Towards

Ab Initio Nuclear Structure Calculations Beyond the p-Shell

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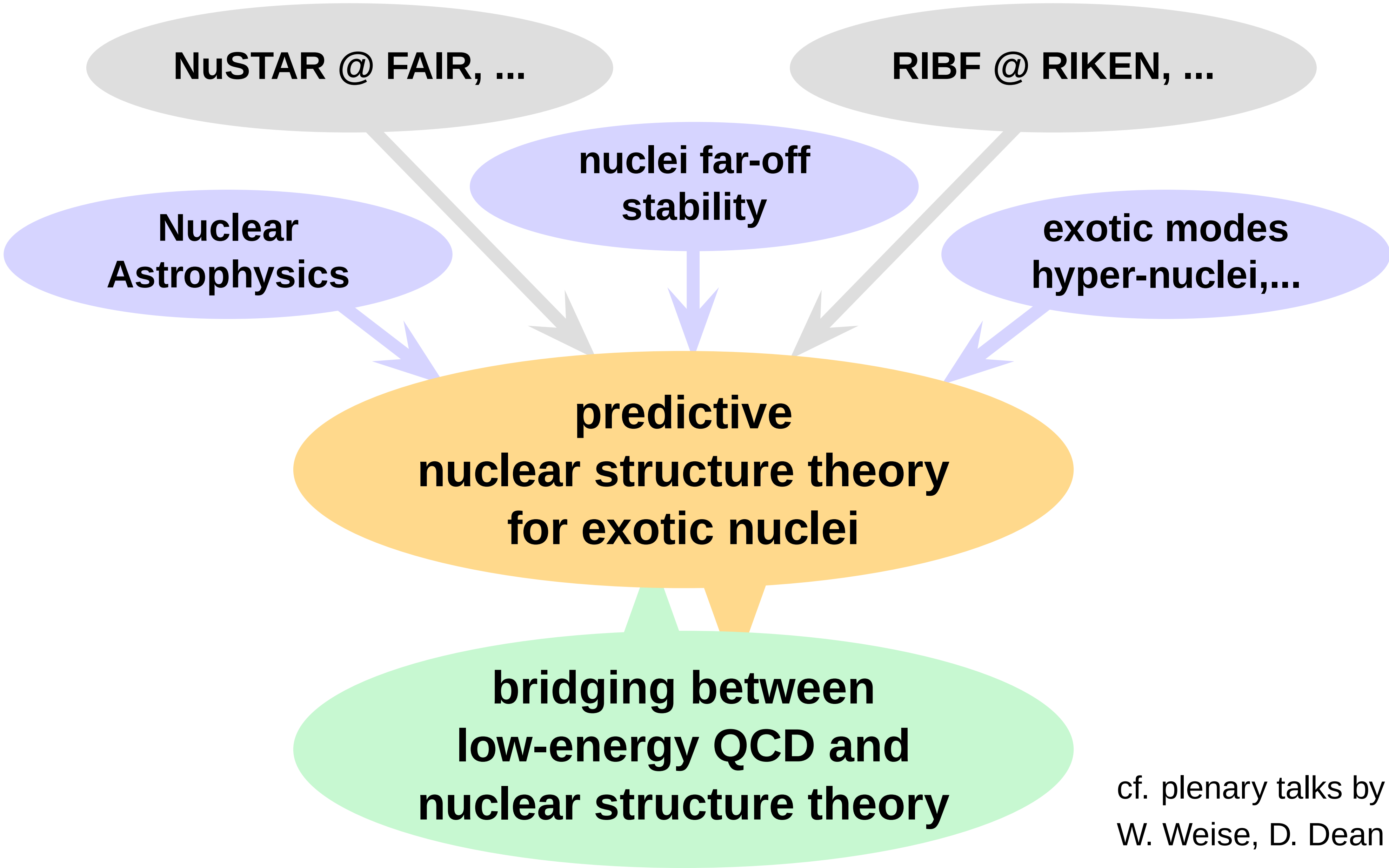
Overview

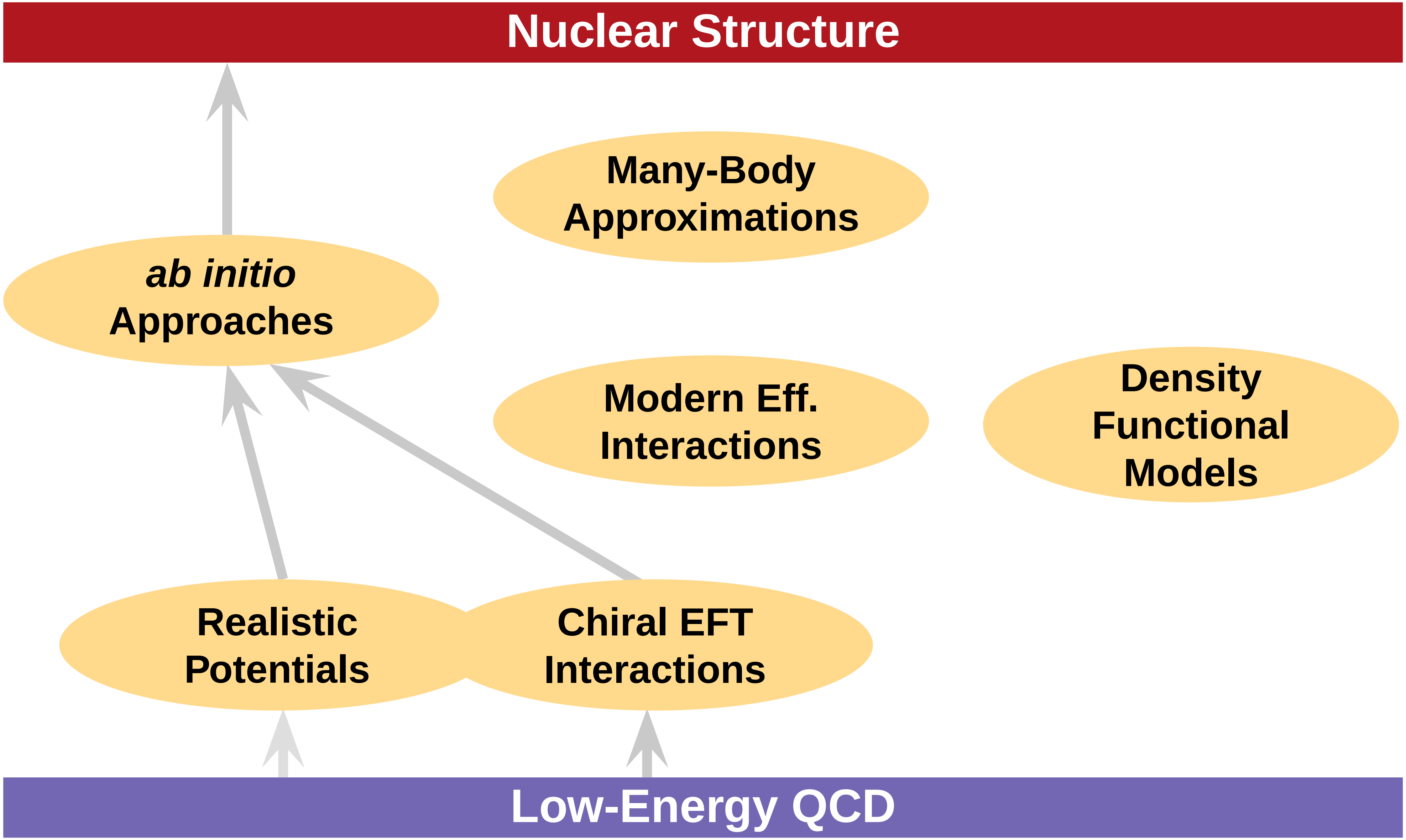
- Motivation
- Modern Effective Interactions
  - Unitary Correlation Operator Method
  - Similarity Renormalization Group
- Innovative Many-Body Methods
  - No-Core Shell Model
  - Importance Truncated NCSM
  - Beyond Hartree-Fock
- Perspectives

Nuclear Structure in the 21st Century

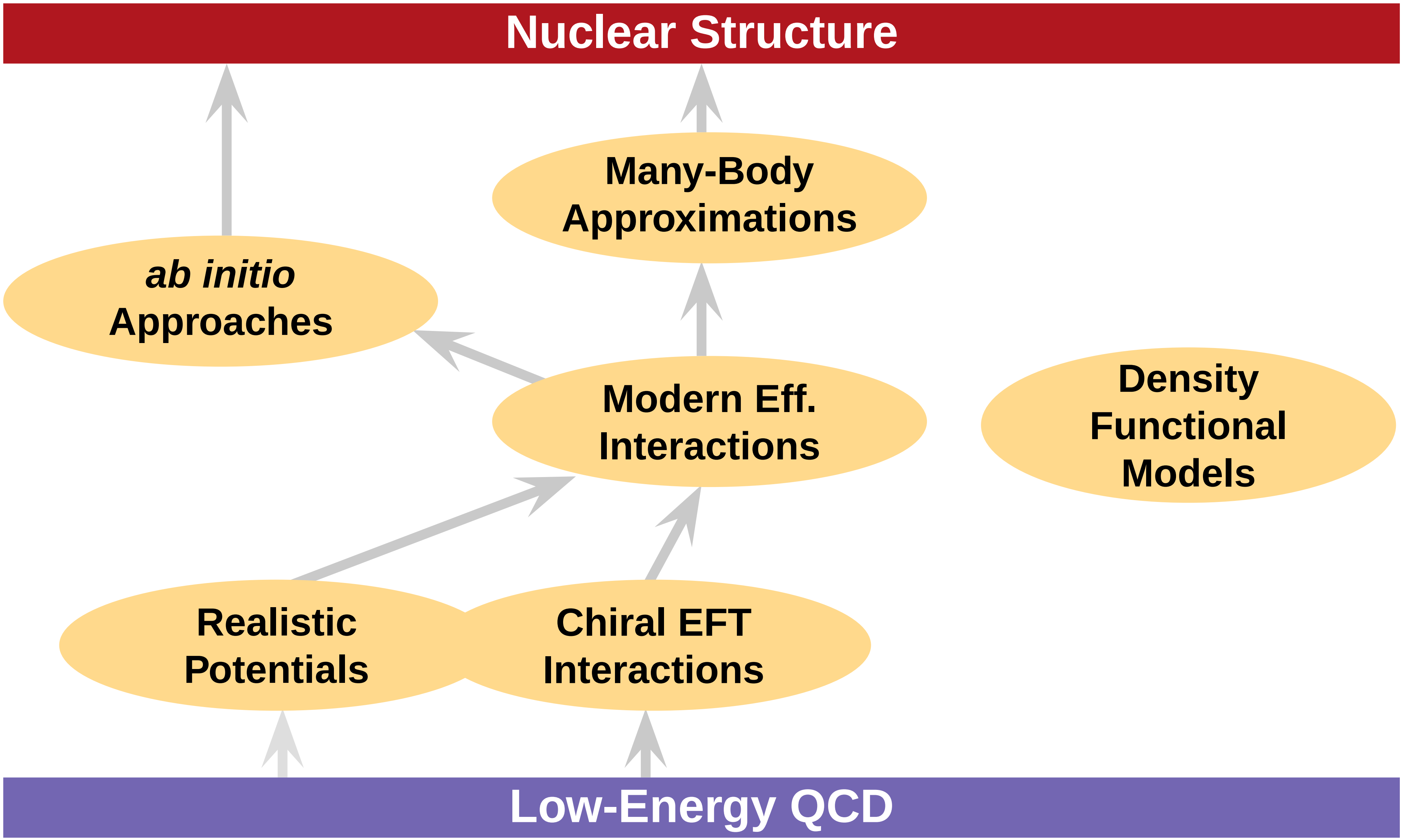


cf. plenary talks by
W. Weise, D. Dean

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

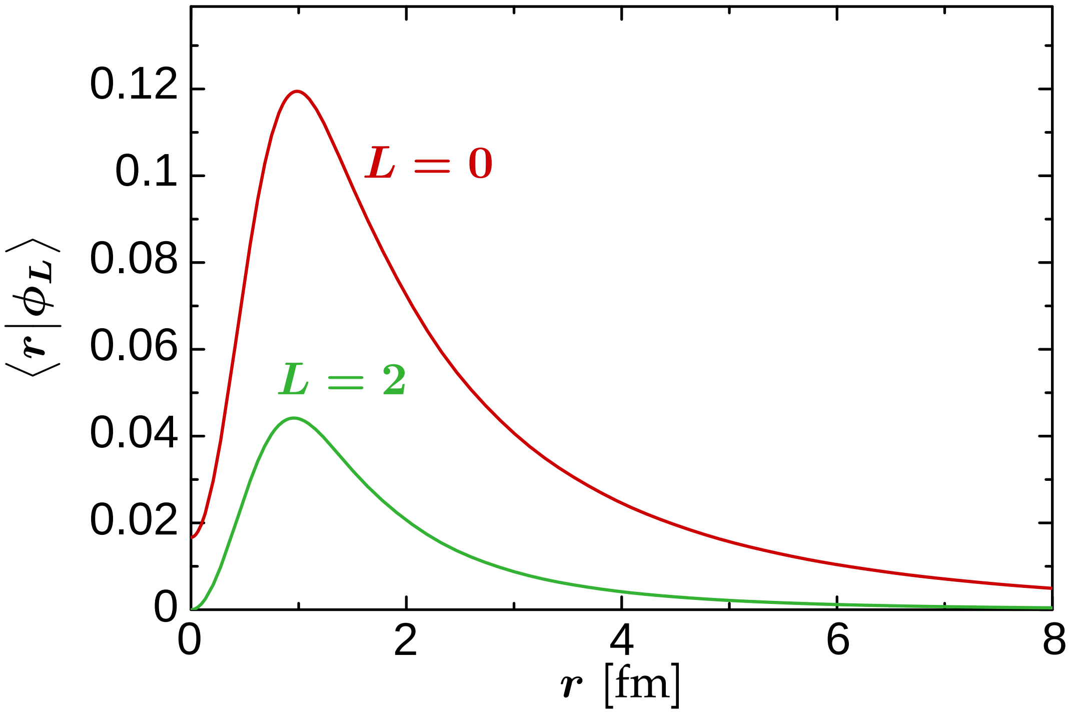
- rely on truncated many-nucleon Hilbert spaces (model space)
- not capable of describing short-range correlations
- extreme: Hartree-Fock based on single Slater determinant

Modern Effective Interactions

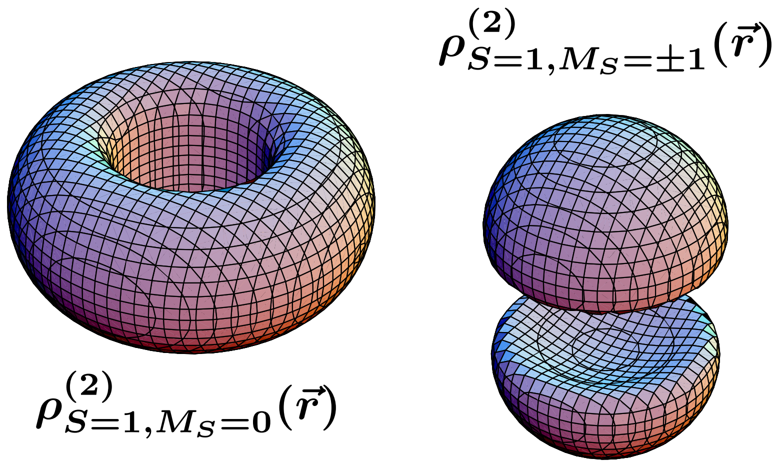
- adapt realistic potential to the available model space
- conserve experimentally constrained properties (phase shifts)

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 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 and all other observables to uncorrelated many-body space

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

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

Unitary Correlation Operator Method

explicit ansatz for 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

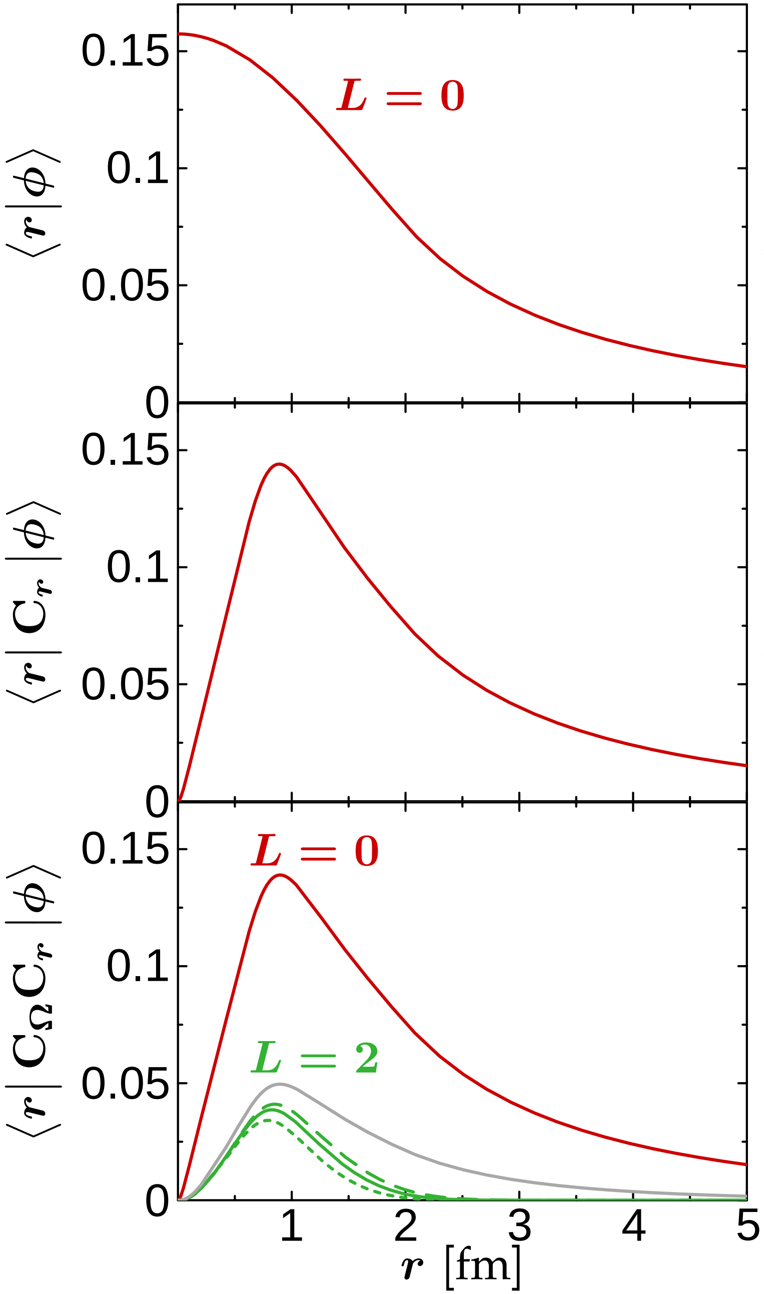
- angular shift depending on the orientation of spin and relative coordinate of a nucleon pair

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

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

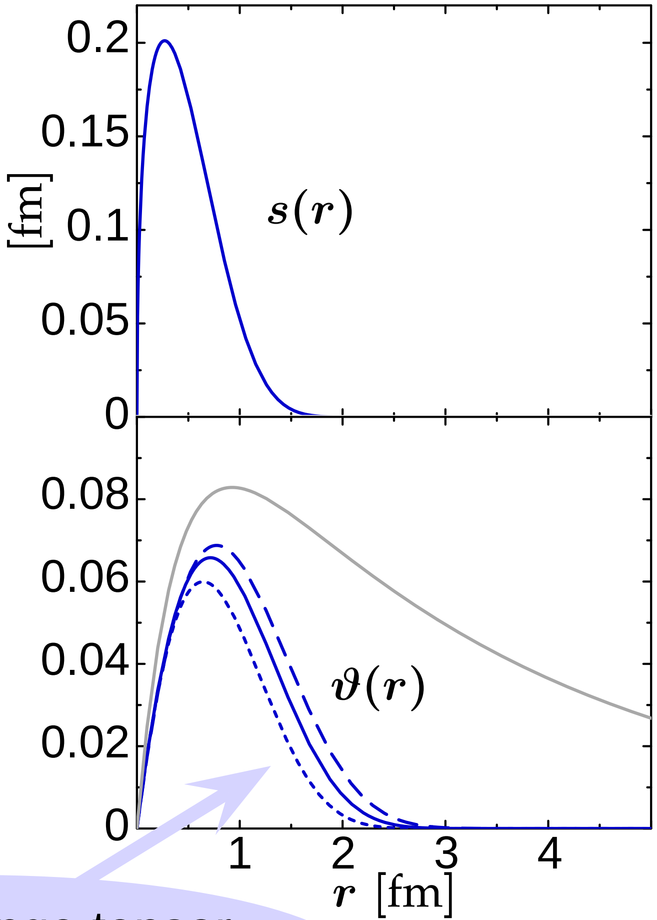
- $s(r)$ and $\vartheta(r)$ for given potential determined by energy minimization in the two-body system (for each S, T)

Correlated States: The Deuteron



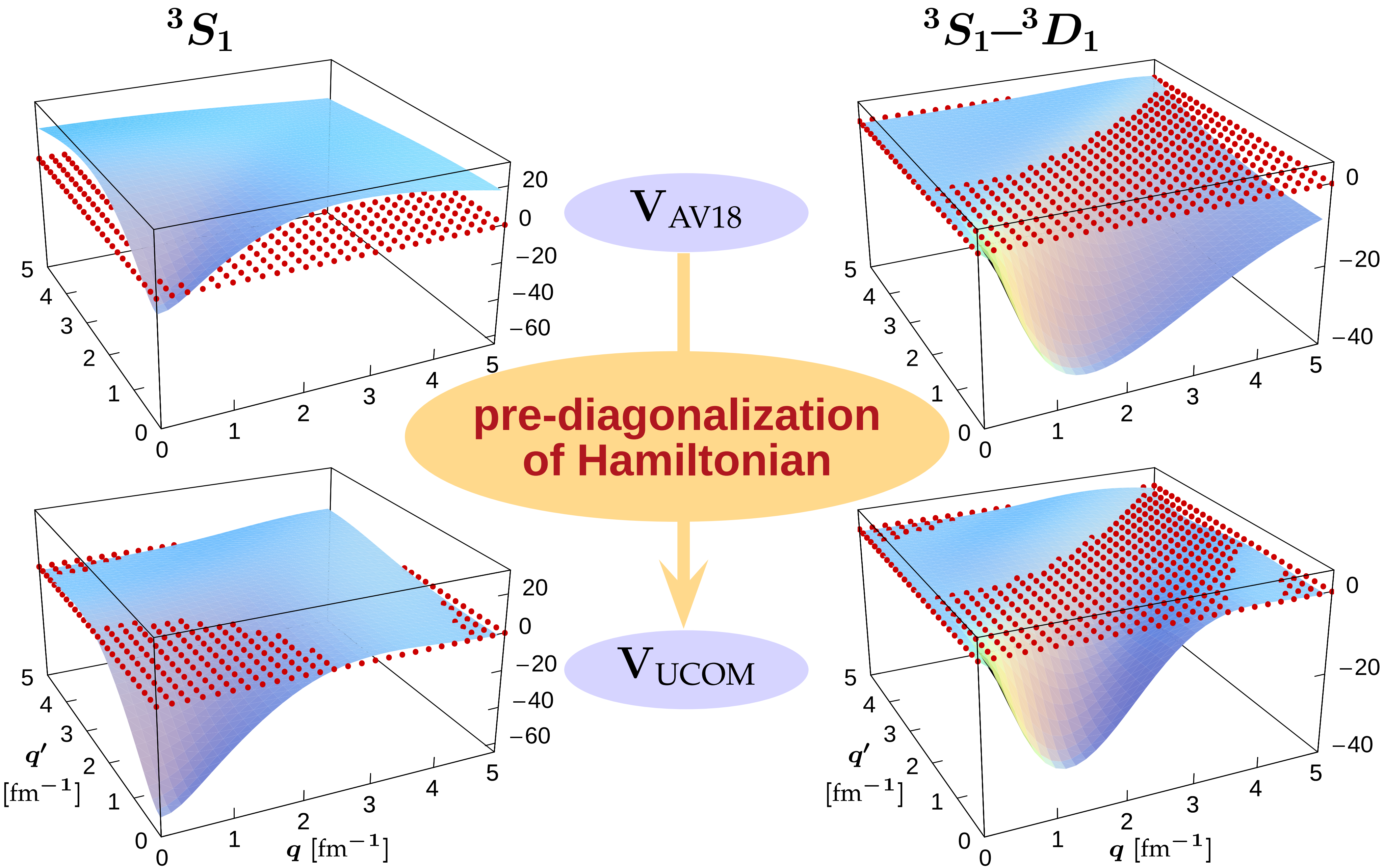
central correlations

tensor correlations



only short-range tensor correlations treated by C_Ω

Correlated Interaction: V_{UCOM}



Modern Effective Interactions

Similarity Renormalization Group (SRG)

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

Bogner et al. — arXiv: nucl-th/0611045

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

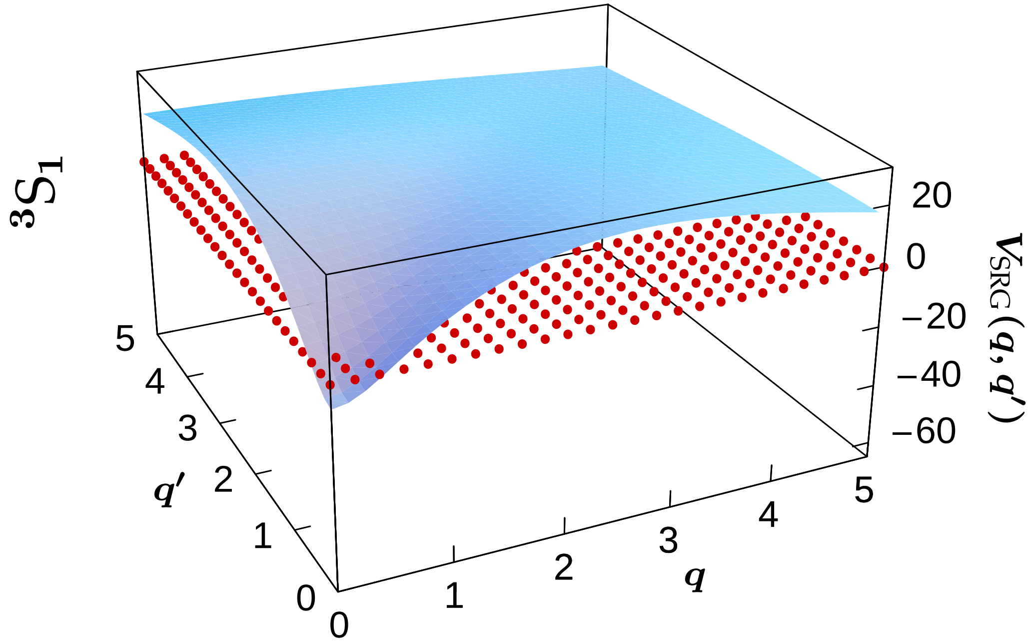
$$\widetilde{\mathrm{H}}(\alpha) = \mathrm{C}^{\dagger}(\alpha)\,\mathrm{H}\,\mathrm{C}(\alpha) \qquad \longrightarrow \qquad \frac{\mathrm{d}}{\mathrm{d}\alpha}\widetilde{\mathrm{H}}(\alpha) = \left[\eta(\alpha), \widetilde{\mathrm{H}}(\alpha)\right]$$

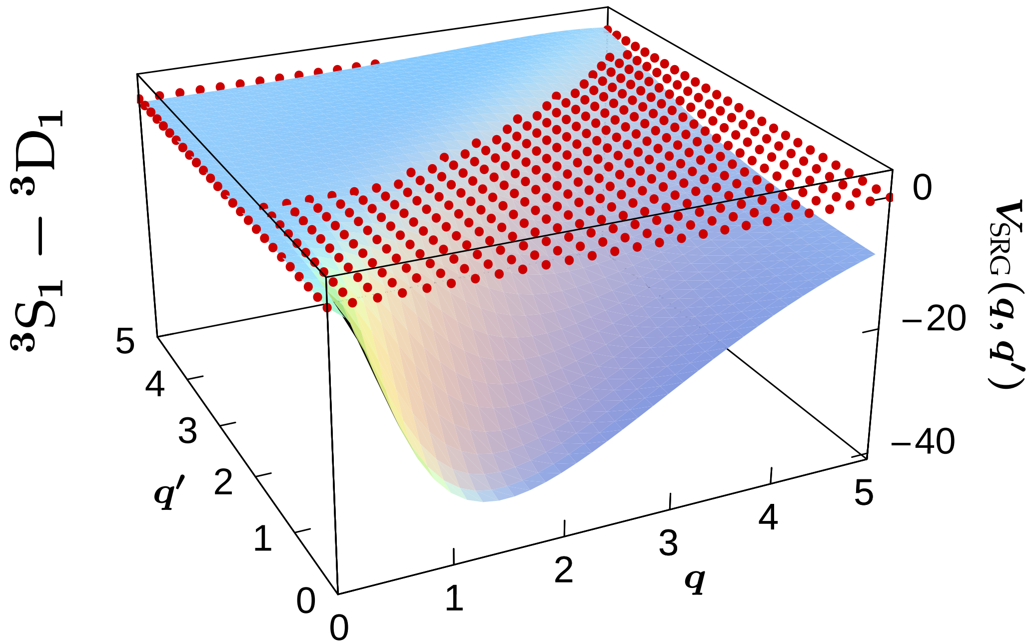
- dynamical generator defined as commutator with the operator in whose eigenbasis H shall be diagonalized

$$\eta(\alpha) = \left[\mathrm{T}_{\mathrm{int}}, \widetilde{\mathrm{H}}(\alpha)\right] \overset{\mathrm{2B}}{=} \frac{1}{2\mu}\left[\vec{\mathrm{q}}^{2}, \widetilde{\mathrm{H}}(\alpha)\right]$$

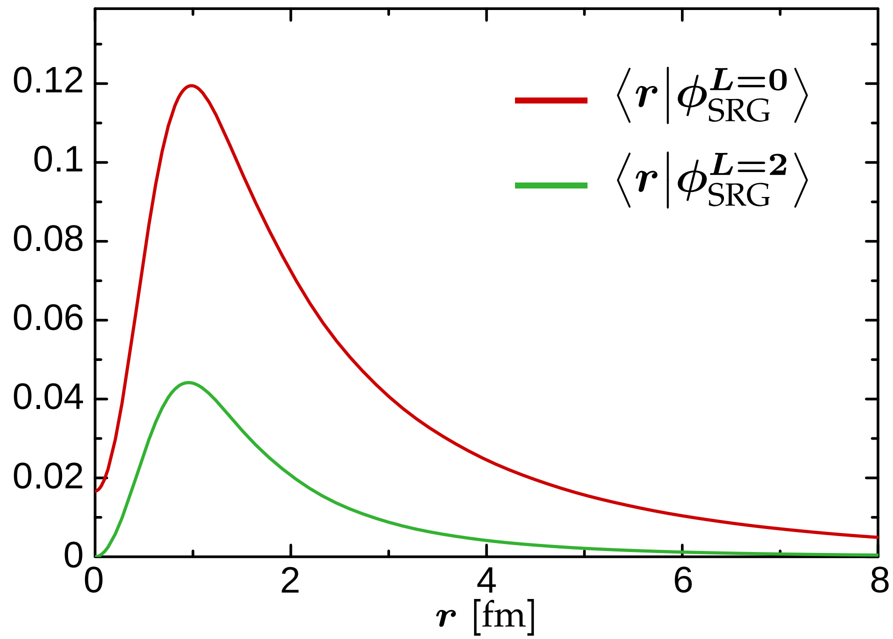
- $\eta(0)$ has the same structure as the UCOM generators g_r and g_Ω

SRG Evolution: The Deuteron

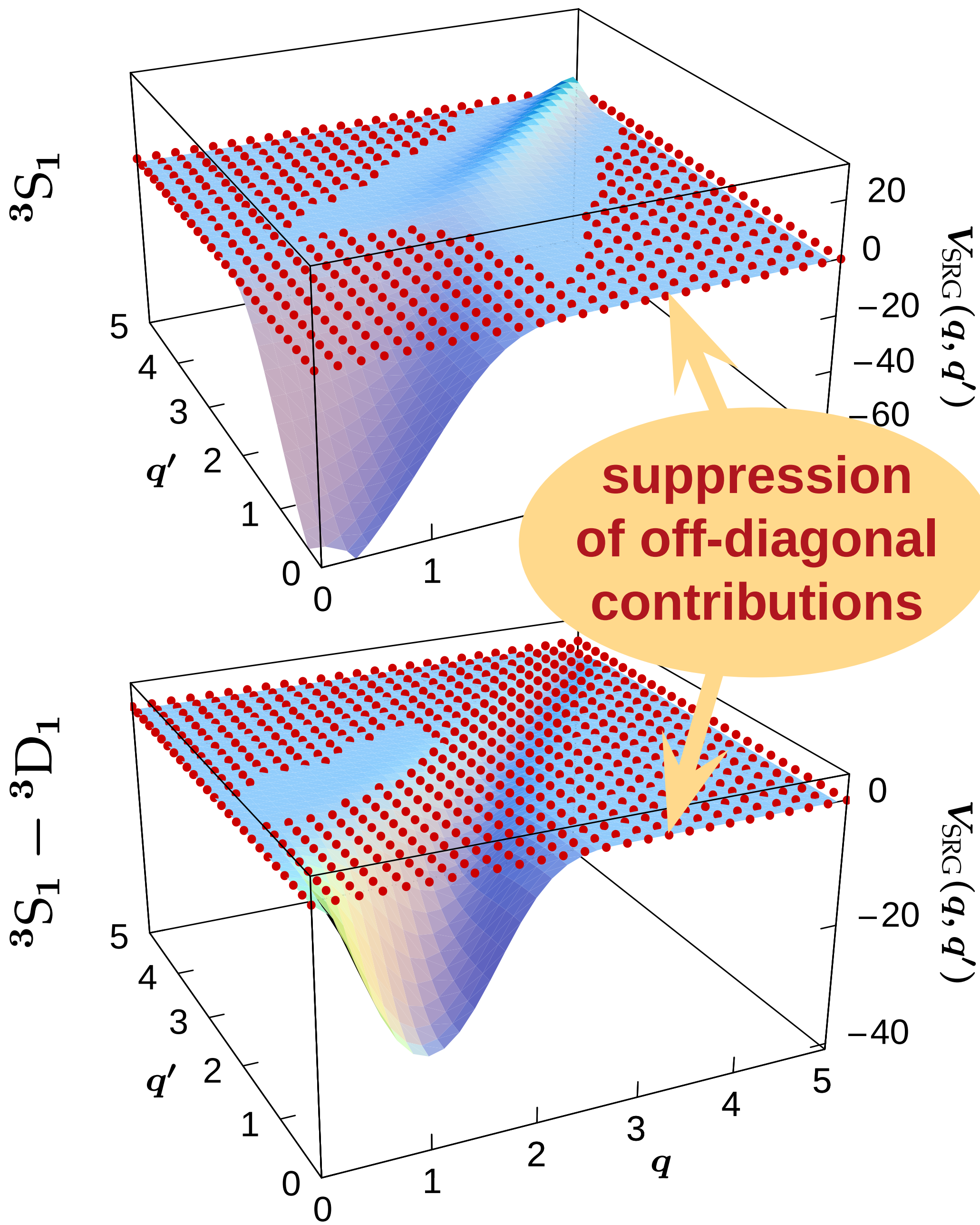




Argonne V18

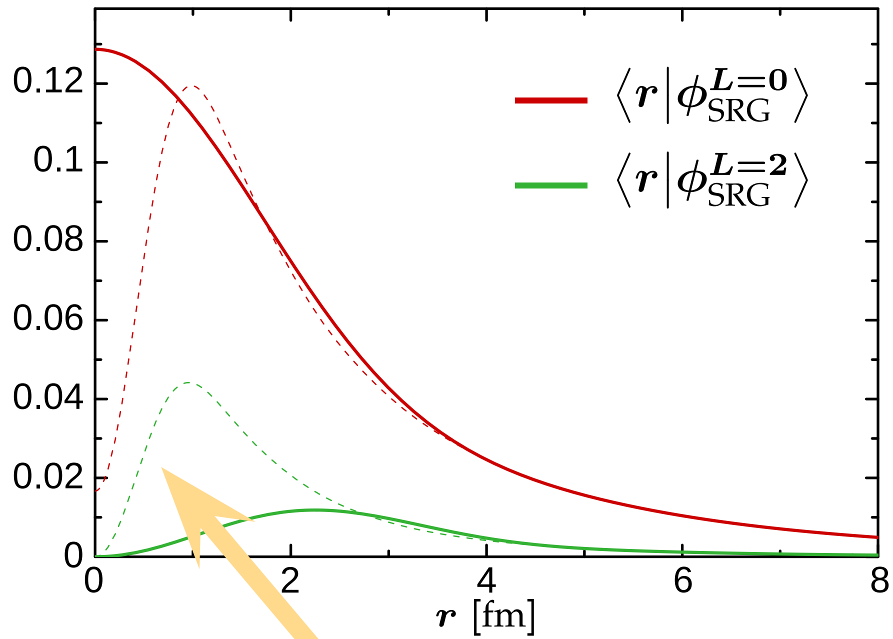


SRG Evolution: The Deuteron



suppression of off-diagonal contributions

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



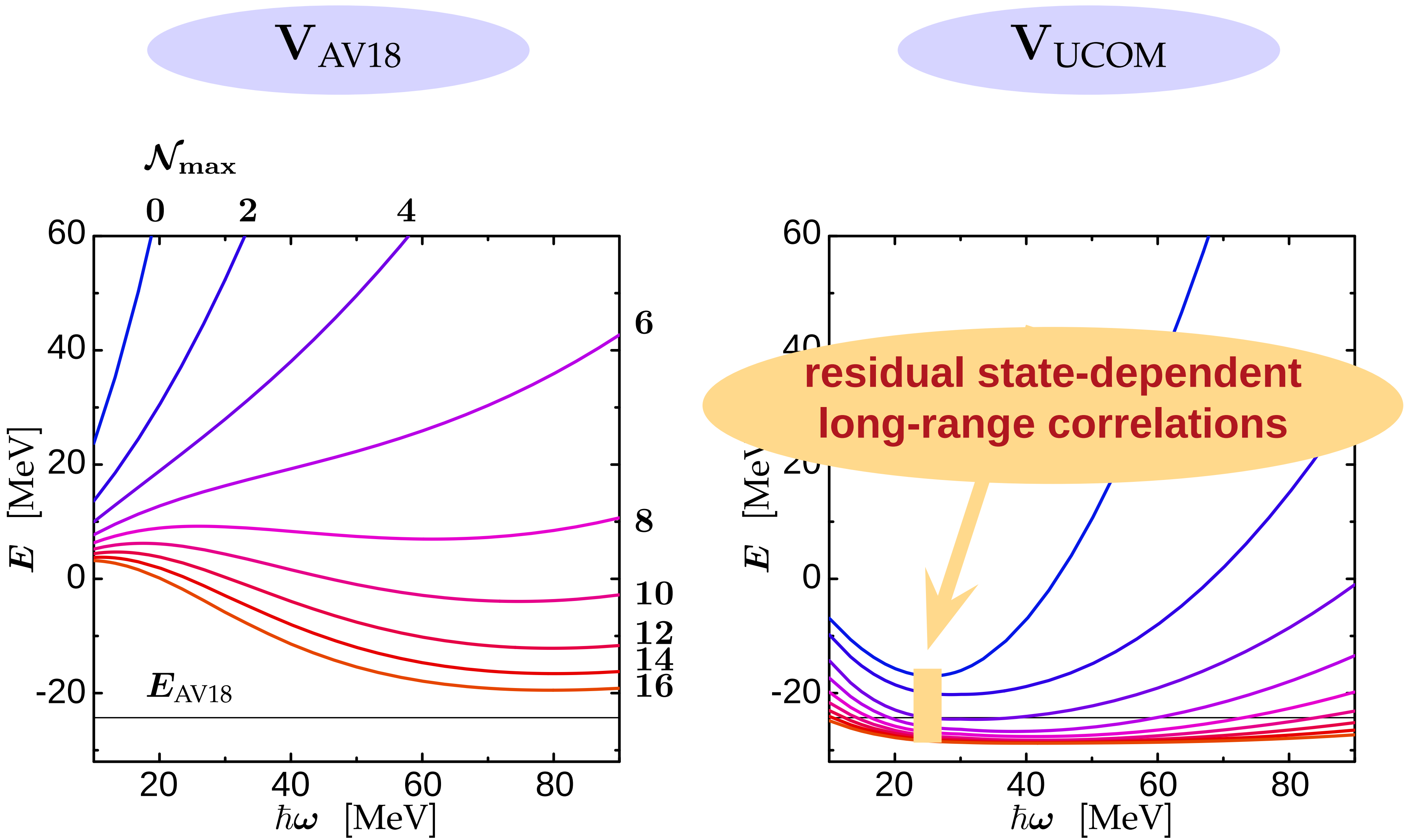
elimination of short-range correlations

Many-Body Methods

No-Core Shell Model

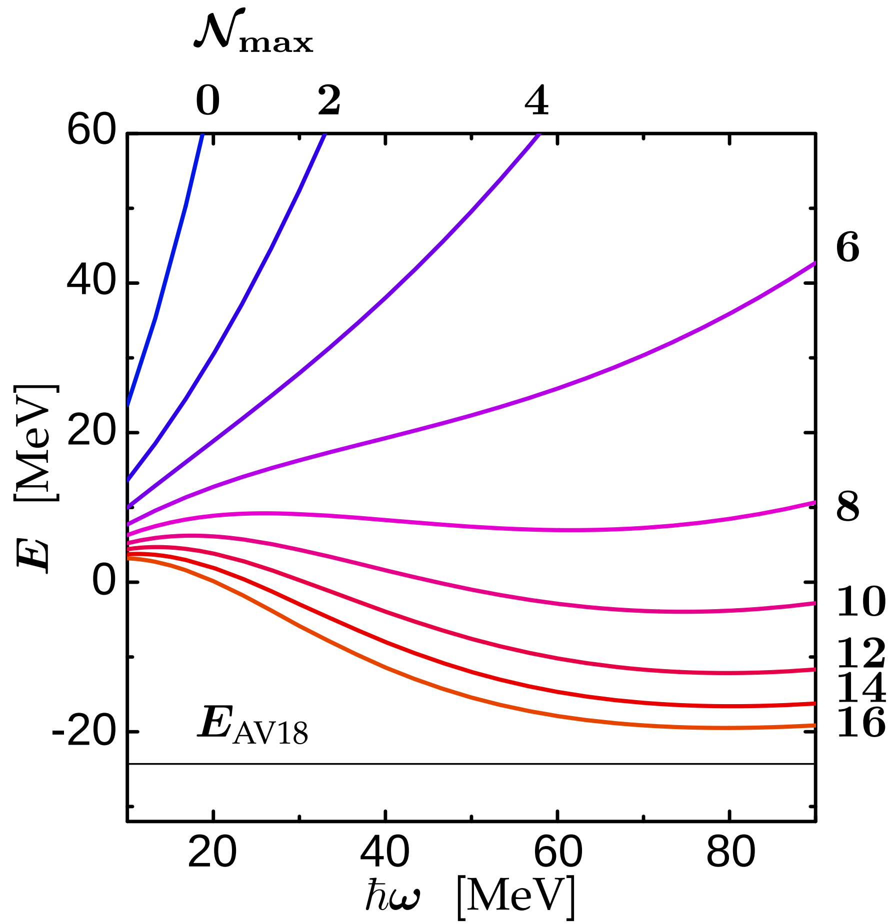
Roth et al. — Phys. Rev. C 72, 034002 (2005)
Roth & Navrátil — in preparation

^{4}He: Convergence

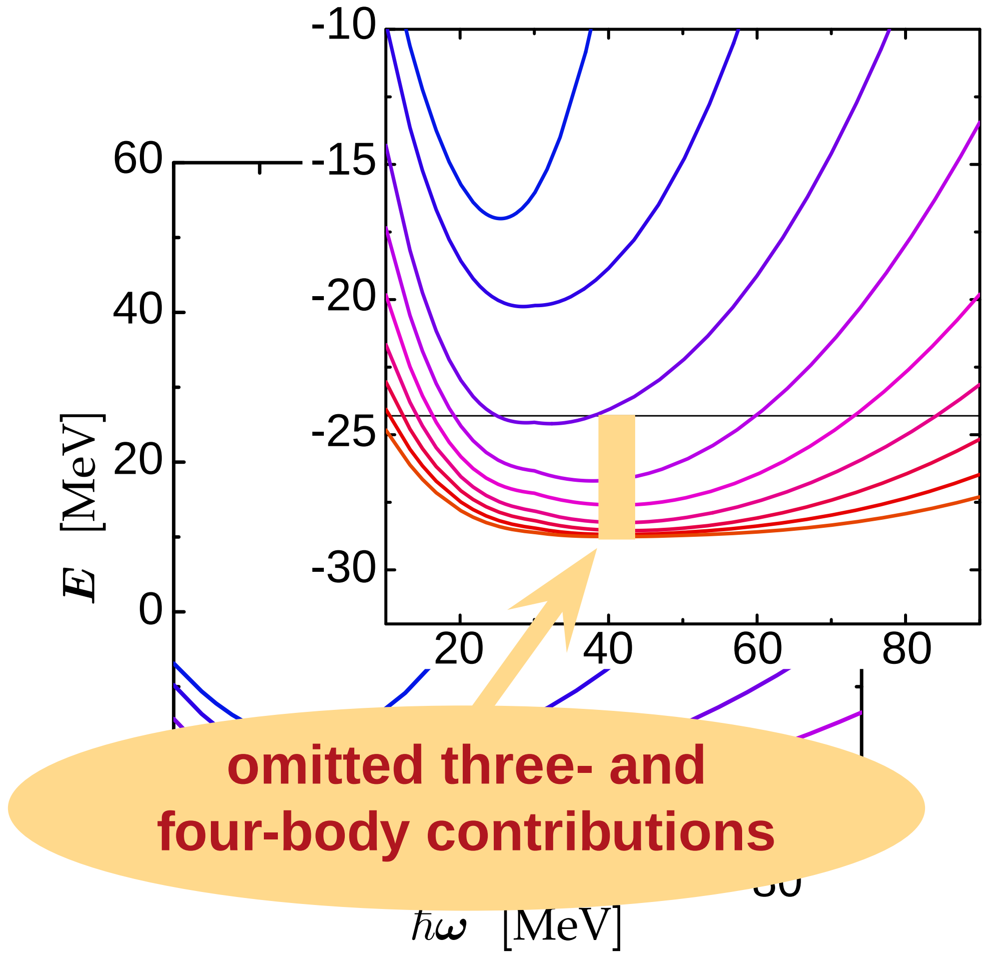


^{4}He: Convergence

V_{AV18}



V_{UCOM}



Three-Body Interactions — Strategies

Correlated Hamiltonian in Many-Body Space

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

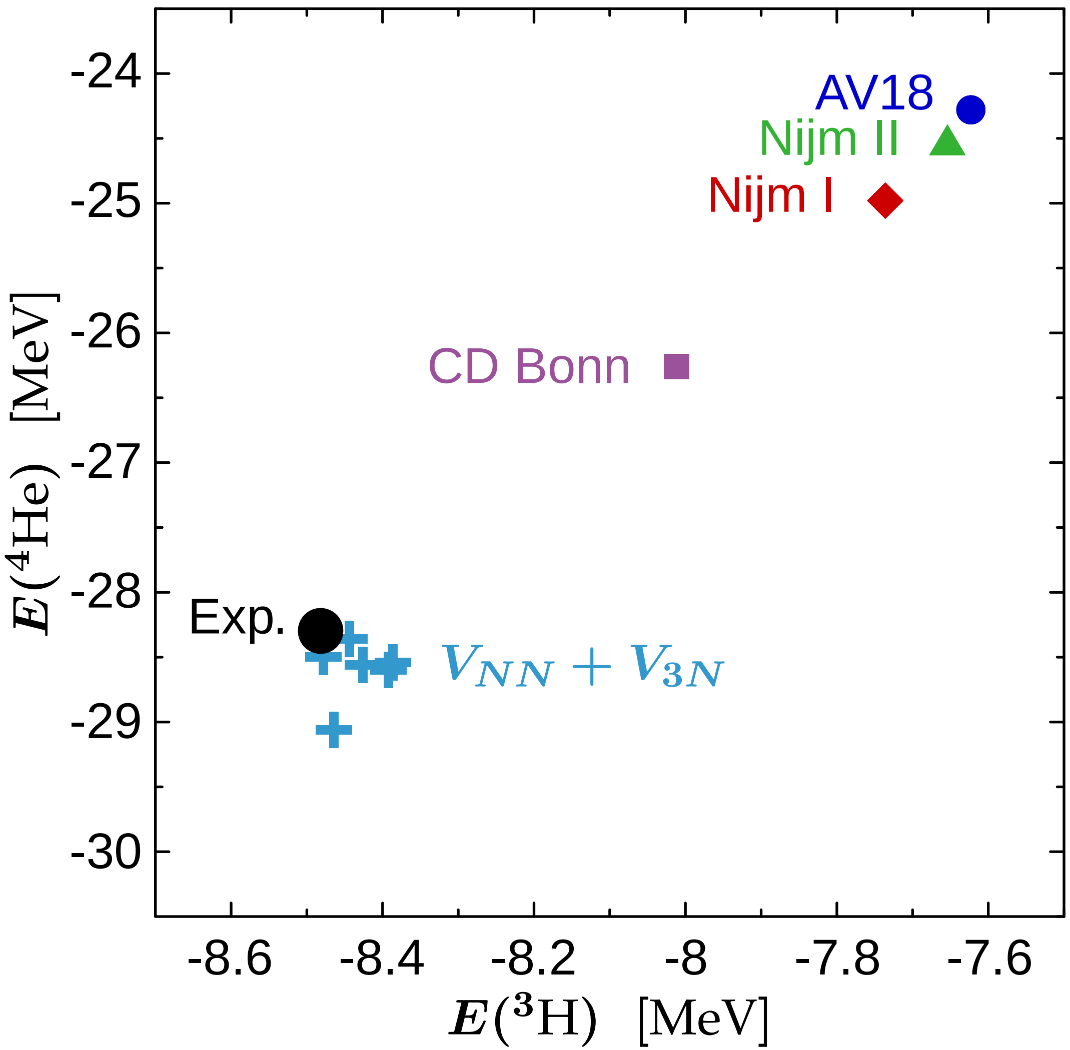
- strategies for treating the three-body contributions:

  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

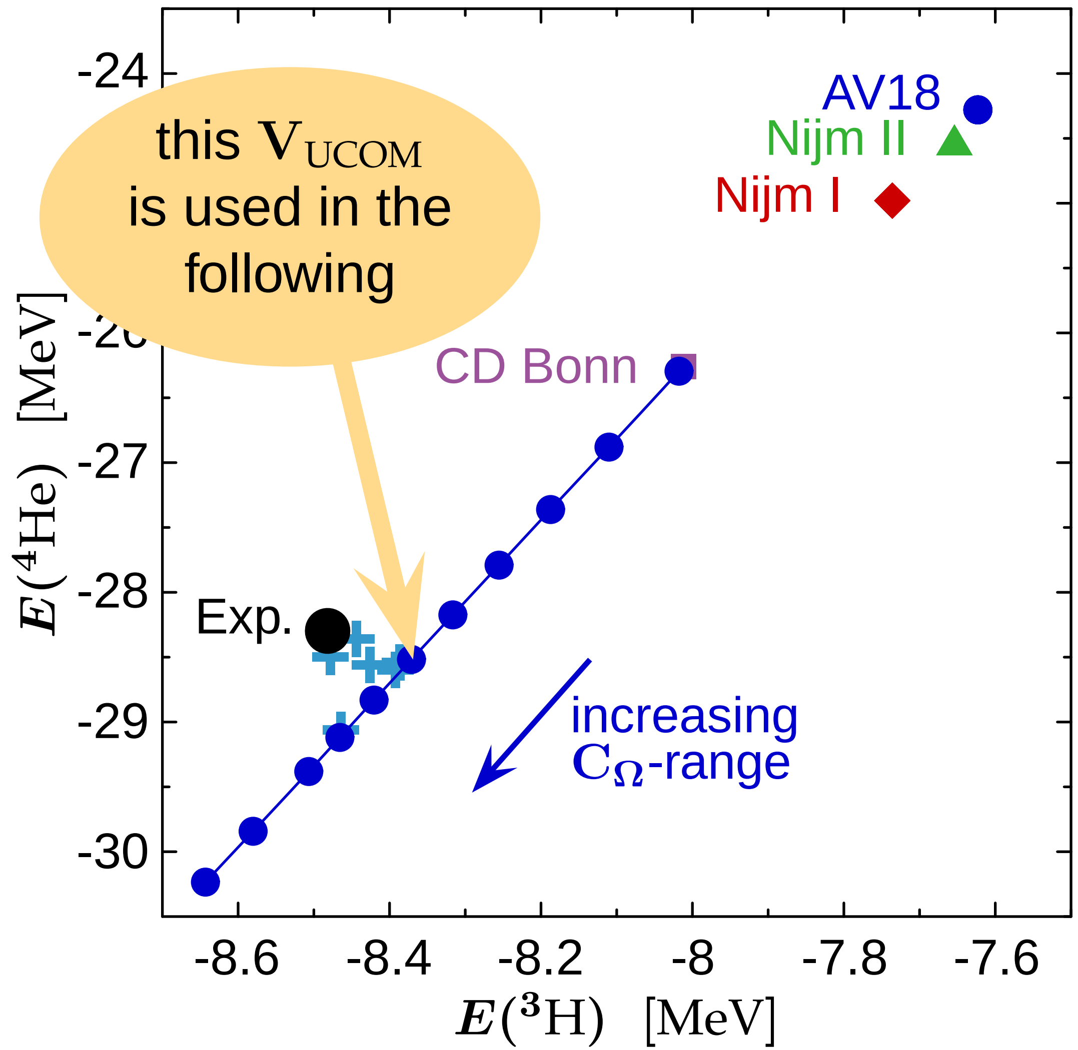
  ❸ **minimize $\mathrm{V}_{\mathrm{UCOM}}^{[3]}$** by proper choice of unitary transformation

Three-Body Interactions — Tjon Line



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

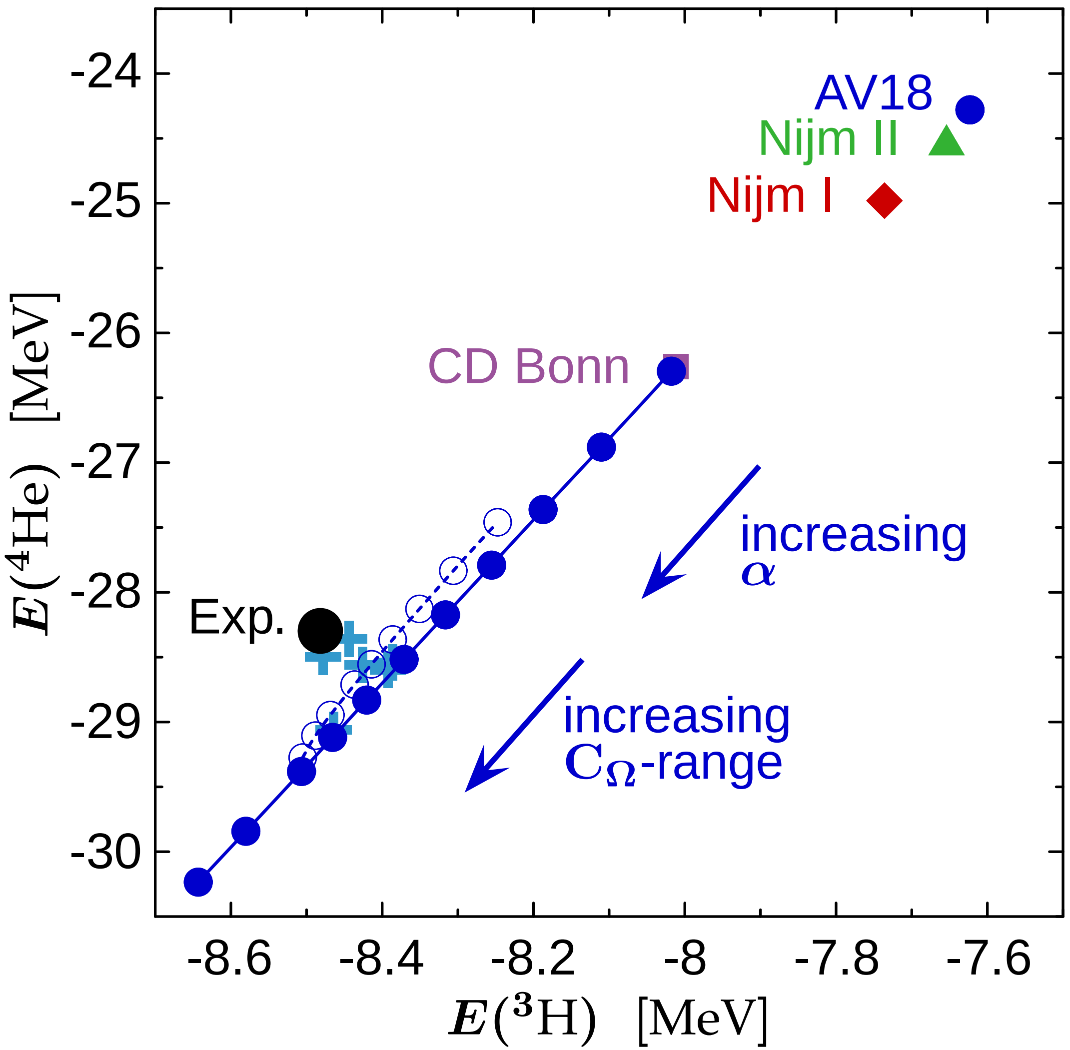
Three-Body Interactions — Tjon Line



- **Tjon-line**: $E(^4\text{He})$ vs. $E(^3\text{H})$ 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

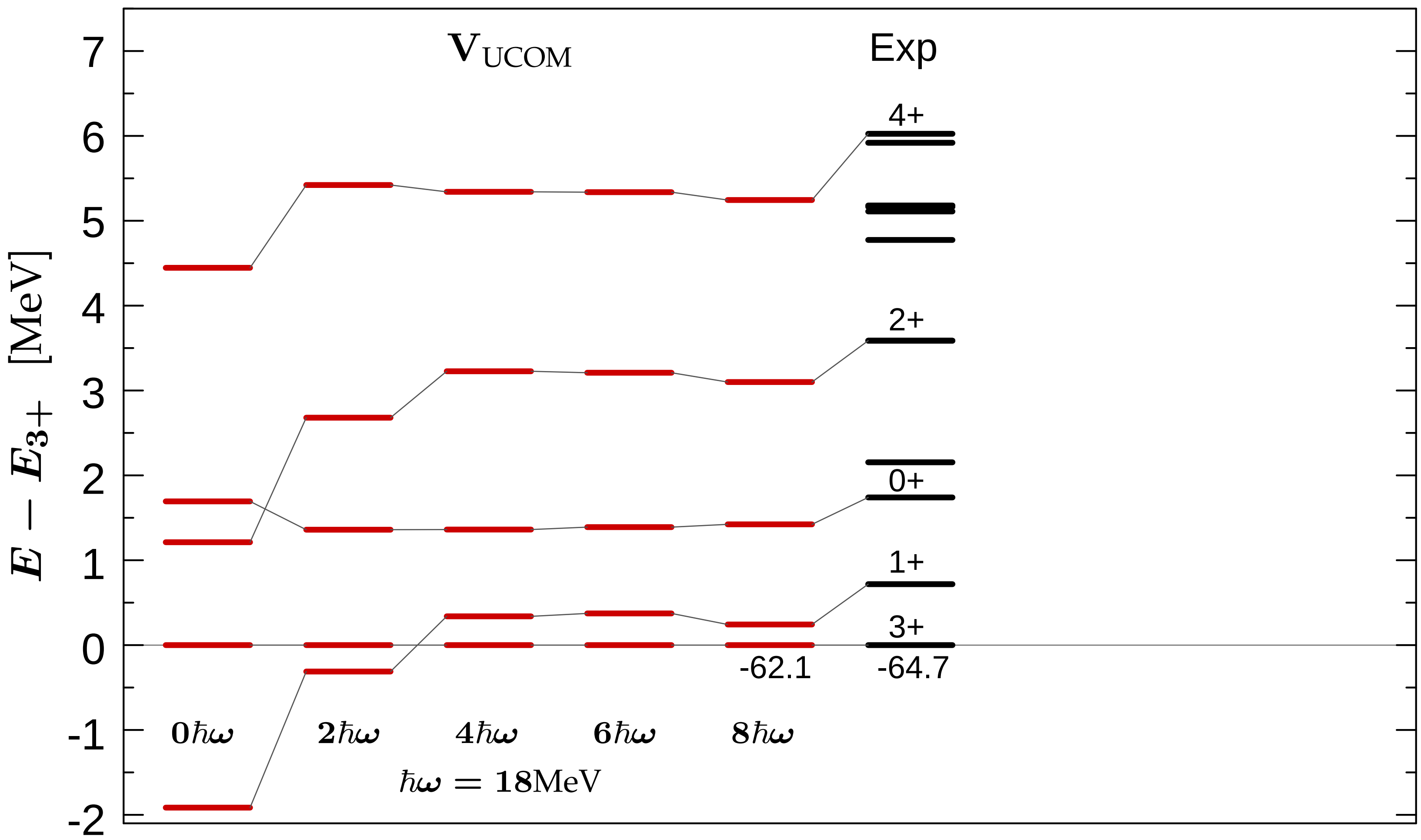
Three-Body Interactions — Tjon Line



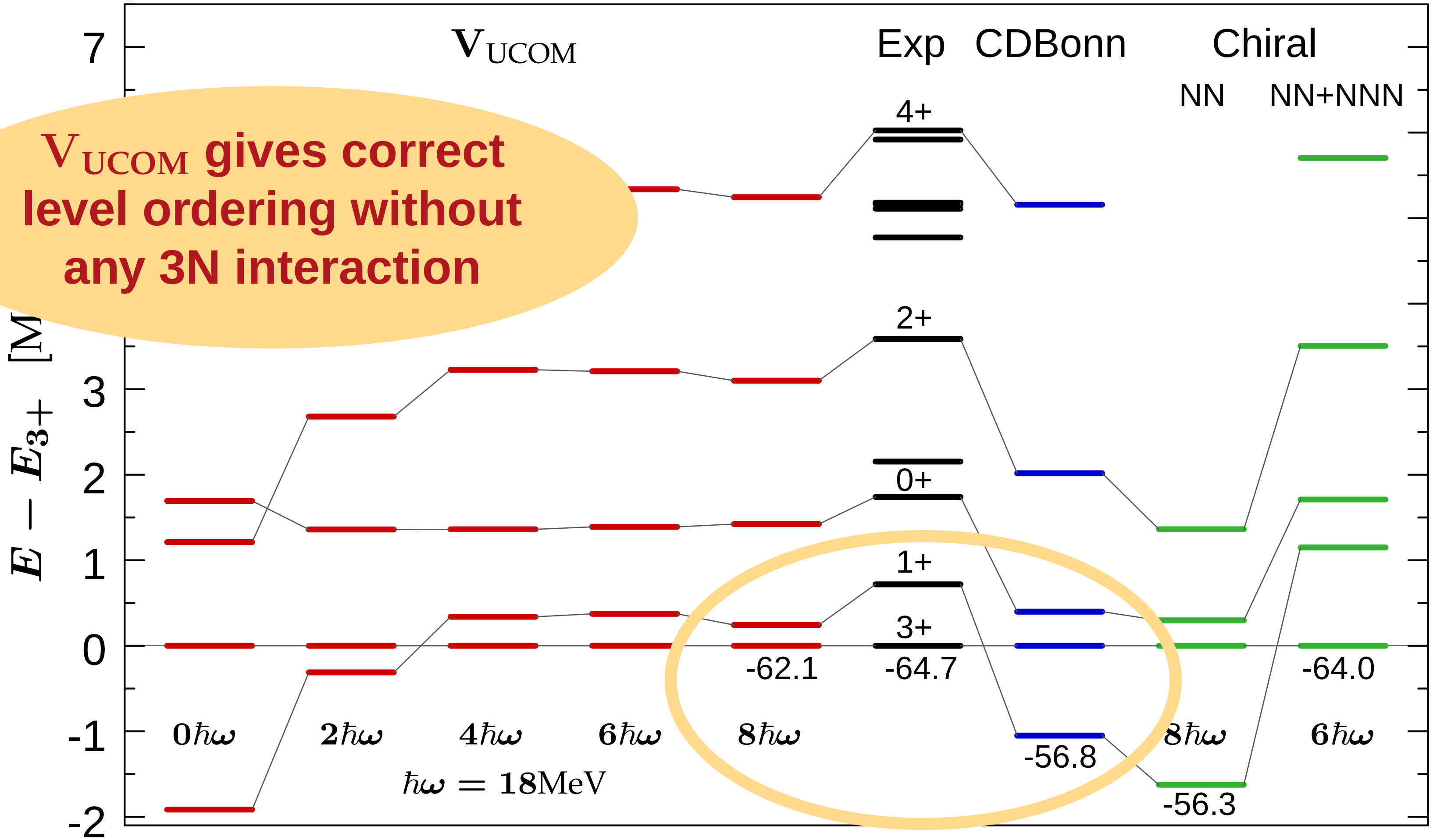
- **Tjon-line**: $E(^4\mathrm{He})$ vs. $E(^3\mathrm{H})$ for phase-shift equivalent NN-interactions
- same behavior for the SRG interaction as function of α

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

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



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



V_{UCOM} gives correct level ordering without any 3N interaction

Many-Body Methods

Importance Truncated No-Core Shell Model

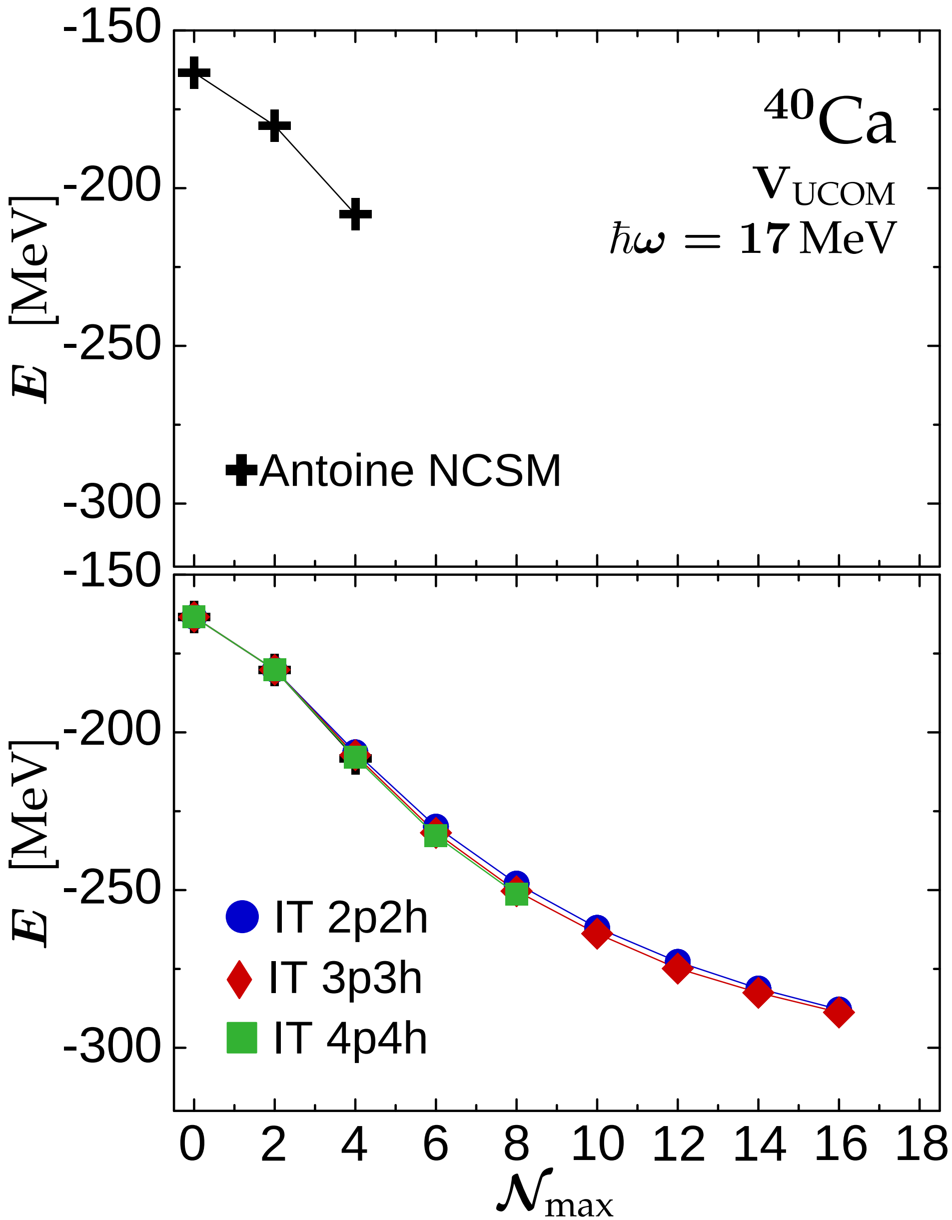
Roth & Navrátil — arXiv: 0705.4069

Importance Truncated NCSM

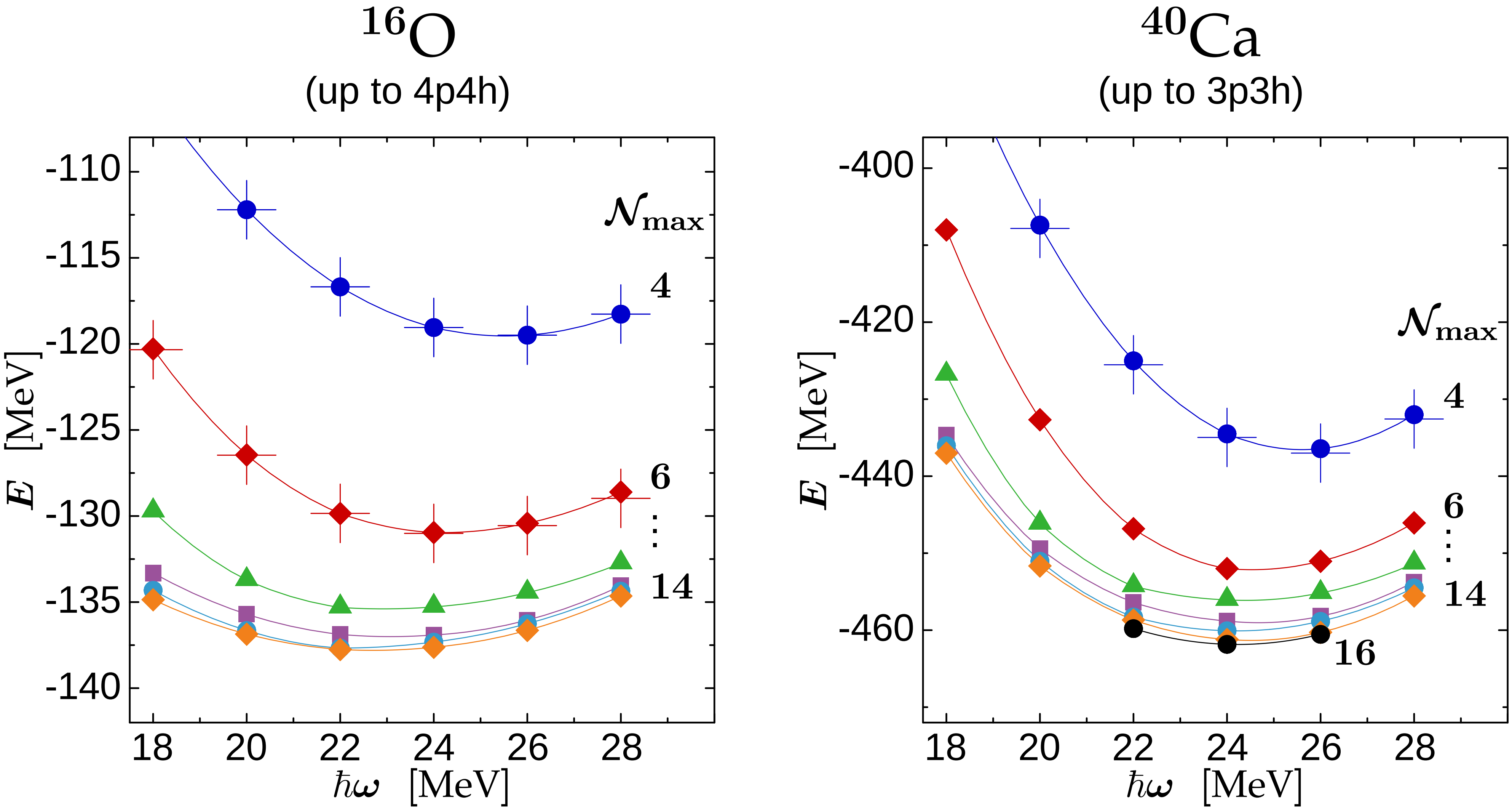
- converged NCSM calculations essentially restricted to p-shell
- full $6\hbar\omega$ calculation for $^{40}\mathrm{Ca}$ presently not feasible (basis dimension $\sim 10^{10}$)

Importance Truncation

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



Converged IT-NCSM using $V_{\text{low}k}$



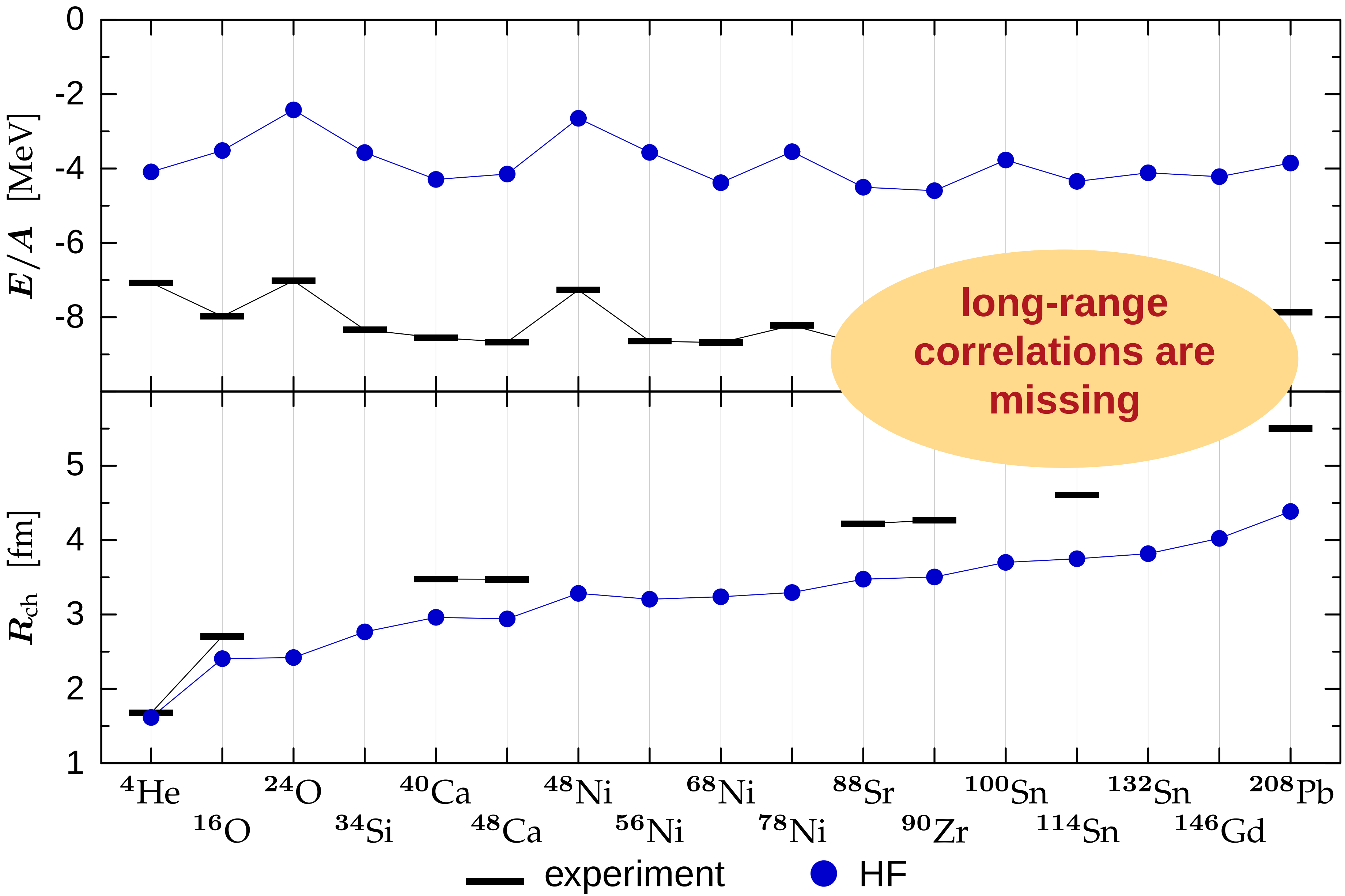
$\mathbf{V}_{\text{low-}k}$
(AV18, $\Lambda = 2.1\,\text{fm}^{-1}$)

Many-Body Methods

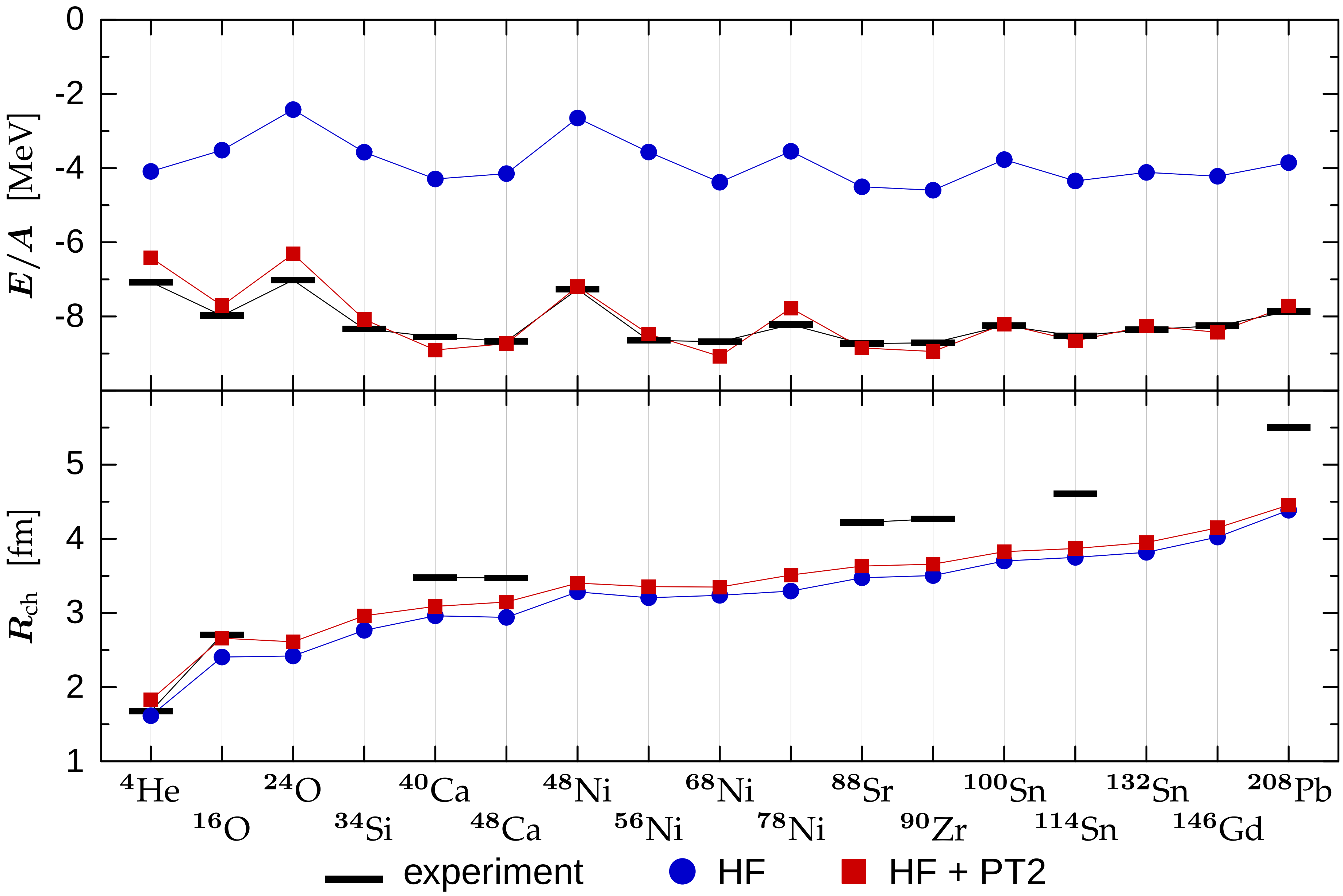
Beyond Hartree-Fock

R. Roth et al. — Phys. Rev. C 73, 044312 (2006)
C. Barbieri et al. — arXiv: nucl-th/0608011

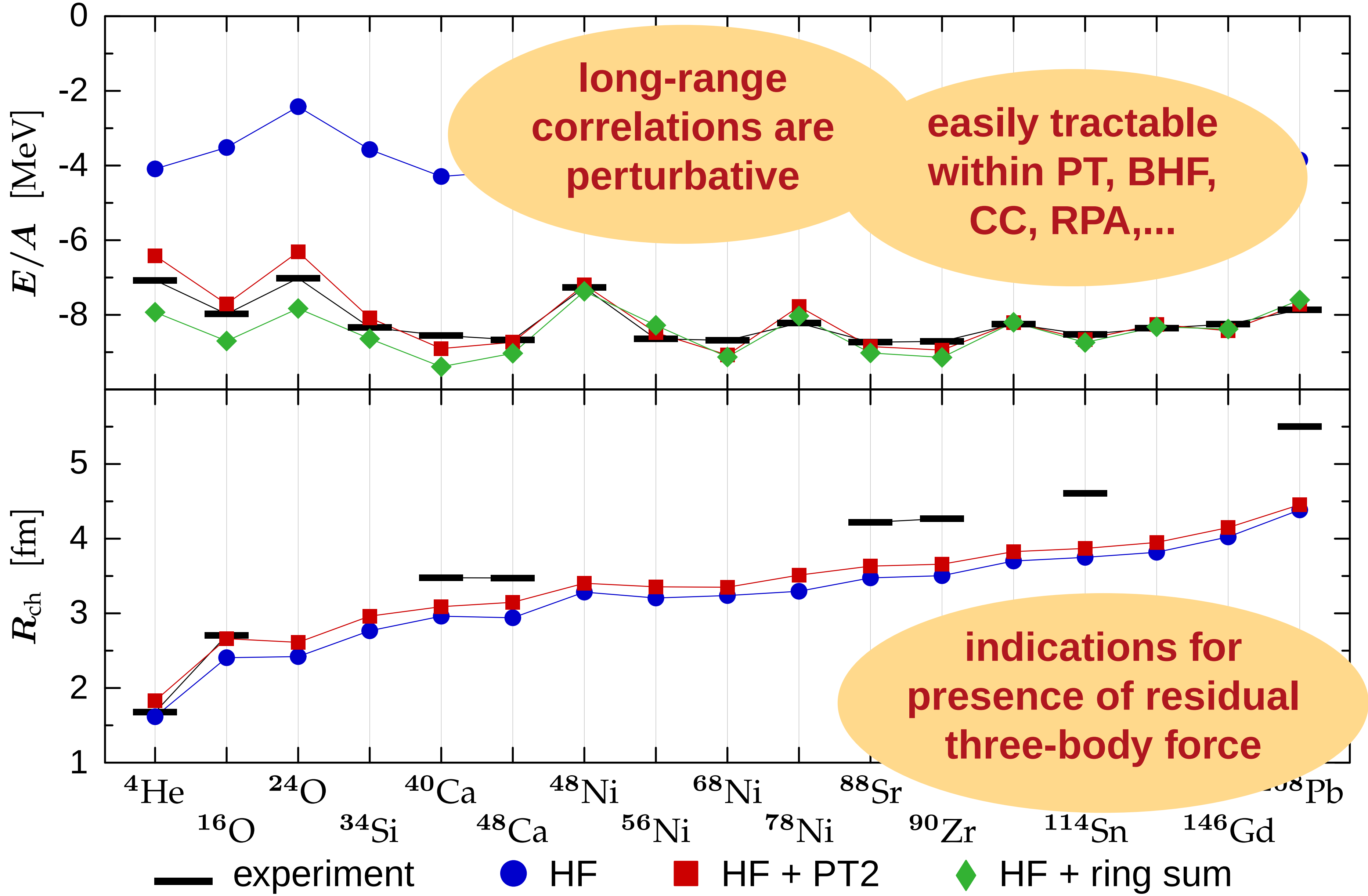
Hartree-Fock with V_{UCOM}



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 NCSM
  - Coupled Cluster Method, Unitary Model Operator Approach,...
  - Hartree-Fock plus MBPT, Padé Resummed MBPT, 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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  - N. Paar

    University of Zagreb, Croatia
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