From QCD to Nuclear Structure:
Interactions and Many-Body Techniques

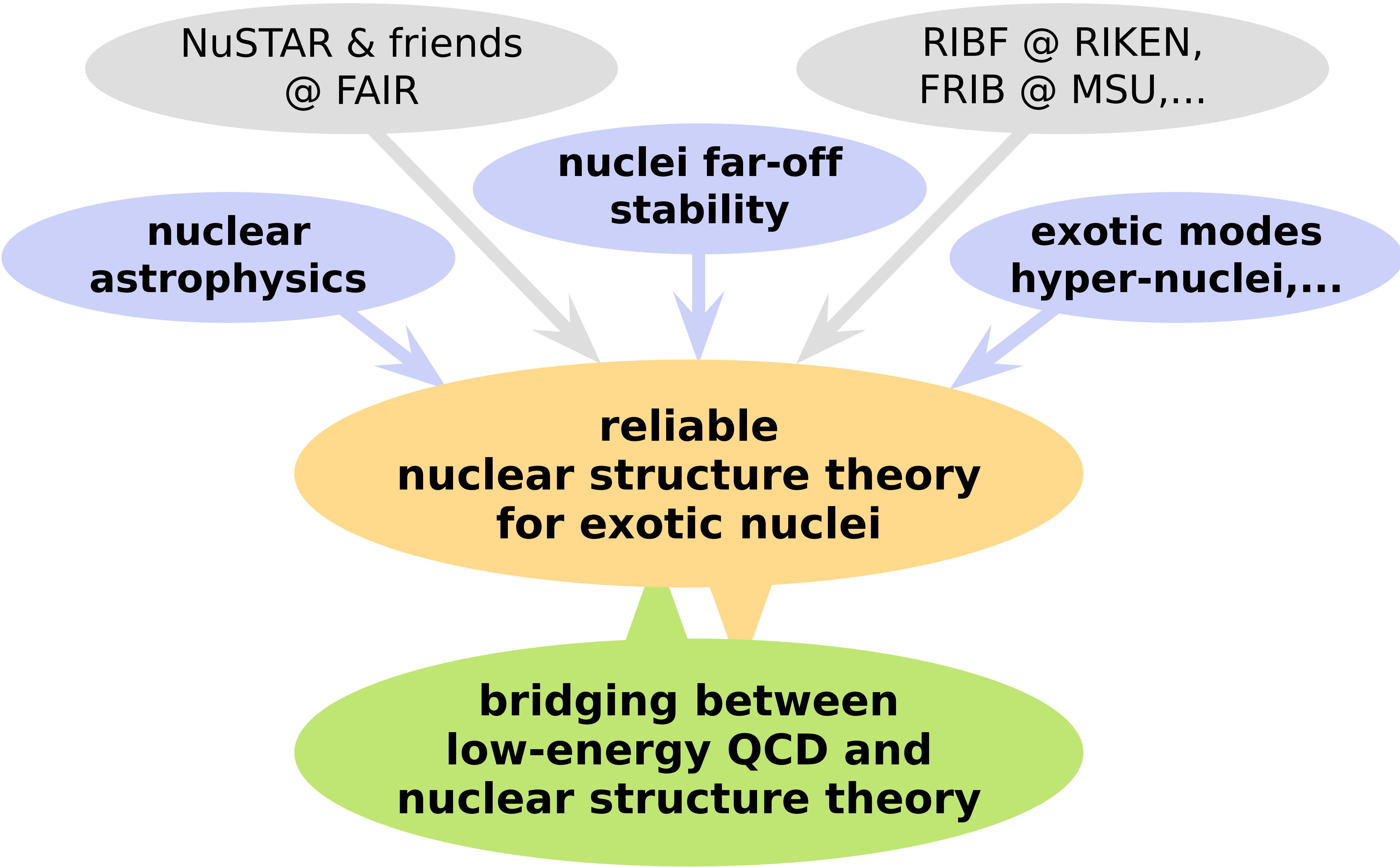
Robert Roth
Institut für Kernphysik

TECHNISCHE UNIVERSITÄT DARMSTADT

Overview

- Motivation
- Nuclear Interactions from QCD
- Similarity Transformed Interactions
  - Unitary Correlation Operator Method
  - Similarity Renormalization Group
- Computational Many-Body Methods
  - No-Core Shell Model
  - Importance Truncated NCSM

Nuclear Structure in the 21st Century

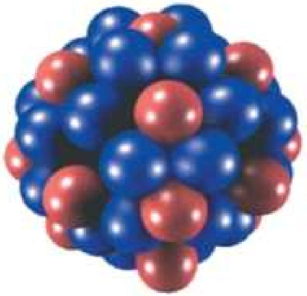


Theoretical Context

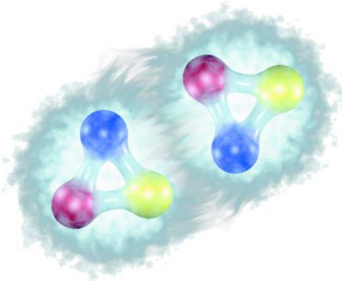
better resolution / more fundamental

Quantum Chromo Dynamics

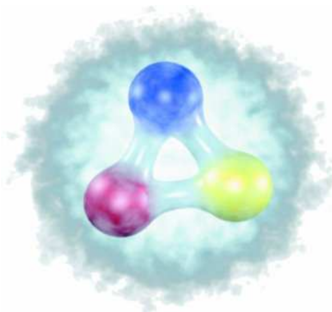
Nuclear Structure



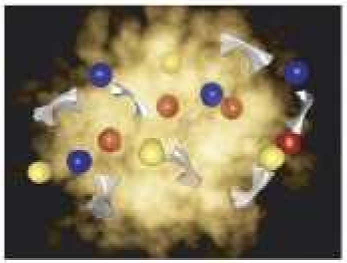
- finite nuclei



- few-nucleon systems
- nucleon-nucleon interaction



- hadron structure



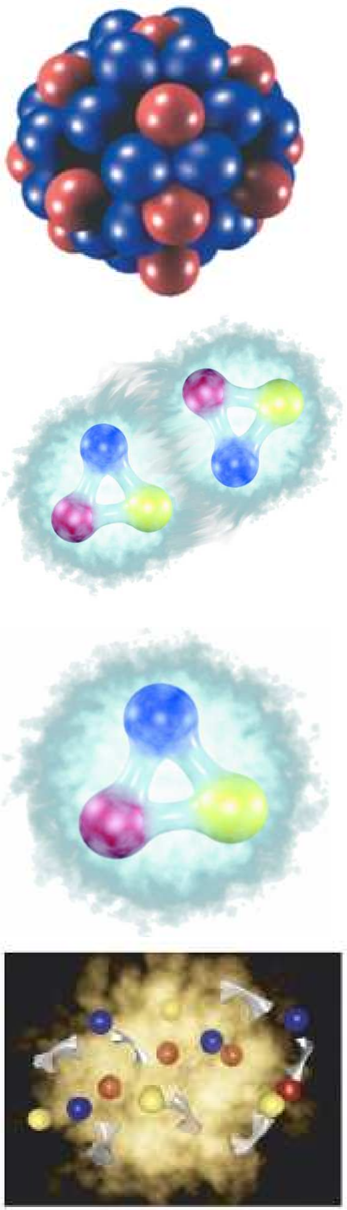
- quarks & gluons
- deconfinement

Theoretical Context

better resolution / more fundamental

Quantum Chromo Dynamics

Nuclear Structure

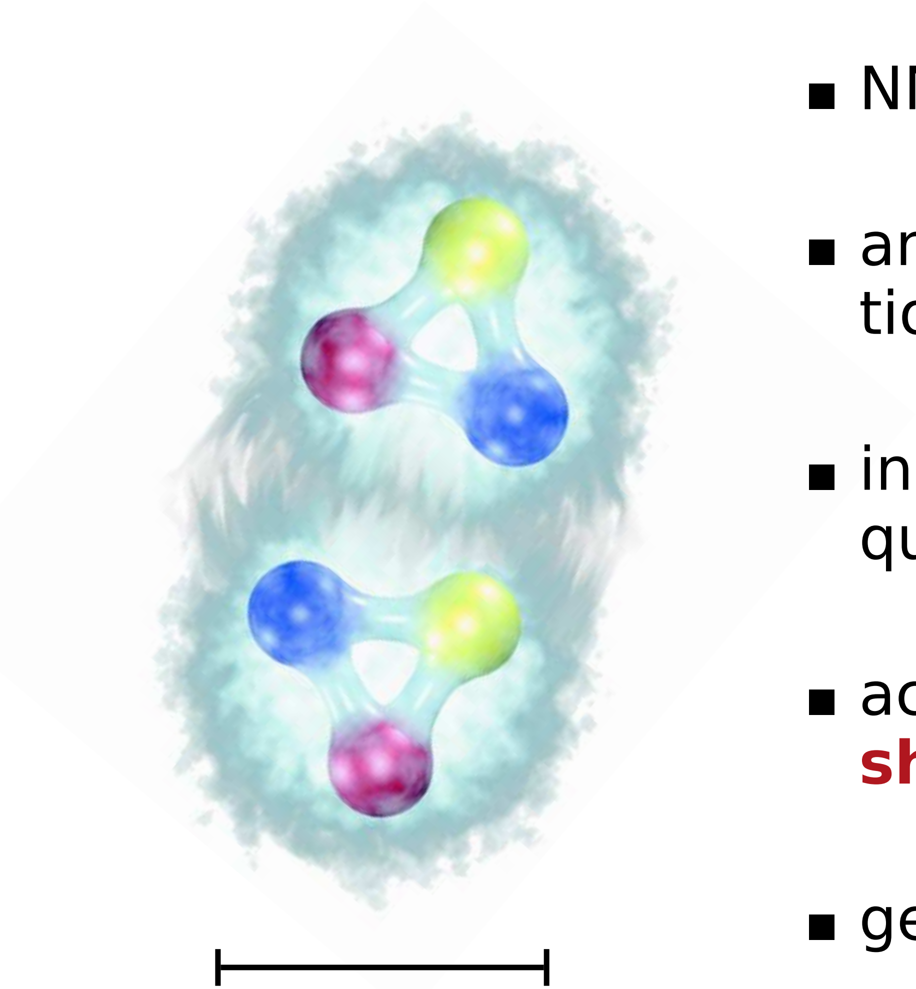


How to solve the quantum many-body problem?

How to derive the nuclear interaction from QCD?

Nuclear Interactions from QCD

Nature of the Nuclear Interaction

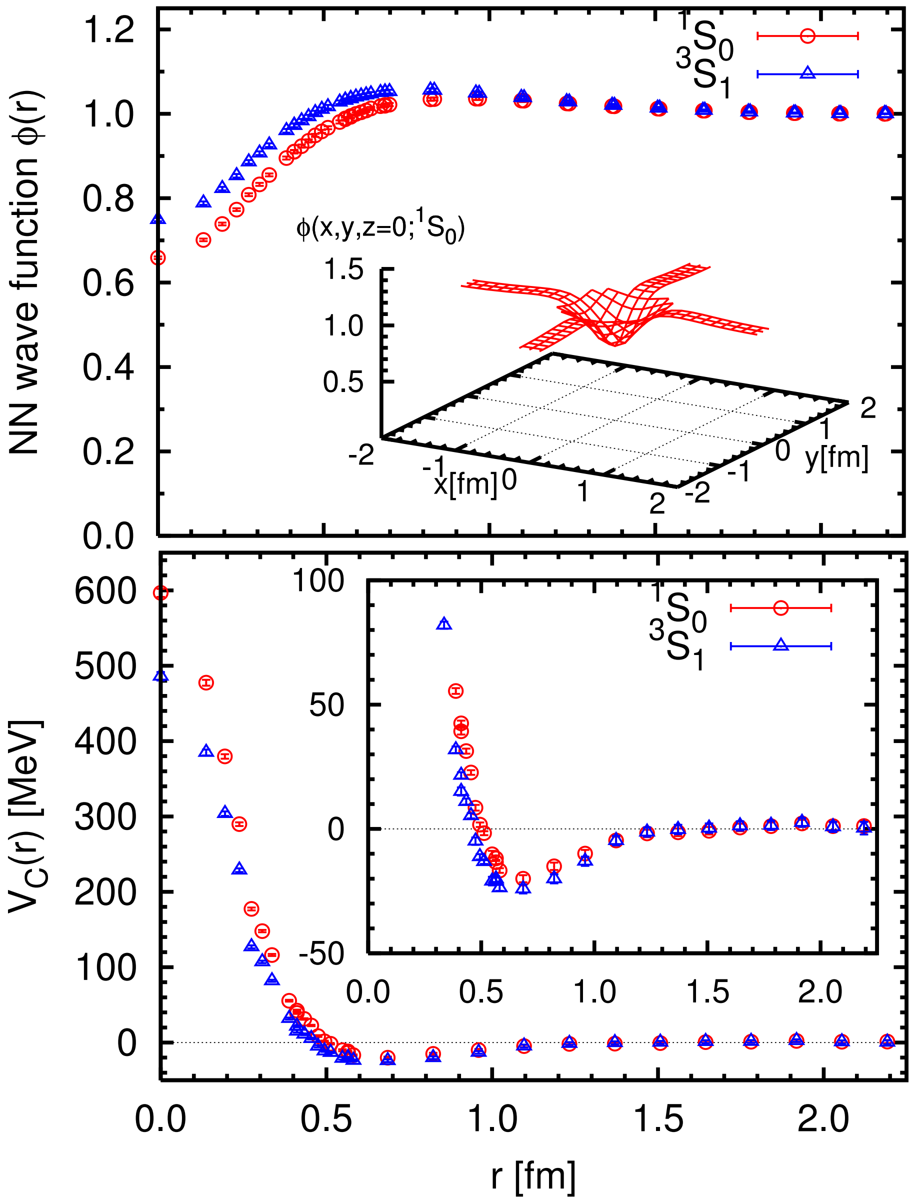


$\sim 1.6\text{fm}$

$\rho_0^{-1/3} = 1.8\text{fm}$

- NN-interaction is **not fundamental**
- analogous to **van der Waals** interaction between neutral atoms
- induced via mutual **polarization** of quark & gluon distributions
- acts only if the nucleons overlap, i.e. at **short ranges**
- genuine **3N-interaction** is important

Nuclear Interaction from Lattice QCD

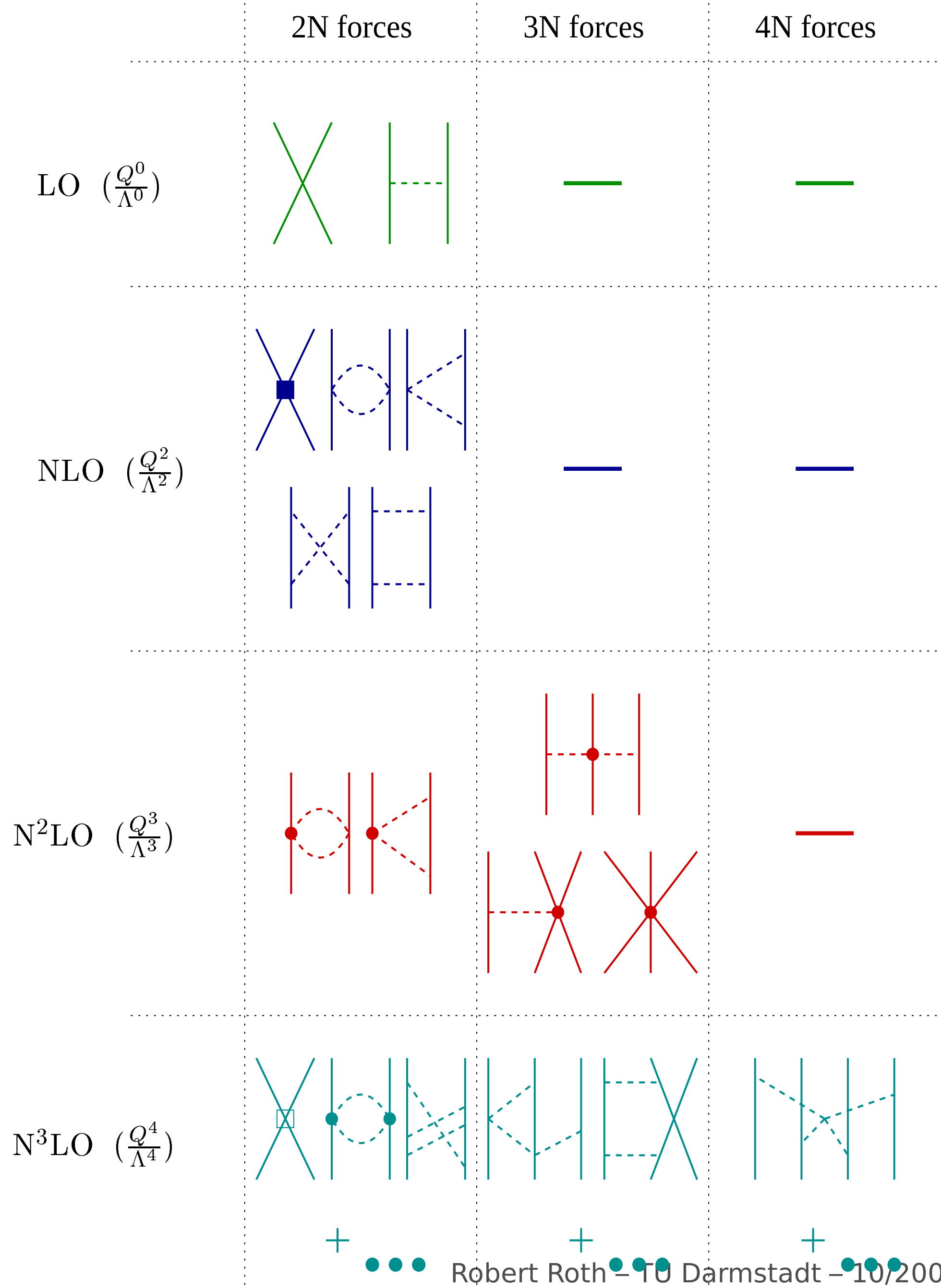


N. Ishii et al., PRL 99, 022001 (2007)

- first steps towards construction of a nuclear interaction through **lattice QCD simulations**
- compute relative **two-nucleon wavefunction** on the lattice
- invert Schrödinger equation to obtain **local 'effective' two-nucleon potential**
- schematic results so far (unphysical quark masses, S-wave interactions only,...)

Nuclear Interaction from Chiral EFT

- **EFT for relevant degrees of freedom (*π*,*N*)** based on symmetries of QCD
- long-range **pion dynamics** treated explicitly
- short-range physics absorbed in **contact terms**
- low-energy constants fitted to experimental data (*NN*, *πN*)
- hierarchy of **consistent NN, 3N,... interactions** (including current operators)



Meißner, NPA 751 (2005) 149c

Realistic Nuclear Interactions

- **QCD ingredients**
  - chiral effective field theory
  - meson-exchange theory
- **short-range phenomenology**
  - contact terms or parameterization of short-range potential
- **experimental two-body data**
  - scattering phase-shifts & deuteron properties reproduced with high precision
- **supplementary 3N interaction**
  - adjusted to spectra of light nuclei

Argonne V18

CD Bonn

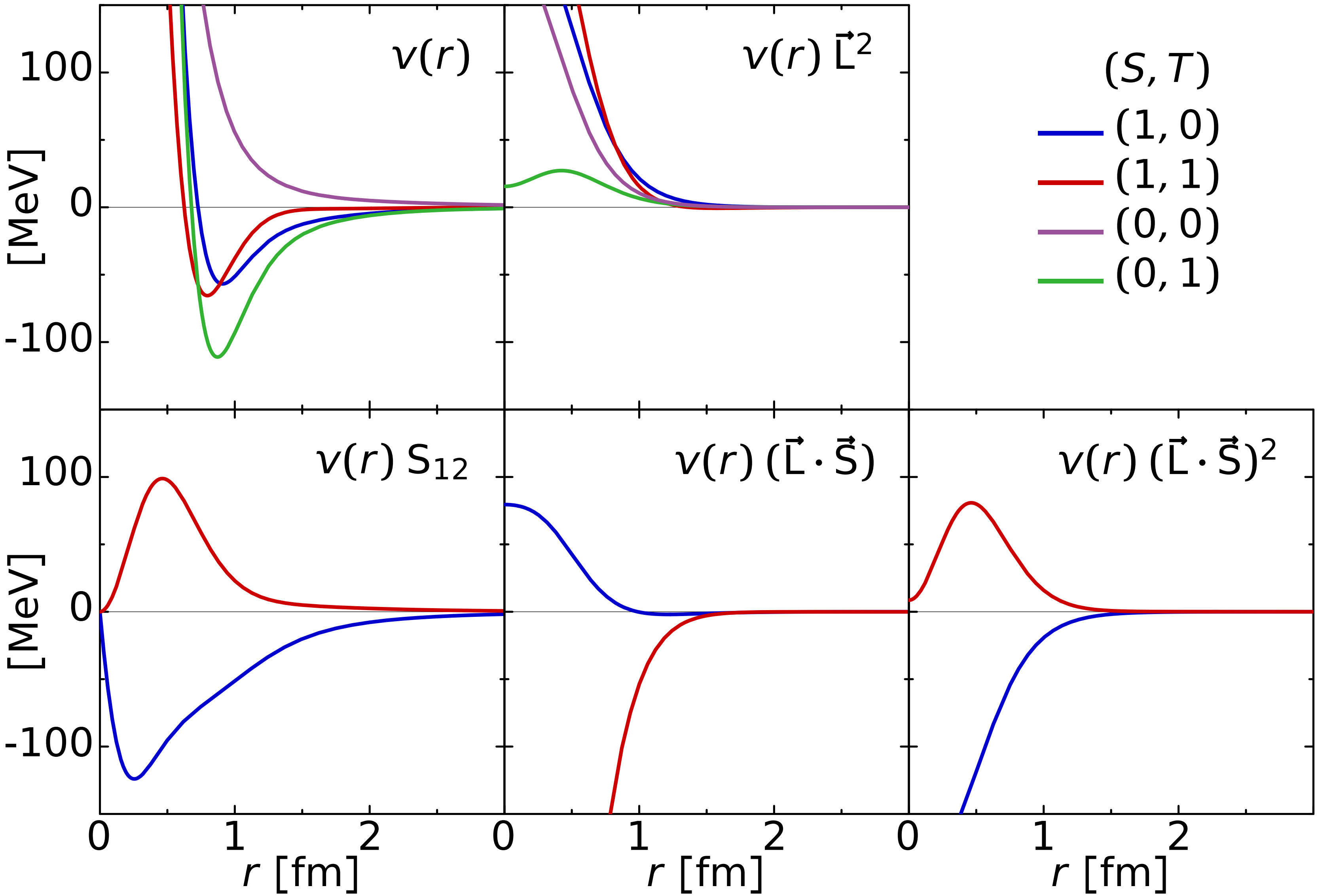
Nijmegen I/II

Chiral N3LO

Argonne V18 + **Illinois 2**

Chiral N3LO + **N2LO**

Argonne V18 Potential



Similarity Transformed Interactions

Why Transformed Interactions?

Realistic Interactions

- generate strong correlations in many-body states
- short-range central & tensor correlations most important

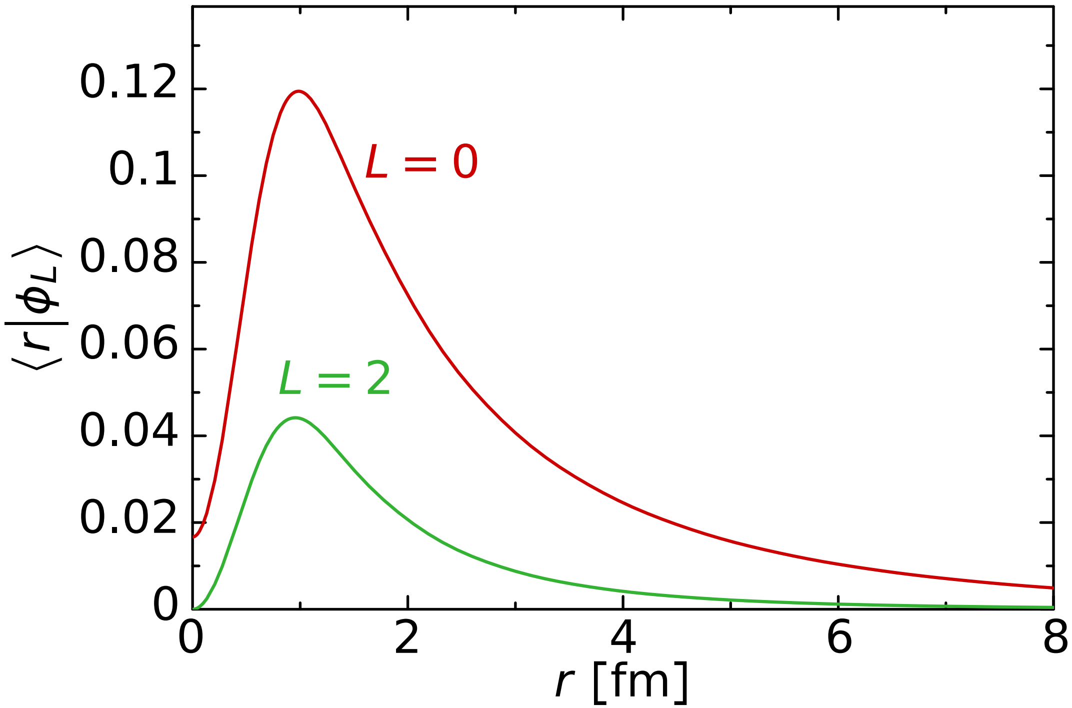
Similarity Transformation

- adapt realistic potential to the available model space
- conserve experimentally constrained properties (phase shifts)

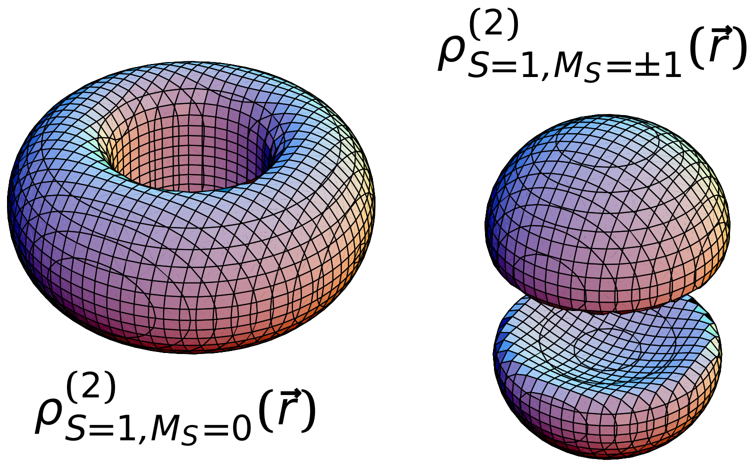
Many-Body Methods

- rely on truncated many-nucleon Hilbert spaces
- not capable of describing short-range correlations
- extreme: Hartree-Fock based on single Slater determinant

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 L=2 admixture to ground state

tensor correlations

Similarity 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

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

Correlated States

imprint short-range cor-
relations onto uncorre-
lated 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

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

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

Tensor Correlator C_Ω

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

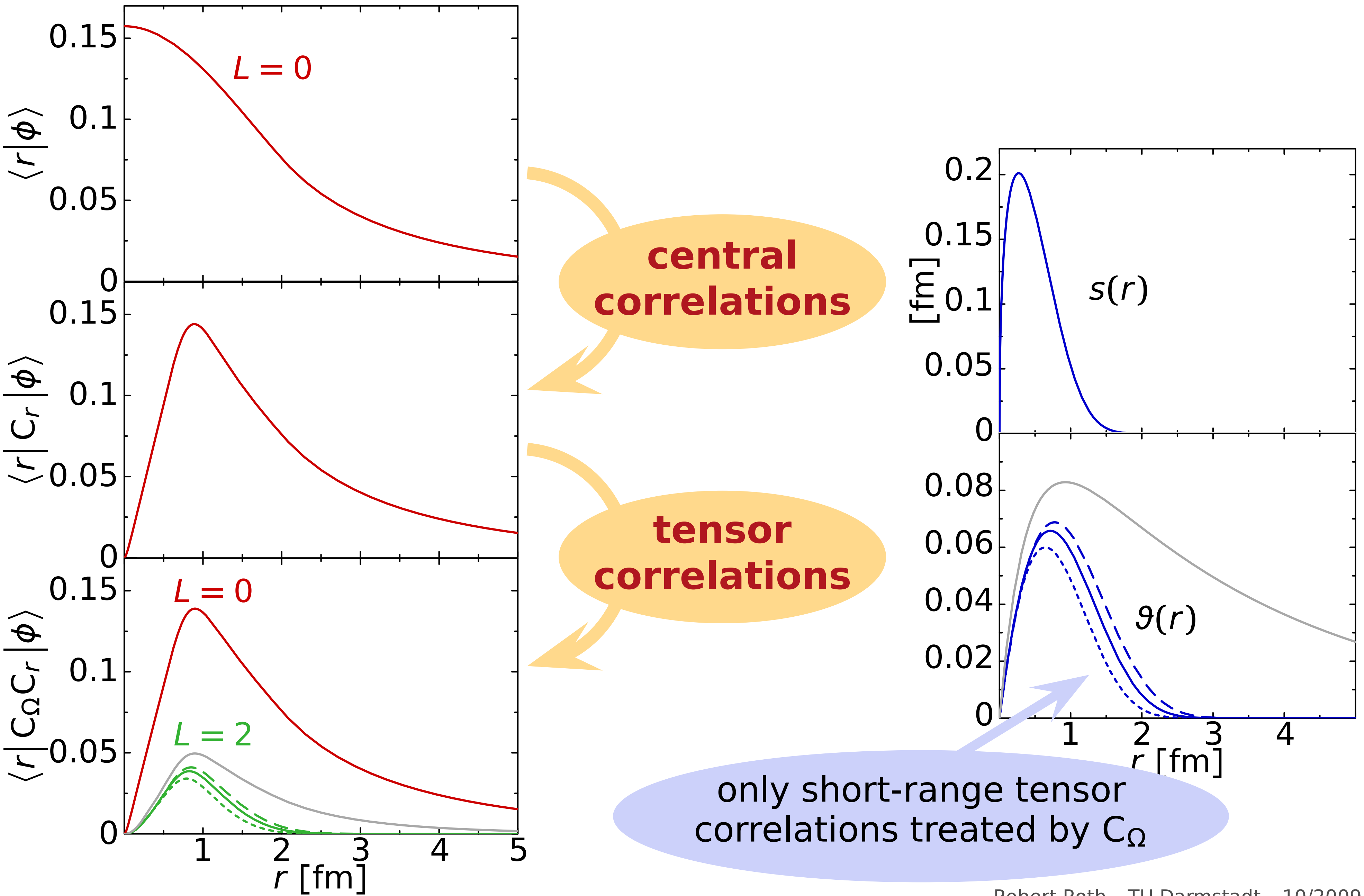
$$g_\Omega = \frac{3}{2}\vartheta(r)\big[(\vec{\sigma}_1\cdot\vec{q}_\Omega)(\vec{\sigma}_2\cdot\vec{r}) + (\vec{r}\leftrightarrow\vec{q}_\Omega)\big]$$

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

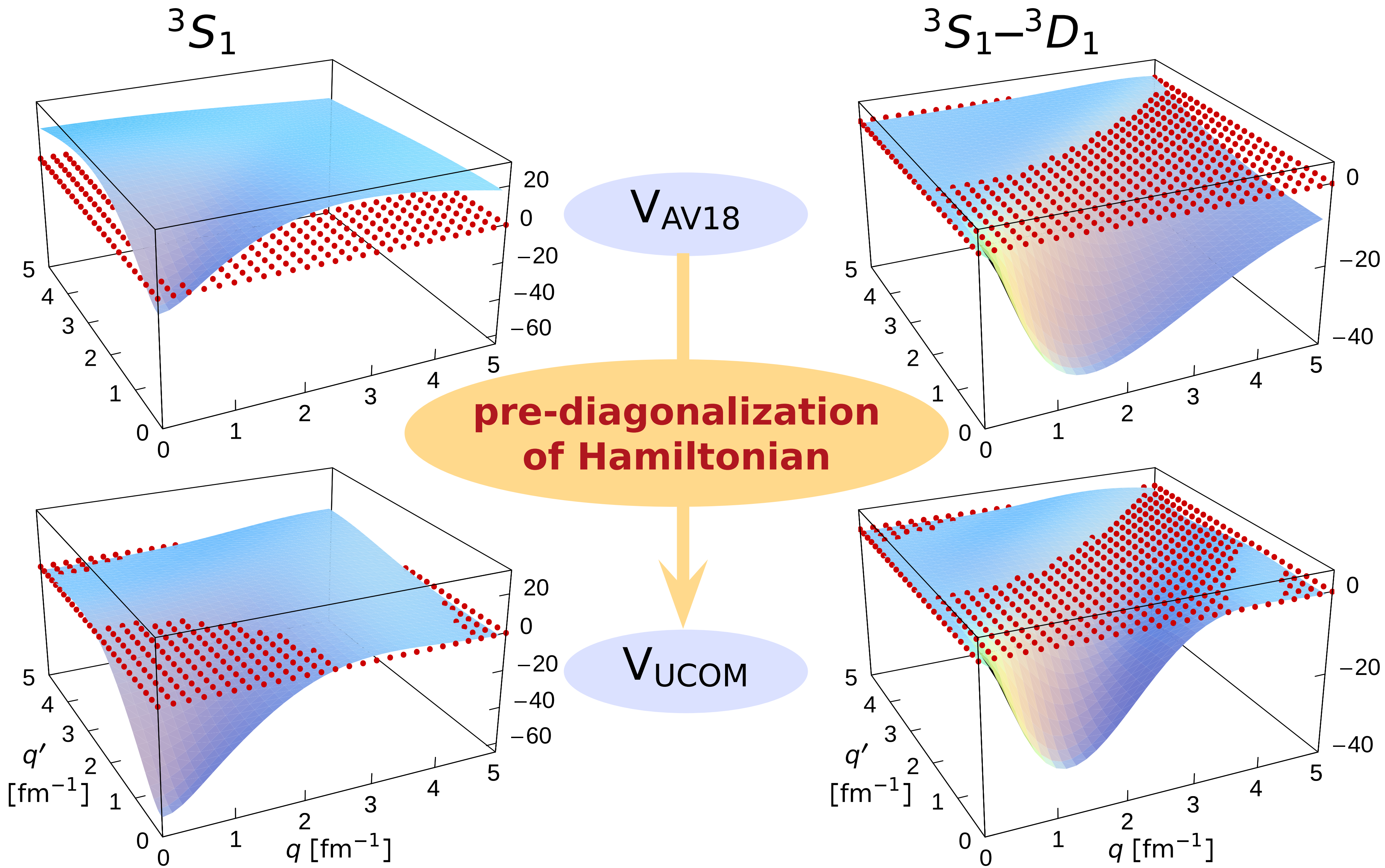
$$C = C_\Omega C_r = \exp\Big(-i\sum_{i<j} g_{\Omega,ij}\Big)\exp\Big(-i\sum_{i<j} g_{r,ij}\Big)$$

- $s(r)$ and $\vartheta(r)$ are optimized for the initial potential

Correlated States: The Deuteron



Correlated Interaction: V_{UCOM}



Similarity 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

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

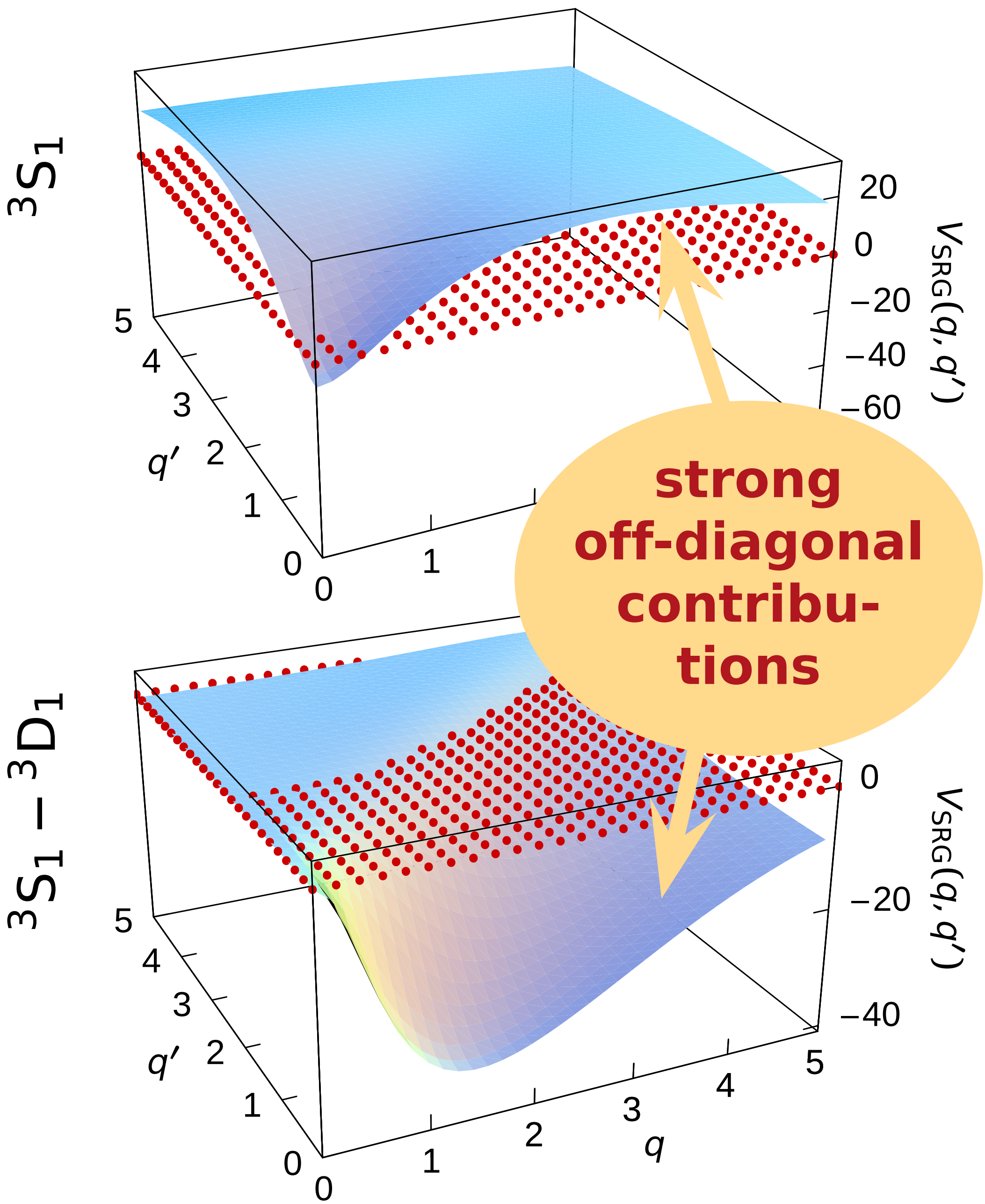
- dynamical generator defined as commutator with the operator in whose eigenbasis H shall be diagonalized

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

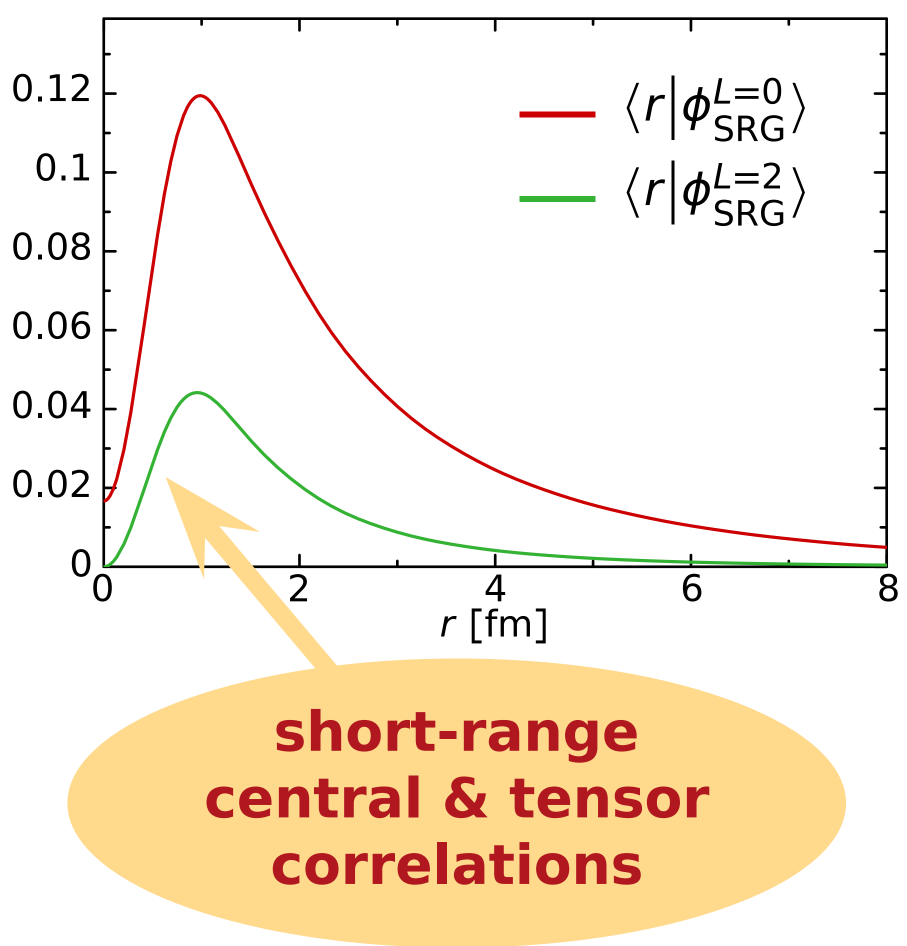
UCOM vs. SRG

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

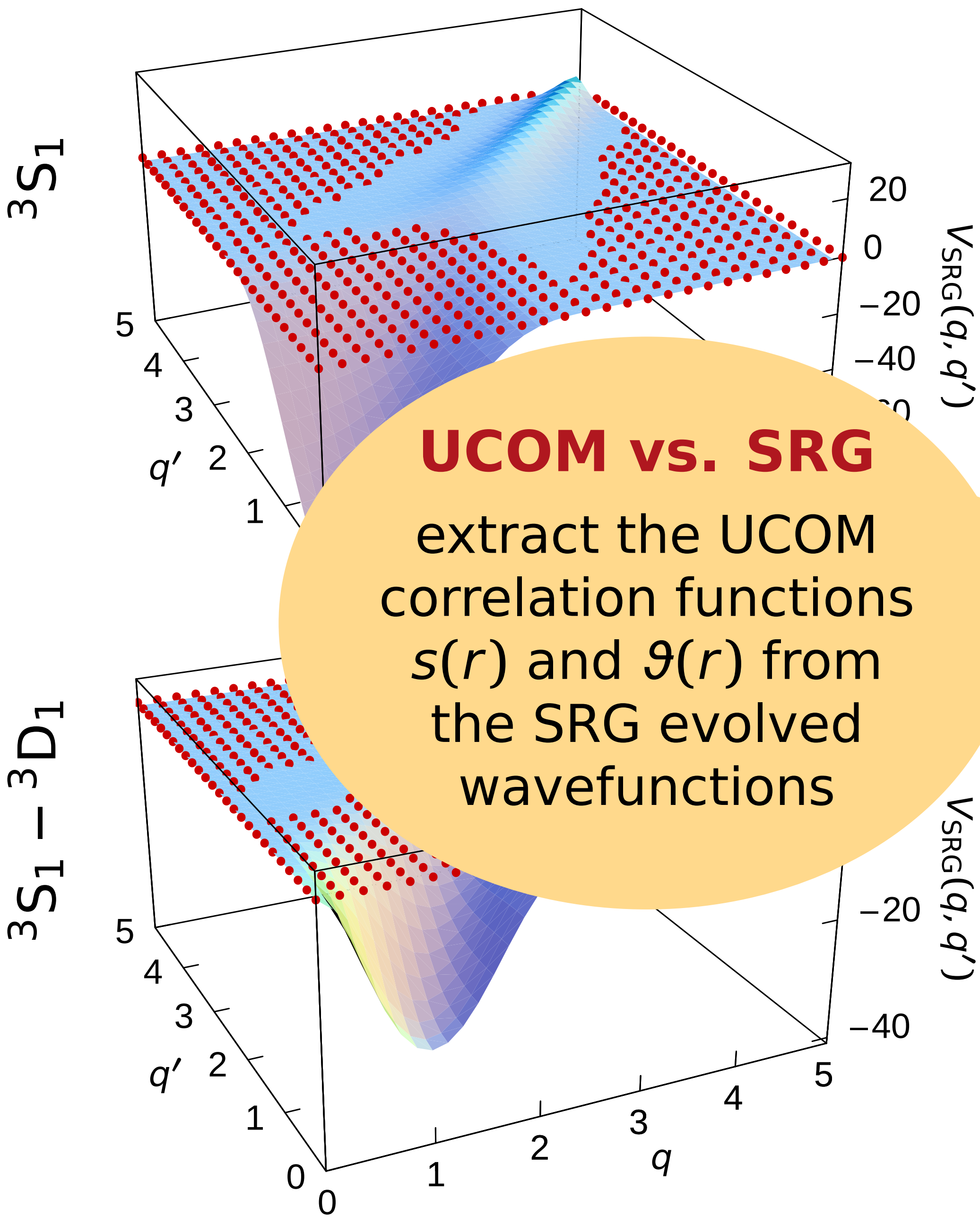
SRG Evolution: The Deuteron



Argonne V18



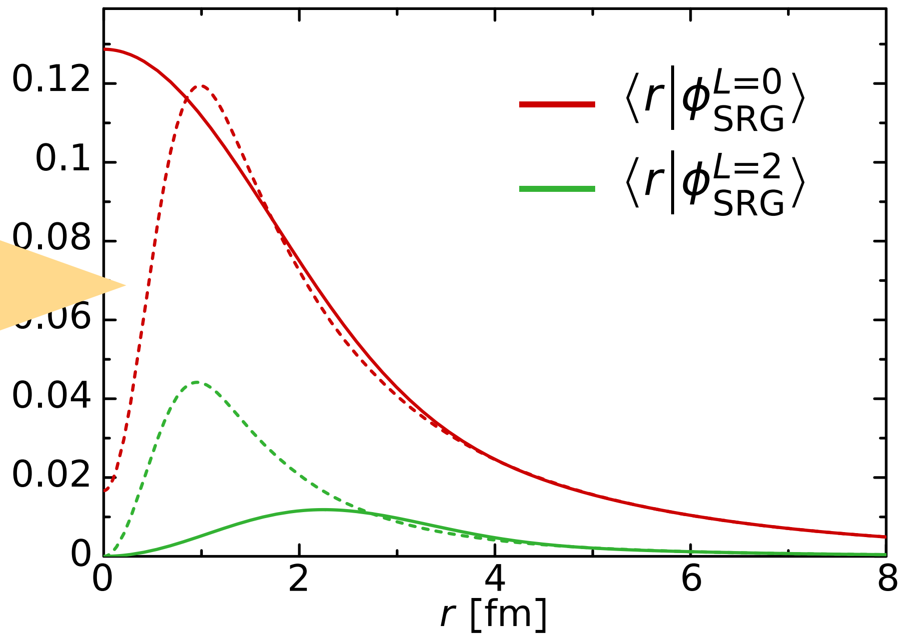
SRG Evolution: The Deuteron



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

UCOM vs. SRG

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



Computational Many-Body Methods

No-Core Shell Model

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

No-Core Shell Model: Basics

- special case of a **full configuration interaction (CI)** scheme
- **many-body basis**: Slater determinants $|\Phi_\nu\rangle$ composed of harmonic oscillator single-particle states

$$|\Psi\rangle = \sum_\nu C_\nu |\Phi_\nu\rangle$$

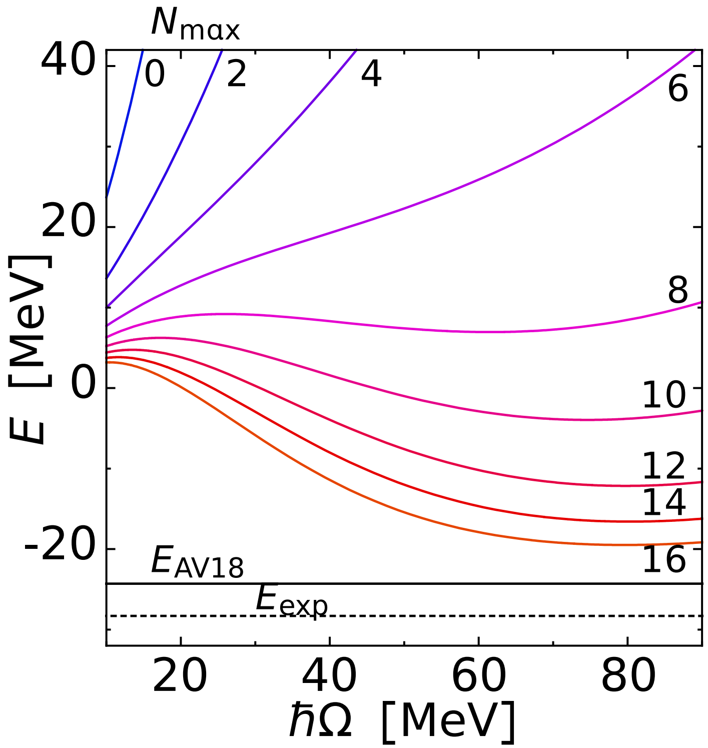
- **model space**: spanned by basis states $|\Phi_\nu\rangle$ with unperturbed excitation energies of up to $N_{\max}\hbar\Omega$
  - ▸ **exact factorization** of intrinsic and CM component is possible
- numerical solution of **eigenvalue problem** for $\mathrm{H}_{\mathrm{int}}$ within $N_{\max}\hbar\Omega$ model space via Lanczos methods
  - ▸ model spaces of **up to 10^9 basis states** are used routinely
- increase $N_{\max}$ until **convergence** is observed

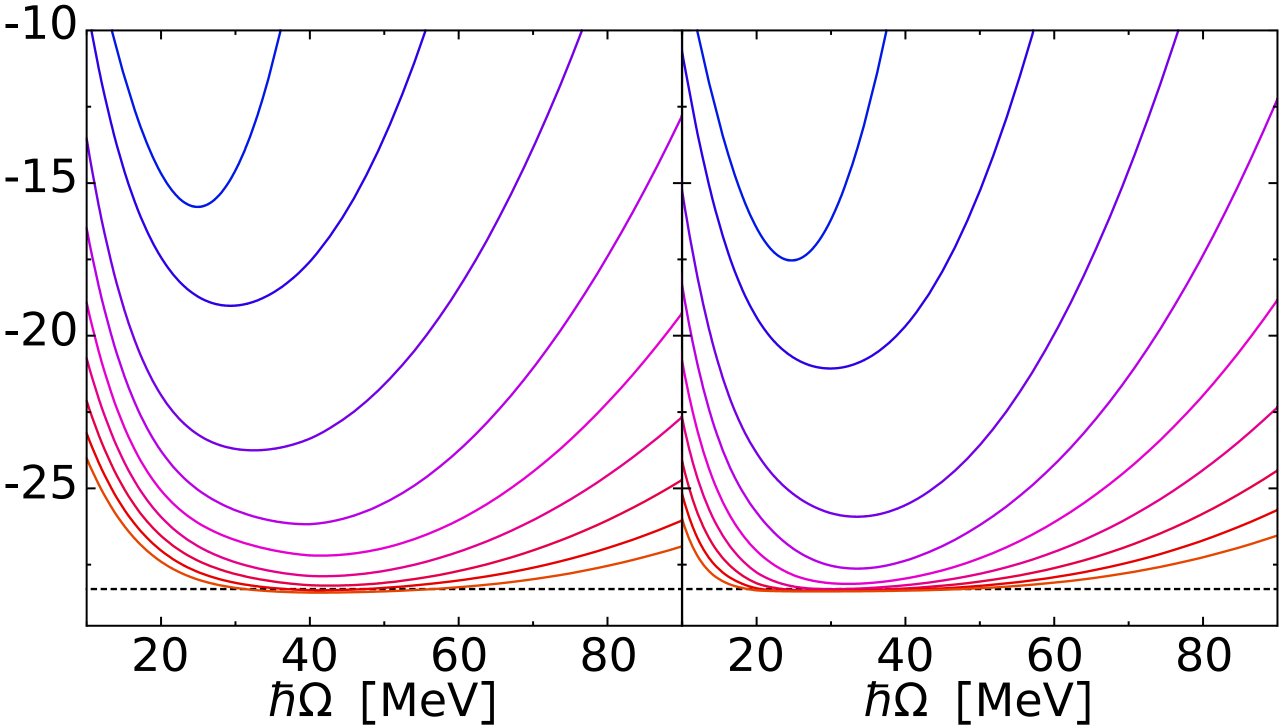
^{4}He: NCSM Convergence

V_{AV18}

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

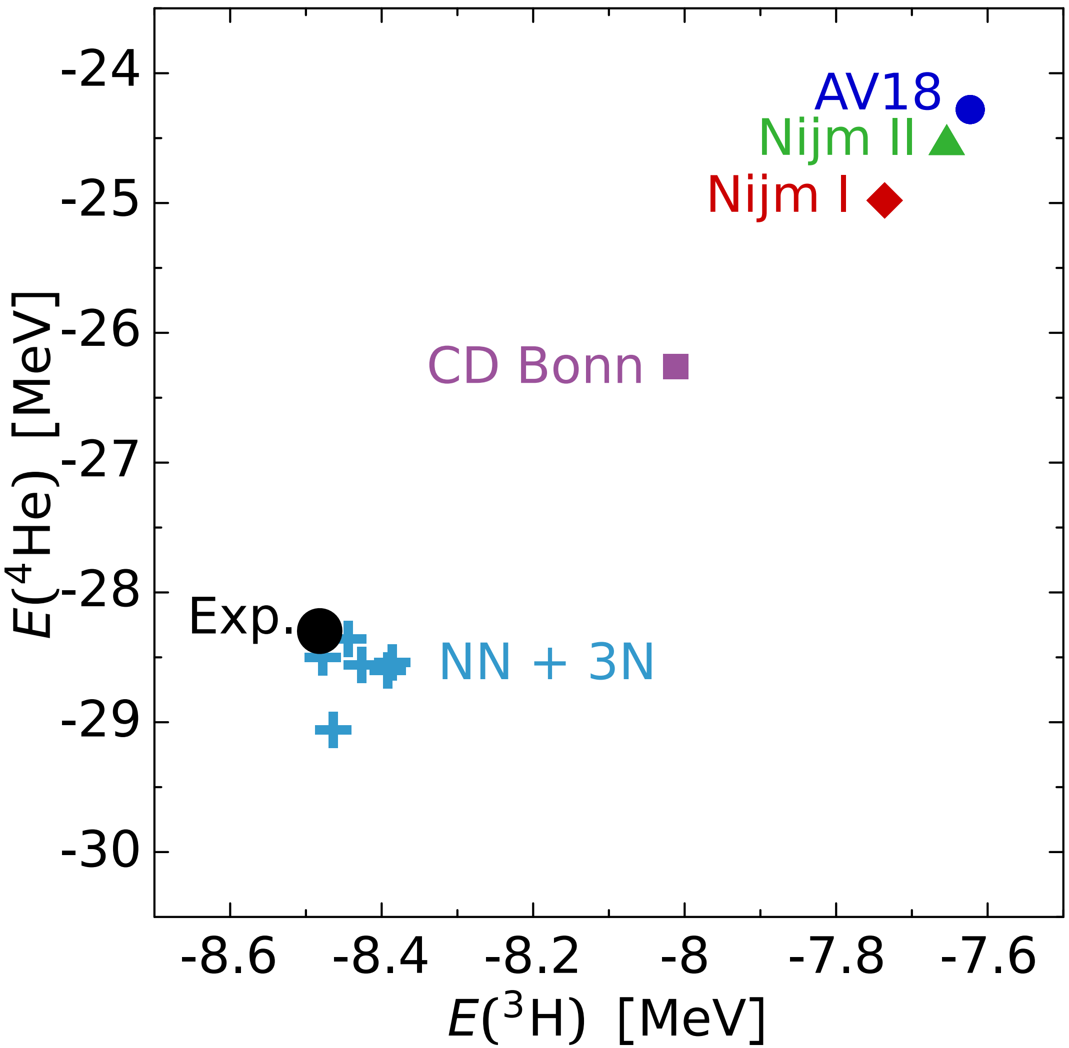
V_{SRG}
$\bar{\alpha} = 0.03\,\text{fm}^4$





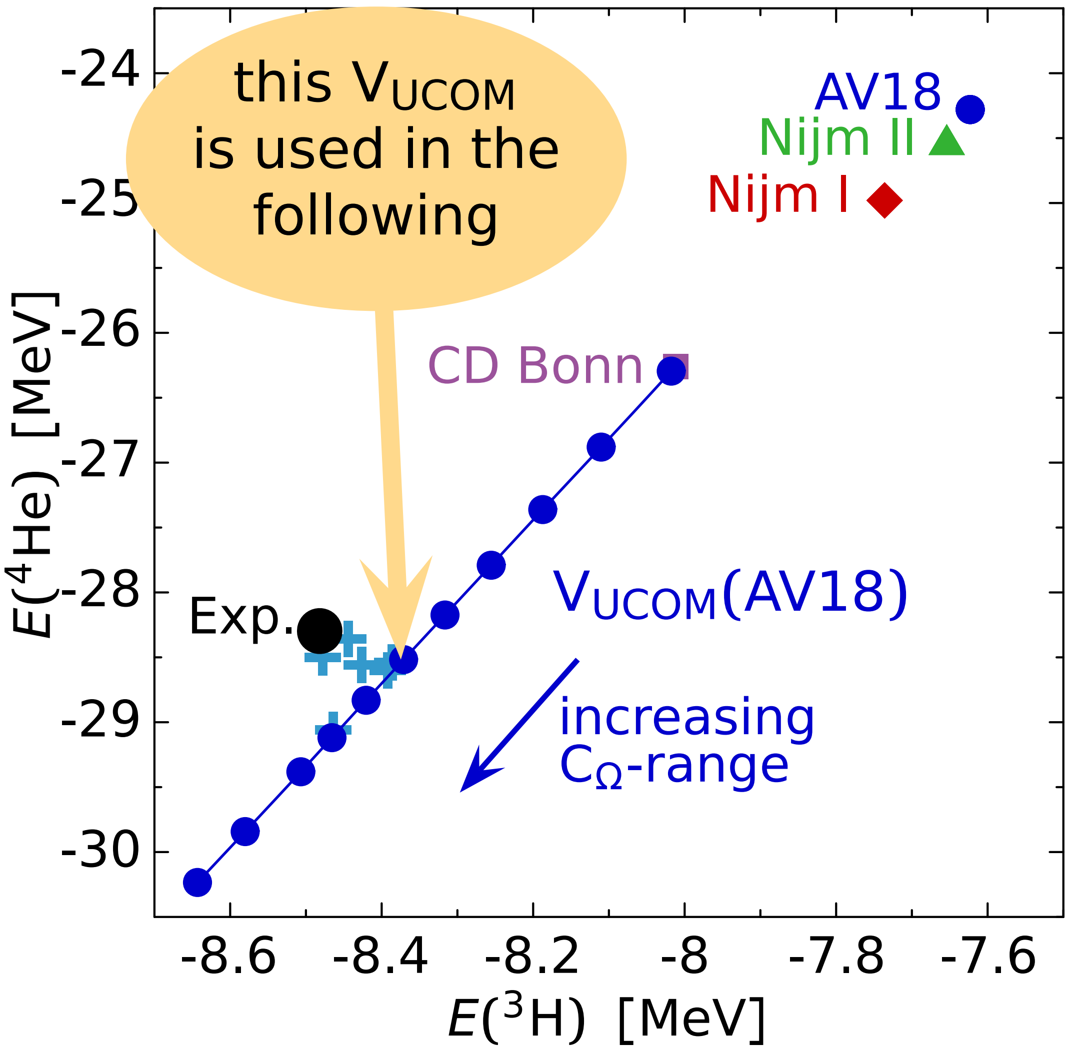
- I_ϑ or $\bar{\alpha}$ adjusted such that ^{4}He binding energy is reproduced

Tjon-Line and Correlator Range



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

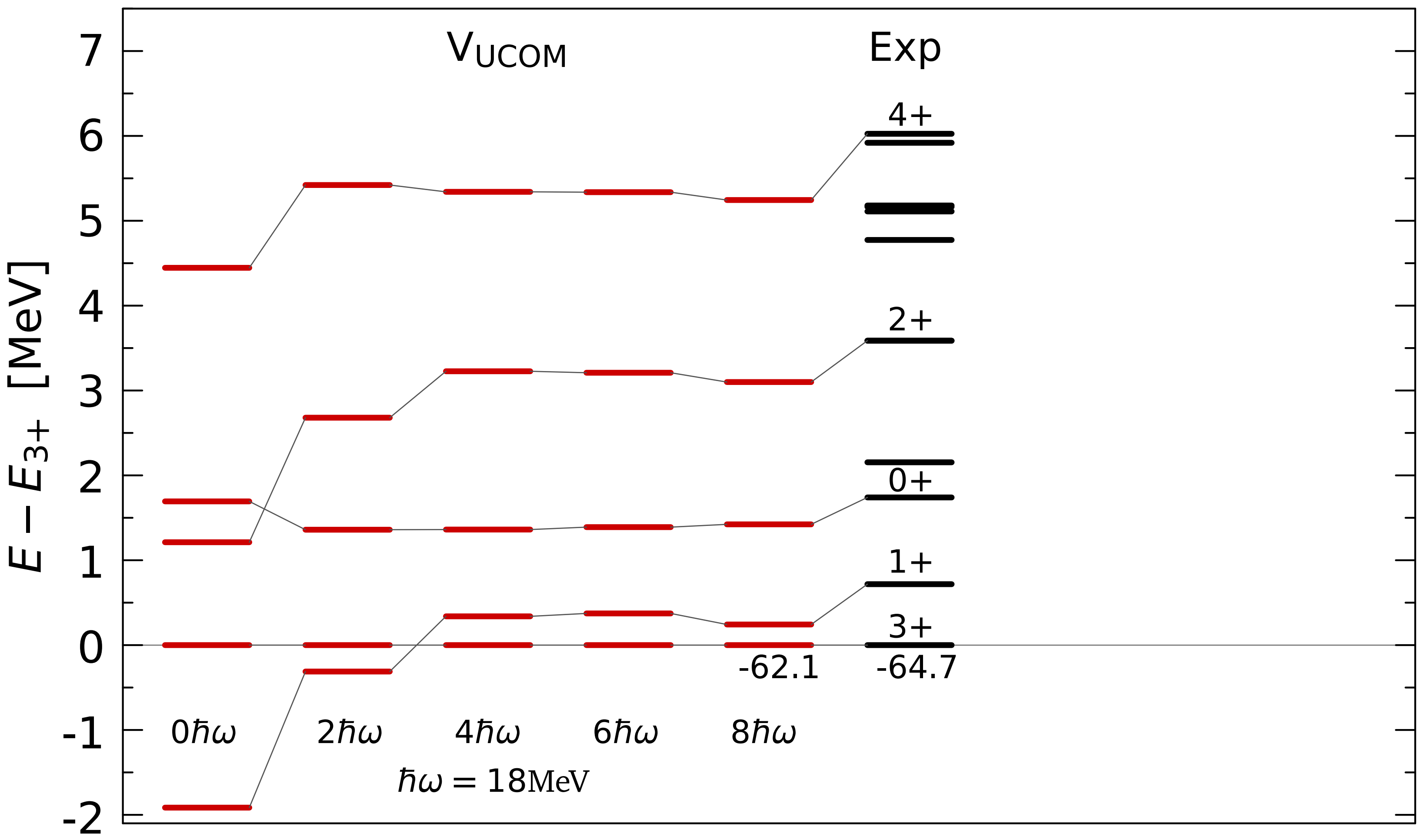
Tjon-Line and Correlator Range



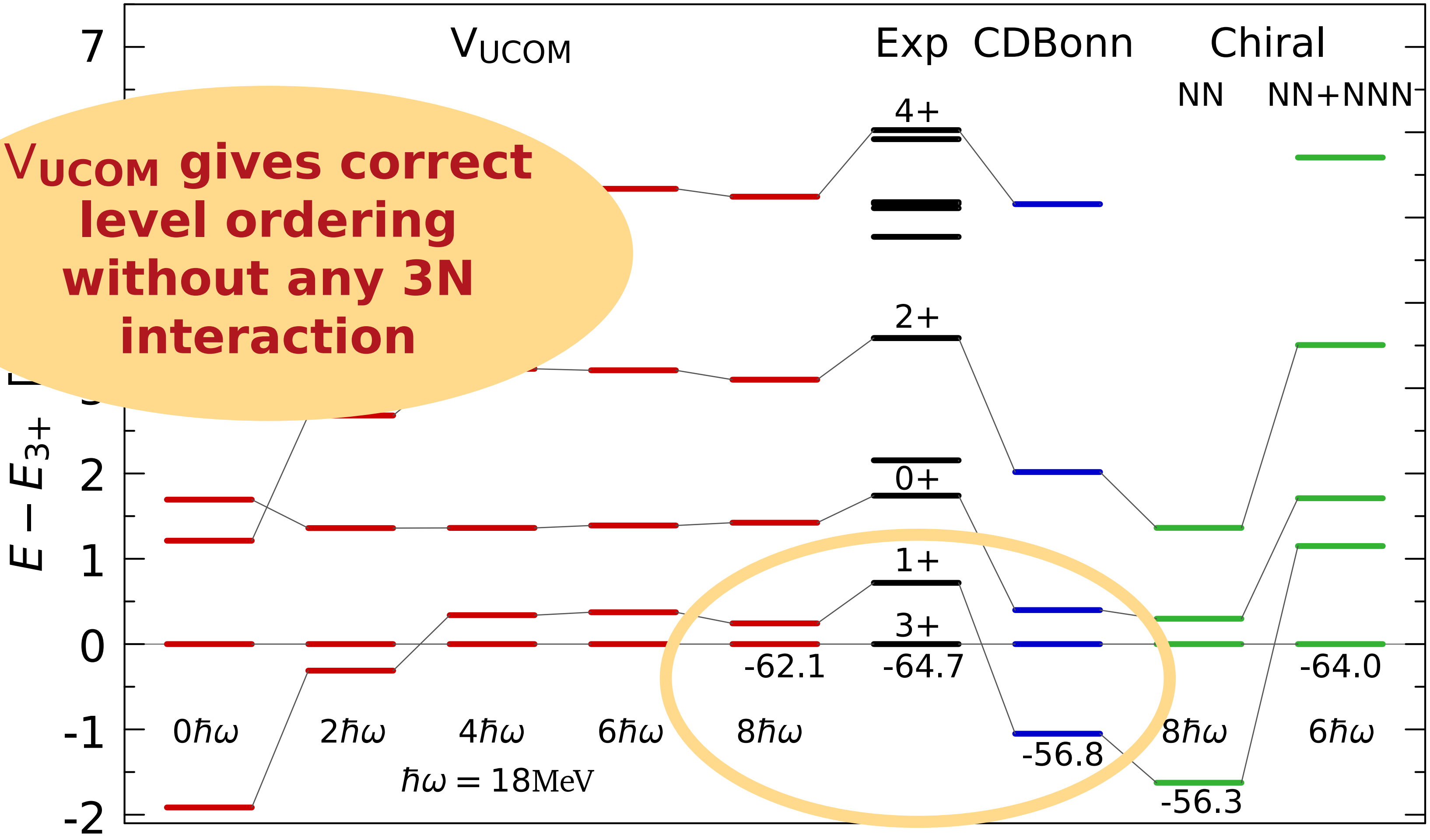
- **Tjon-line**: $E(^4\text{He})$ vs. $E(^3\text{H})$ for phase-shift equivalent NN-interactions
- change of C_{Ω}-correlator range results in shift along Tjon-line

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

^{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 — Phys. Rev. C 79, 064324 (2009)
Roth, Gour & Piecuch — Phys. Lett. B 679, 334 (2009)
Roth, Gour & Piecuch — Phys. Rev. C 79, 054325 (2009)
Roth & Navrátil — Phys. Rev. Lett. 99, 092501 (2007)

Importance Truncated NCSM

- converged NCSM calculations are essentially re… stricted to p-s…
- full 10 o… for ^{16}O r… (basis dim…

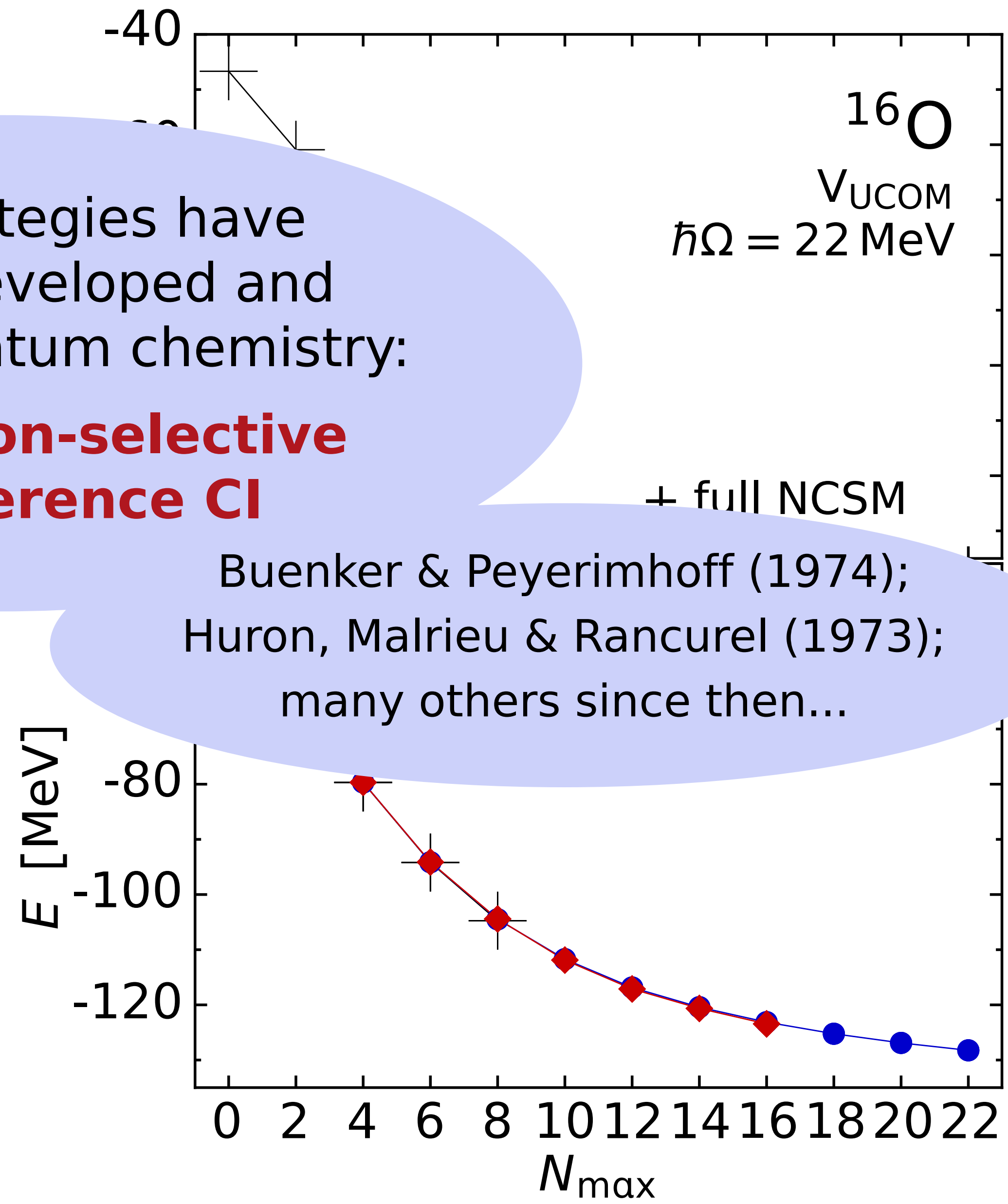
similar strategies have first been developed and applied in quantum chemistry:

configuration-selective multireference CI

Buenker & Peyerimhoff (1974);
Huron, Malrieu & Rancurel (1973);
many others since then...

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

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

- 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] or IT-CI[i]

- simple iterative scheme for arbitrary many-body model spaces

✪ 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 $|\Psi_{\text{ref}}\rangle$

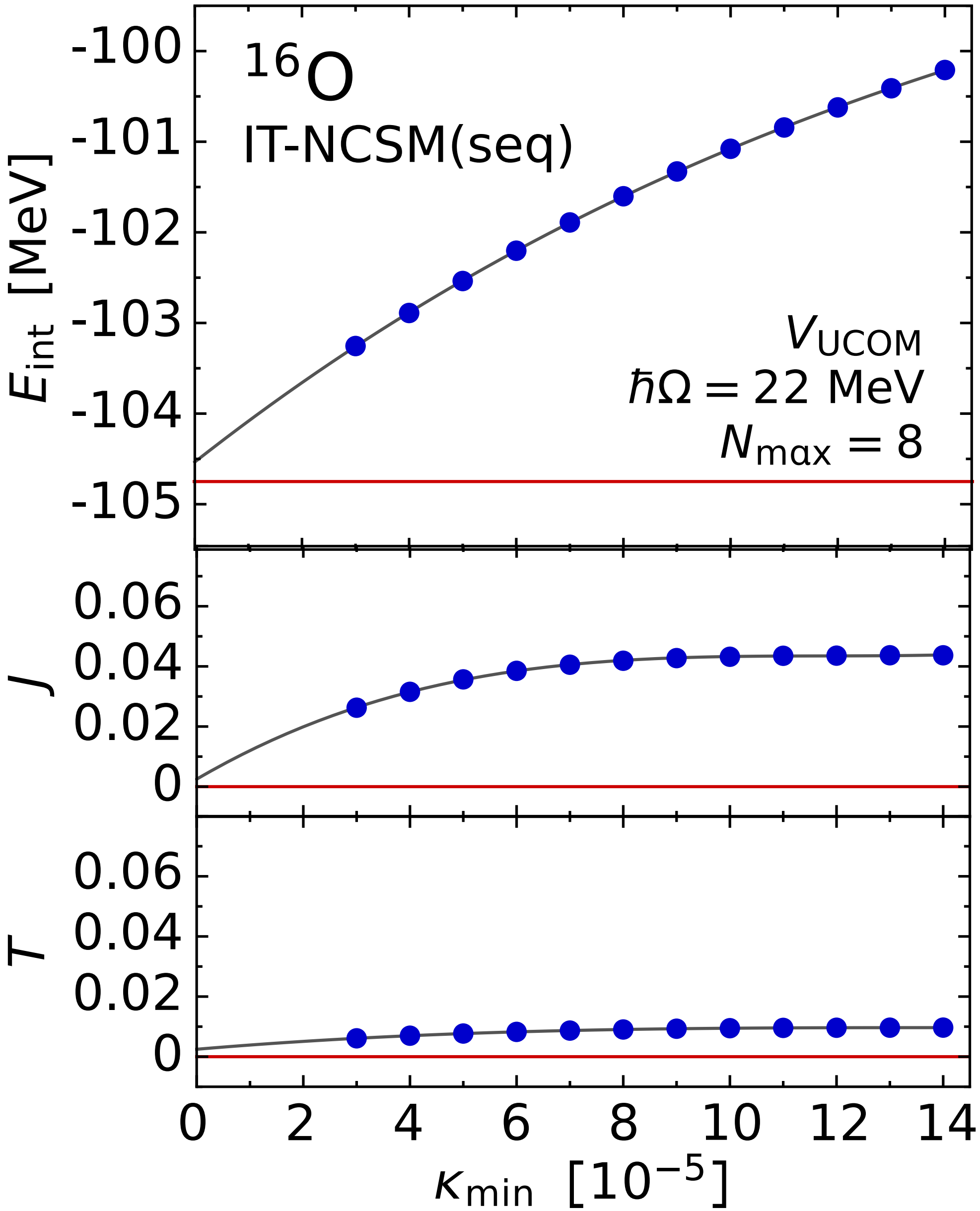
❶ construct importance truncated ... r $N_{\max} + 2$

... 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 Dependence

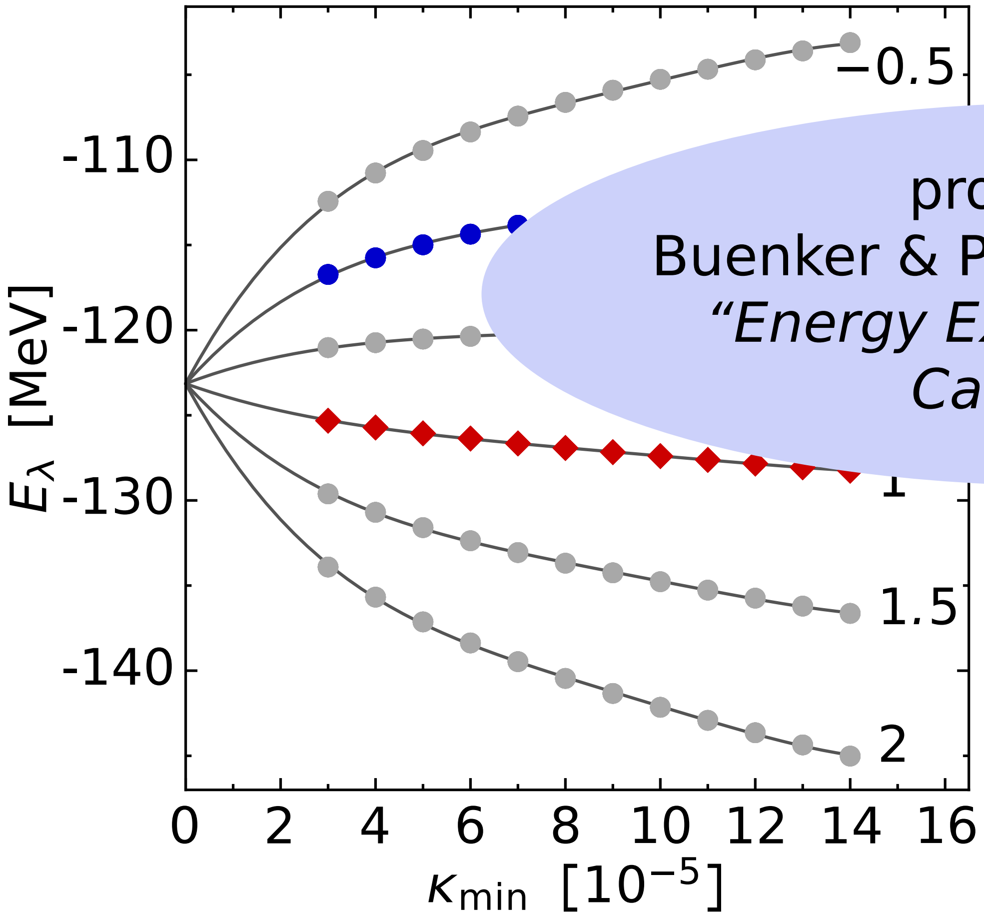


- do calculations for a **sequence of importance thresholds** κ_{min}
- observables show smooth threshold dependence
- systematic approach to the **full NCSM limit**
- use **a posteriori extrapolation** $\kappa_{min} \to 0$ of observables to account for effect of excluded configurations

Constrained Threshold Extrapolation

^{16}O, IT-NCSM(seq)

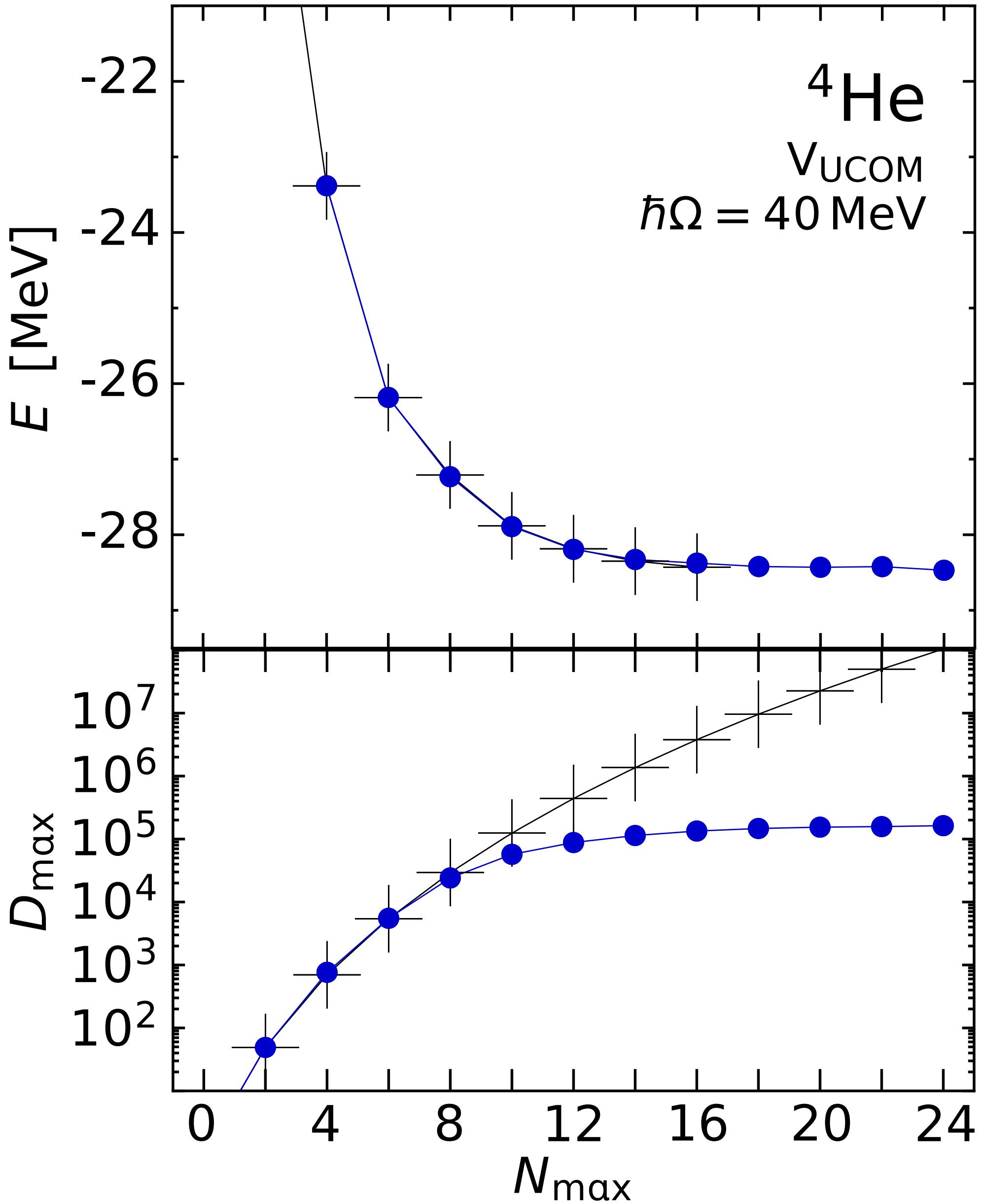
V_{UCOM}, $\hbar\Omega = 22\,\text{MeV}$, $N_{max} = 16$



- estimate energy contribution of **excluded states** perturbatively ➔ $\Delta_{excl}(\kappa_{min})$
- ...**neous fit** of combined ... $\lambda\Delta_{excl}(\kappa_{min})$ for set of λ-values with the constraint $E_\lambda(0) = E_{extrap}$
- **robust threshold extrapolation** with error bars determined by variation of the λ set

proposed by
Buenker & Peyerimhoff (1975):
"Energy Extrapolation in CI Calculation"

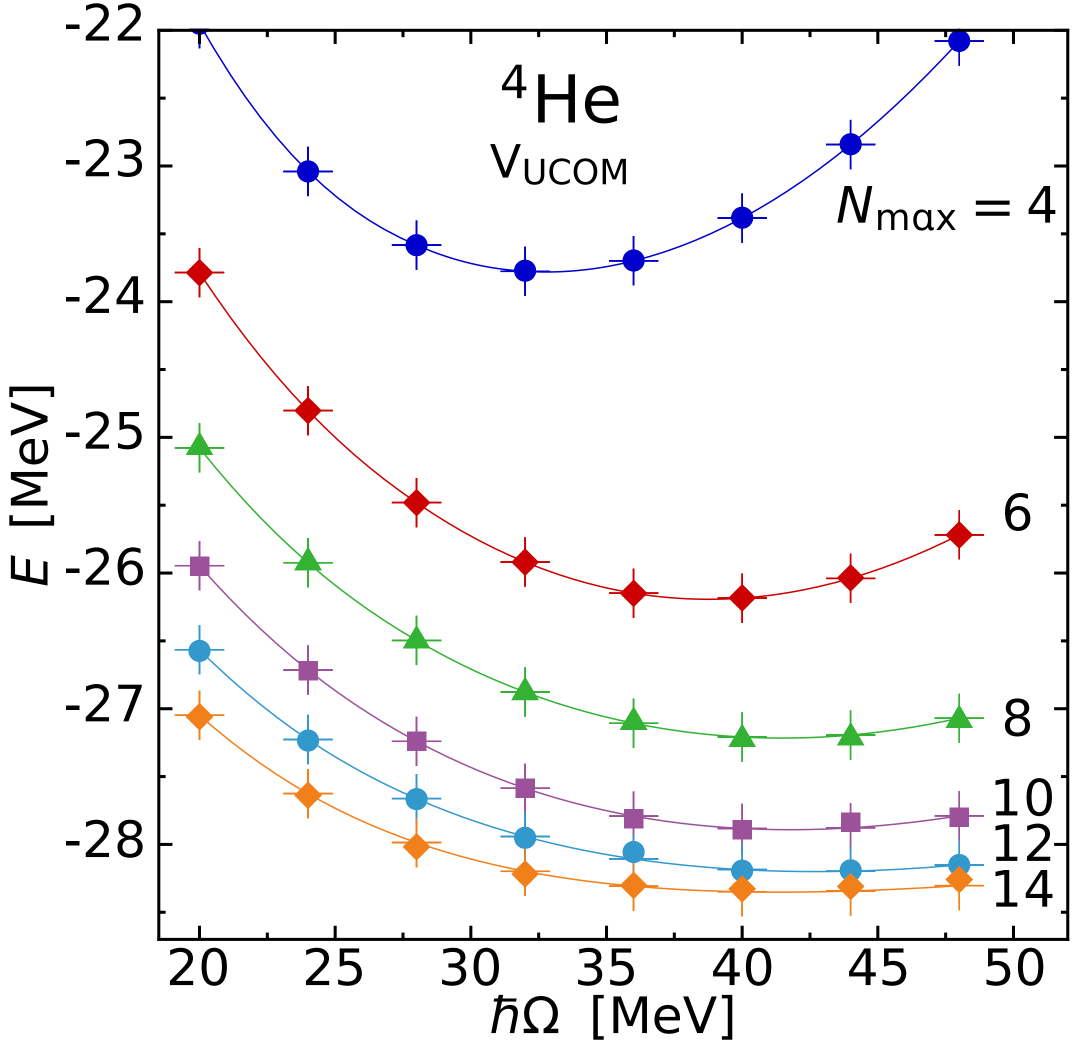
^{4}He: Importance-Truncated NCSM



- **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)

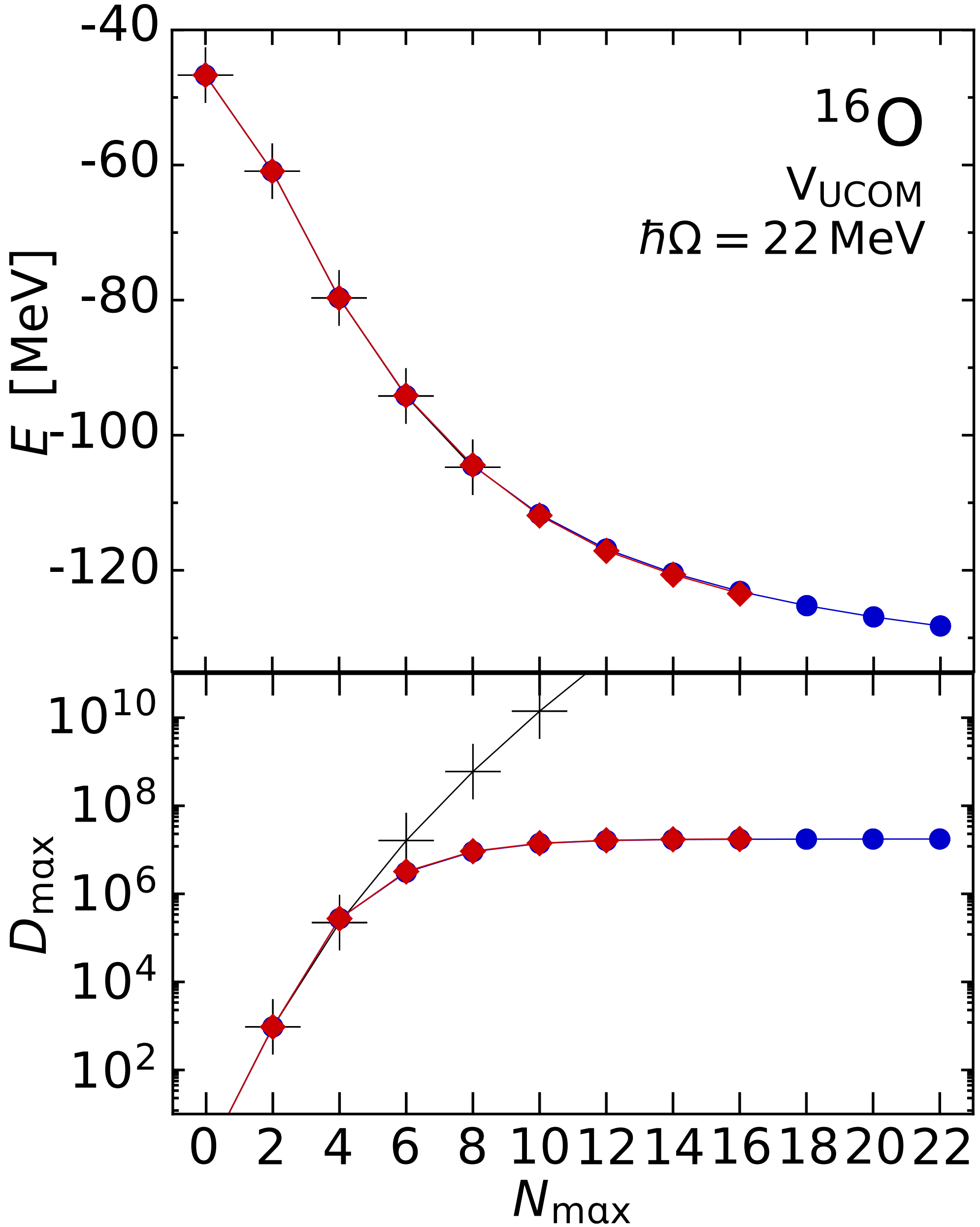
^{4}He: Importance-Truncated NCSM



- **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 $\hbar\Omega$

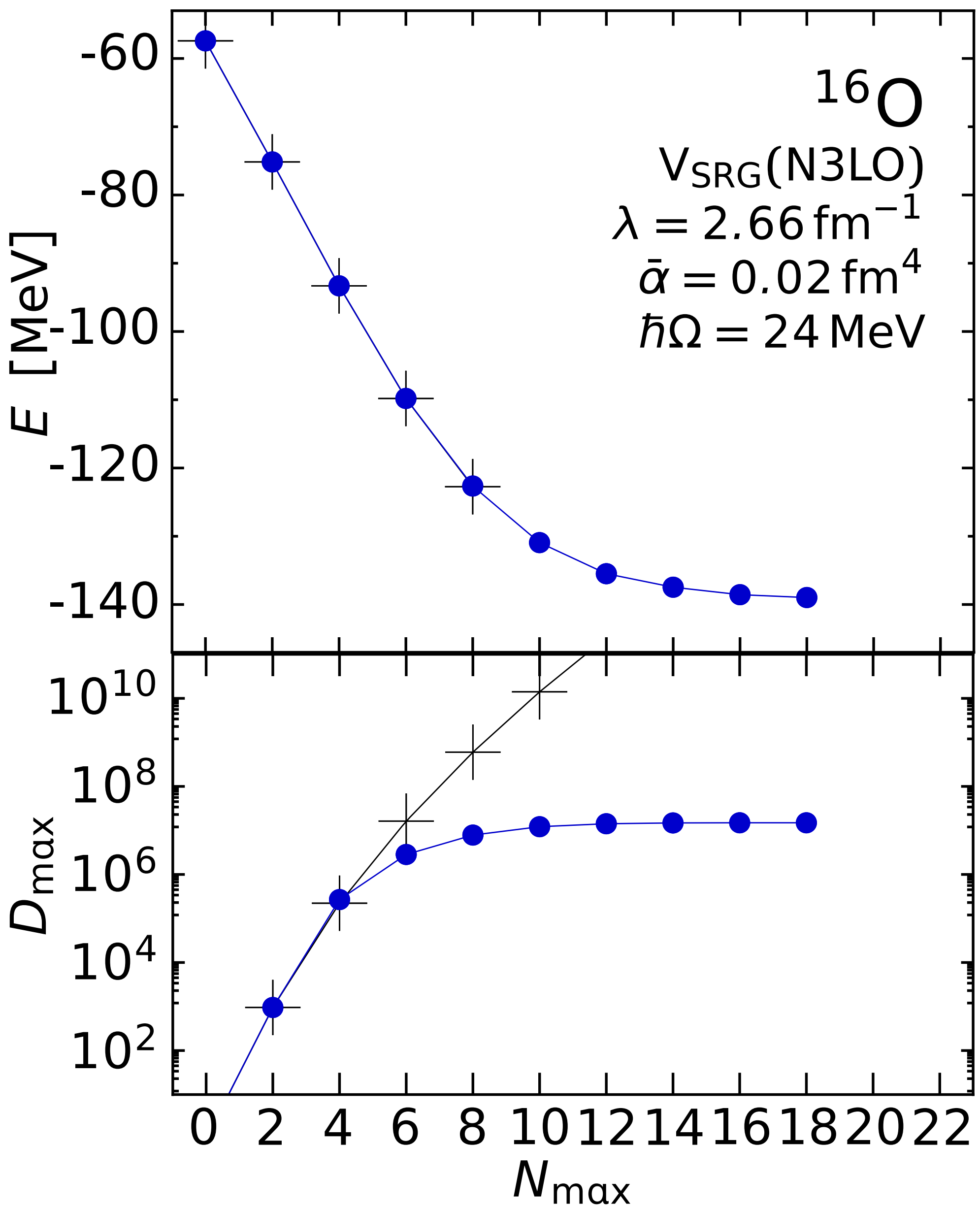
+ full NCSM
● IT-NCSM(seq)

^{16}O: Importance-Truncated NCSM



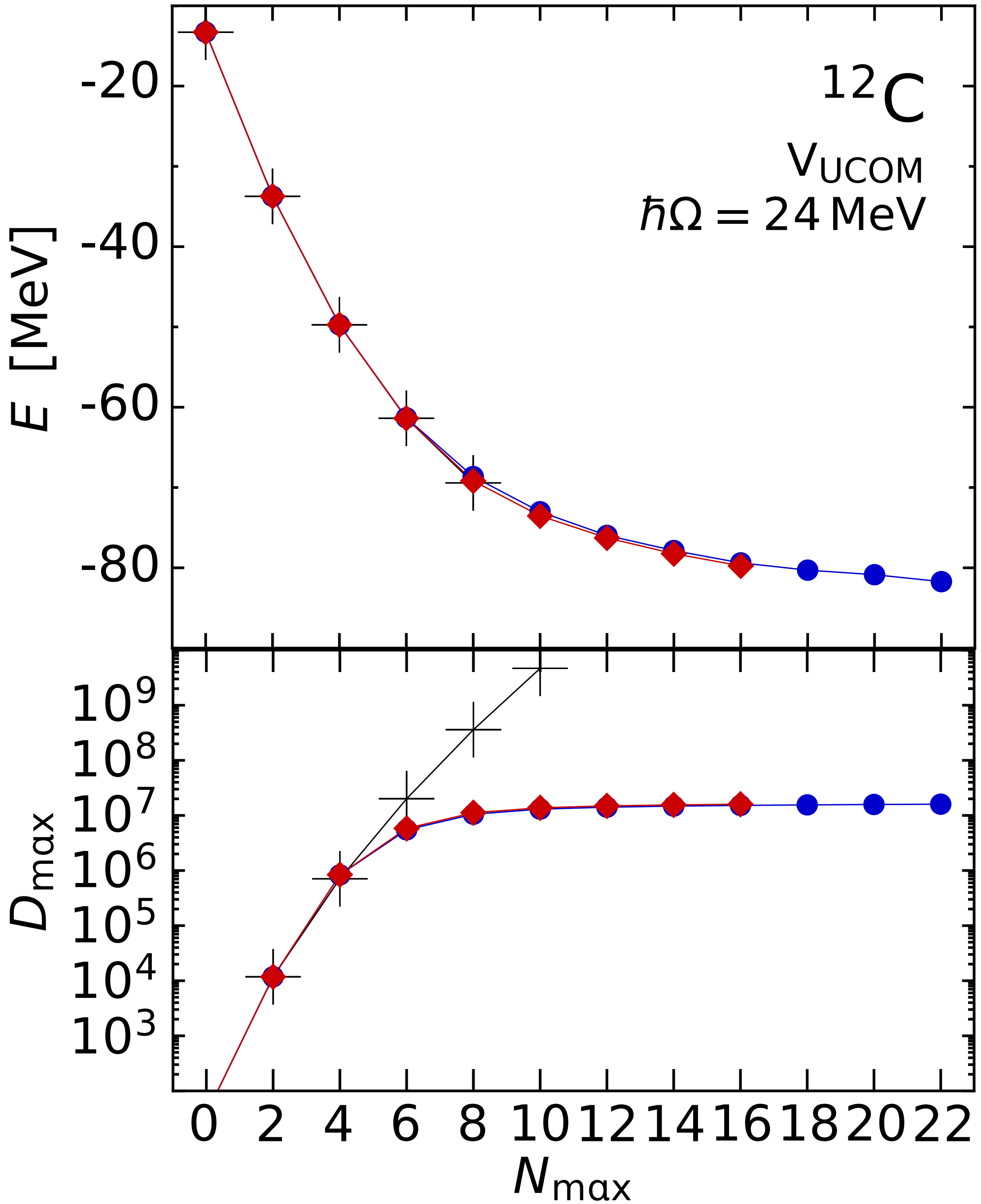
- IT-NCSM(seq) provides **excellent agreement with full NCSM** calculation
- dimension reduced by **several orders of magnitude**
- possibility to go **way beyond** the domain of the full NCSM

^{16}O: Importance-Truncated NCSM



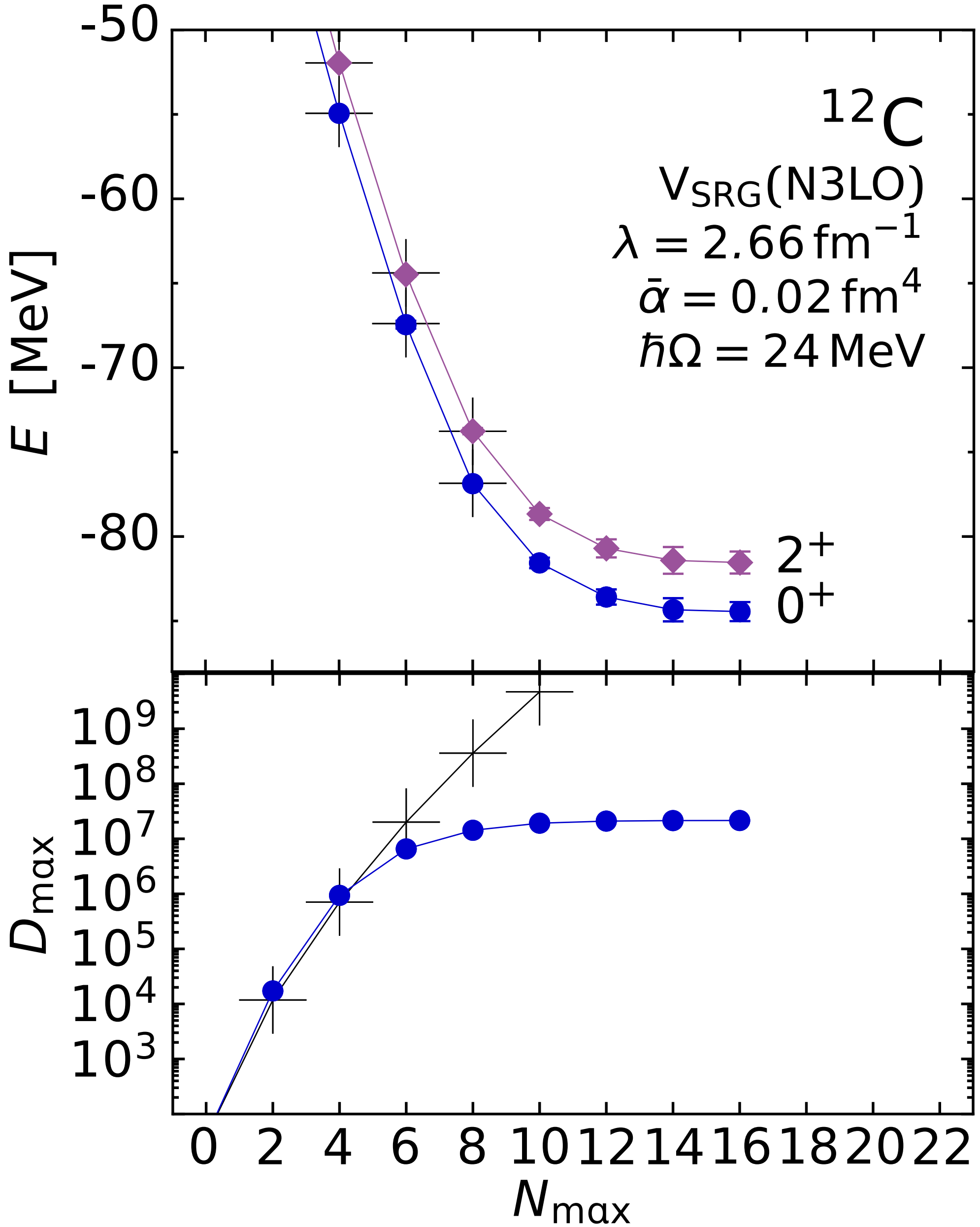
- **SRG-evolved N3LO potential** provides a much better convergence behavior
- nevertheless, $N_{max} \leq 8$ calculations are not sufficient
- non-exponential behavior observed with V_{UCOM} is really due to interaction

^{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

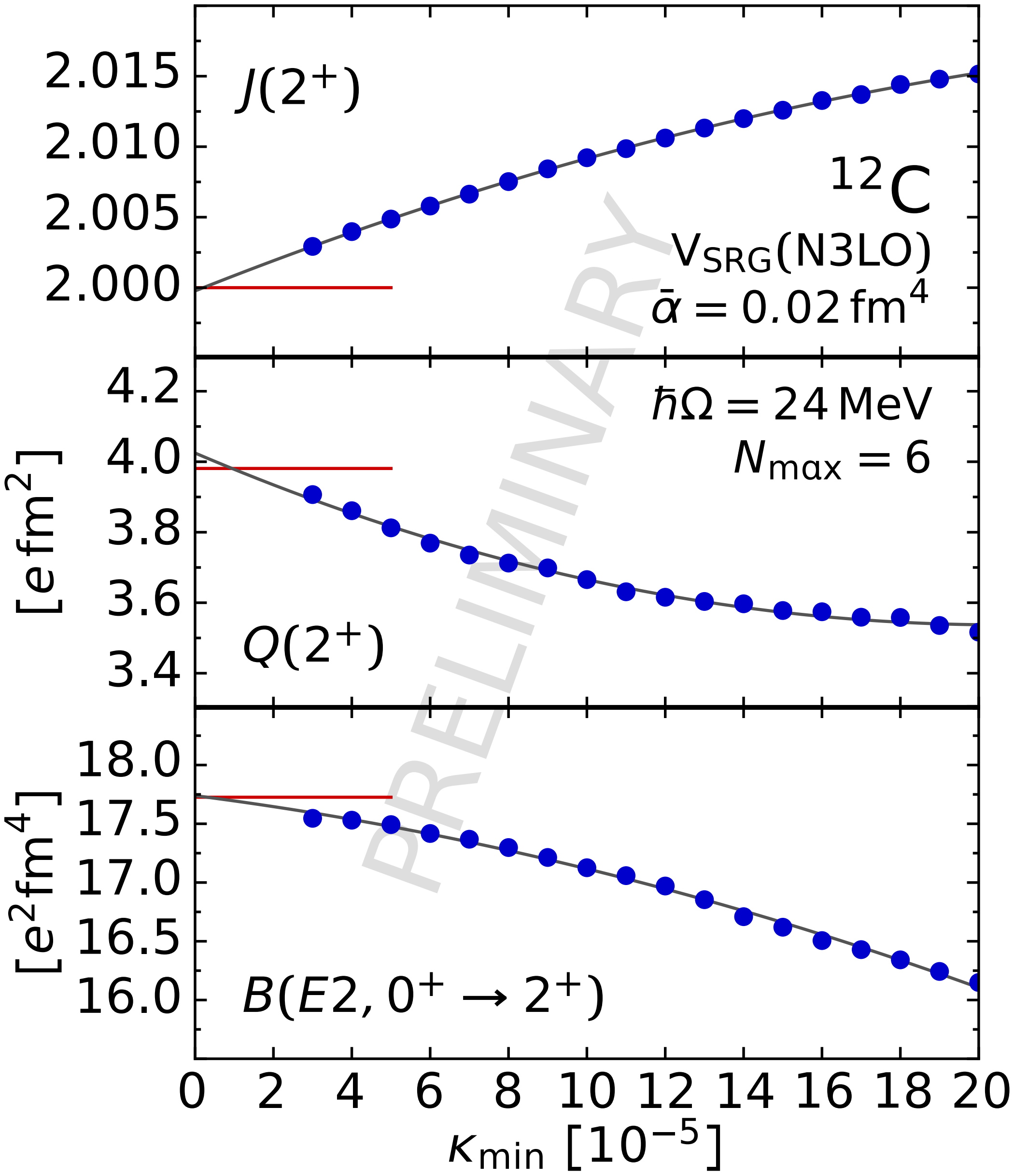
^{12}C: IT-NCSM for Excited States



- **target ground & excited states** simultaneously
  - separate importance measure $\kappa_\nu^{(n)}$ for each target state
  - basis state is included if $|\kappa_\nu^{(n)}| \geq \kappa_{\text{min}}$ for any n
- dimension of importance truncated space **grows linearly** with # of target states

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

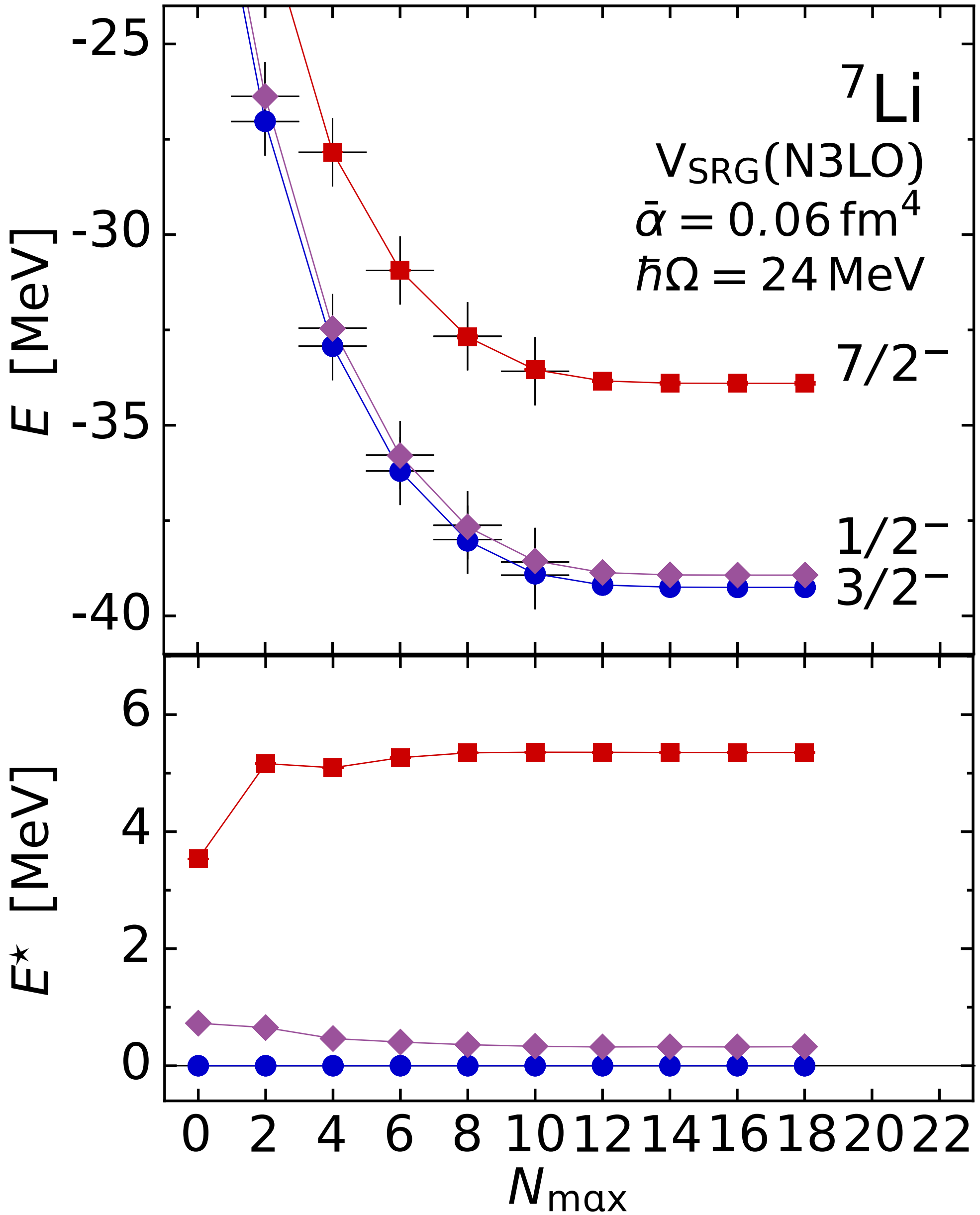
^{12}C: IT-NCSM for Spectroscopy



- access to **spectroscopic observables** via eigenstates
- multipole moments, transition strengths, transition formfactors, densities,...
- simple threshold extrapolation essentially **reproduces full NCSM results**

systematic spectroscopy in p- and sd-shell with large $N_{max}\hbar\Omega$ spaces

^{7}Li: IT-NCSM for Odd Nuclei



- IT-NCSM(seq) treats a ground state & low-lying excited states for open- and closed-shell nuclei **on the same footing**
- **excellent agreement with full NCSM** calculations in all cases

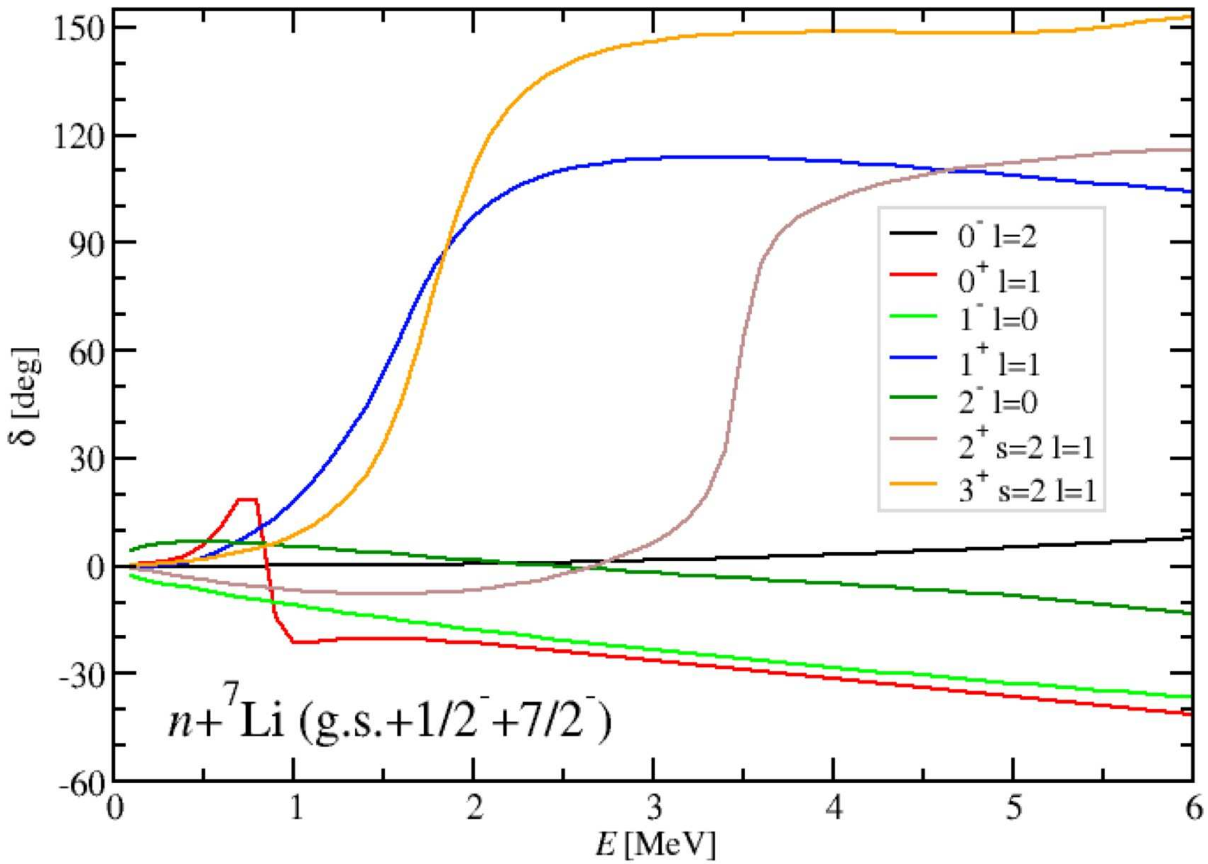
+ full NCSM

●♦■ IT-NCSM(seq), $C_{min} = 0.0002$

RGM & IT-NCSM: Ab Initio Reactions

with Petr Navrátil & Sofia Quaglioni (LLNL)

- **IT-NCSM wave function as input for RGM** (Resonating Group Method) calculations of low-energy nucleon-nucleus scattering



- using 3 lowest ^{7}Li states
- so-far up to $N_{max} = 14$, here $N_{max} = 8$
- phase-shifts with full NCSM and IT-NCSM input agree
- 2 bound states for ^{8}Li
- 4 resonances: 3^+ and 1^+ are known, 0^+ and 2^+ resonances are predictions

IT-NCSM: Pros and Cons

- ✔ **fulfills variational principle** & Hylleraas-Undheim theorem
- ✔ **no center-of-mass contamination** induced by importance truncation in $N_{\text{max}}\hbar\Omega$ space
- ✔ constrained **threshold extrapolation** $\kappa_{\text{min}} \to 0$ 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
- **approximate size-extensivity** after threshold extrapolation in IT-NCSM(seq) or IT-NCSM[i_{conv}] – **no explicit *npnh* truncation**
- ✘ computationally still demanding

Computational Many-Body Methods

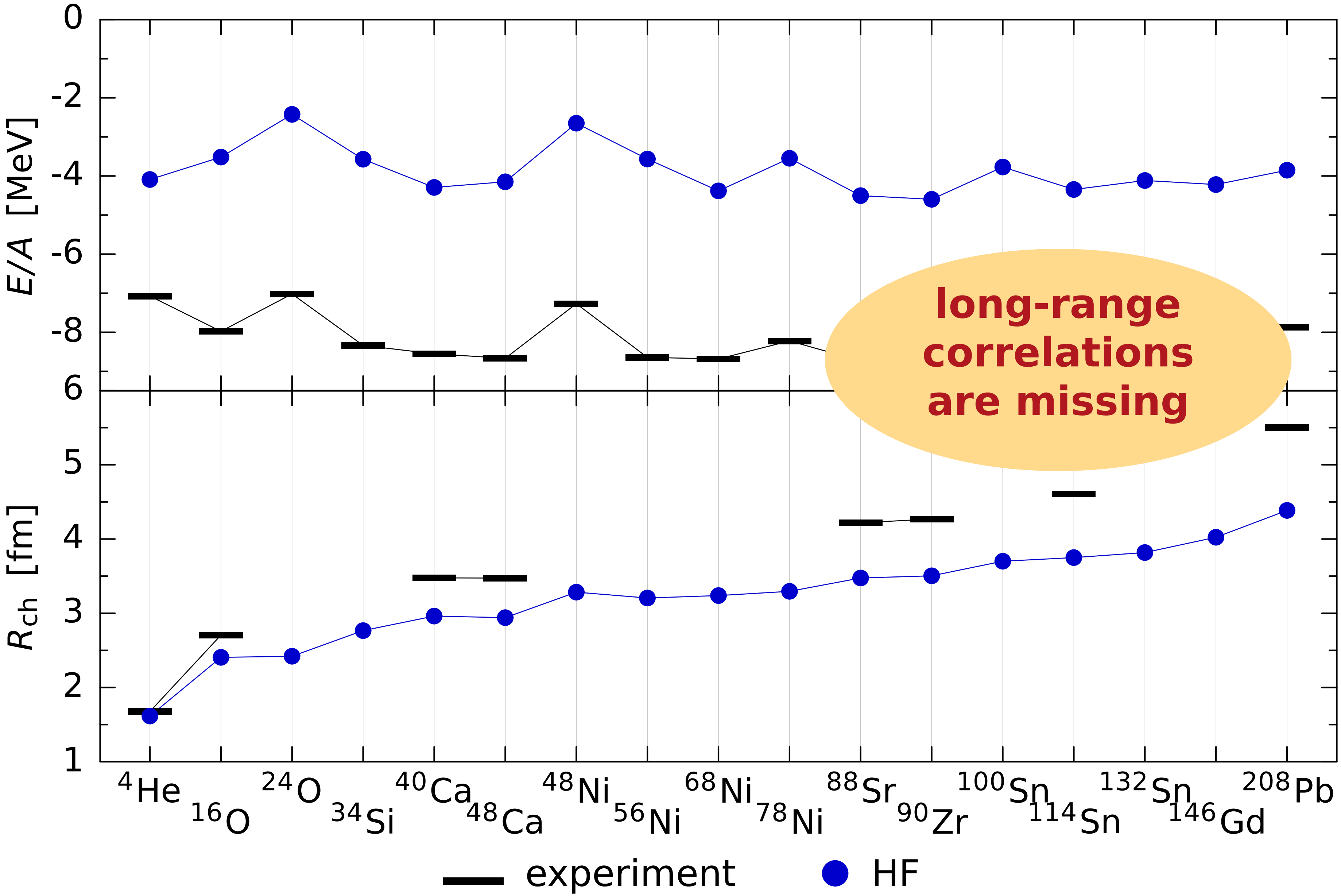
Other Options...

Other Options...

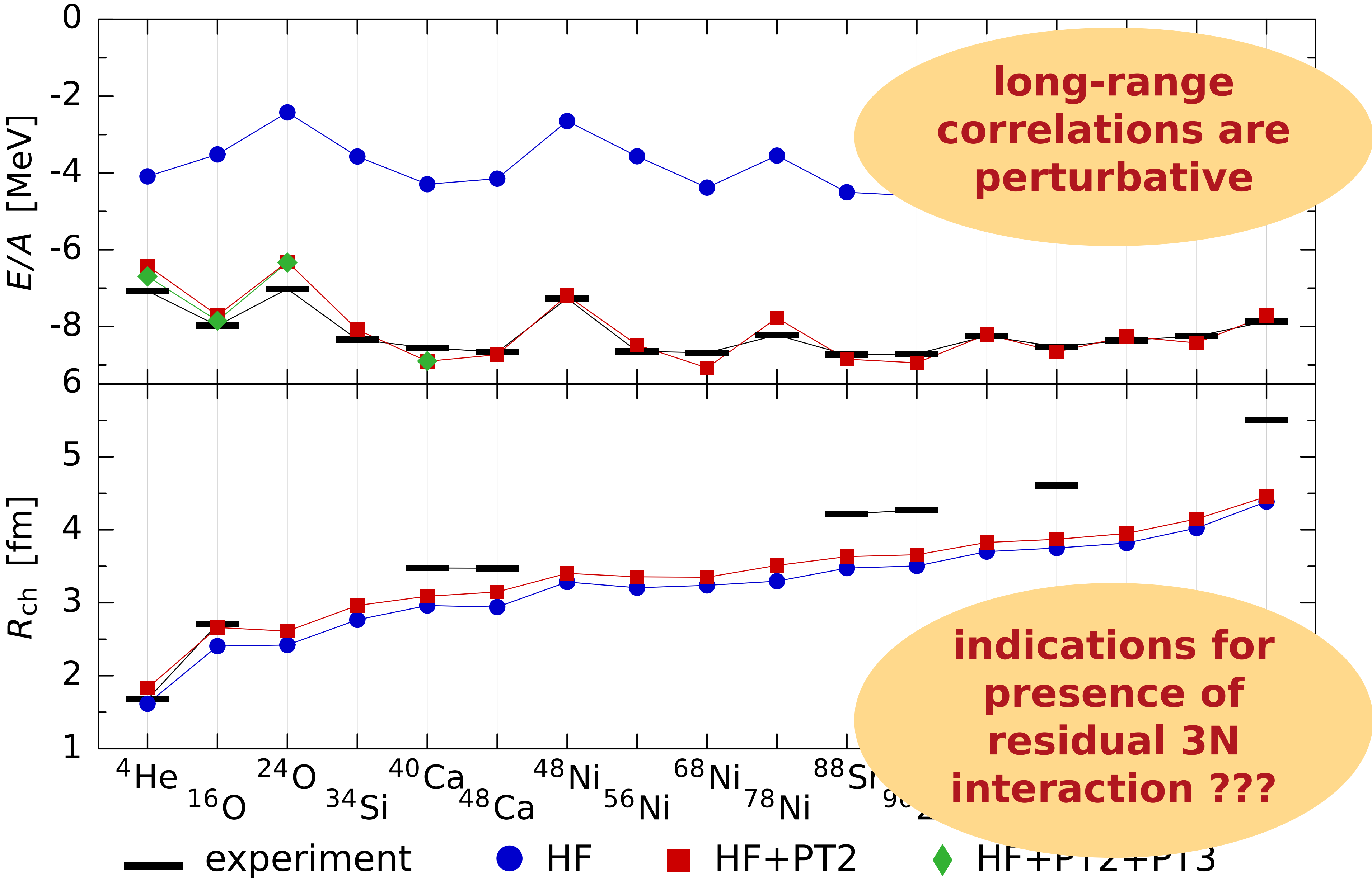
similarity transformed interactions (e.g. V_{UCOM}) provide universal input for various many-body methods

- exact few-body methods
- coupled-cluster method
- Hartree-Fock & many-body perturbation theory
- RPA & Second-RPA
- FMD with projection & configuration mixing
- NCSM + Resonating Group Method

Hartree-Fock with V_{UCOM}



Perturbation Theory with V_{UCOM}



Conclusions

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

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

Epilogue

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    Institut für Kernphysik, TU Darmstadt
  - P. Navrátil, S. Quaglioni

    Lawrence Livermore National Laboratory, USA
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