New Frontiers in Nuclear Structure Theory

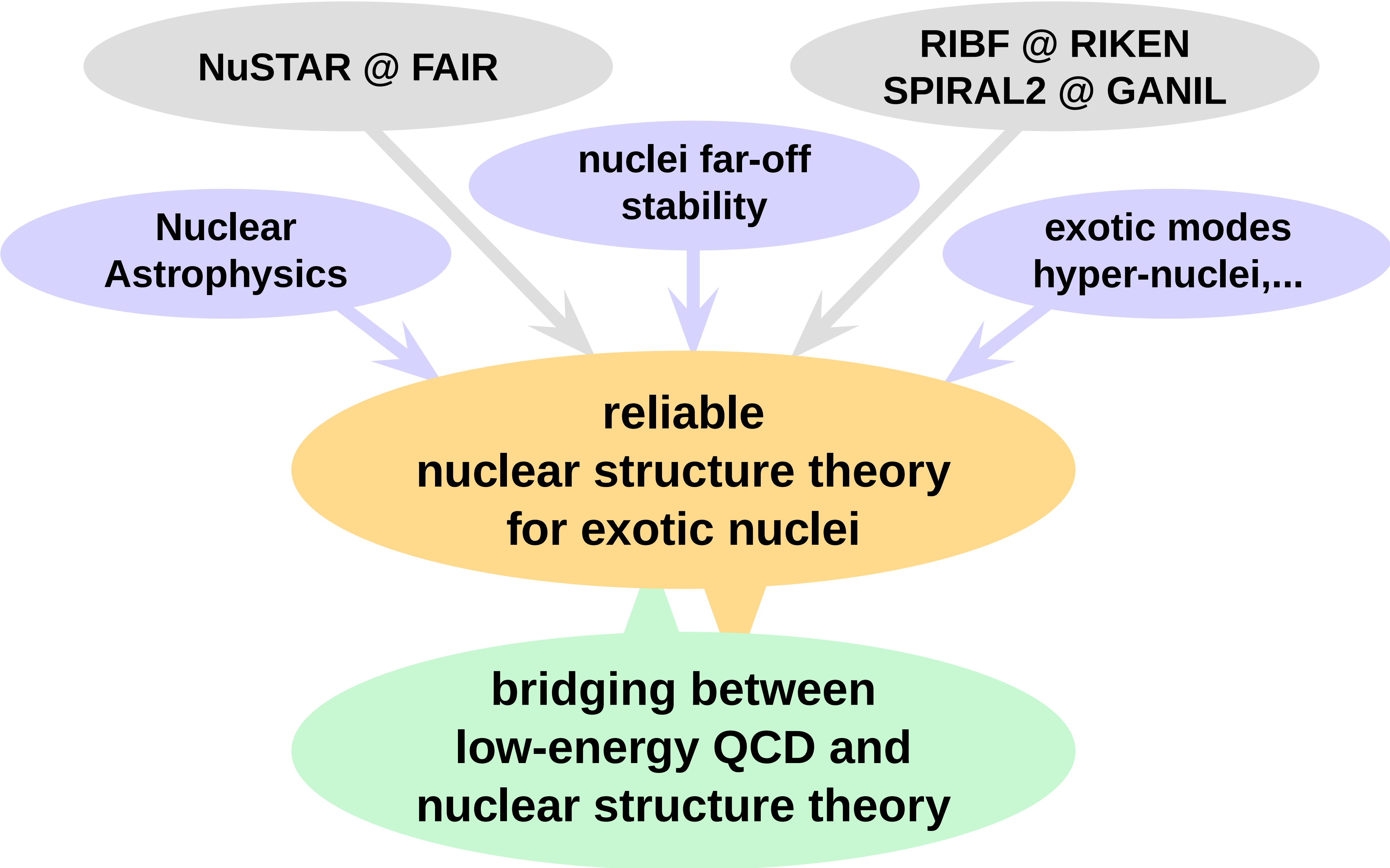
Robert Roth

Institut für Kernphysik
Technische Universität Darmstadt

Overview

- Motivation
- Modern Effective Interactions
  - Unitary Correlation Operator Method
  - Similarity Renormalization Group
- Many-Body Methods I
  - No Core Shell Model & Beyond
- Many-Body Methods II
  - Hartree-Fock & Beyond

Nuclear Structure in the 21st Century



Modern Nuclear Structure Theory

Nuclear Structure

Many-Body Approximations

***ab initio* Approaches**

Effective Interactions

Density Functional Models

Realistic Potentials

Chiral Interactions

Low-Energy QCD

Realistic Interactions

- **QCD motivated**
  - symmetries, meson-exchange picture
  - chiral effective field theory
- **short-range phenomenology**
  - short-range parametrisation or contact terms
- **experimental two-body data**
  - scattering phase-shifts & deuteron properties reproduced with high precision
- **supplementary three-nucleon force**
  - adjusted to spectra of light nuclei

Argonne V18

CD Bonn

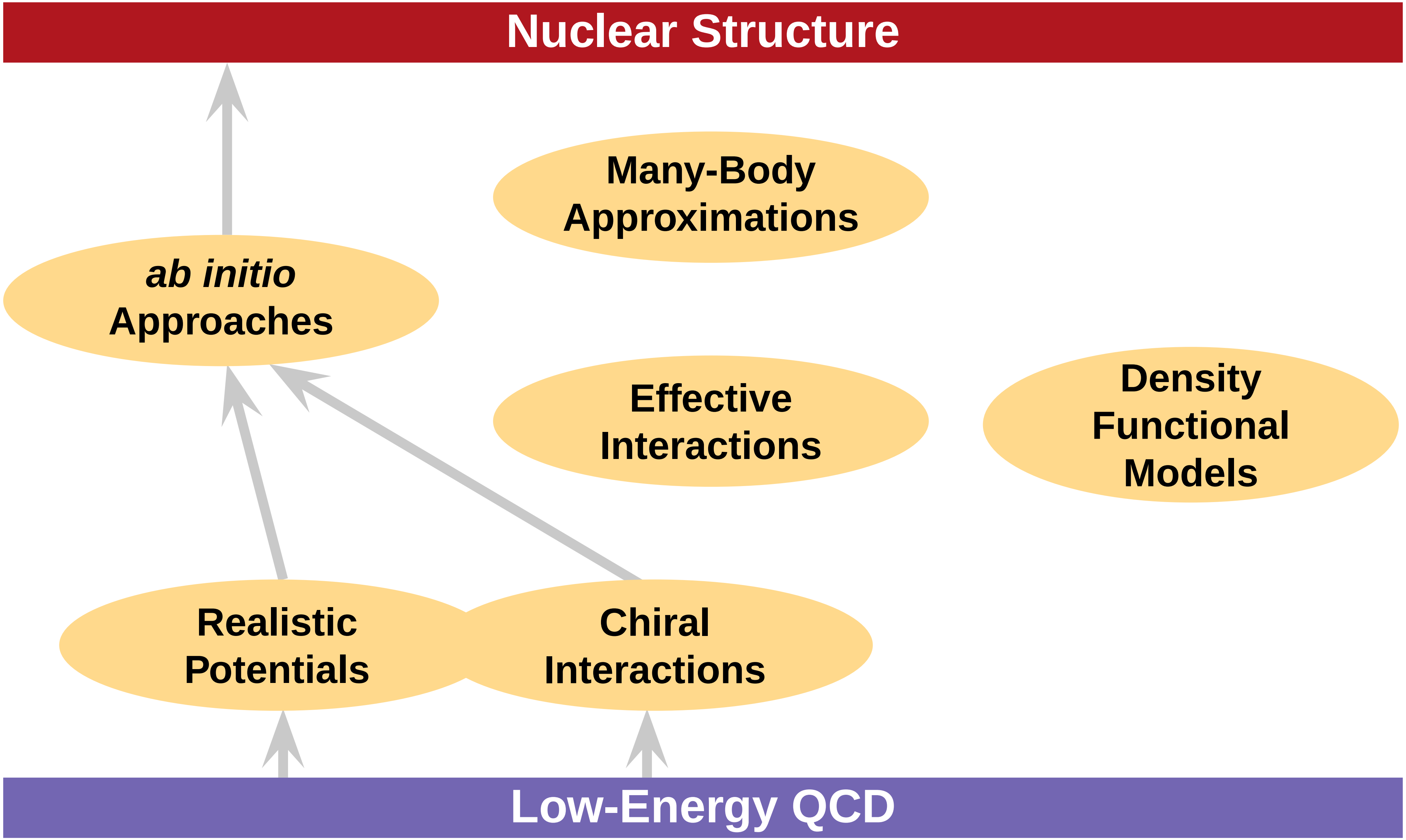
Nijmegen I/II

Chiral N3LO

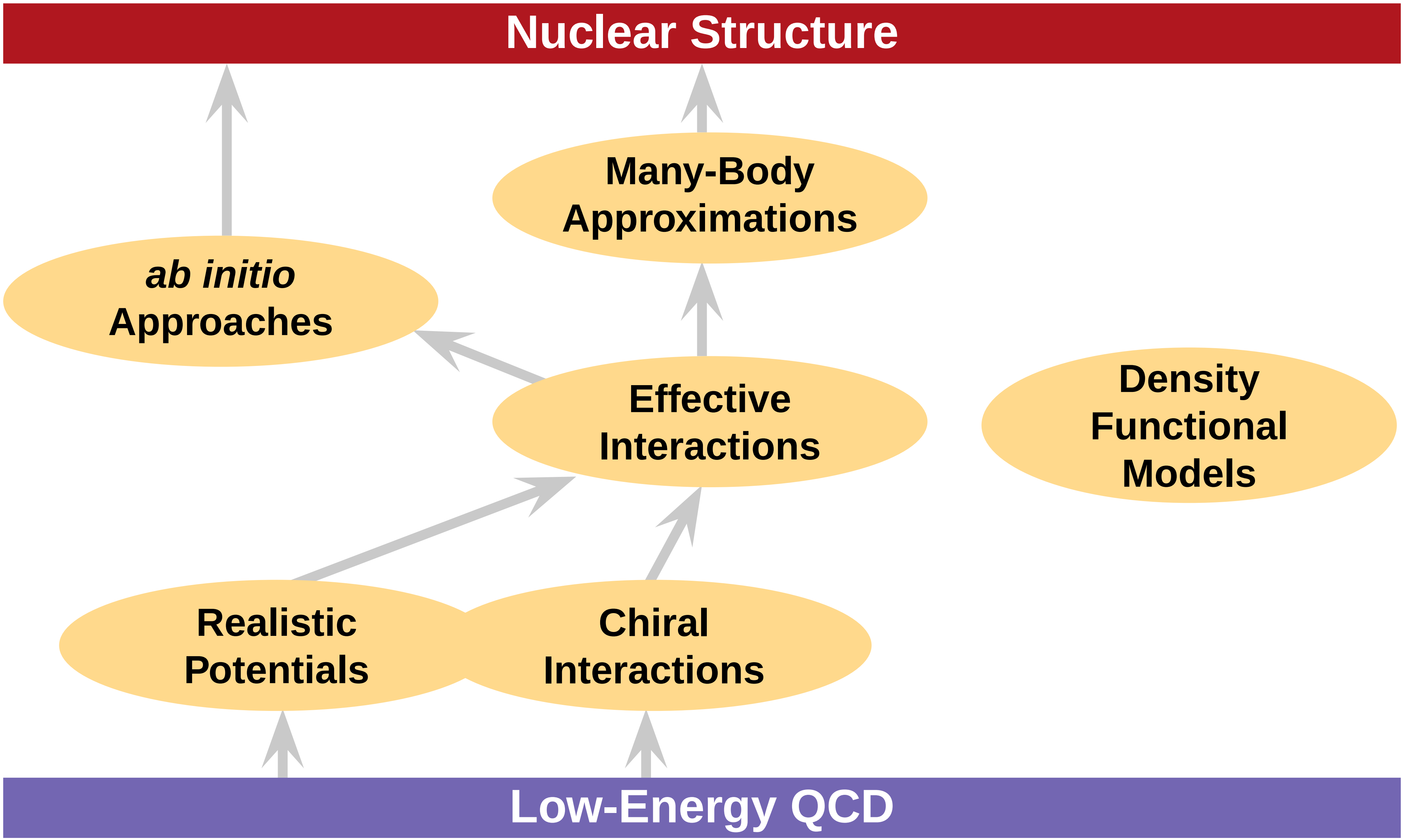
Argonne V18 +
Illinois 2

Chiral N3LO +
N2LO

Modern Nuclear Structure Theory



Modern Nuclear Structure Theory



Why Effective Interactions?

Realistic Potentials

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

Modern Effective Interactions

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

can be viewed as new realistic interaction

Many-Body Approximations

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

Modern Effective Interactions

UCOM vs. SRG

Modern Effective Interactions

Unitary Transformation

define a unitary operator C to describe the effect of correlations that cannot be handled by the model space

Correlated States

imprint short-range correlations onto uncorrelated many-body states

$$|\widetilde{\psi}\rangle = \mathrm{C}\ |\psi\rangle$$

Correlated Operators

adapt Hamiltonian and all other observables to uncorrelated many-body space

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

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

Unitary Correlation Operator Method

explicit ansatz for the correlation operator motivated by the **physics of short-range central and tensor correlations**

Central Correlator C_r

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

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

$$\mathrm{g}_r = \frac{1}{2}\big[s(\mathrm{r})\,\mathrm{q}_r + \mathrm{q}_r\,s(\mathrm{r})\big]$$

Tensor Correlator C_Ω

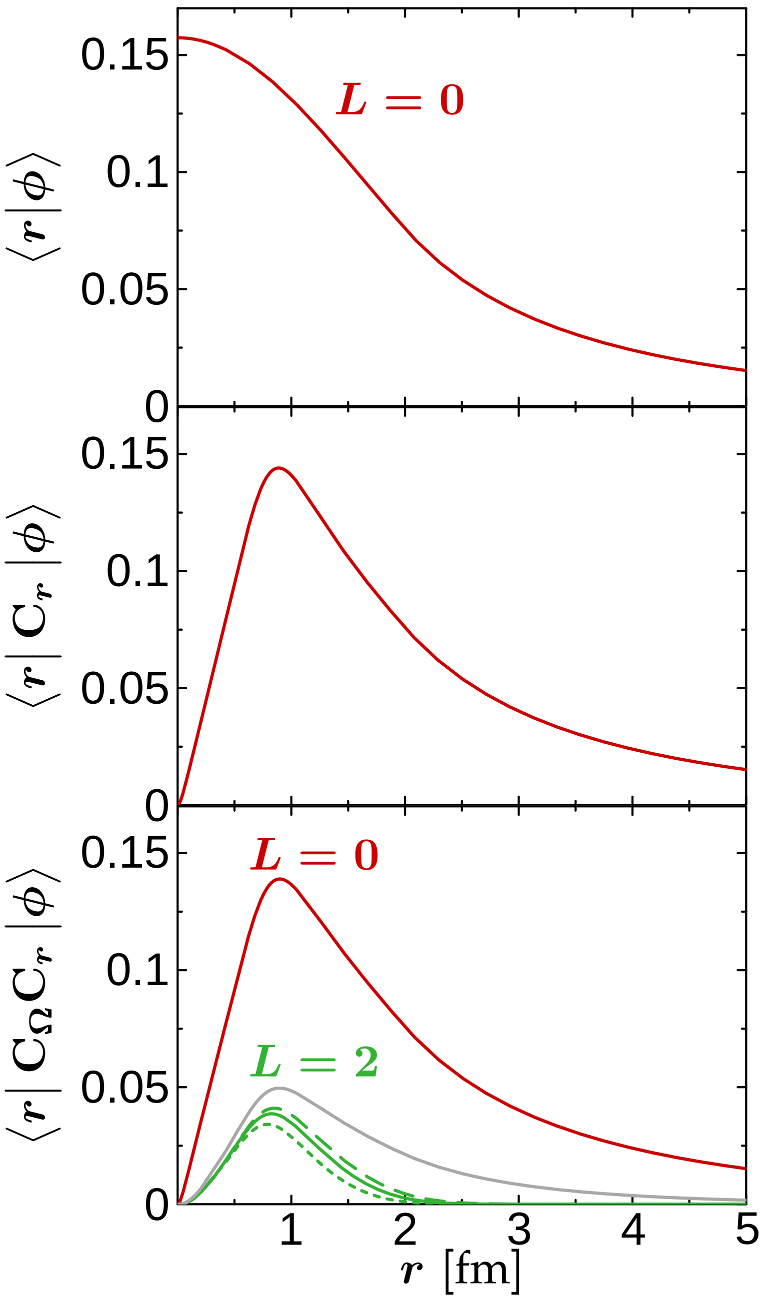
- angular shift depending on the orientation of spin and relative coordinate of a nucleon pair

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

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

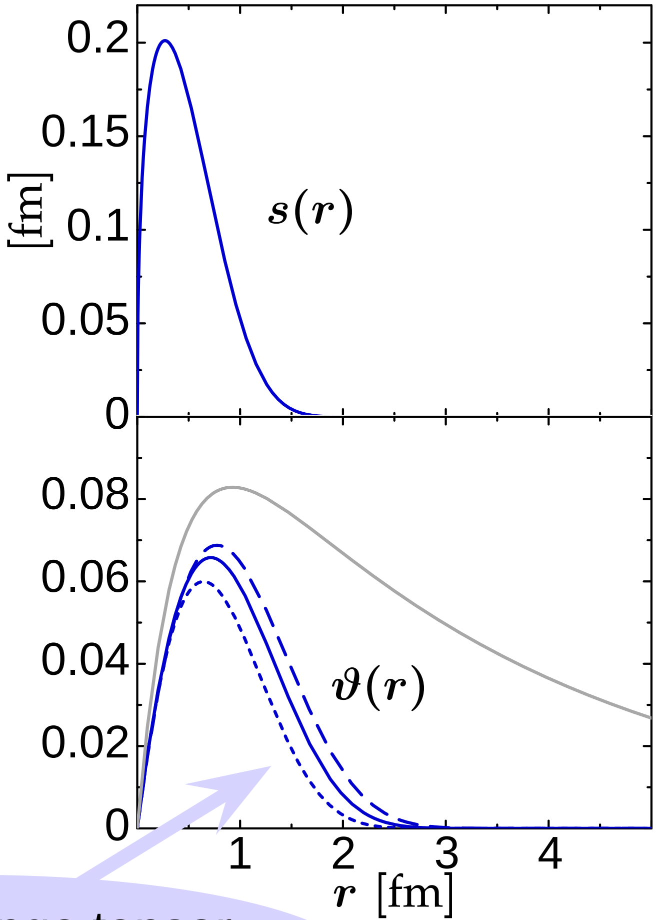
- $s(r)$ and $\vartheta(r)$ for given potential determined by energy minimization in the two-body system (for each S, T)

Correlated States: The Deuteron



central correlations

tensor correlations



only short-range tensor correlations treated by C_Ω

Similarity Renormalization Group

unitary transformation of the **Hamiltonian to a band-diagonal form** with respect to a given uncorrelated many-body basis

Flow Equation for Hamiltonian

- evolution equation for Hamiltonian

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

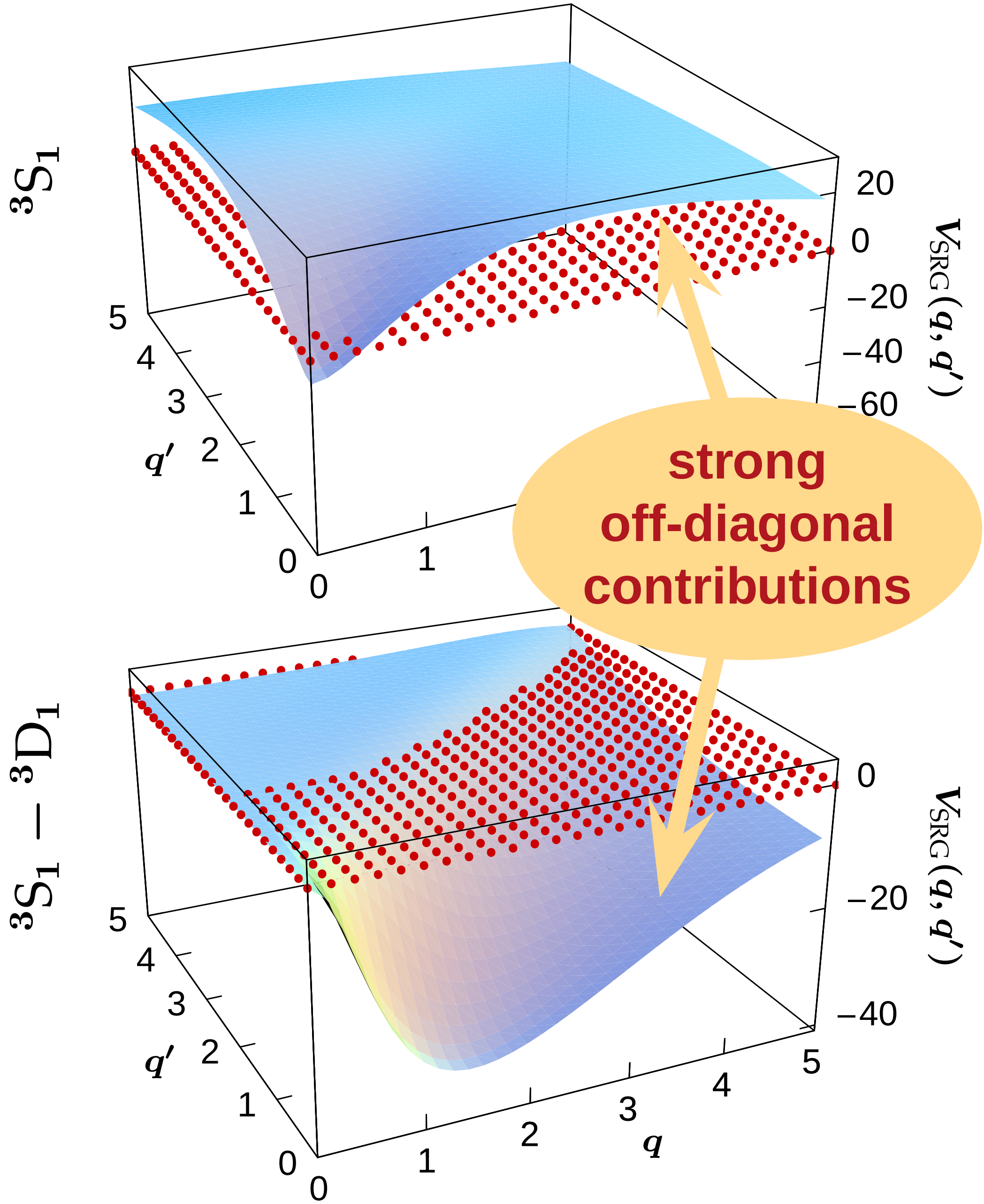
- dynamical generator defined as commutator with the operator in whose eigenbasis H shall be diagonalized

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

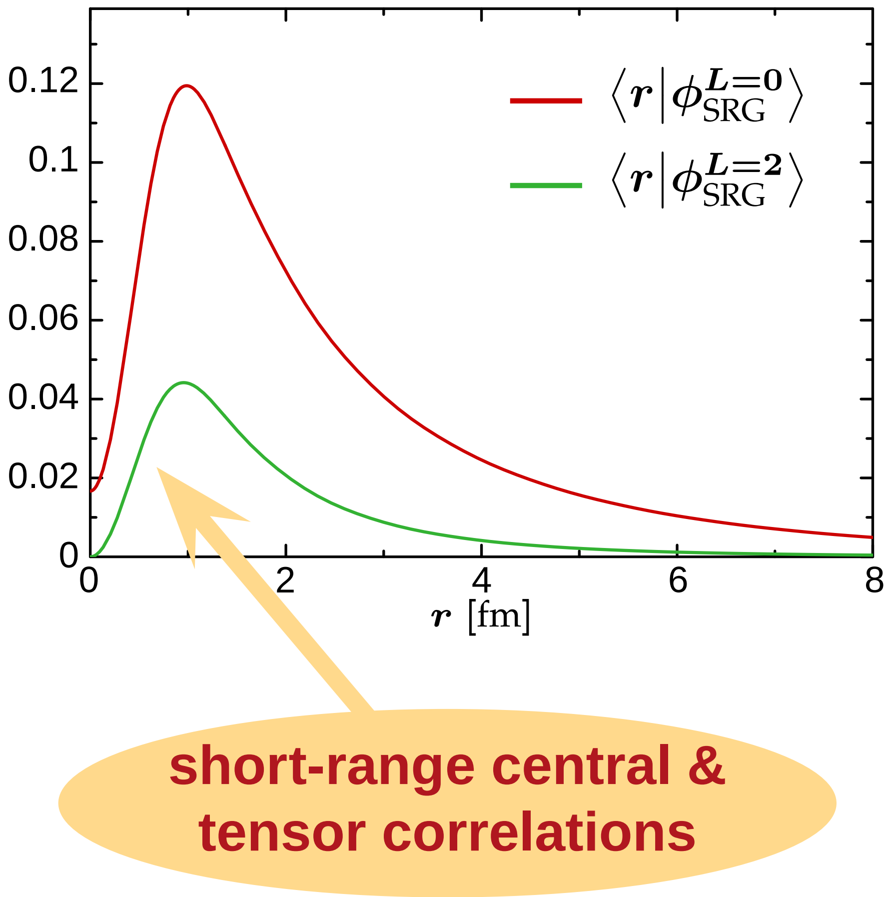
- $\eta(0)$ has the same structure as the UCOM generators g_r and g_Ω

[Bogner et al., nucl-th/0611045; Hergert et al., nucl-th/0703006]

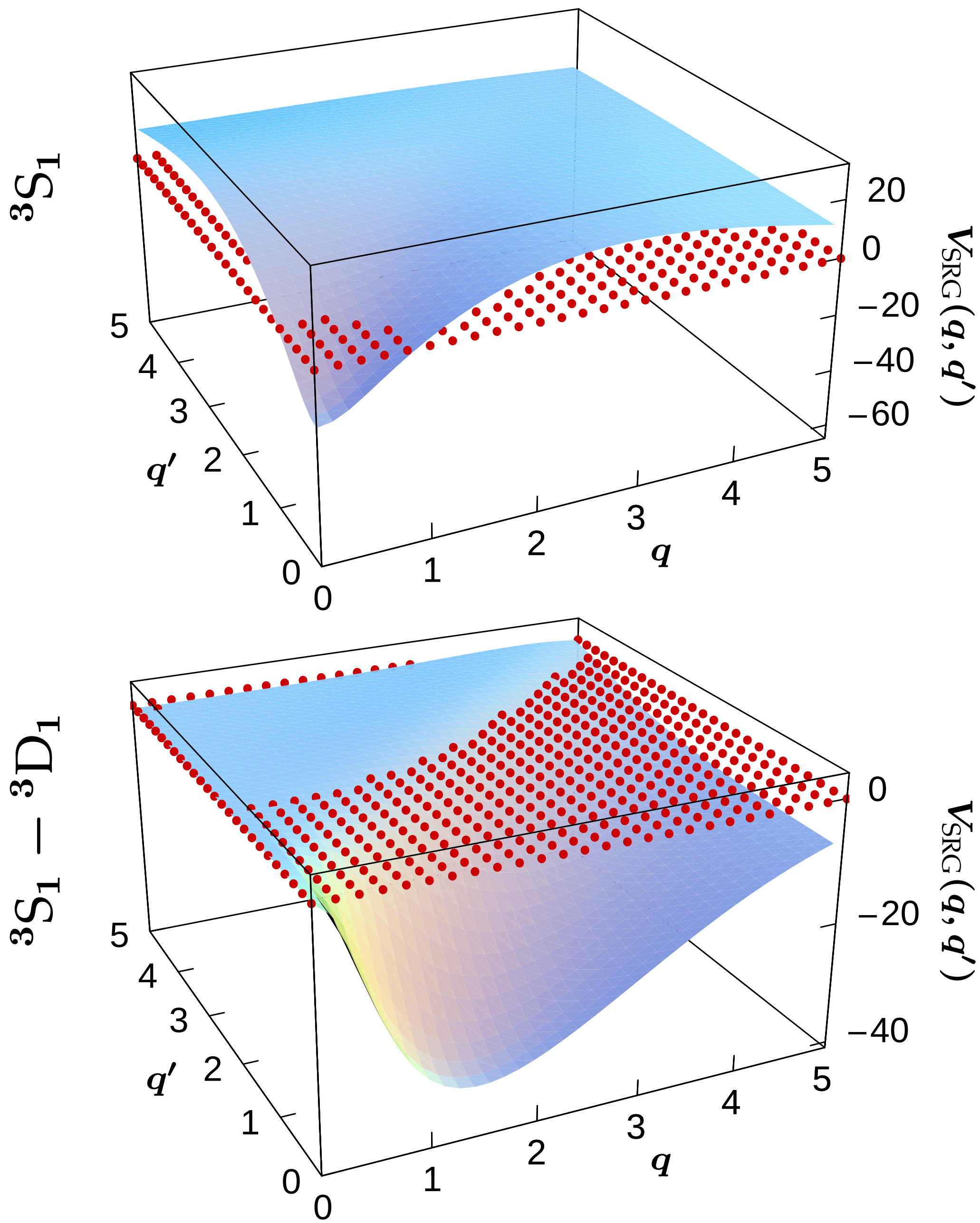
SRG Evolution: The Deuteron



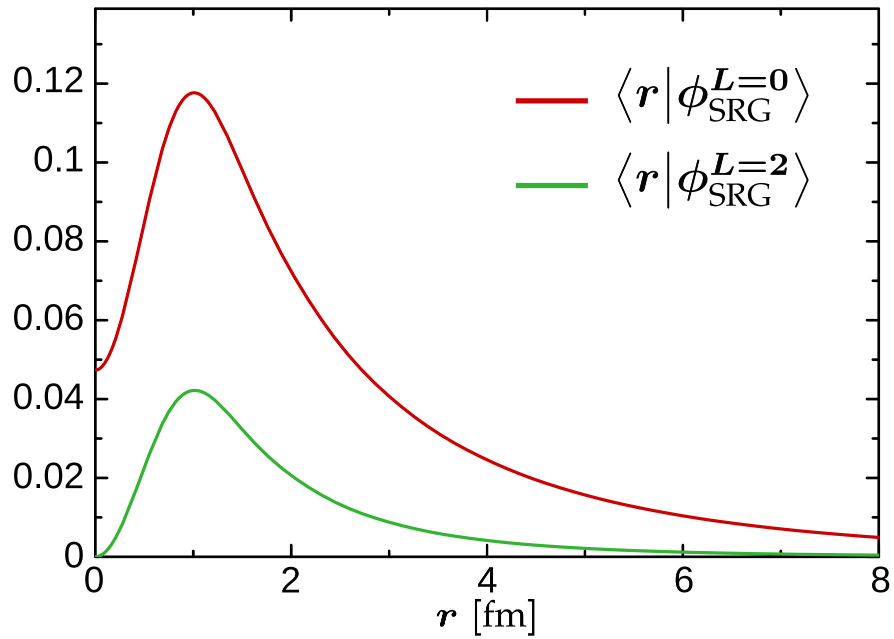
bare AV18



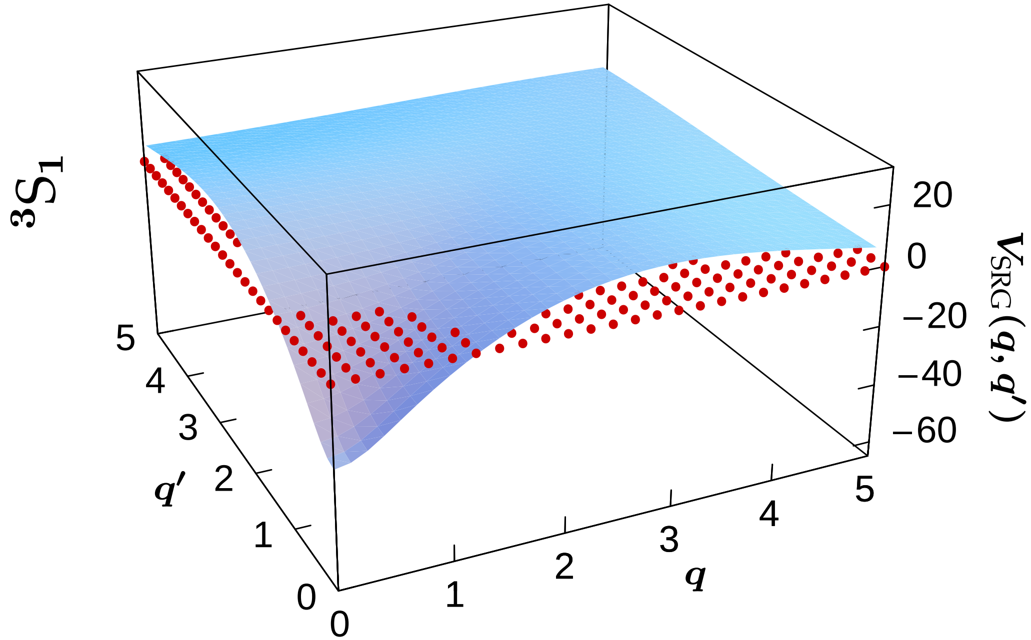
SRG Evolution: The Deuteron

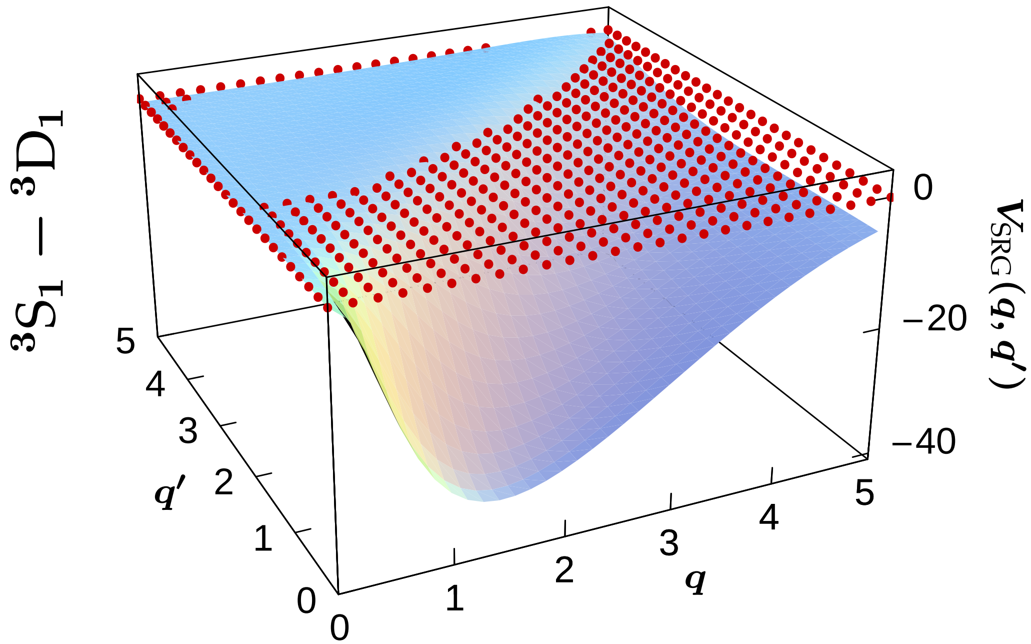


$\alpha = 0.0004\,\mathrm{fm}^4$

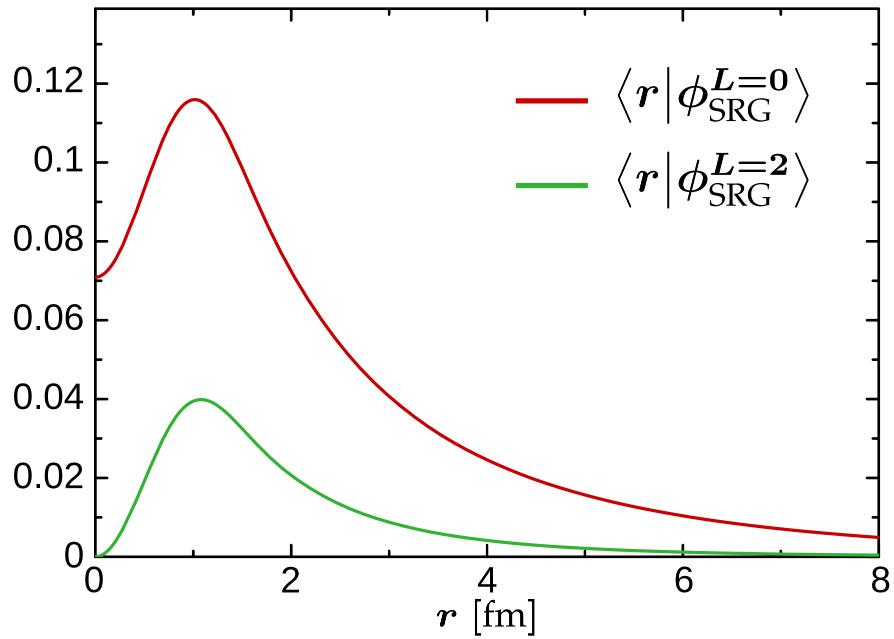


SRG Evolution: The Deuteron

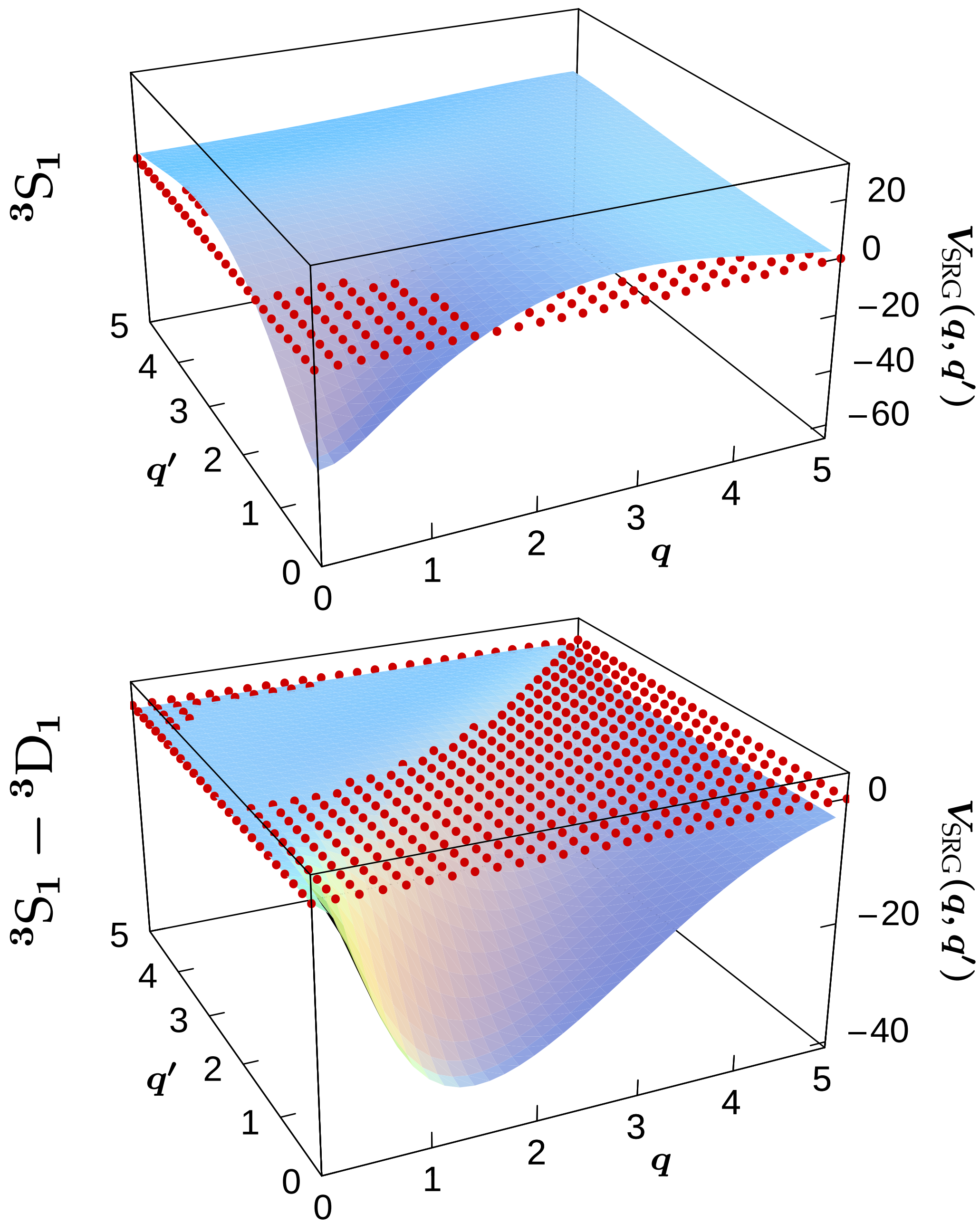




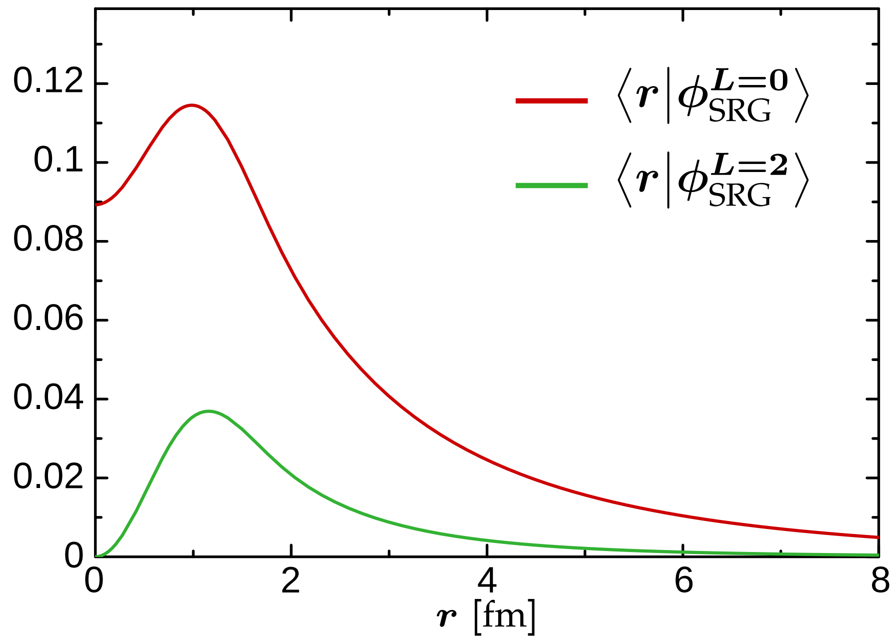
$$\alpha = 0.0010\,\text{fm}^4$$



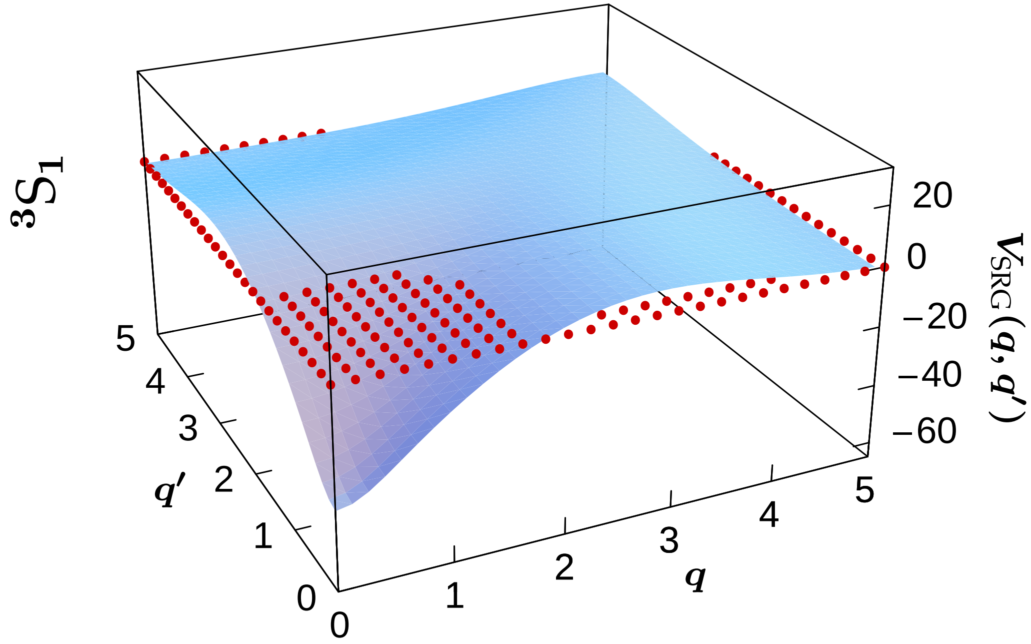
SRG Evolution: The Deuteron

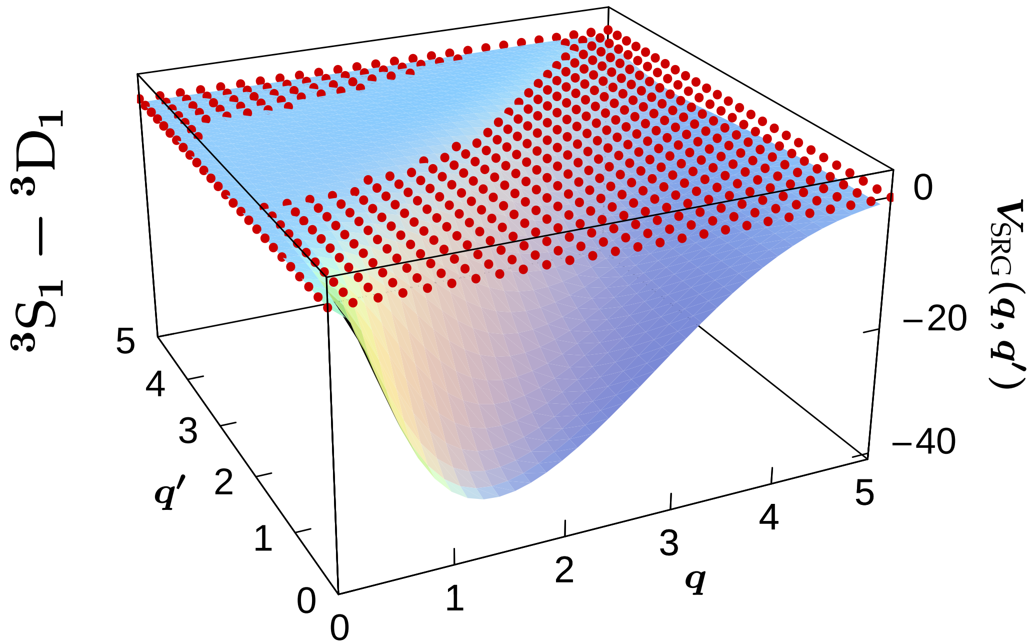


$\alpha = 0.0020\,\mathrm{fm}^4$

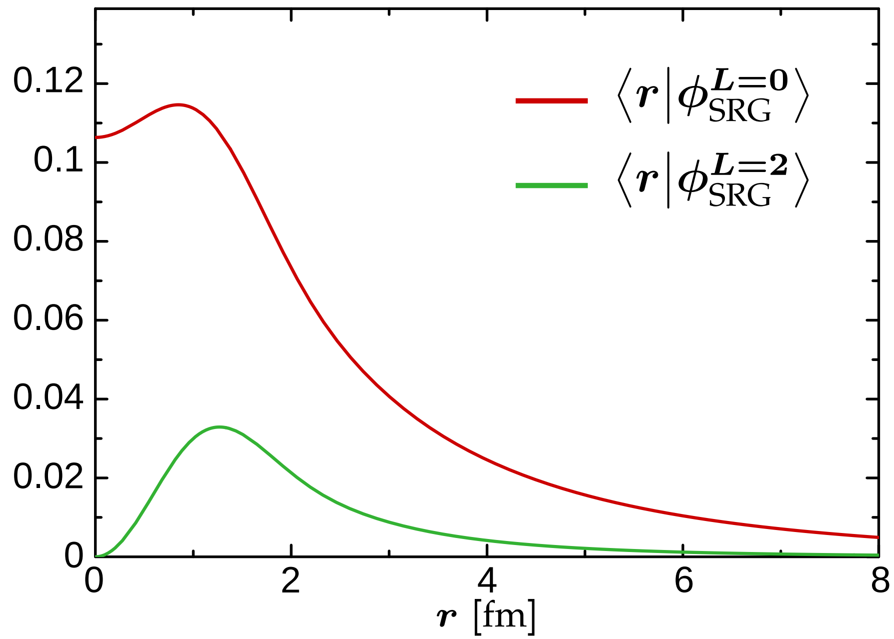


SRG Evolution: The Deuteron

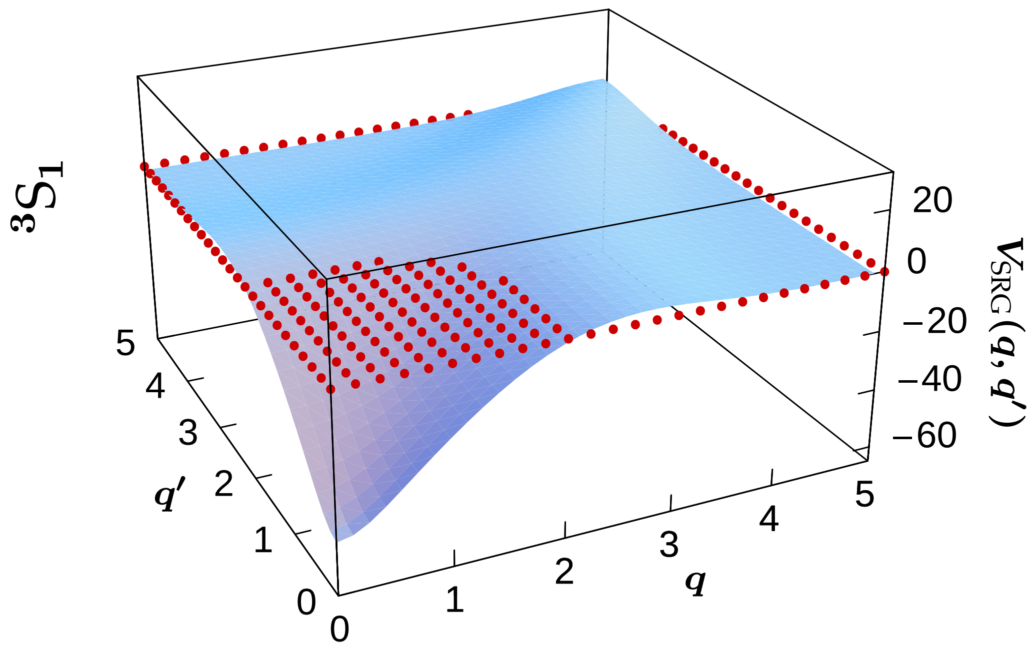


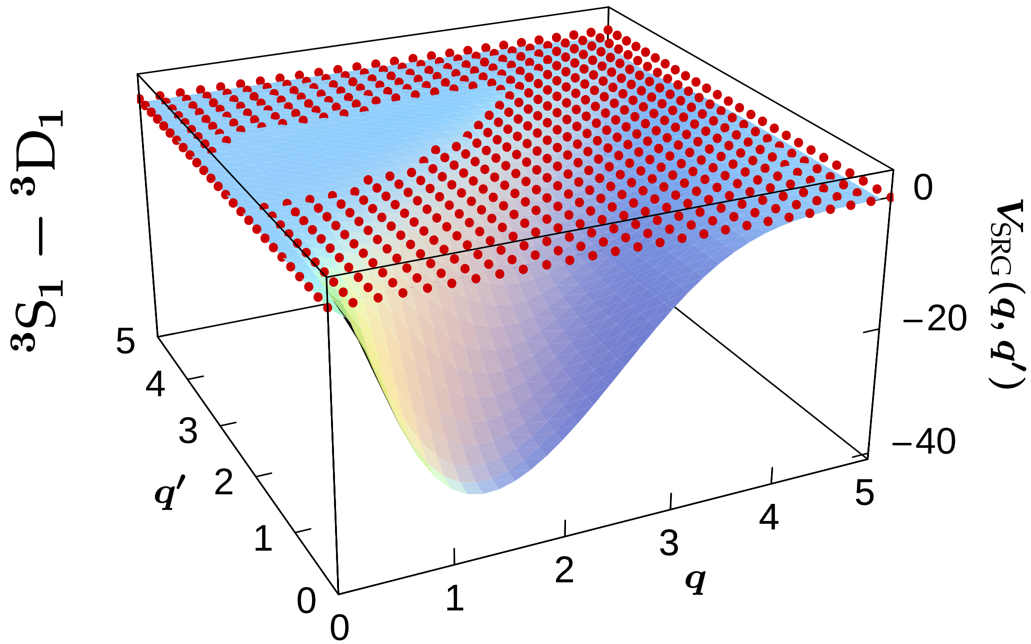


$$\alpha = 0.0040\,\text{fm}^4$$

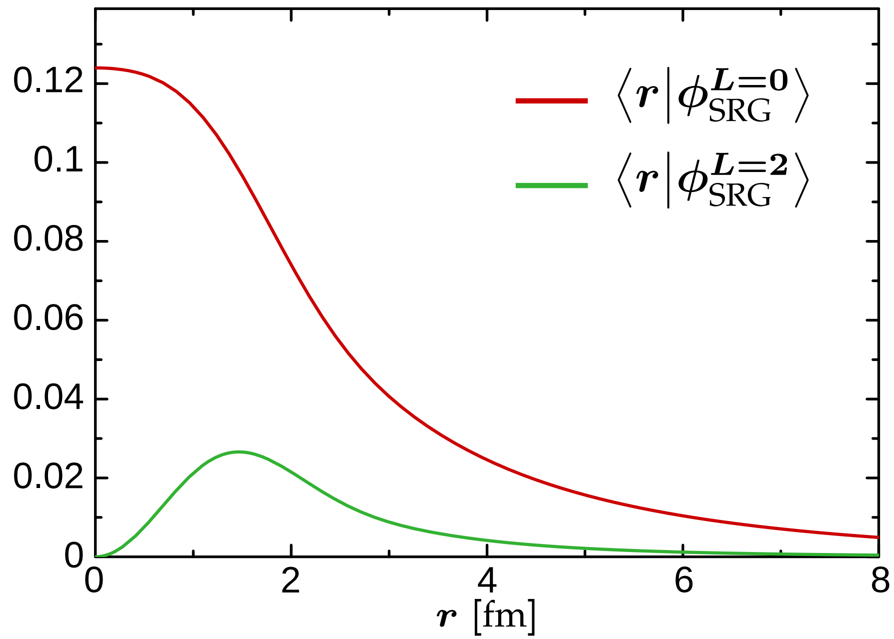


SRG Evolution: The Deuteron

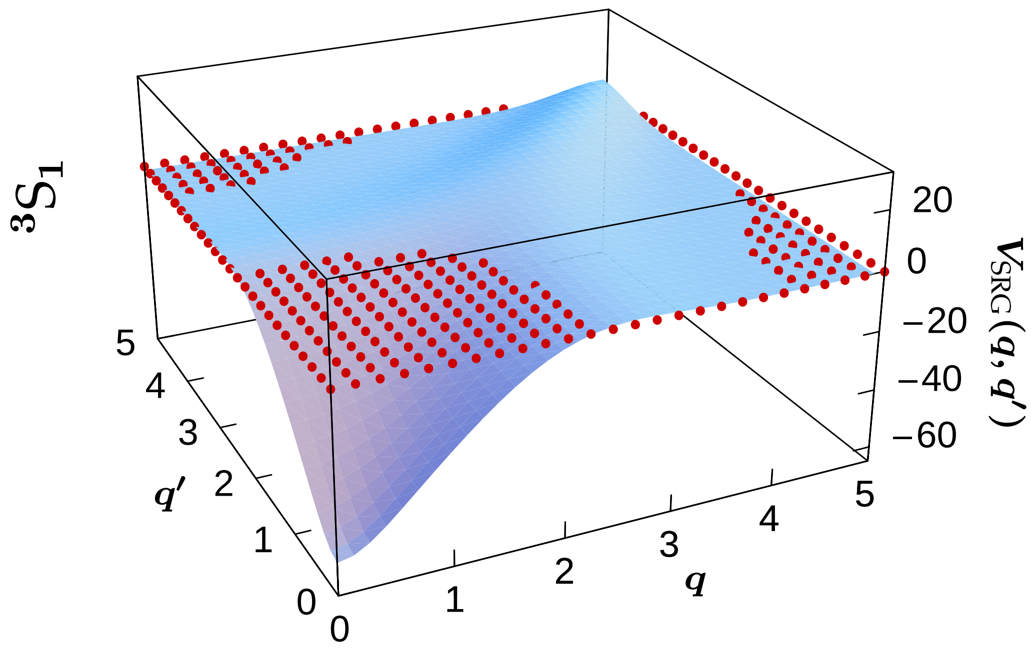


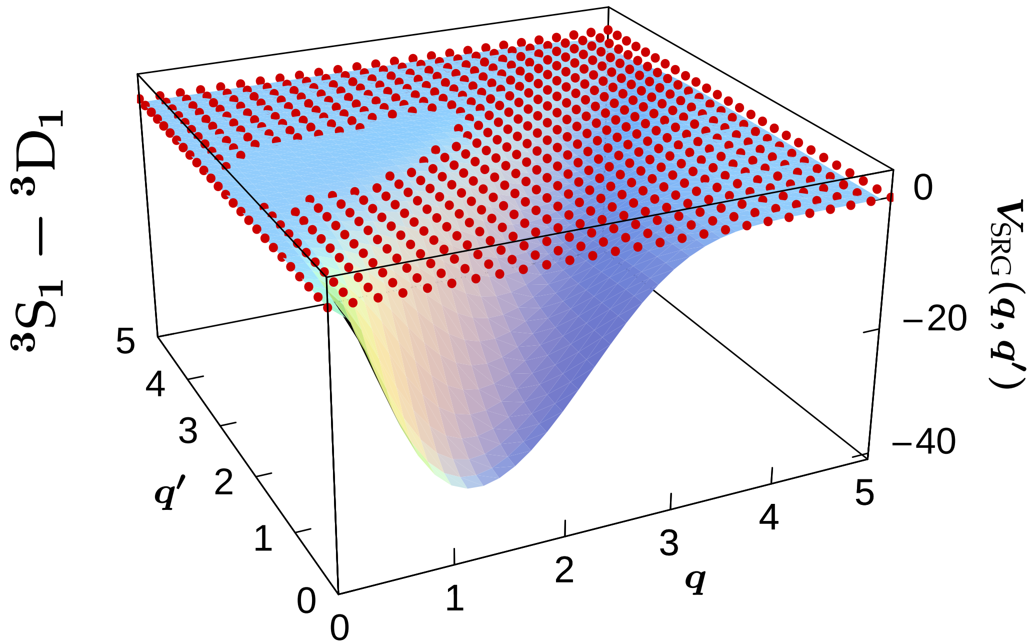


$$\alpha = 0.0100\,\mathrm{fm}^4$$

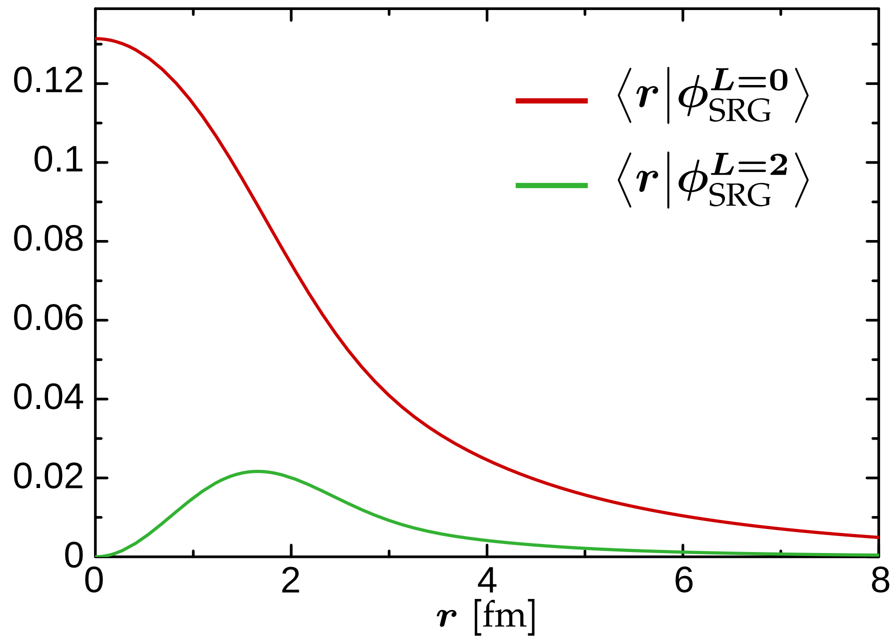


SRG Evolution: The Deuteron

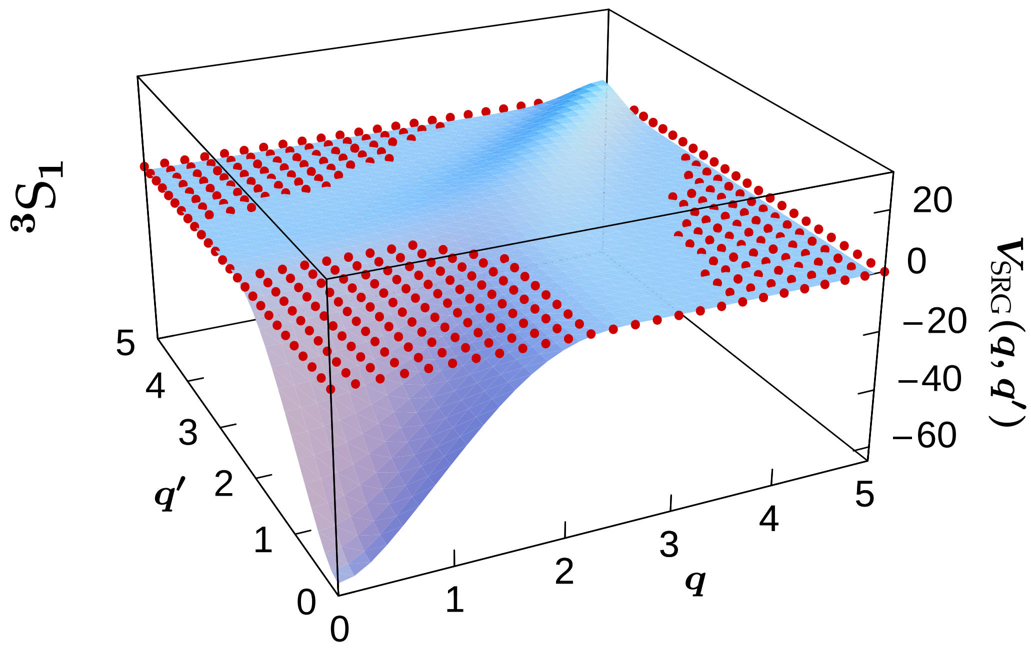


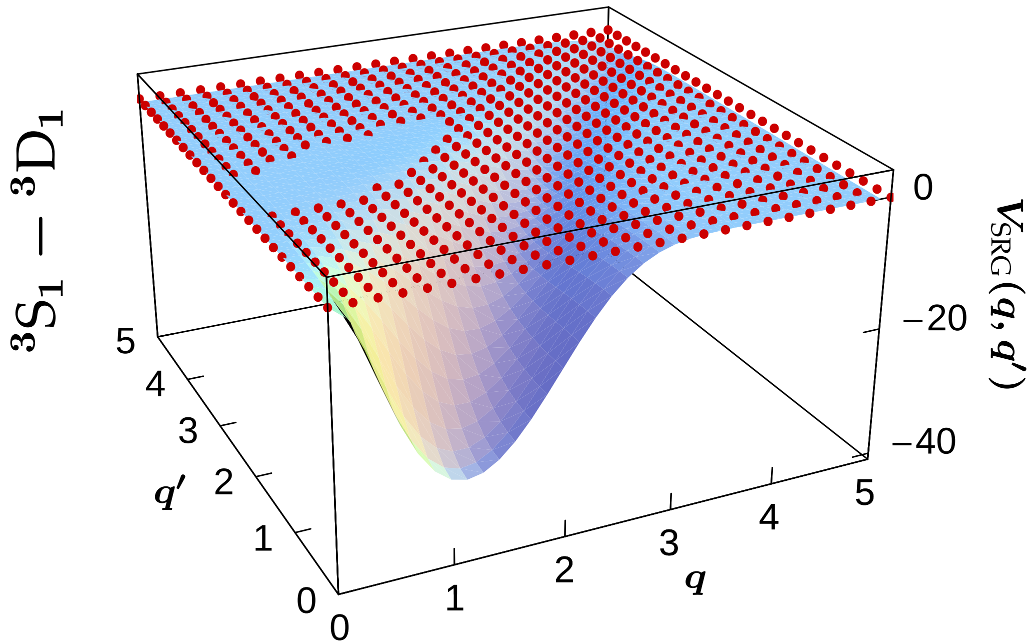


$$\alpha = 0.0200\,\mathrm{fm}^4$$

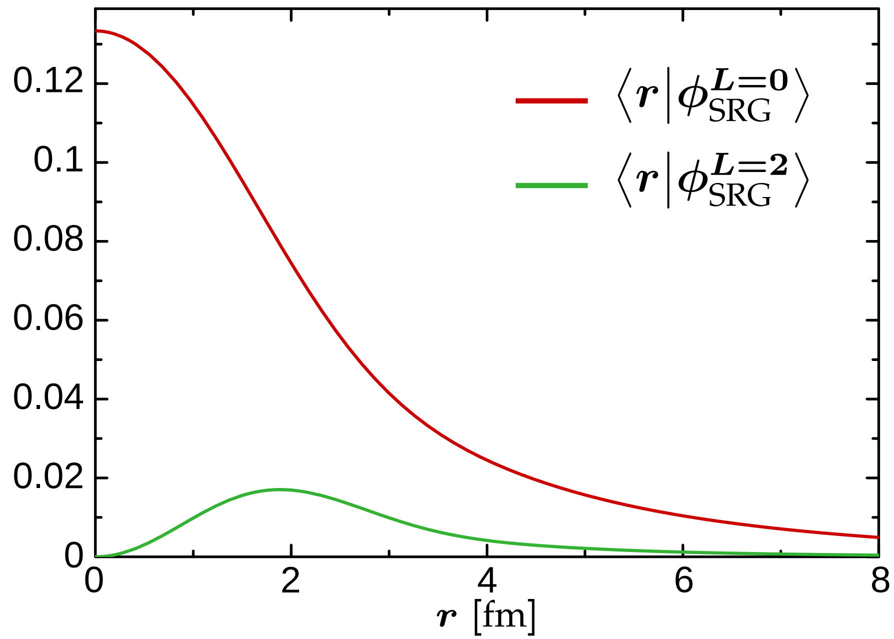


SRG Evolution: The Deuteron

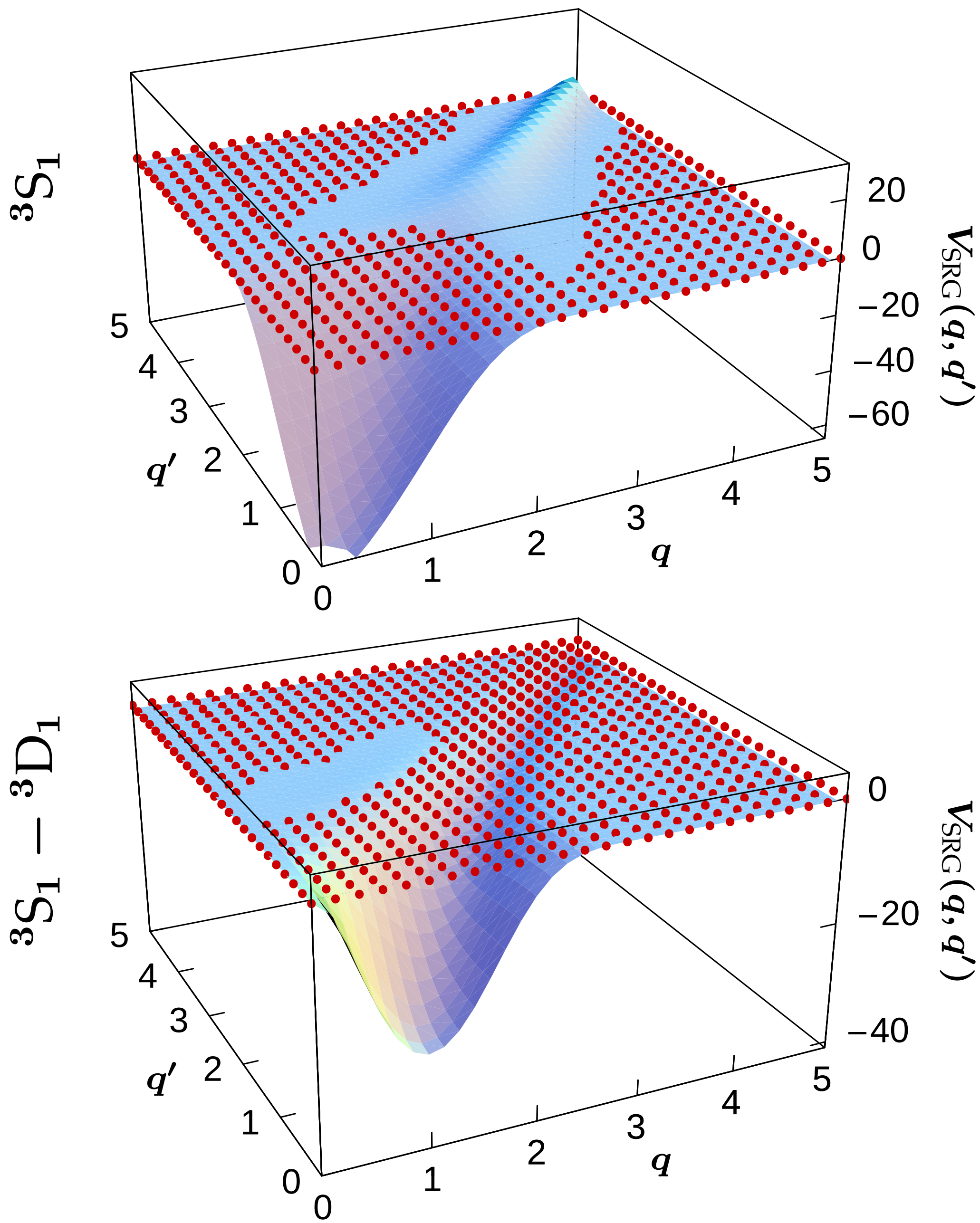




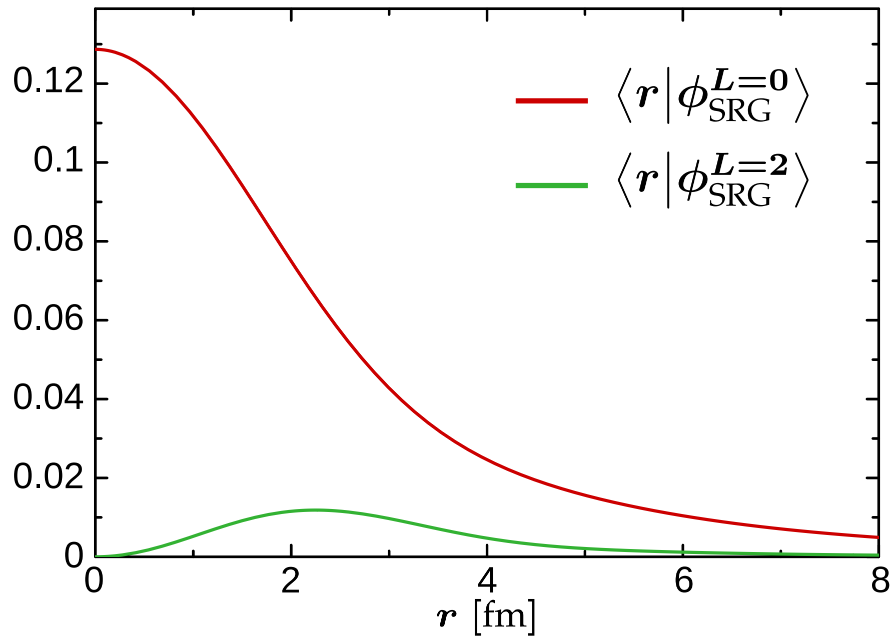
$$\alpha = 0.0400\,\mathrm{fm}^4$$



SRG Evolution: The Deuteron

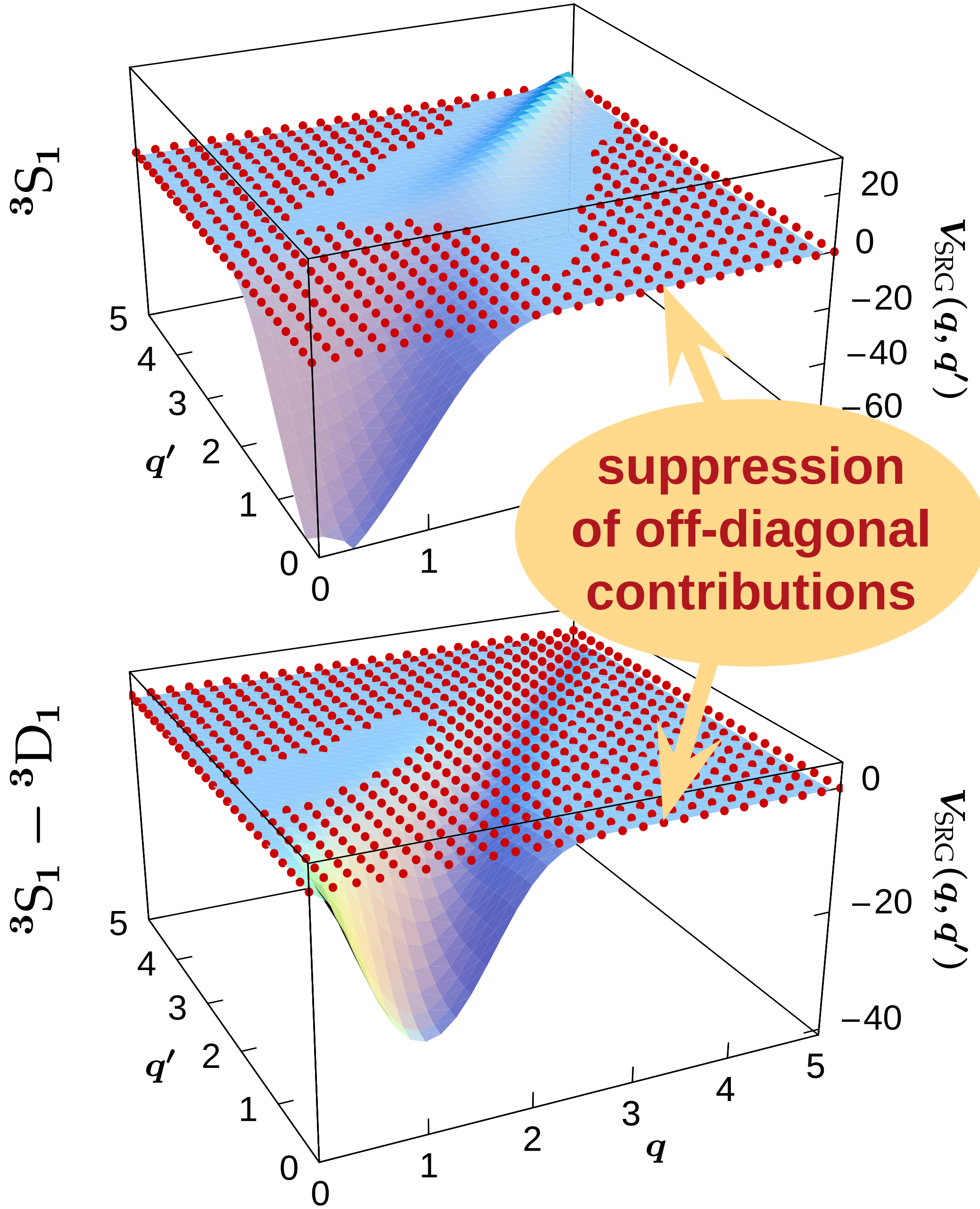


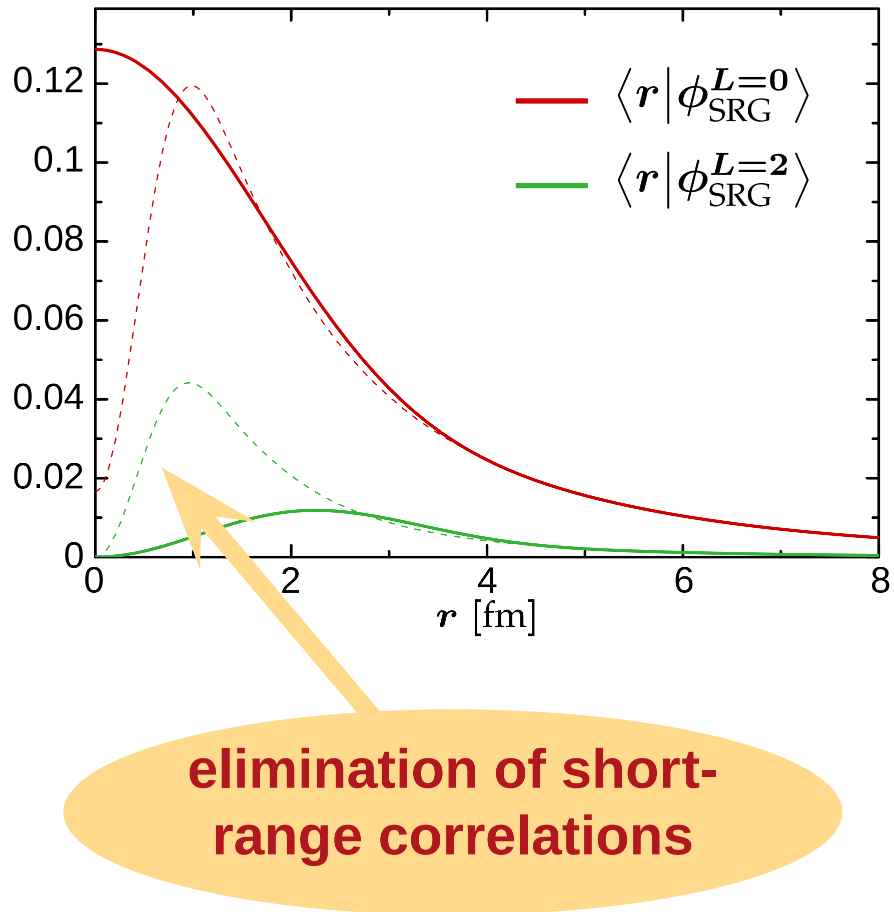
$\alpha = 0.1000\,\text{fm}^4$



SRG Evolution: The Deuteron

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





Many-Body Methods I

No-Core Shell Model

in collaboration with

Petr Navrátil (LLNL)

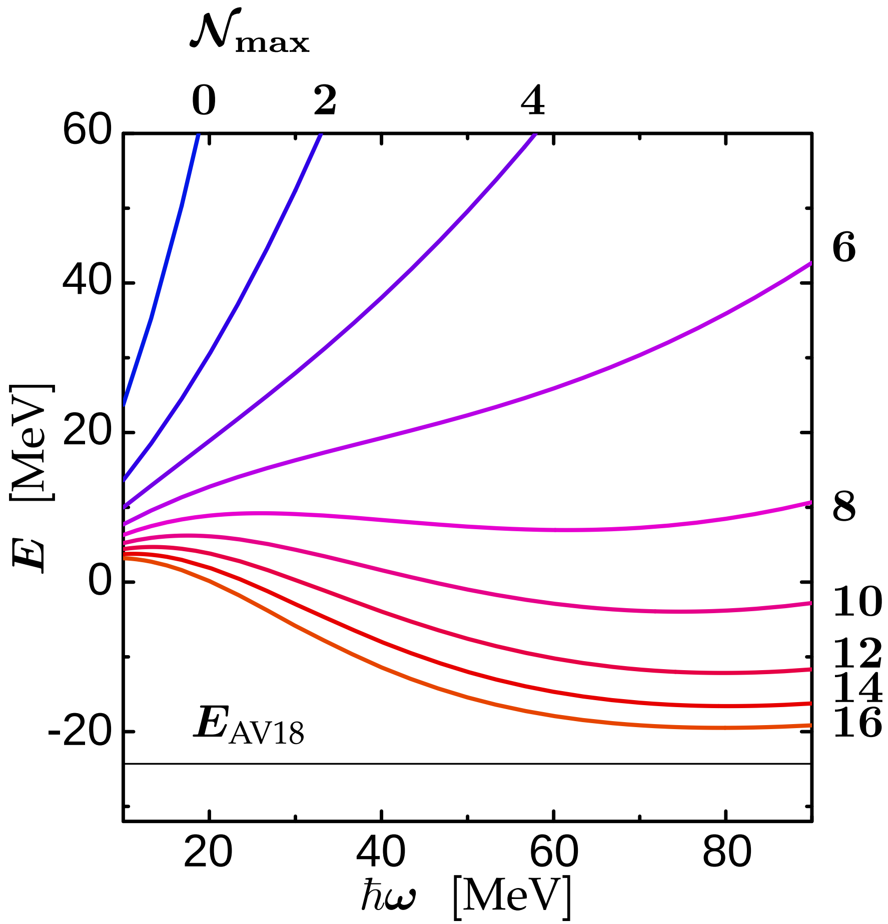
NCSM + Correlated Interaction

No-Core Shell Model
+
Matrix Elements of Correlated Realistic Interaction V_{UCOM}

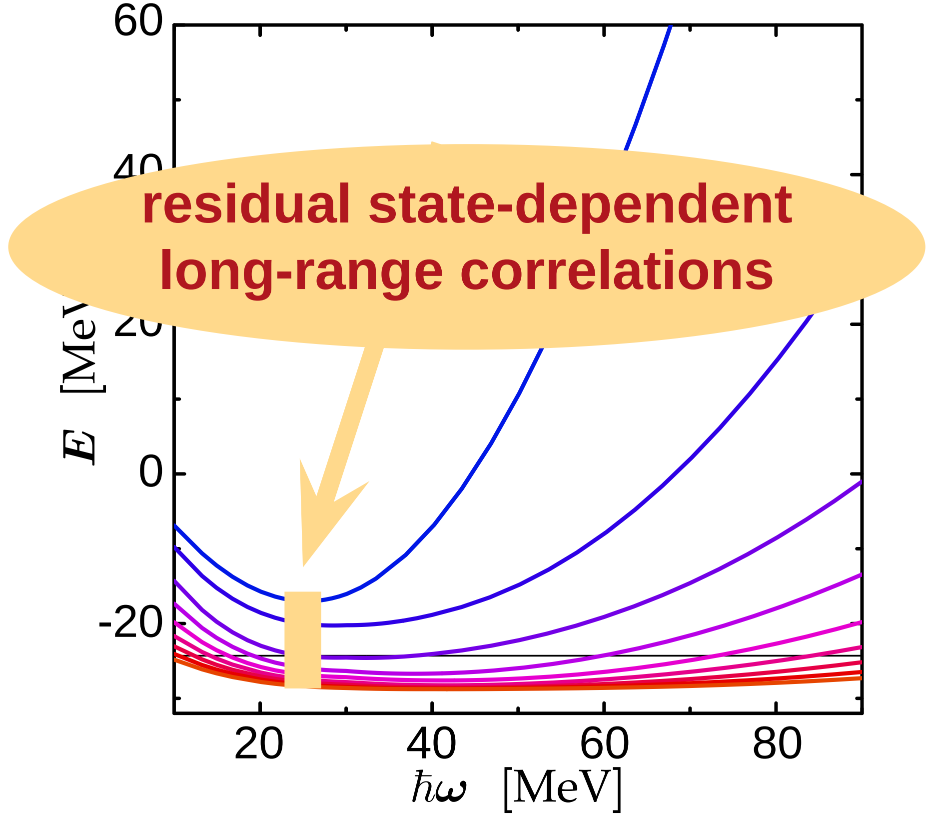
- many-body state is expanded in Slater determinants of harmonic oscillator single-particle states
- large scale diagonalization of Hamiltonian within a truncated model space ($\mathcal{N}\hbar\omega$ truncation)
- assessment of short- and long-range correlations

^{4}He: Convergence

$\mathbf{V}_{\mathrm{AV18}}$

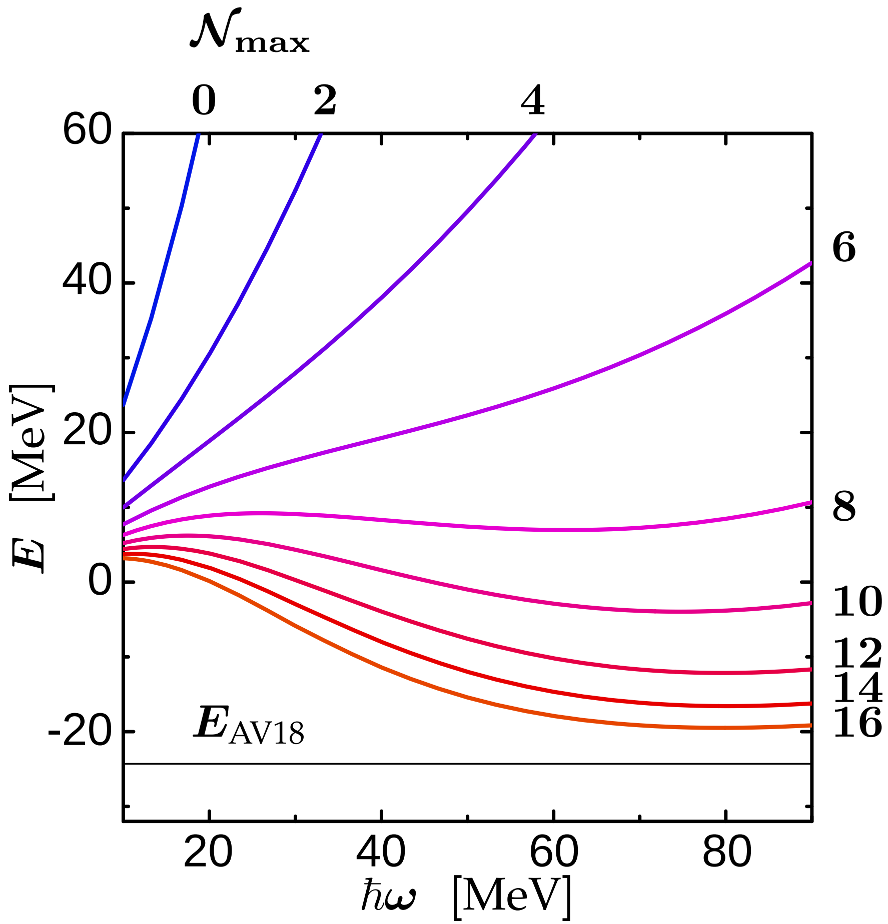


$\mathbf{V}_{\mathrm{UCOM}}$

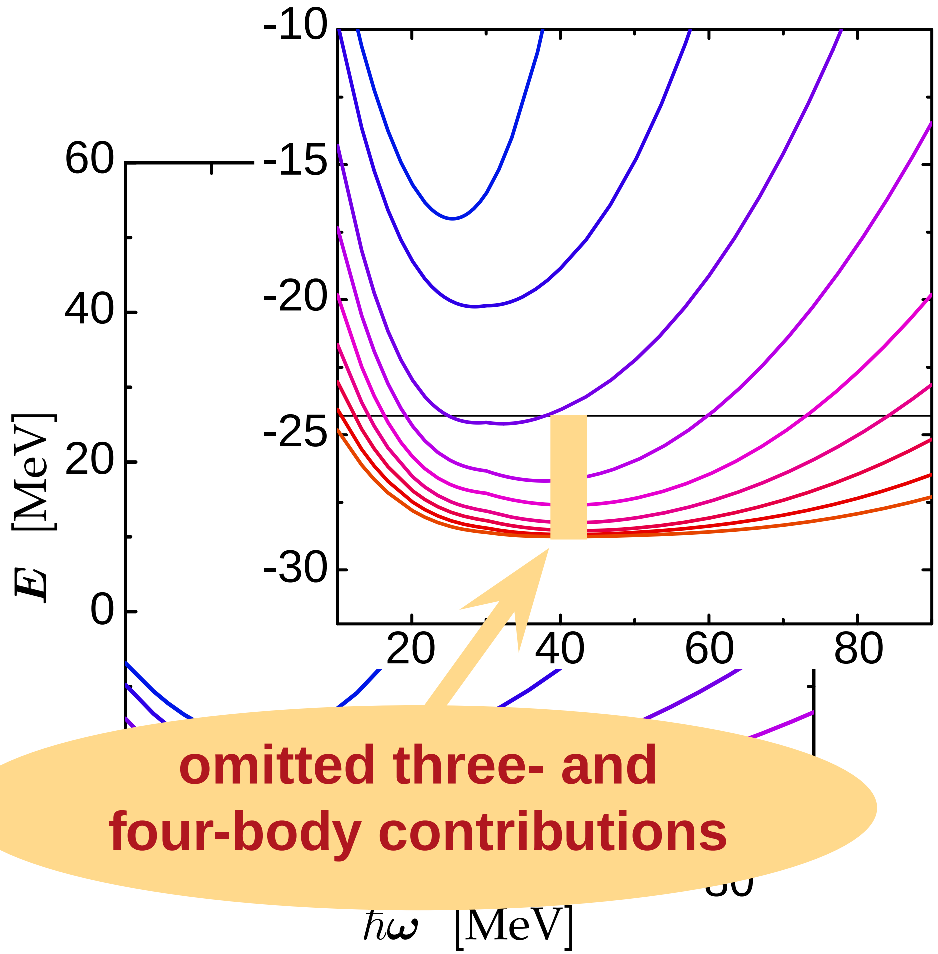


^{4}He: Convergence

V_{AV18}



V_{UCOM}



omitted three- and four-body contributions

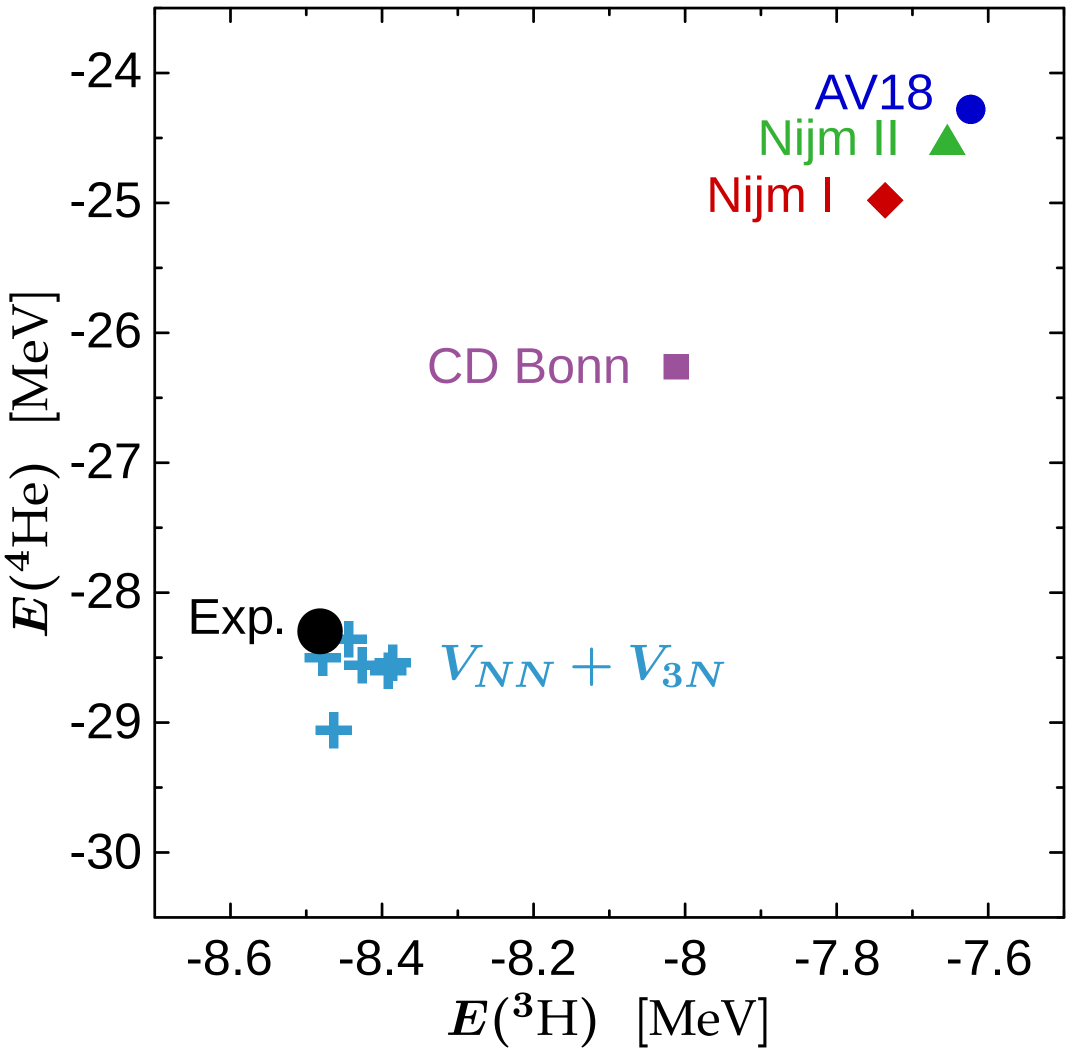
Three-Body Interactions — Strategies

Correlated Hamiltonian in Many-Body Space

$$
\begin{aligned}
\widetilde{\mathrm{H}} &= \mathrm{C}^\dagger\,(\mathrm{T} + \mathrm{V}_{NN} + \mathrm{V}_{3N})\,\mathrm{C} \\
&= \widetilde{\mathrm{T}}^{[1]} + (\widetilde{\mathrm{T}}^{[2]} + \widetilde{\mathrm{V}}^{[2]}_{NN}) + (\widetilde{\mathrm{T}}^{[3]} + \widetilde{\mathrm{V}}^{[3]}_{NN} + \widetilde{\mathrm{V}}^{[3]}_{3N}) + \cdots \\
&= \mathrm{T} + \mathrm{V}_{\mathrm{UCOM}} + \mathrm{V}^{[3]}_{\mathrm{UCOM}} + \cdots
\end{aligned}
$$

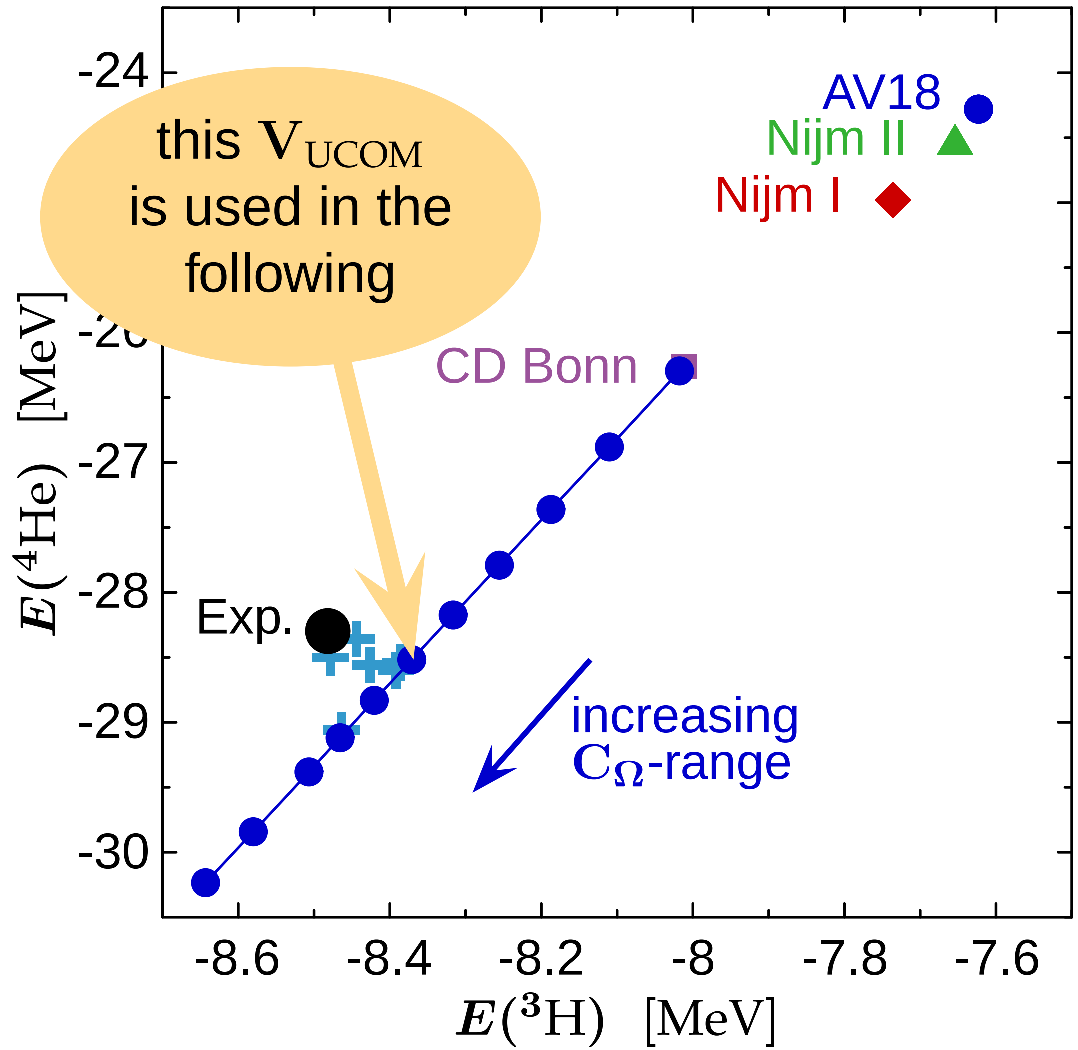
- **include full $\mathrm{V}^{[3]}_{\mathrm{UCOM}}$** consisting of genuine and induced 3N terms
  (not really feasible beyond lightest isotopes)
- **replace $\mathrm{V}^{[3]}_{\mathrm{UCOM}}$** by phenomenological three-body force
  (tractable also for heavier nuclei)
- **minimize $\mathrm{V}^{[3]}_{\mathrm{UCOM}}$**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

Three-Body Interactions — Tjon Line



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

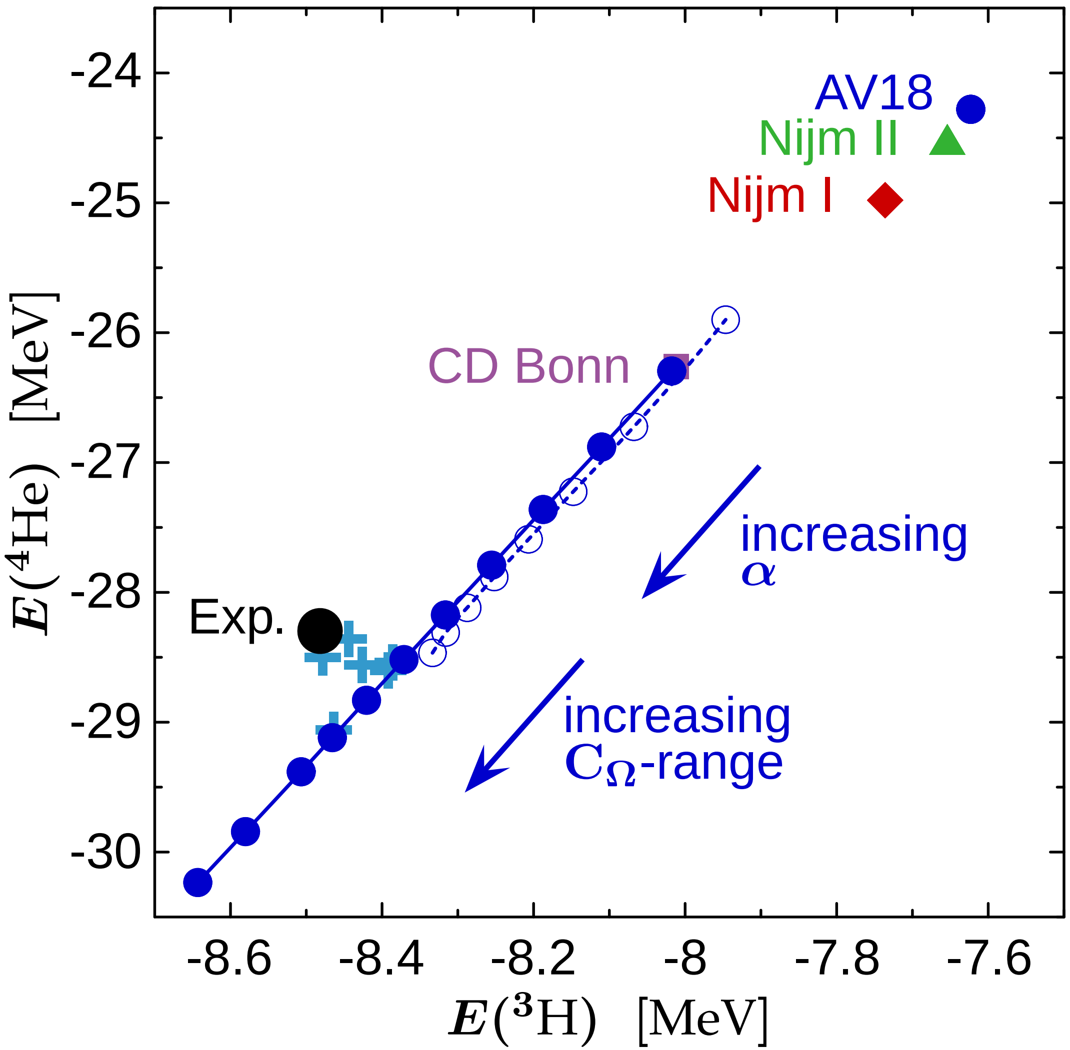
Three-Body Interactions — Tjon Line



- **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 three-body force by choosing correlator with energies close to experimental value

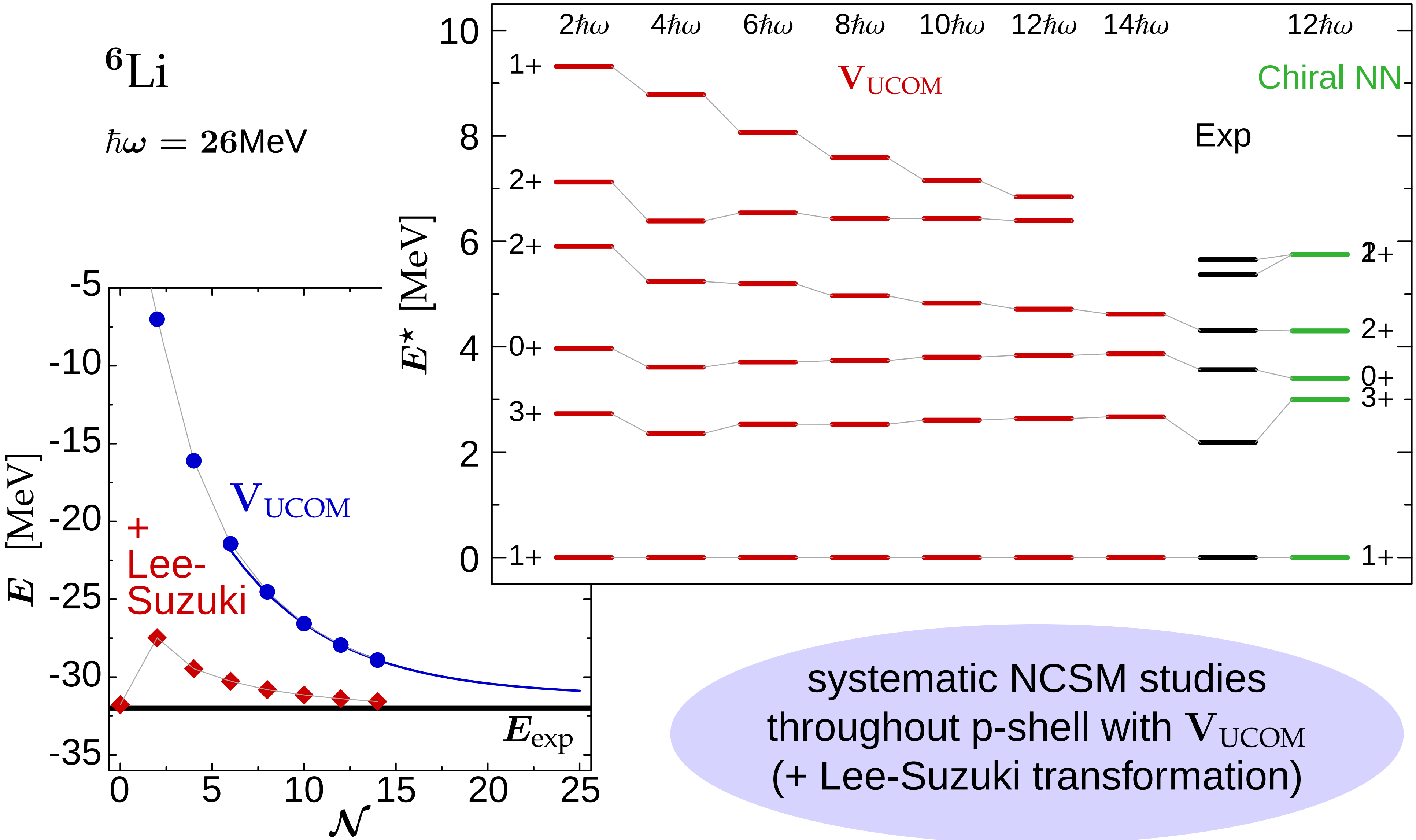
Three-Body Interactions — Tjon Line



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

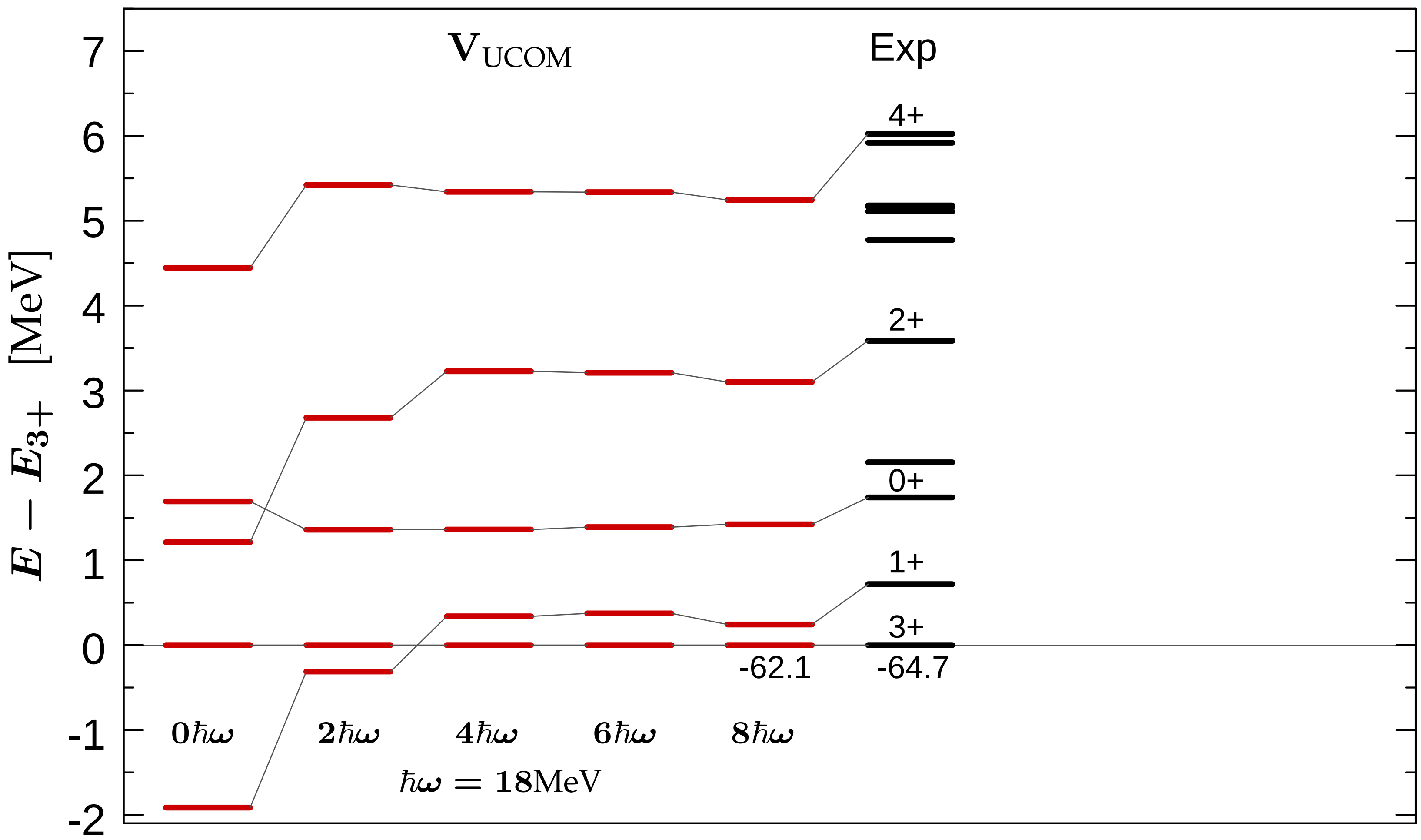
minimize net three-body force by choosing correlator with energies close to experimental value

^{6}Li: NCSM throughout the p-Shell

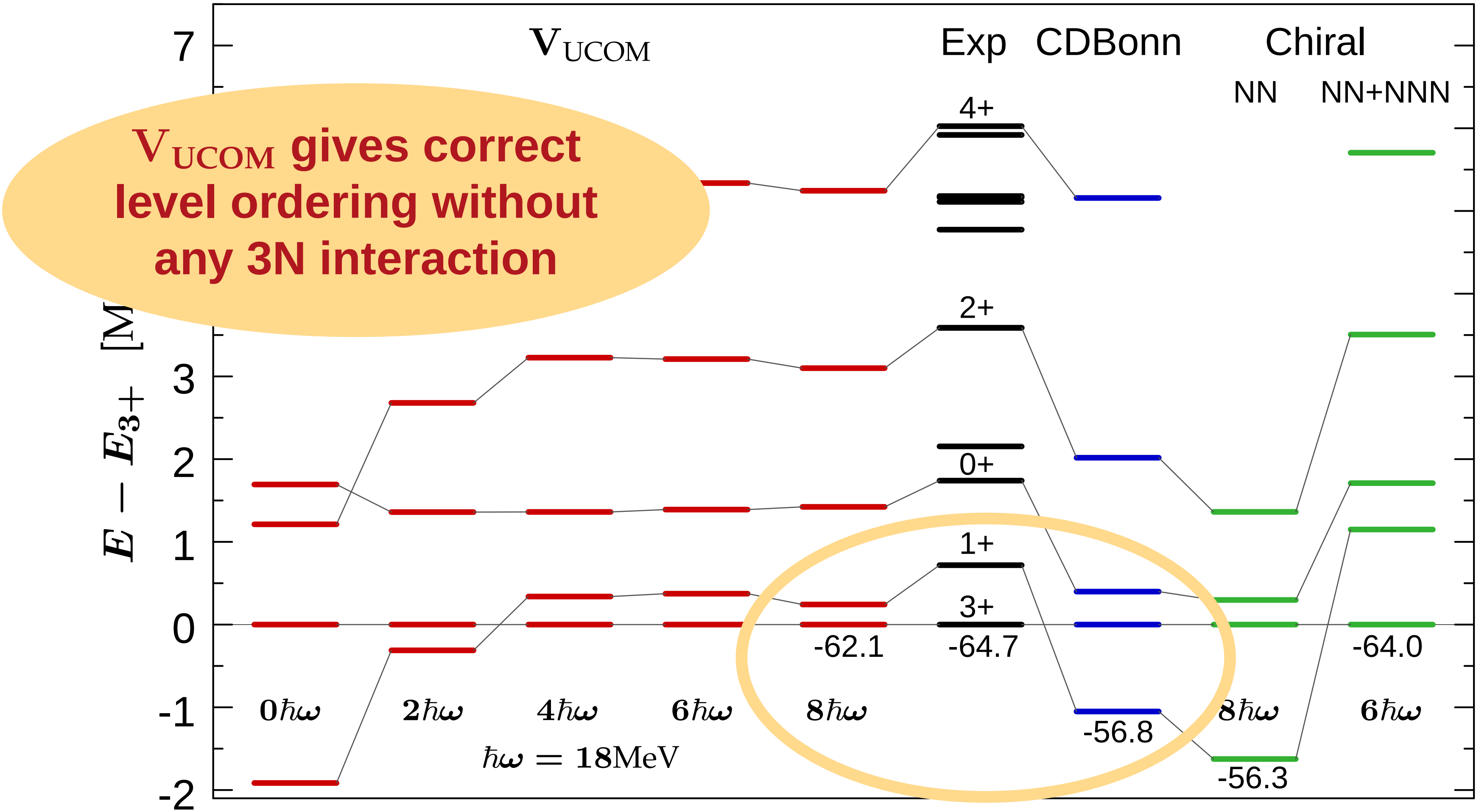


systematic NCSM studies throughout p-shell with V$_{UCOM}$ (+ Lee-Suzuki transformation)

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



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



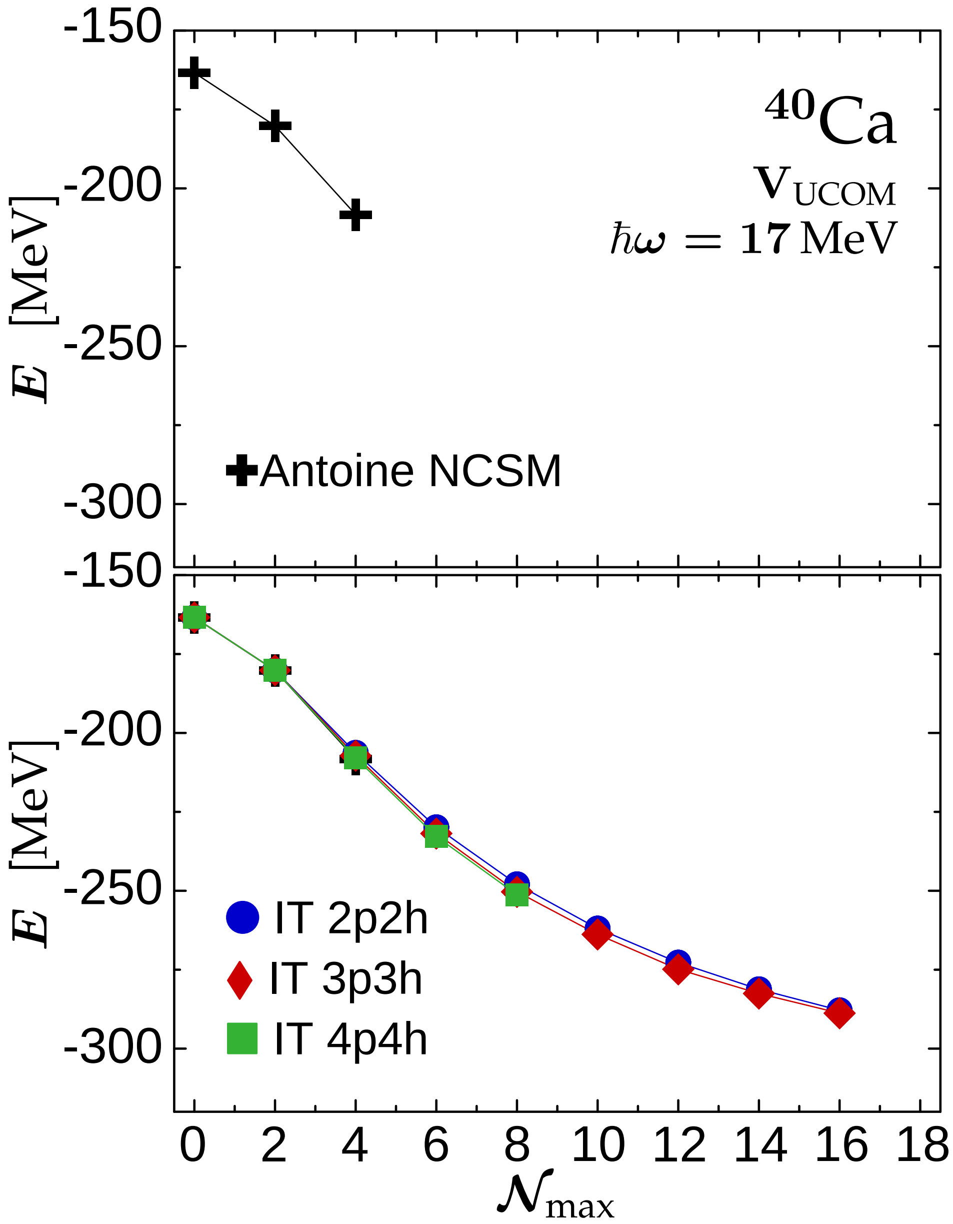
Importance Truncated NCSM

NCSM

- converged calculations essentially restricted to p-shell
- $6\hbar\omega$ for ^{40}Ca presently not feasible ($\sim 10^{10}$ states)

Importance Truncation

- diagonalization in space of **important** configurations
- **a priori importance measure** given by perturbation theory



Many-Body Methods II:

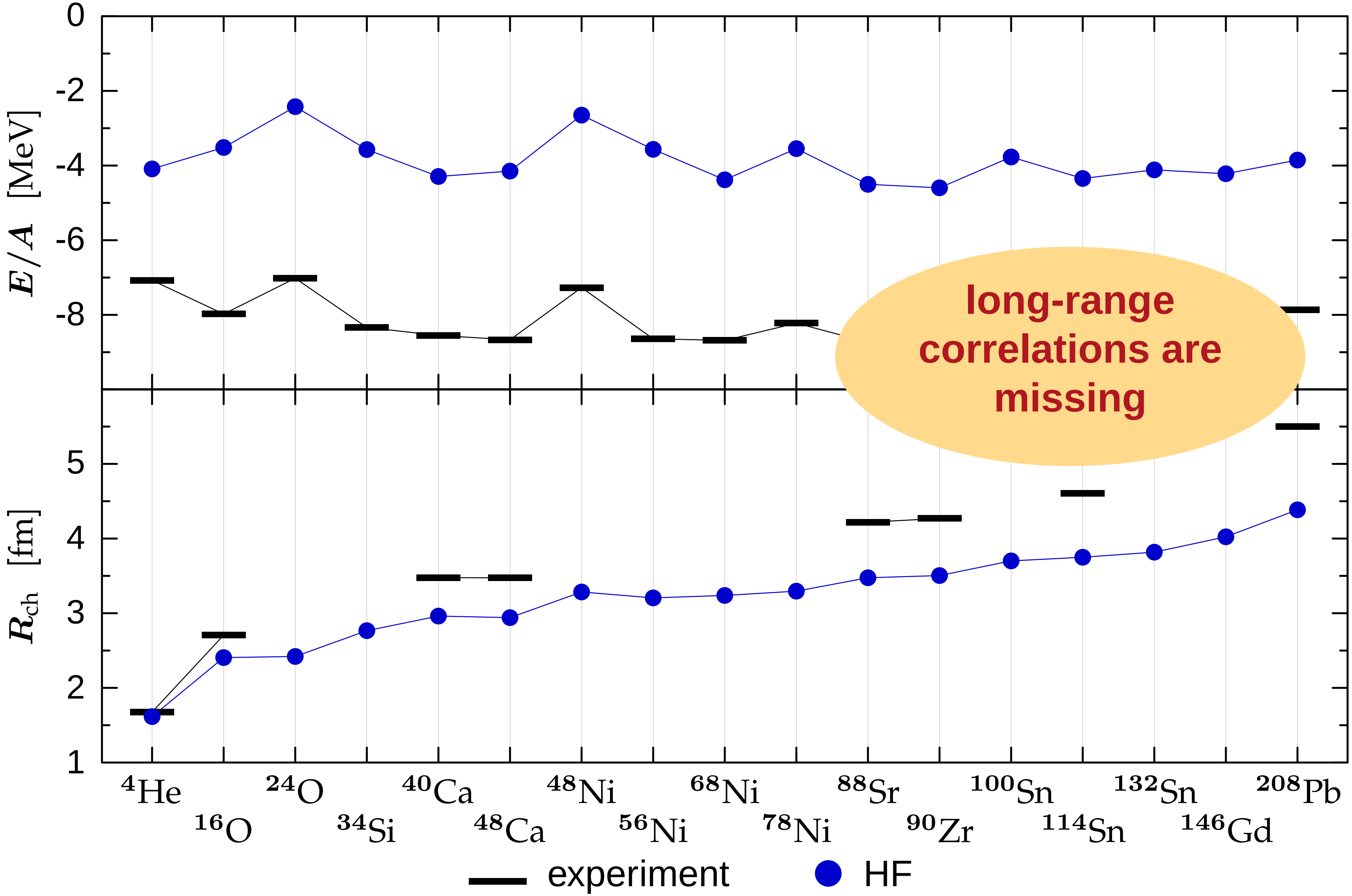
Hartree-Fock & Beyond

HF + Realistic Interactions

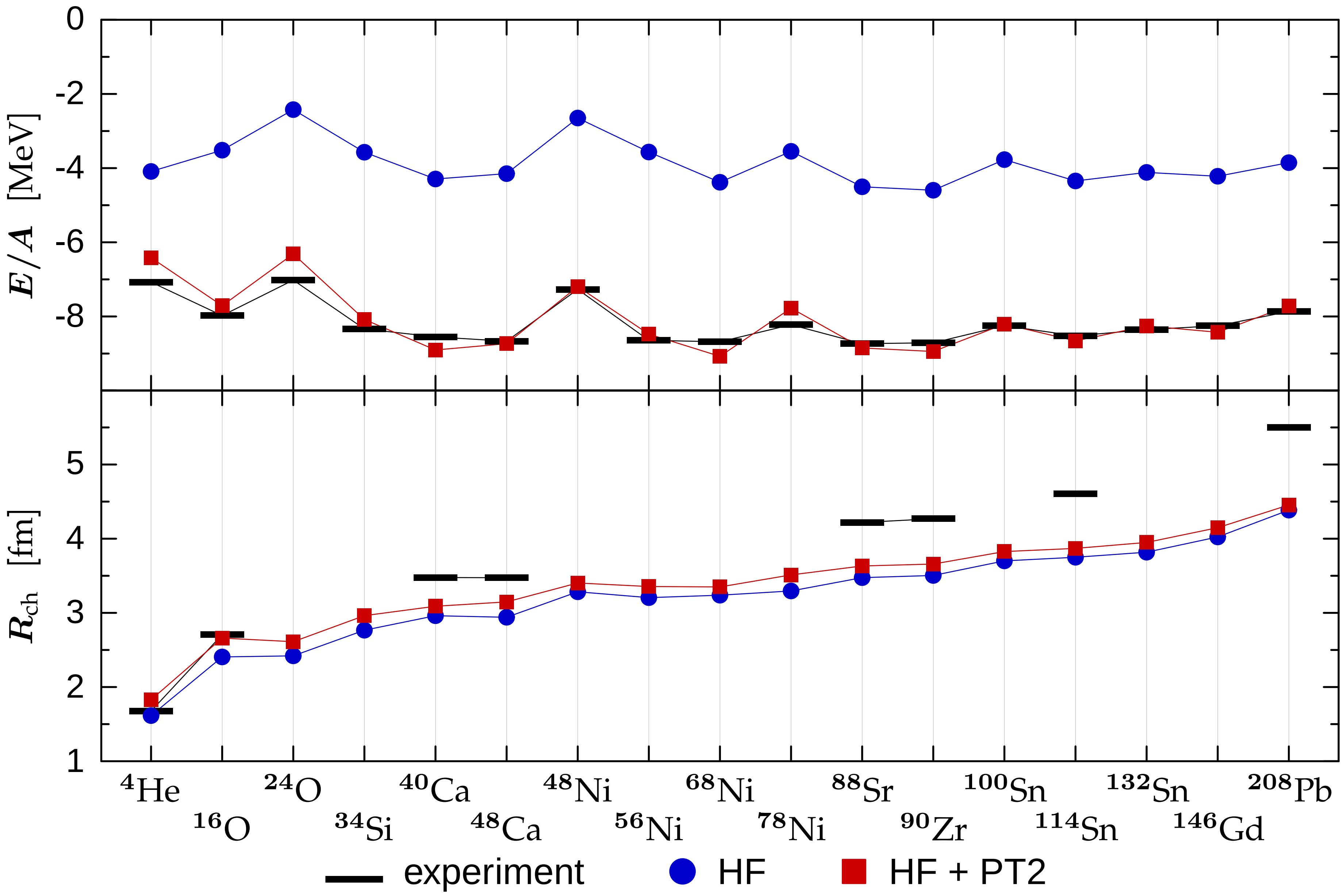
Standard Hartree-Fock
+
Matrix Elements of Correlated Realistic Interaction V_{UCOM}

- many-body state is a **Slater determinant** of single-particle states expanded in oscillator basis (∼13 major shells)
- **correlations cannot be described** by Hartree-Fock states
- starting point for **improved many-body calculations**: MBPT, RPA, SM/CI, CC,...

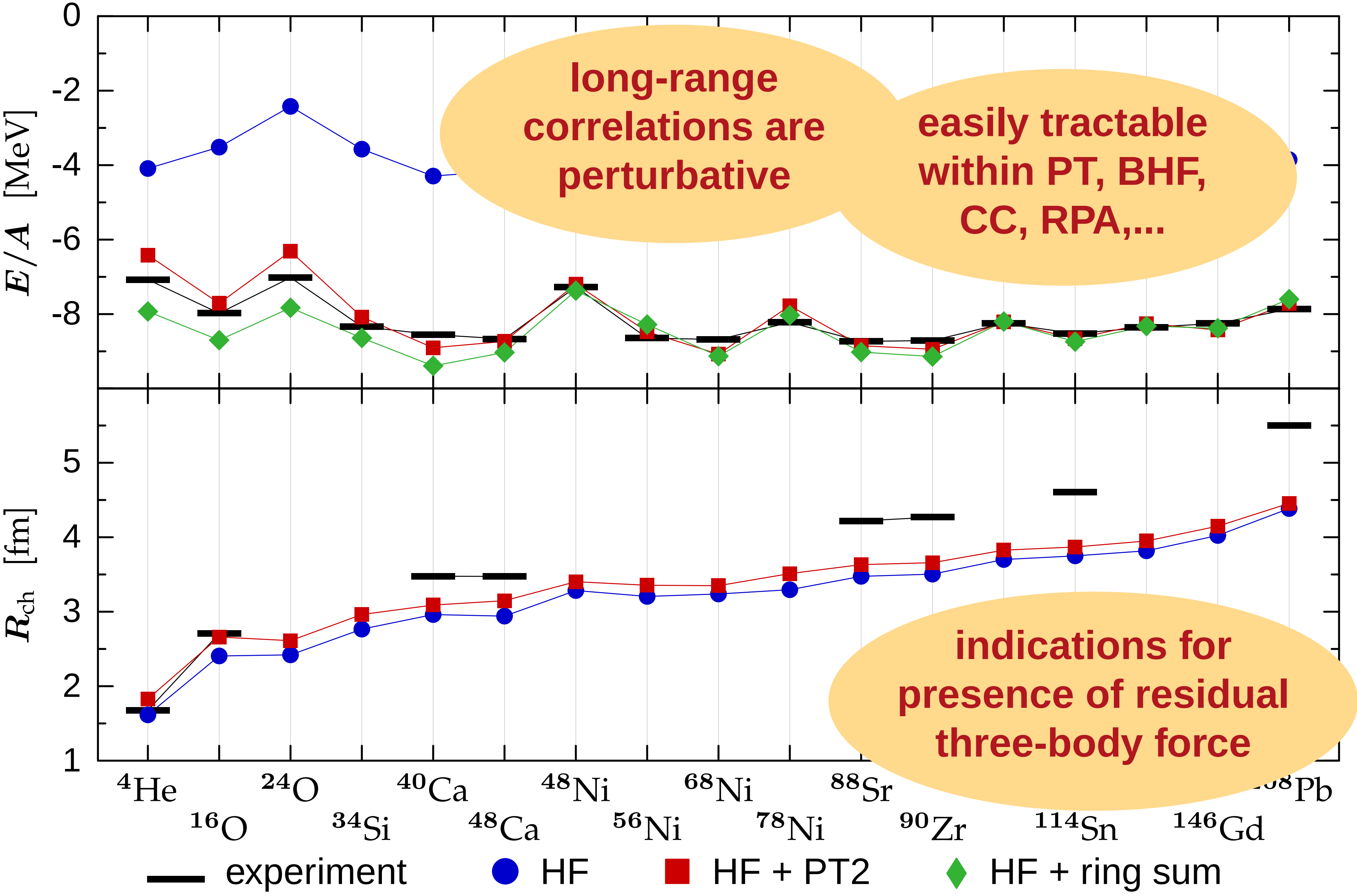
Hartree-Fock with V_{UCOM}



Perturbation Theory with V_{UCOM}



Perturbation Theory with V_{UCOM}

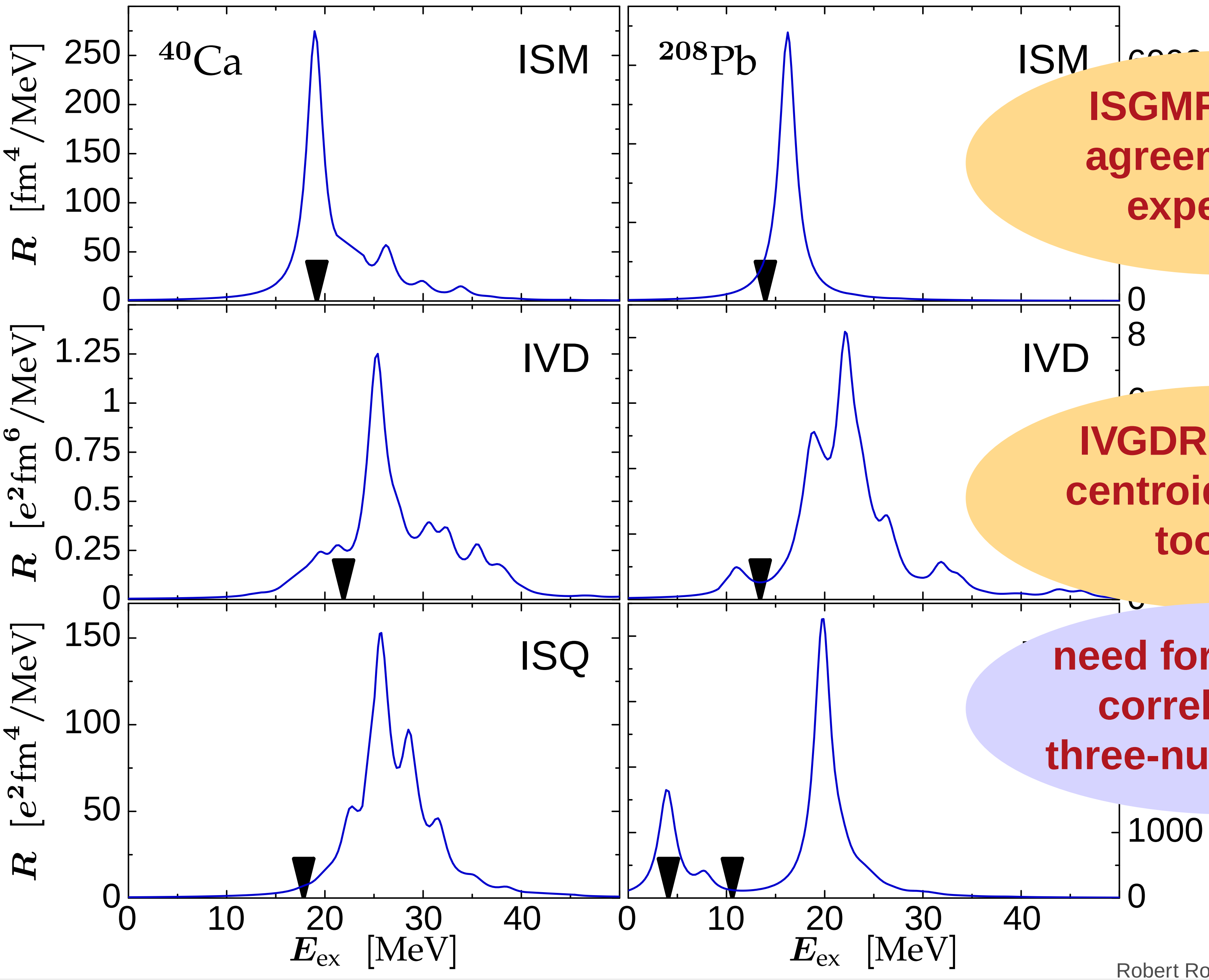


RPA + Realistic Interactions

RPA, ERPA & SRPA
+
Matrix Elements of Correlated Realistic Interaction V_{UCOM}

- **fully self-consistent RPA** based on the Hartree-Fock orbits using the same V_{UCOM}
- recovering sum rules with high precision, spurious center-of-mass mode fully decoupled at ~ 10 keV
- **Extended-RPA and Second-RPA** to include effects of ground state correlations and complex configurations

RPA with V_{UCOM}

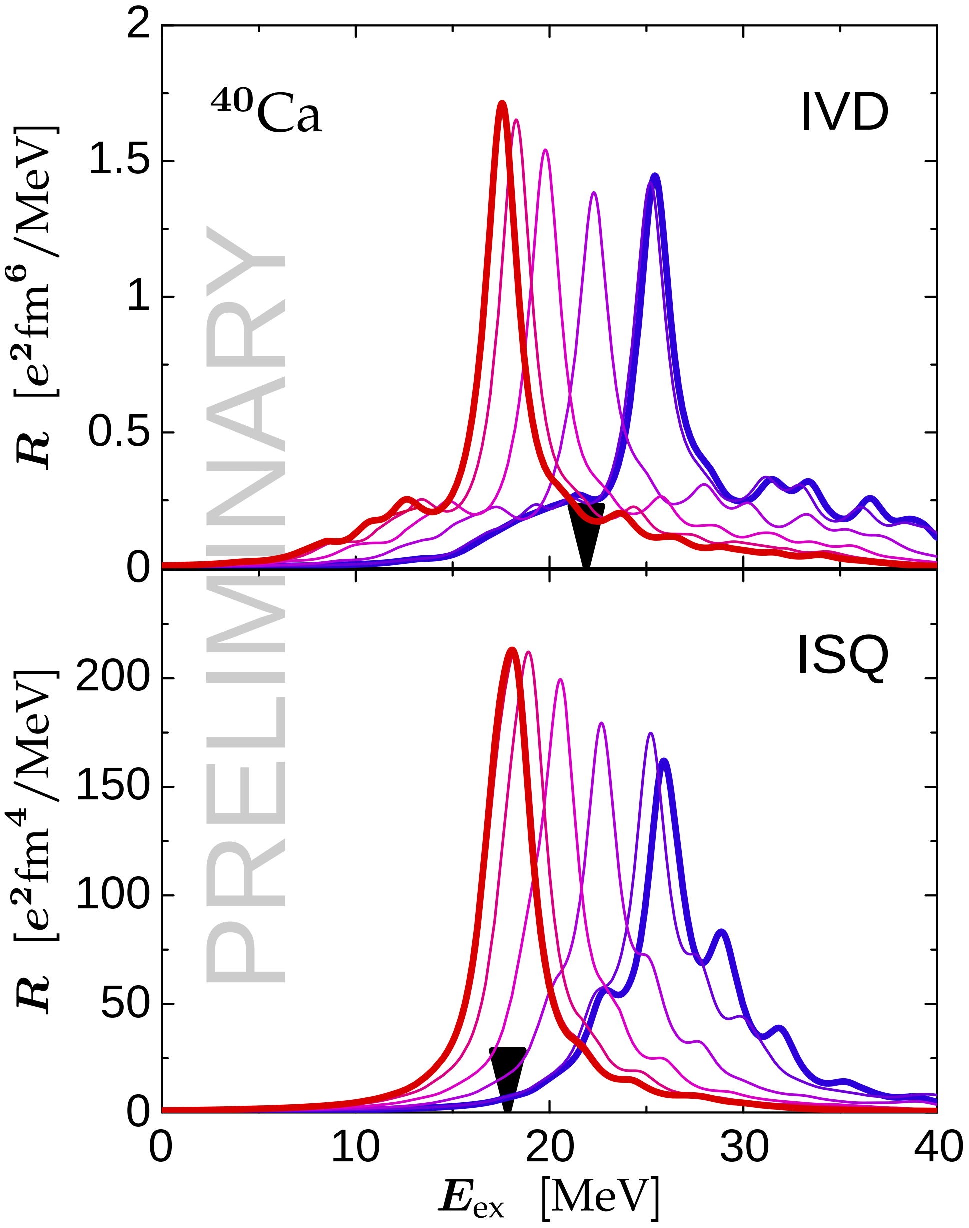


ISGMR in good agreement with experiment

IVGDR & ISGQR centroid energies too high

need for additional correlations & three-nucleon force

SRPA: Complex Configurations



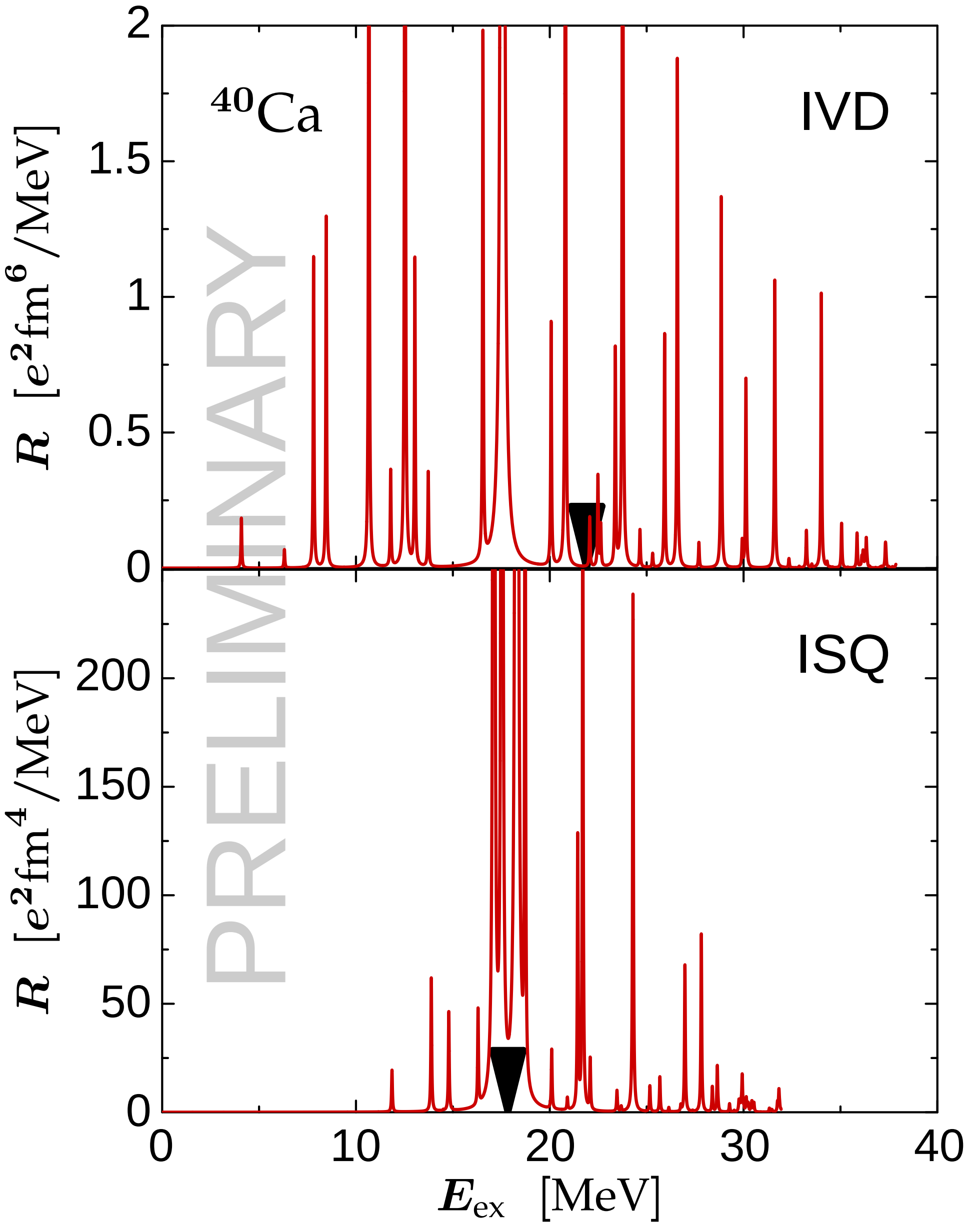
RPA (full 1p1h space)

SRPA (full 1p1h+2p2h space)

(11 major shells, $\Gamma = 2\,\text{MeV}$)

complex configurations have significant impact on response

SRPA: Complex Configurations



RPA (full 1p1h space)

SRPA (full 1p1h+2p2h space)

(11 major shells, $\Gamma = 50\,\mathrm{keV}$)

complex configurations have significant impact on response

possibility to investigate fine structure

Conclusions

- **Modern Effective Interactions**
  - treatment of short-range central and tensor correlations by unitary transformations: UCOM, SRG, Lee-Suzuki,...
  - universal phase-shift equivalent correlated interaction $\mathbf{V}_{\text{UCOM}}$

- **Innovative Many-Body Methods**
  - No-Core Shell Model, Importance Truncation
  - Hartree-Fock, MBPT, CC, RPA, ERPA, SRPA,...
  - Fermionic Molecular Dynamics

unified description of nuclear structure across the whole nuclear chart is within reach

Epilogue

- **thanks to my group & my collaborators**
  - T. Böhlen, P. Hedfeld, H. Hergert, M. Hild, P. Papakonstantinou, F. Schmitt, I. Türschmann, A. Zapp

    Institut für Kernphysik, TU Darmstadt
  - P. Navrátil

    Lawrence Livermore National Laboratory, USA
  - N. Paar

    University of Zagreb, Croatia
  - H. Feldmeier, T. Neff, C. Barbieri, S. Bacca, C. Özen,...

    Gesellschaft für Schwerionenforschung (GSI)

supported by the DFG through SFB 634 “Nuclear Structure, Nuclear Astrophysics and Fundamental Experiments...”