Ab Initio Nuclear Structure beyond the p-Shell

Importance Truncated No-Core Shell Model

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

From QCD to Nuclear Structure

Nuclear Structure

Low-Energy QCD

From QCD to Nuclear Structure

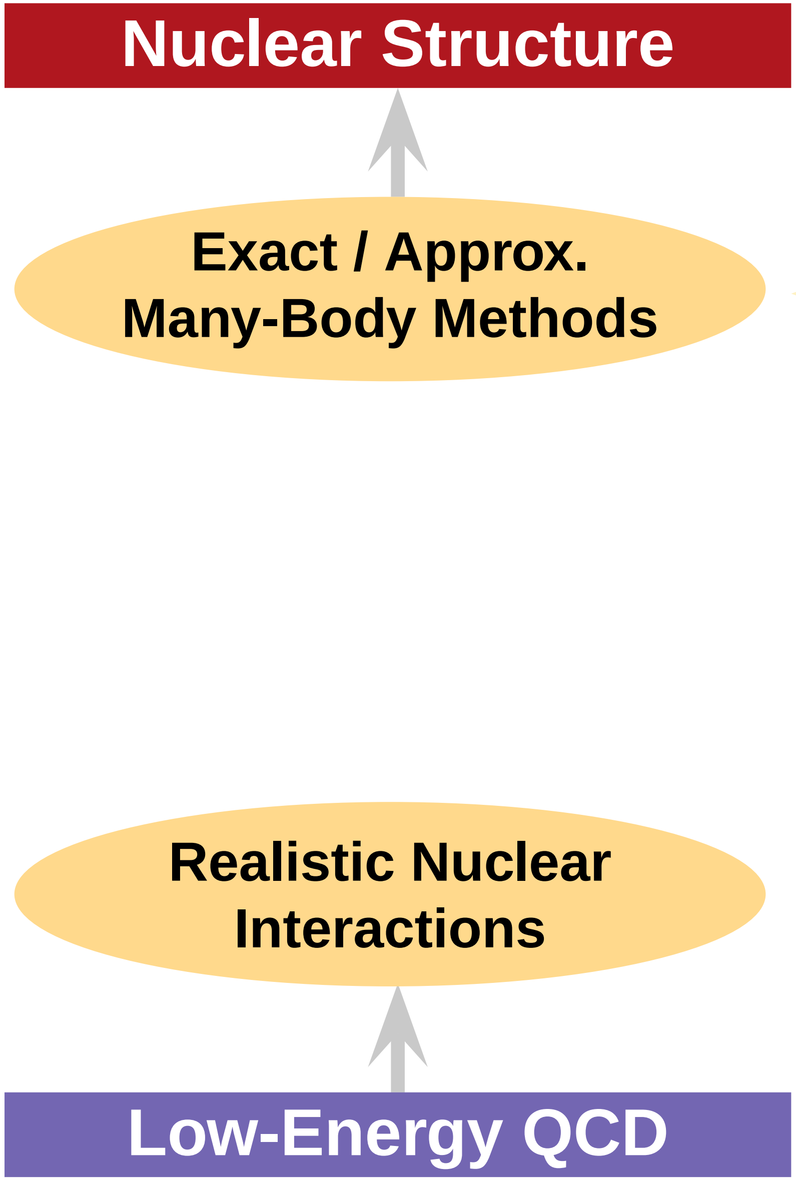
Nuclear Structure

Realistic Nuclear Interactions

- 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

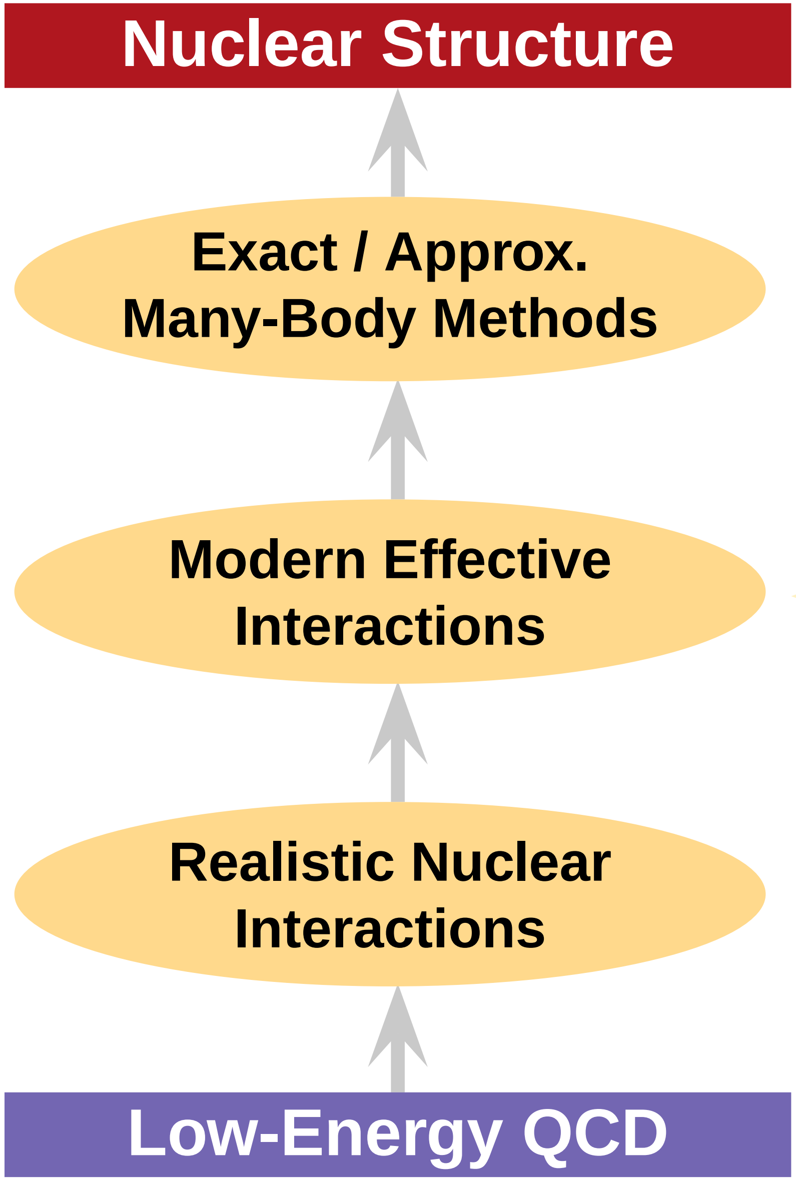
Low-Energy QCD

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



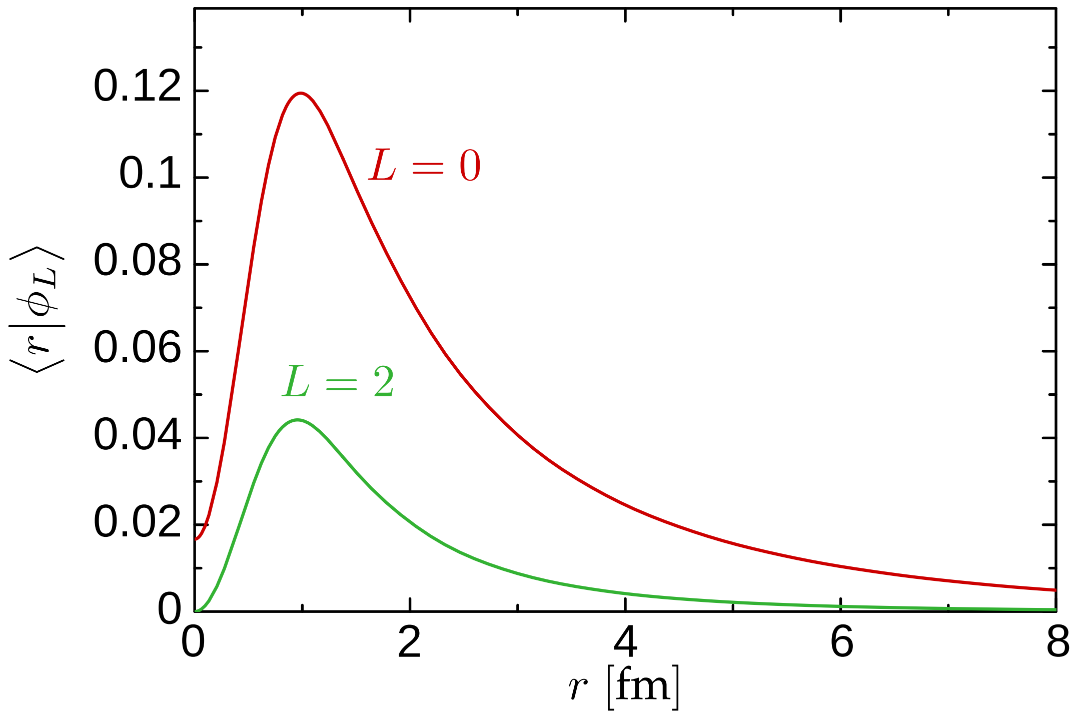
- adapt realistic potential to the available model space
  - tame short-range correlations
  - improve convergence behavior
- conserve experimentally constrained properties (phase shifts)
  - generate new realistic interaction
- provide consistent effective interaction & effective operators
- unitary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

Modern Effective Interactions

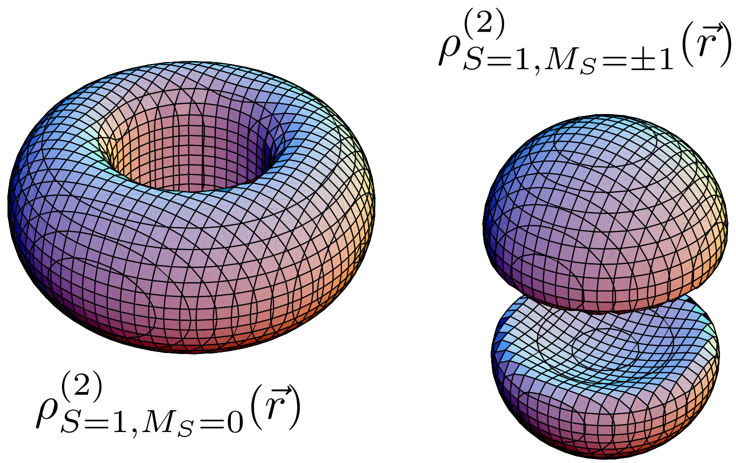
Unitary Correlation Operator Method (UCOM)

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)

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 unitary transformation operator **motivated by the physics of short-range central & 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

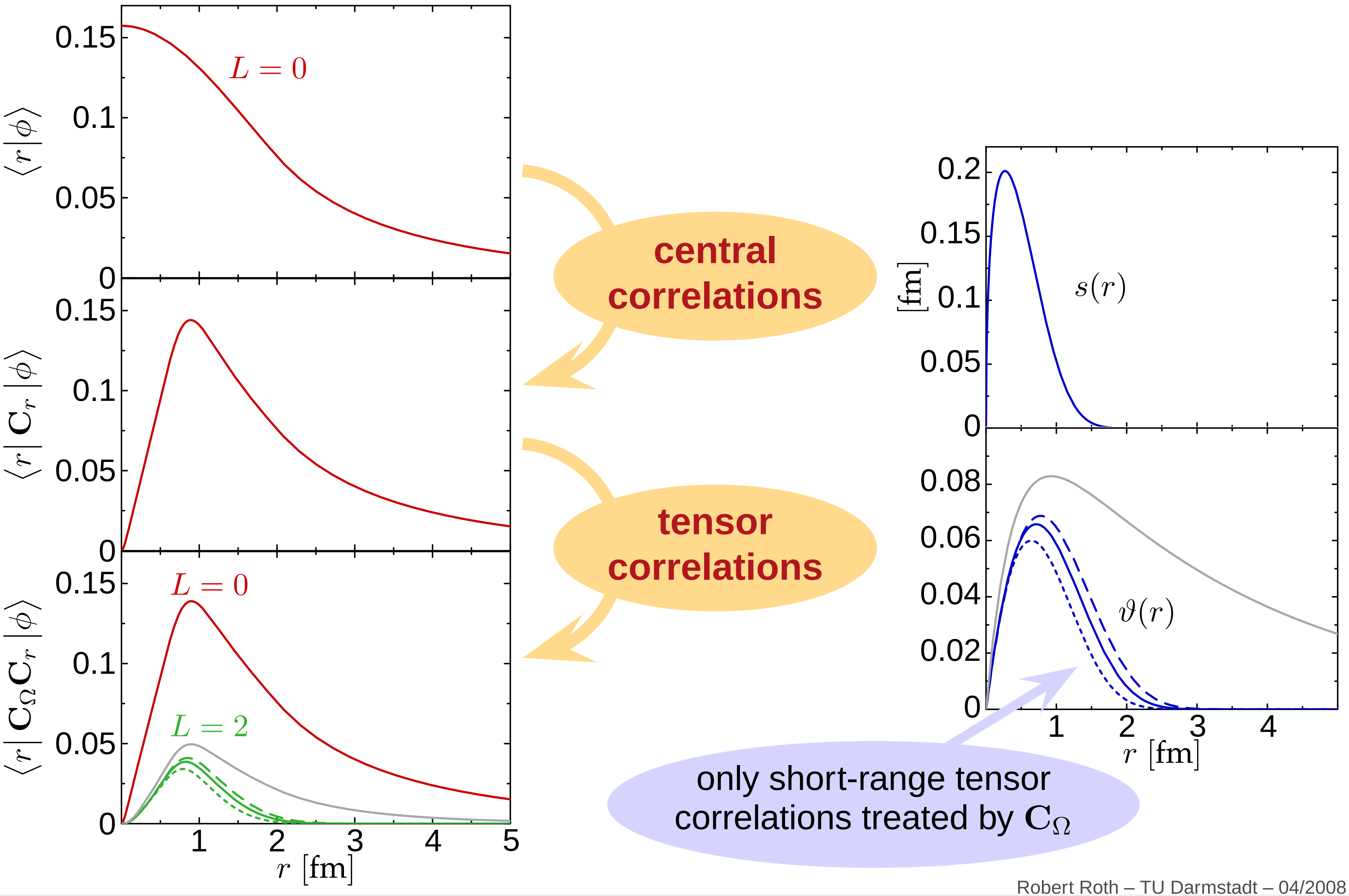
$$\mathbf{g}_\Omega = \frac{3}{2}\vartheta(\mathbf{r})\big[(\vec{\boldsymbol{\sigma}}_1 \cdot \vec{\mathbf{q}}_\Omega)(\vec{\boldsymbol{\sigma}}_2 \cdot \vec{\mathbf{r}}) + (\vec{\mathbf{r}} \leftrightarrow \vec{\mathbf{q}}_\Omega)\big]$$

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

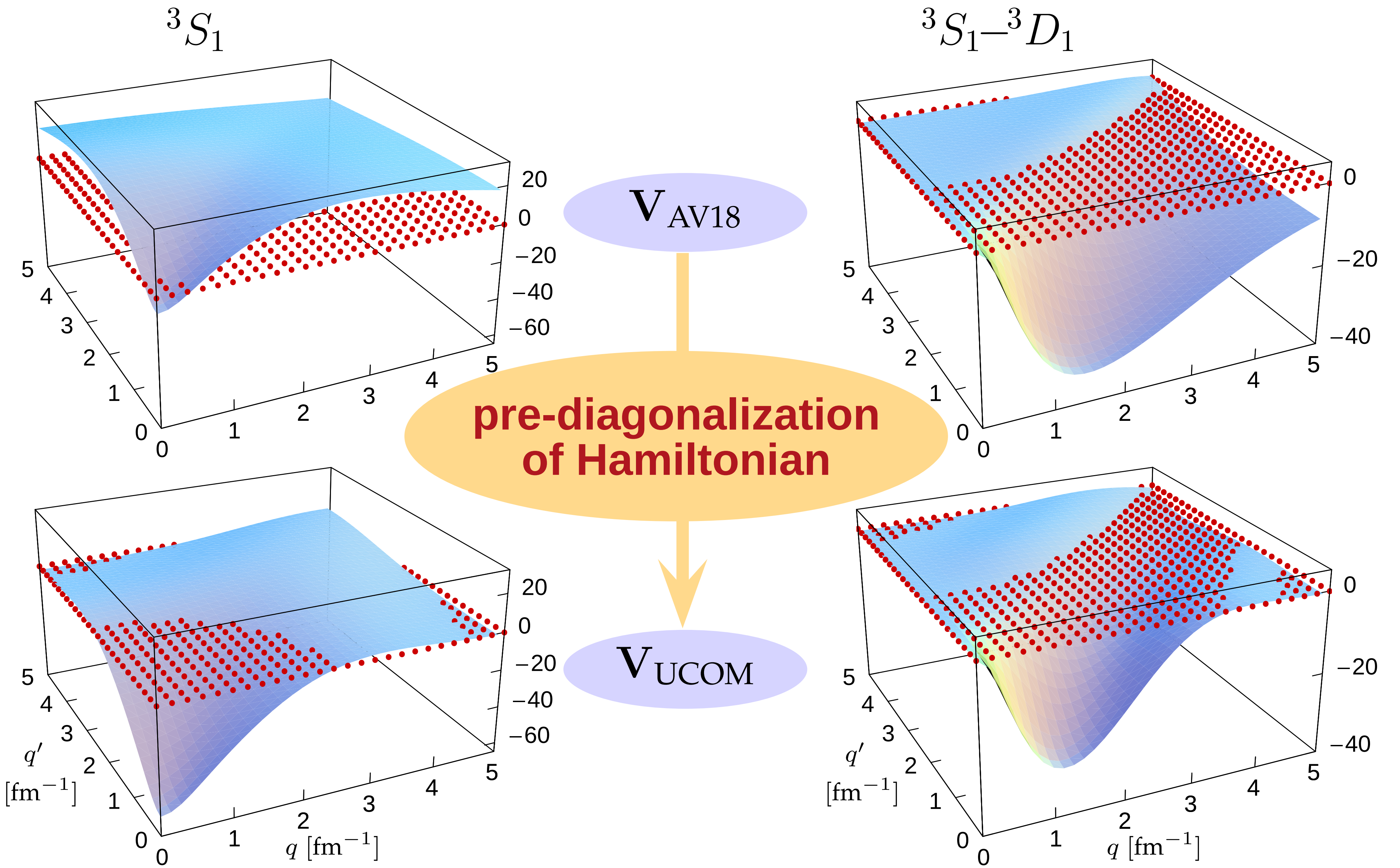
$$\mathbf{C} = \mathbf{C}_\Omega \mathbf{C}_r = \exp\Big(-\,\mathrm{i}\sum\nolimits_{i<j} \mathbf{g}_{\Omega,ij}\Big)\exp\Big(-\,\mathrm{i}\sum\nolimits_{i<j} \mathbf{g}_{r,ij}\Big)$$

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

Correlated States: The Deuteron



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)
Roth, Reinhardt, Hergert — arXiv:0802.4239

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

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

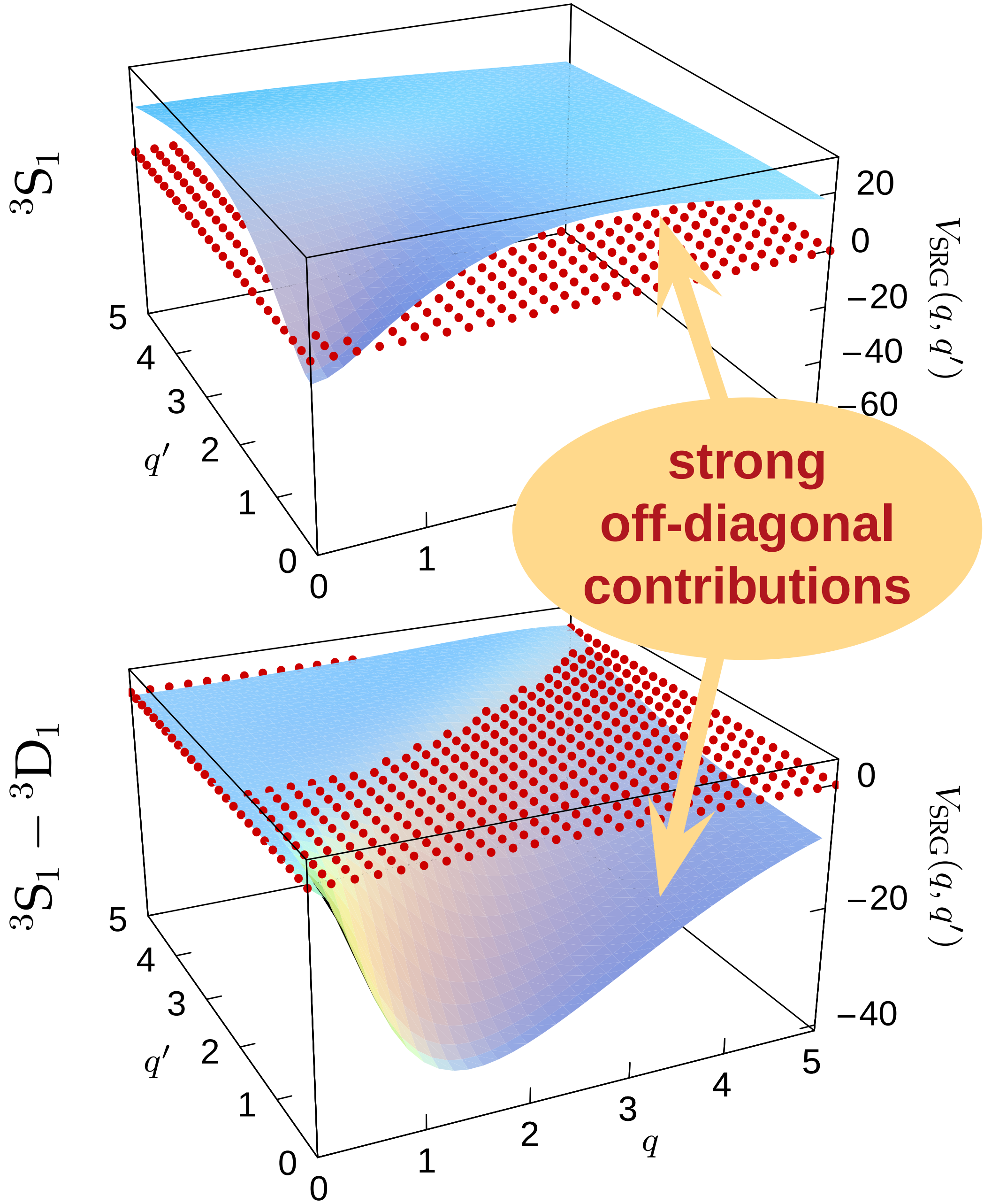
- dynamical generator defined as commutator with the operator in whose eigenbasis $\mathbf{H}$ shall be diagonalized

$$\boldsymbol{\eta}(\alpha) \stackrel{2B}{=} \tfrac{1}{2\mu}\left[\vec{\mathbf{q}}^{2}, \widetilde{\mathbf{H}}(\alpha)\right]$$

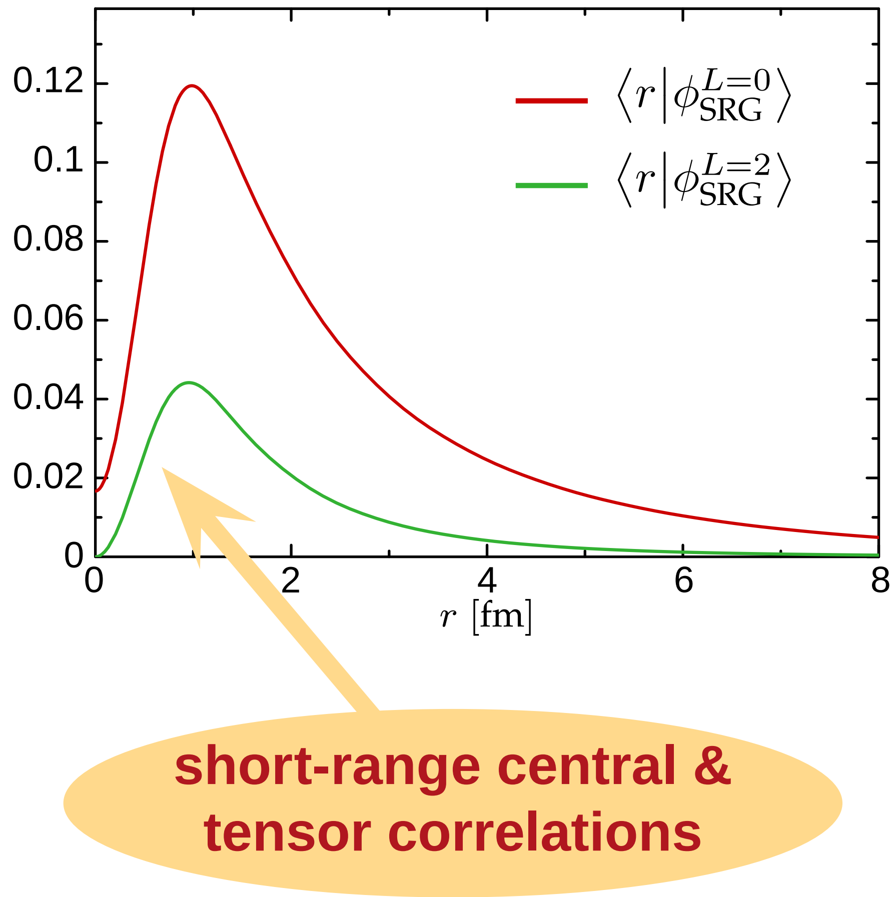
UCOM vs. SRG

$\boldsymbol{\eta}(0)$ has the same structure as the UCOM generators $\mathbf{g}_r$ and $\mathbf{g}_\Omega$

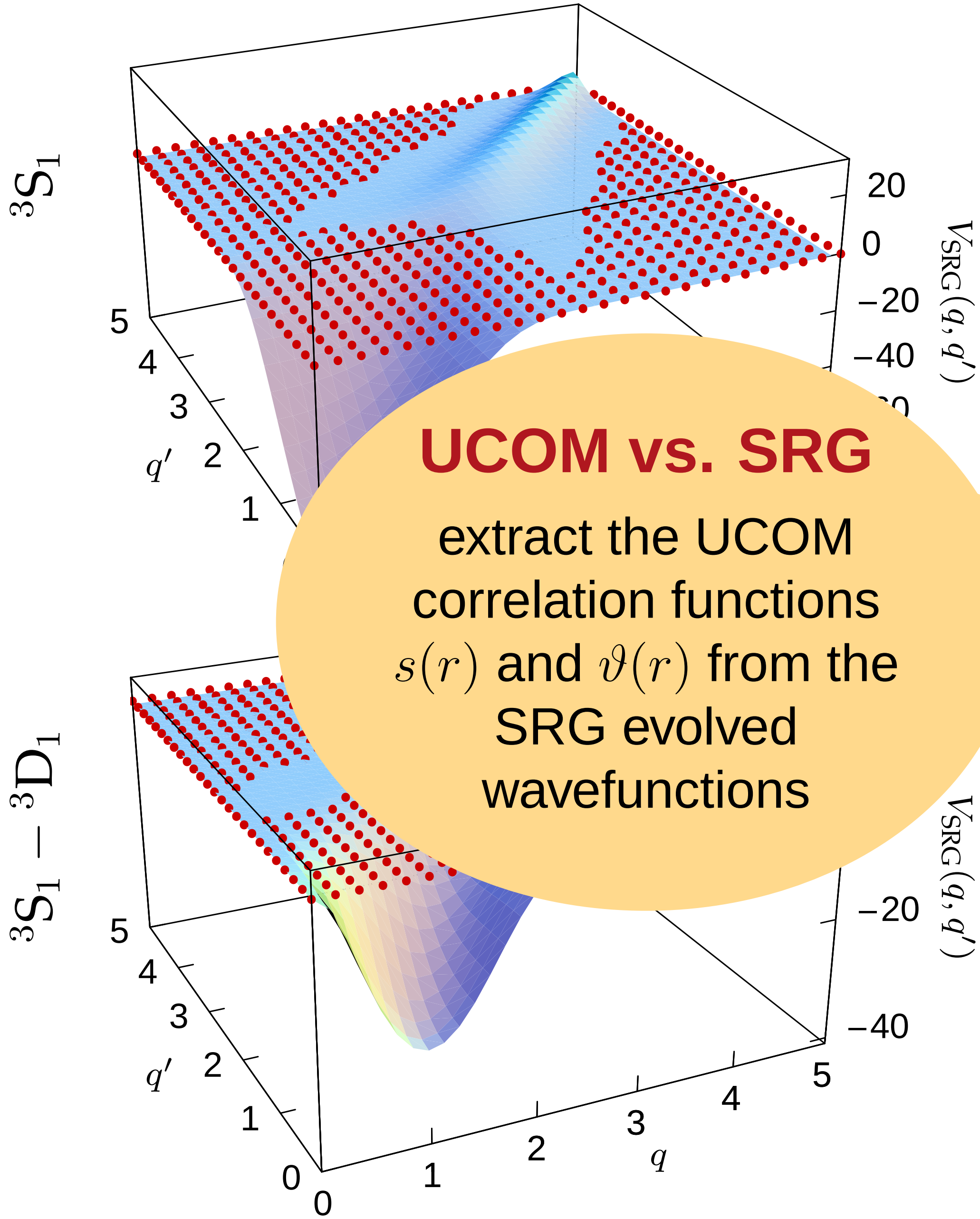
SRG Evolution: The Deuteron



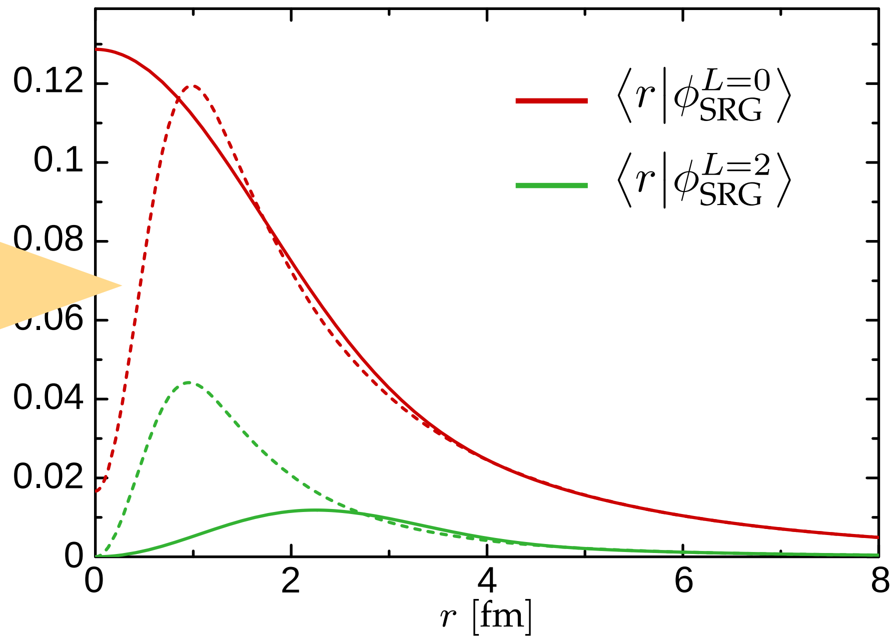
Argonne V18



SRG Evolution: The Deuteron



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



UCOM vs. SRG

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

Exact Many-Body Methods

No-Core Shell Model

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

Reminder: No-Core Shell Model

- many-body state is **expanded in Slater determinants** $|\Phi_\nu\rangle$ composed of harmonic oscillator single-particle states

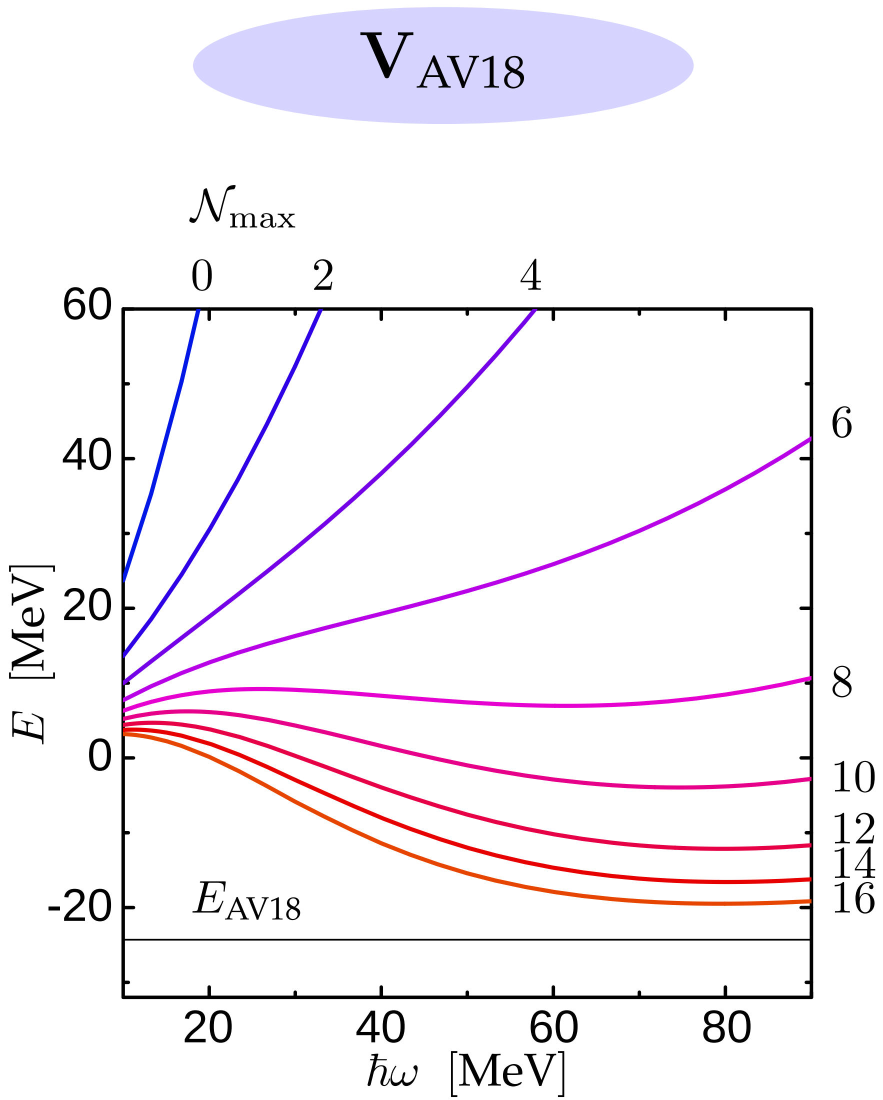
$$|\Psi\rangle = \sum_\nu C_\nu |\Phi_\nu\rangle$$

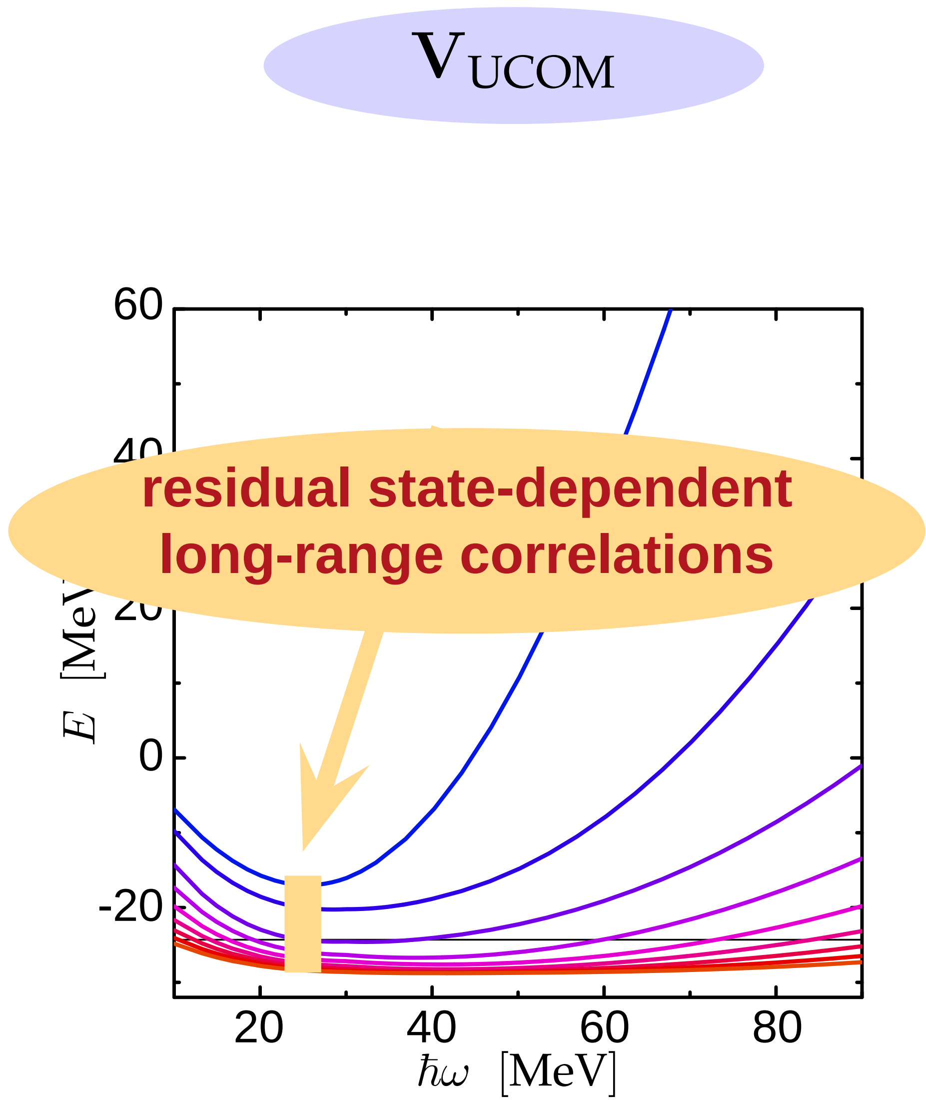
- $\mathcal{N}_{\text{max}}\hbar\omega$ **model space**: truncate basis of Slater determinants with respect to number of oscillator quanta (unperturbed excitation energy)

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

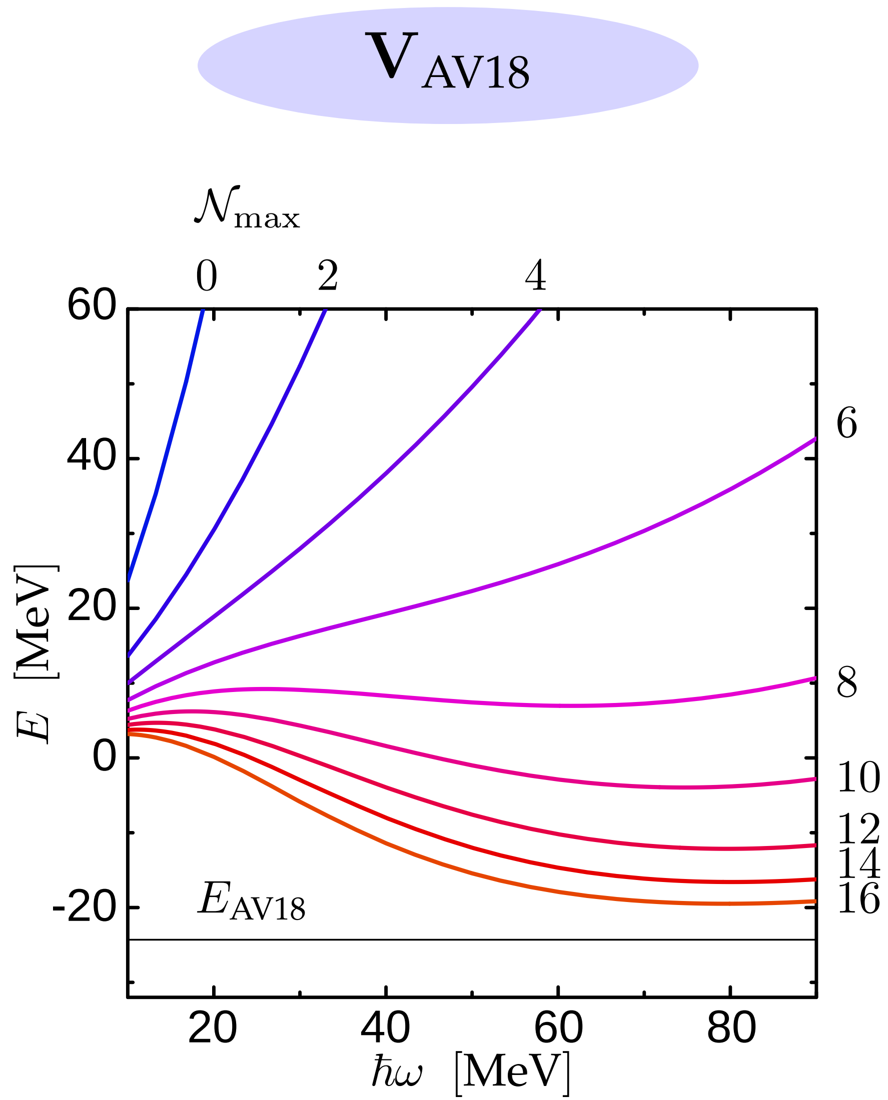
facilitates systematic study of short- and long-range correlations

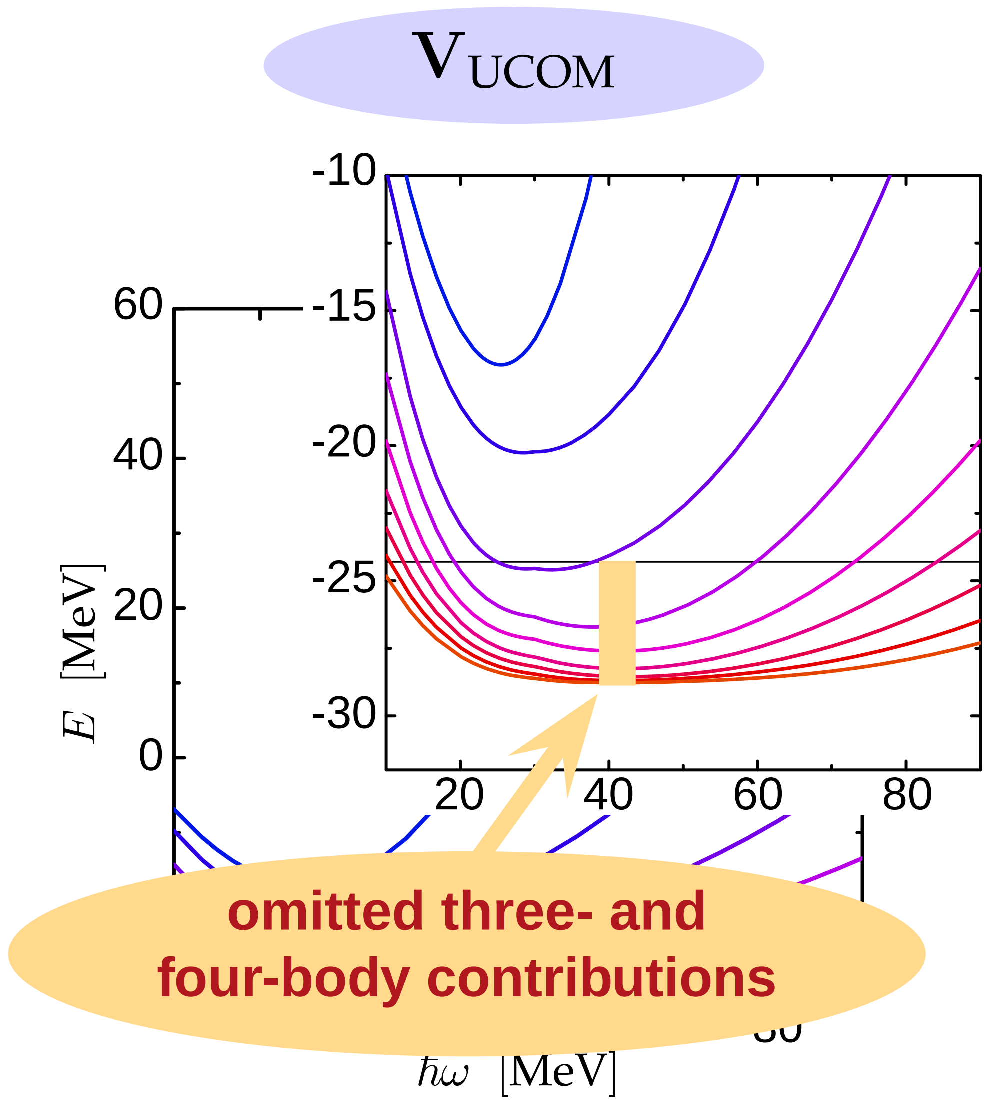
^{4}He: Convergence



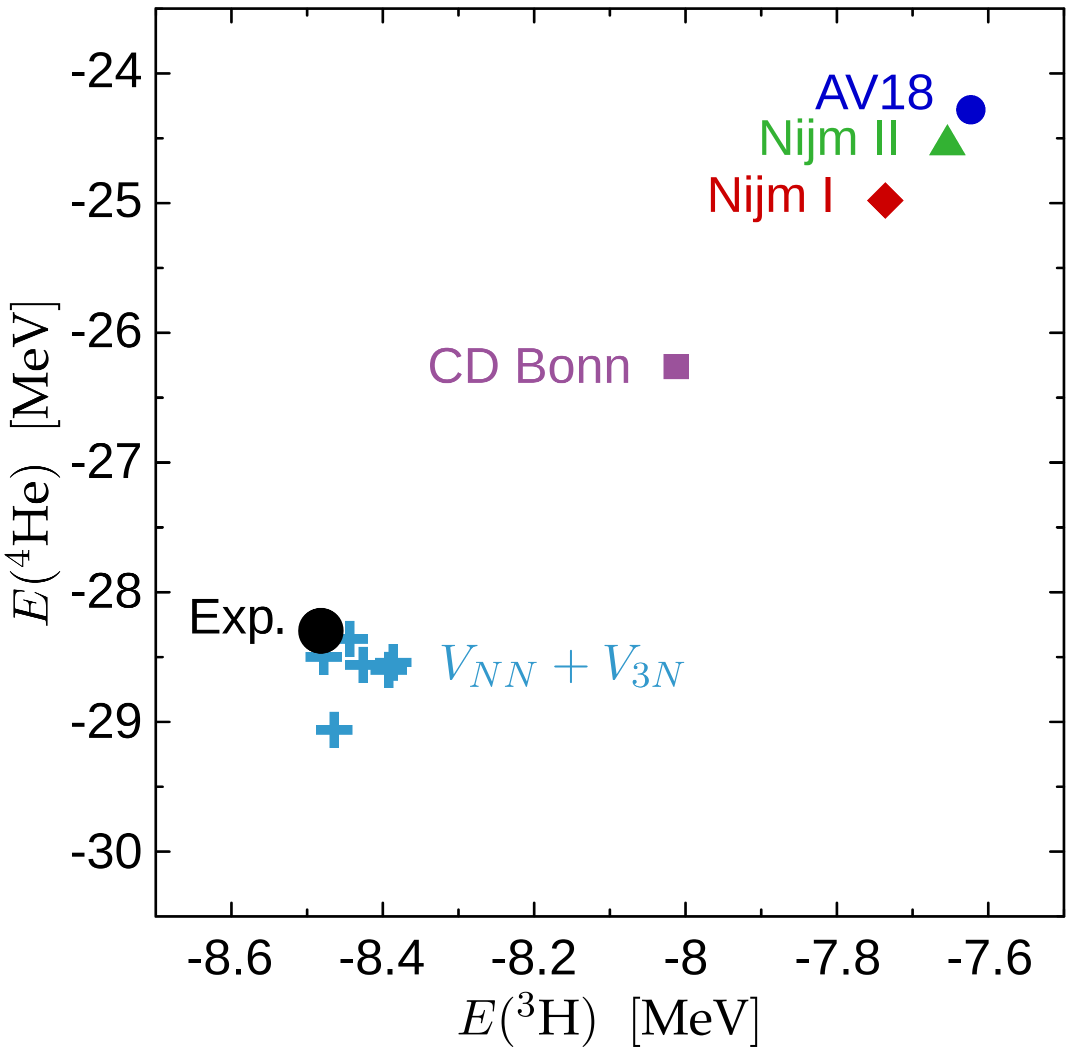


^{4}He: Convergence



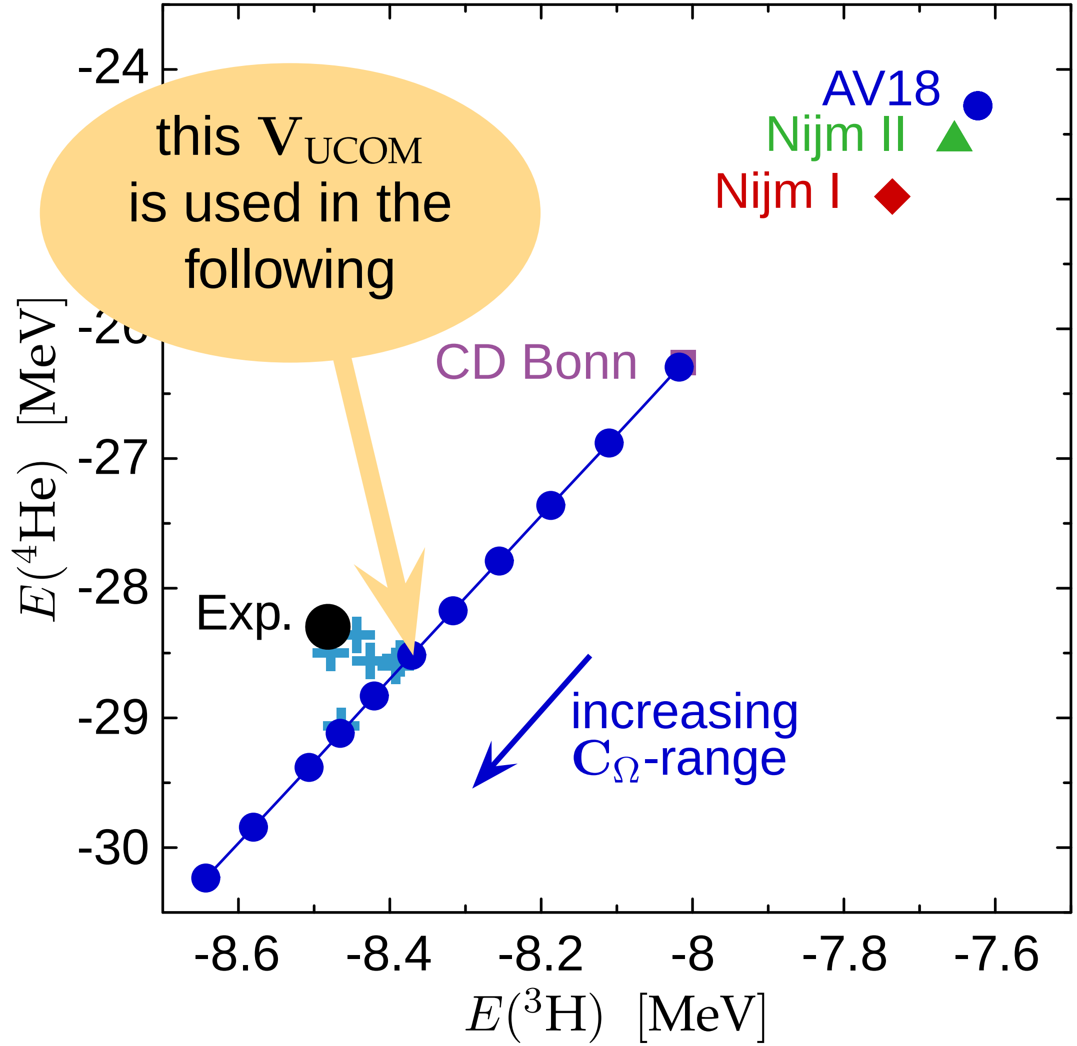


Three-Body Interactions — Tjon Line



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

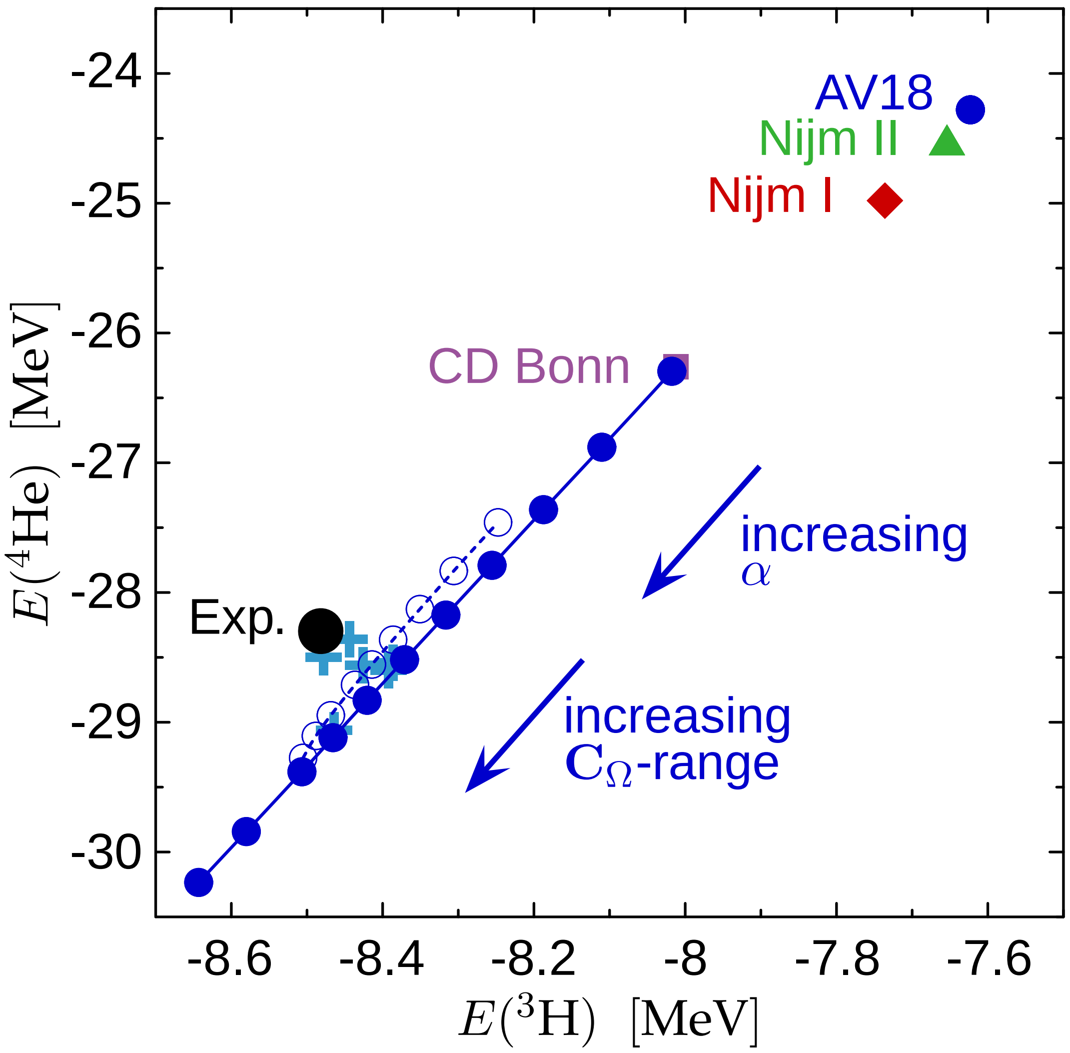
Three-Body Interactions — Tjon Line



- **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

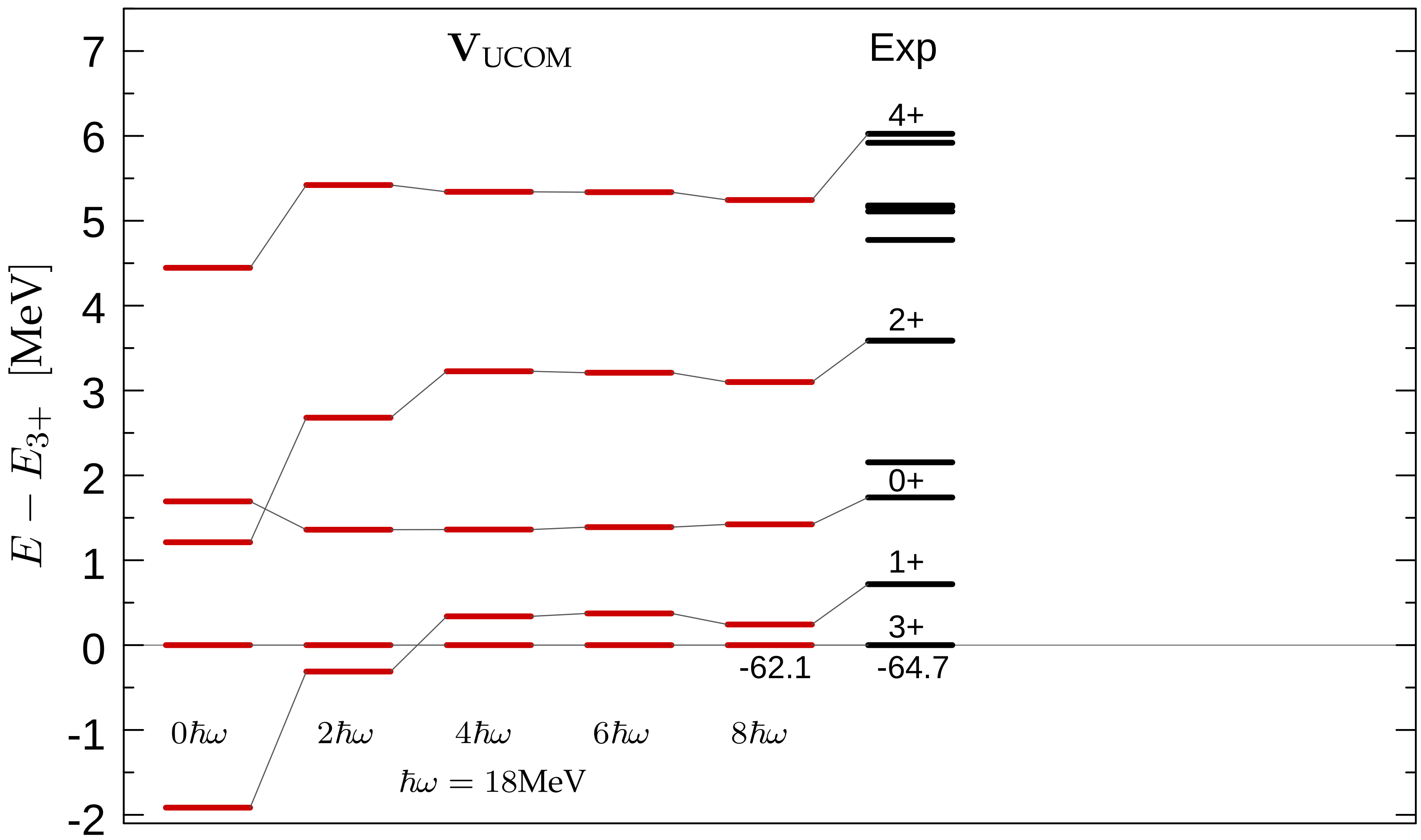
Three-Body Interactions — Tjon Line



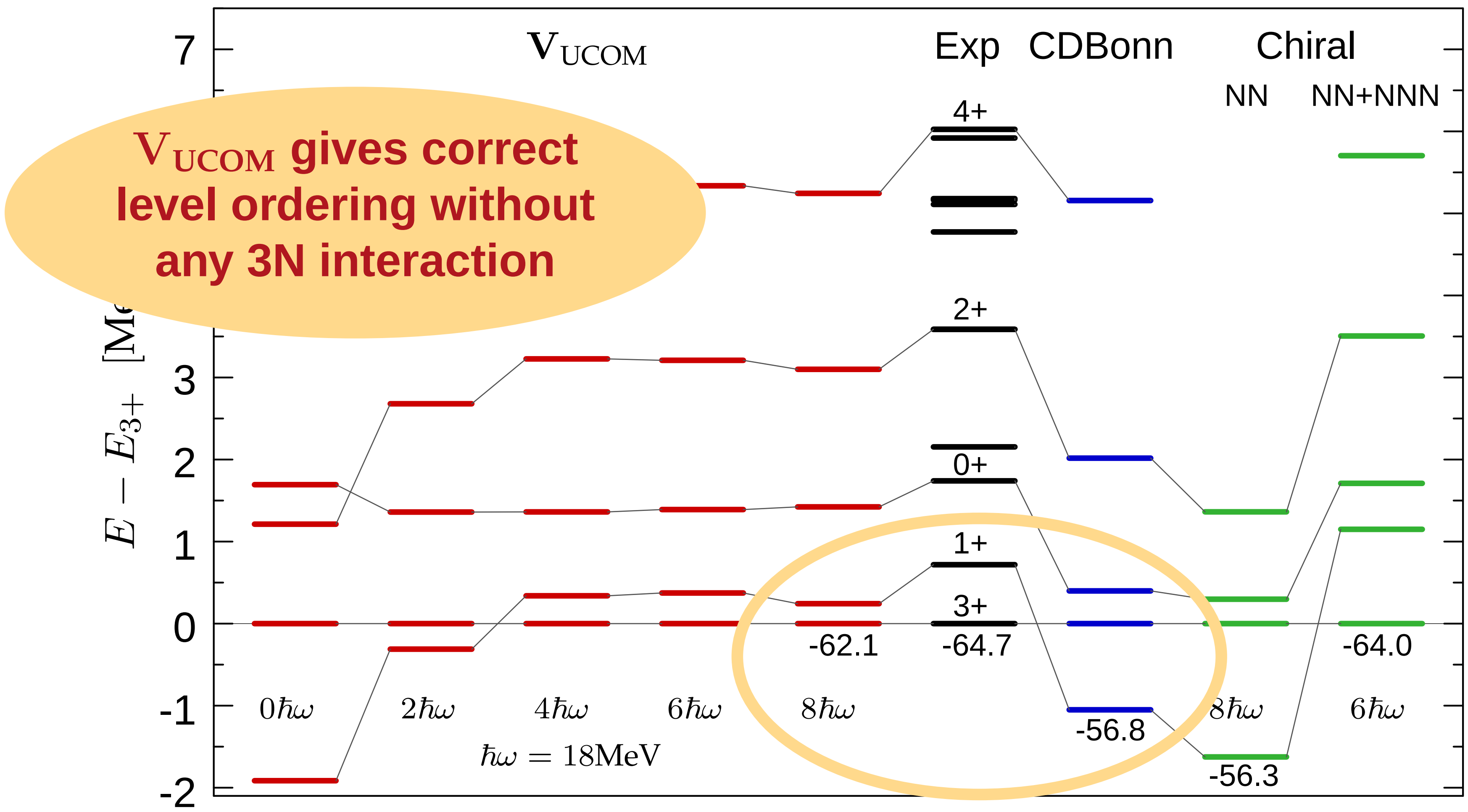
- **Tjon-line**: $E(^4\mathrm{He})$ vs. $E(^3\mathrm{H})$ for phase-shift equivalent NN-interactions
- same behavior for the SRG interaction as function of α

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, Piecuch, Gour — in preparation

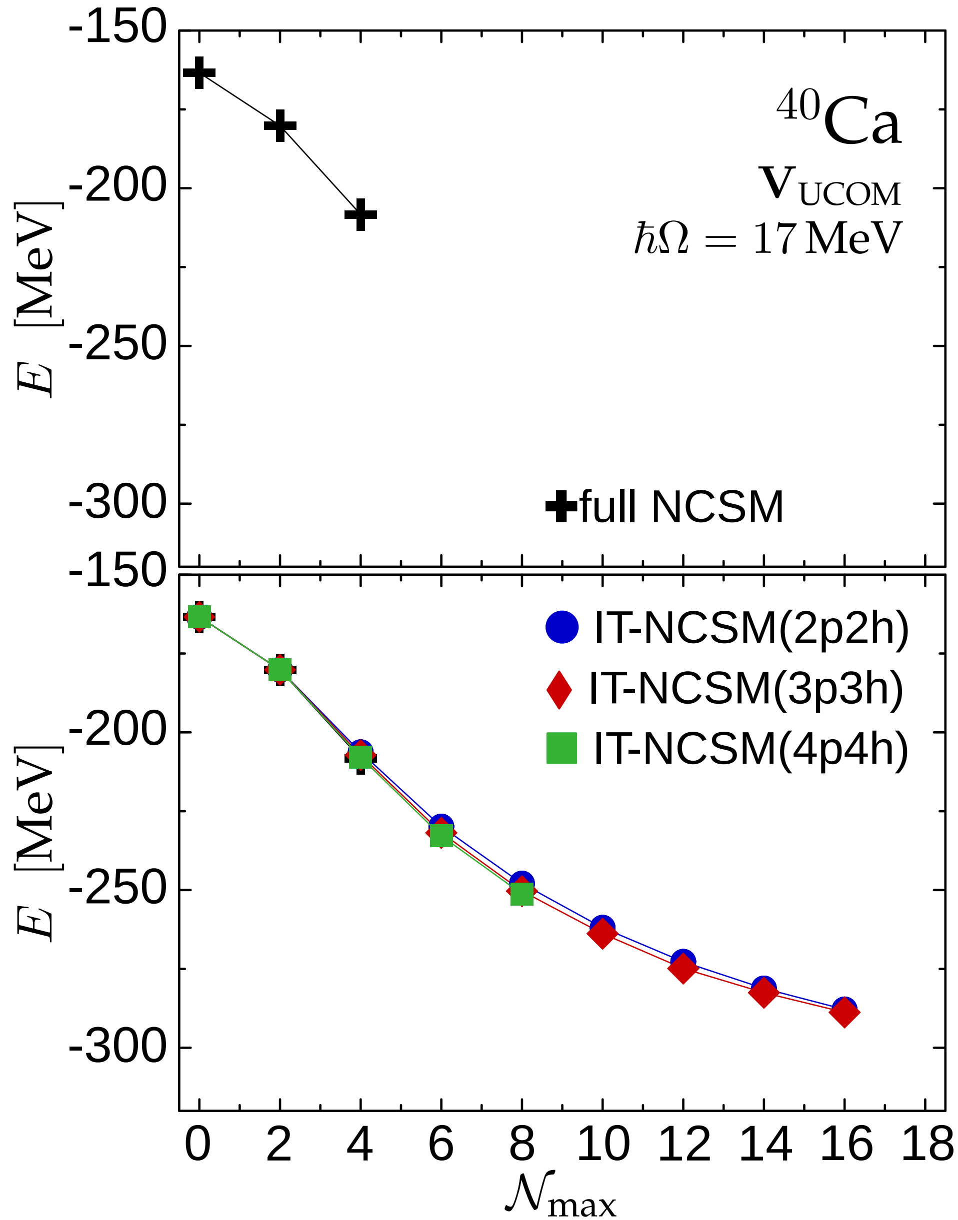
Roth — in preparation

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 Truncation: General Idea

- start with $\mathcal{N}_{\max}\hbar\omega$ **space** of the NCSM
  - ➔ separation of intrinsic and center-of-mass component of state

- **importance measure**: identify important basis states $|\Phi_\nu\rangle$ via first-order multiconfigurational perturbation theory

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

- **importance truncation**: starting from approximation $|\Psi_{\text{ref}}\rangle$ of target state, construct importance truncated space spanned by basis states with $|\kappa_\nu| \geq \kappa_{\min}$
  - ➔ contains 2p2h excitations with respect to $|\Psi_{\text{ref}}\rangle$ at most
  - ➔ perturbative measure entails NpNh hierarchy, i.e., higher-order NpNh states only enter in higher orders of PT

Importance Truncation: General Idea

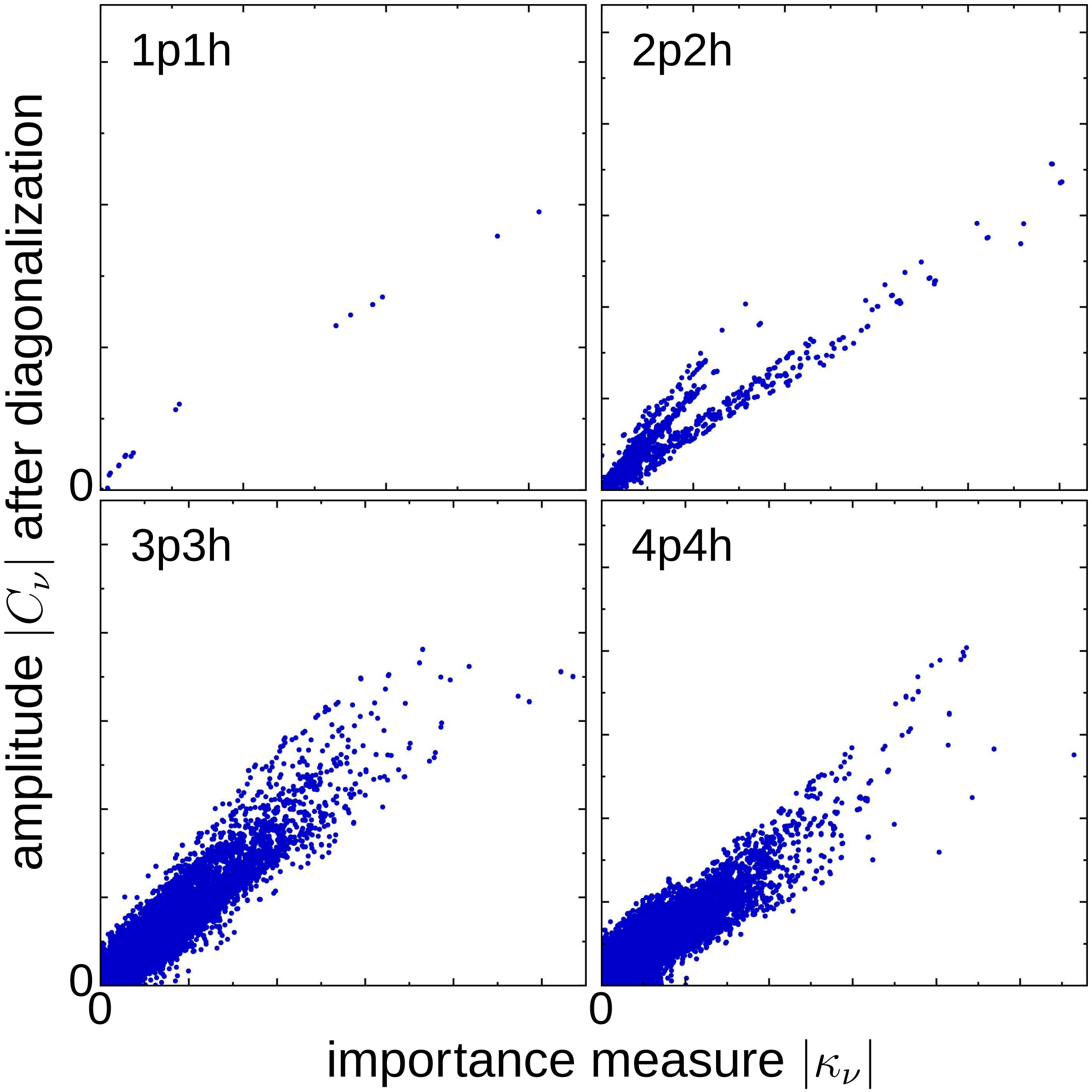
- solve **eigenvalue problem** in importance truncated space
  - ➔ rigorous variational upper bound

- **iterative scheme**: repeat construction of importance truncated model space using eigenstate as improved reference $|\Psi_{\text{ref}}\rangle$
  - ➔ recovers full $\mathcal{N}_{\max}\hbar\omega$ space after $A/2$ iterations in the limit $\kappa_{\min} \to 0$
  - ➔ typically 2 or 3 iterations to convergence

- **threshold extrapolation**: constrained extrapolation $\kappa_{\min} \to 0$ of energies recovers contribution of excluded configurations

- **perturbative estimates** and **Davidson corrections** for the contribution of the next iteration also possible

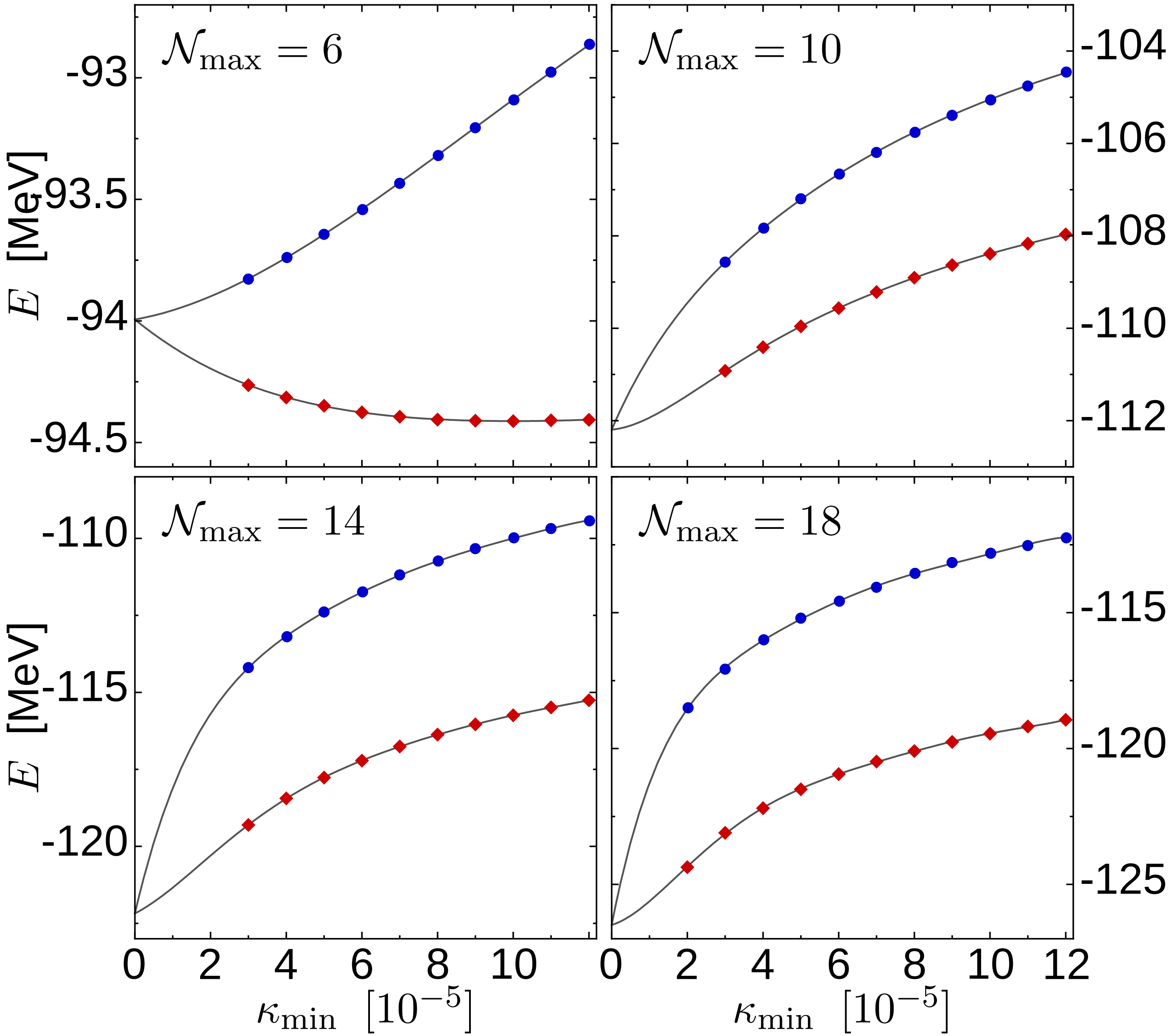
Technicalities: Importance Measure



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

^{16}O
$\mathbf{V}_{\mathrm{UCOM}}$
$\hbar\Omega = 22\,\mathrm{MeV}$
$\mathcal{N}_{\max} = 6$

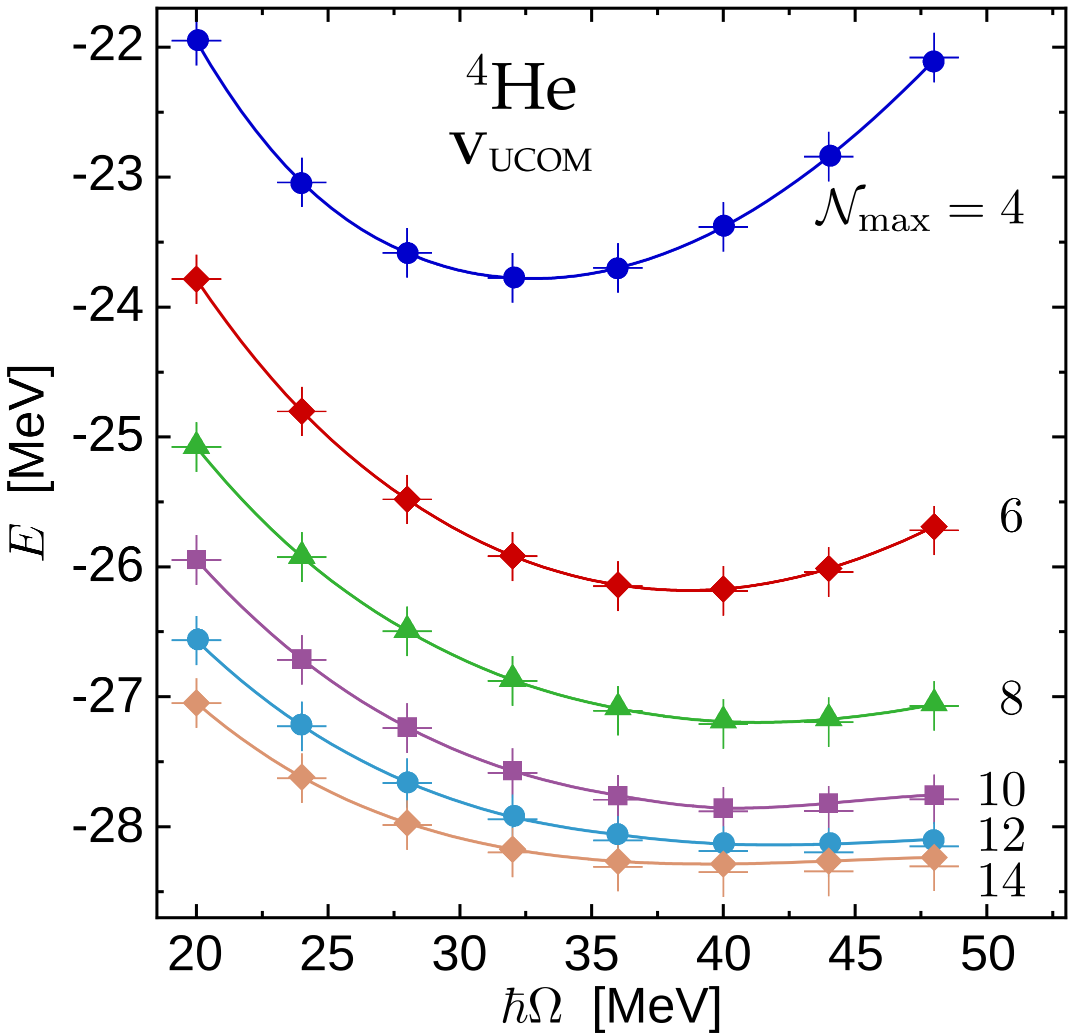
Technicalities: Threshold Extrapolation



- **smooth $\kappa_{\min}$-dependence** allows for robust extrapolation
- include perturbative estimate of excluded configurations for simultaneous **constrained extrapolation $\kappa_{\min} \to 0$**

^{16}O
$\mathbf{V}_{\text{UCOM}}$
$\hbar\Omega = 22\,\text{MeV}$

^{4}He: Importance Truncated NCSM

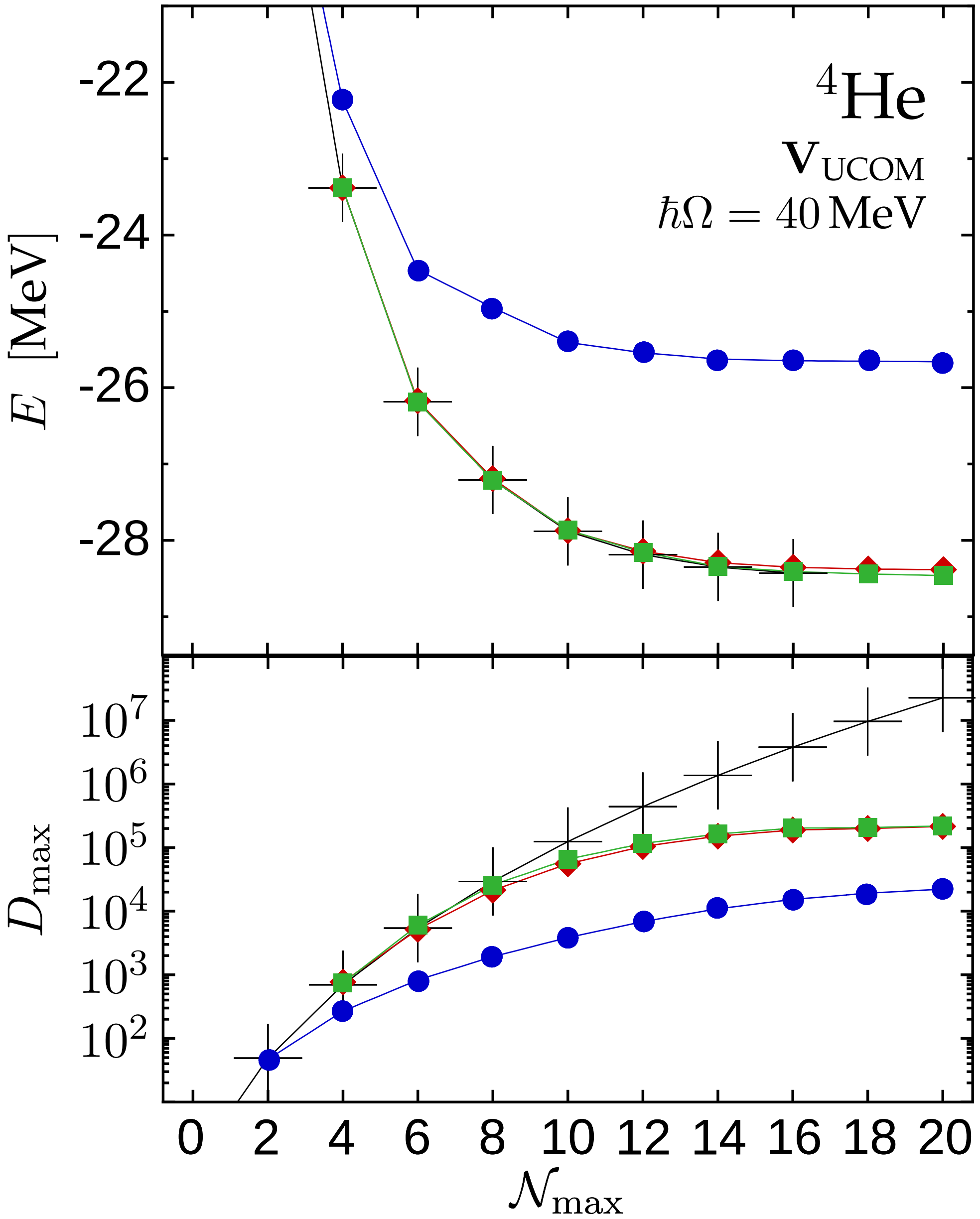


- **reproduces exact NCSM result** for all $\hbar\omega$ and $\mathcal{N}_{\max}$
- importance measure and threshold extrapolation are reliable
- no center-of-mass contamination of states

+ + · · · full NCSM

● ♦ · · · IT-NCSM(2 iter, 4p4h)

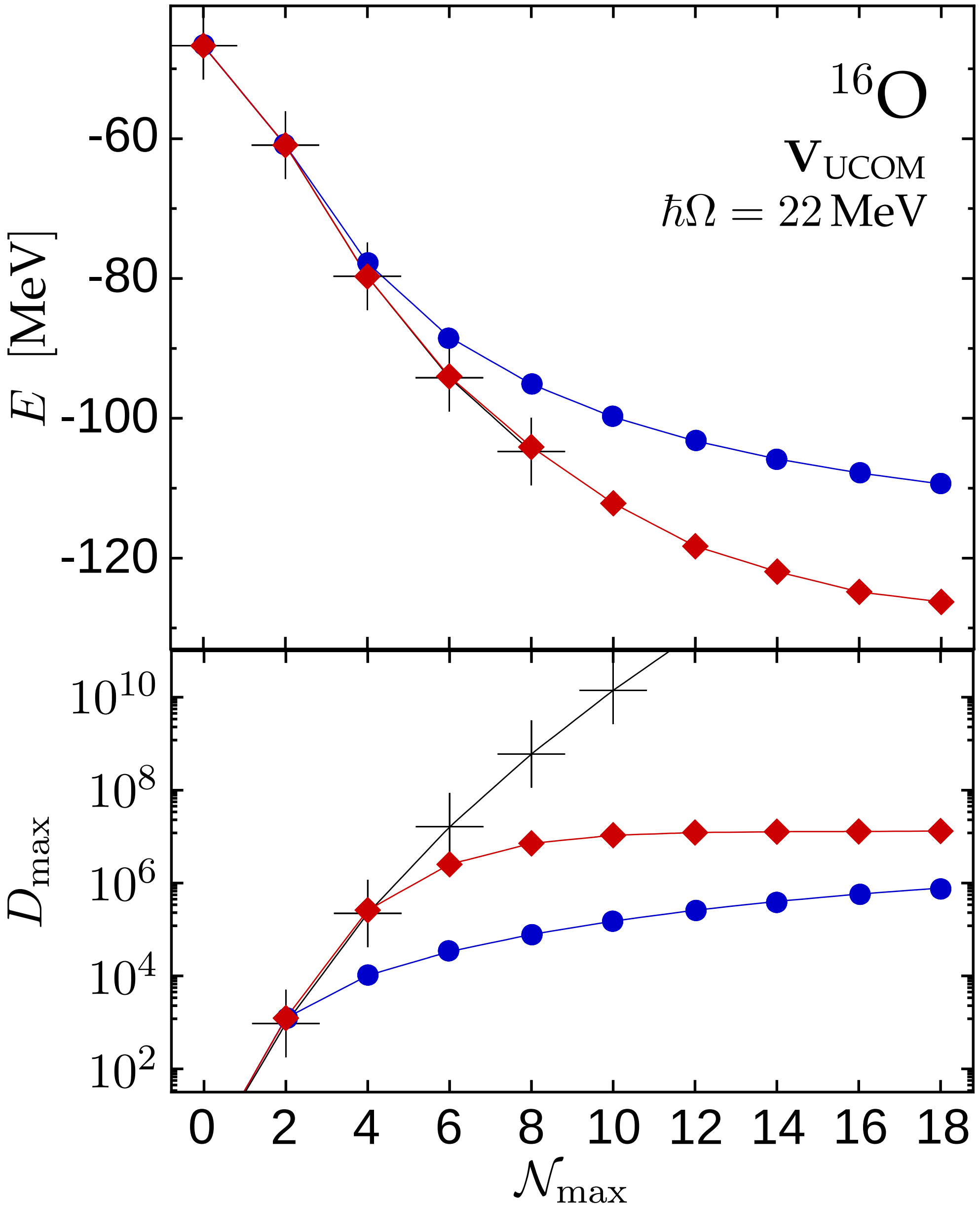
^{4}He: Importance Truncated NCSM



- **reproduces exact NCSM result** for all $\hbar\omega$ and $\mathcal{N}_{\text{max}}$
- iterations converge very fast
- reduction of basis by more than two orders of magnitude w/o loss of precision
- saturation of IT-NCSM dimension indicates convergence

+ full NCSM
● IT-NCSM(1 iter, 2p2h)
♦ IT-NCSM(2 iter, 4p4h)
■ IT-NCSM(3 iter, 4p4h)

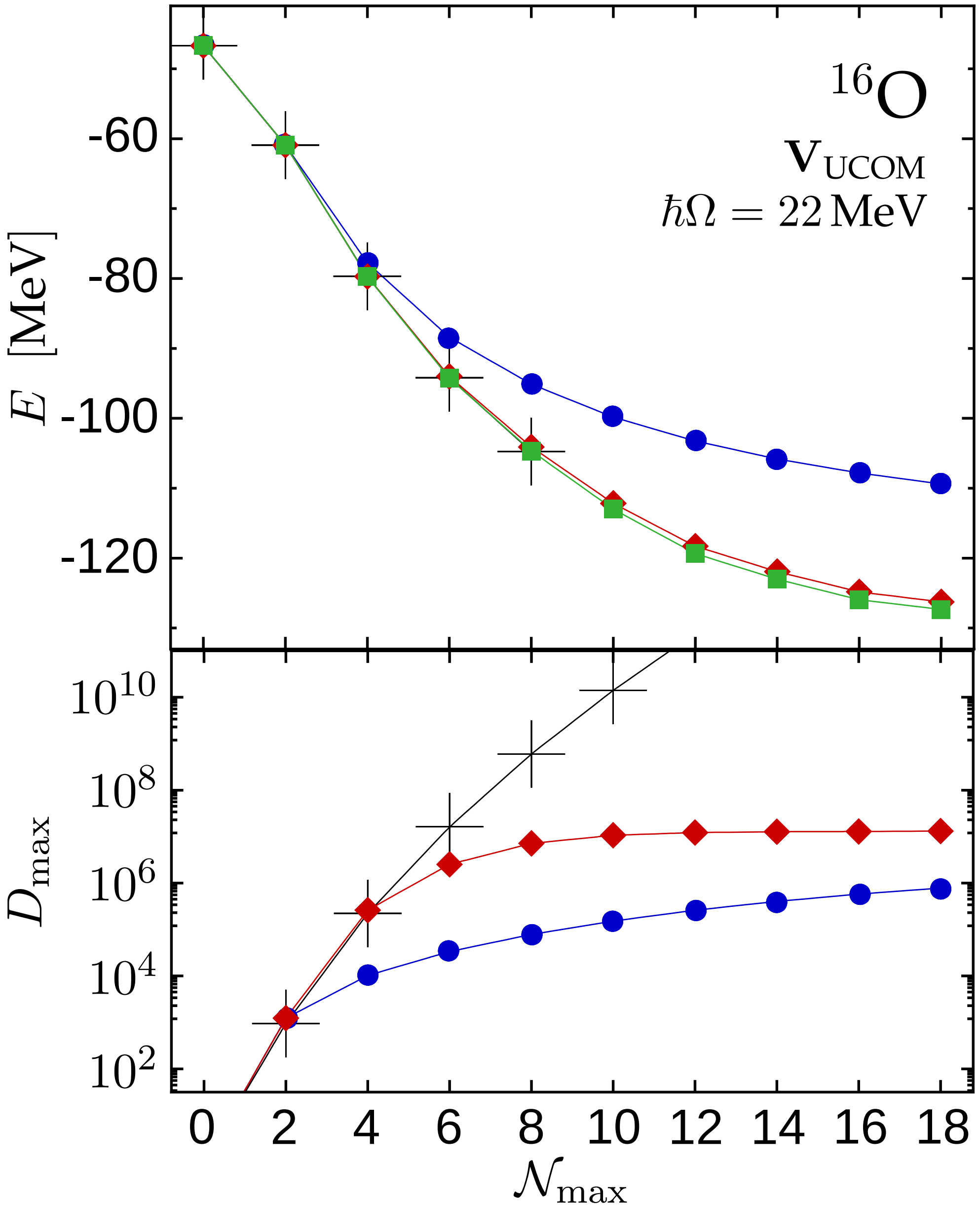
^{16}O: Importance Truncated NCSM



- **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

^{16}O: Importance Truncated NCSM



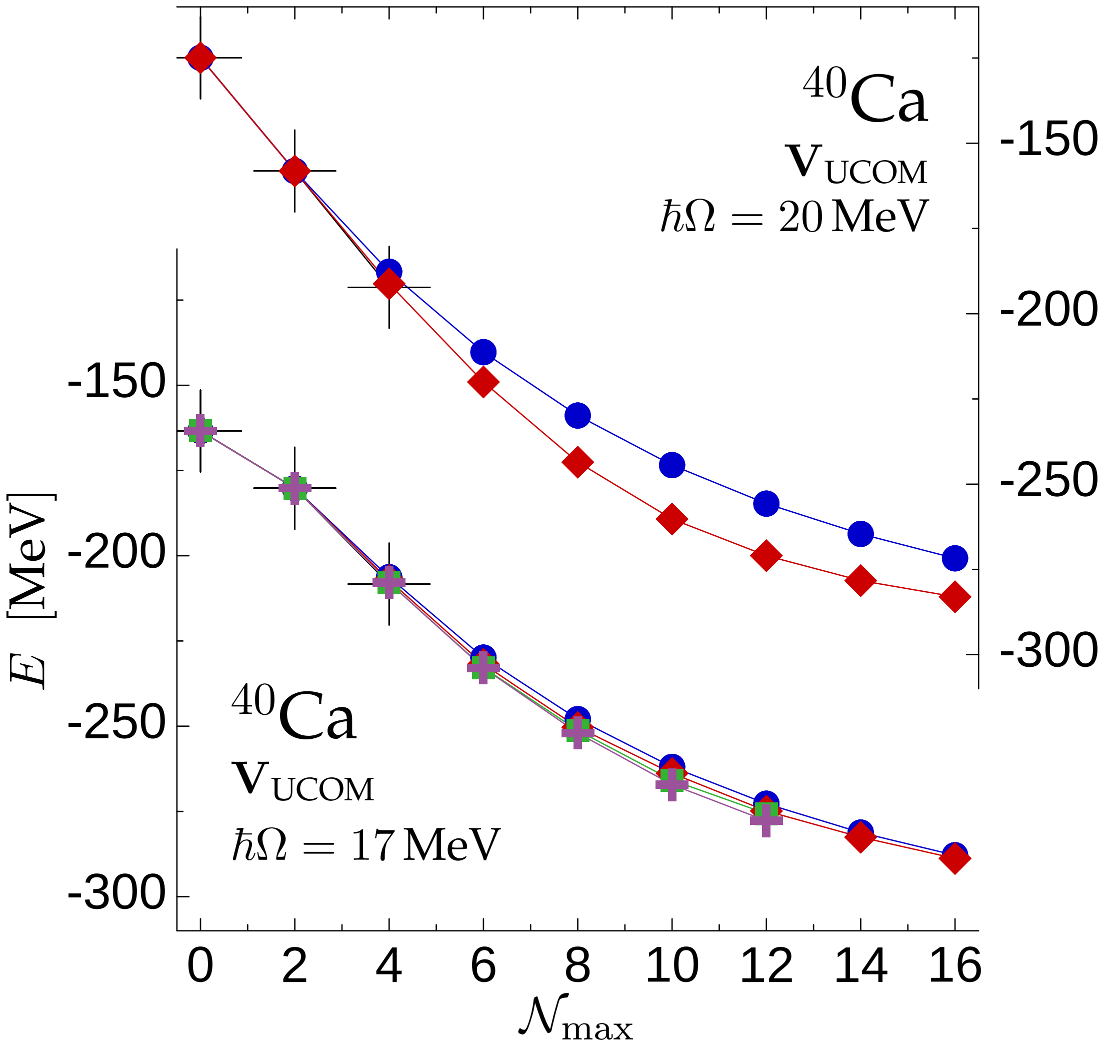
- extrapolation to $\mathcal{N}_{\text{max}} \to \infty$

$$E_{\text{IT-NCSM(2 iter)}} \approx -129 \pm 1\,\text{MeV}$$
$$E_{\text{IT-NCSM(2 iter)+MRD}} \approx -130 \pm 1\,\text{MeV}$$
$$E_{\text{exp}} = -127.6\,\text{MeV}$$

- $\mathbf{V}_{\text{UCOM}}$ predicts **reasonable binding energies** also for heavier nuclei

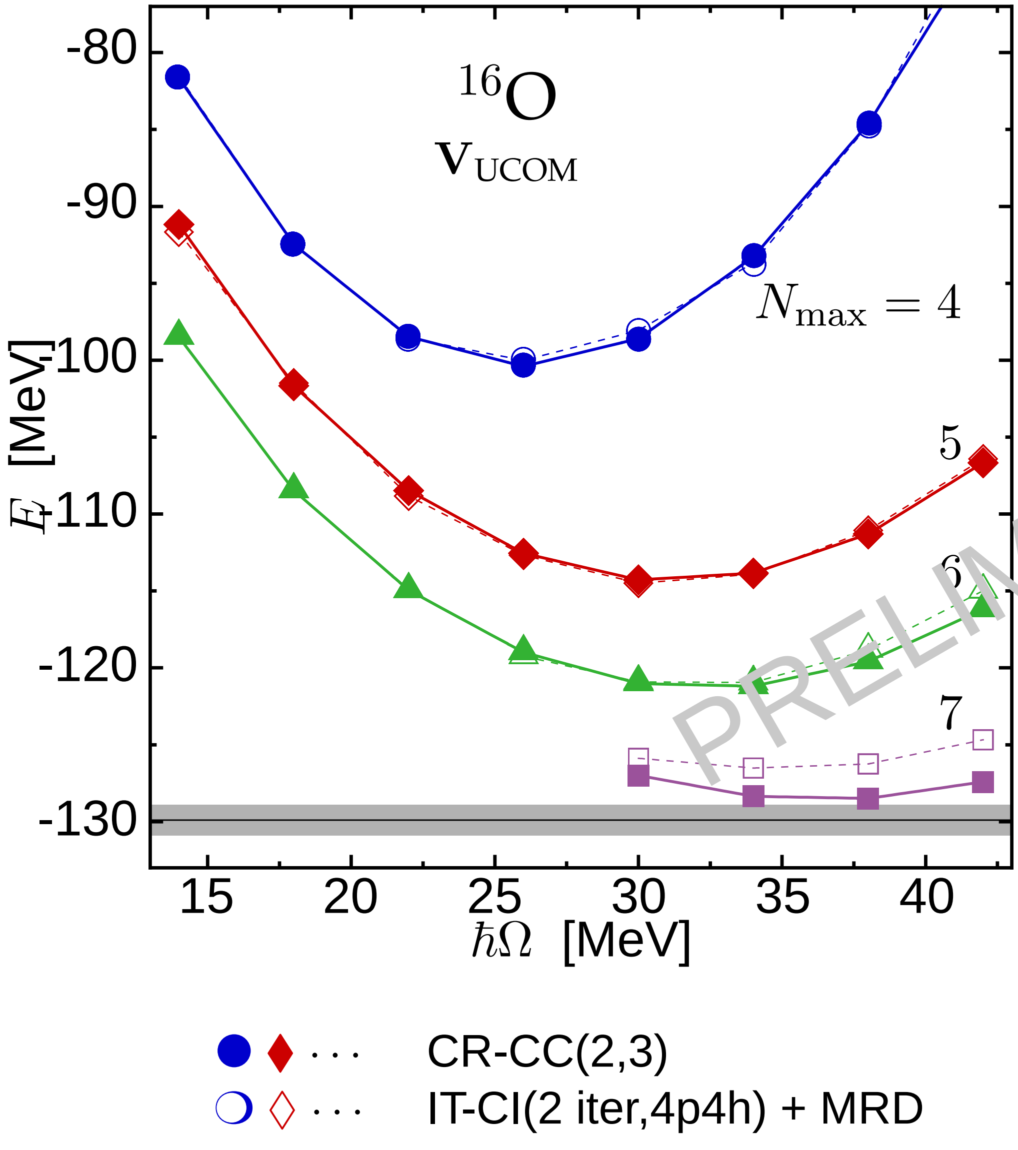
+ full NCSM
● IT-NCSM(1 iter, 2p2h)
♦ IT-NCSM(2 iter, 4p4h)
■ IT-NCSM(2 iter, 4p4h) + MRD

^{40}Ca: Importance Truncated NCSM



- **$16\hbar\Omega$ and more are feasible** for ^{40}Ca in IT-NCSM(2 iter)
- size of individual NpNh-contributions depends on $\hbar\Omega$
- result consistent with experimental binding energy

Direct Comparison: CC vs. IT-CI



in collaboration with J. Gour & P. Piecuch (MSU)

- **CR-CC vs. IT-CI**:
  - good agreement for all $\hbar\Omega$ and models spaces
  - lack of strict size extensivity in the IT-CI is irrelevant
- **CR-CC/IT-CI vs. IT-NCSM**:
  - CC/CI seems to tend to a lower binding energy than IT-NCSM
  - CC/CI suffer from center-of-mass contamination

IT-NCSM: Pros and Cons

- ✔ rigorously fulfills **variational principle** and Hylleraas-Undheim theorem
- ✔ **no sizable center-of-mass contamination** induced by IT in $\mathcal{N}_{\max}\hbar\Omega$ space
- ✔ constrained **threshold extrapolation** $\kappa_{\min} \to 0$ recovers contribution of excluded configurations efficiently and accurately
- ✔ **perturbative correction** and Davidson correction for perturbative energy correction can be used
- ✔ **compatible with shell-model**: excited states and angular-momentum projection via Lanczos, eigenstates in shell-model representation, computation of observables

- ✘ only **approximate size-extensivity** if working with few iterations
- ✘ computationally still demanding

Perspectives

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

■ thanks to my group & my collaborators

- S. Binder, H. Hergert, M. Hild, J. Langhammer, P. Papakonstantinou, A. Popa, S. Reinhardt, F. Schmitt, F. Wagner, A. Zapp

  Institut für Kernphysik, TU Darmstadt

- P. Navrátil

  Lawrence Livermore National Laboratory, USA

- P. Piecuch, J. Gour

  Michigan State University, USA

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

  Gesellschaft für Schwerionenforschung (GSI)

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