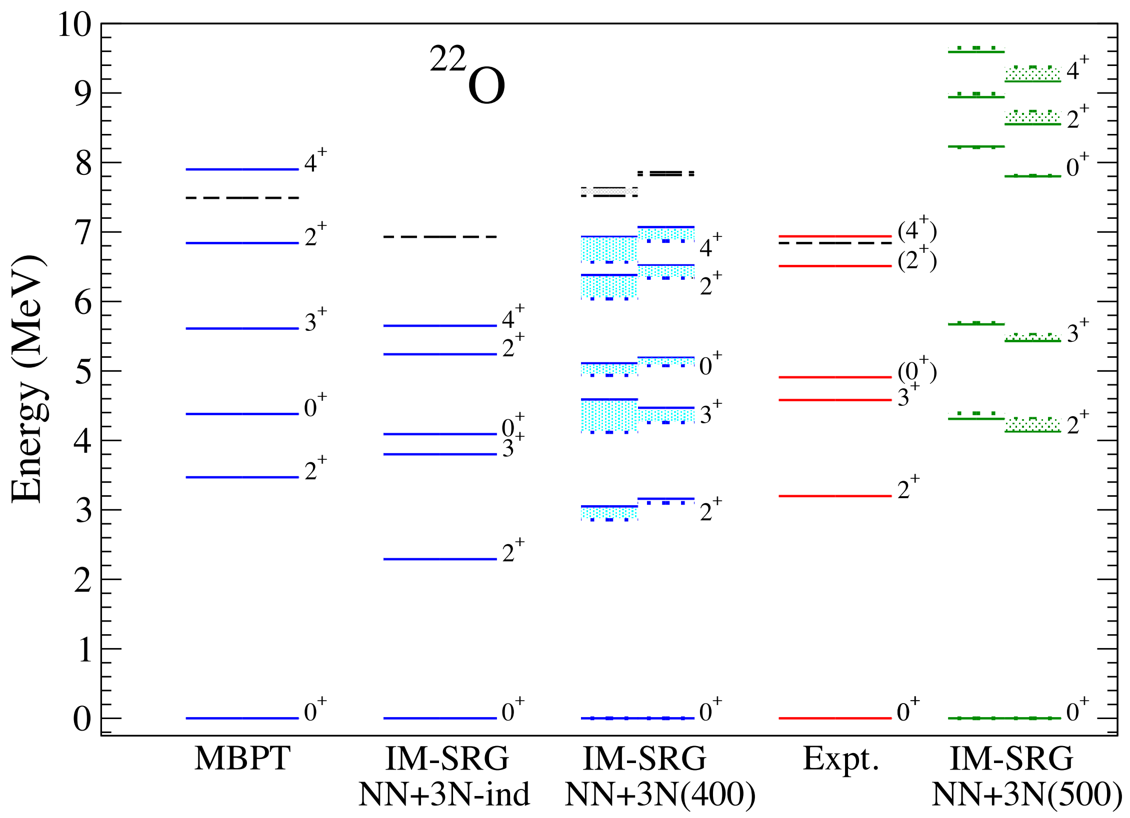
s=0.2 MeV^{-1}

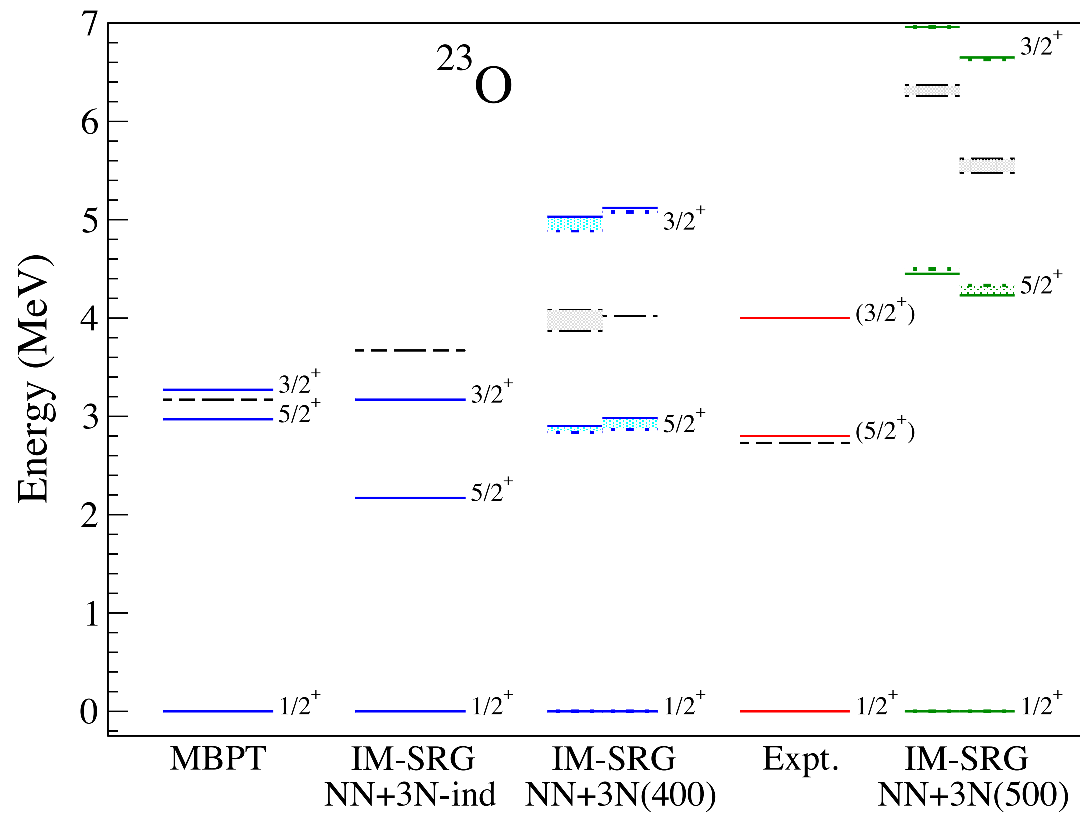
- **promising starting point** for ab initio studies of arbitrary open-shell nuclei

Back to Phenomenology

Tsukiyama, et al., PRC 85, 061304(R) (2012); Bogner el al.; PRL 113, 142501 (2014)...

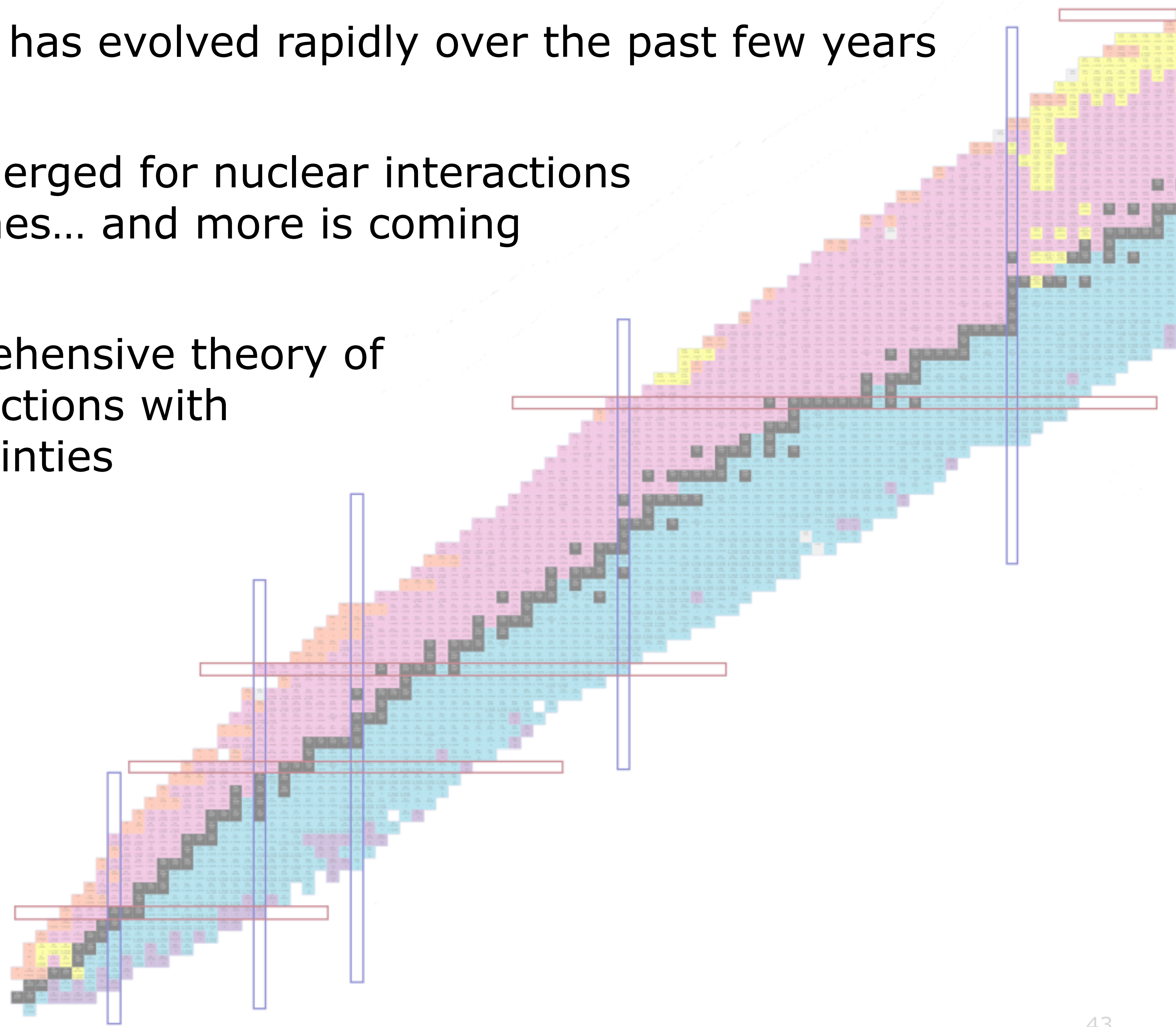
- the decoupling concept can also be used to **connect ab initio methods to traditional phenomenological approaches**
- **valence-space shell model**: construct a valence-space interaction by decoupling core and excluded space from valence space though IM-SRG or Lee-Suzuki transformation
- **unification** of nuclear structure approaches and their interpretation





New Era of Nuclear Structure Physics

- nuclear structure physics has evolved rapidly over the past few years
- many new ideas have emerged for nuclear interactions and many-body approaches… and more is coming
- moving towards a comprehensive theory of nuclear structure and reactions with quantified theory uncertainties
- it’s fun to be part of it…



Epilogue

- **thanks to my group and my collaborators**
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    NSCL / Michigan State University
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    Iowa State University
  - S. Quaglioni
    Lawrence Livermore National Laboratory
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    Universität Bochum, …

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