Ab-Initio Nuclear Structure beyond the p-Shell:

Interactions and Many-Body Techniques

Robert Roth
Institut für Kernphysik

TECHNISCHE UNIVERSITÄT DARMSTADT

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

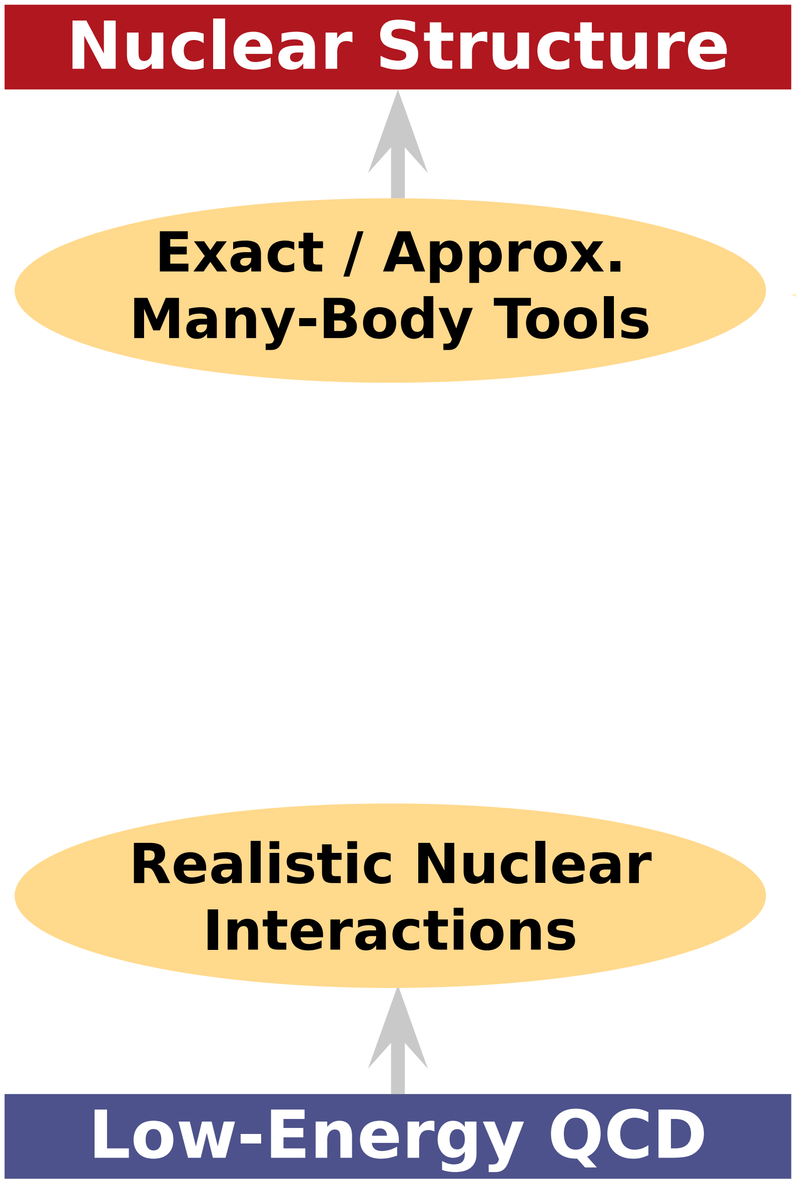
Nuclear Structure

Realistic Nuclear Interactions

Low-Energy QCD

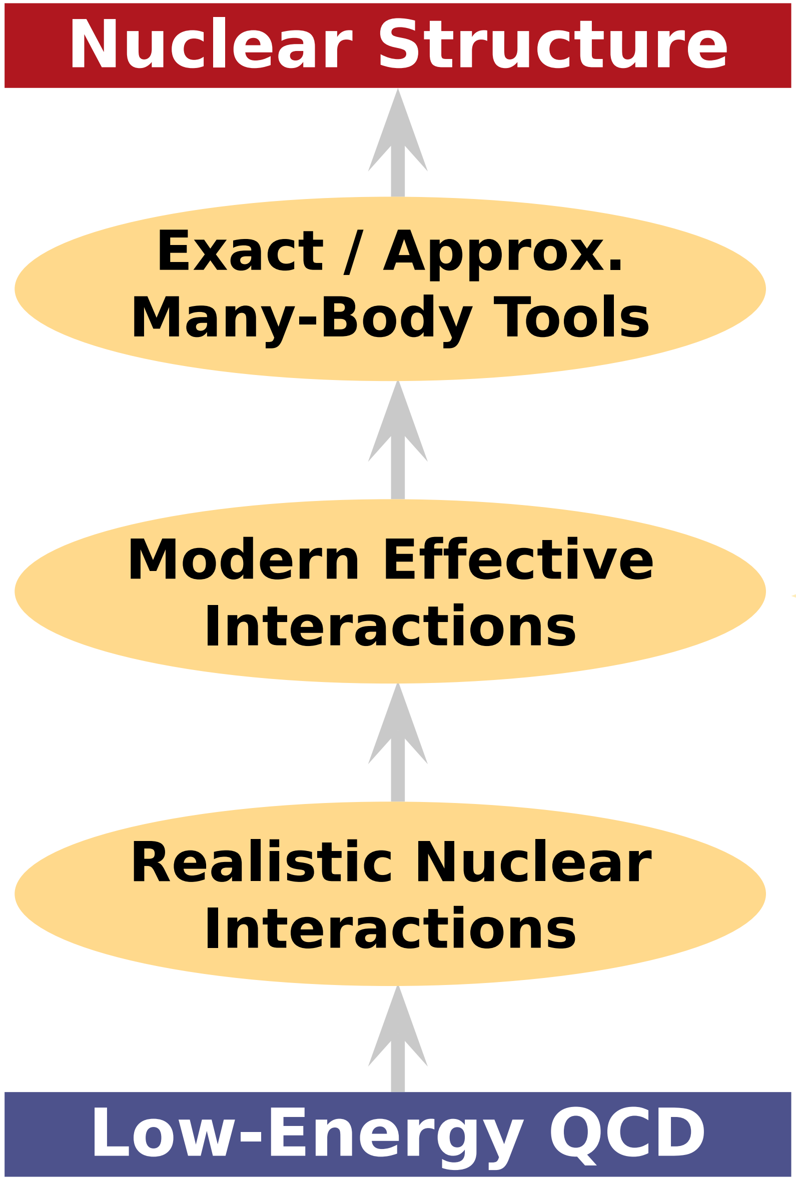
- chiral EFT interactions: consistent NN & 3N interaction derived within χEFT
- traditional NN-interactions: Argonne V18, CD Bonn,...
- reproduce experimental two-body data with high precision
- induce strong short-range central & tensor correlations

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



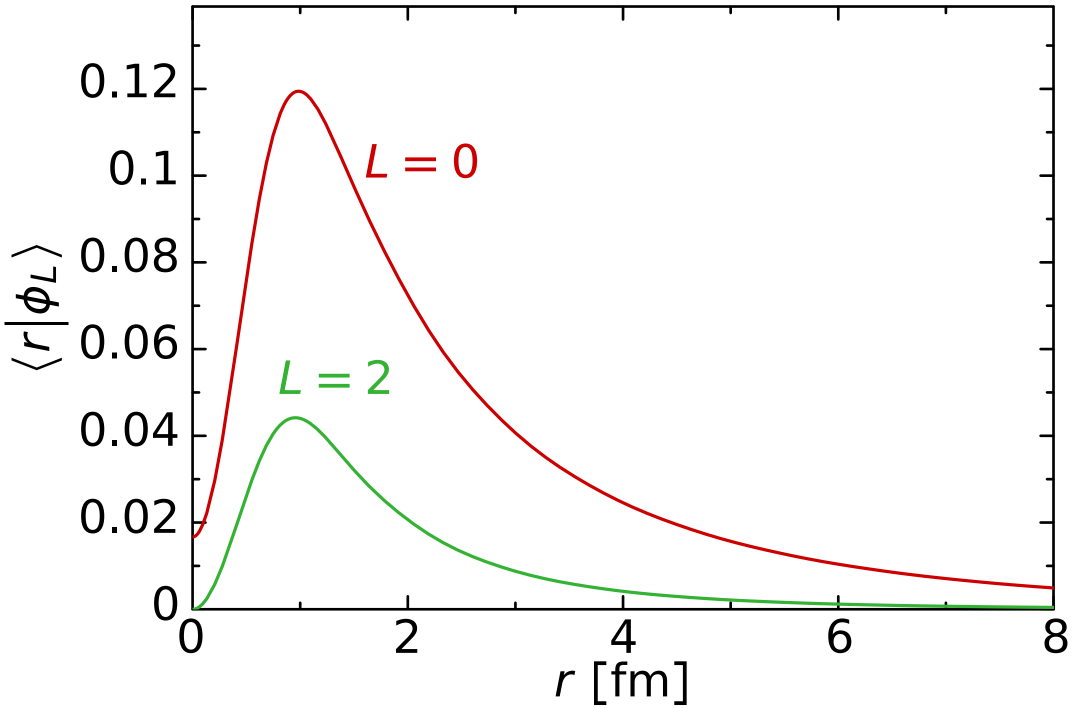
- adapt realistic potential to the available model space
  - tame short-range correlations
  - improve convergence behavior
- conserve experimentally constrained properties (phase shifts & deuteron)
  - generate new realistic int.
- need consistent effective interaction & effective operators
- unitary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

Unitarily Transformed Interactions

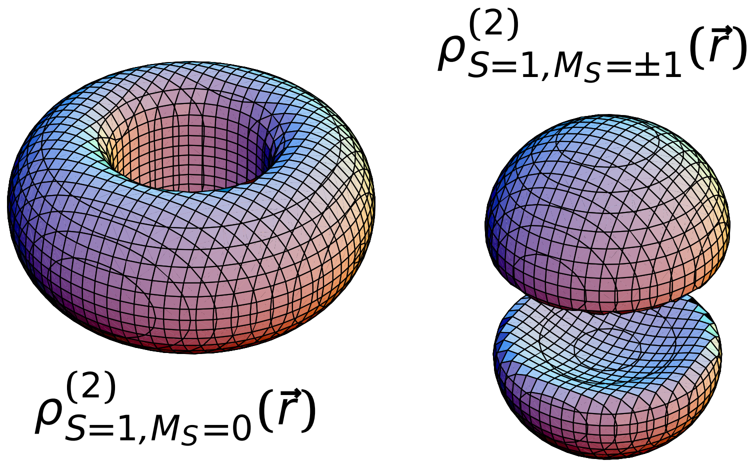
Unitary Correlation Operator Method (UCOM)

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

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

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

Tensor Correlator C_Ω

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

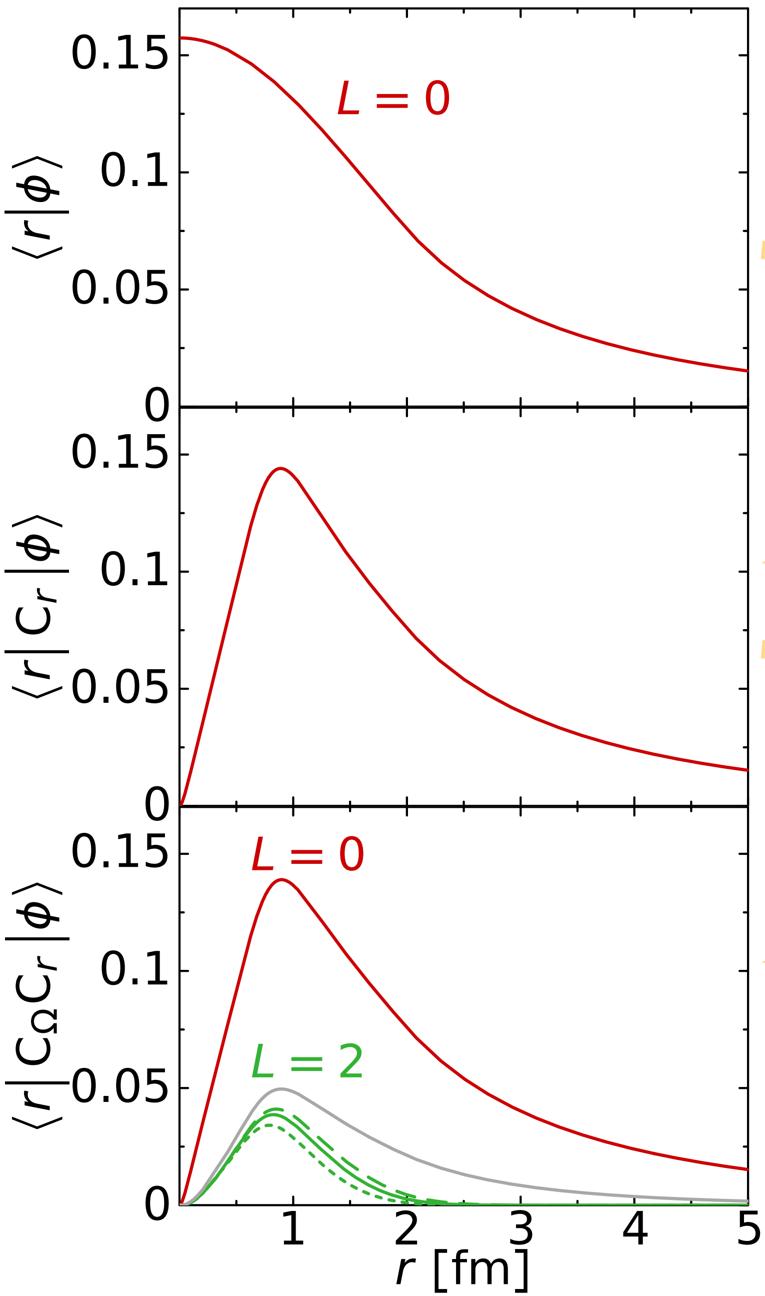
$$g_\Omega = \frac{3}{2}\vartheta(r)\big[(\vec{\sigma}_1\cdot\vec{q}_\Omega)(\vec{\sigma}_2\cdot\vec{r}) + (\vec{r}\leftrightarrow\vec{q}_\Omega)\big]$$

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

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

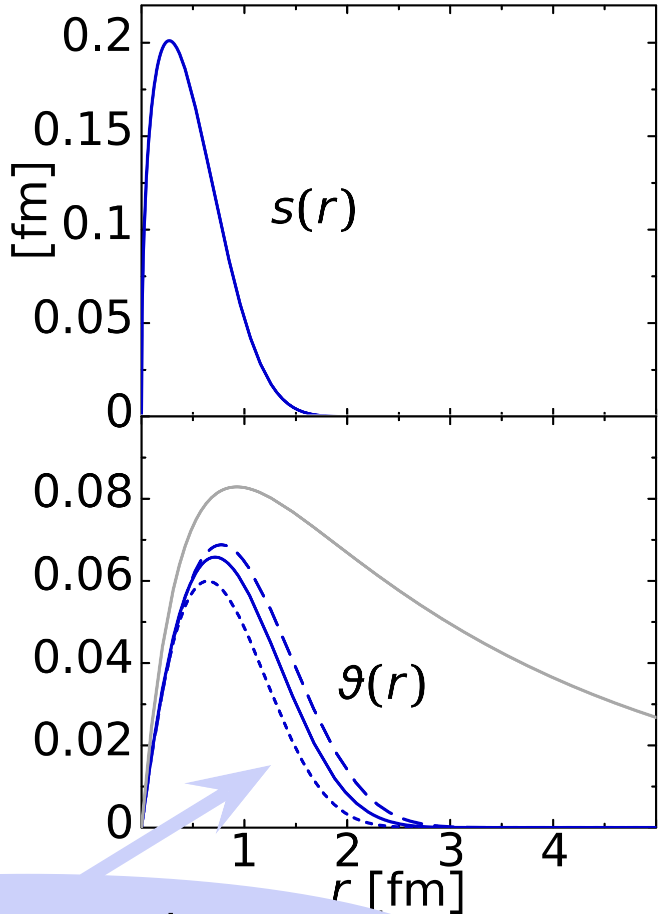
- $s(r)$ and $\vartheta(r)$ depend on & are optimized for initial potential

Correlated States: The Deuteron



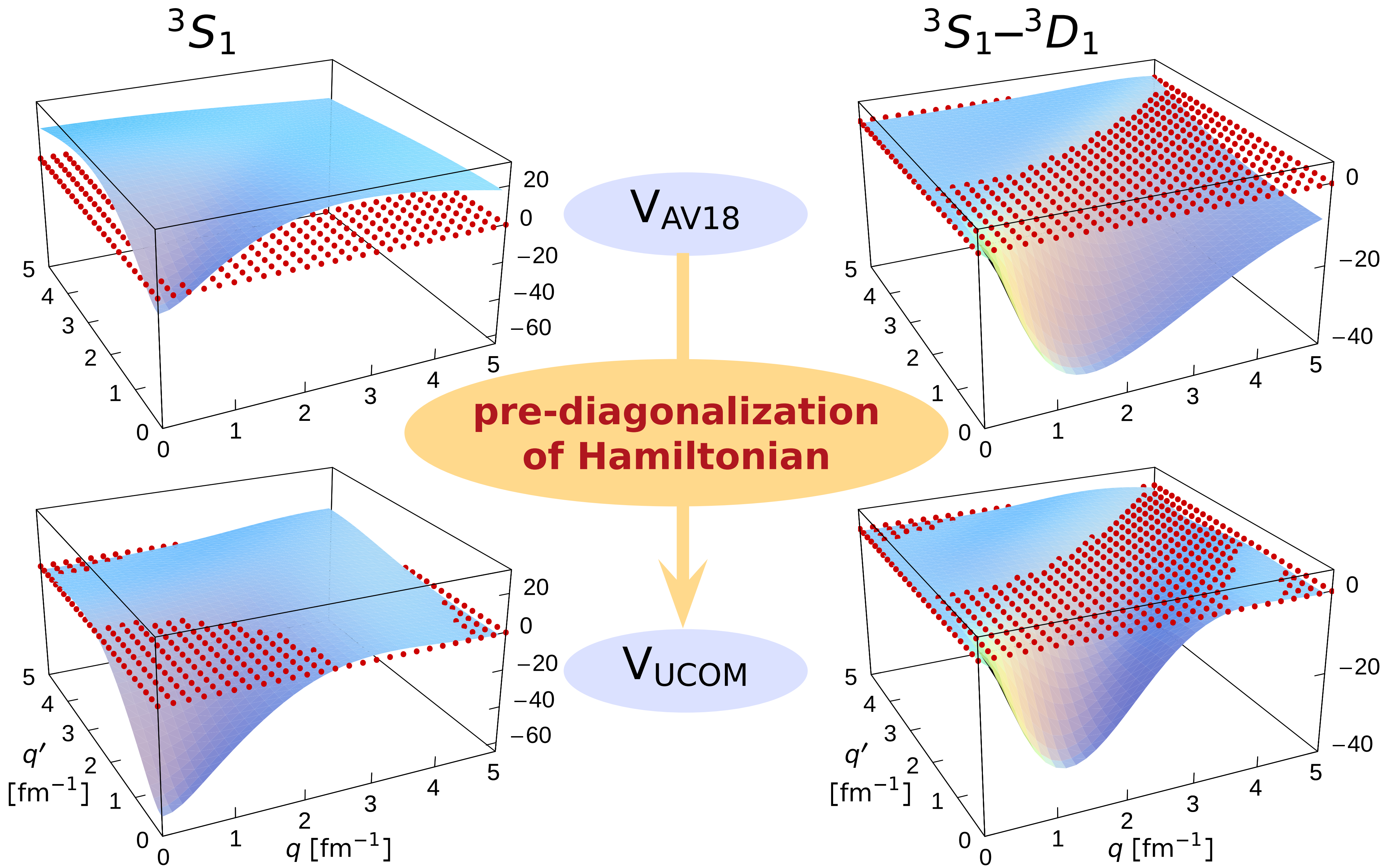
central correlations

tensor correlations



only short-range tensor correlations treated by C_Ω

Correlated Interaction: V_{UCOM}



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

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

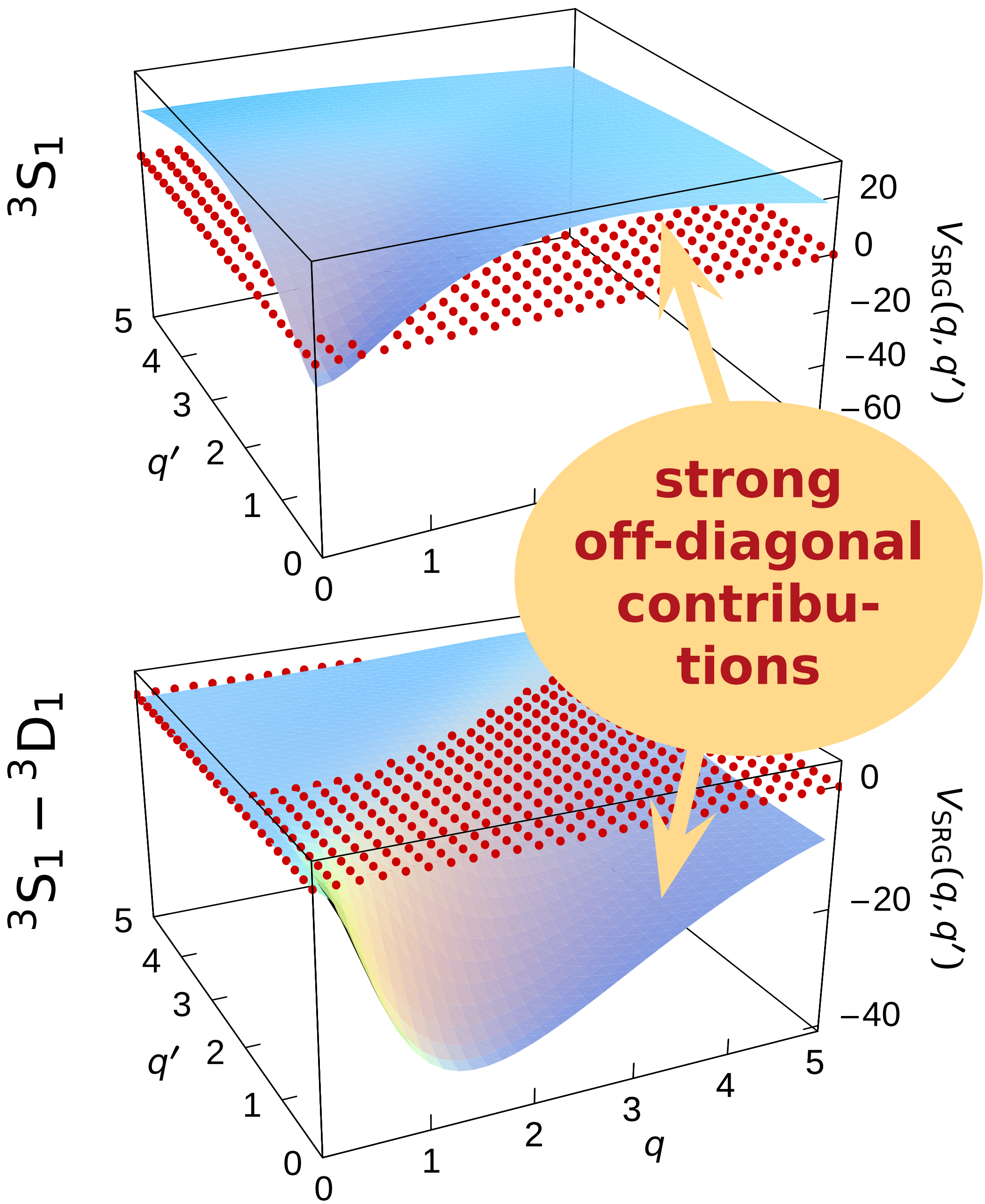
- dynamical generator defined as commutator with the operator in whose eigenbasis H shall be diagonalized

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

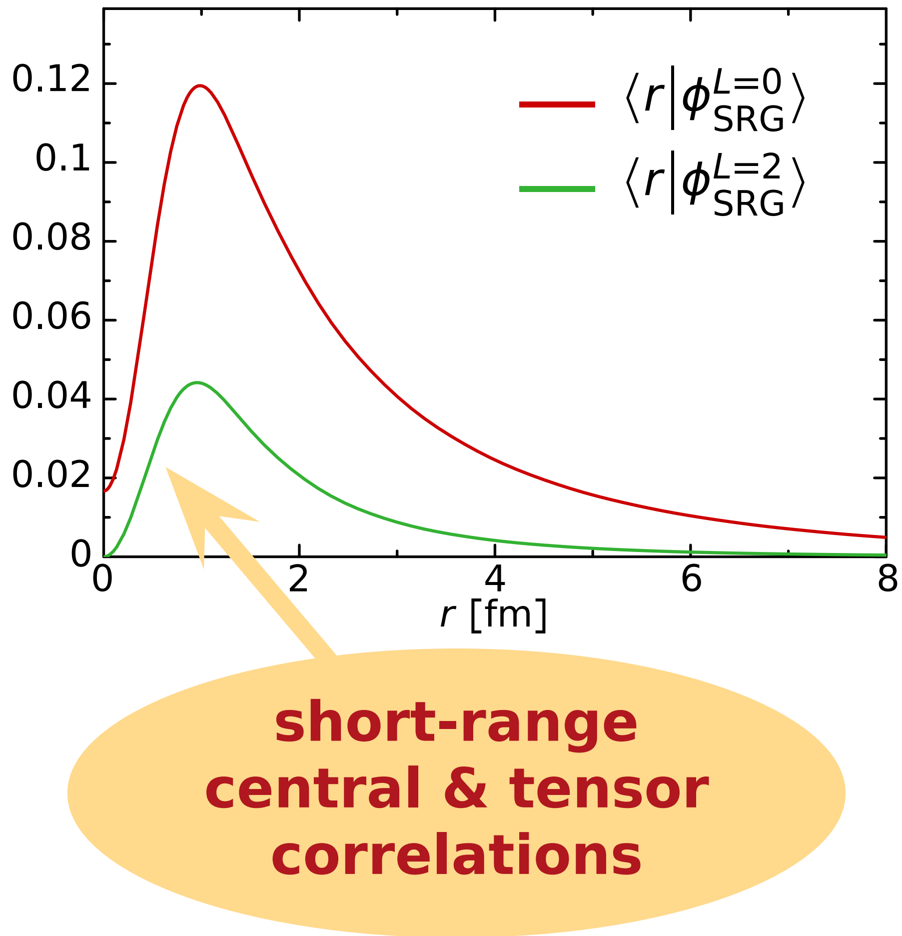
UCOM vs. SRG

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

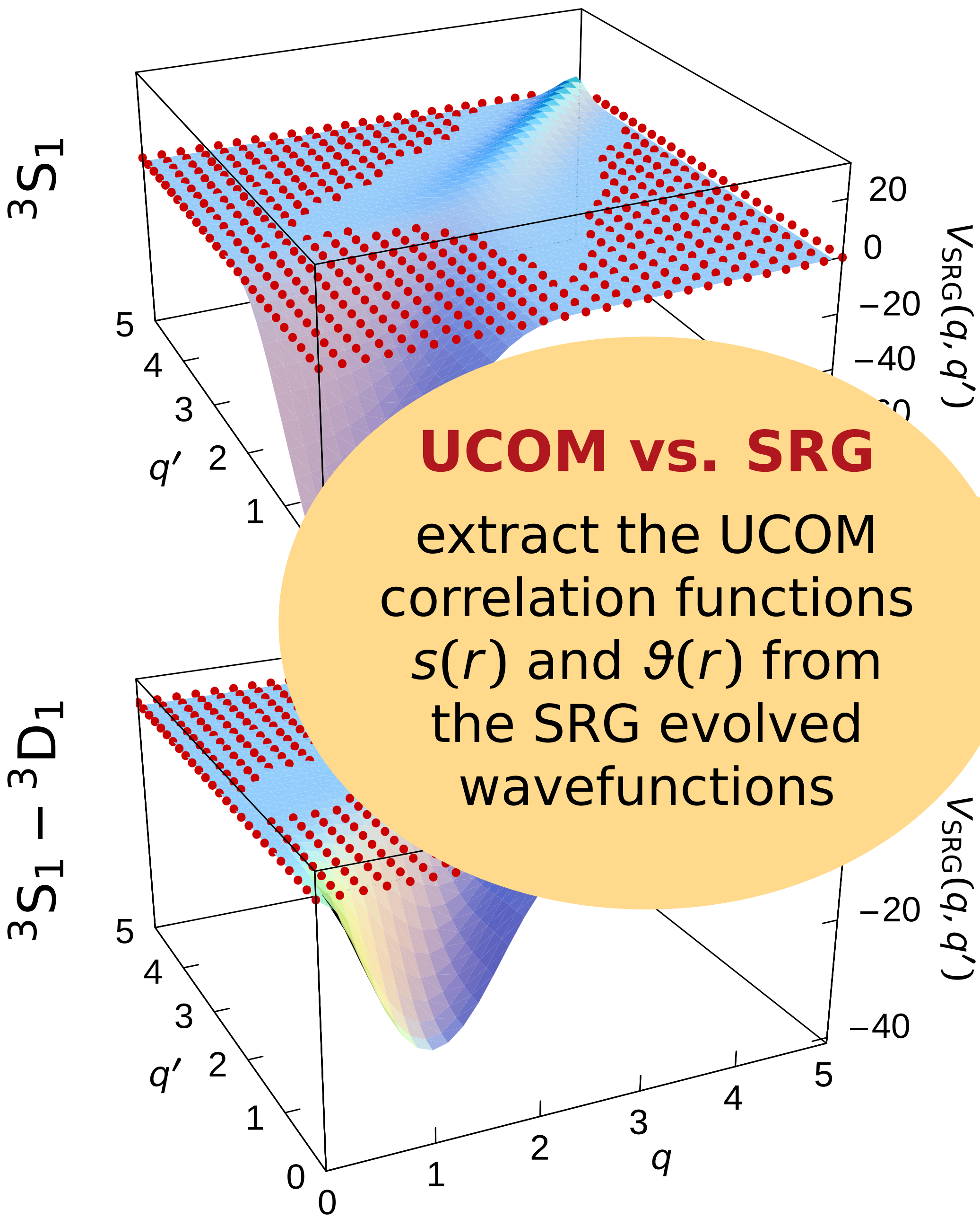
SRG Evolution: The Deuteron



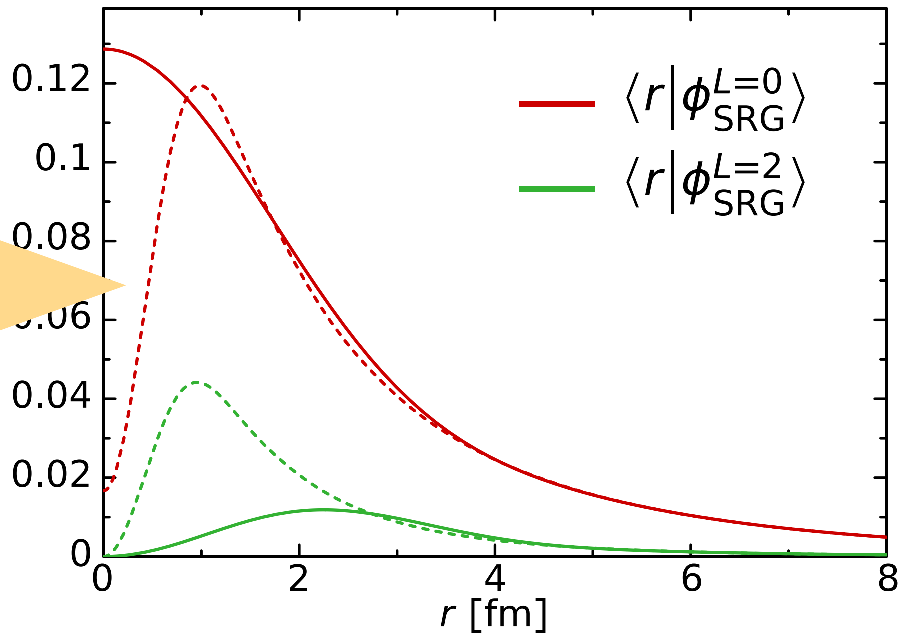
Argonne V18



SRG Evolution: The Deuteron



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



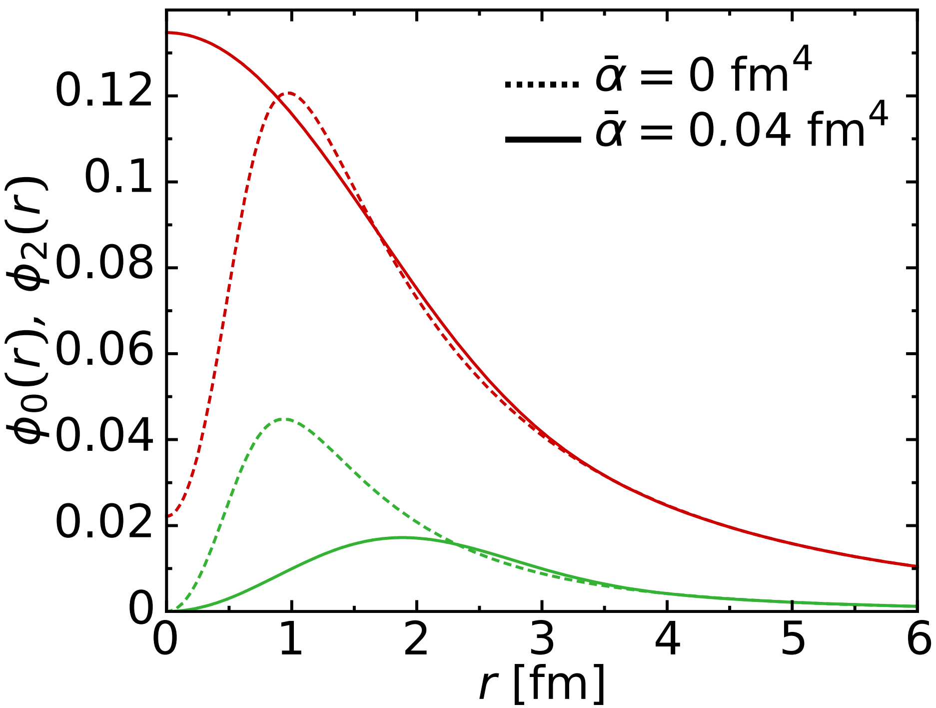
UCOM vs. SRG

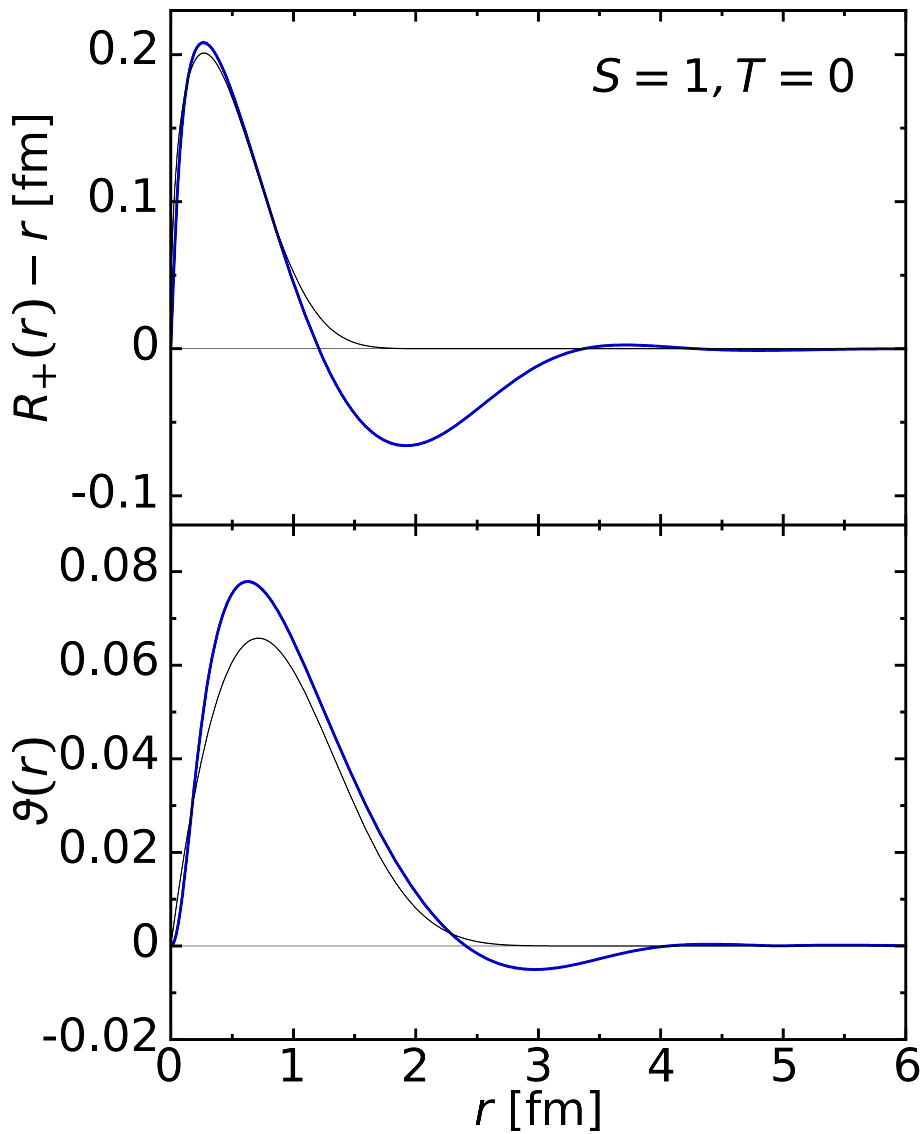
extract the UCOM correlation functions $s(r)$ and $\vartheta(r)$ from the SRG evolved wavefunctions

SRG-Generated UCOM Correlators: AV18

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

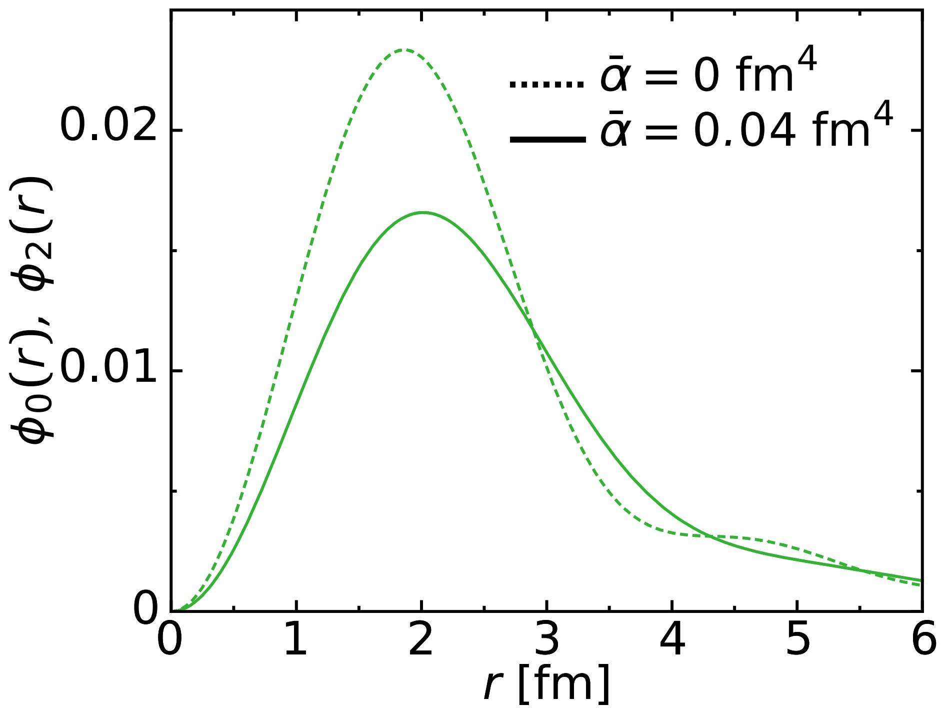
$$\left|\Phi_{\mathrm{SRG}}^{(0)}\right\rangle \stackrel{!}{=} \mathrm{C} \left|\Phi_{\mathrm{SRG}}^{(\bar{\alpha})}\right\rangle$$

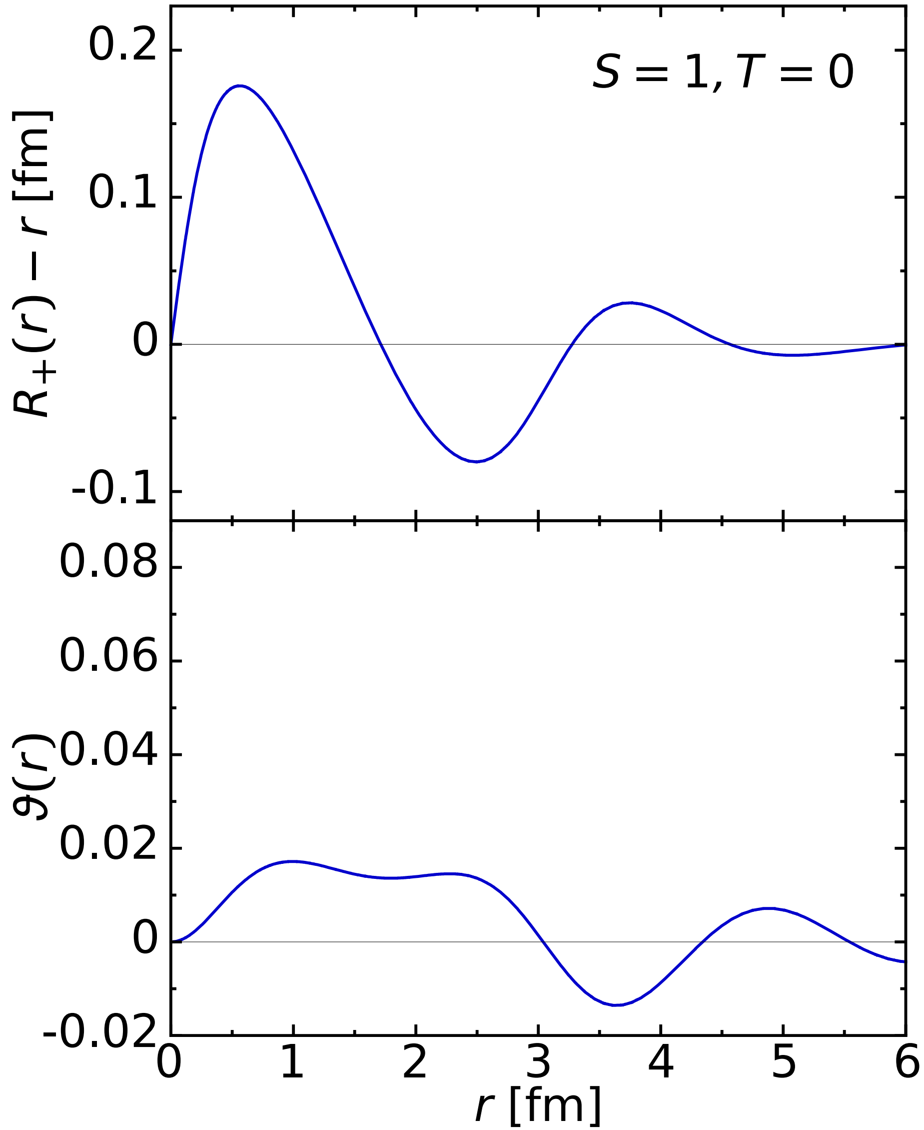




SRG-Generated UCOM Correlators: N3LO

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



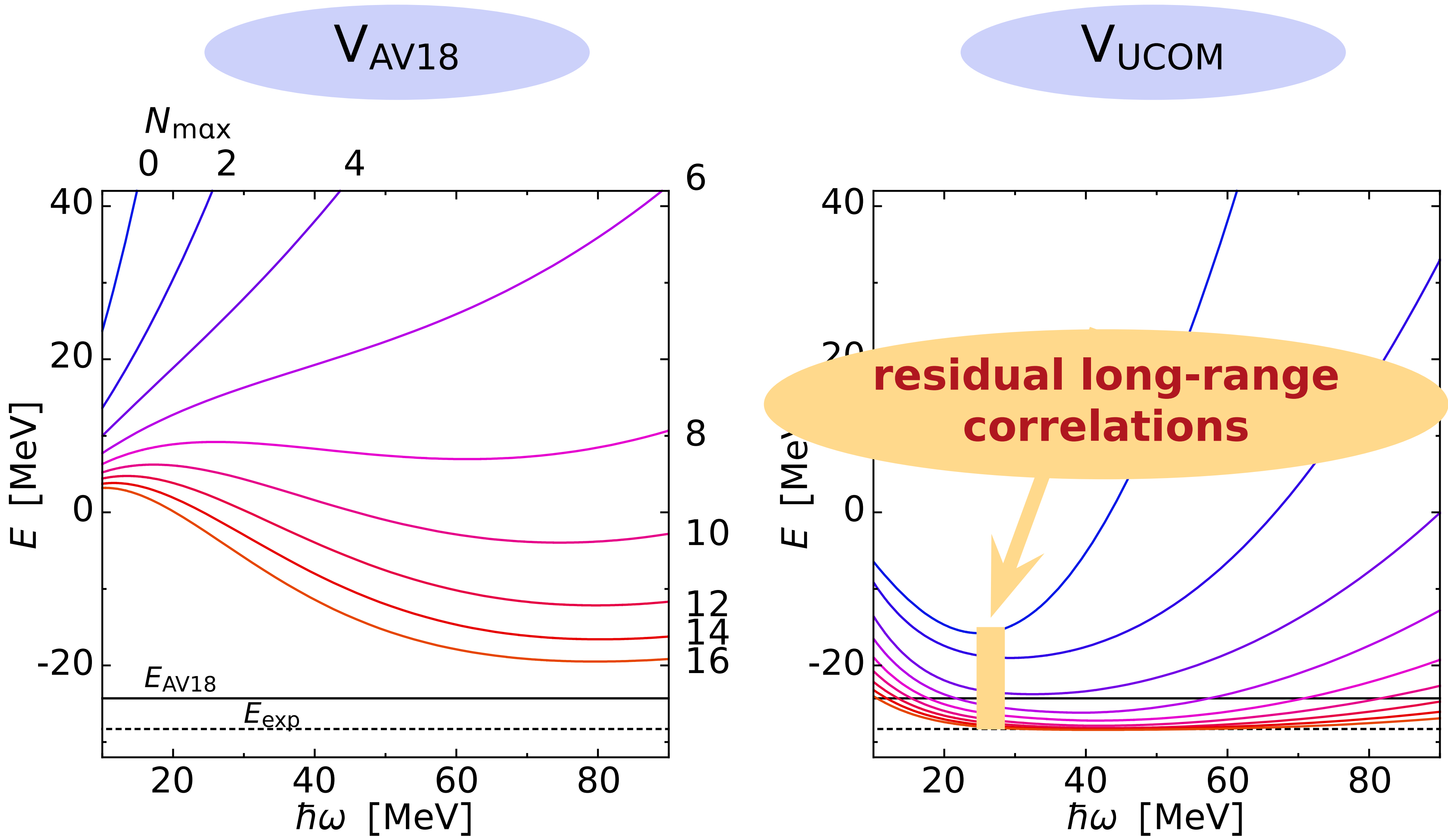


Computational Many-Body Methods

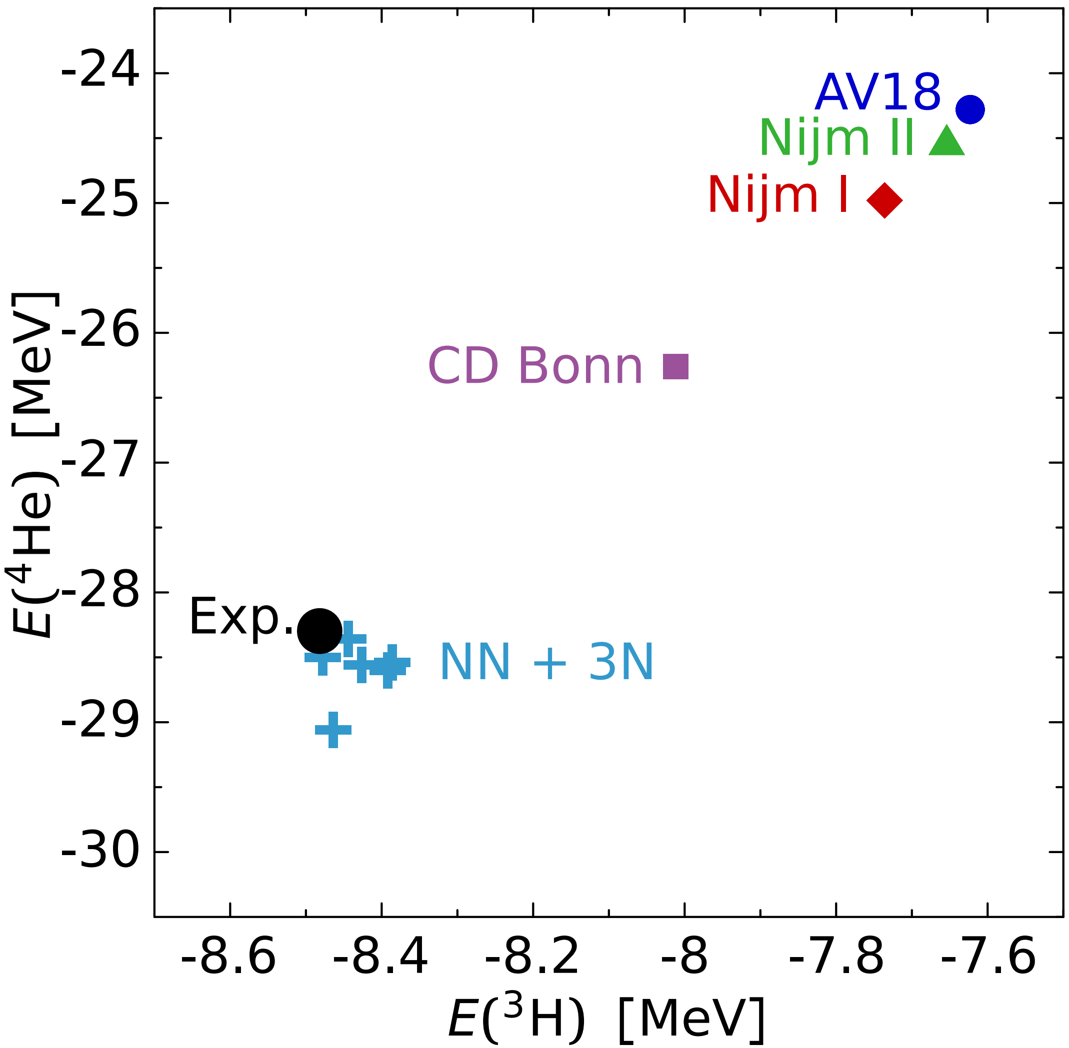
No-Core Shell Model

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

^{4}He: Convergence

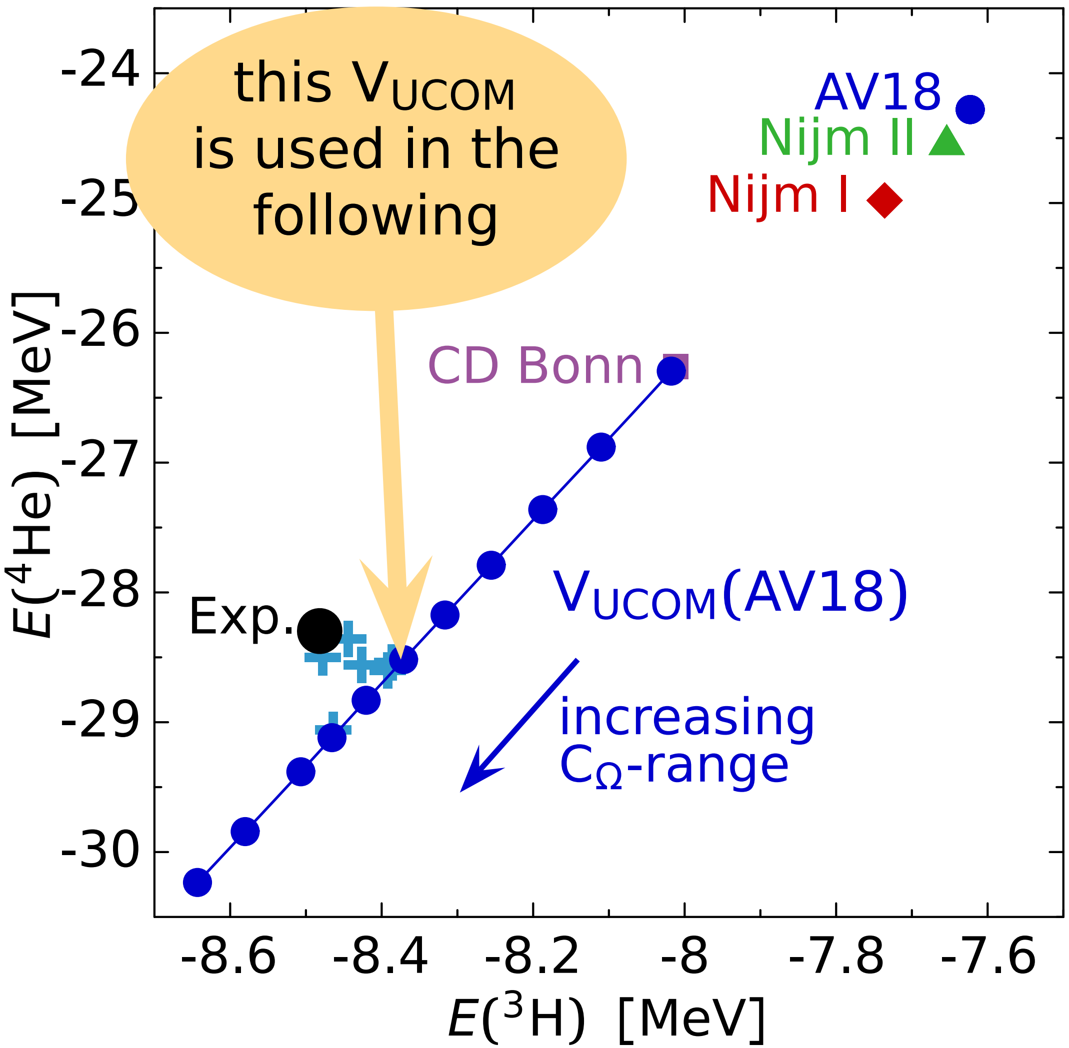


Tjon-Line and Correlator Range



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

Tjon-Line and Correlator Range



- **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

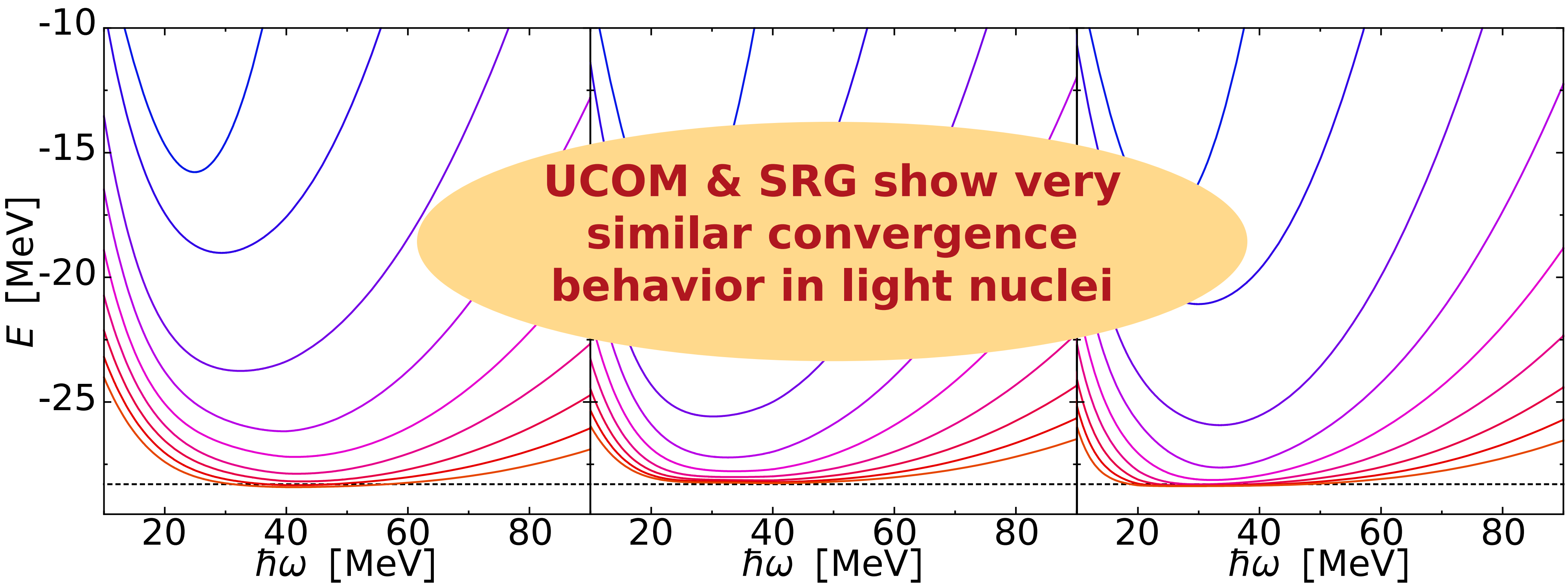
minimize net 3N interaction by choosing correlator close to experimental point

UCOM vs. SRG: ^{4}He Convergence

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

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

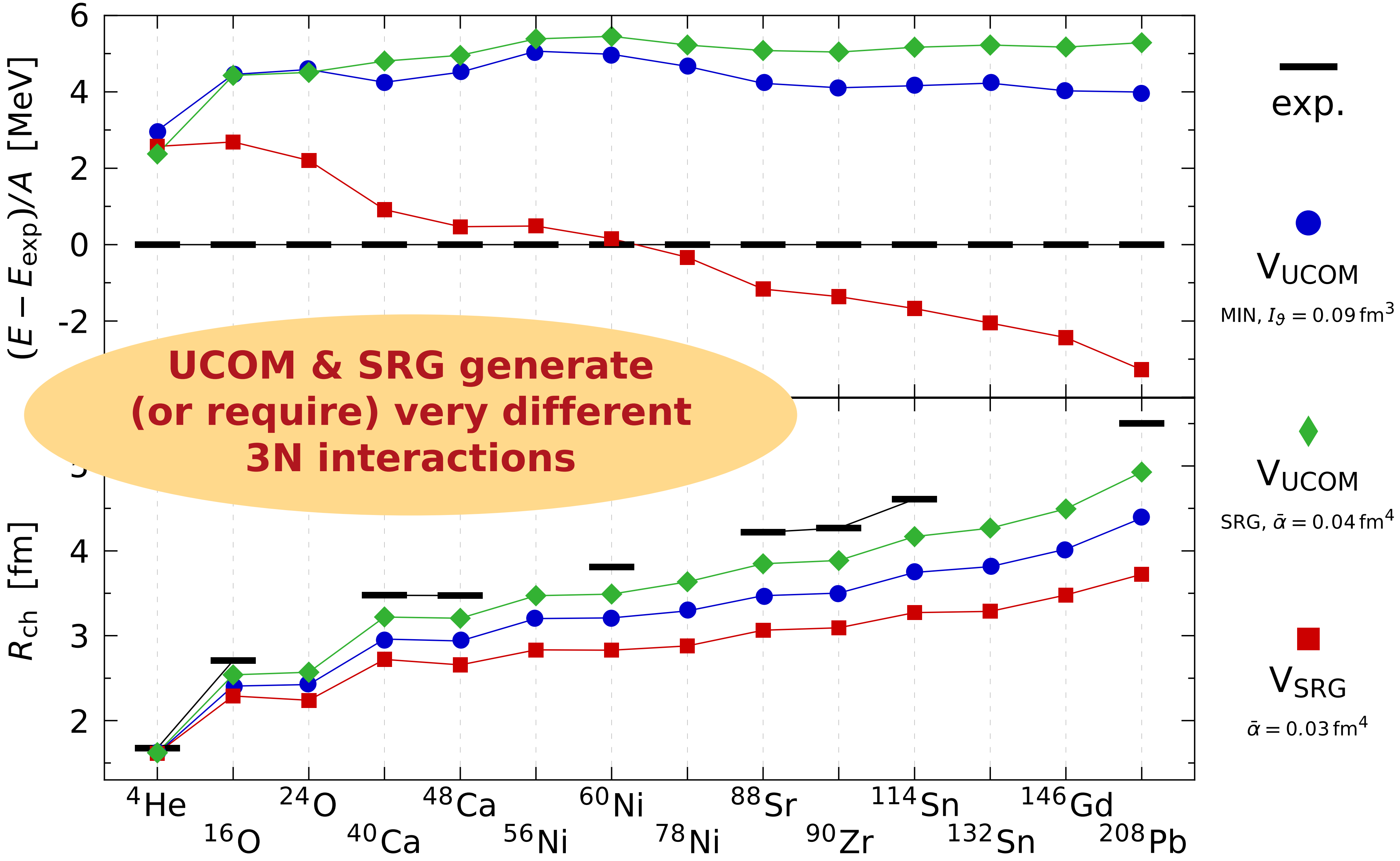
V_{SRG}
$\bar{\alpha} = 0.03\,\text{fm}^4$



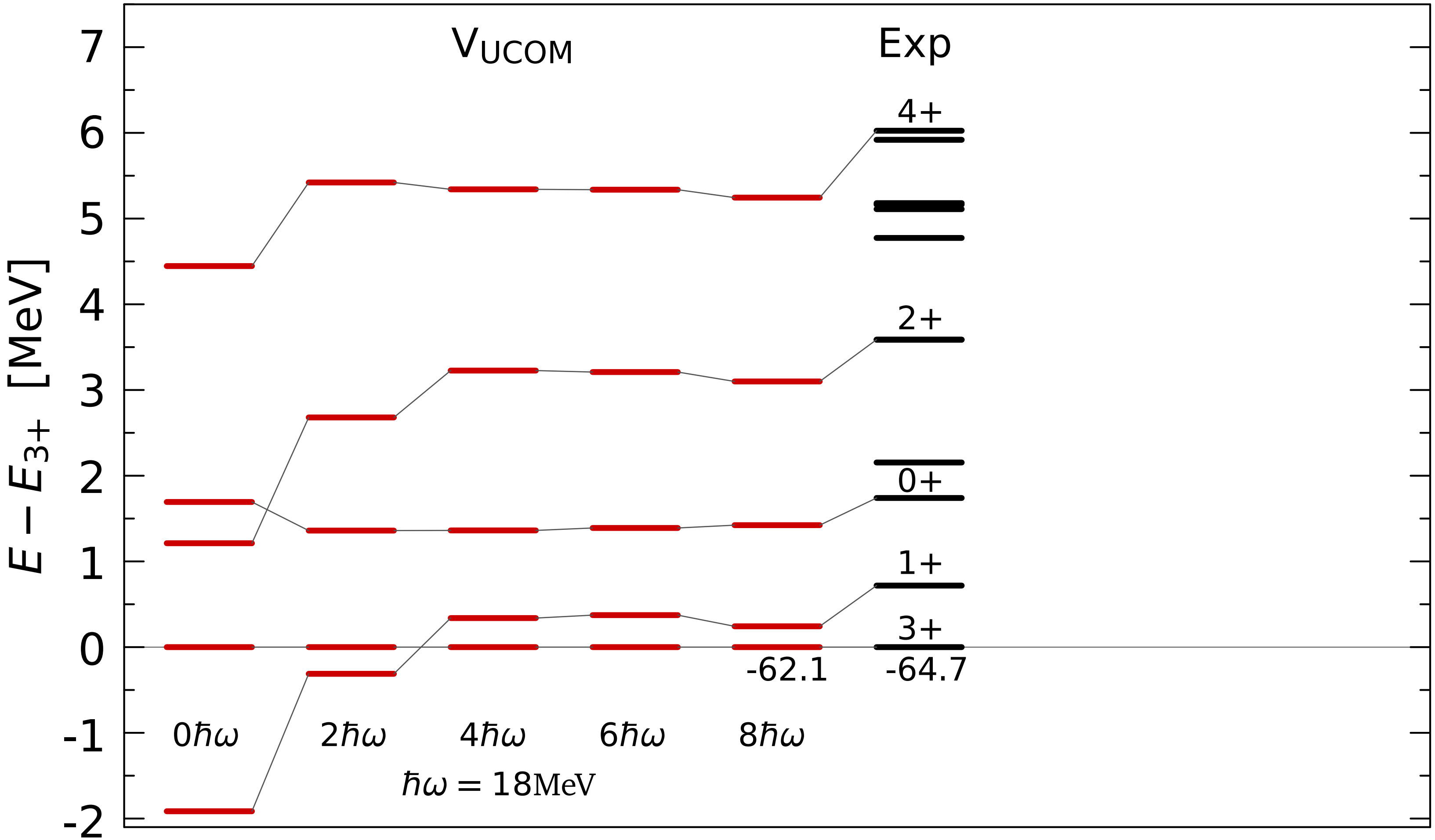
UCOM & SRG show very similar convergence behavior in light nuclei

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

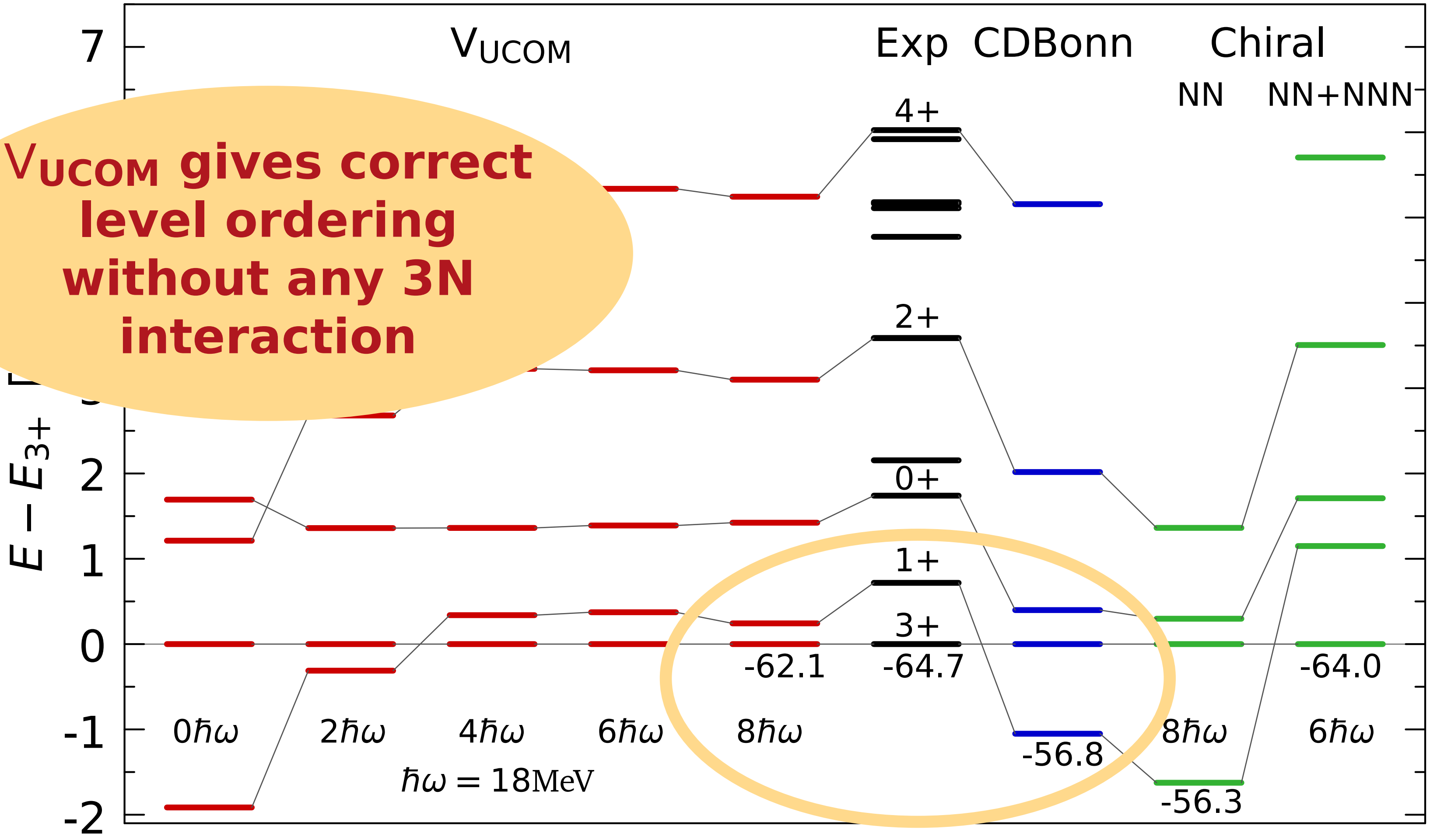
UCOM vs. SRG: Hartree-Fock Systematics



^{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

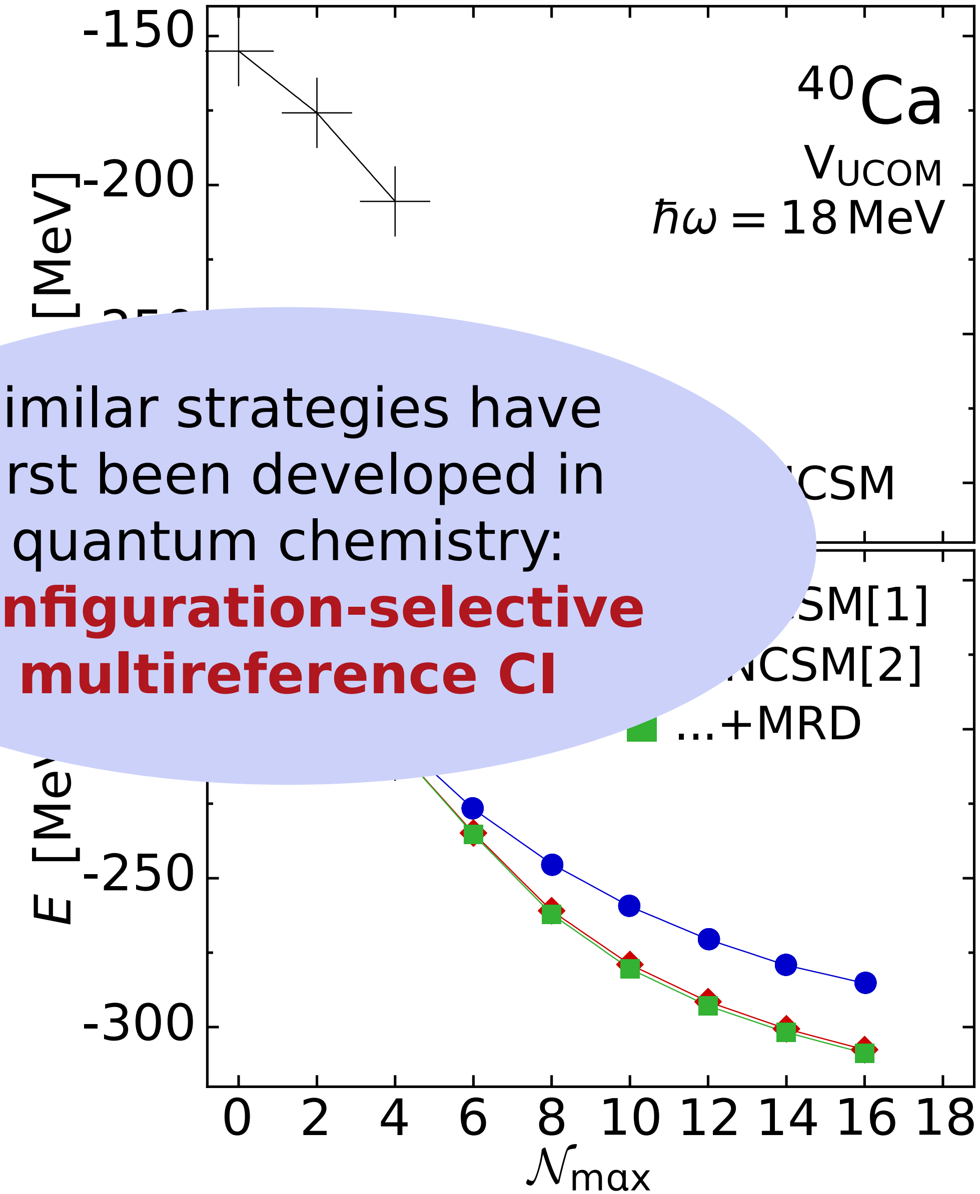
Roth & Navrátil — Phys. Rev. Lett. 99, 092501 (2007)

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** 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

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

- 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

Iterative Scheme: IT-NCSM[i]

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

- simple **iterative construction** of importance truncated model space:

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

  ❶ construct model space of states with $|\kappa_\nu| \geq \kappa_{\min}$

  ❷ solve eigenvalue problem

  ❸ use dominant components of eigenstate as new $|\Psi_{\text{ref}}\rangle$, goto ❶

- **need $n/2$ iterations** to recover full space with $npnp$ excitations in the limit $\kappa_{\min} \to 0$

Sequential Scheme: IT-NCSM(seq)

- **special property of $N_{\max}\hbar\omega$ space**: step from $N_{\max}$ to $N_{\max}+2$ requires 2p2h excitations at most
  - combine importance update with increase of $N_{\max}$ by 2

- **sequential calculation** for set of $N_{\max}\hbar\omega$ spaces:

  ✪ complete NCSM calculation for $N_{\max}=0$ or 2 to obtain $|\Psi_{\text{ref}}\rangle$

  ❶ construct importance-truncated space with $N_{\max}+2$ of states with $|\kappa_\nu| \geq \kappa_{\min}$

  ❷ solve eigenvalue problem

  ❸ use dominant components of eigenstate as new $|\Psi_{\text{ref}}\rangle$, goto ❶

- **only one importance update** for each value of $N_{\max}$ needed to recover full space in the limit $\kappa_{\min} \to 0$

Threshold Extrapolation

- all calculations done for a **sequence of importance thresholds** ➔ $E(\kappa_{\min})$

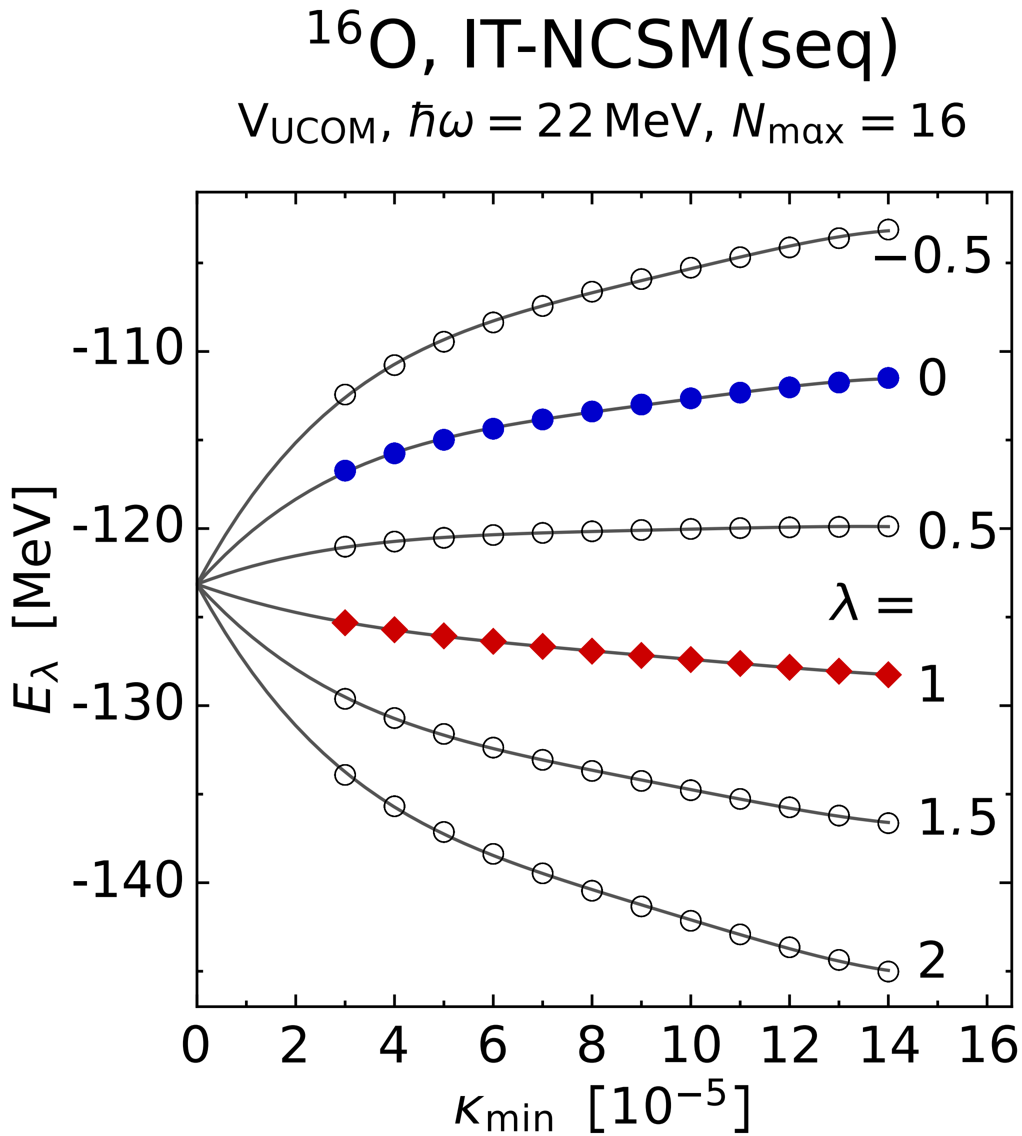
- contribution of **excluded states** estimated perturbatively ➔ $\Delta_{\text{excl}}(\kappa_{\min})$

- **simultaneous extrapolation** of combined energy

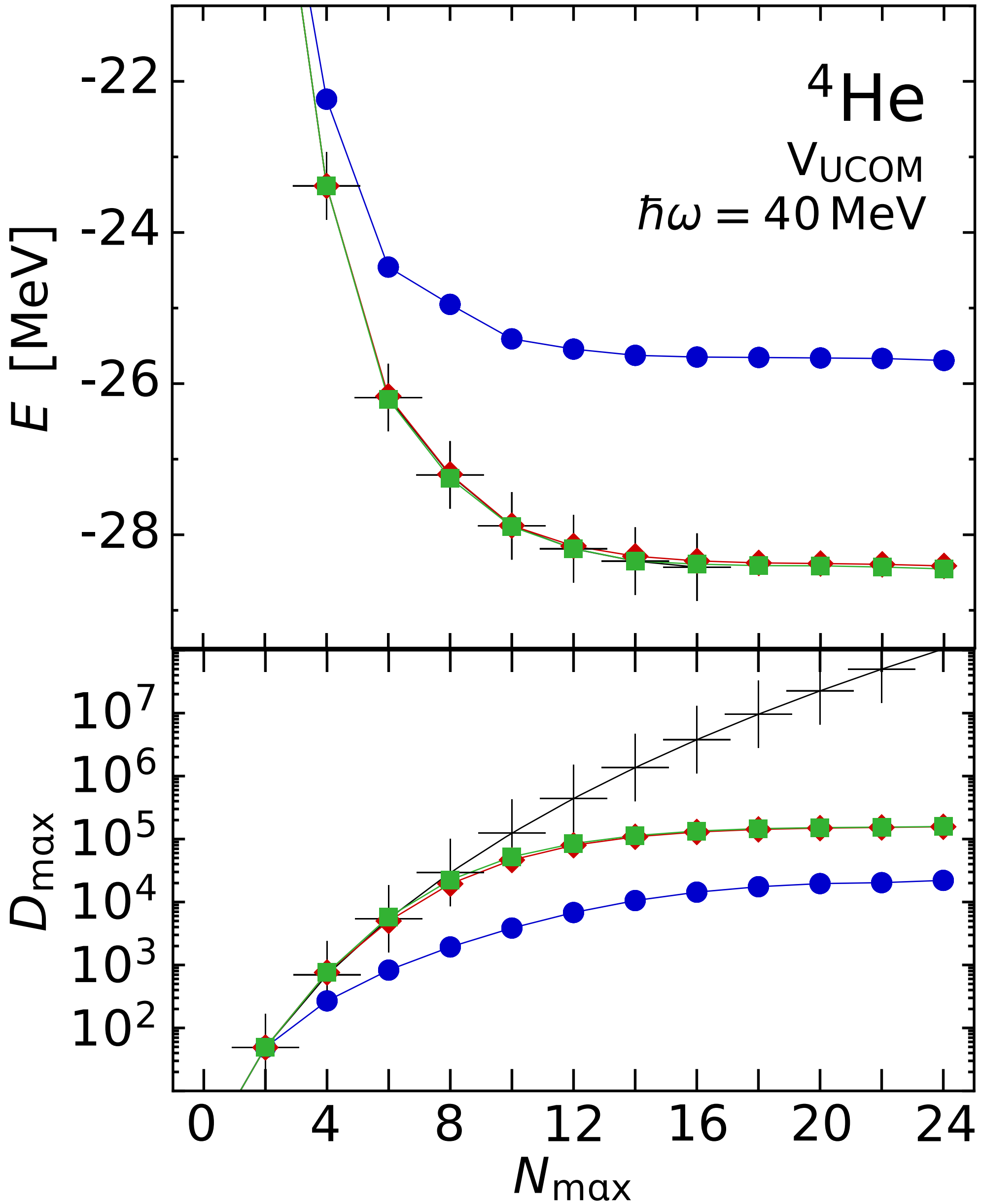
$$E_\lambda(\kappa_{\min}) = E(\kappa_{\min}) + \lambda\Delta_{\text{excl}}(\kappa_{\min})$$

  to $\kappa_{\min} = 0$ for set of λ-values

- all IT-NCSM energies shown are threshold extrapolated

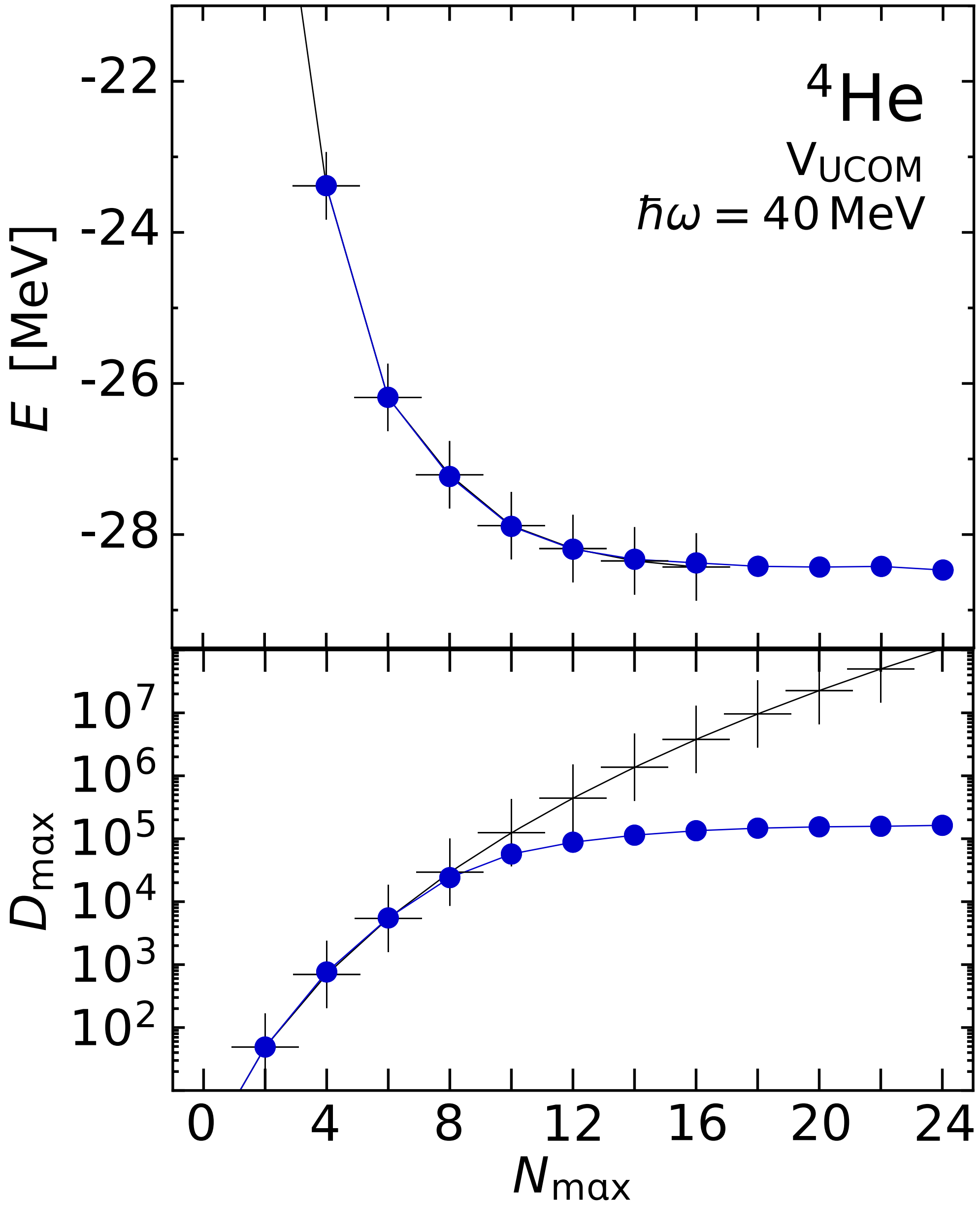


^{4}He: Importance-Truncated NCSM



- **iterative IT-NCSM(*i*)** 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

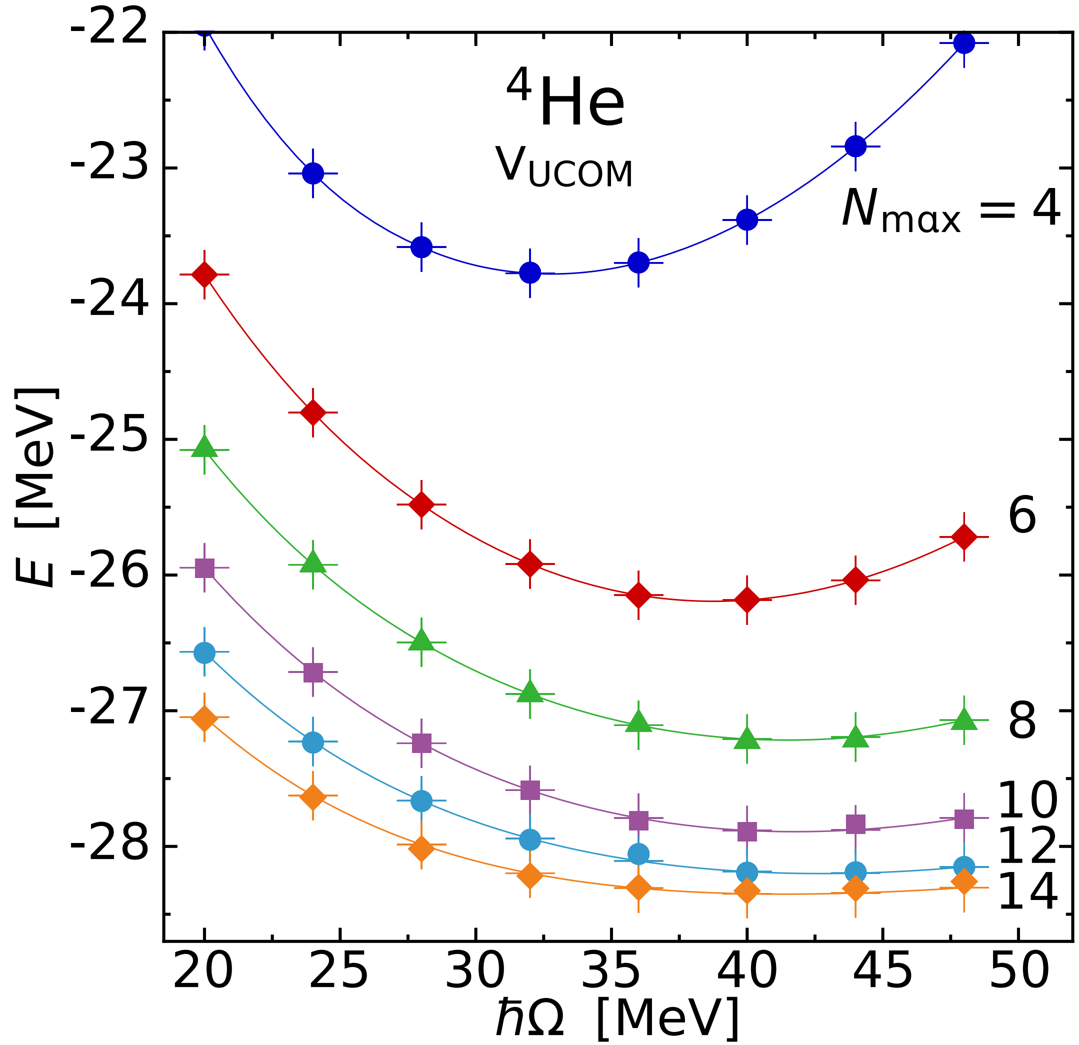
^{4}He: Importance-Truncated NCSM



- **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)

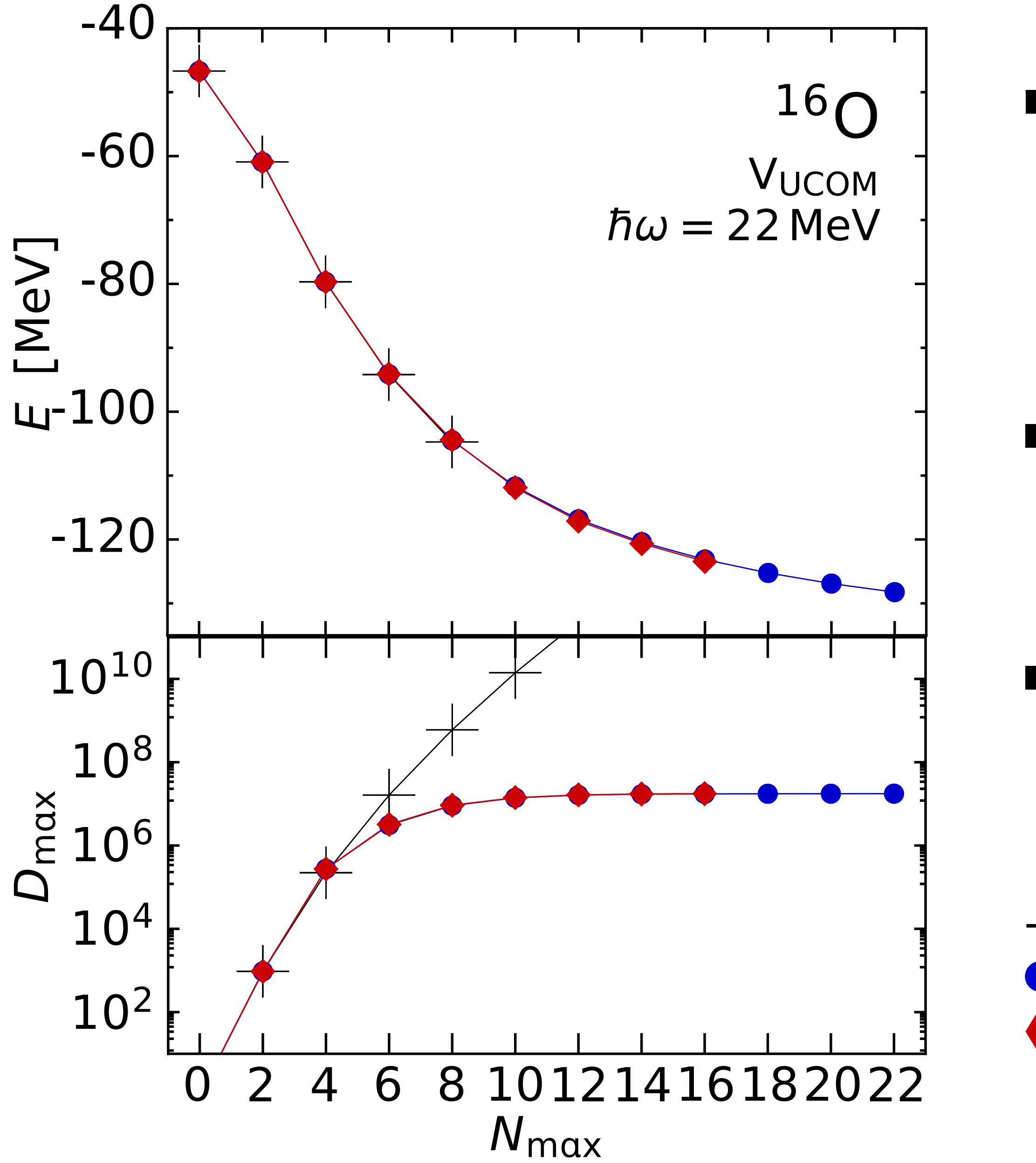
^{4}He: Importance-Truncated NCSM



- **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

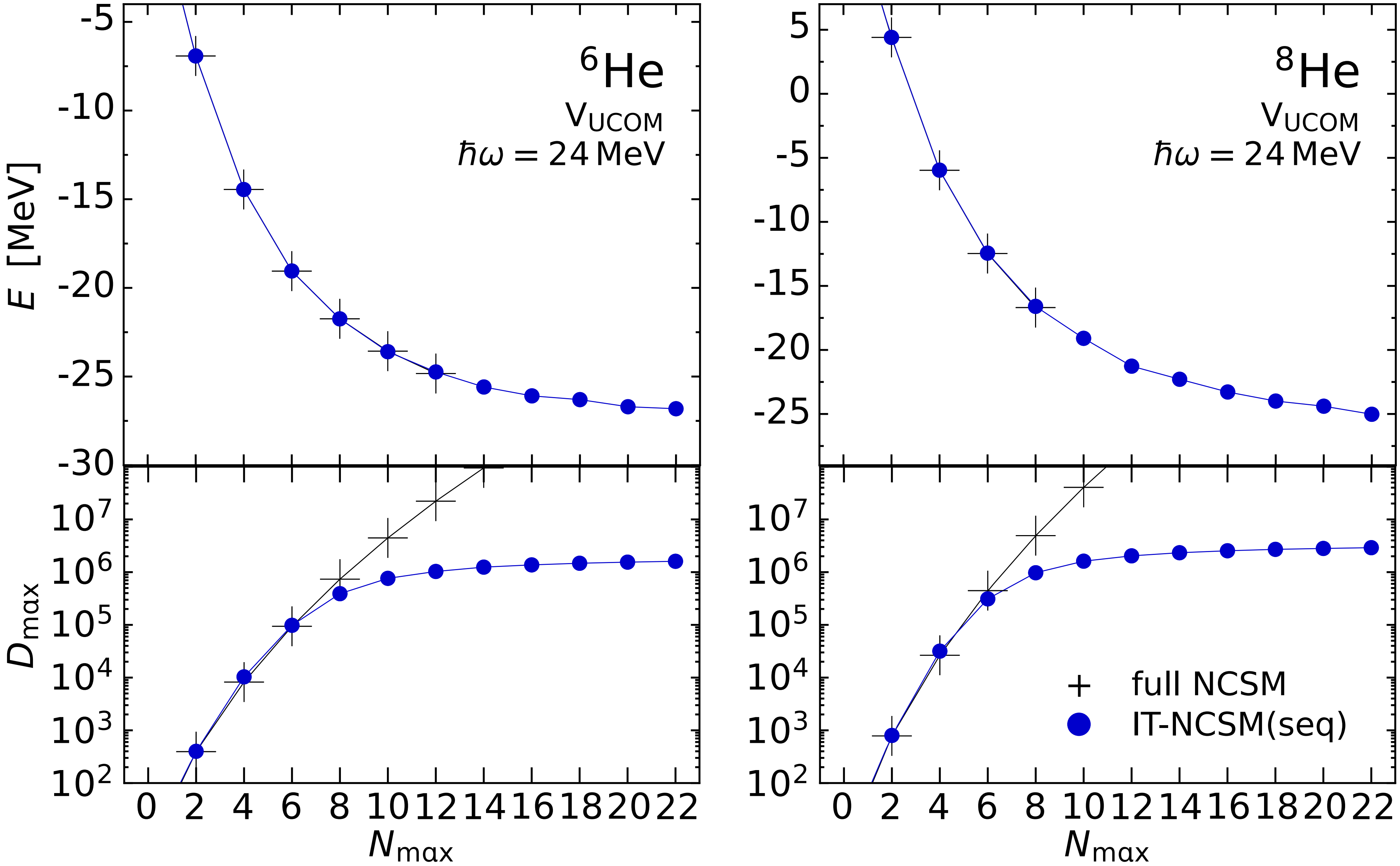


- extrapolation to $N_{max} \to \infty$

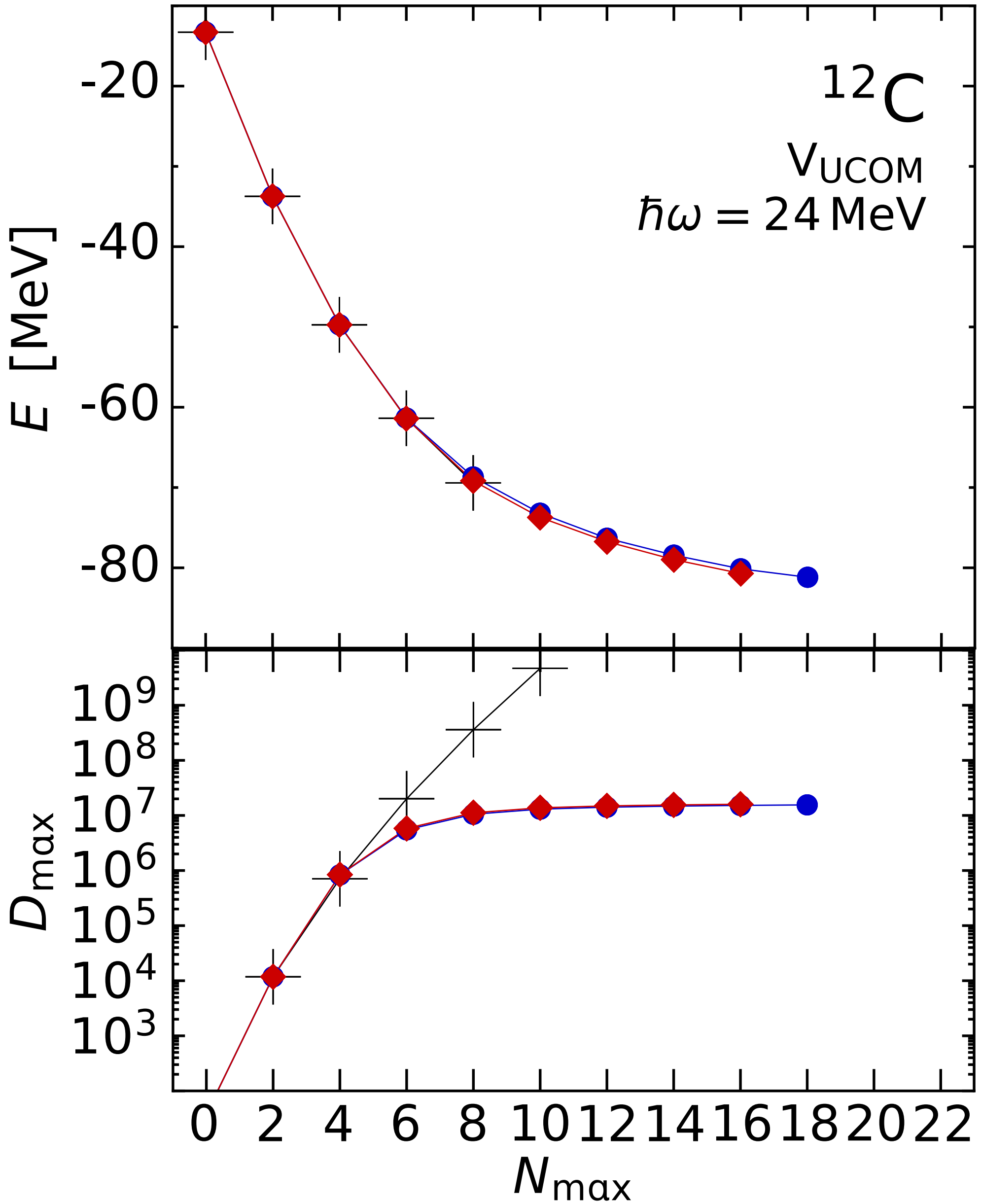
$$E_{\text{IT-NCSM(seq)}} = -132(3)\,\text{MeV}$$
$$E_{\text{exp}} = -127.6\,\text{MeV}$$

- V_{UCOM} predicts **reasonable binding energies** also for heavier nuclei
- slow non-exponential convergence makes precise extrapolation difficult

^{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

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

Computational Many-Body Methods

Coupled-Cluster vs. Configuration Interaction

Roth, Piecuch, Gour — arXiv: 0806.0333

Coupled-Cluster vs. IT-CI/NCSM

- How does importance truncation perform in one-to-one comparison with coupled-cluster calculations?

- **coupled-cluster calculations** [J. Gour & P. Piecuch @ MSU]
  - using harmonic oscillator and Hartree-Fock single-particle basis
  - CCSD and CR-CC(2,3)

- **importance-truncated CI**
  - use same basis and single-particle-truncated model space as CC
  - IT-CI[2](4p4h) and IT-CI[2](4p4h)+MRD

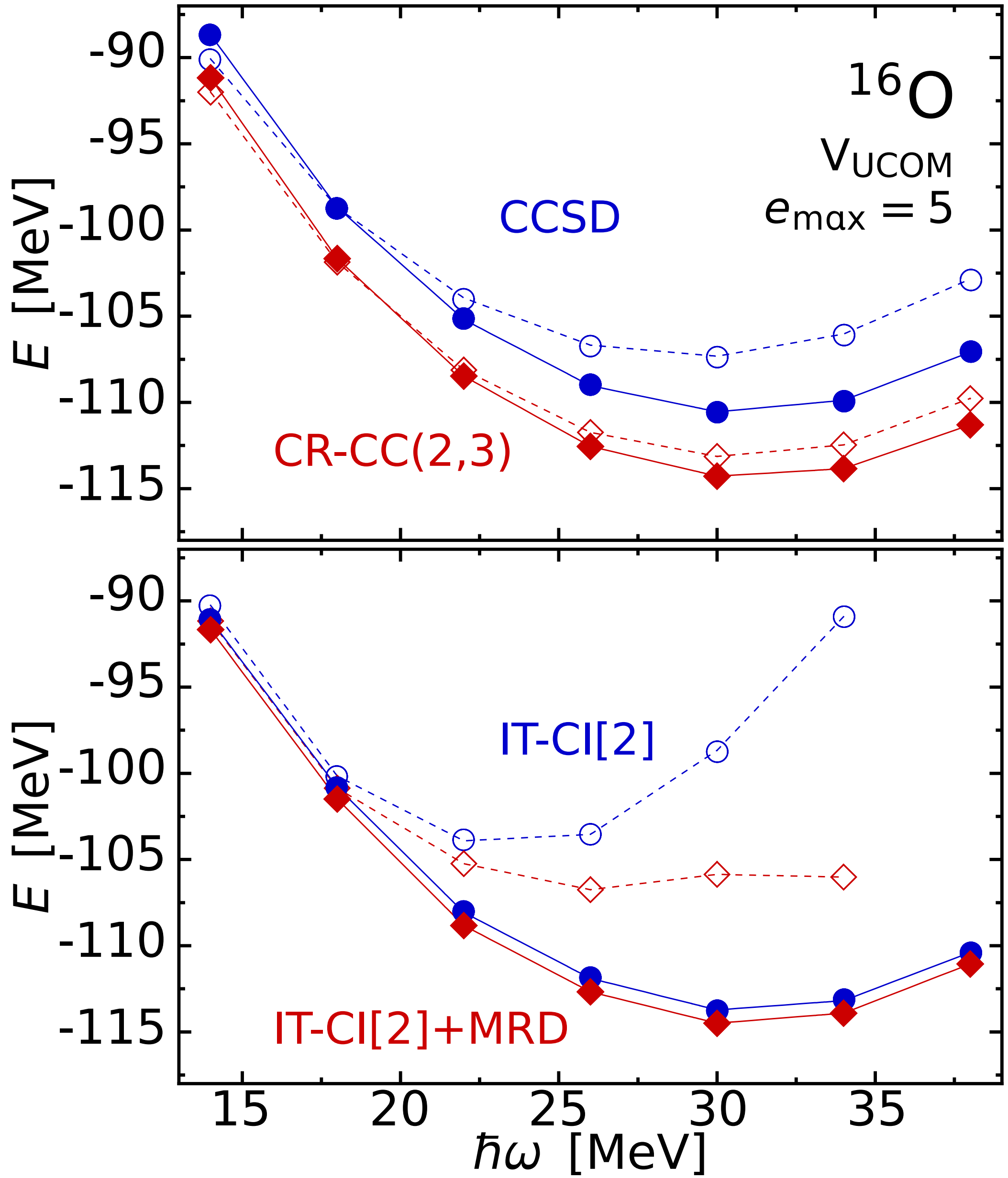
- **importance-truncated NCSM**
  - can only compare extrapolated energy due to different model space

^{16}O: Center-of-Mass Contamination

- only the $N_{\text{max}}\hbar\omega$ space built from HO basis allows for **exact separation of intrinsic and CM motion** ▶ translational invariance
- any other single-particle basis or model-space truncation induces a coupling of intrinsic and CM sates ▶ **CM contamination**
- use Lawson Hamiltonian $\text{H} = \text{H}_{\text{int}} + \beta \text{H}_{\text{cm}}$ to assess CM contamination of intrinsic state

		$\beta = 0$		$\beta = 10$	
		$\langle \text{H}_{\text{int}} \rangle$	$\langle \text{H}_{\text{cm}} \rangle$	$\langle \text{H}_{\text{int}} \rangle$	$\langle \text{H}_{\text{cm}} \rangle$
CCSD	$e_{\text{max}} = 5$	-107.32	5.88	-104.84	0.24
CR-CC(2,3)	$\hbar\omega = 30\,\text{MeV}$	-113.14	5.38	-111.23	0.20
IT-CI[2]		-98.67	1.37	-96.73	0.19
IT-NCSM[2]	$N_{\text{max}} = 8$	-104.10	0.08	-104.01	0.02
full NCSM	$\hbar\omega = 22\,\text{MeV}$	-104.75	—	-104.75	0.00

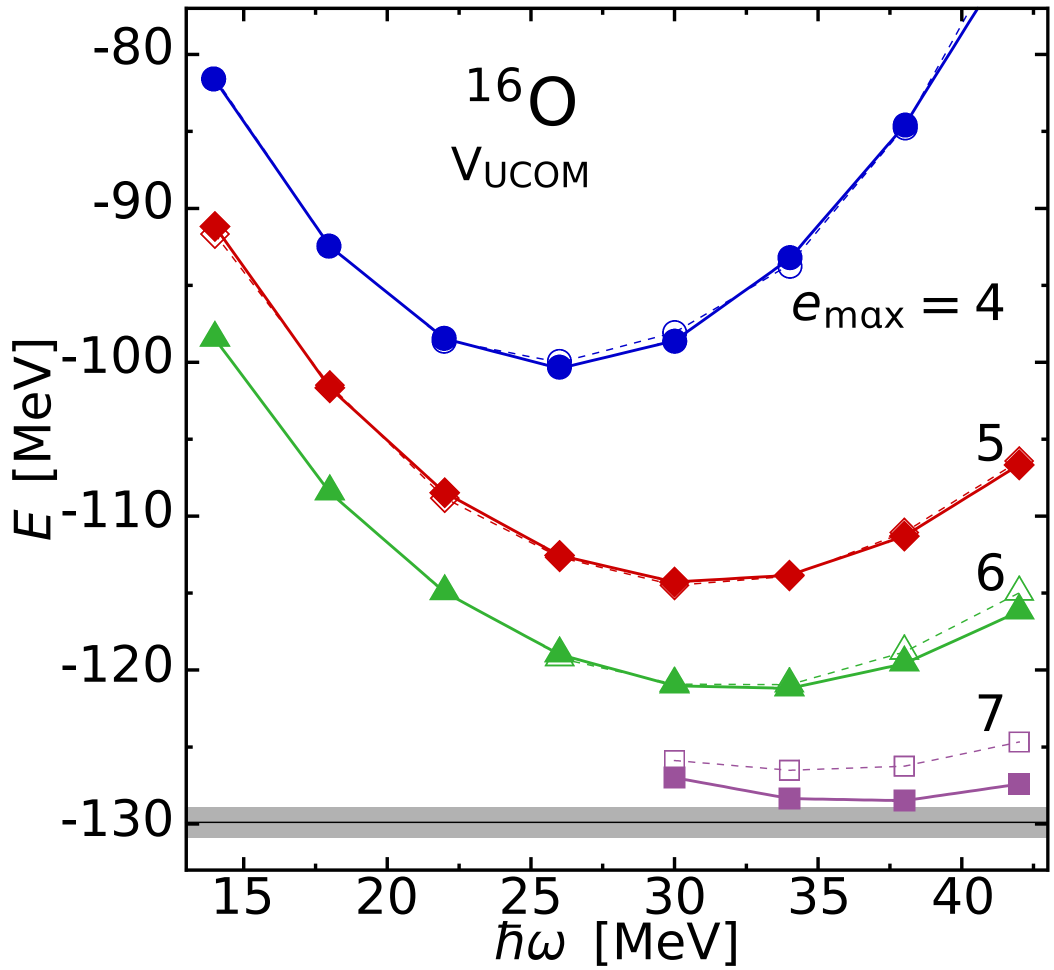
^{16}O: Role of Single-Particle Basis

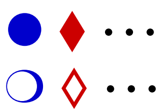


- compare **harmonic oscillator** with **Hartree-Fock basis** obtained for $e_{max} = 5$
- **CC** is largely insensitive to basis optimization due to $\exp(T_1)$ terms
- **IT-CI** benefits much more from optimized basis
- Davidson correction and C_1 amplitudes indicate where basis becomes inadequate

○ / ◇ harmonic oscillator basis
● / ◆ Hartree-Fock basis

^{16}O: Direct Comparison CC vs. IT-CI





- **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

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

    Institut für Kernphysik, TU Darmstadt
  - P. Navrátil

    Lawrence Livermore National Laboratory, USA
  - P. Piecuch, J. Gour

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

    Gesellschaft für Schwerionenforschung (GSI)

Deutsche Forschungsgemeinschaft DFG

SFB 634

HIC for FAIR

LOEWE – Landes-Offensive zur Entwicklung Wissenschaftlich-ökonomischer Exzellenz