Unitarily Transformed Interactions for Ab-Initio Nuclear Structure

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Overview

- Motivation
- Unitarily Transformed Interactions
  - Unitary Correlation Operator Method
  - Similarity Renormalization Group
- Computational Many-Body Methods
  - No-Core Shell Model
  - Importance Truncated NCSM & CI
  - Coupled-Cluster Method

From QCD to Nuclear Structure

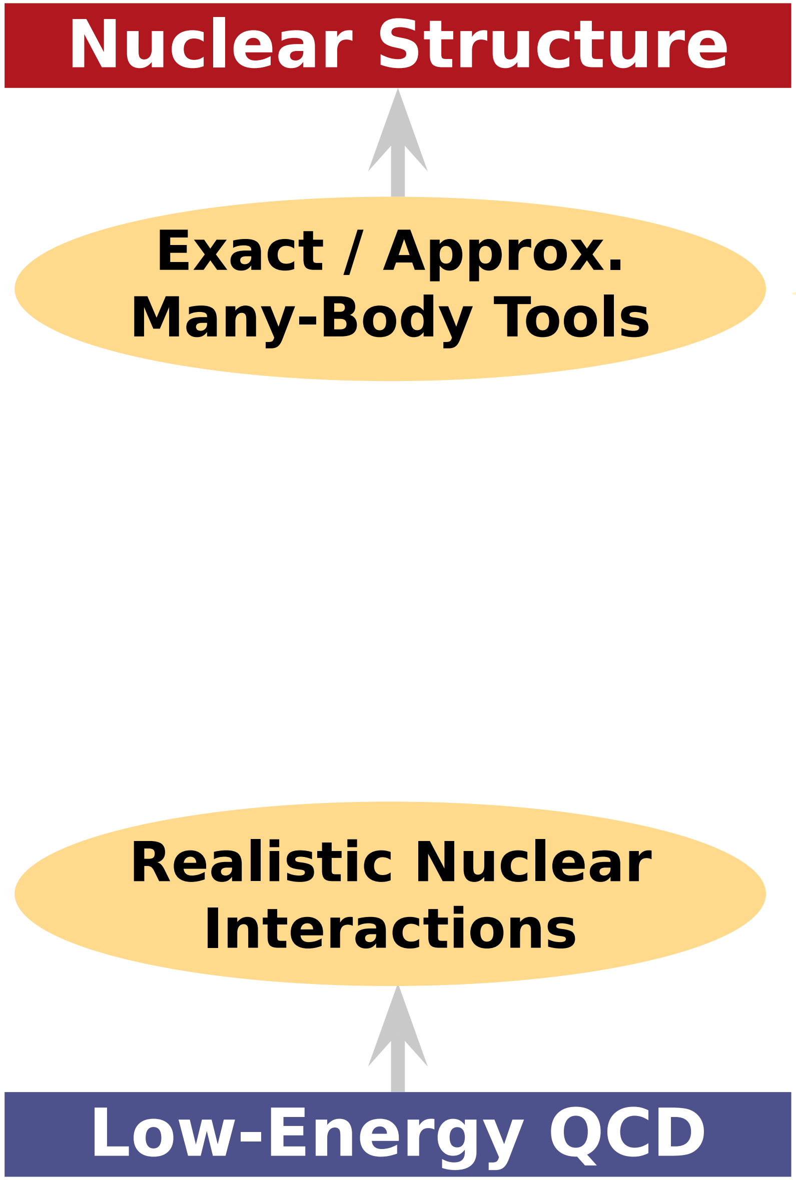
Nuclear Structure

Realistic Nuclear Interactions

Low-Energy QCD

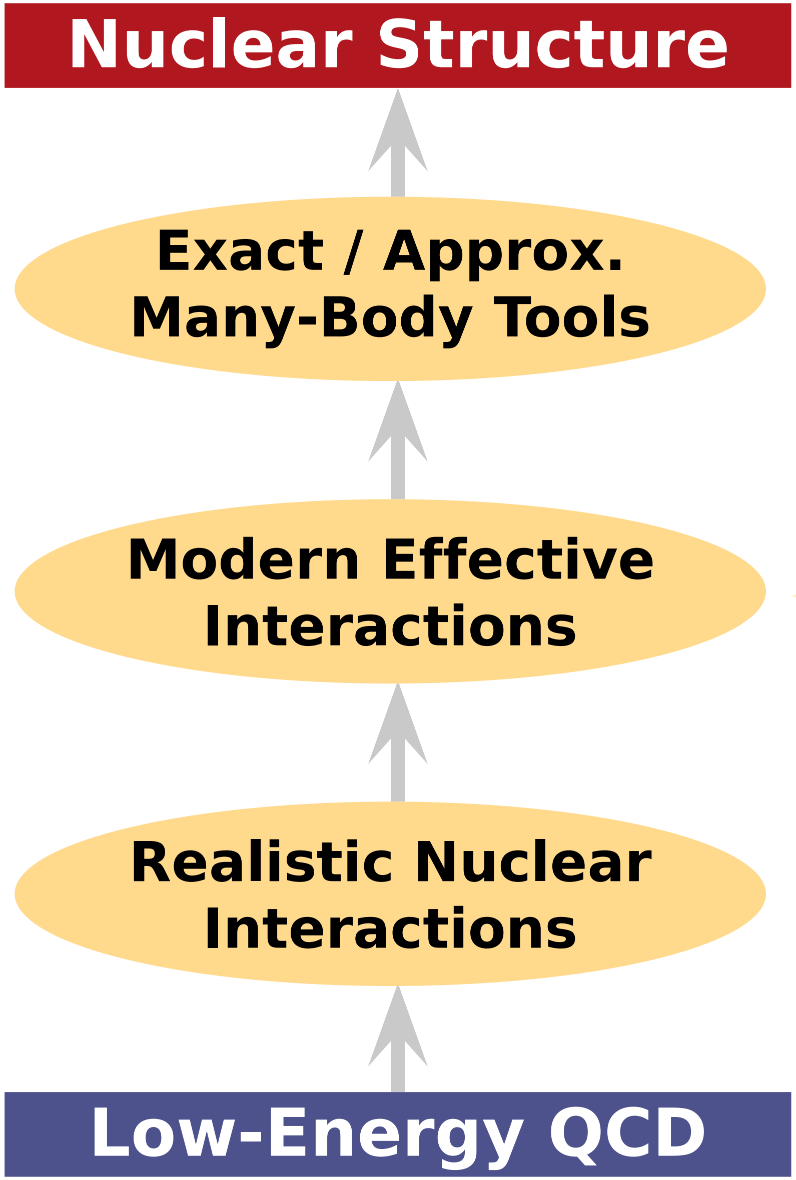
- chiral EFT interactions: consistent NN & 3N interaction derived within χEFT
- traditional NN-interactions: Argonne V18, CD Bonn,...
- reproduce experimental two-body data with high precision
- induce strong short-range central & tensor correlations

From QCD to Nuclear Structure



- ‘exact’ solution of the many-body problem for light & intermediate masses (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 con-strained properties (phase shifts & deuteron)
  - generate new realistic int.
- need consistent effective inter-action & effective operators
- unitary transformations most convenient

Unitarily Transformed Interactions

Unitary Correlation Operator Method (UCOM)

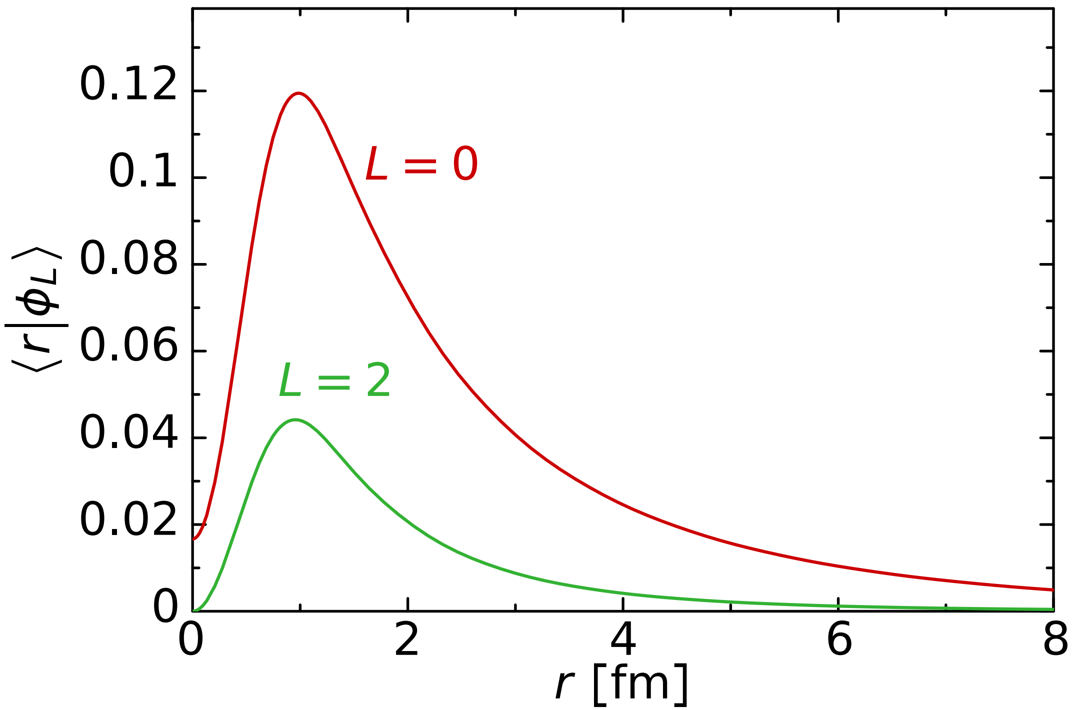
H. Feldmeier et al. — Nucl. Phys. A 632 (1998) 61

T. Neff et al. — Nucl. Phys. A713 (2003) 311

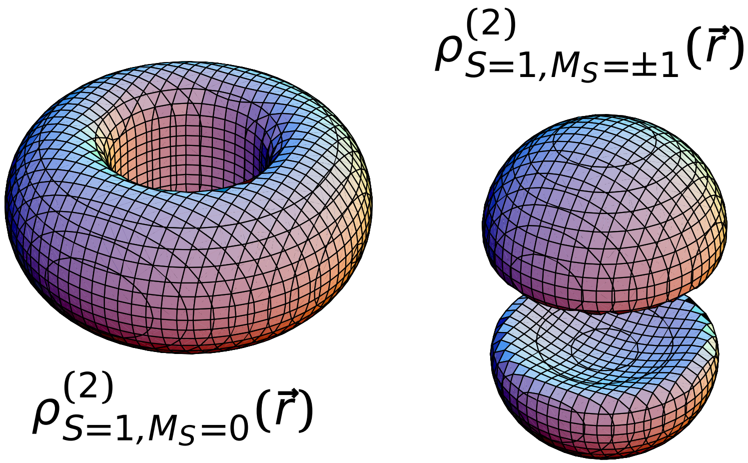
R. Roth et al. — Nucl. Phys. A 745 (2004) 3

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 wave function at small distances r

central correlations

tensor interaction generates L=2 admixture to ground state

tensor correlations

Unitary Correlation Operator Method

Correlation Operator

define a 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

$$|\tilde{\psi}\rangle = \mathrm{C}\,|\psi\rangle$$

Correlated Operators

adapt Hamiltonian to uncorrelated states (pre-diagonalization)

$$\tilde{\mathrm{O}} = \mathrm{C}^{\dagger}\,\mathrm{O}\,\mathrm{C}$$

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

Unitary Correlation Operator Method

explicit ansatz for unitary transformation operator **motivated by the physics of short-range correlations**

Central Correlator C_r

- radial distance-dependent shift in the relative coordinate of a nucleon pair

$$g_r = \frac{1}{2}\left[s(r)\, q_r + q_r\, s(r)\right]$$

$$q_r = \tfrac{1}{2}\left[\tfrac{\vec{r}}{r}\cdot\vec{q} + \vec{q}\cdot\tfrac{\vec{r}}{r}\right]$$

Tensor Correlator C_Ω

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

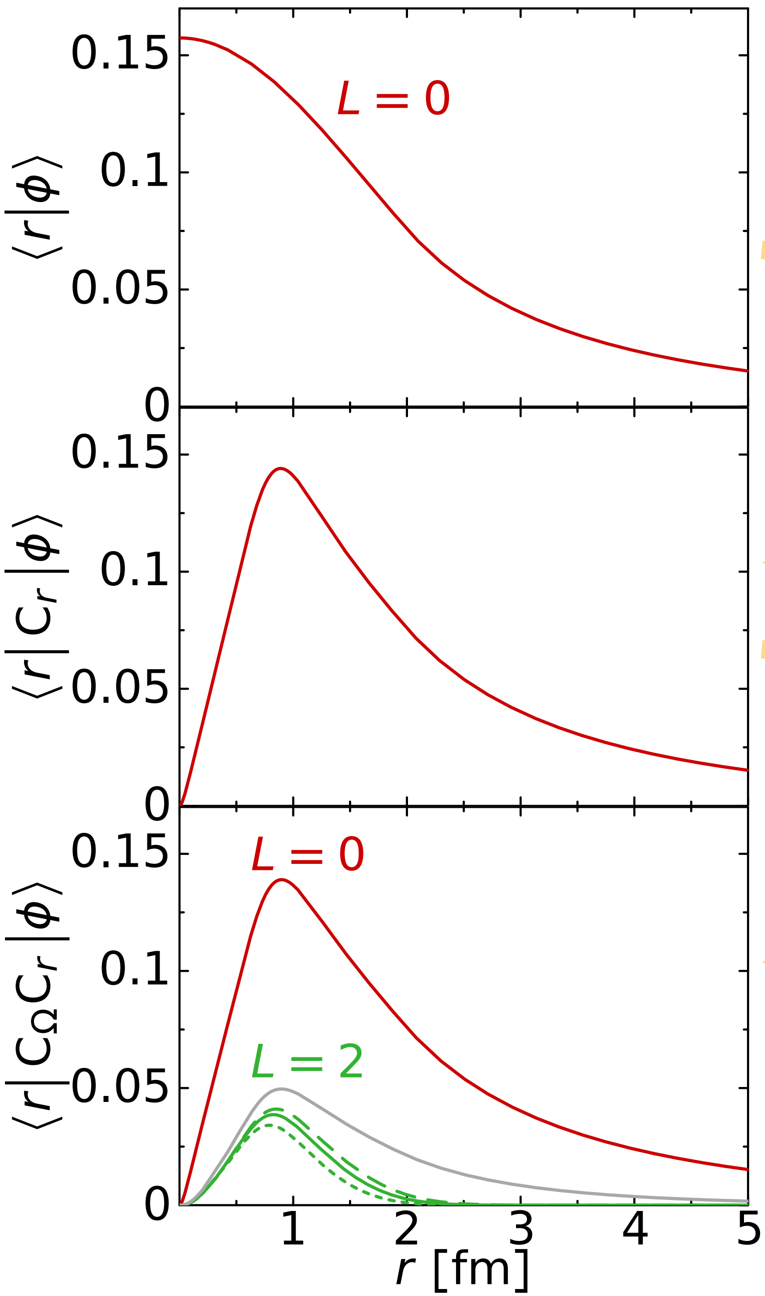
$$g_\Omega = \frac{3}{2}\vartheta(r)\left[(\vec{\sigma}_1\cdot\vec{q}_\Omega)(\vec{\sigma}_2\cdot\vec{r}) + (\vec{r}\longleftrightarrow\vec{q}_\Omega)\right]$$

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

$$C = C_\Omega C_r = \exp\Big(-\,i\sum_{i<j} g_{\Omega,ij}\Big)\, \exp\Big(-\,i\sum_{i<j} g_{r,ij}\Big)$$

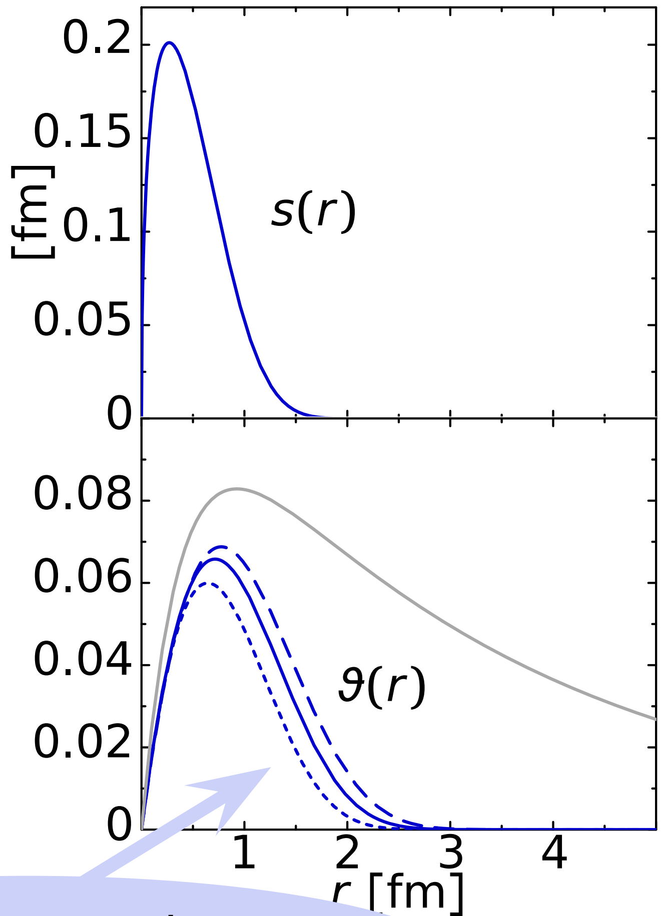
- $s(r)$ and $\vartheta(r)$ depend on & are optimized for initial potential

Correlated States: The Deuteron



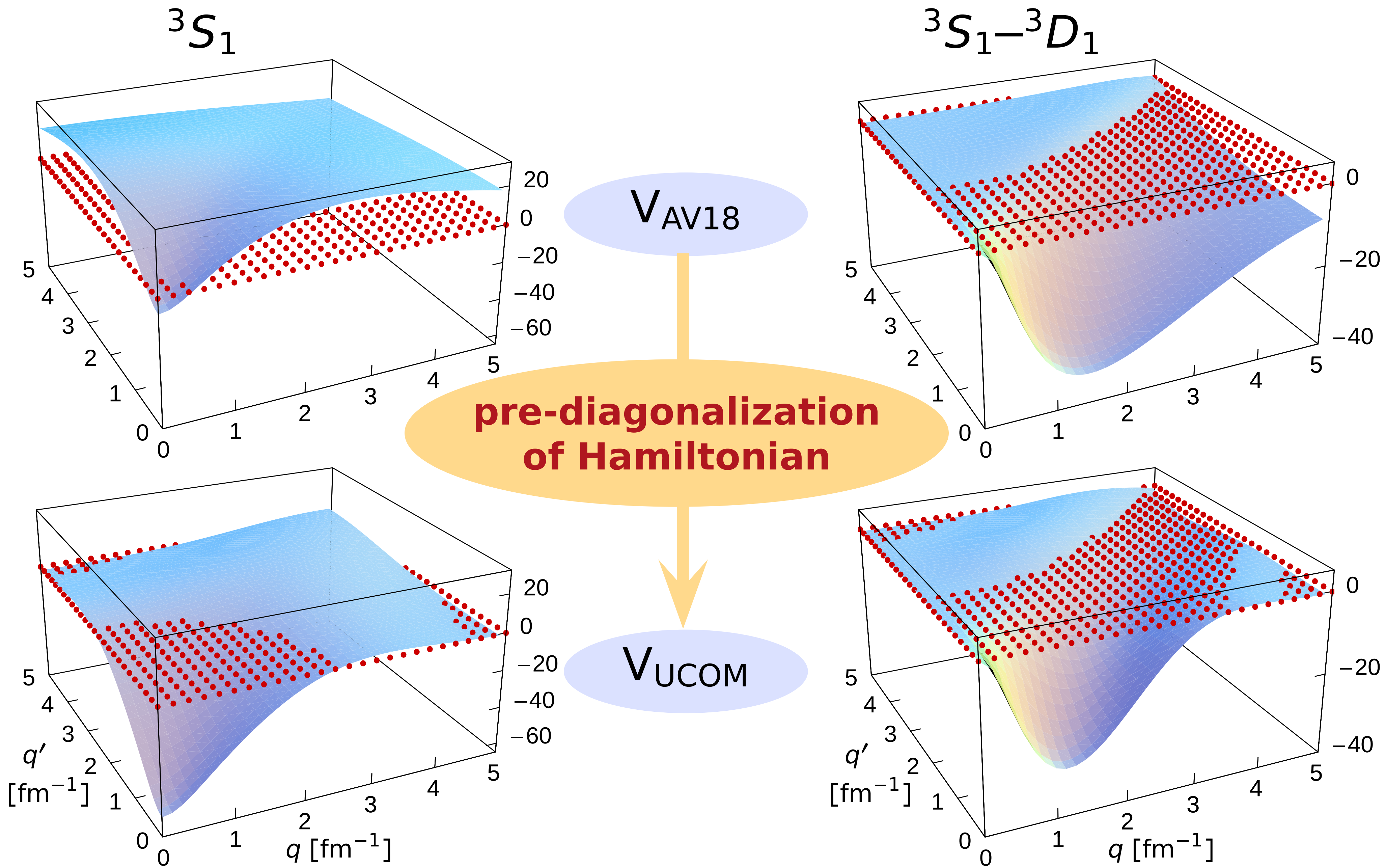
central correlations

tensor correlations



only short-range tensor correlations treated by C_Ω

Correlated Interaction: V_{UCOM}



Correlated Interaction: V_{UCOM}

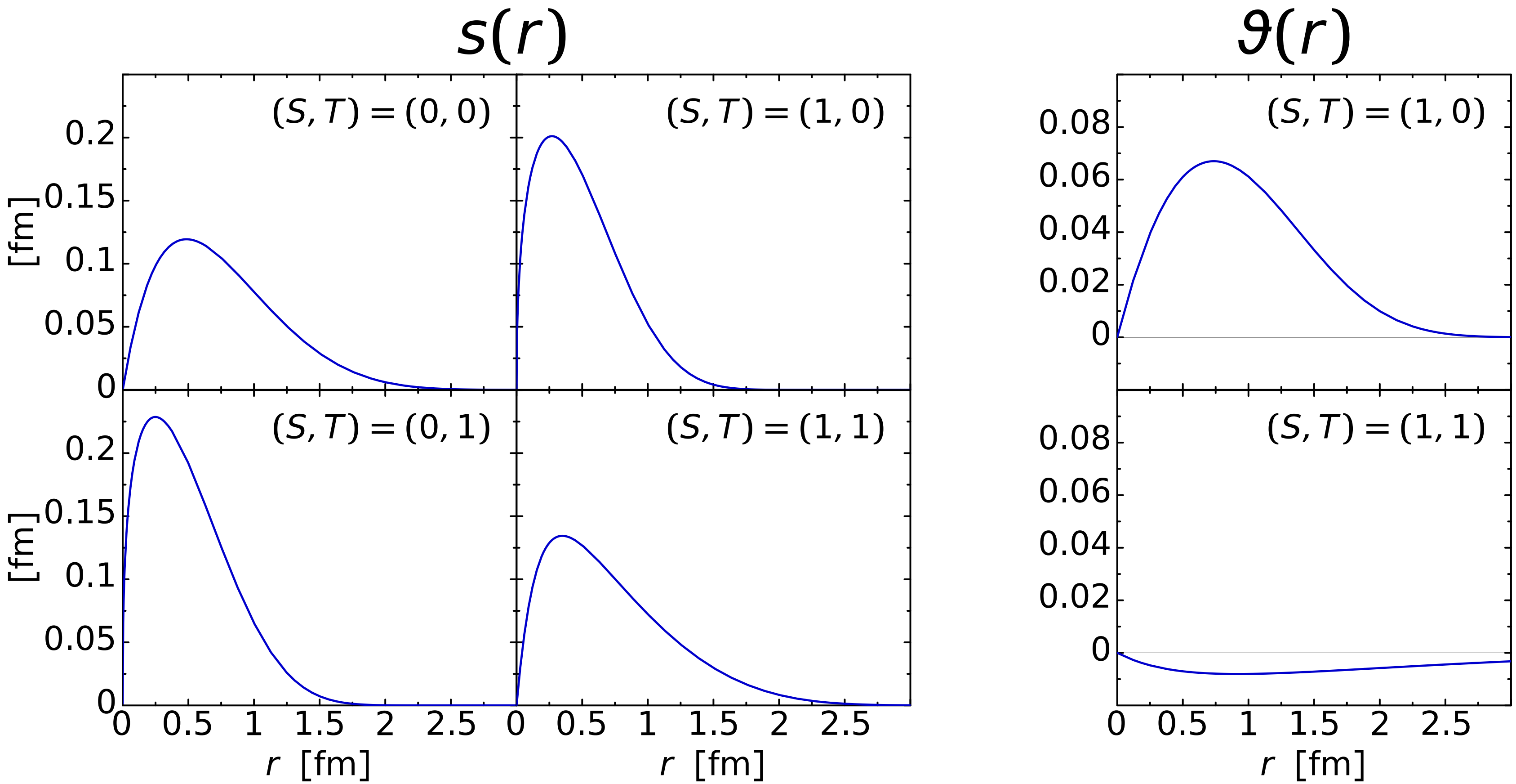
$$V_{UCOM} = \sum_p \frac{1}{2}\left[\tilde{v}_p(r)\, O_p + O_p\, \tilde{v}_p(r)\right]$$

$$\begin{aligned} O = \{1,\ &(\vec{\sigma}_1\cdot\vec{\sigma}_2),\ \vec{q}^{\,2},\ \vec{q}^{\,2}(\vec{\sigma}_1\cdot\vec{\sigma}_2),\ \vec{L}^2,\ \vec{L}^2(\vec{\sigma}_1\cdot\vec{\sigma}_2), \\ &(\vec{L}\cdot\vec{S}),\ S_{12}(\vec{r},\vec{r}),\ S_{12}(\vec{L},\vec{L}), \\ &\bar{S}_{12}(\vec{q}_\Omega,\vec{q}_\Omega),\ q_r\, S_{12}(\vec{r},\vec{q}_\Omega),\ \vec{L}^2(\vec{L}\cdot\vec{S}), \\ &\vec{L}^2\bar{S}_{12}(\vec{q}_\Omega,\vec{q}_\Omega),\ \dots\} \otimes \{1,\ (\vec{\tau}_1\cdot\vec{\tau}_2)\} \end{aligned}$$

- C_r-transformation evaluated directly
- C_Ω-transformation through Baker-Campell-Hausdorff expansion
- $\tilde{v}_p(r)$ determined by bare potential and correlation functions

Optimal Correlation Functions

- $s(r)$ and $\vartheta(r)$ determined by two-body **energy minimisation**
- constraint on range of the tensor correlators $\vartheta(r)$ to isolate state independent **short-range correlations**



Unitarily Transformed 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 — Phys. Rev. C 77, 064033 (2008)

Similarity Renormalization Group

flow evolution of the **Hamiltonian to band-diagonal form** with respect to uncorrelated many-body basis

Flow Equation for Hamiltonian

- evolution equation for Hamiltonian

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

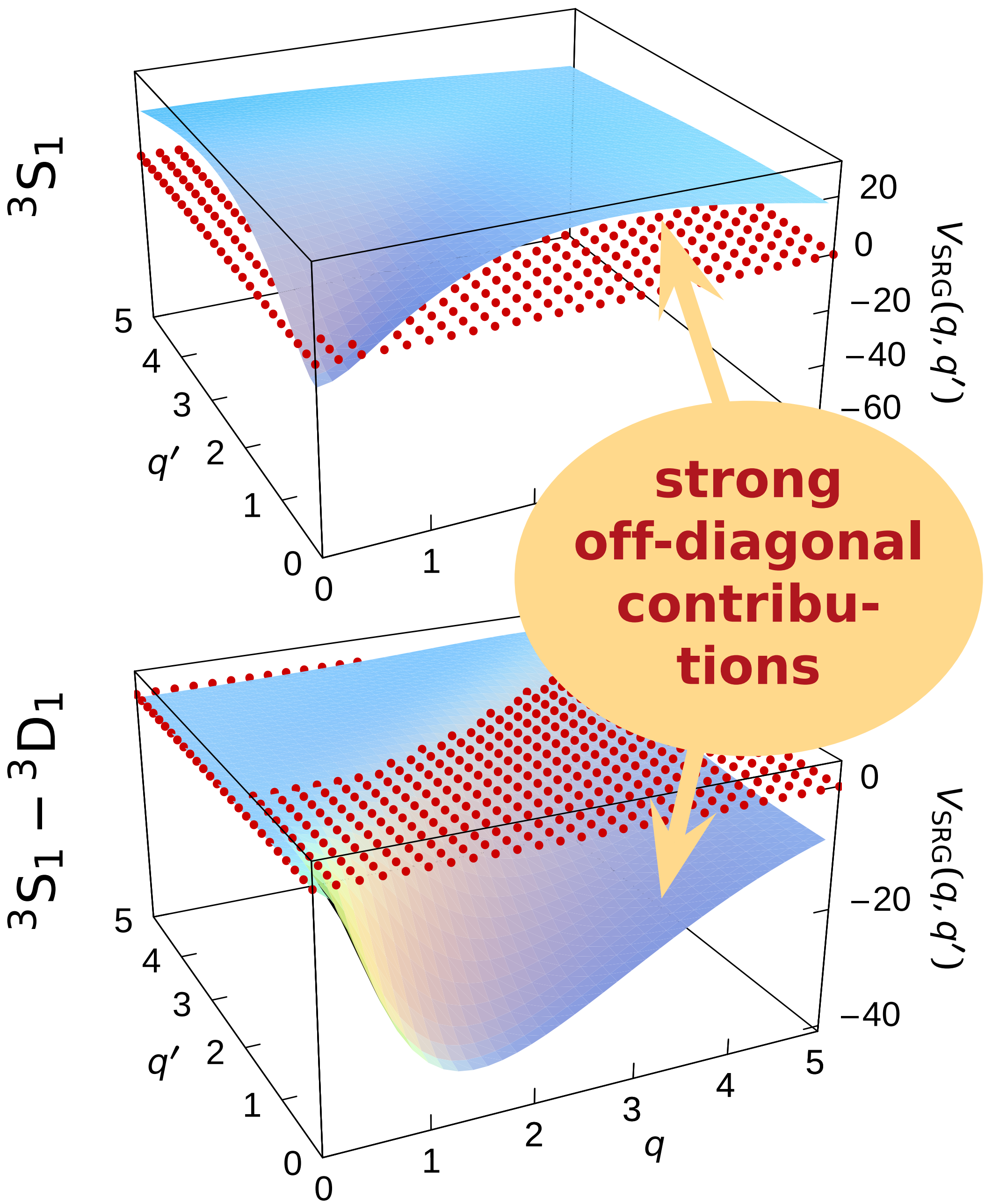
- dynamical generator defined as commutator with the operator in whose eigenbasis H shall be diagonalized

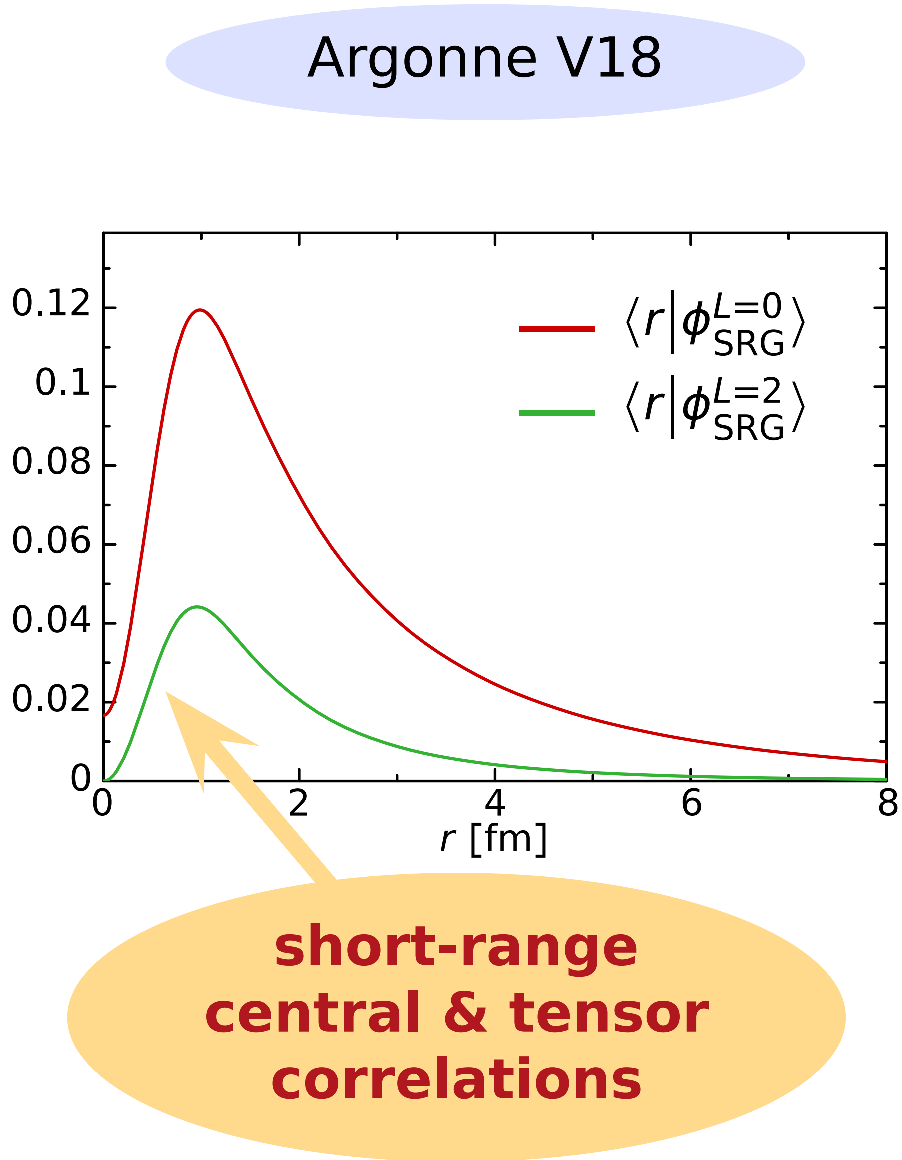
$$\eta(\alpha) \overset{2B}{=} \frac{1}{2\mu}\left[\vec{q}^{\,2}, \widetilde{H}(\alpha)\right]$$

UCOM vs. SRG

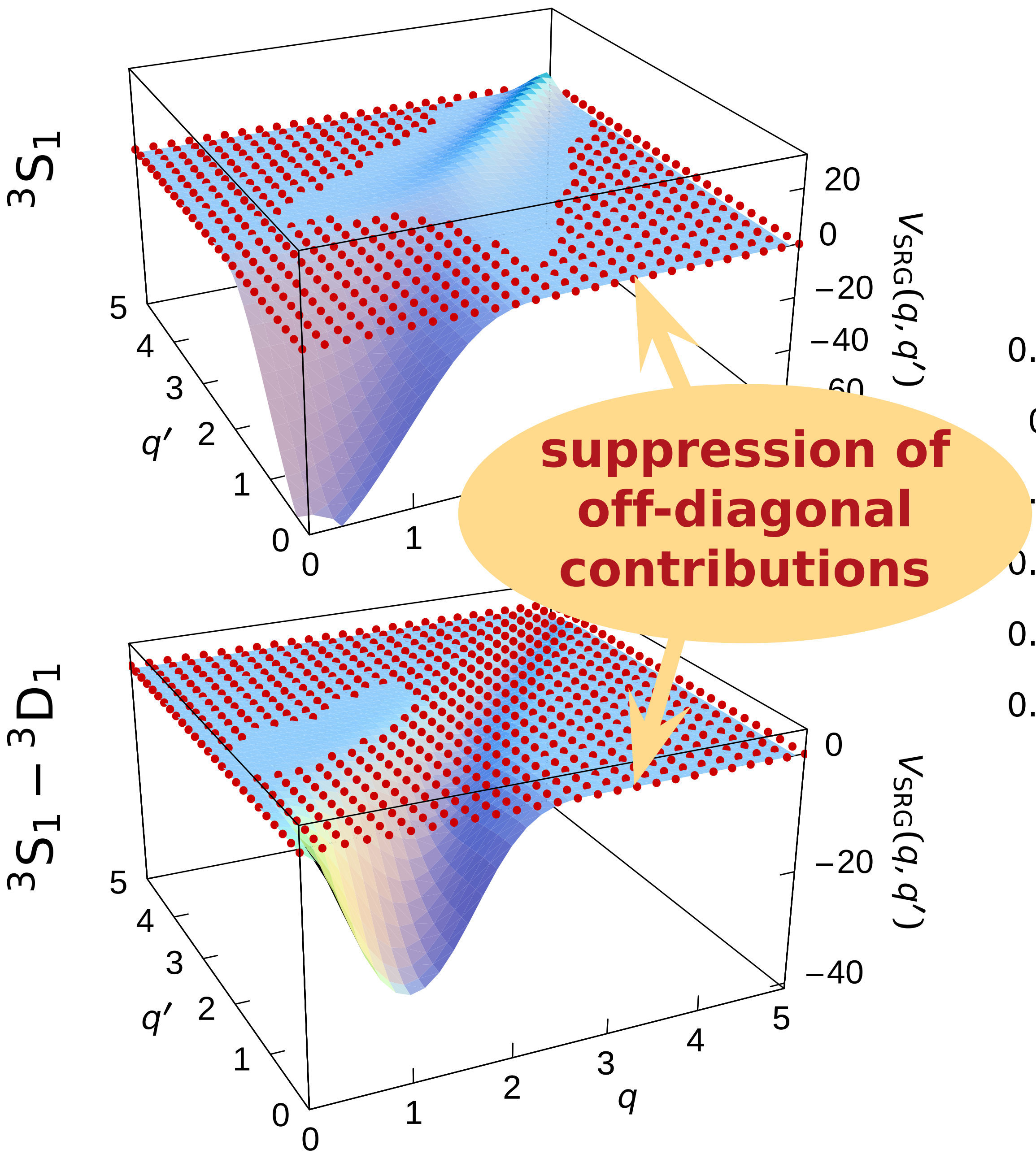
$\eta(0)$ has the same structure as UCOM generators g_r & g_{Ω}

SRG Evolution: The Deuteron

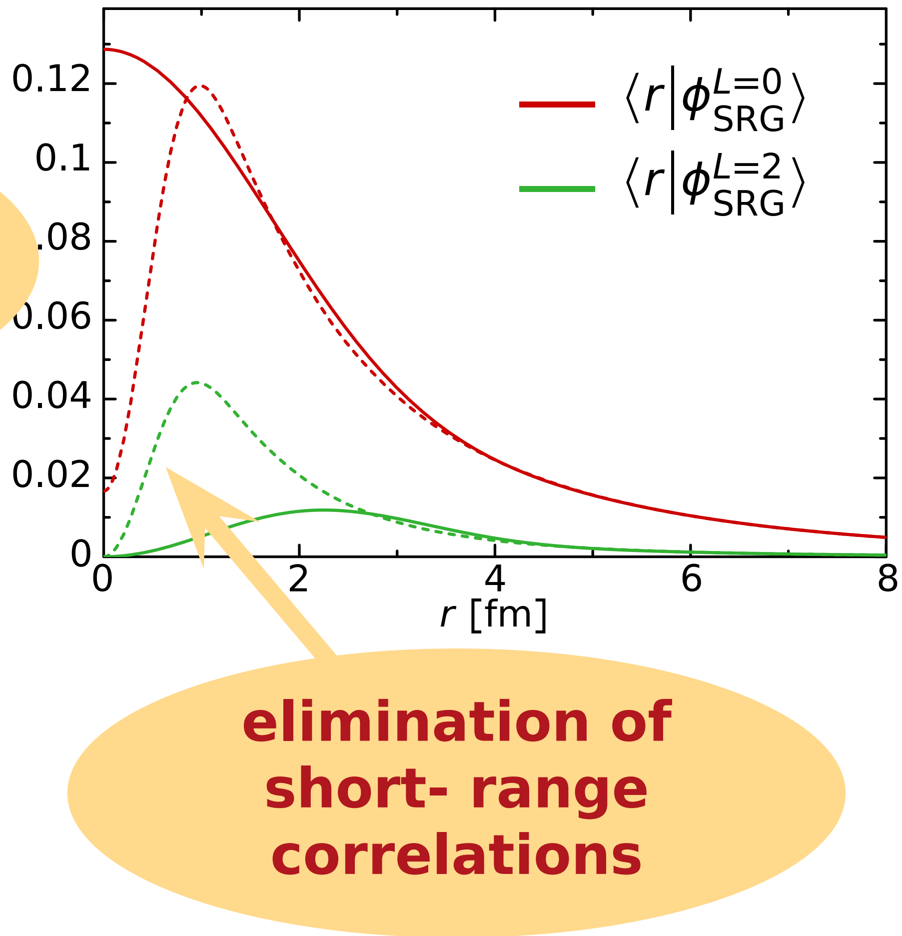




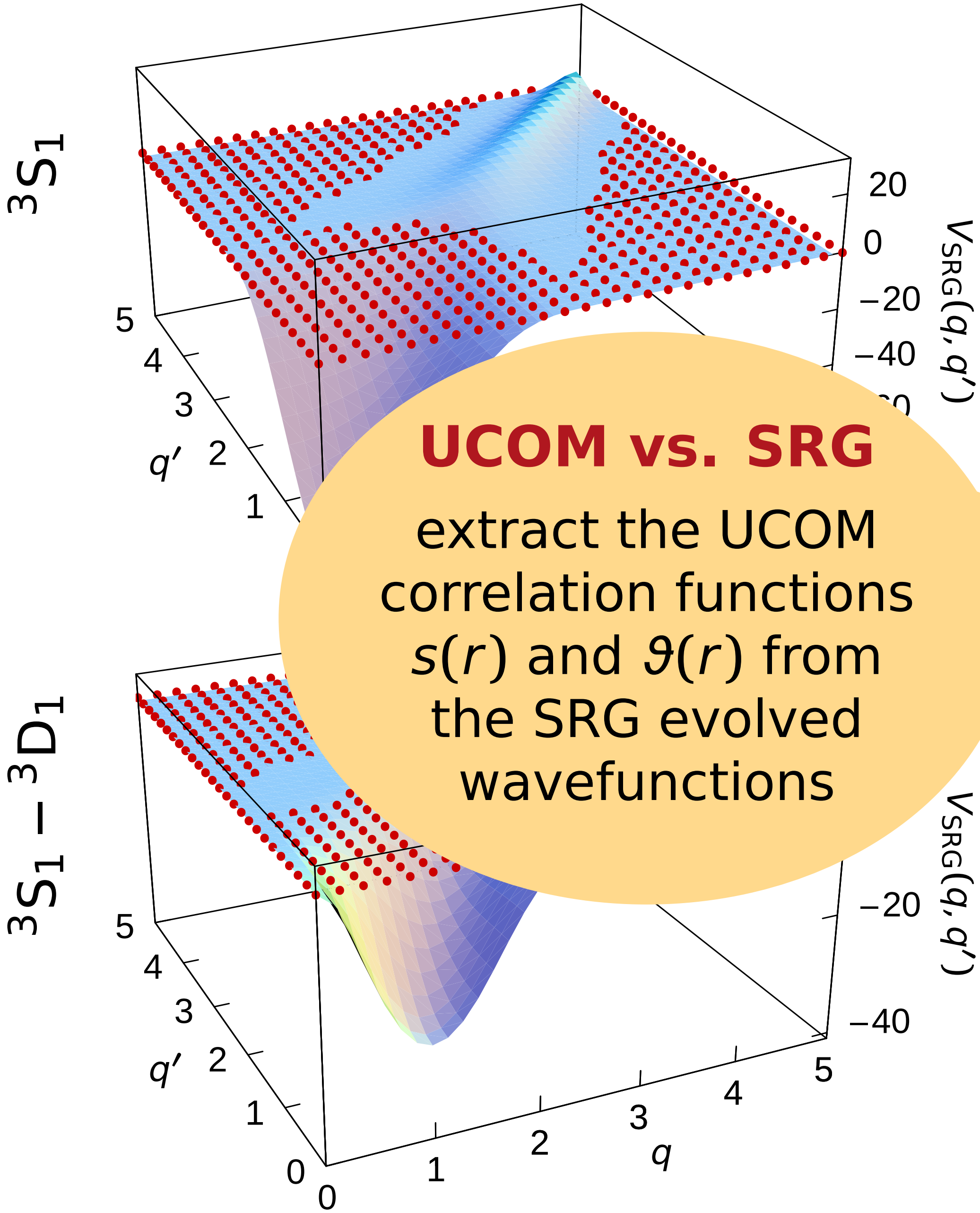
SRG Evolution: The Deuteron



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



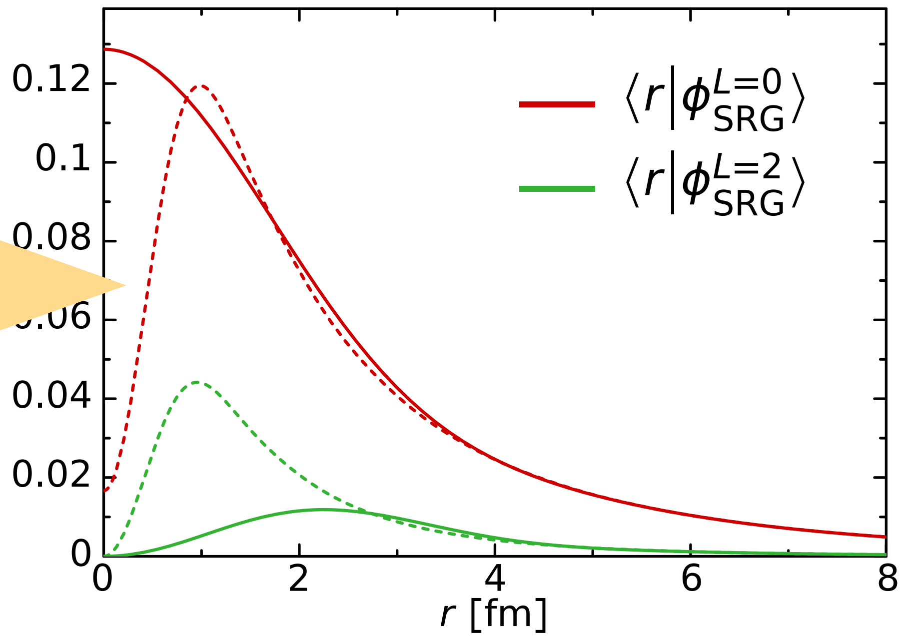
SRG Evolution: The Deuteron



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

UCOM vs. SRG

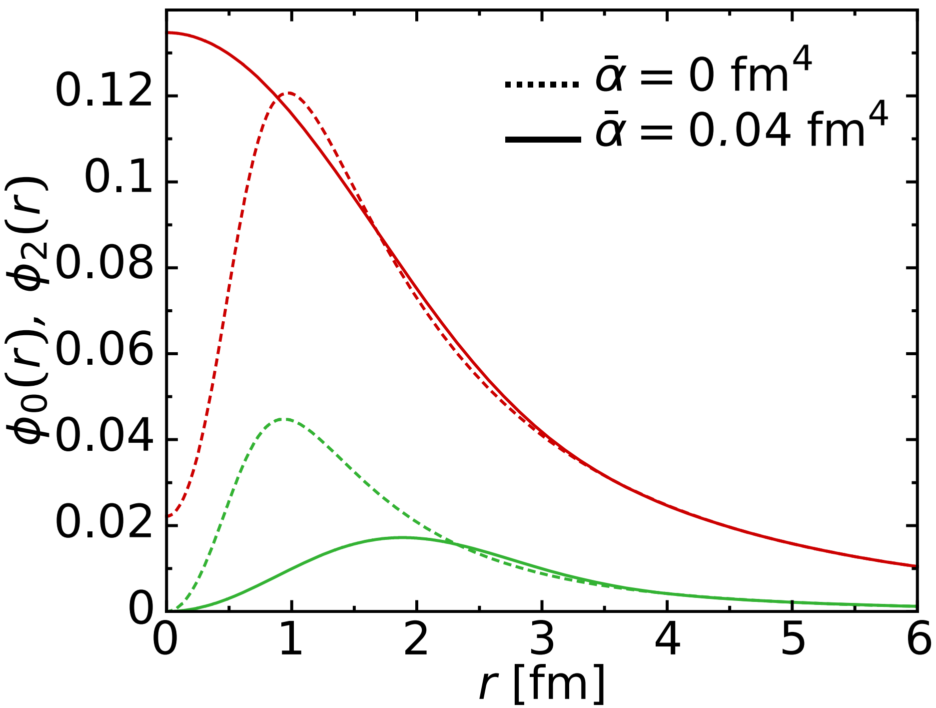
extract the UCOM correlation functions $s(r)$ and $\vartheta(r)$ from the SRG evolved wavefunctions

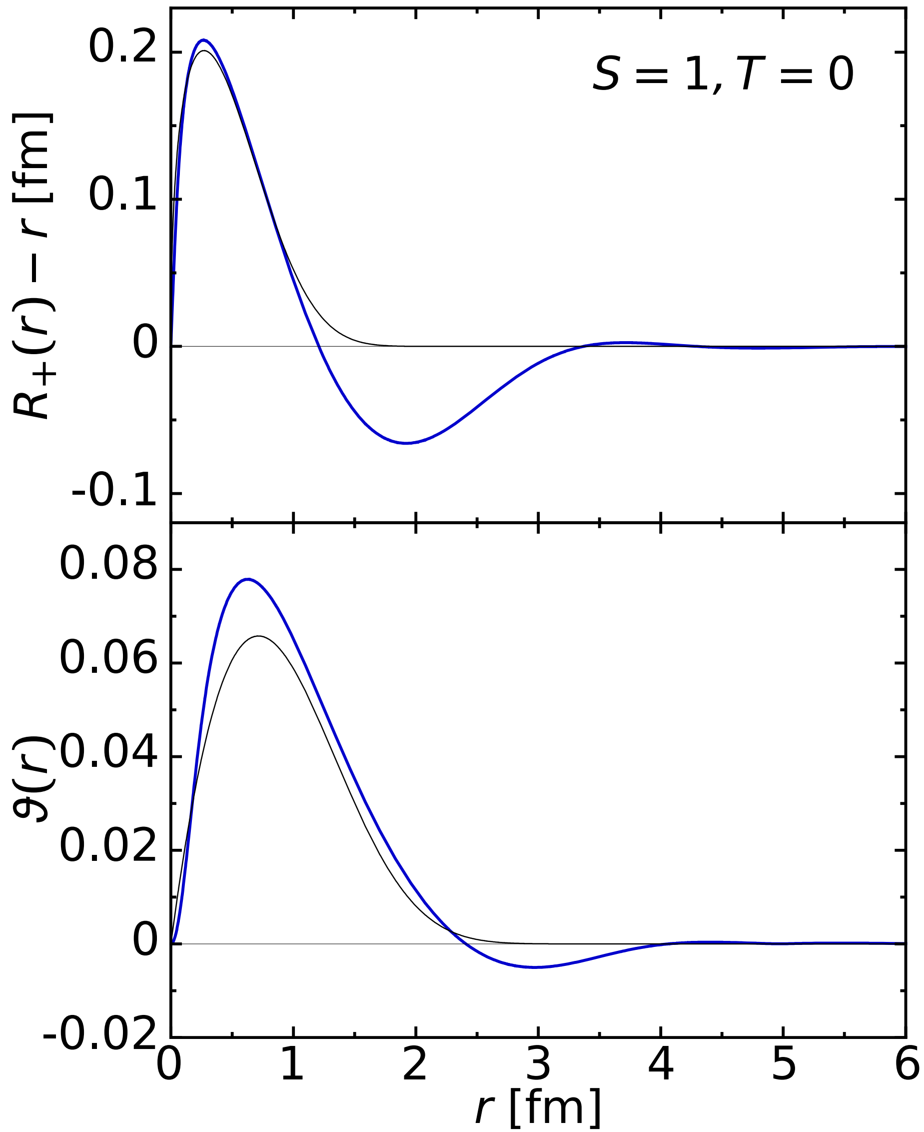


SRG-Generated UCOM Correlators: AV18

- determine UCOM correlators from SRG-evolved two-body wave functions via

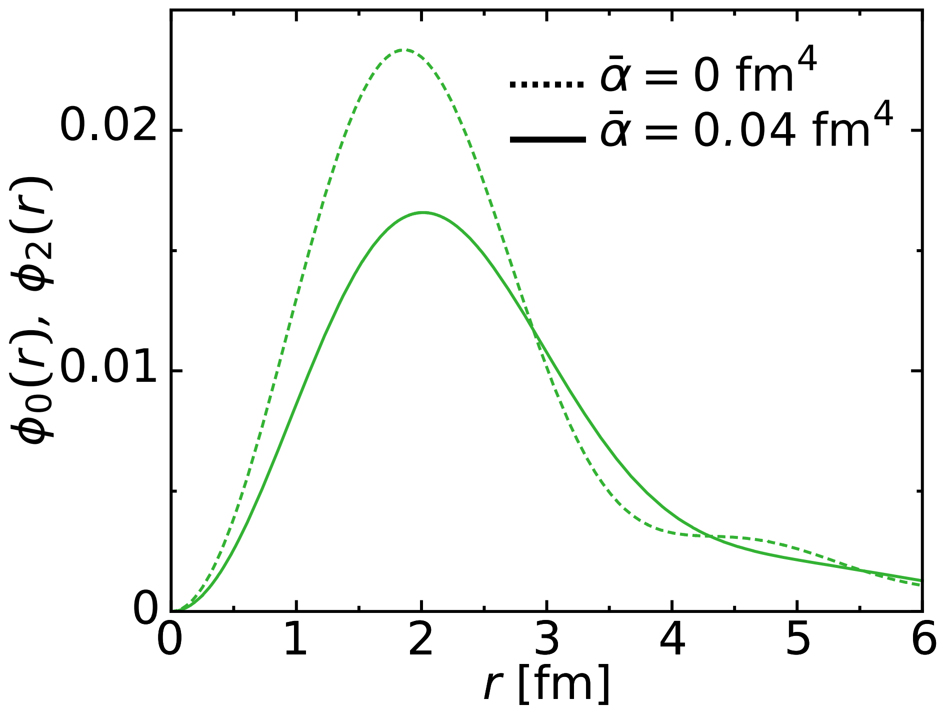
$$\left|\Phi^{(0)}_{\text{SRG}}\right\rangle \stackrel{!}{=} \mathrm{C} \left|\Phi^{(\bar{\alpha})}_{\text{SRG}}\right\rangle$$

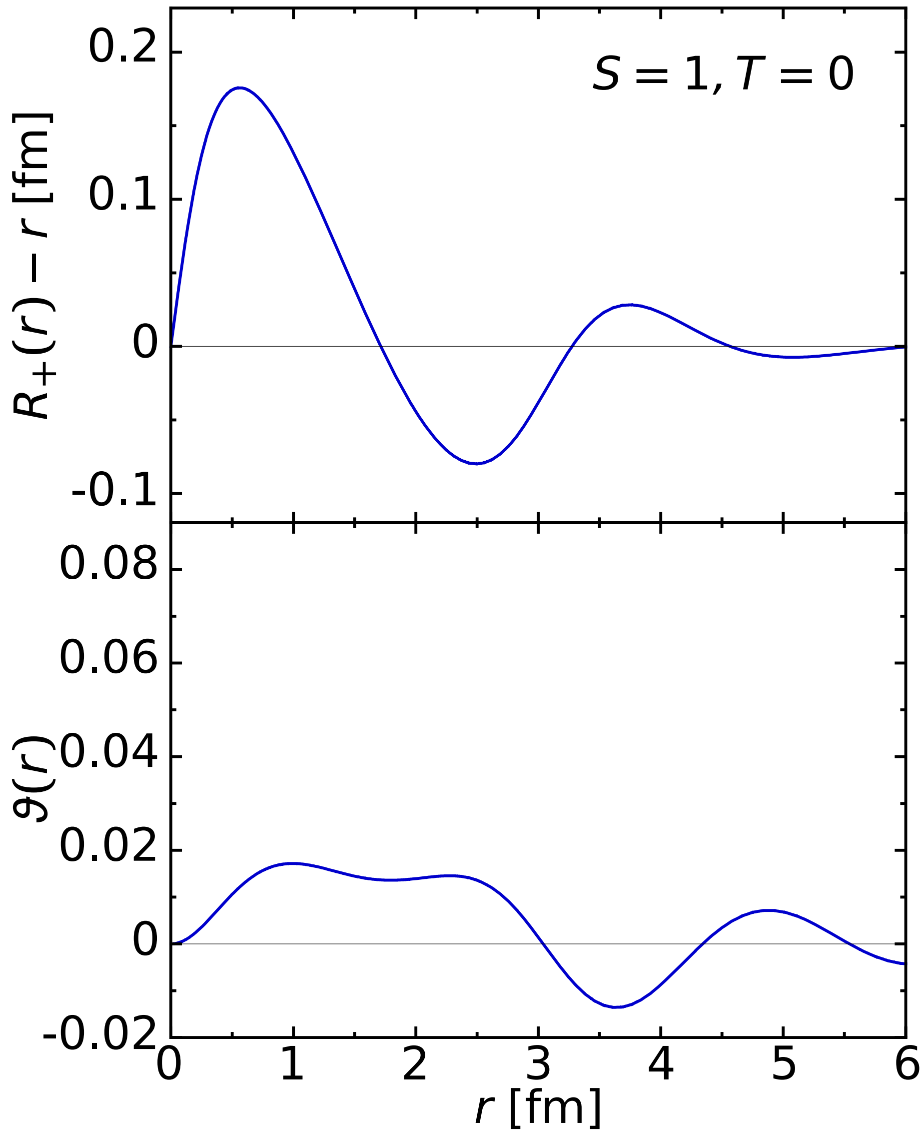




SRG-Generated UCOM Correlators: N3LO

- oscillatory behavior of wave function leads to long-range correlators
- **cutoff artifact?**



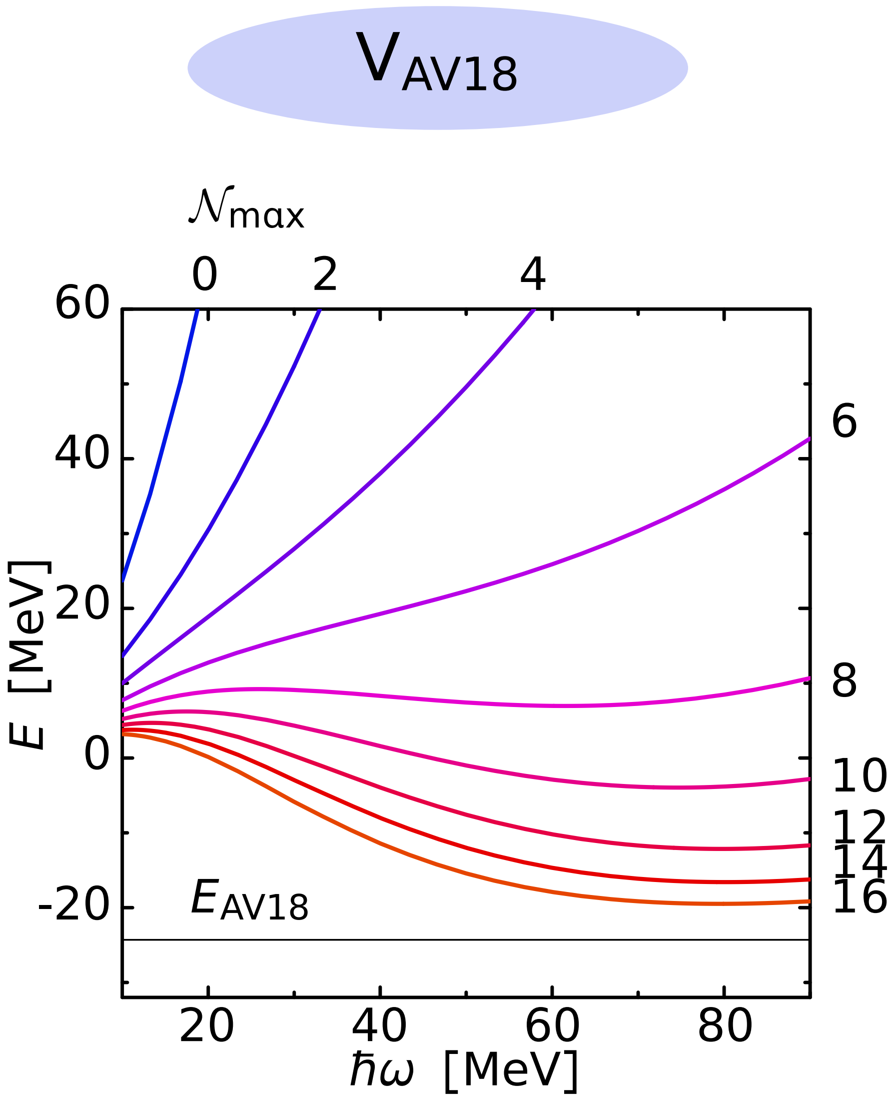


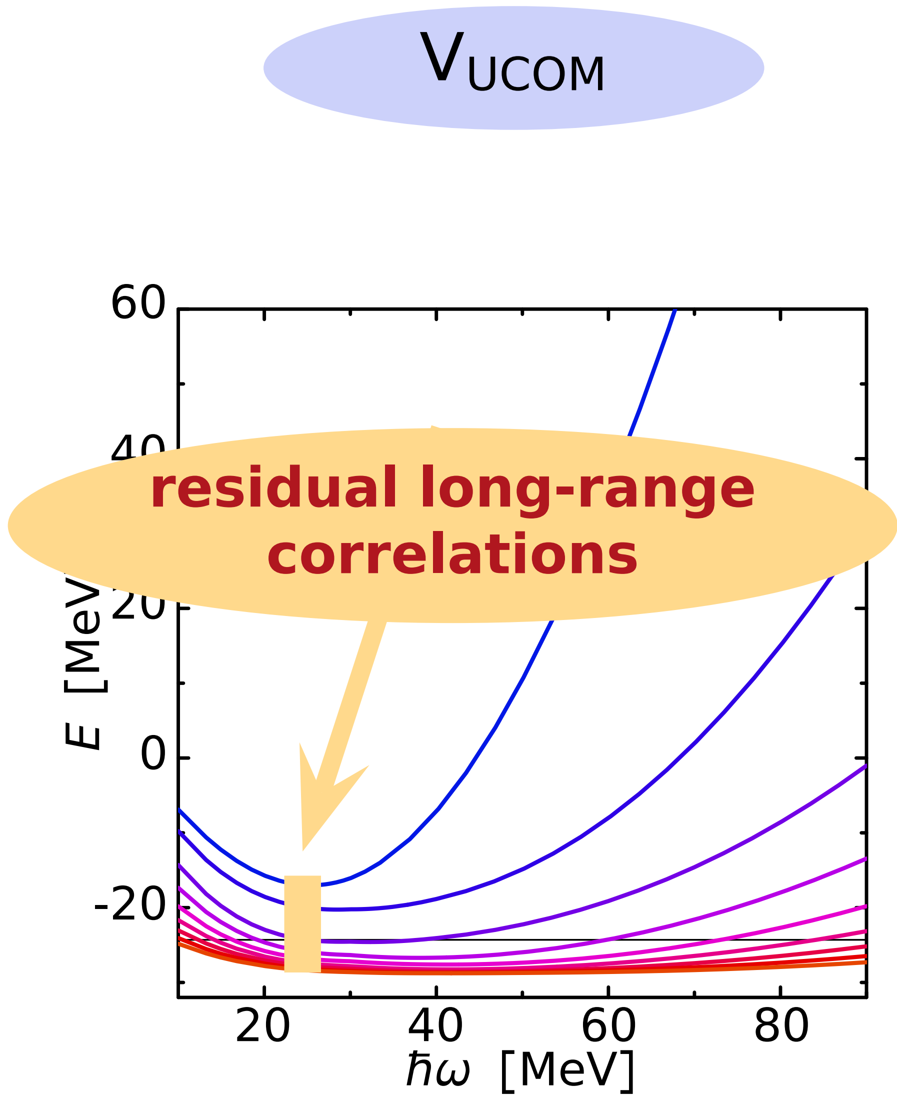
Computational Many-Body Methods

No-Core Shell Model

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

^{4}He: Convergence





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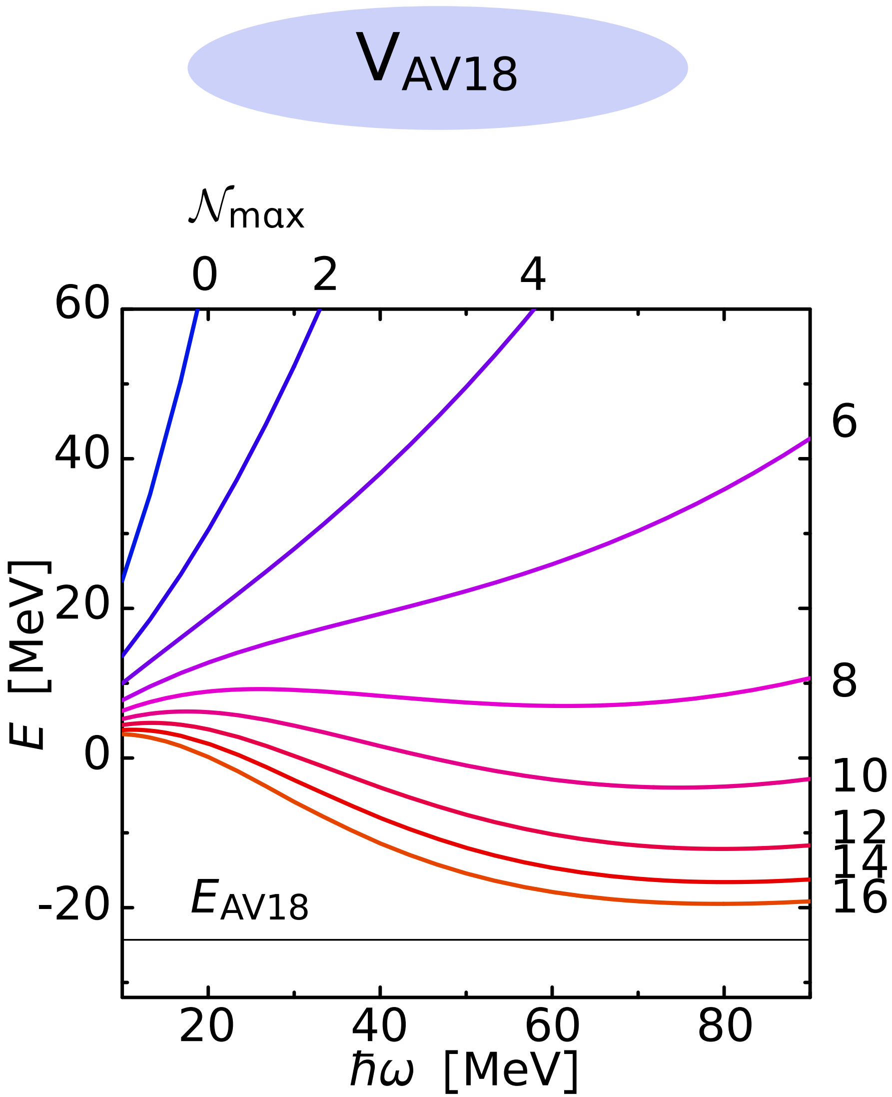
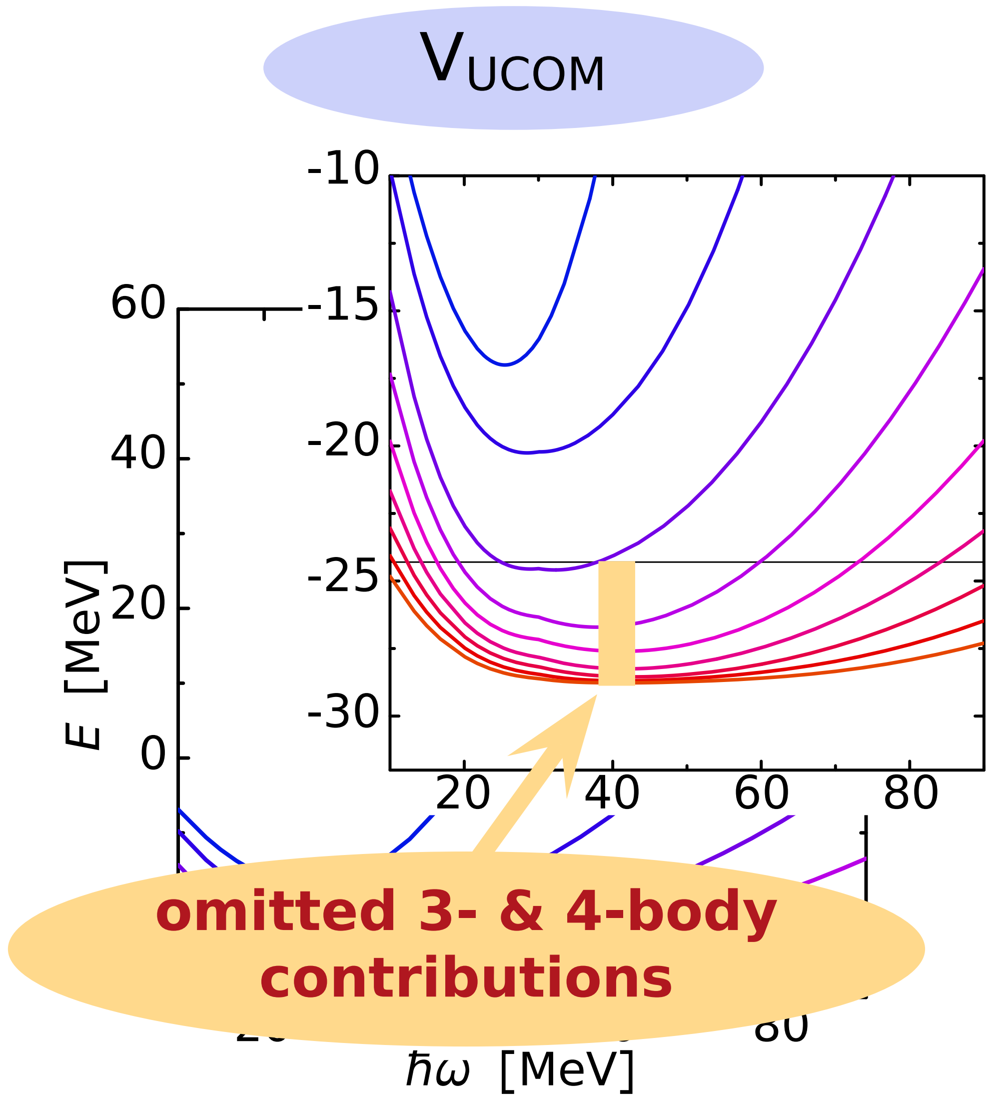




Three-Body Interactions — Strategies

Correlated Hamiltonian in Many-Body Space

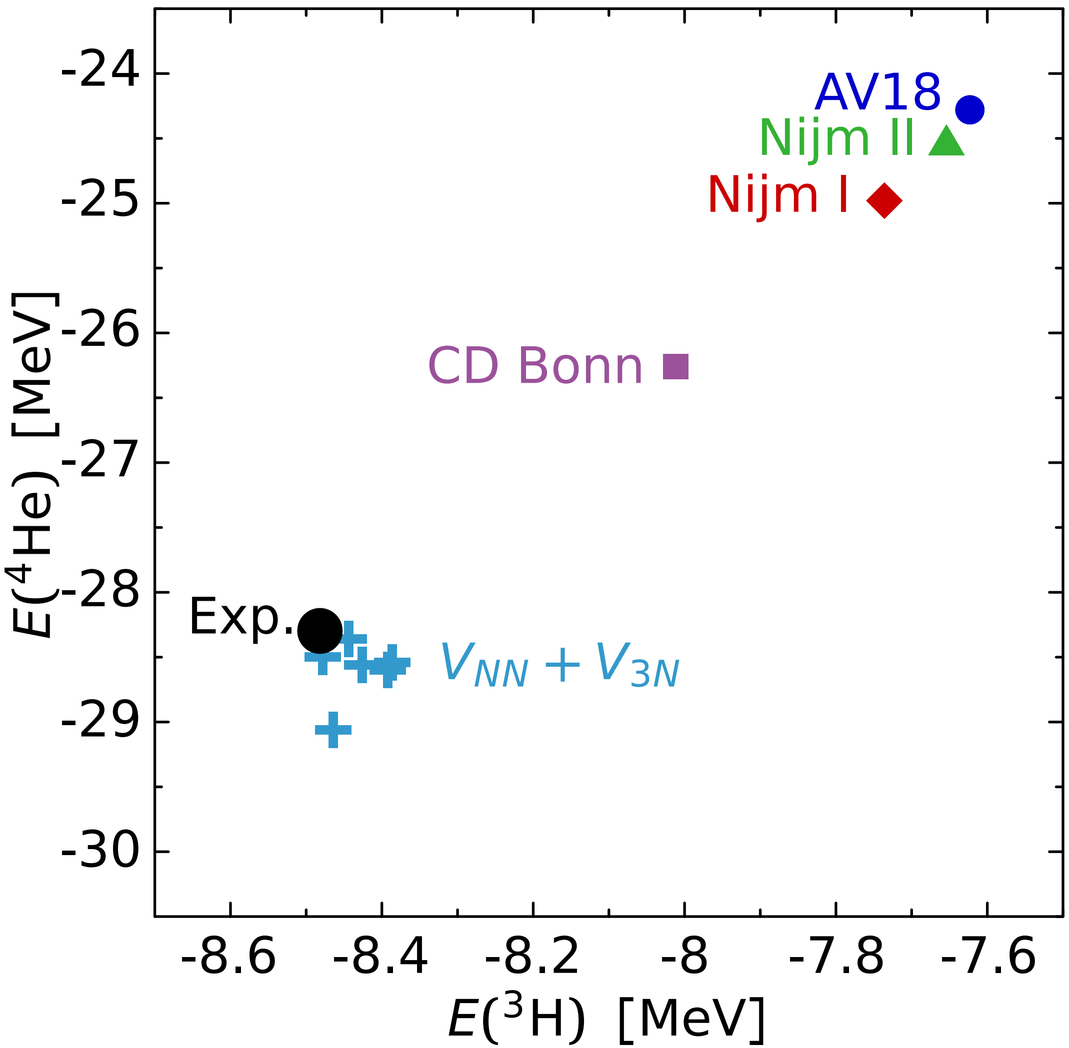
$$\widetilde{\mathrm{H}} = \mathrm{C}^\dagger\,(\mathrm{T} + \mathrm{V}_{NN} + \mathrm{V}_{3N})\,\mathrm{C}$$

$$= \widetilde{\mathrm{T}}^{[1]} + (\widetilde{\mathrm{T}}^{[2]} + \widetilde{\mathrm{V}}_{NN}^{[2]}) + (\widetilde{\mathrm{T}}^{[3]} + \widetilde{\mathrm{V}}_{NN}^{[3]} + \widetilde{\mathrm{V}}_{3N}^{[3]}) + \cdots$$

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

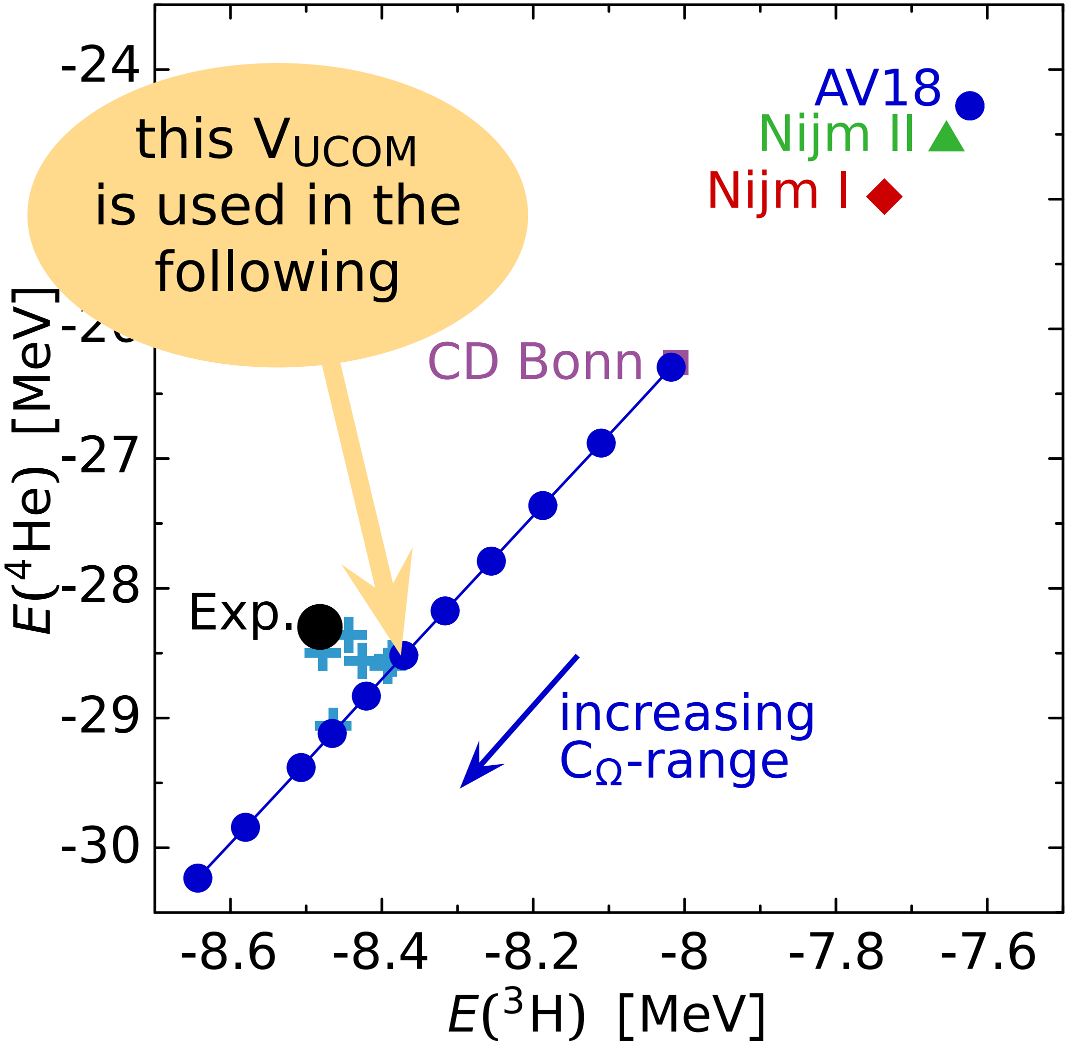
- **include full** $\mathrm{V}_{\mathbf{UCOM}}^{[3]}$ consisting of genuine and induced 3N terms
  (not really feasible beyond lightest isotopes)
- **replace** $\mathrm{V}_{\mathbf{UCOM}}^{[3]}$ by phenomenological three-body force
  (tractable also for heavier nuclei)
- **minimize** $\mathrm{V}_{\mathbf{UCOM}}^{[3]}$ by proper choice of unitary transformation
  (calculation with a pure two-body interaction)

Three-Body Interactions — Tjon Line



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

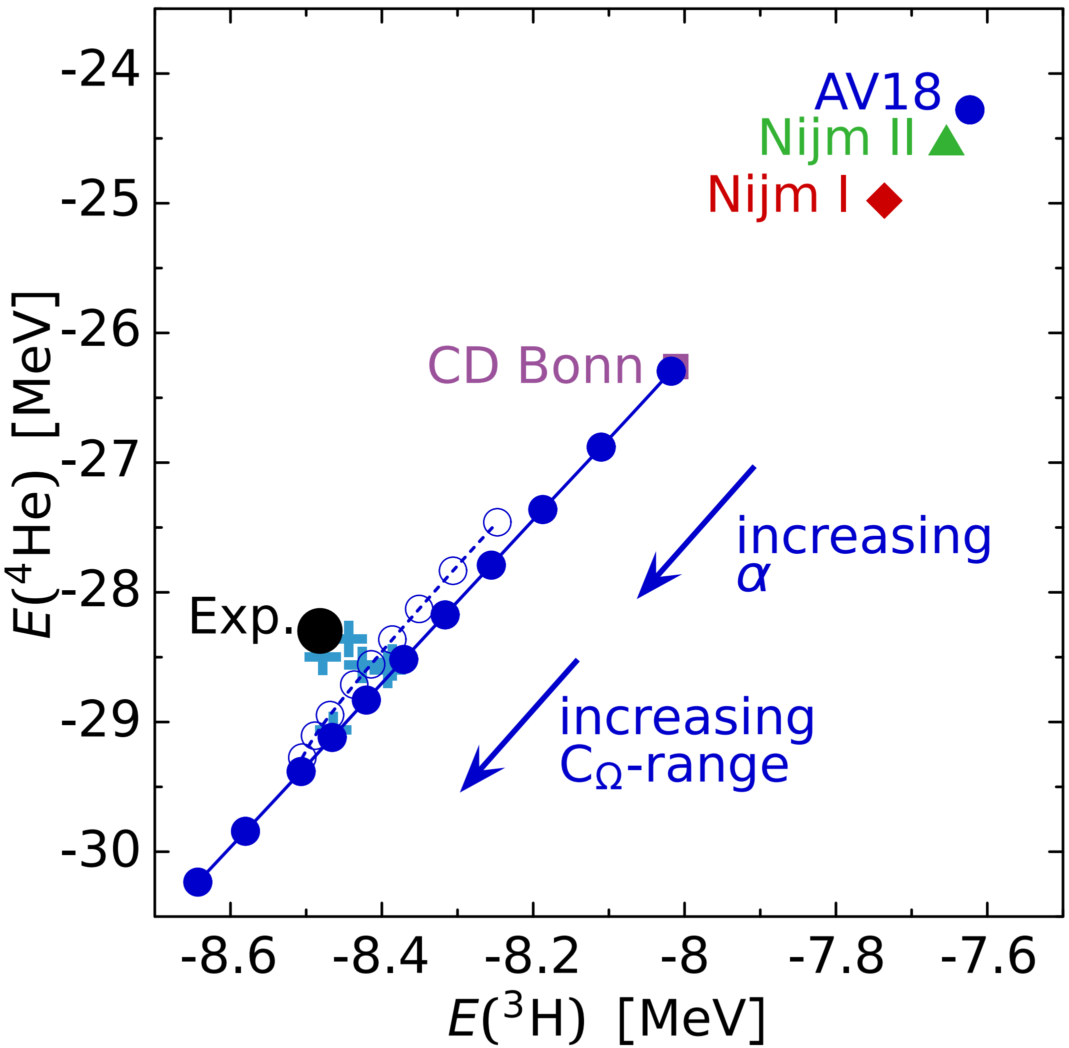
Three-Body Interactions — Tjon Line



- **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 3N interaction by choosing correlator close to experimental point

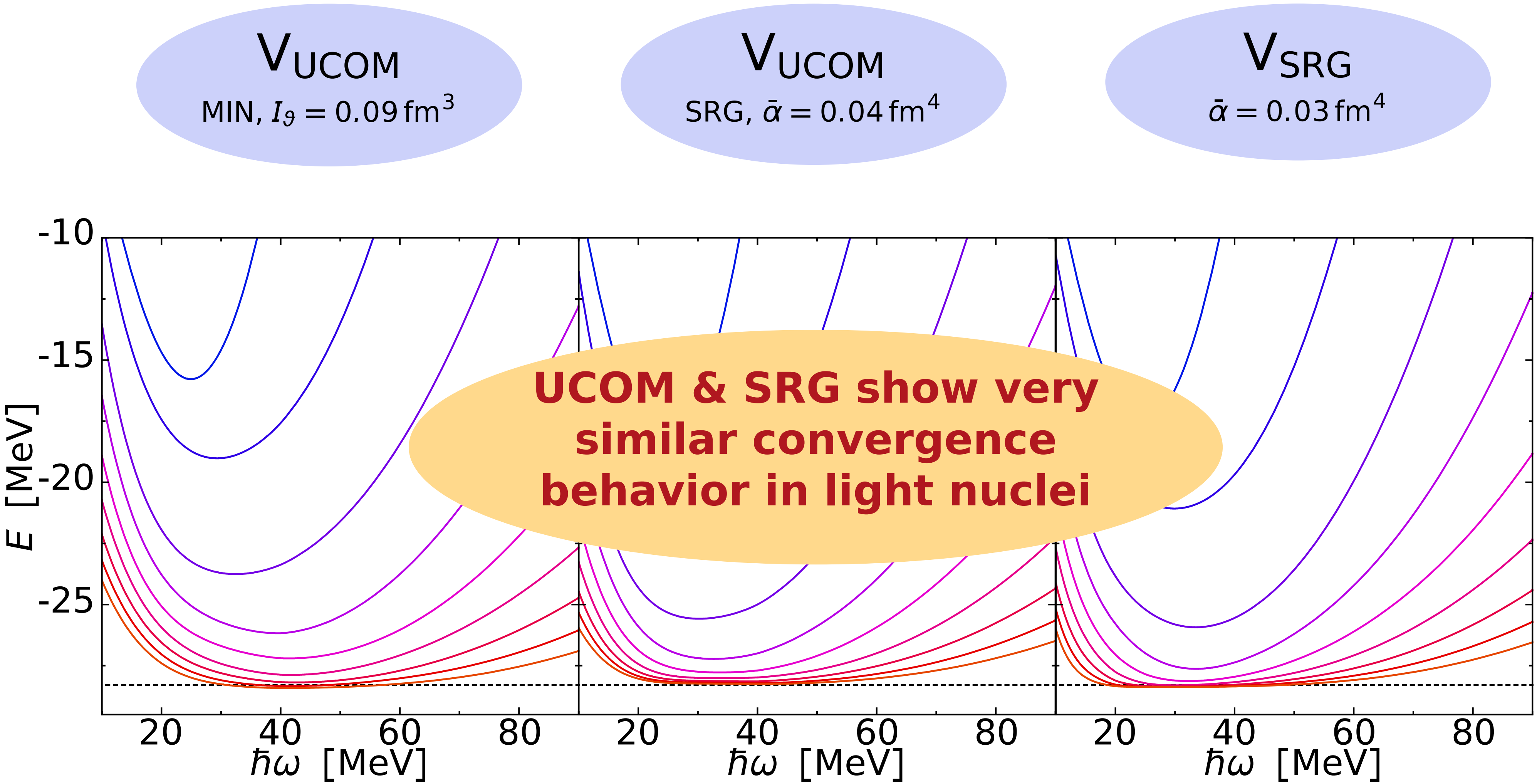
Three-Body Interactions — Tjon Line



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

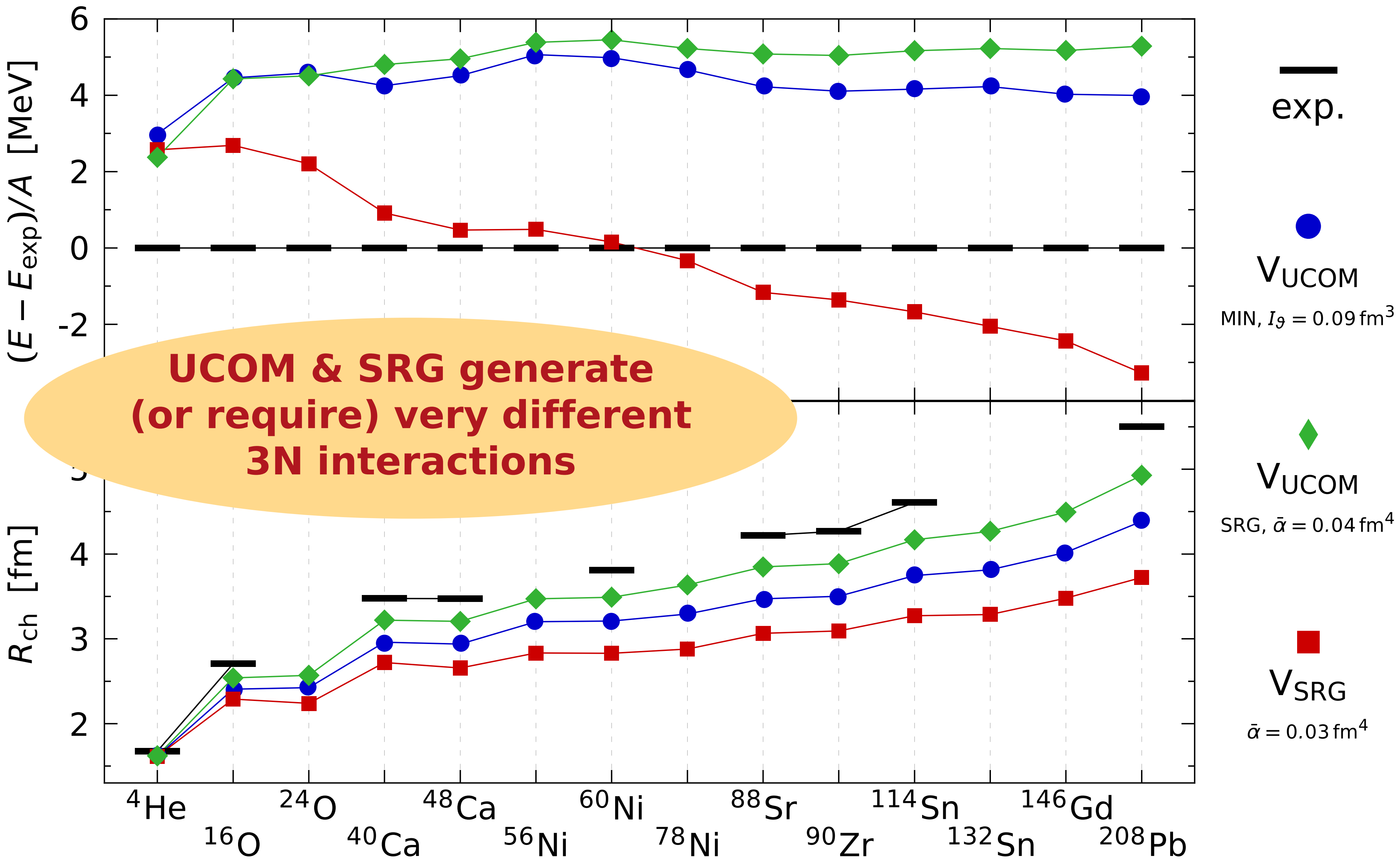
minimize net 3N interaction by choosing correlator close to experimental point

UCOM vs. SRG: ^{4}He Convergence

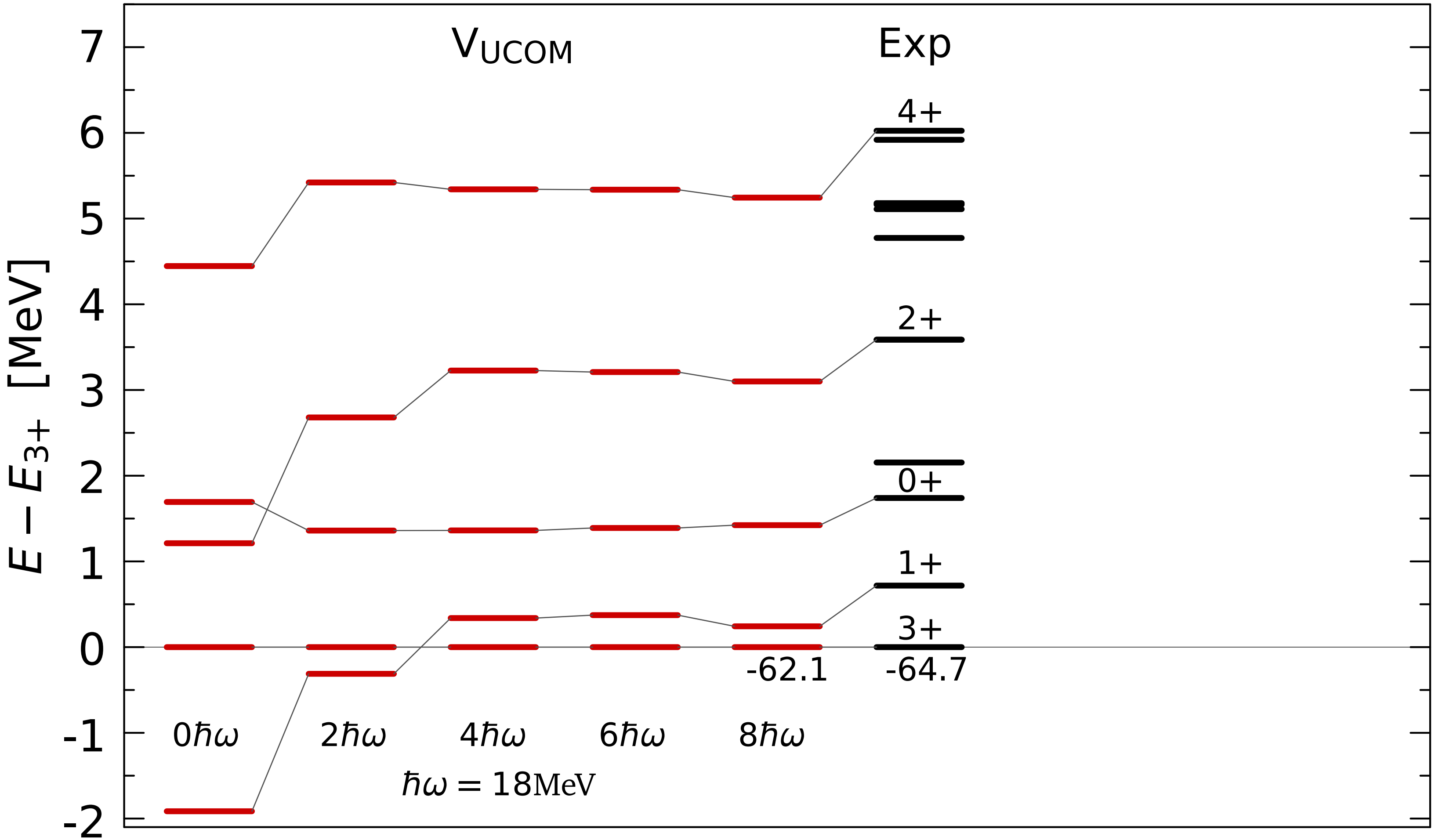


- I_ϑ or $\bar{\alpha}$ adjusted such that ^{4}He binding energy is reproduced

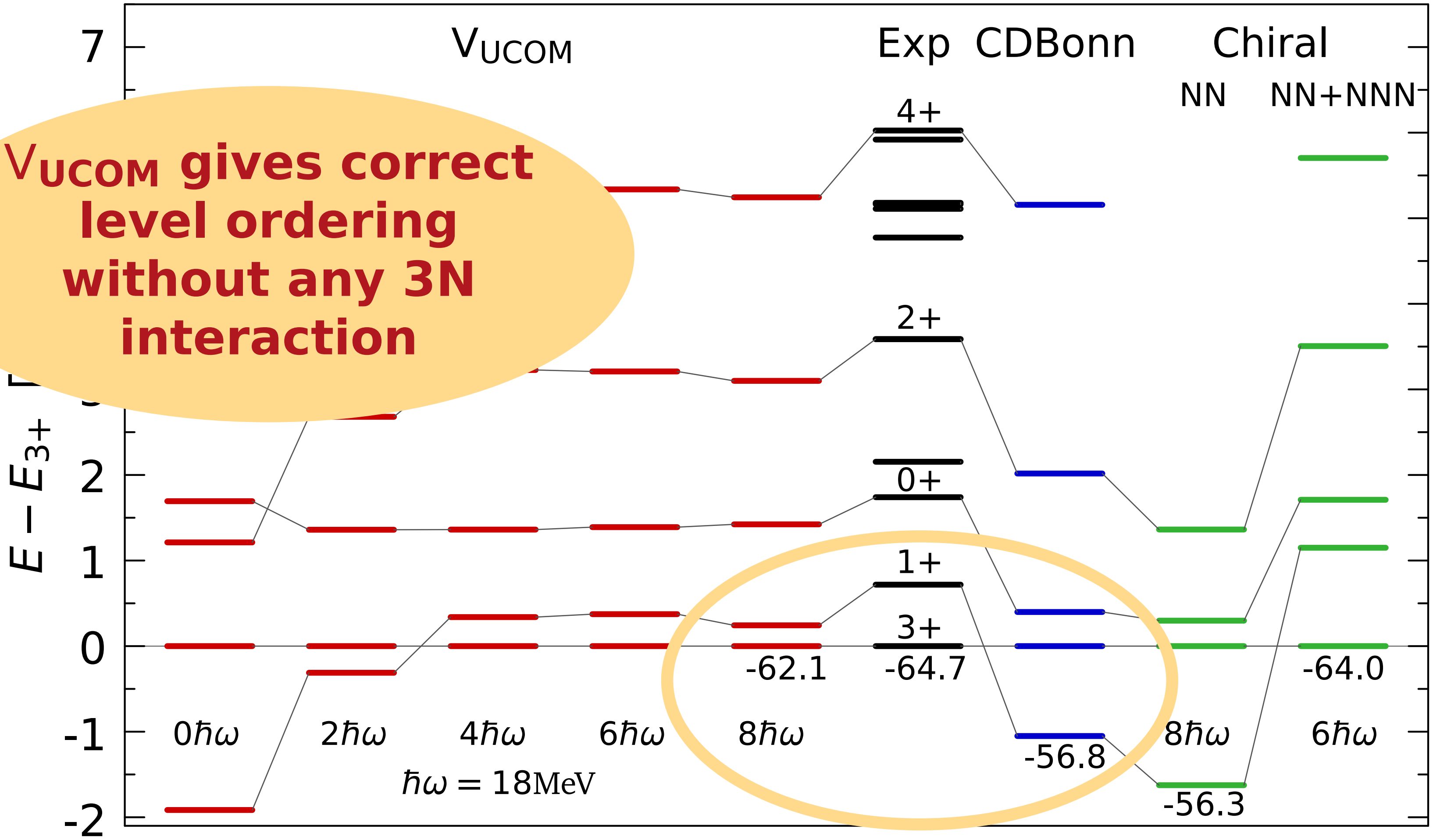
UCOM vs. SRG: Hartree-Fock Systematics



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



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



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

Computational Many-Body Methods

Importance-Truncated No-Core Shell Model

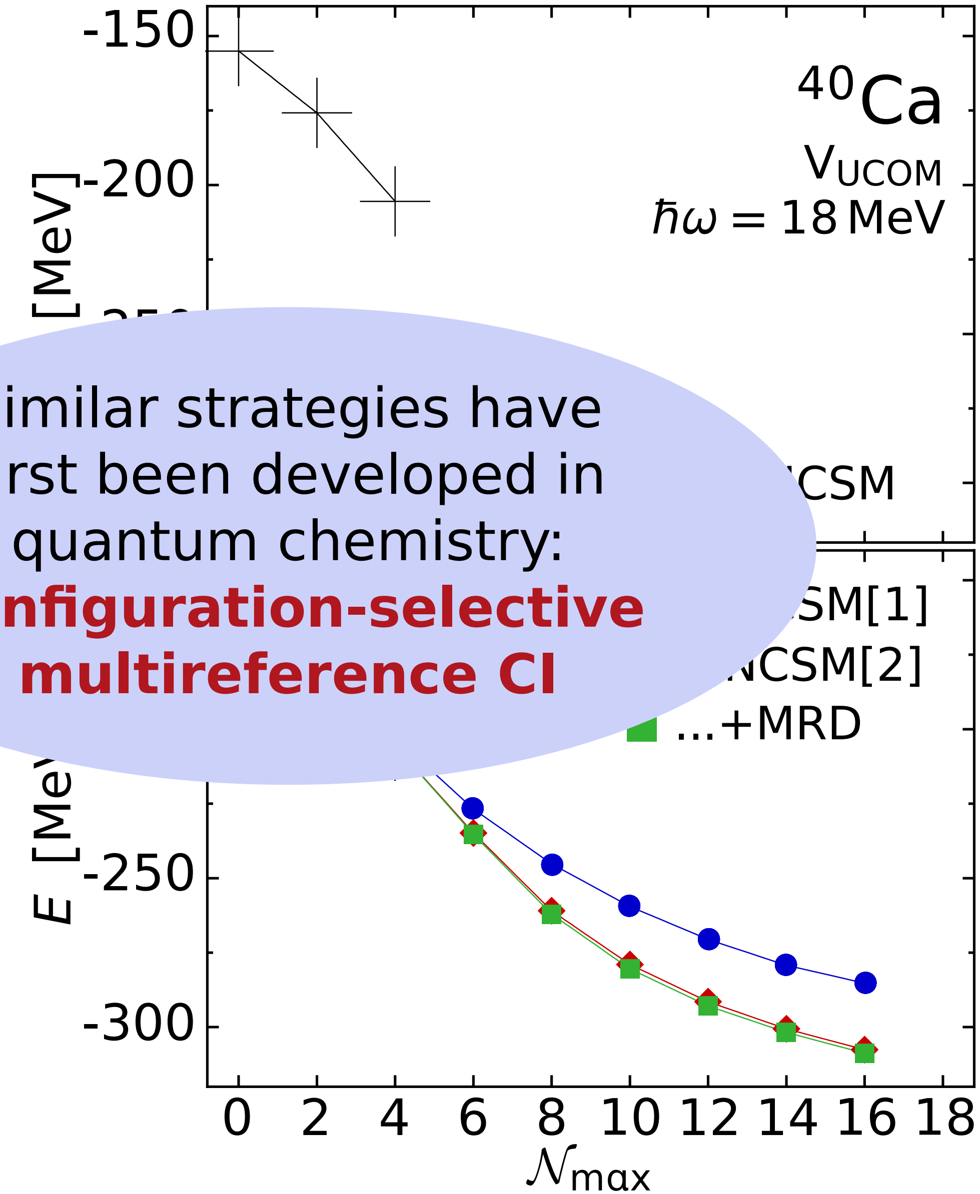
Roth & Navrátil — Phys. Rev. Lett. 99, 092501 (2007)

Roth, Piecuch, Gour — arXiv: 0806.0333

Roth — in preparation

Importance-Truncated NCSM

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



Importance Truncation

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

similar strategies have first been developed in quantum chemistry: **configuration-selective multireference CI**

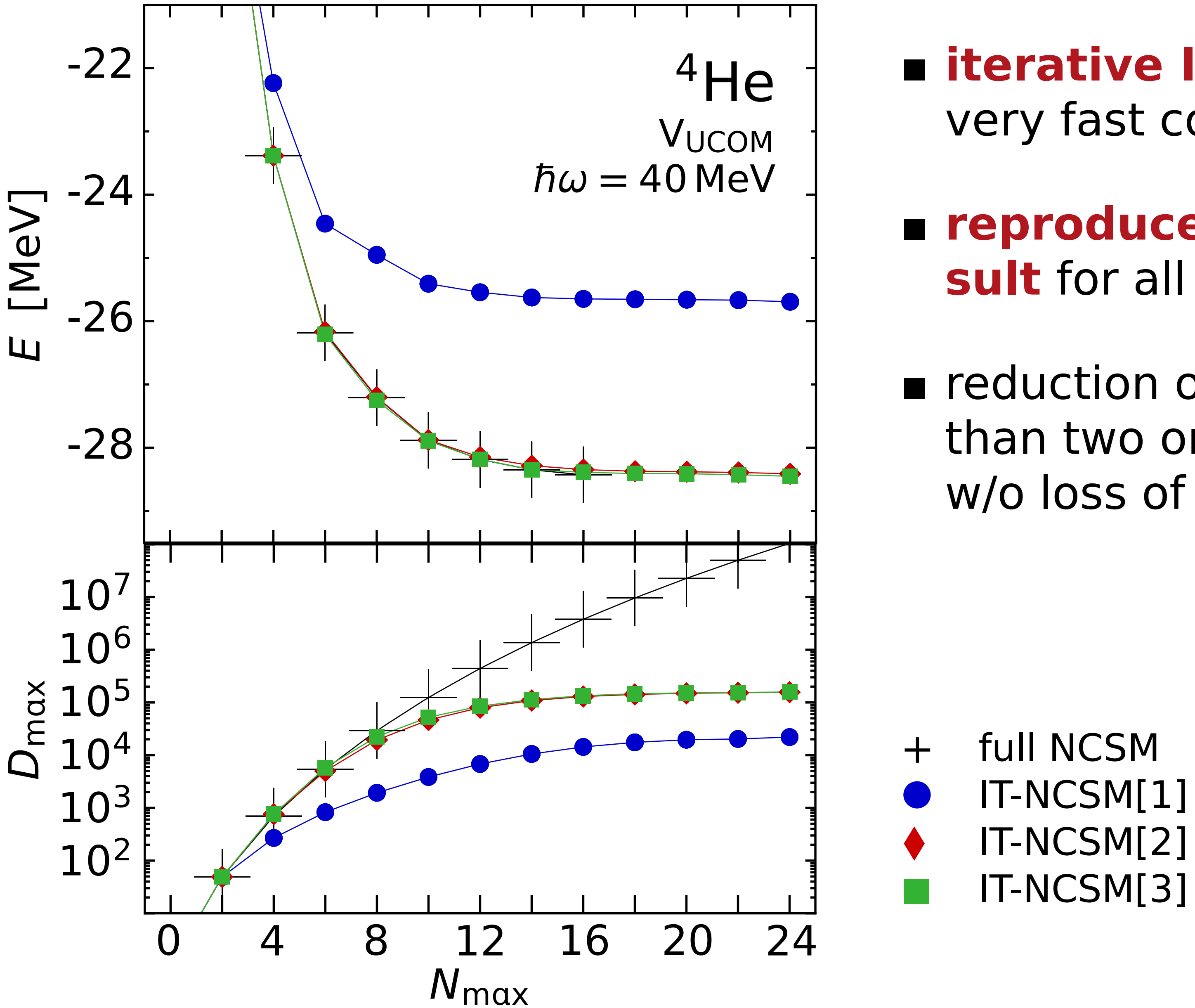
Importance Truncation: General Idea

- given an initial approximation $|\Psi_{\text{ref}}\rangle$ for the **target state**
- **measure the importance** of individual basis state $|\Phi_\nu\rangle$ via first-order multiconfigurational perturbation theory

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

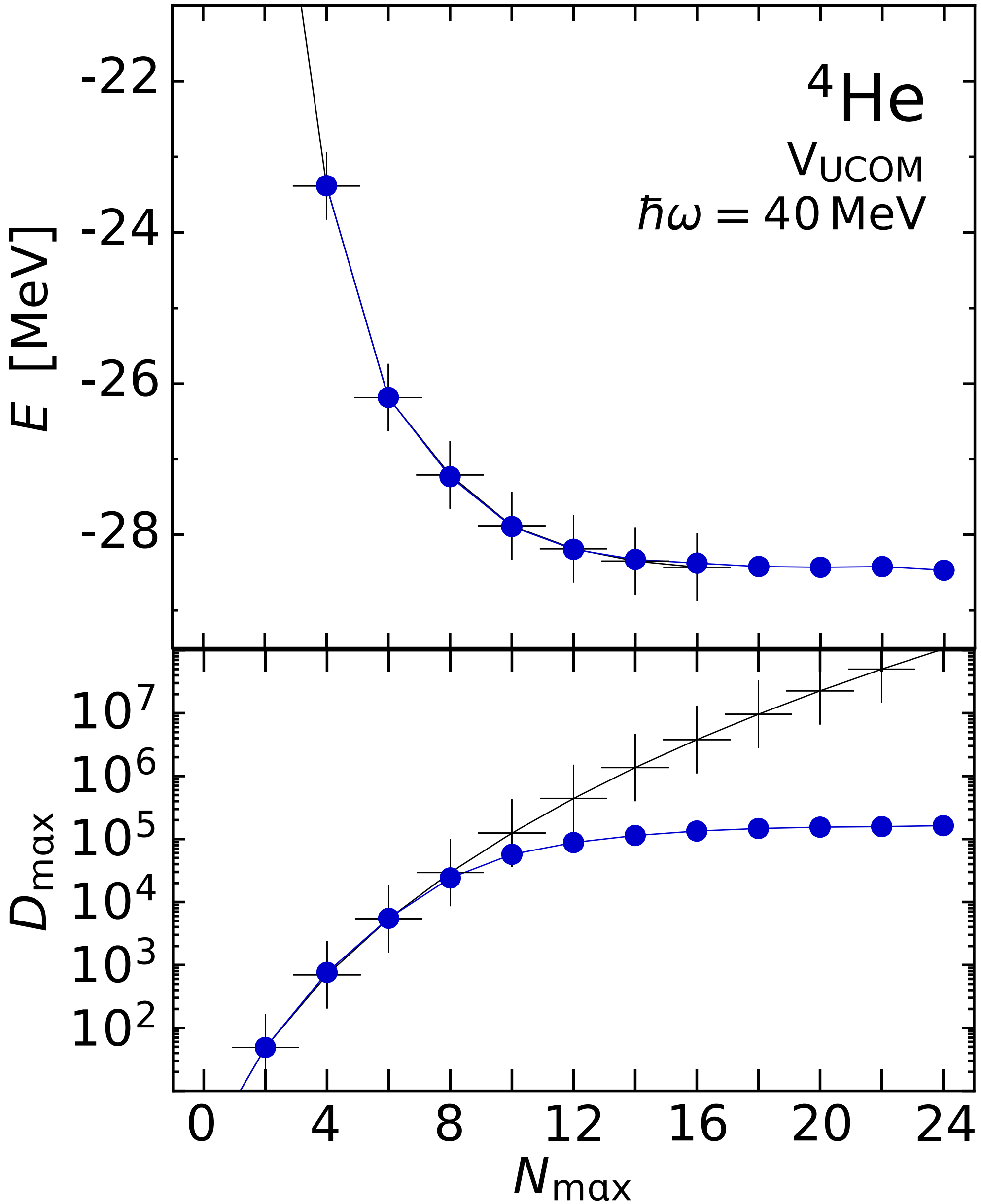
- construct **importance-truncated space** spanned by basis states with $|\kappa_\nu| \geq \kappa_{\text{min}}$ and solve eigenvalue problem
- **iterative scheme**: repeat construction of importance-truncated model space using eigenstate as improved reference $|\Psi_{\text{ref}}\rangle$
- **threshold extrapolations** and **perturbative corrections** can be used to account for discarded basis states

^{4}He: Importance-Truncated NCSM



- **iterative IT-NCSM(*i*)** shows very fast convergence
- **reproduces exact NCSM result** for all N_{max}
- reduction of basis by more than two orders of magnitude w/o loss of precision

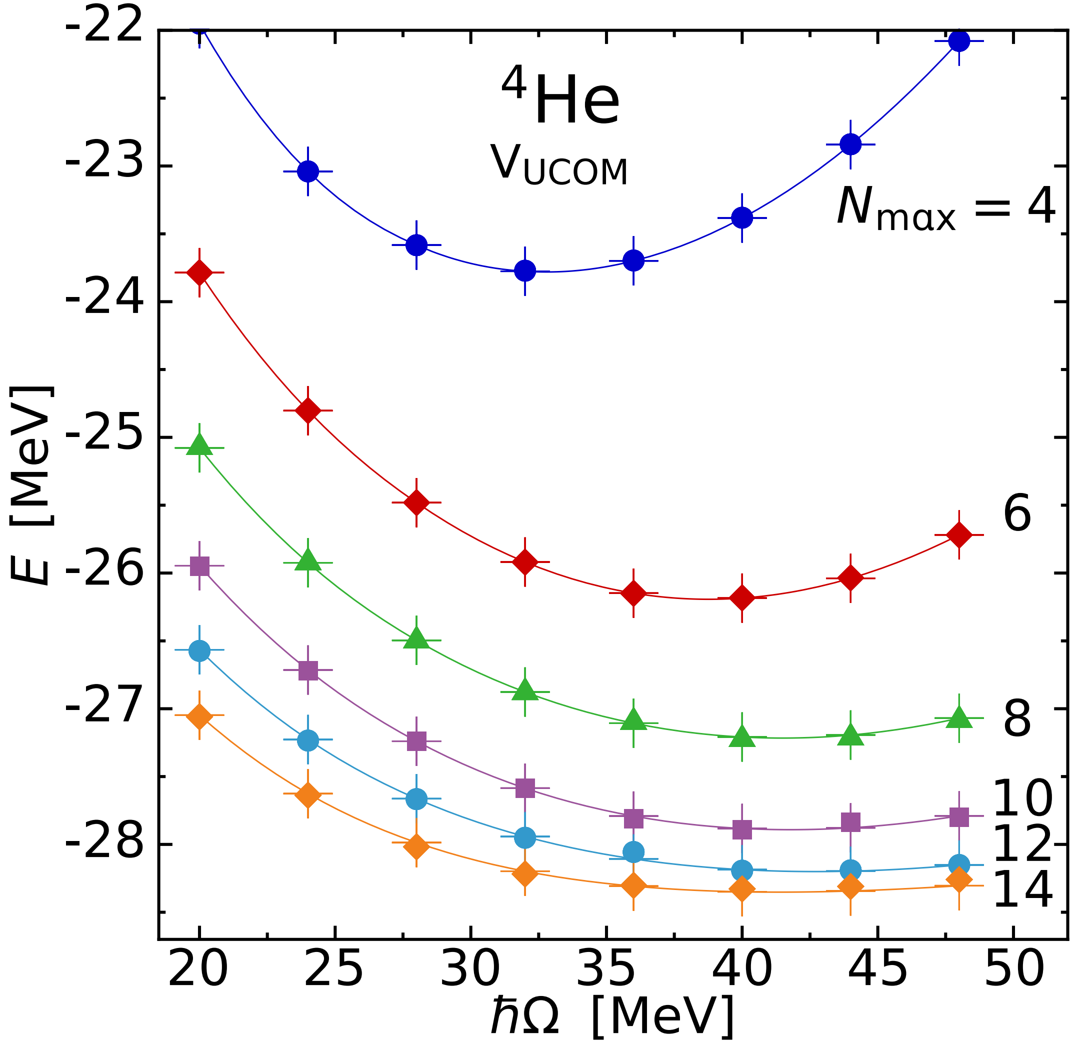
^{4}He: Importance-Truncated NCSM



- **sequential IT-NCSM(seq)** provides same results as IT-NCSM(3) with just one update per N_{max}
- **reproduces exact NCSM result** for all N_{max}
- reduction of basis by more than two orders of magnitude w/o loss of precision

+ full NCSM
● IT-NCSM(seq)

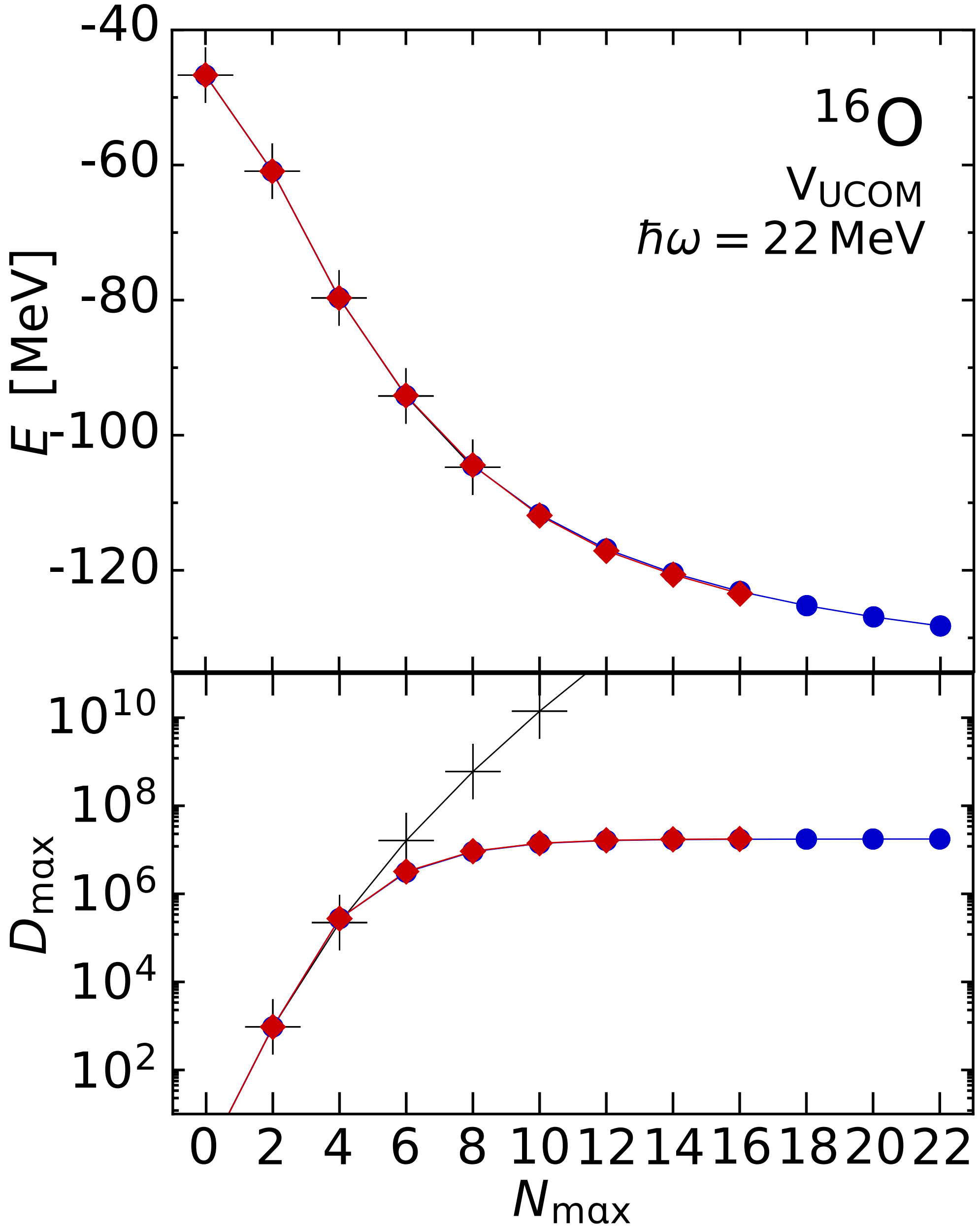
^{4}He: Importance-Truncated NCSM



- **reproduces exact NCSM result** for all $\hbar\omega$ and N_{max}
- importance truncation & threshold extrapolation is robust
- no problem with center of mass

+ full NCSM
● IT-NCSM(seq)

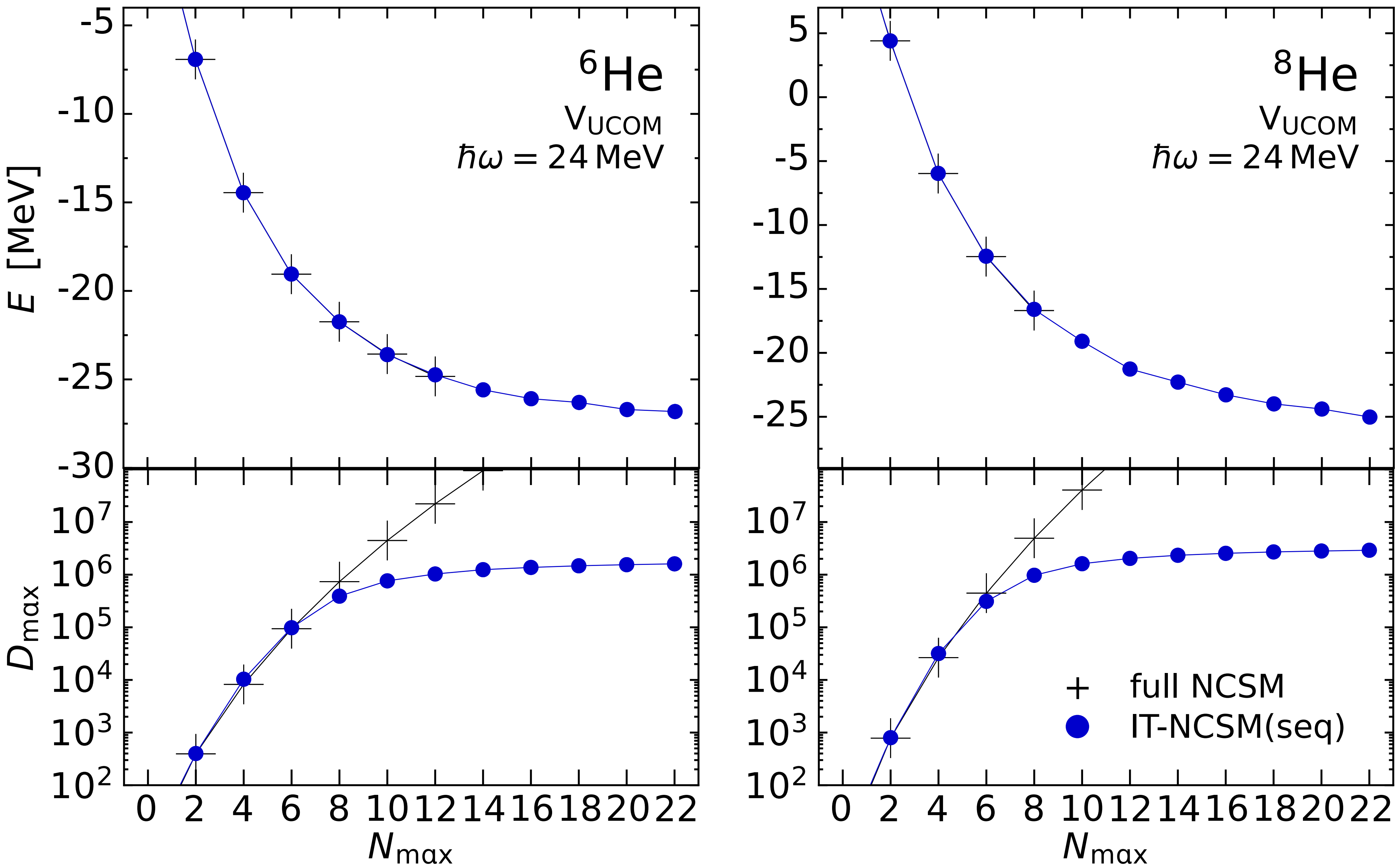
^{16}O: Importance-Truncated NCSM



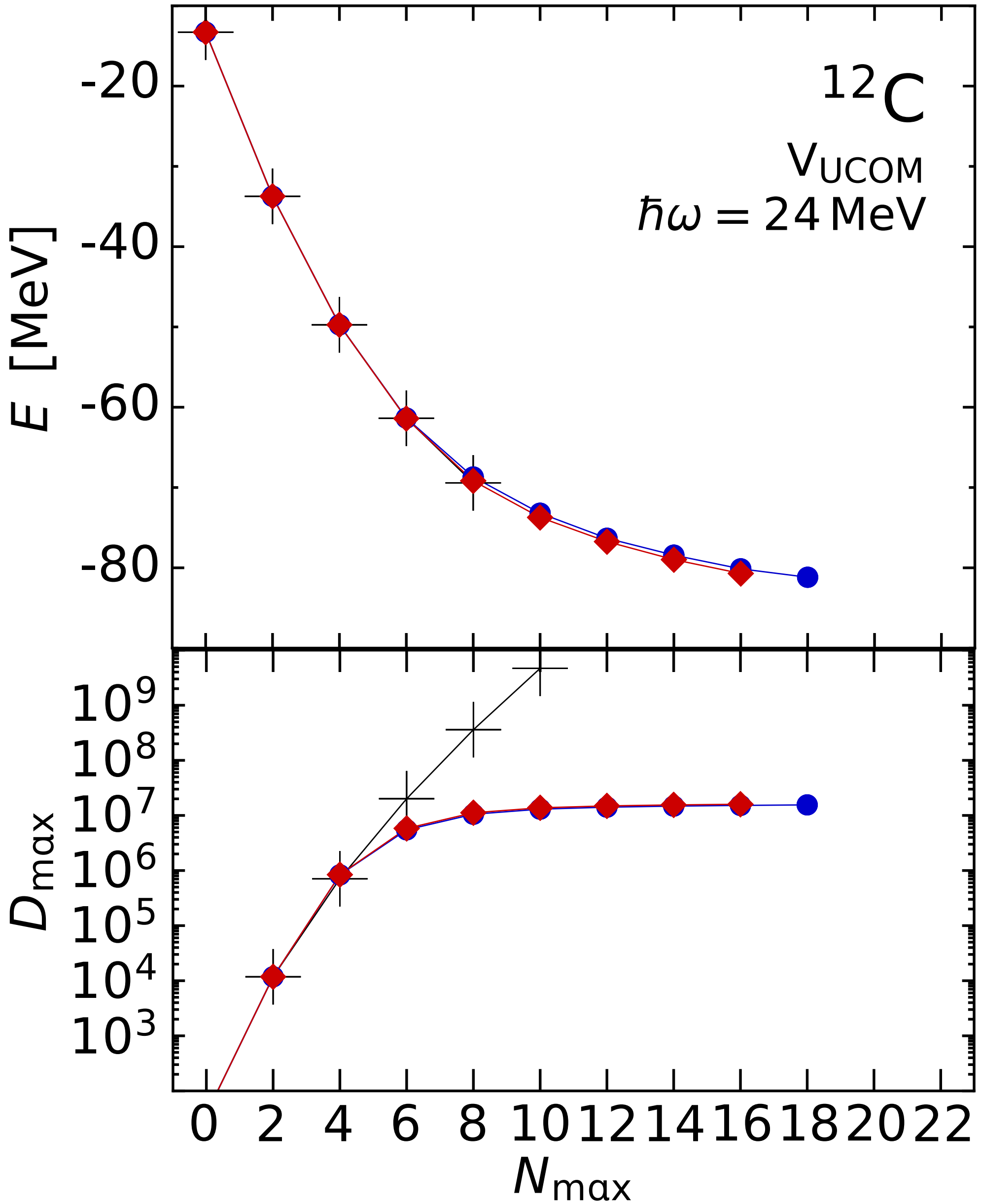
- IT-NCSM(seq) provides **excellent agreement with full NCSM** calculation
- dimension reduced by **several orders of magnitude**
- possibility to go **way beyond** the domain of the full NCSM

+ full NCSM
● IT-NCSM(seq), $C_{min} = 0.0005$
♦ IT-NCSM(seq), $C_{min} = 0.0003$

^{6}He & ^{8}He: IT-NCSM for Open-Shell Nuclei



^{12}C: IT-NCSM for Open-Shell Nuclei



- **excellent agreement with full NCSM** calculations
- IT-NCSM(seq) works just as well for **non-magic / open-shell nuclei**
- all calculations limited by CPU-time only

+ full NCSM
● IT-NCSM(seq), $C_{min} = 0.0005$
♦ IT-NCSM(seq), $C_{min} = 0.0003$

IT-NCSM: Pros and Cons

- ✔ rigorously fulfills **variational principle** and Hylleraas-Undheim theorem
- ✔ **no sizable center-of-mass contamination** induced by IT in $N_{\max}\hbar\Omega$ space
- ✔ constrained **threshold extrapolation** $\kappa_{\min} \to 0$ recovers contribution of excluded configurations efficiently and accurately
- ✔ **open and closed-shell nuclei** with **ground and excited states** can be treated on the same footing
- ✔ **compatible with shell-model**: excited states and angular-momentum projection via Lanczos, eigenstates in shell-model representation, computation of observables
- ✘ computationally still demanding

Perspectives

- three steps from QCD to the nuclear chart
  - QCD-based nuclear interactions
  - unitarily transformed interactions (UCOM, SRG,...)
  - computational many-body methods
- exciting new developments in all three sectors
- alternative route using density functional methods

QCD-based description of nuclear structure across the whole nuclear chart is within reach

Epilogue

- **thanks to my group & my collaborators**
  - S. Binder, B. Erler, A. Günther, H. Hergert, M. Hild, H. Krutsch, J. Langhammer, P. Papakonstantinou, S. Reinhardt, F. Schmitt, N.Vogelmann, F. Wagner

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  - P. Navrátil

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  - P. Piecuch, J. Gour

    Michigan State University, USA
  - H. Feldmeier, T. Neff,...

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Deutsche Forschungsgemeinschaft
DFG

SFB 634

HIC for FAIR

LOEWE – Landes-Offensive zur Entwicklung Wissenschaftlich-ökonomischer Exzellenz