Towards Nuclear Structure from Consistent Chiral NN+3N Interactions

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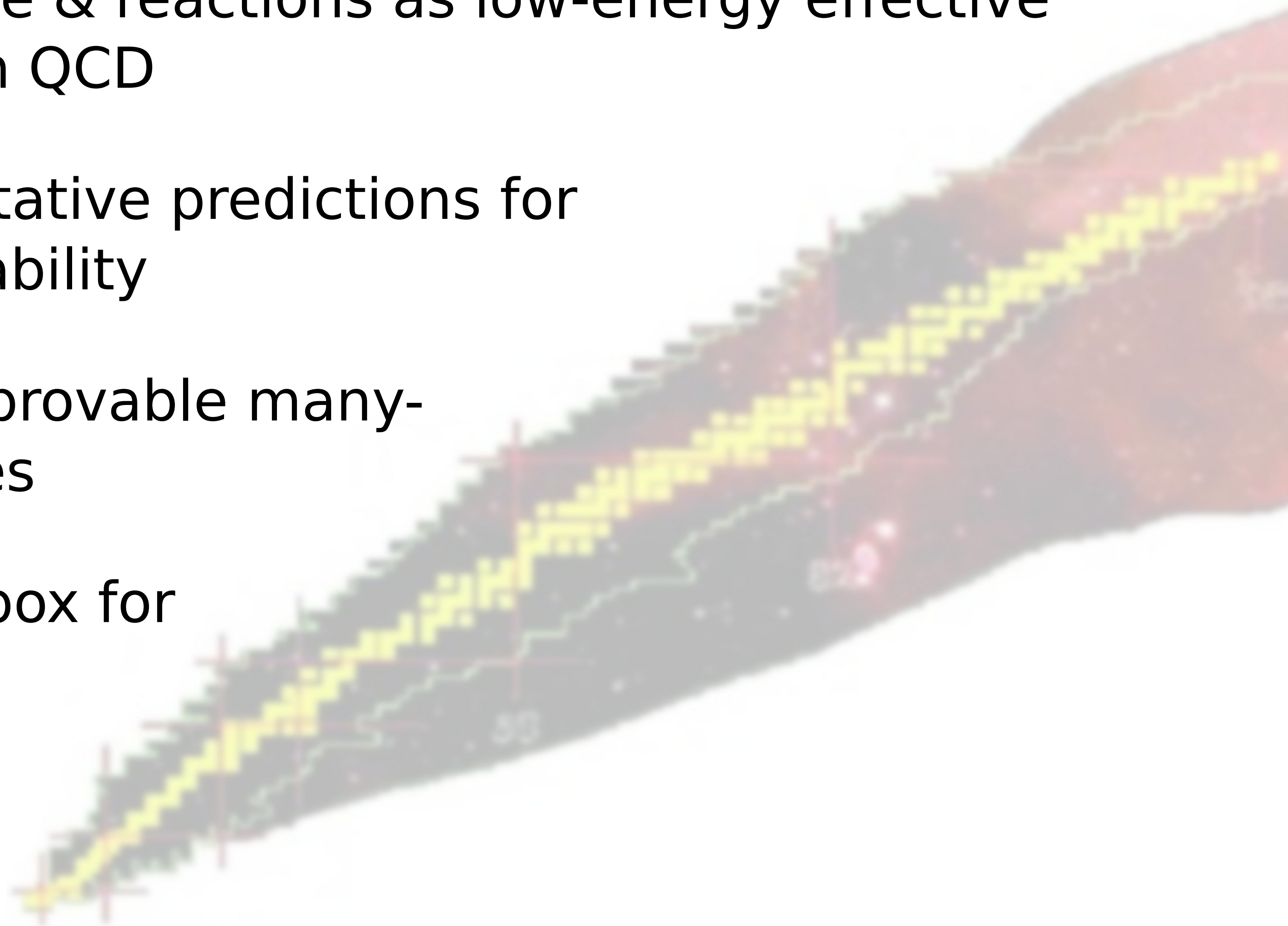
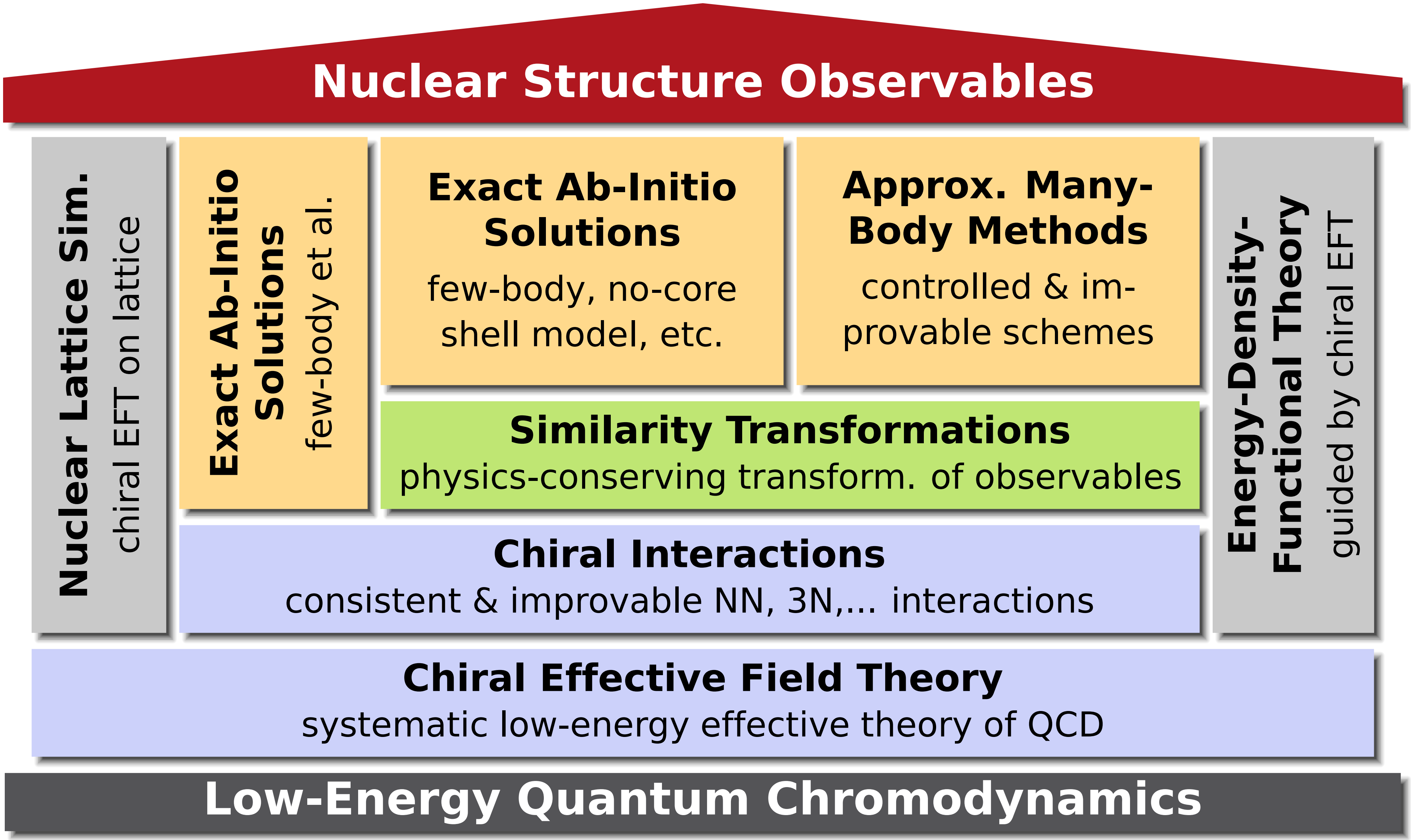
Nuclear Structure Theory — Wish List



- nuclear structure & reactions as low-energy effective theory based on QCD
- robust & quantitative predictions for nuclei far-off stability
- controlled & improvable many-body approaches
- theoretical toolbox for all masses and observables

Ab Initio Nuclear Structure



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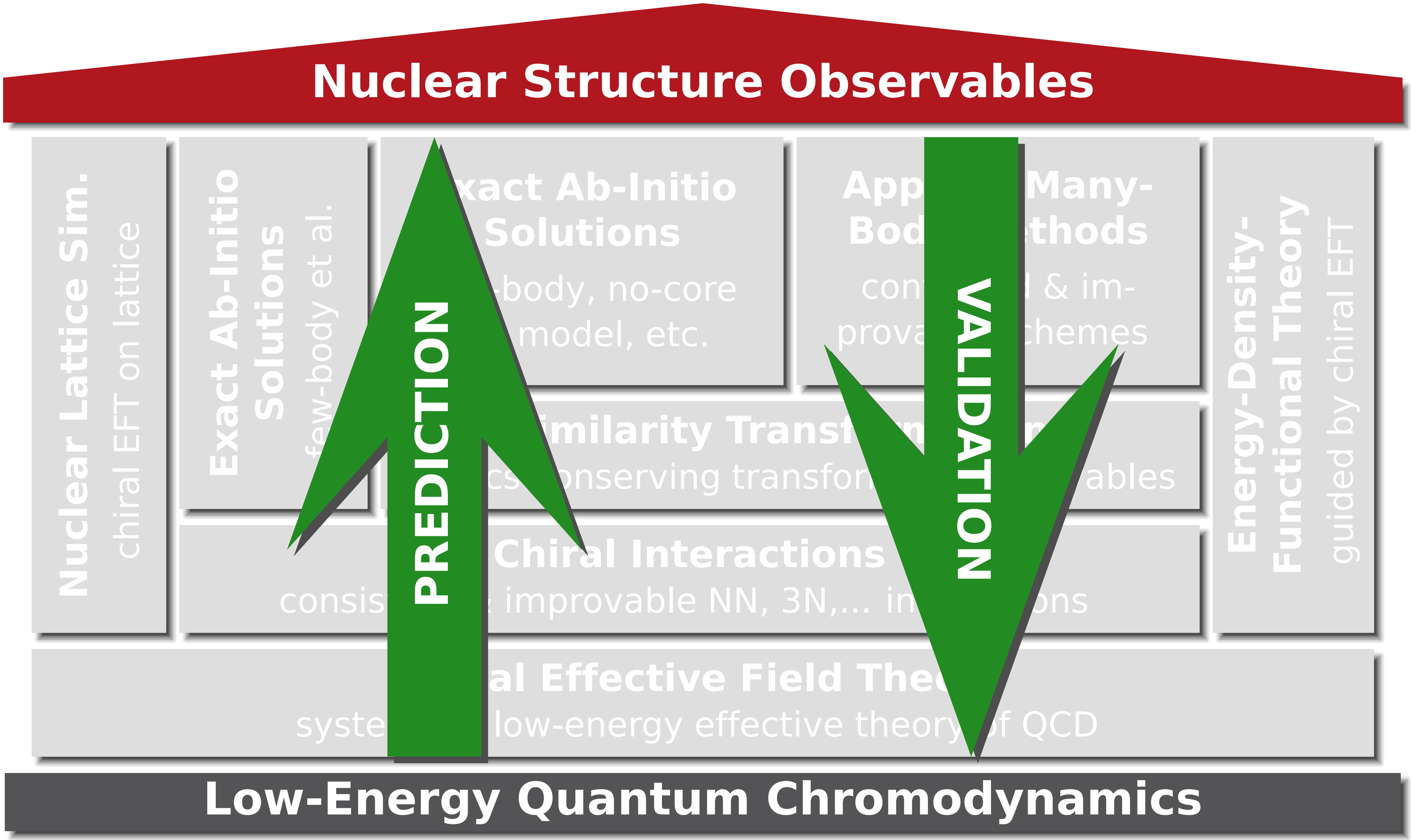

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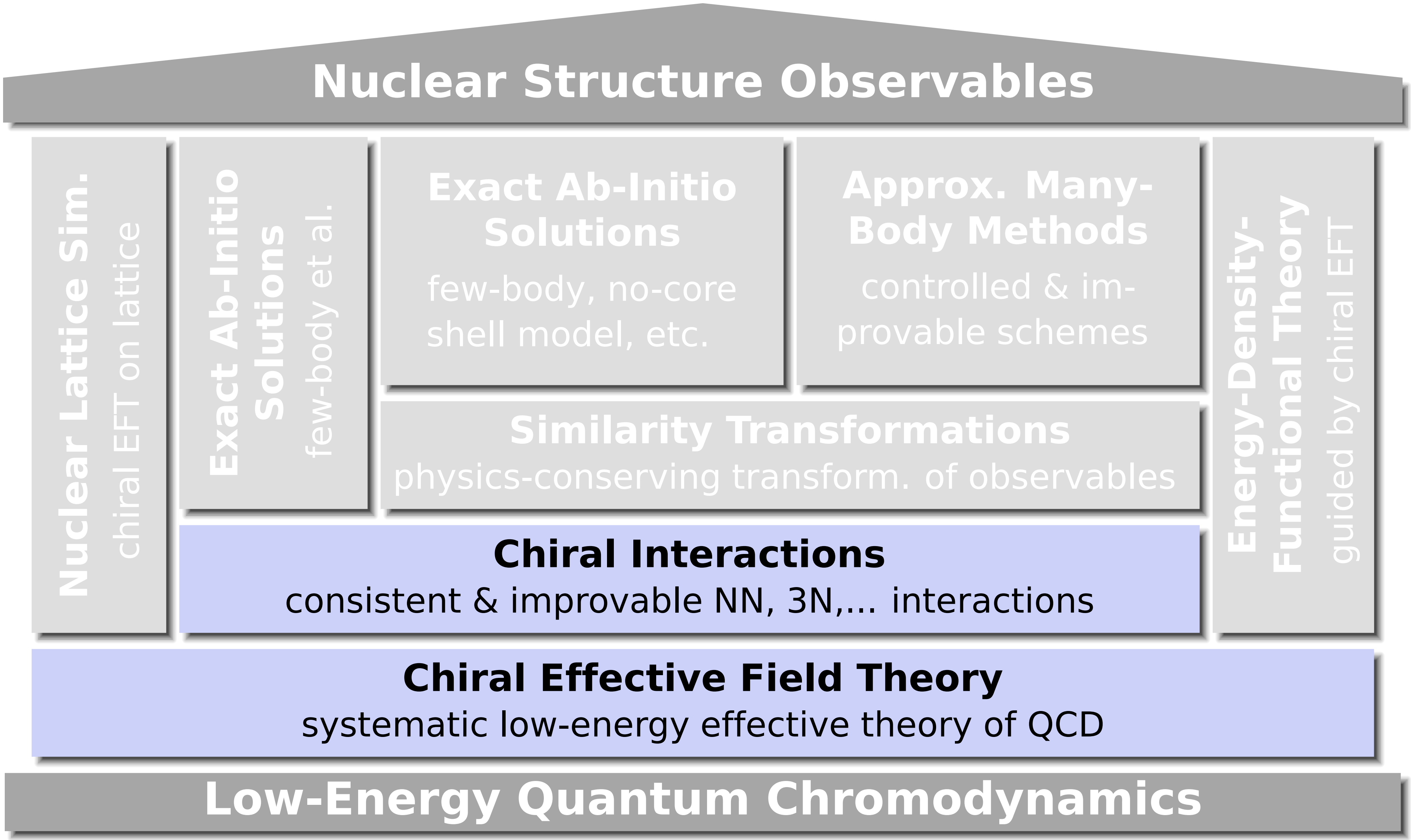
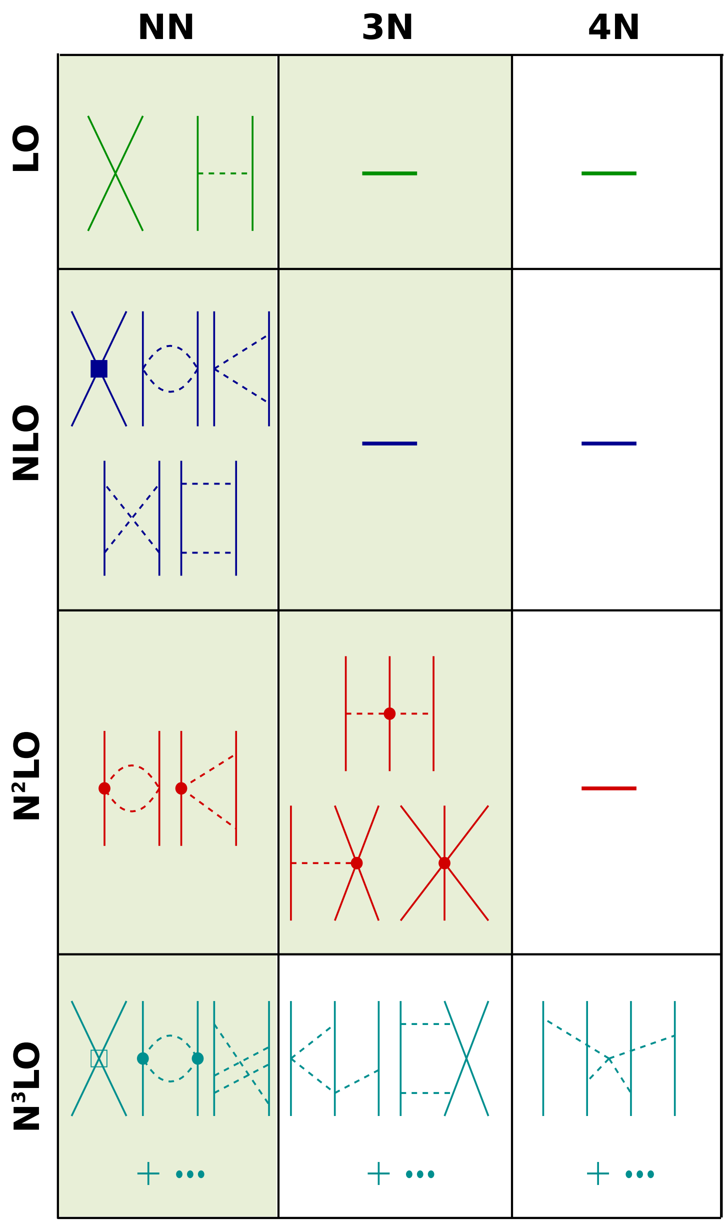


Nuclear Interactions from Chiral EFT

- 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^3LO
  - explicit inclusion of Δ-resonance
  - formal issues: power counting, renormalization, cutoff choice,...



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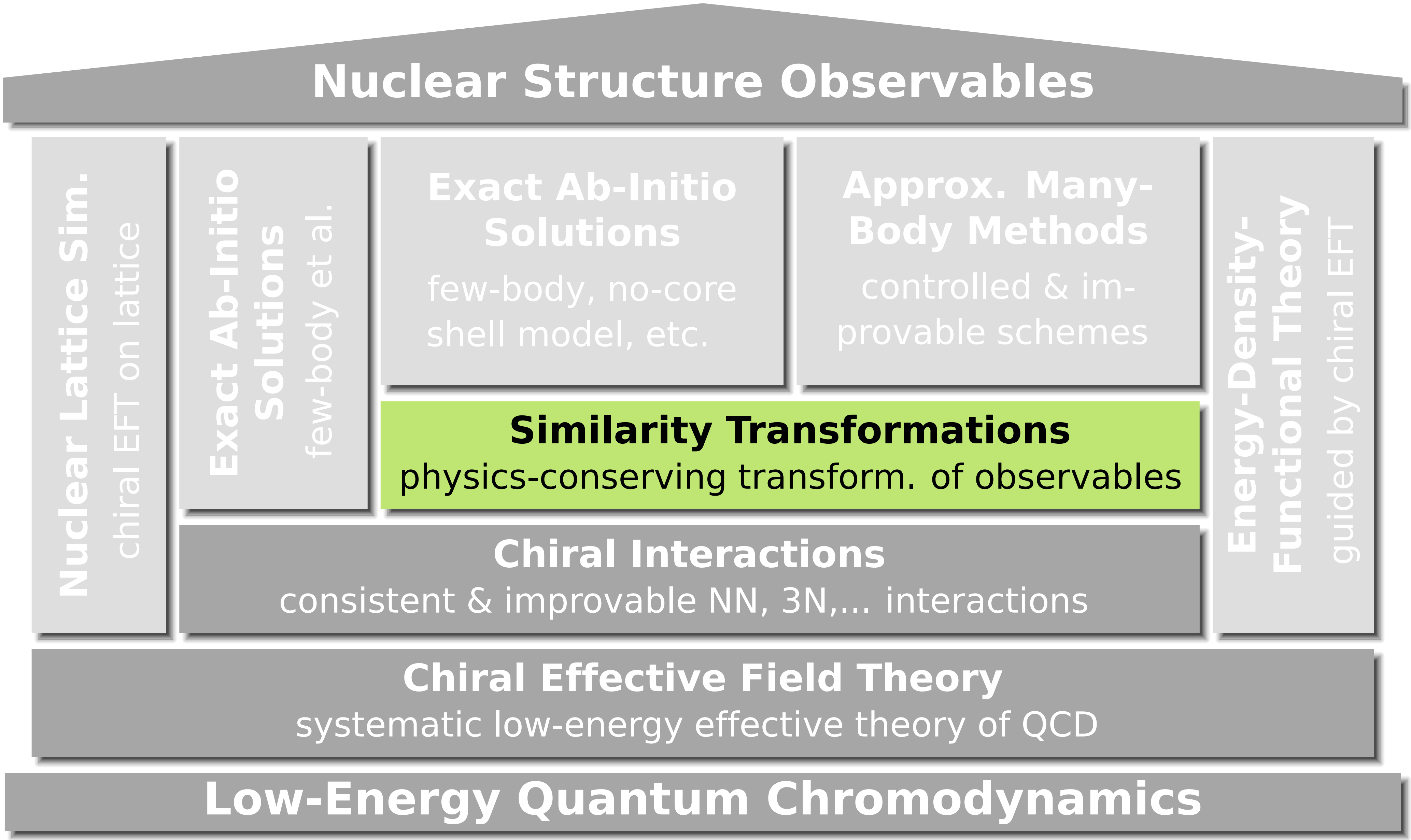
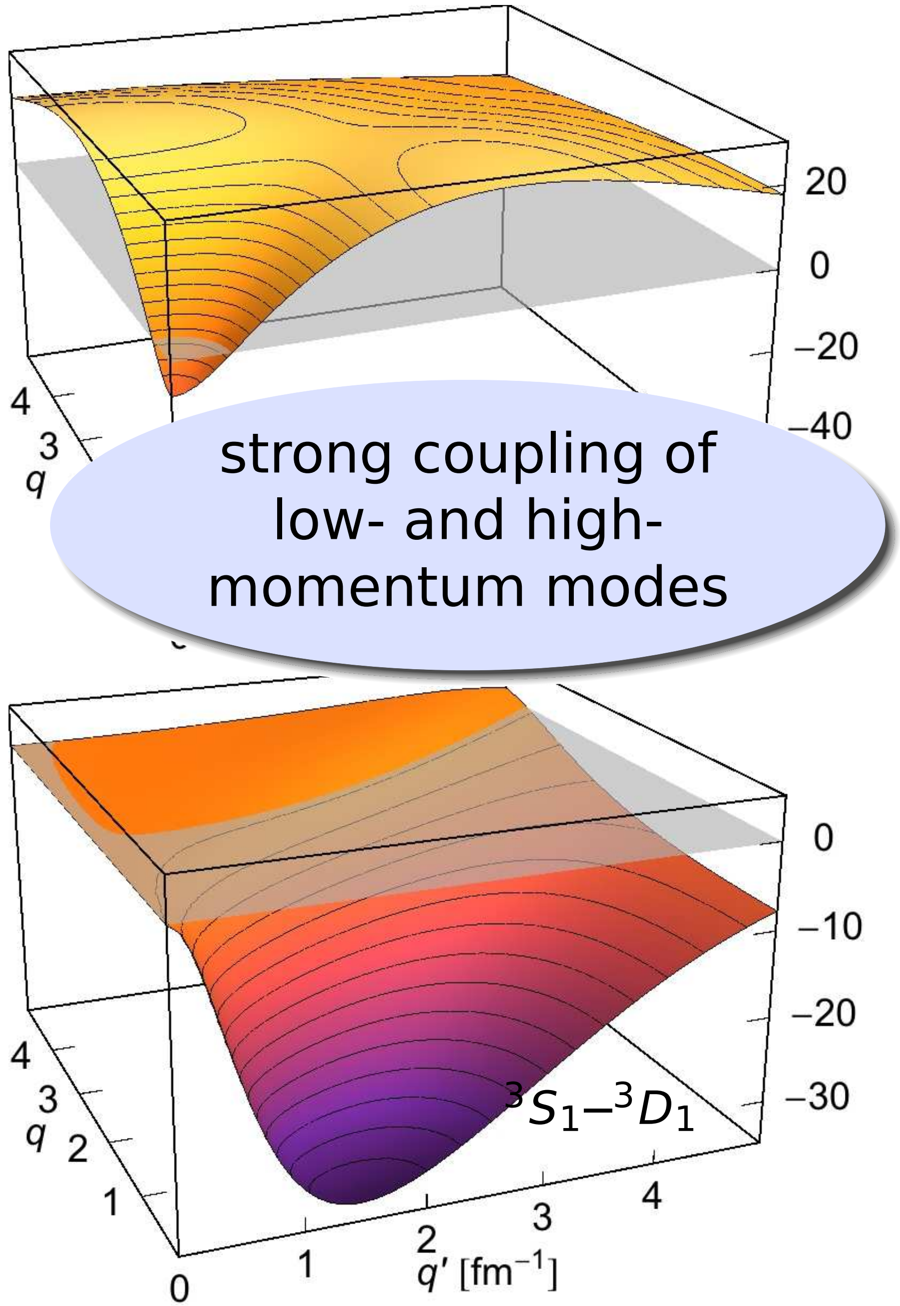


Why Similarity Transformations?

momentum-space matrix elements

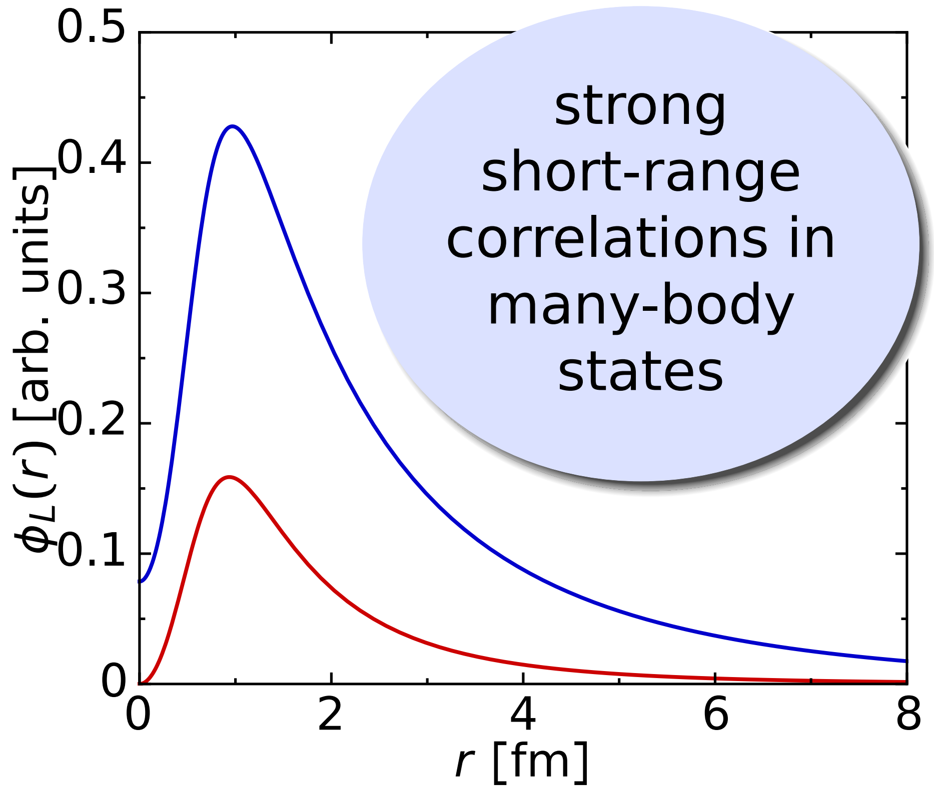


strong coupling of low- and high-momentum modes

Argonne V18

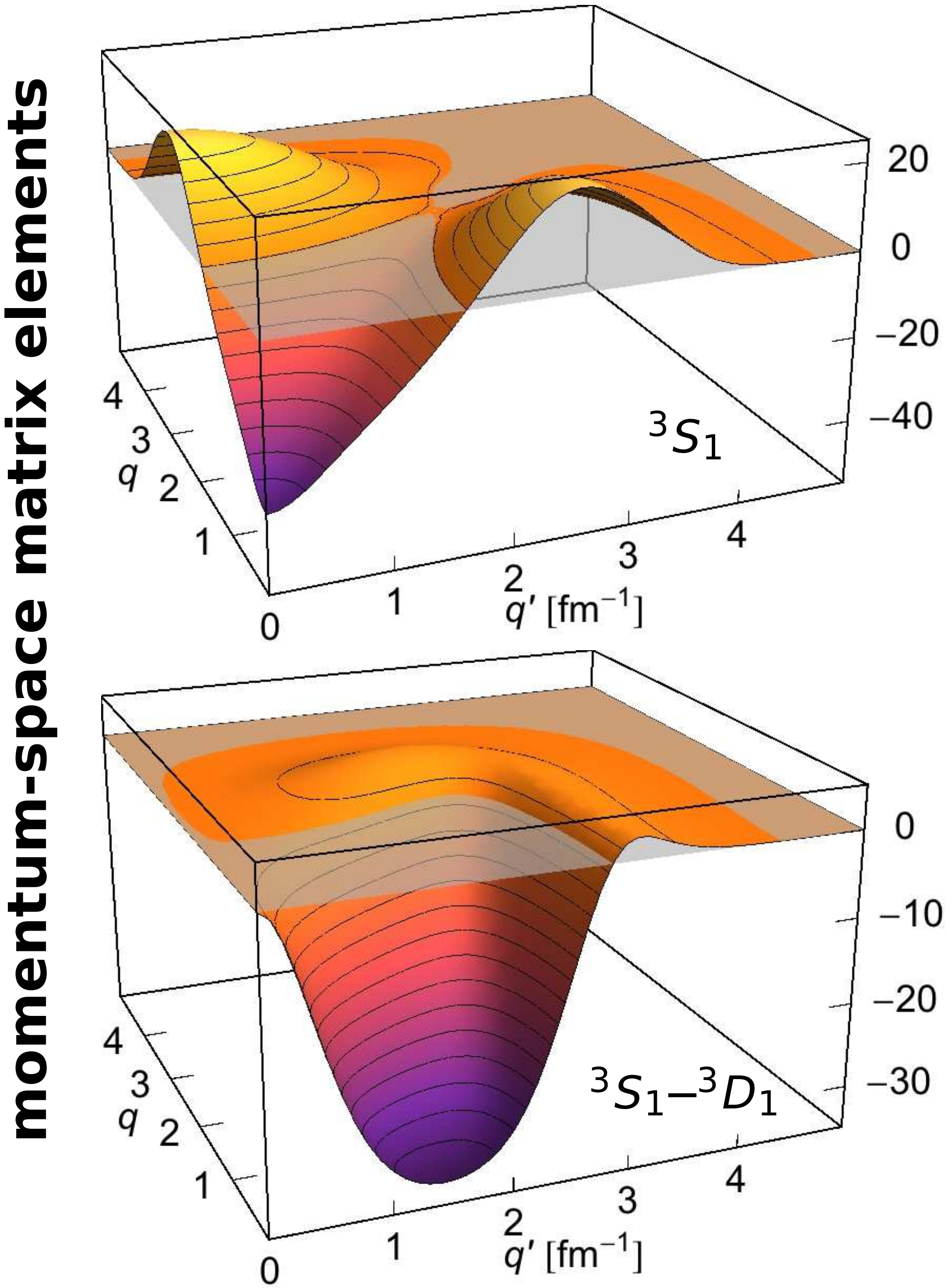
$J^\pi = 1^+, T = 0$

deuteron wave-function



strong short-range correlations in many-body states

Why Similarity Transformations?

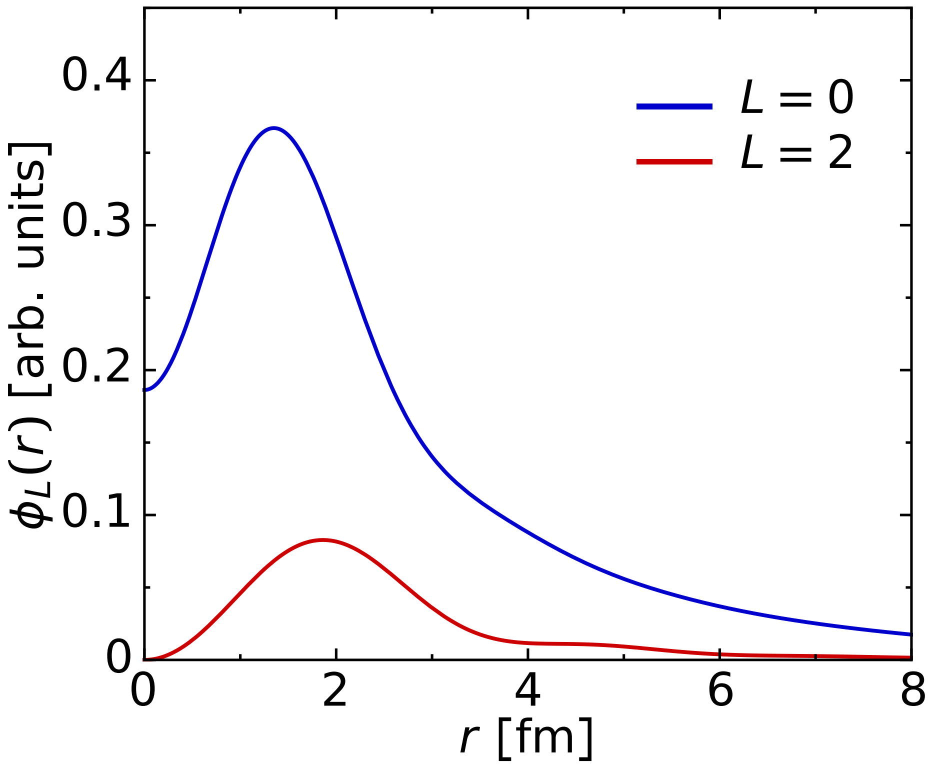


chiral N^{3}LO

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

simplicity and flexibility are great advantages of the SRG approach

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

- **unitary transformation** of Hami

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

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

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

- **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 of Matrix Elements

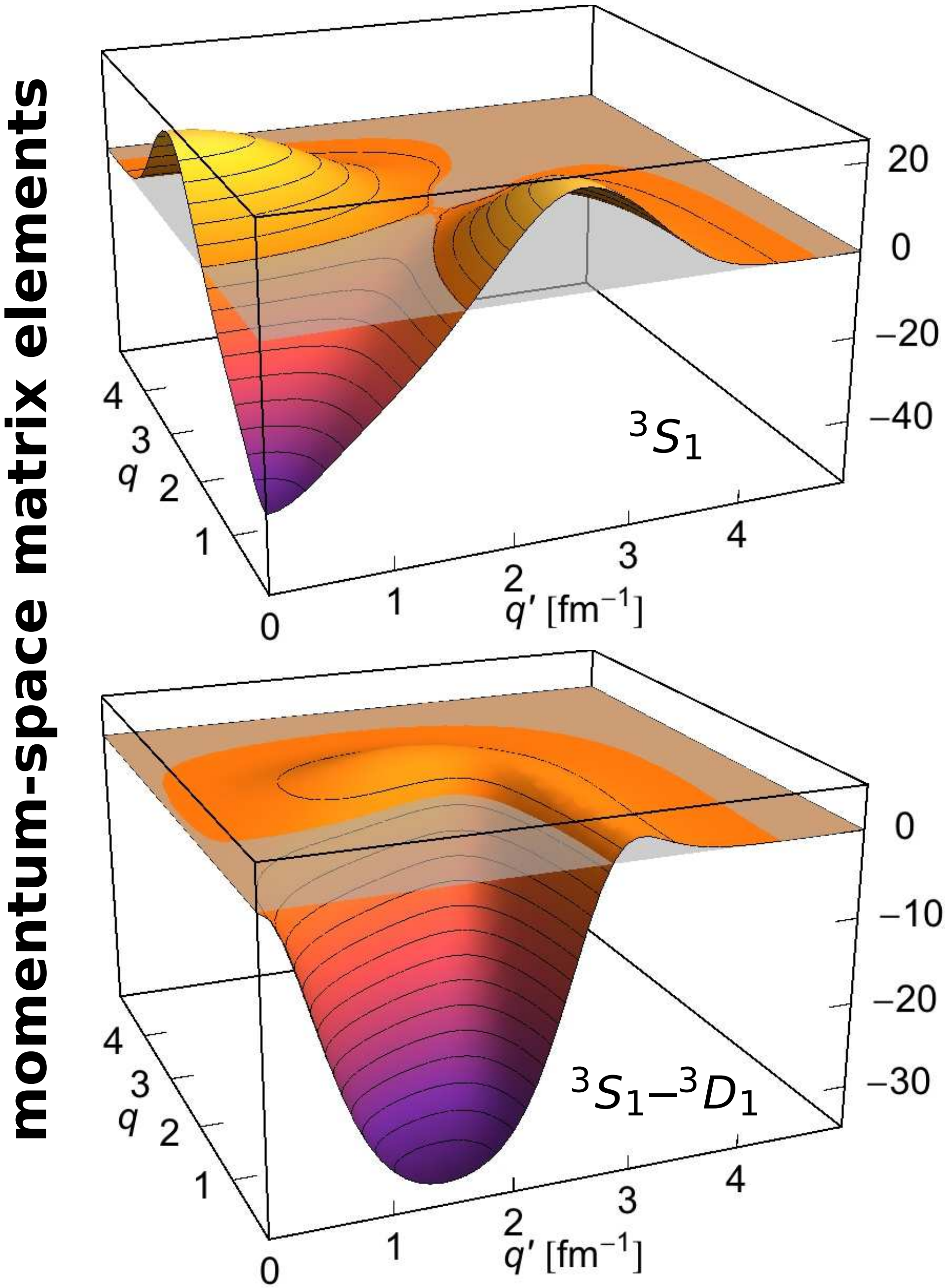
- convert Fock-space operator equations into **coupled evolution equations for matrix elements** in n-body Hilbert space

- $n = 2$: use **antisym. relative LS-coupled two-body states**
  - momentum space: $\left|q(LS)JT\right\rangle$
  - harmonic oscillator: $\left|n(LS)JT\right\rangle$

- system of **coupled evolution equations** for each $J^{\pi}ST$-block

$$\frac{\mathrm{d}}{\mathrm{d}\alpha}\langle n(LS)JT|\,\widetilde{\mathrm{H}}_{\alpha}\,|n'(L'S)JT\rangle = (2\mu)^2 \sum_{n''L''}\sum_{n'''L'''}\Big[\langle nL\ldots|\,\mathrm{T}_{\text{int}}\,|n''L''\ldots\rangle\,\langle n''L''\ldots|\,\widetilde{\mathrm{H}}_{\alpha}\,|n'''L'''\ldots\rangle\,\langle n'''L'''\ldots|\,\widetilde{\mathrm{H}}_{\alpha}\,|n'L'\ldots\rangle$$
$$-2\langle nL\ldots|\,\widetilde{\mathrm{H}}_{\alpha}\,|n''L''\ldots\rangle\,\langle n''L''\ldots|\,\mathrm{T}_{\text{int}}\,|n'''L'''\ldots\rangle\,\langle n'''L'''\ldots|\,\widetilde{\mathrm{H}}_{\alpha}\,|n'L'\ldots\rangle$$
$$+\langle nL\ldots|\,\widetilde{\mathrm{H}}_{\alpha}\,|n''L''\ldots\rangle\,\langle n''L''\ldots|\,\widetilde{\mathrm{H}}_{\alpha}\,|n'''L'''\ldots\rangle\,\langle n'''L'''\ldots|\,\mathrm{T}_{\text{int}}\,|n'L'\ldots\rangle\Big]$$

SRG Evolution in Two-Body Space

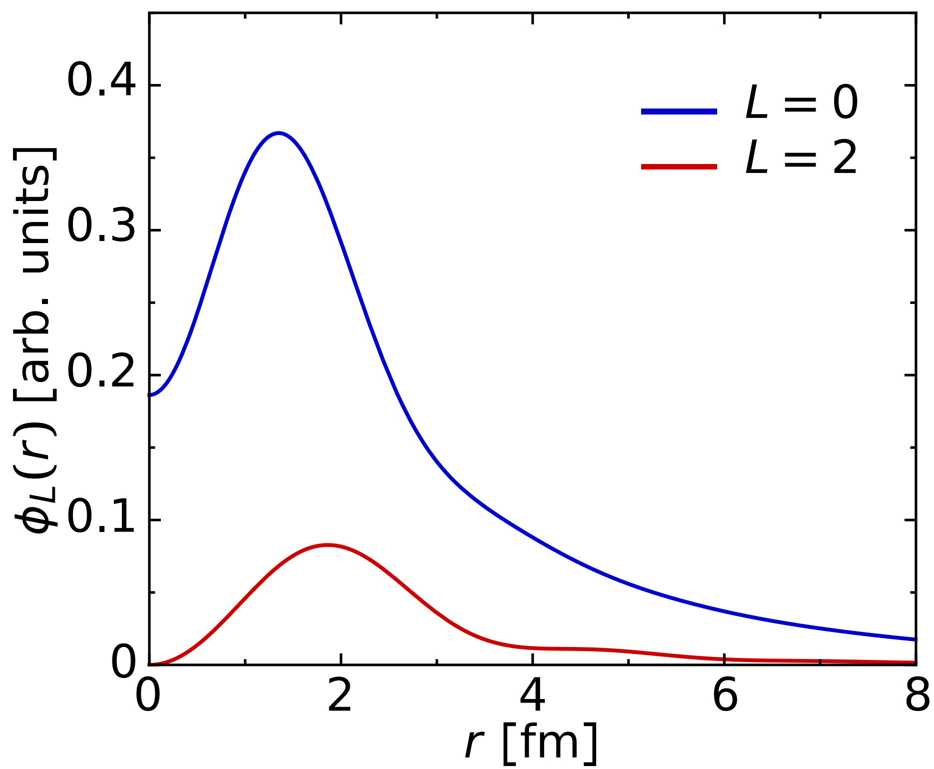


$\alpha = 0.000\,\mathrm{fm}^4$

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

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

deuteron wave-function



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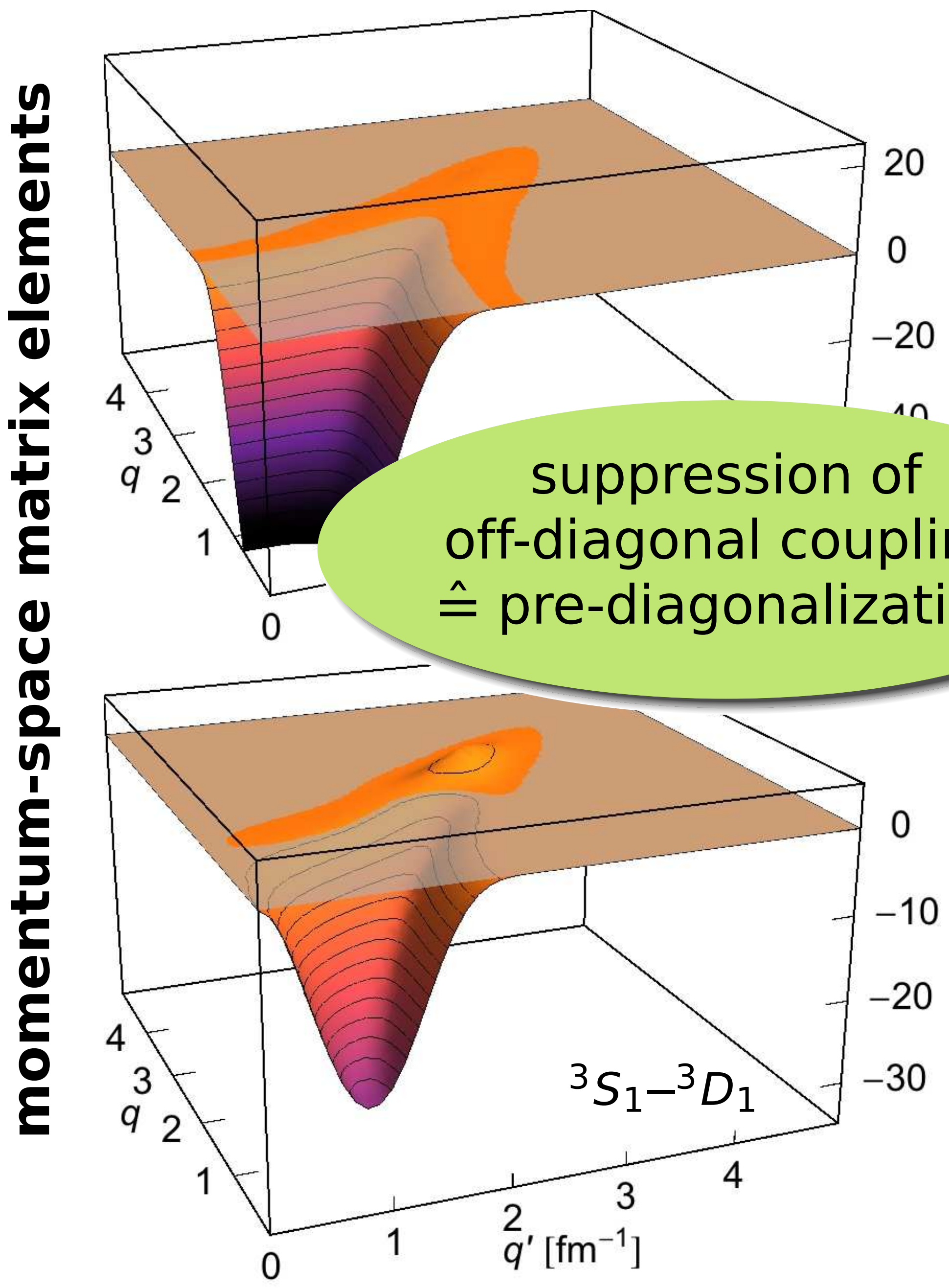


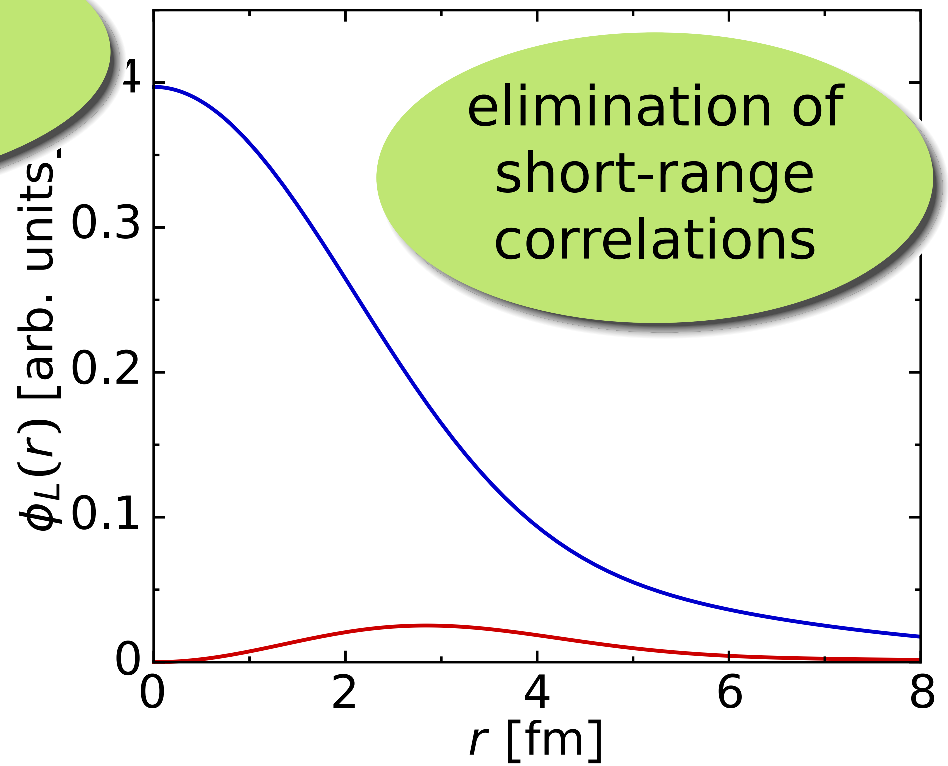
suppression of
off-diagonal coupling
≙ pre-diagonalization

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

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

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

deuteron wave-function



elimination of
short-range
correlations

SRG Evolution of Matrix Elements

- convert Fock-space operator equations into **coupled evolution equations for matrix elements** in n-body Hilbert space

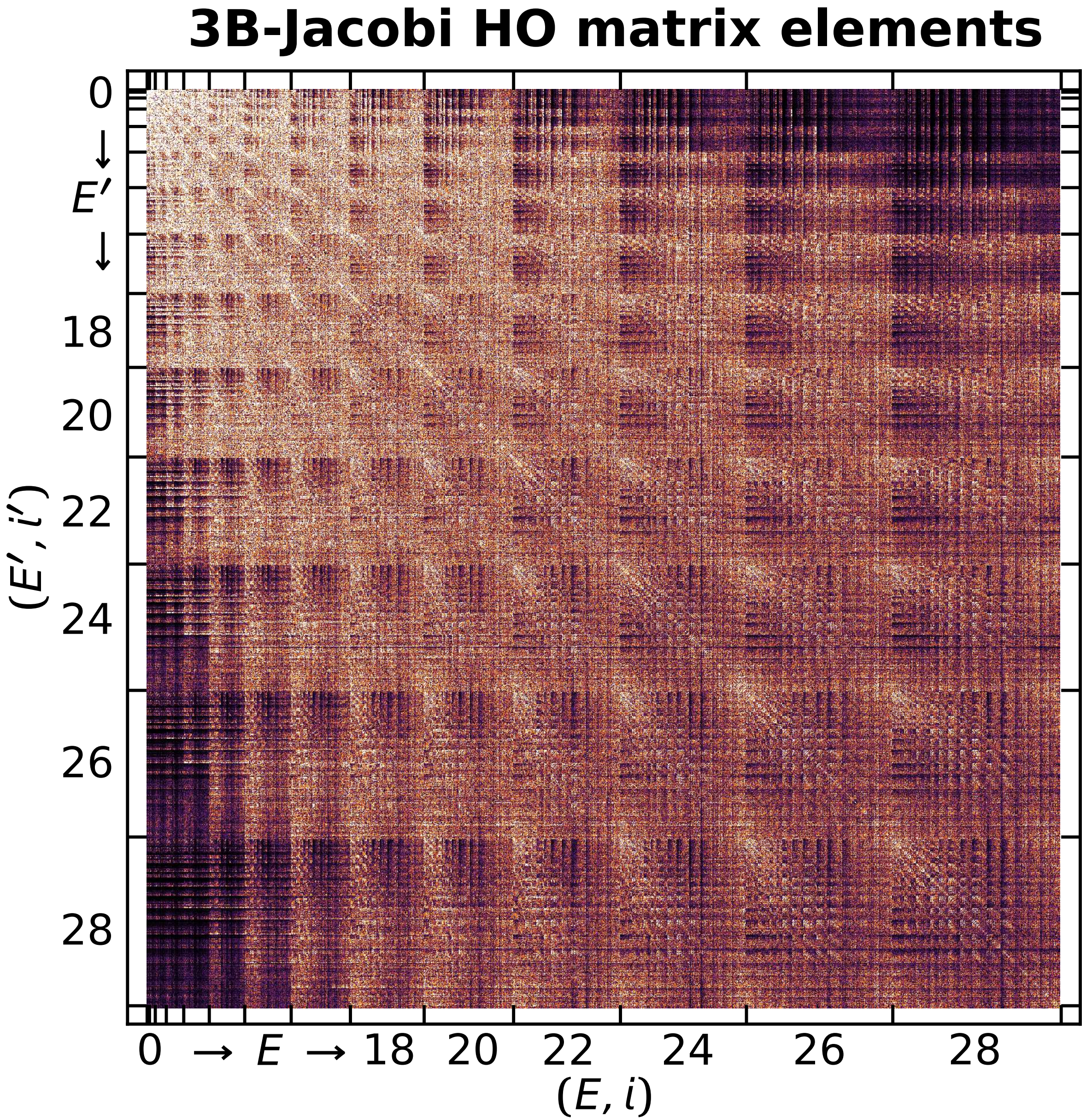
- $n = 3$: use **antisym. Jacobi-coordinate three-body states**
  - harmonic oscillator: $|E i J^\pi T\rangle$

- system of **coupled evolution equations** for each $J^\pi T$-block

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

- we use $E_{\mathrm{SRG}} = 40$ for $J \leq 5/2$ and ramp down to 24 in steps of 4 (sufficient to converge the intermediate sums for $\hbar\Omega \gtrsim 16\,\mathrm{MeV}$)

SRG Evolution in Three-Body Space



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

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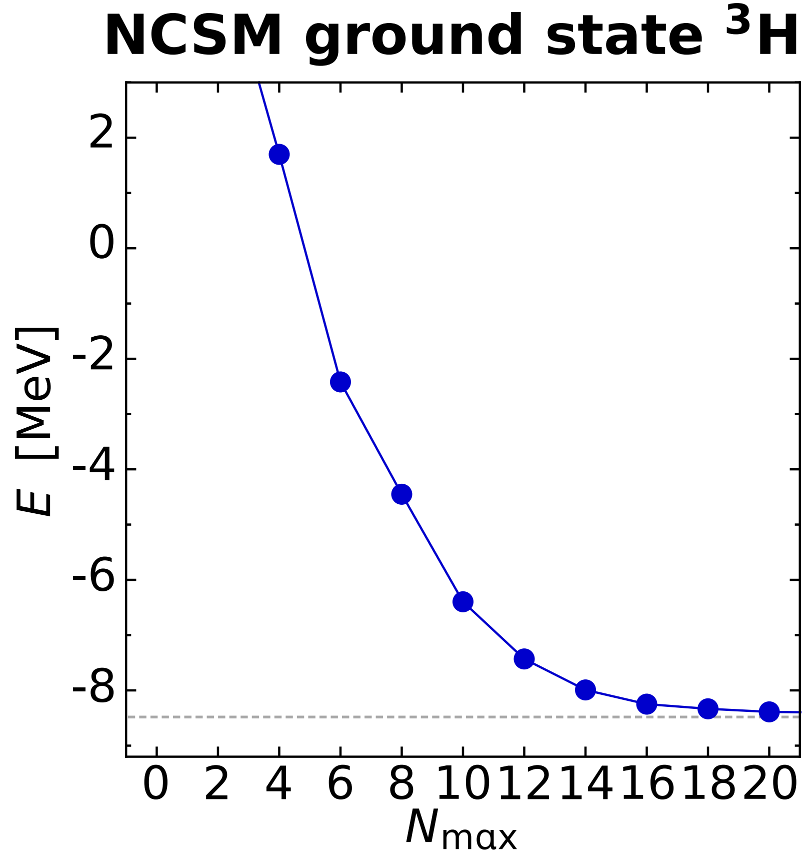
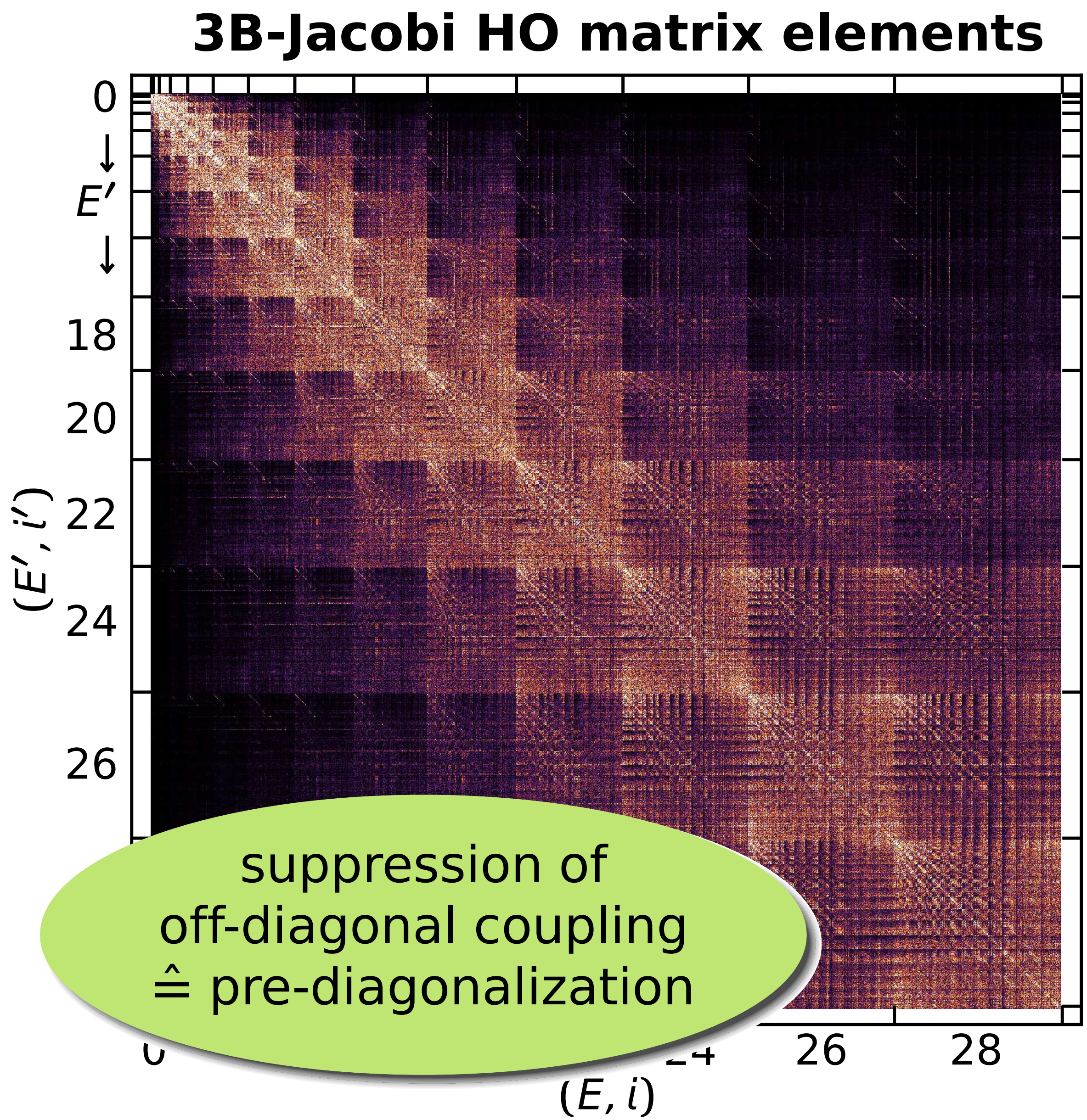
$J^\pi = \frac{1}{2}^+, T = \frac{1}{2}, \hbar\Omega = 28\,\mathrm{MeV}$



SRG Evolution in Three-Body Space



suppression of
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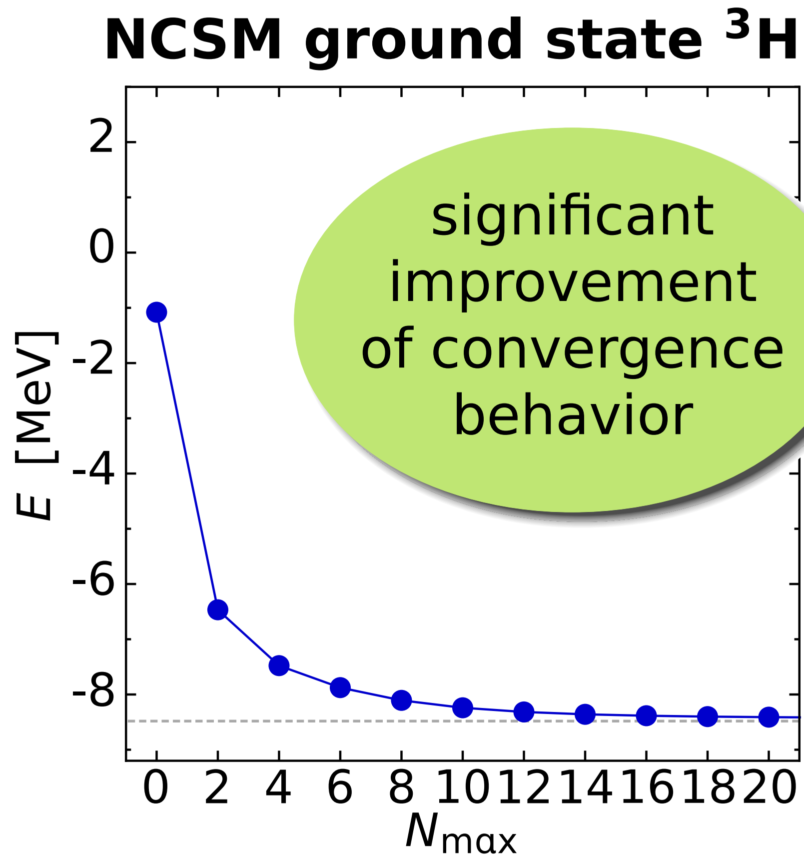

significant
improvement
of convergence
behavior

Calculations in A-Body Space

- **cluster decomposition**: decompose evolved Hamiltonian from 2B/3B space into irreducible n-body contributions $\widetilde{H}_\alpha^{[n]}$

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

- **cluster truncation**: can construct cluster-orders up to $n = 3$ from evolution in 2B and 3B space, have to discard $n > 3$
  - only the **full evolution in A-body space** is formally unitary and conserves A-body energy eigenvalues (independent of α)
  - α-dependence of eigenvalue **milto-** **nian** measures impact of s

α-variation provides a **diagnostic tool** to assess the omitted induced 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 & BLAS; 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

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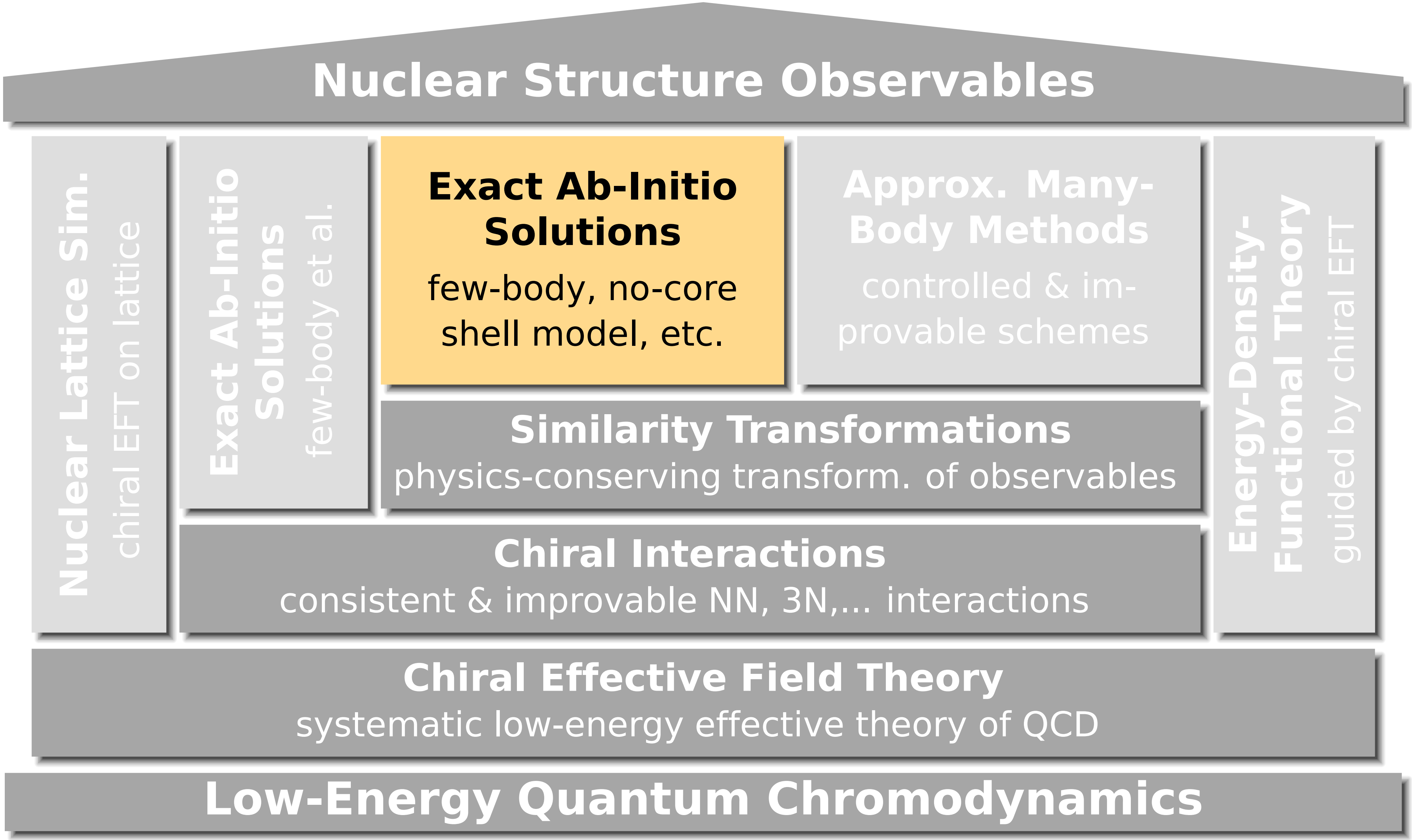


No-Core Shell Model (NCSM)

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

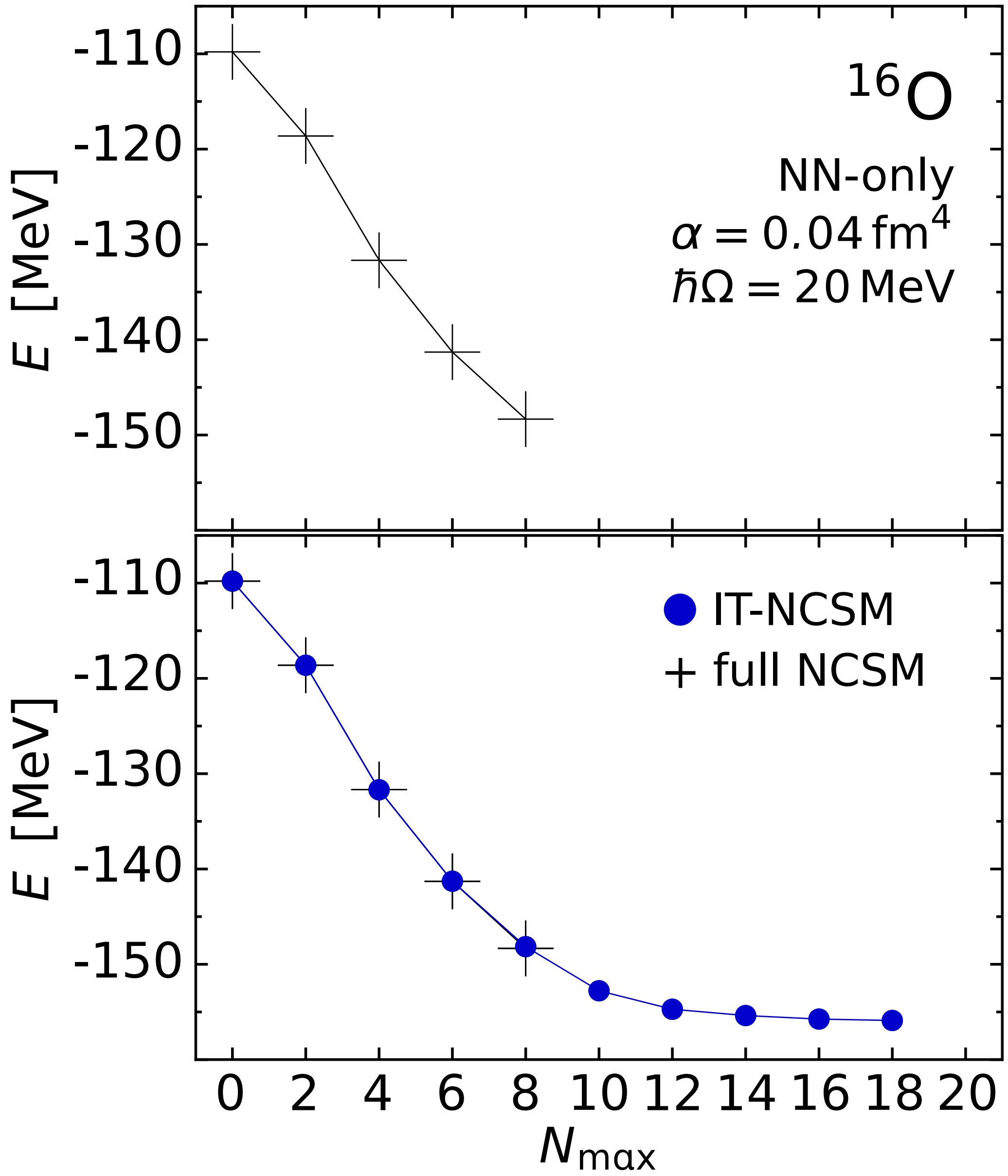
- construct matrix representation of Hamiltonian using a **basis of HO Slater determinants** truncated w.r.t. HO excitation energy $N_{max}\hbar\Omega$
- solve **large-scale eigenvalue problem** for a few extremal eigenvalues
- **all relevant observables** can be computed from the eigenstates
- range 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

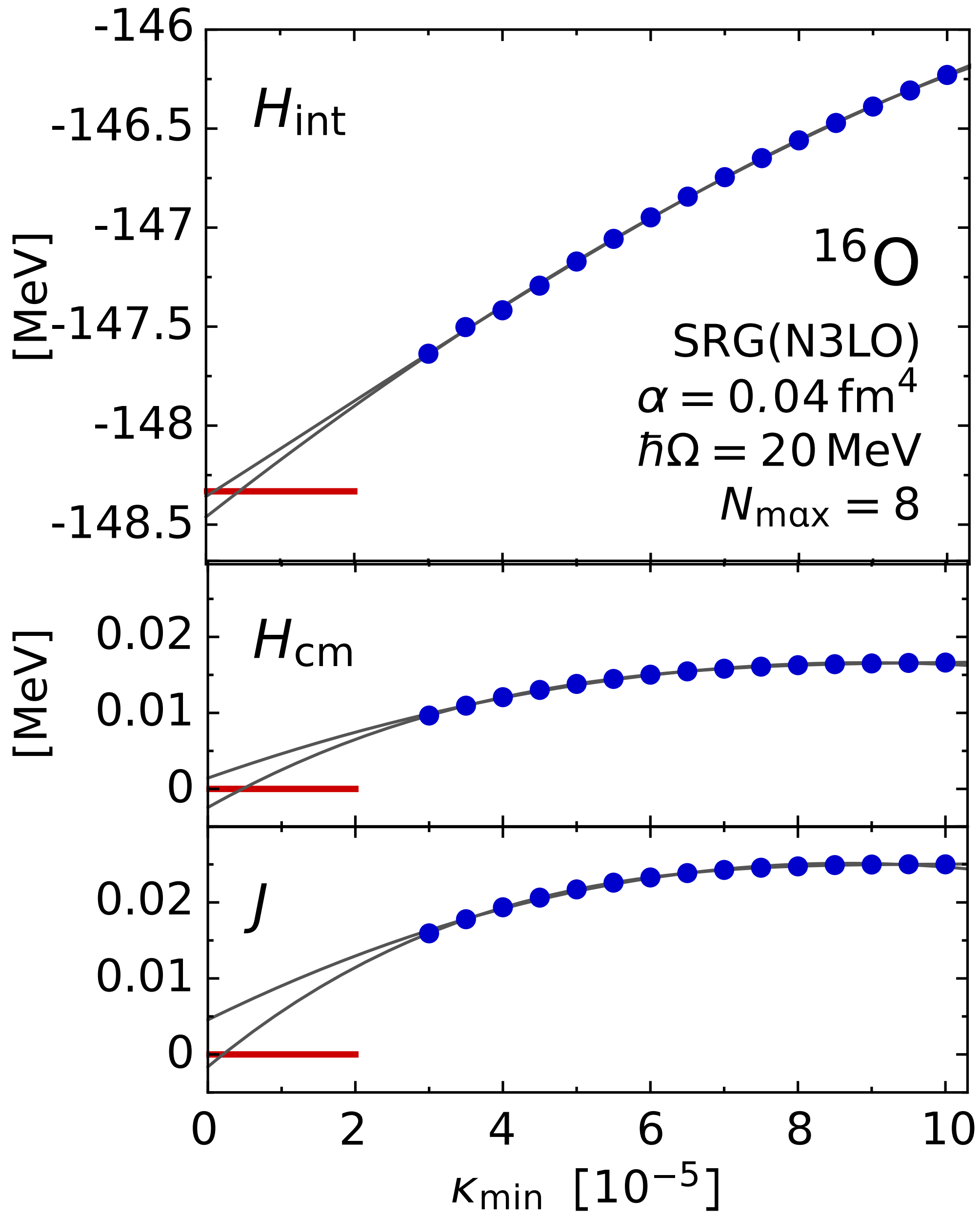
- given an initial approximation $|\Psi_{\text{ref}}^{(m)}\rangle$ for the **target states**
- **measure the importance** of individual basis state $|\Phi_\nu\rangle$ via first-order multiconfigurational perturbation theory

$$\kappa_\nu^{(m)} = -\frac{\langle \Phi_\nu | H | \Psi_{\text{ref}}^{(m)} \rangle}{\epsilon_\nu - \epsilon_{\text{ref}}}$$

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

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

Threshold Extrapolation



- do calculations for a **sequence of importance thresholds κ_{min}**
- observables show smooth threshold dependence
- systematic approach to the **full NCSM limit**
- use **a posteriori extrapolation $\kappa_{min} \rightarrow 0$** of observables to account for effect of excluded configurations

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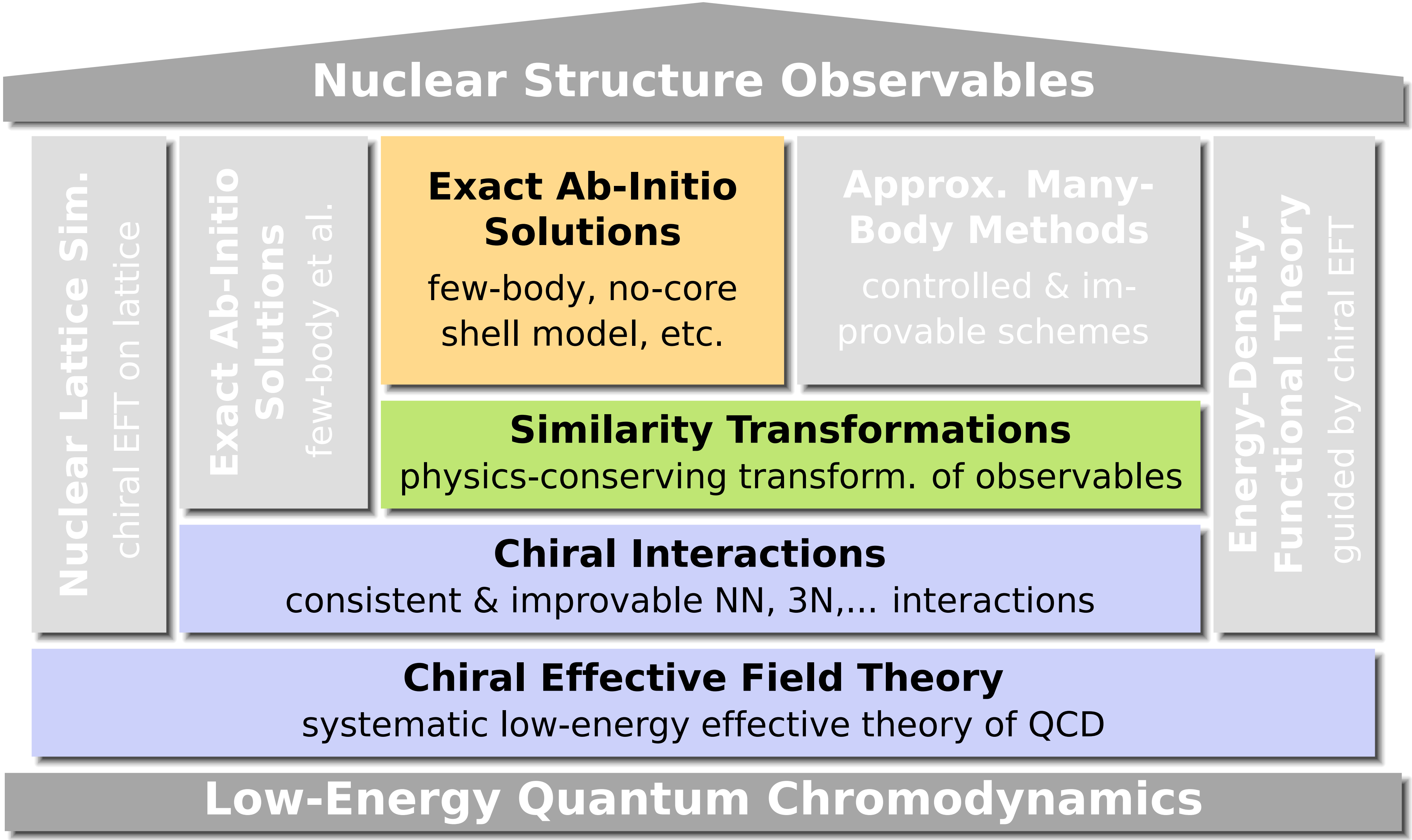


A Tale of Three Hamiltonians

Initial Hamiltonian

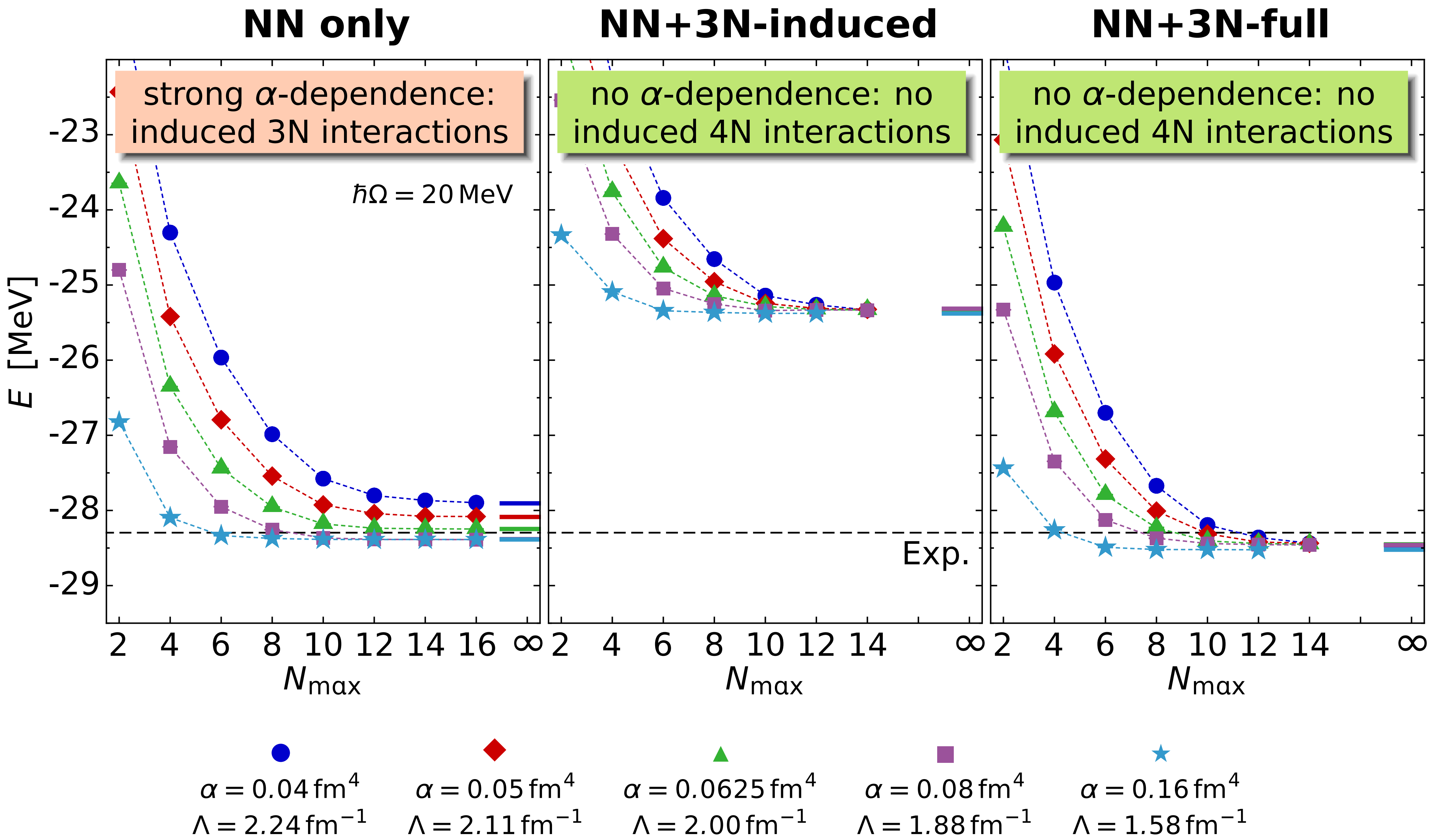
- NN: chiral interaction at N^3LO (Entem & Machleidt, 500 MeV)
- 3N: chiral interaction at N^2LO (c_D, c_E from ^3H binding & half-life)

SRG-Evolved Hamiltonians

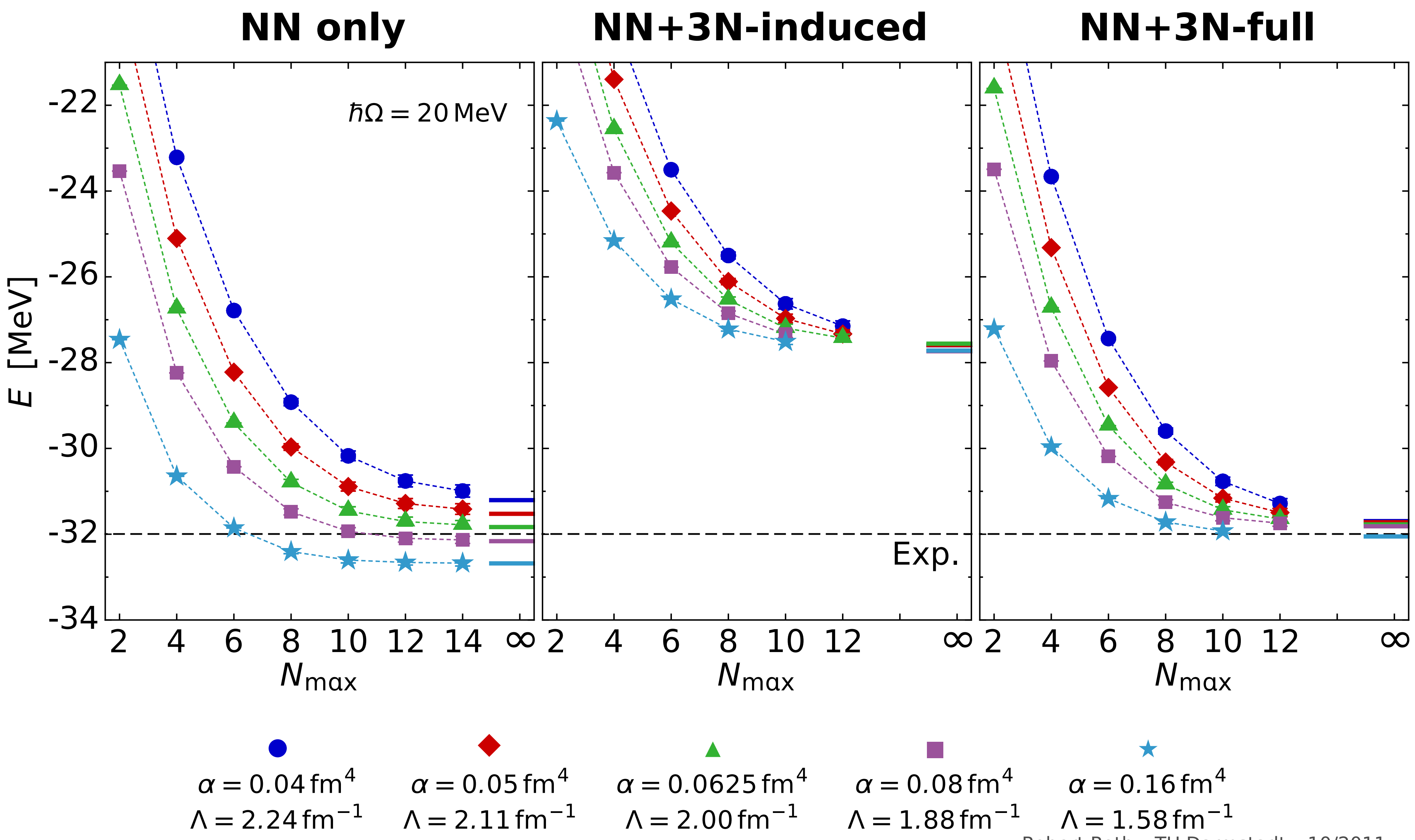
- **NN only**: start with NN initial Hamiltonian and keep two-body terms only
- **NN+3N-induced**: start with NN initial Hamiltonian and keep two- and three-body terms
- **NN+3N-full**: start with NN+3N in[...] two- and three-body terms

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

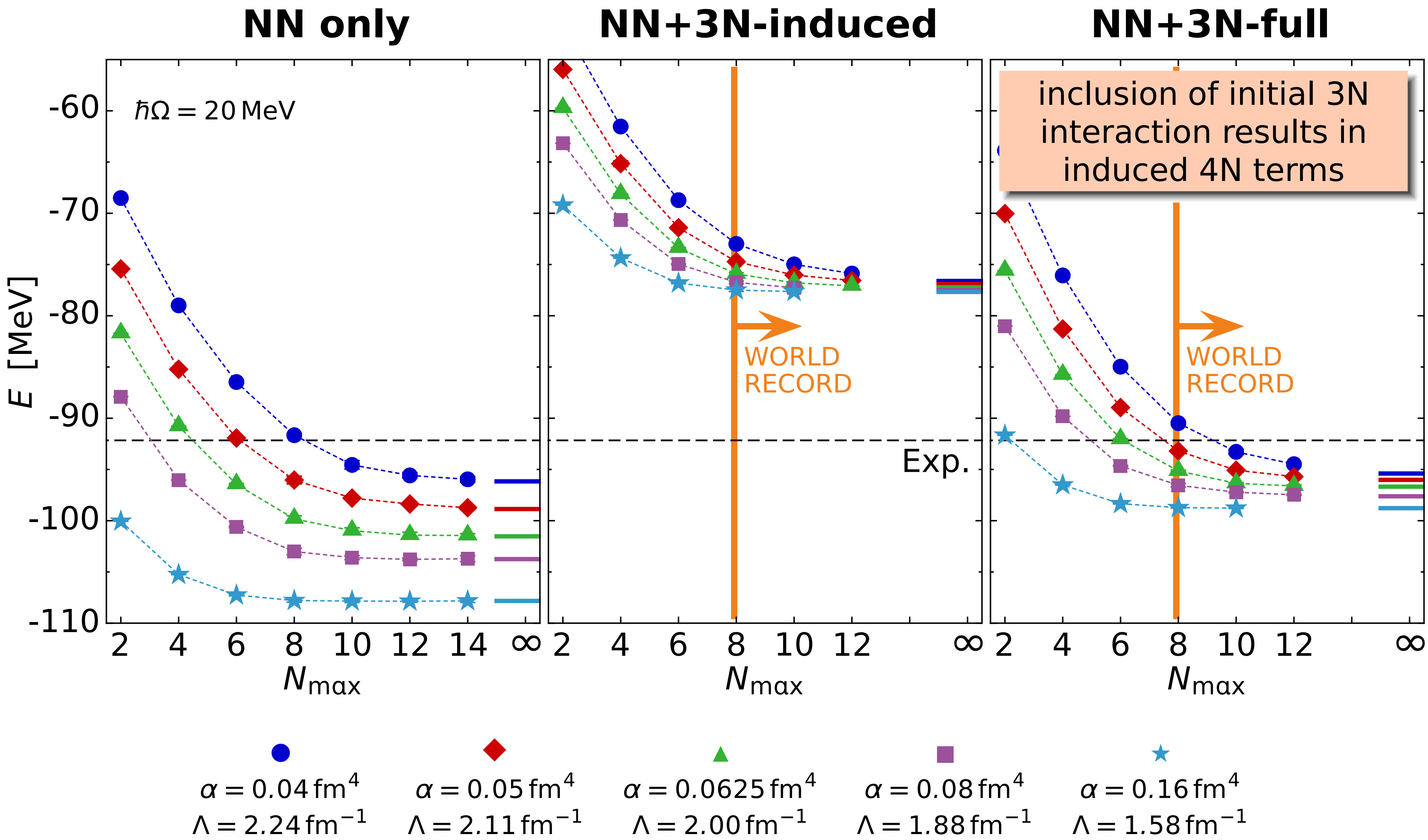
^{4}He: Ground-State Energies



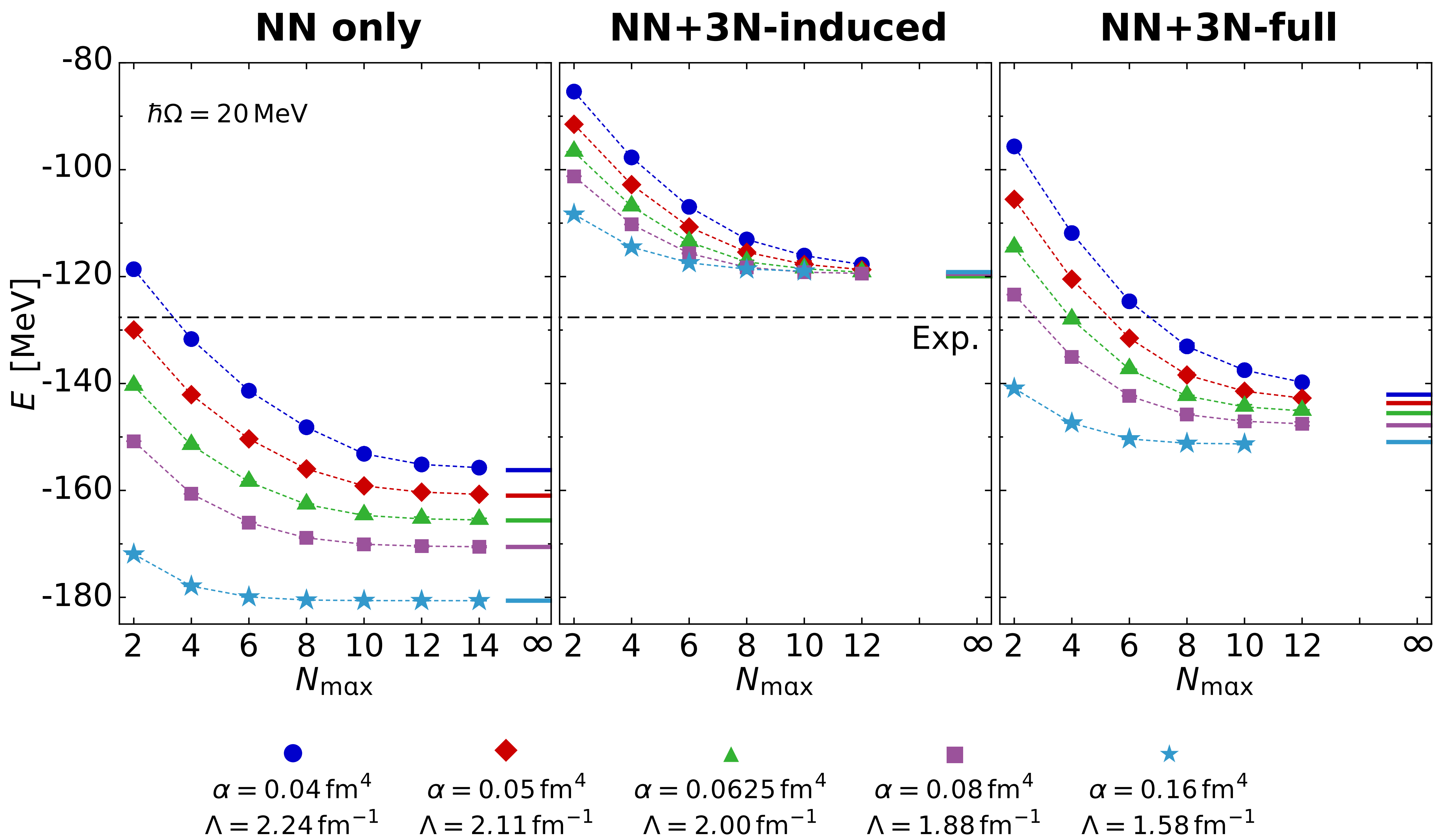
^{6}Li: Ground-State Energies



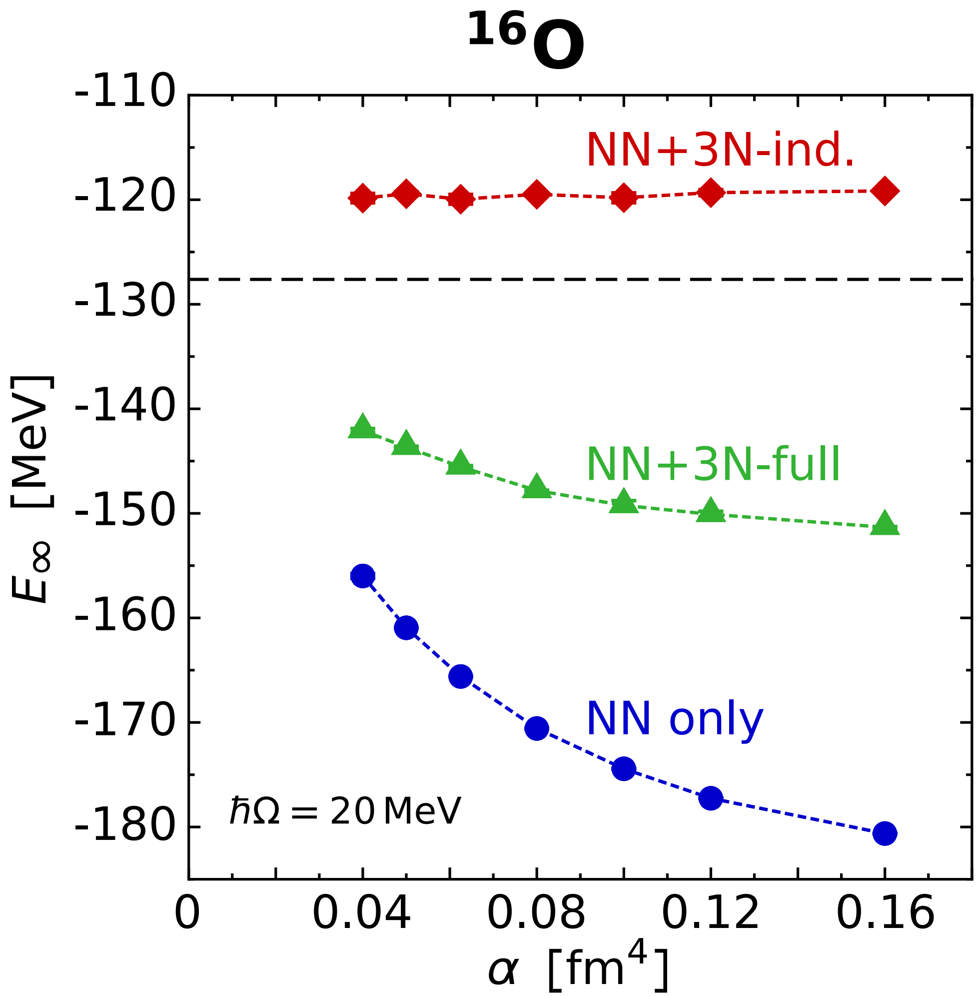
^{12}C: Ground-State Energies



^{16}O: Ground-State Energies

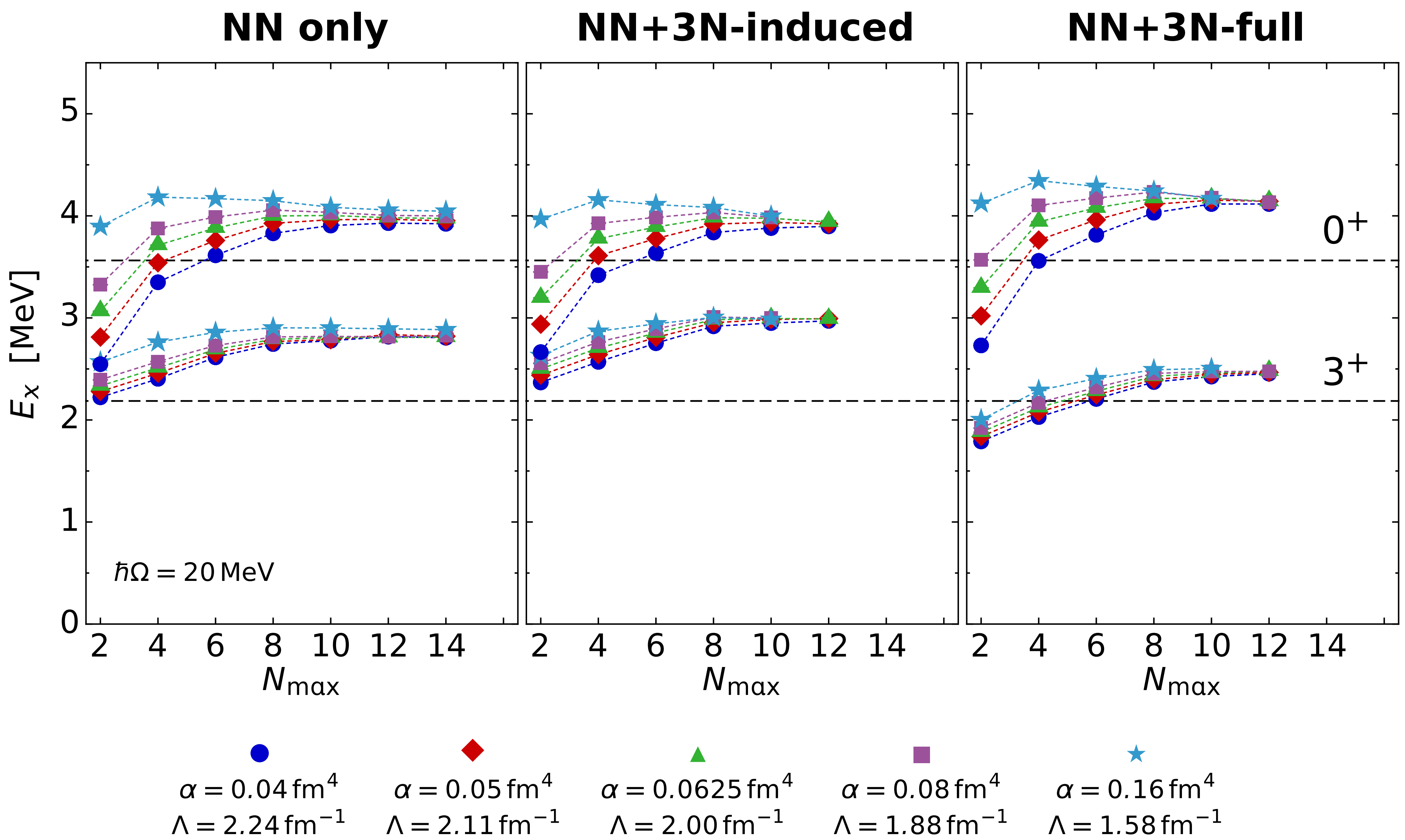


^{16}O: Energy vs. Flow Parameter

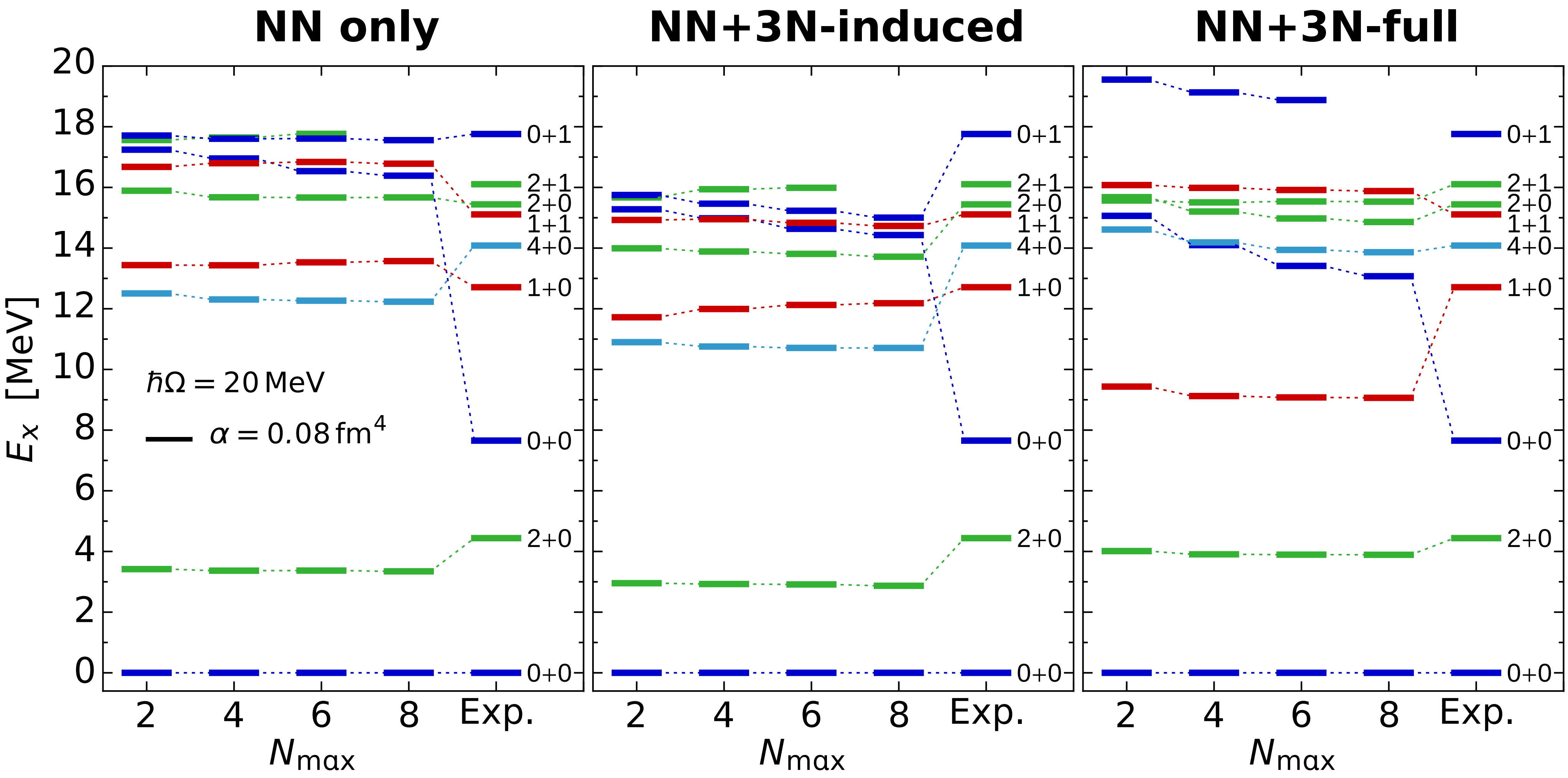


- **initial NN Hamiltonian**
  - induced 3N interactions are significant
  - no indication of induced 4N
  - NN+3N-induced unitarily equivalent to initial NN
- **initial NN+3N Hamiltonian**
  - induced 4N interactions are sizable in upper p-shell
  - generated by long-range 2π terms of initial 3N interaction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

^{6}Li: 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

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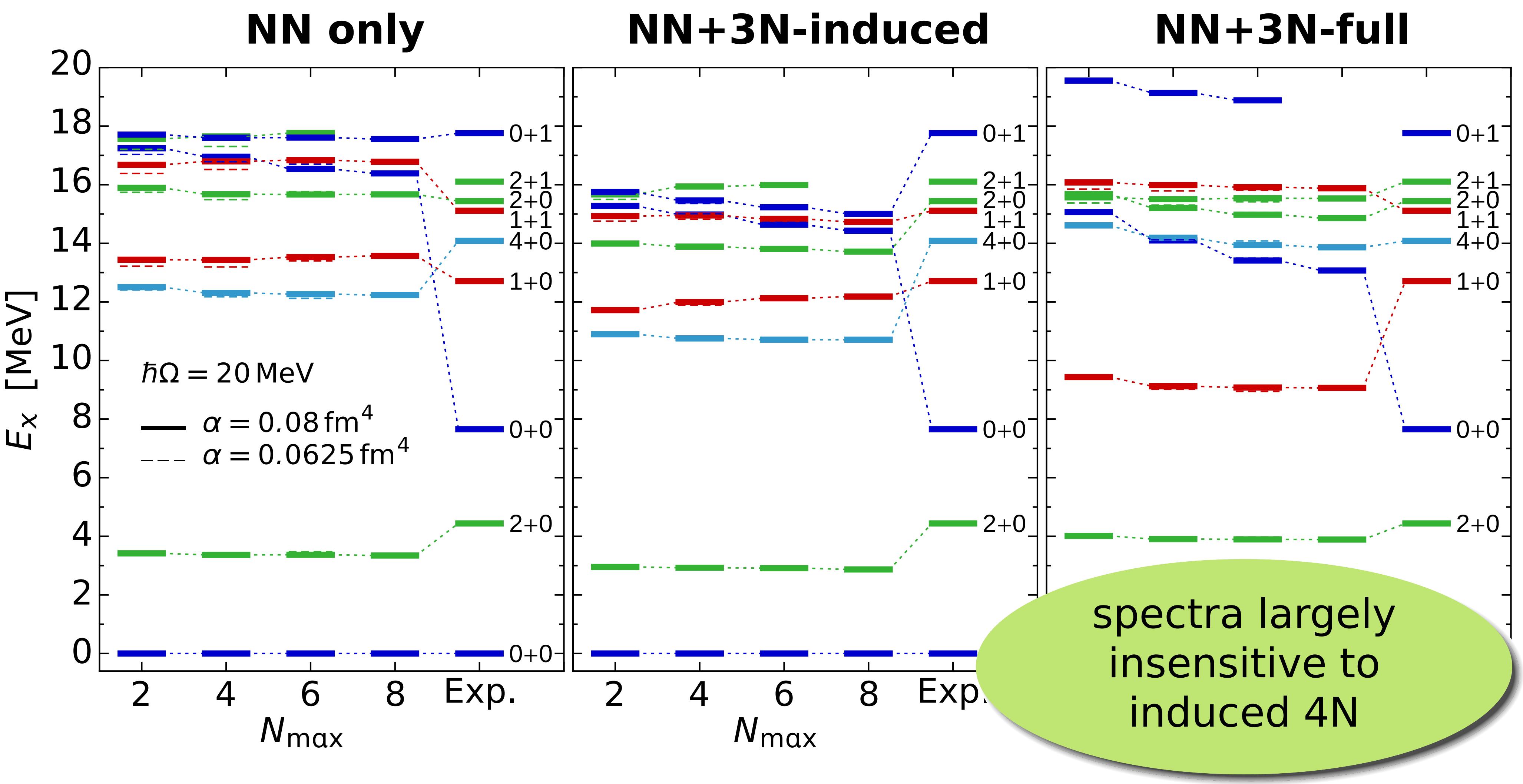

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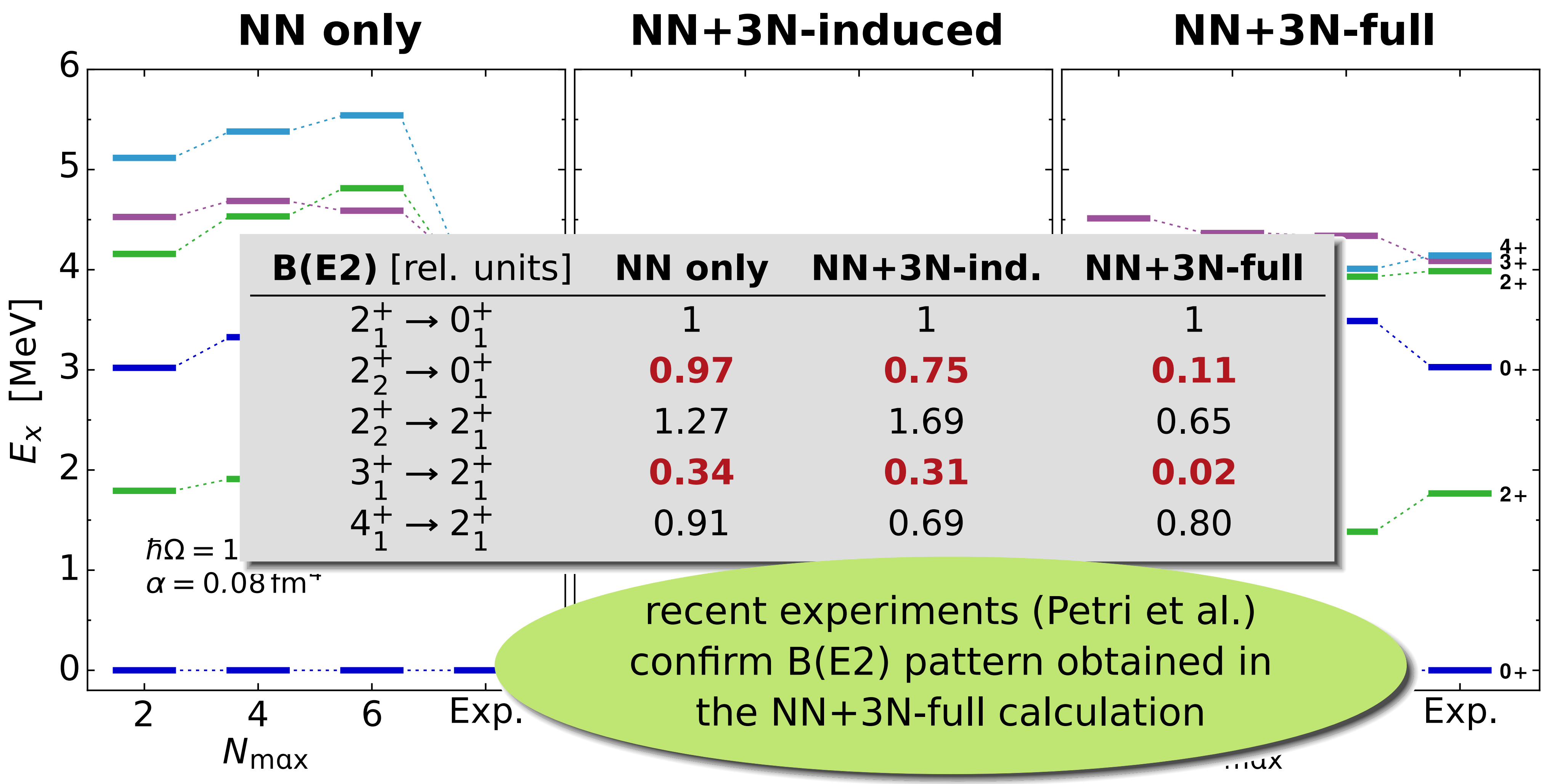

B(E2) [rel. units]	NN only	NN+3N-ind.	NN+3N-full
$2^+_1 \rightarrow 0^+_1$	1	1	1
$2^+_2 \rightarrow 0^+_1$	**0.97**	**0.75**	**0.11**
$2^+_2 \rightarrow 2^+_1$	1.27	1.69	0.65
$3^+_1 \rightarrow 2^+_1$	**0.34**	**0.31**	**0.02**
$4^+_1 \rightarrow 2^+_1$	0.91	0.69	0.80

recent experiments (Petri et al.) confirm B(E2) pattern obtained in the NN+3N-full calculation

Conclusions

Conclusions

- new era of **ab-initio nuclear structure and reaction theory** connected to QCD via chiral EFT
  - chiral EFT as universal starting point... some 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...

Epilogue

- **thanks to my group & my collaborators**
  - **S. Binder**, **A. Calci**, B. Erler, A. Günther, H. Krutsch, **J. Langhammer**, P. Papakonstantinou, S. Reinhardt, C. Stumpf, R. Trippel, K. Vobig
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    LLNL Livermore, USA
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  - C. Forssén
    Chalmers University, Sweden
  - H. Feldmeier, T. Neff,...
    GSI Helmholtzzentrum

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