Introduction to

Ab Initio Nuclear Structure Theory

Part I: Hamiltonian

Robert Roth

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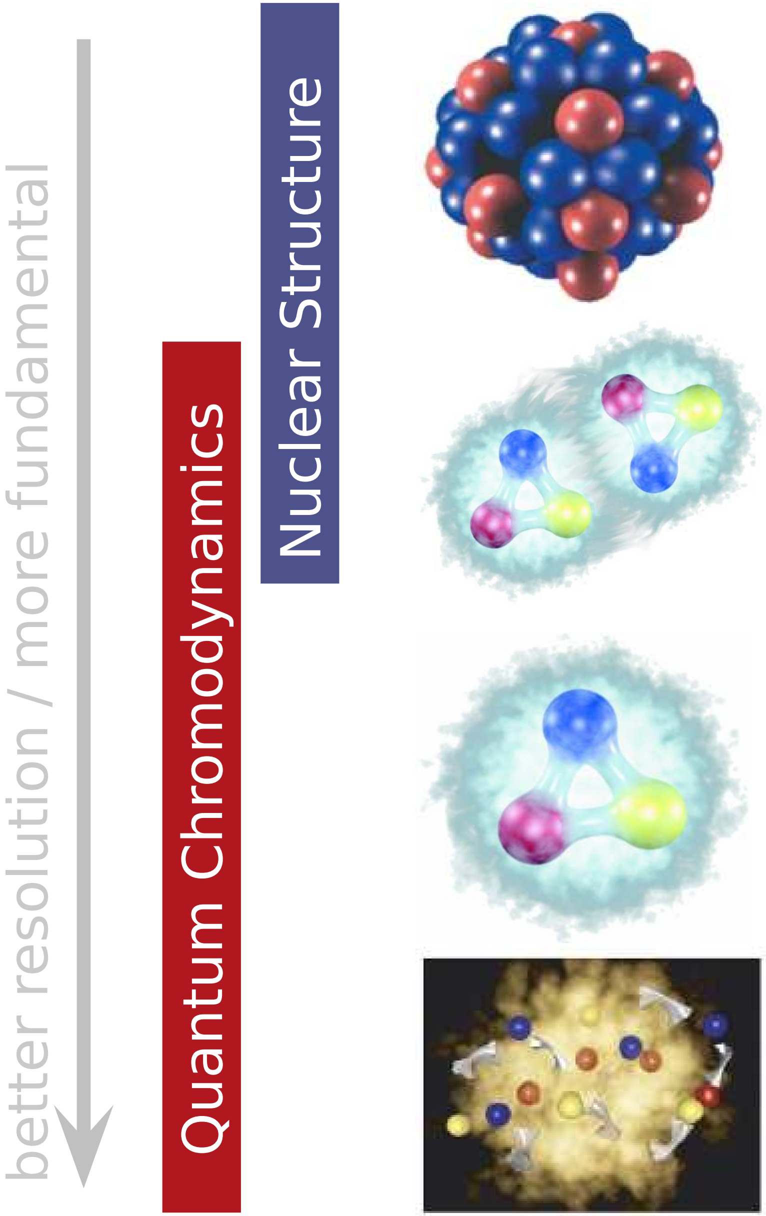
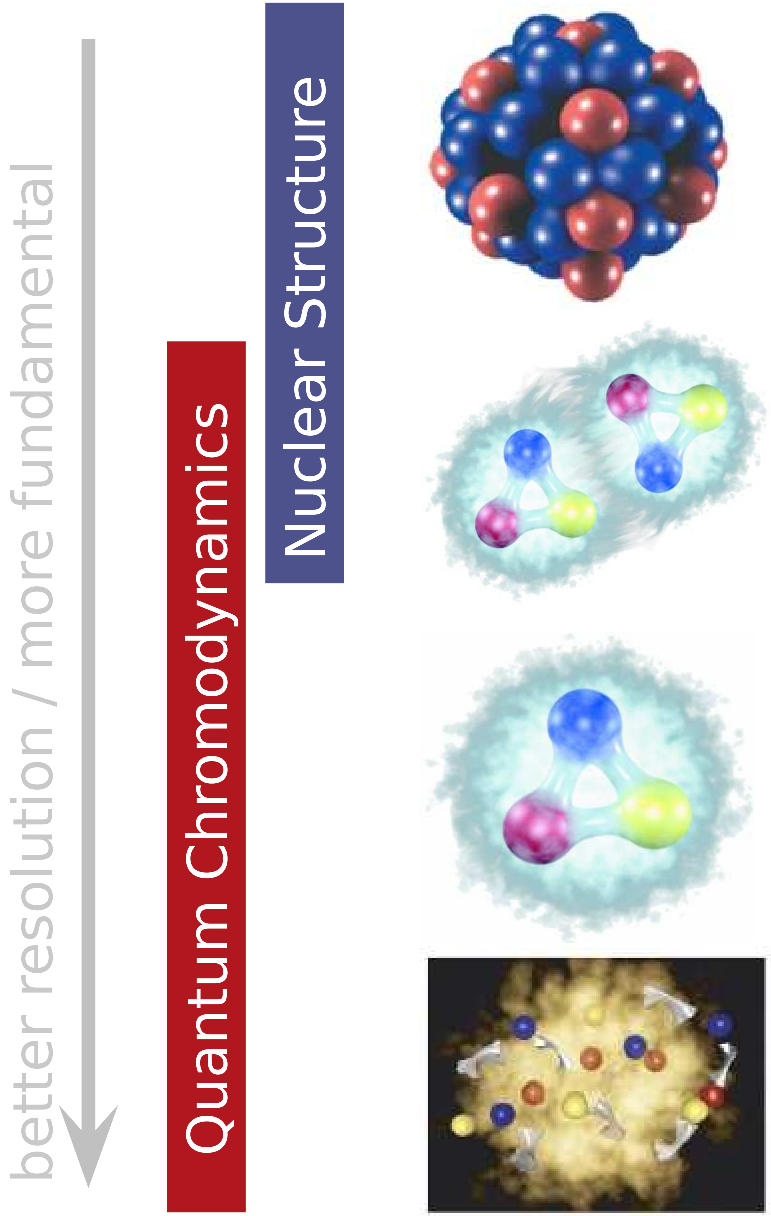
Theoretical Context



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

Theoretical Context



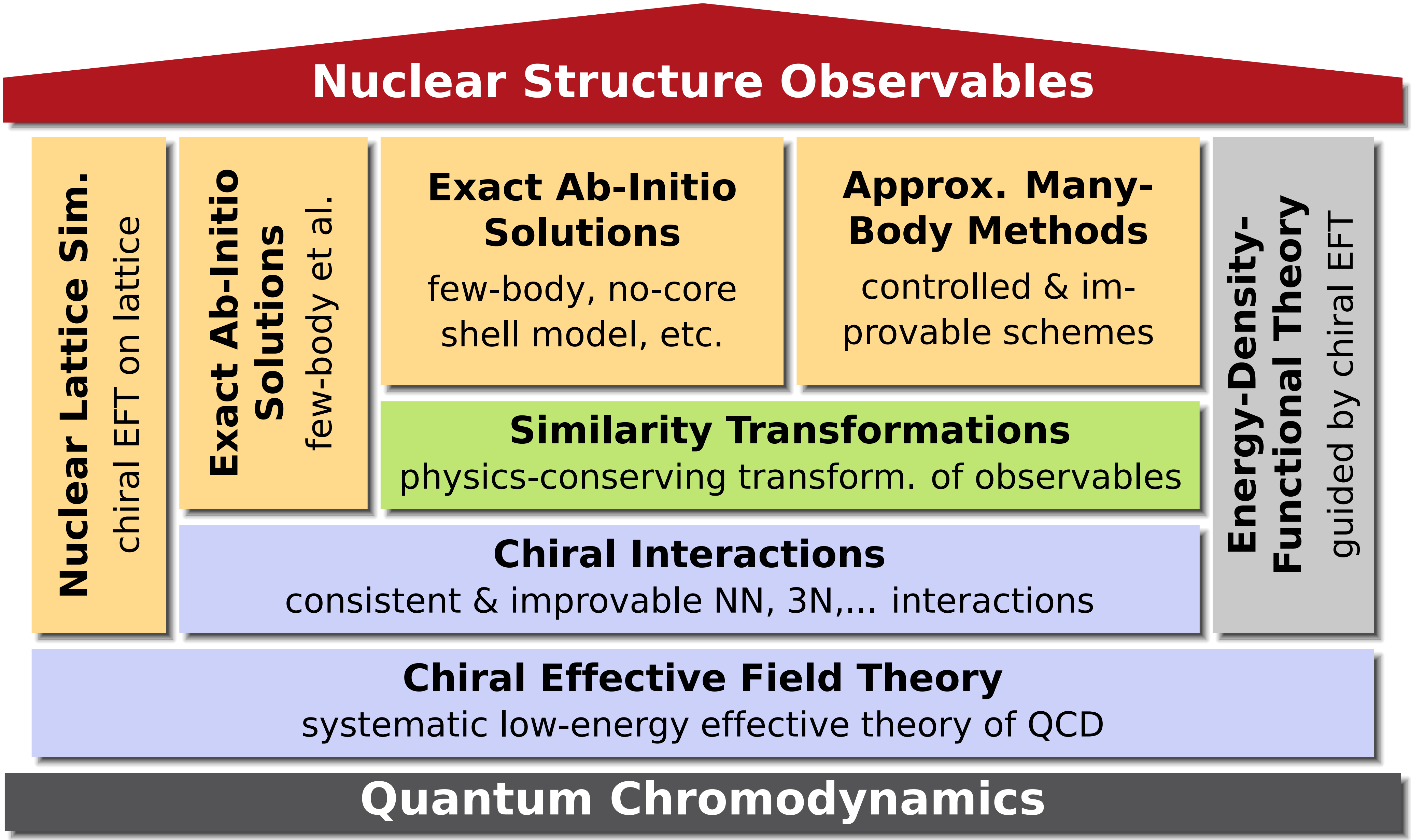
How to solve the quantum many-body problem?

How to derive the nuclear interaction from QCD?

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**

Building Blocks



Building Blocks — Anno 2000

Nuclear Structure Observables

Exact Ab-Initio Solutions
few-body et al.

Exact Ab-Initio Solutions
few-body, no-core shell model

Approx. Many-Body Methods
uncontrolled ad hoc approximations

Energy-Density-Functional Theory
pure phenomenology

Effective Interactions
adapting Hamiltonian to model space

Realistic Interactions
phenomenology with input from meson exchange

??? Connection to QCD ???

Quantum Chromodynamics

Nuclear Interactions from QCD

Building Blocks

Nuclear Structure Observables

Nuclear Lattice Sim.
chiral EFT on lattice

Exact Ab-Initio Solutions
few-body et al.

Exact Ab-Initio Solutions
few-body, no-core shell model, etc.

Approx. Many-Body Methods
controlled & improvable schemes

Energy-Density-Functional Theory
guided by chiral EFT

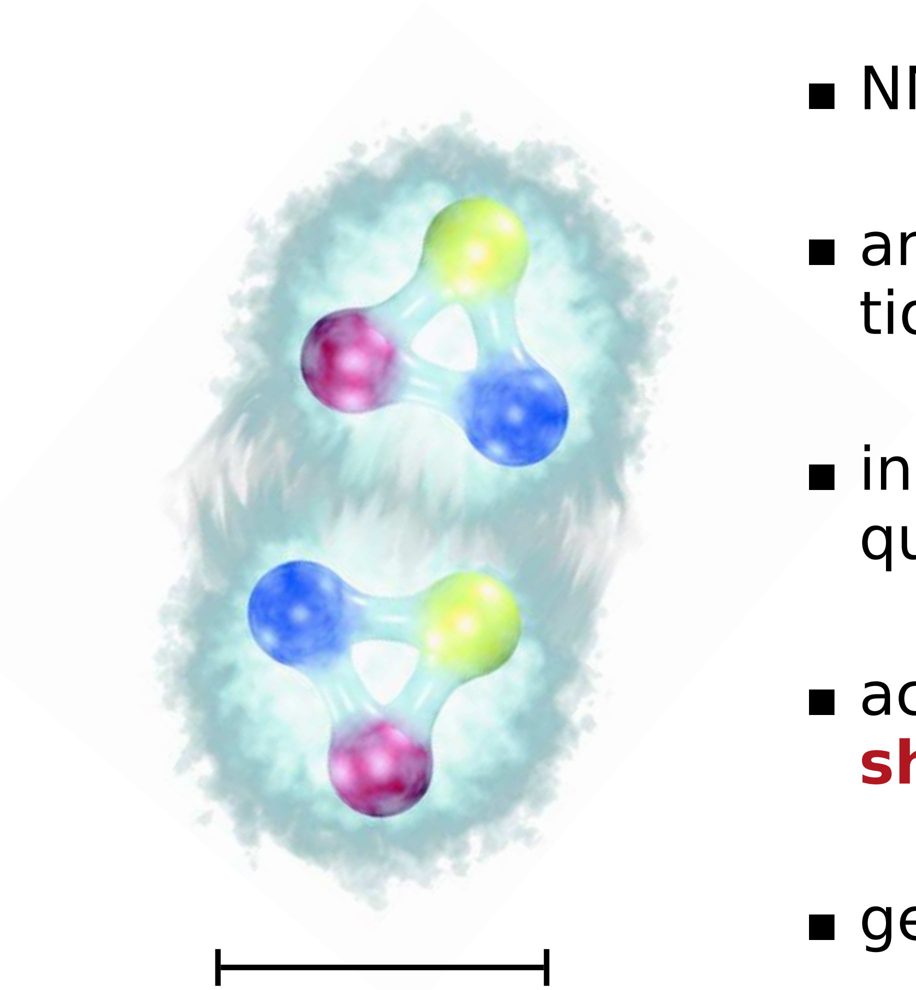
Similarity Transformations
physics-conserving transform. of observables

Chiral Interactions
consistent & improvable NN, 3N,... interactions

Chiral Effective Field Theory
systematic low-energy effective theory of QCD

Quantum Chromodynamics

Nature of the Nuclear Interaction

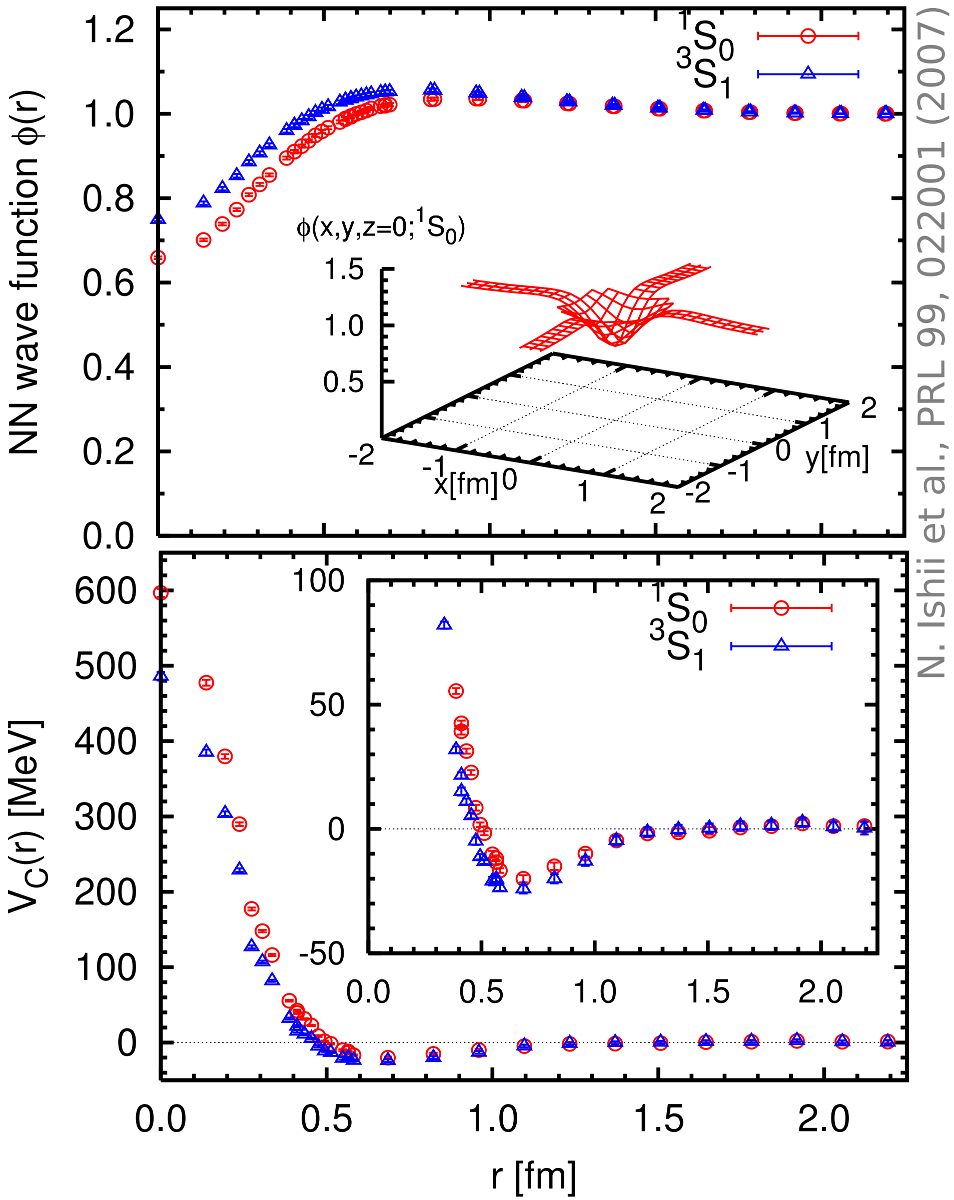


$\sim 1.6\text{fm}$

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

- NN-interaction is **not fundamental**
- analogous to **van der Waals** interaction between neutral atoms
- induced via mutual **polarization** of quark & gluon distributions
- acts only if the nucleons overlap, i.e. at **short ranges**
- genuine **3N-interaction** is important

Nuclear Interaction from Lattice QCD



- first steps towards construction of a nuclear interaction through **lattice QCD simulations**
- compute relative **two-nucleon wavefunction** on the lattice
- invert Schrödinger equation to obtain **local 'effective' two-nucleon potential**
- schematic results so far (unphysical quark masses, S-wave interactions only,...)

Realistic Nuclear Interactions

- **QCD ingredients**
  - chiral effective field theory
  - meson-exchange theory
- **short-range phenomenology**
  - contact terms or parameterization of short-range potential
- **experimental two-body data**
  - scattering phase-shifts & deuteron properties reproduced with high precision
- **supplementary 3N interaction**
  - adjusted to spectra of light nuclei

Argonne V18

CD Bonn

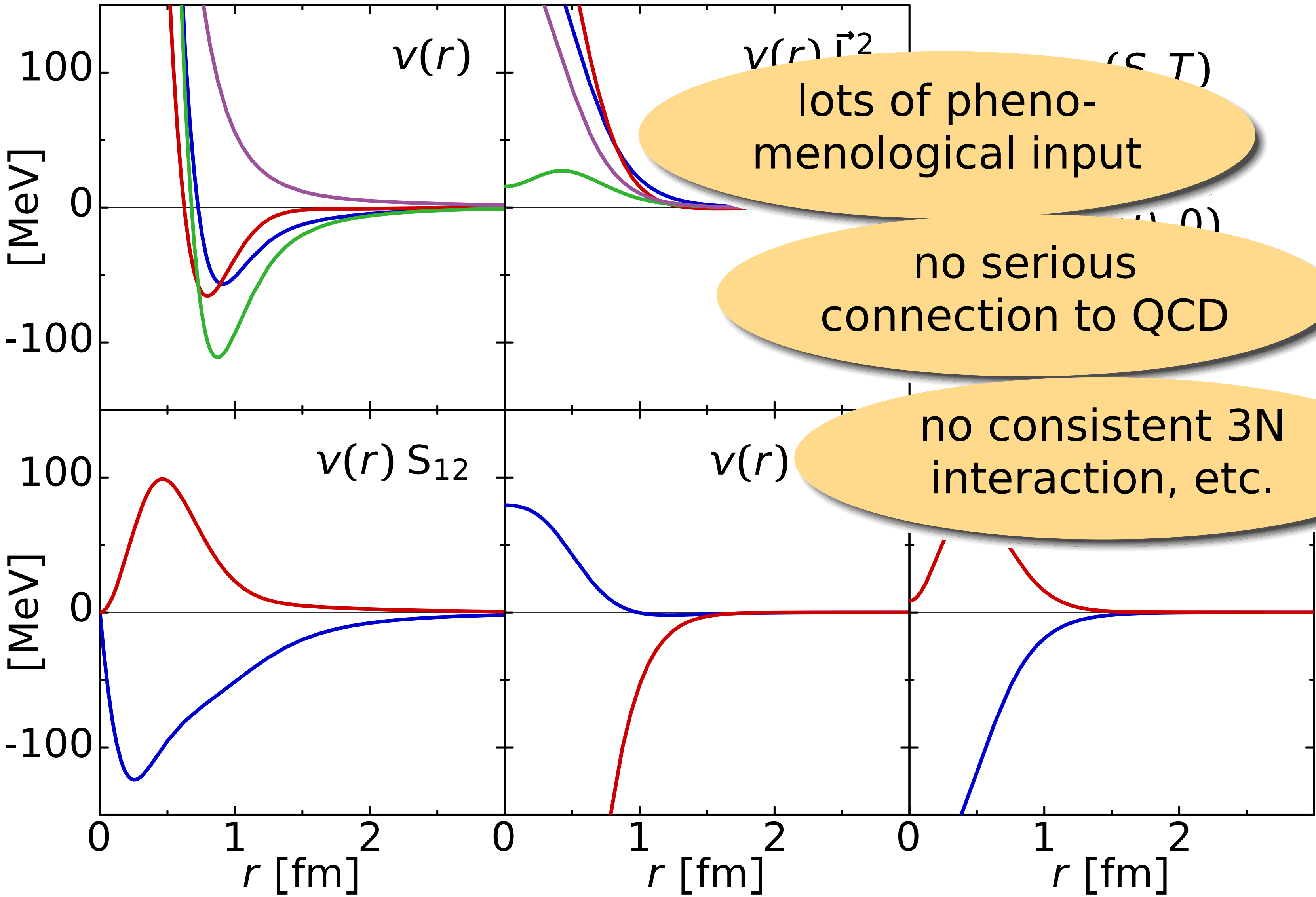
Nijmegen I/II

Chiral N3LO

Argonne V18 + **Illinois X**

Chiral N3LO + **N2LO**

Argonne V18 Potential



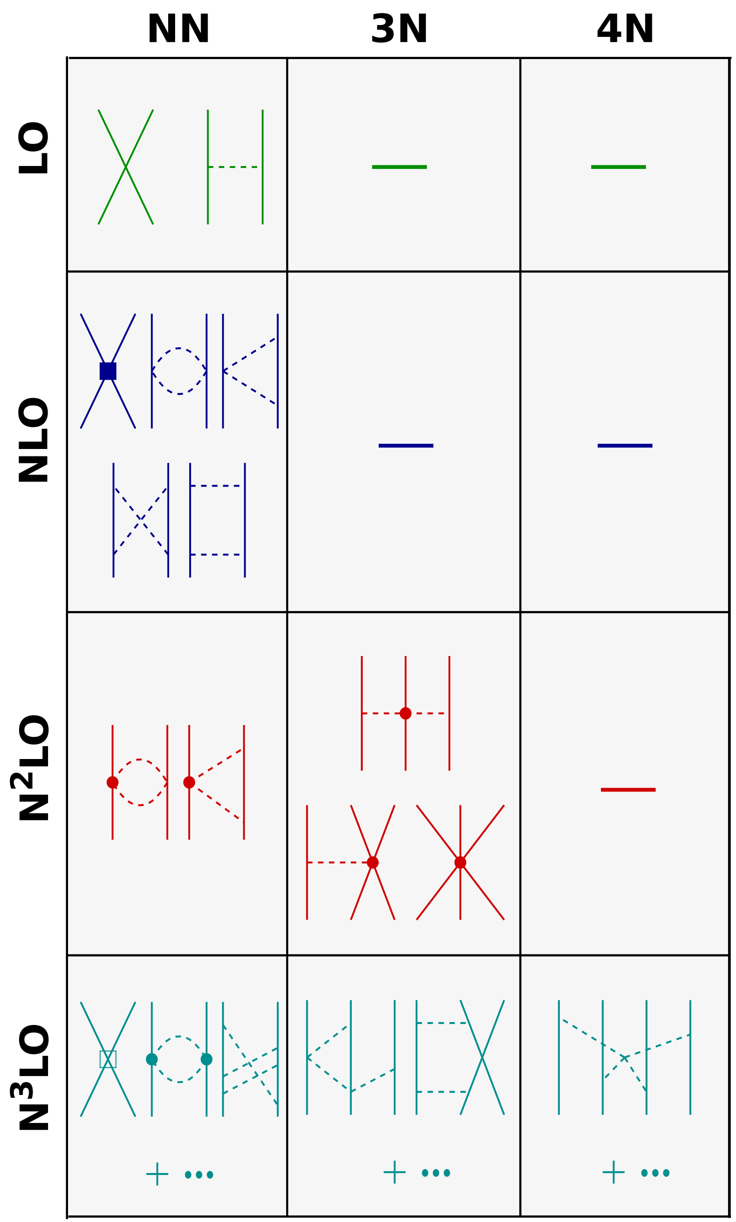
lots of pheno-
menological input

no serious
connection to QCD

no consistent 3N
interaction, etc.

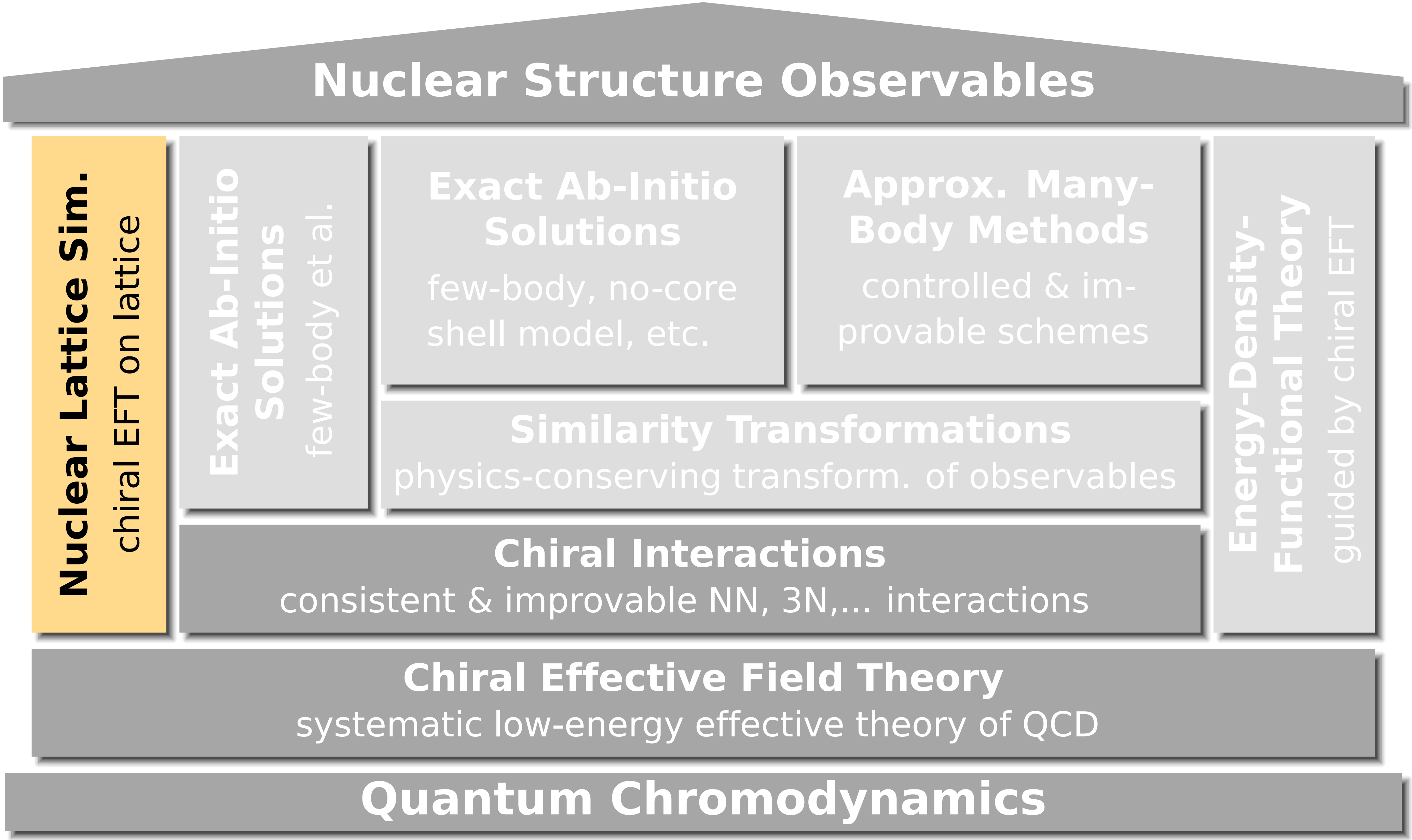
Nuclear Interactions from Chiral EFT

- 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,...



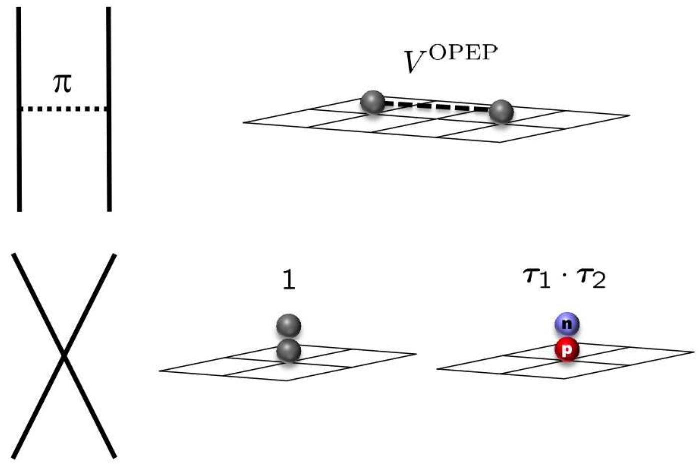
adapted from Meißner (2005)

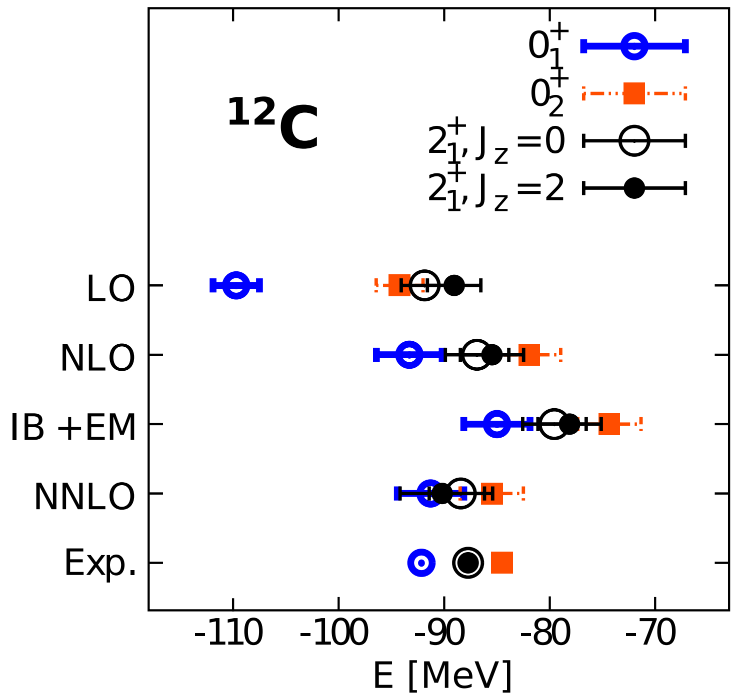
Building Blocks



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)

Similarity Transformations

Building Blocks

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Why Similarity Transformations?

Realistic Interactions

- generate strong correlations in many-body states
- short-range central & tensor correlations most important

Similarity Transformation

- adapt realistic potential to the available model space
- conserve experimentally constrained properties (phase shifts, deuteron properties)

Many-Body Methods

- rely on truncated many-nucleon Hilbert spaces
- not capable of describing short-range correlations
- extreme: Hartree-Fock based on single Slater determinant

What are Correlations?

correlations:
everything beyond the
independent-particle picture

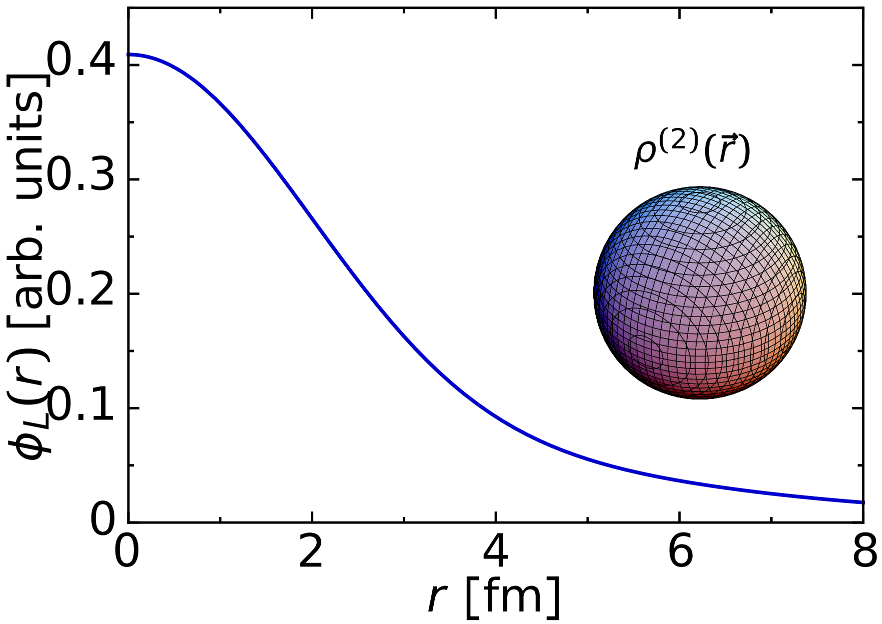
- the quantum state of A independent (non-interacting) fermions is a **Slater determinant**

$$\left|\Phi^{\mathrm{SD}}\right\rangle \propto \sum_{\pi} \mathrm{sgn}(\pi)\, \mathrm{P}_{\pi} \; \left|\phi_1\right\rangle \otimes \left|\phi_2\right\rangle \otimes \cdots \otimes \left|\phi_A\right\rangle$$

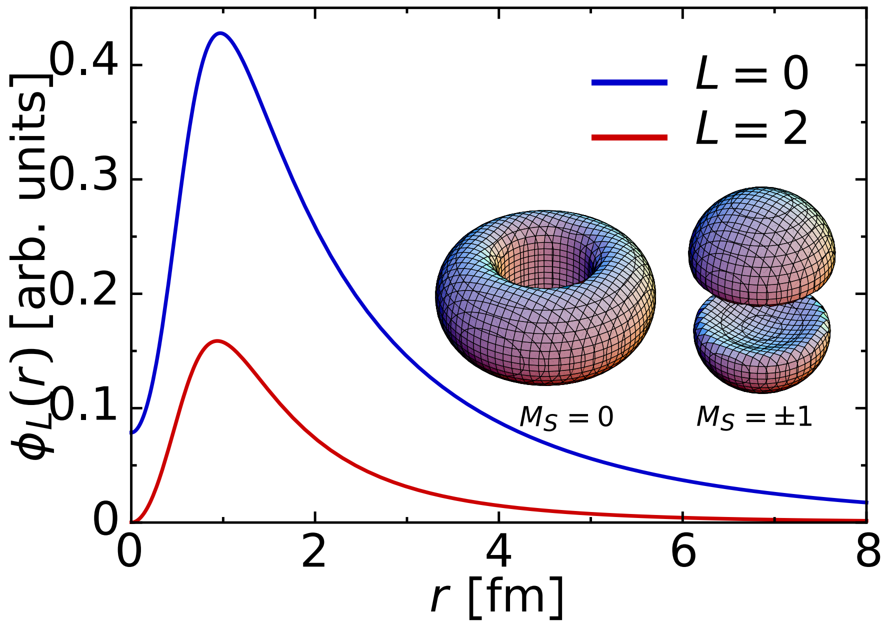
- **any two-body interaction induces correlations** which cannot be described by a single Slater determinant

Deuteron: Manifestation of Correlations

independent n+p in a trap



realistic deuteron solution



short-range repulsion supresses wavefunction at small distances r

central correlations

tensor interaction generates L=2 admixture to ground state

tensor correlations

Similarity Transformations

Unitary Correlation Operator Method

Unitary Correlation Operator Method

Correlation Operator

define a unitary operator C to describe the effect of short-range correlations

$$\mathrm{C} = \exp[-\mathrm{i}\,\mathrm{G}] = \exp\Big[-\mathrm{i}\sum_{i<j}\mathrm{g}_{ij}\Big]$$

Correlated States

imprint short-range correlations onto uncorrelated many-body states

$$|\widetilde{\psi}\rangle = \mathrm{C}\,|\psi\rangle$$

Correlated Operators

adapt Hamiltonian to uncorrelated states (pre-diagonalization)

$$\widetilde{\mathrm{O}} = \mathrm{C}^{\dagger}\,\mathrm{O}\,\mathrm{C}$$

$$\langle\widetilde{\psi}|\,\mathrm{O}\,|\widetilde{\psi}'\rangle = \langle\psi|\,\mathrm{C}^{\dagger}\,\mathrm{O}\,\mathrm{C}\,|\psi'\rangle = \langle\psi|\,\widetilde{\mathrm{O}}\,|\psi'\rangle$$

Unitary Correlation Operator Method

explicit ansatz for unitary transformation operator **motivated by the physics of short-range correlations**

- **explicit unitary transformation** with correlation operator C

$$C = C_\Omega C_r = \exp\Big(-\mathrm{i}\sum_{i<j} g_{\Omega,ij}\Big)\exp\Big(-\mathrm{i}\sum_{i<j} g_{r,ij}\Big)$$

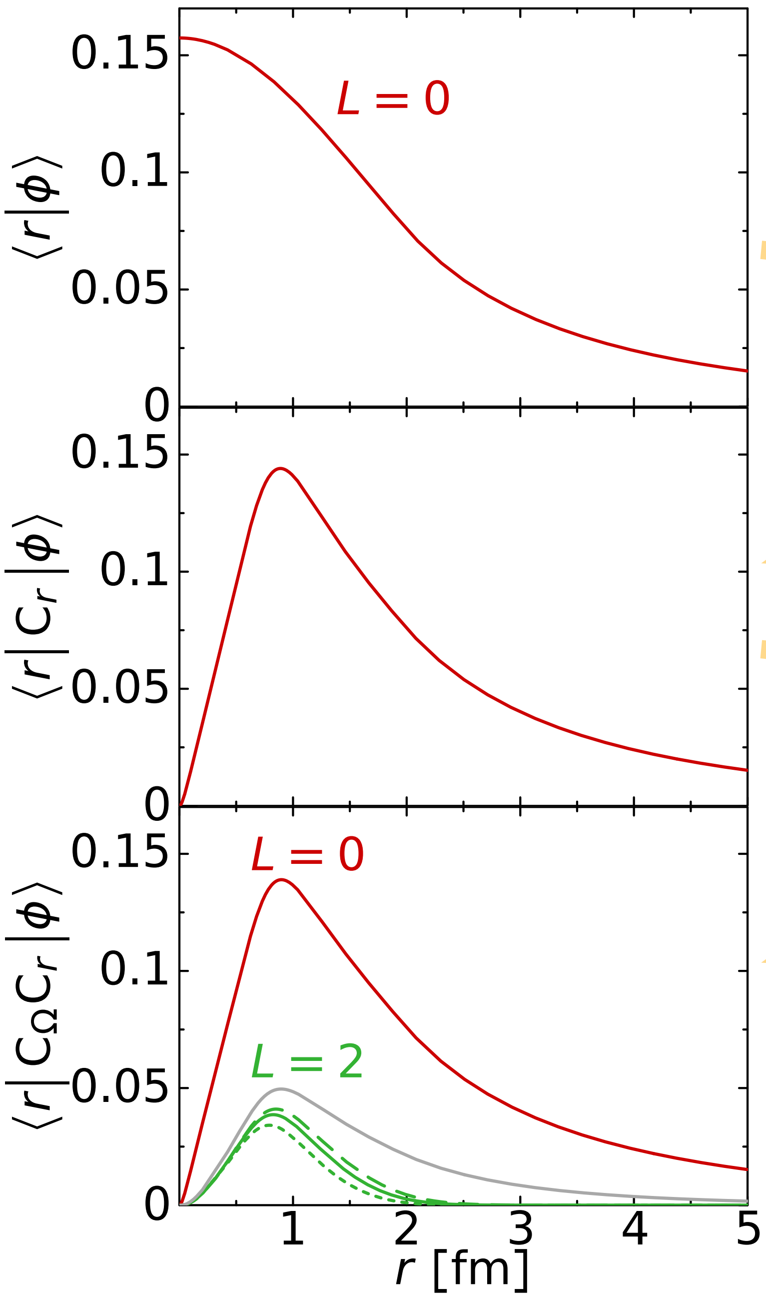
- **central correlator** C_r: radial distance-dependent shift in the relative coordinate of a nucleon pair

$$g_r = \frac{1}{2}\big[s(r)\,q_r + q_r\,s(r)\big] \qquad q_r = \tfrac{1}{2}\big[\tfrac{\vec{r}}{r}\cdot\vec{q} + \vec{q}\cdot\tfrac{\vec{r}}{r}\big]$$

- **tensor correlator** C_Ω: angular shift depending on the orientation of spin and relative coordinate of a nucleon pair

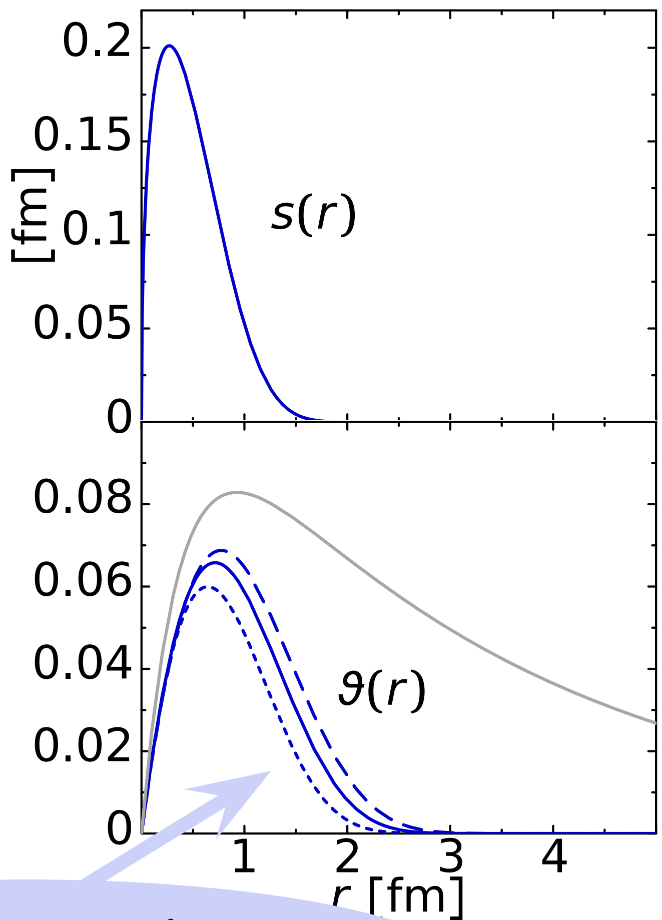
$$g_\Omega = \frac{3}{2}\vartheta(r)\big[(\vec{\sigma}_1\cdot\vec{q}_\Omega)(\vec{\sigma}_2\cdot\vec{r}) + (\vec{r}\leftrightarrow\vec{q}_\Omega)\big] \qquad \vec{q}_\Omega = \vec{q} - \tfrac{\vec{r}}{r}\,q_r$$

Correlated States: The Deuteron



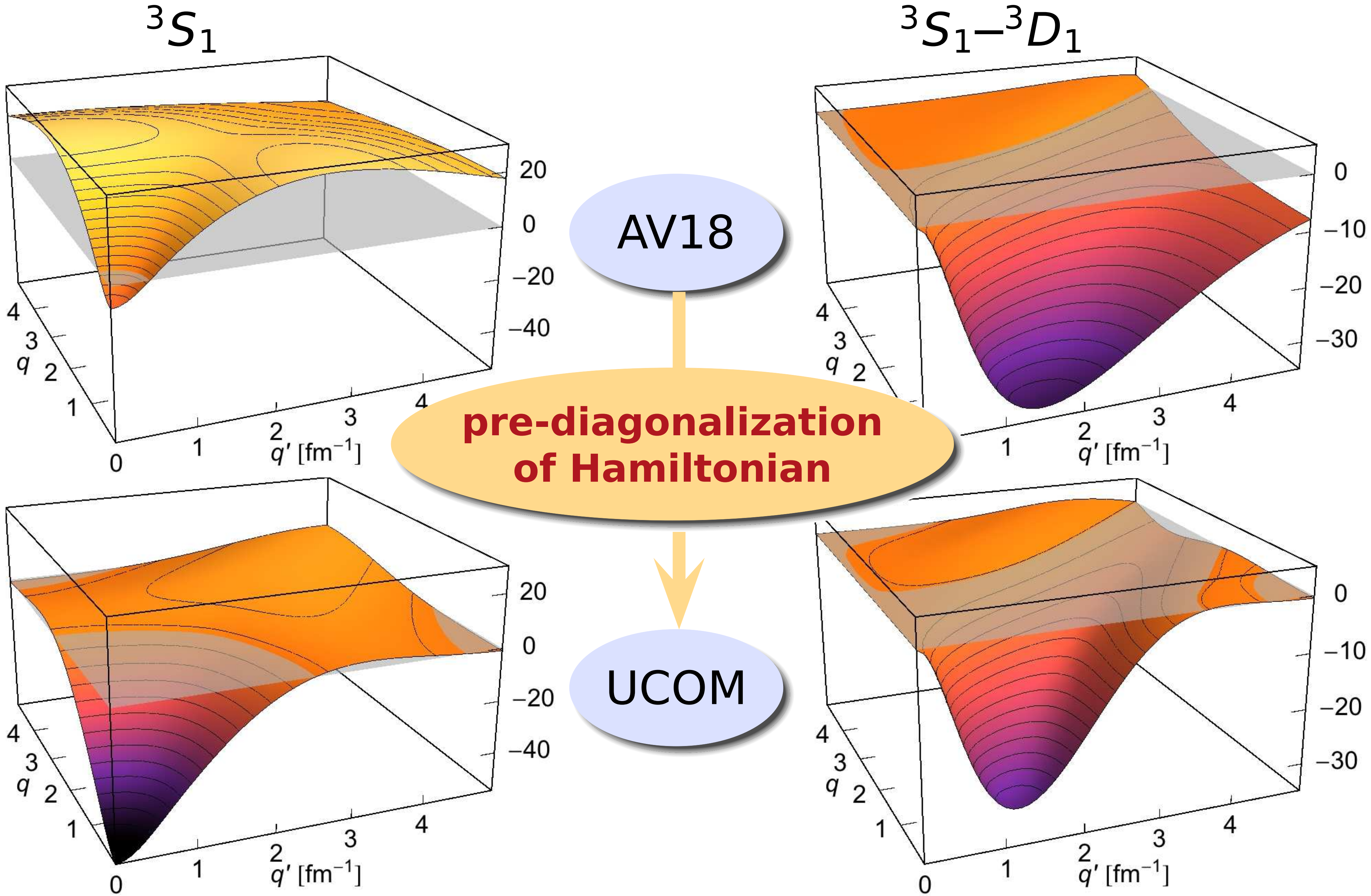
central correlations

tensor correlations



only short-range tensor correlations treated by C_Ω

Correlated Operators: V_{UCOM}



Similarity Renormalization Group

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

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

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

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

- **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

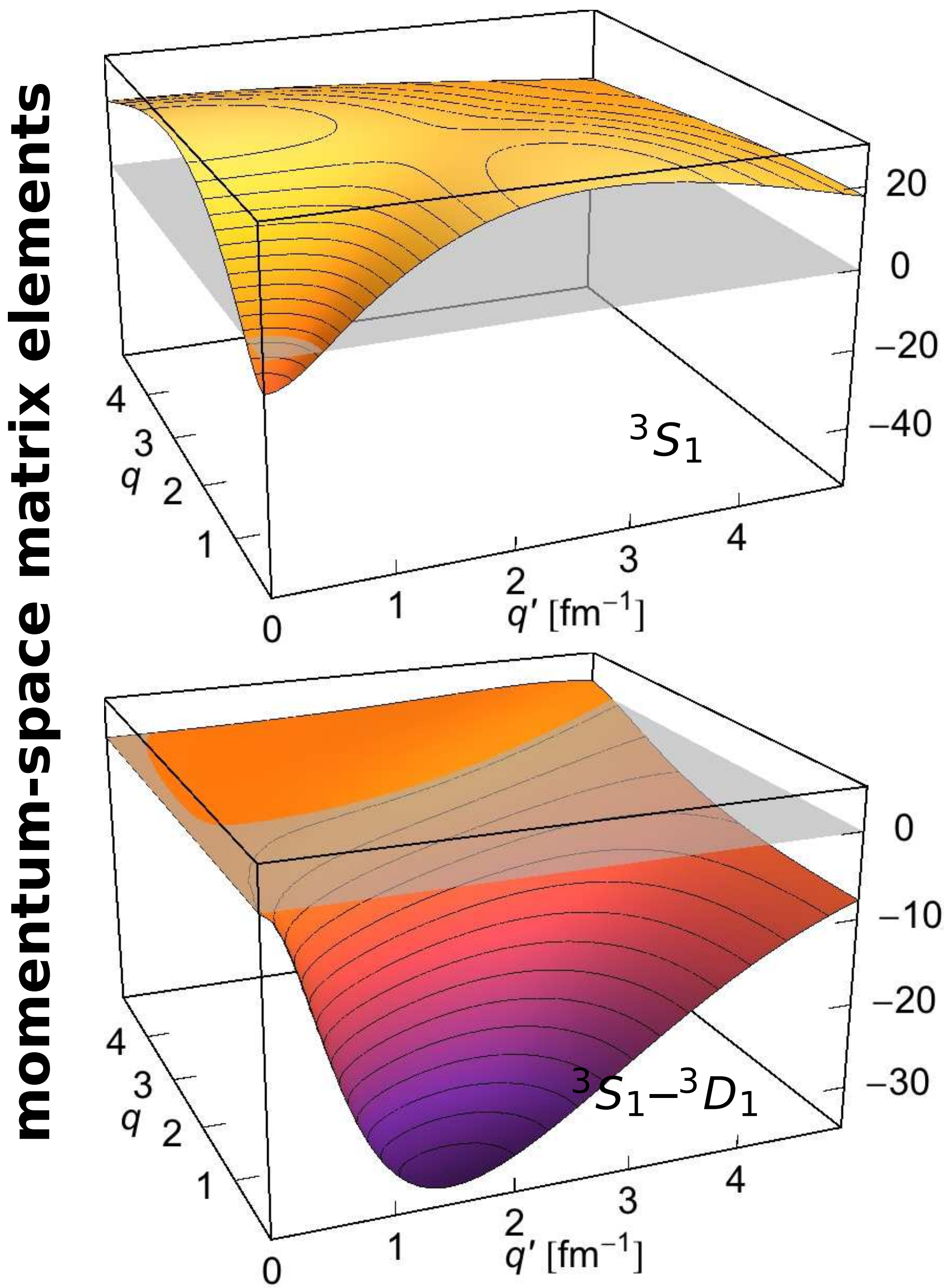
$$\frac{\mathrm{d}}{\mathrm{d}\alpha}\langle n(LS)JT|\,\widetilde{\mathrm{H}}_\alpha\,|n'(L'S)JT\rangle = (2\mu)^2 \sum_{n''L''}\sum_{n'''L'''}\Big[$$

$$\langle nL\ldots|\,\mathrm{T}_{\mathrm{int}}\,|n''L''\ldots\rangle\,\langle n''L''\ldots|\,\widetilde{\mathrm{H}}_\alpha\,|n'''L'''\ldots\rangle\,\langle n'''L'''\ldots|\,\widetilde{\mathrm{H}}_\alpha\,|n'L'\ldots\rangle$$

$$-2\langle nL\ldots|\,\widetilde{\mathrm{H}}_\alpha\,|n''L''\ldots\rangle\,\langle n''L''\ldots|\,\mathrm{T}_{\mathrm{int}}\,|n'''L'''\ldots\rangle\,\langle n'''L'''\ldots|\,\widetilde{\mathrm{H}}_\alpha\,|n'L'\ldots\rangle$$

$$+\langle nL\ldots|\,\widetilde{\mathrm{H}}_\alpha\,|n''L''\ldots\rangle\,\langle n''L''\ldots|\,\widetilde{\mathrm{H}}_\alpha\,|n'''L'''\ldots\rangle\,\langle n'''L'''\ldots|\,\mathrm{T}_{\mathrm{int}}\,|n'L'\ldots\rangle\Big]$$

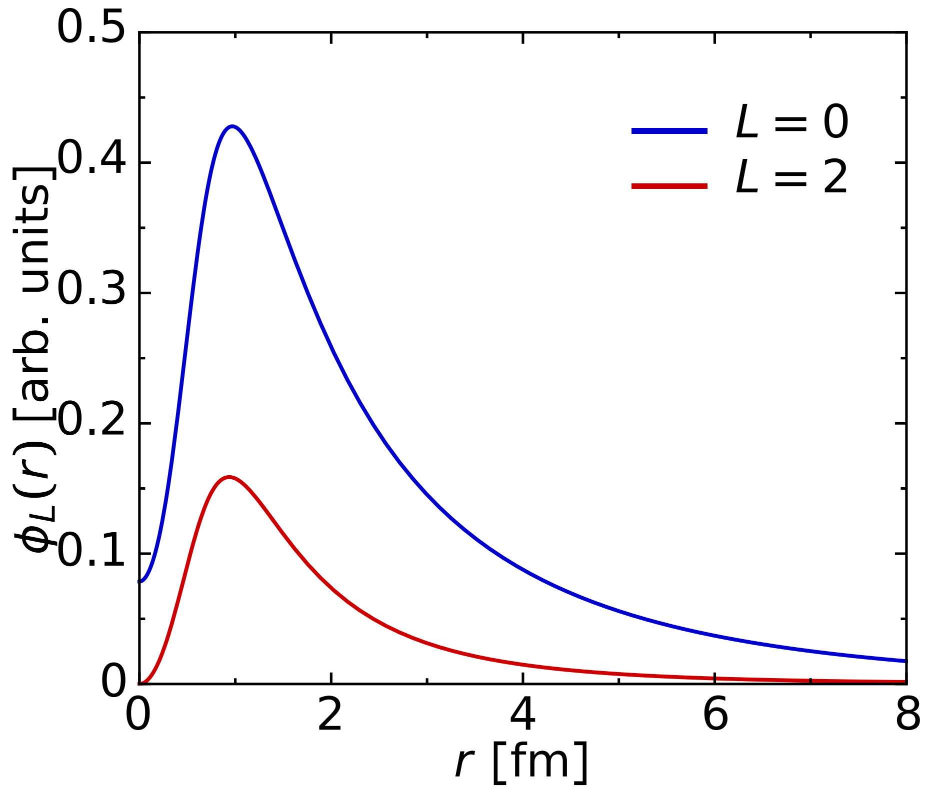
SRG Evolution in Two-Body Space



Argonne V18

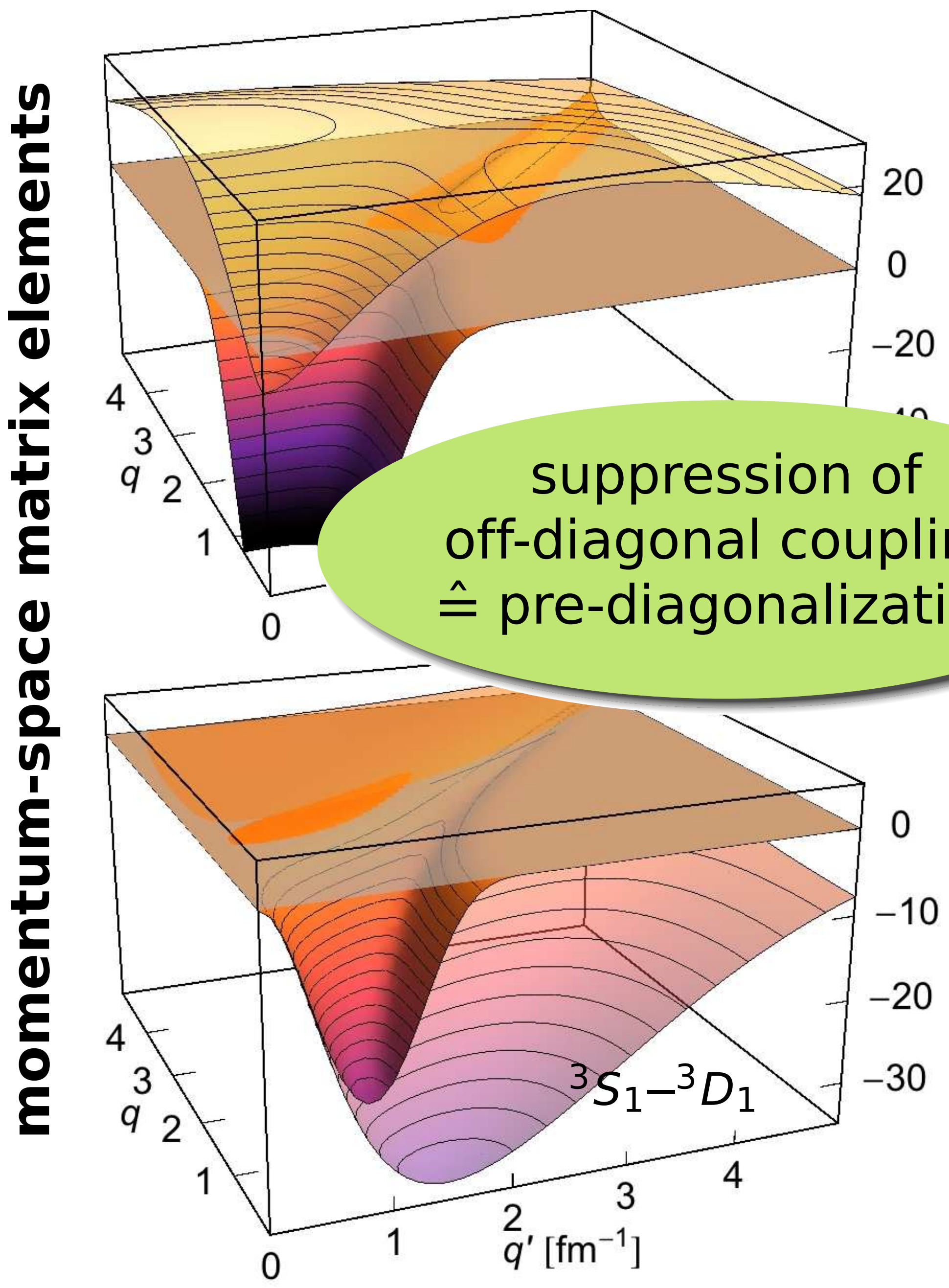
$J^\pi = 1^+, T = 0$

deuteron wave-function



SRG Evolution in Two-Body Space

momentum-space matrix elements



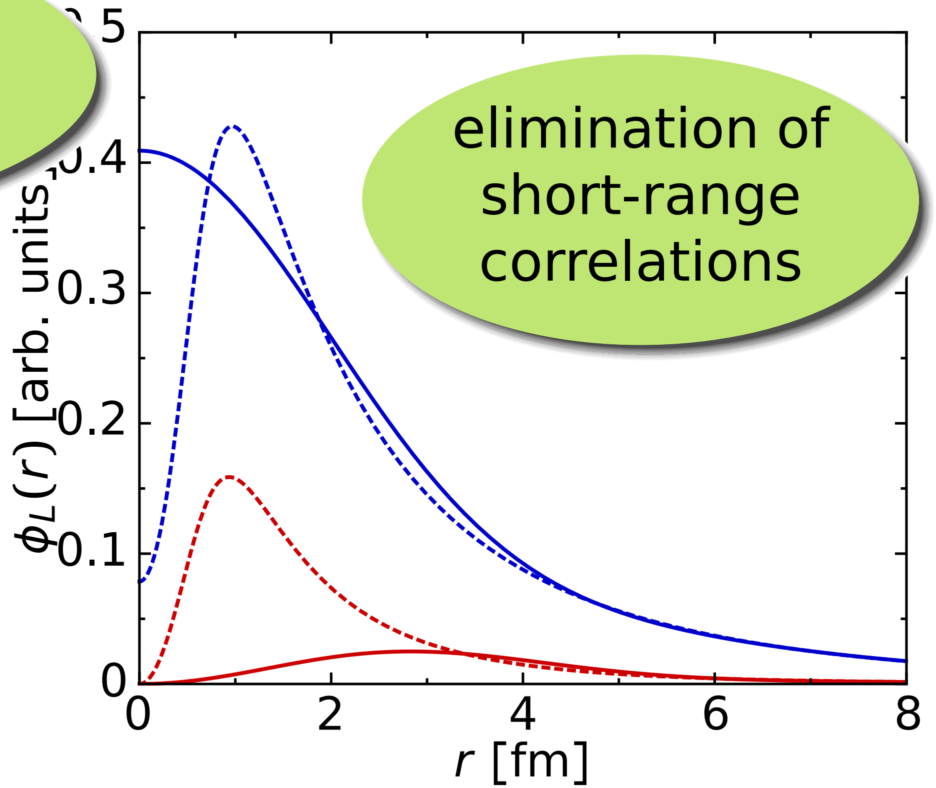
$\alpha = 0.320\,\text{fm}^4$

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

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

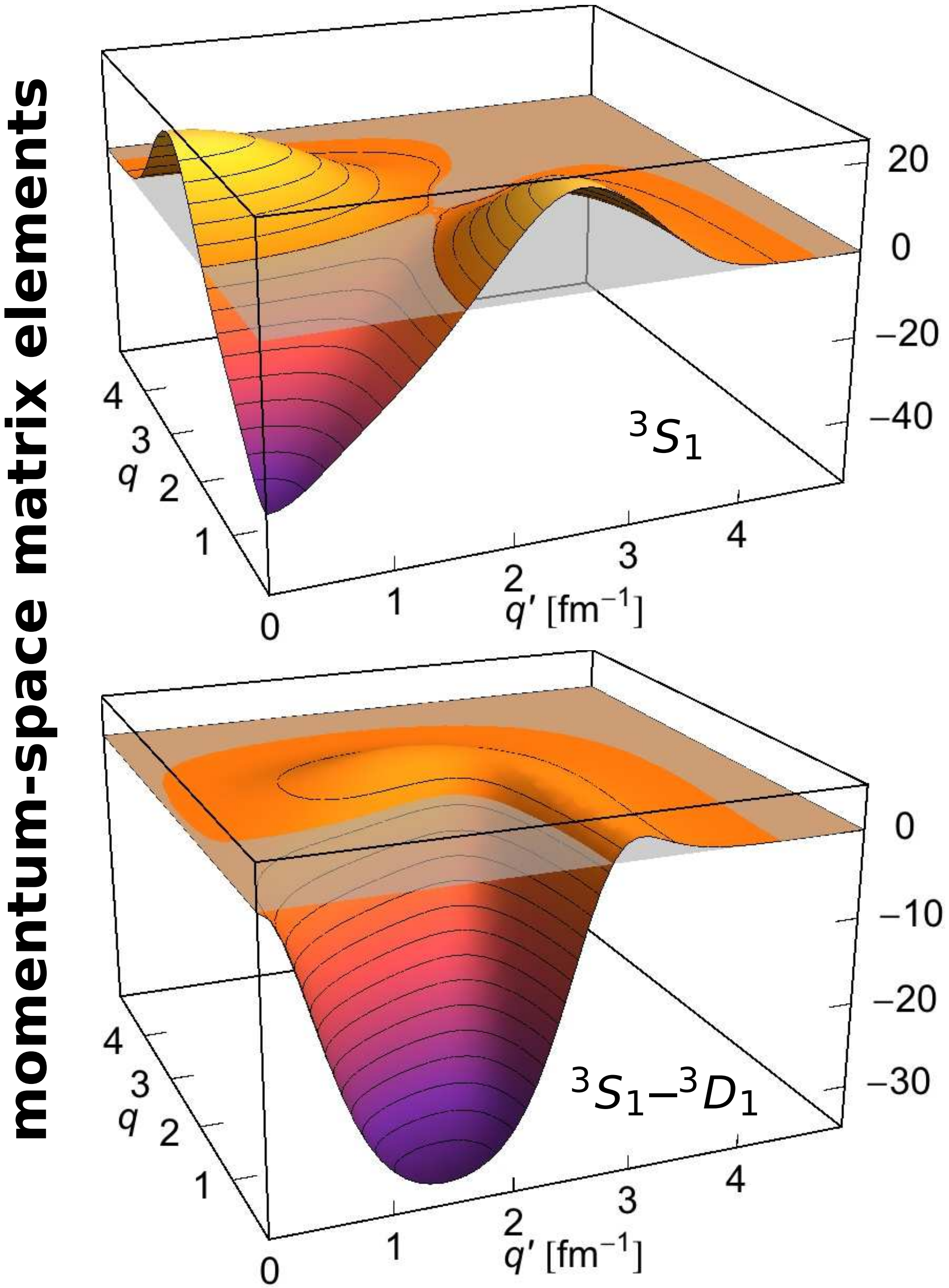
suspension of
off-diagonal coupling
≙ pre-diagonalization

deuteron wave-function



elimination of
short-range
correlations

SRG Evolution in Two-Body Space

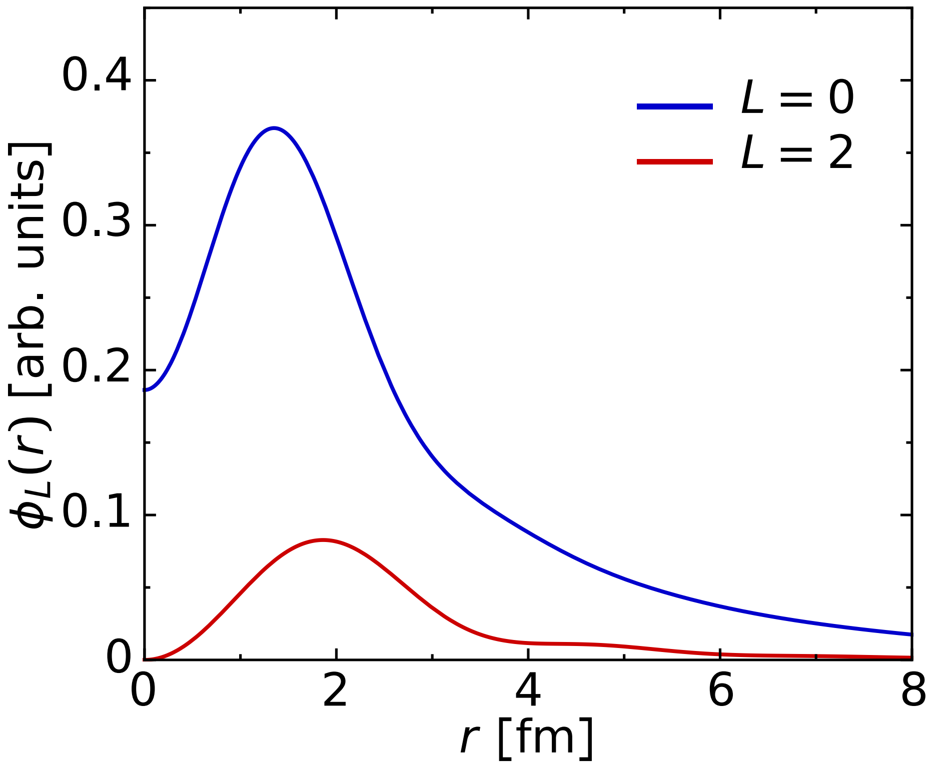


chiral NN

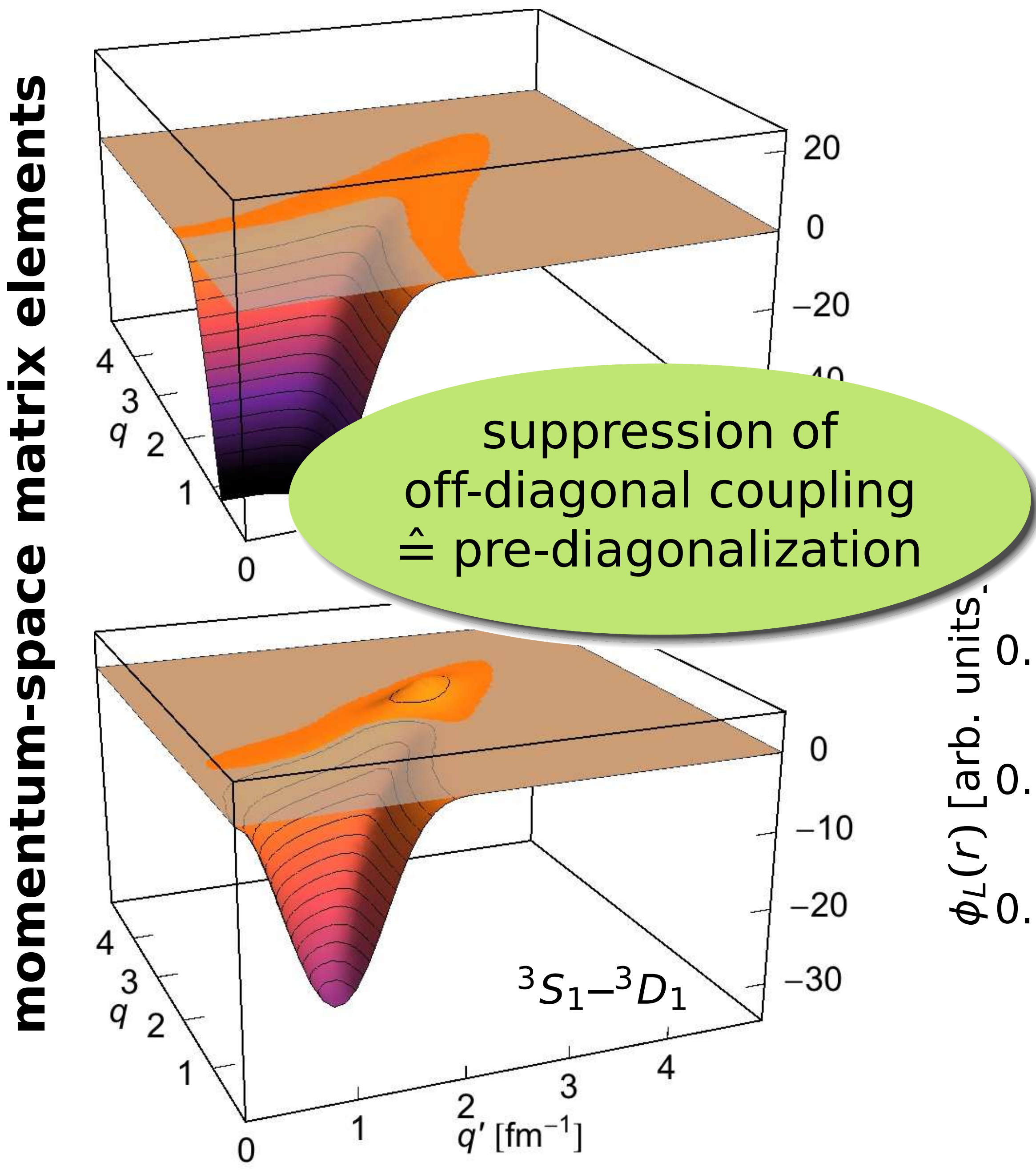
Entem & Machleidt. N^{3}LO, 500 MeV

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

deuteron wave-function



SRG Evolution in Two-Body Space



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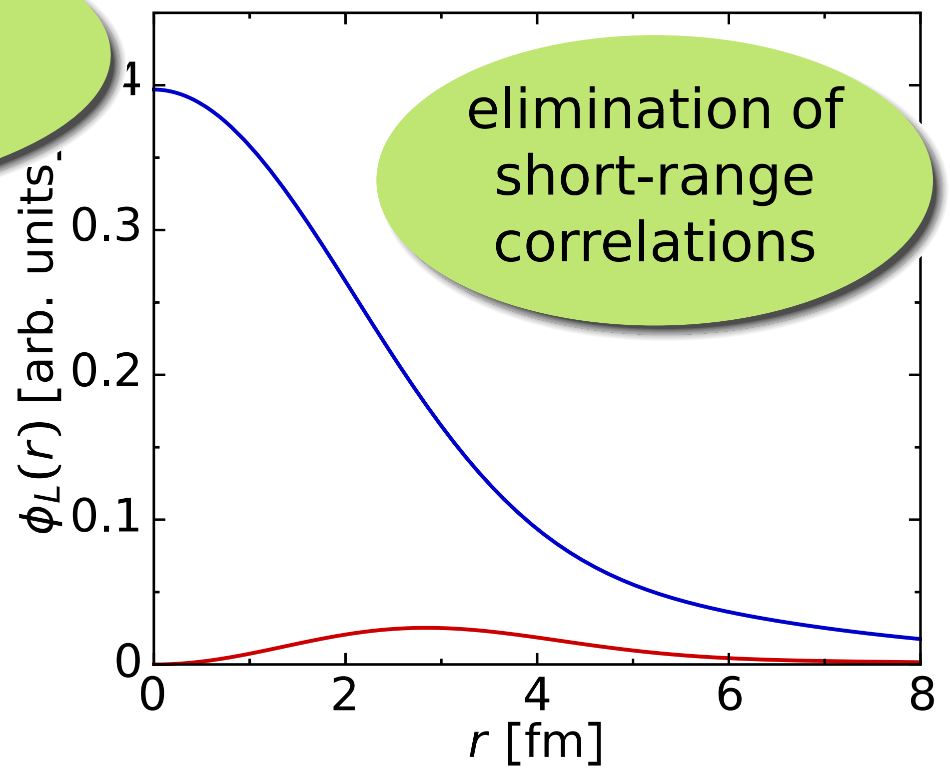


SRG Evolution of Matrix Elements

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

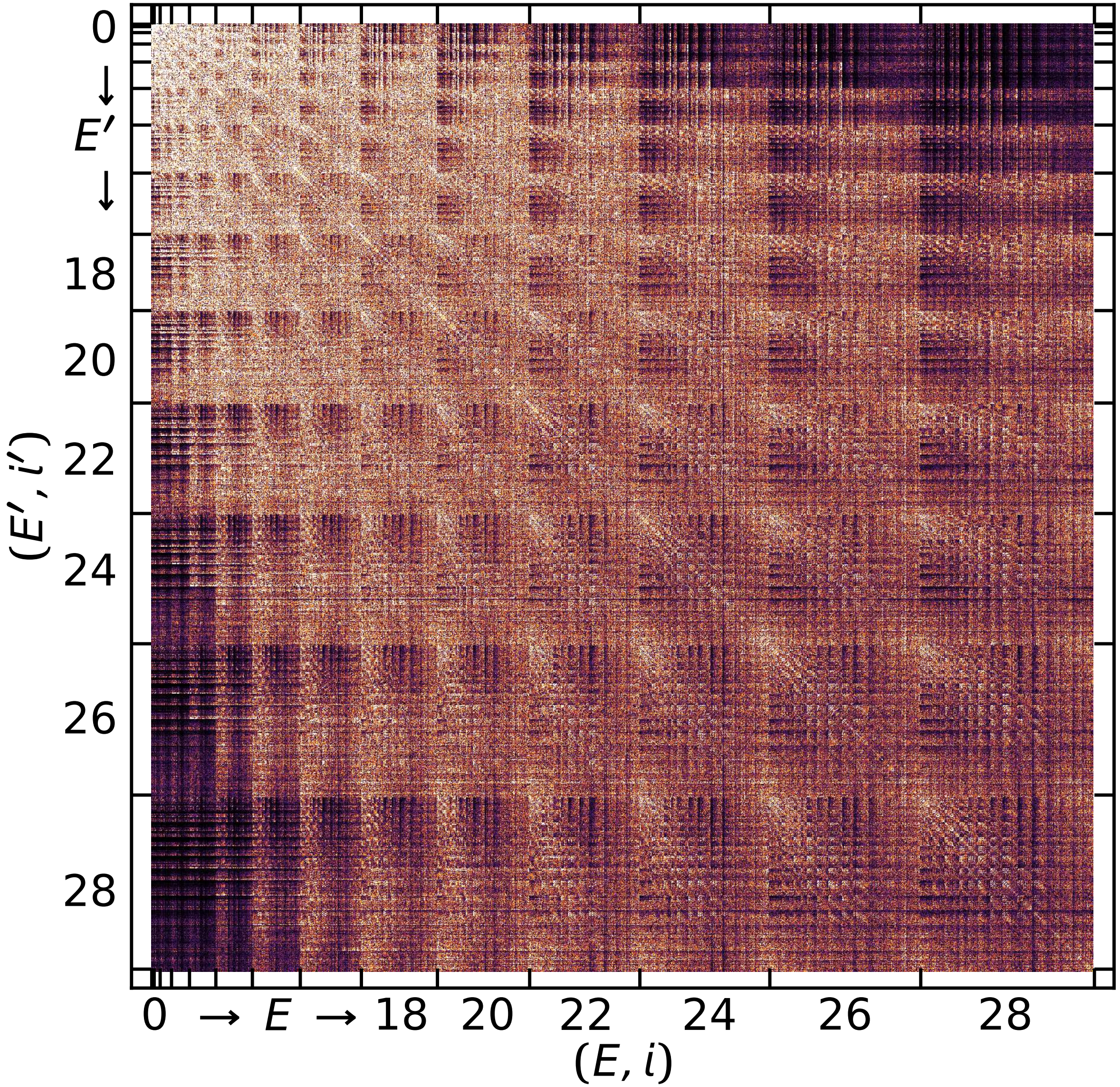
- $n = 3$: use **antisym. Jacobi-coordinate three-body states**
  - harmonic oscillator: $\left|E i J^{\pi} T\right\rangle$

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

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

SRG Evolution in Three-Body Space

3B-Jacobi HO matrix elements

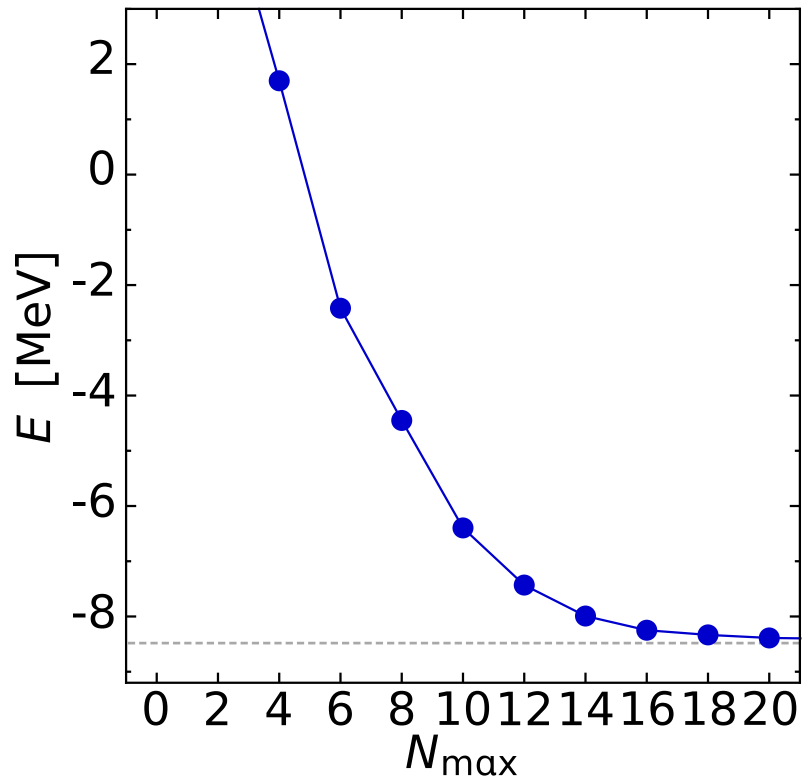


chiral NN+3N

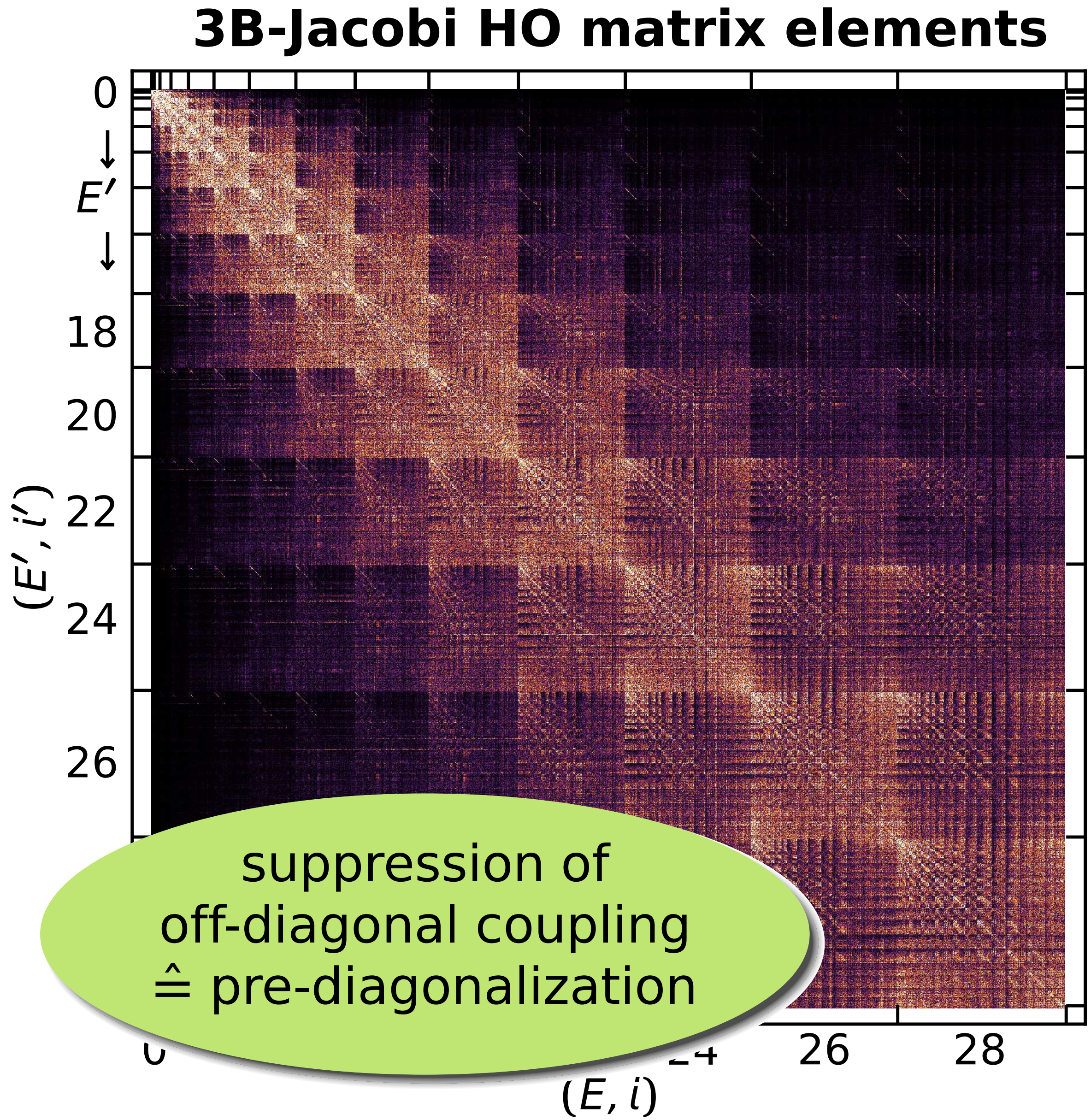
$N^3LO + N^2LO$, triton-fit, 500 MeV

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

NCSM ground state ^3H



SRG Evolution in Three-Body Space



suppression of
off-diagonal coupling
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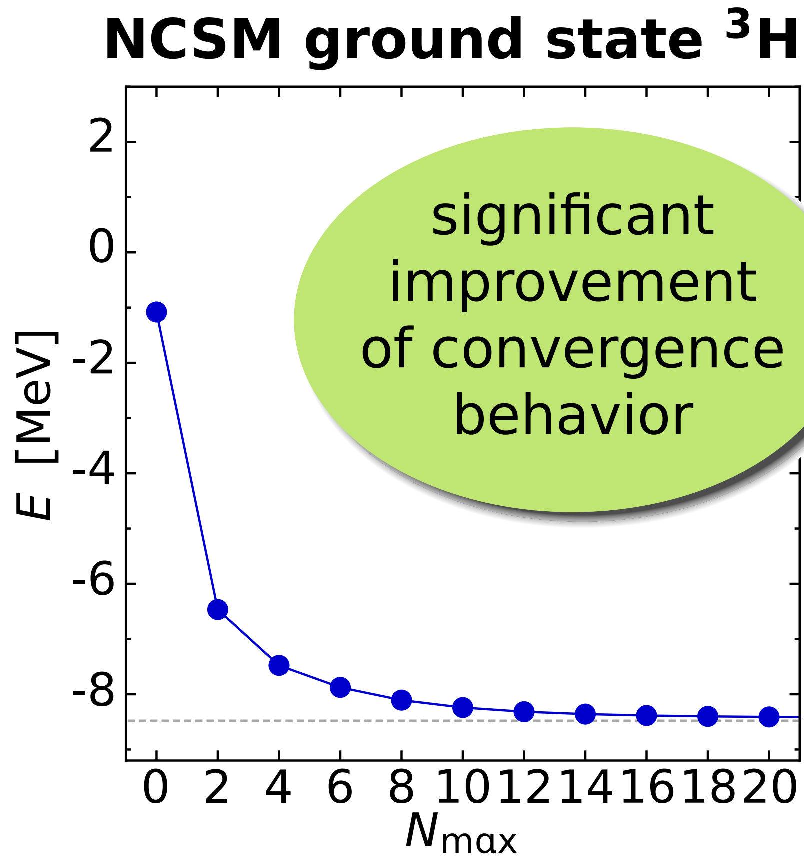

significant
improvement
of convergence
behavior

SRG Evolution in A-Body Space

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

$$\widetilde{H}_0 = \sum \dots a^\dagger a^\dagger a a \,, \qquad T_{\text{int}} = T - T_{\text{cm}} = \sum \dots a^\dagger a^\dagger a a$$

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

$$\begin{aligned} \widetilde{H}_{\Delta\alpha} &= \widetilde{H}_0 + \Delta\alpha \left[\left[T_{\text{int}}, \widetilde{H}_0 \right], \widetilde{H}_0 \right] \\ &= \sum \dots a^\dagger a^\dagger a a \\ &\quad + \Delta\alpha \left(\sum \dots a^\dagger a^\dagger a a \right) \left(\sum \dots a^\dagger a^\dagger a a \right) \left(\sum \dots a^\dagger a^\dagger a a \right) + \dots \end{aligned}$$

- unitary transformation **induces many-body contributions** in the Hamiltonian

Hamiltonian in A-Body Space

- **cluster decomposition**: decompose evolved Hamiltonian into irreducible n-body contributions $\widetilde{\text{H}}_\alpha^{[n]}$

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

- ***A*-body unitarity**: transformation is unitary only if all terms up to $n = A$ are kept, then all eigenvalues are independent of α

- **cluster truncation**: can construct contributions up to $n = 3$ from evolution in 2B and 3B space, but have to discard $n > 3$

- α-dependence of eigenvalu **nian**
  measures impact of discar

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

Introduction to

Ab Initio Nuclear Structure Theory

Part II: Many-Body Problem

Robert Roth

TECHNISCHE
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DARMSTADT

Ab Initio Many-Body Methods

No-Core Shell Model

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No-Core Shell Model — Basics

- **many-body basis**: Slater determinants $|\Phi_\nu^{\text{SD}}\rangle$ composed of harmonic oscillator single-particle states (m-scheme)

$$|\Psi\rangle = \sum_\nu C_\nu |\Phi_\nu^{\text{SD}}\rangle$$

- **model space**: spanned by basis states $|\Phi_\nu^{\text{SD}}\rangle$ with unperturbed excitation energies of up to $N_{\text{max}}\hbar\Omega$

with increasing model space size more and more **correlations can be described** by the model space

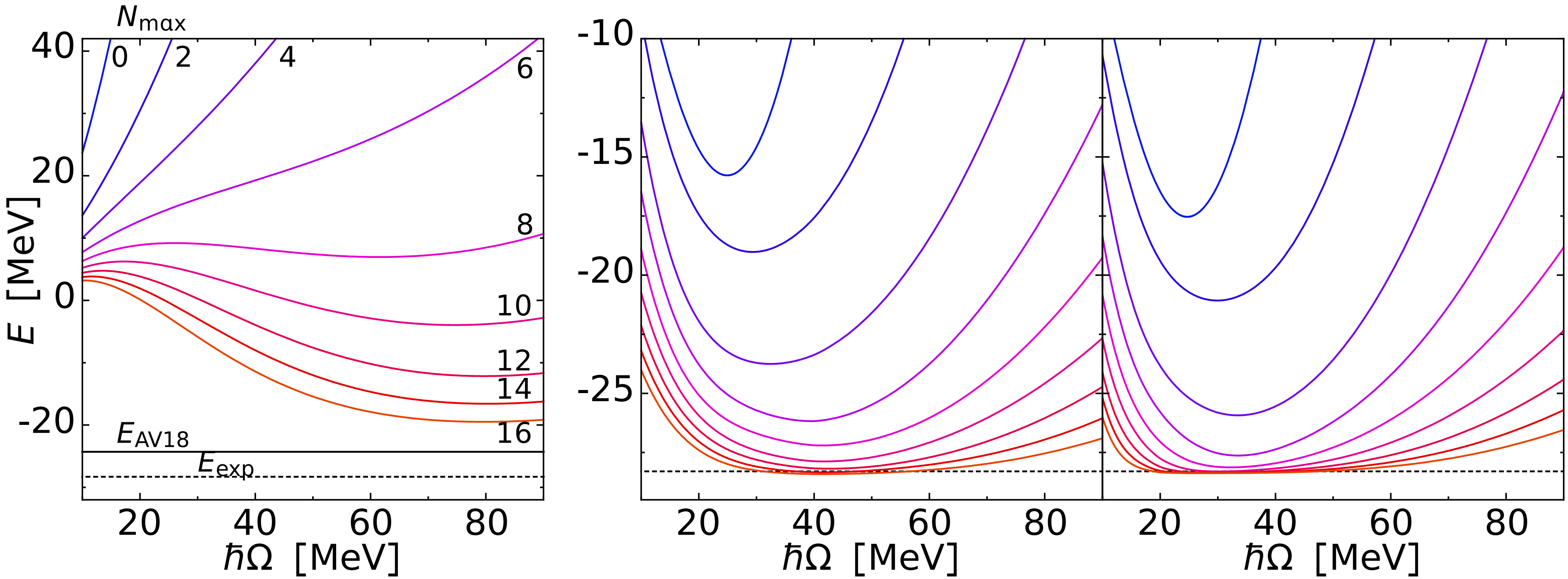
convergence of observables with N_{max} has to be investigated and is crucial

^{4}He: NCSM Convergence

V_{AV18}

V_{UCOM}
MIN, $I_\vartheta = 0.09\,\mathrm{fm}^3$

V_{SRG}
$\alpha = 0.03\,\mathrm{fm}^4$



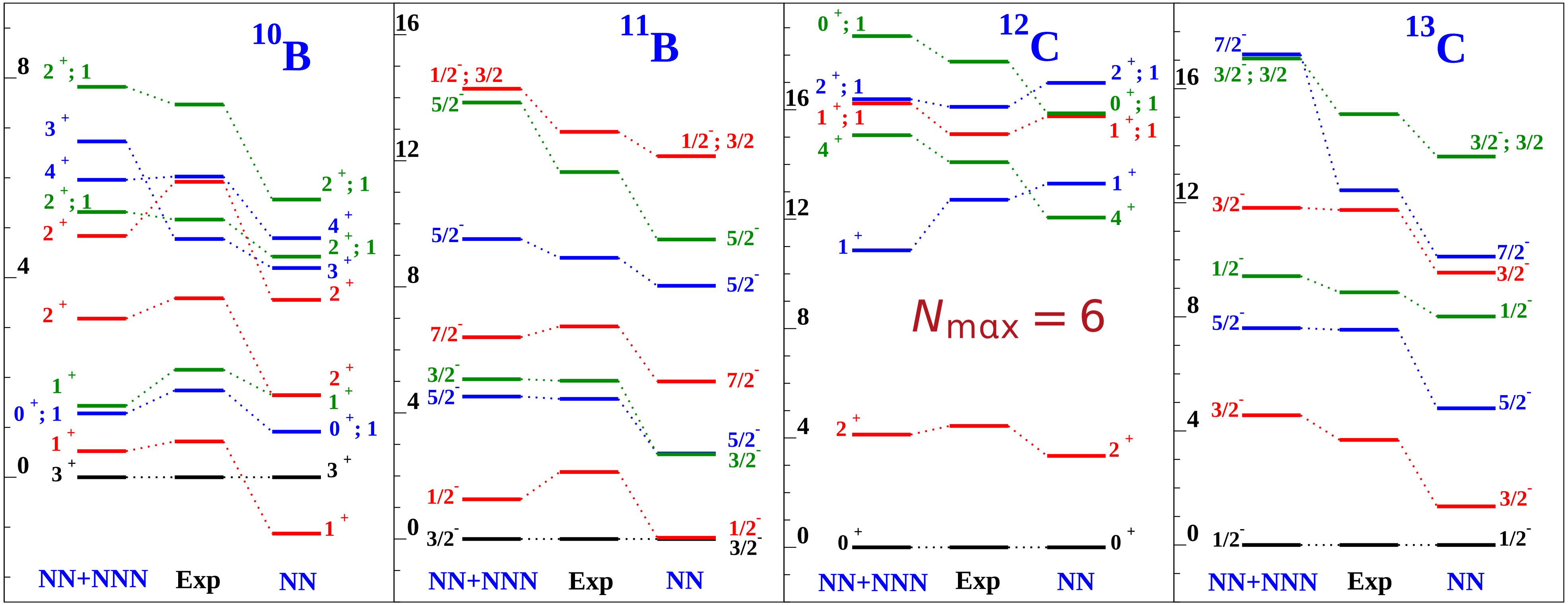
- I_ϑ or $\bar{\alpha}$ adjusted such that ^{4}He binding energy is reproduced

High-End Applications

PRL 99, 042501 (2007) PHYSICAL REVIEW LETTERS week ending 27 JULY 2007

Structure of A = 10–13 Nuclei with Two- Plus Three-Nucleon Interactions from Chiral Effective Field Theory

P. Navrátil,[1] V. G. Gueorguiev,[1,*] J. P. Vary,[1,2] W. E. Ormand,[1] and A. Nogga[3]

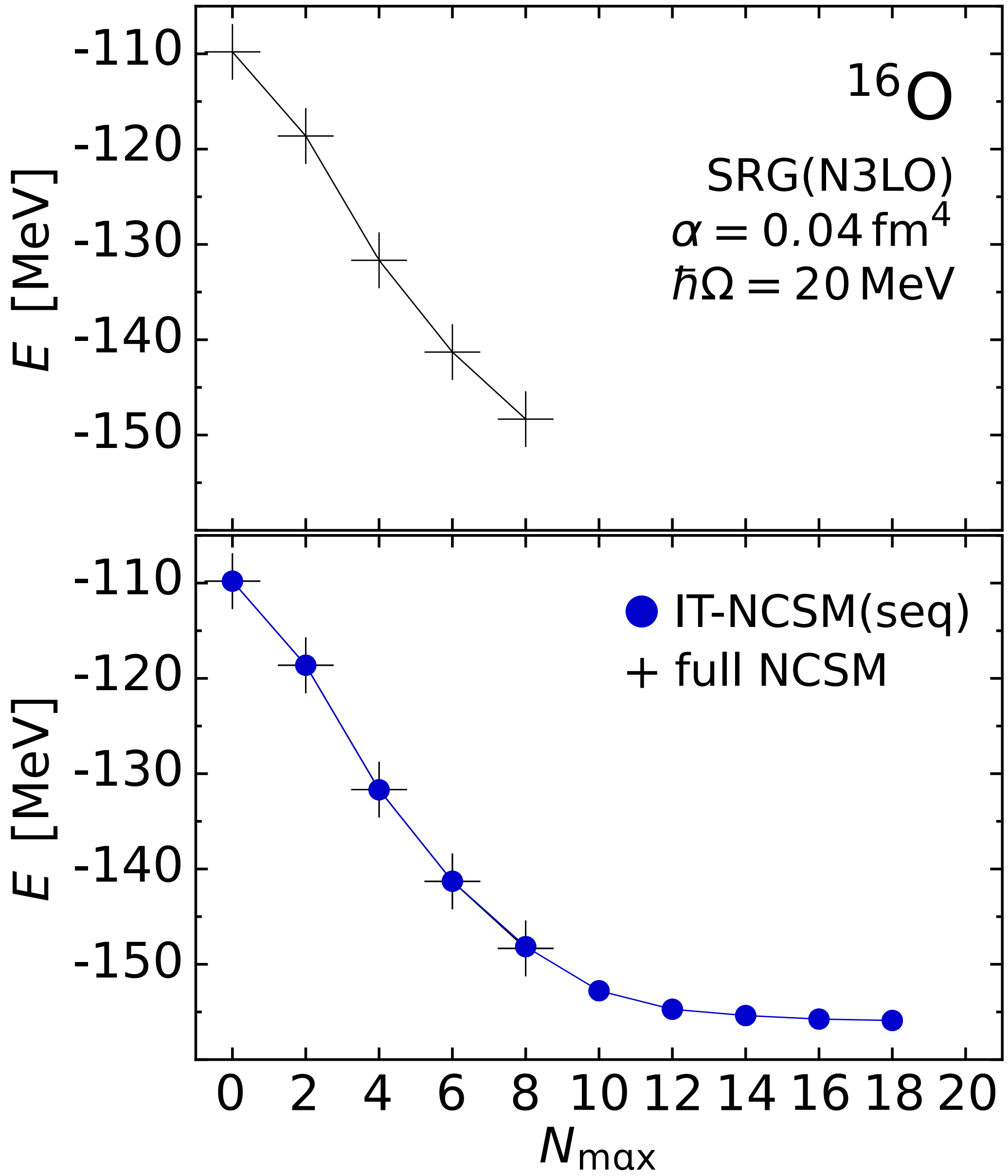


Importance Truncated NCSM

- 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



A Tale of Three Hamiltonians

Initial Hamiltonian

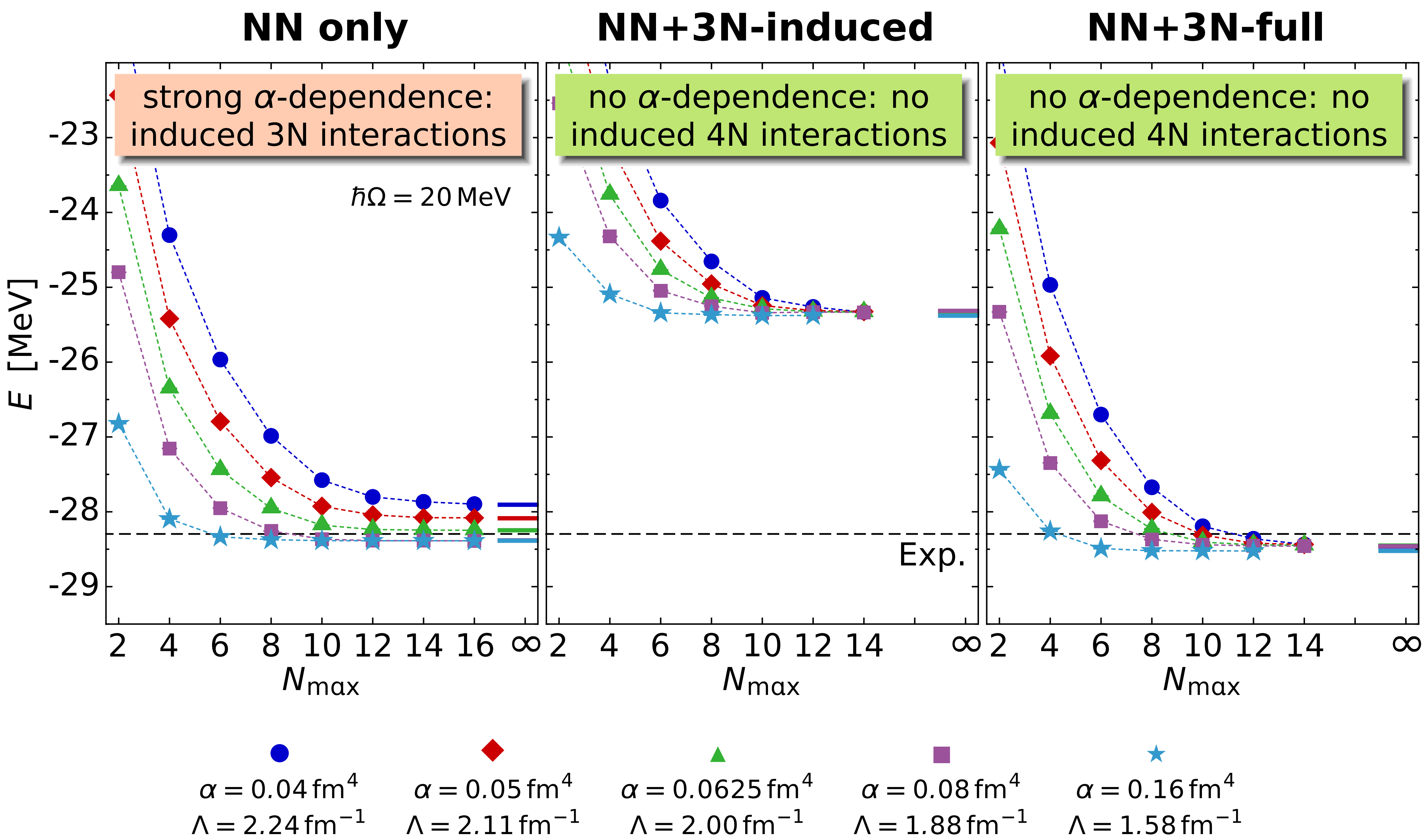
- NN: chiral interaction at N^3LO (Entem & Machleidt, 500 MeV)
- 3N: chiral interaction at N^2LO (c_D, c_E from ^3H binding & half-live)

SRG-Evolved Hamiltonians

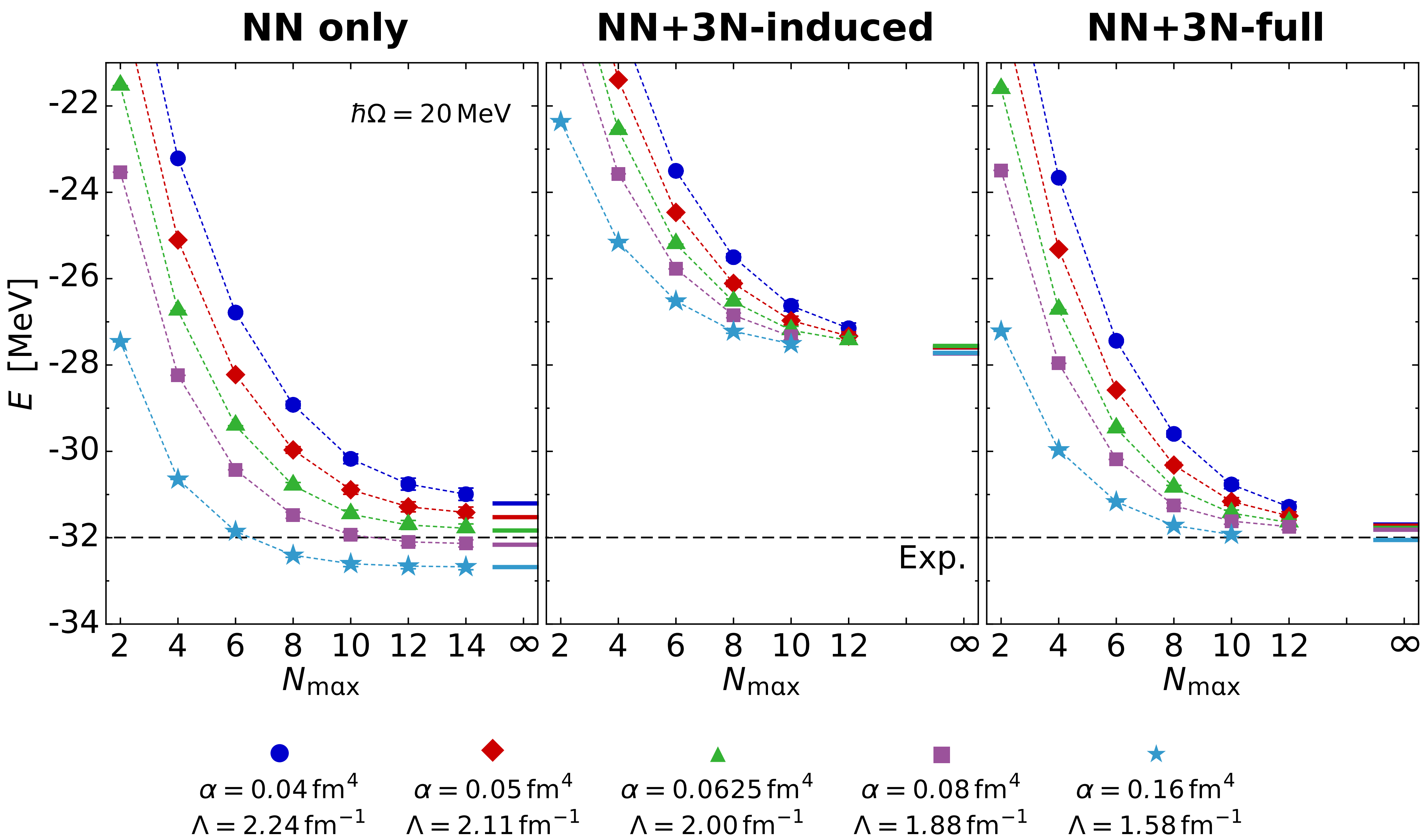
- **NN only**: start with NN initial Hamiltonian and keep two-body terms only
- **NN+3N-induced**: start with NN initial Hamiltonian and keep two- and three-body terms
- **NN+3N-full**: start with NN+3N in[...] two- and three-body terms

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

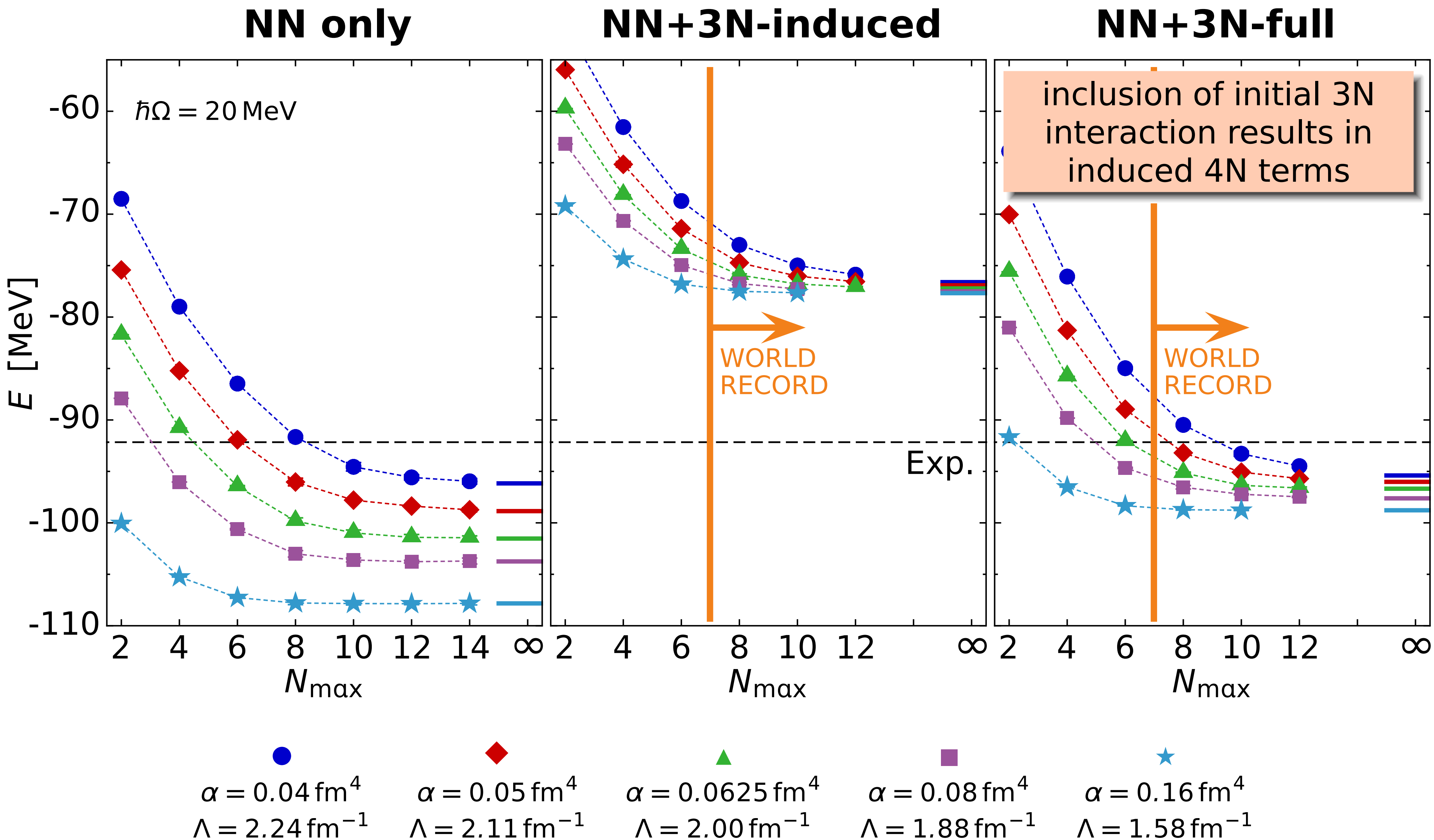
^{4}He: Ground-State Energies



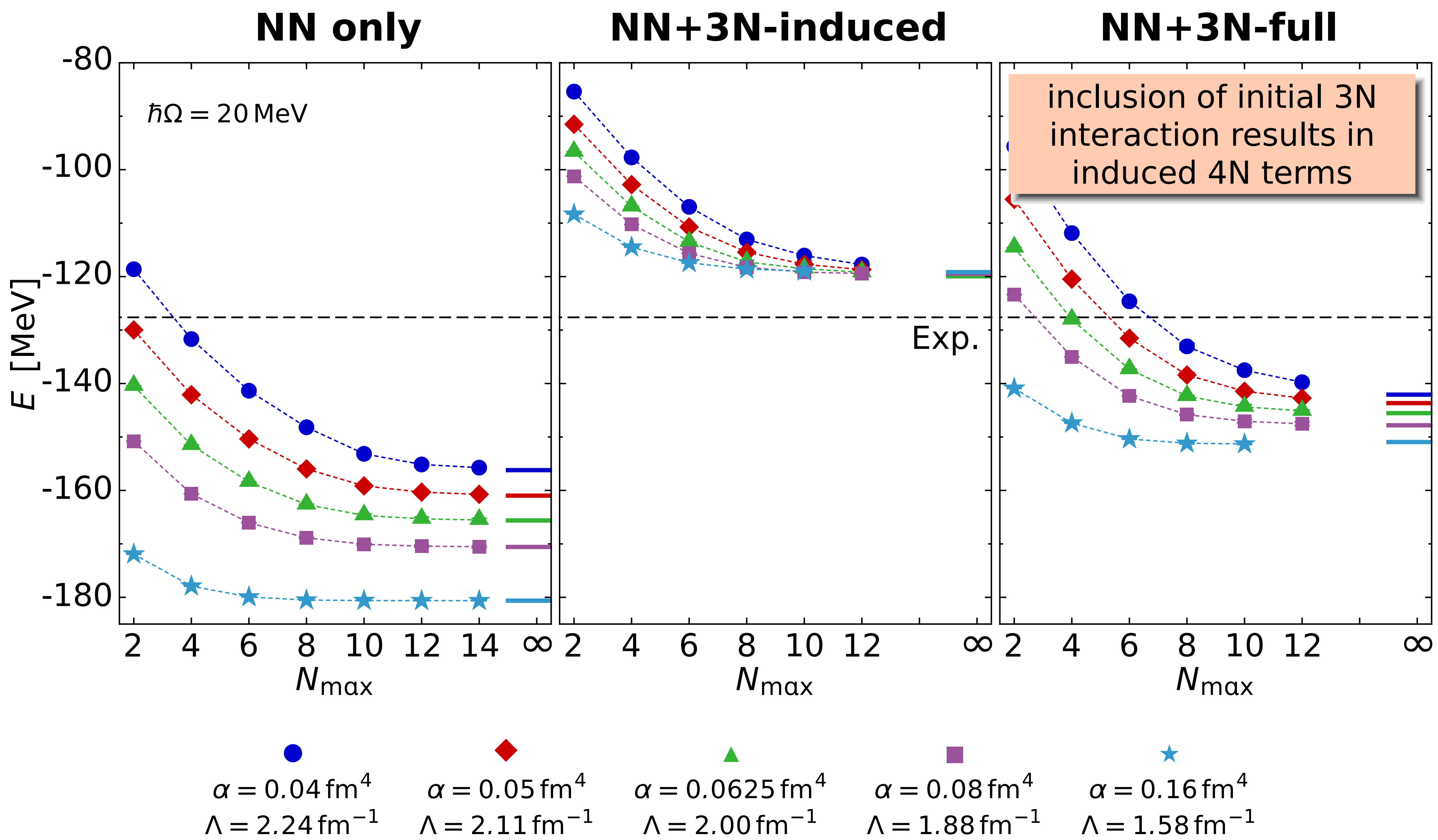
^{6}Li: Ground-State Energies



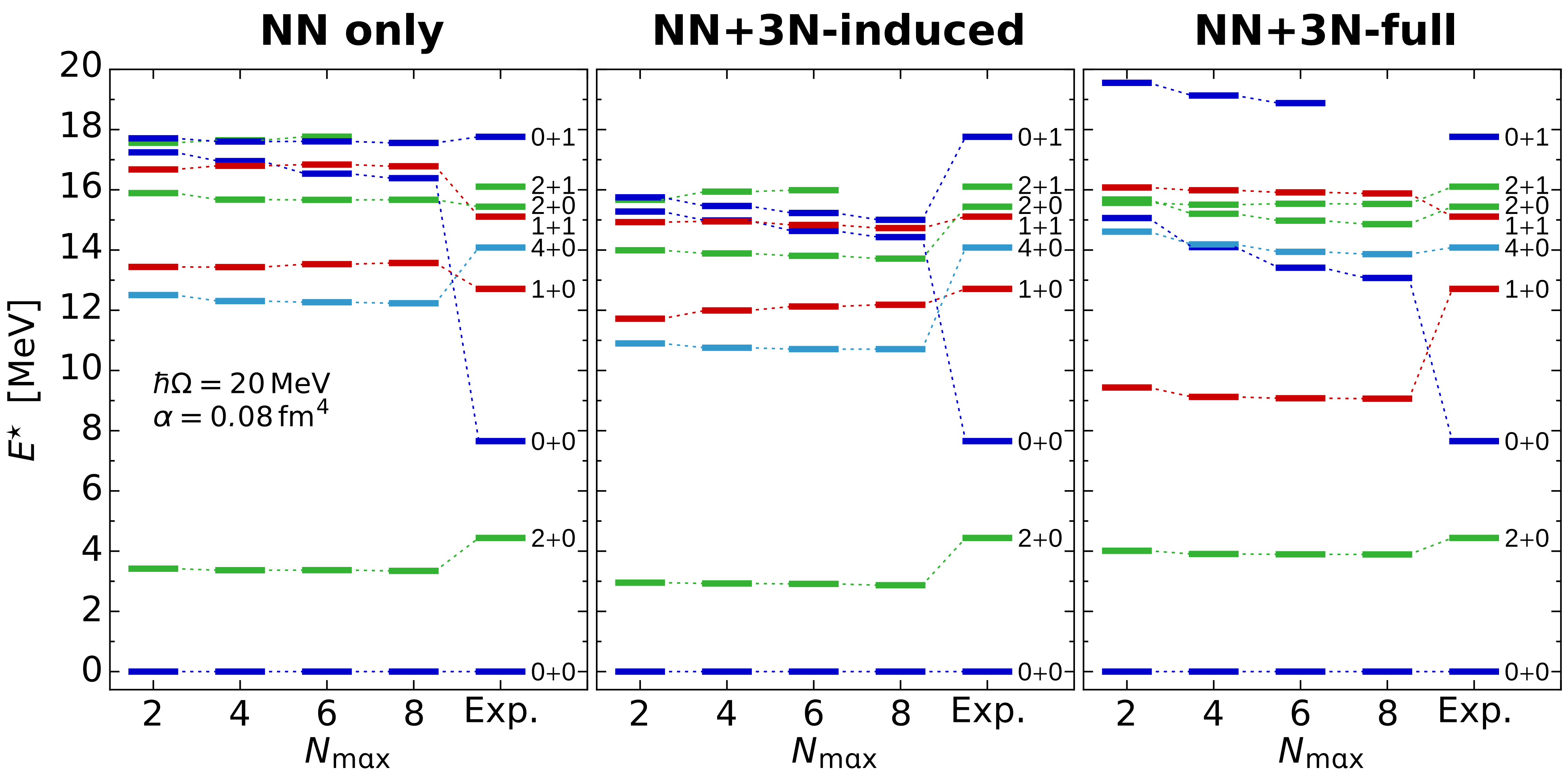
^{12}C: Ground-State Energies



^{16}O: Ground-State Energies



Spectroscopy of ^{12}C

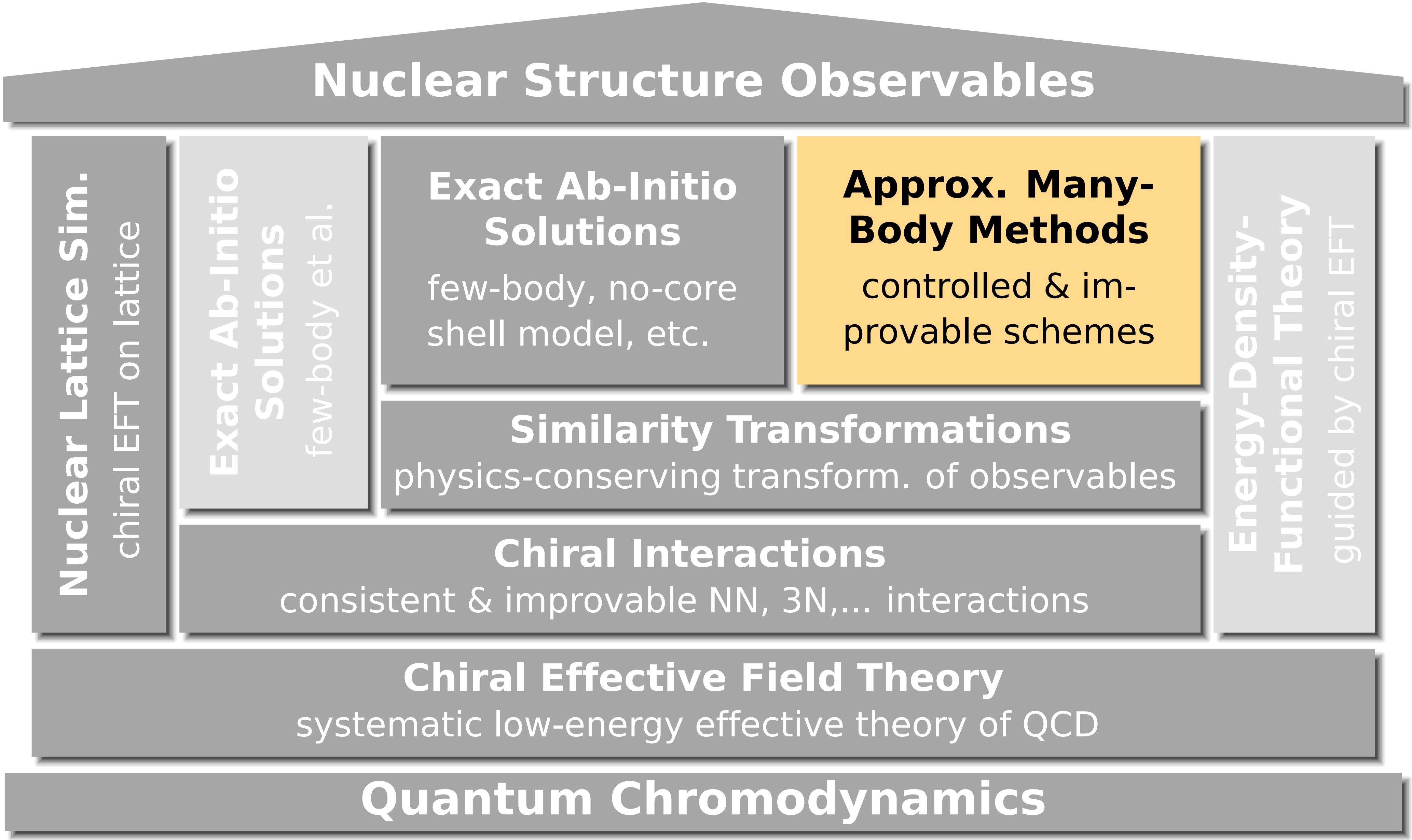


- IT-NCSM gives access to **complete spectroscopy of p- and sd-shell nuclei** starting from chiral NN+3N interactions

Approximate Many-Body Methods

Hartree-Fock & Beyond

Building Blocks



Hartree-Fock Approximation — Basics

- ground state $|\Psi\rangle$ approximated by a **single Slater determinant**

$$|\mathrm{HF}\rangle = |\phi_1, \phi_2, \dots, \phi_A\rangle_a = \sum_\pi \mathrm{sgn}(\pi)\, \mathrm{P}_\pi \; |\phi_1\rangle \otimes |\phi_2\rangle \otimes \cdots \otimes |\phi_A\rangle$$

- **variational calculation**: single-particle states $|\phi_i\rangle$ determined by minimizing the energy expectation value

$$E_{\mathrm{HF}} = \langle \mathrm{HF} | \mathrm{H}_{\mathrm{int}} | \mathrm{HF} \rangle = \frac{1}{2} \sum_{i,j=1}^{A} {}_a\langle \phi_i \phi_j | (\mathrm{T}_{\mathrm{int}} + \mathrm{V}_{\mathrm{NN}}) | \phi_i \phi_j \rangle_a$$

single Slater determinant by definition **cannot describe any correlations**

Hartree-Fock solution is **starting point for improved calculations**

Perturbation Theory — Basics

- start from HF state as zeroth-order 'unperturbed' state and construct **perturbative corrections** to the state and the energy

$$\left|\Psi\right\rangle = \left|\text{HF}\right\rangle + \lambda \left|\Delta\Psi^{(1)}\right\rangle + \lambda^2 \left|\Delta\Psi^{(2)}\right\rangle + \lambda^3 \left|\Delta\Psi^{(3)}\right\rangle + \cdots$$

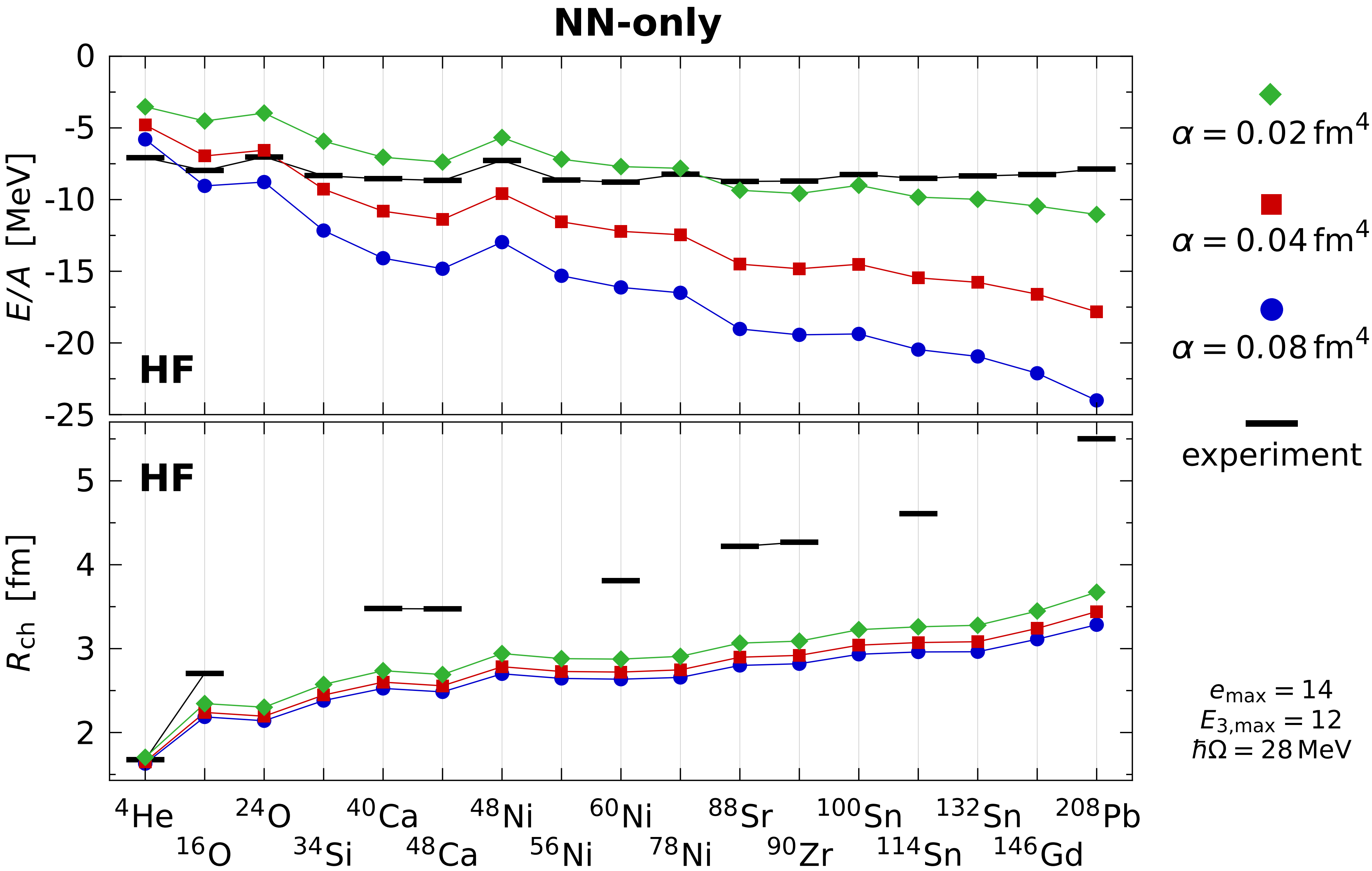
$$E = E_{\text{HF}} + \lambda \Delta E^{(1)} + \lambda^2 \Delta E^{(2)} + \lambda^3 \Delta E^{(3)} + \cdots$$

- **second-order energy correction** gives estimate for influence of correlations

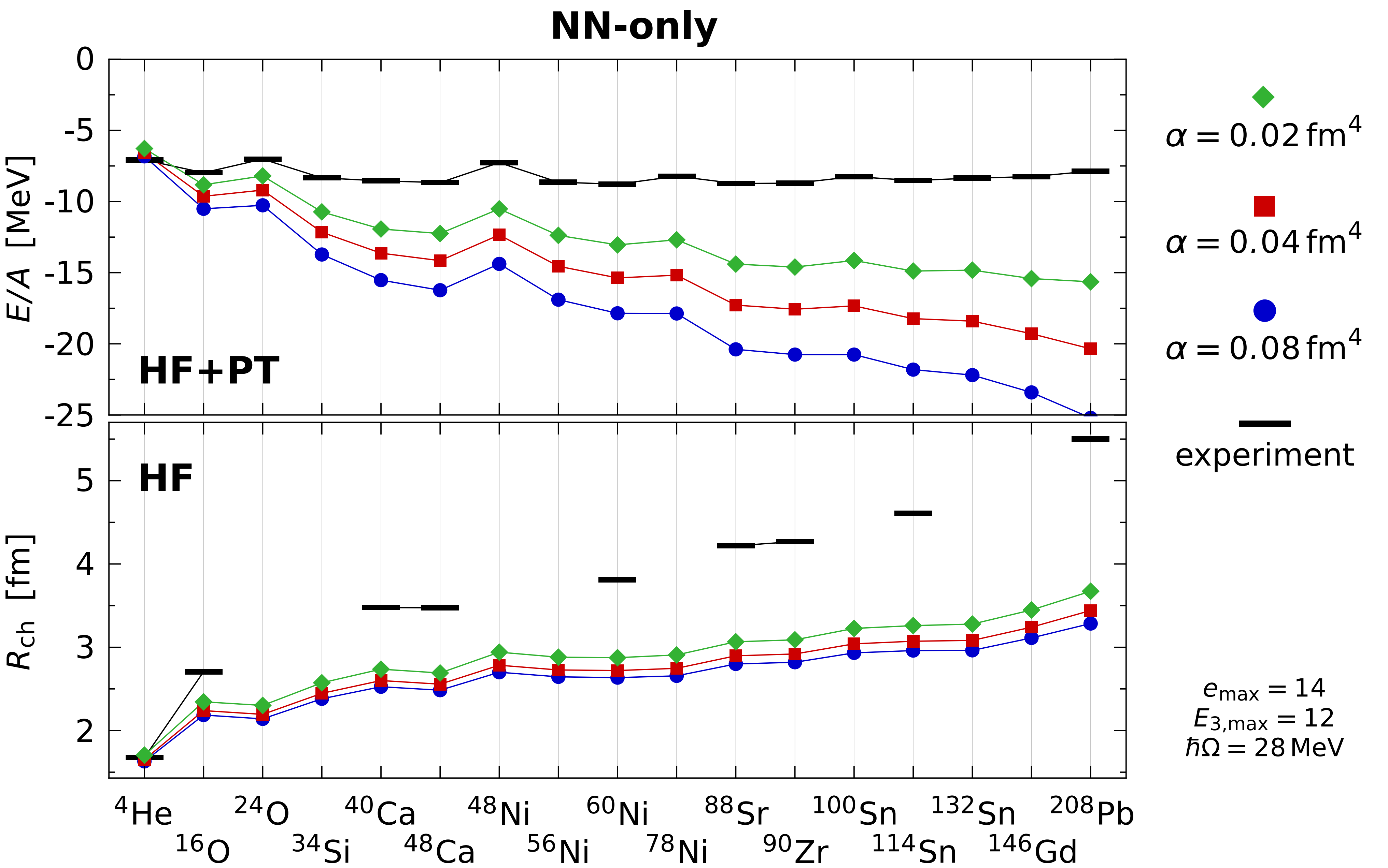
$$\Delta E^{(2)} = -\frac{1}{4} \sum_{i,j}^{\text{occu.}} \sum_{k,l}^{\text{unoccu.}} \frac{\left|{}_a\left\langle \phi_k \phi_l \right| (\text{T}_{\text{int}} + \text{V}_{\text{NN}}) \left| \phi_i \phi_j \right\rangle_a\right|^2}{\epsilon_k + \epsilon_l - \epsilon_i - \epsilon_j}$$

- higher orders or partial all-order summations can be evaluated
- eventually, at high-order (with appropriate resummations) perturbation theory will **recover the exact result**

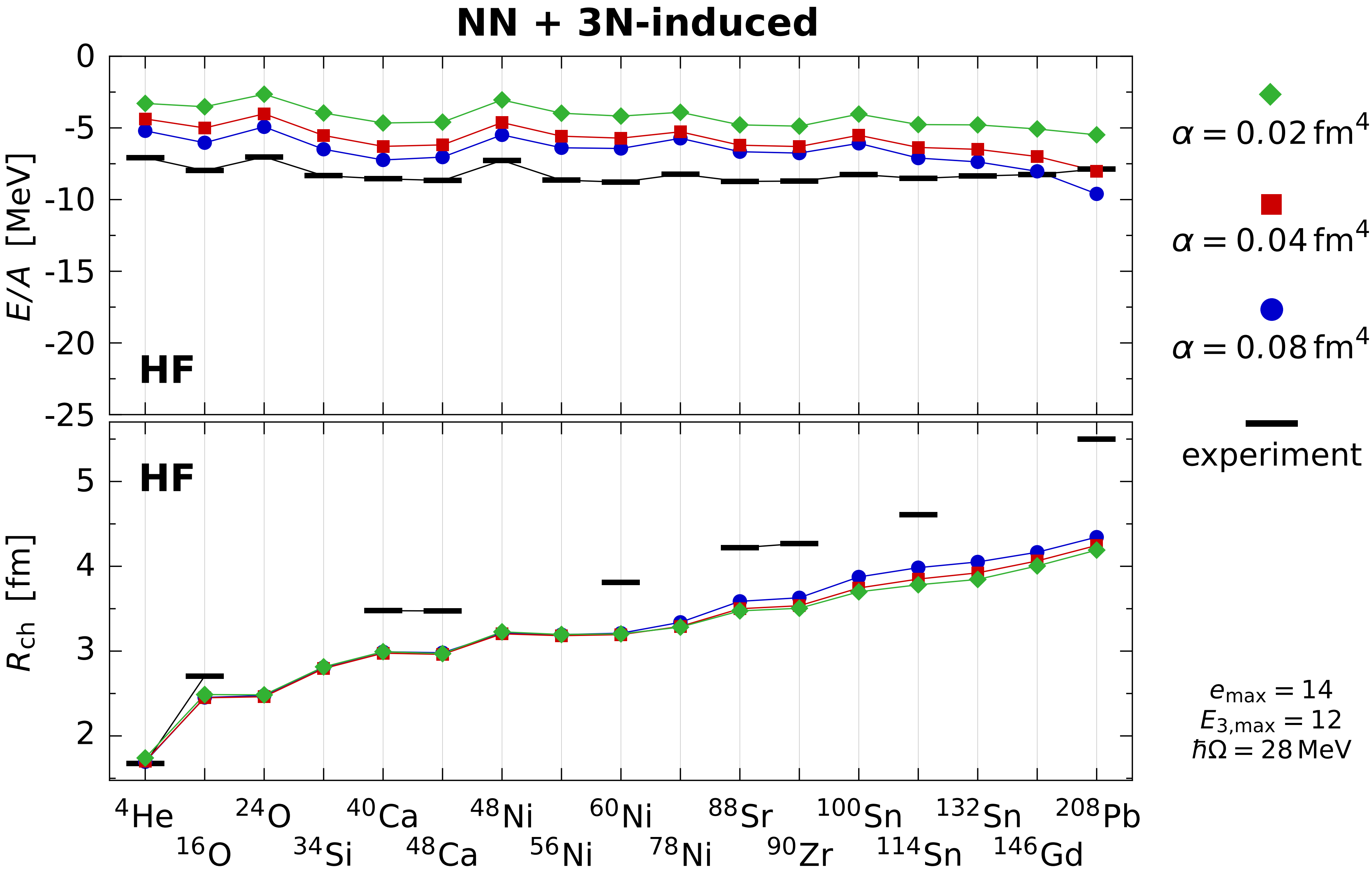
Systematics: E/A and R_{ch}



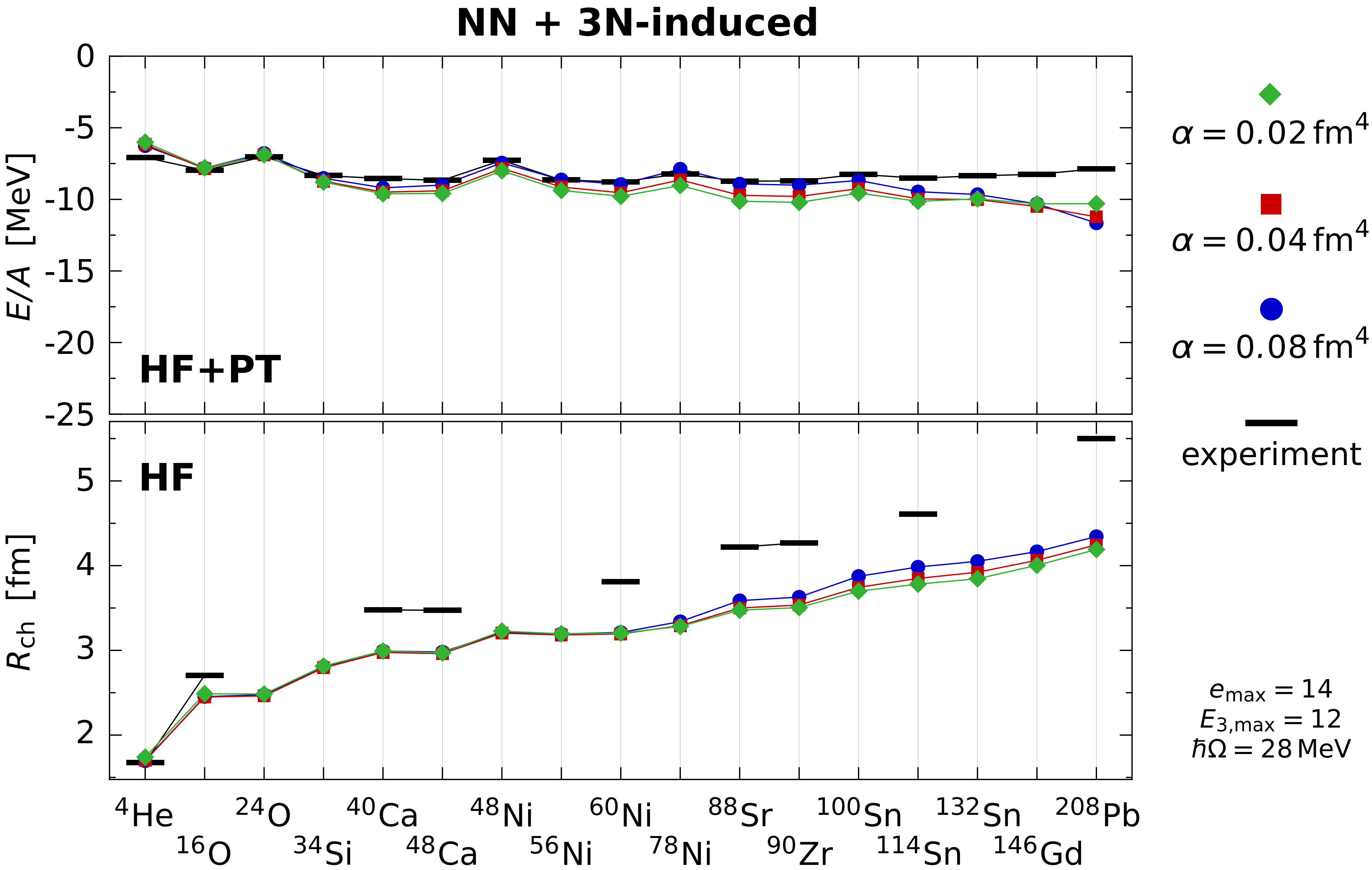
Systematics: E/A and R_{ch}



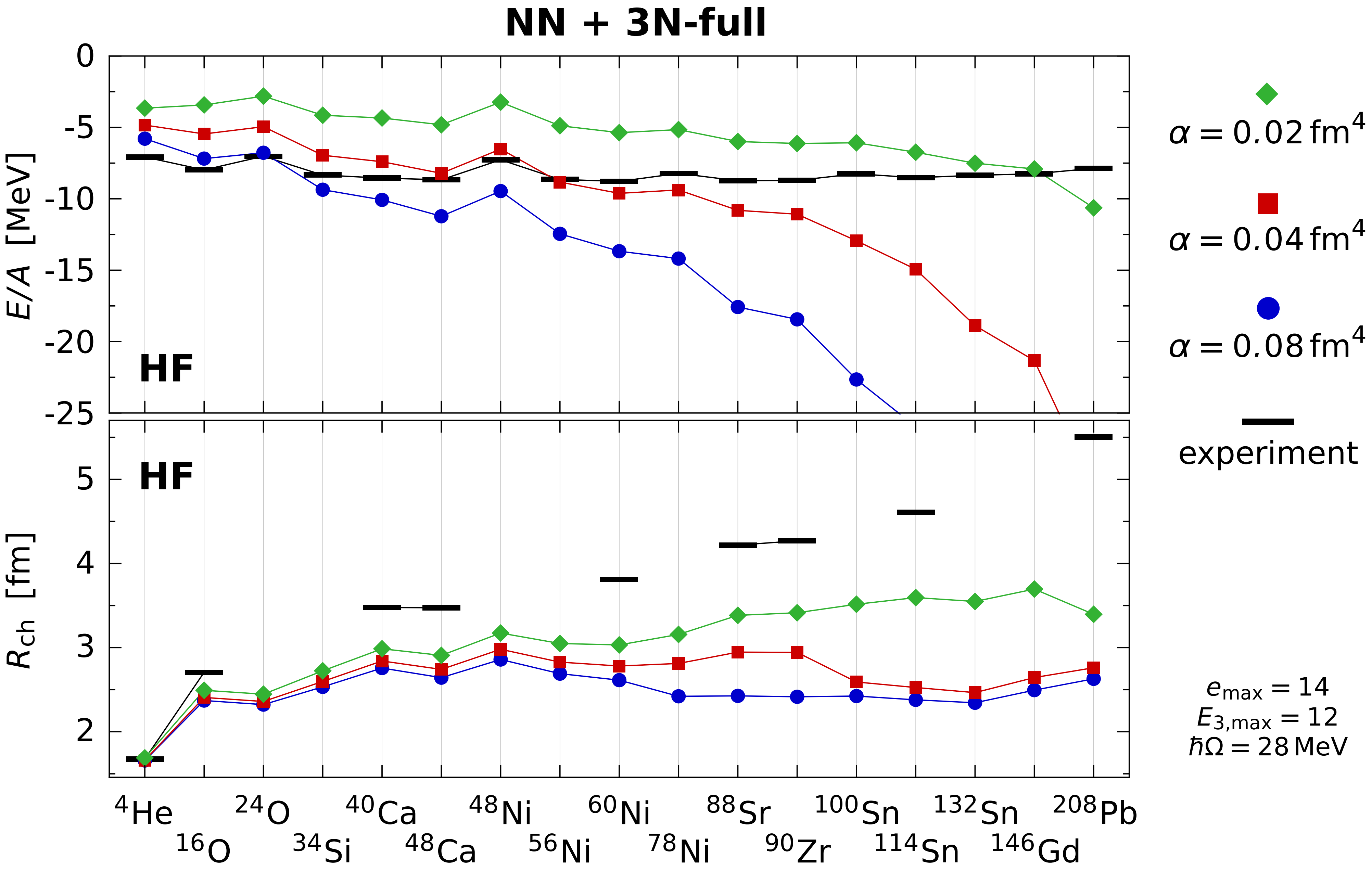
Systematics: E/A and R_{ch}



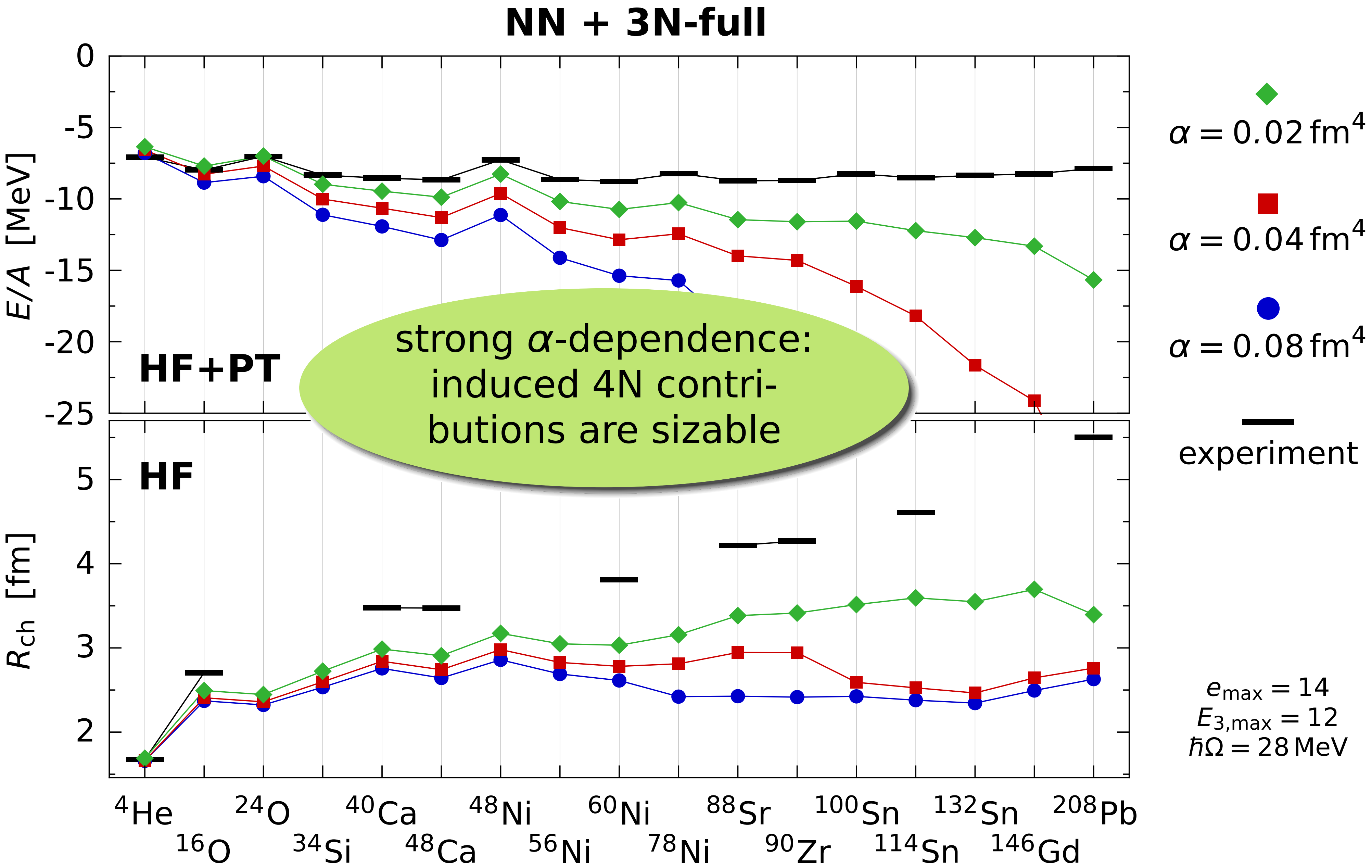
Systematics: E/A and R_{ch}



Systematics: E/A and R_{ch}



Systematics: E/A and R_{ch}



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 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...

Epilogue

- **thanks to my group & my collaborators**
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    GSI Helmholtzzentrum

COMPUTING TIME

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Center for Scientific Computing Frankfurt

SFB 634

Deutsche Forschungsgemeinschaft DFG

HIC for FAIR Helmholtz International Center

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