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

From QCD to Nuclear Structure

Nuclear Structure

Low-Energy QCD

From QCD to Nuclear Structure

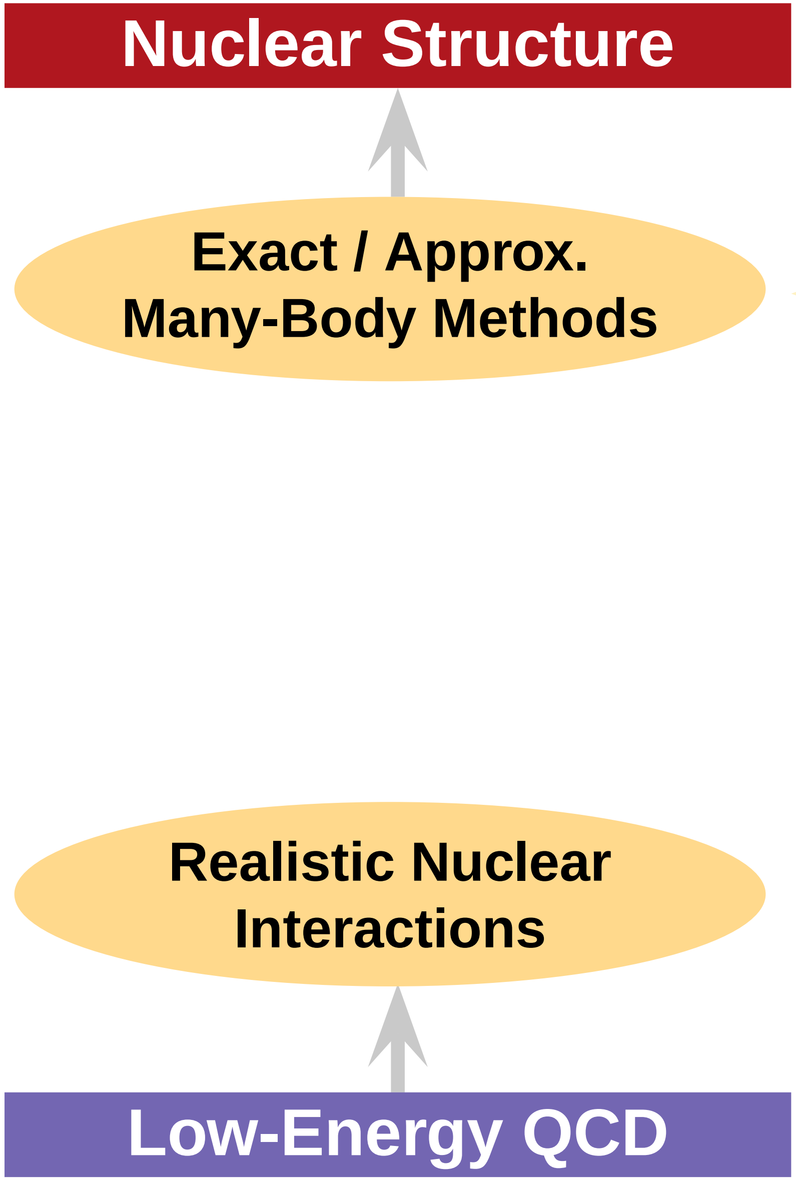
Nuclear Structure

Realistic Nuclear Interactions

Low-Energy QCD

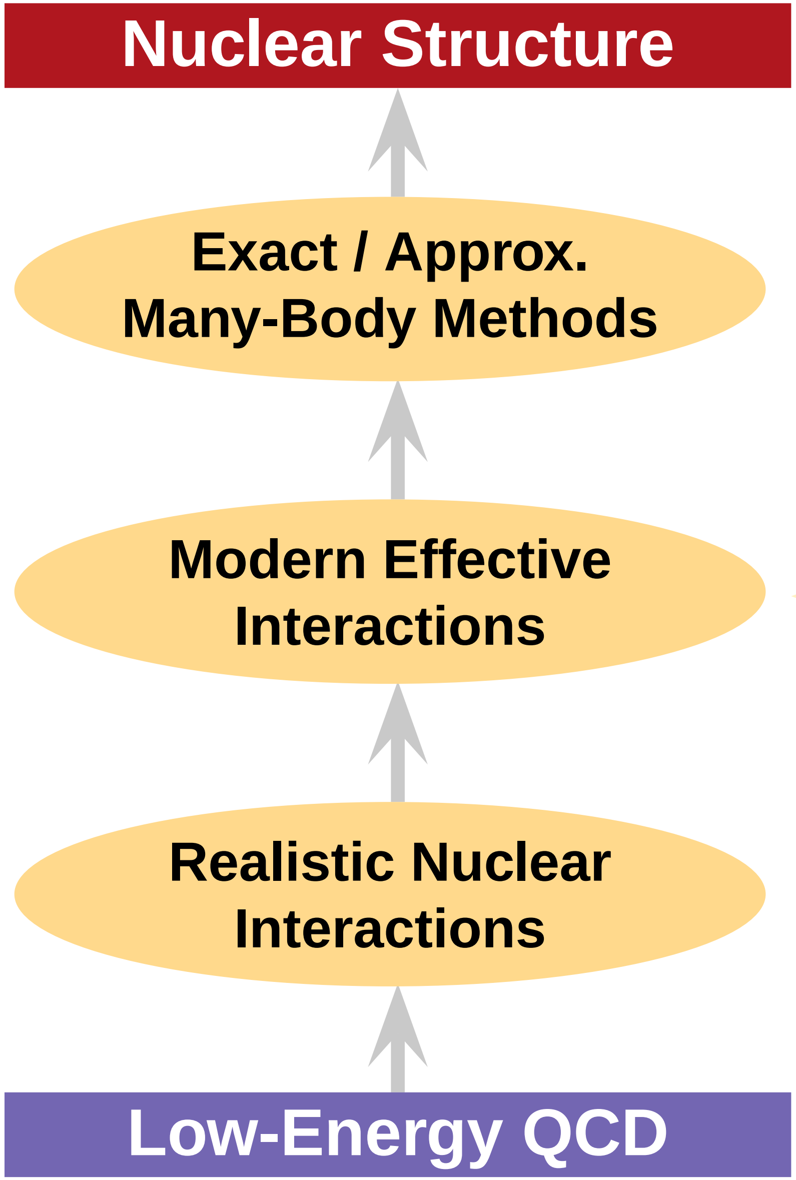
- chiral interactions: consistent NN & 3N interaction derived within χEFT
- traditional NN-interactions: Argonne V18, CD Bonn,...
- reproduce experimental NN phase-shifts with high precision
- induce strong short-range central & tensor correlations

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
- 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)

... also known as

Project 'Bohrloch'

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
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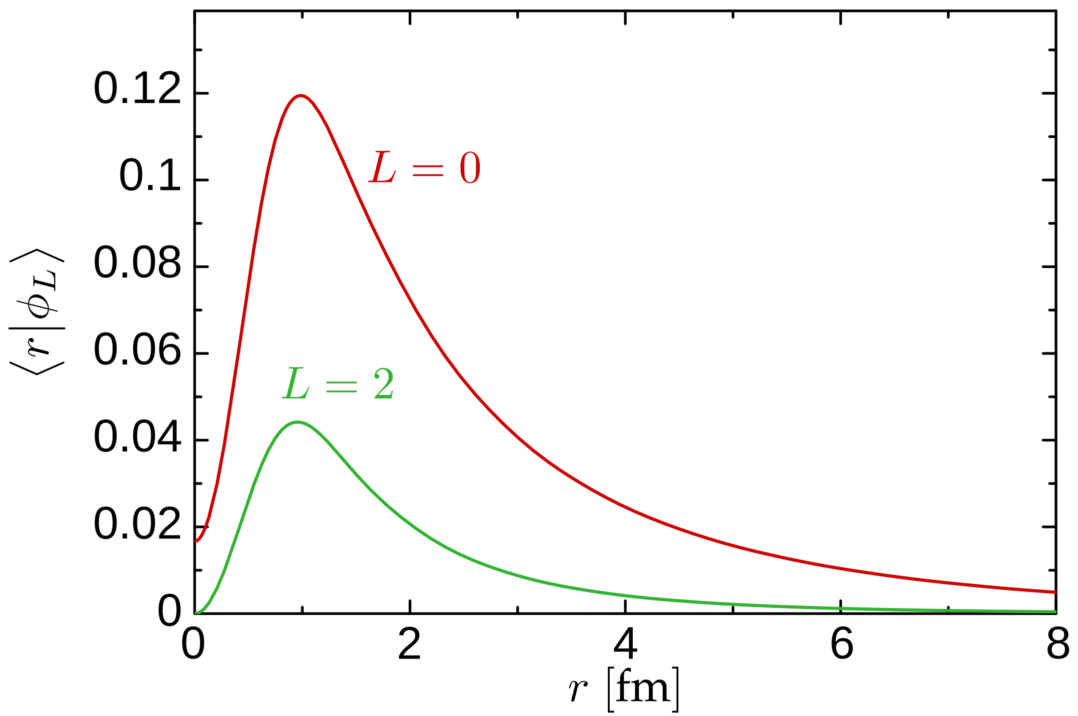
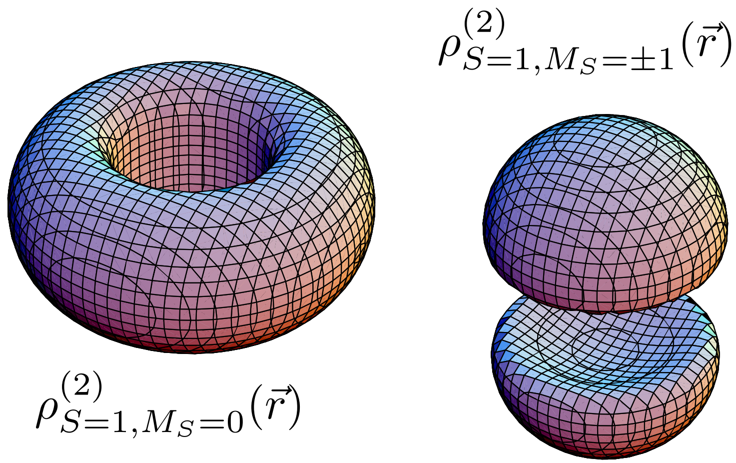
Deuteron: Manifestation of Correlations



- **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

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

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

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

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)

Bohrloch – 14

Hans Feldmeier
early 1996

Korrelierte Wellenfunktion (Index ℓm weggelassen)

$$x\,\chi(x) = \left(\frac{dR_-}{dx}\right)^{1/2} R_-(x)\,\varphi(R_-(x))$$

$$\left.\begin{aligned} R_-(x) &:= R\big(Y(x)-1\big) \\ R_+(r) &:= R\big(Y(r)+1\big) \end{aligned}\right\} \rightsquigarrow \left\{\begin{aligned} R_-\big(R_+(r)\big) &= r \\ R_+\big(R_-(x)\big) &= x \end{aligned}\right.$$

R_+ invers zu R_-

$$\left.\begin{aligned} R'_-(x) &:= \frac{dR_-(x)}{dx} = \frac{S(R_-(x))}{S(x)} \\ R'_+(r) &:= \frac{dR_+(r)}{dr} = \frac{S(R_+(r))}{S(r)} \end{aligned}\right\} \rightsquigarrow R'_-(x) = \frac{1}{R'_+(r)}$$

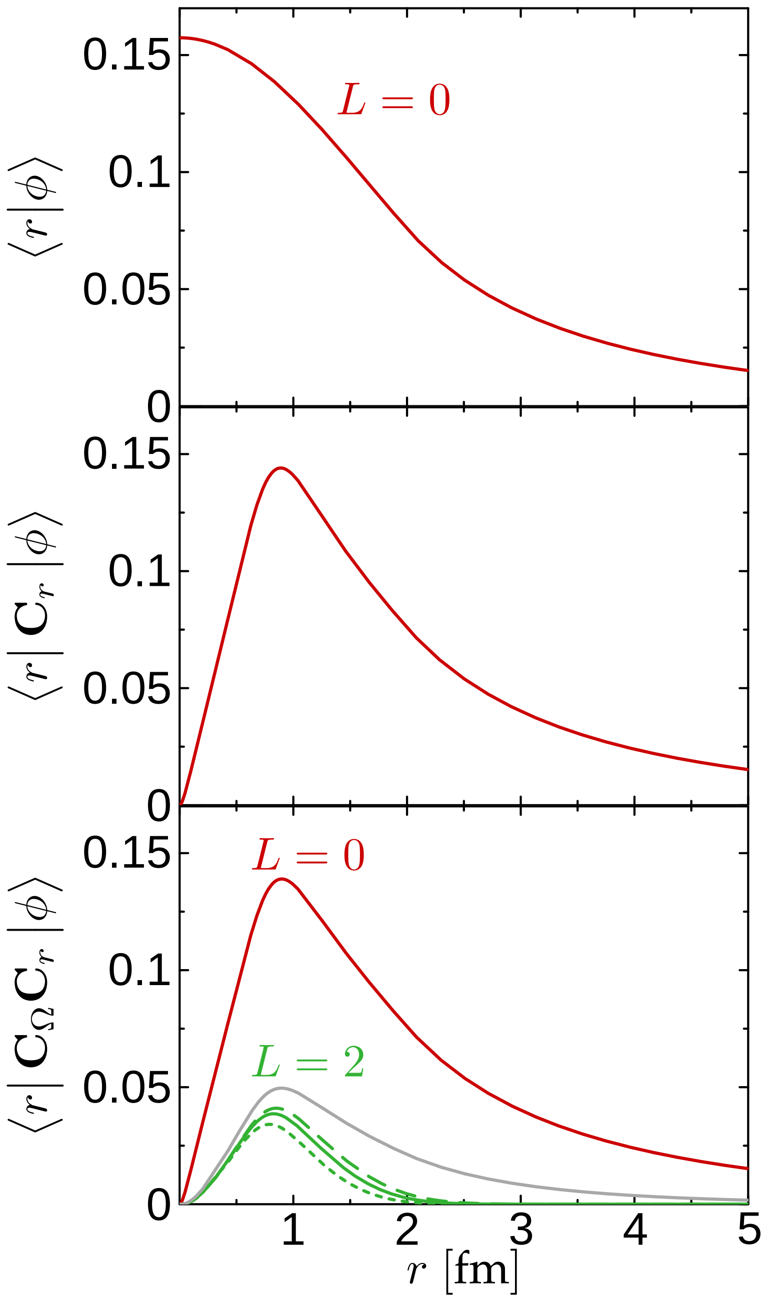
wobei $r = R_-(x)$

Koordinatentransformation:

$r = R_-(x)$

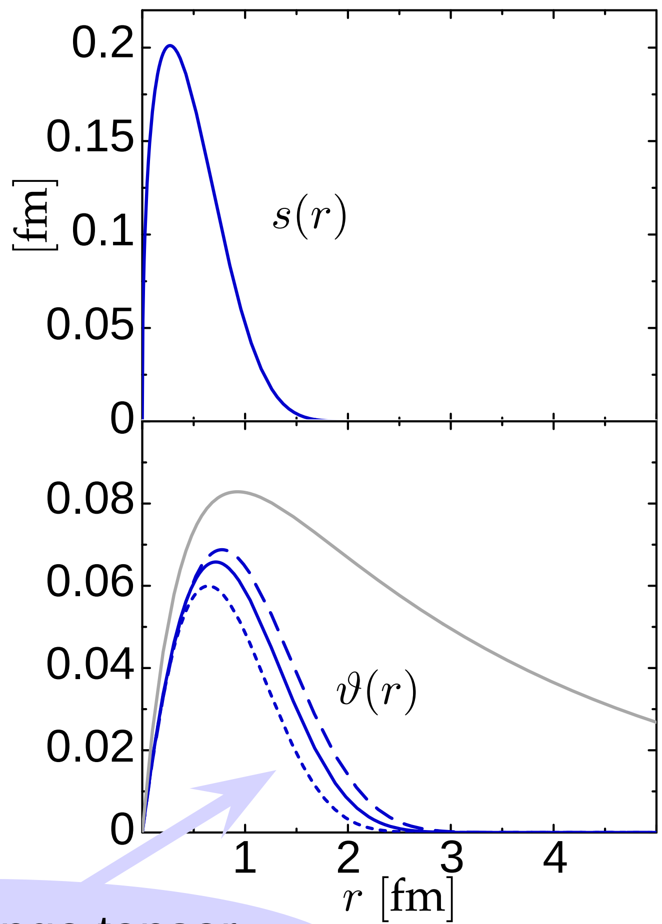
$x = R_+(r) \qquad dx = R'_+(r)\,dr$

Correlated States: The Deuteron



central correlations

tensor correlations



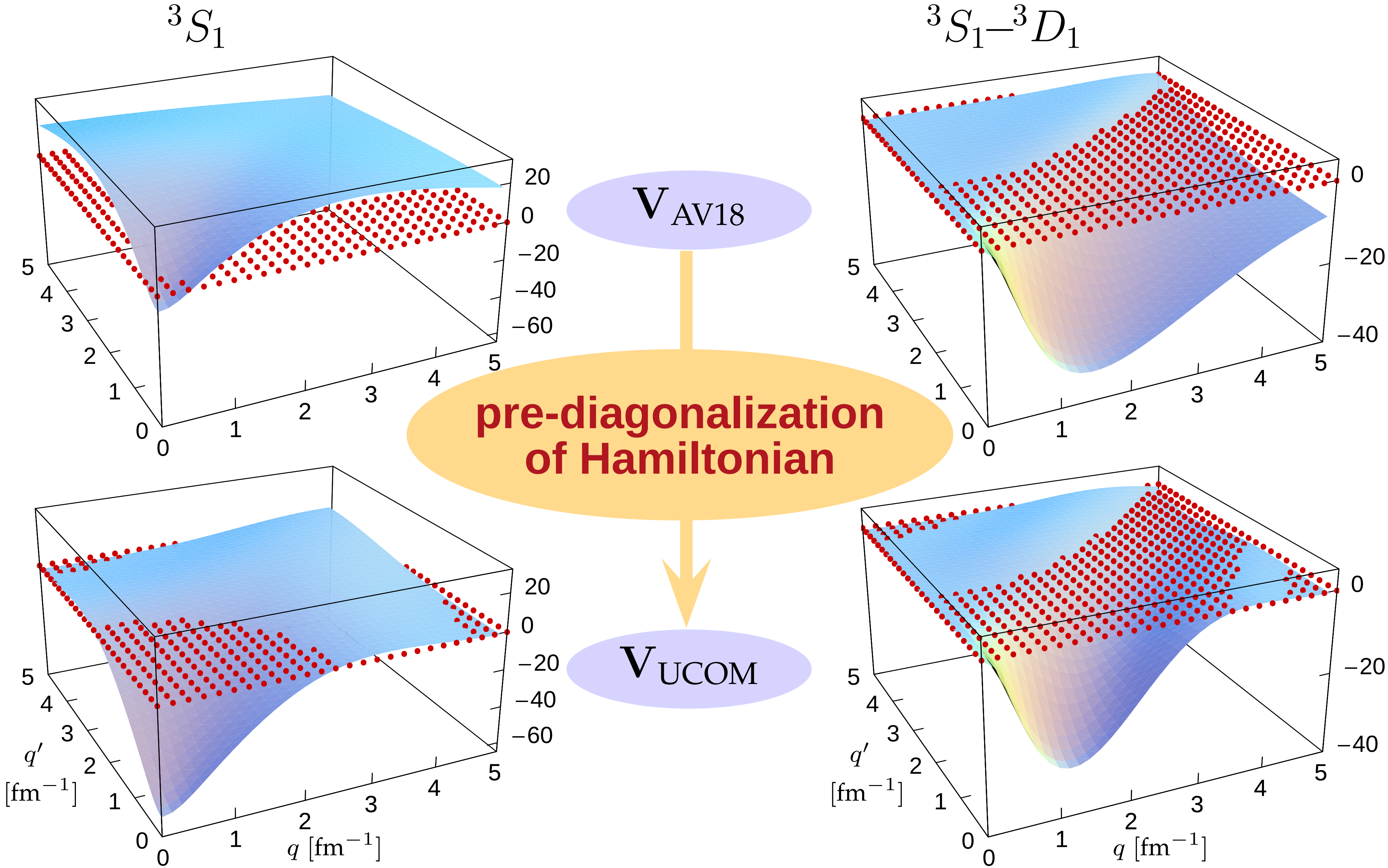
only short-range tensor correlations treated by $\mathbf{C}_\Omega$

Correlated Interaction: V_{UCOM}

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

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

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

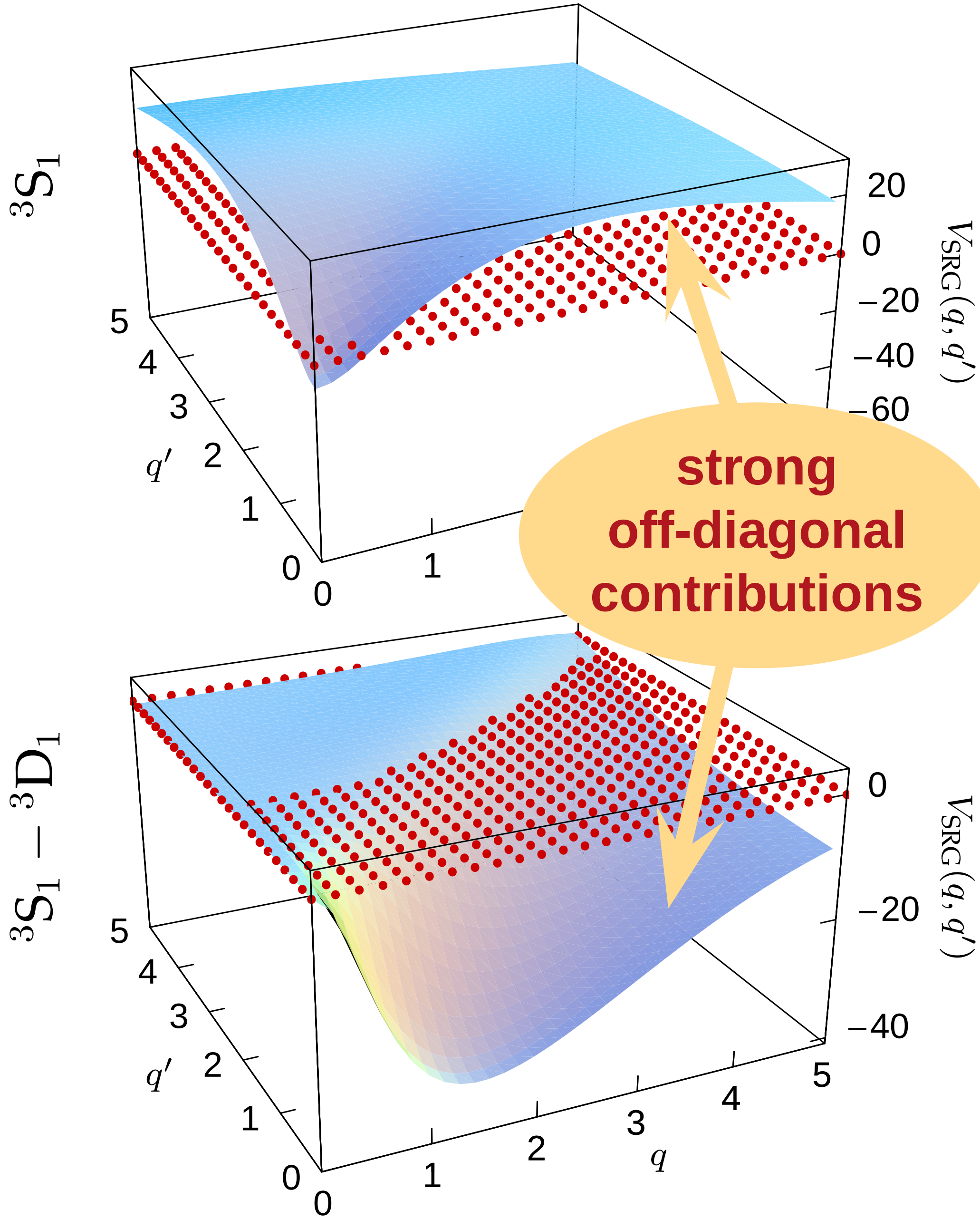
- dynamical generator defined as commutator with the operator in whose eigenbasis $\mathbf{H}$ shall be diagonalized

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

UCOM vs. SRG

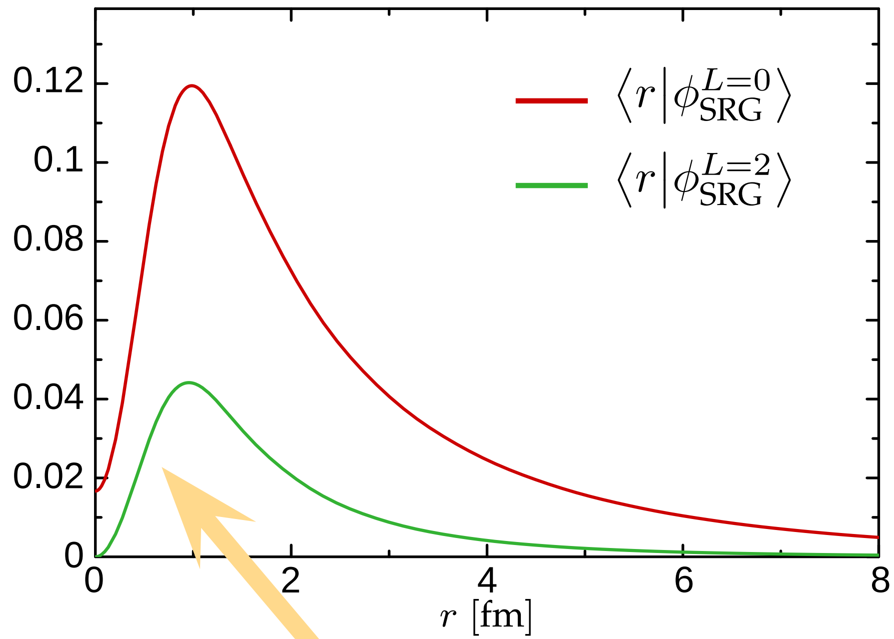
$\boldsymbol{\eta}(0)$ has the same structure as the UCOM generators g_r and g_Ω

SRG Evolution: The Deuteron



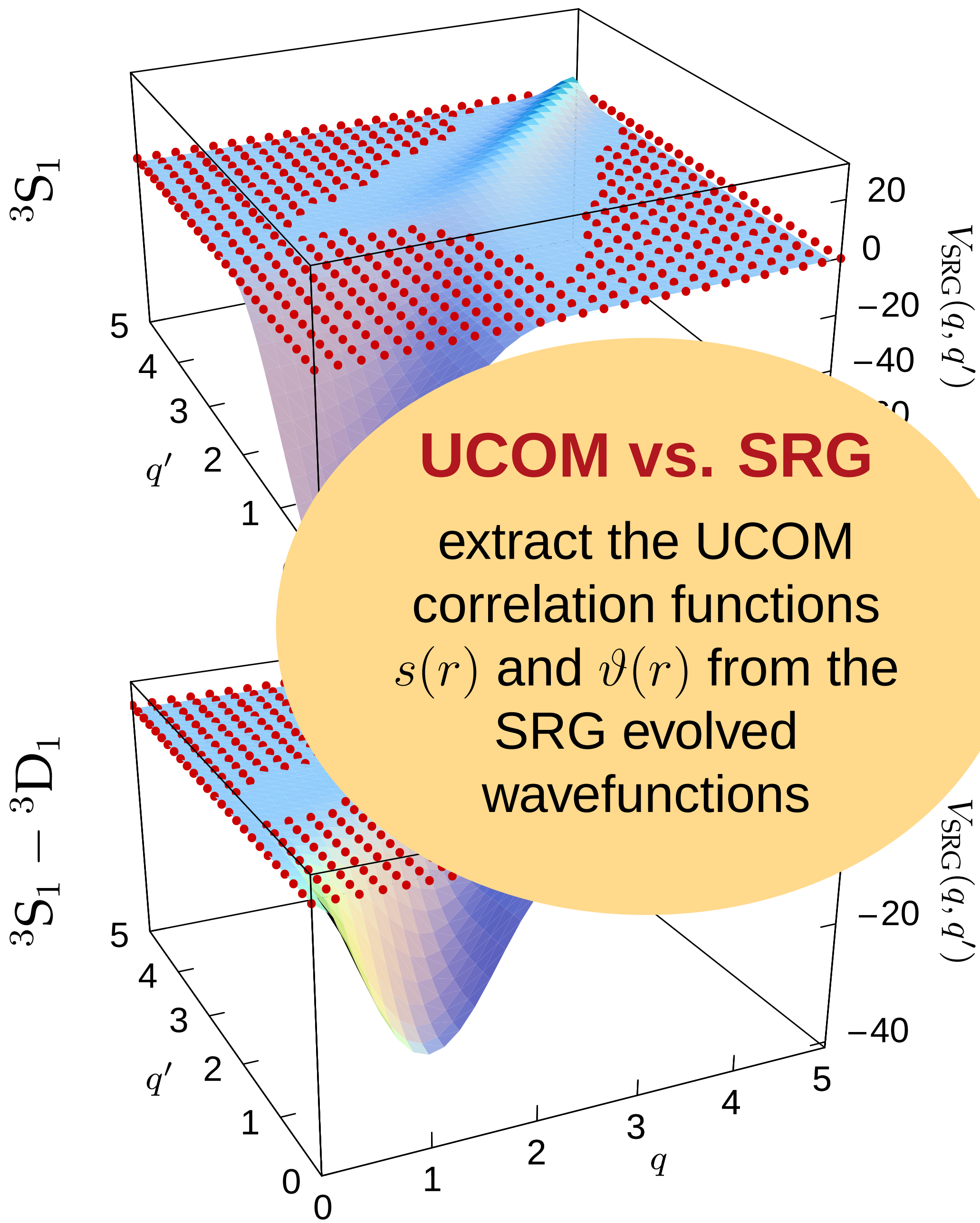
strong off-diagonal contributions

Argonne V18



short-range central & tensor correlations

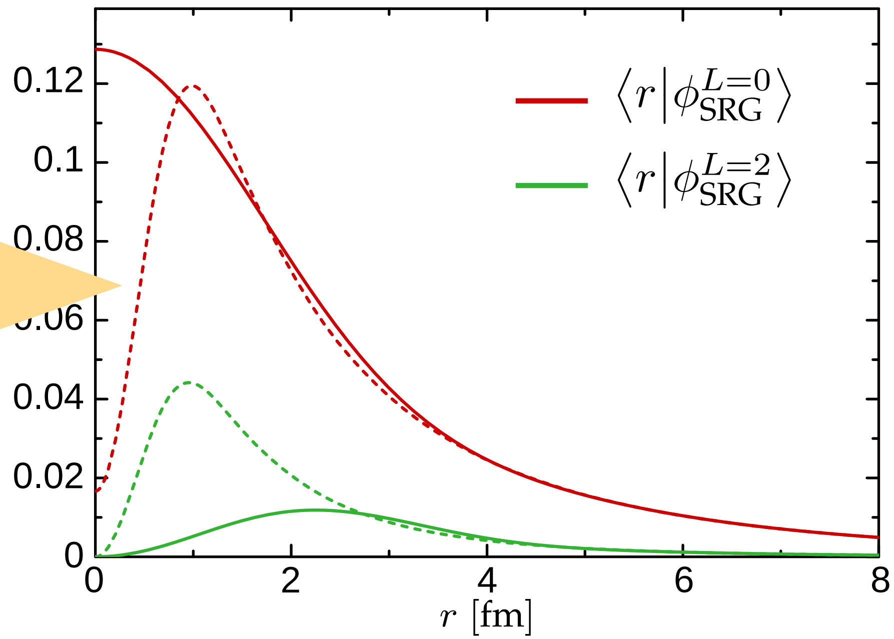
SRG Evolution: The Deuteron



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

UCOM vs. SRG

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



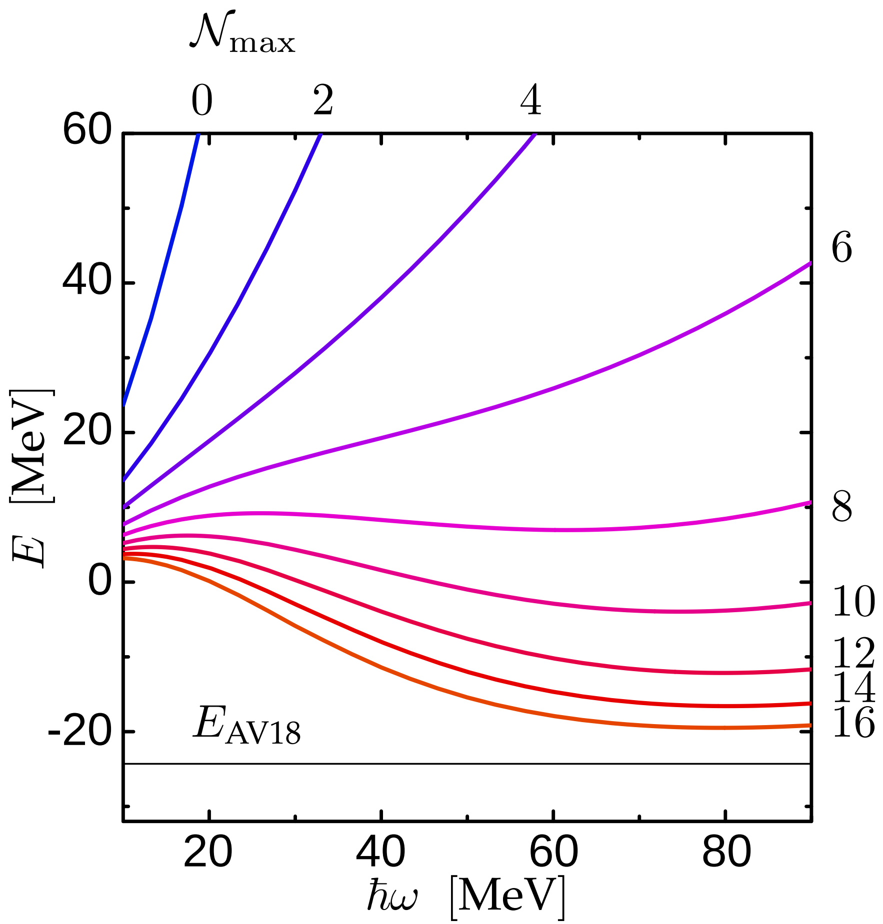
Exact Many-Body Methods

No-Core Shell Model

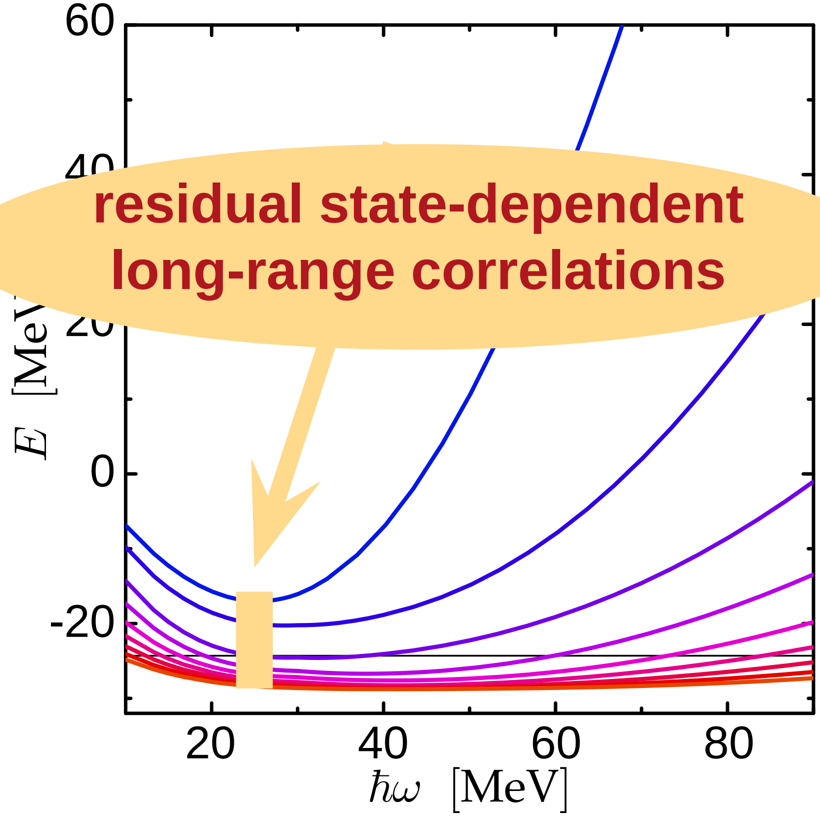
Roth et al. — Phys. Rev. C 72, 034002 (2005)
Roth & Navrátil — in preparation

^{4}He: Convergence

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

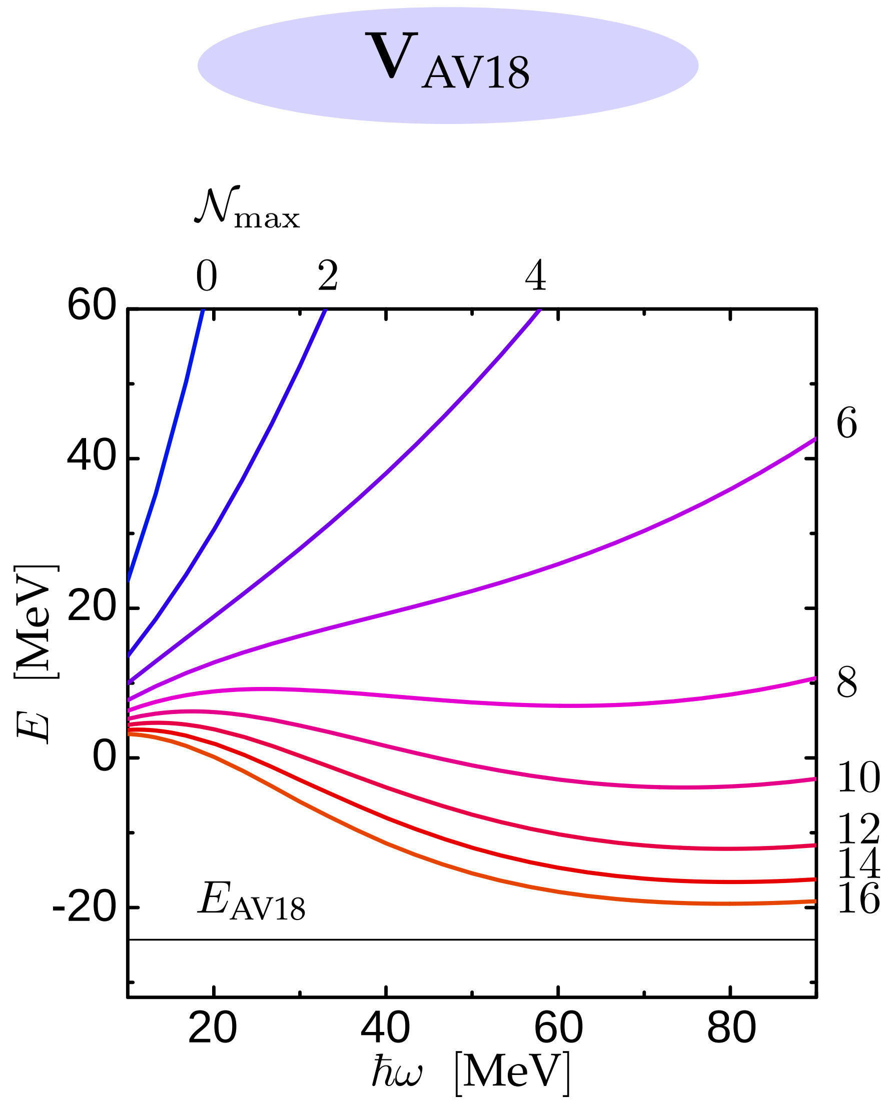


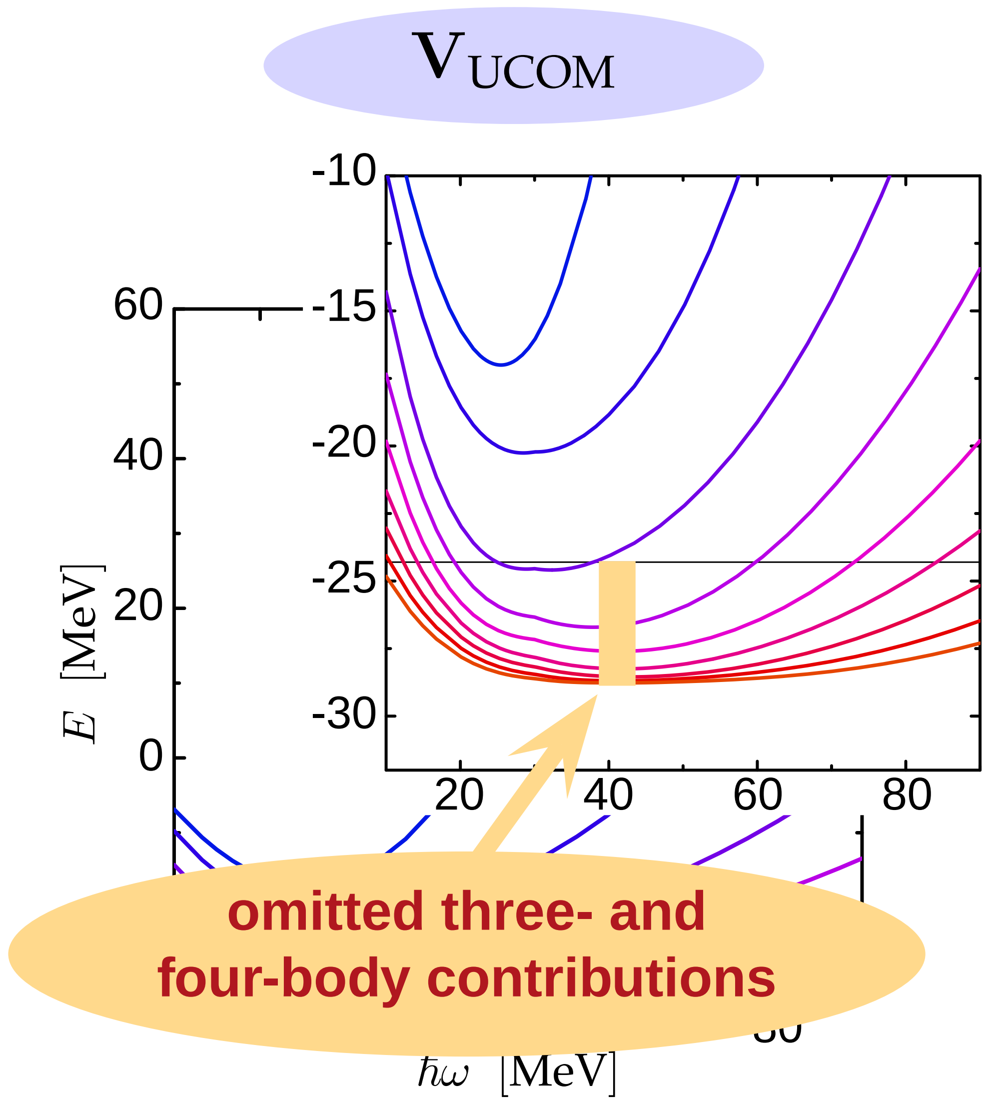
$\mathbf{V}_{\mathrm{UCOM}}$



residual state-dependent long-range correlations

^{4}He: Convergence





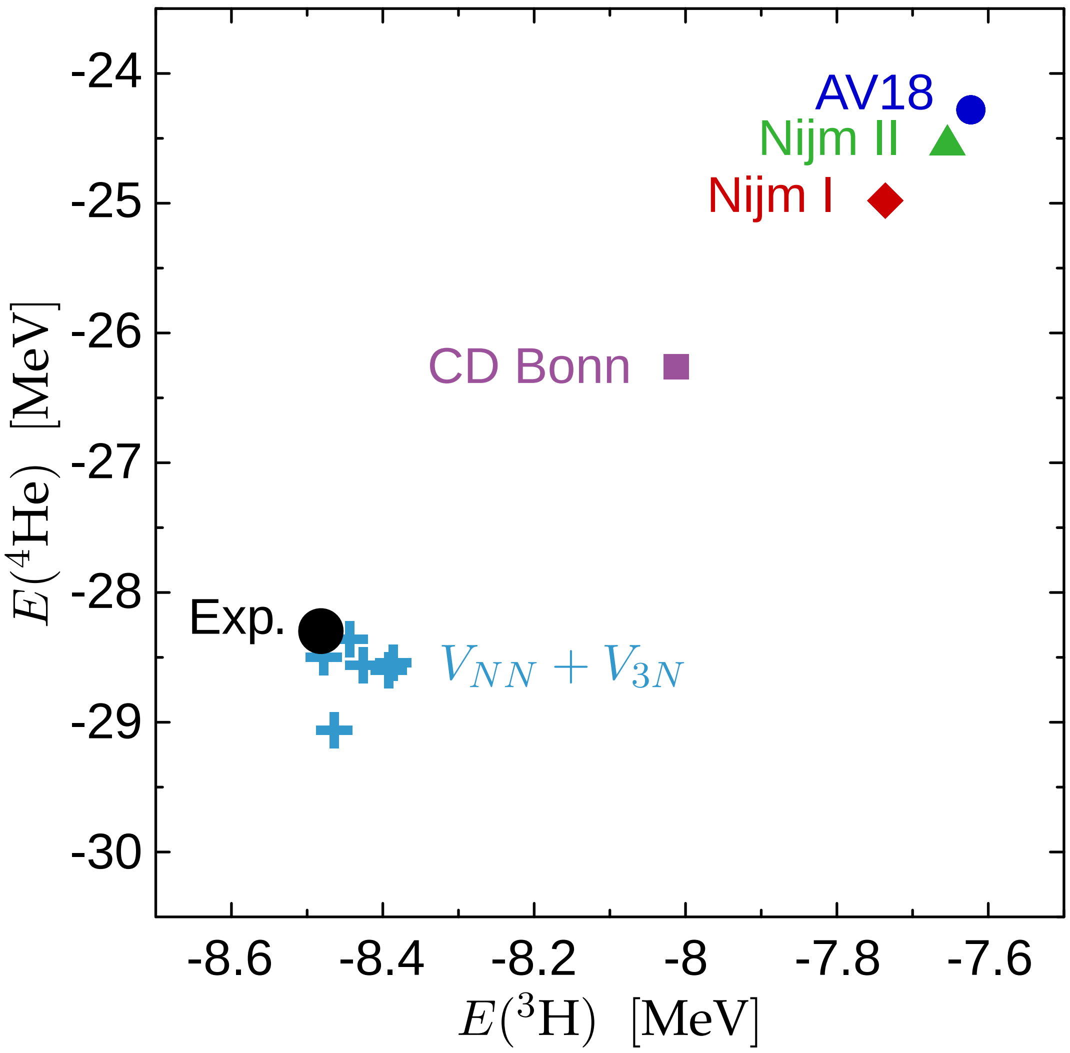
Three-Body Interactions — Remarks

Correlated Hamiltonian in Many-Body Space

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

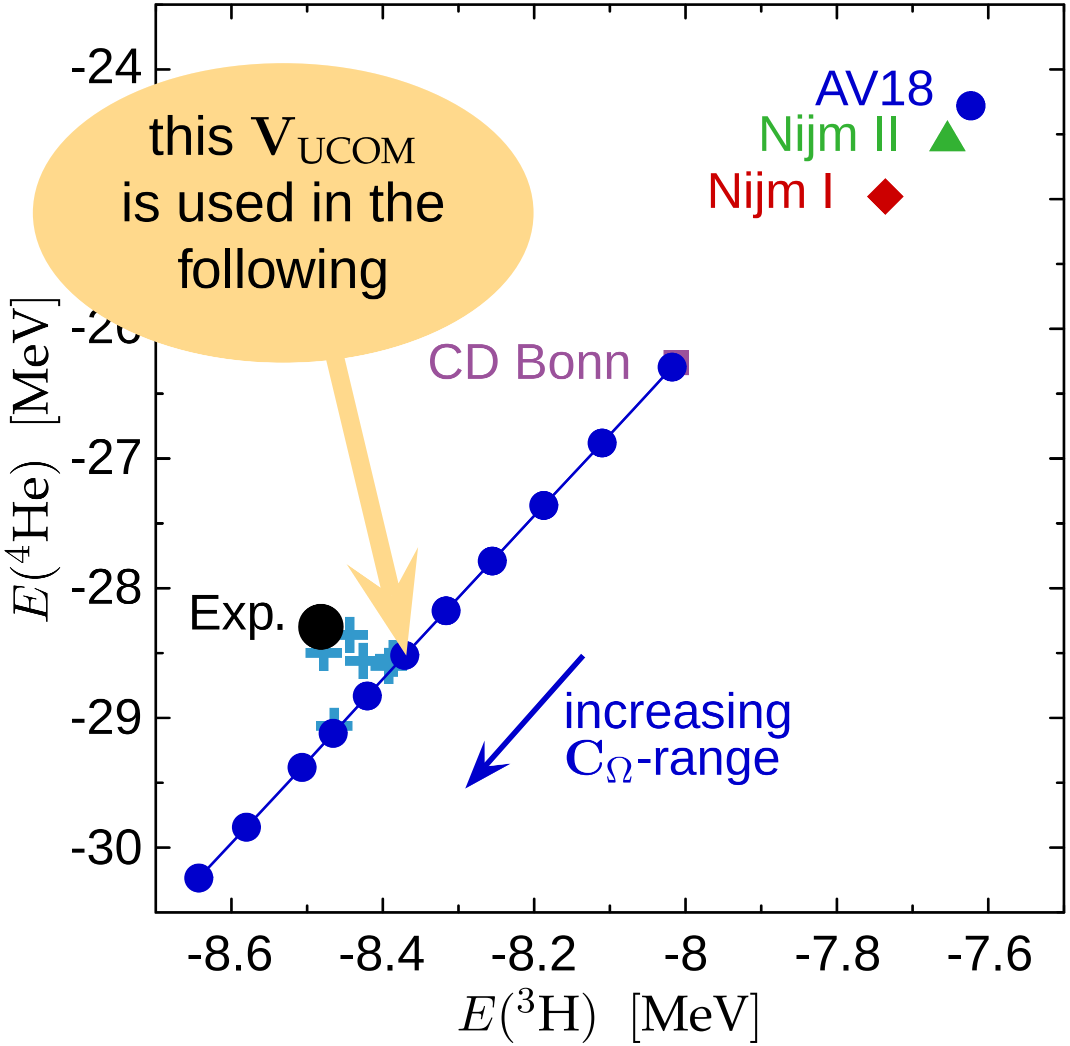
- there is no ‘the three-body interaction’
- phase-shift conserving unitary transformations can be used to **convert between two- and three-body interactions**
- we can try to **minimize the net contribution** of three-body terms, e.g., to the energies

Three-Body Interactions — Tjon Line



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

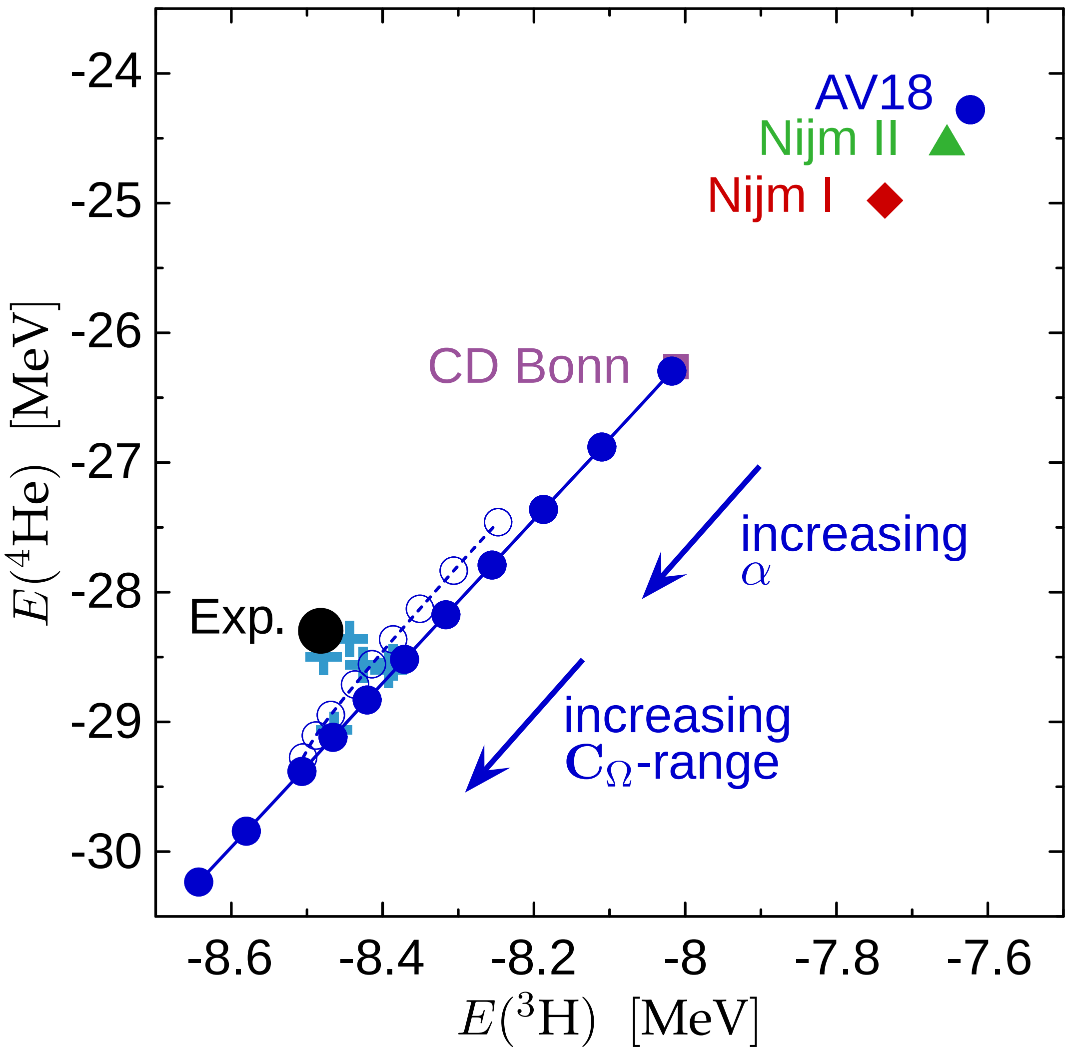
Three-Body Interactions — Tjon Line



- **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

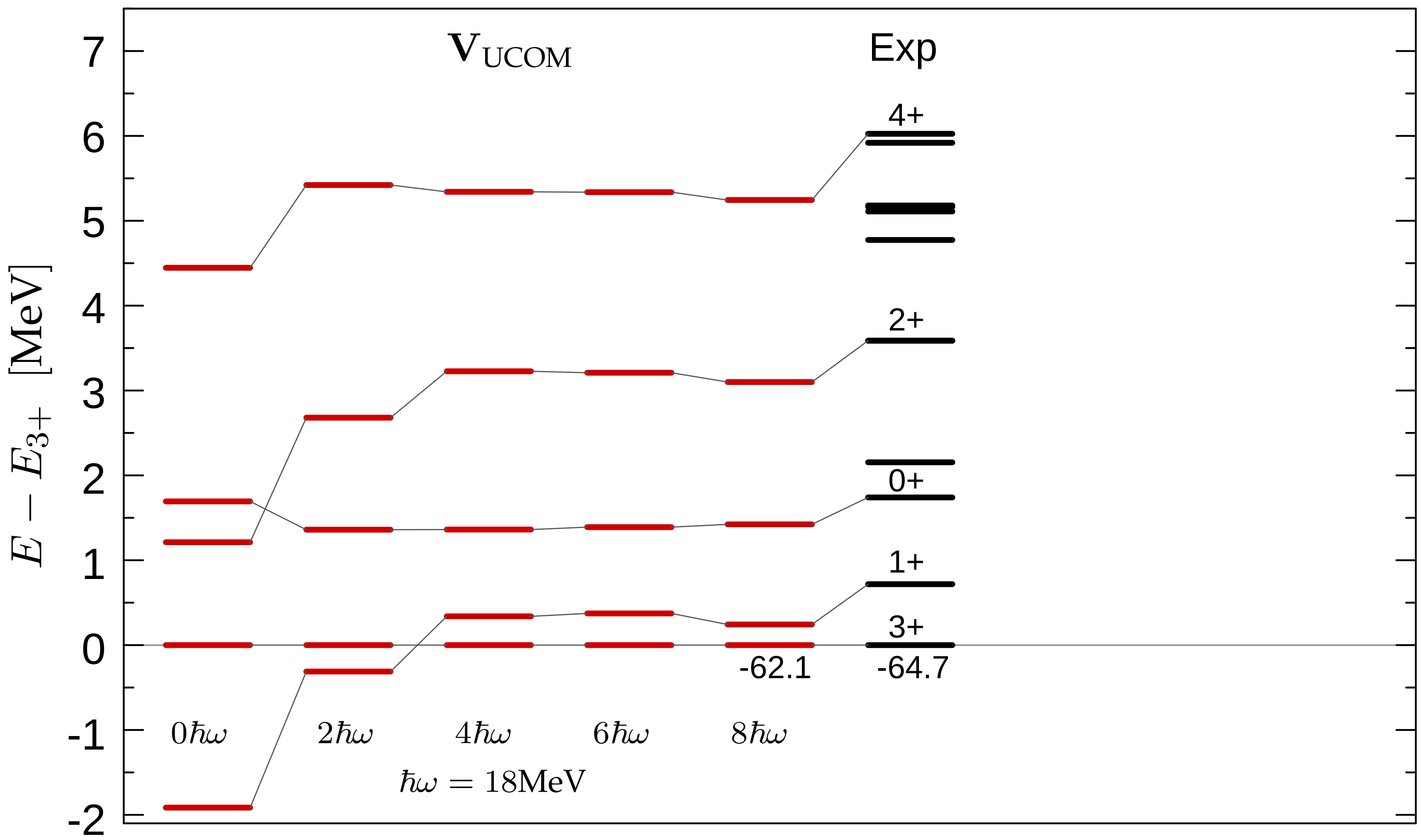
Three-Body Interactions — Tjon Line



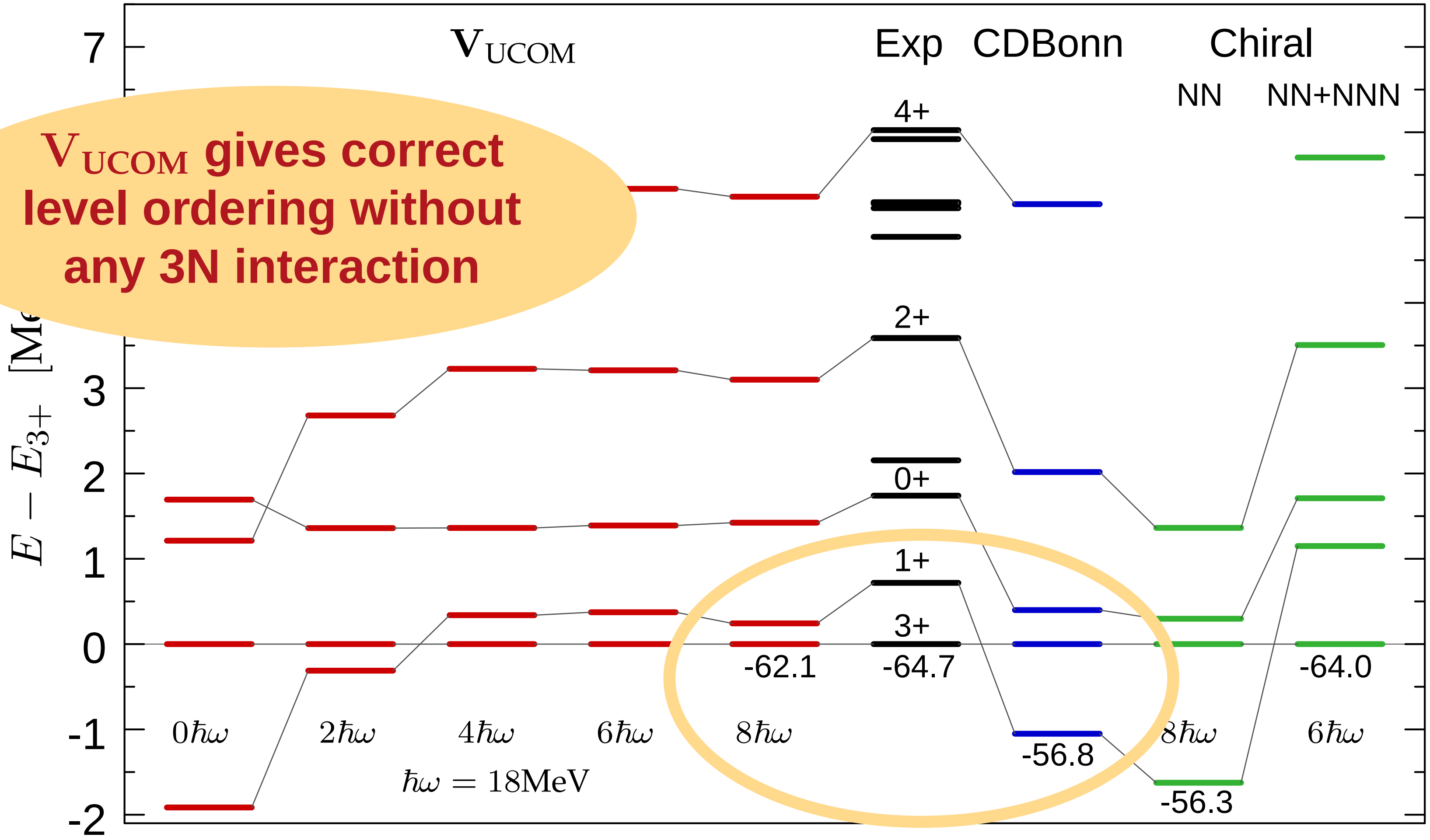
- **Tjon-line**: $E(^4\mathrm{He})$ vs. $E(^3\mathrm{H})$ for phase-shift equivalent NN-interactions
- same behavior for the SRG interaction as function of α

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?



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

Exact Many-Body Methods

Importance Truncated No-Core Shell Model

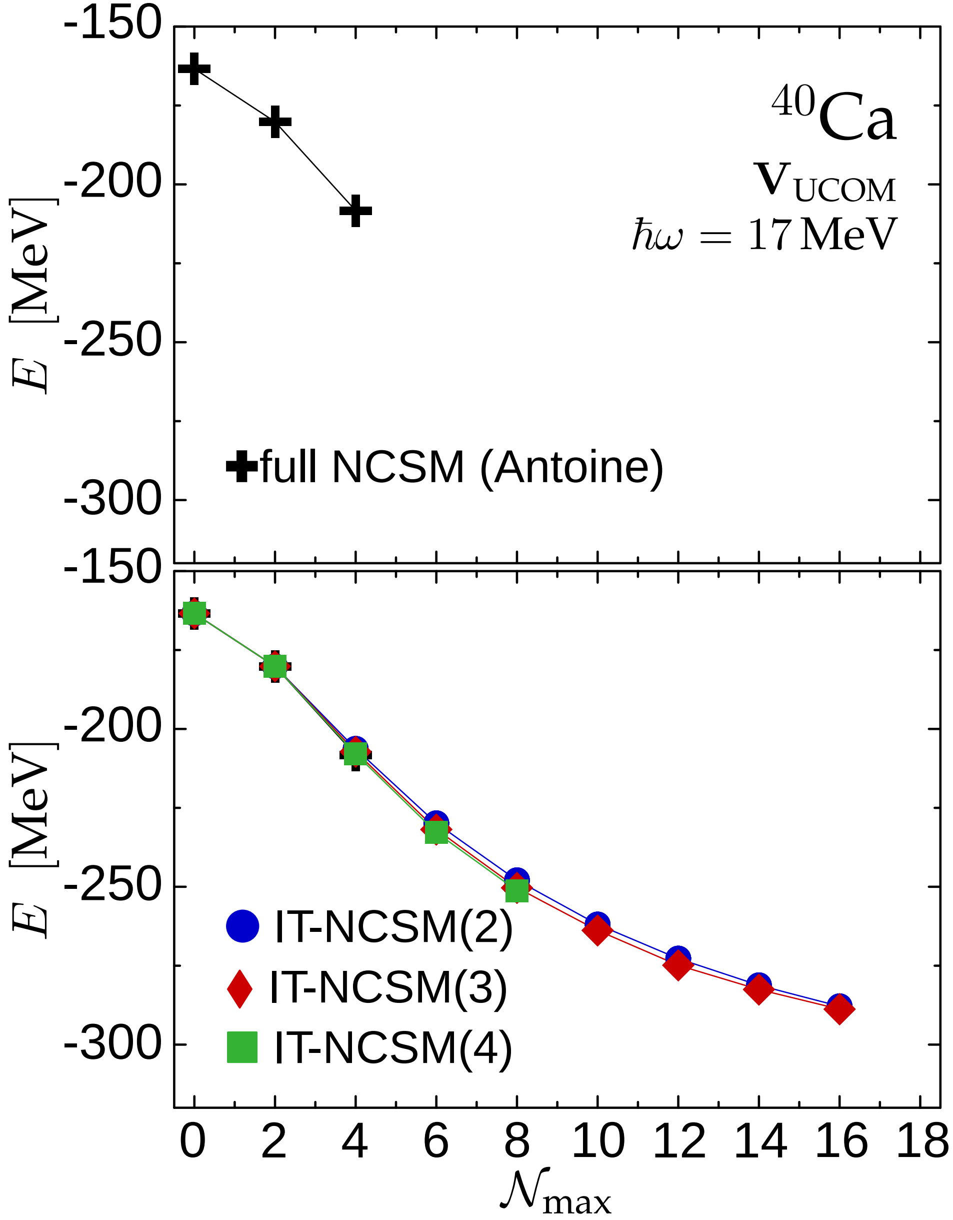
Roth & Navrátil — Phys. Rev. Lett. 99, 092501 (2007)
Roth — in preparation

Importance Truncated NCSM

- converged NCSM calculations essentially restricted to p-shell
- full $6\hbar\omega$ calculation for $^{40}\mathrm{Ca}$ 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 $\left|\Phi_\nu\right\rangle$ via first-order multiconfigurational perturbation theory

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

- **importance truncation**: starting from approximation $\left|\Psi_{\text{ref}}\right\rangle$ of target state, construct importance truncated space with $|\kappa_\nu| \geq \kappa_{\min}$

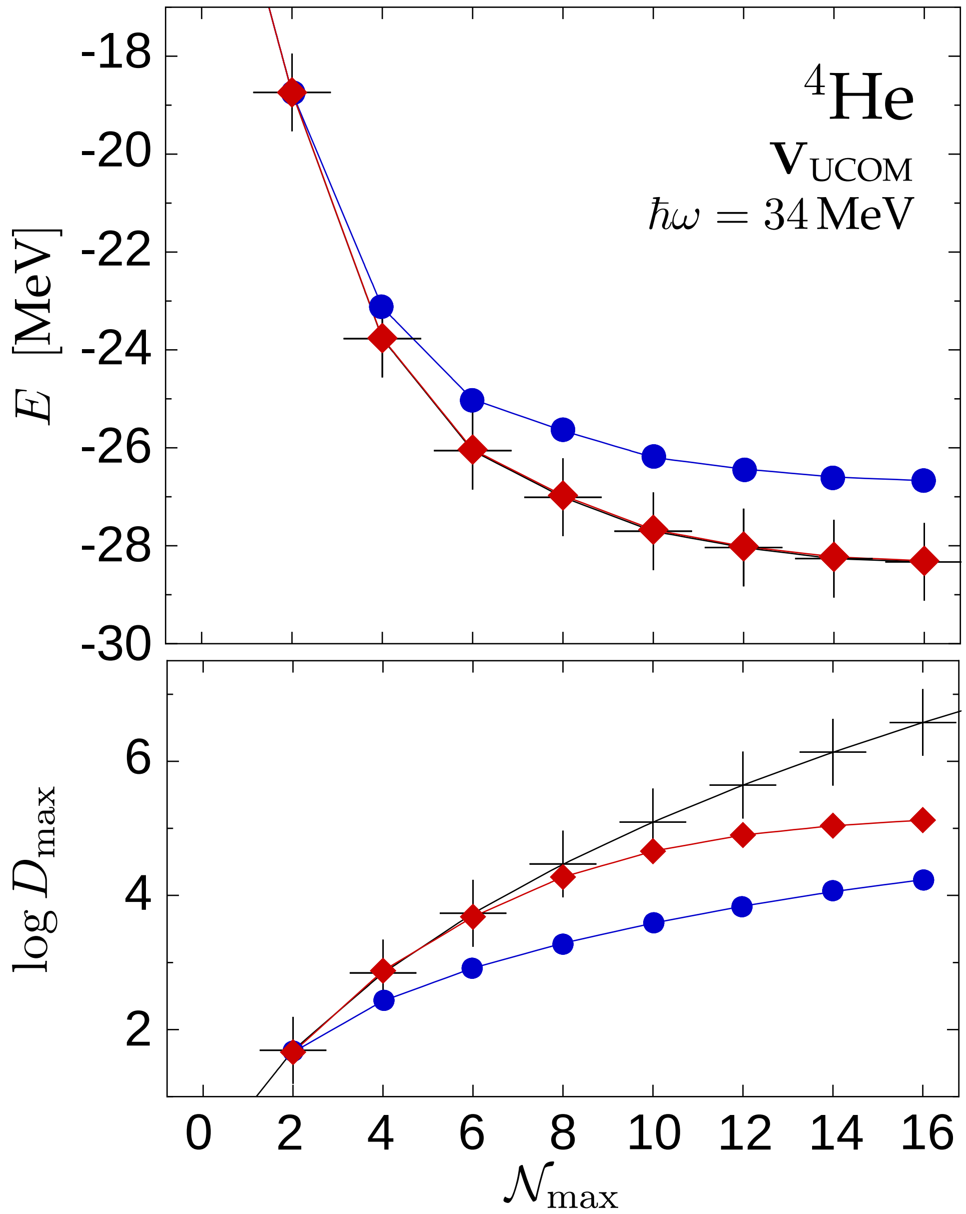
  ➜ contains 2p2h excitations w.r.t. $\left|\Psi_{\text{ref}}\right\rangle$ at most

  ➜ 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 new $|\Psi_{\text{ref}}\rangle$
  - → convergence to full $\mathcal{N}_{\text{max}}\hbar\omega$ space in the limit $\kappa_{\text{min}} \to 0$
  - → convergence w.r.t. iterations implies approximate size extensivity
- multiconfiguration PT can be used to directly correct for contribution of excluded configurations

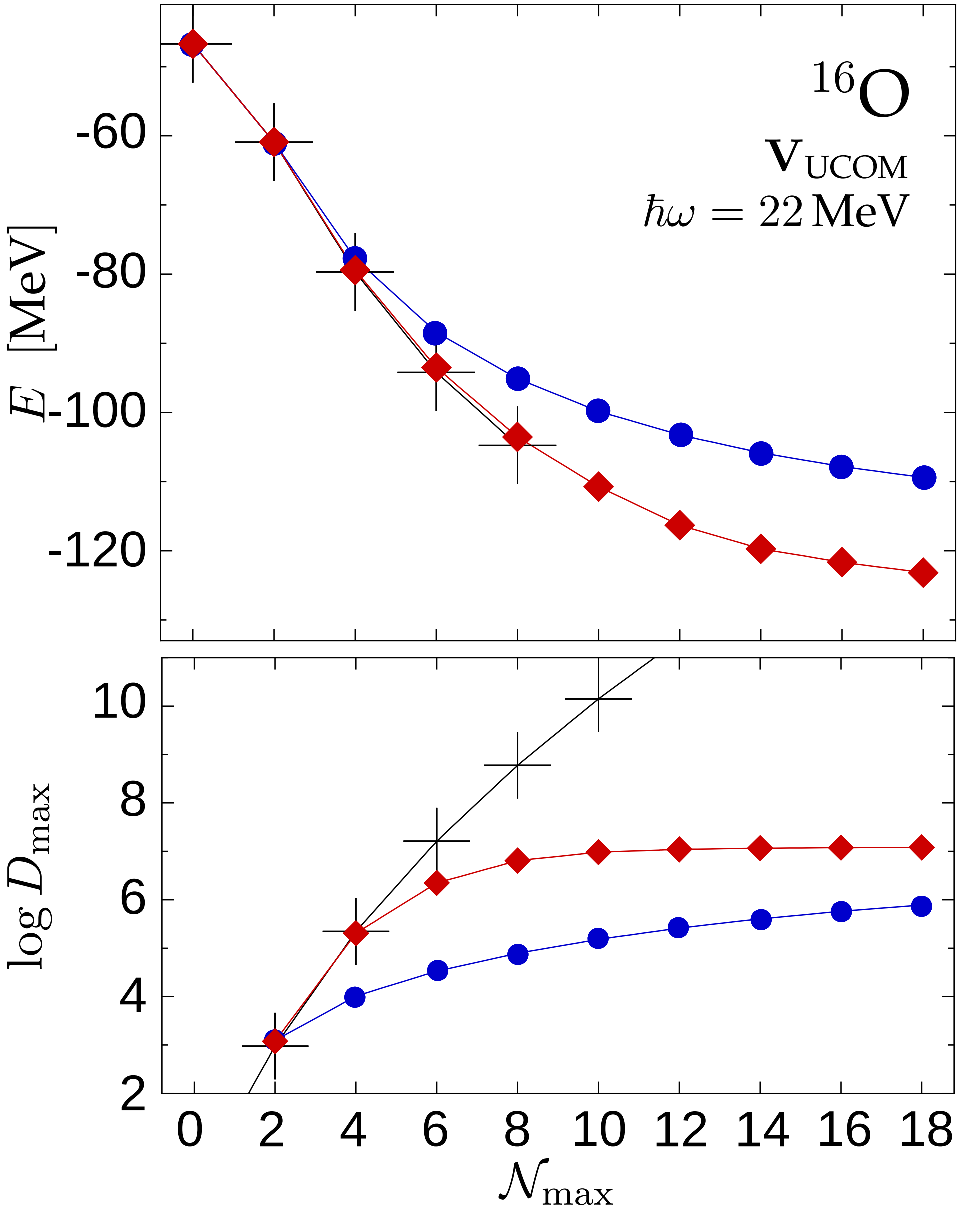
^{4}He: Importance Truncated NCSM



- **reproduces exact NCSM result** for all $\hbar\omega$ and $\mathcal{N}_{\max}$
- importance truncation scheme and $\kappa_{\min} \rightarrow 0$ extrapolation are reliable
- no center-of-mass contamination
- reduction of basis by up to two orders of magnitude

$+$ full NCSM (Antoine)
● IT-NCSM(2p2h)
♦ IT-NCSM(4p4h)

^{16}O: Importance Truncated NCSM

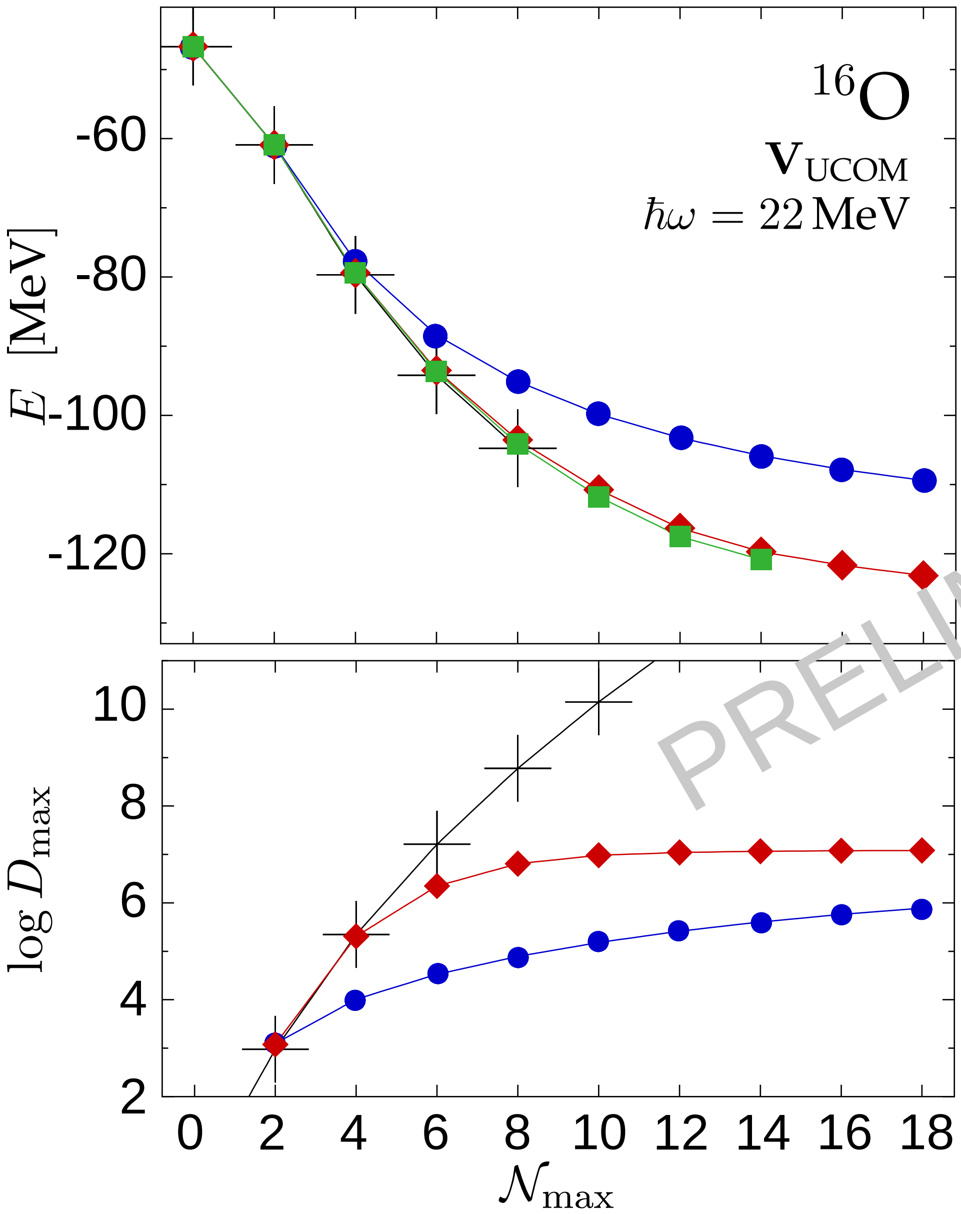


- **excellent agreement with full NCSM** calculation although configurations beyond 4p4h are not included

- dimension reduced by **several orders of magnitude**; possibility to go way beyond the domain of the full NCSM

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

^{16}O: Importance Truncated NCSM

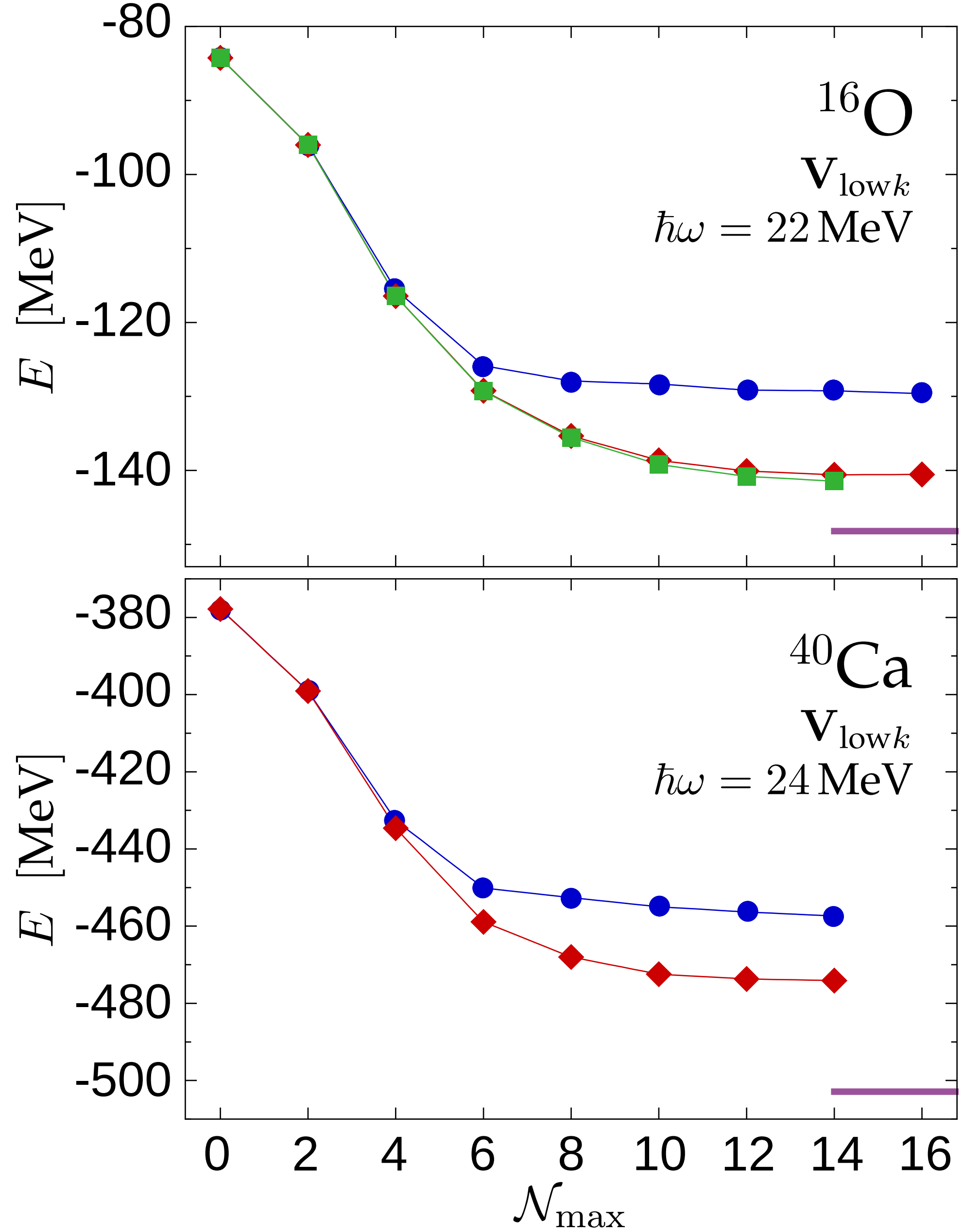


- **perturbative correction** up to 6p6h on top of IT-NCSM(4p4h) eigenstate
- small contribution of configurations beyond 4p4h level
- extrapolation to $\mathcal{N}_{\max} \to \infty$

$$E_{\text{IT-NCSM(4p4h)}} \approx -127.5 \pm 2\,\text{MeV}$$
$$E_{\text{IT-NCSM(4p4h)+PT}} \approx -128.5 \pm 2\,\text{MeV}$$
$$E_{\text{exp}} = -127.6\,\text{MeV}$$

$+$ full NCSM (Antoine)
● IT-NCSM(2p2h)
♦ IT-NCSM(4p4h)
■ IT-NCSM(4p4h)+MCPT(6p6h)

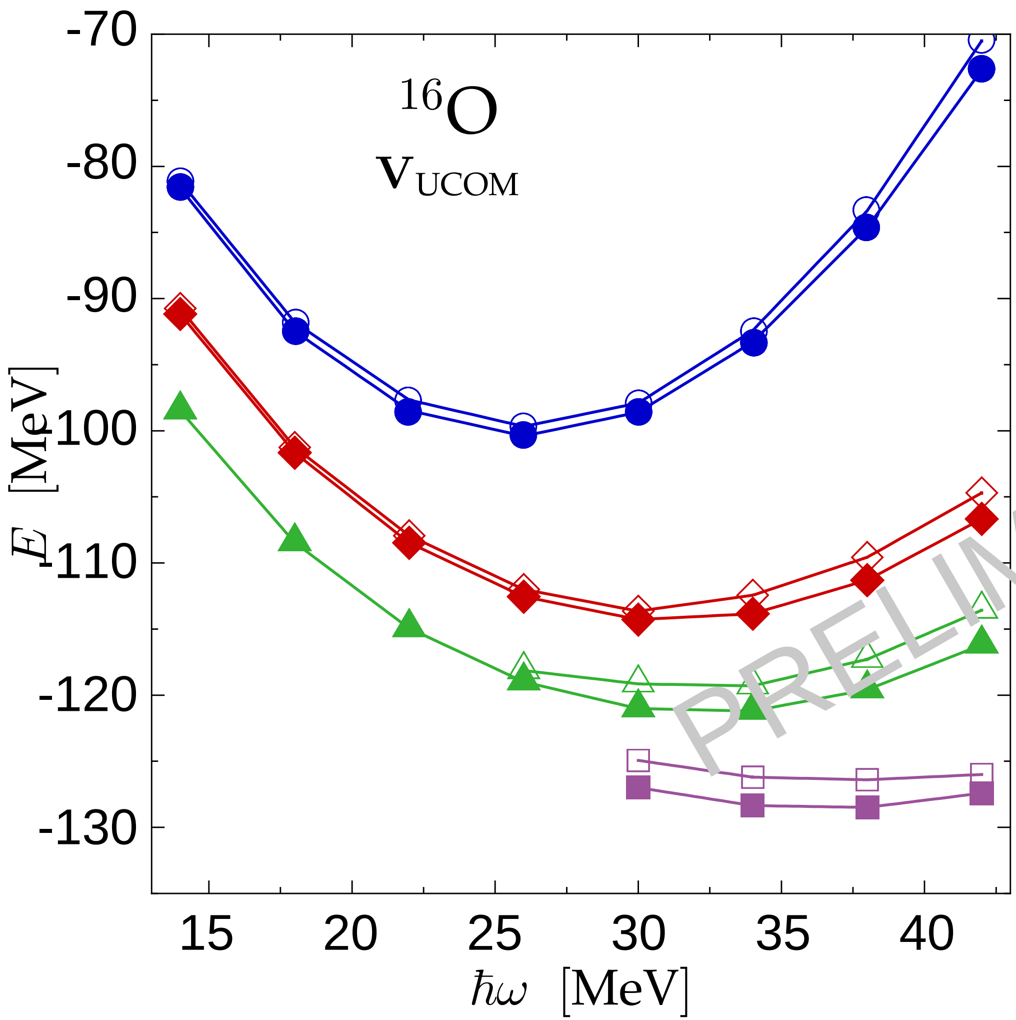
^{16}O & ^{40}Ca: Benchmark using $V_{\mathrm{low}k}$



- faster convergence with $\mathbf{V}_{\mathrm{low}k}$ but unrealistic binding energy
- systematic deviation from coupled-cluster CCSD(T) results of Hagen, Dean, et al. [PRC 76, 044305 (2007)]

+ full NCSM (Antoine)
● IT-NCSM(2p2h)
♦ IT-NCSM(4p4h)
■ IT-NCSM(4p4h)+MCPT(6p6h)
— CCSD(T) Hagen et al.

Direct Comparison: CC vs. IT-CI



solid symbols: CR-CC(2,3)
open symbols: IT-CI(4p4h)+MRD

- HF single-particle basis with truncation to 5,6,7,8 shells
- violation of translational invariance from the outset
- **coupled-cluster calculation** with non-perturbative triples correction: CR-CC(2,3)
- **importance-truncated configuration interaction** up to 4p4h plus multi-reference Davidson correction ($\lesssim 3$ MeV)

CC by J. Gour & P. Piecuch (MSU)

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

- **thanks to my group & my collaborators**
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    Michigan State University, USA
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Epilogue

special thanks to

Hans Feldmeier

...for so many things