Towards

Ab Initio Nuclear Structure beyond the p-Shell

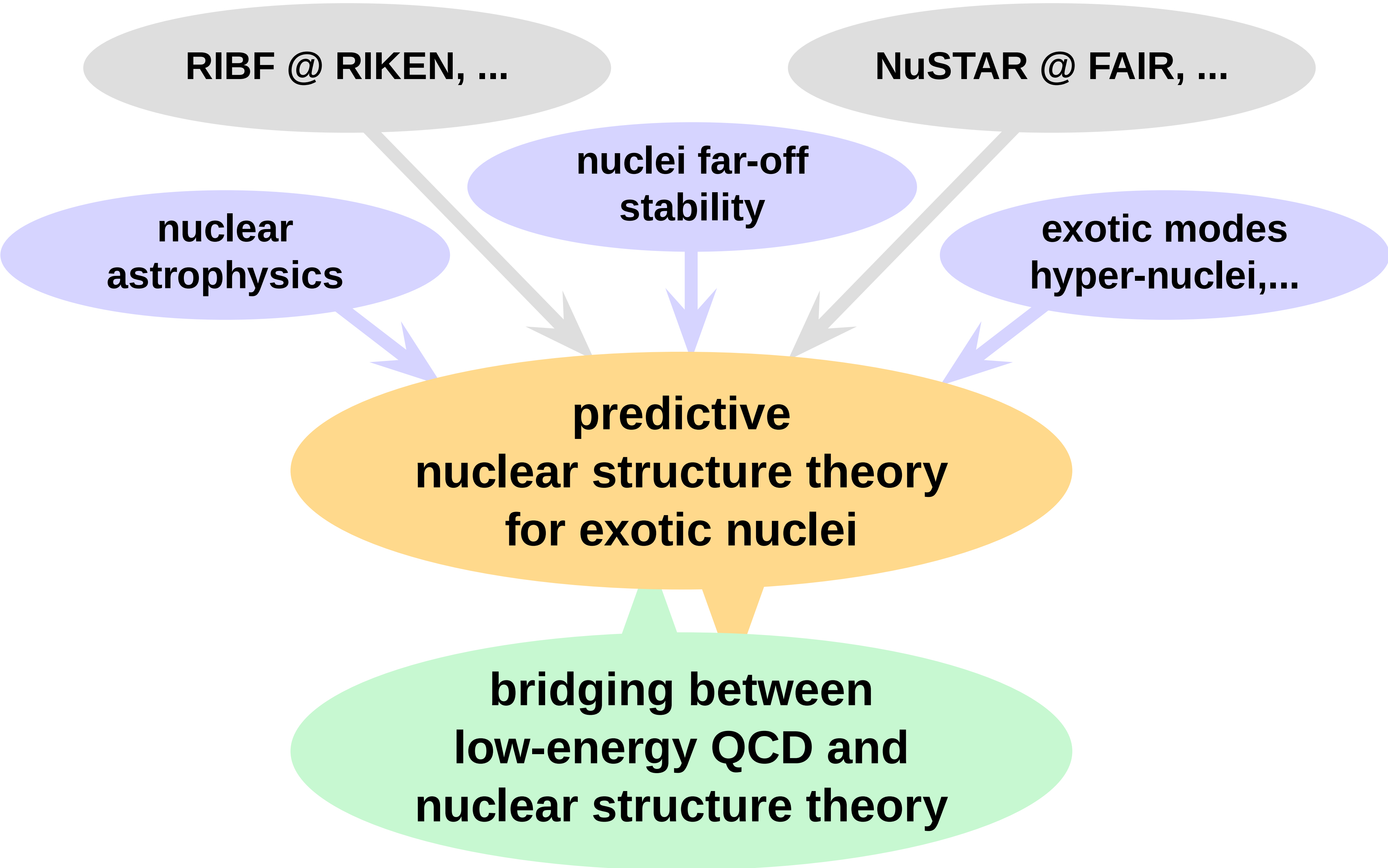
Robert Roth

Institut für Kernphysik
Technische Universität Darmstadt

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 in the 21^{st} Century



From QCD to Nuclear Structure

Nuclear Structure

Low-Energy QCD

From QCD to Nuclear Structure

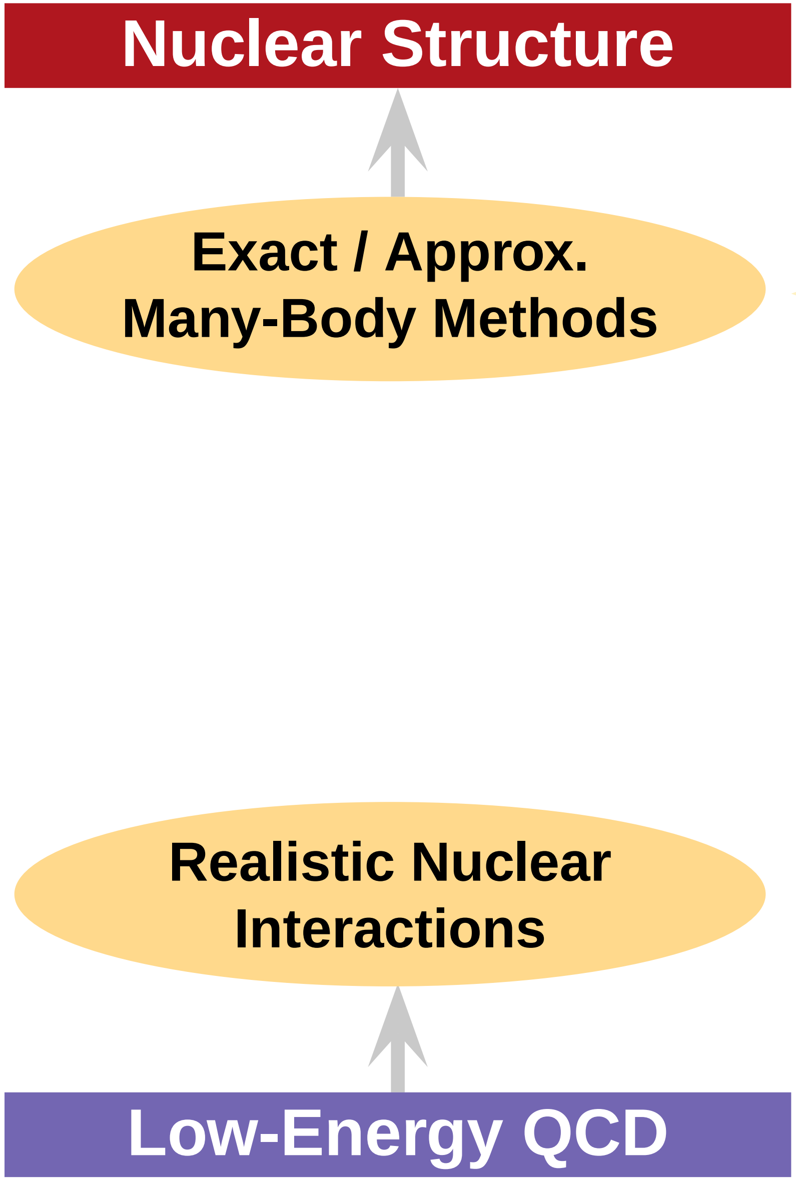
Nuclear Structure

Realistic Nuclear Interactions

Low-Energy QCD

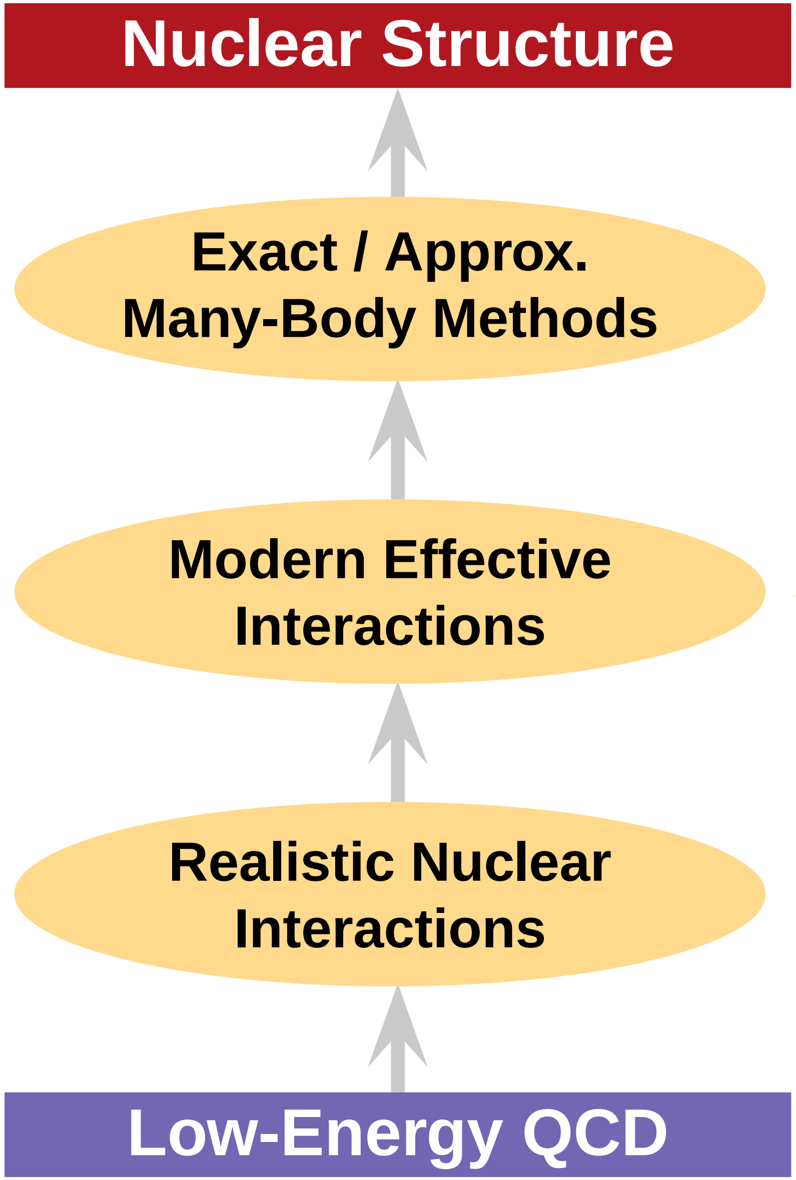
- chiral interactions: consistent NN & 3N interaction derived within χEFT
- traditional NN-interactions: Argonne V18, CD Bonn,...
- reproduce experimental NN phase-shifts with high precision
- induce strong short-range central & tensor correlations

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
- need 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

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

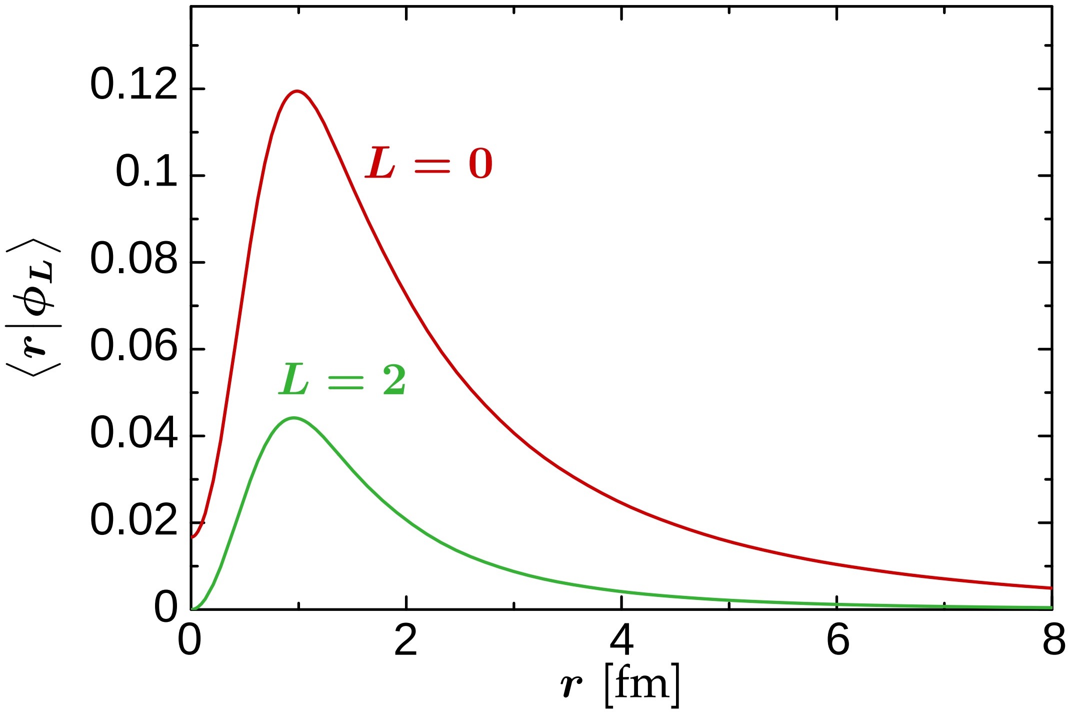
Correlated Operators

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

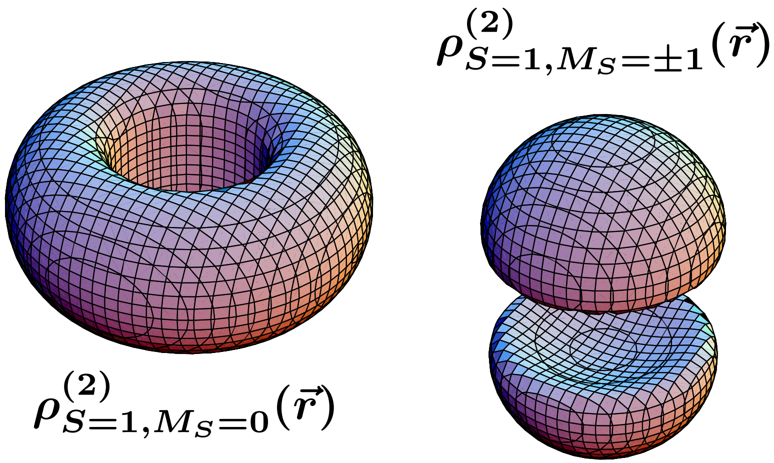
$$\widetilde{\mathrm{O}} = \mathrm{C}^{\dagger}\;\mathrm{O}\;\mathrm{C}$$

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

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

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

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

Tensor Correlator C_Ω

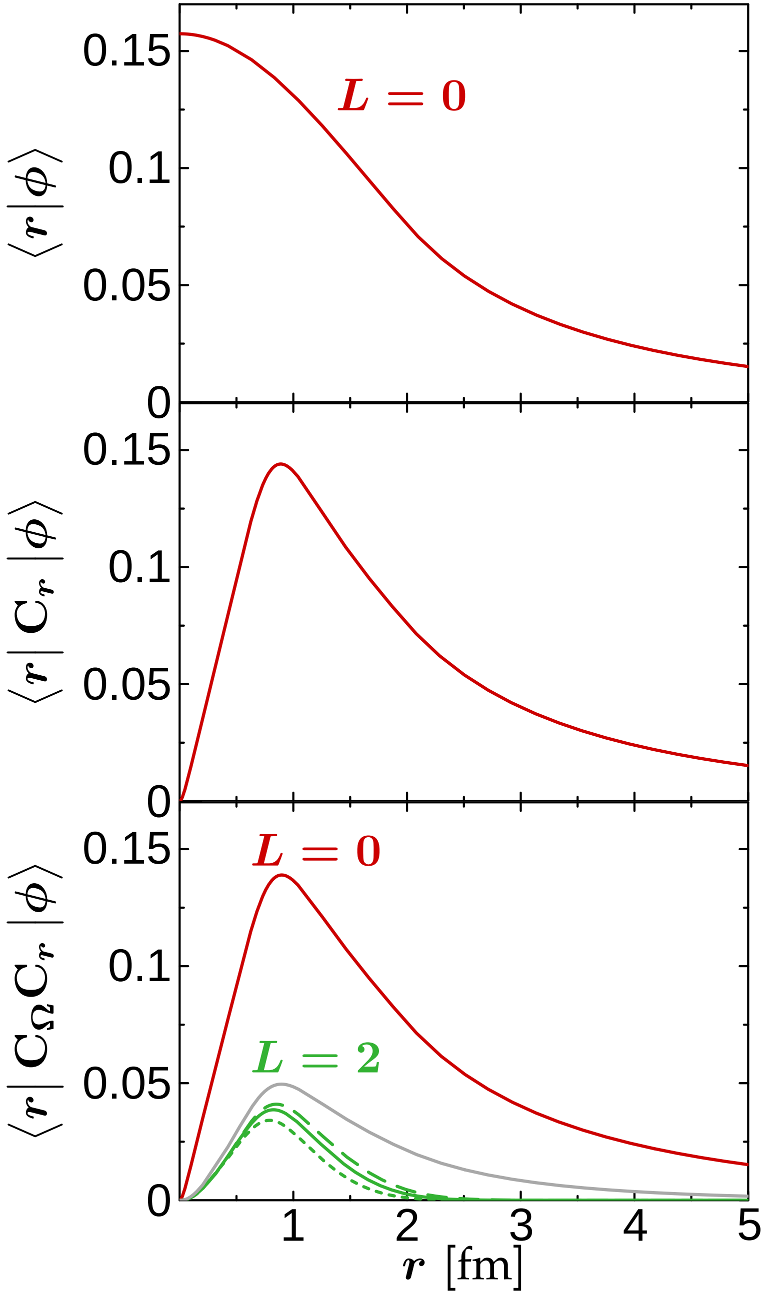
- angular shift depending on the orientation of spin and relative coordinate of a nucleon pair

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

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

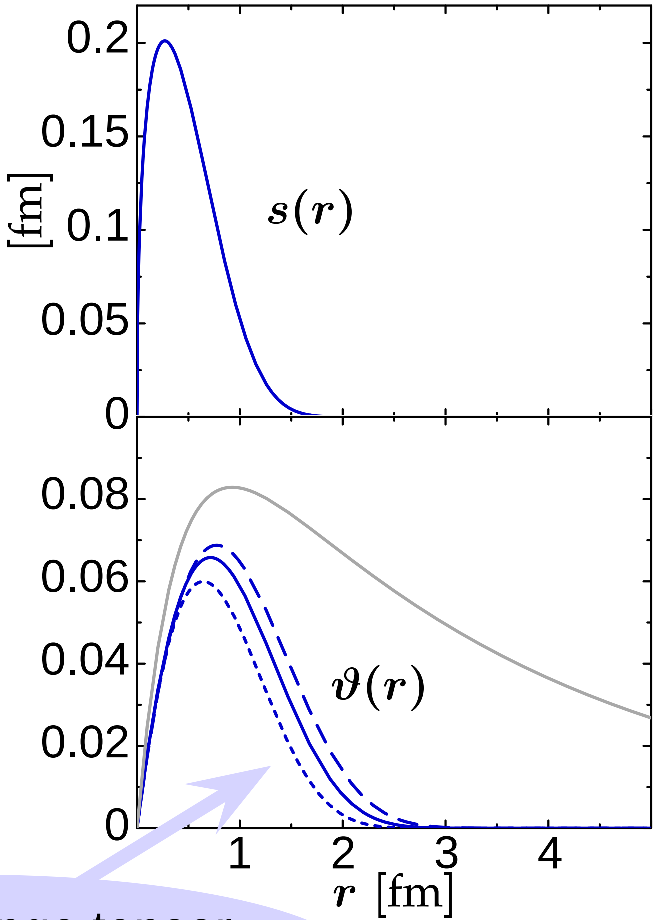
- $s(r)$ and $\vartheta(r)$ for given potential determined by energy minimization in the two-body system (for each S, T)

Correlated States: The Deuteron



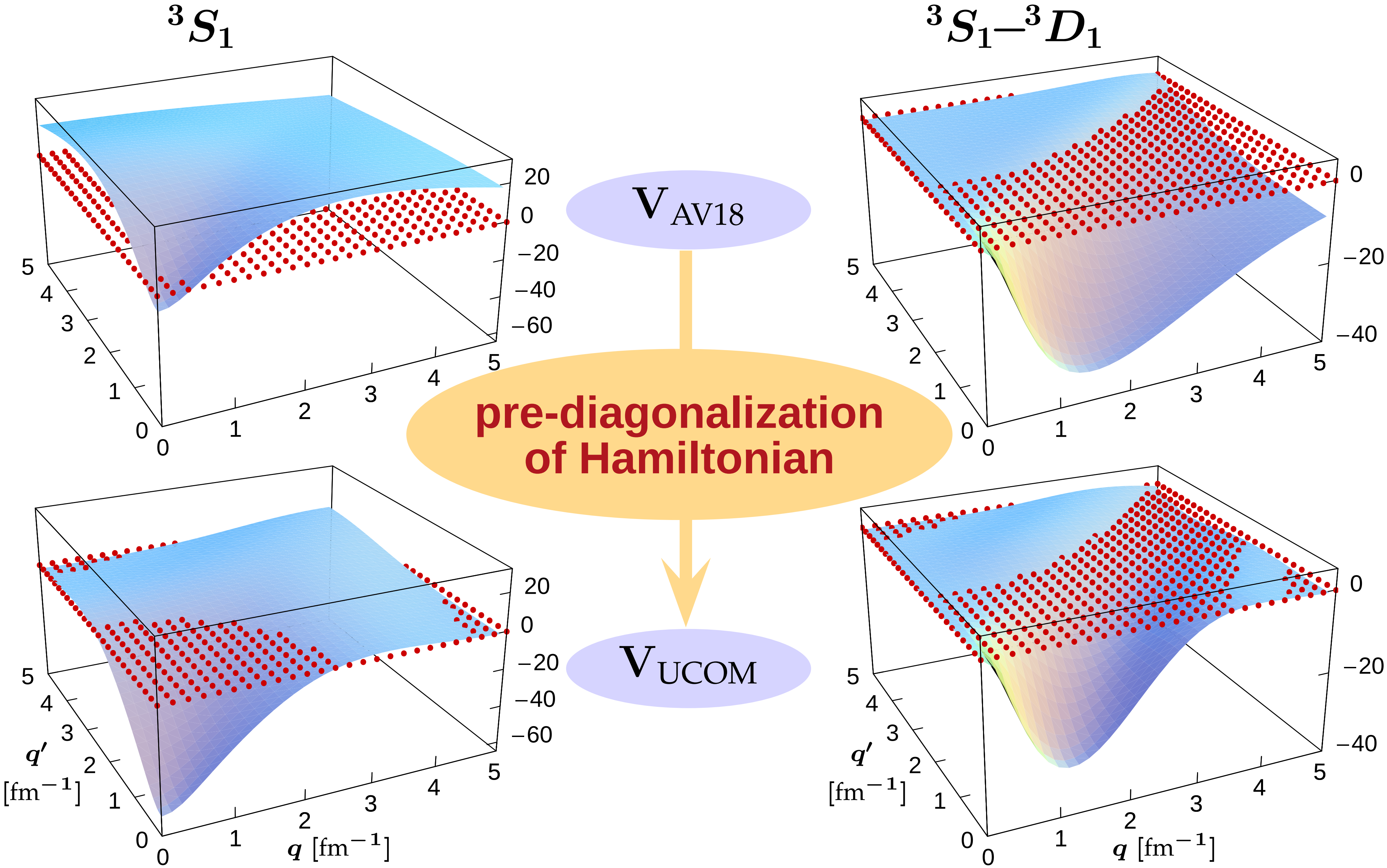
central correlations

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. — 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

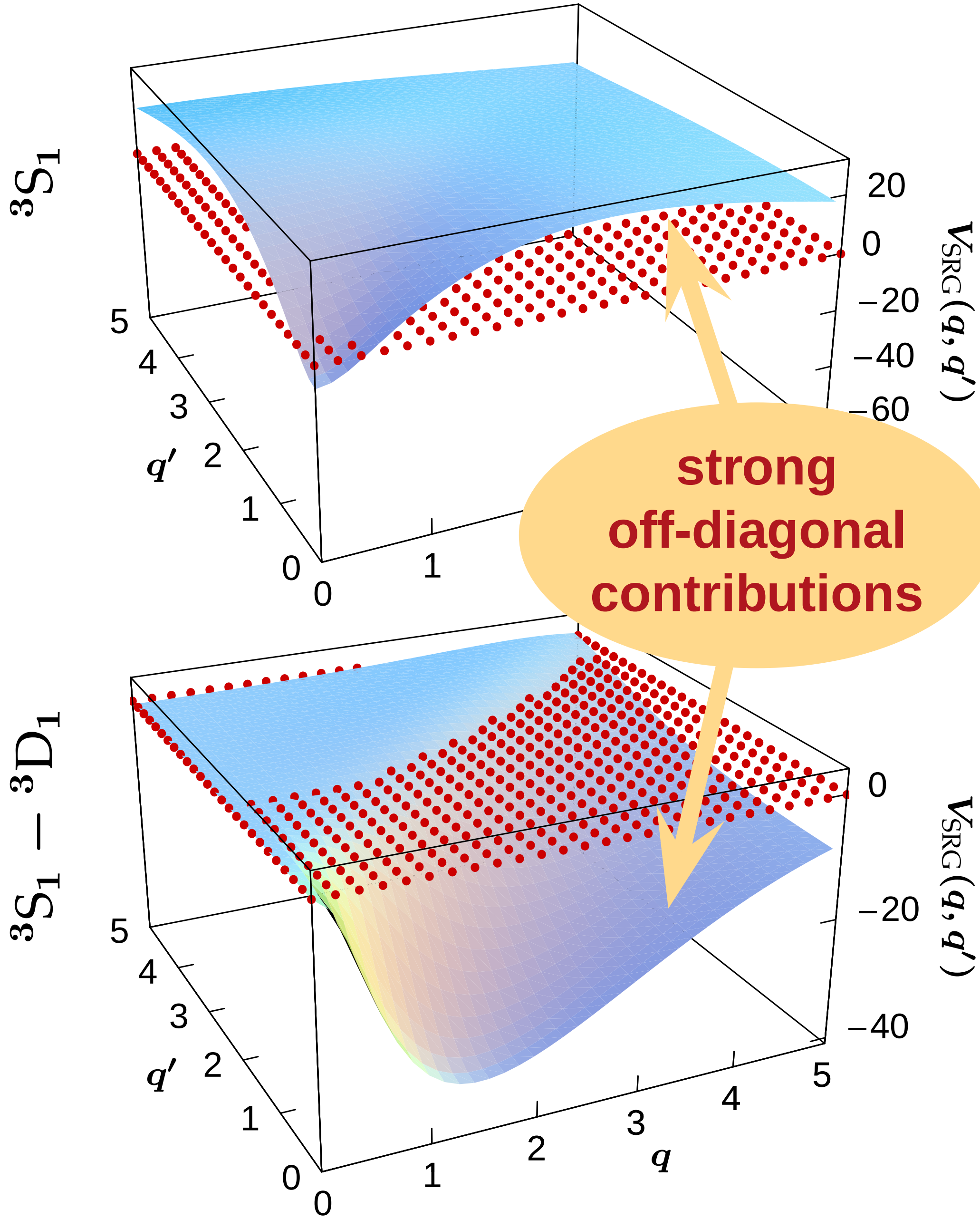
$$\widetilde{\mathrm{H}}(\alpha) = \mathrm{C}^{\dagger}(\alpha)\,\mathrm{H}\,\mathrm{C}(\alpha) \qquad \rightarrow \qquad \frac{\mathrm{d}}{\mathrm{d}\alpha}\widetilde{\mathrm{H}}(\alpha) = \left[\eta(\alpha), \widetilde{\mathrm{H}}(\alpha)\right]$$

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

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

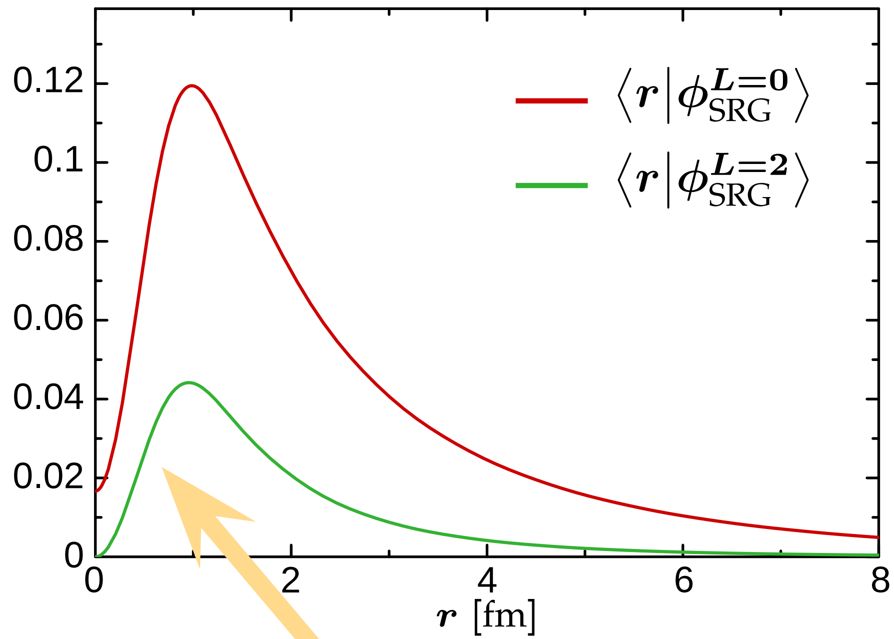
- $\eta(0)$ has the same structure as the UCOM generators g_r and g_Ω

SRG Evolution: The Deuteron



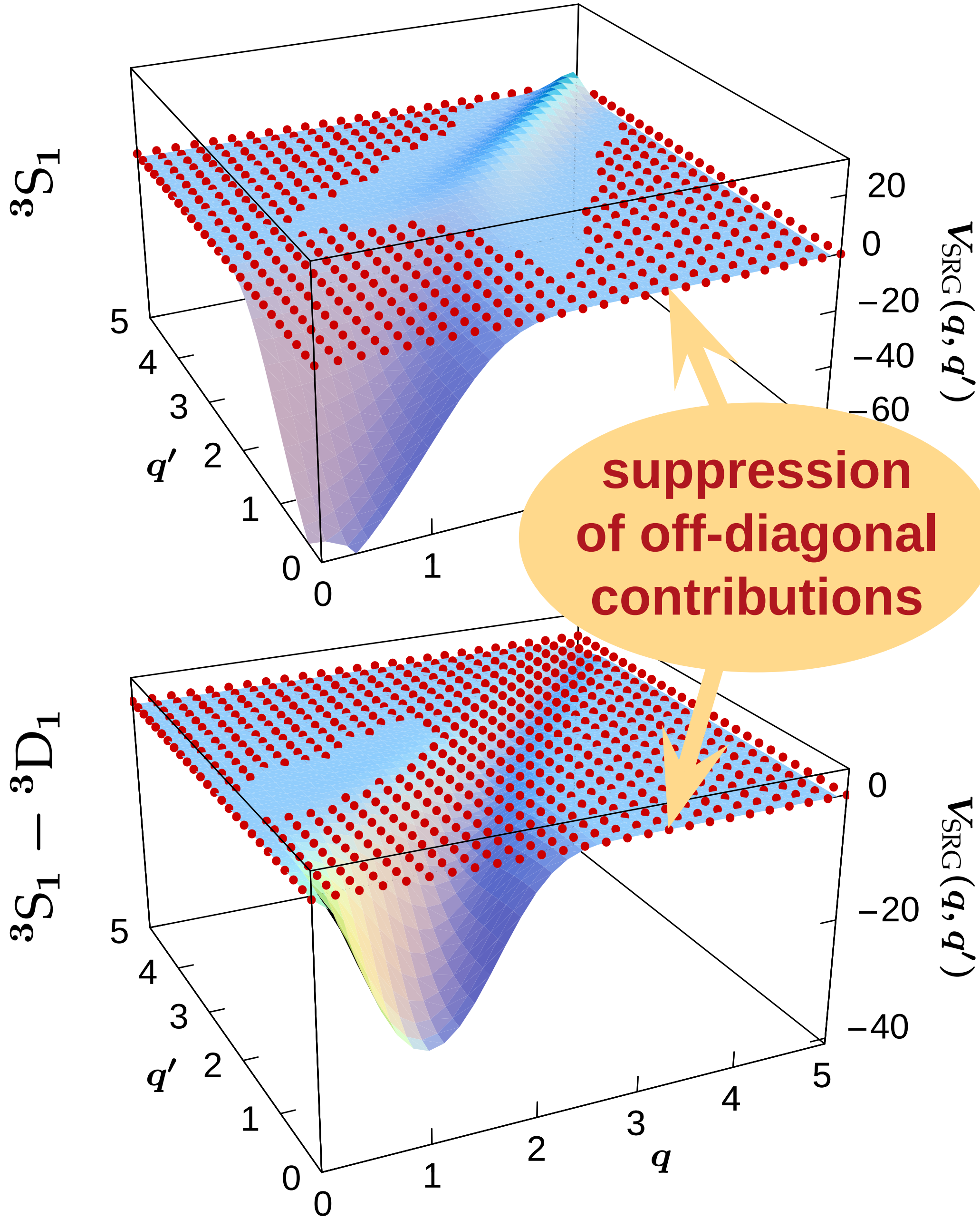
strong off-diagonal contributions

Argonne V18

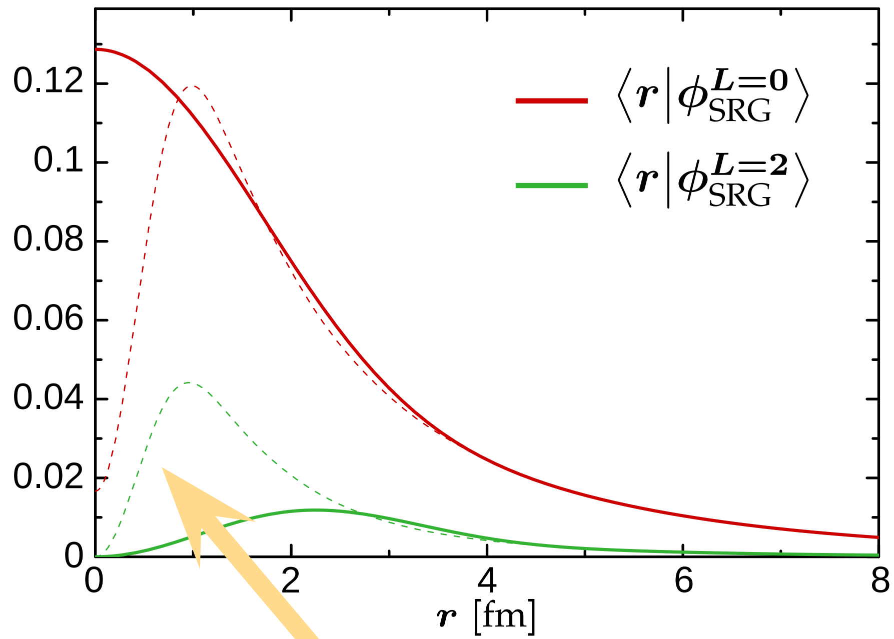


short-range central & tensor correlations

SRG Evolution: The Deuteron



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



suppression of off-diagonal contributions

elimination of short-range correlations

Exact Many-Body Methods

No-Core Shell Model

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

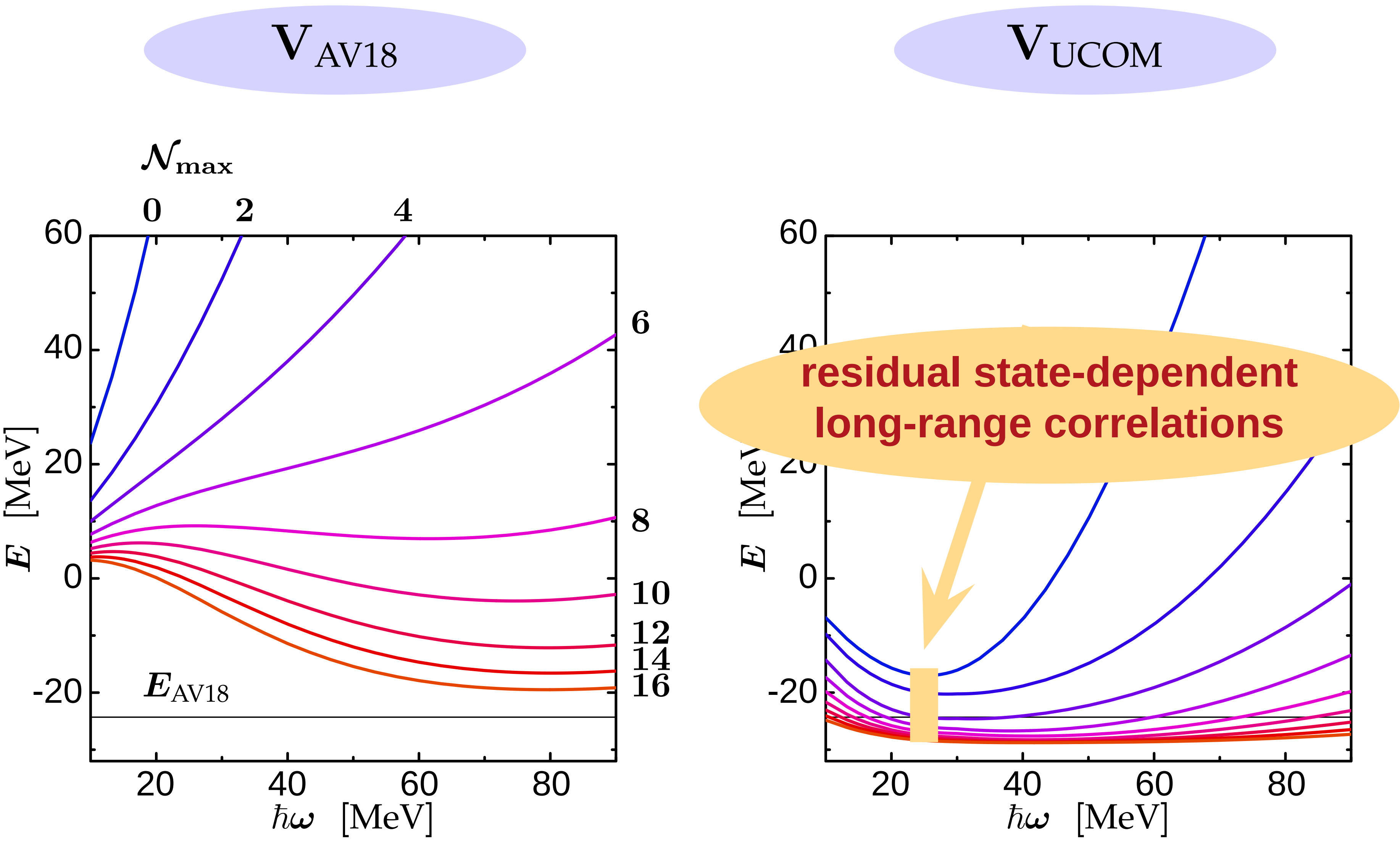
Roth & Navrátil — in preparation

NCSM + Correlated Interactions

No-Core Shell Model
+
Matrix Elements of Correlated Realistic Interaction V_{UCOM}

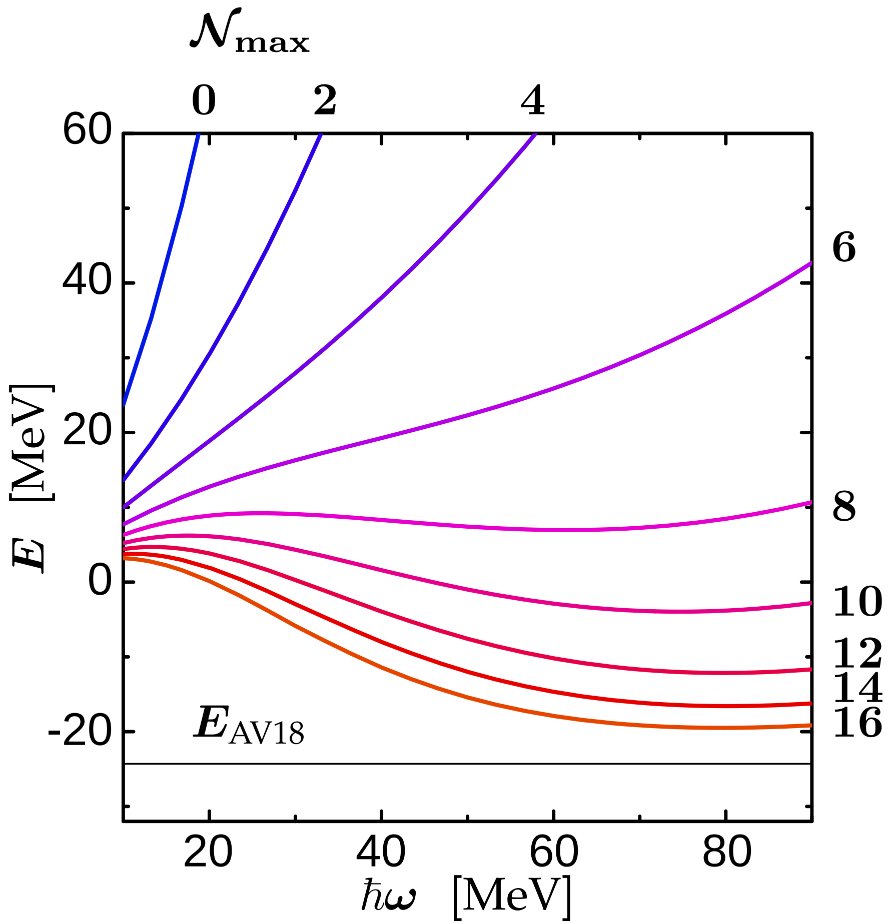
- many-body state is expanded in Slater determinants of harmonic oscillator single-particle states
- large-scale diagonalization of Hamiltonian within a **truncated model space** ($\mathcal{N}\hbar\omega$ truncation)
- assessment of **short- and long-range correlations**
- role of **three-nucleon interactions**

^{4}He: Convergence

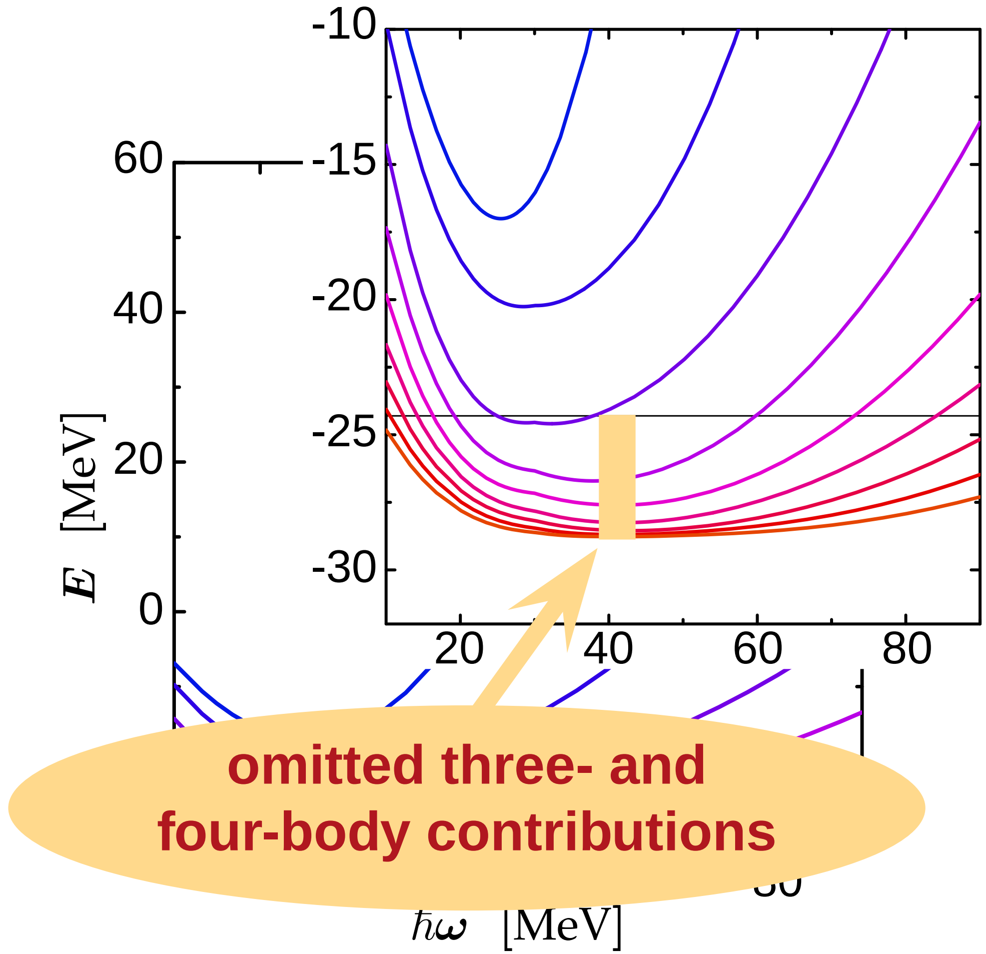


^{4}He: Convergence

V_{AV18}



V_{UCOM}



Three-Body Interactions — Strategies

Correlated Hamiltonian in Many-Body Space

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

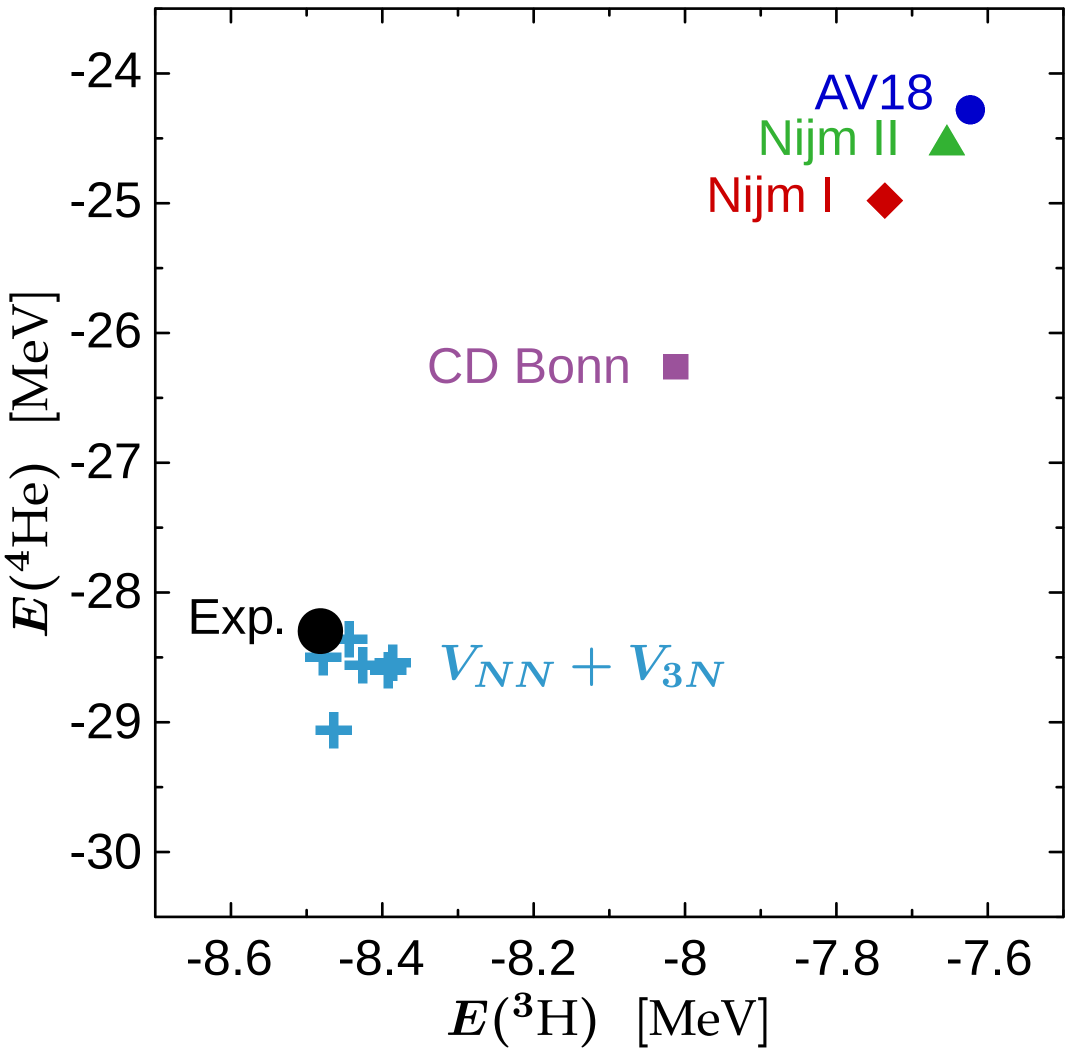
- strategies for treating the three-body contributions:

  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

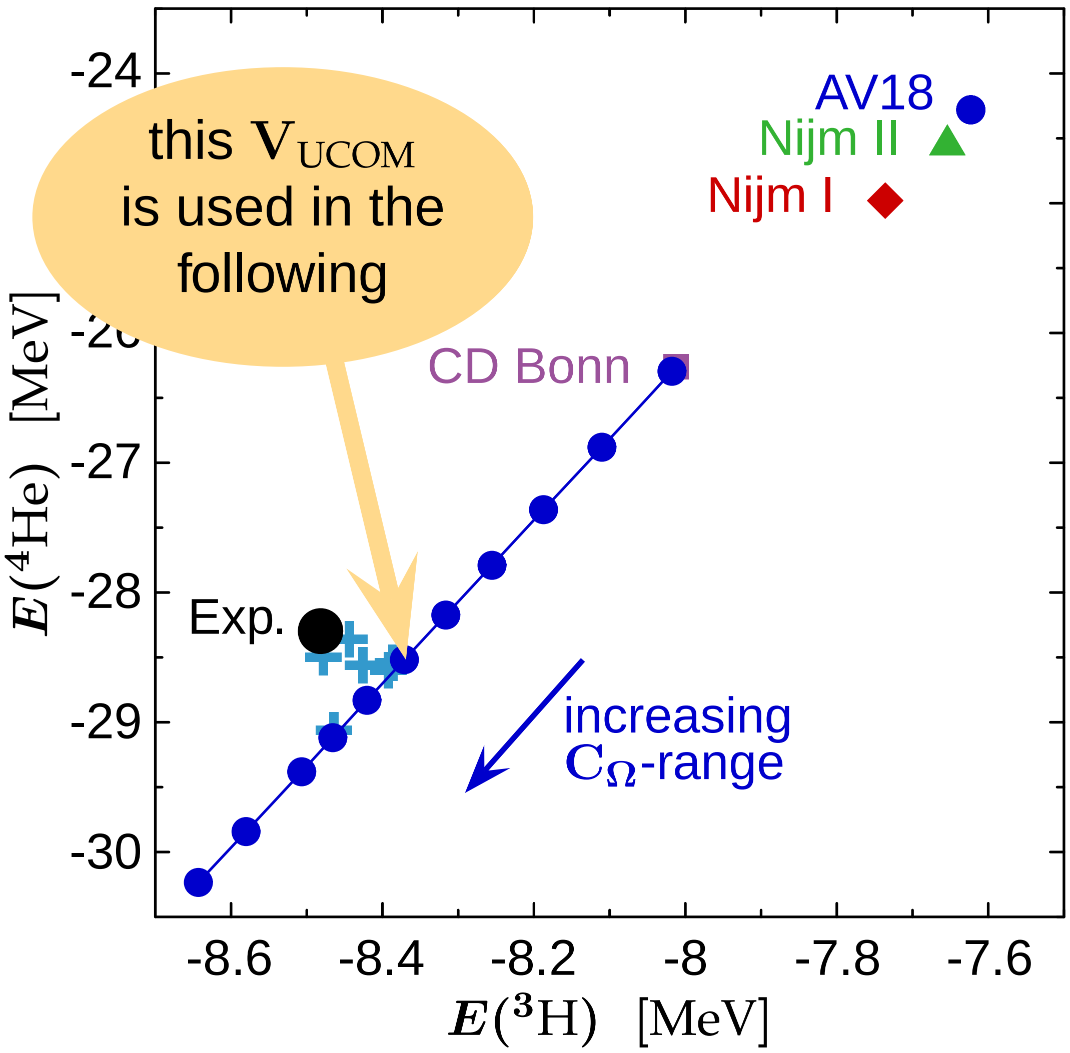
  ❸ **minimize $\mathrm{V}_{\mathrm{UCOM}}^{[3]}$** by proper choice of unitary transformation

Three-Body Interactions — Tjon Line



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

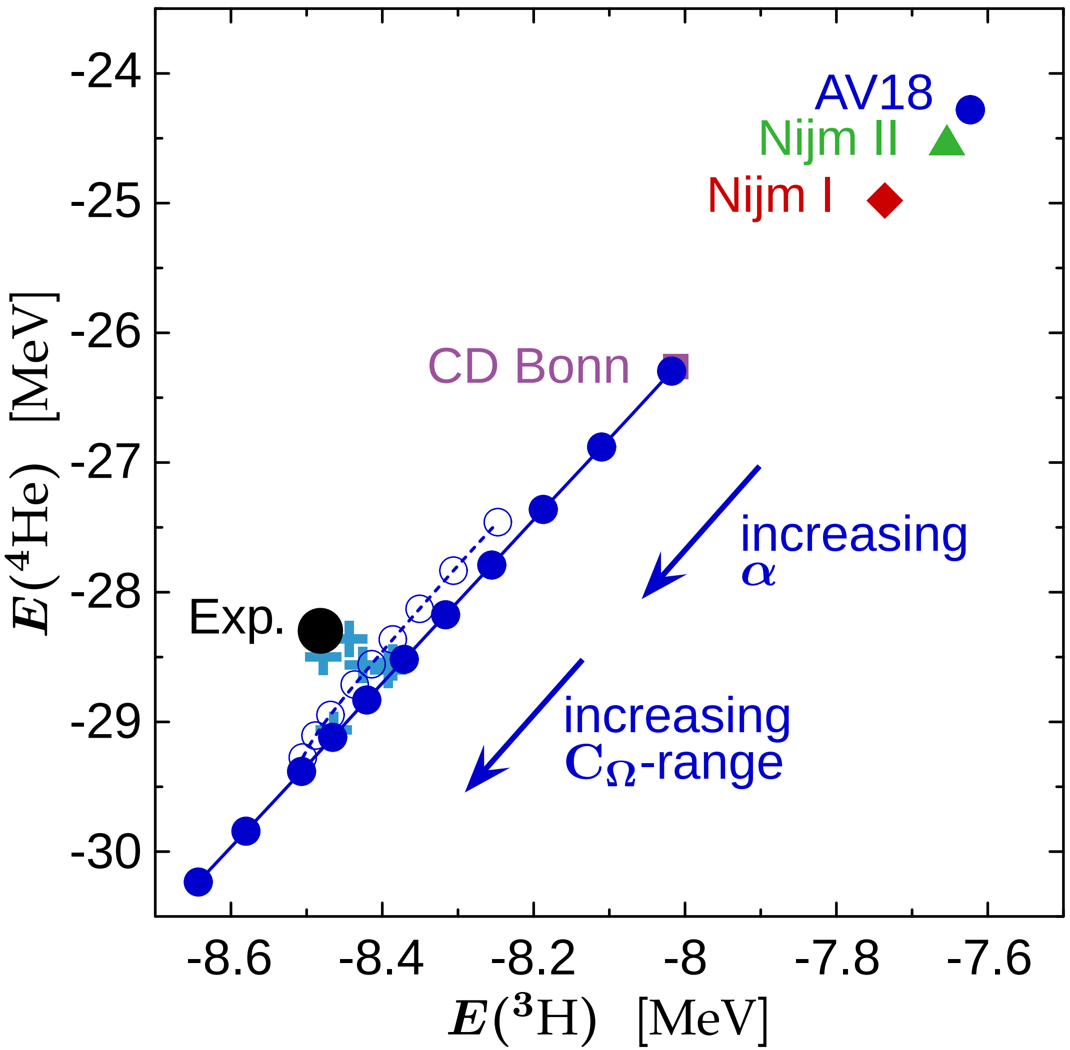
Three-Body Interactions — Tjon Line



- **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

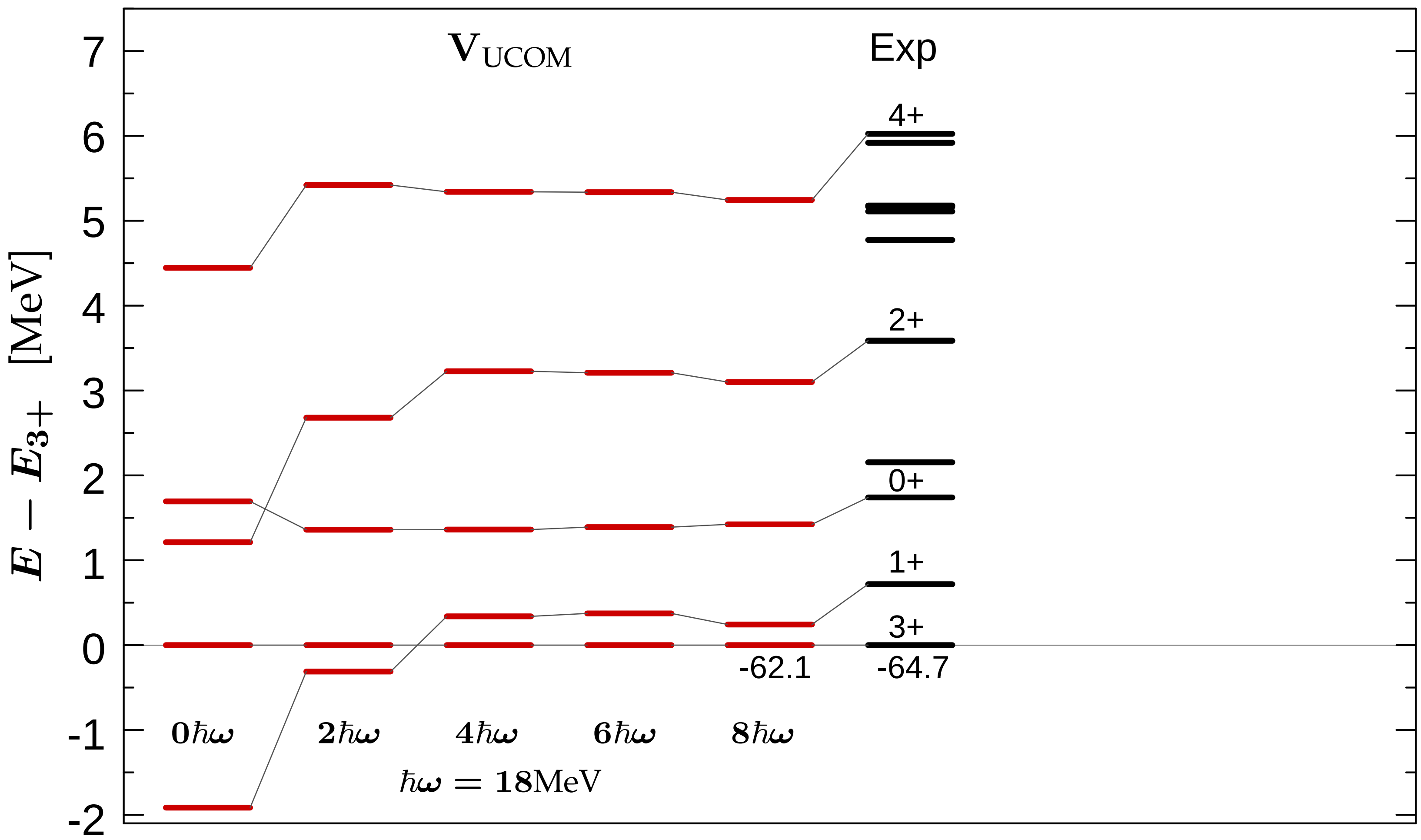
Three-Body Interactions — Tjon Line



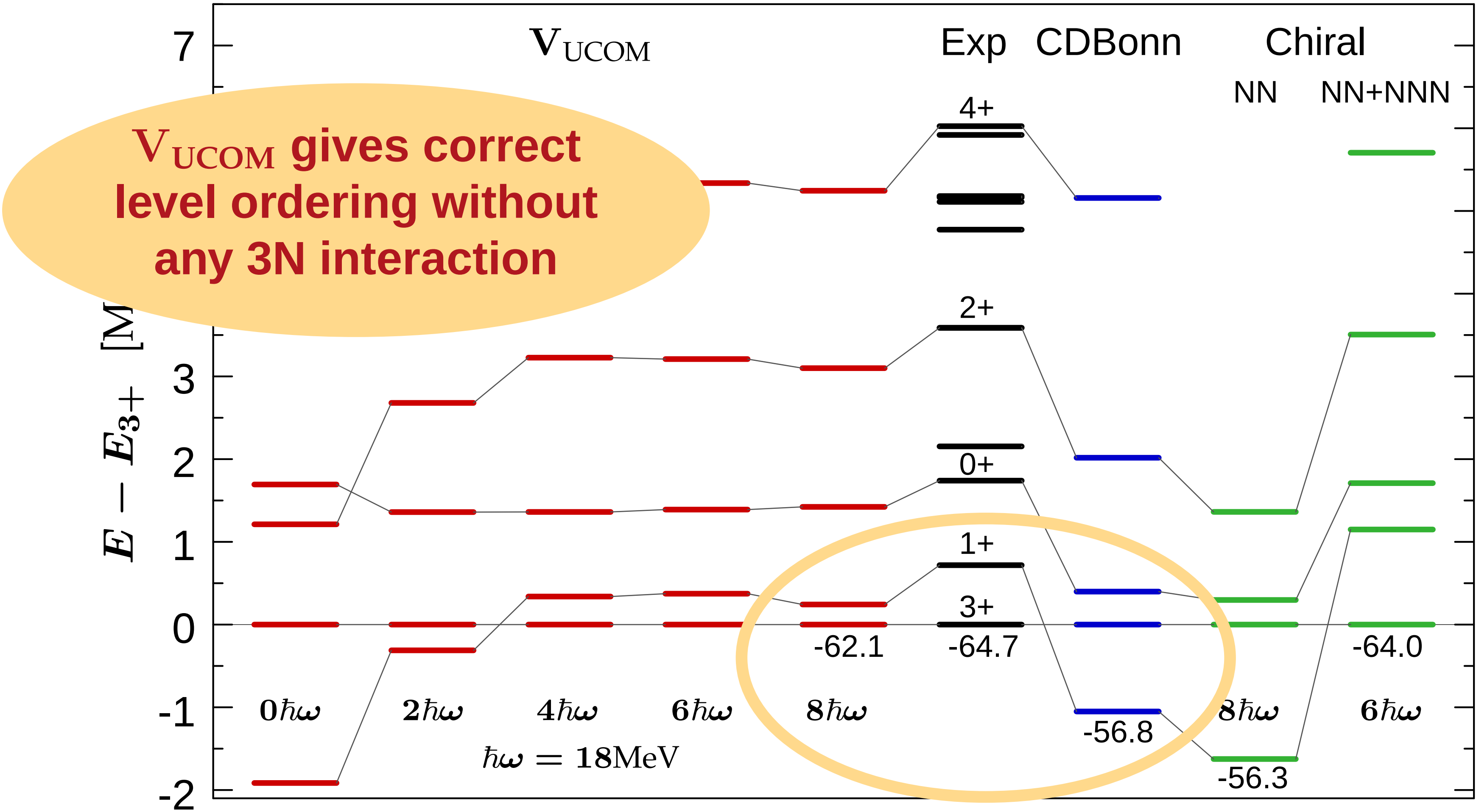
- **Tjon-line**: $E(^4\mathrm{He})$ vs. $E(^3\mathrm{H})$ for phase-shift equivalent NN-interactions
- same behavior for the SRG interaction as function of α

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?



Exact Many-Body Methods

Importance Truncated No-Core Shell Model

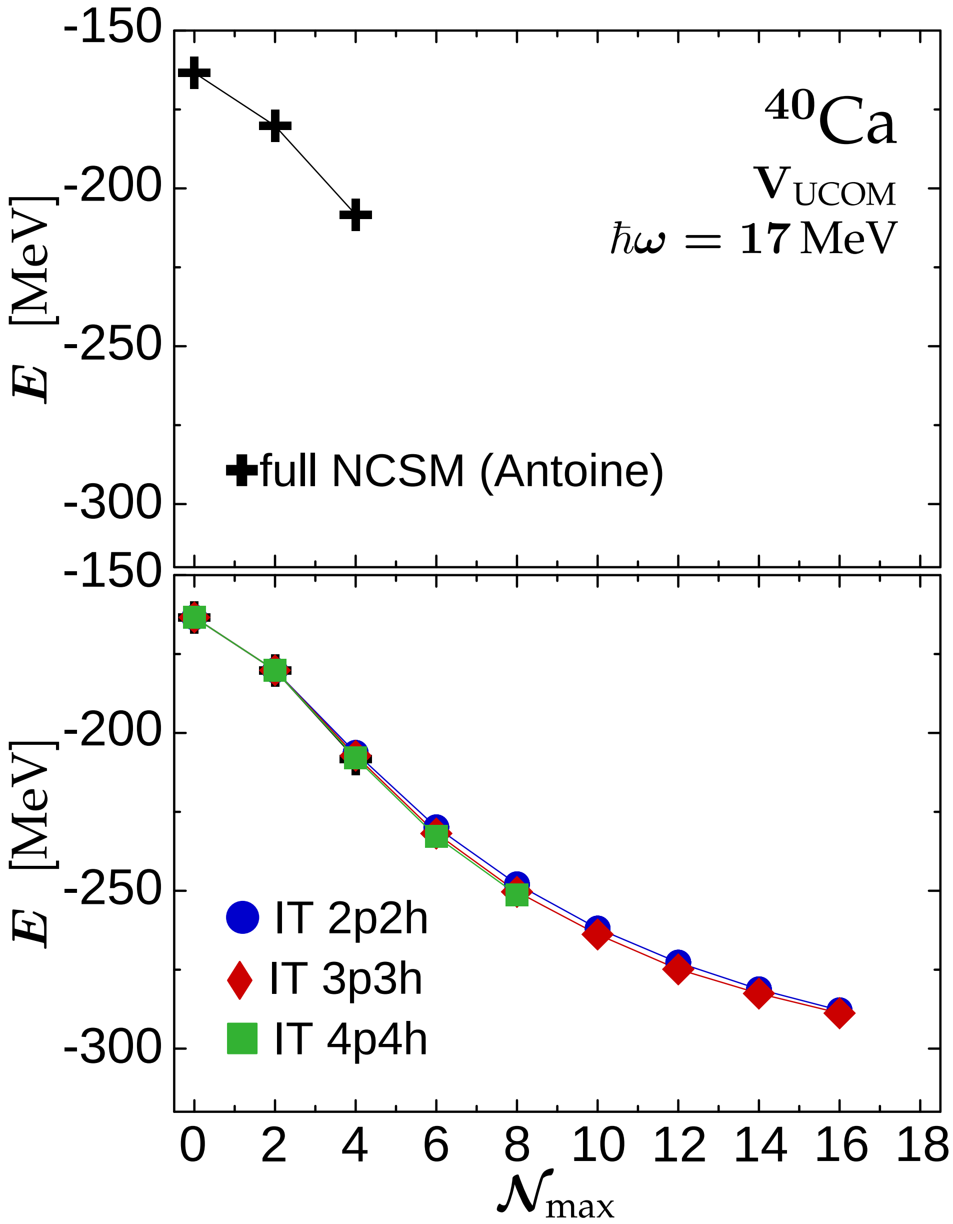
Roth & Navrátil — Phys. Rev. Lett. 99, 092501 (2007)

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

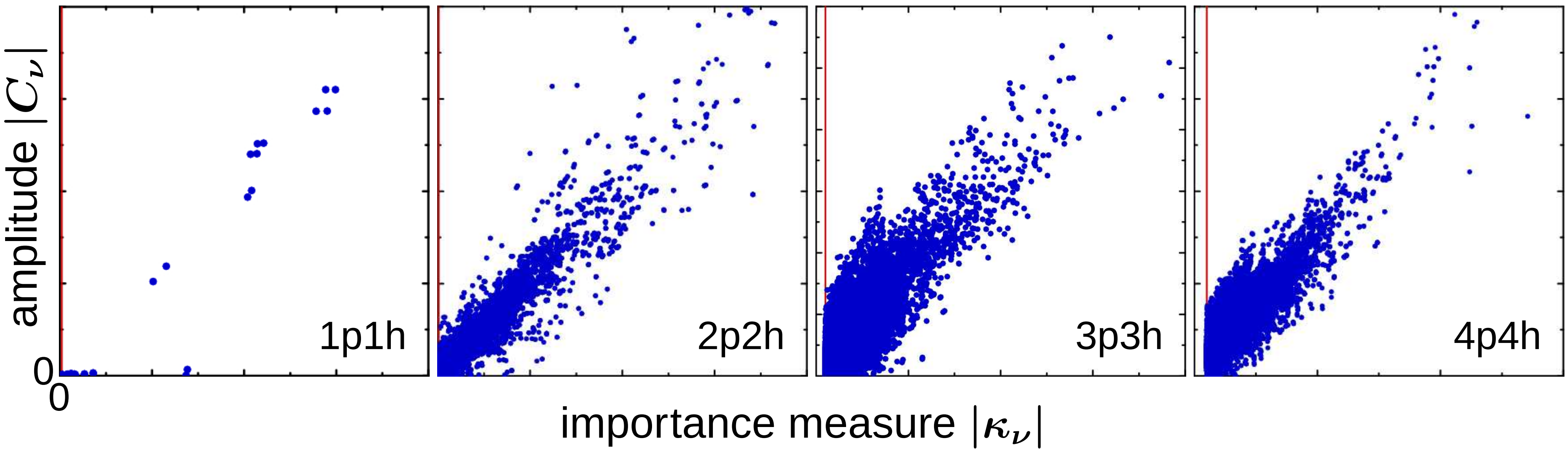


Importance Measure from MBPT

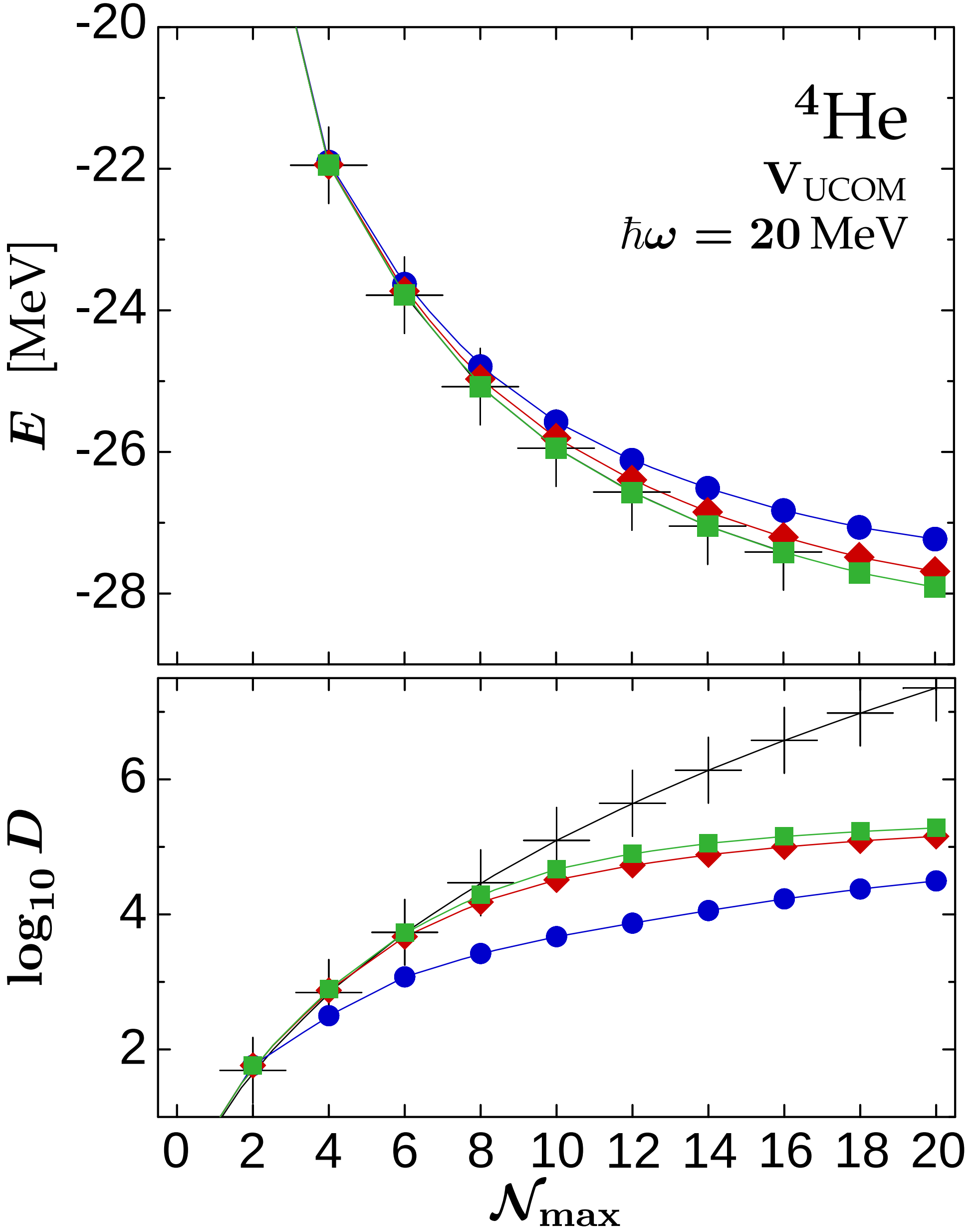
- estimate **a posteriori amplitude C_ν** of shell model configuration $|\Phi_\nu\rangle$ via **a priori perturbative weight κ_ν** starting from a reference state $|\Psi_{\text{ref}}\rangle$:

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

- iterative procedure for construction of **importance truncated model space**



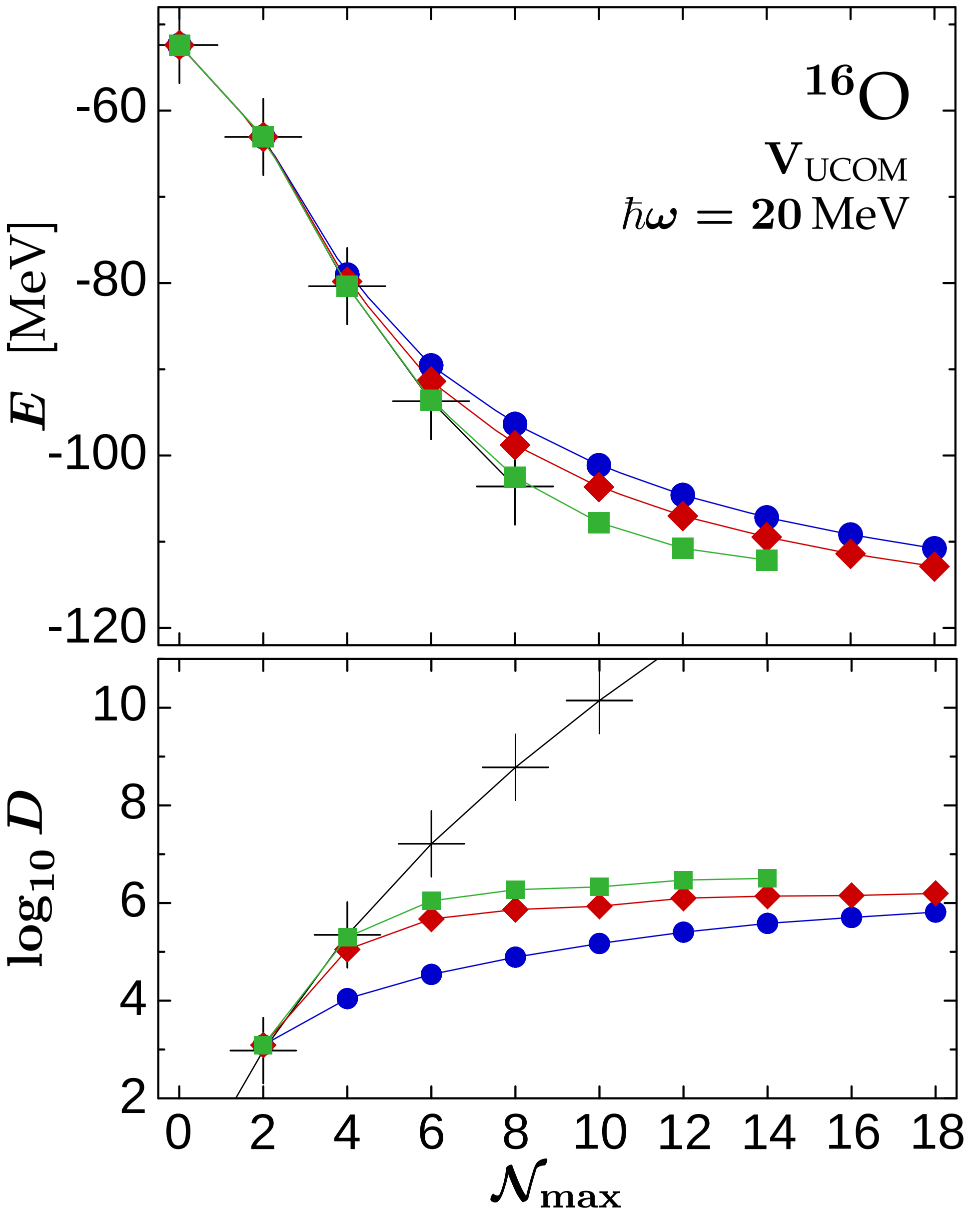
Benchmark: ^{4}He



- **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

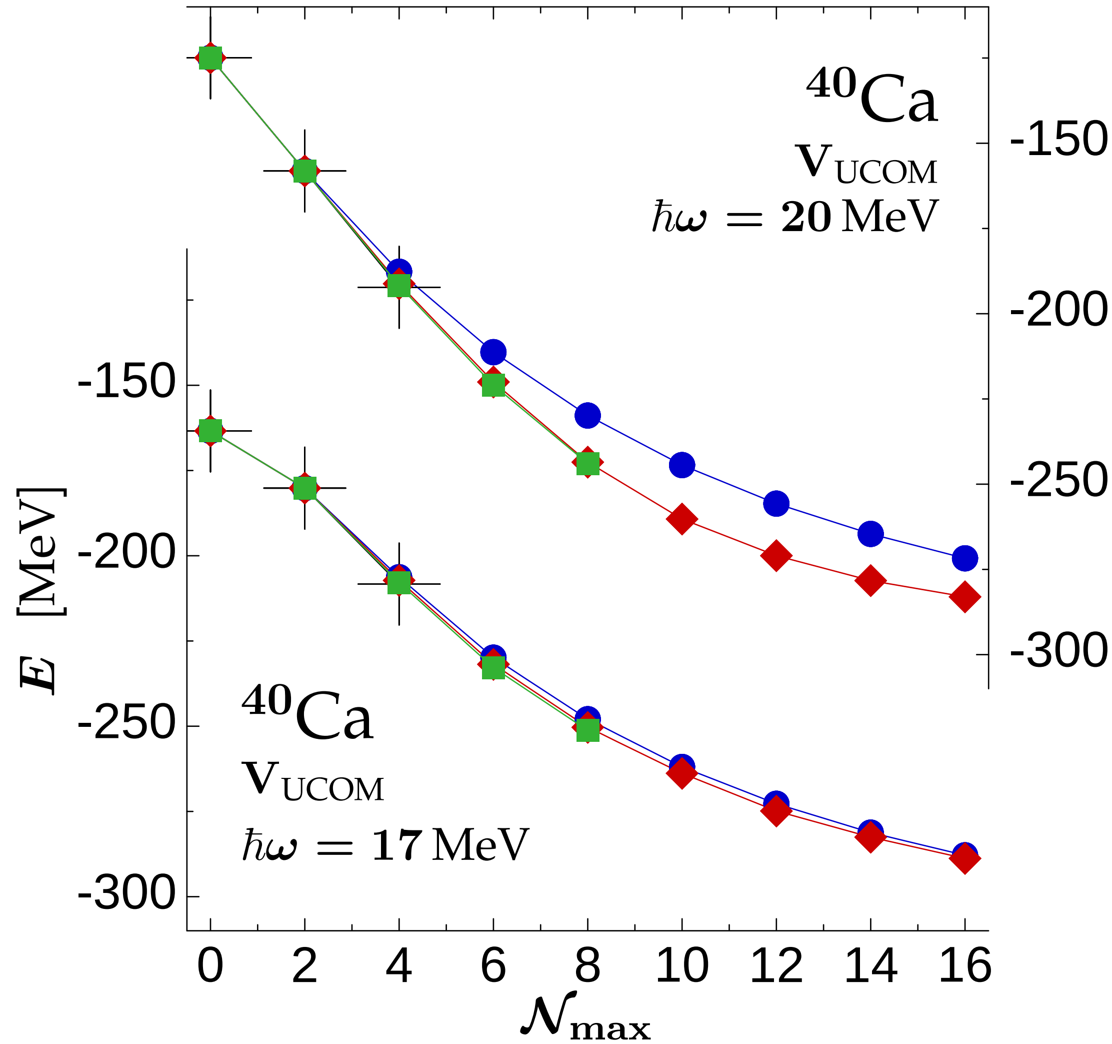
Benchmark: ^{16}O



- **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

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

- **Innovative Many-Body Methods**
  - No-Core Shell Model,...
  - Importance Truncated NCSM, 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

  Institut für Kernphysik, TU Darmstadt

- P. Navrátil

  Lawrence Livermore National Laboratory, USA

- N. Paar

  University of Zagreb, Croatia

- H. Feldmeier, T. Neff, C. Barbieri,...

  Gesellschaft für Schwerionenforschung (GSI)

supported by the DFG through SFB 634
“Nuclear Structure, Nuclear Astrophysics and Fundamental Experiments...”