Towards Ab Initio Nuclear Structure 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
- Perspectives

Nuclear Structure

Low-Energy QCD

From QCD to Nuclear Structure

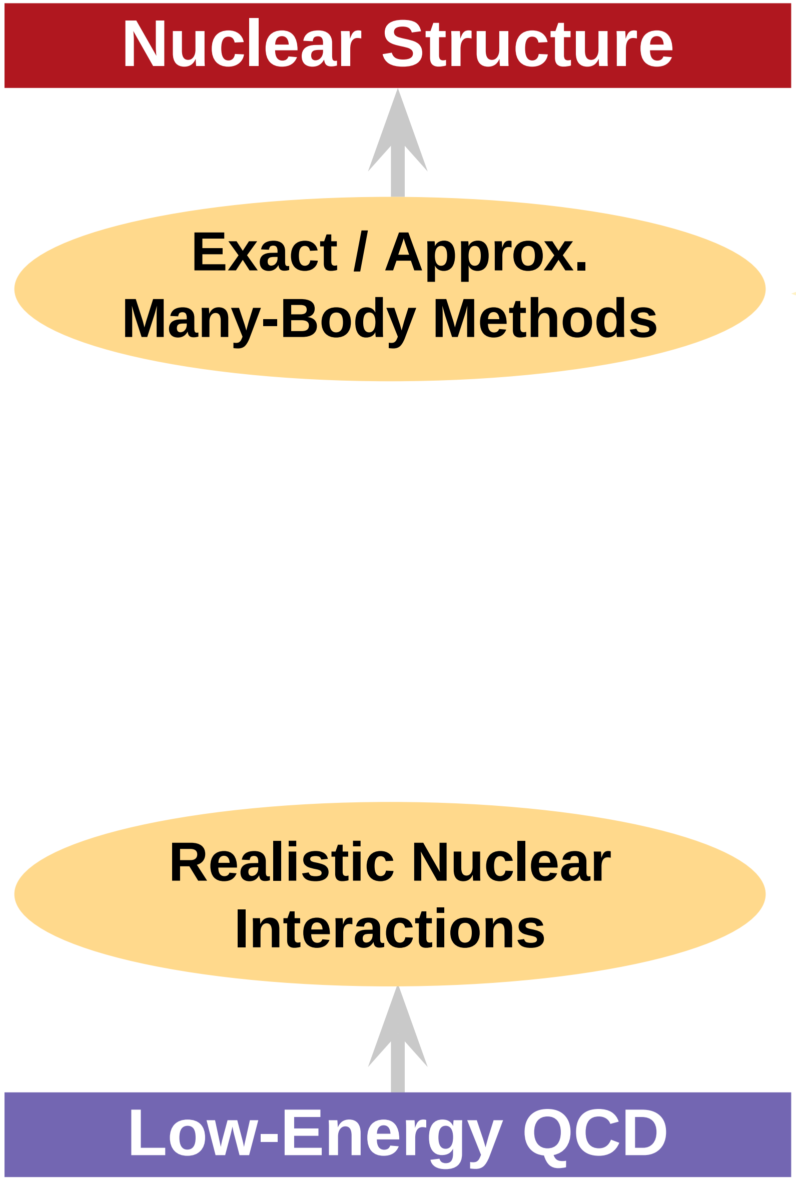
Nuclear Structure

Realistic Nuclear Interactions

Low-Energy QCD

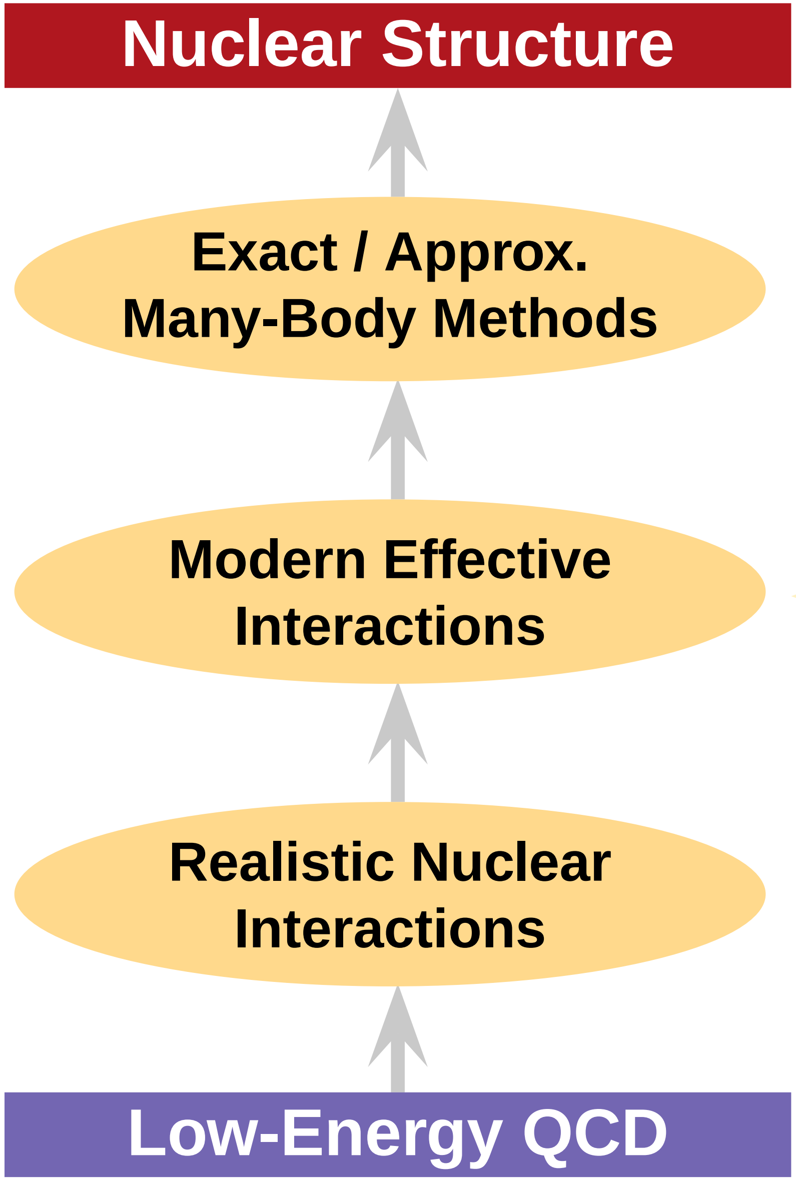
- chiral interactions: consistent NN & 3N interaction derived within χEFT
- traditional NN-interactions: Argonne V18, CD Bonn,...
- reproduce experimental NN phase-shifts with high precision
- induce strong short-range central & tensor correlations

From QCD to Nuclear Structure



- ‘exact’ solution of the many-body problem for light and intermediate masses (GFMC, NCSM, CC,...)
- controlled approximations for heavier nuclei (HF & MBPT,...)
- rely on restricted model spaces of tractable size
- not suitable for the description of short-range correlations

From QCD to Nuclear Structure



- adapt realistic potential to the available model space
  - tame short-range correlations
  - improve convergence behavior
- conserve experimentally constrained properties (phase shifts)
  - generate new realistic interaction
- provide consistent effective interaction & effective operators
- unitary transformations most convenient

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

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

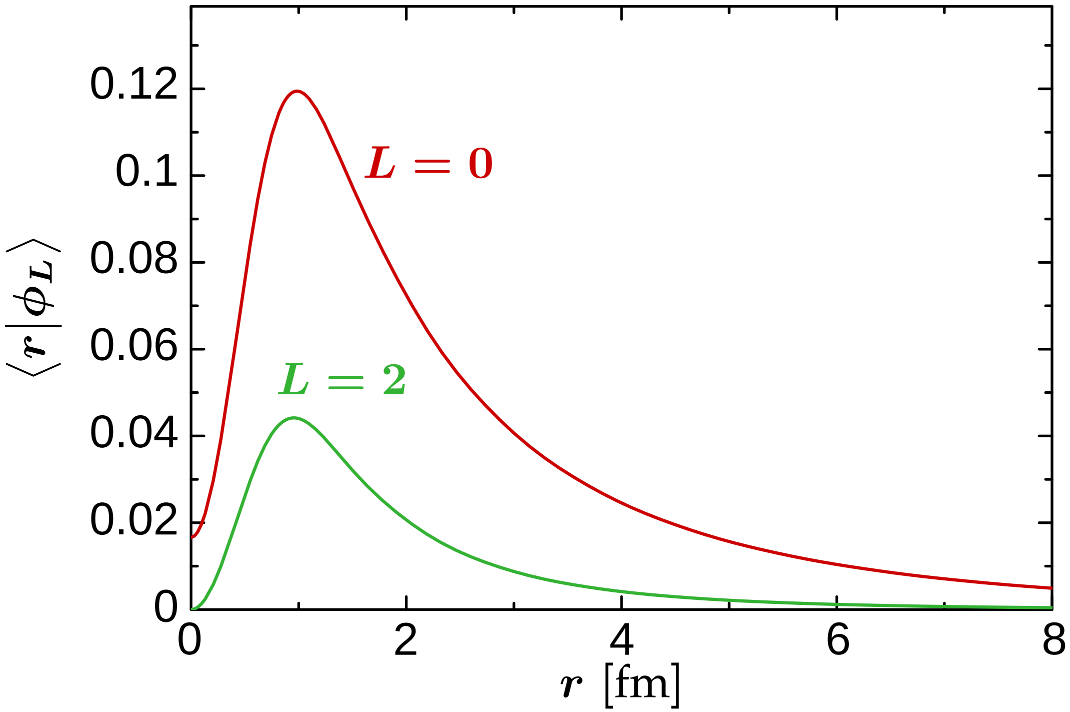
Correlated Operators

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

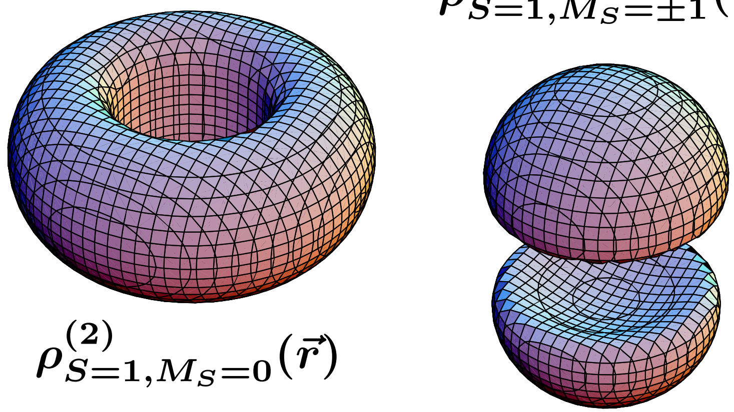
$$\widetilde{\mathrm{O}} = \mathrm{C}^\dagger\ \mathrm{O}\ \mathrm{C}$$

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

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

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

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

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

Tensor Correlator C_Ω

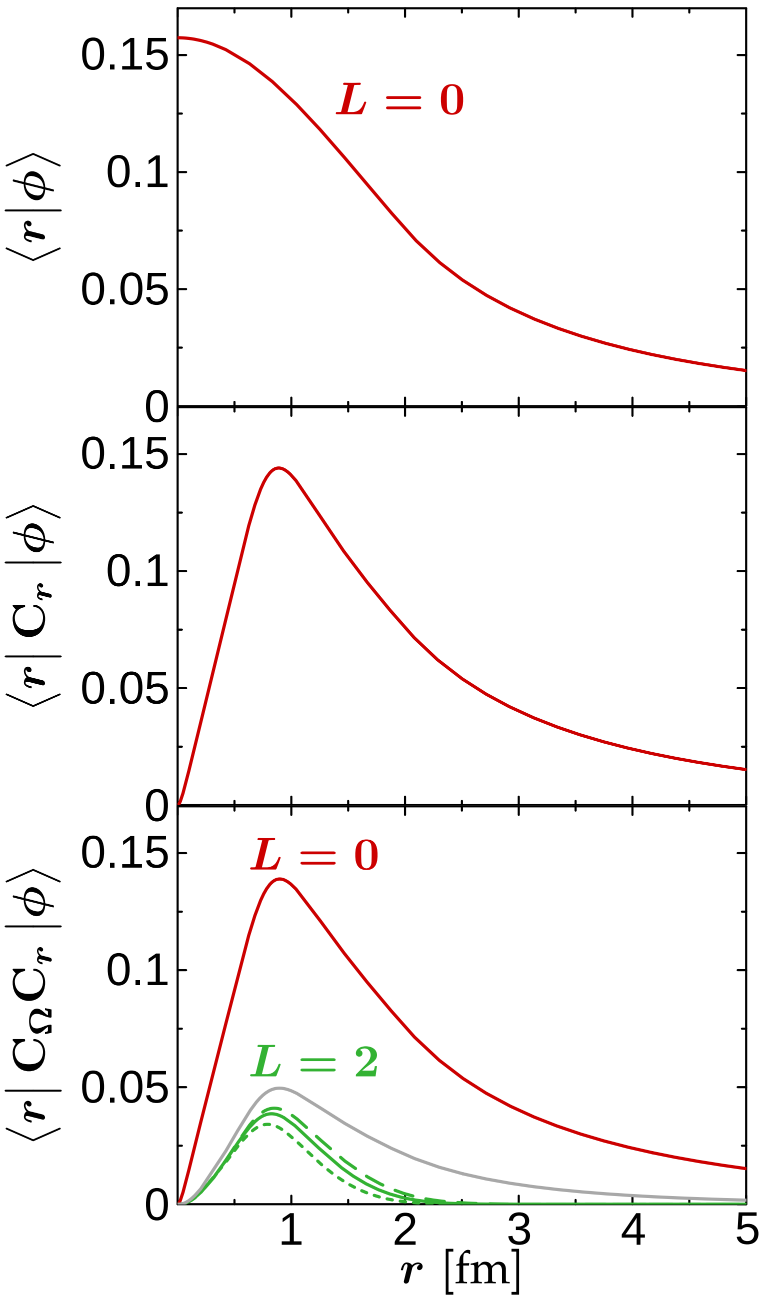
- angular shift depending on the orientation of spin and relative coordinate of a nucleon pair

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

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

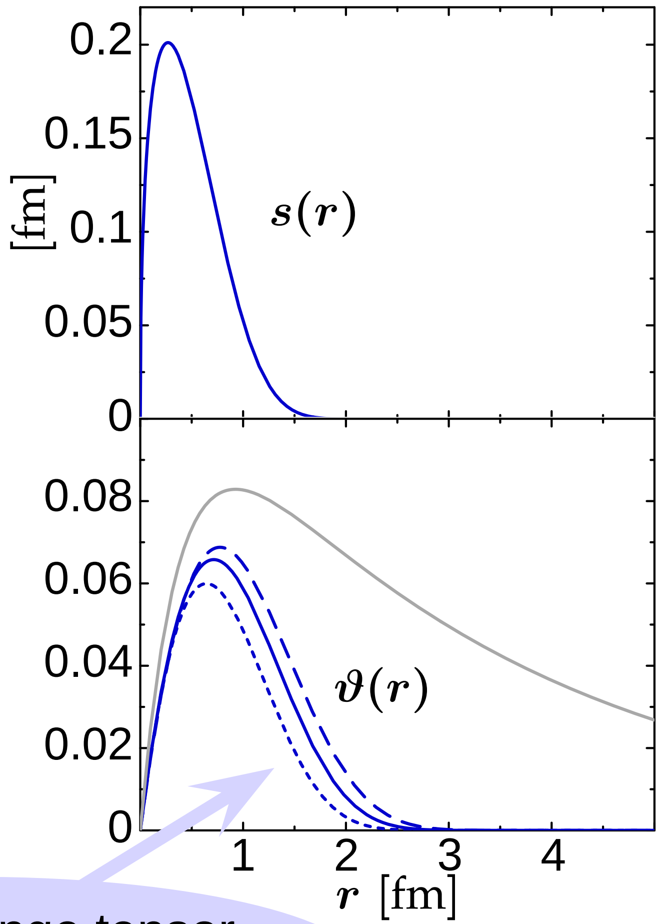
- $s(r)$ and $\vartheta(r)$ for given potential determined by energy minimization in the two-body system (for each S, T)

Correlated States: The Deuteron



central correlations

tensor correlations



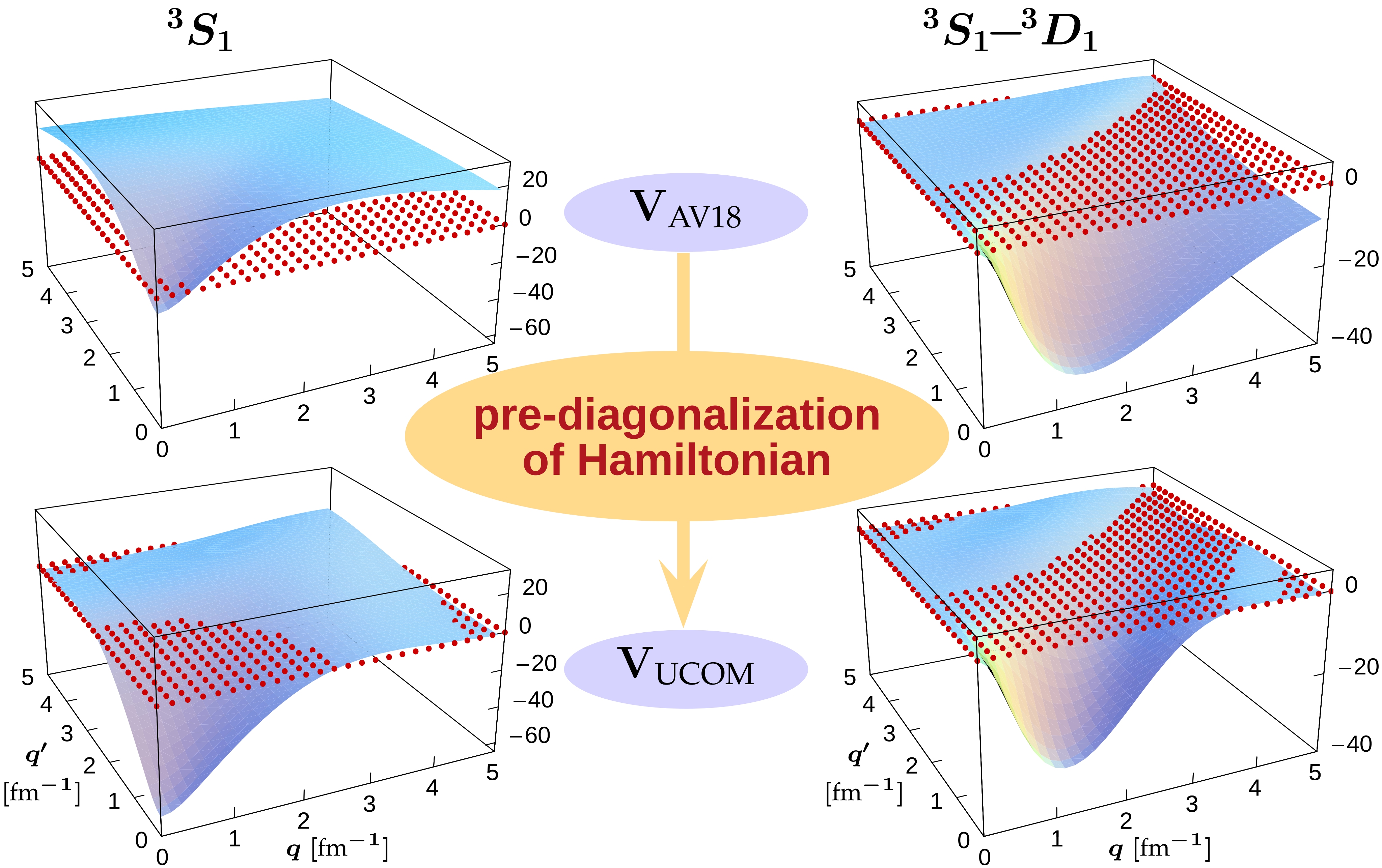
only short-range tensor correlations treated by C_Ω

Correlated Interaction: V_{UCOM}

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

- **closed operator expression** for the correlated interaction $\mathbf{V}_{\text{UCOM}}$ 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

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

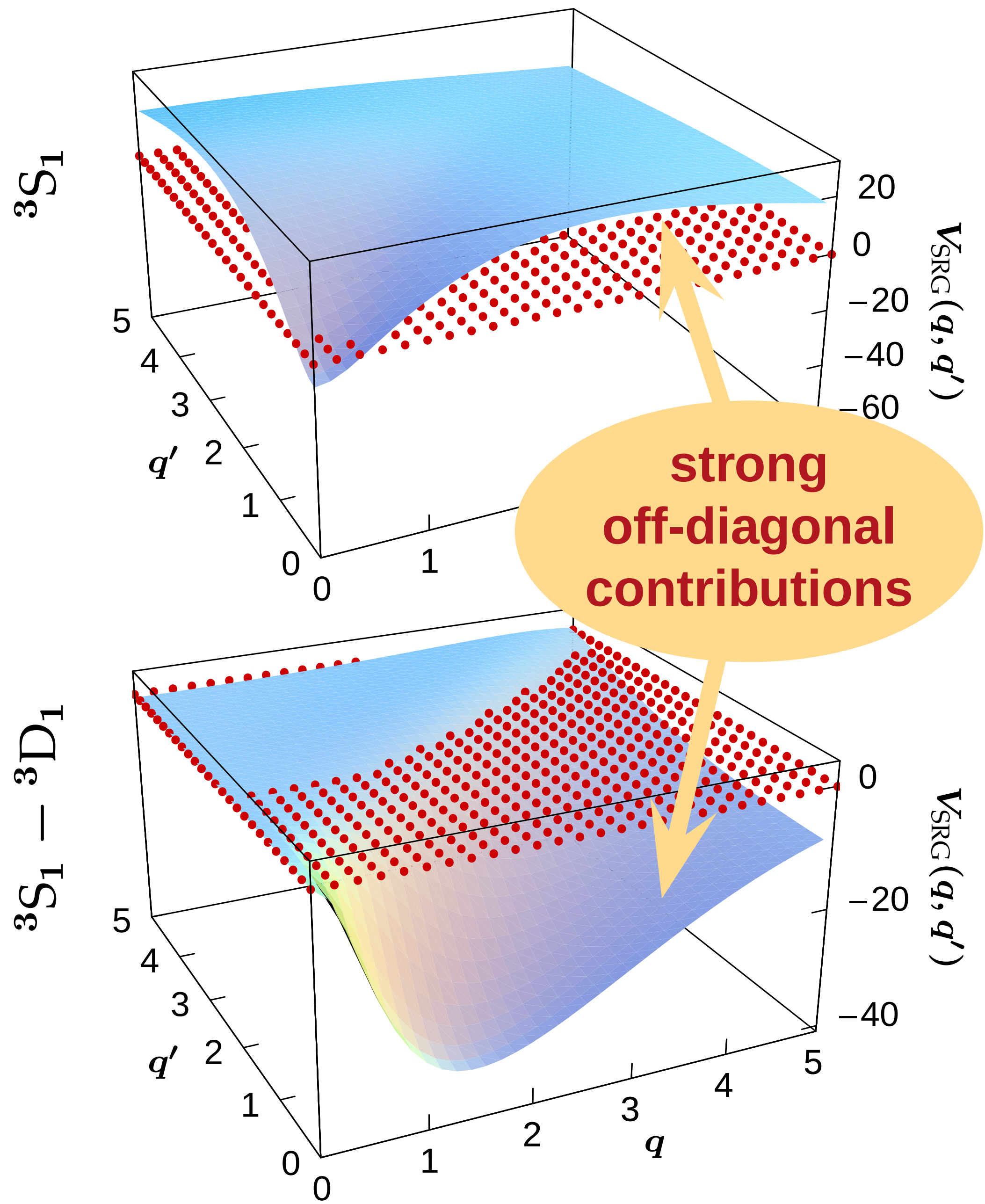
- dynamical generator defined as commutator with the operator in whose eigenbasis H shall be diagonalized

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

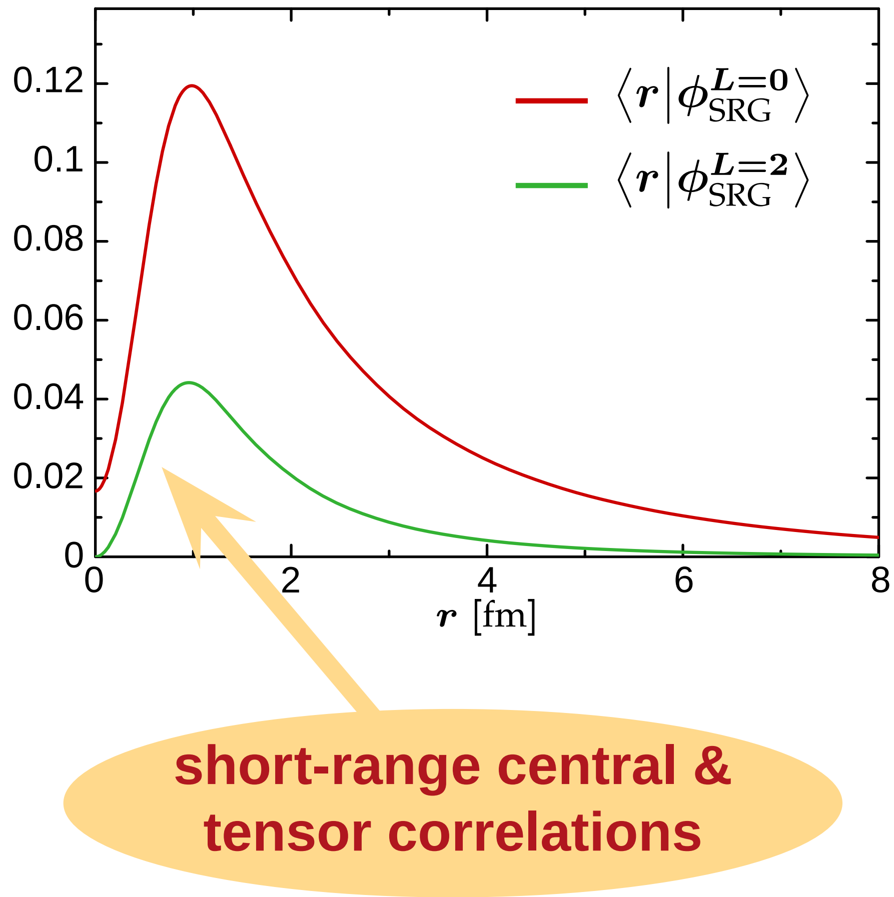
UCOM vs. SRG

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

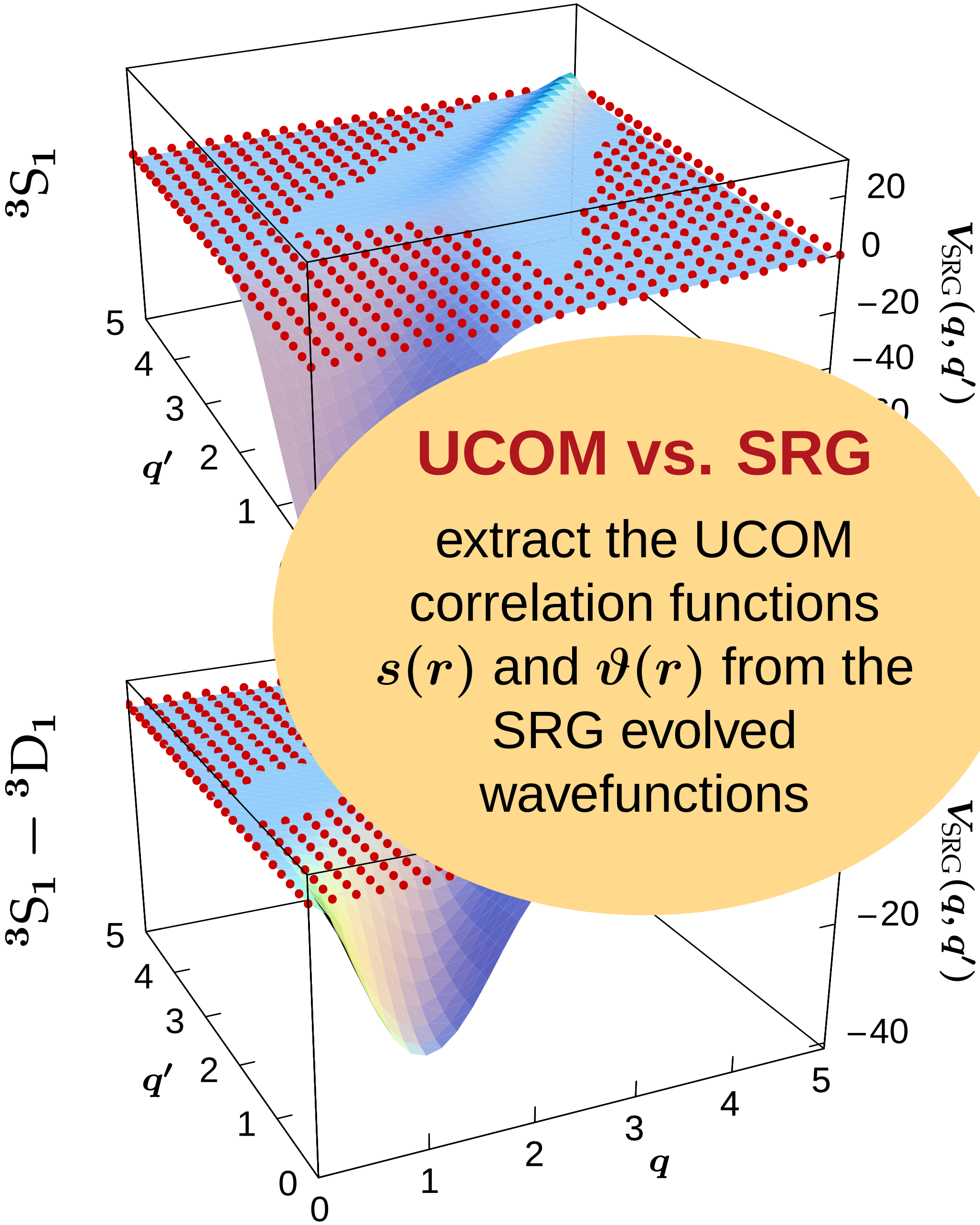
SRG Evolution: The Deuteron



Argonne V18



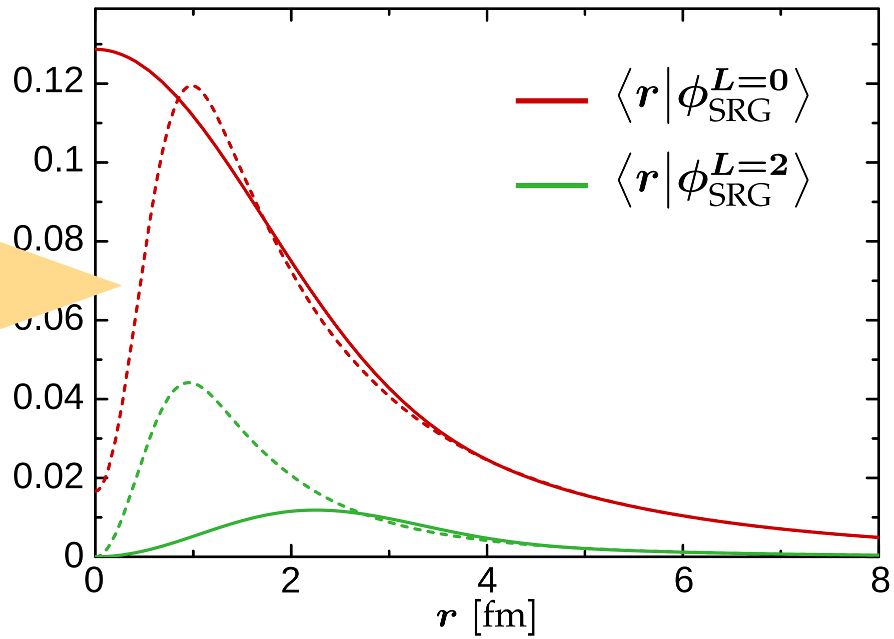
SRG Evolution: The Deuteron



UCOM vs. SRG

extract the UCOM correlation functions $s(r)$ and $\vartheta(r)$ from the SRG evolved wavefunctions

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



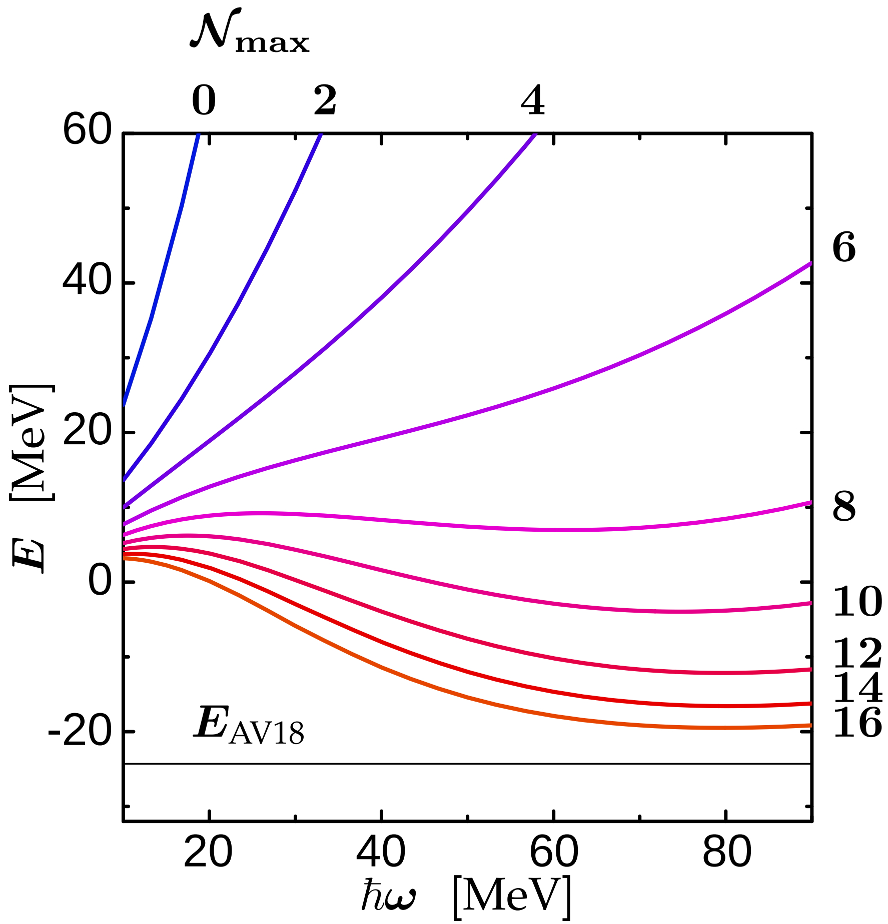
Exact Many-Body Methods

No-Core Shell Model

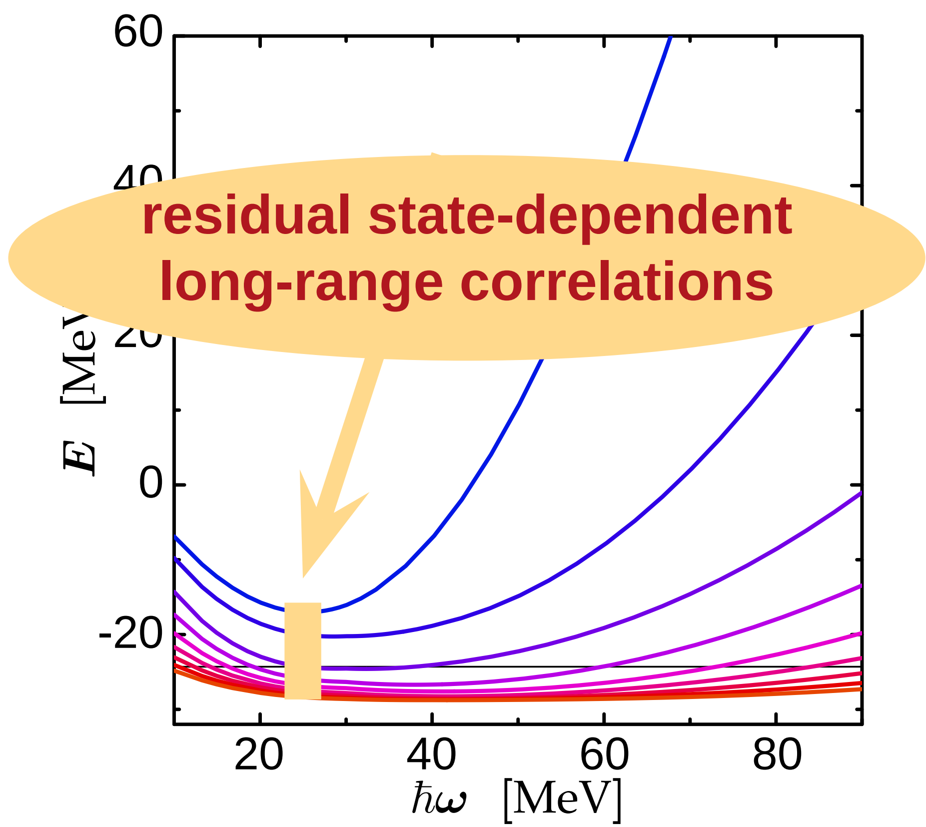
Roth et al. — Phys. Rev. C 72, 034002 (2005)
Roth & Navrátil — in preparation

^{4}He: Convergence

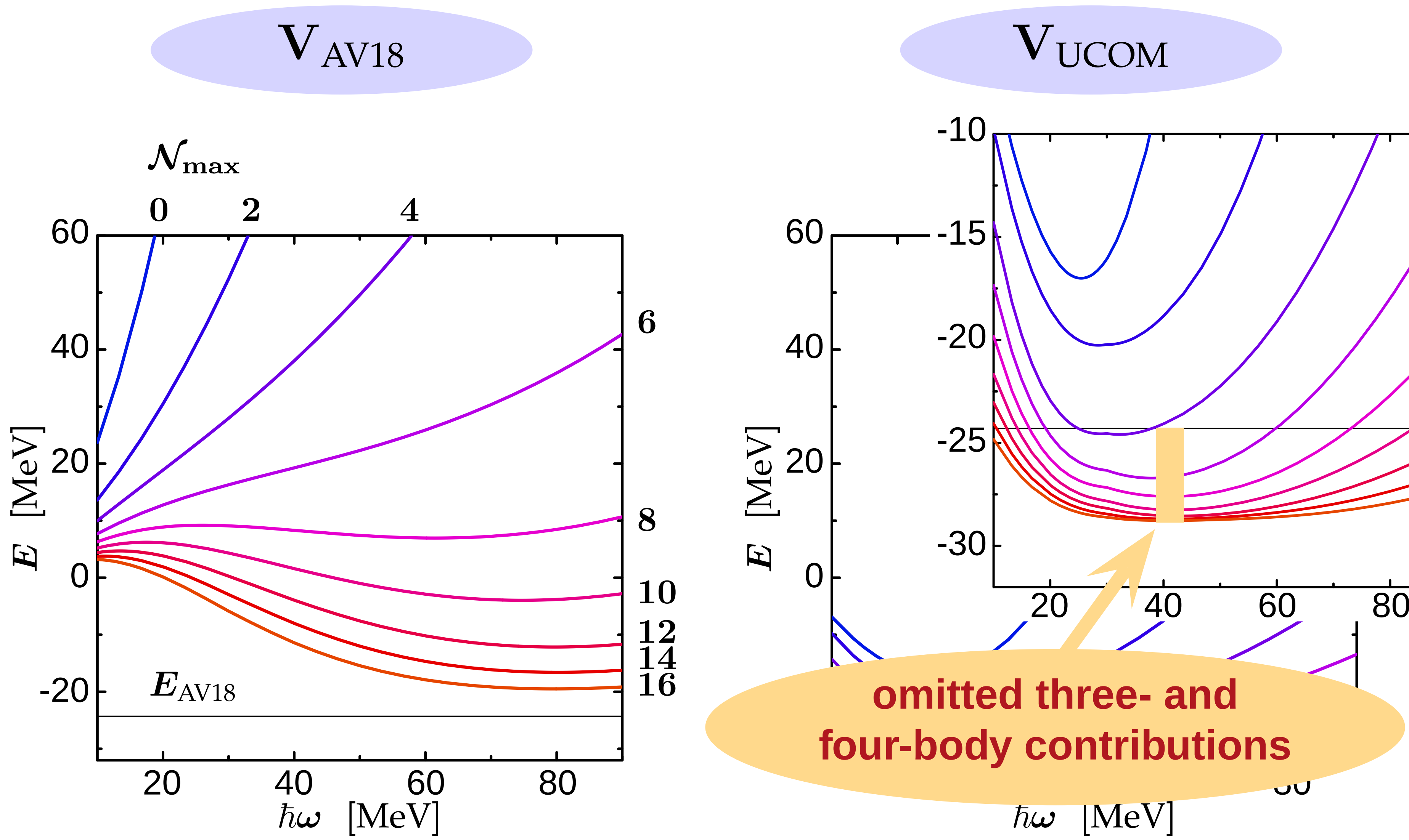
V_{AV18}



V_{UCOM}



^{4}He: Convergence



Three-Body Interactions — Strategies

Correlated Hamiltonian in Many-Body Space

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

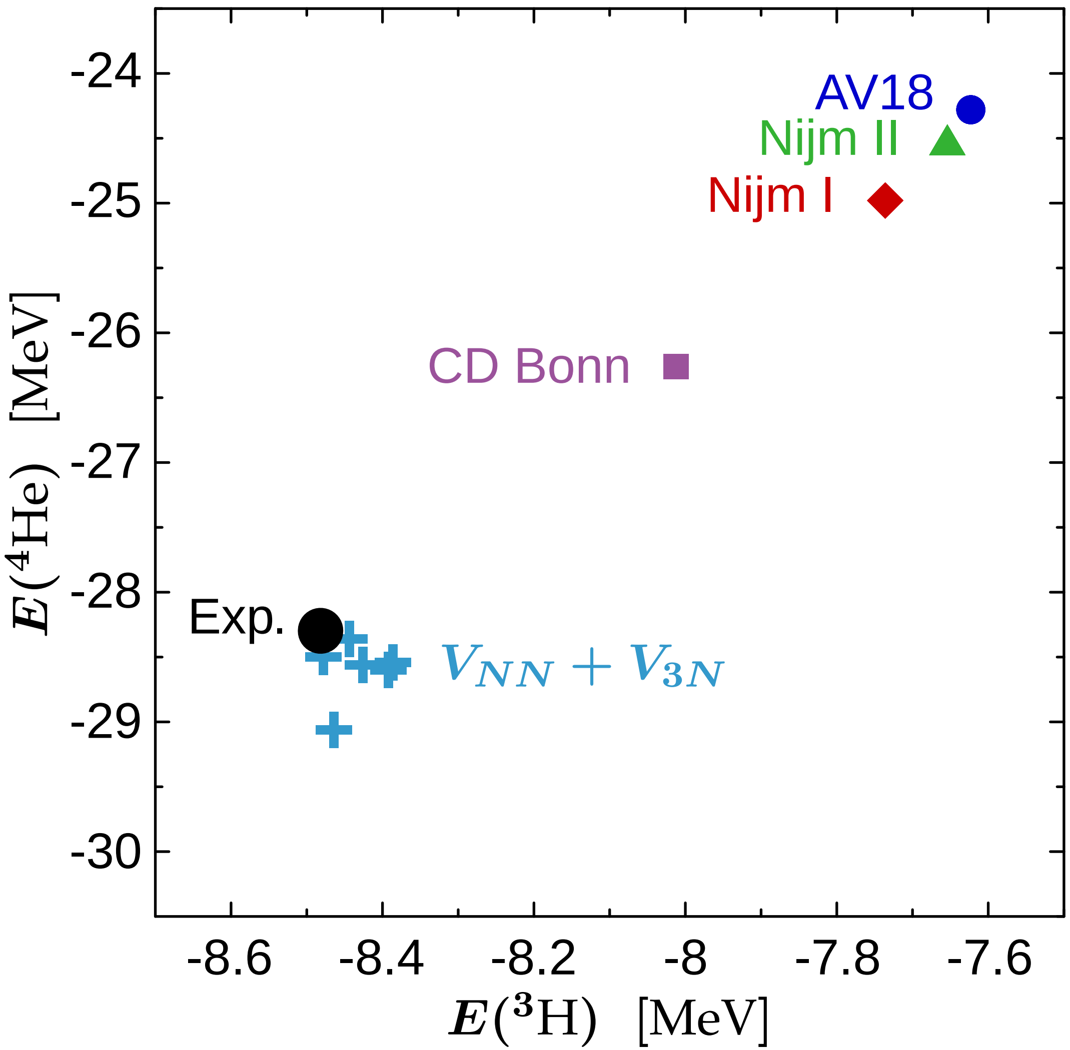
- strategies for treating the three-body contributions:

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

  ❷ **replace $\mathrm{V}^{[3]}_{\mathrm{UCOM}}$** by simplified 3N force (no consistent transformation)

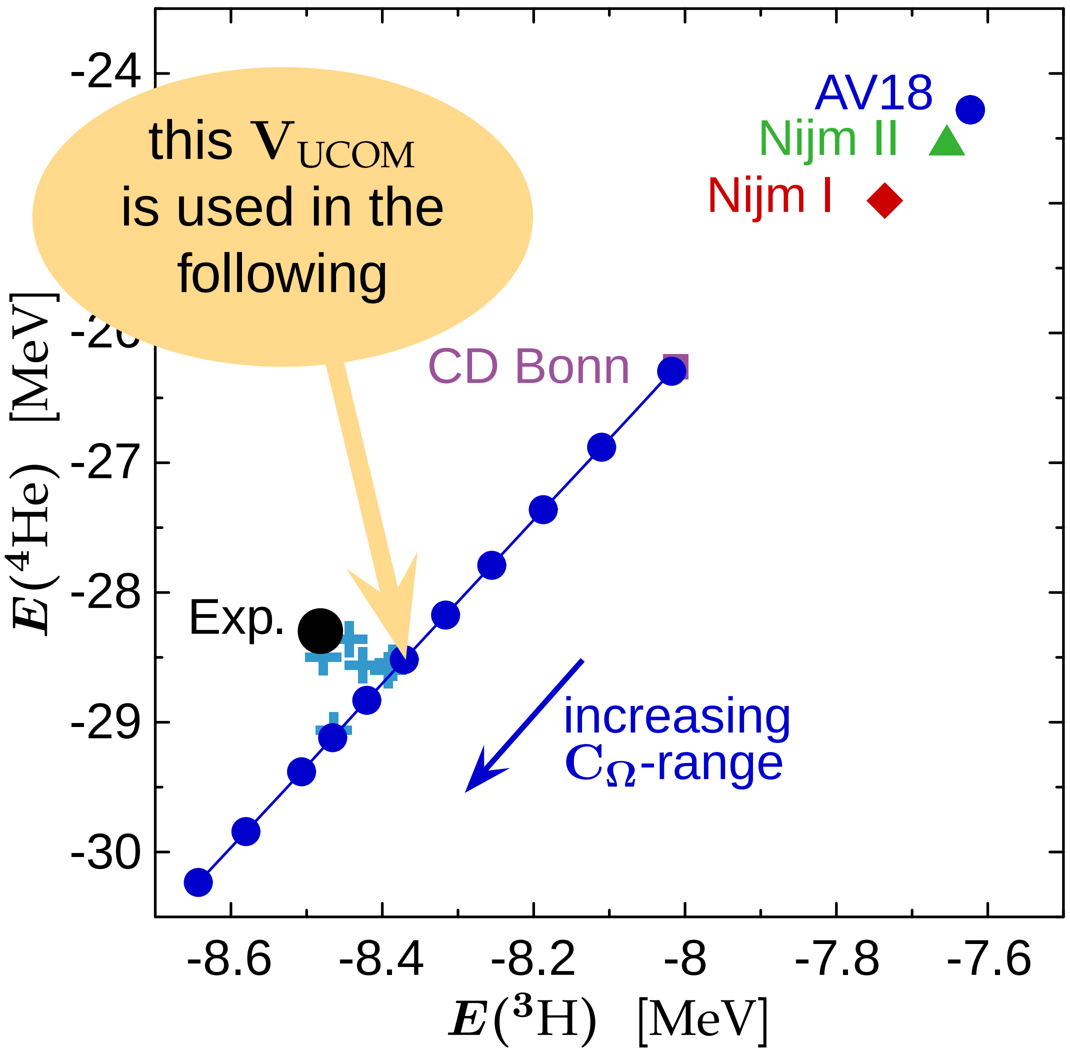
  ❸ **minimize $\mathrm{V}^{[3]}_{\mathrm{UCOM}}$** by proper choice of unitary transformation

Three-Body Interactions — Tjon Line



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

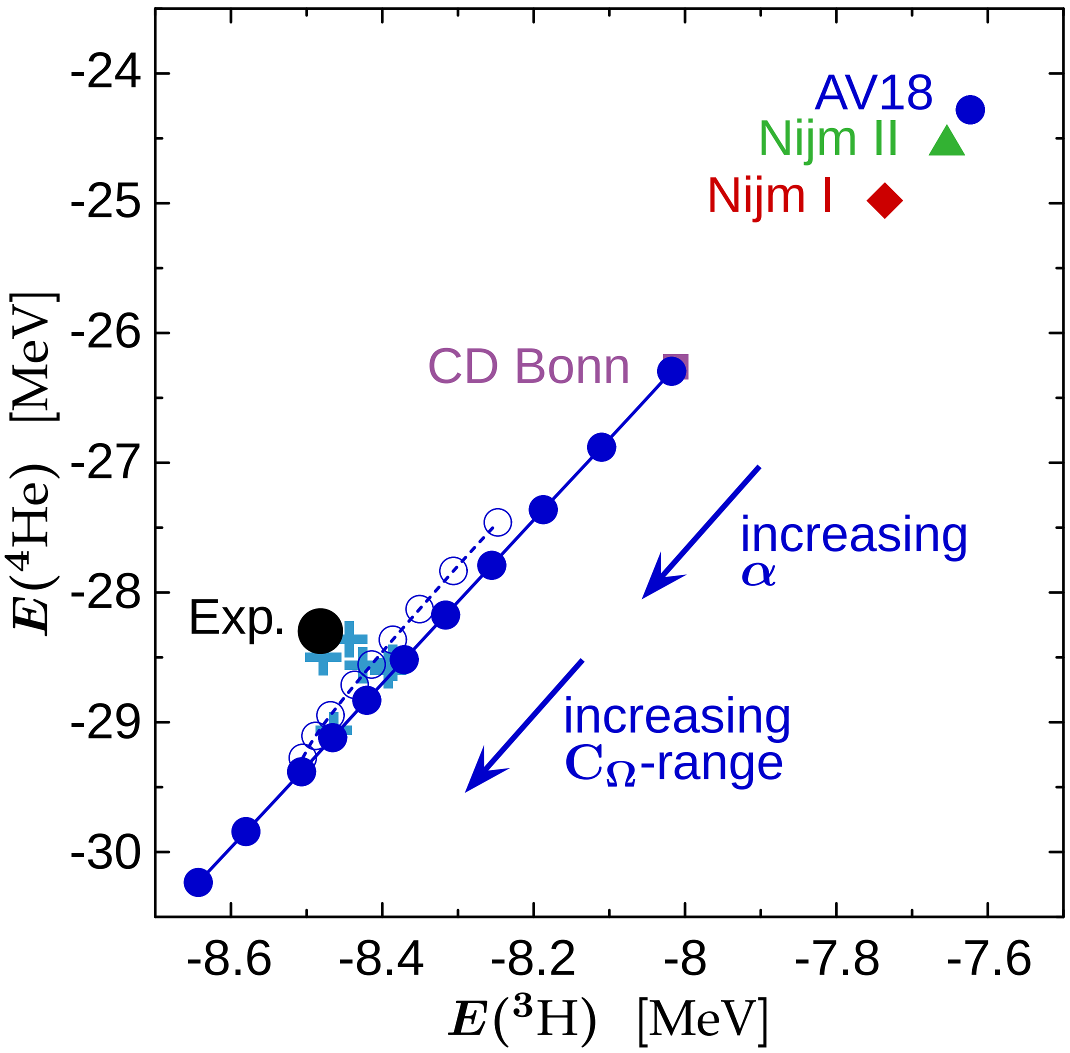
Three-Body Interactions — Tjon Line



- **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

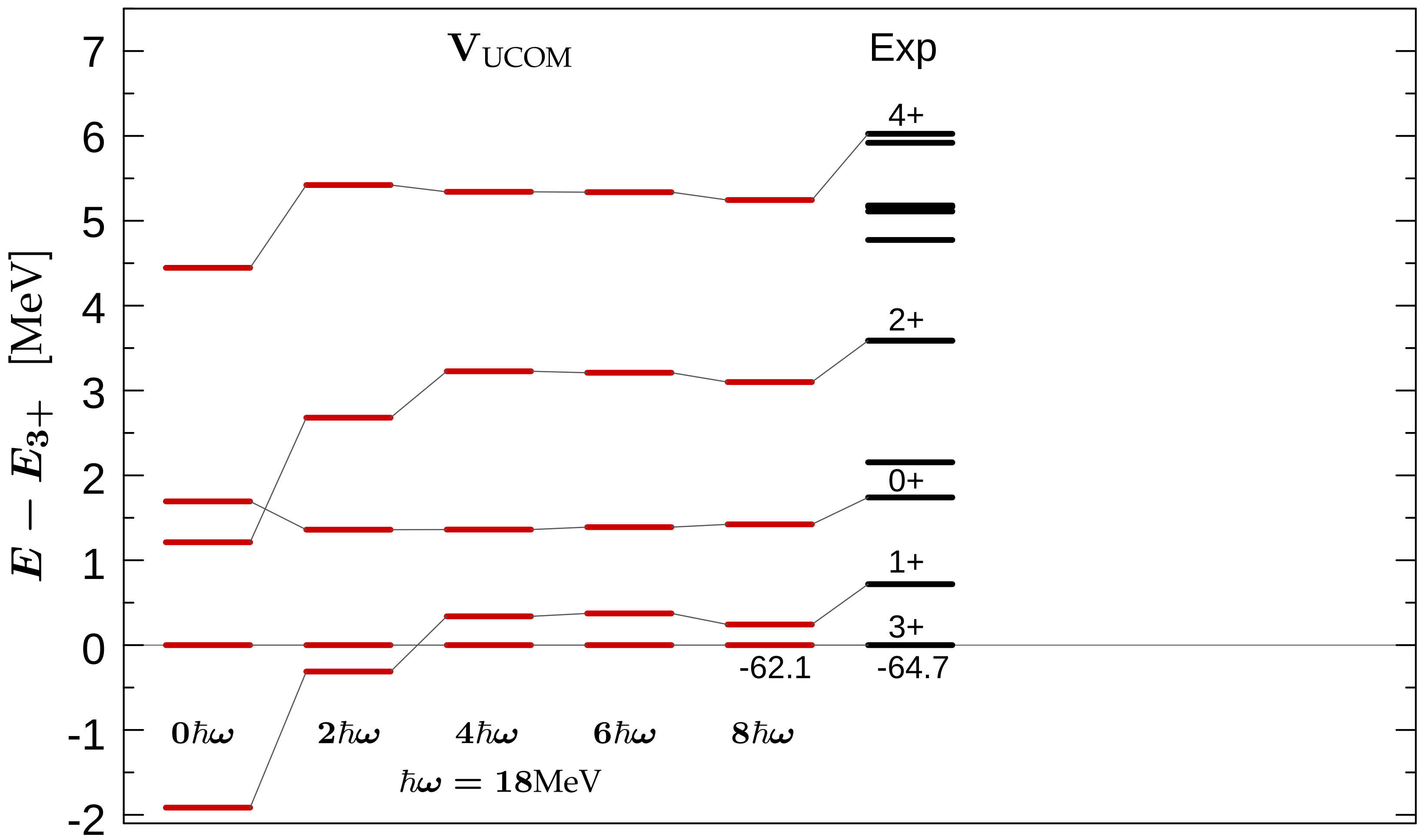
Three-Body Interactions — Tjon Line



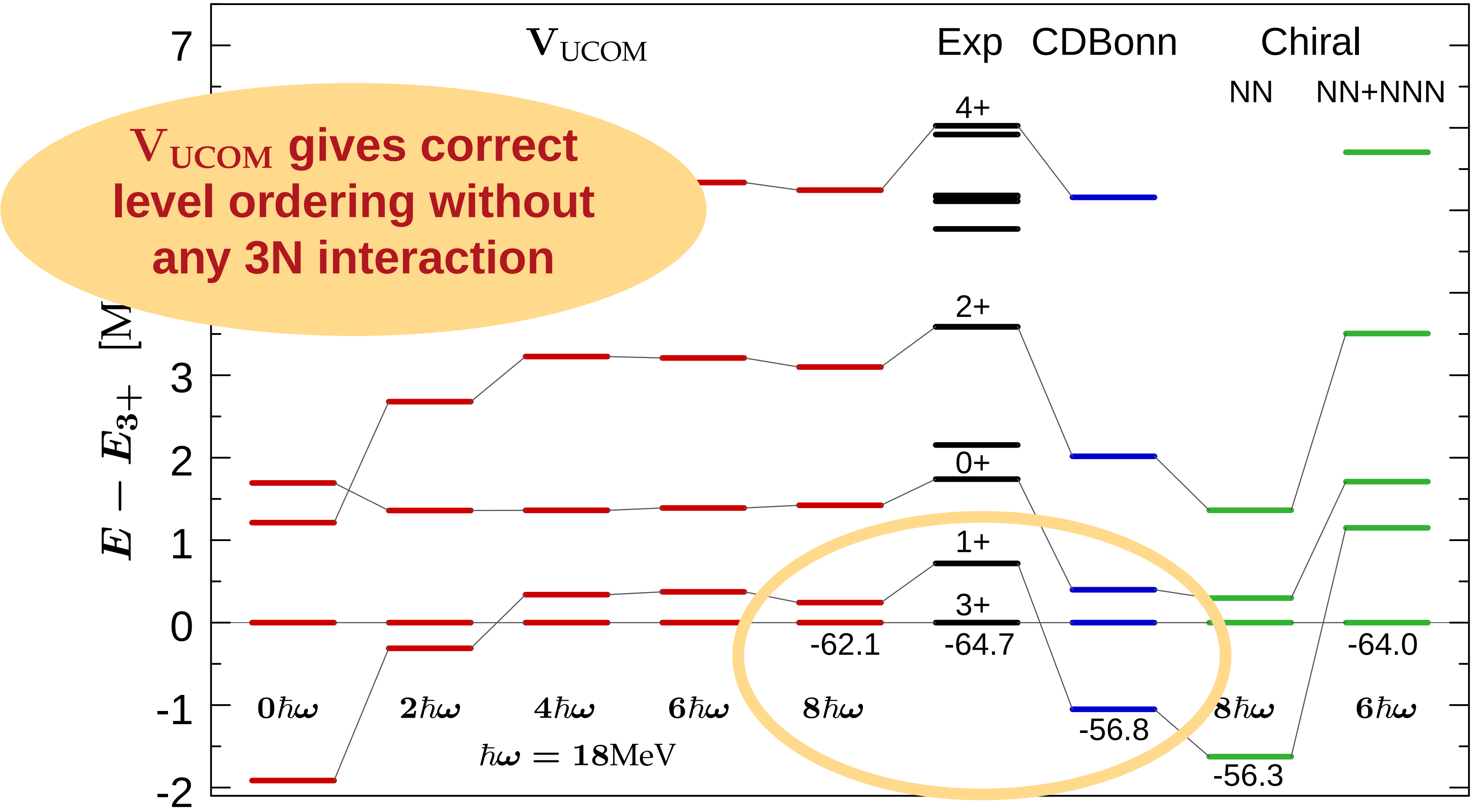
- **Tjon-line**: $E(^4\mathrm{He})$ vs. $E(^3\mathrm{H})$ for phase-shift equivalent NN-interactions
- same behavior for the SRG interaction as function of α

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

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



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



Exact Many-Body Methods

Importance Truncated No-Core Shell Model

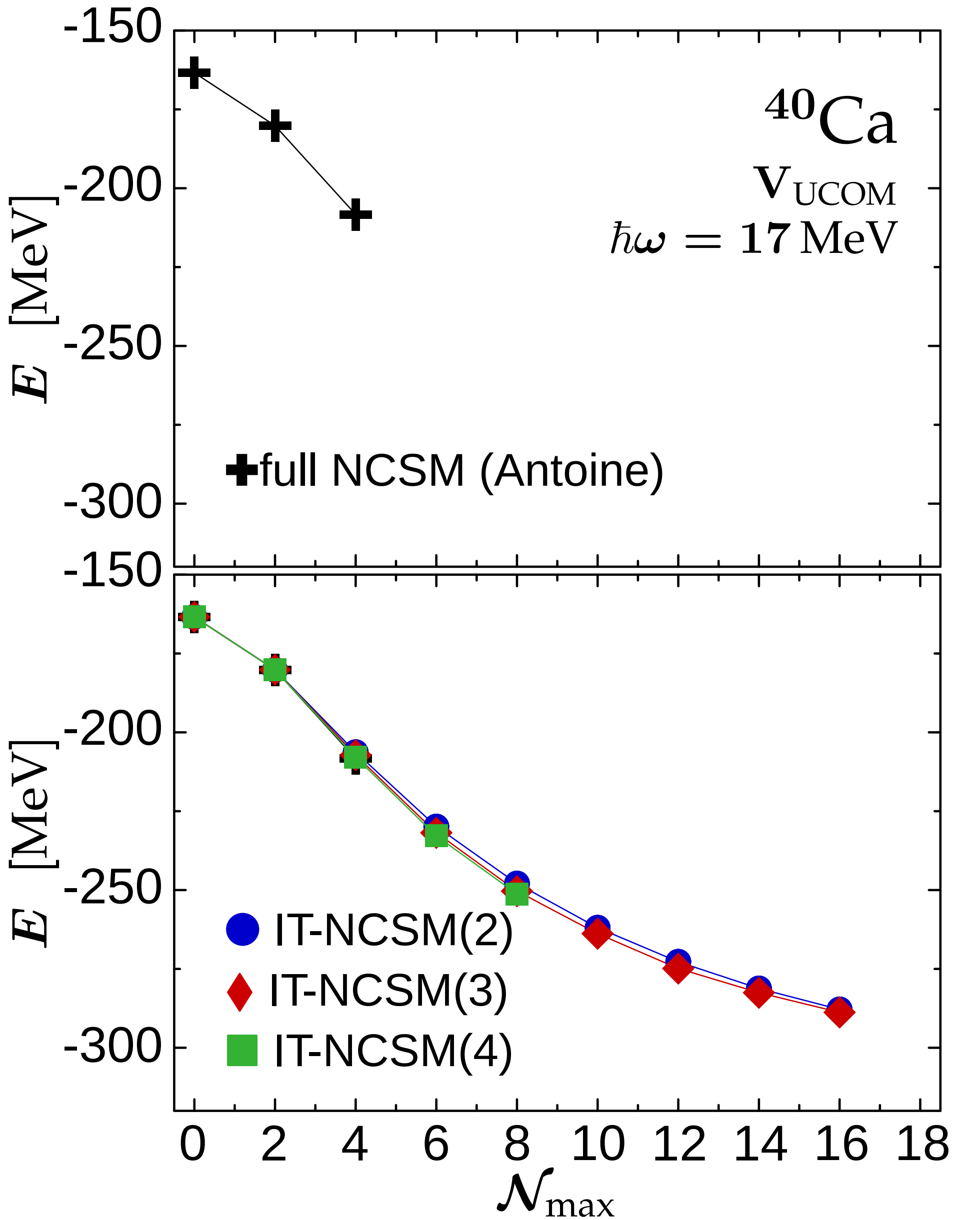
Roth & Navrátil — Phys. Rev. Lett. 99, 092501 (2007)
Roth — in preparation

Importance Truncated NCSM

- converged NCSM calculations essentially restricted to p-shell
- full $6\hbar\omega$ calculation for ^{40}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

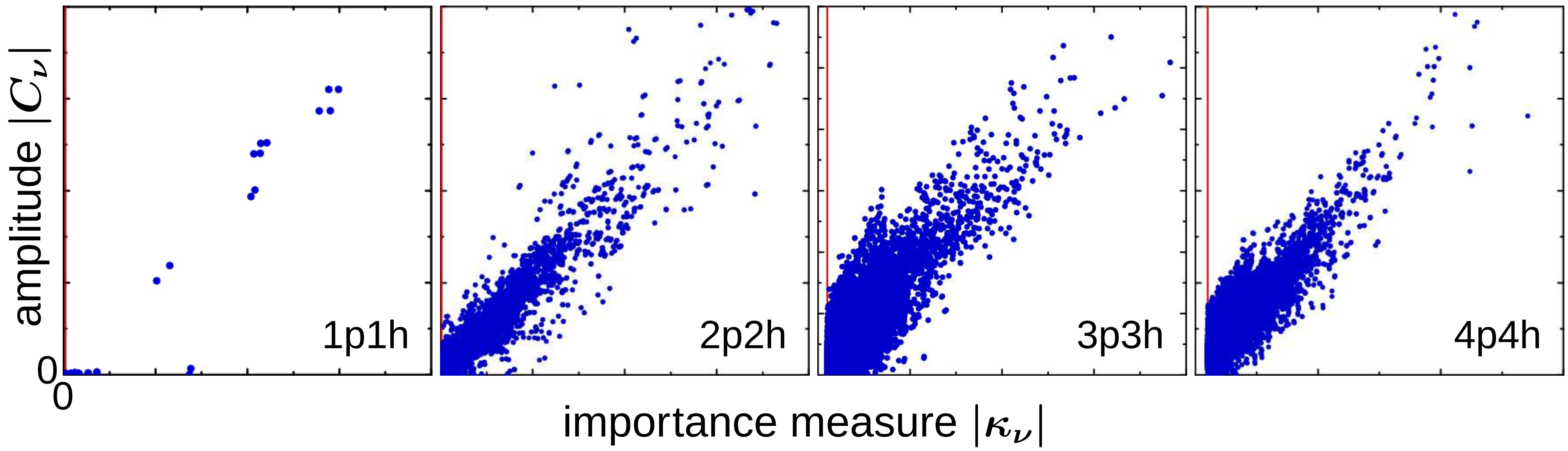


Importance Measure from MBPT

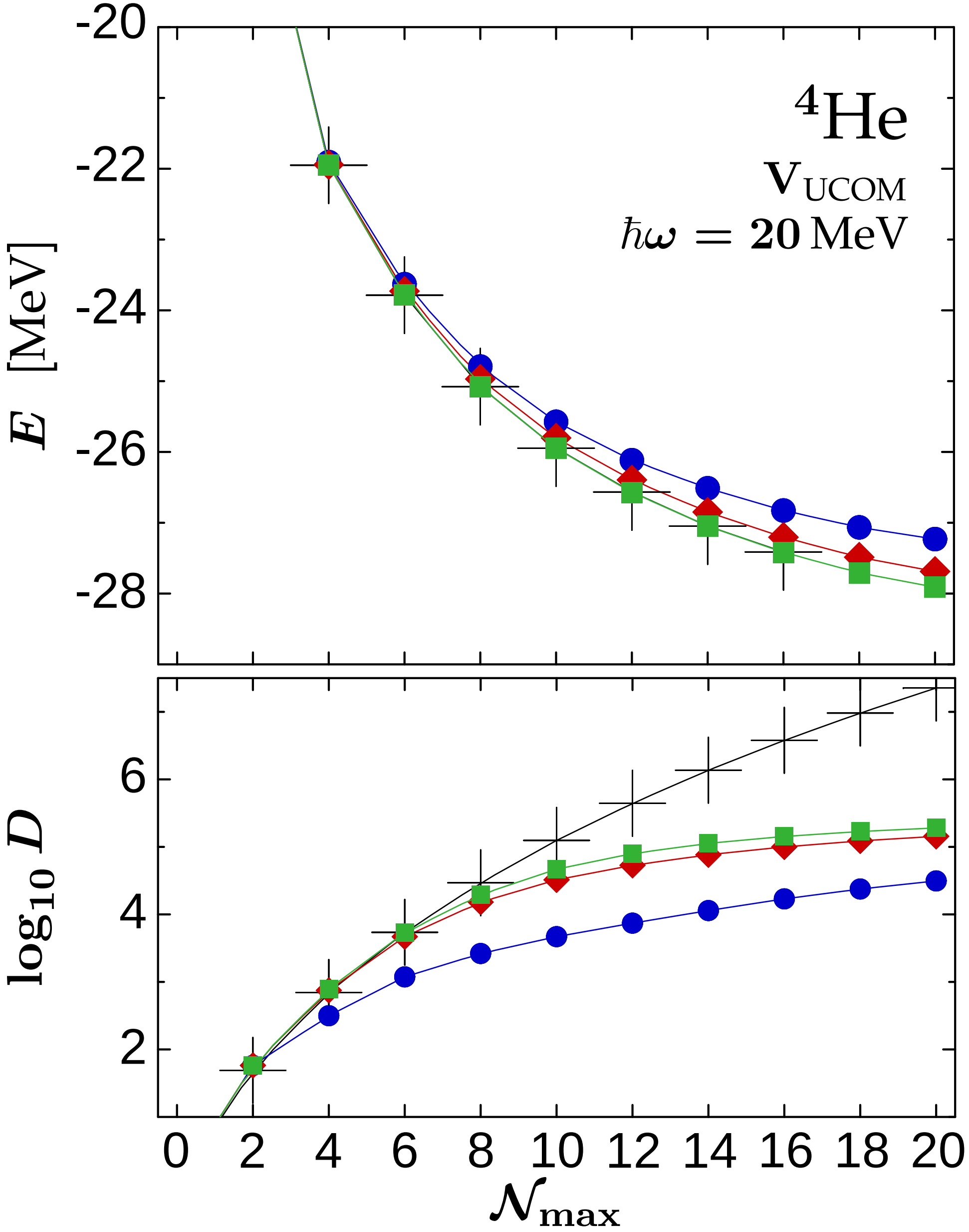
- **importance measure κ_ν**: a priori estimate for amplitude C_ν of shell-model configuration $|\Phi_\nu\rangle$ from multiconfigurational perturbation theory based on reference state $|\Psi_{\text{ref}}\rangle$:

$$\kappa_\nu = -\frac{\langle \Phi_\nu | \mathbf{H}' | \Psi_{\text{ref}} \rangle}{\epsilon_\nu - \epsilon_{\text{ref}}}$$

- iterative procedure for construction of **importance truncated model space** with reference states of increasing complexity



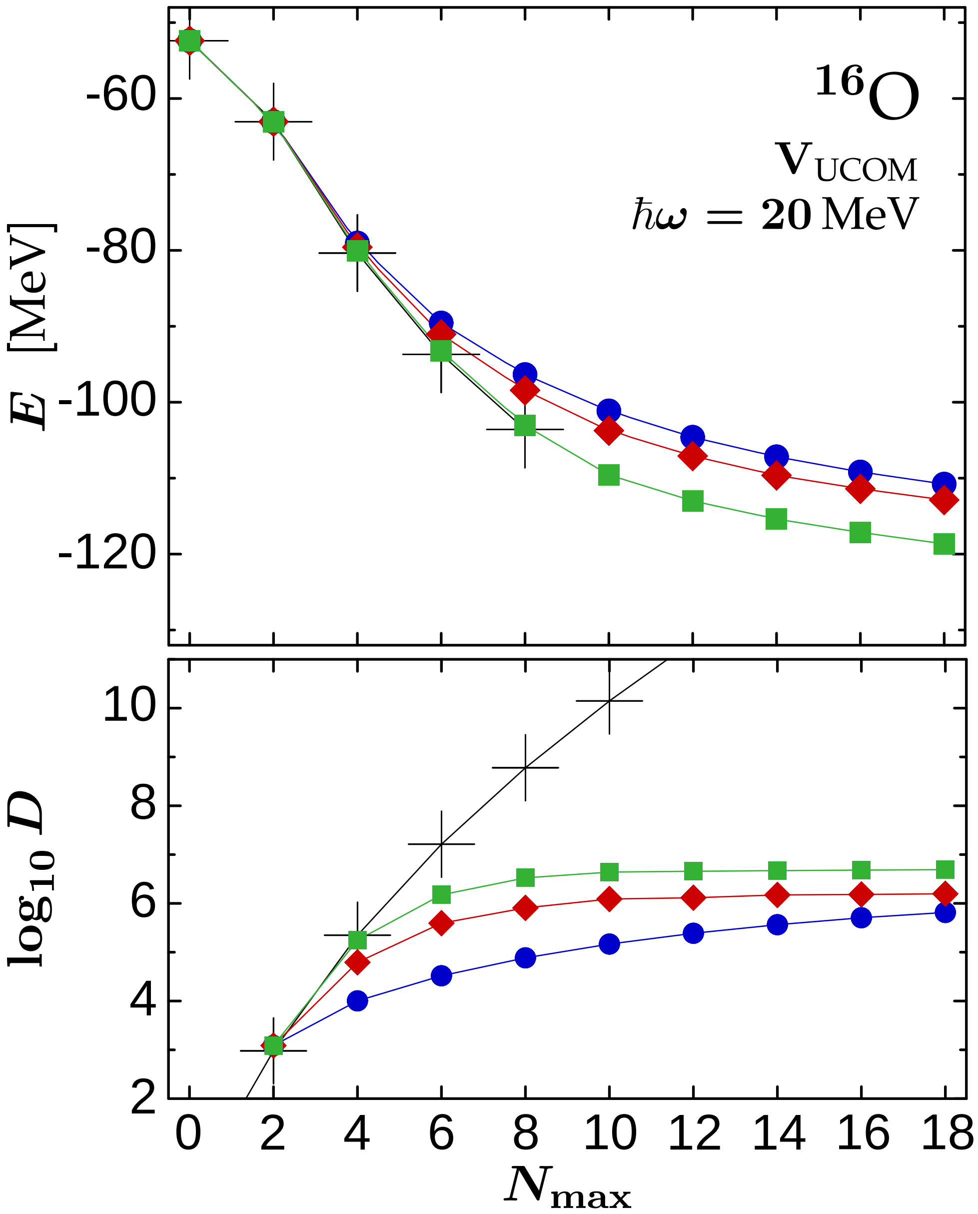
^{4}He: Importance Truncated NCSM



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

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

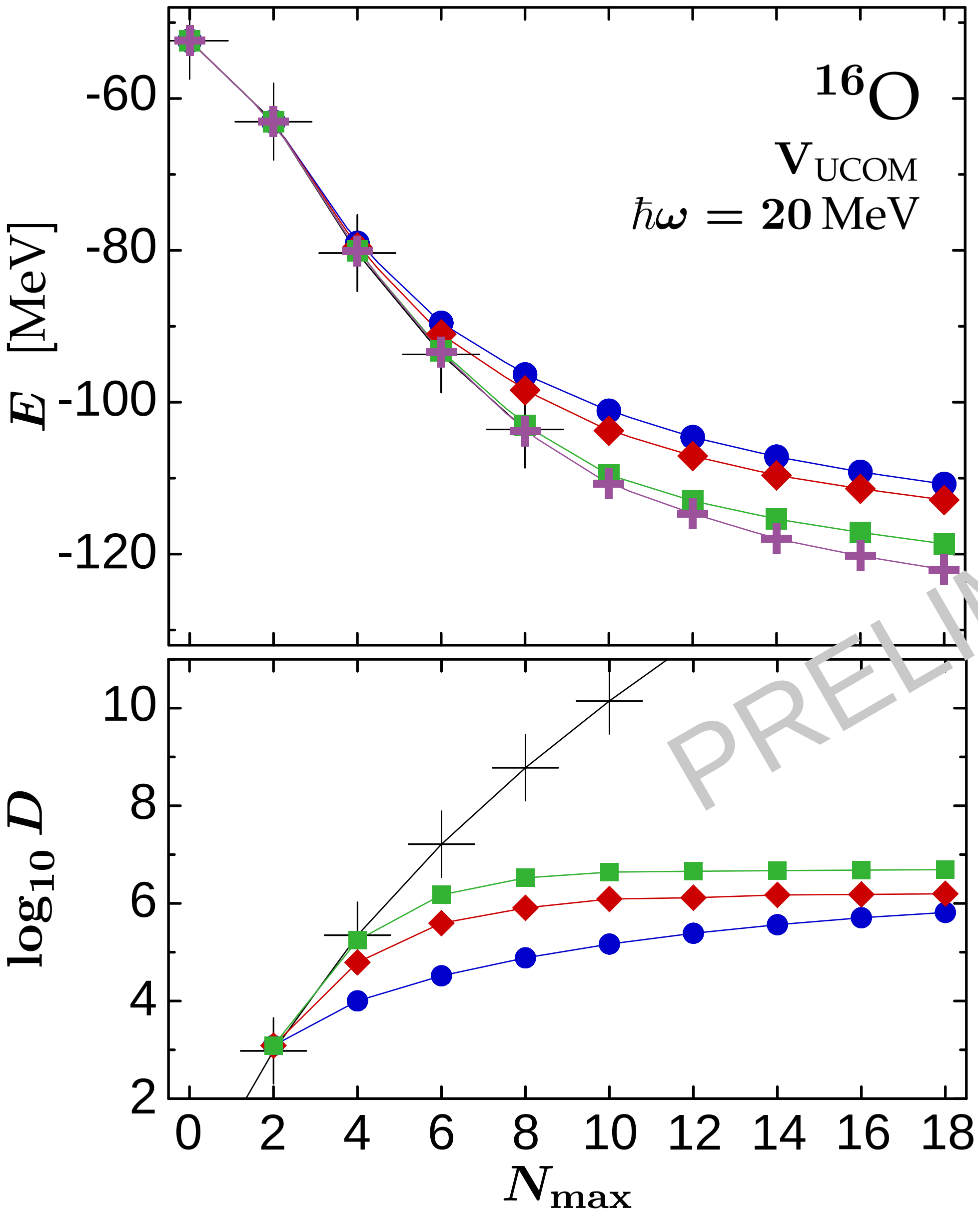
^{16}O: Importance Truncated NCSM



- **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(2)
♦ IT-NCSM(3)
■ IT-NCSM(4)

^{16}O: Importance Truncated NCSM



- beyond 4p4h contributions and size-extensivity via **multi-reference Davidson correction**

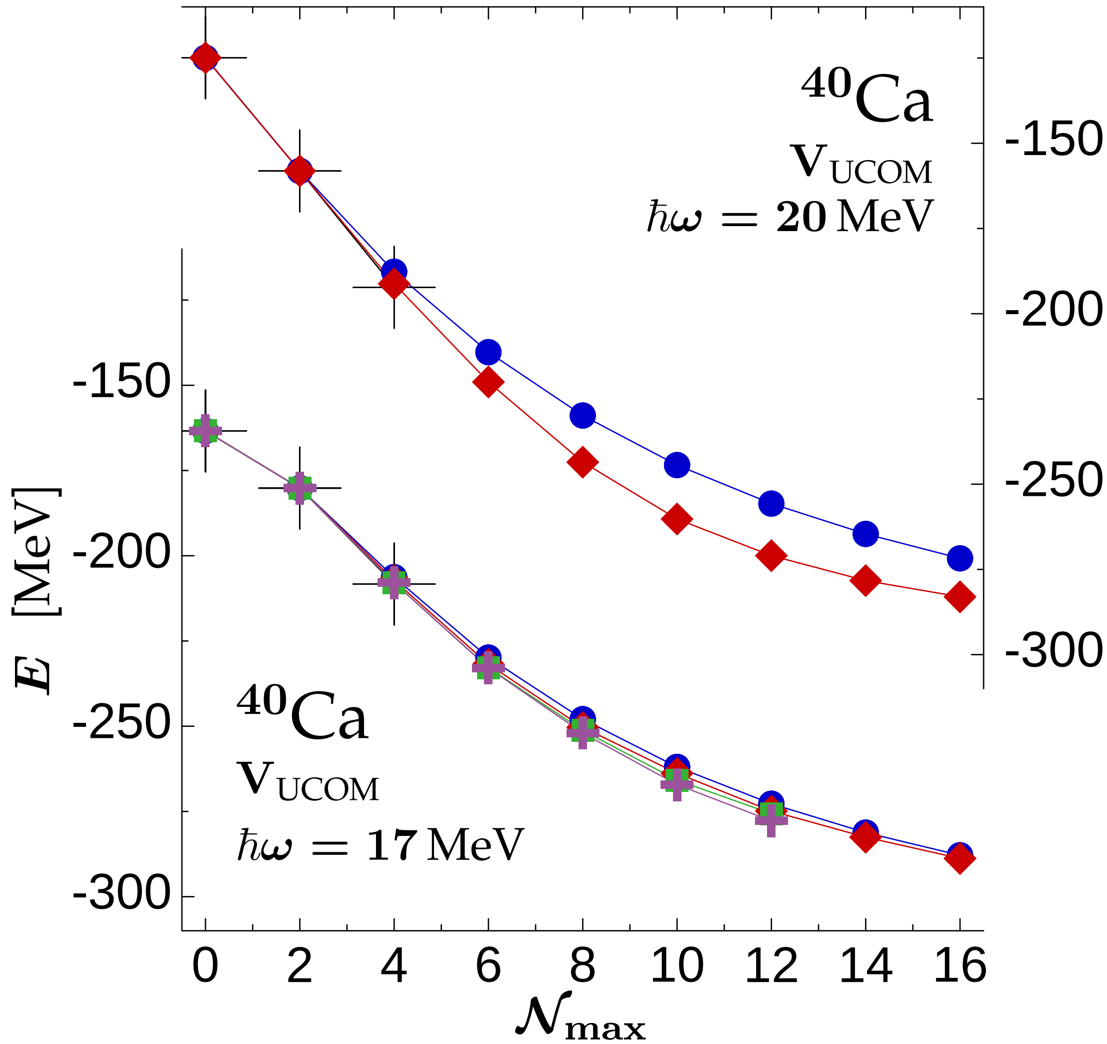
- extrapolation to $N_{max} \to \infty$

$$E_{\text{IT-NCSM(4)D}} = -127.9 \pm 2\,\text{MeV}$$

$$E_{\text{exp}} = -127.6\,\text{MeV}$$

the two-body interaction V_{UCOM} does predict **correct binding energies** for heavier nuclei

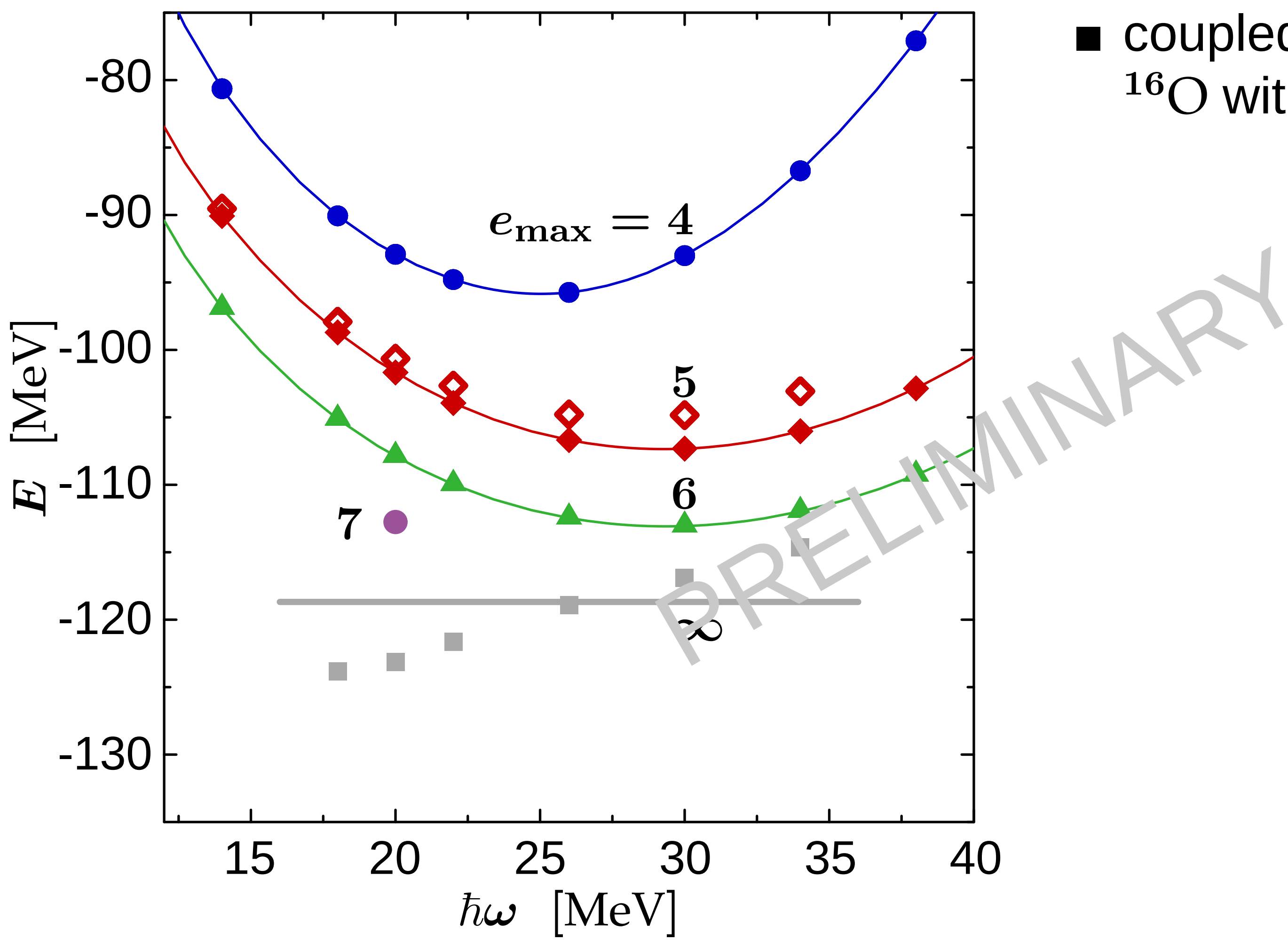
^{40}Ca: Importance Truncated NCSM



- **$16\hbar\omega$ and more are feasible** for ^{40}Ca in IT-NCSM(4)D
- size of individual npnh-contributions depends on oscillator frequency
- result consistent with experimental binding energy

^{16}O: Coupled Cluster Method

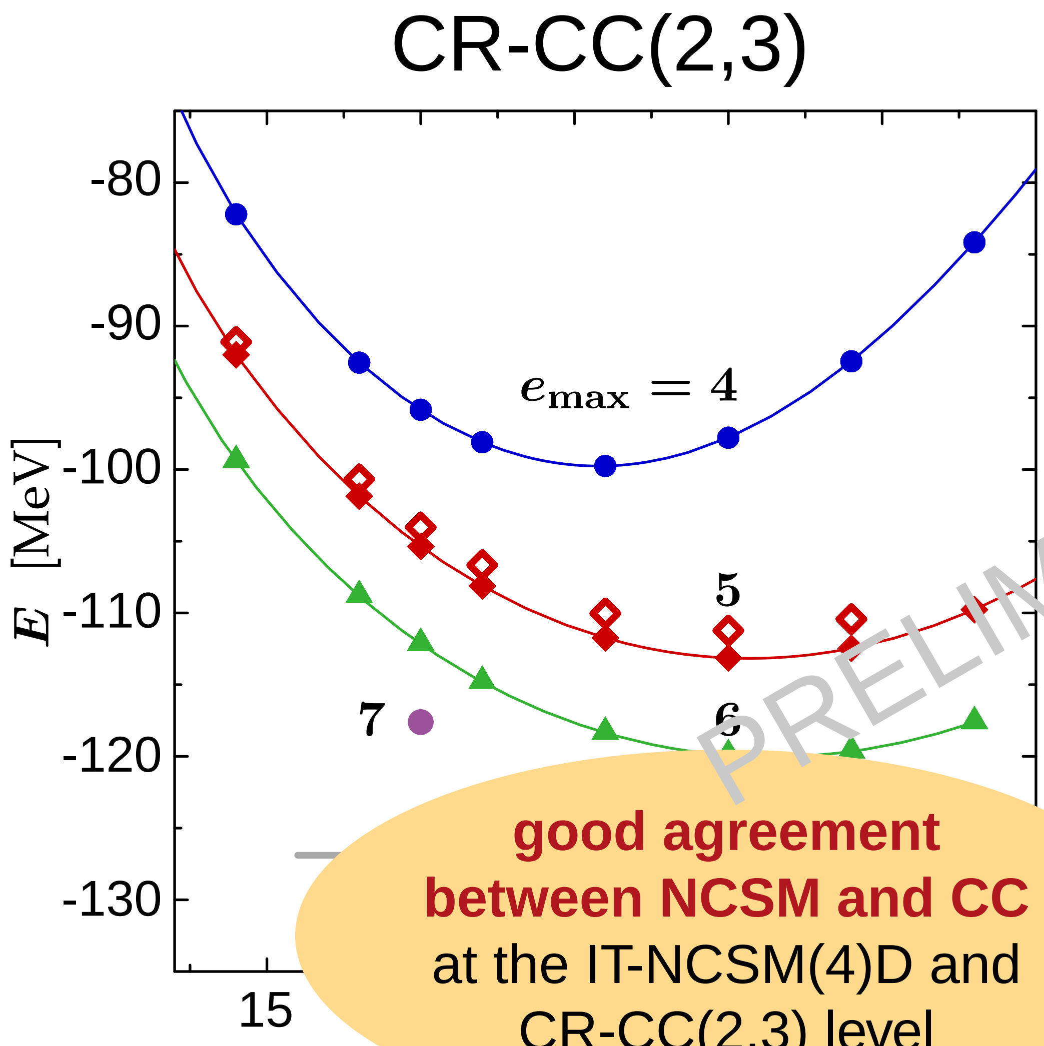
CCSD



calculations by J. Gour & P. Piecuch

- coupled-cluster calculation for ^{16}O with V_{UCOM}

^{16}O: Coupled Cluster Method



good agreement between NCSM and CC at the IT-NCSM(4)D and CR-CC(2,3) level

calculations by J. Gour & P. Piecuch

- coupled-cluster calculation for ^{16}O with V_{UCOM}
- including non-perturbative triples correction (completely renormalized CC)
- extrapolated ground-state energies

$$E_{\text{CR-CC(2,3)}} = -126.9 \pm 5\,\text{MeV}$$
$$E_{\text{IT-NCSM(4)D}} = -127.9 \pm 2\,\text{MeV}$$
$$E_{\text{exp}} = -127.6\,\text{MeV}$$

Perspectives

- **Modern Effective Interactions**
  - treatment of short-range central and tensor correlations by unitary transformations: UCOM, SRG, Lee-Suzuki,...
  - phase-shift equivalent correlated interaction $\mathbf{V}_{\mathrm{UCOM}}$ which is soft and requires minimal three-body forces
  - universal input for...
- **Innovative Many-Body Methods**
  - No-Core Shell Model,...
  - Importance Truncated NCSM, Coupled Cluster Method,...
  - Hartree-Fock plus MBPT, Padé Resummed MBPT, BHF, HFB, RPA,...
  - Fermionic Molecular Dynamics,...

Epilogue

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