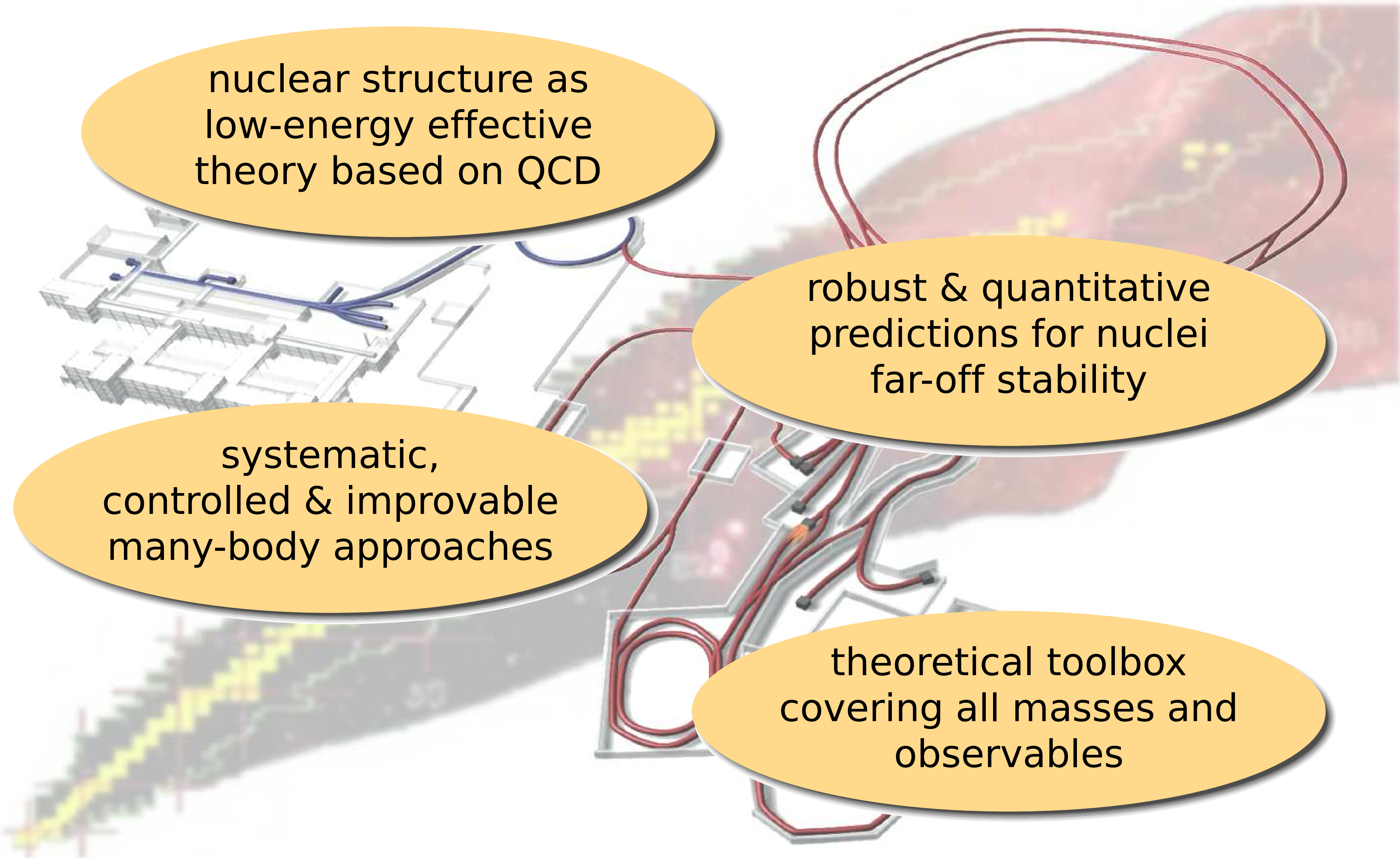
Ab Initio Nuclear Structure Theory with Chiral NN plus 3N Interactions

Robert Roth
Institut für Kernphysik

TECHNISCHE UNIVERSITÄT DARMSTADT

Nuclear Theory — Wish List



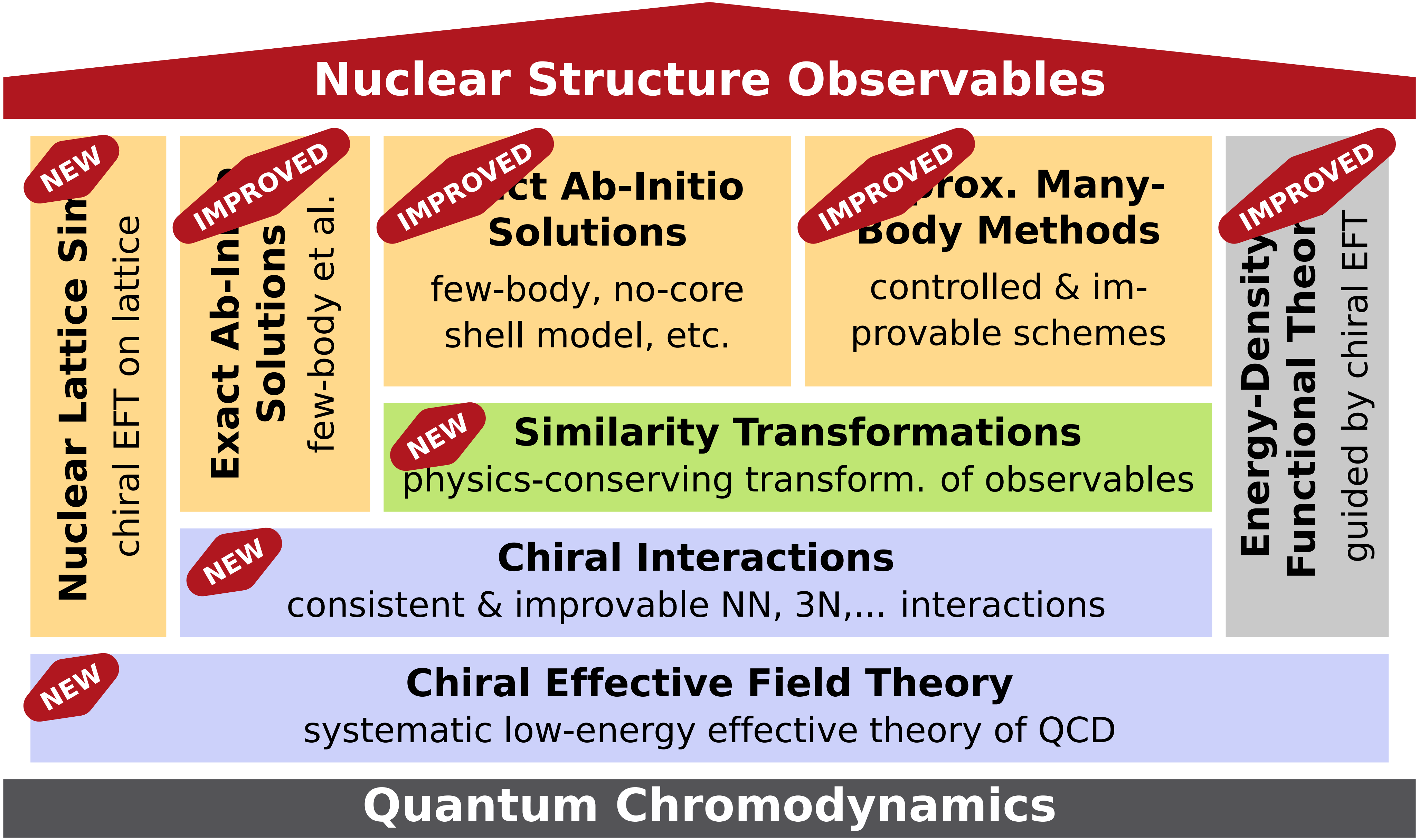
nuclear structure as low-energy effective theory based on QCD

robust & quantitative predictions for nuclei far-off stability

systematic, controlled & improvable many-body approaches

theoretical toolbox covering all masses and observables

Ab Initio Building Blocks



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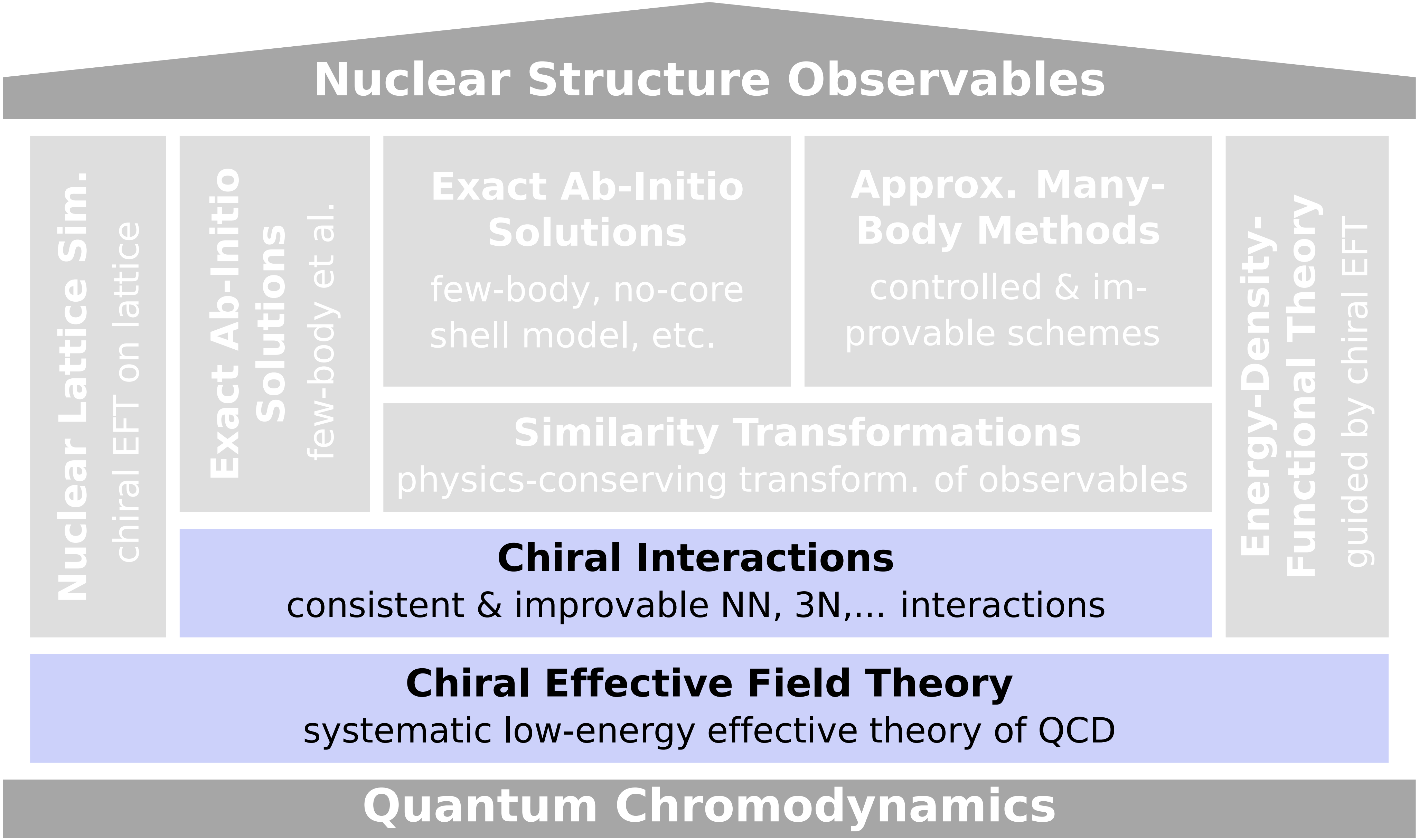
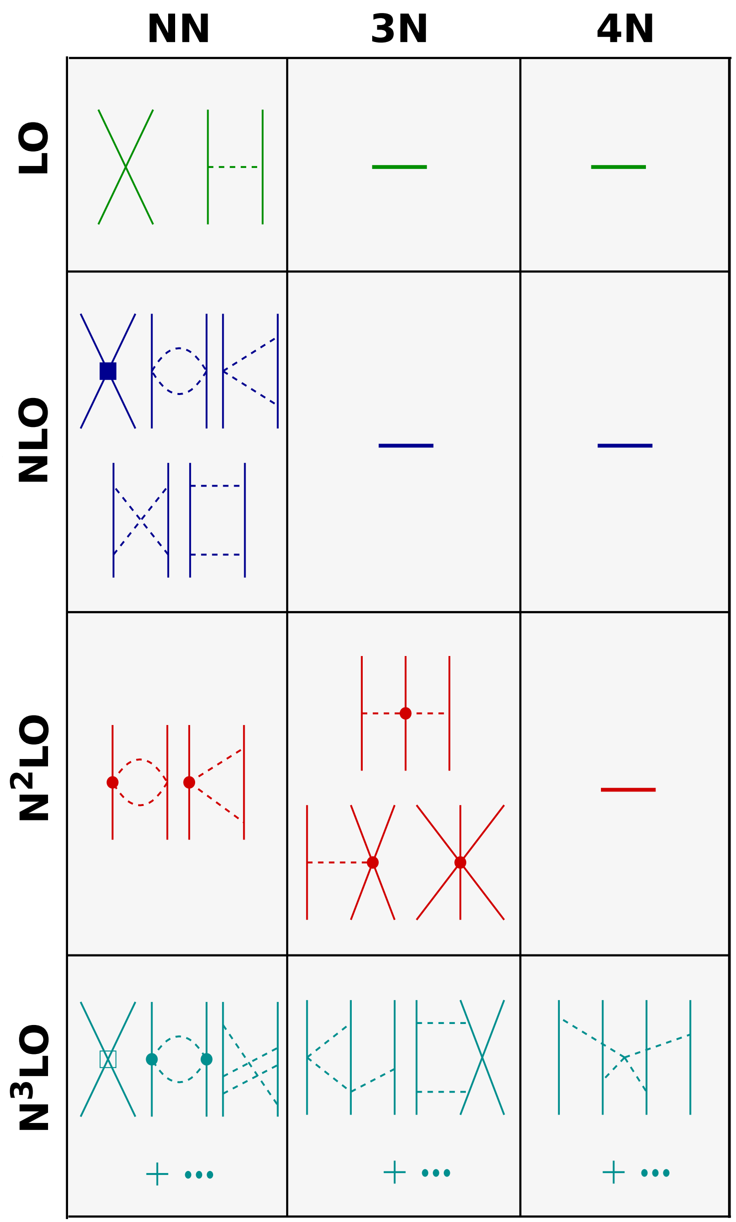


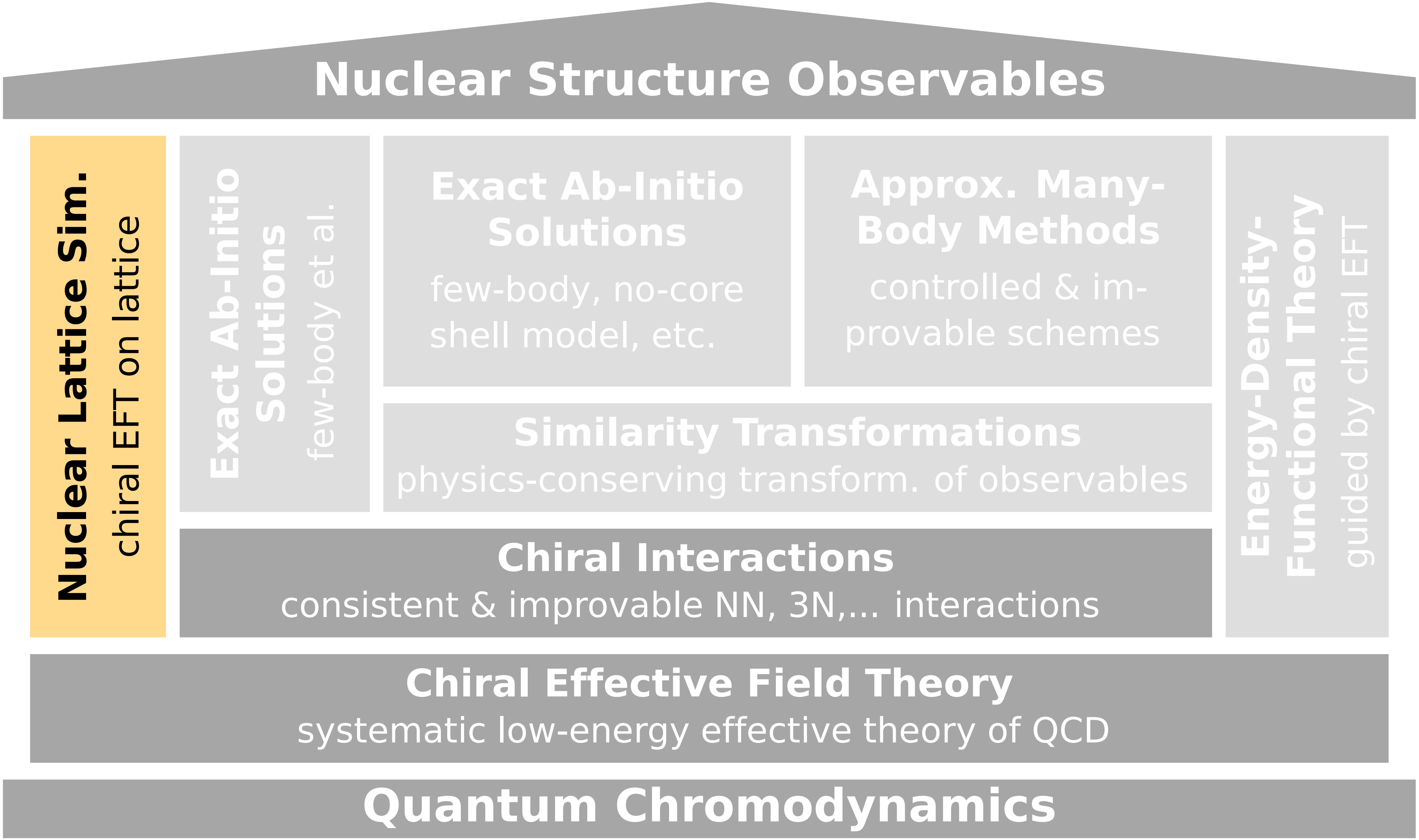
Chiral EFT for Nuclear Interactions

- low-energy **effective field theory** for relevant degrees of freedom (π,N) based on symmetries of QCD
- long-range **pion dynamics** explicitly
- short-range physics absorbed in **contact terms**, low-energy constants fitted to experiment (NN, πN,...)
- hierarchy of **consistent NN, 3N,... interactions** (plus currents)
- many **ongoing developments**
  - 3N interaction at N^{3}LO
  - explicit inclusion of Δ-resonance
  - formal issues: power counting, renormalization, cutoff choice,...



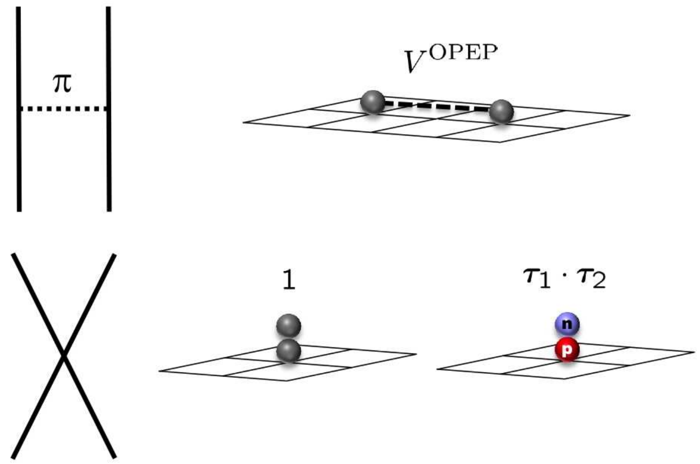
adapted from Meißner (2005)

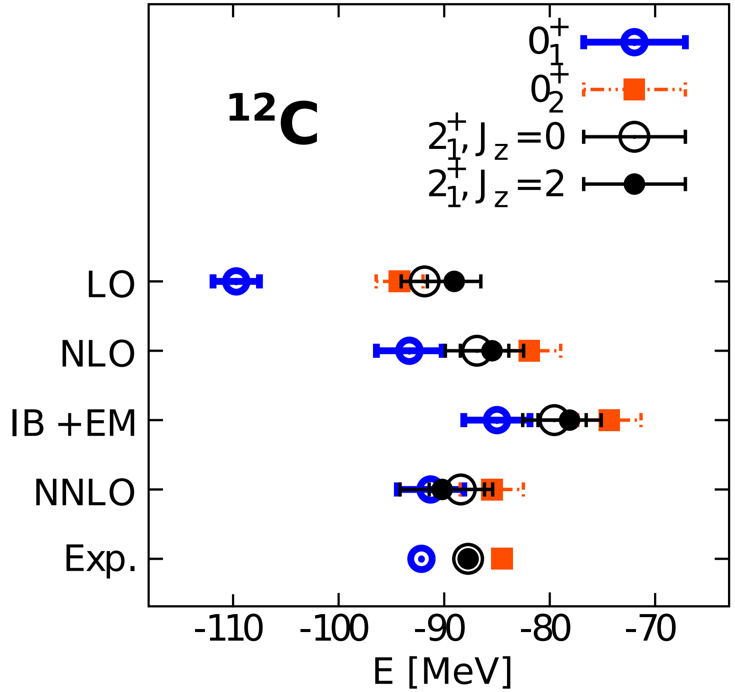
Ab Initio Building Blocks



Nuclear Lattice Simulations

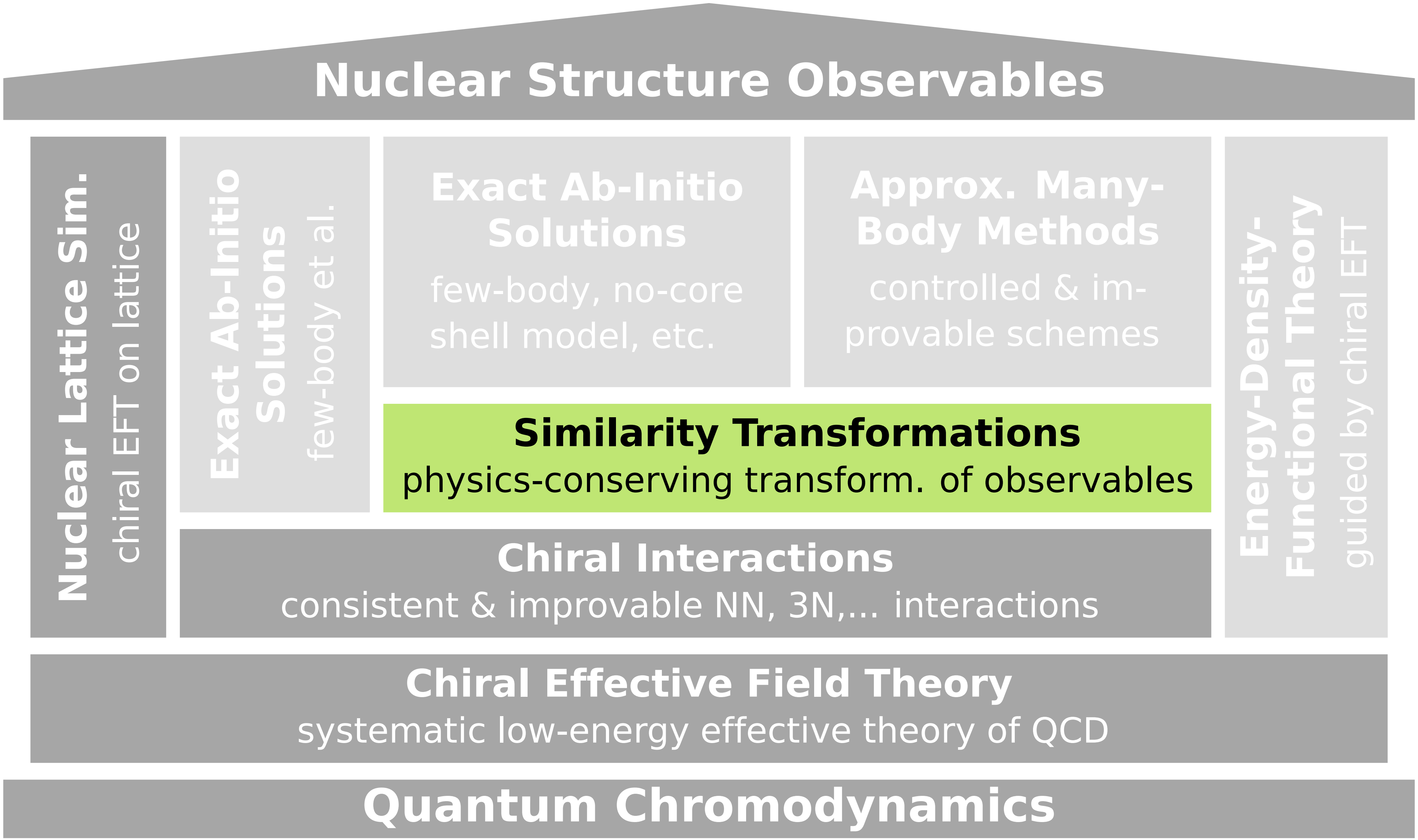
- put **chiral EFT on a space-time lattice** and use Lattice-QCD technology
- lattice defines IR and UV cutoffs
- fit LECs to scattering and ground-state observables on the lattice
- **Euclidean time projection** to extract ground and excited states
- ground states of ^{4}He, ^{8}Be, ^{12}C,...
- highlight: **Hoyle state in ^{12}C**
- **statistical and extrapolation errors** still too large for spectroscopy



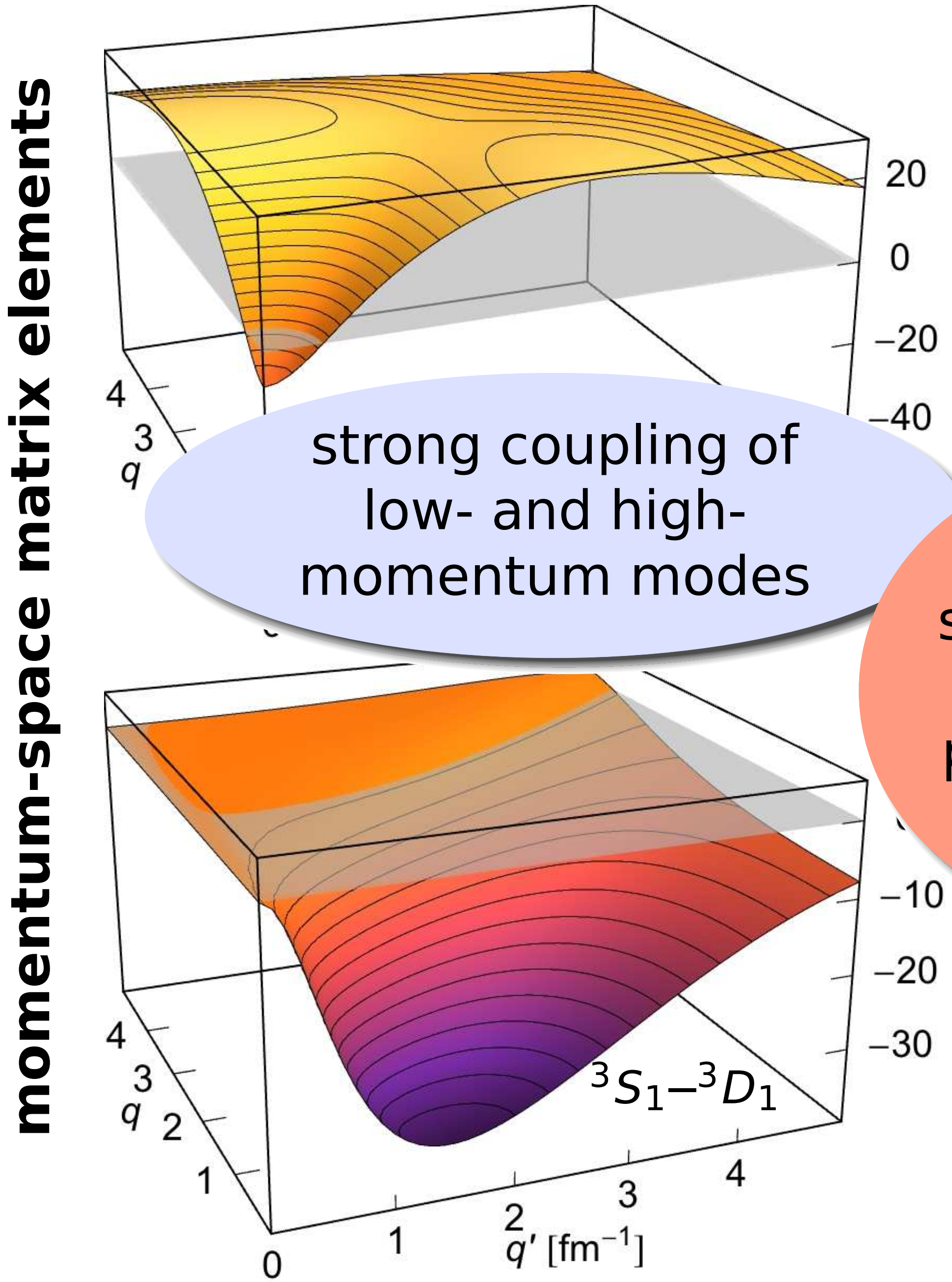


Epelbaum, Krebs, Lee, Meißner (2011)

Ab Initio Building Blocks



Why Similarity Transformations?



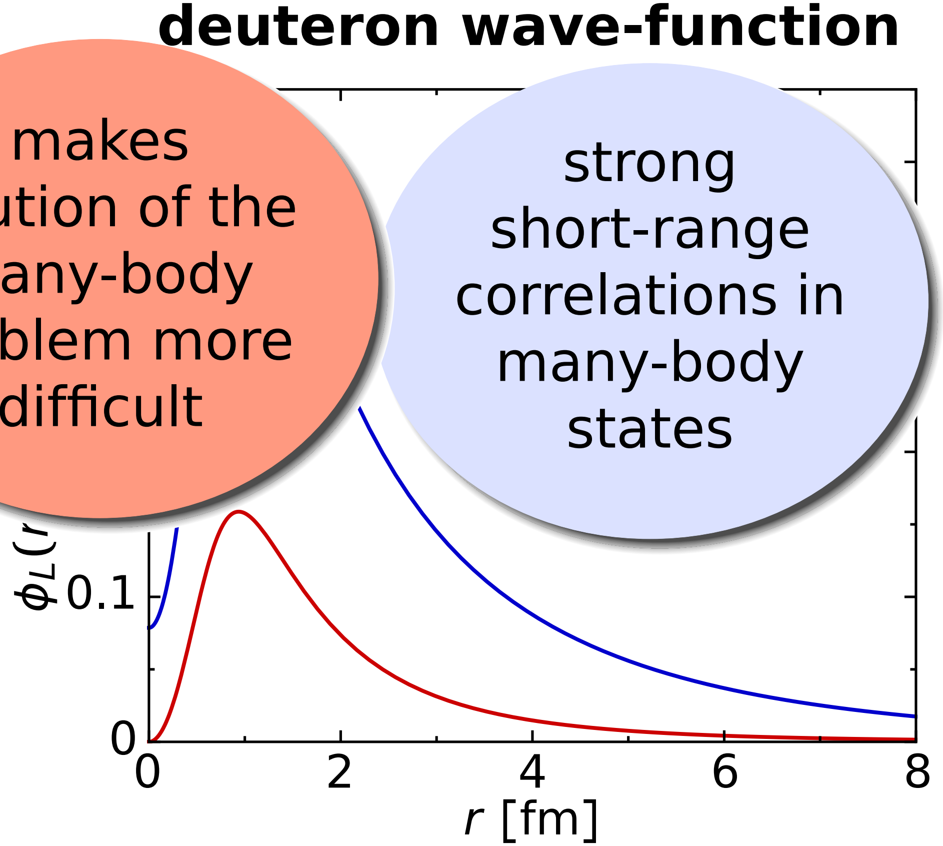
Argonne V18

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

strong coupling of low- and high-momentum modes

makes solution of the many-body problem more difficult

strong short-range correlations in many-body states



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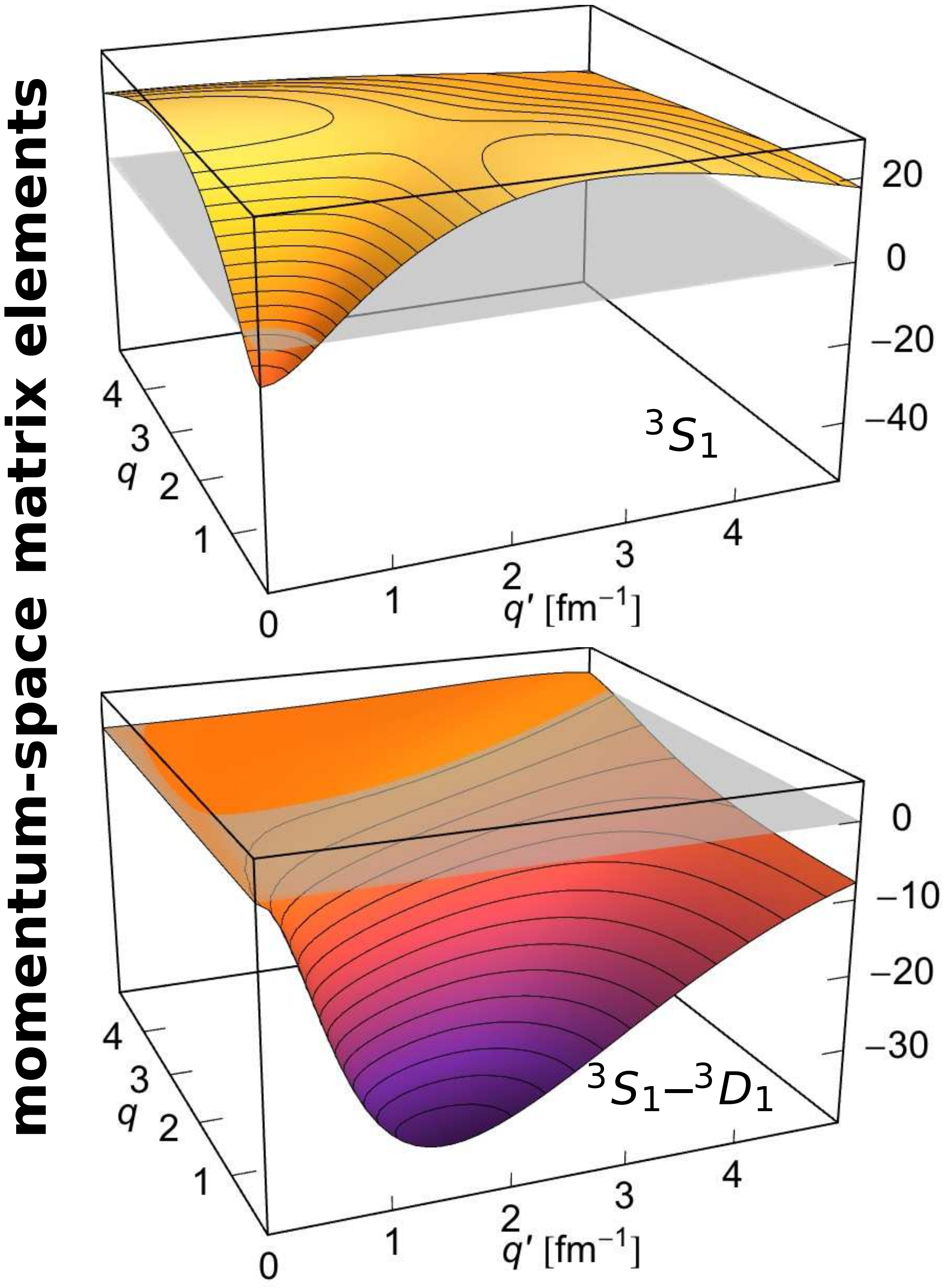
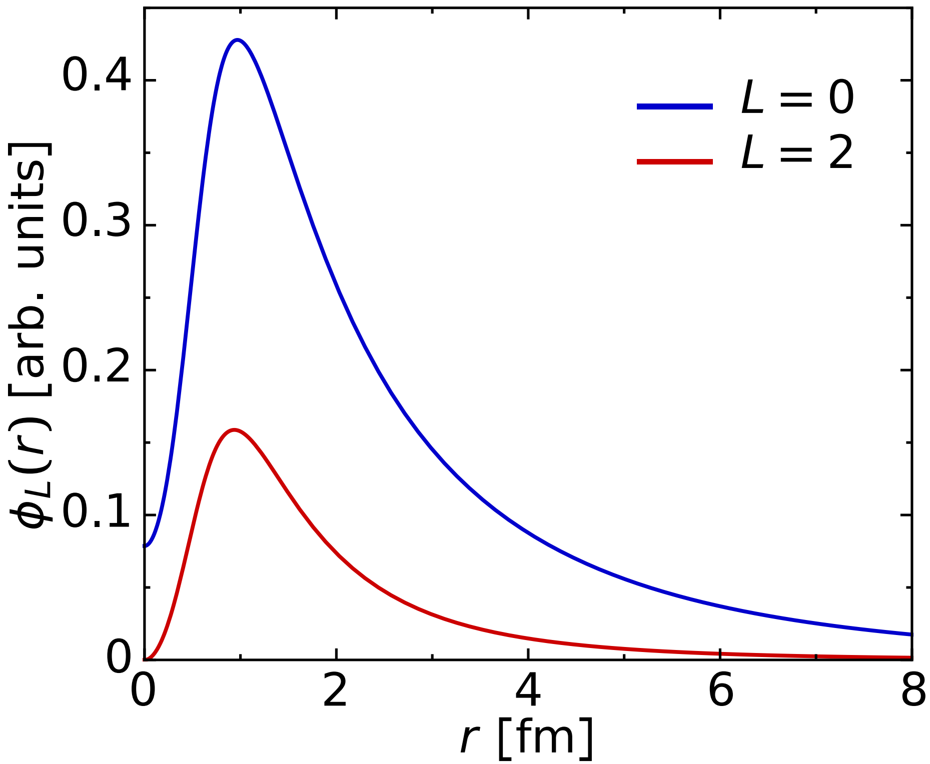


Argonne V18

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

deuteron wave-function



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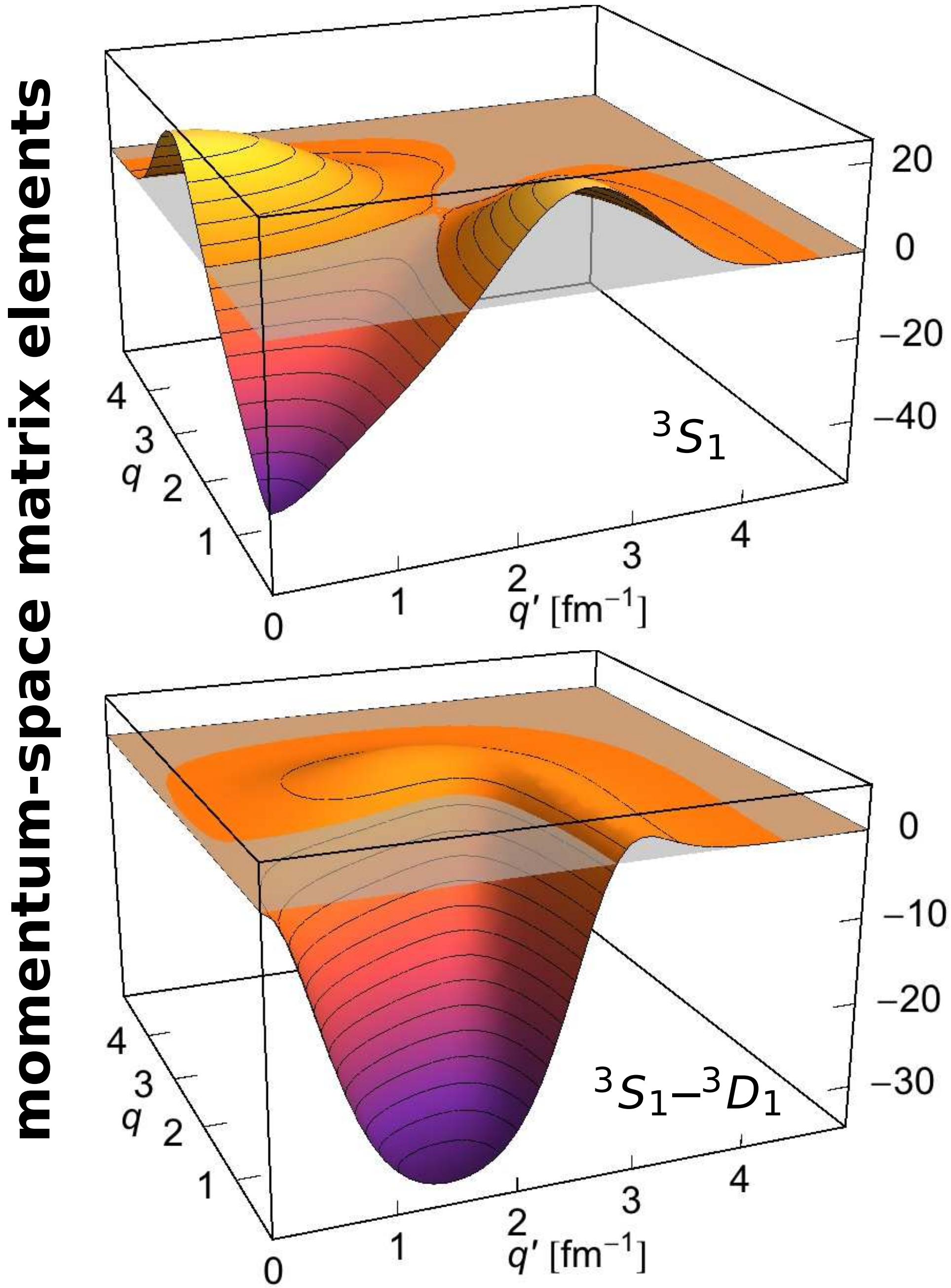
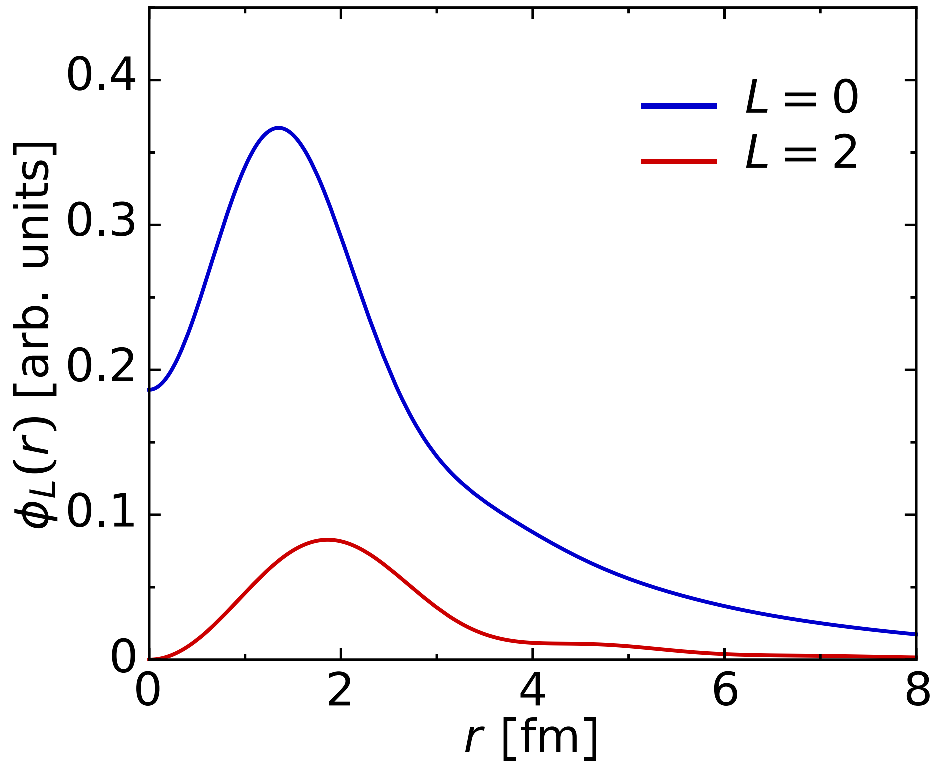


chiral N^{3}LO

Entem & Machleidt, 500 MeV

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

deuteron wave-function



Similarity Renormalization Group

continuous transformation driving
Hamiltonian to band-diagonal form
with respect to a chosen basis

- **unitary transformation** of Hami

$$\widetilde{H}_\alpha = U_\alpha^\dagger H U_\alpha$$

simplicity and flexibility
are great advantages of
the SRG approach

- **evolution equations** for $\widetilde{H}_\alpha$ and

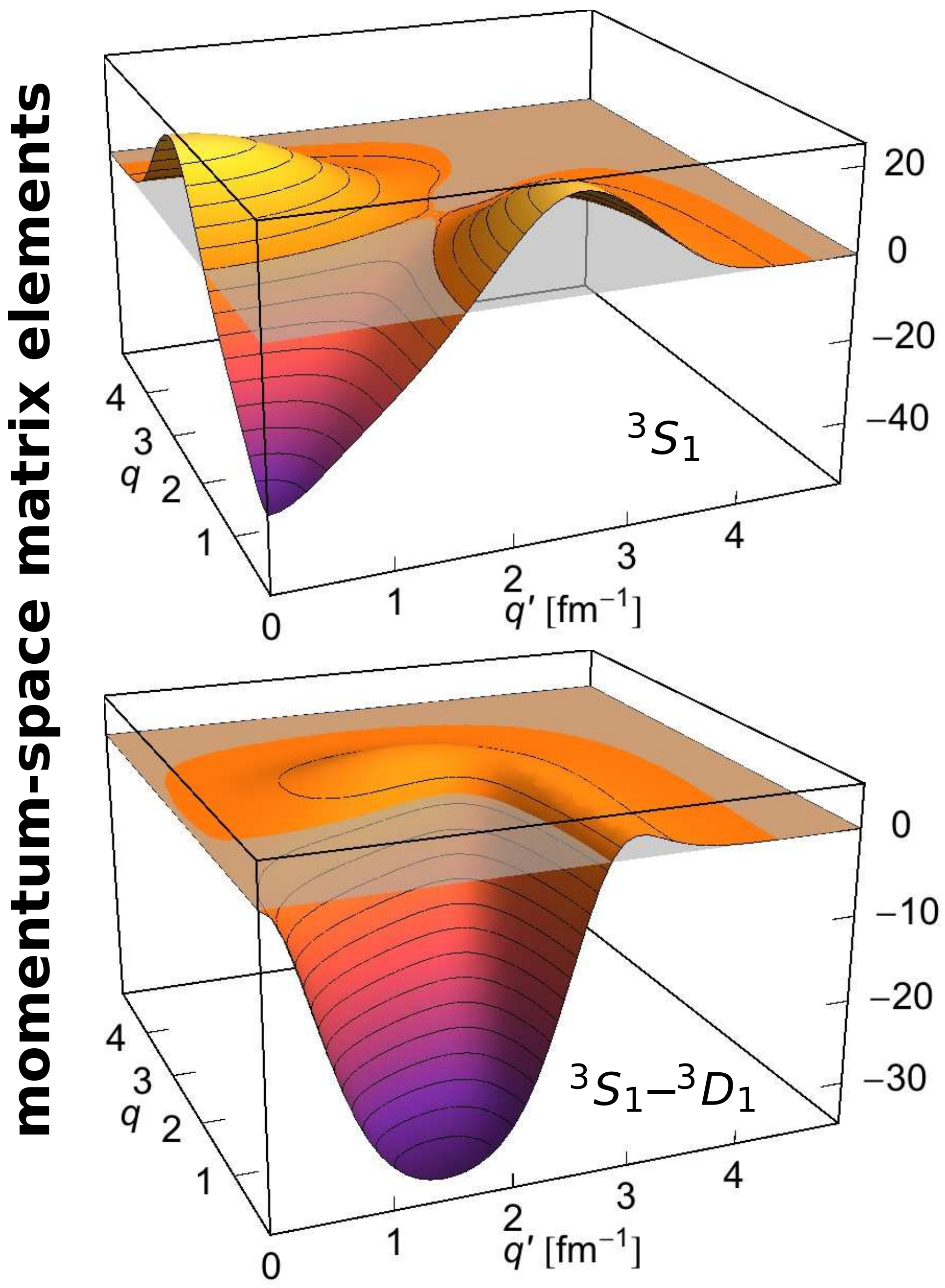
$$\frac{d}{d\alpha}\widetilde{H}_\alpha = [\eta_\alpha, \widetilde{H}_\alpha]$$

other transformation
approaches (UCOM, $V_{\text{low}k}$)
follow as special cases

- **dynamic generator**: commutator with the operator in whose eigenbasis H shall be diagonalized

$$\eta_\alpha = (2\mu)^2 [T_{\text{int}}, \widetilde{H}_\alpha]$$

SRG Evolution in Two-Body Space

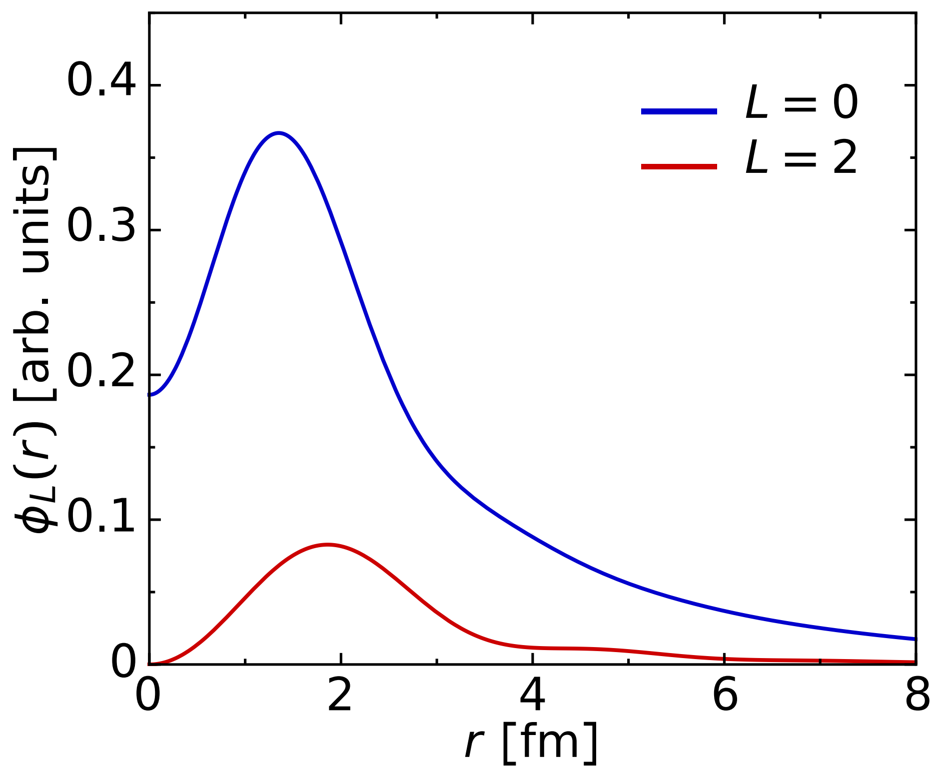


$\alpha = 0.000\,\mathrm{fm}^4$

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

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

deuteron wave-function

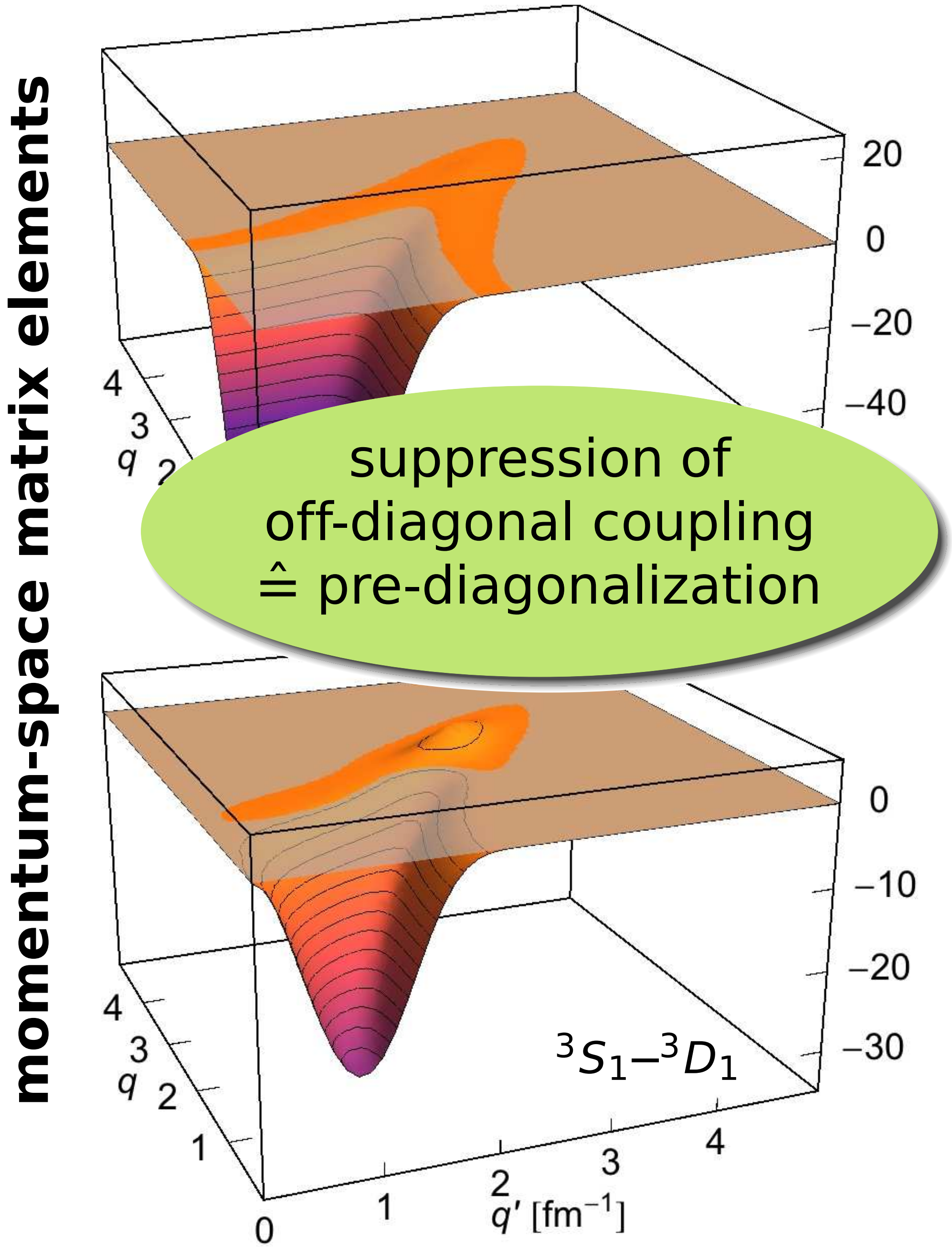


SRG Evolution in Two-Body Space

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

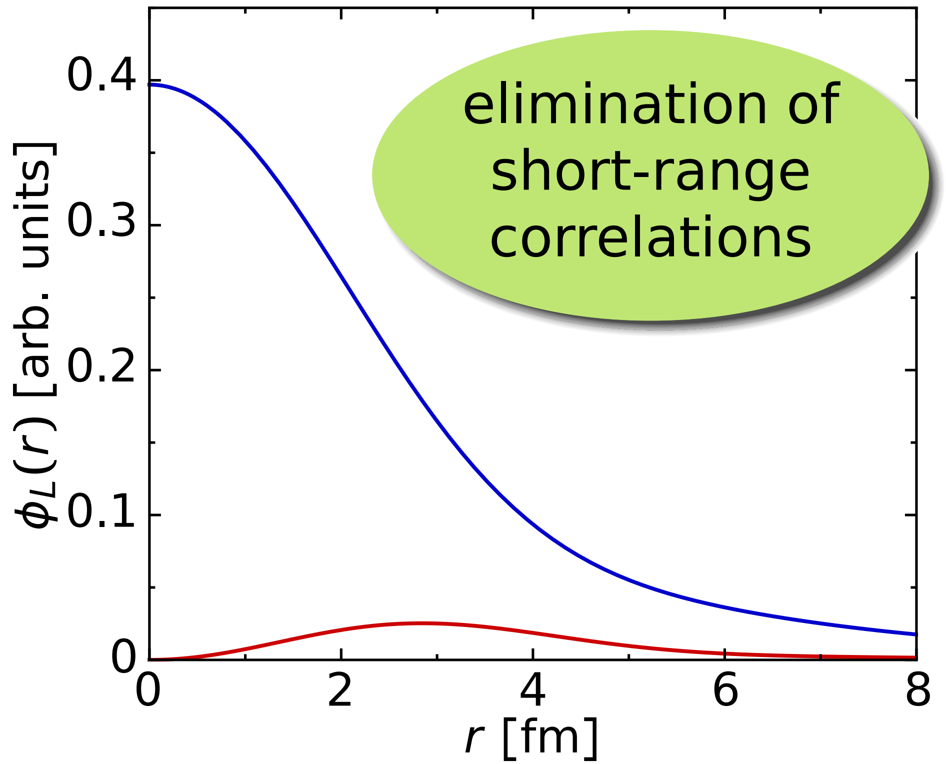
$\Lambda = 1.33\,\mathrm{fm}^{-1}$

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



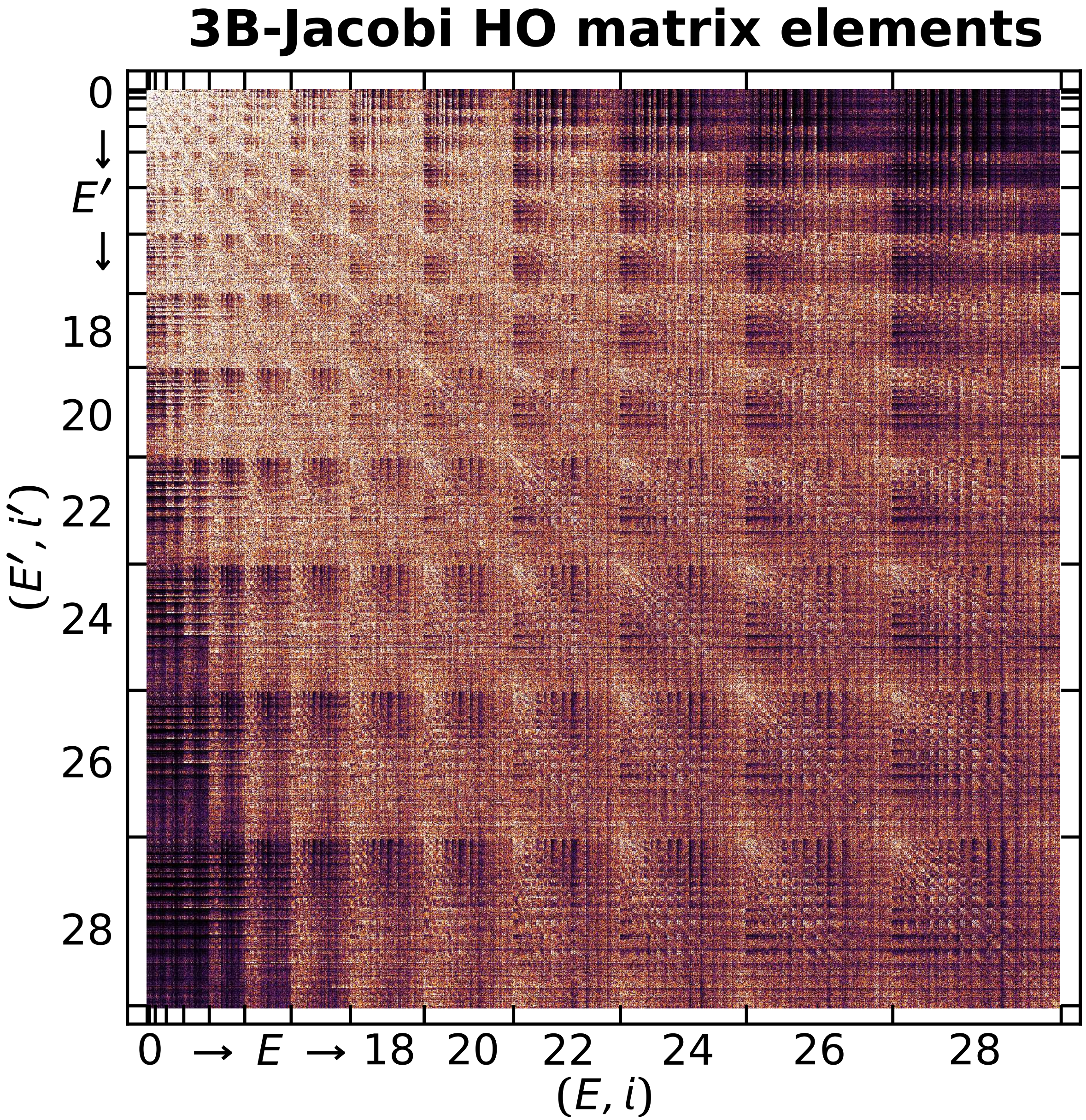
suppression of
off-diagonal coupling
≙ pre-diagonalization

deuteron wave-function



elimination of
short-range
correlations

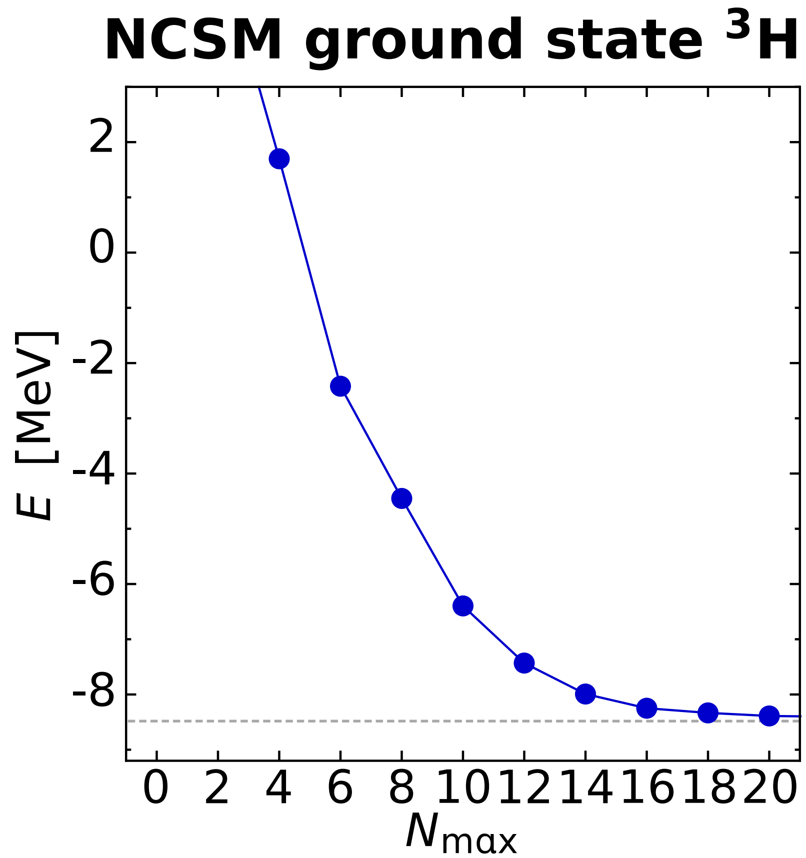
SRG Evolution in Three-Body Space



$$\alpha = 0.000\,\text{fm}^4$$

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

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



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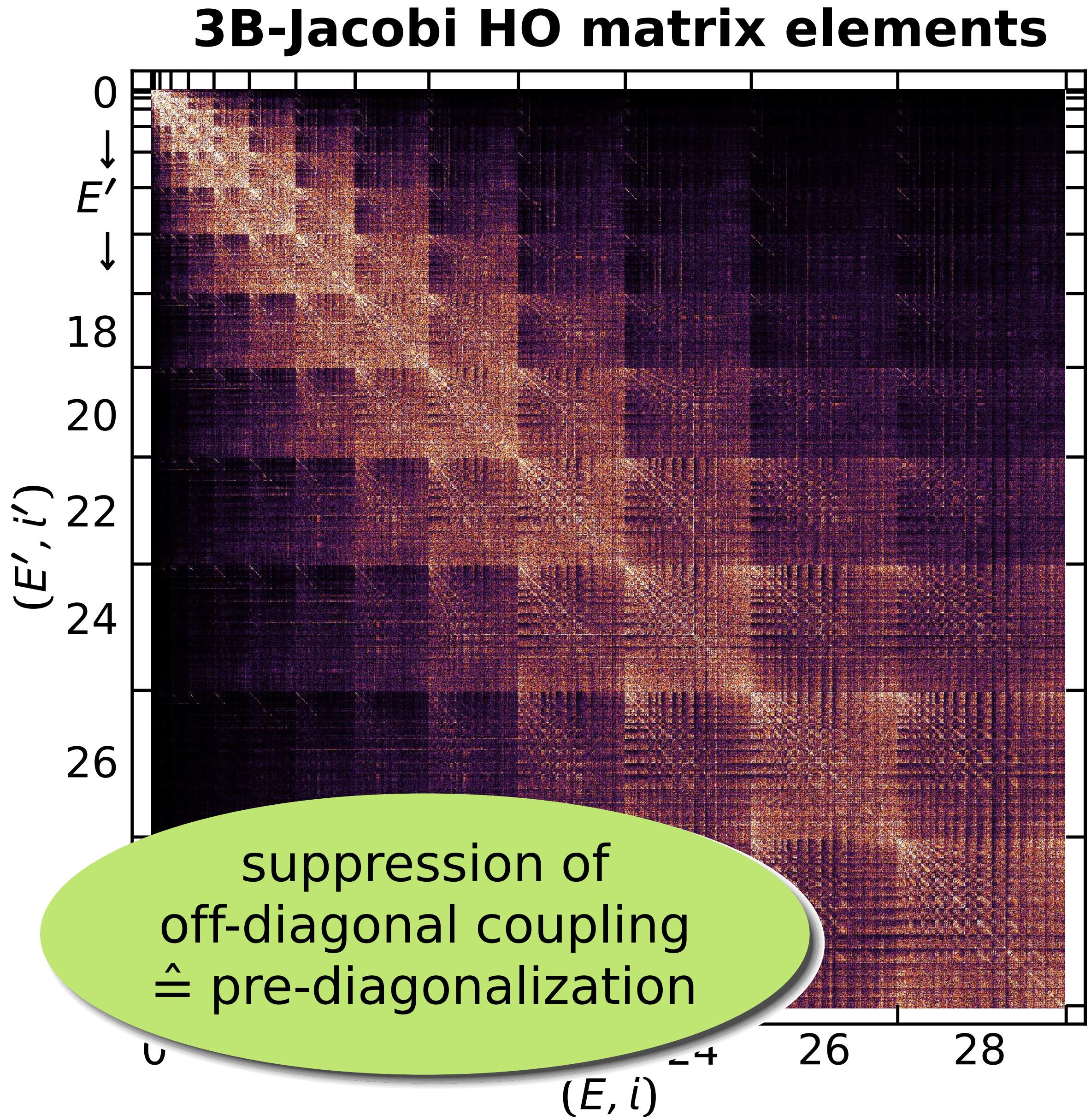

$\alpha = 0.320\,\mathrm{fm}^4$

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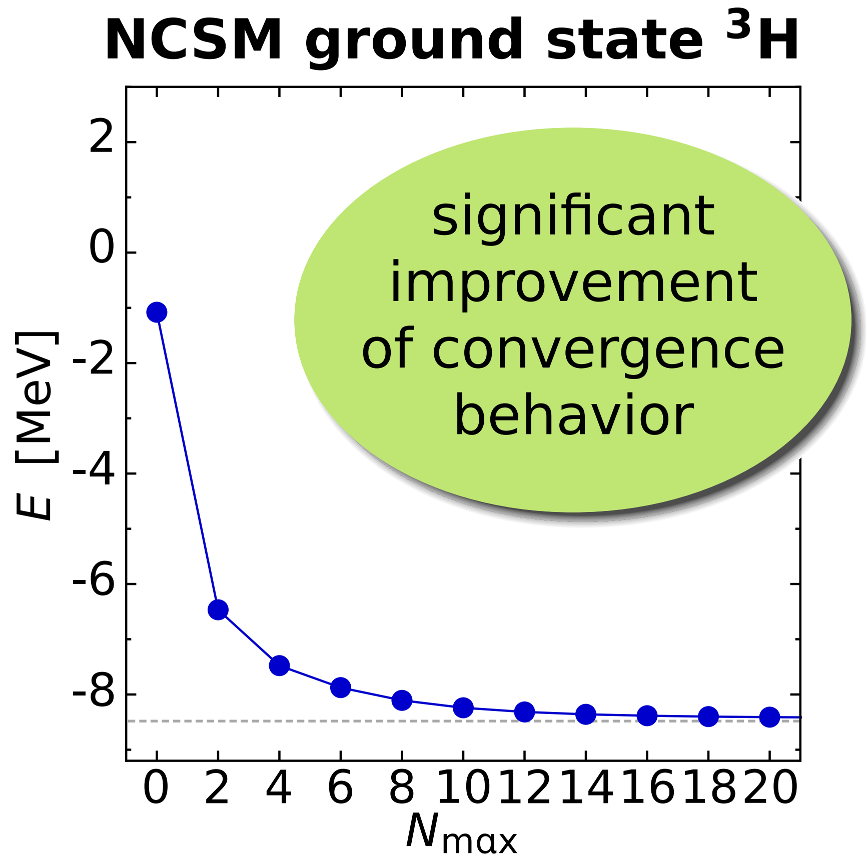


Hamiltonian in A-Body Space

- unitary transformation **induces n-body contributions** $\widetilde{H}_\alpha^{[n]}$ in the Hamiltonian

$$\widetilde{H}_\alpha = \widetilde{H}_\alpha^{[1]} + \widetilde{H}_\alpha^{[2]} + \widetilde{H}_\alpha^{[3]} + \cdots + \widetilde{H}_\alpha^{[A]}$$

- **cluster truncation**: can construct contributions up to $n = 3$ from evolution in 2B and 3B space, but have to discard $n > 3$
  - only the **full evolution in A-body space** conserves A-body energy eigenvalues and, thus, independence of α
  - α-dependence of eigenvalues ... **milto-nian** measures impact of ...

α-variation provides a **diagnostic tool** to assess the contributions of omitted many-body interactions

Sounds easy, but...

❶ computation of initial 2B/3B-Jacobi HO matrix elements of chiral NN+3N interactions

- we use Petr Navratil's ManyEff code for computing 3B-Jacobi matrix elements and corresponding CFPs

❷ SRG evolution in 2B/3B space and cluster decomposition

- efficient implementation using adaptive ODE solver; largest block takes a few hours on single node

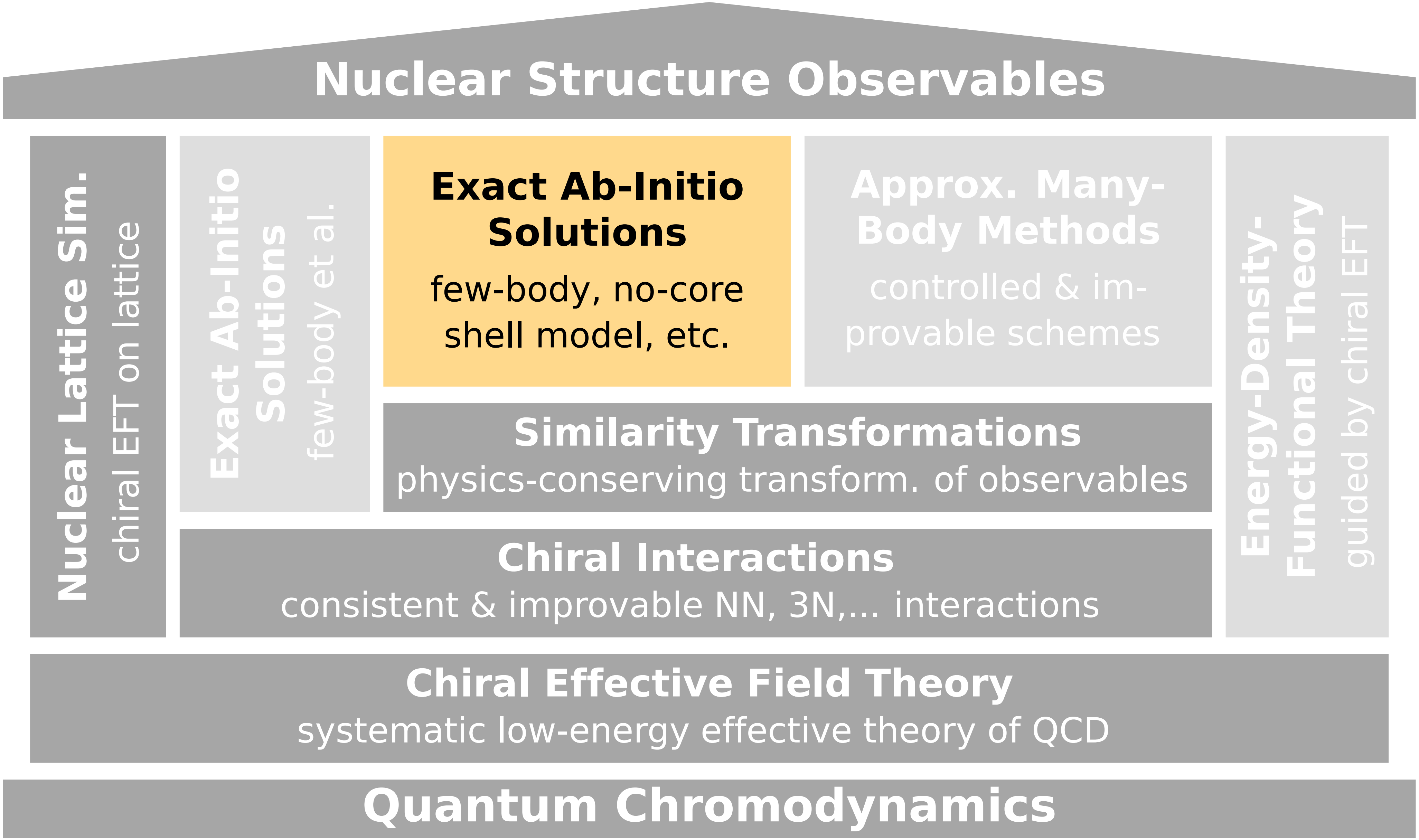
❸ transformation of 2B/3B Jacobi HO matrix elements into JT-coupled representation

- formulated transformation directly into JT-coupled scheme; highly efficient implementation; can handle $E_{3\,max} = 16$ in JT-coupled scheme

❹ data management and on-the-fly decoupling in many-body codes

- invented optimized storage scheme for fast on-the-fly decoupling; can keep all matrix elements up to $E_{3\,max} = 16$ in memory

Ab Initio Building Blocks



No-Core Shell Model (NCSM)

NCSM is one of the most powerful and universal exact ab-initio methods

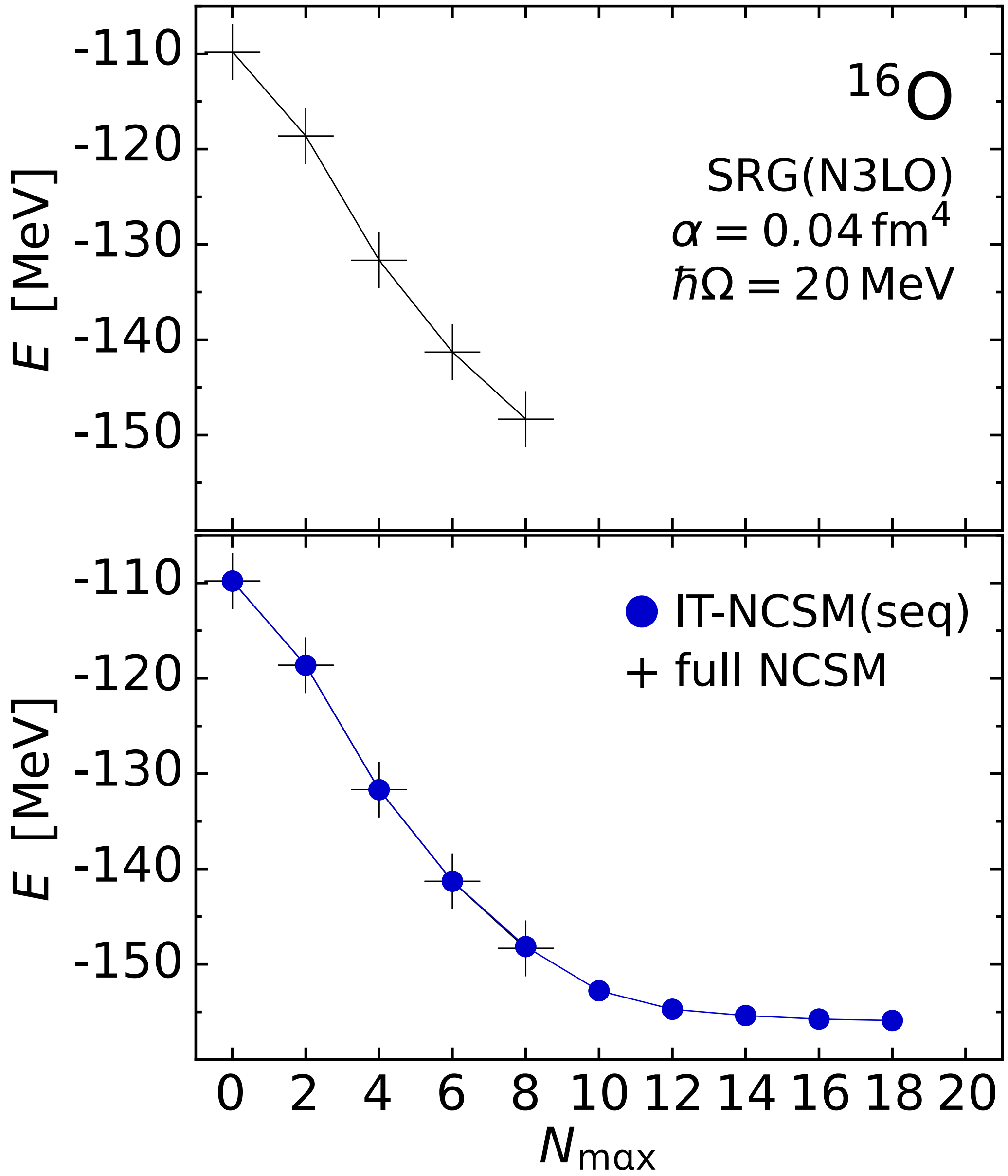
- construct matrix representation of Hamiltonian using a **basis of HO Slater determinants** truncated w.r.t. HO excitation energy $N_{\max}\hbar\Omega$
- solve **large-scale eigenvalue problem** for a few extremal eigenvalues
- **all relevant observables** can be computed from the eigenstates
- range of applicability limited by **factorial growth** of basis with $N_{\max}$ & A
- adaptive **importance truncation** extends the range of NCSM by reducing the model space to physically relevant states
- we have developed a **parallelized IT-NCSM/NCSM code** capable of handling 3N matrix elements up to $E_{3\max} = 16$

Importance Truncated NCSM

- converged NCSM calculations essentially restricted to lower/mid p-shell
- full 10 or 12$\hbar\Omega$ calculation for ^{16}O not really feasible (basis dimension > 10^{10})

Importance Truncation

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



Importance Truncation: General Idea

- given an initial approximation $\left|\Psi^{(m)}_{\text{ref}}\right\rangle$ for the **target states**
- **measure the importance** of individual basis state $\left|\Phi_\nu\right\rangle$ via first-order multiconfigurational perturbation theory

$$\kappa^{(m)}_\nu = -\frac{\left\langle \Phi_\nu \middle| \text{H} \middle| \Psi^{(m)}_{\text{ref}} \right\rangle}{\epsilon_\nu - \epsilon_{\text{ref}}}$$

- construct **importance truncated space** spanned by basis states with $|\kappa^{(m)}_\nu| \geq \kappa_{\text{min}}$ and solve eigenvalue problem
- **sequential scheme**: constru… next N_{max} using previous eigen…
- a posteriori **threshold extrapolation** and **perturbative correction** used to recover contributions from discarded basis states

for $\kappa_{\text{min}} \rightarrow 0$ the full NCSM model space and thus the **exact solution is recovered**

A Tale of Three Hamiltonians

Initial Hamiltonian

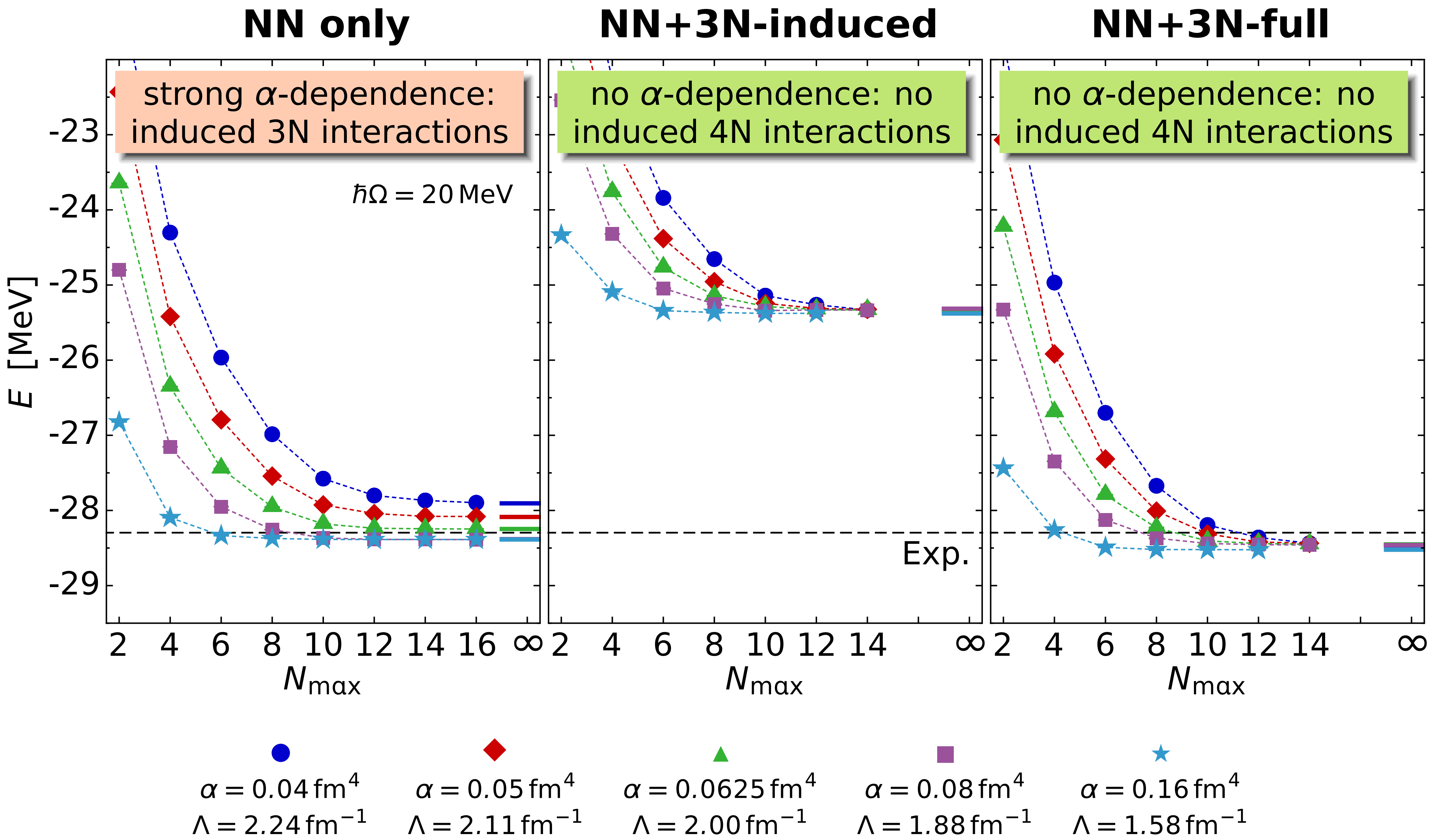
- NN: chiral interaction at N^3LO (Entem & Machleidt, 500 MeV)
- 3N: chiral interaction at N^2LO (c_D, c_E from ^{3}H binding & half-live)

SRG-Evolved Hamiltonians

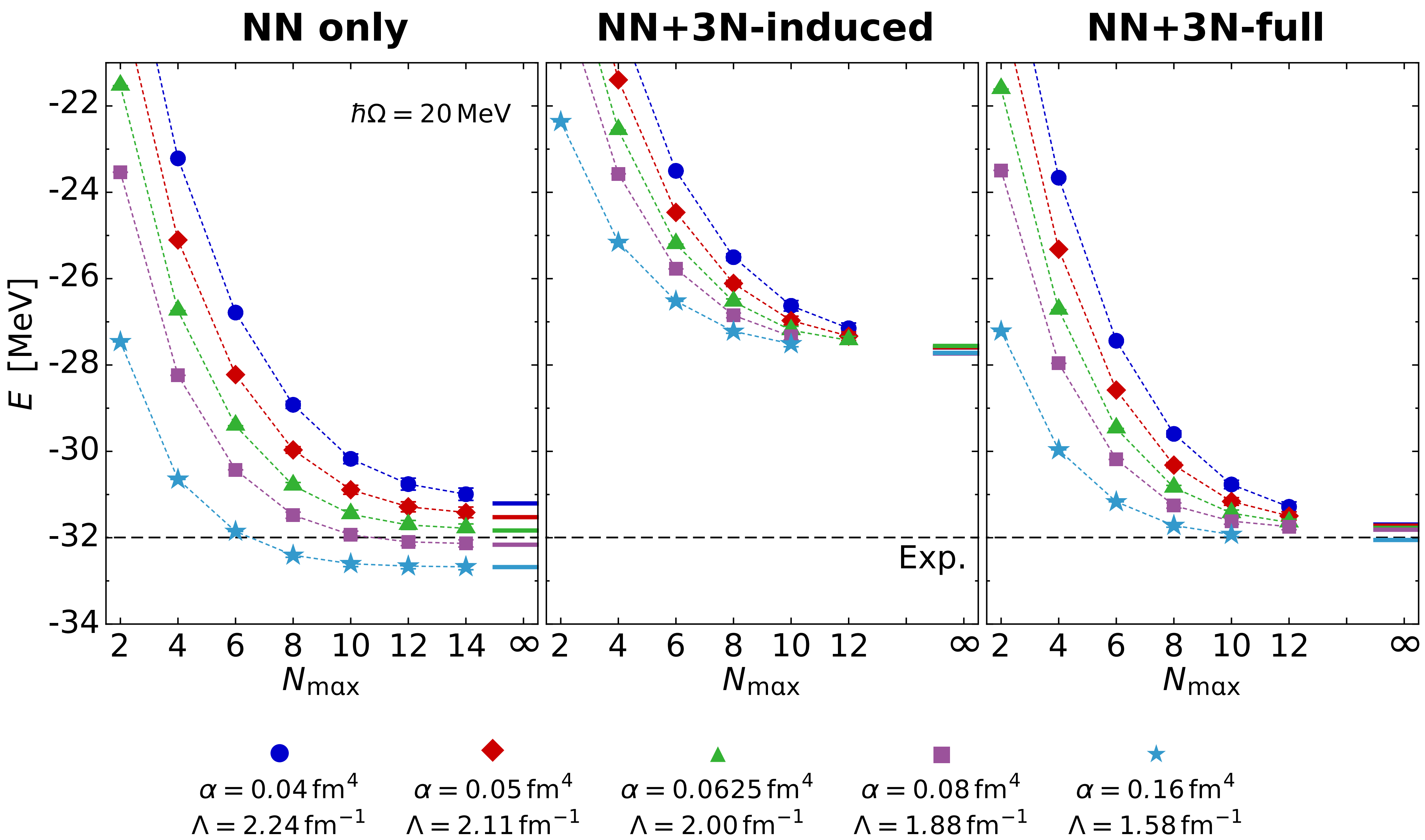
- **NN only**: start with NN initial Hamiltonian and keep two-body terms only
- **NN+3N-induced**: start with NN initial Hamiltonian and keep two- and three-body terms
- **NN+3N-full**: start with NN+3N in[...] two- and three-body terms

α-variation provides a **diagnostic tool** to assess the contributions of omitted many-body interactions

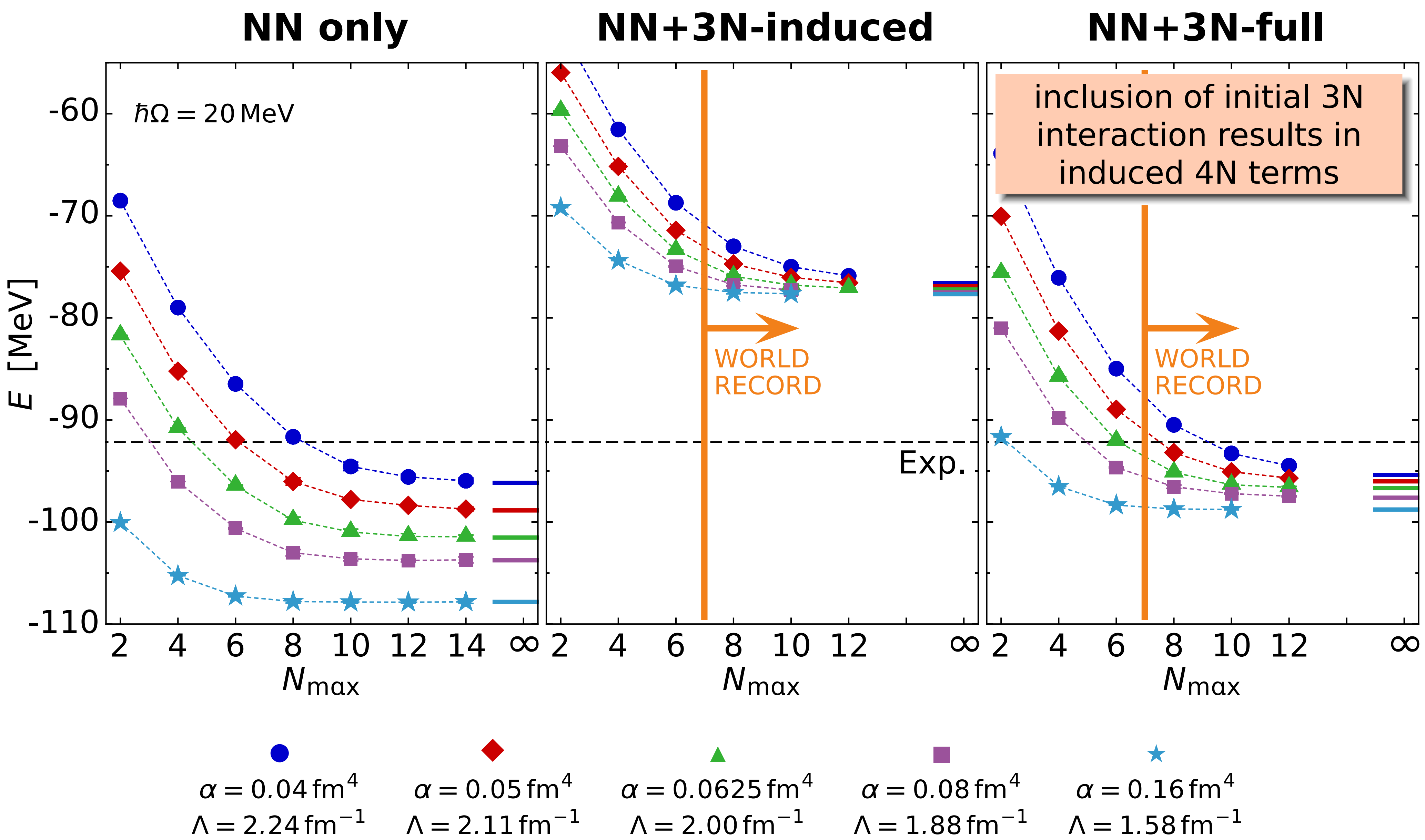
^{4}He: Ground-State Energies



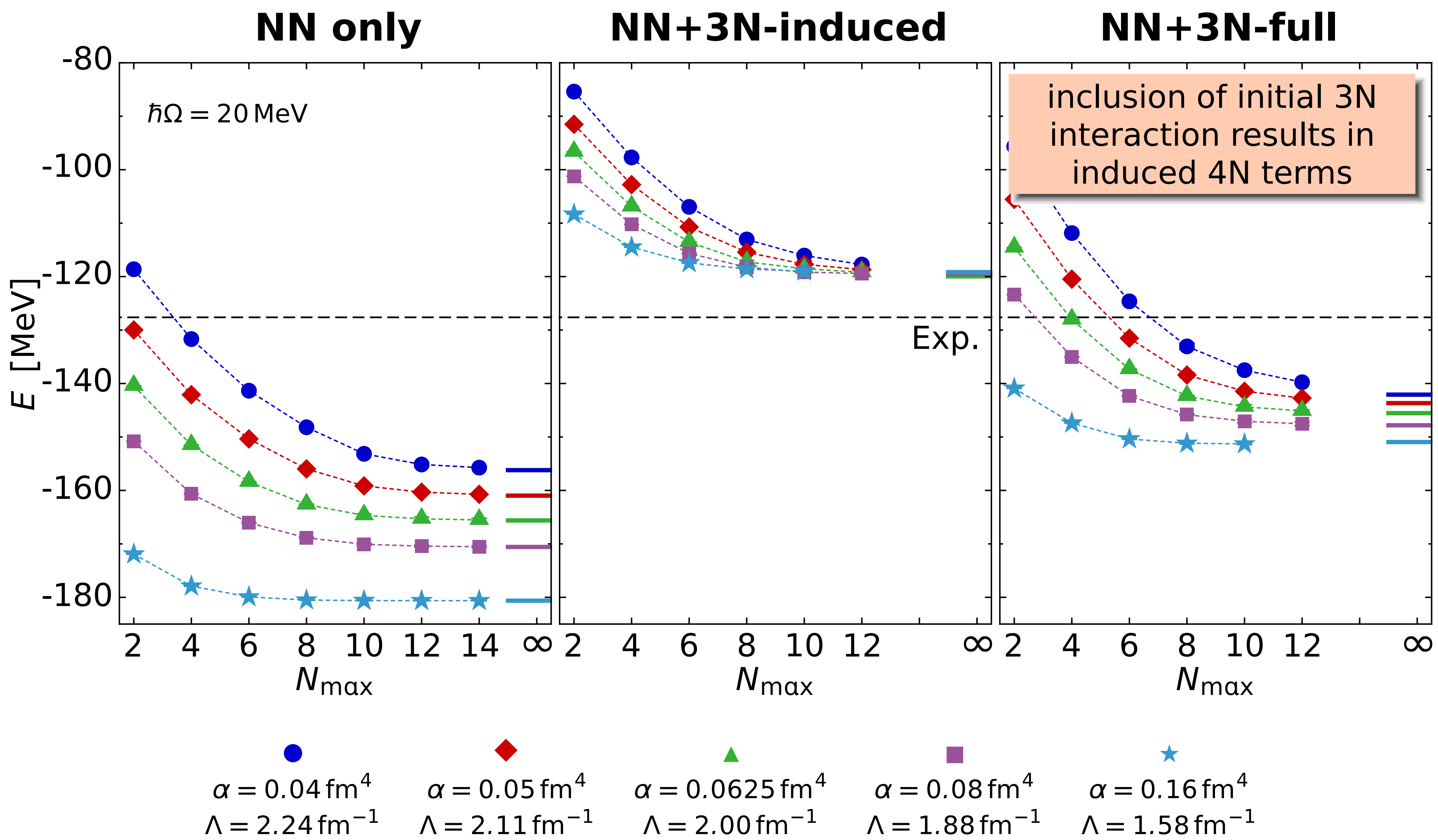
^{6}Li: Ground-State Energies



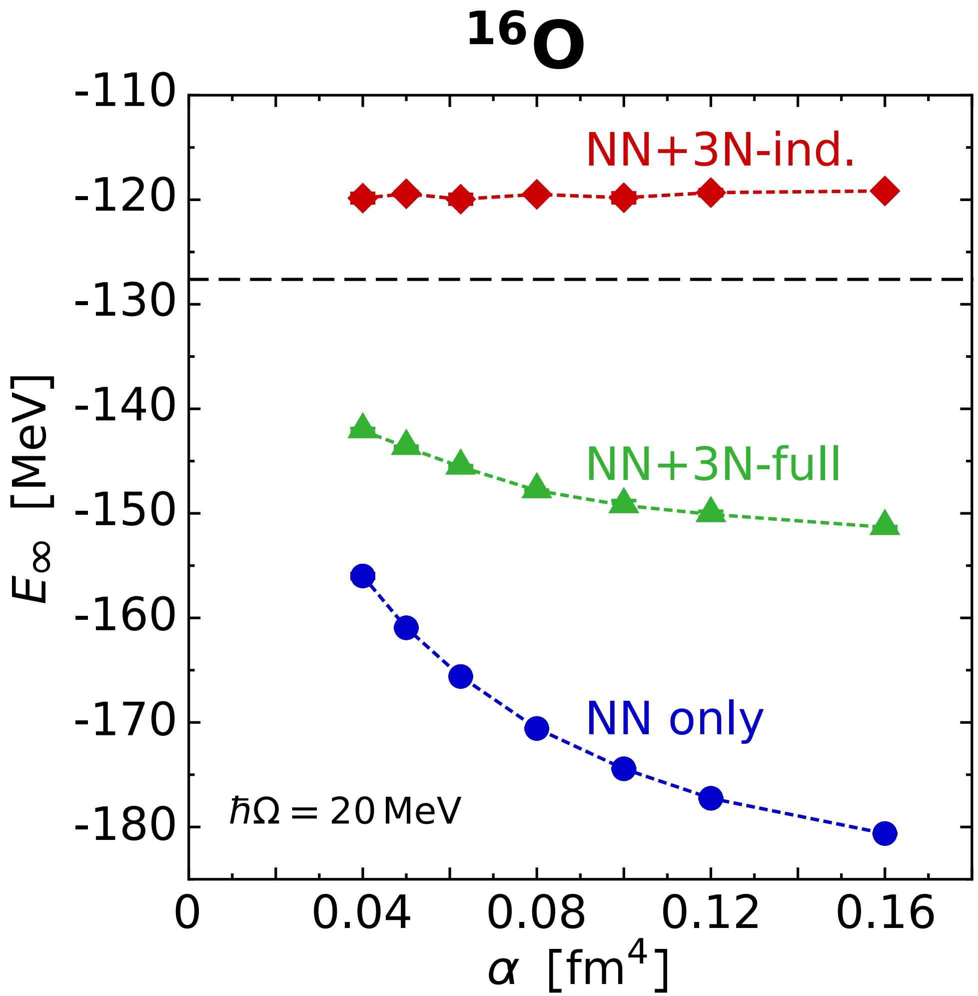
^{12}C: Ground-State Energies



^{16}O: Ground-State Energies

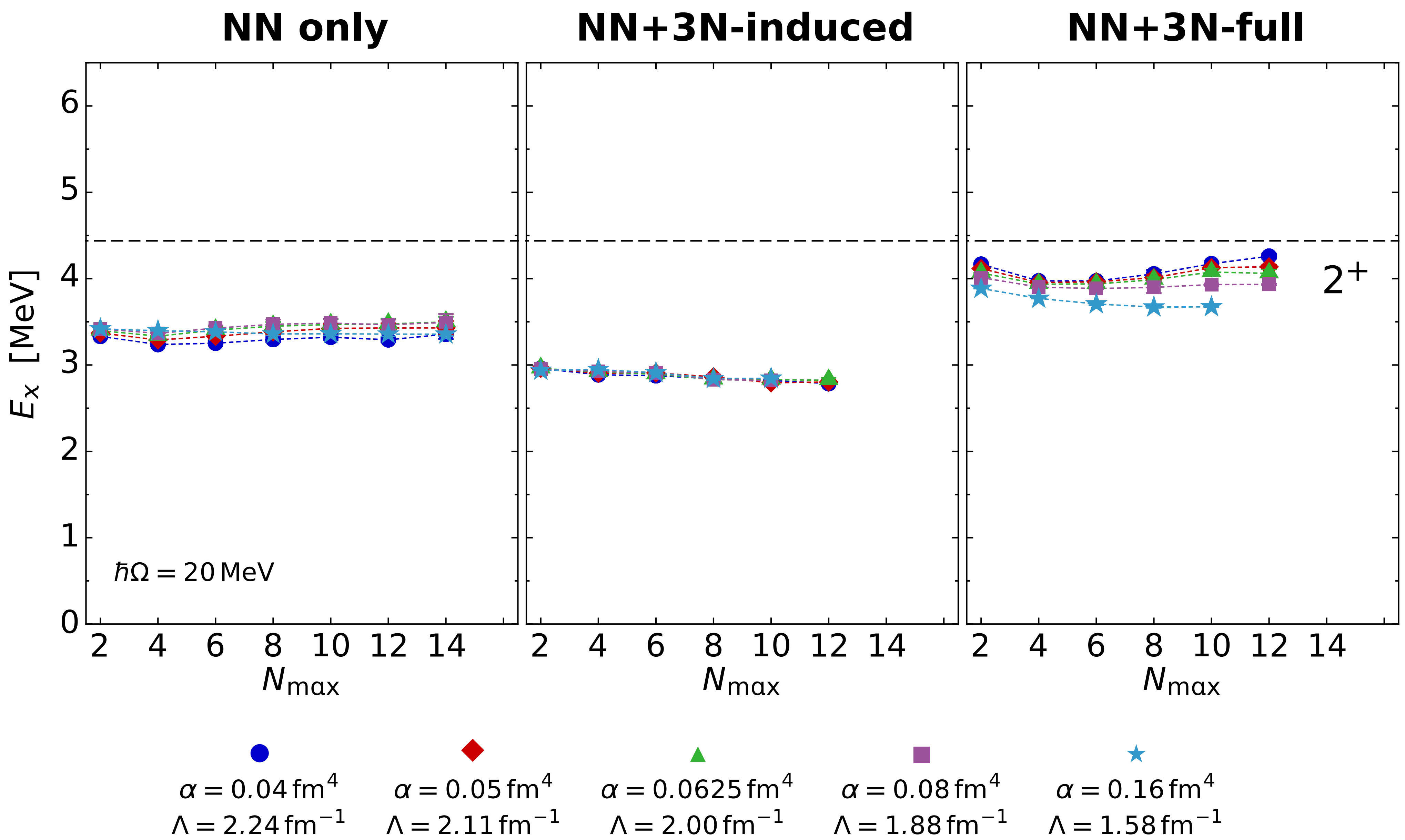


^{16}O: Energy vs. Flow Parameter

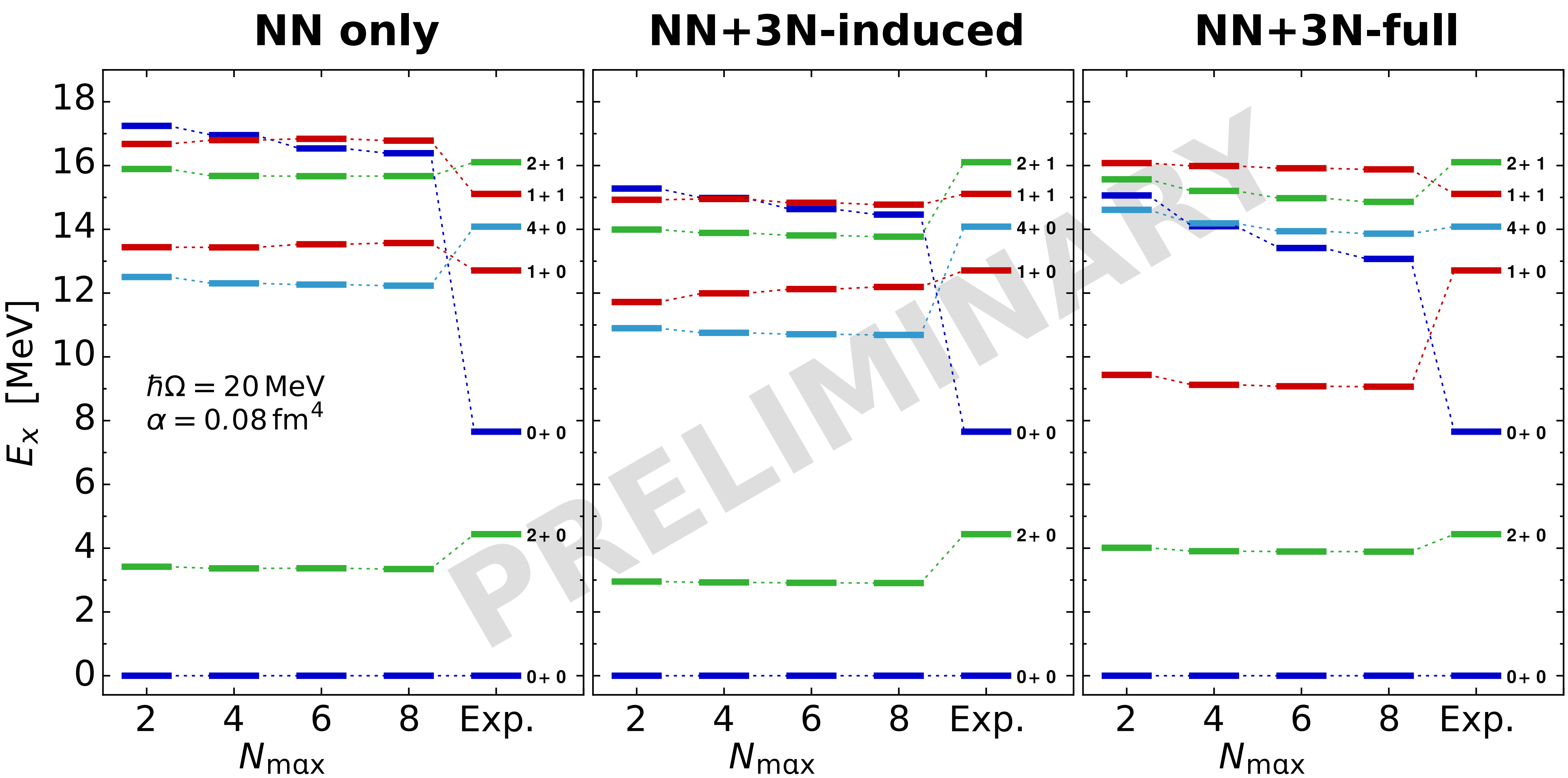


- **initial NN Hamiltonian**
  - induced 3N interactions are significant
  - no indication of induced 4N
  - NN+3N-induced unitarily equivalent to initial NN
- **initial NN+3N Hamiltonian**
  - induced 4N interactions are sizable in upper p-shell
  - generated by long-range 2π terms of initial 3N interaction
  - design modified SRG generator to suppress induced 4N

^{12}C: 2^+ Excitation Energies

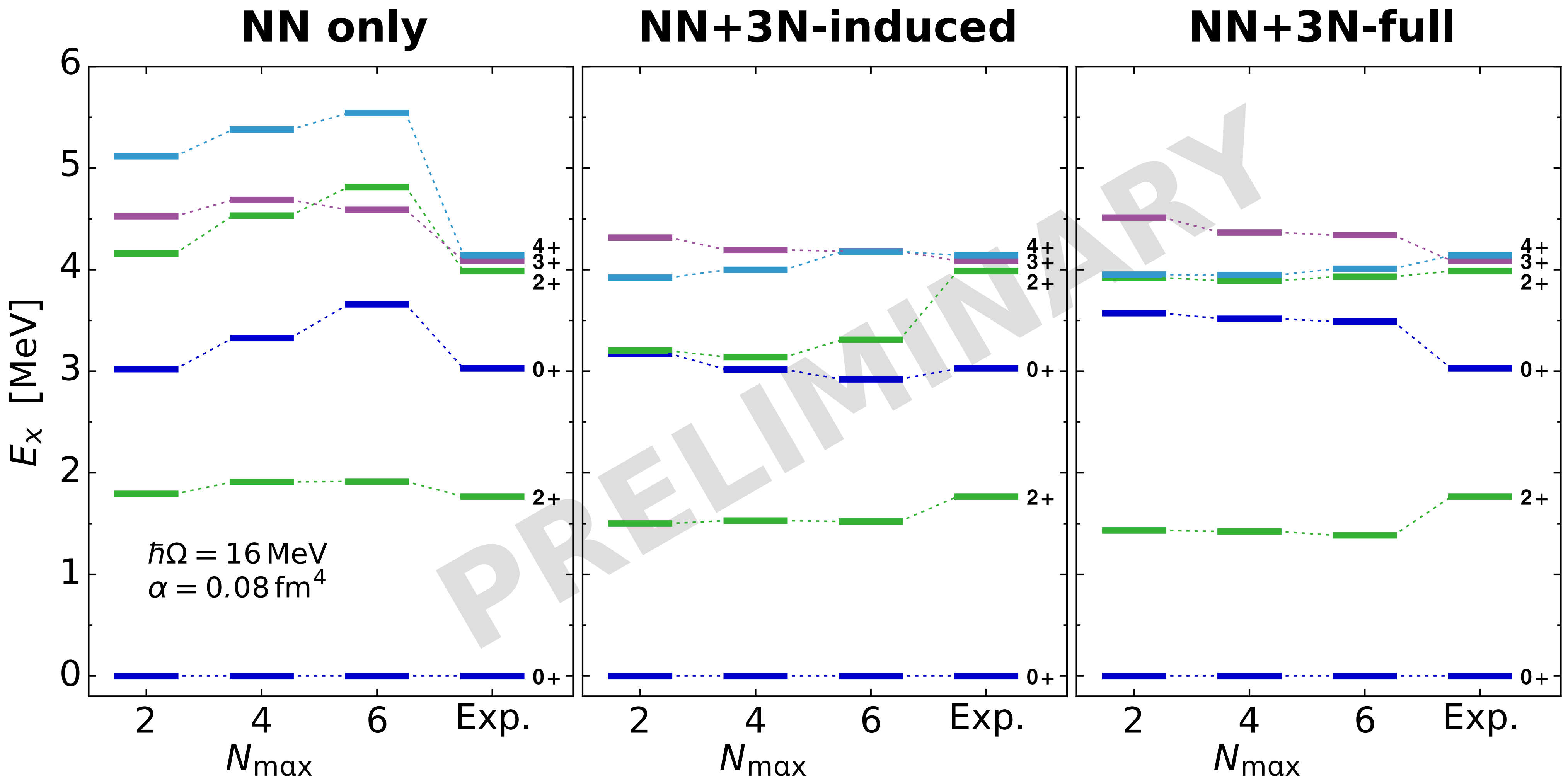


Spectroscopy of ^{12}C



- IT-NCSM gives access to **complete spectroscopy of p- and sd-shell nuclei** starting from chiral NN+3N interactions

Spectroscopy of ^{16}C

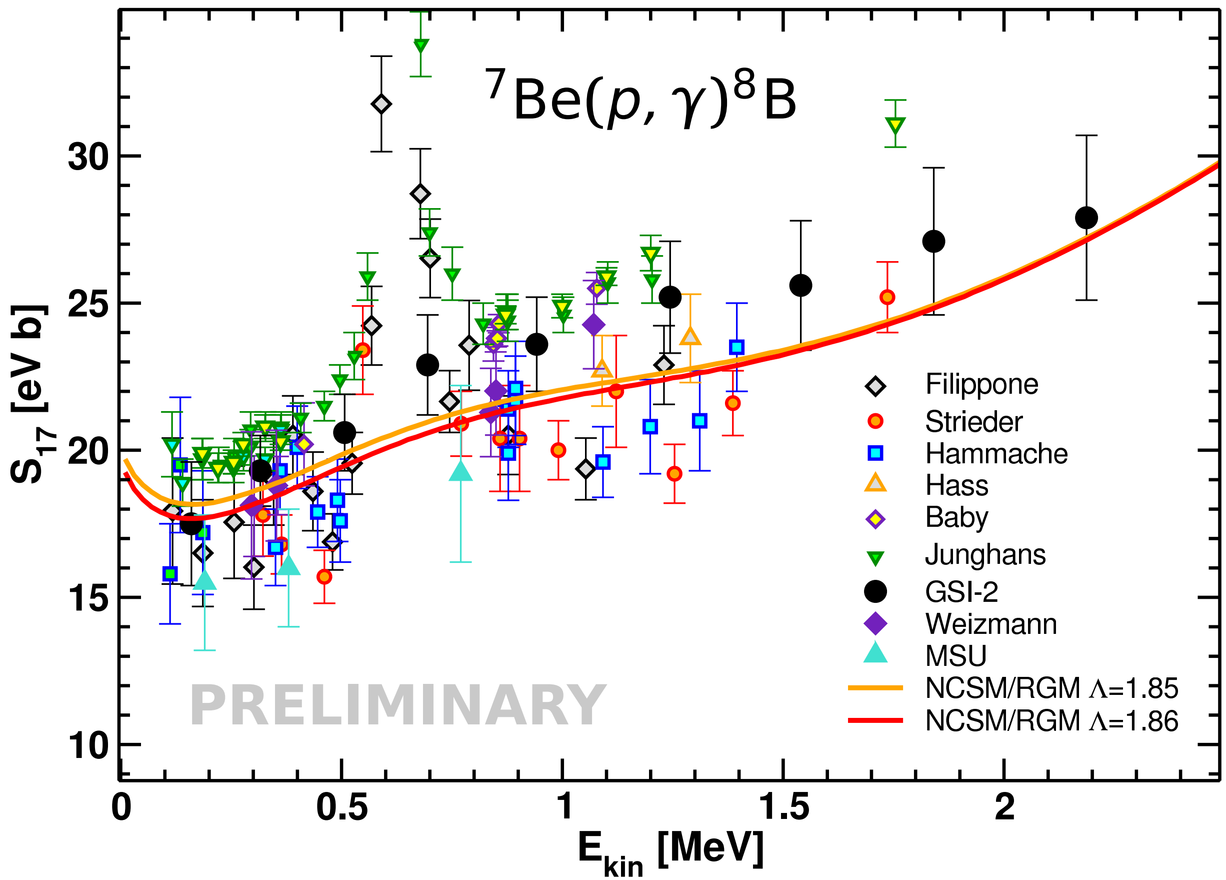


- IT-NCSM gives access to **complete spectroscopy of p- and sd-shell nuclei** starting from chiral NN+3N interactions

Bridge to Ab-Initio Reaction Theory

with P. Navrátil (TRIUMF) & S. Quaglioni (LLNL)

- **NCSM/RGM**: combine Resonating Group Method for description of relative projective-target motion with IT-NCSM for the description of target nucleus



- astrophysical S-factor for proton capture on ^{7}Be
- IT-NCSM wave functions for ^{7}Be for up to 8 eigenstates
- solution of the RGM with kernels involving the full many-body information
- SRG-evolved chiral NN interaction with α adjusted to reproduce ^{8}B energy relative to threshold

Conclusions

- new era of **ab-initio nuclear structure and reaction theory** connected to QCD via chiral EFT
  - chiral EFT as universal starting point... some formal issues remain
- consistent **inclusion of 3N interactions** in similarity transformations & many-body calculations
  - breakthrough in computation & handling of 3N matrix elements
- **innovations in many-body theory**: extended reach of exact methods & improved control over approximations
  - versatile toolbox for different observables & mass ranges
- many **exciting applications** ahead...
- see also: HK23.4, HK23.6, HK33.3, HK41.5

Epilogue

- **thanks to my group & my collaborators**
  - **S. Binder**, **A. Calci**, B. Erler, A. Günther, M. Hild, H. Krutsch, **J. Langhammer**, P. Papakonstantinou, S. Reinhardt, F. Schmitt, C. Stumpf, K. Vobig, R. Wirth
    Institut für Kernphysik, TU Darmstadt
  - **P. Navrátil**
    TRIUMF Vancouver, Canada
  - S. Quaglioni
    LLNL Livermore, USA
  - H. Hergert, P. Piecuch
    Michigan State University, USA
  - C. Forssén
    Chalmers University, Sweden
  - H. Feldmeier, T. Neff,...
    GSI Helmholtzzentrum

COMPUTING TIME

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SFB 634

Deutsche Forschungsgemeinschaft DFG

HIC for FAIR
Helmholtz International Center

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