Nuclear Structure based on Correlated Realistic NN Potentials

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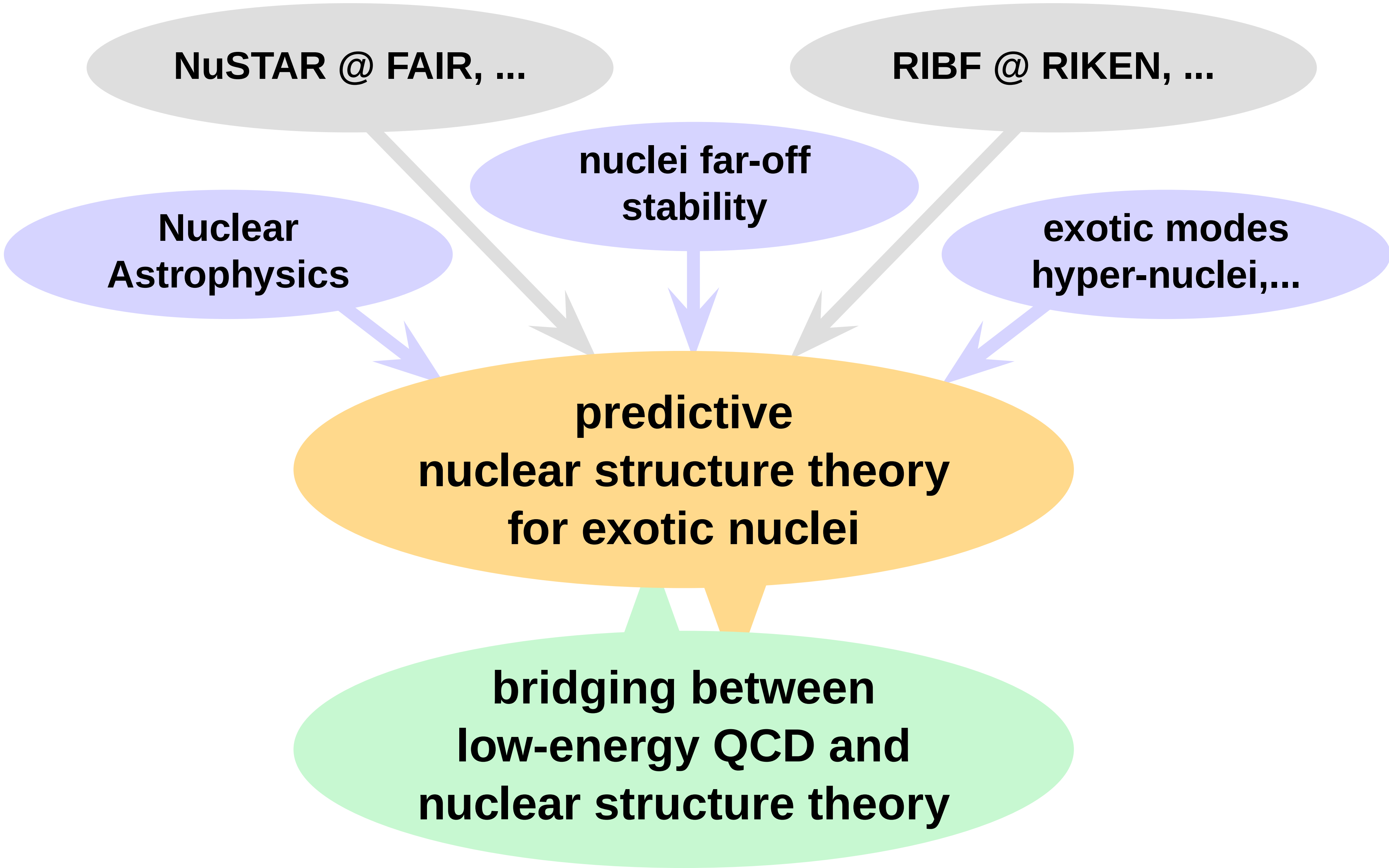
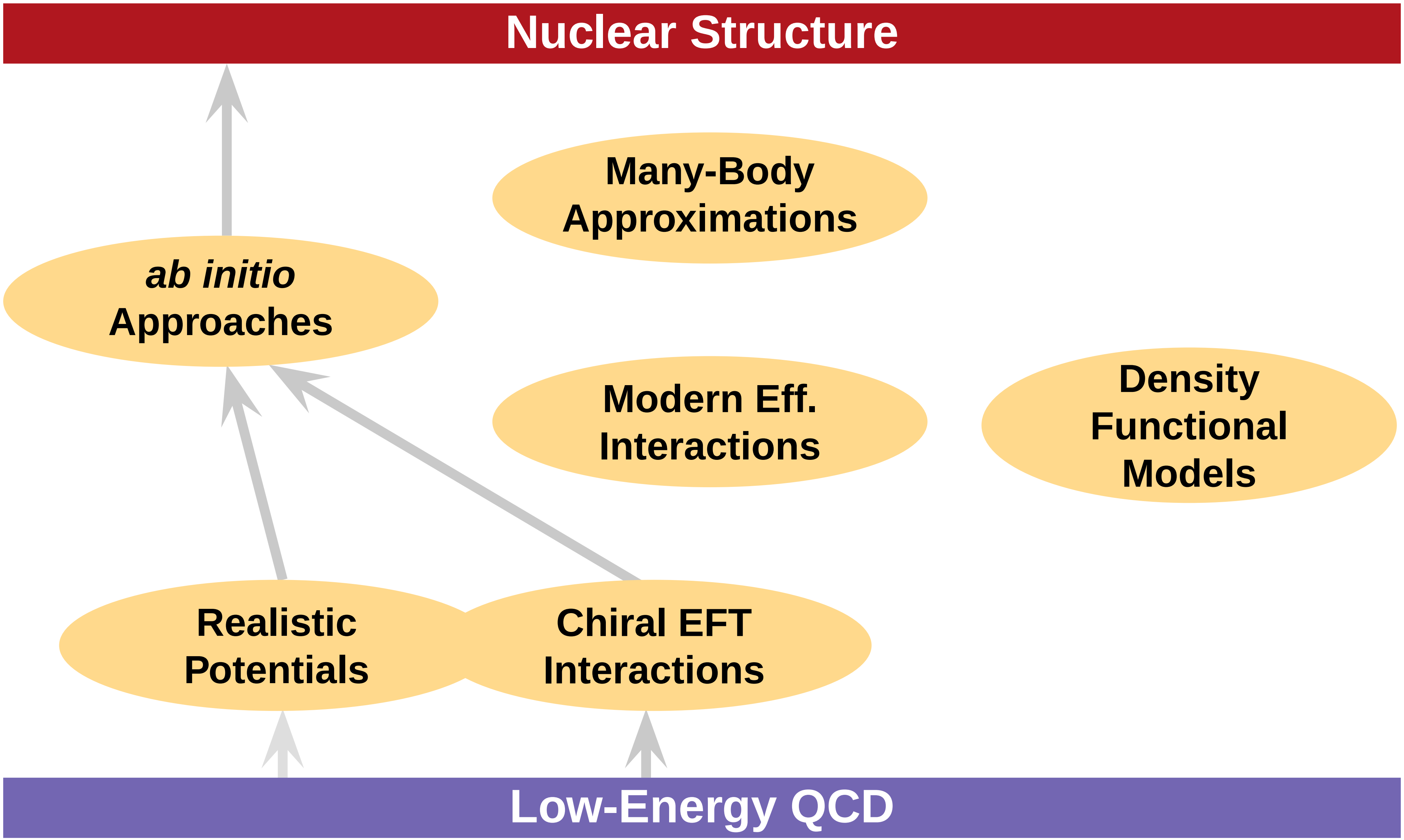
Overview

- Motivation
- Correlations & Modern Effective Interactions
  - Unitary Correlation Operator Method
  - Similarity Renormalization Group
- Innovative Many-Body Methods
  - No-Core Shell Model
  - Importance Truncated NCSM
  - Hartree-Fock & Beyond
- Perspectives

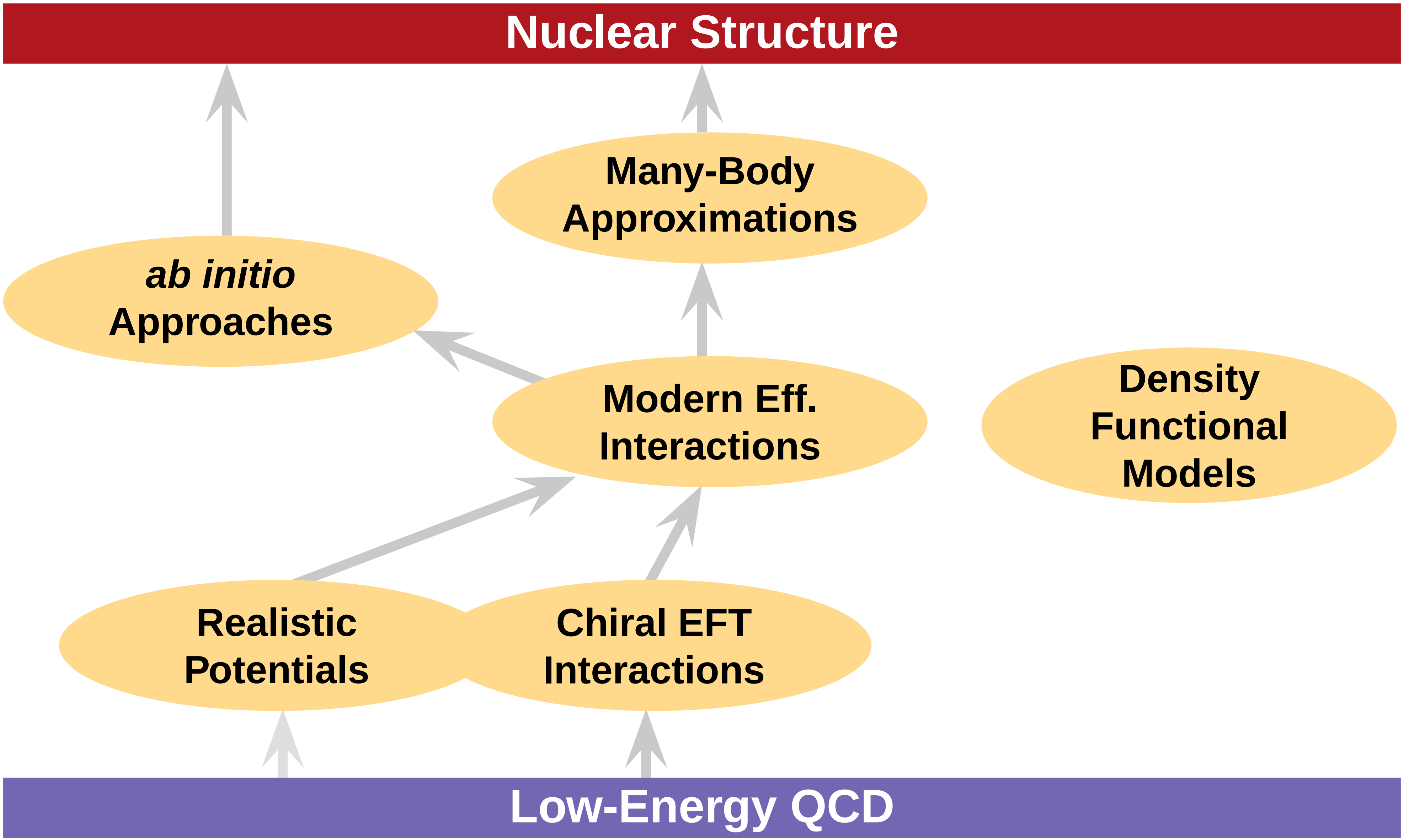
Nuclear Structure in the 21st Century



Modern Nuclear Structure Theory



Modern Nuclear Structure Theory



Why Effective Interactions?

Realistic Potentials

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

Many-Body Approximations

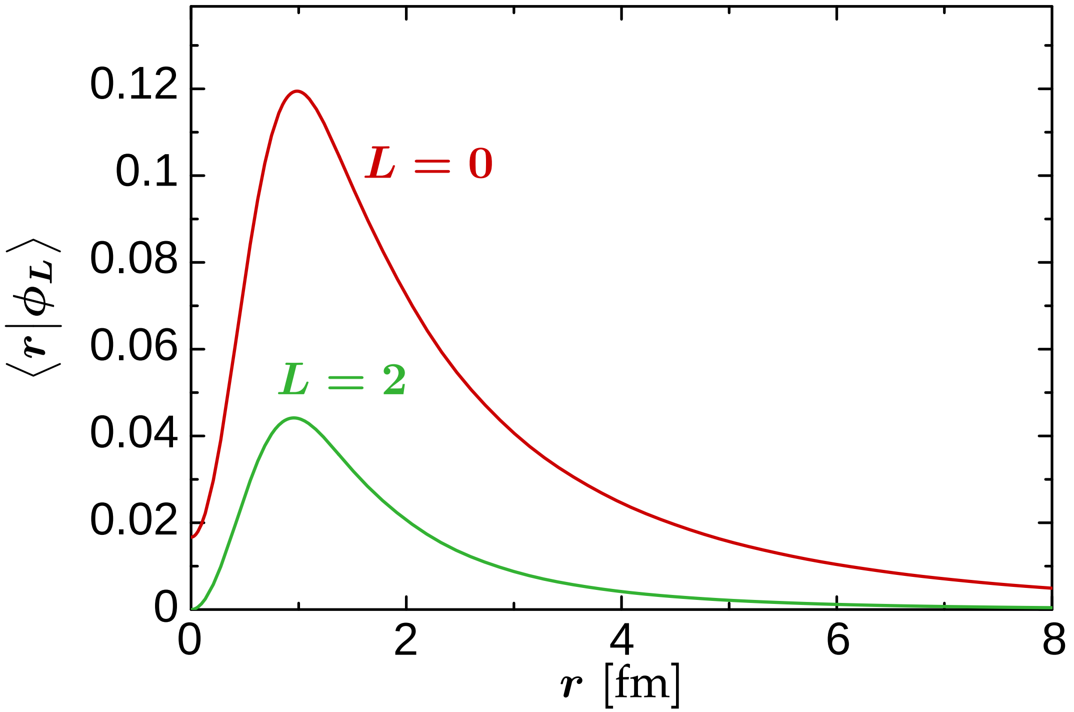
- rely on truncated many-nucleon Hilbert spaces (model space)
- not capable of describing short-range correlations
- extreme: Hartree-Fock based on single Slater determinant

Modern Effective Interactions

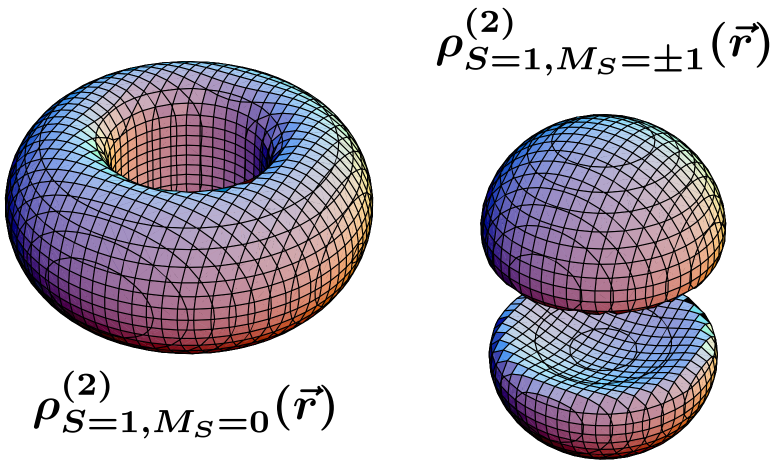
- adapt realistic potential to the available model space
- conserve experimentally constrained properties (phase shifts)

can be viewed as realistic interactions

Deuteron: Manifestation of Correlations



- **exact deuteron solution** for Argonne V18 potential



short-range repulsion supresses wavefunction at small distances r

central correlations

tensor interaction generates D-wave admixture in the ground state

tensor correlations

Modern Effective Interactions

Unitary Correlation Operator Method (UCOM)

H. Feldmeier et al. — Nucl. Phys. A 632 (1998) 61

T. Neff et al. — Nucl. Phys. A713 (2003) 311

R. Roth et al. — Nucl. Phys. A 745 (2004) 3

R. Roth et al. — Phys. Rev. C 72, 034002 (2005)

Unitary Correlation Operator Method

Correlation Operator

define an unitary operator $\mathbf{C}$ to describe the effect of short-range correlations

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

Correlated States

imprint short-range correlations onto uncorrelated many-body states

$$|\widetilde{\psi}\rangle = \mathbf{C}\ |\psi\rangle$$

Correlated Operators

adapt Hamiltonian and all other observables to uncorrelated many-body space

$$\widetilde{\mathbf{O}} = \mathbf{C}^{\dagger}\ \mathbf{O}\ \mathbf{C}$$

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

Unitary Correlation Operator Method

explicit ansatz for the correlation operator motivated by the **physics of short-range central and tensor correlations**

Central Correlator C_r

- radial distance-dependent shift in the relative coordinate of a nucleon pair

$$\mathrm{g}_r = \frac{1}{2}\big[s(\mathrm{r})\ \mathrm{q}_r + \mathrm{q}_r\ s(\mathrm{r})\big]$$

$$\mathrm{q}_r = \tfrac{1}{2}\big[\tfrac{\vec{\mathrm{r}}}{\mathrm{r}} \cdot \vec{\mathrm{q}} + \vec{\mathrm{q}} \cdot \tfrac{\vec{\mathrm{r}}}{\mathrm{r}}\big]$$

Tensor Correlator C_Ω

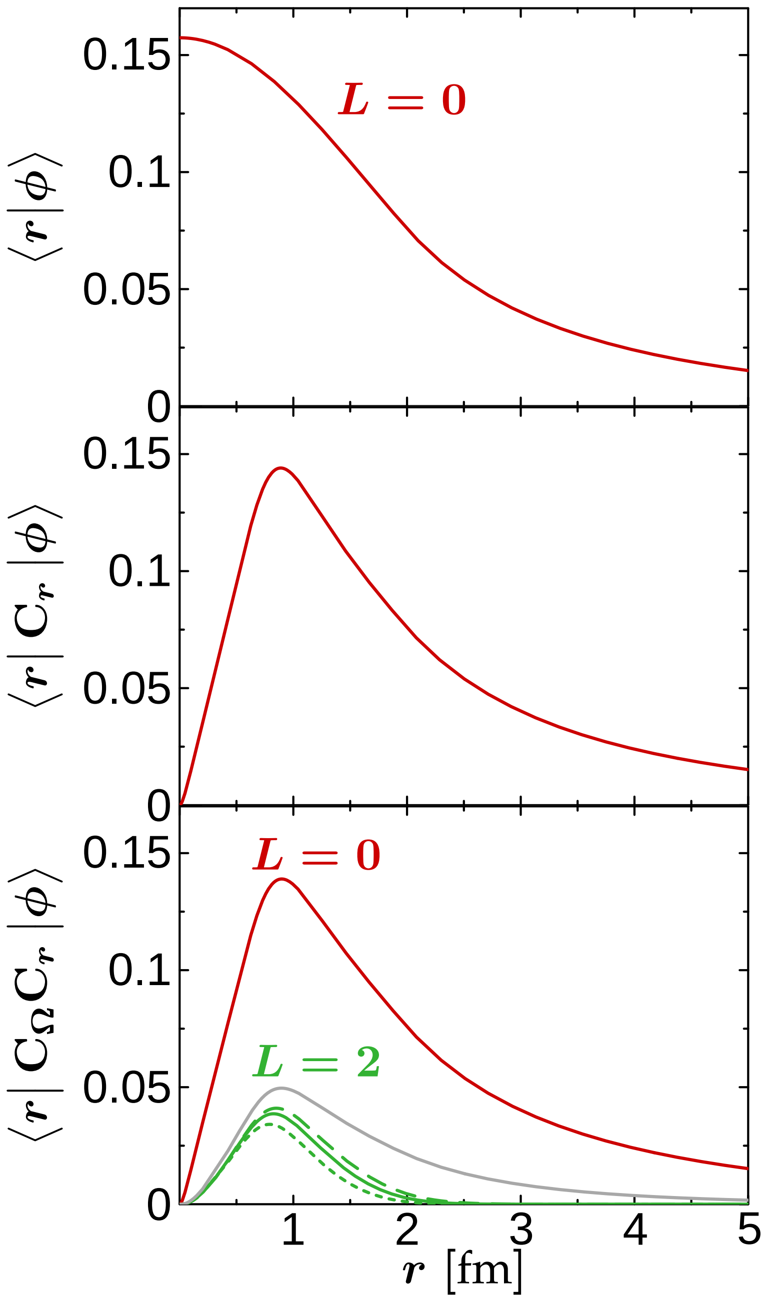
- angular shift depending on the orientation of spin and relative coordinate of a nucleon pair

$$\mathrm{g}_\Omega = \frac{3}{2}\vartheta(\mathrm{r})\big[(\vec{\sigma}_1 \cdot \vec{\mathrm{q}}_\Omega)(\vec{\sigma}_2 \cdot \vec{\mathrm{r}}) + (\vec{\mathrm{r}} \leftrightarrow \vec{\mathrm{q}}_\Omega)\big]$$

$$\vec{\mathrm{q}}_\Omega = \vec{\mathrm{q}} - \tfrac{\vec{\mathrm{r}}}{\mathrm{r}}\ \mathrm{q}_r$$

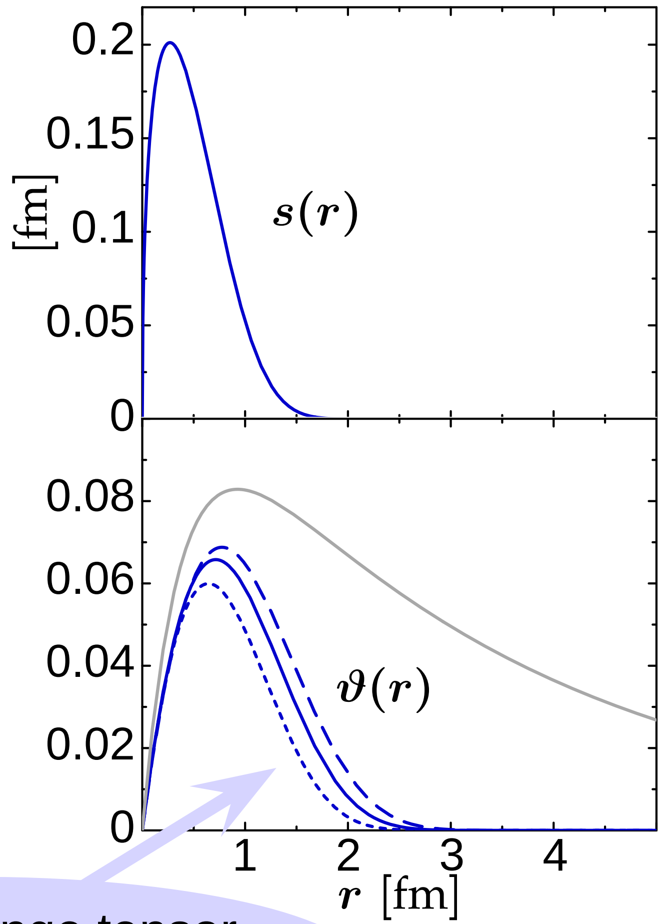
- $s(r)$ and $\vartheta(r)$ for given potential determined by energy minimization in the two-body system (for each S, T)

Correlated States: The Deuteron



central correlations

tensor correlations



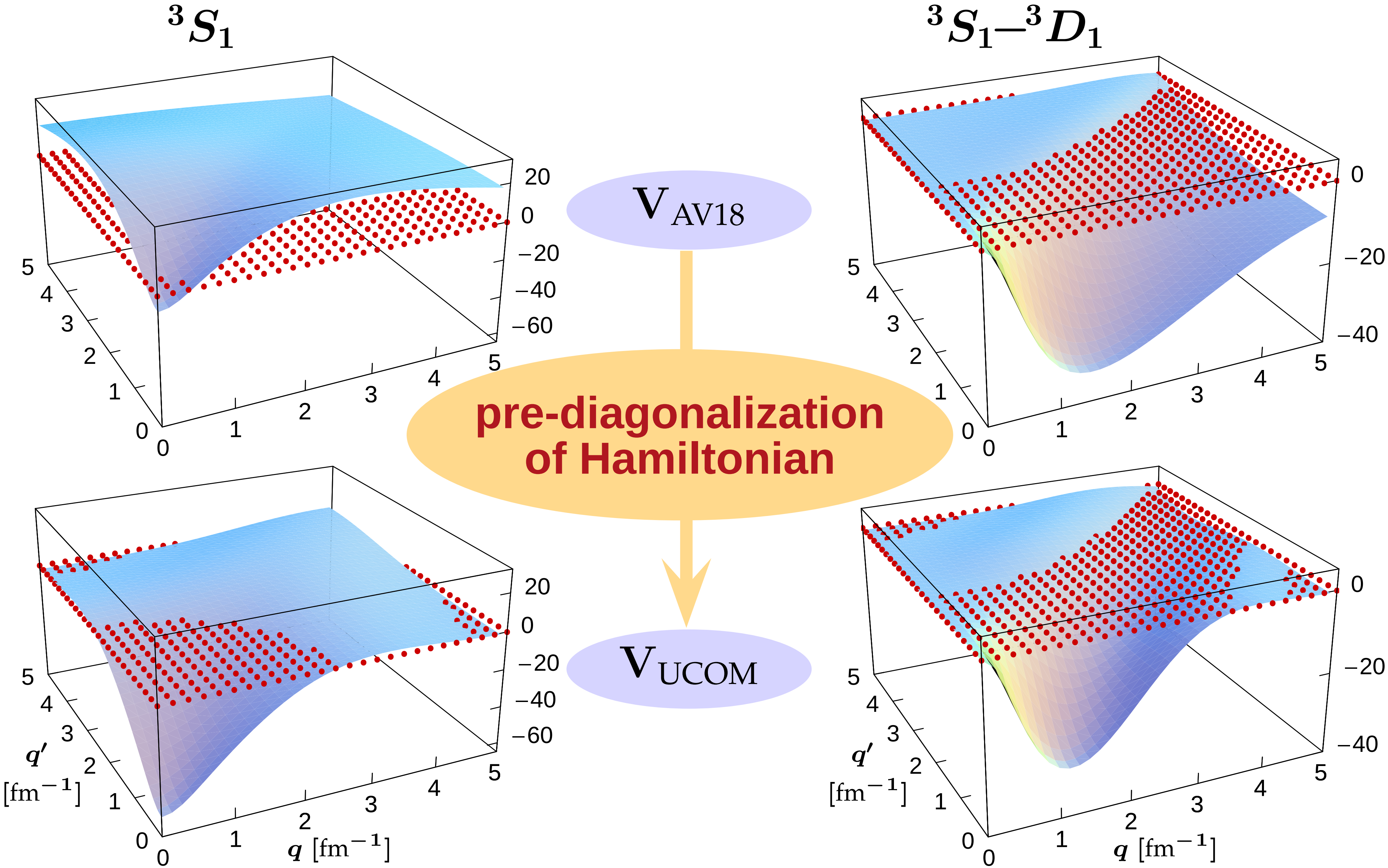
only short-range tensor correlations treated by C_Ω

Correlated Interaction: V_{UCOM}

$$\widetilde{\mathrm{H}} = \mathrm{T} + \mathrm{V}_{\text{UCOM}} + \mathrm{V}_{\text{UCOM}}^{[3]} + \cdots$$

- **closed operator expression** for the correlated interaction V_{UCOM} in two-body approximation
- correlated interaction and original NN-potential are **phase shift equivalent** by construction
- unitary transformation results in a **pre-diagonalization** of Hamiltonian (similar to renormalization group methods)
- operators of **all observables** (densities, transitions) have to be and can be **transformed consistently**

Correlated Interaction: V_{UCOM}



Modern Effective Interactions

Similarity Renormalization Group (SRG)

Hergert & Roth — Phys. Rev. C 75, 051001(R) (2007)

Bogner et al. — Phys. Rev. C 75, 061001(R) (2007)

Similarity Renormalization Group

unitary transformation of the **Hamiltonian to a band-diagonal form** with respect to a given uncorrelated many-body basis

Flow Equation for Hamiltonian

- evolution equation for Hamiltonian

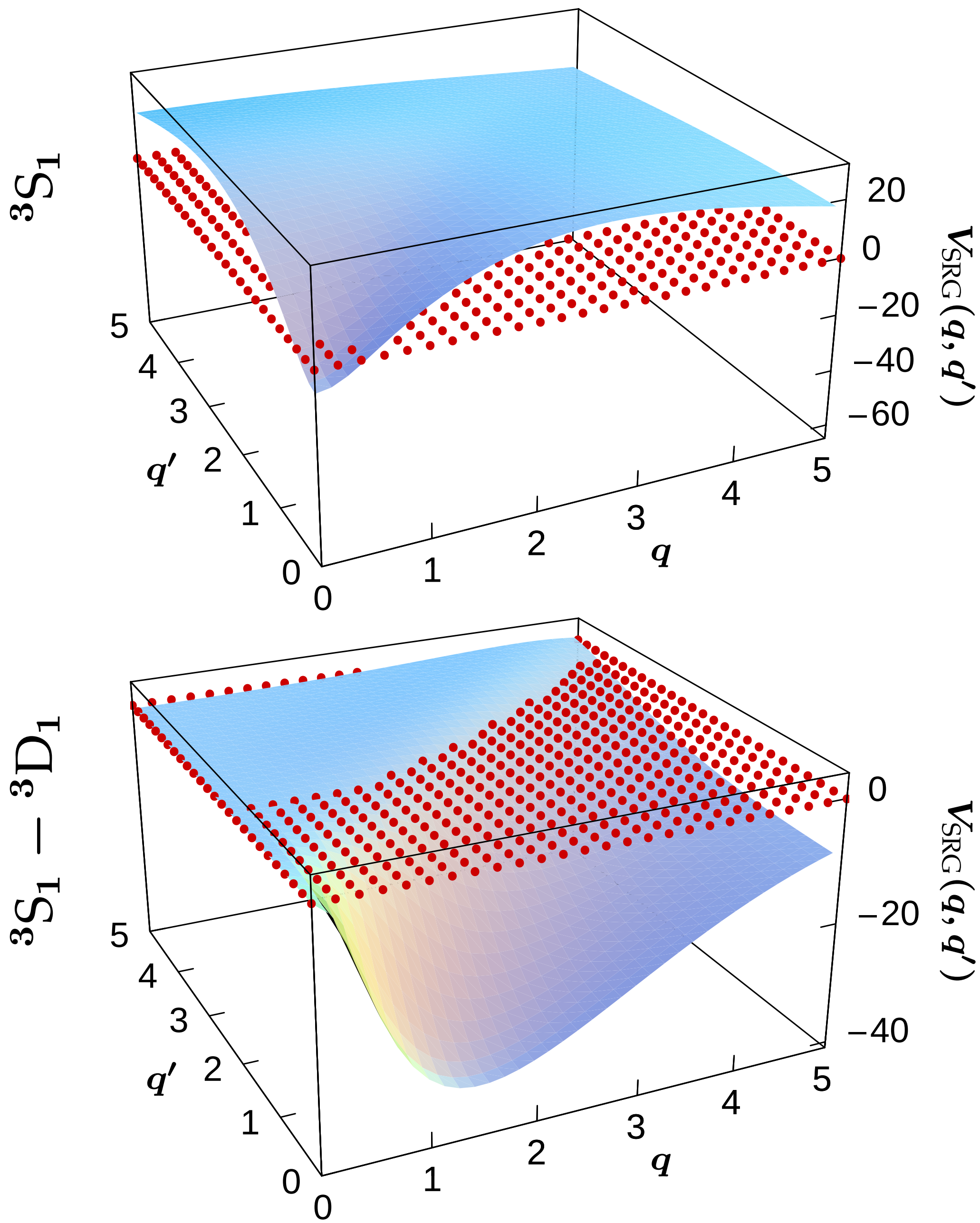
$$\widetilde{H}(\alpha) = C^{\dagger}(\alpha)\, H\, C(\alpha) \qquad \rightarrow \qquad \frac{d}{d\alpha}\widetilde{H}(\alpha) = \left[\eta(\alpha), \widetilde{H}(\alpha)\right]$$

- dynamical generator defined as commutator with the operator in whose eigenbasis H shall be diagonalized

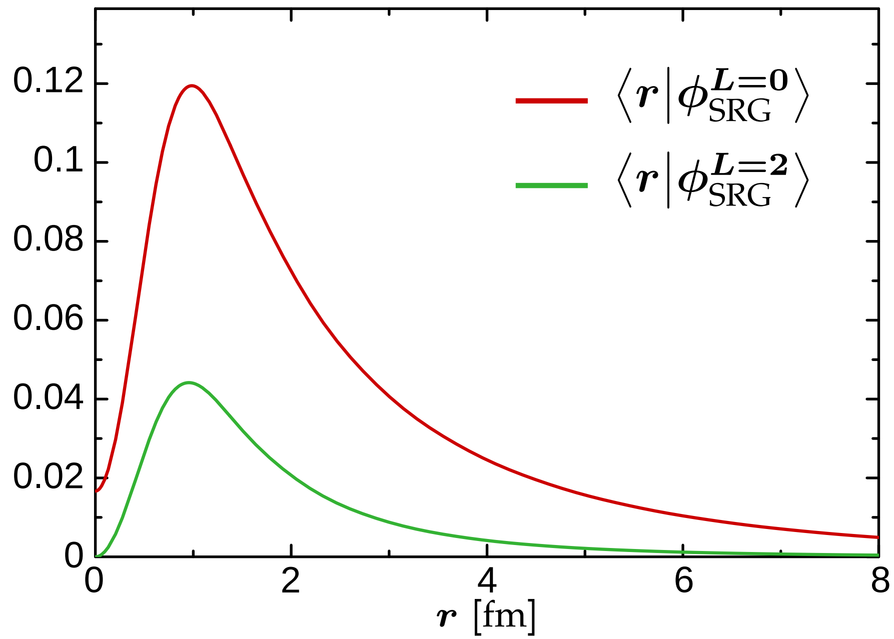
$$\eta(\alpha) = \left[T_{\text{int}}, \widetilde{H}(\alpha)\right] \stackrel{2B}{=} \frac{1}{2\mu}\left[\vec{q}^{\,2}, \widetilde{H}(\alpha)\right]$$

- $\eta(0)$ has the same structure as the UCOM generators g_r and g_Ω

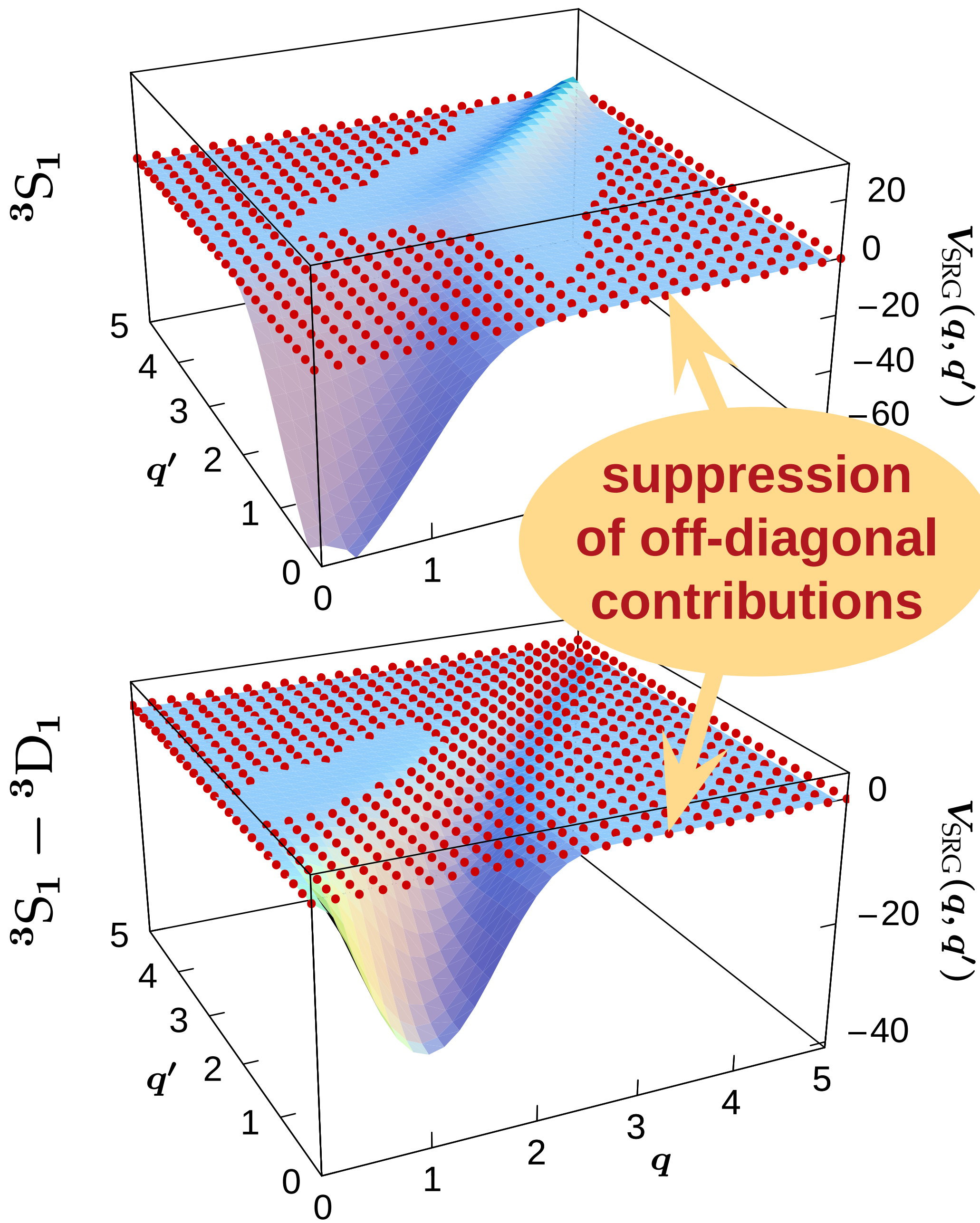
SRG Evolution: The Deuteron



Argonne V18

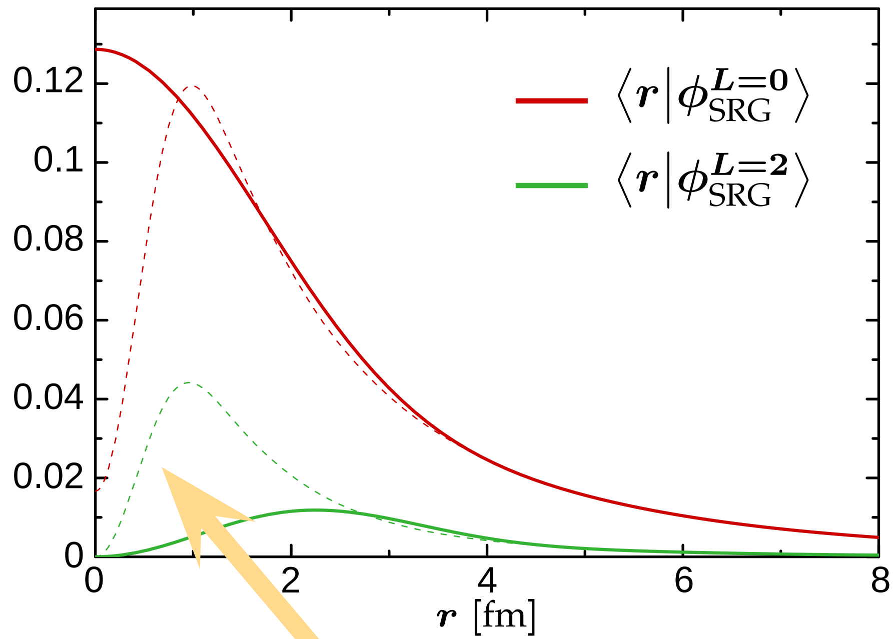


SRG Evolution: The Deuteron



suppression of off-diagonal contributions

$\alpha = 0.1000\,\mathrm{fm}^4$



elimination of short-range correlations

Many-Body Methods

No-Core Shell Model

Roth et al. — Phys. Rev. C 72, 034002 (2005)

Roth & Navrátil — in preparation

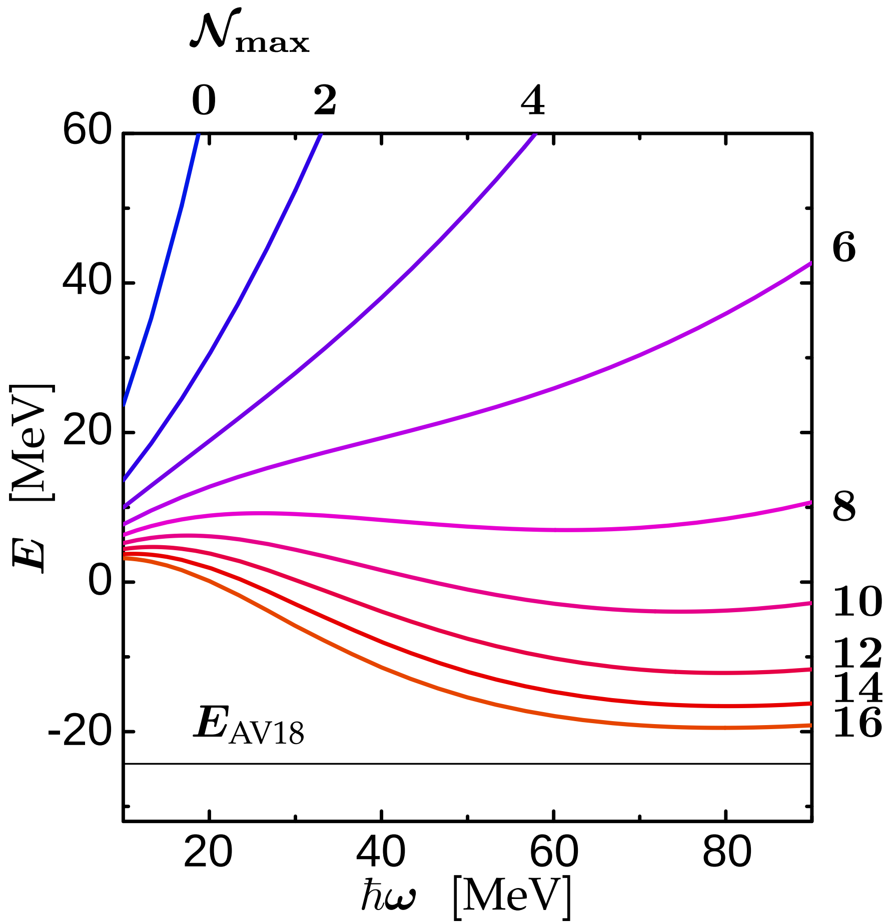
NCSM + Correlated Interactions

No-Core Shell Model
+
Matrix Elements of Correlated Realistic Interaction $\mathrm{V}_{\mathrm{UCOM}}$

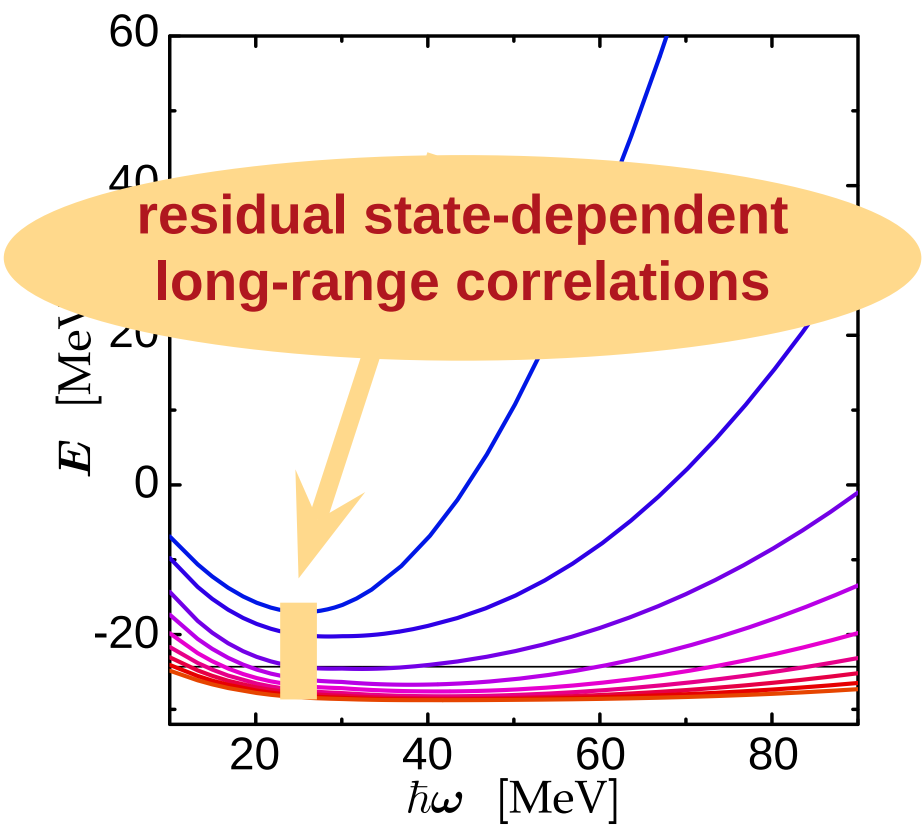
- many-body state is expanded in Slater determinants of harmonic oscillator single-particle states
- large-scale diagonalization of Hamiltonian within a **truncated model space** ($\mathcal{N}\hbar\omega$ truncation)
- assessment of **short- and long-range correlations**
- role of **three-nucleon interactions**

^{4}He: Convergence

$\mathbf{V}_{\mathrm{AV18}}$

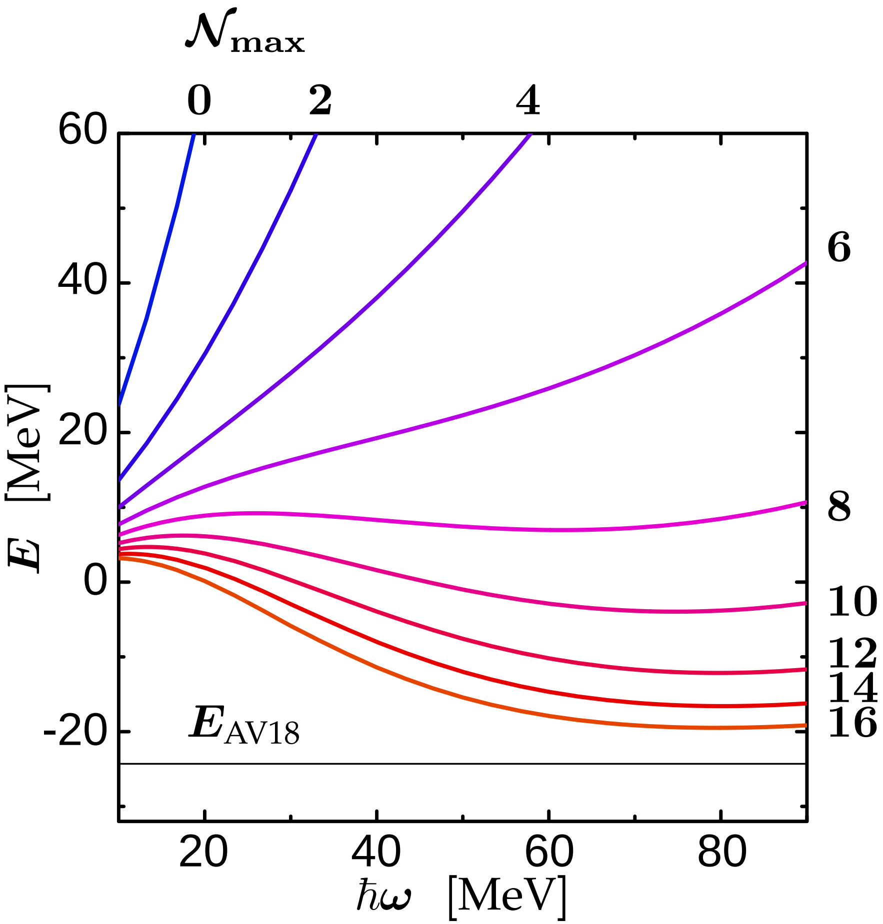


$\mathbf{V}_{\mathrm{UCOM}}$

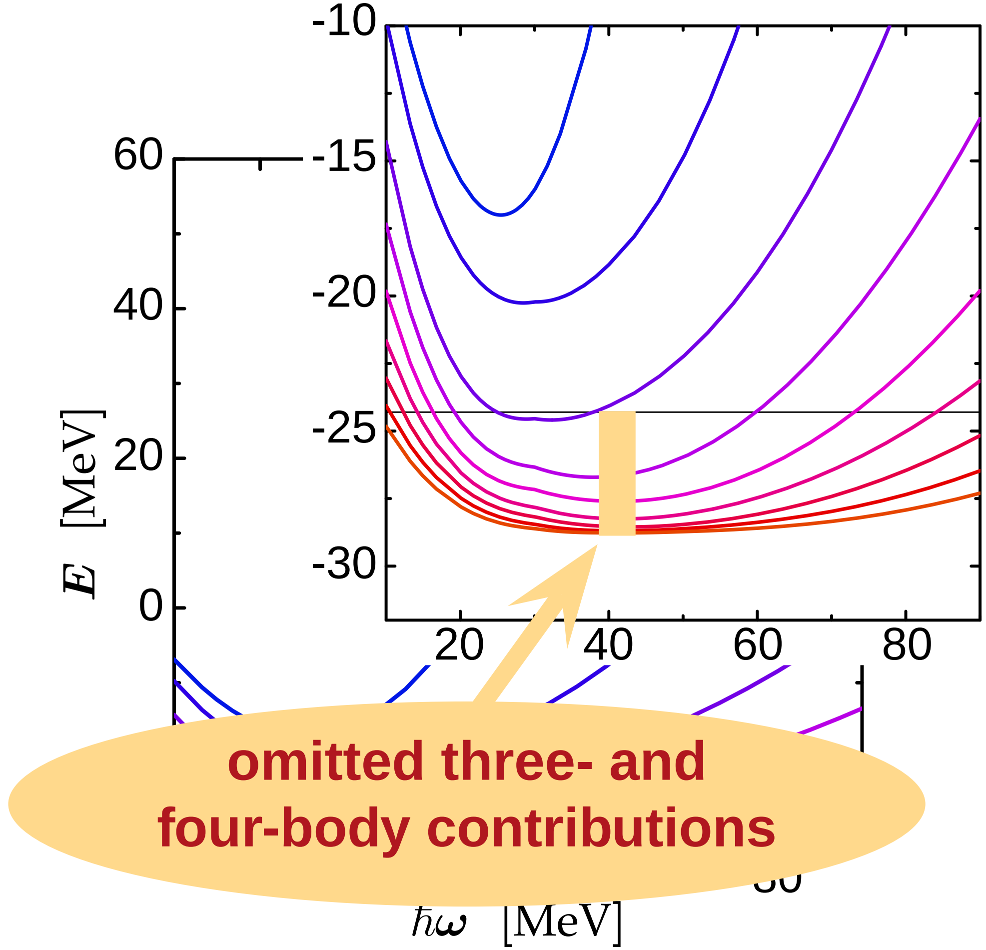


^{4}He: Convergence

V_{AV18}



V_{UCOM}



Three-Body Interactions — Strategies

Correlated Hamiltonian in Many-Body Space

$$\begin{aligned}\widetilde{\mathrm{H}} &= \mathrm{C}^\dagger\,(\mathrm{T} + \mathrm{V}_{NN} + \mathrm{V}_{3N})\,\mathrm{C} \\ &= \widetilde{\mathrm{T}}^{[1]} + (\widetilde{\mathrm{T}}^{[2]} + \widetilde{\mathrm{V}}_{NN}^{[2]}) + (\widetilde{\mathrm{T}}^{[3]} + \widetilde{\mathrm{V}}_{NN}^{[3]} + \widetilde{\mathrm{V}}_{3N}^{[3]}) + \cdots \\ &= \mathrm{T} + \mathrm{V}_{\mathrm{UCOM}} + \mathrm{V}_{\mathrm{UCOM}}^{[3]} + \cdots\end{aligned}$$

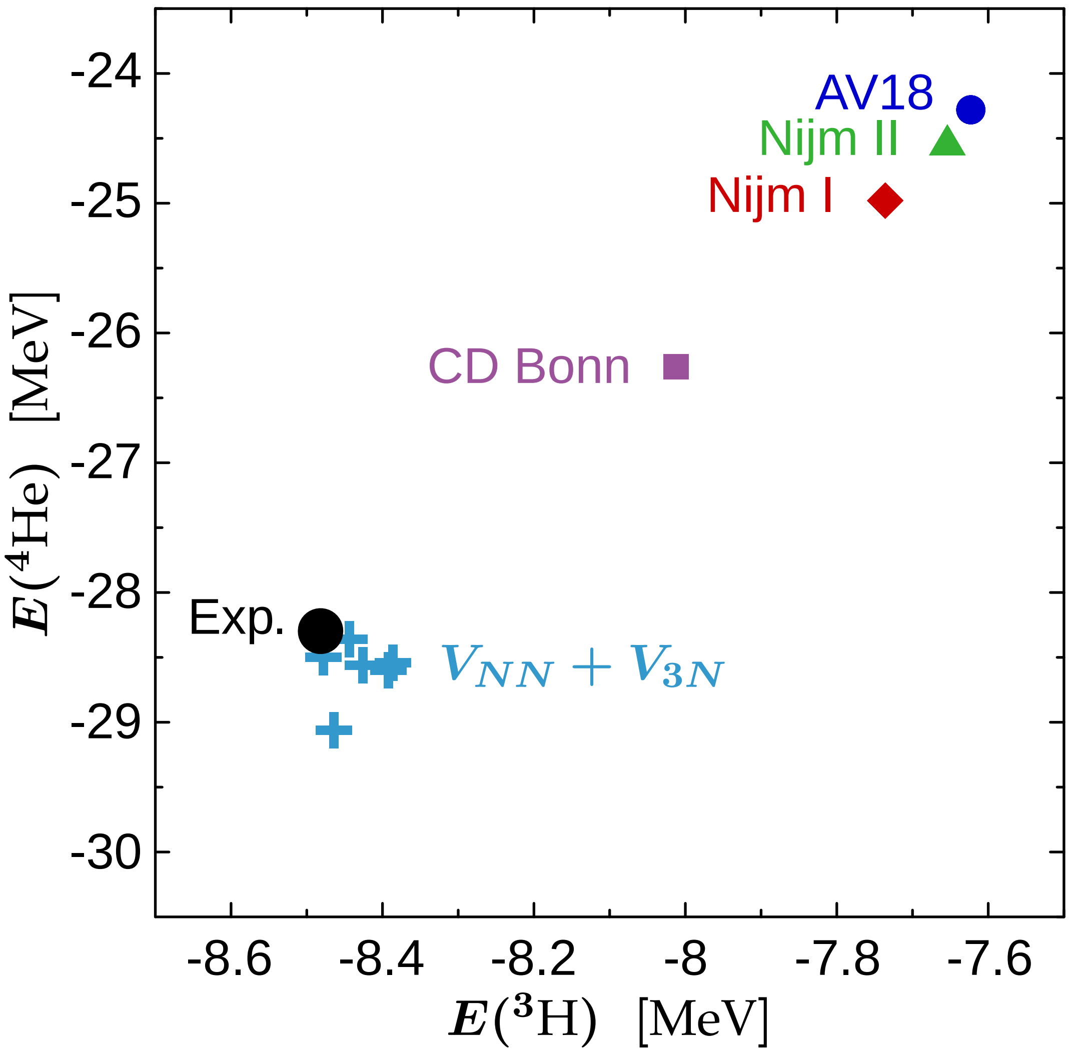
- strategies for treating the three-body contributions:

❶ **include full $\mathrm{V}_{\mathrm{UCOM}}^{[3]}$** consisting of genuine and induced 3N terms

❷ **replace $\mathrm{V}_{\mathrm{UCOM}}^{[3]}$** by phenomenological three-body force

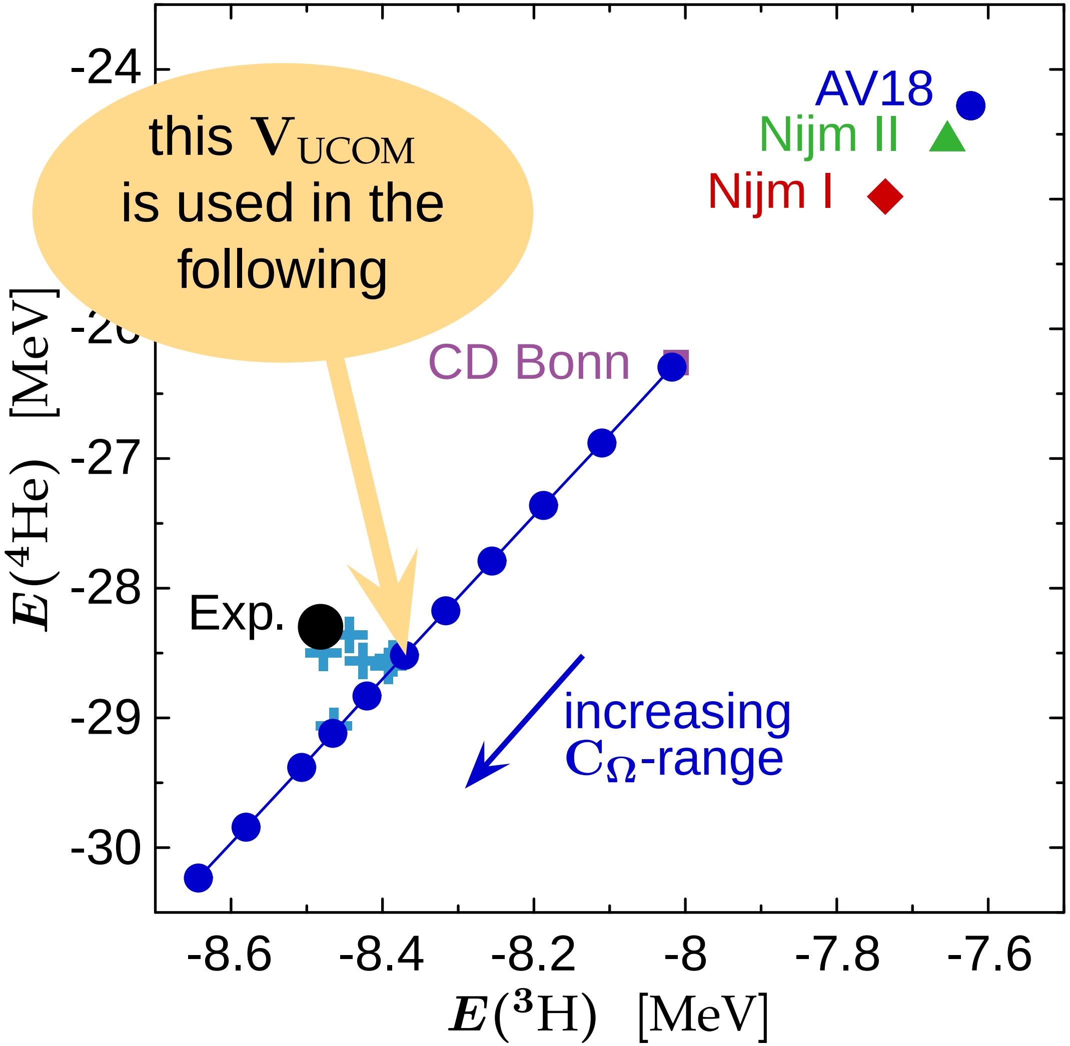
❸ **minimize $\mathrm{V}_{\mathrm{UCOM}}^{[3]}$** by proper choice of unitary transformation

Three-Body Interactions — Tjon Line



- **Tjon-line**: $E(^4\mathrm{He})$ vs. $E(^3\mathrm{H})$ for phase-shift equivalent NN-interactions

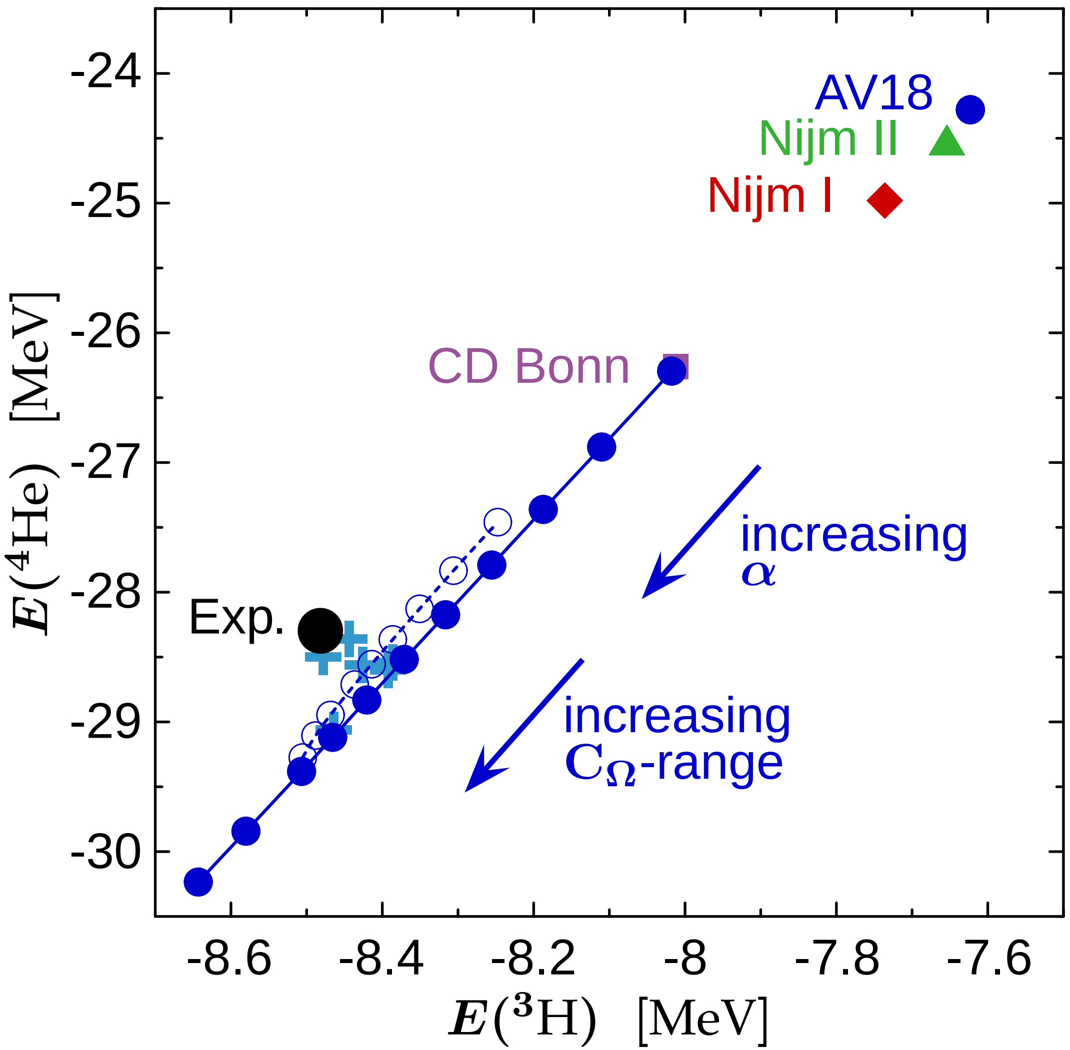
Three-Body Interactions — Tjon Line



- **Tjon-line**: $E(^4\mathrm{He})$ vs. $E(^3\mathrm{H})$ for phase-shift equivalent NN-interactions
- change of C_{Ω}-correlator range results in shift along Tjon-line

minimize net three-body force
by choosing correlator with energies close to experimental value

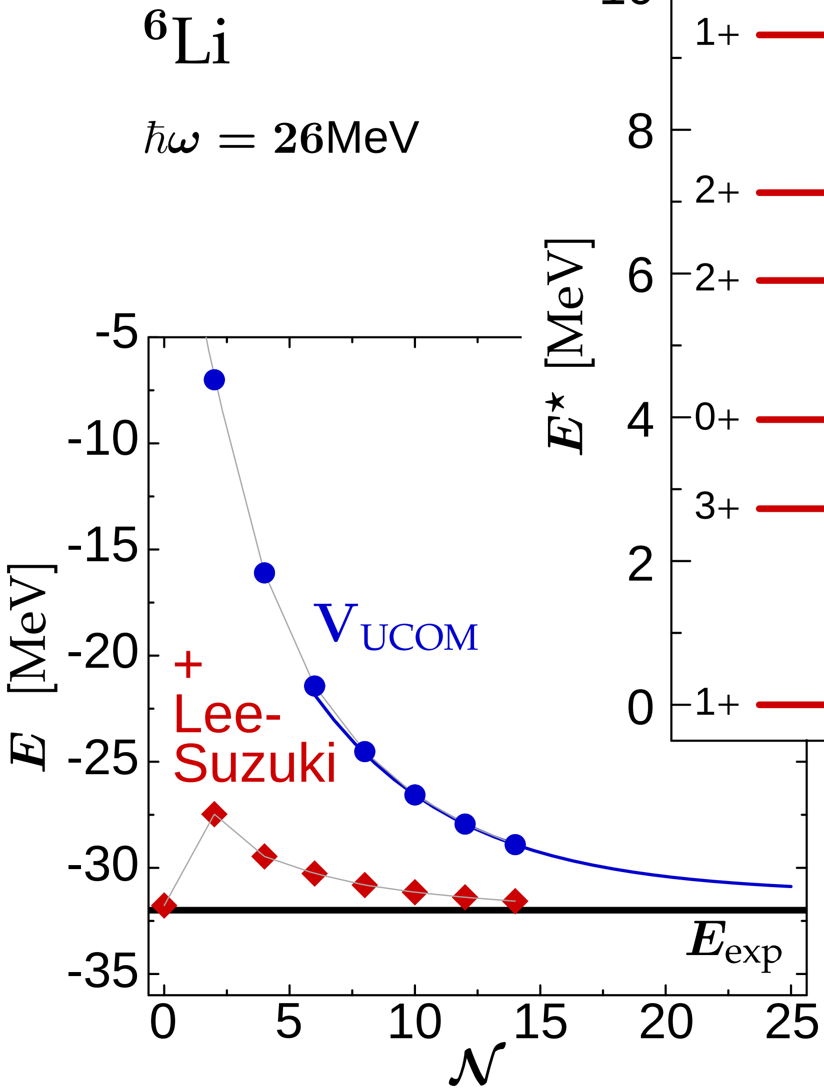
Three-Body Interactions — Tjon Line

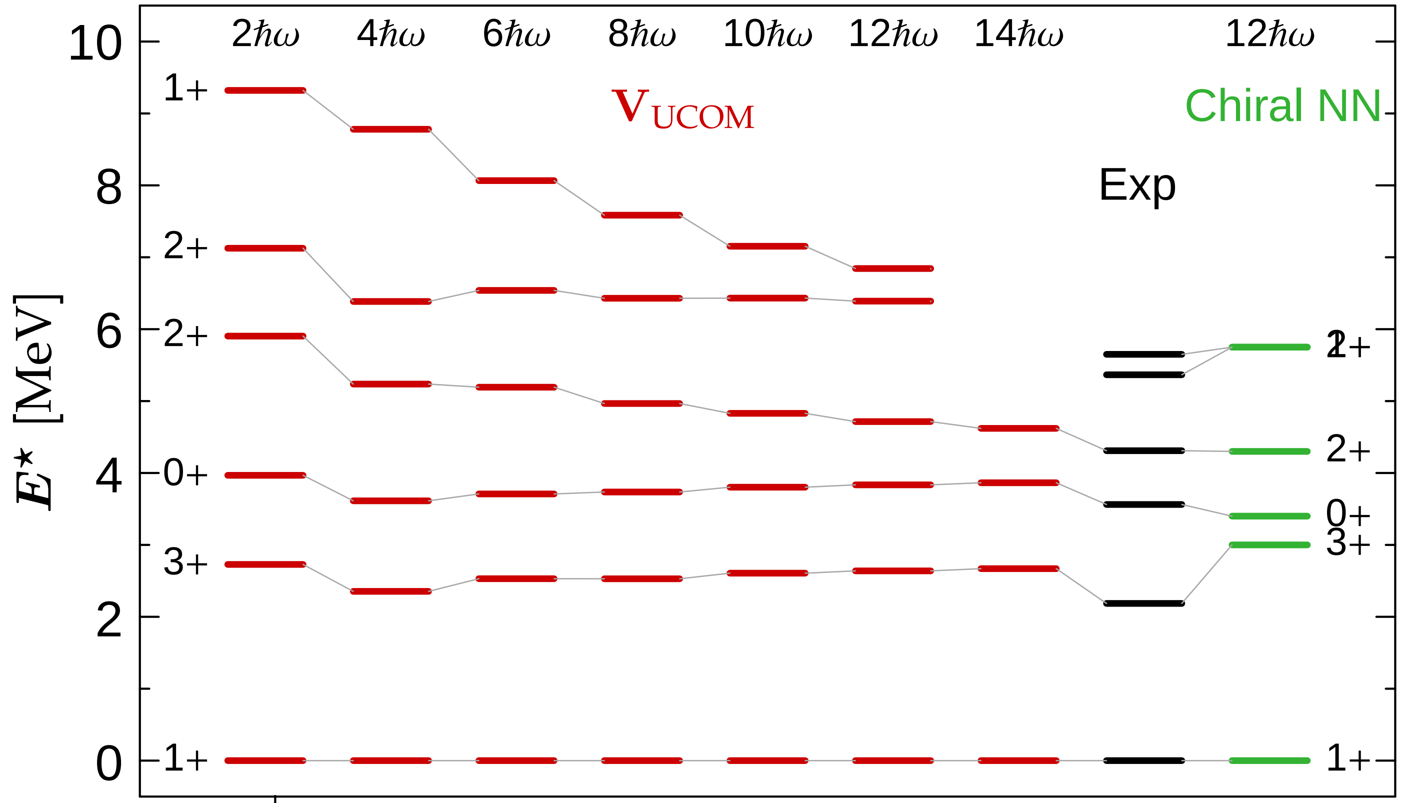


- **Tjon-line**: $E(^4\mathrm{He})$ vs. $E(^3\mathrm{H})$ for phase-shift equivalent NN-interactions
- same behavior for the SRG interaction as function of α

minimize net three-body force by choosing correlator with energies close to experimental value

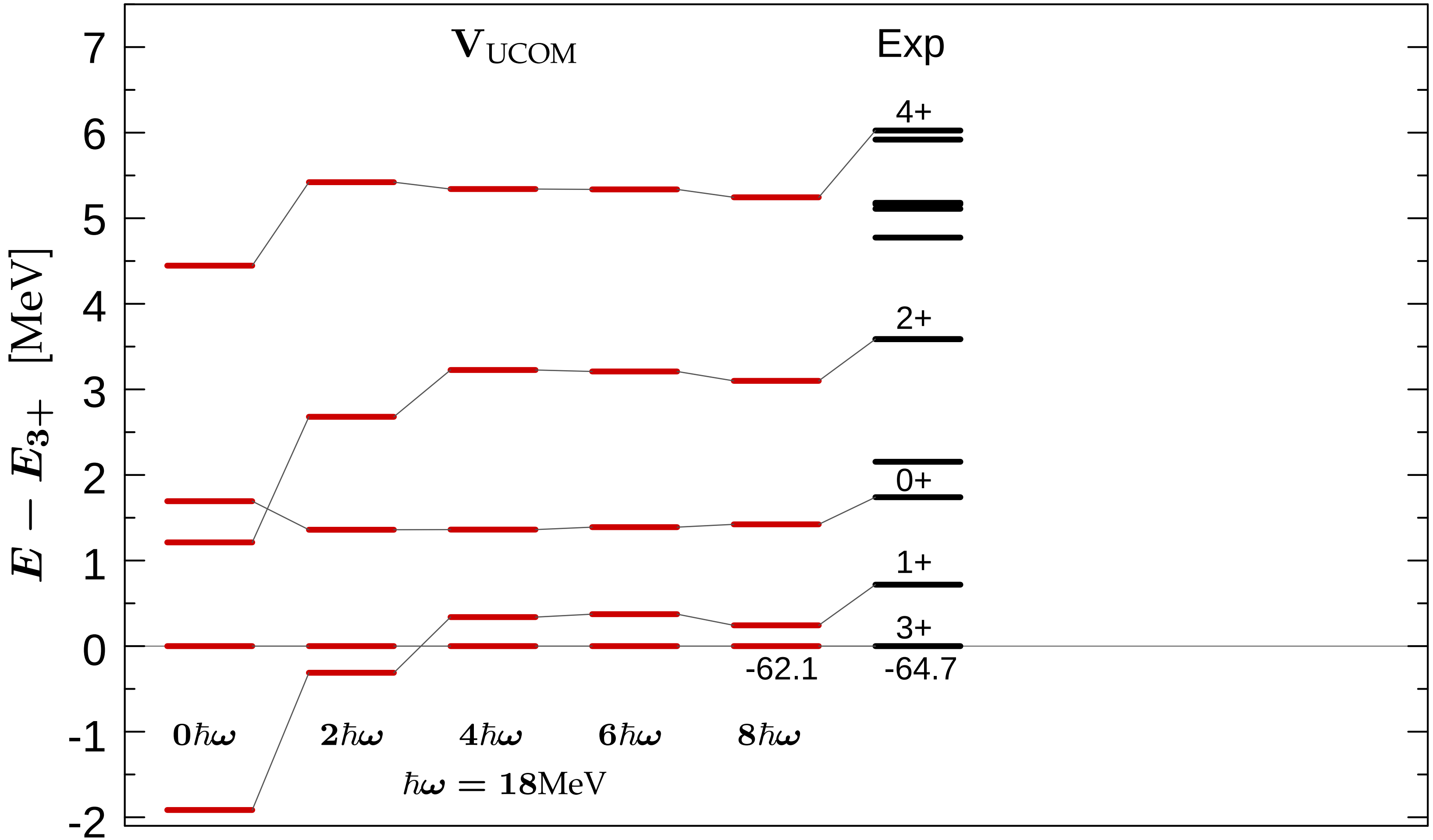
^{6}Li: NCSM throughout the p-Shell



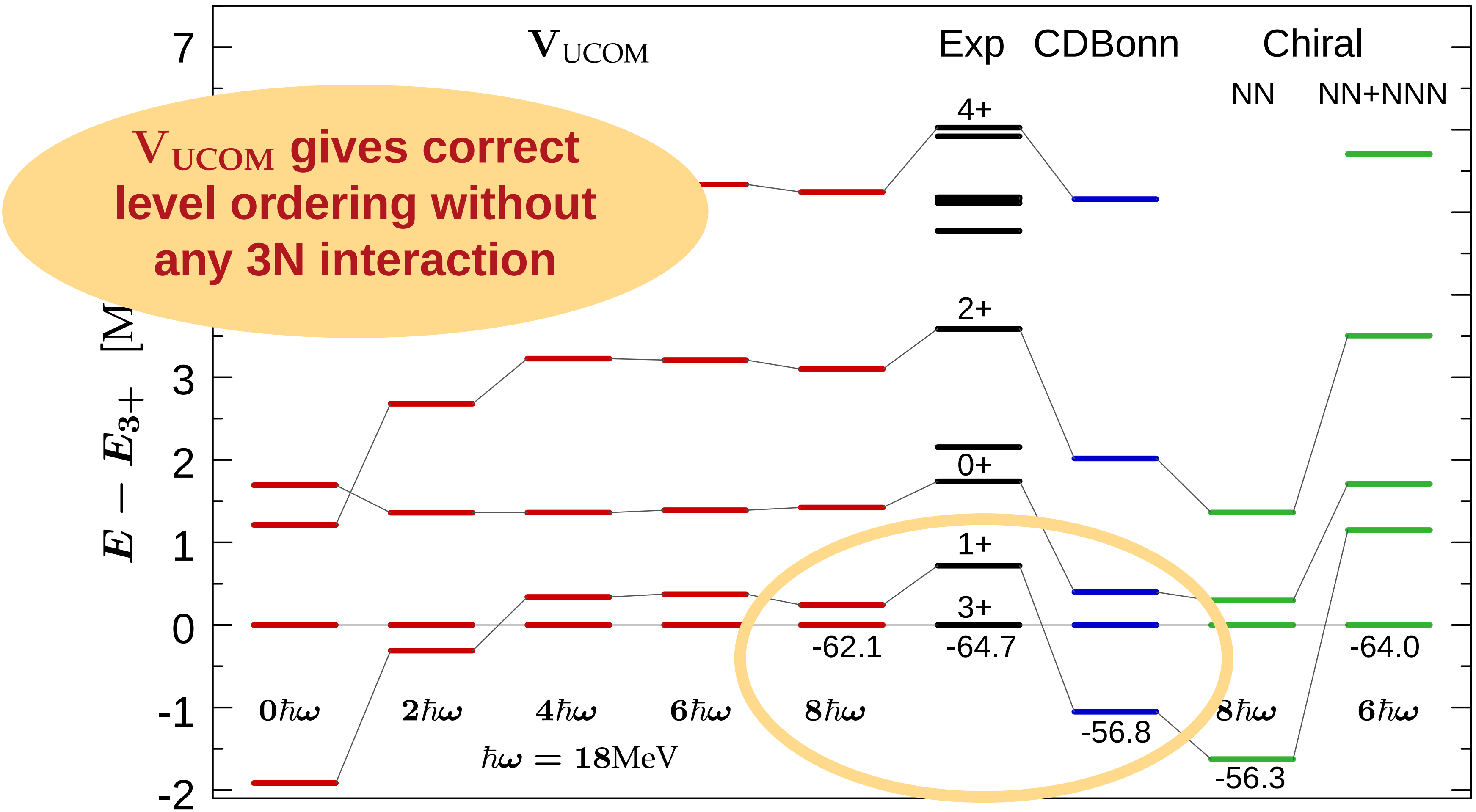


systematic NCSM studies throughout p-shell with V_{UCOM} (+ Lee-Suzuki transformation)

^{10}B: Hallmark of a 3N Interaction?



^{10}B: Hallmark of a 3N Interaction?



Importance Truncated No-Core Shell Model

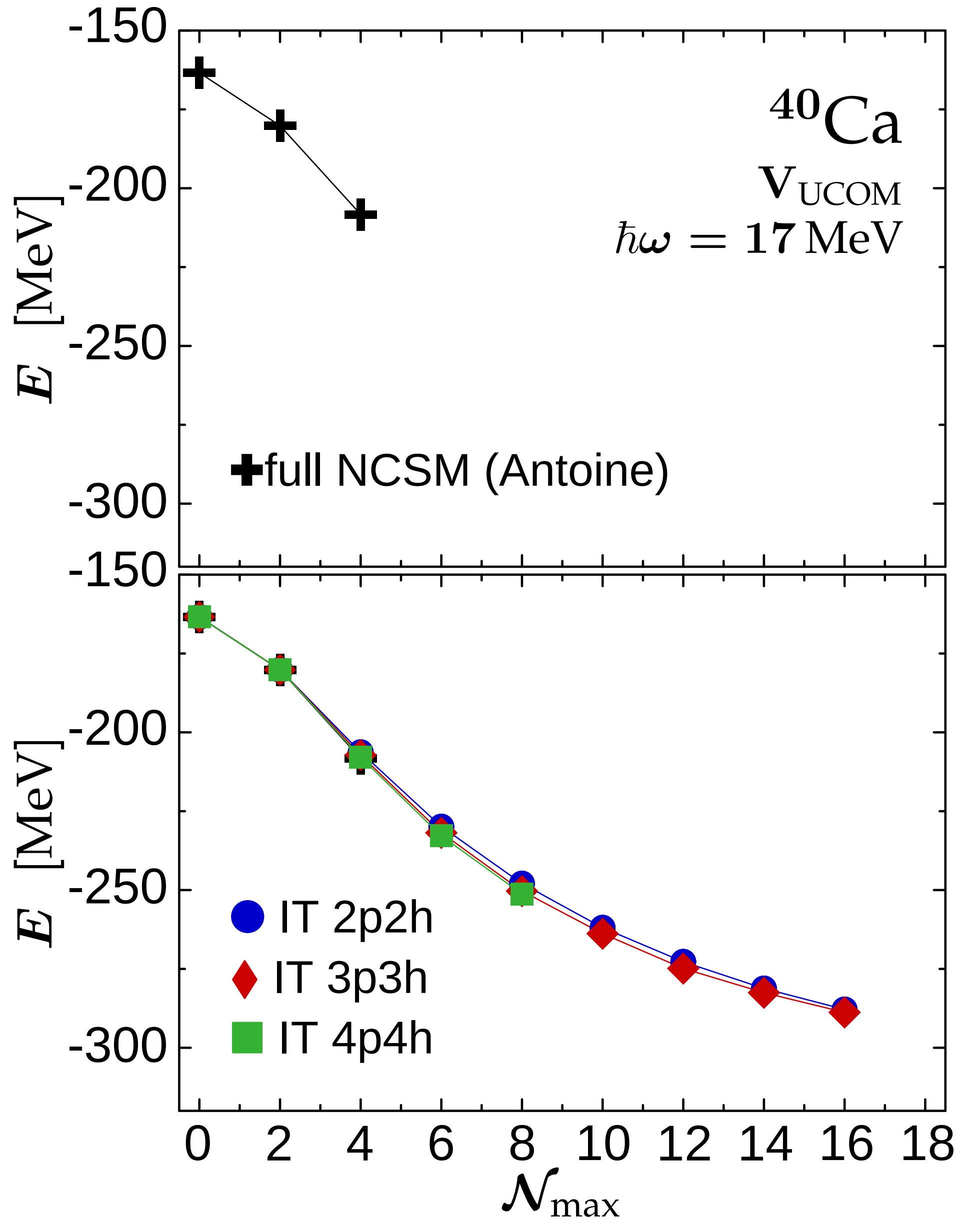
Roth & Navrátil — arXiv: 0705.4069

Importance Truncated NCSM

- converged NCSM calculations essentially restricted to p-shell
- full $6\hbar\omega$ calculation for $^{40}\mathrm{Ca}$ presently not feasible (basis dimension $\sim\mathbf{10^{10}}$)

Importance Truncation

reduce NCSM space to relevant states using an **a priori importance measure** derived from MBPT



General Idea

- given an intrinsic Hamiltonian

$$\mathbf{H}_{\text{int}} = \mathbf{T} - \mathbf{T}_{\text{cm}} + \mathbf{V} = \mathbf{H}_0 + \mathbf{H}'$$

  and an unperturbed Hamiltonian $\mathbf{H}_0$ with eigenstates $|\Phi_\nu\rangle$

- consider lowest-order **perturbation theory** to construct a correction $|\Psi^{(1)}\rangle$ to the unperturbed reference state $|\Psi^{(0)}\rangle$

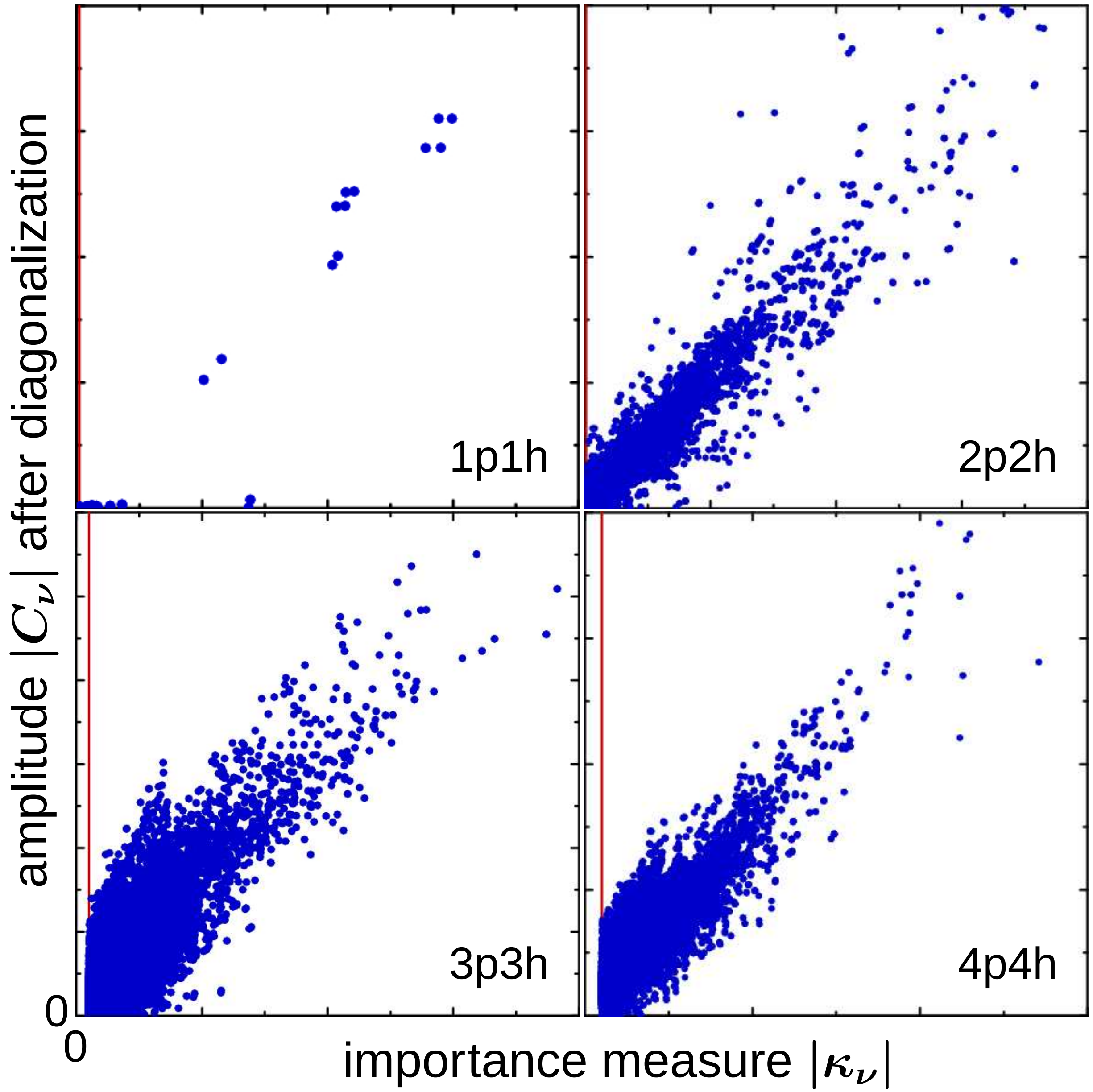
$$|\Psi^{(0)}\rangle = |\Psi_{\text{ref}}\rangle = |\Phi_0\rangle \qquad |\Psi^{(1)}\rangle = \sum_{\nu \neq \text{ref}} \kappa_\nu |\Phi_\nu\rangle$$

- perturbative estimate of amplitudes serves as **measure for importance of individual basis states $|\Phi_\nu\rangle$**

$$\kappa_\nu = -\frac{\langle\Phi_\nu|\,\mathbf{H}'\,|\Psi_{\text{ref}}\rangle}{E_\nu^{(0)} - E_{\text{ref}}^{(0)}}$$

- restrict model space to **important configurations with $|\kappa_\nu| \geq \kappa_{\min}$** and solve eigenvalue problem

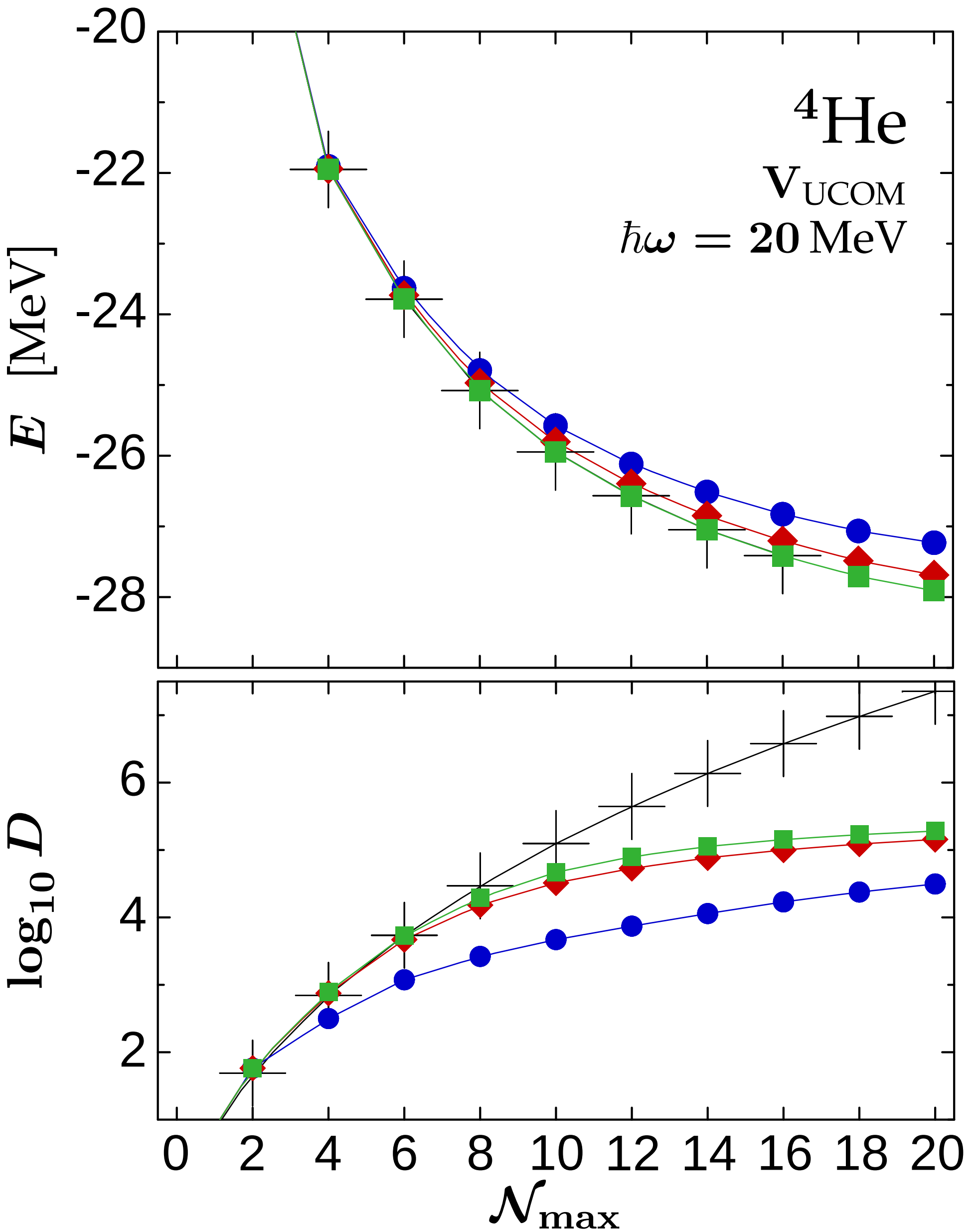
Importance Measure



- importance measure κ_ν provides **reliable a priori estimate** of the a posteriori amplitude C_ν obtained from diagonalization

^{16}O
$\mathbf{V}_{\text{UCOM}}$
$\hbar\omega = 20\,\text{MeV}$
$\mathcal{N}_{\max} = 6$

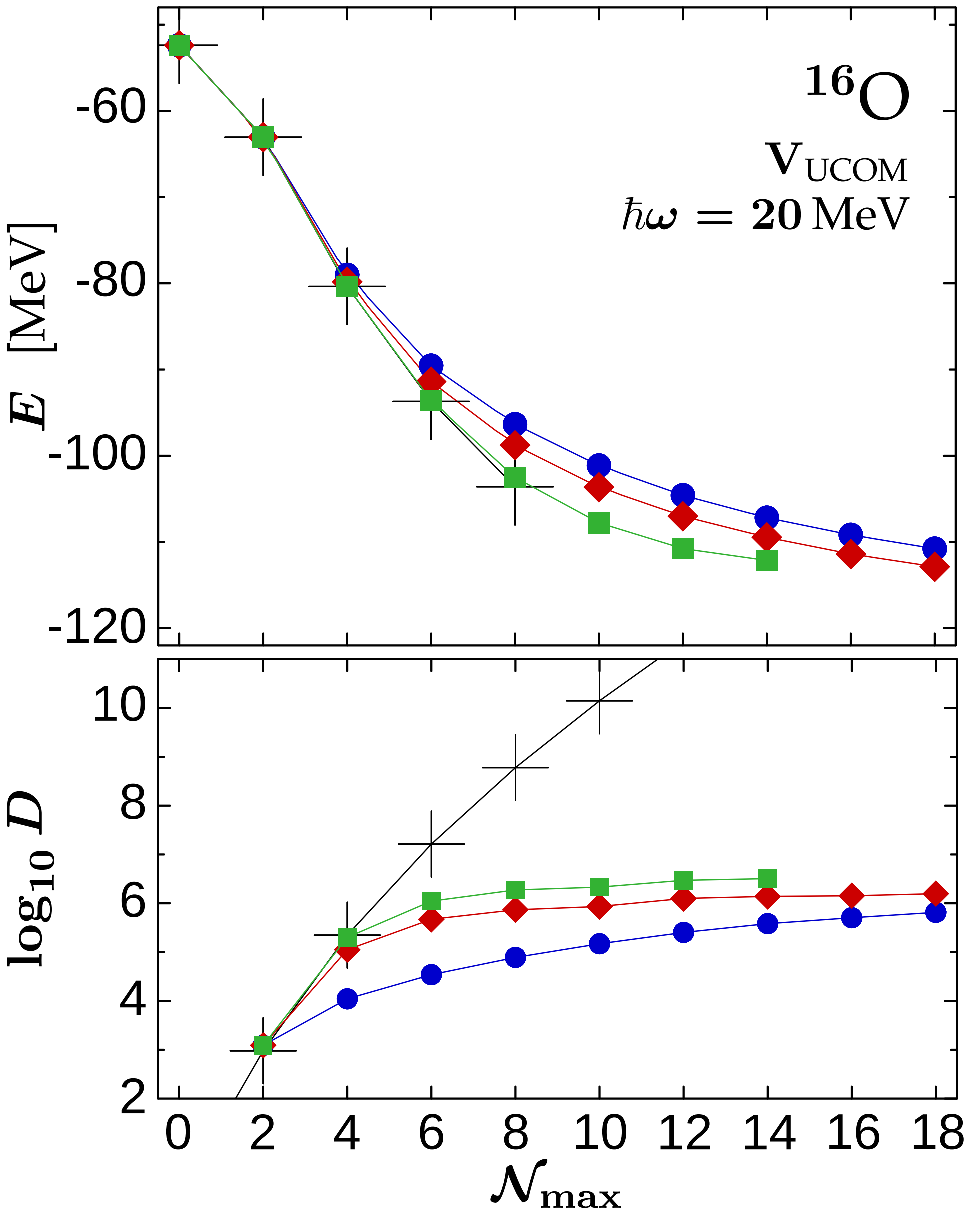
Benchmark: ^{4}He



- **reproduces exact NCSM result** with an importance truncated basis that is 2 orders of magnitude smaller than the full $\mathcal{N}_{max}\hbar\omega$ space

+ full NCSM (Antoine)
● IT-NCSM 2p2h
♦ IT-NCSM 3p3h
■ IT-NCSM 4p4h

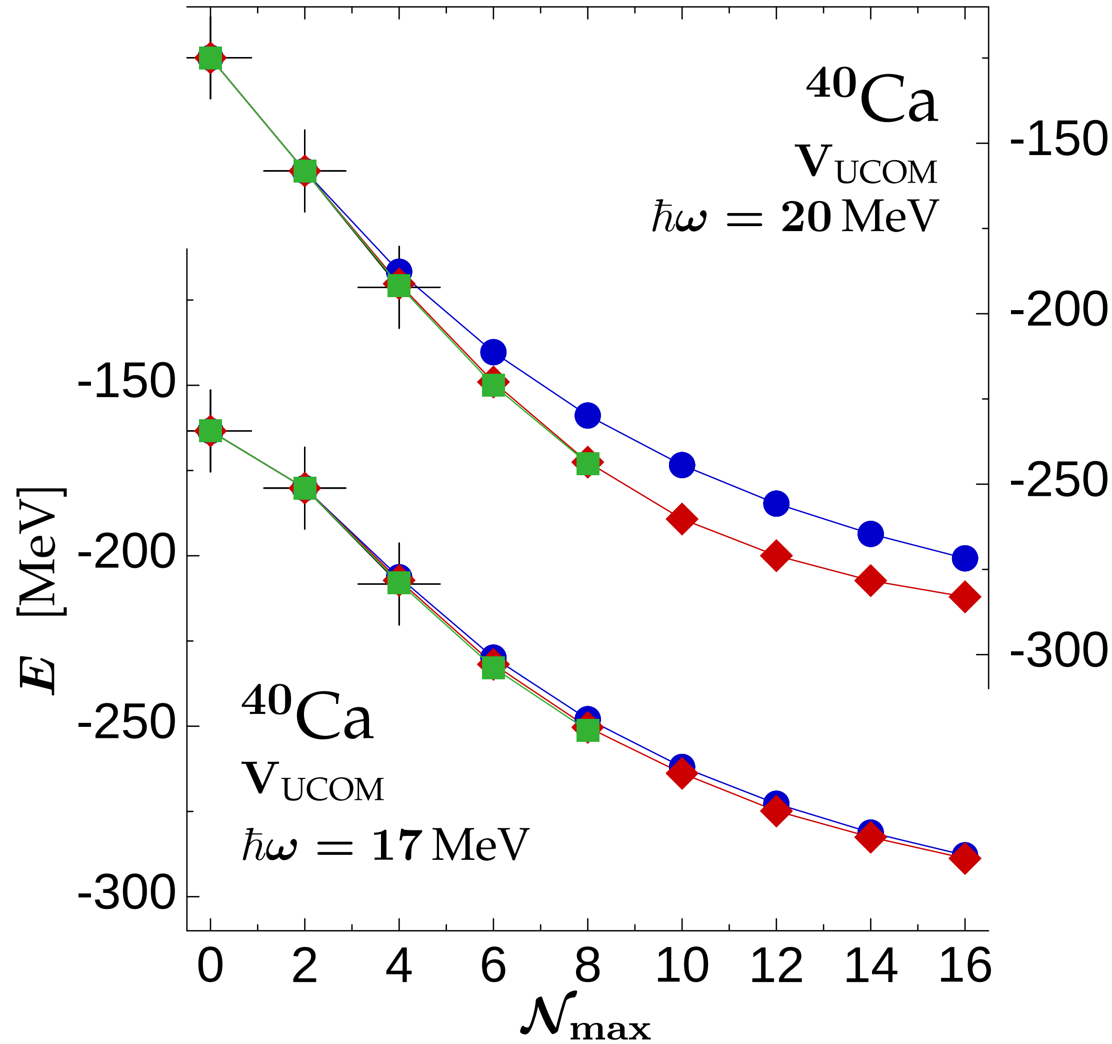
Benchmark: ^{16}O



- **excellent agreement with full NCSM** calculation although configurations beyond 4p4h are not included
- dimension reduced by **several orders of magnitude**; possibility to go way beyond the domain of the full NCSM

+ full NCSM (Antoine)
● IT-NCSM 2p2h
♦ IT-NCSM 3p3h
■ IT-NCSM 4p4h

Benchmark: ^{40}Ca



- $\mathbf{16}\hbar\omega$ calculations for ^{40}Ca are feasible
- extrapolation of ground state energy (3p3h, $\hbar\omega = \mathbf{17}\,\text{MeV}$) yields

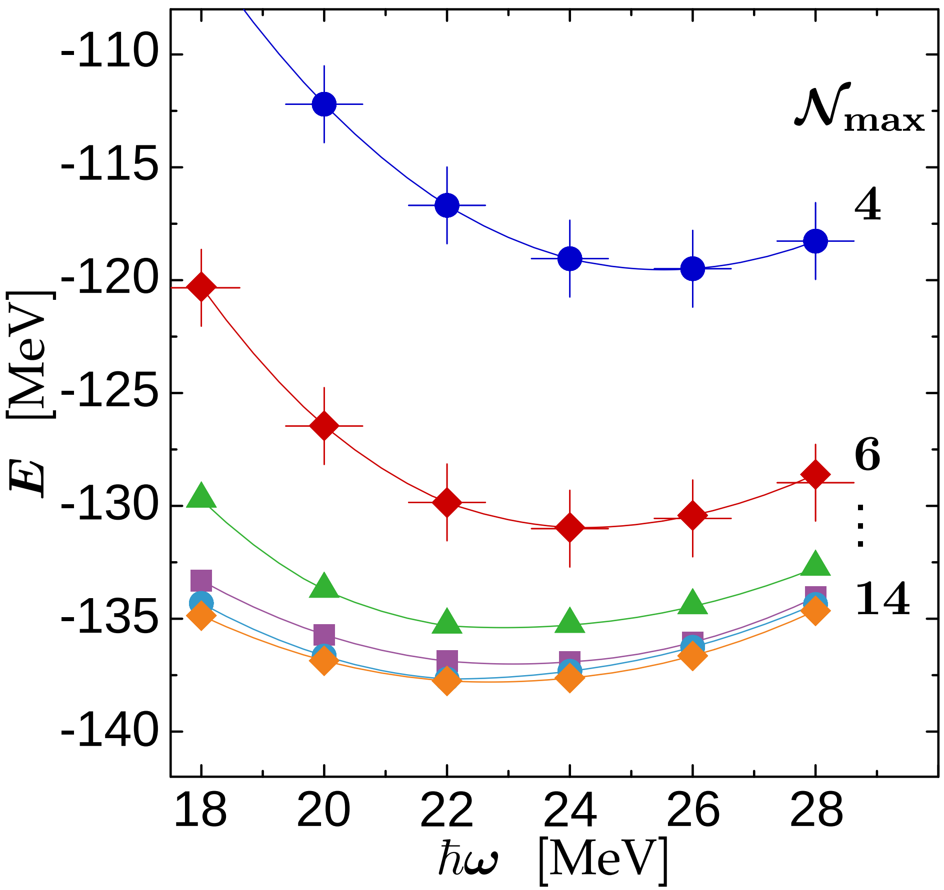
$$E_\infty \approx -\mathbf{316}\,\text{MeV}$$
$$E_{\text{exp}} = -\mathbf{342.05}\,\text{MeV}$$

+ full NCSM (Antoine)
● IT-NCSM 2p2h
♦ IT-NCSM 3p3h
■ IT-NCSM 4p4h

Benchmark Results for $V_{\mathrm{low}k}$

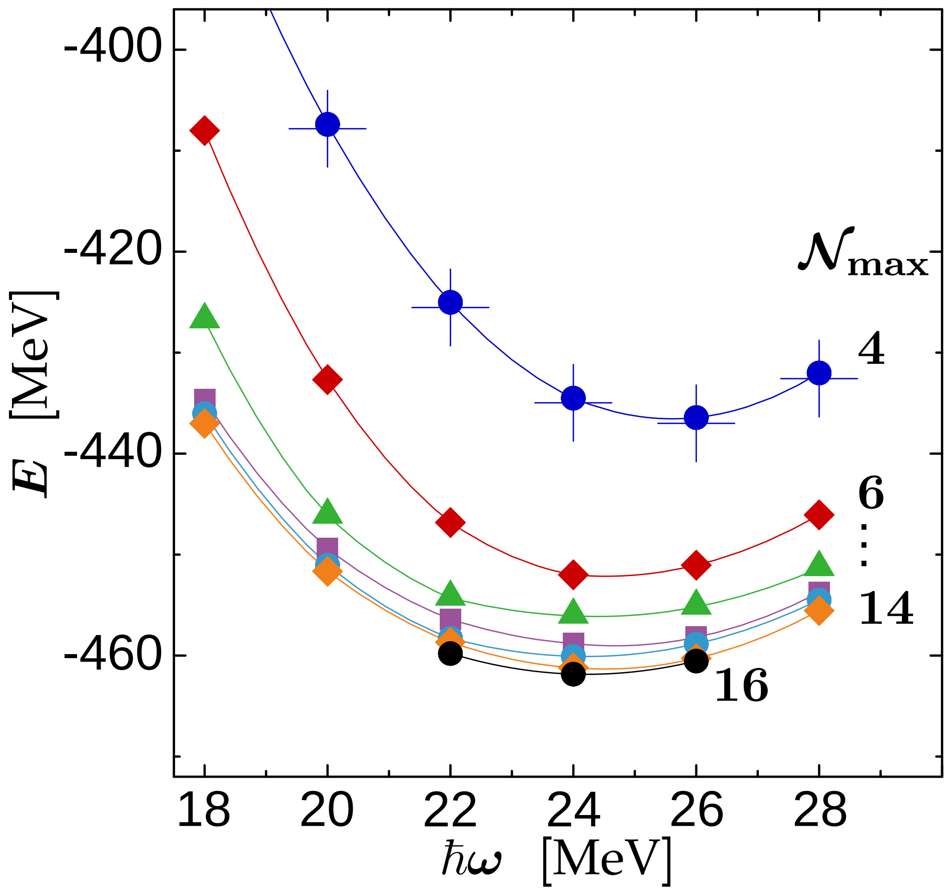
$\mathrm{V}_{\text{low-}k}$
(AV18, $\Lambda = 2.1\,\mathrm{fm}^{-1}$)

$^{16}\mathrm{O}$
(up to 4p4h)



E_∞(4p4h) $\approx -138\,\mathrm{MeV}$
R_{rms}(4p4h) $= 2.03\,\mathrm{fm}$

$^{40}\mathrm{Ca}$
(up to 3p3h)



E_∞(3p3h) $\approx -463\,\mathrm{MeV}$
R_{rms}(3p3h) $= 2.27\,\mathrm{fm}$

Many-Body Methods

Hartree-Fock & Beyond

R. Roth et al. — Phys. Rev. C 73, 044312 (2006)

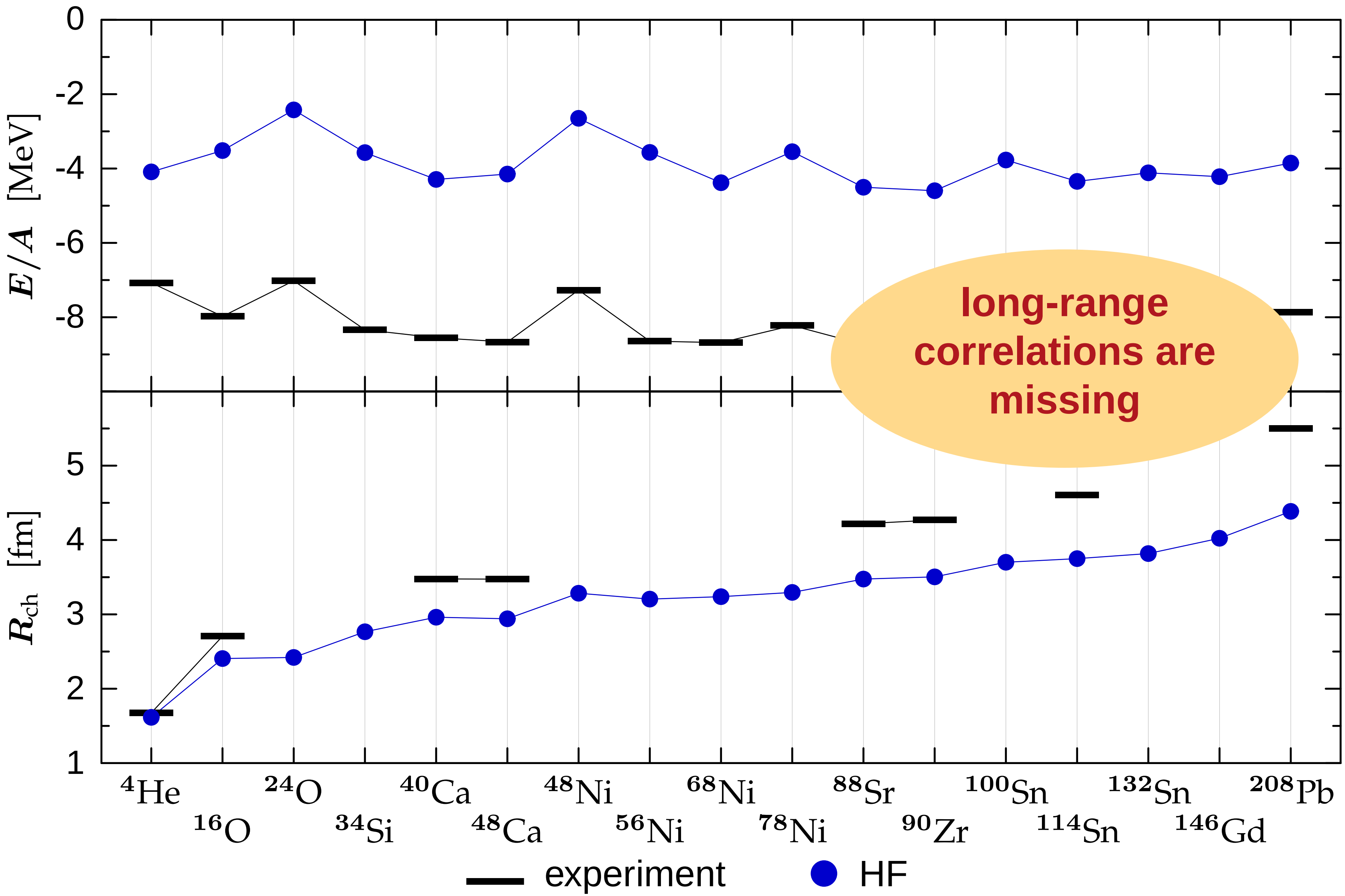
C. Barbieri et al. — arXiv: nucl-th/0608011

HF + Correlated Interactions

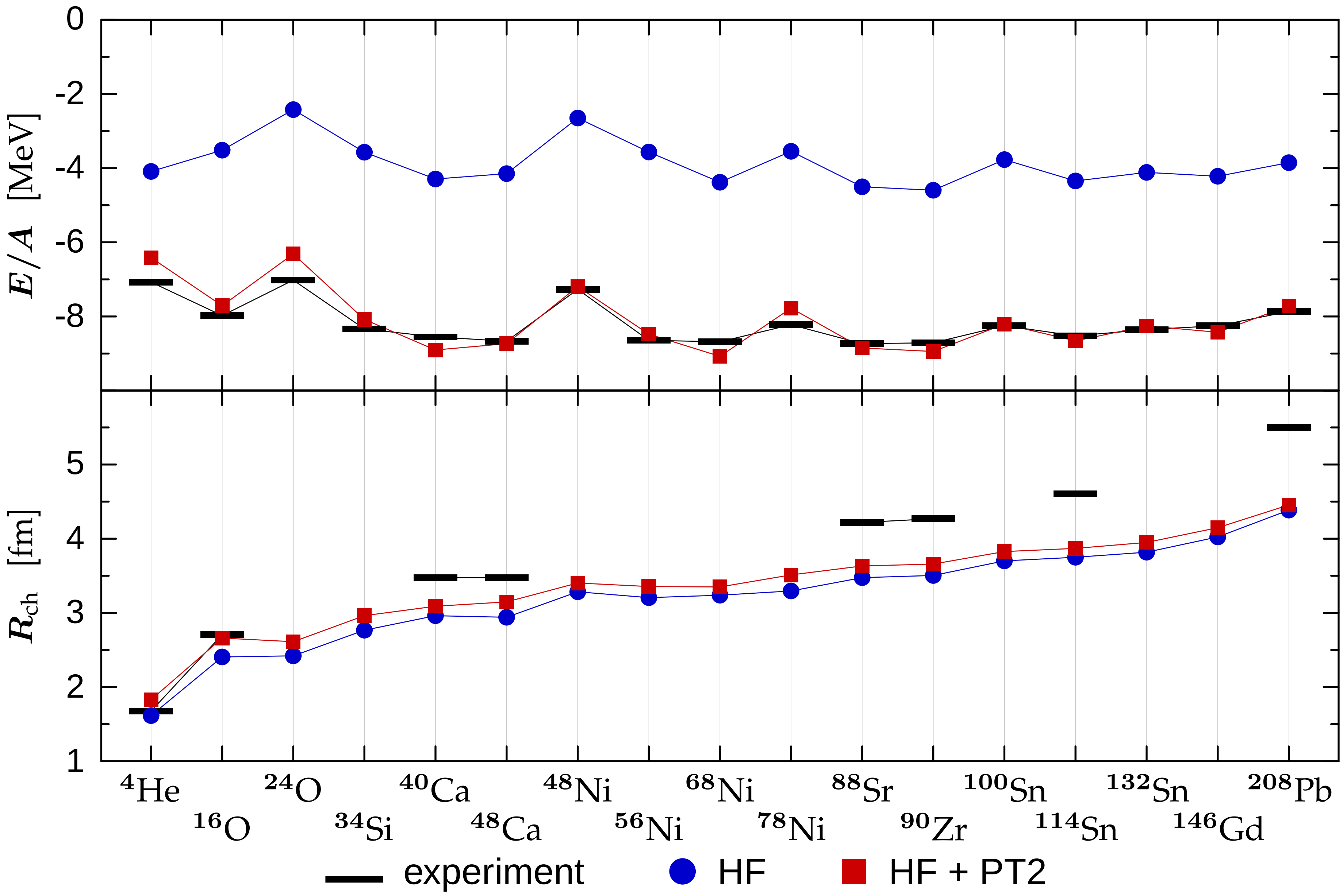
Standard Hartree-Fock
+
Matrix Elements of Correlated Realistic Interaction $\mathrm{V}_{\mathrm{UCOM}}$

- many-body state is a **Slater determinant** of single-particle states expanded in oscillator basis ($\sim$13 major shells)
- **correlations cannot be described** by Hartree-Fock states
- starting point for **improved many-body calculations**: MBPT, RPA, SM/CI, CC,...

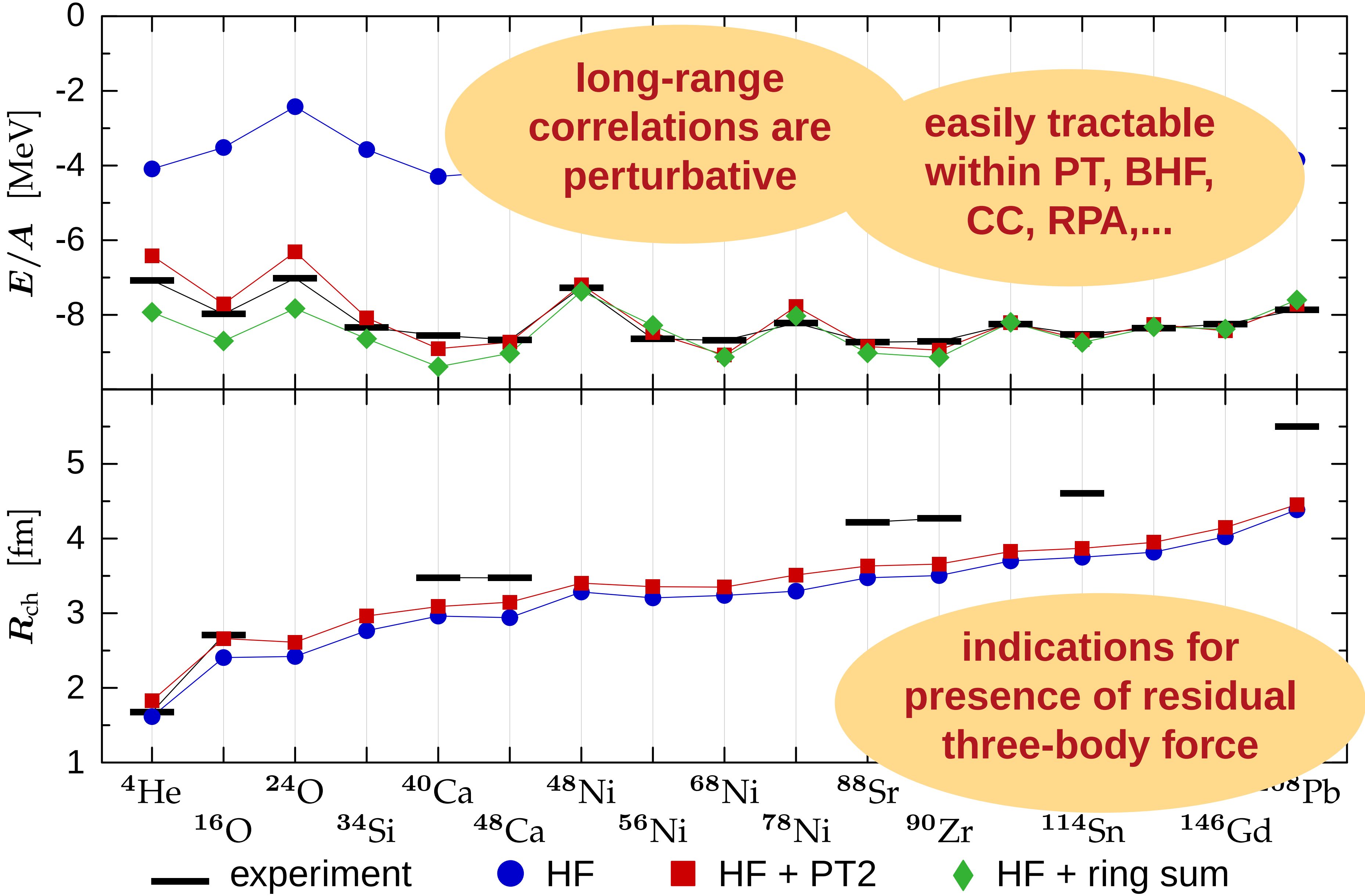
Hartree-Fock with V_{UCOM}



Perturbation Theory with V_{UCOM}



RPA Ring Summation with V_{UCOM}



Perspectives

Modern Effective Interactions

- treatment of short-range central and tensor correlations by unitary transformations: UCOM, SRG, Lee-Suzuki,...
- universal phase-shift equivalent correlated interaction $\mathbf{V}_{\mathrm{UCOM}}$

Innovative Many-Body Methods

- No-Core Shell Model,...
- Importance Truncated CI, Coupled Cluster Method,...
- Hartree-Fock plus MBPT, Padé Resummed MBPT, BHF, RPA,...

unified description of nuclear structure across the whole nuclear chart is within reach

Epilogue

- **thanks to my group & my collaborators**
  - S. Binder, P. Hedfeld, H. Hergert, M. Hild, P. Papakonstantinou, S. Reinhardt, F. Schmitt, I. Türschmann, A. Zapp

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  - P. Navrátil

    Lawrence Livermore National Laboratory, USA
  - N. Paar

    University of Zagreb, Croatia
  - H. Feldmeier, T. Neff, C. Barbieri,...

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