

Ab-Initio Nuclear Structure beyond the p-Shell:

Interactions & Many-Body Techniques

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DARMSTADT

Overview

- Motivation
- Unitarily Transformed Interactions
 - Unitary Correlation Operator Method
 - Similarity Renormalization Group
- Computational Many-Body Methods
 - Testing UCOM & SRG in Nuclei: NCSM & HF+MBPT
 - Importance Truncated NCSM

From QCD to Nuclear Structure

Nuclear Structure

Low-Energy QCD

From QCD to Nuclear Structure

Nuclear Structure

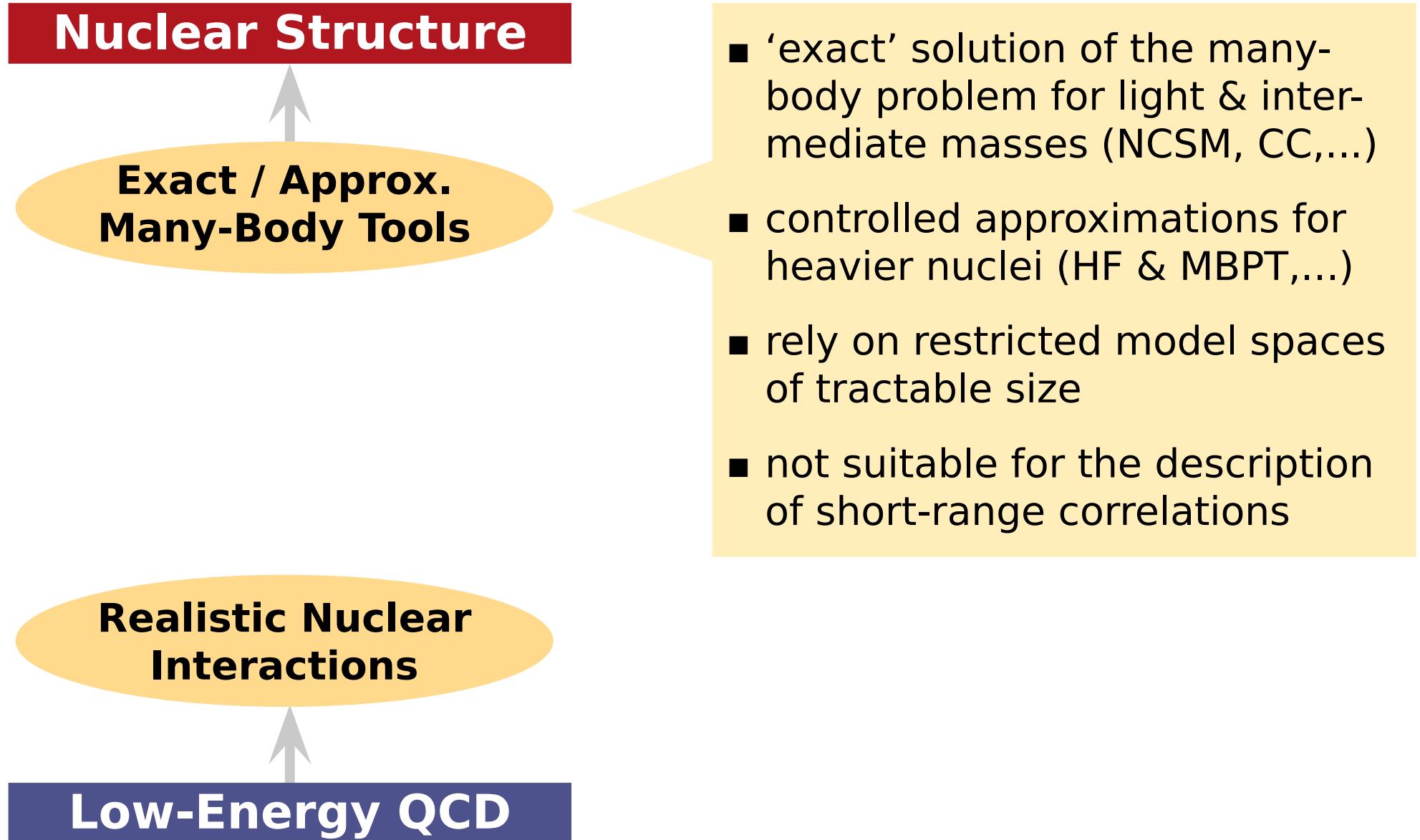
**Realistic Nuclear
Interactions**

Low-Energy QCD

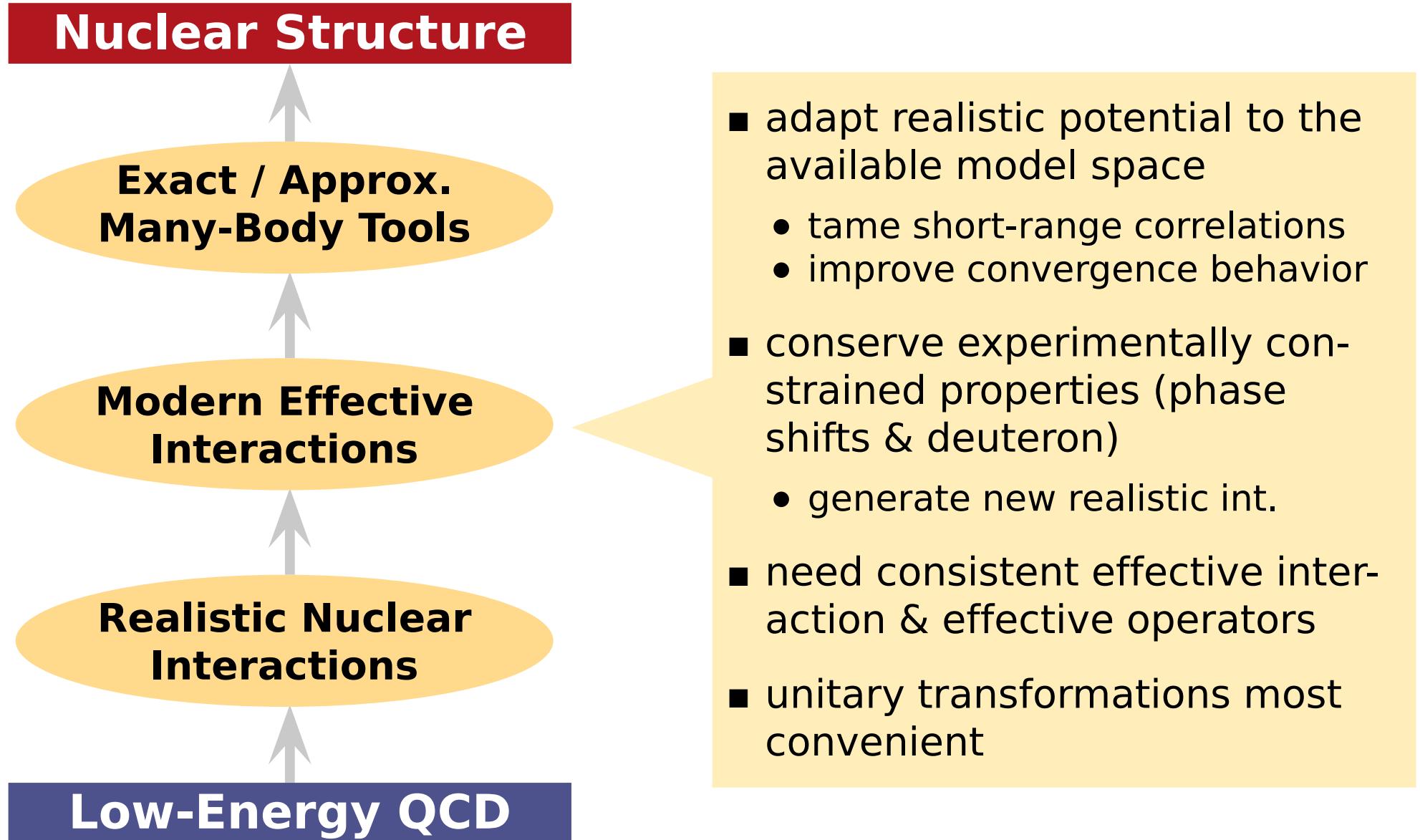


- chiral EFT interactions: consistent NN & 3N interaction derived within χ EFT
- traditional NN-interactions: Argonne V18, CD Bonn,...
- reproduce experimental two-body data with high precision
- induce strong short-range central & tensor correlations

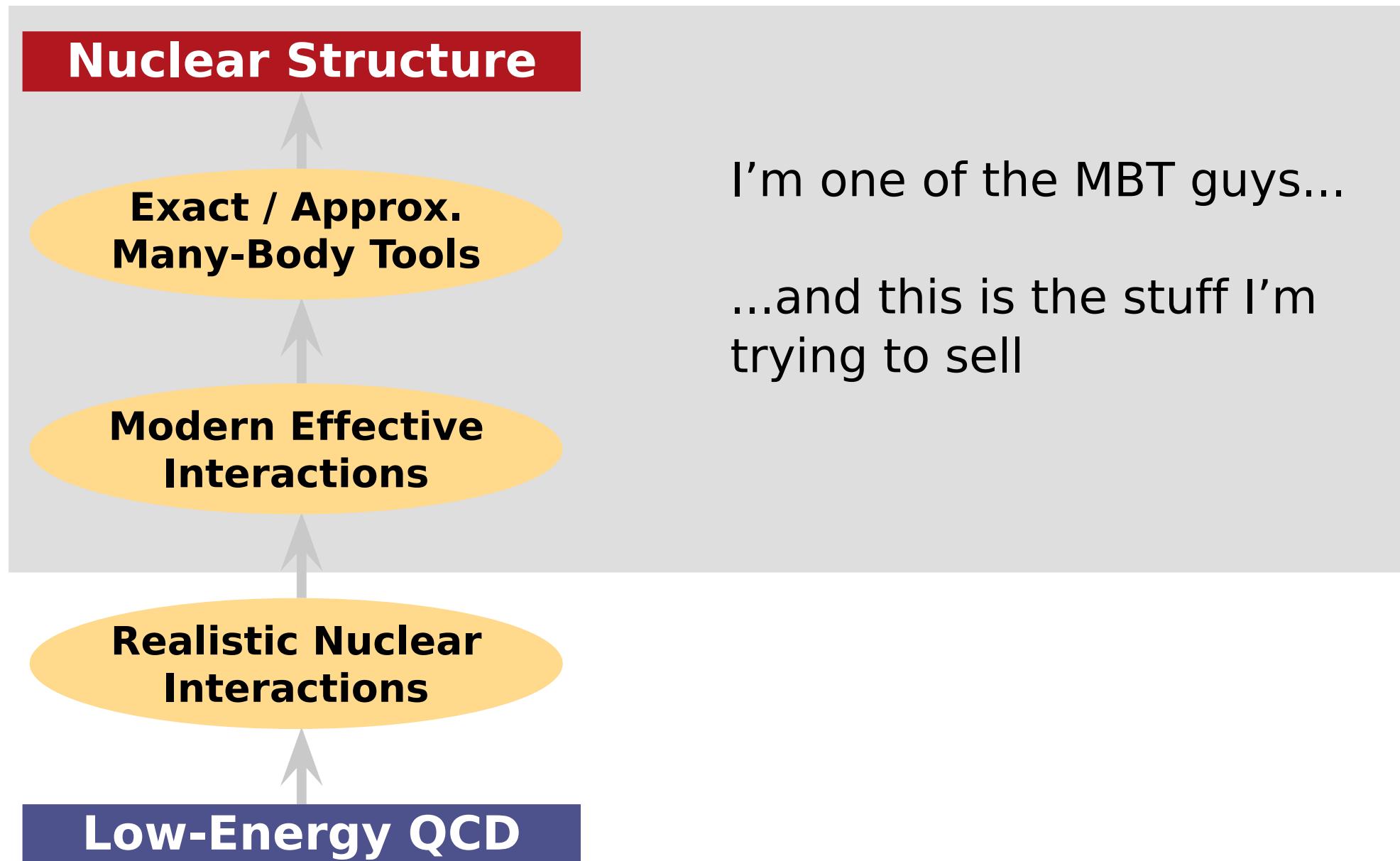
From QCD to Nuclear Structure



From QCD to Nuclear Structure



From QCD to Nuclear Structure



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)

Unitary Correlation Operator Method

Correlation Operator

define a unitary operator C to describe the effect of short-range correlations

$$C = \exp[-iG] = \exp\left[-i\sum_{i < j} g_{ij}\right]$$

Correlated States

imprint short-range correlations onto uncorrelated many-body states

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

Correlated Operators

adapt Hamiltonian to uncorrelated states (pre-diagonalization)

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

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

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

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

$$q_r = \frac{1}{2} [\vec{r} \cdot \vec{q} + \vec{q} \cdot \vec{r}]$$

Tensor Correlator C_Ω

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

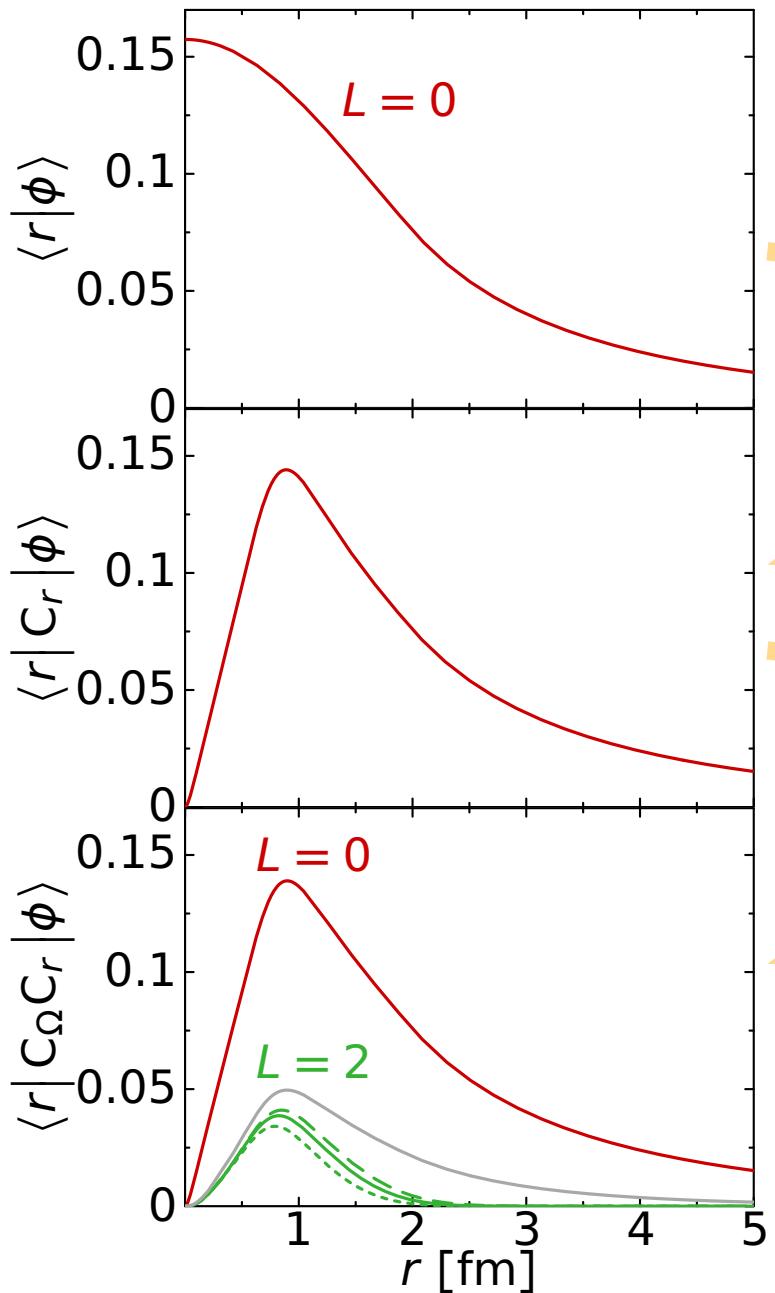
$$g_\Omega = \frac{3}{2} \vartheta(r) [(\vec{\sigma}_1 \cdot \vec{q}_\Omega)(\vec{\sigma}_2 \cdot \vec{r}) + (\vec{r} \leftrightarrow \vec{q}_\Omega)]$$

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

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

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

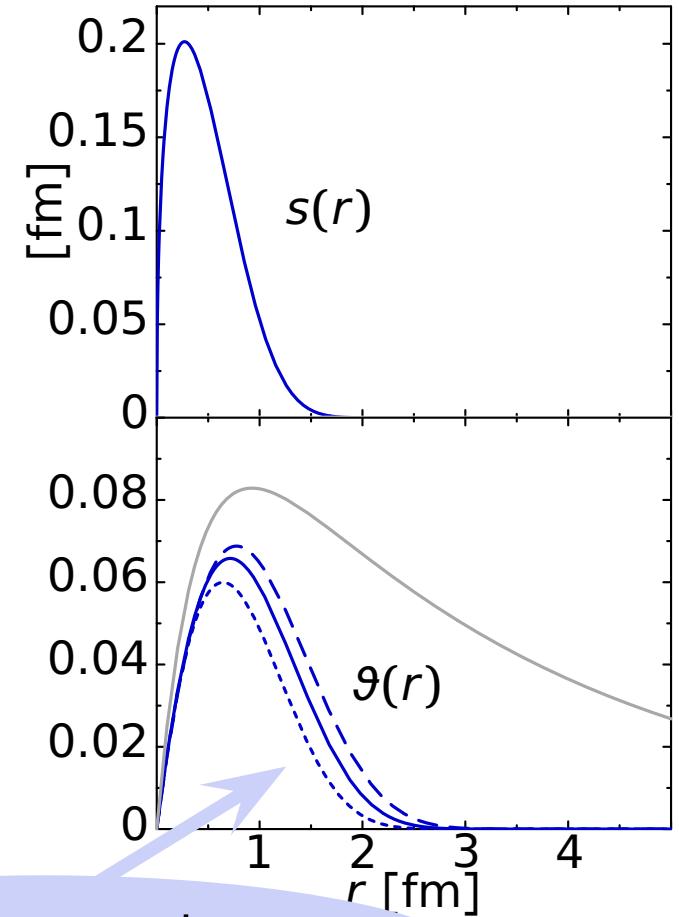
Correlated States: The Deuteron



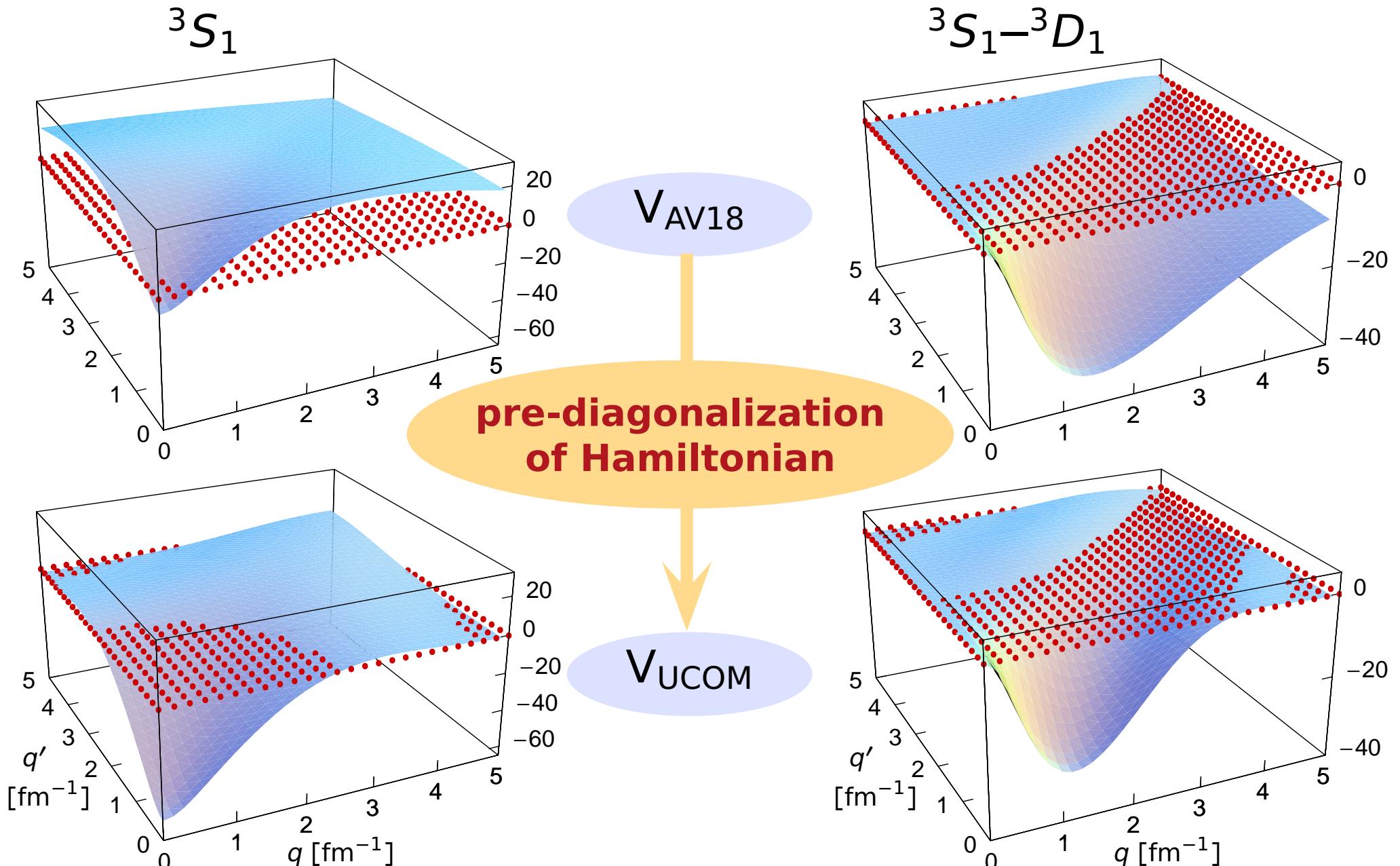
central correlations

tensor correlations

only short-range tensor correlations treated by C_Ω



Correlated Interaction: V_{UCOM}



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

$$\tilde{H}(\alpha) = C^\dagger(\alpha) H C(\alpha) \quad \rightarrow \quad \frac{d}{d\alpha} \tilde{H}(\alpha) = [\eta(\alpha), \tilde{H}(\alpha)]$$

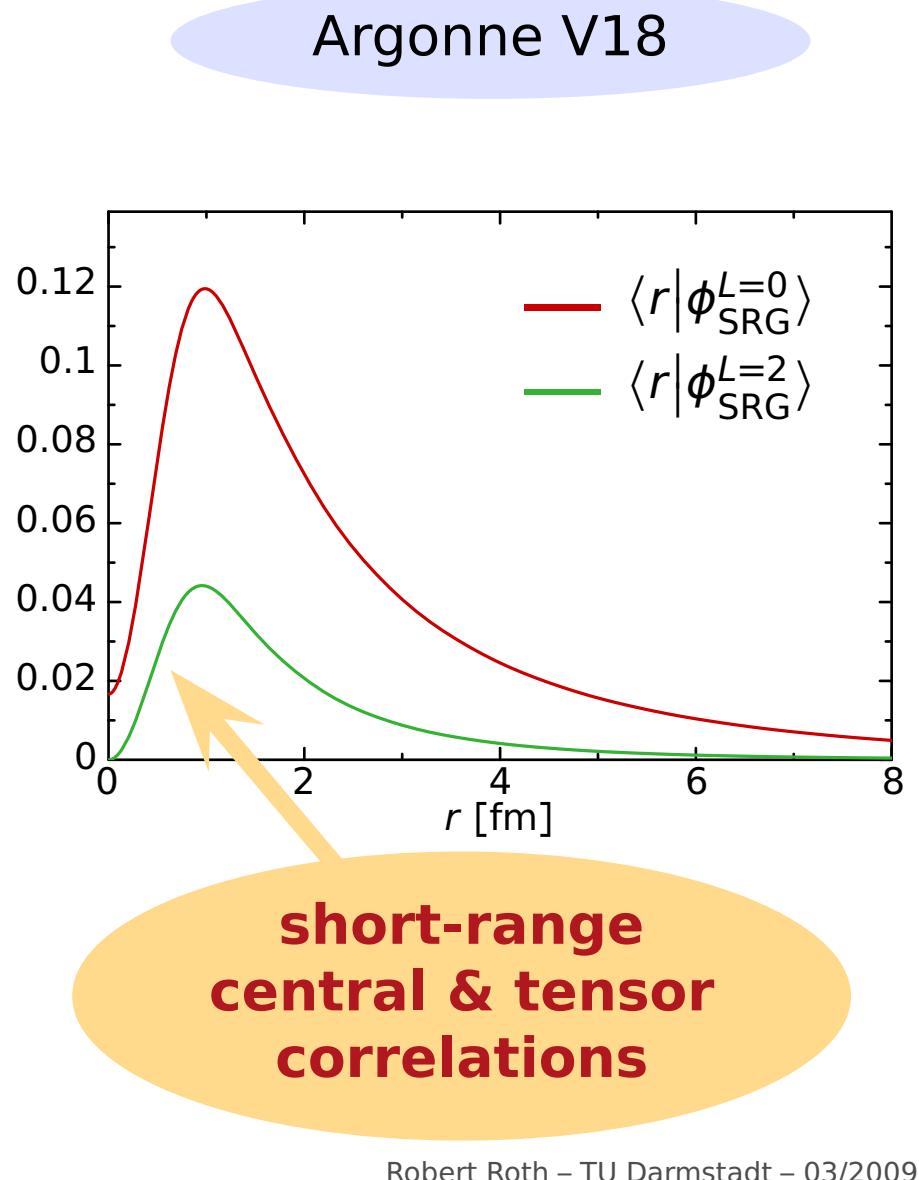
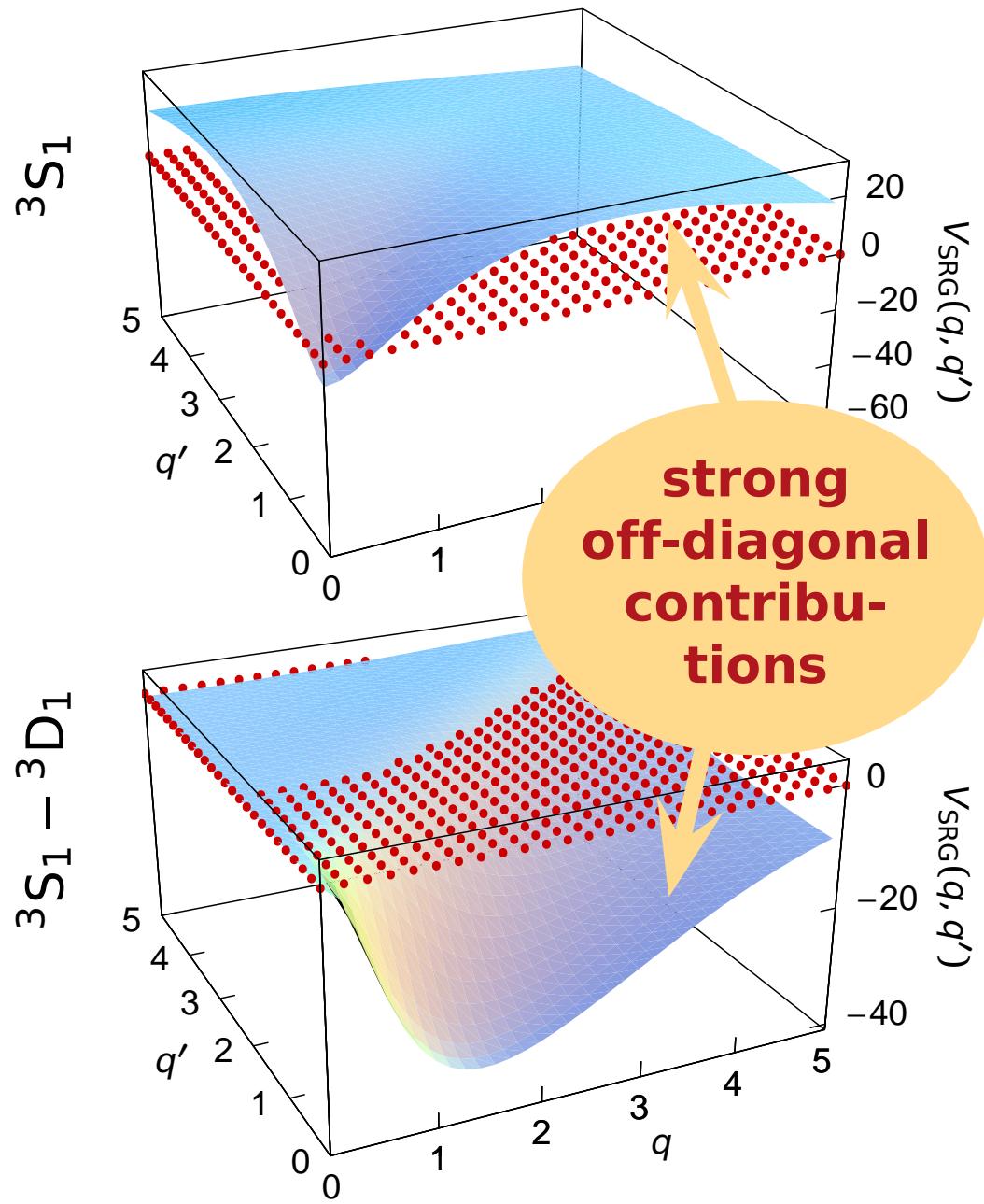
- dynamical generator defined as commutator with the operator in whose eigenbasis H shall be diagonalized

$$\eta(\alpha) \stackrel{2B}{=} \frac{1}{2\mu} [\vec{q}^2, \tilde{H}(\alpha)]$$

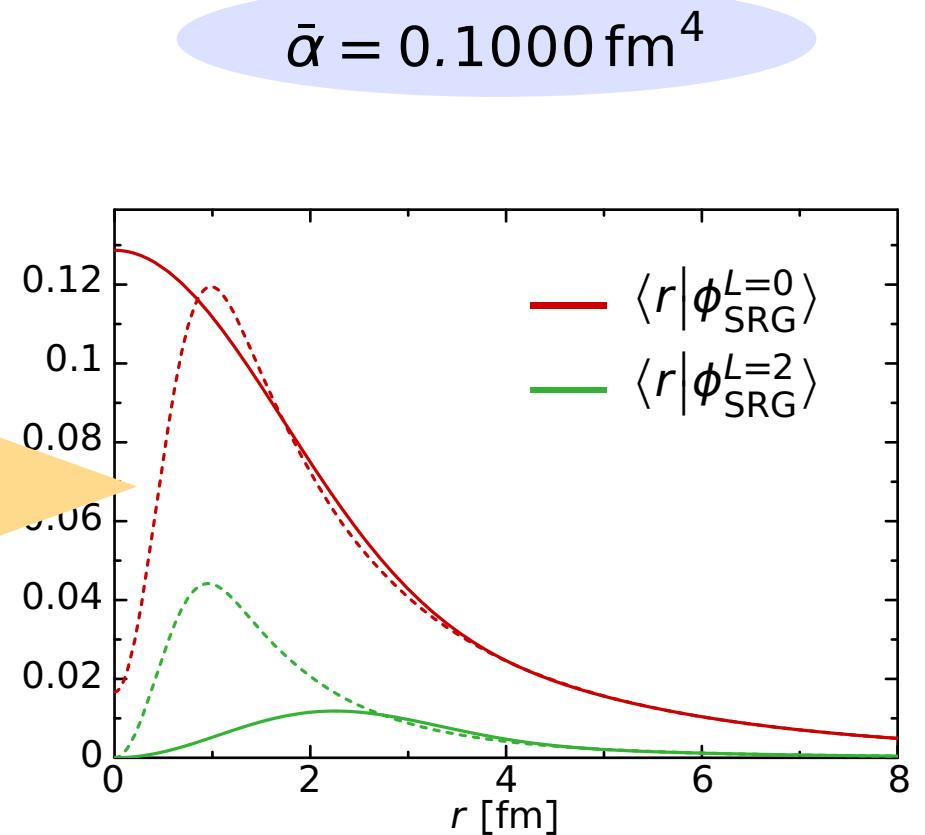
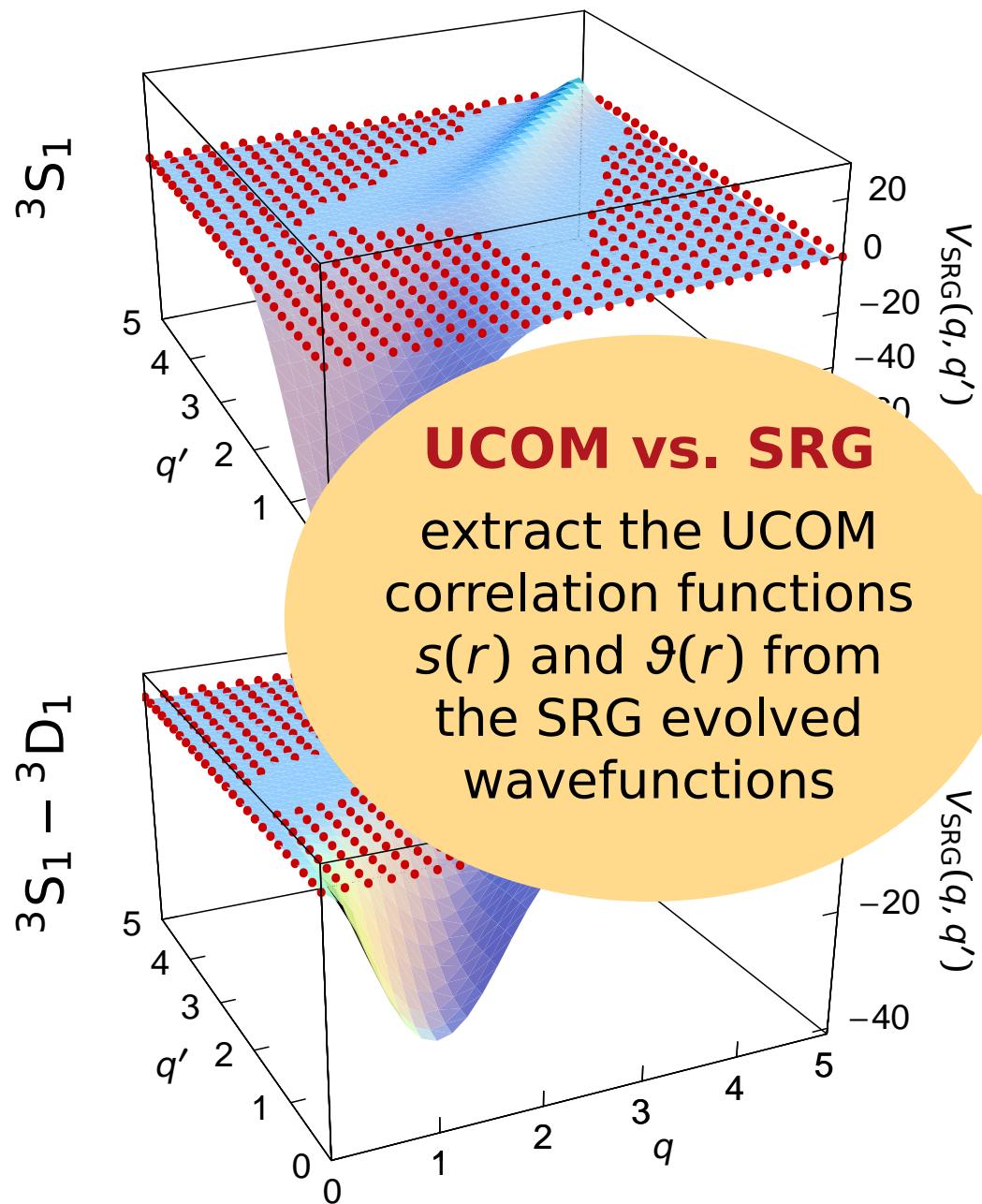
UCOM vs. SRG

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

SRG Evolution: The Deuteron



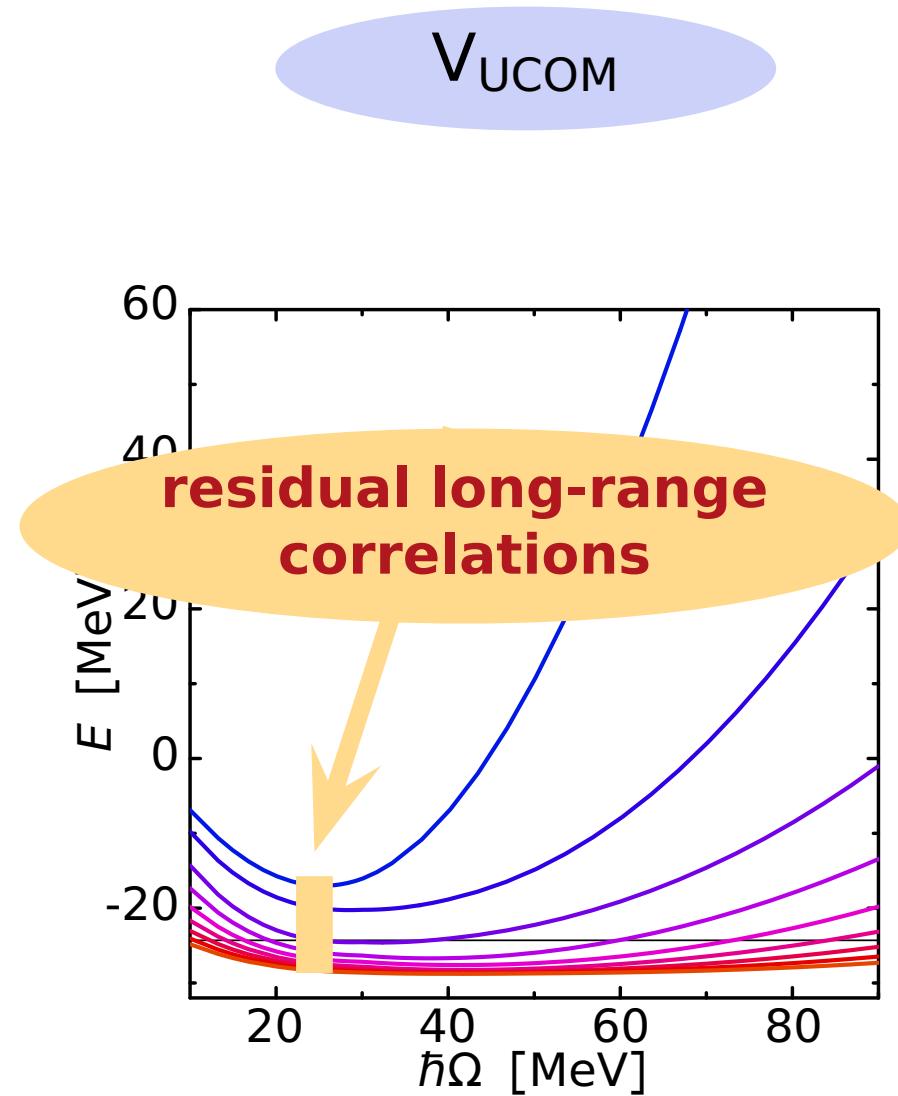
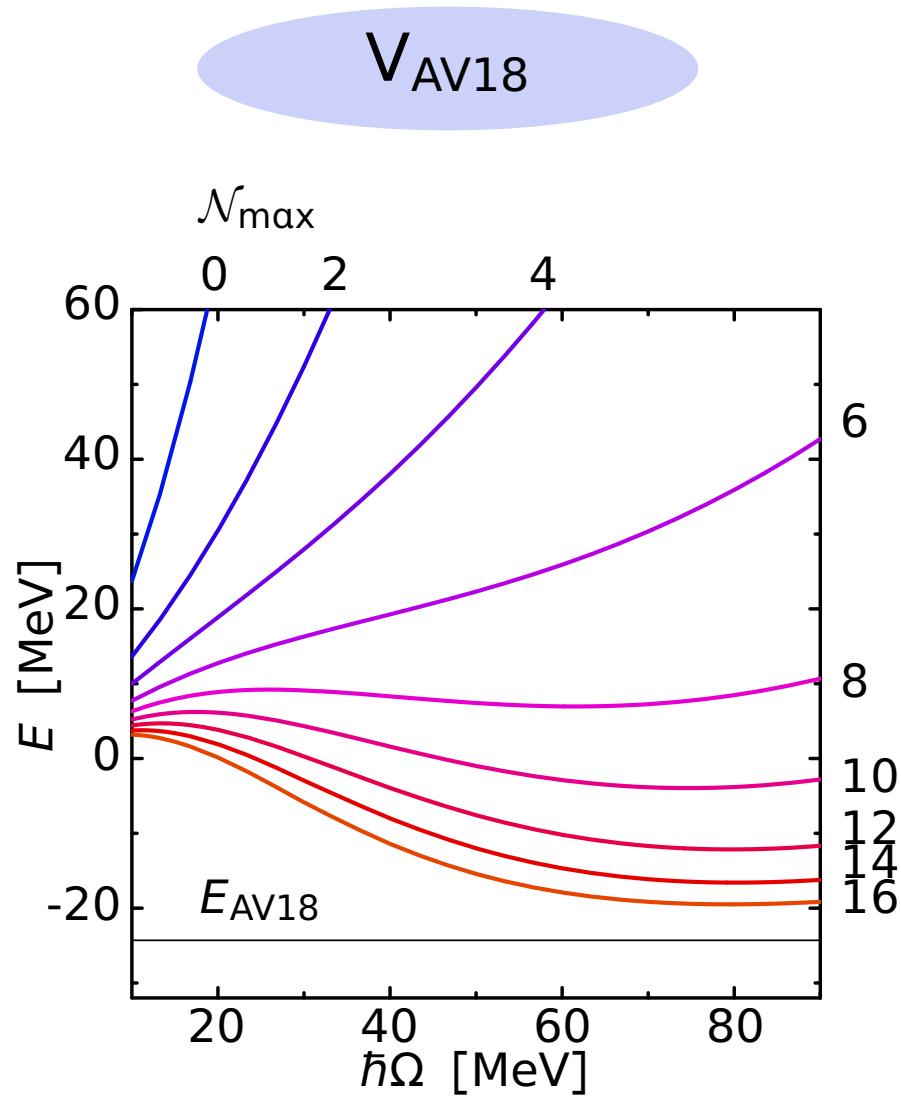
SRG Evolution: The Deuteron



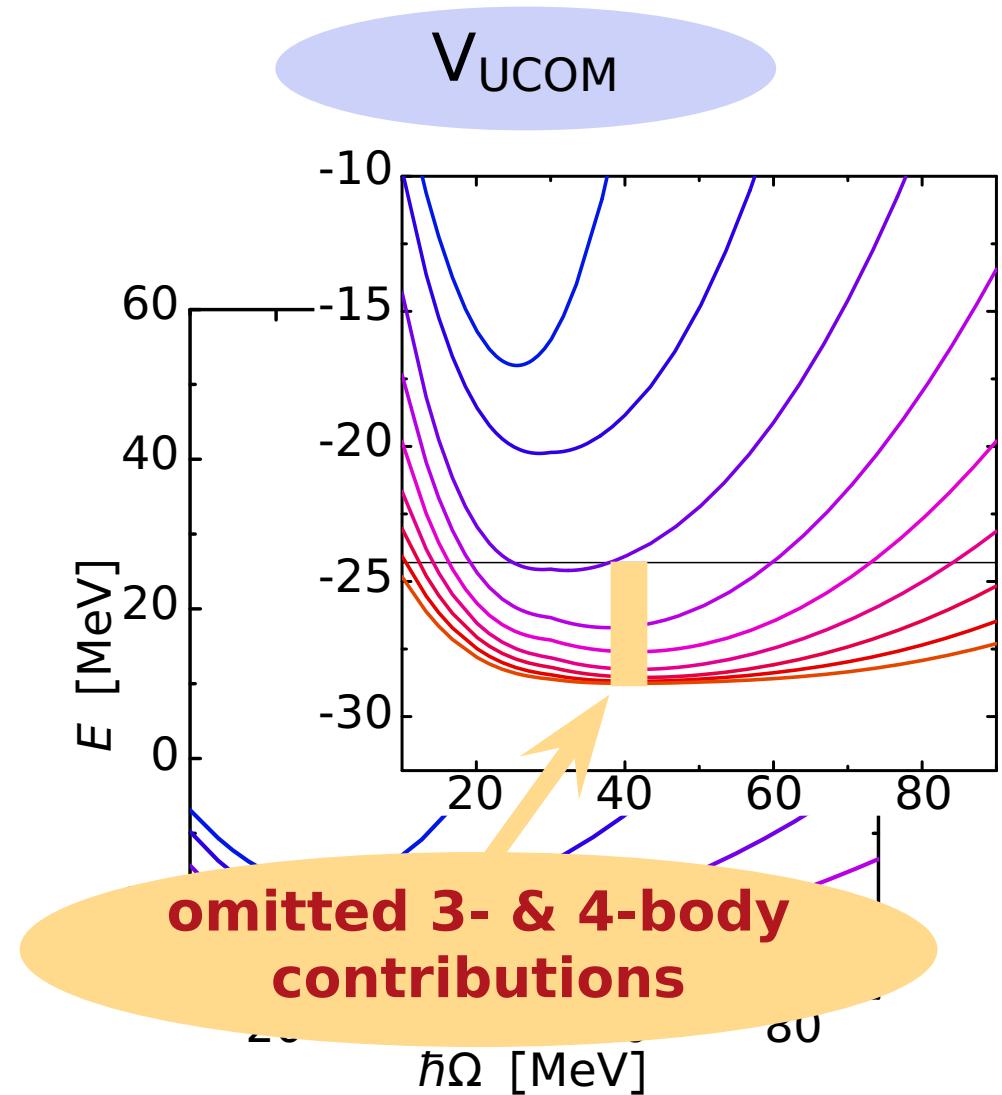
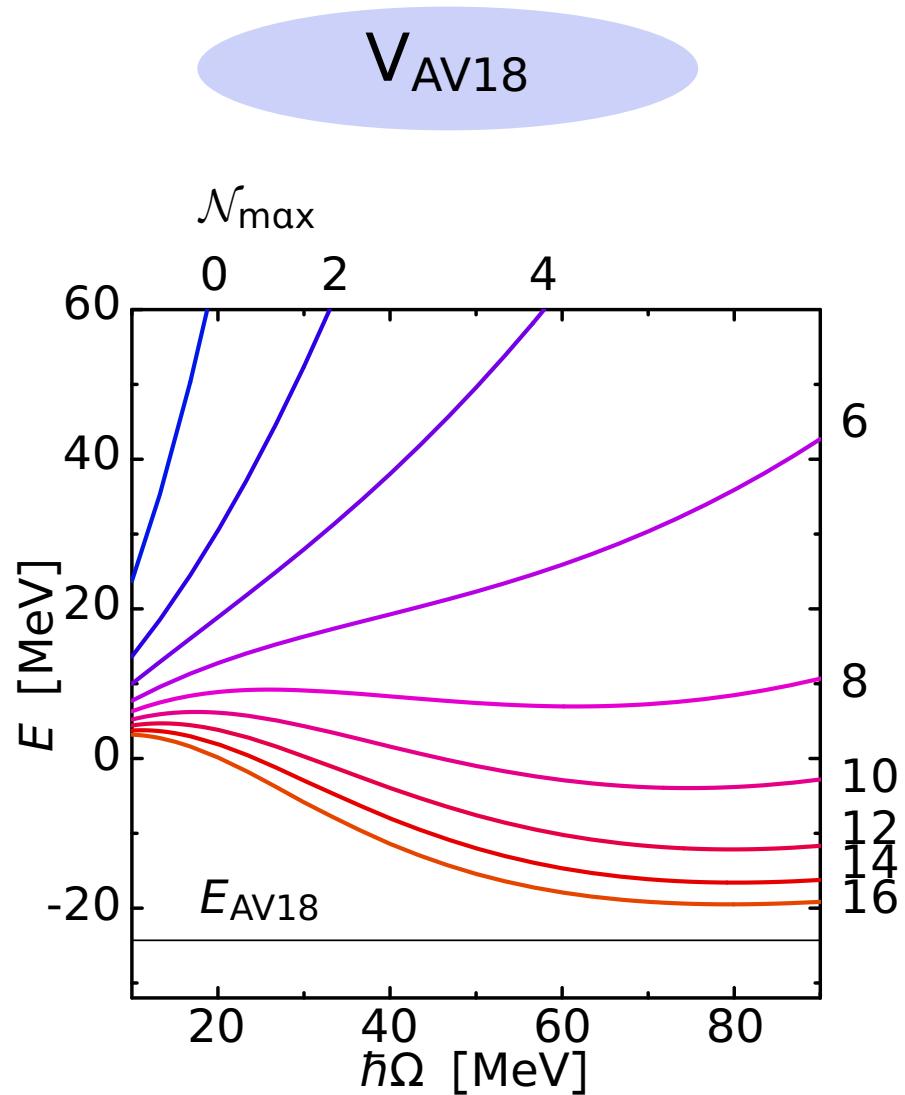
Computational Many-Body Methods

Testing UCOM & SRG
Interactions in Nuclei

NCSM: ^4He Convergence



NCSM: ^4He Convergence



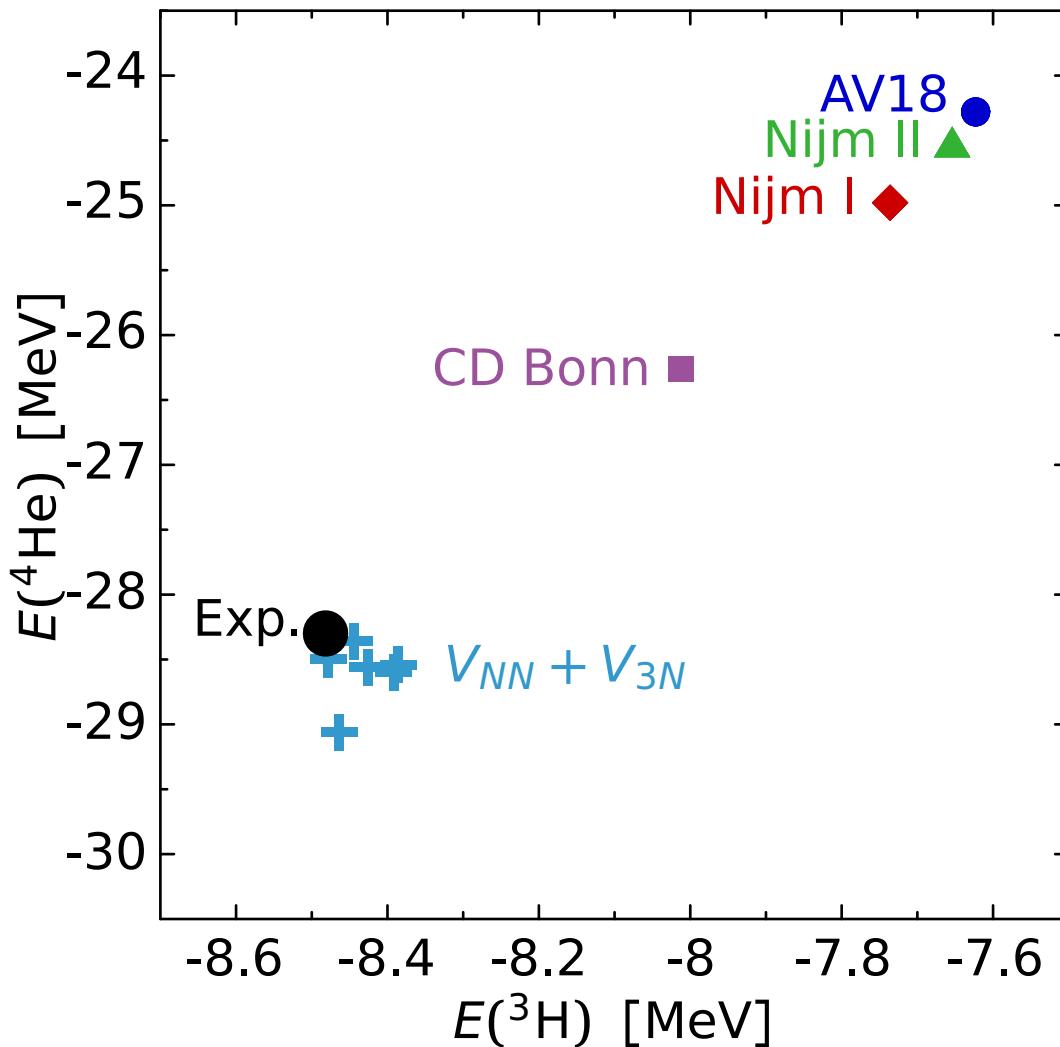
Three-Body Interactions — Strategies

Correlated Hamiltonian in Many-Body Space

$$\begin{aligned}\tilde{H} &= C^\dagger (T + V_{NN} + V_{3N}) C \\ &= \tilde{T}^{[1]} + (\tilde{T}^{[2]} + \tilde{V}_{NN}^{[2]}) + (\tilde{T}^{[3]} + \tilde{V}_{NN}^{[3]} + \tilde{V}_{3N}^{[3]}) + \dots \\ &= T + V_{UCOM} + V_{UCOM}^{[3]} + \dots\end{aligned}$$

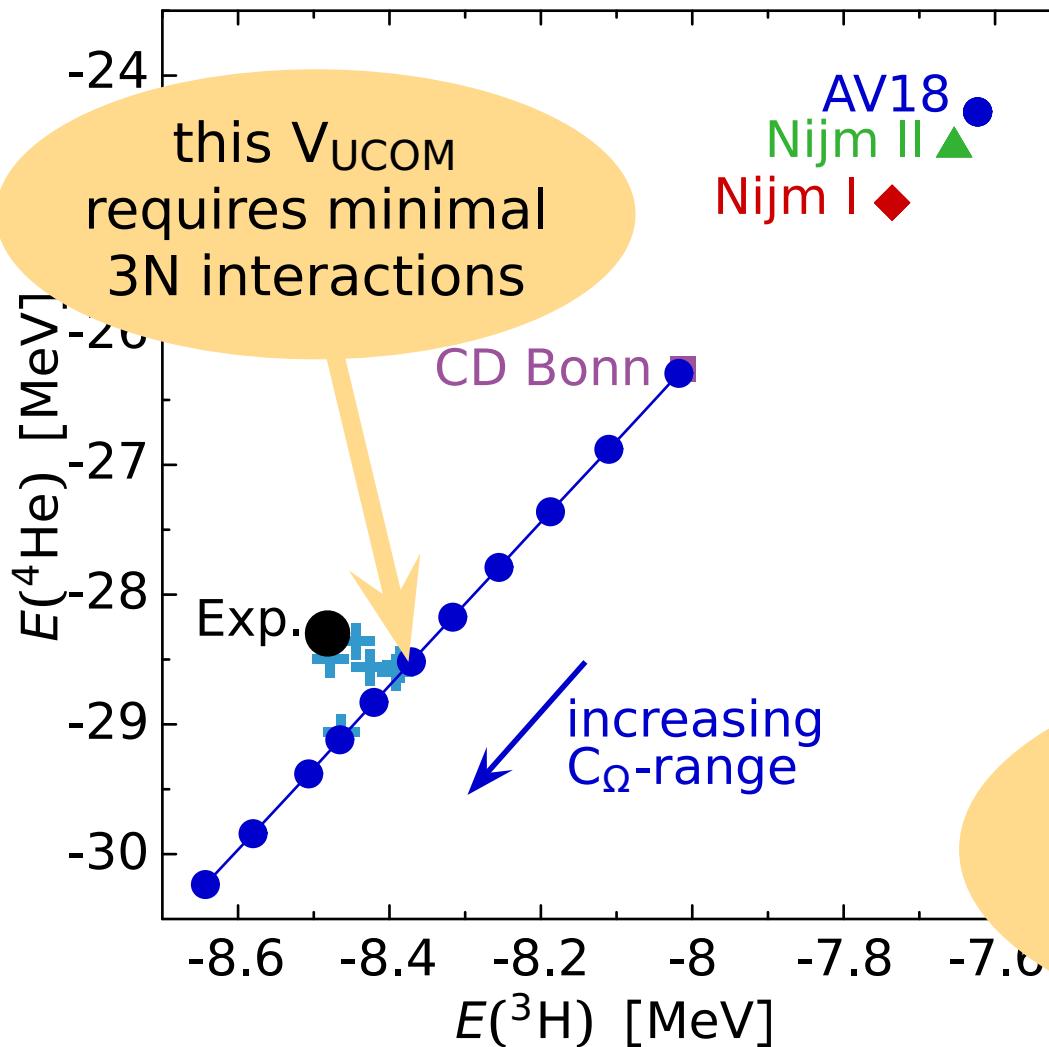
- **include full $V_{UCOM}^{[3]}$** consisting of genuine and induced 3N terms
(very hard in UCOM, but Dick can do it in SRG)
- **replace $V_{UCOM}^{[3]}$** by phenomenological three-body force
(easily tractable also for heavier nuclei)
- **minimize $V_{UCOM}^{[3]}$** by proper choice of unitary transformation
(cheap calculation with a pure two-body interaction)

Three-Body Interactions — Tjon Line



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

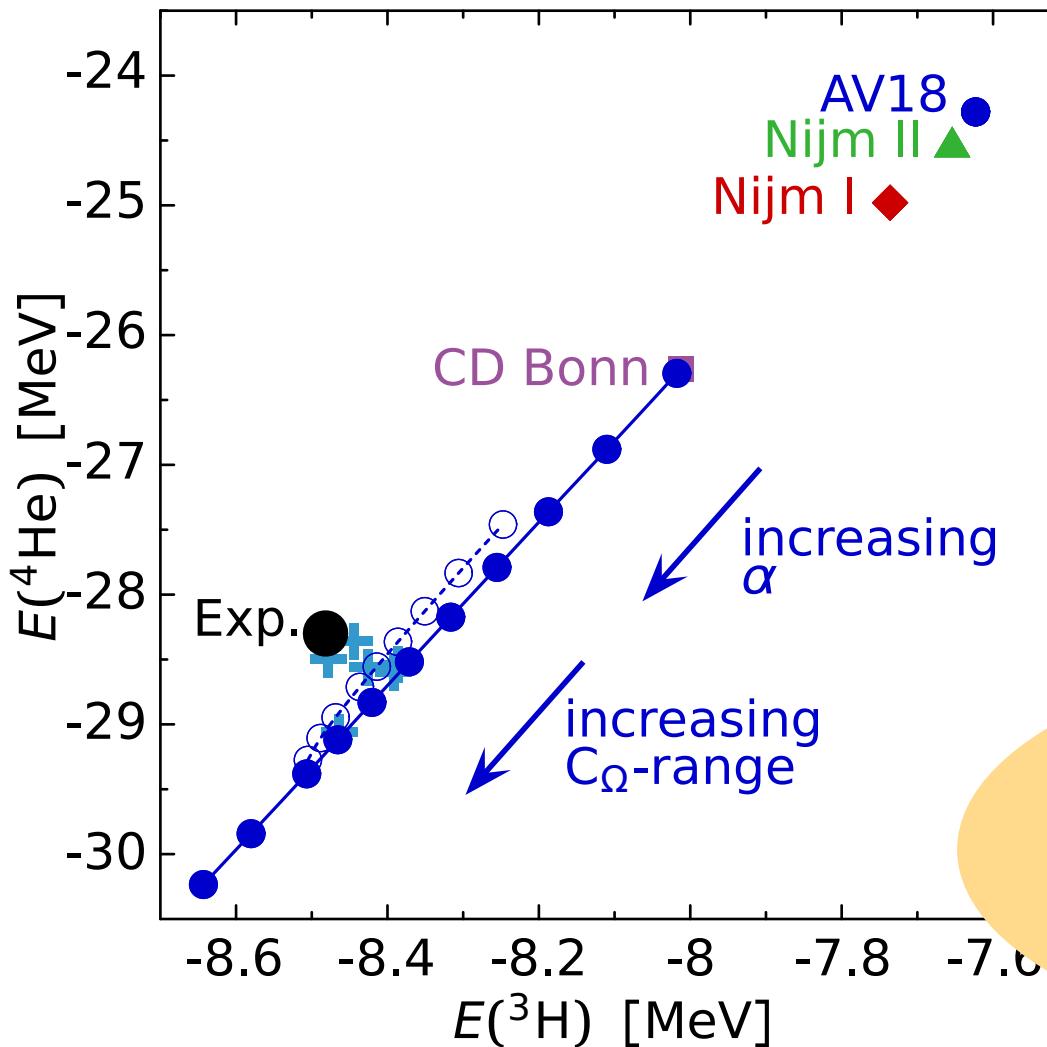
Three-Body Interactions — Tjon Line



- **Tjon-line**: $E(^4\text{He})$ vs. $E(^3\text{H})$ for phase-shift equivalent NN-interactions
- change of C_Ω -correlator range results in shift along Tjon-line

control the strength of the net 3N interaction
through the parameters of the unitary transformation

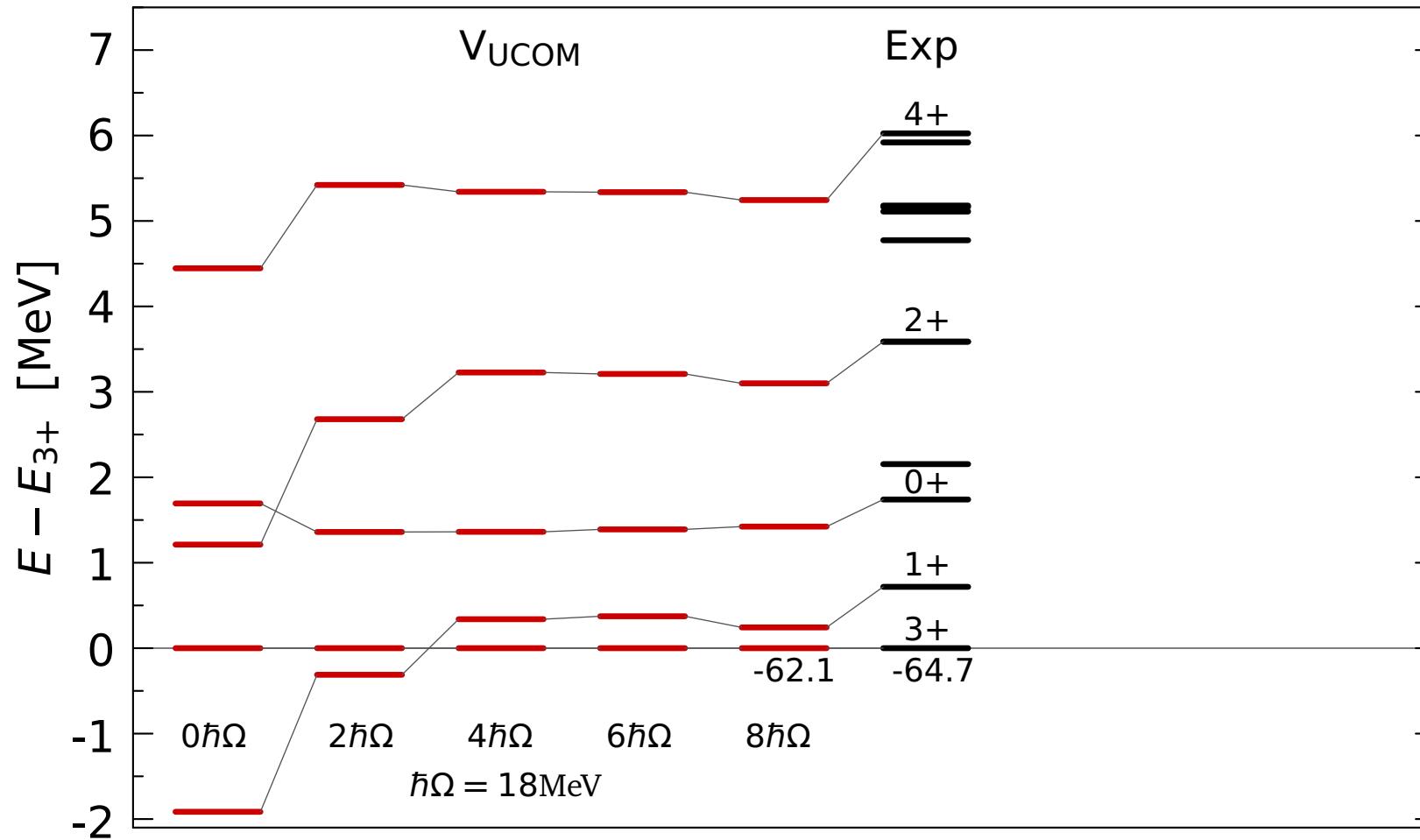
Three-Body Interactions — Tjon Line



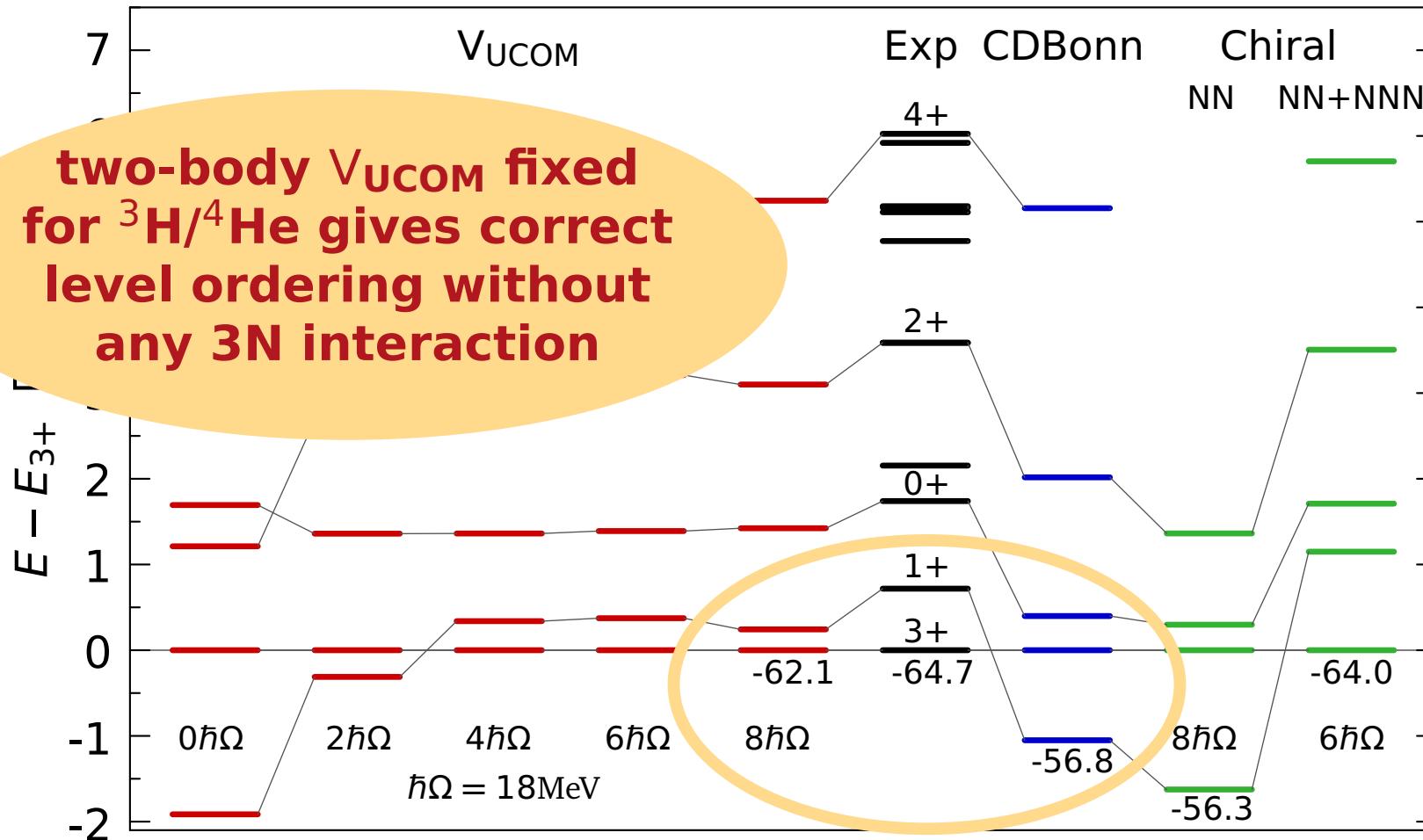
- **Tjon-line:** $E(^4\text{He})$ vs. $E(^3\text{H})$ for phase-shift equivalent NN-interactions
- same behavior for the SRG interaction as function of α

control the strength of the net 3N interaction
through the parameters of the unitary transformation

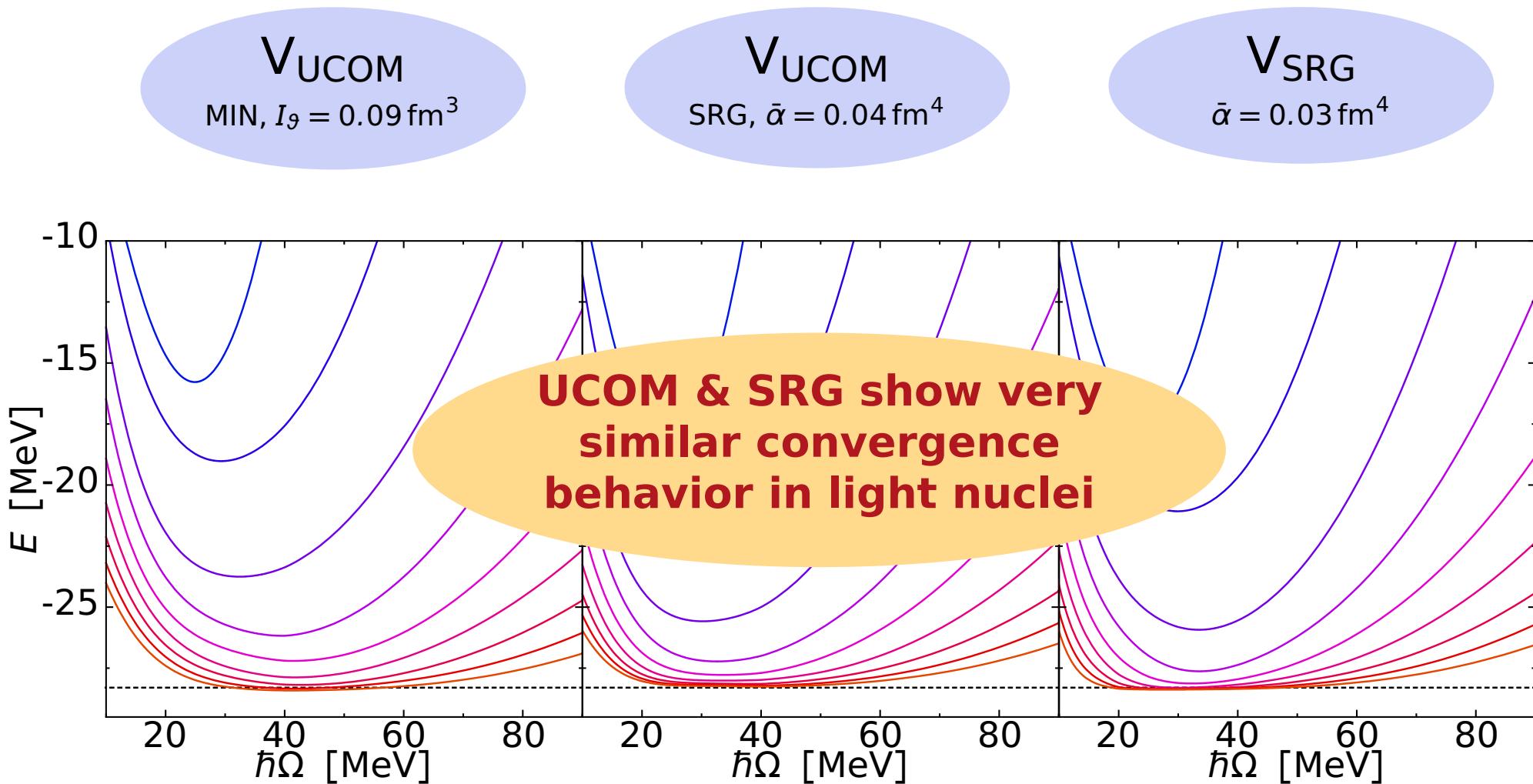
^{10}B : Hallmark of a 3N Interaction?



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

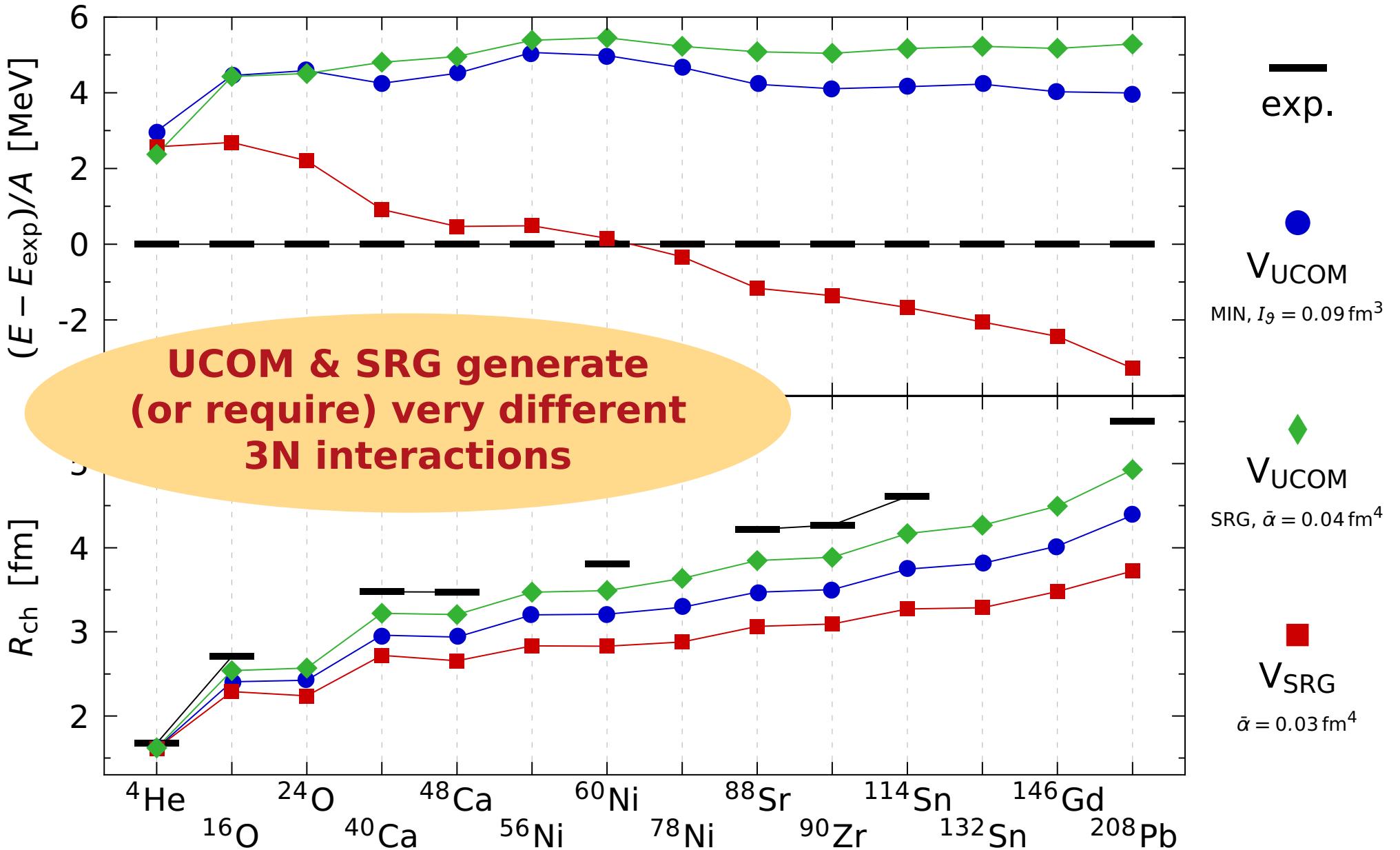


UCOM vs. SRG: ^4He Convergence

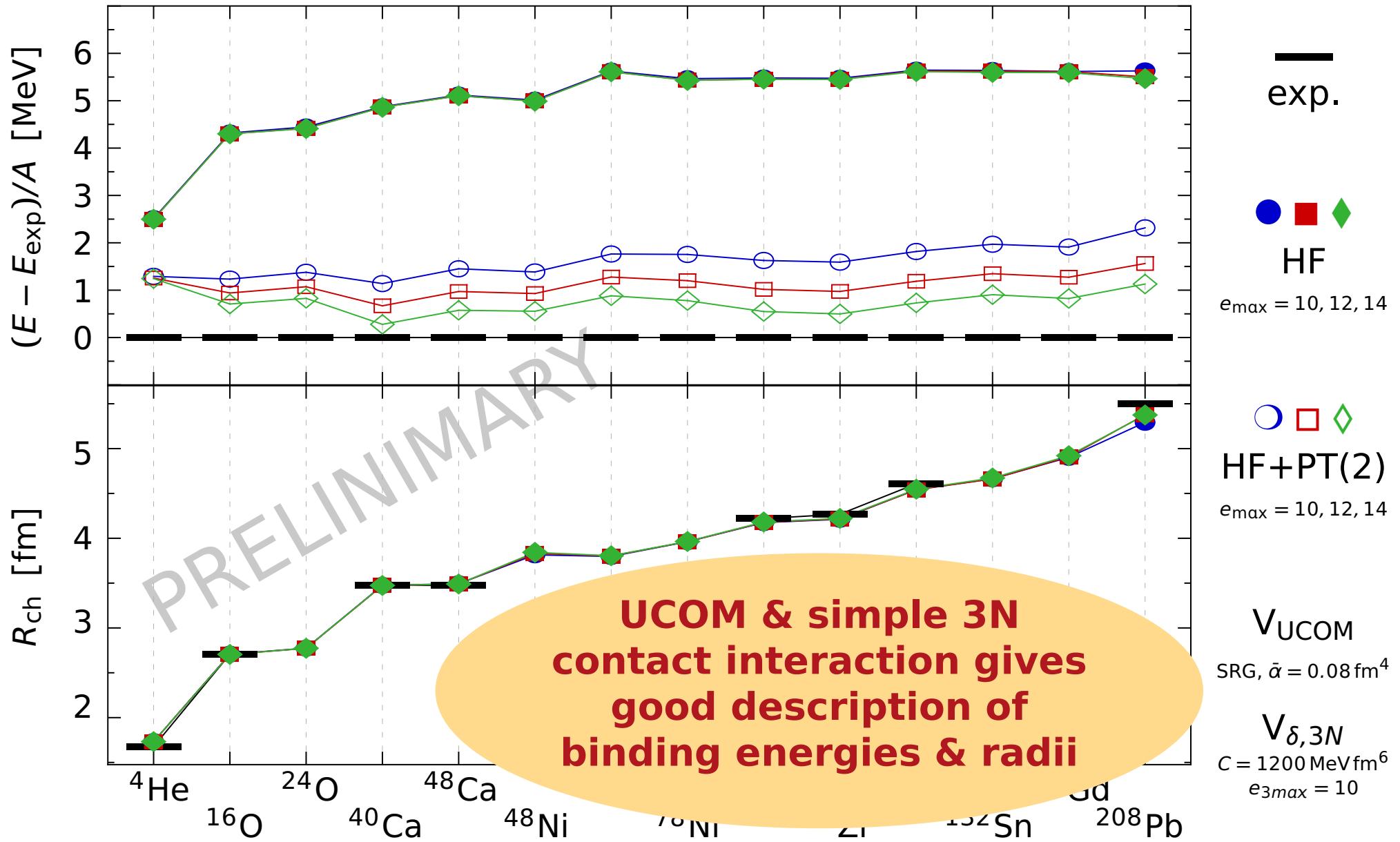


- I_9 or $\bar{\sigma}$ adjusted such that ^4He binding energy is reproduced

UCOM vs. SRG: Hartree-Fock Systematics



UCOM plus 3N Contact 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

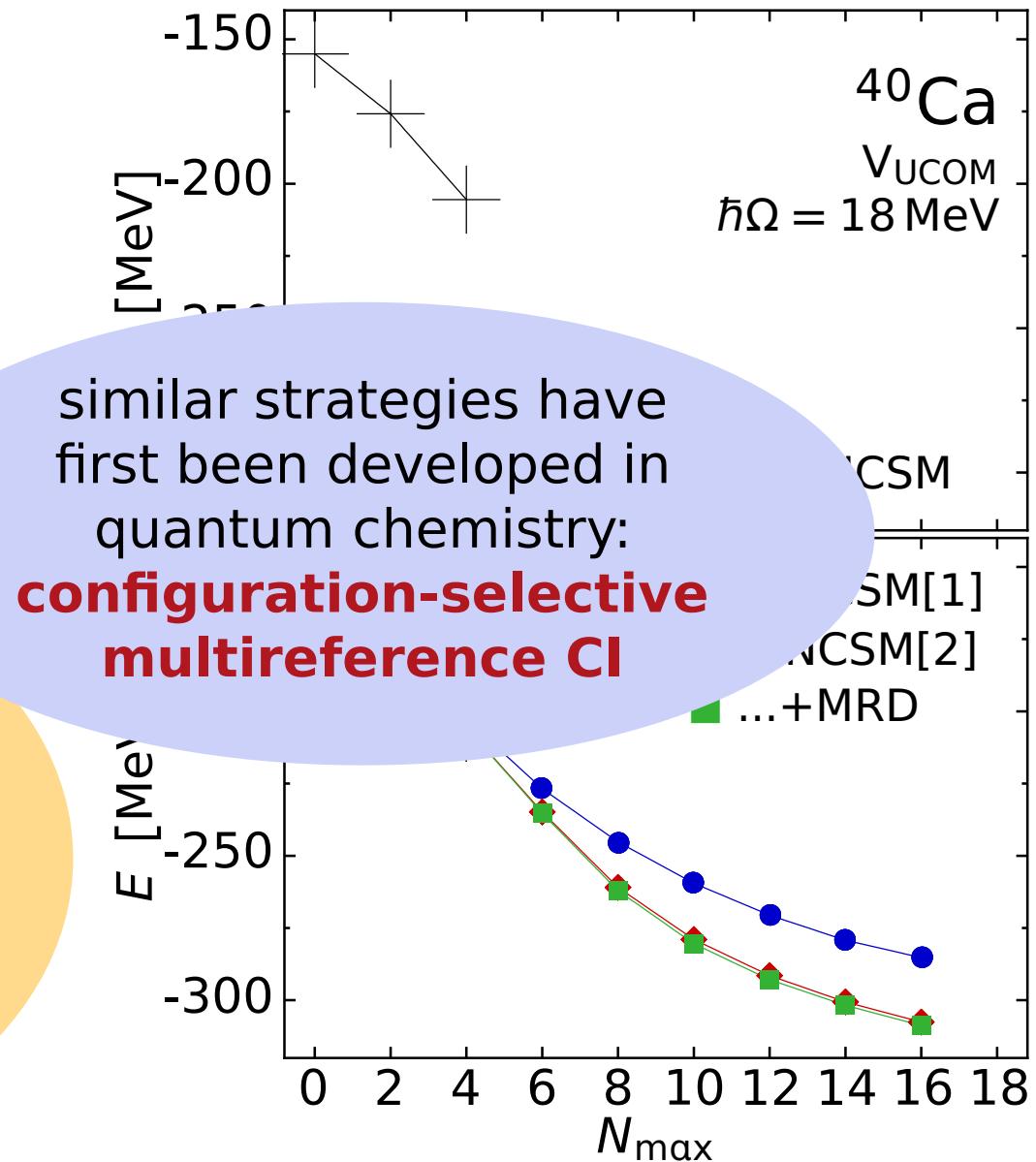
Roth — arXiv: 0903.4605

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 $\sim 10^{10}$)

Importance Truncation

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



Importance Truncation: General Idea

- given an initial approximation $|\Psi_{\text{ref}}\rangle$ for the **target state** within a limited **reference space** \mathcal{M}_{ref}

$$|\Psi_{\text{ref}}\rangle = \sum_{\nu \in \mathcal{M}_{\text{ref}}} C_{\nu}^{(\text{ref})} |\Phi_{\nu}\rangle$$

- **measure the importance** of individual basis state $|\Phi_{\nu}\rangle \notin \mathcal{M}_{\text{ref}}$ 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** $\mathcal{M}(\kappa_{\min})$ spanned by basis states with $|\kappa_{\nu}| \geq \kappa_{\min}$
- **solve eigenvalue problem** in importance truncated space $\mathcal{M}(\kappa_{\min})$ and obtain improved approximation of target state

Importance Truncation: Iterative Scheme

- non-zero importance measure κ_ν only for states which **differ from $|\Psi_{\text{ref}}\rangle$ by 2p2h excitation** at most

IT-NCSM[i]

- simple iterative scheme for a single $N_{\max}\hbar\Omega$ model space

★ start with $|\Psi_{\text{ref}}\rangle = |\Phi_0\rangle$

① construct importance truncated space containing up to 2p2h on top of $|\Psi_{\text{ref}}\rangle$

② solve eigenvalue problem

③ use dominant component of eigenstate ($|C_\nu| \geq C_{\min}$) as new $|\Psi_{\text{ref}}\rangle$, goto ①

IT-NCSM(seq)

- sequential update scheme for a set of $N_{\max}\hbar\Omega$ spaces

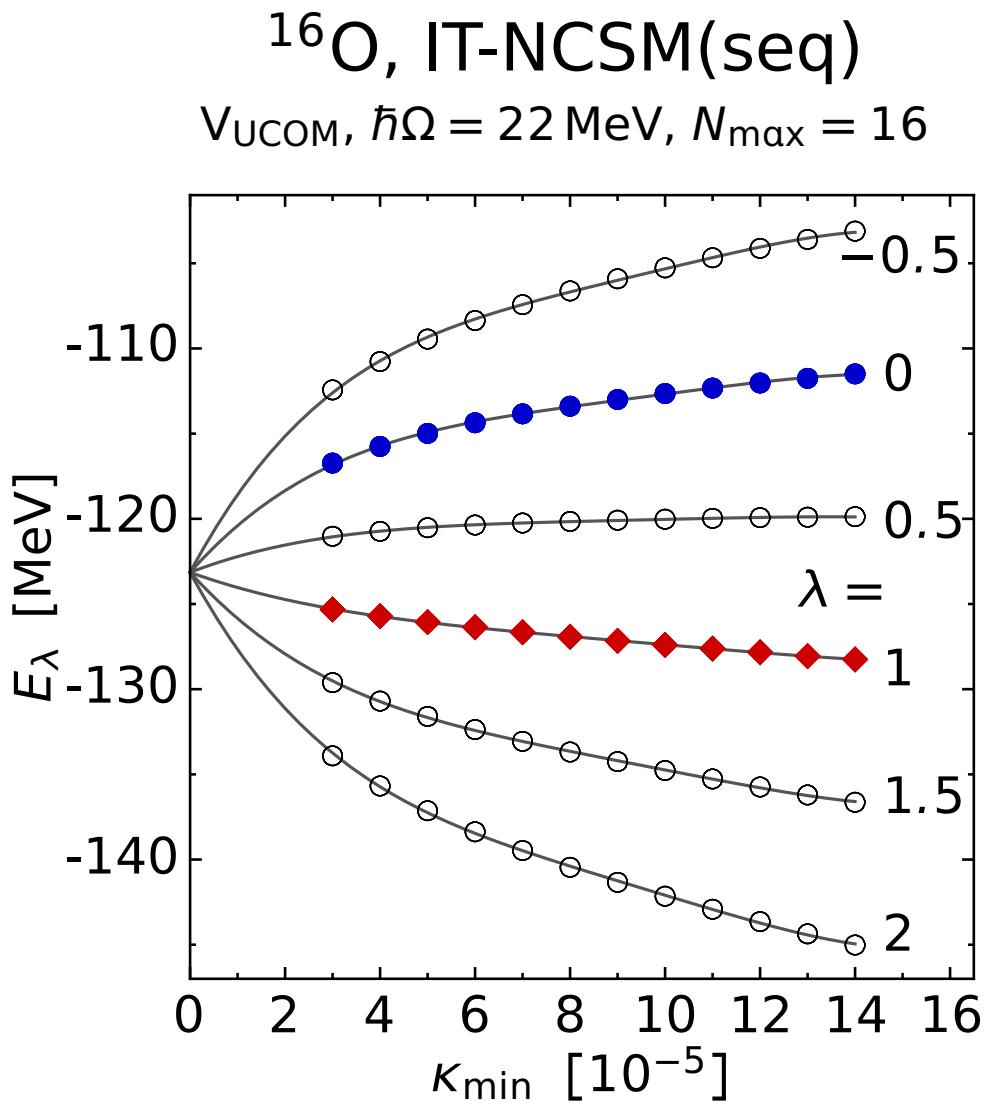
★ start with $N_{\max} = 2$ eigenstate from full NCSM as initial $|\Psi_{\text{ref}}\rangle$

① construct importance truncated space for $N_{\max} + 2$

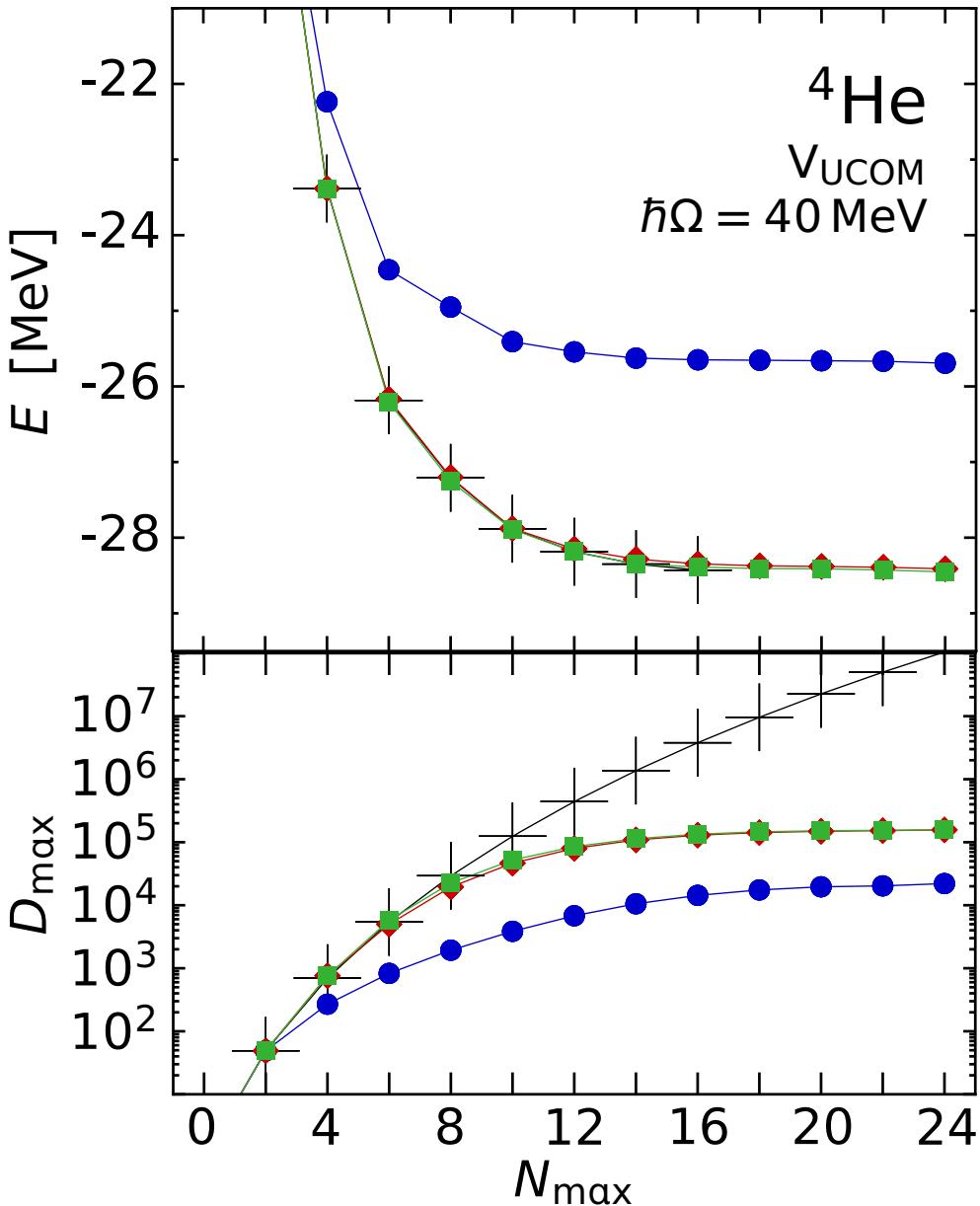
full NCSM model space is recovered in the limit $(K_{\min}, C_{\min}) \rightarrow 0$ in IT-NCSM(seq) and IT-NCSM[i_{conv}]

Threshold Extrapolation

- all calculations done for a **sequence of importance thresholds** $\rightarrow E(\kappa_{\min})$
- contribution of **excluded states** estimated perturbatively $\rightarrow \Delta_{\text{excl}}(\kappa_{\min})$
- **simultaneous extrapolation** of combined energy $E_\lambda(\kappa_{\min}) = E(\kappa_{\min}) + \lambda \Delta_{\text{excl}}(\kappa_{\min})$ to $\kappa_{\min} = 0$ for set of λ -values
- all IT-NCSM energies shown are threshold extrapolated



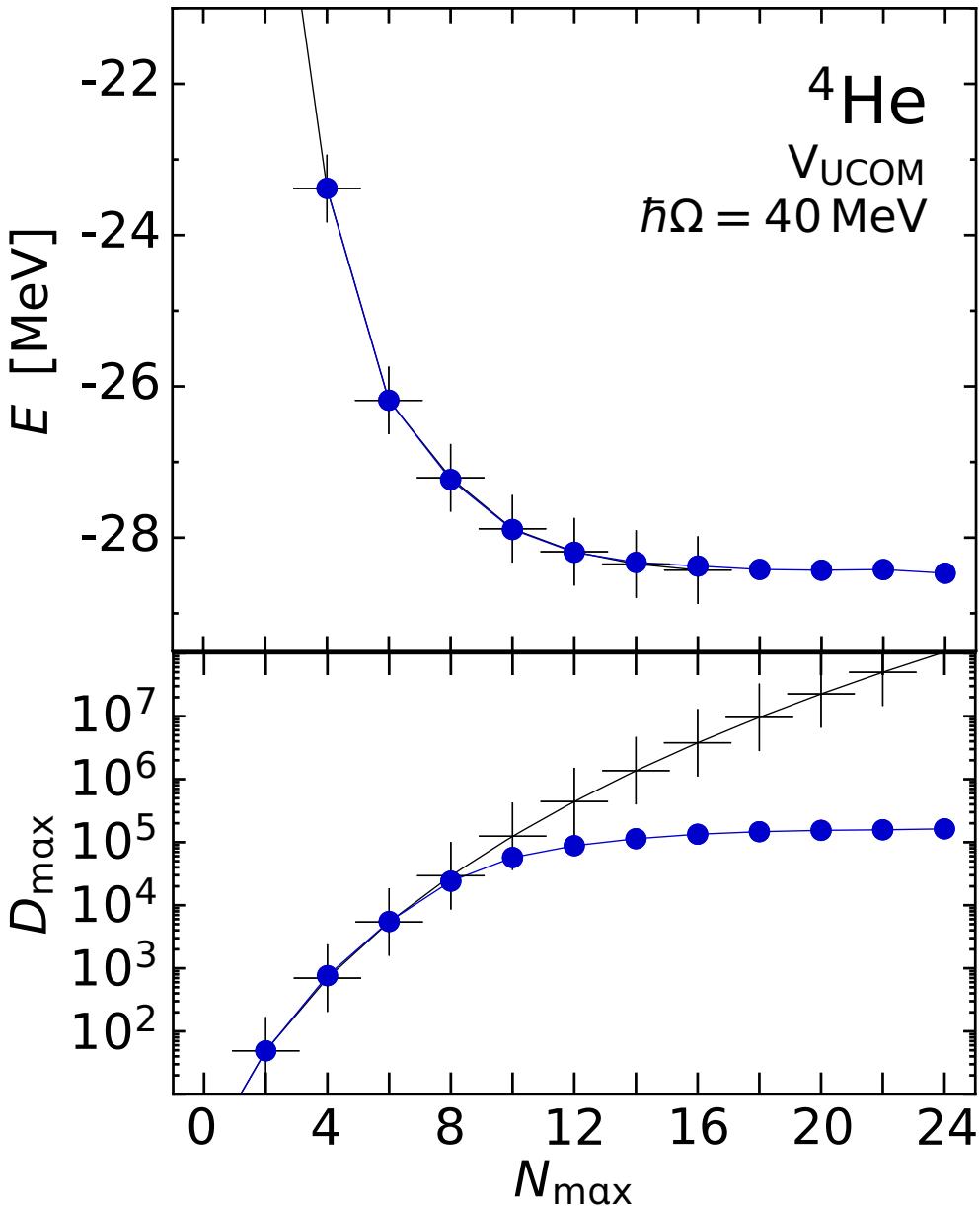
^4He : Importance-Truncated NCSM



- **iterative IT-NCSM[i]**: few iterations with $0\hbar\Omega$ determinant as initial reference
- **reproduces exact NCSM result** for all N_{\max}
- reduction of basis by more than two orders of magnitude w/o loss of precision

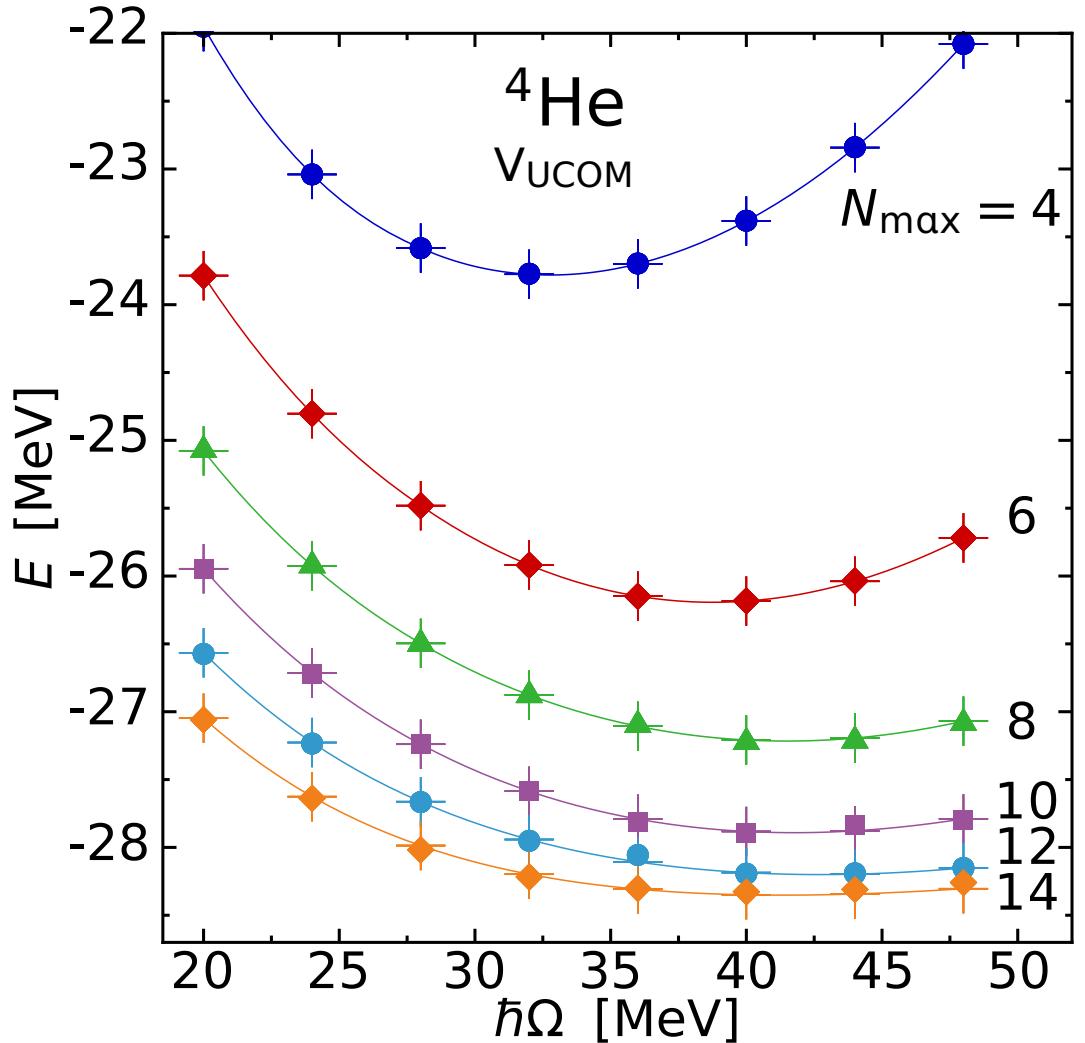
- + full NCSM
- IT-NCSM[1]
- ◆ IT-NCSM[2]
- IT-NCSM[3]

^4He : Importance-Truncated NCSM



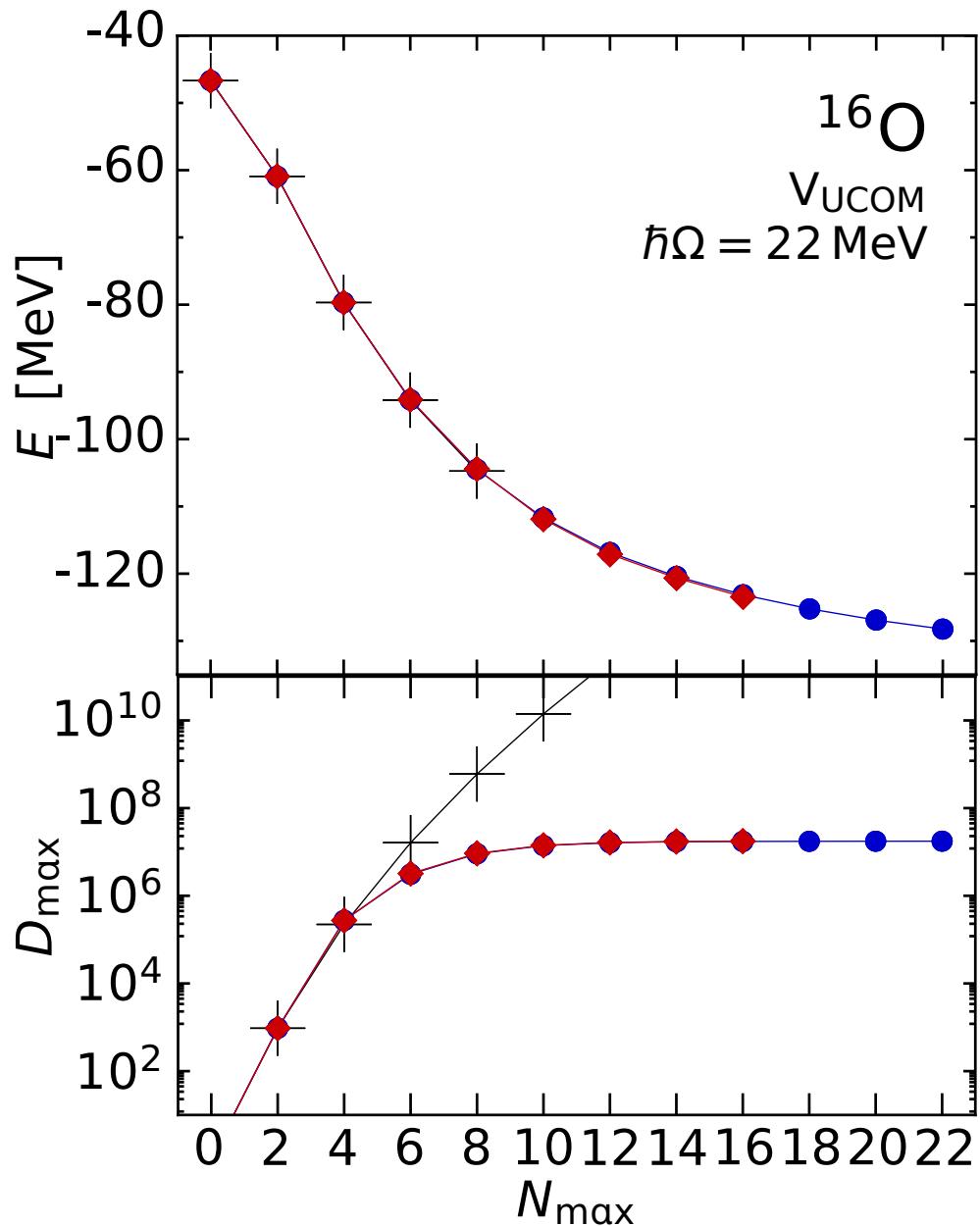
- **sequential IT-NCSM(seq):** single importance update using $(N_{\max} - 2)\hbar\Omega$ eigenstate as reference
 - **reproduces exact NCSM result** for all N_{\max}
 - reduction of basis by more than two orders of magnitude w/o loss of precision
- + full NCSM
● IT-NCSM(seq)

^4He : Importance-Truncated NCSM



- **reproduces exact NCSM result** for all $\hbar\Omega$ and N_{\max}
 - importance truncation & threshold extrapolation is robust
 - **no center-of-mass contamination** for any N_{\max} and $\hbar\Omega$
- + full NCSM
● IT-NCSM(seq)

^{16}O : Importance-Truncated NCSM



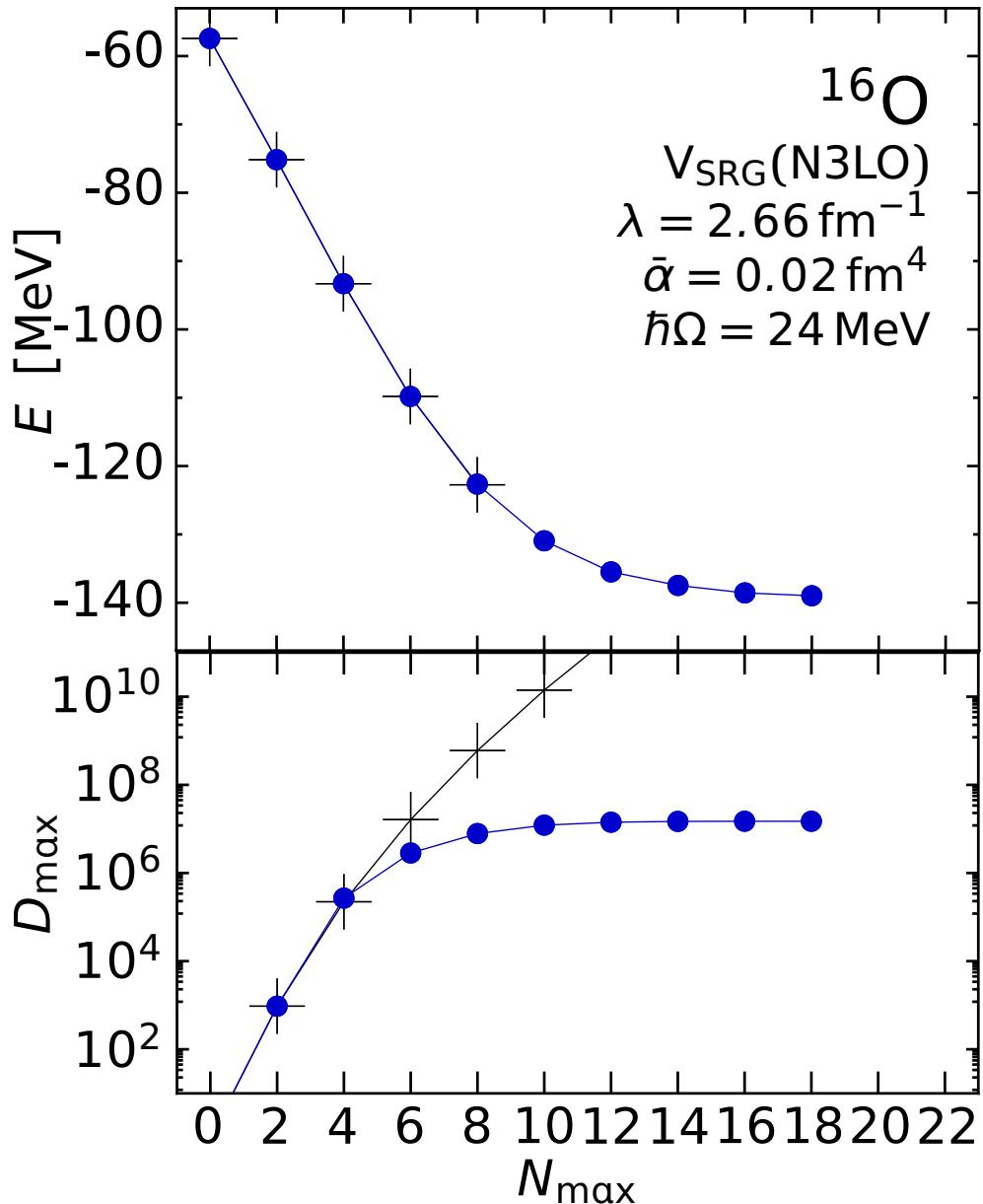
- extrapolation $N_{\max} \rightarrow \infty$ using five consecutive points

N_{\max}	E_{∞} [MeV]
14...22	-133.1
12...20	-132.4
10...18	-130.8
experiment	-127.6

- slow **non-exponential convergence** makes precise extrapolation difficult

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

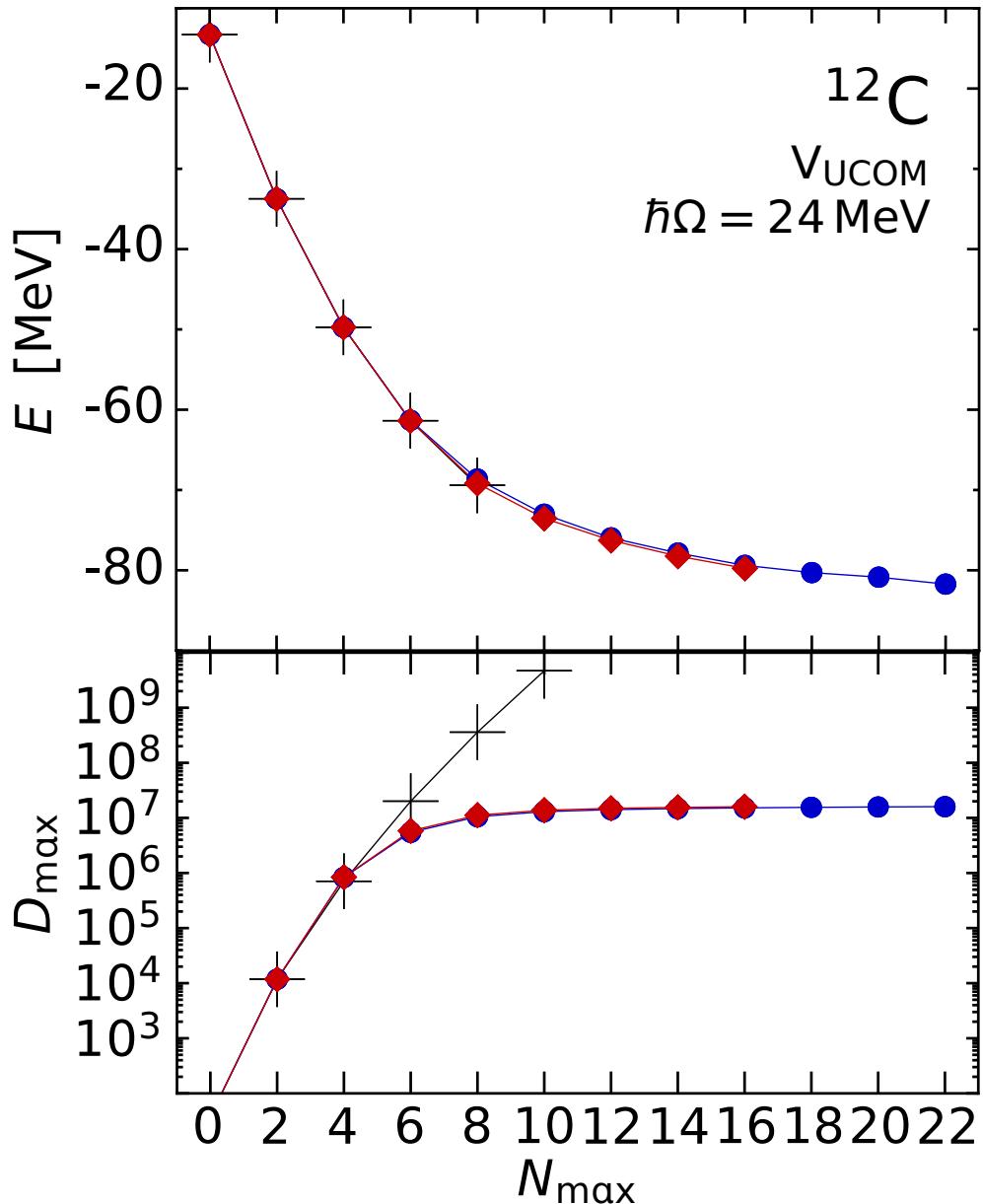
^{16}O : Importance-Truncated NCSM



- **SRG-evolved N3LO potential** provides a much better convergence behavior
- nevertheless, $N_{\text{max}} \leq 8$ calculations are not sufficient
- non-exponential behavior observed with V_{UCOM} is really due to interaction

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

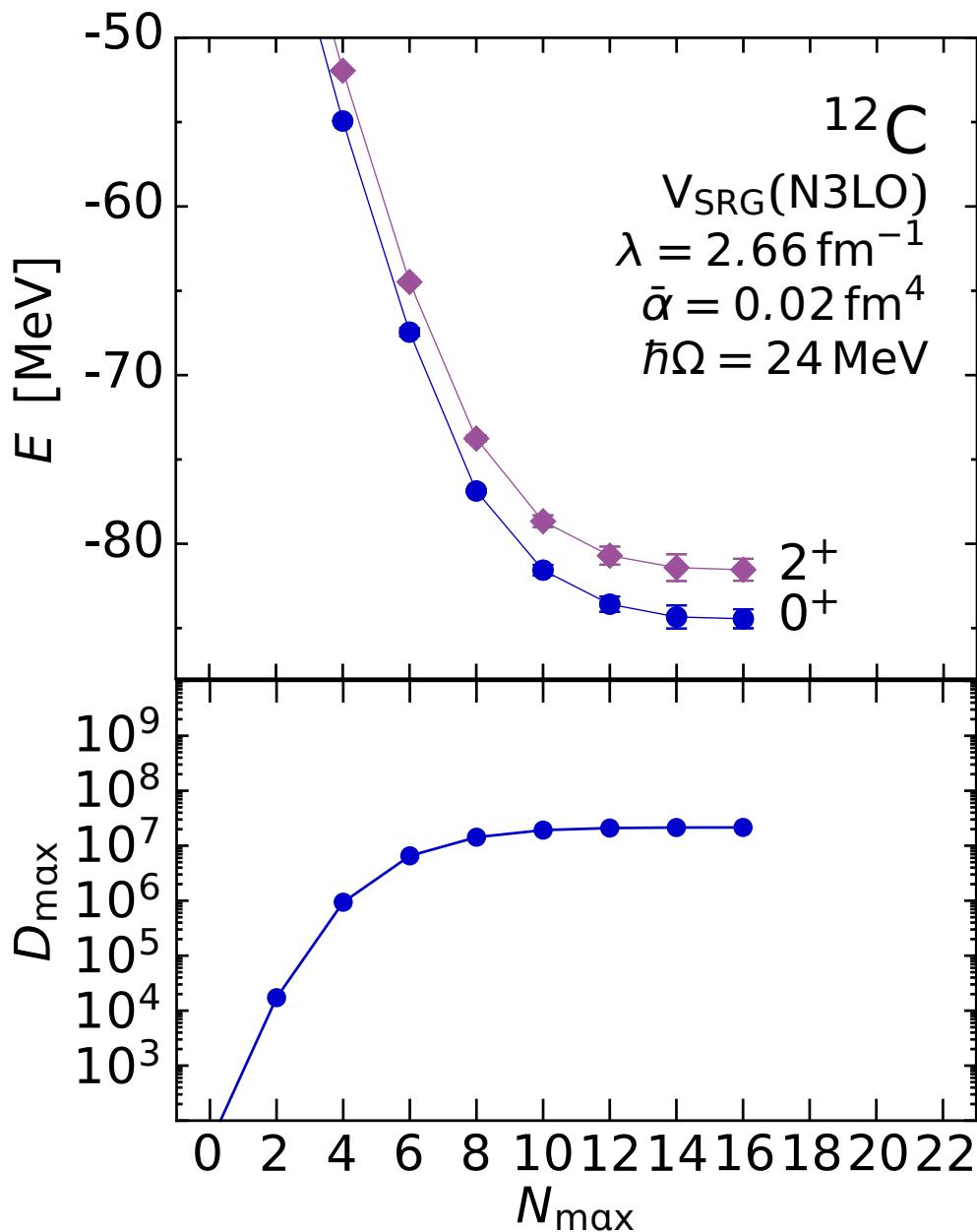
^{12}C : IT-NCSM for Open-Shell Nuclei



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

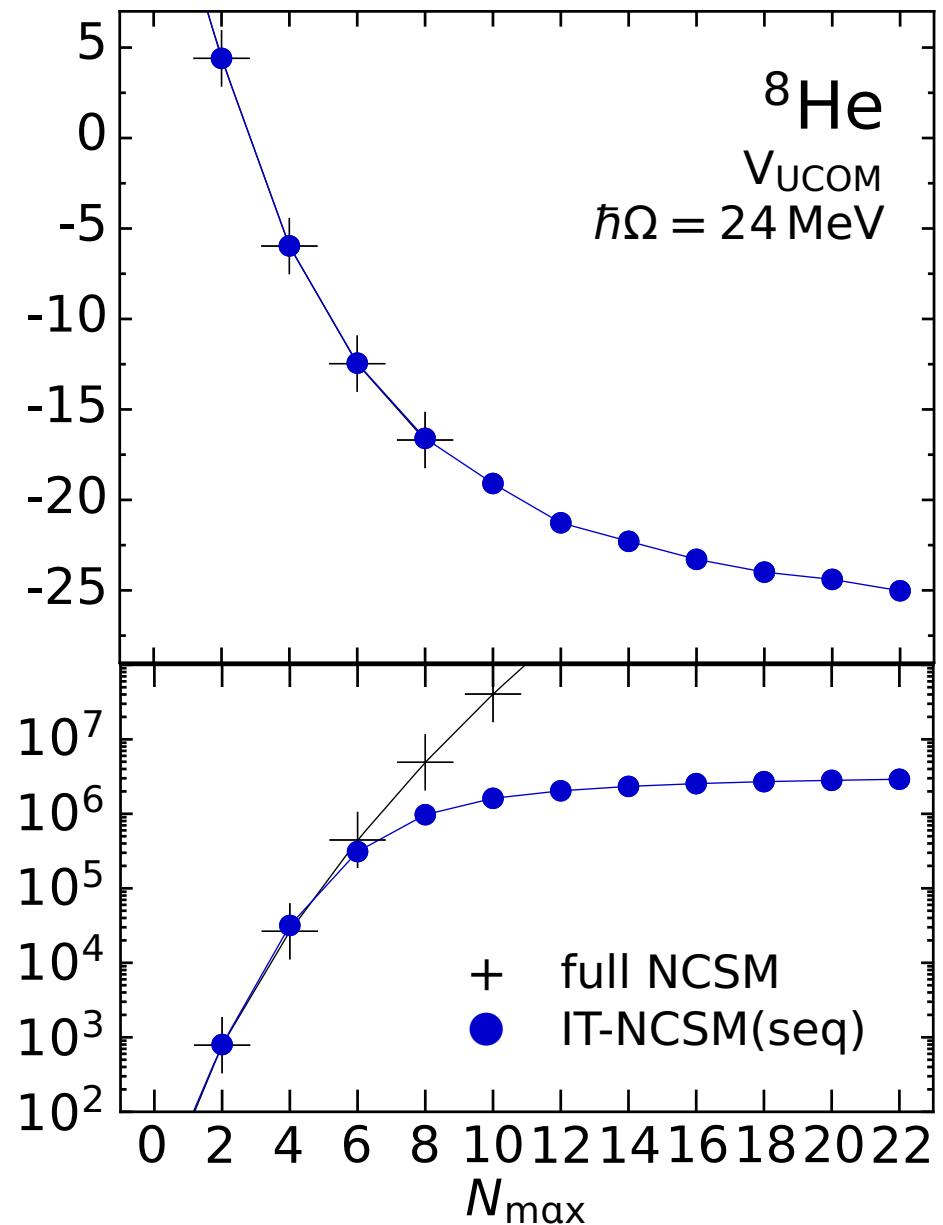
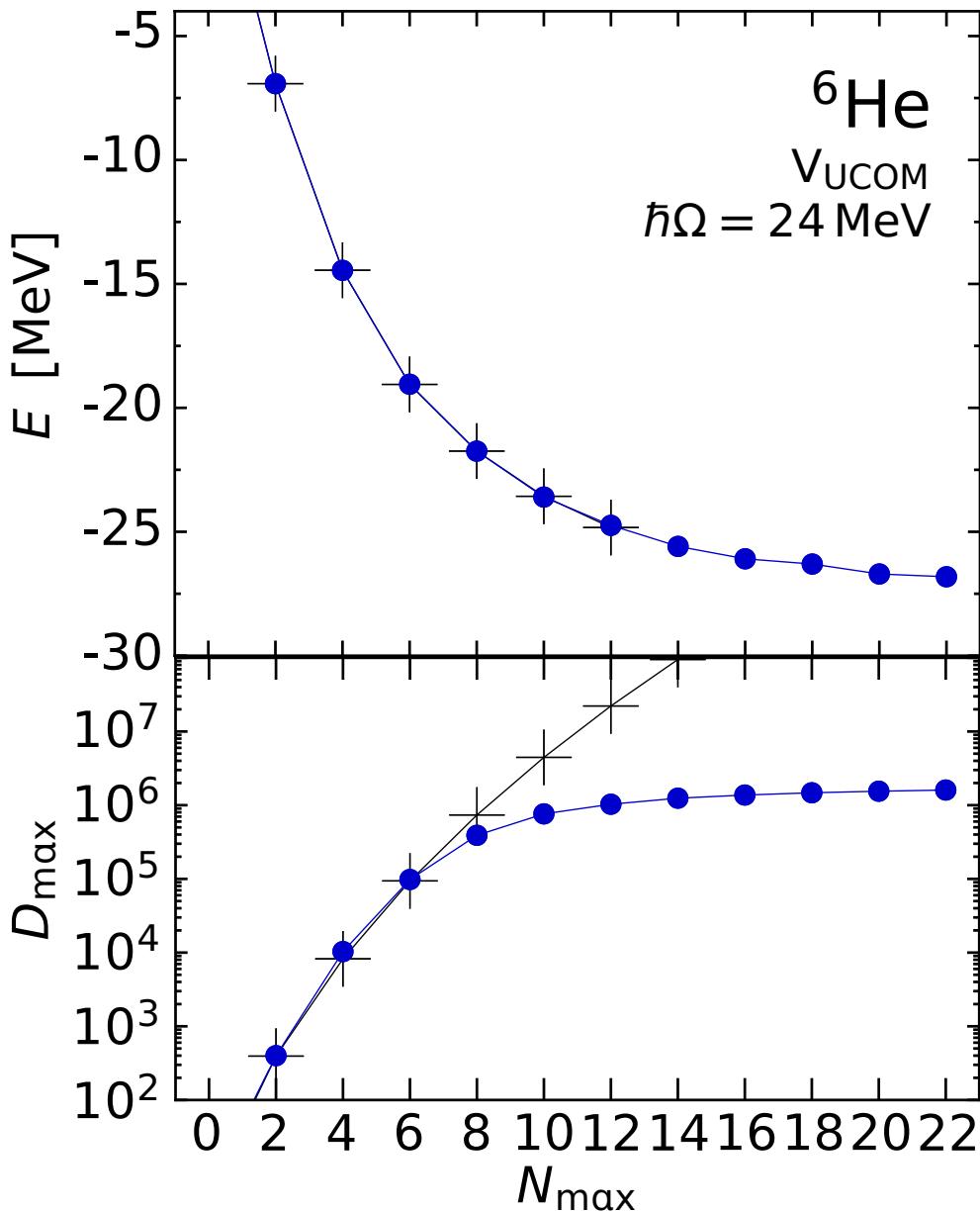
+ full NCSM
● IT-NCSM(seq), $C_{\min} = 0.0005$
◆ IT-NCSM(seq), $C_{\min} = 0.0003$

^{12}C : IT-NCSM for Excited States



- targeting ground & excited states simultaneously via importance measure
 - IT-NCSM(seq) can treat a ground state & few low-lying excited states **on the same footing**
 - full access to **spectroscopy**
- ♦ IT-NCSM(seq), $C_{\min} = 0.0005$

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



IT-NCSM: Pros and Cons

- ✓ **fulfills variational principle** & Hylleraas-Undheim theorem
- ✓ **no center-of-mass contamination** induced by importance truncation in $N_{\max}\hbar\Omega$ space
- ✓ constrained **threshold extrapolation** $K_{\min} \rightarrow 0$ 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**: compute any observable from wave functions in SM representation
- ✗ **only approximate size-extensivity** after threshold extrapolation in IT-NCSM(seq) or IT-NCSM[i_{conv}] – no explicit nph truncation
- ✗ computationally still demanding

Perspectives

■ Unitarily Transformed Interactions

- treatment of short-range central and tensor correlations by unitary transformations: UCOM, SRG,...
- phase-shift equivalent transformed interaction (e.g. V_{UCOM}) as universal input for...

■ Computational Many-Body Methods

- No-Core Shell Model,...
- Importance Truncated NCSM, Coupled Cluster Method,...
- Hartree-Fock plus MBPT, Padé Resummed MBPT, BHF, HFB, RPA, QRPA, Second RPA,...
- Fermionic Molecular Dynamics,...

Epilogue

■ thanks to my group & my collaborators

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DFG



 **LOEWE – Landes-Offensive
zur Entwicklung Wissenschaftlich-
ökonomischer Exzellenz**