Ab-Initio Nuclear Structure beyond the p-Shell:

Interactions & Many-Body Techniques

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Overview

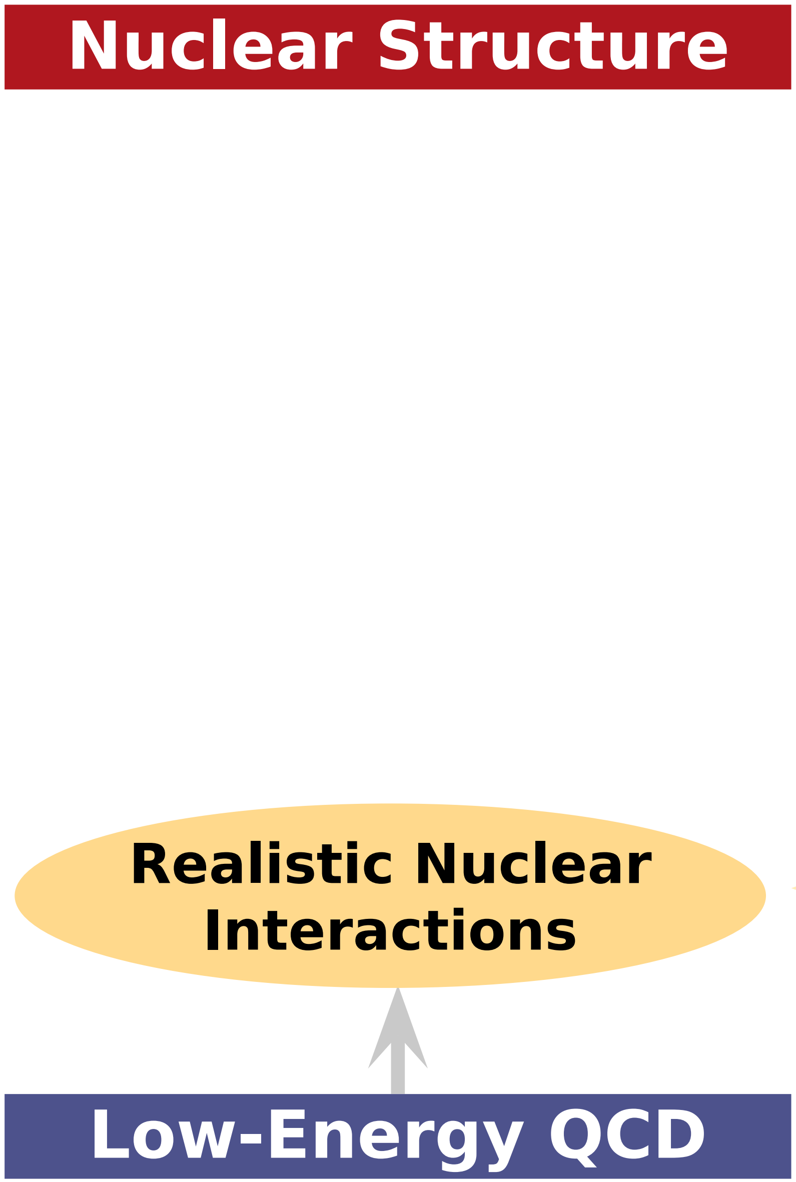
- Motivation
- Unitarily Transformed Interactions
  - Unitary Correlation Operator Method
  - Similarity Renormalization Group
- Computational Many-Body Methods
  - Testing UCOM & SRG in Nuclei: NCSM & HF+MBPT
  - Importance Truncated NCSM

From QCD to Nuclear Structure

Nuclear Structure

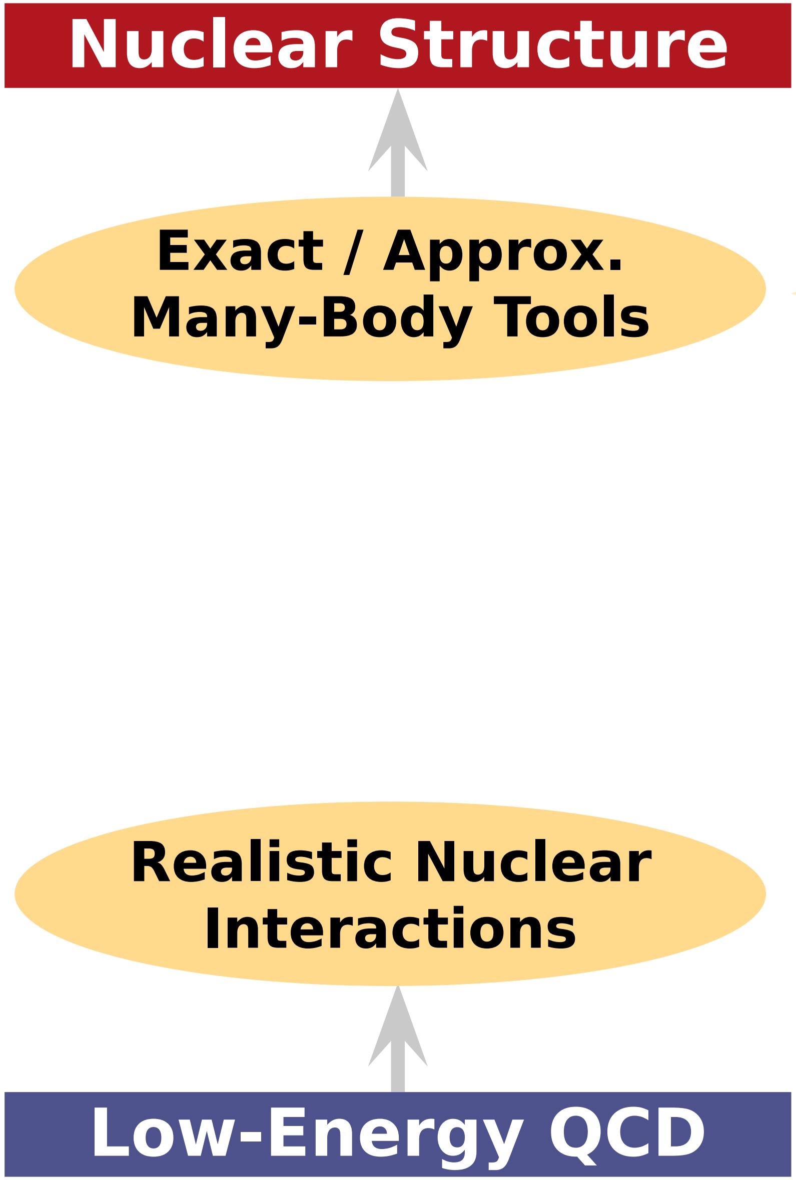
Low-Energy QCD

From QCD to Nuclear Structure



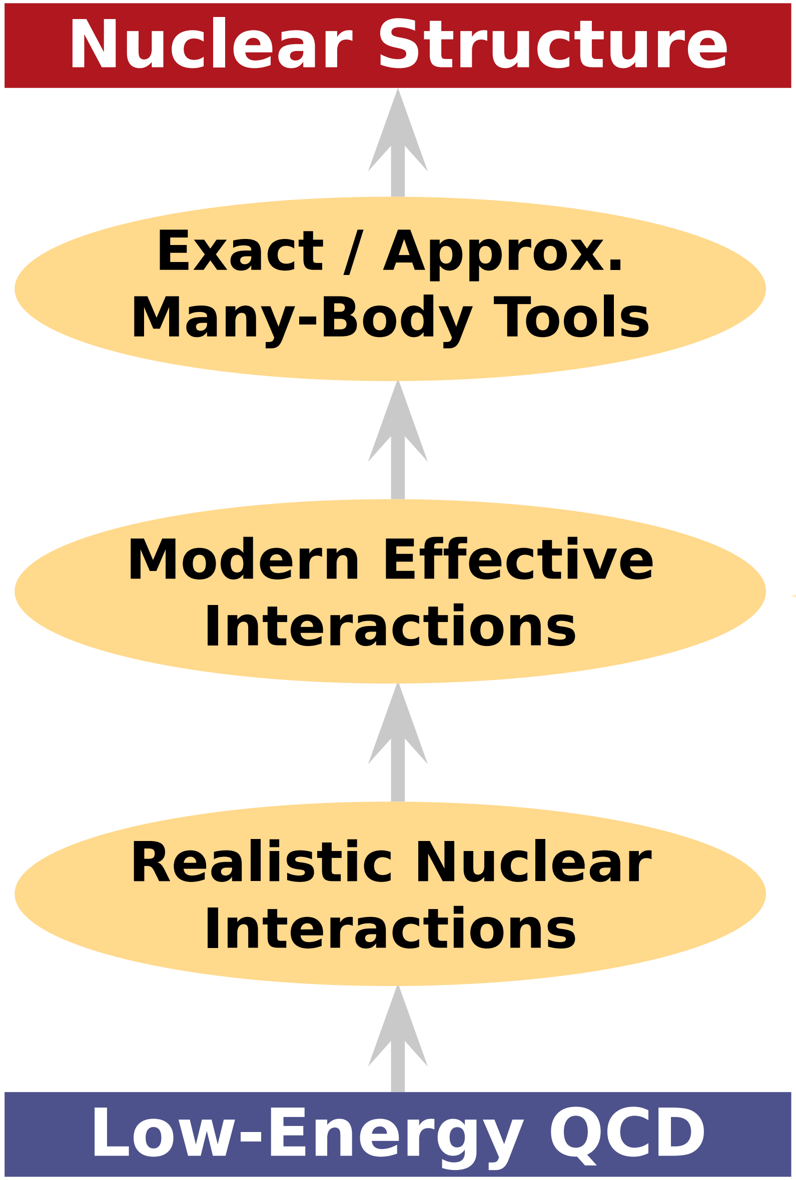
- chiral EFT interactions: consistent NN & 3N interaction derived within χEFT
- traditional NN-interactions: Argonne V18, CD Bonn,...
- reproduce experimental two-body data with high precision
- induce strong short-range central & tensor correlations

From QCD to Nuclear Structure



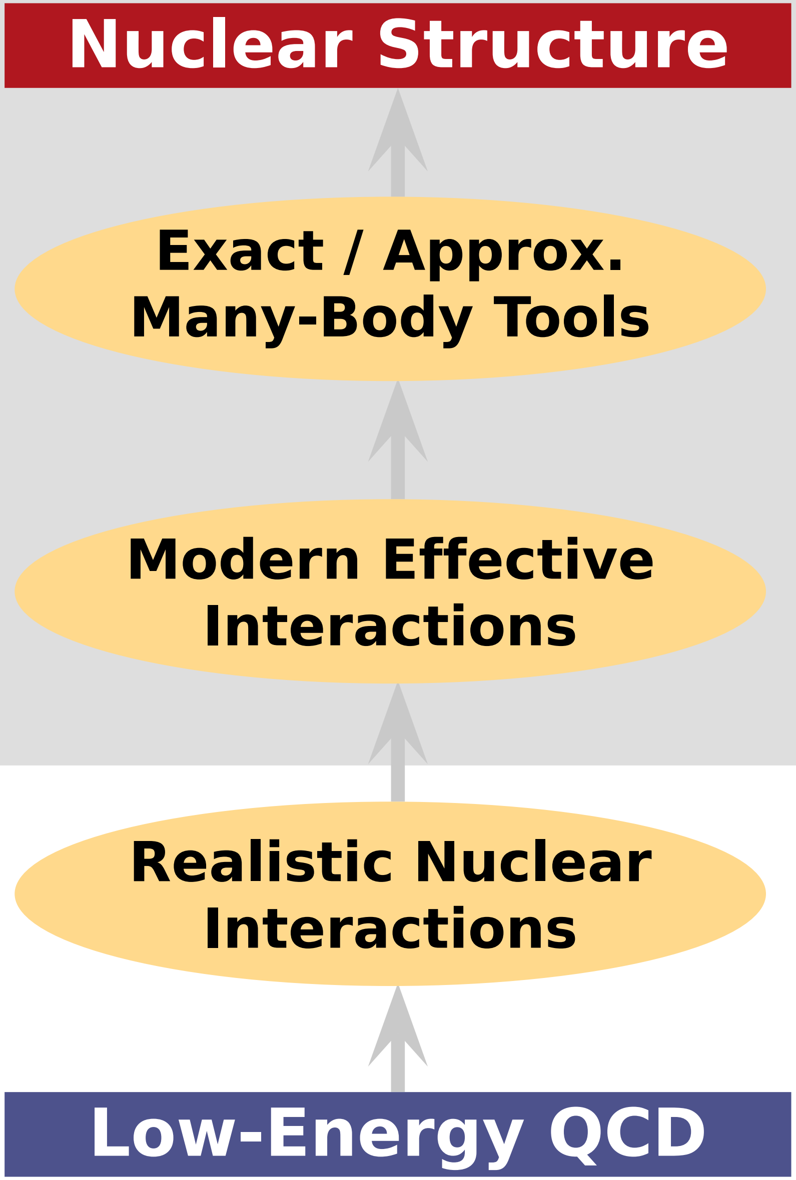
- ‘exact’ solution of the many-body problem for light & intermediate masses (NCSM, CC,...)
- controlled approximations for heavier nuclei (HF & MBPT,...)
- rely on restricted model spaces of tractable size
- not suitable for the description of short-range correlations

From QCD to Nuclear Structure



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

From QCD to Nuclear Structure



I’m one of the MBT guys...

...and this is the stuff I’m trying to sell

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

$$\mathrm{C} = \exp[-\mathrm{i}\,\mathrm{G}] = \exp\Big[-\mathrm{i}\sum_{i<j}\mathrm{g}_{ij}\Big]$$

Correlated States

imprint short-range correlations onto uncorrelated many-body states

$$\left|\widetilde{\psi}\right\rangle = \mathrm{C}\,\left|\psi\right\rangle$$

Correlated Operators

adapt Hamiltonian to uncorrelated states (pre-diagonalization)

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

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

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

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

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

Tensor Correlator C_Ω

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

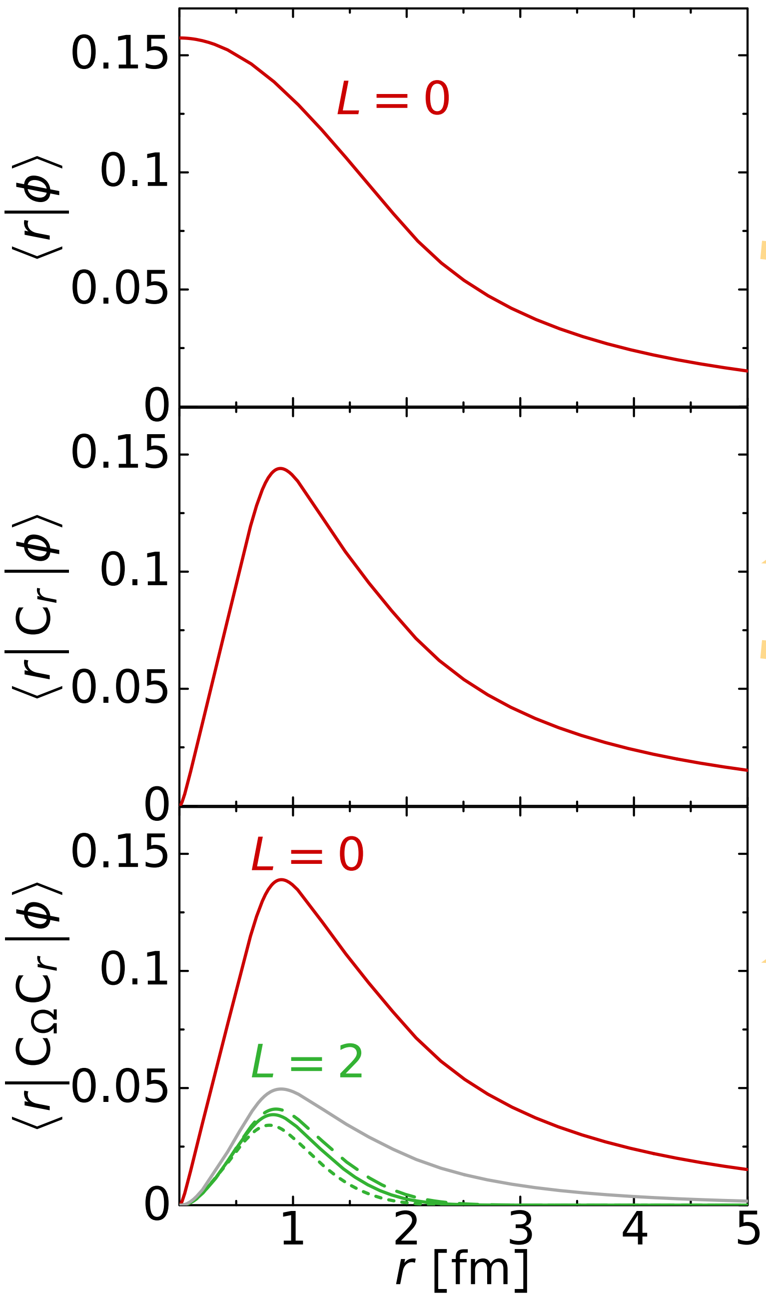
$$g_\Omega = \frac{3}{2}\vartheta(r)\big[(\vec{\sigma}_1\cdot\vec{q}_\Omega)(\vec{\sigma}_2\cdot\vec{r}) + (\vec{r}\longleftrightarrow\vec{q}_\Omega)\big]$$

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

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

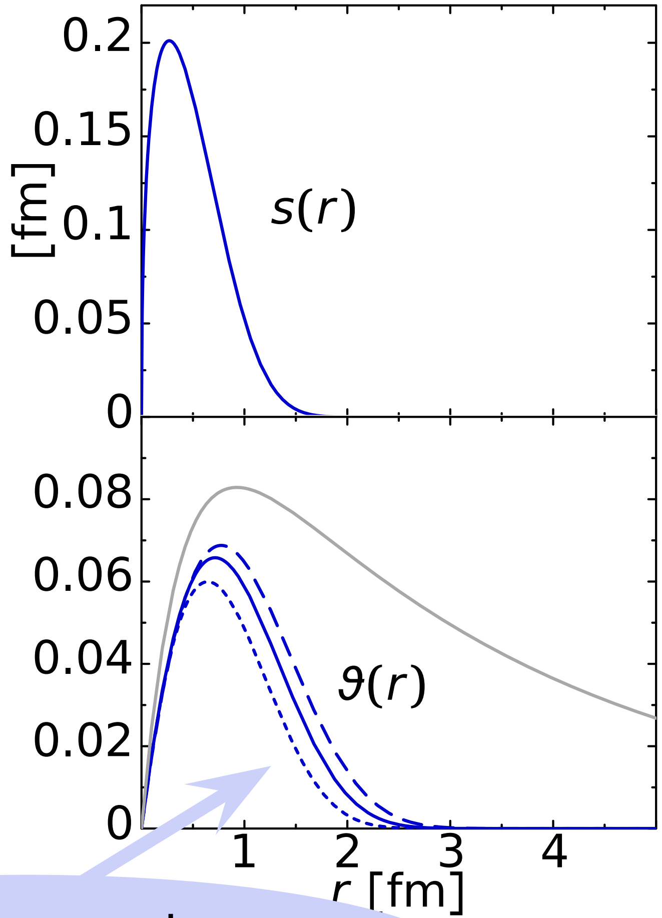
- $s(r)$ and $\vartheta(r)$ depend on & are optimized for initial potential

Correlated States: The Deuteron



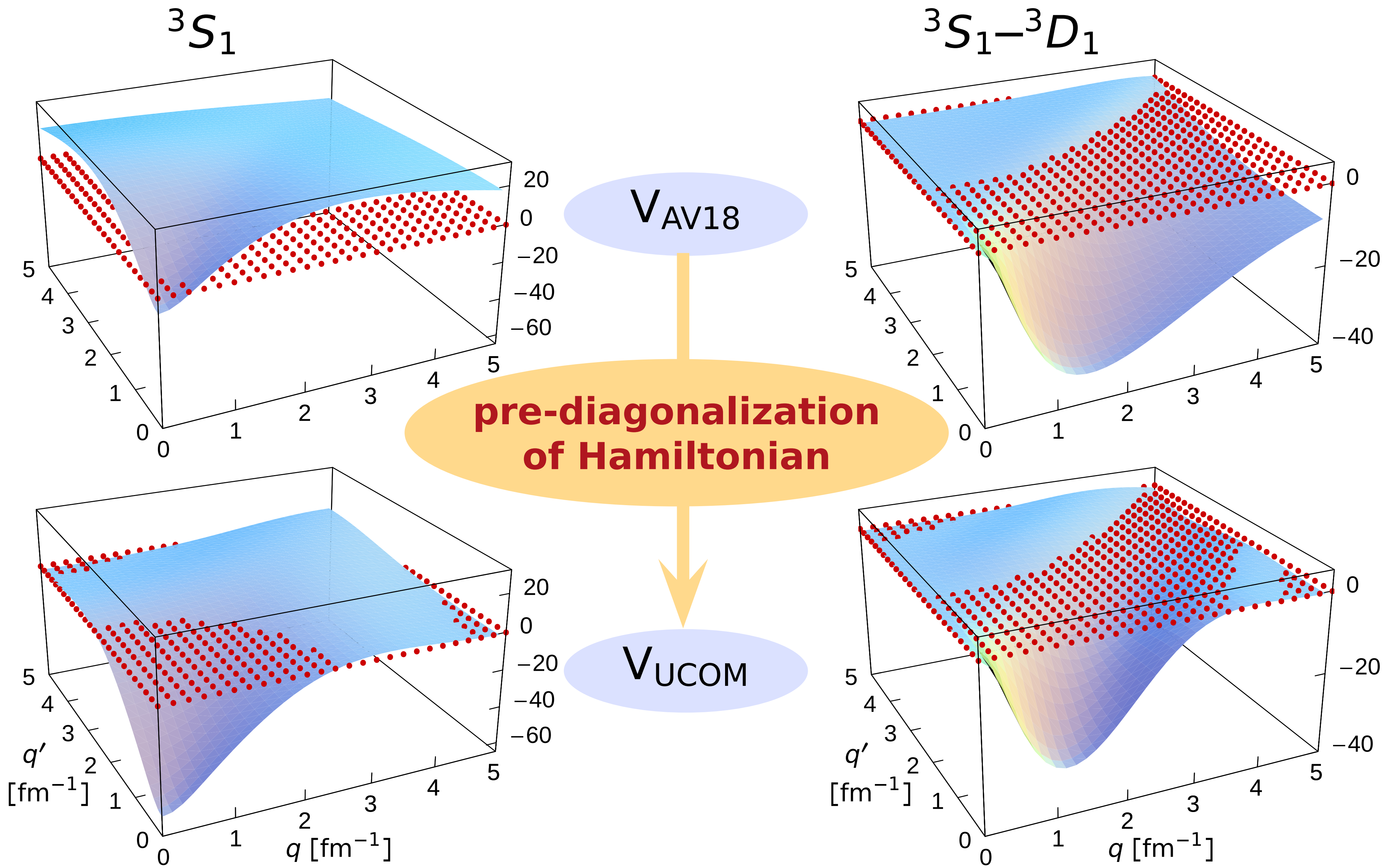
central correlations

tensor correlations



only short-range tensor correlations treated by C_Ω

Correlated Interaction: V_{UCOM}



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

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

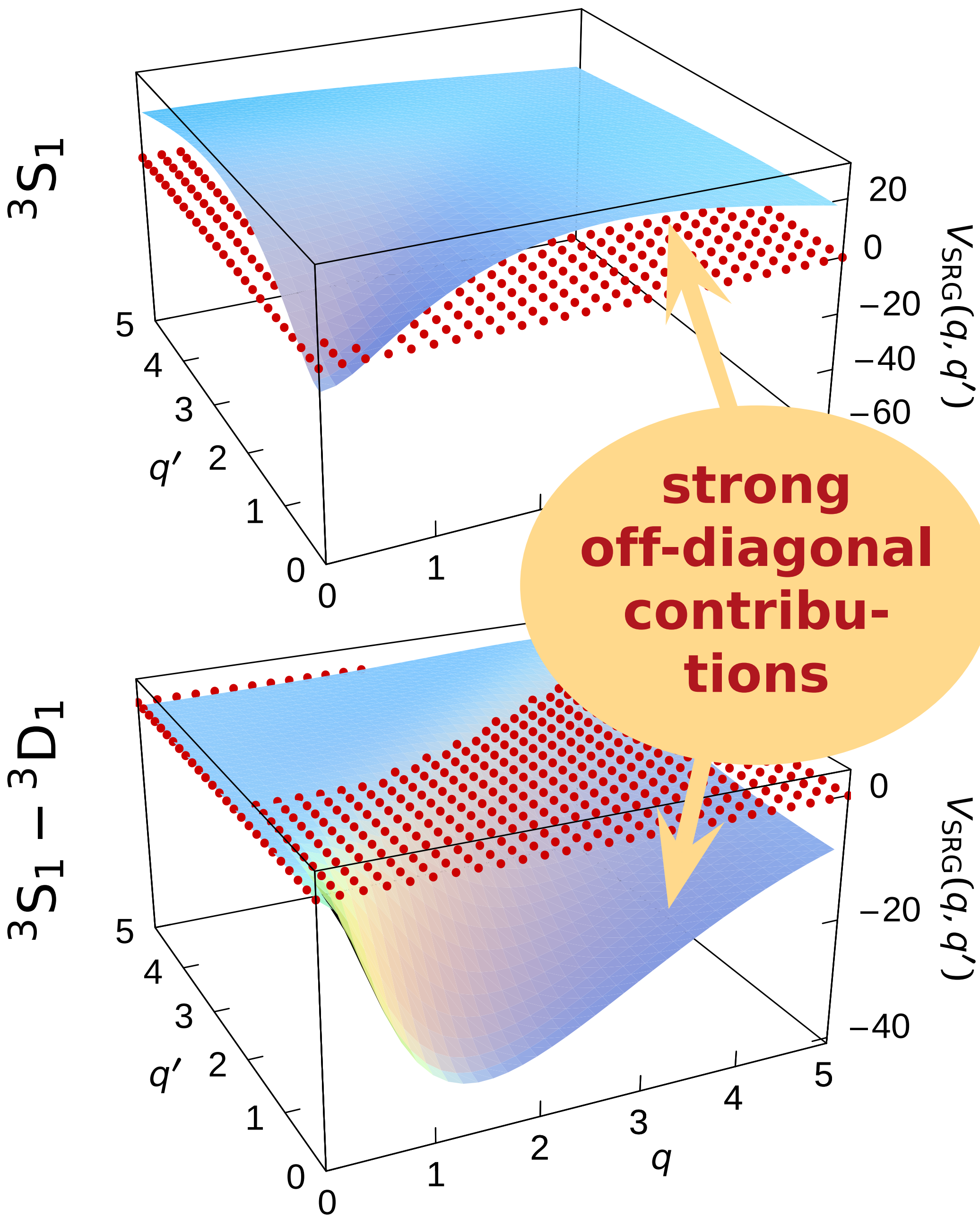
- dynamical generator defined as commutator with the operator in whose eigenbasis H shall be diagonalized

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

UCOM vs. SRG

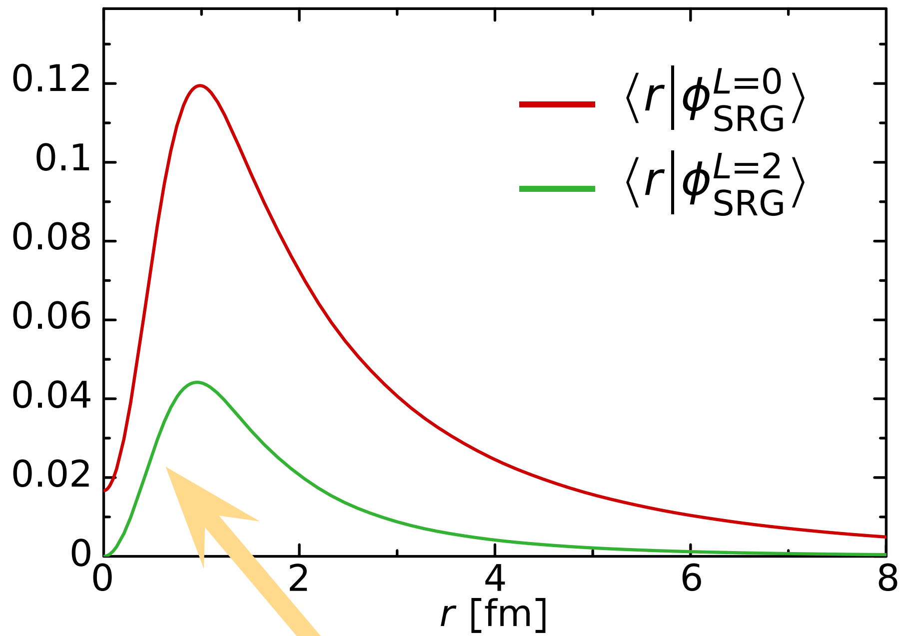
$\eta(0)$ has the same structure as UCOM generators g_r & g_Ω

SRG Evolution: The Deuteron



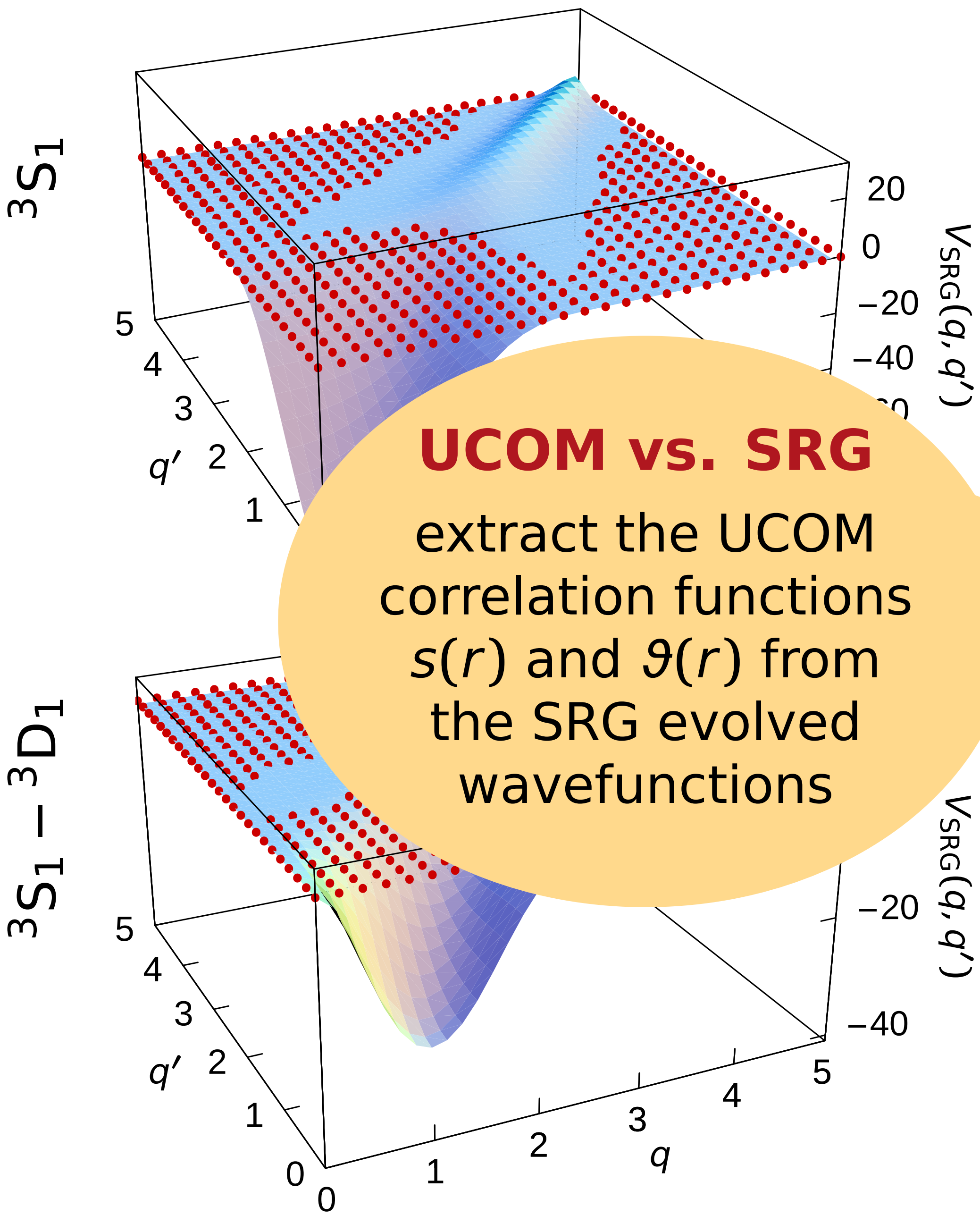
strong off-diagonal contributions

Argonne V18

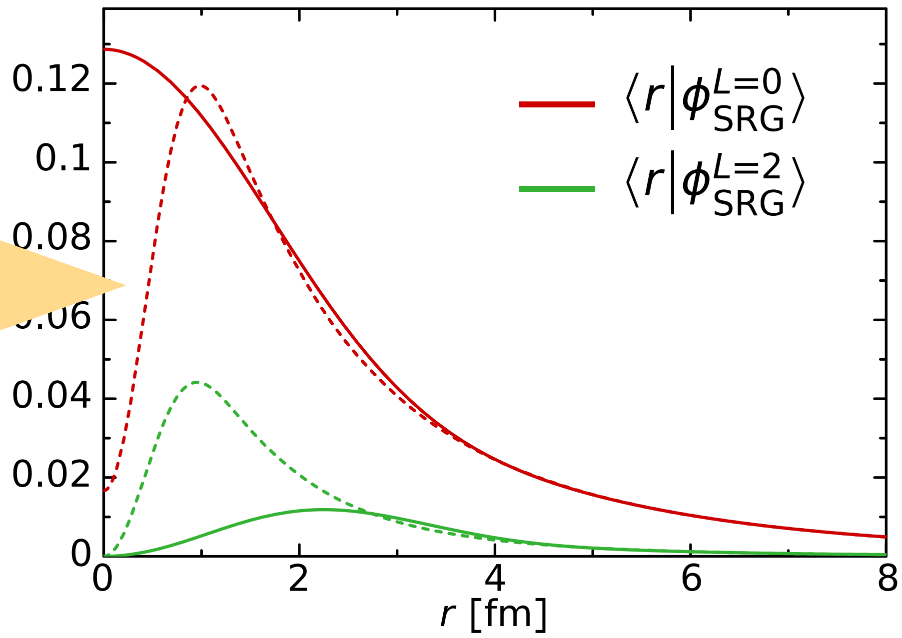


short-range central & tensor correlations

SRG Evolution: The Deuteron



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



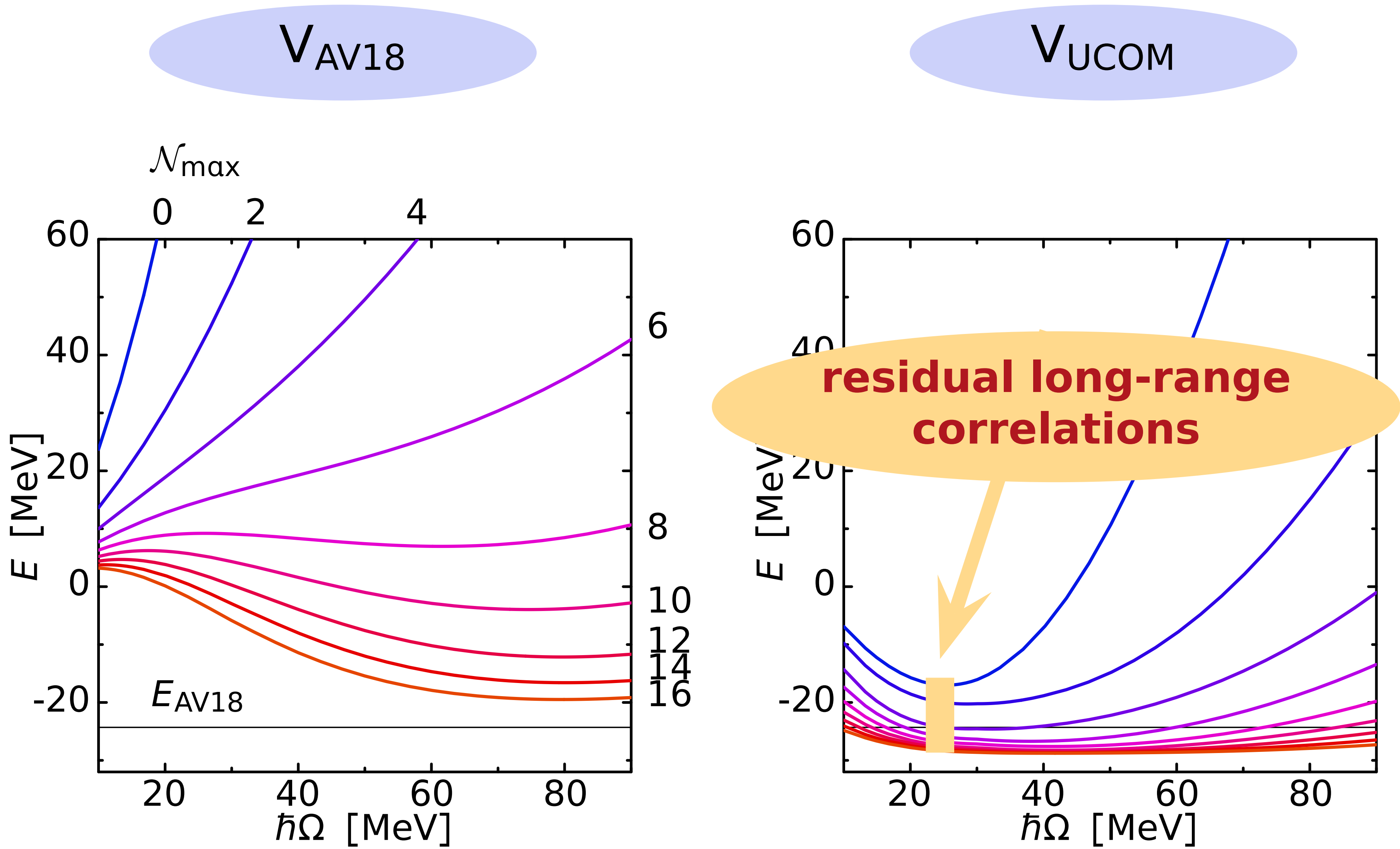
UCOM vs. SRG

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

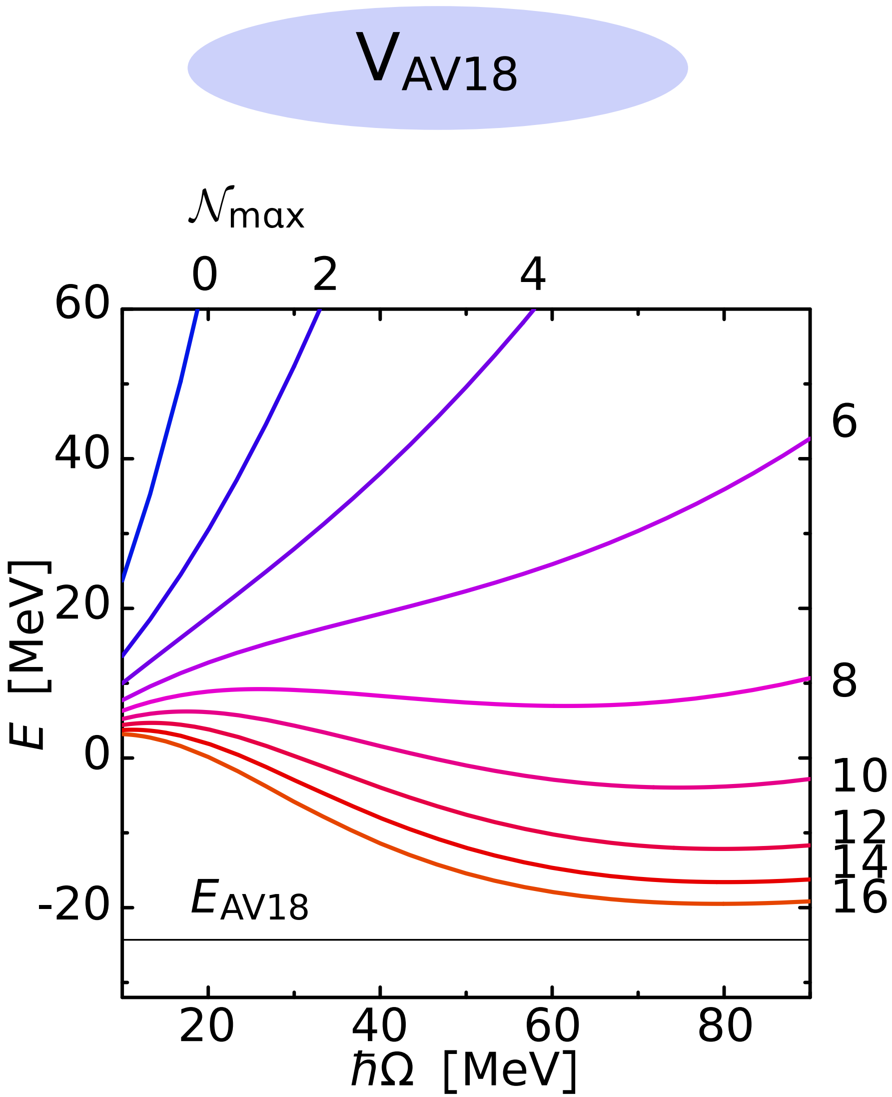
Computational Many-Body Methods

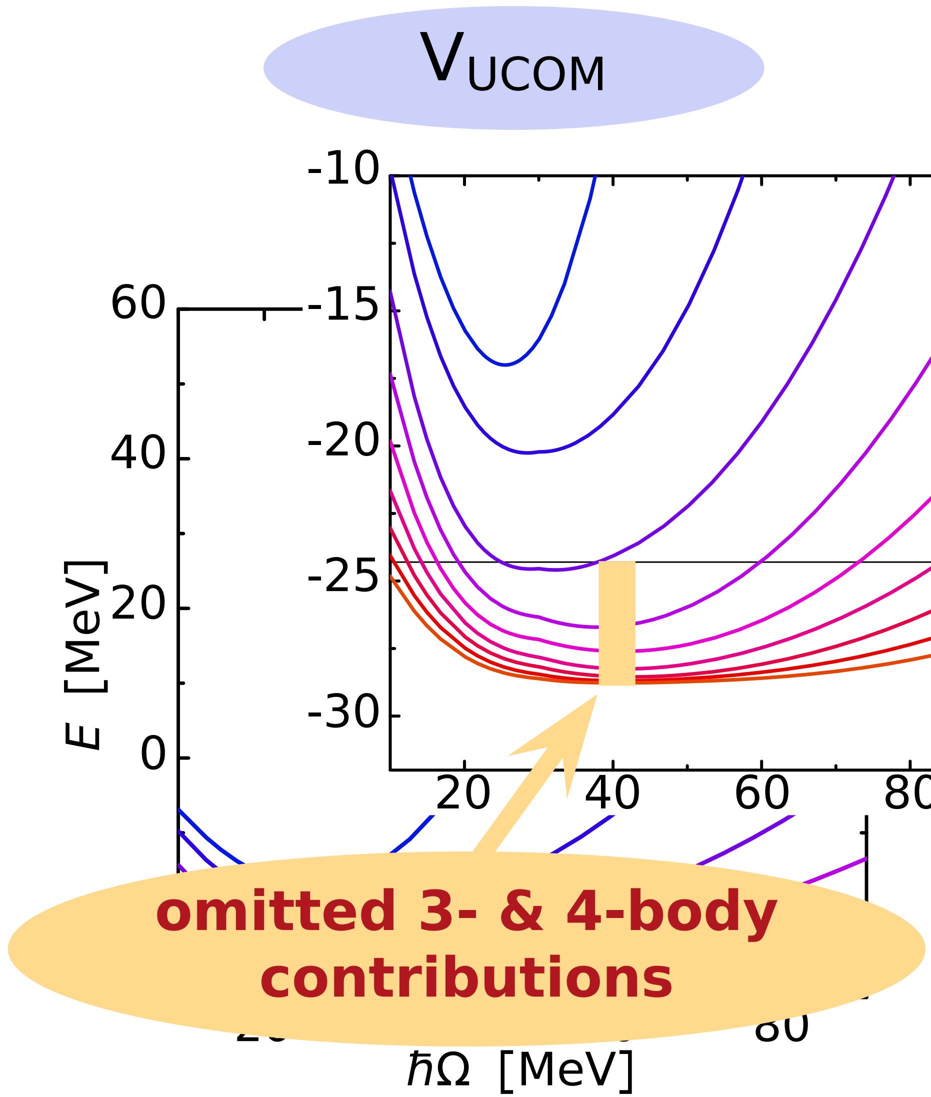
Testing UCOM & SRG Interactions in Nuclei

NCSM: ^{4}He Convergence



NCSM: ^{4}He Convergence





Three-Body Interactions — Strategies

Correlated Hamiltonian in Many-Body Space

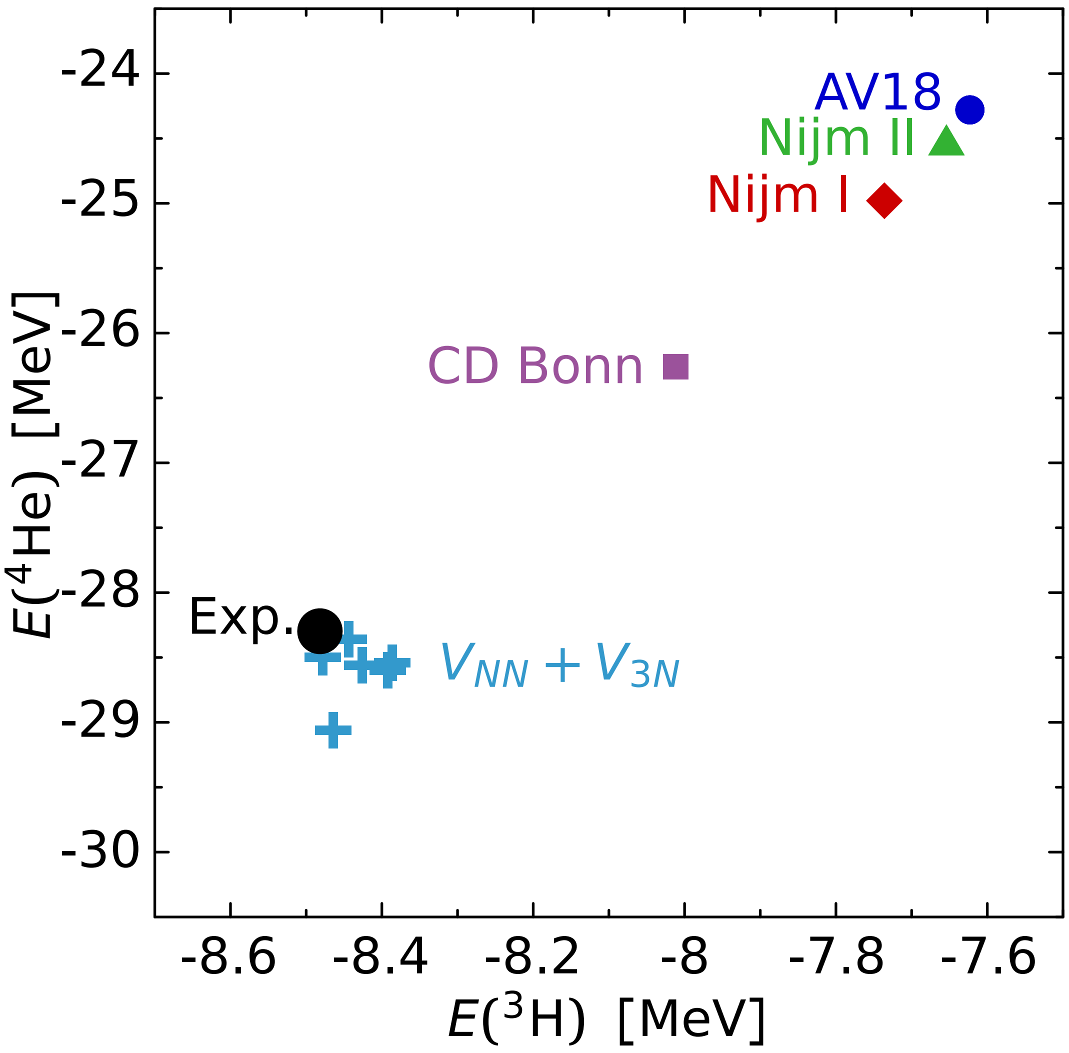
$$\widetilde{H} = C^{\dagger}\,(T + V_{NN} + V_{3N})\,C$$

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

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

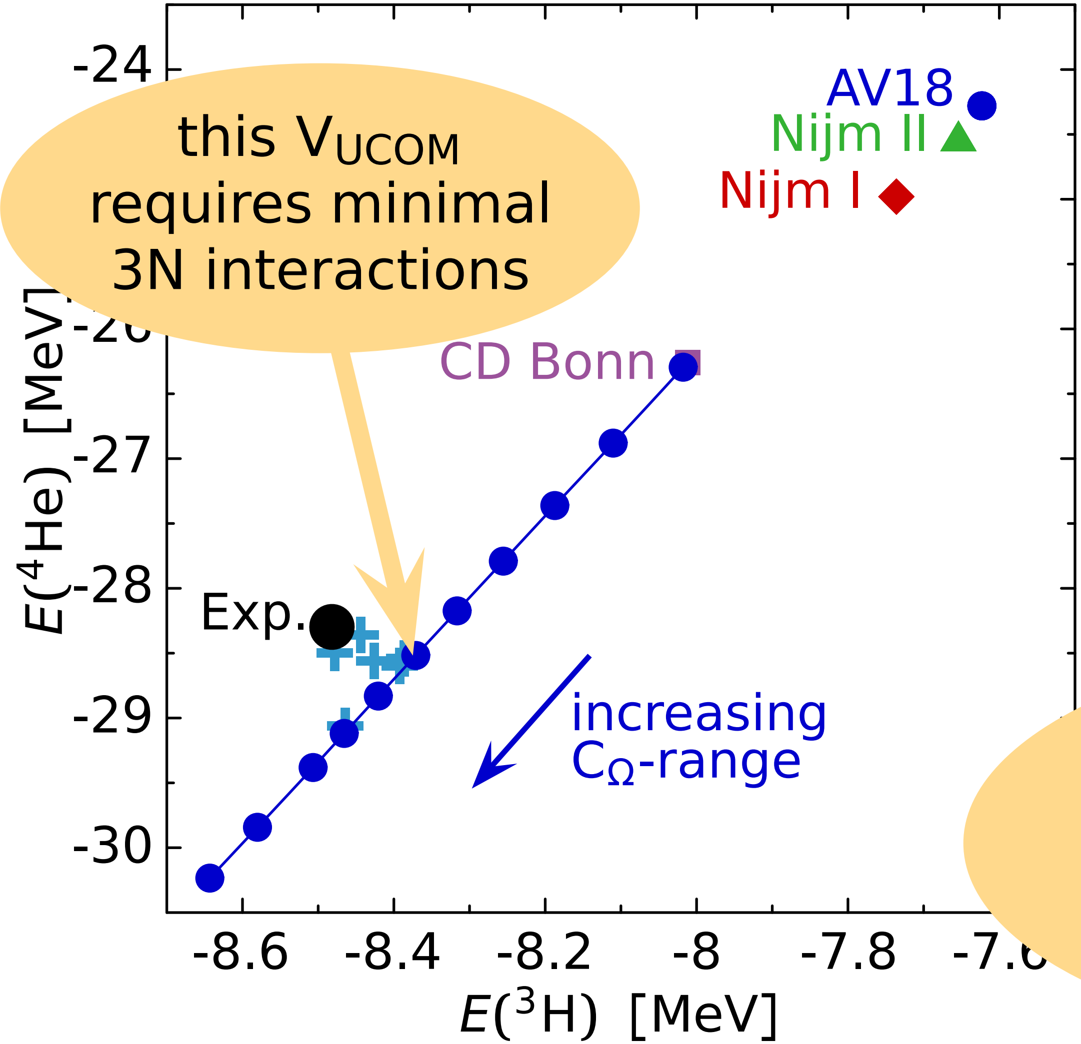
- **include full** $V^{[3]}_{\mathrm{UCOM}}$ consisting of genuine and induced 3N terms
  (very hard in UCOM, but Dick can do it in SRG)
- **replace** $V^{[3]}_{\mathrm{UCOM}}$ by phenomenological three-body force
  (easily tractable also for heavier nuclei)
- **minimize** $V^{[3]}_{\mathrm{UCOM}}$ by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

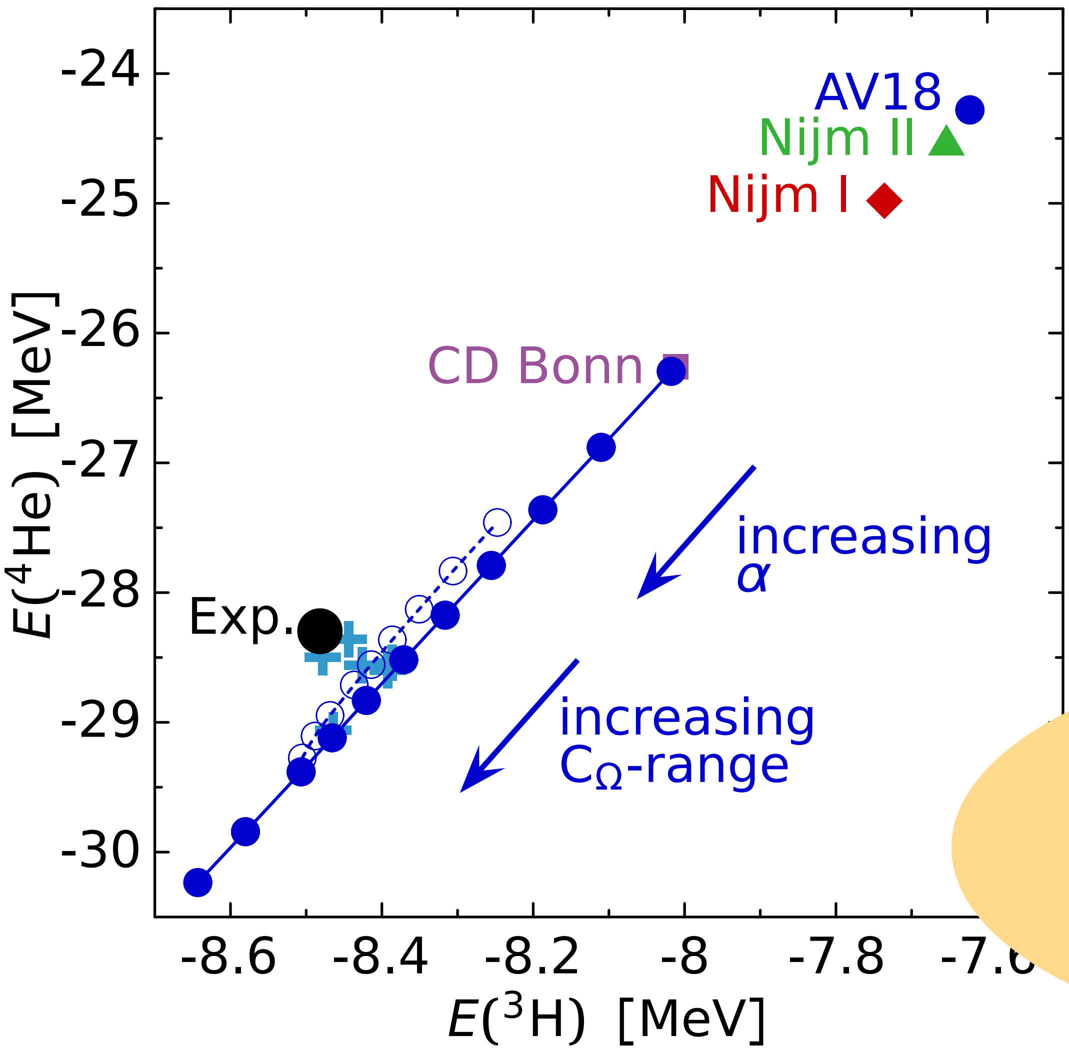
Three-Body Interactions — Tjon Line



- **Tjon-line**: $E(^4He)$ vs. $E(^3H)$ 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

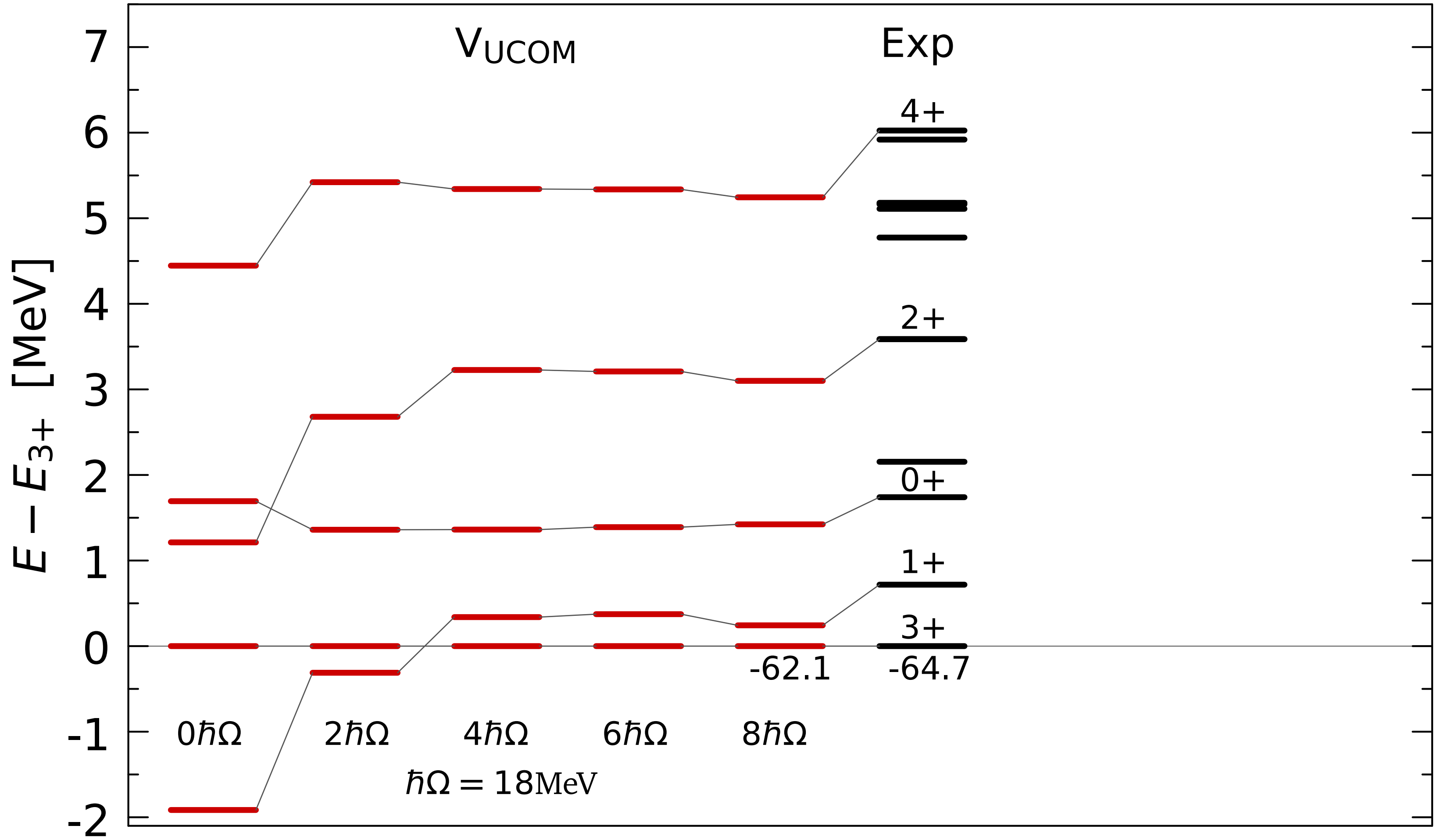
Three-Body Interactions — Tjon Line



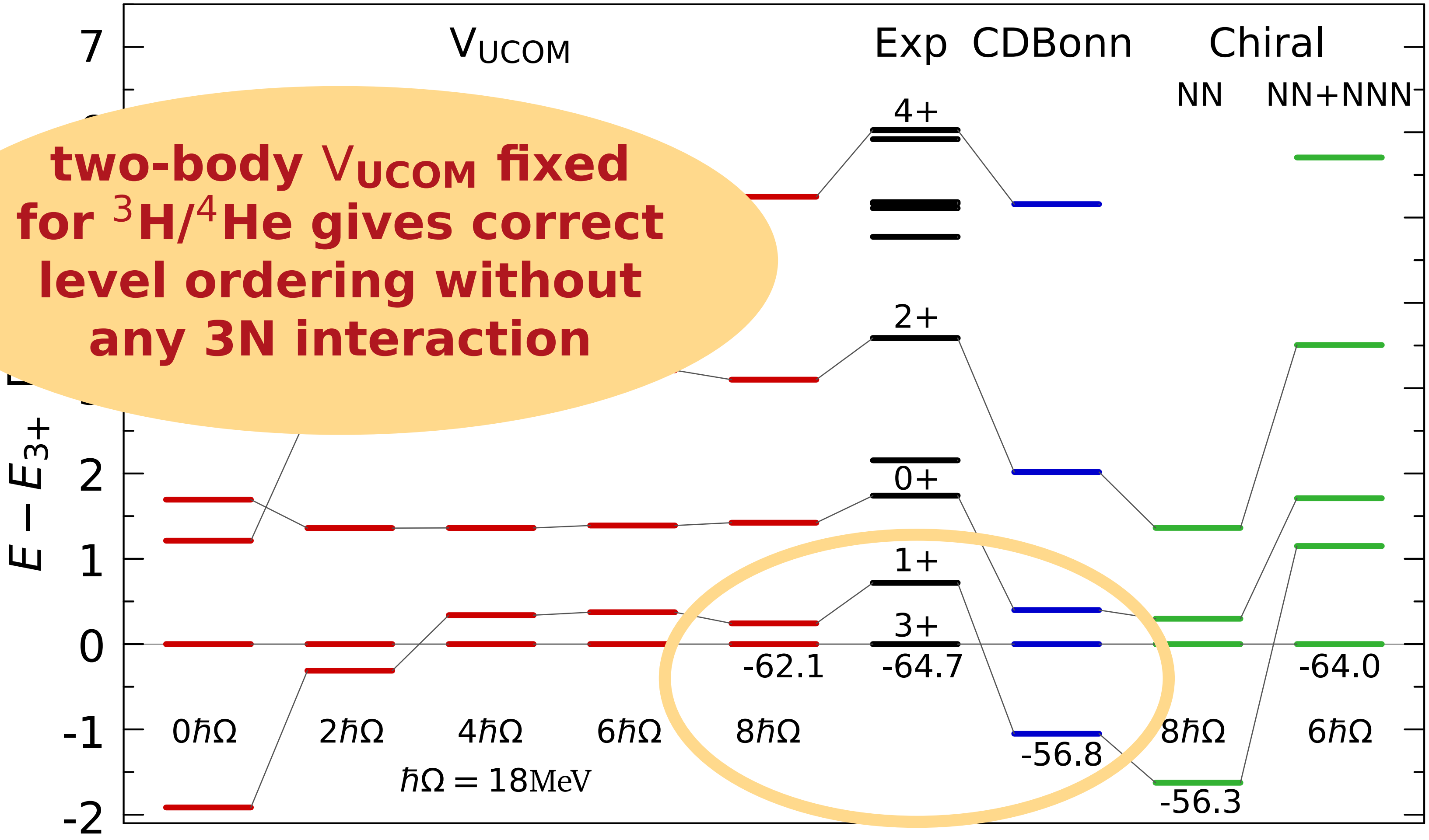
- **Tjon-line**: $E(^4\text{He})$ vs. $E(^3\text{H})$ for phase-shift equivalent NN-interactions
- same behavior for the SRG interaction as function of α

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?



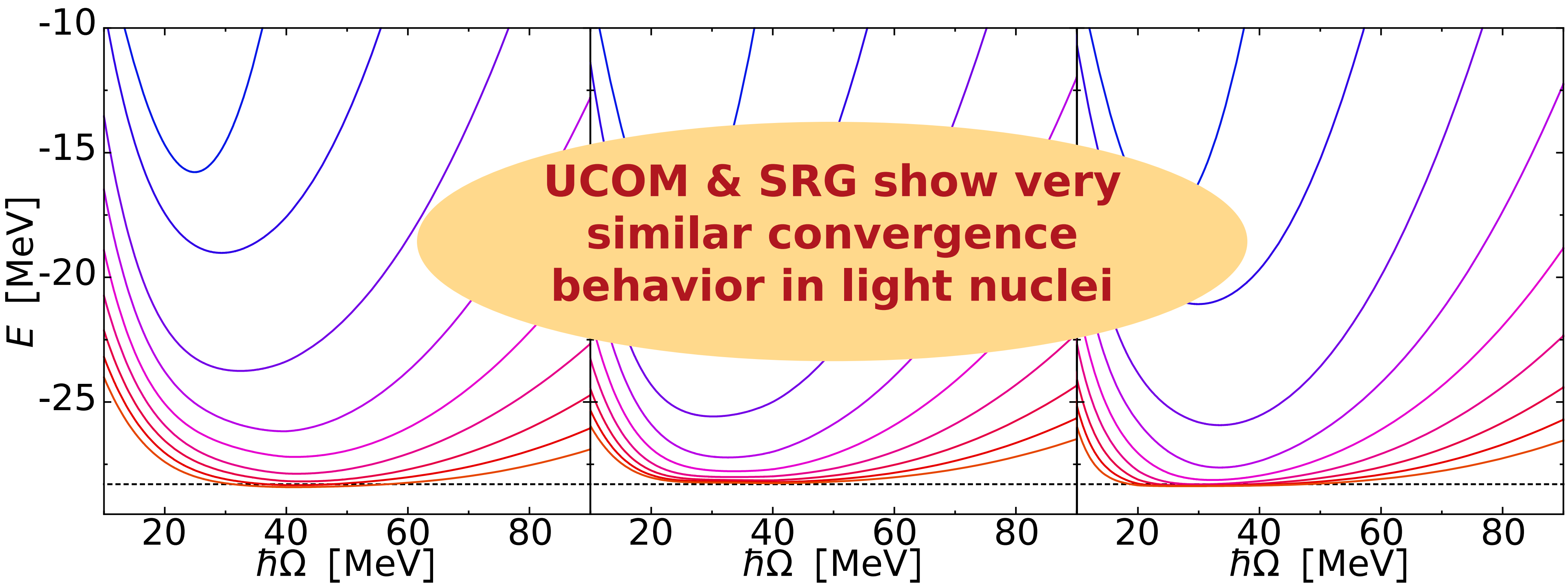
two-body V_{UCOM} fixed for ^{3}H/^{4}He gives correct level ordering without any 3N interaction

UCOM vs. SRG: ^{4}He Convergence

V_{UCOM}
MIN, $I_\vartheta = 0.09\,\mathrm{fm}^3$

V_{UCOM}
SRG, $\bar{\alpha} = 0.04\,\mathrm{fm}^4$

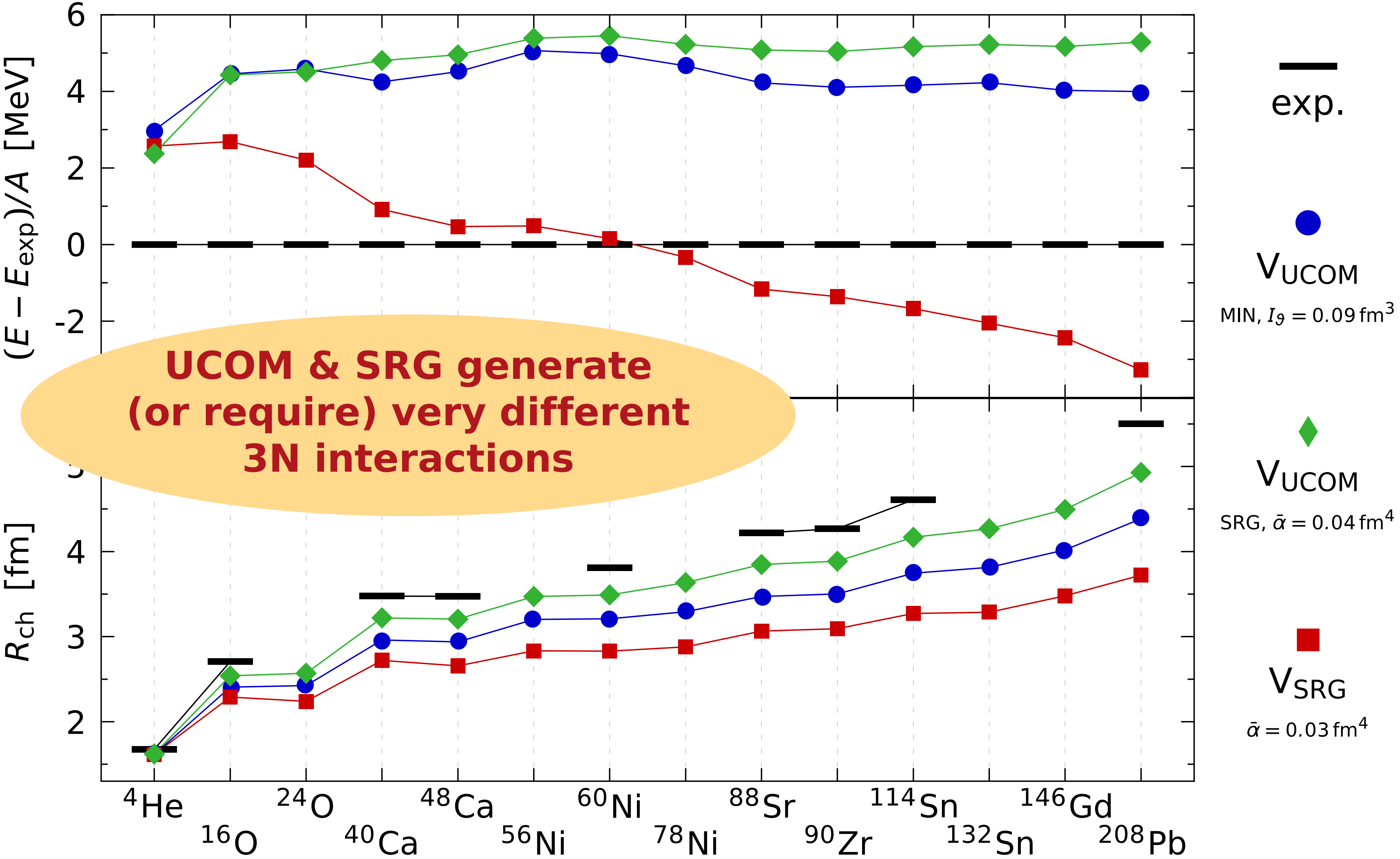
V_{SRG}
$\bar{\alpha} = 0.03\,\mathrm{fm}^4$



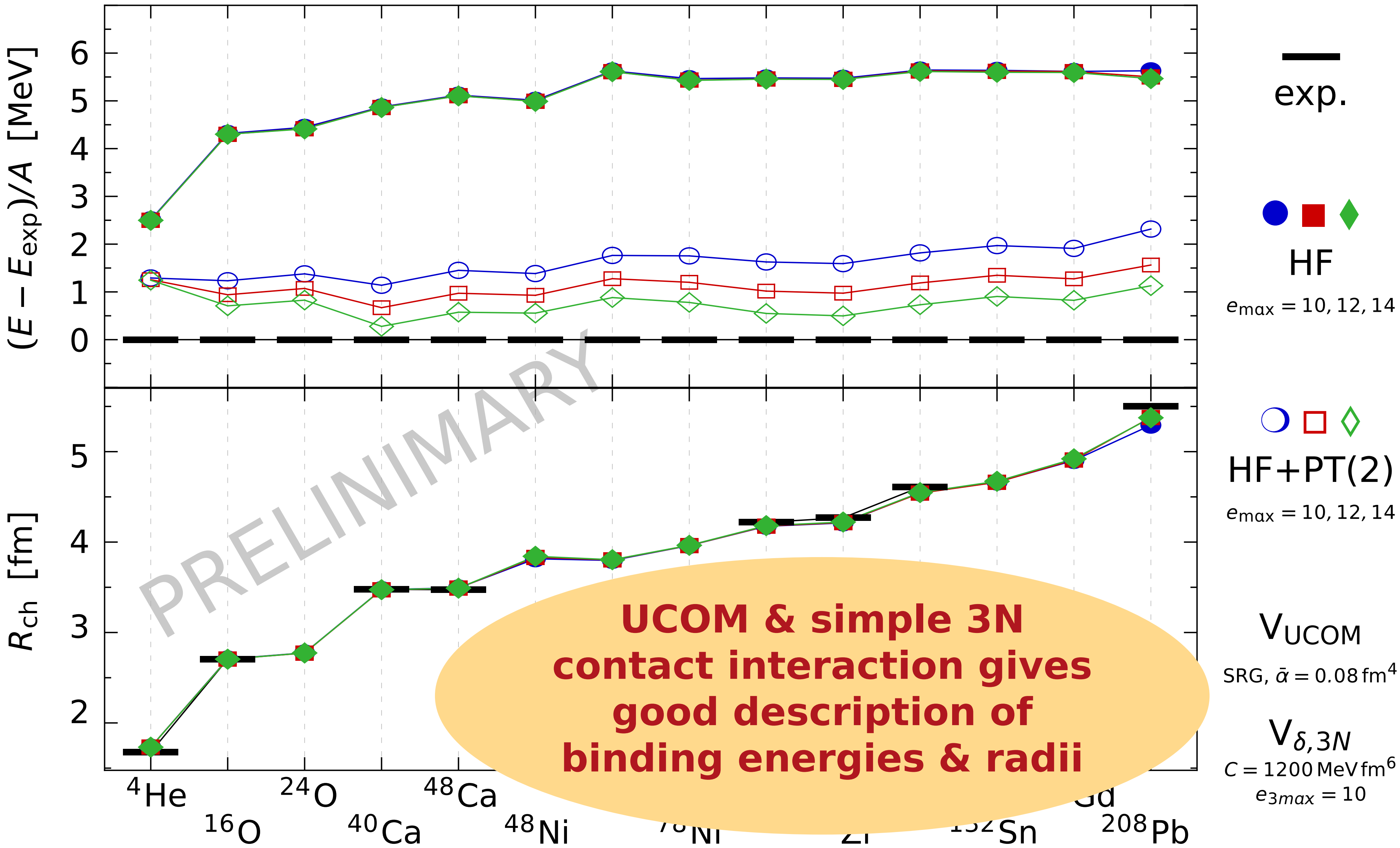
UCOM & SRG show very similar convergence behavior in light nuclei

- I_ϑ or $\bar{\alpha}$ adjusted such that ^{4}He 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

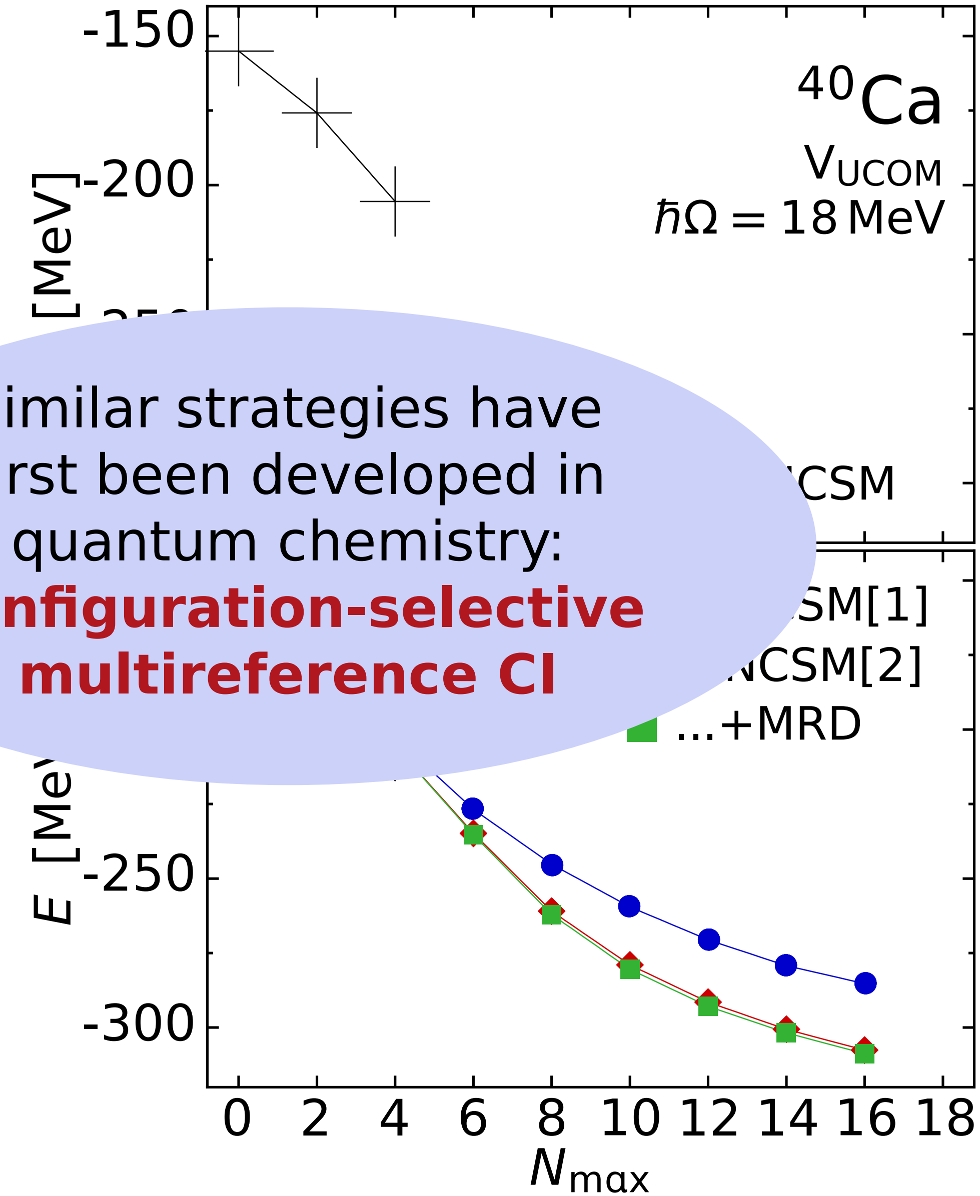
Roth & Navrátil — Phys. Rev. Lett. 99, 092501 (2007)

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 ~10^{10})



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

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 $\mathcal{M}_{\text{ref}}$**

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

- **measure the importance** of individual basis state $|\Phi_{\nu}\rangle \notin \mathcal{M}_{\text{ref}}$ via first-order multiconfigurational perturbation theory

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

- construct **importance-truncated space $\mathcal{M}(\kappa_{\text{min}})$** spanned by basis states with $|\kappa_{\nu}| \geq \kappa_{\text{min}}$

- **solve eigenvalue problem** in importance truncated space $\mathcal{M}(\kappa_{\text{min}})$ 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 $|\Psi_{\text{ref}}\rangle = |\Phi_0\rangle$

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

❷ solve eigenvalue

❸ use dominant c eigenstate ($|C_\nu|$ $|\Psi_{\text{ref}}\rangle$, goto ❶

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 $|\Psi_{\text{ref}}\rangle$

❶ construct importance truncated ... r $N_{\max} + 2$

... e problem

... nponents of ... $\geq C_{\min}$) as new

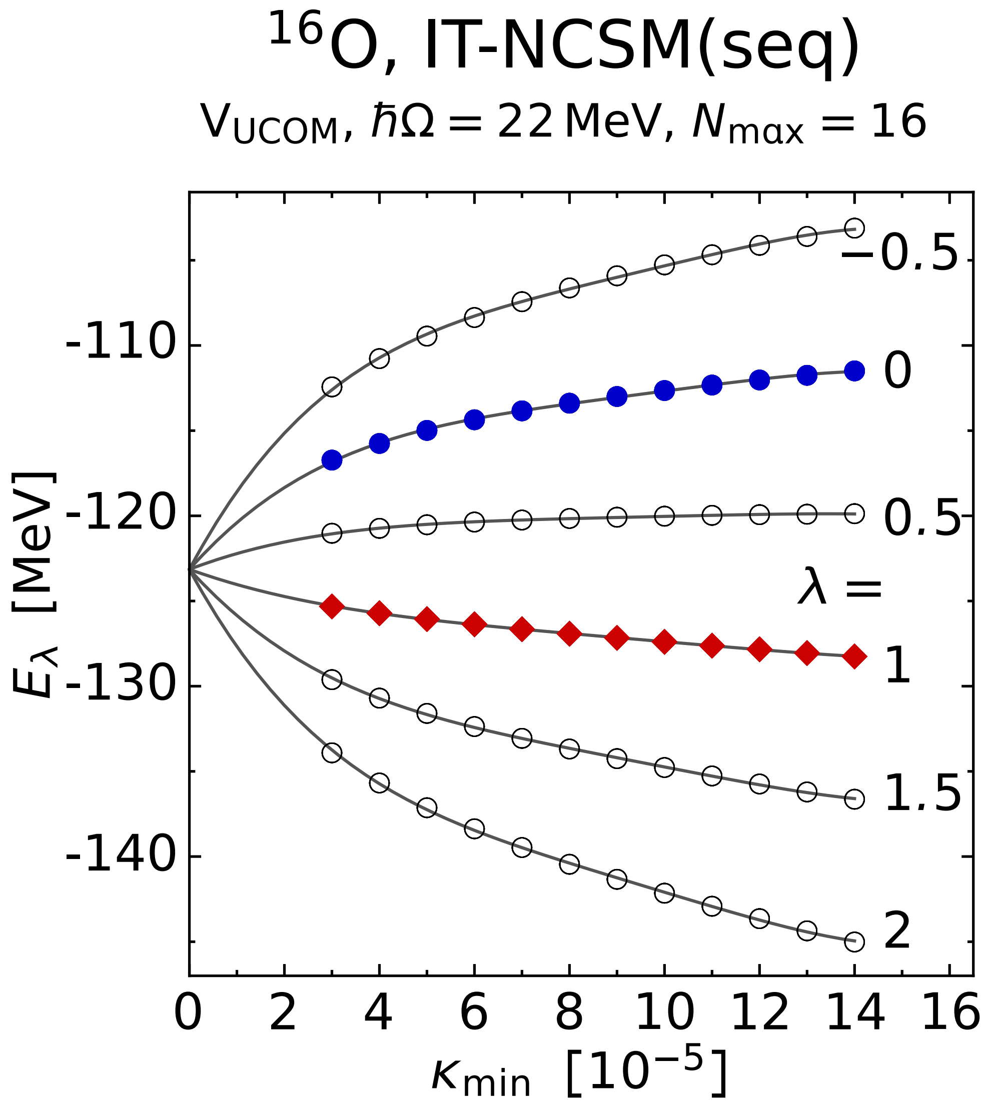
full NCSM model space is recovered in the limit $(\kappa_{\min}, C_{\min}) \to 0$ in IT-NCSM(seq) and IT-NCSM[i_{conv}]

Threshold Extrapolation

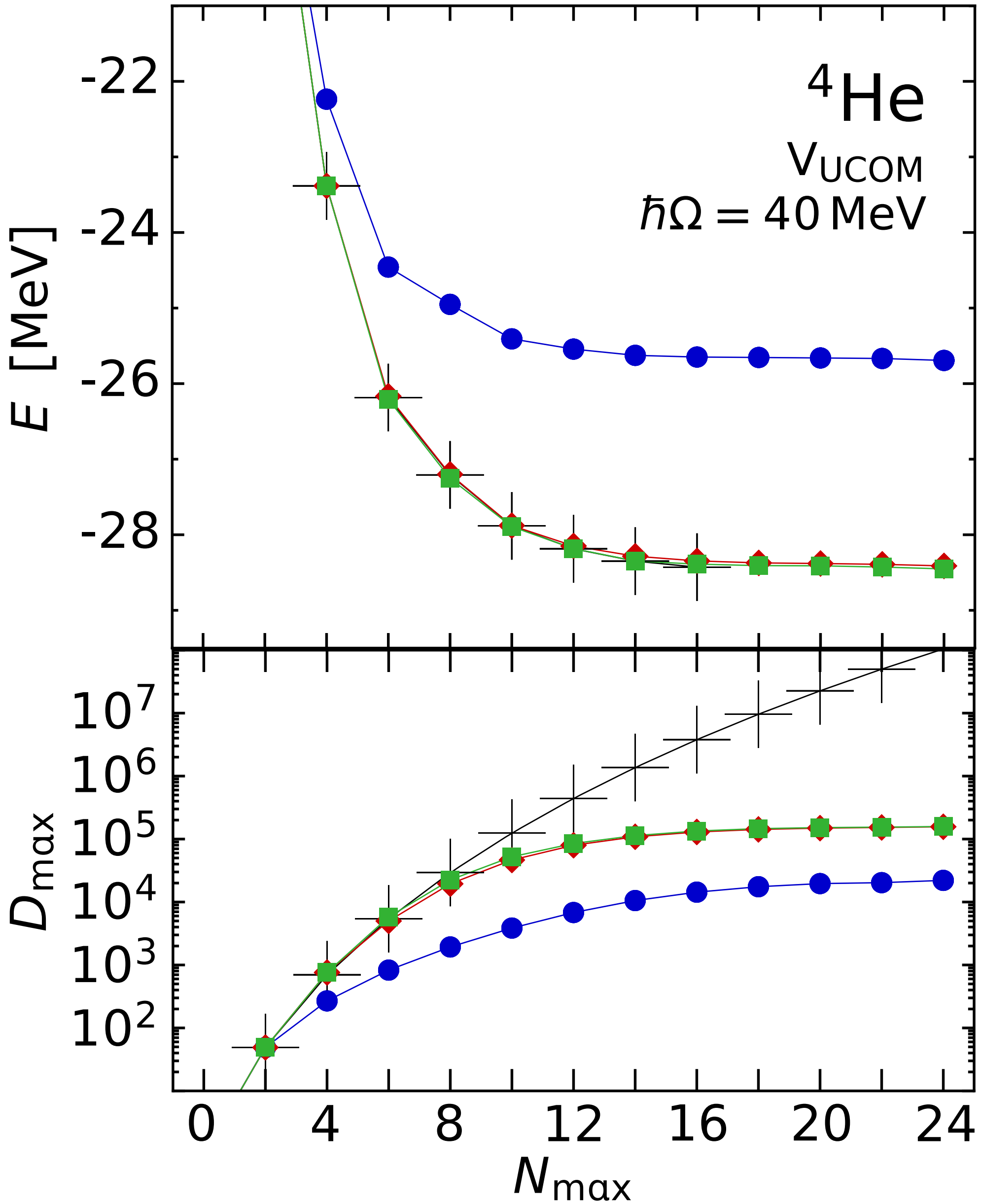
- all calculations done for a **sequence of importance thresholds** ➔ $E(\kappa_{\min})$
- contribution of **excluded states** estimated perturbatively ➔ $\Delta_{\text{excl}}(\kappa_{\min})$
- **simultaneous extrapolation** of combined energy

$$E_\lambda(\kappa_{\min}) = E(\kappa_{\min}) + \lambda \Delta_{\text{excl}}(\kappa_{\min})$$

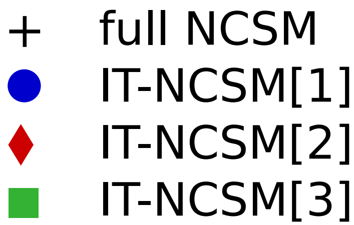
  to $\kappa_{\min} = 0$ for set of λ-values
- all IT-NCSM energies shown are threshold extrapolated



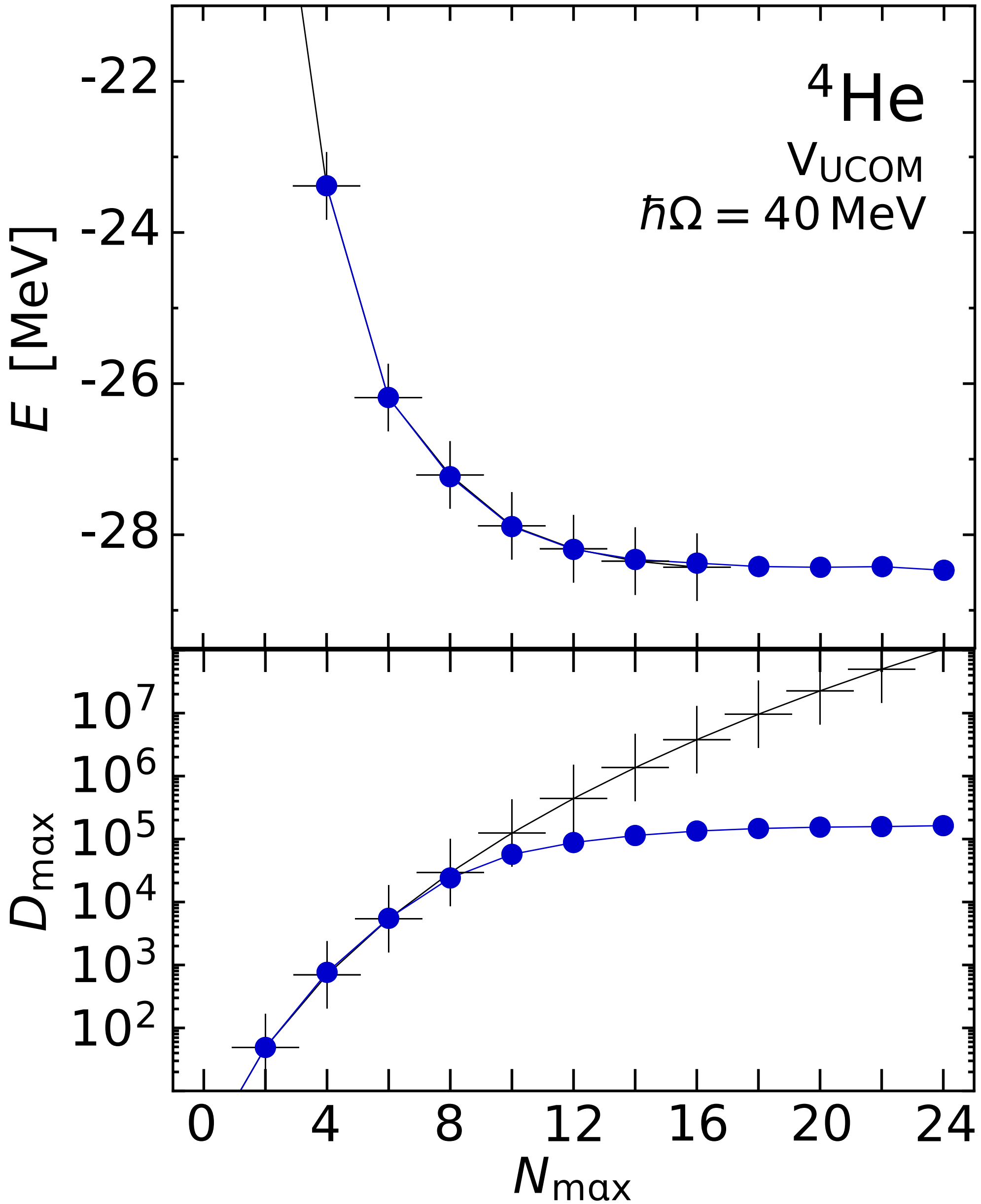
^{4}He: Importance-Truncated NCSM



- **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



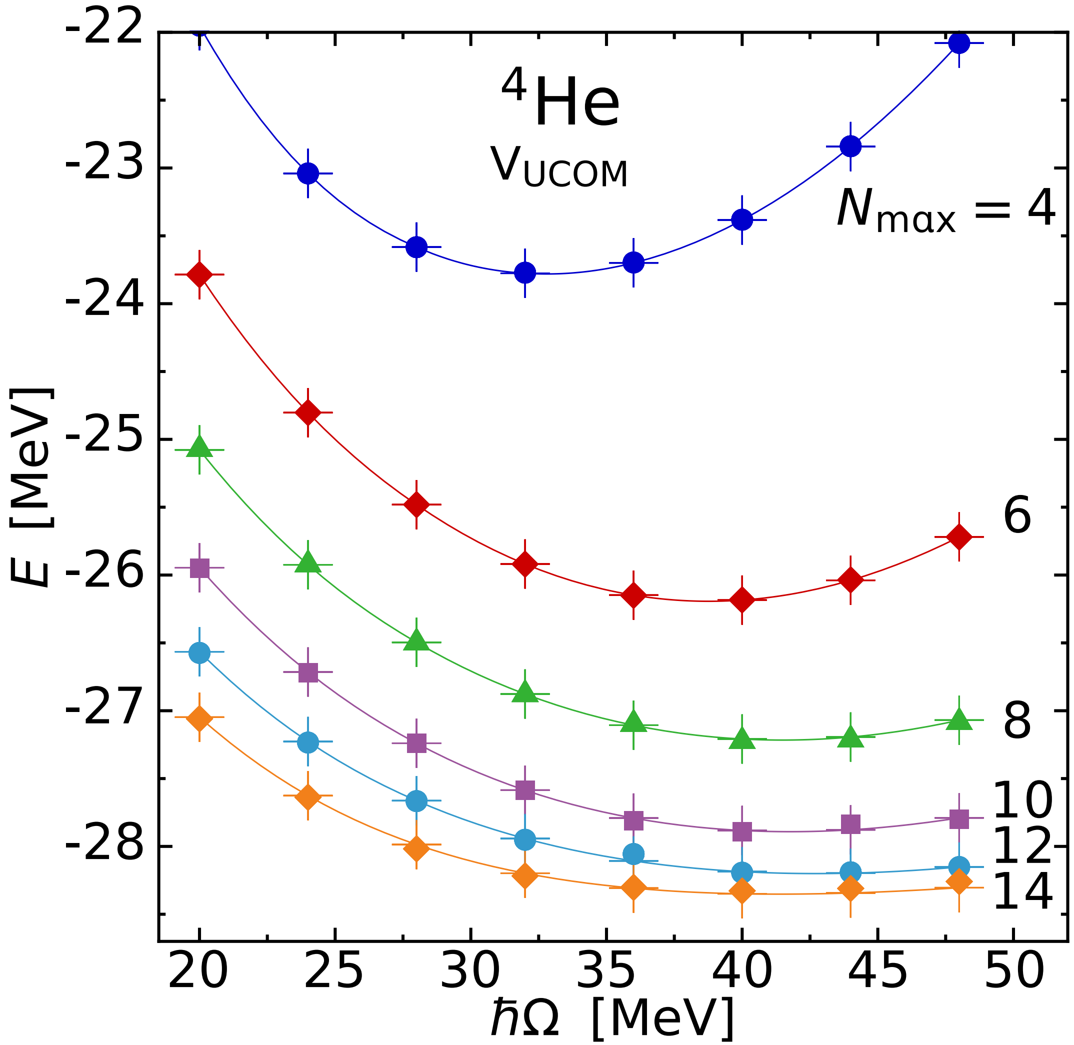
^{4}He: Importance-Truncated NCSM



- **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)

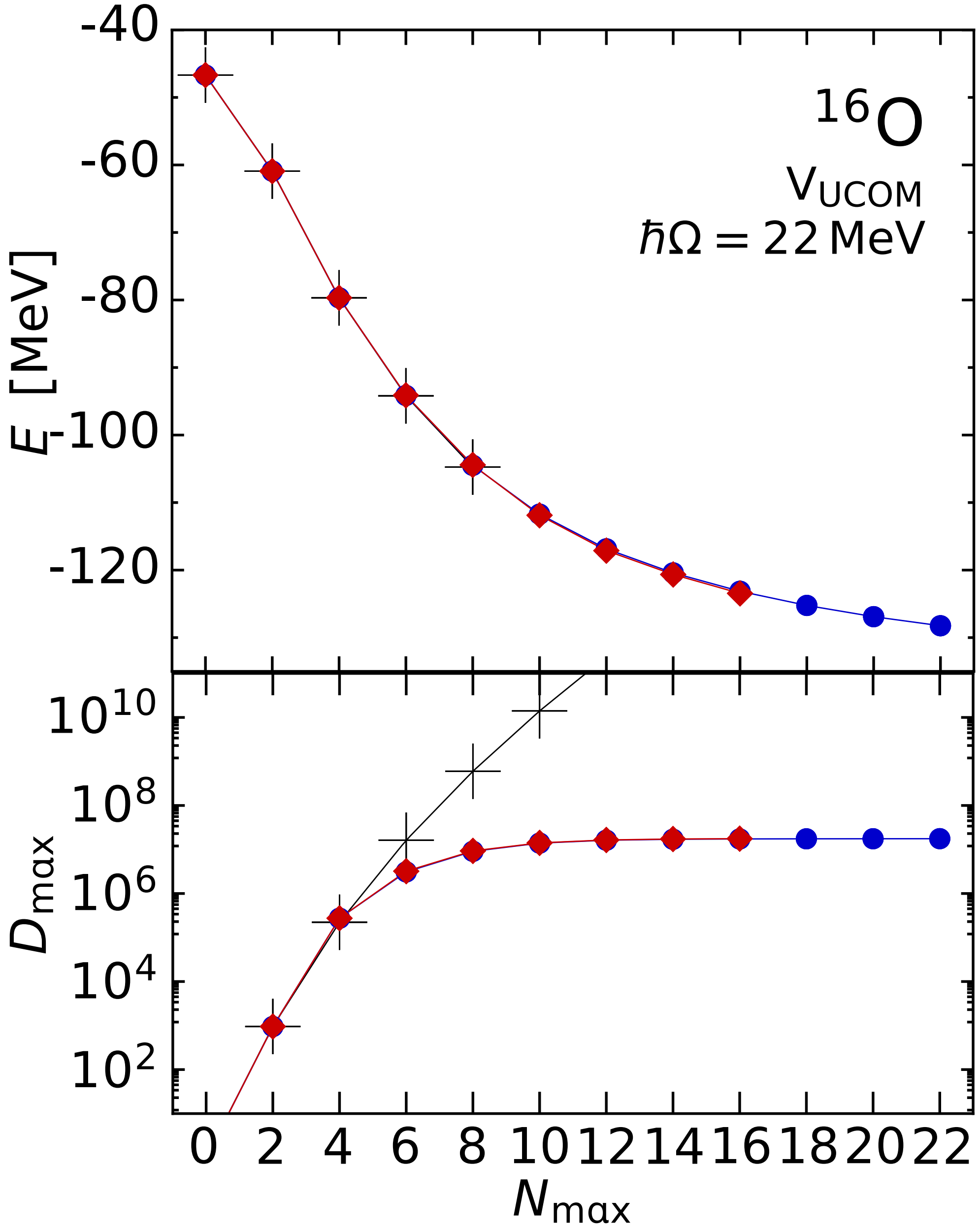
^{4}He: Importance-Truncated NCSM



- **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



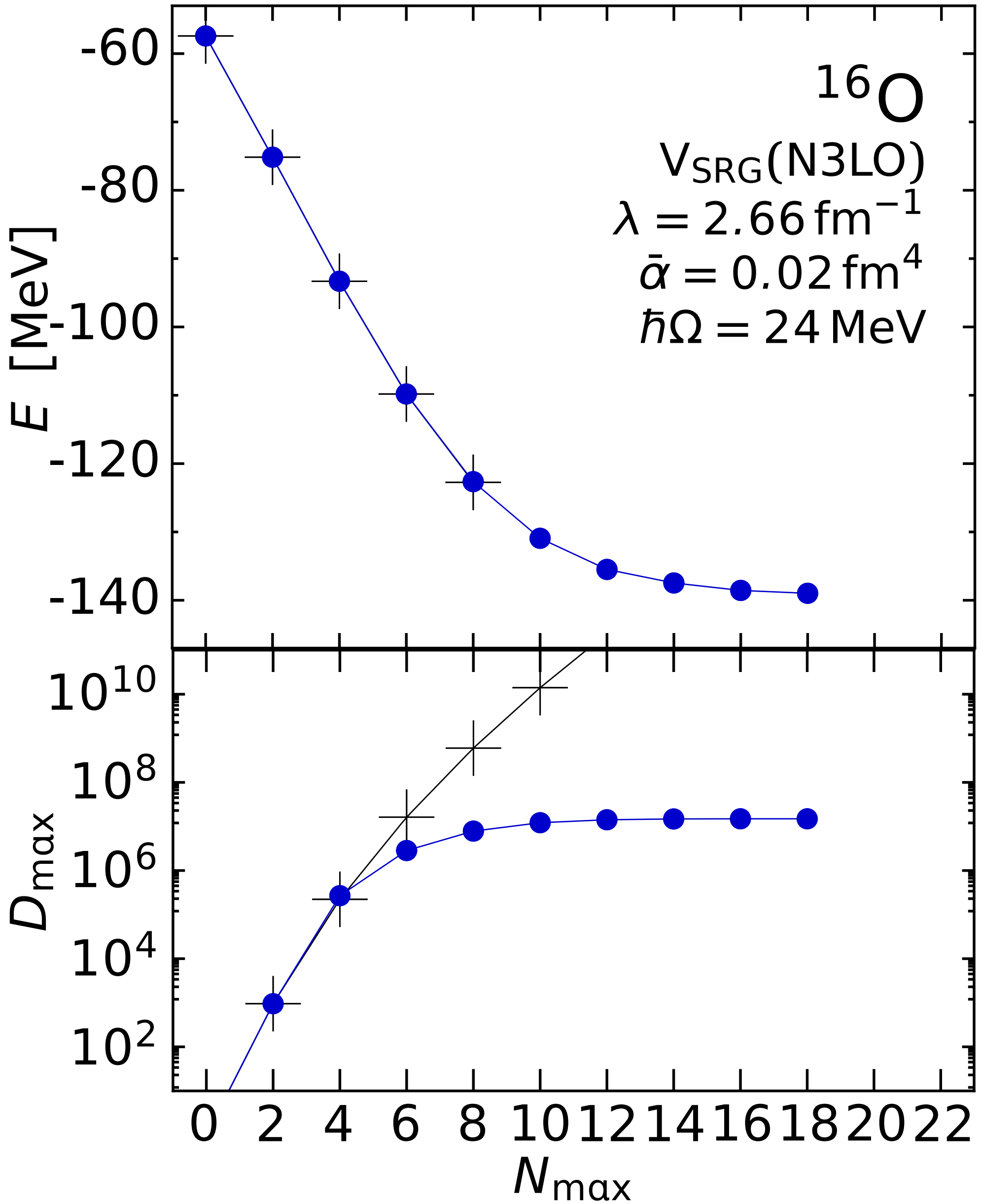
- extrapolation $N_{max} \to \infty$ using five consecutive points

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), $C_{min} = 0.0003$

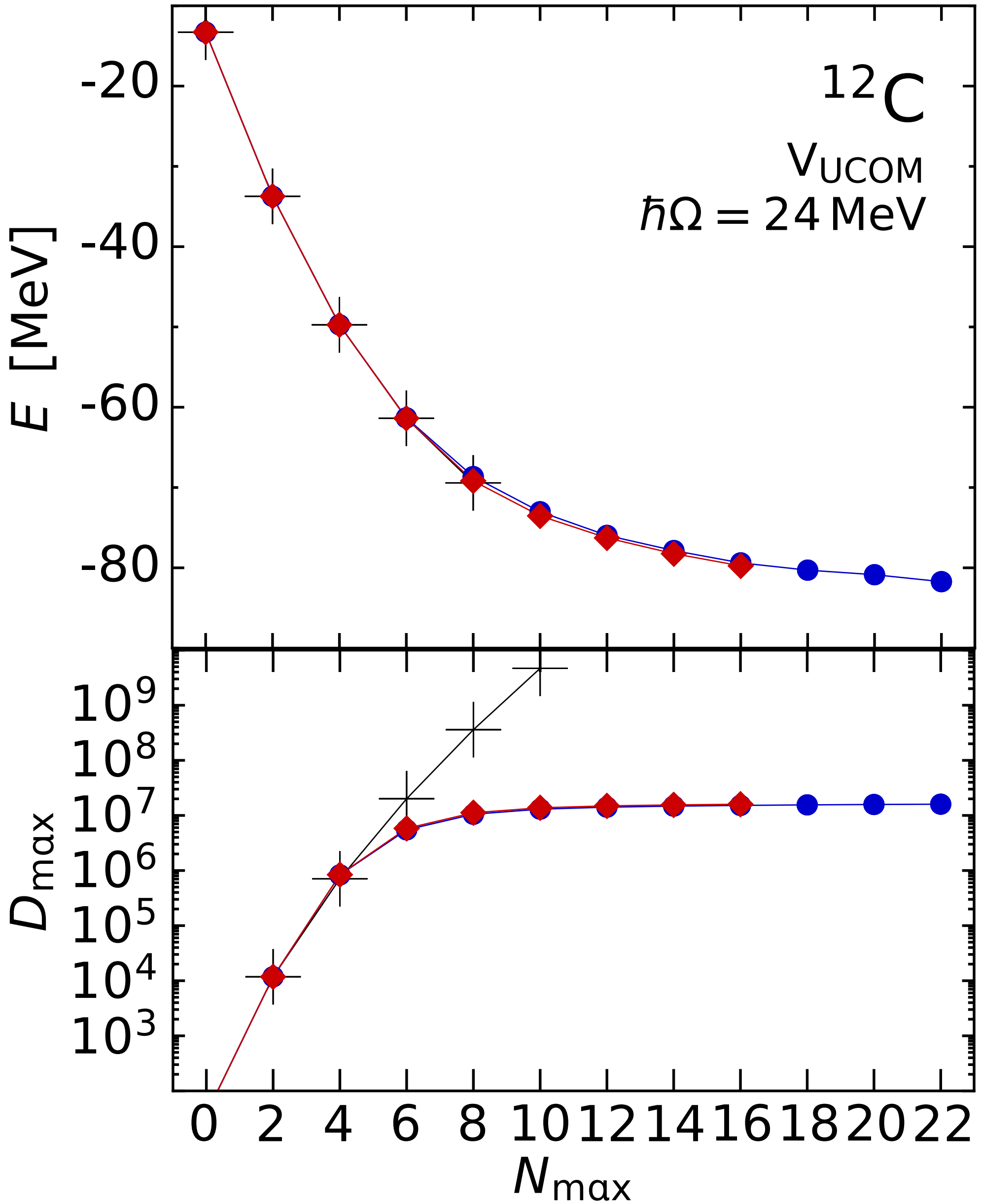
^{16}O: Importance-Truncated NCSM



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

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

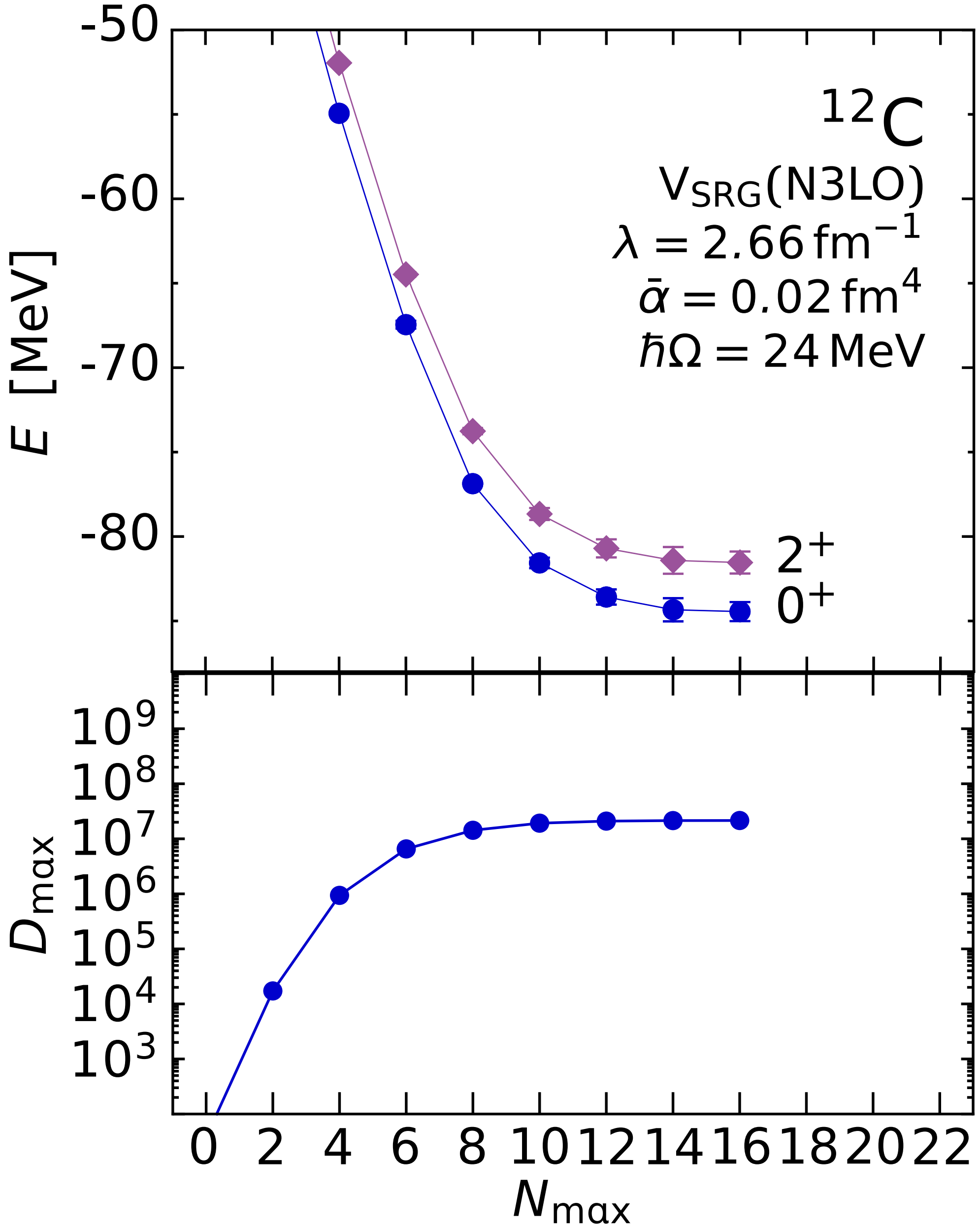
^{12}C: IT-NCSM for Open-Shell Nuclei



- **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), $C_{min} = 0.0003$

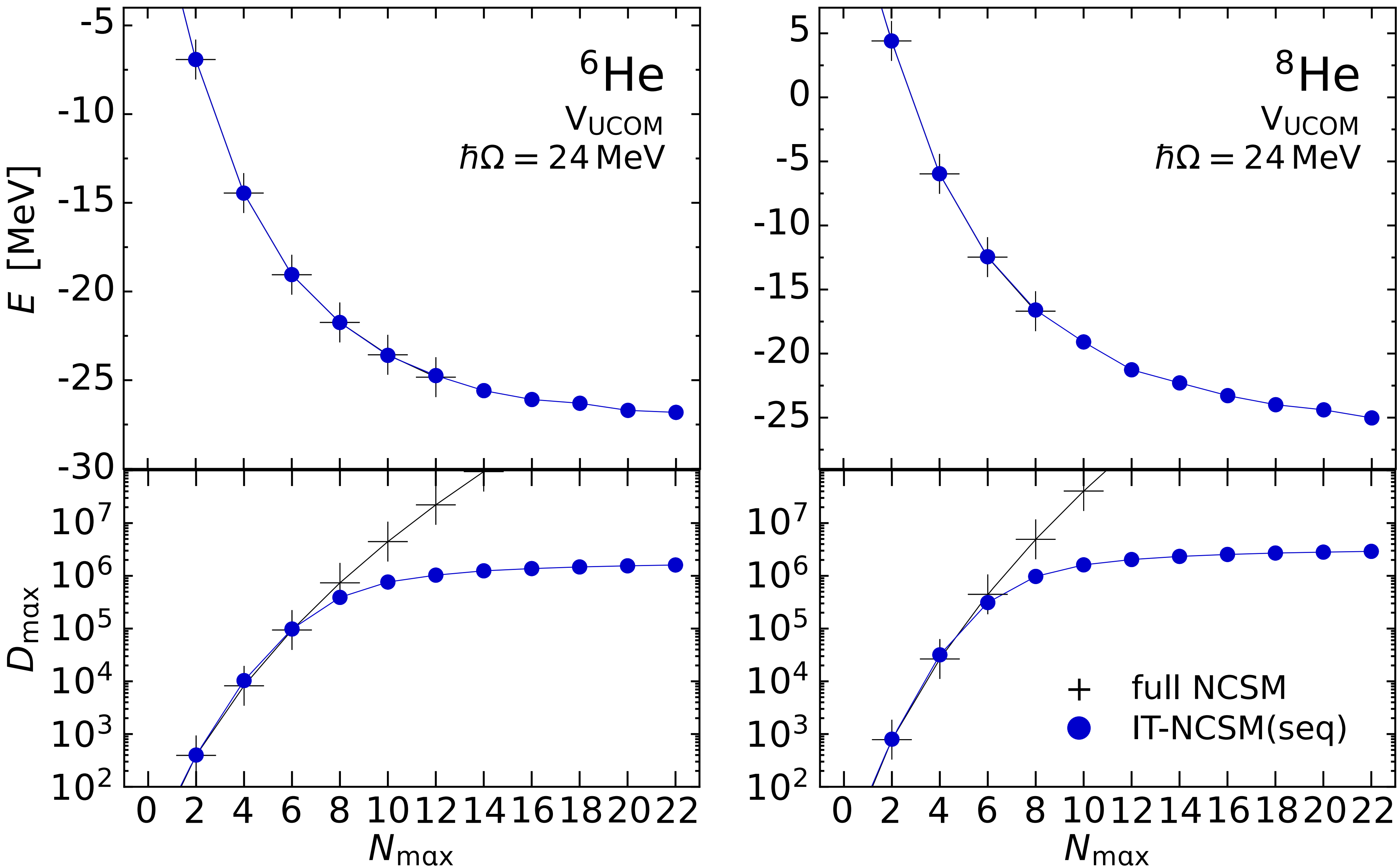
^{12}C: IT-NCSM for Excited States



- **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), $C_{min} = 0.0005$

^{6}He & ^{8}He: 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 $N_{\mathrm{max}}\hbar\Omega$ space
- ✔ constrained **threshold extrapolation** $\kappa_{\mathrm{min}} \to 0$ 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**: 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 *npnh* 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**
  - 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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