From QCD to the Nuclear Chart:

New Concepts in Nuclear Structure Theory

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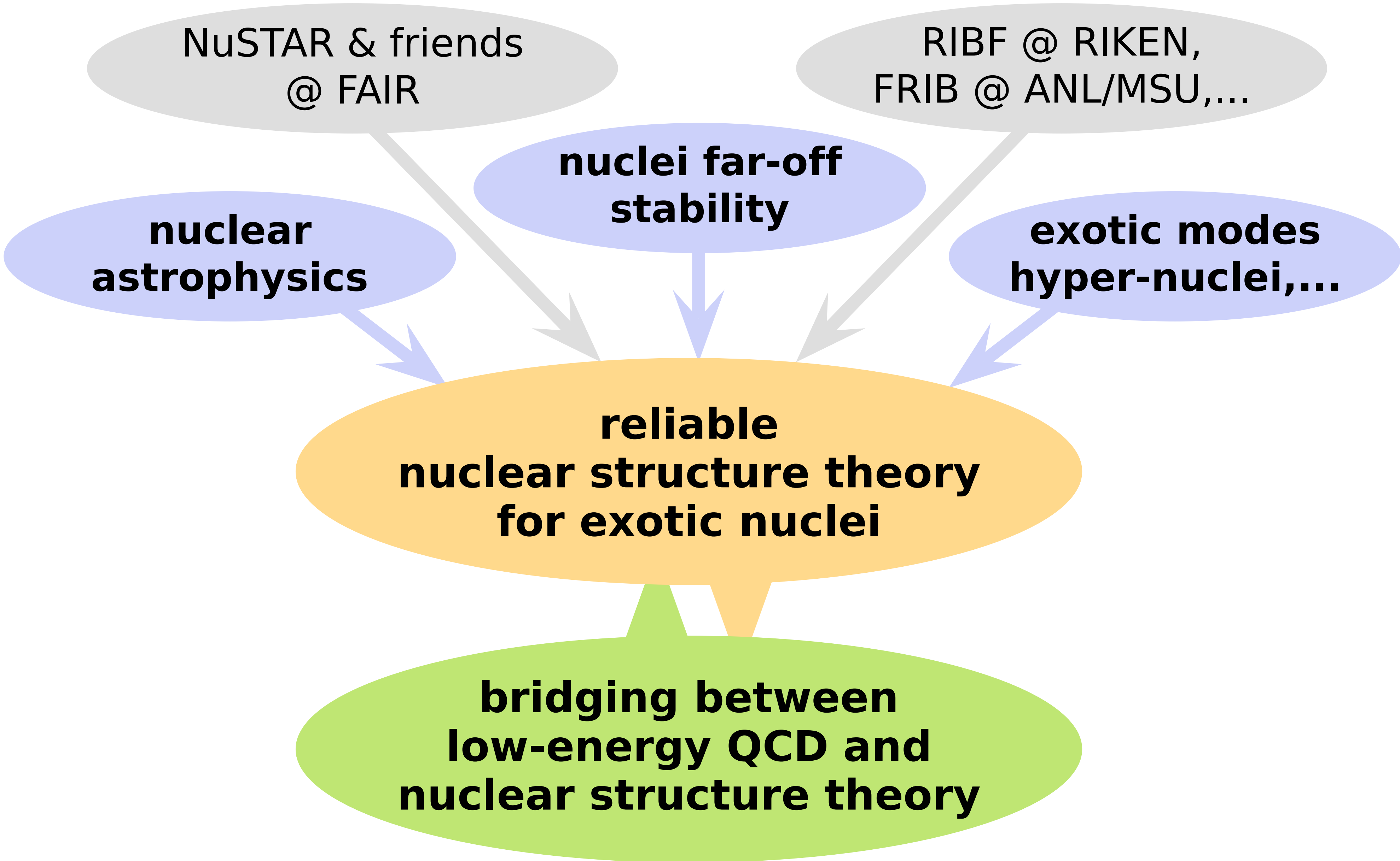
Overview

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

Nuclear Structure in the 21st Century

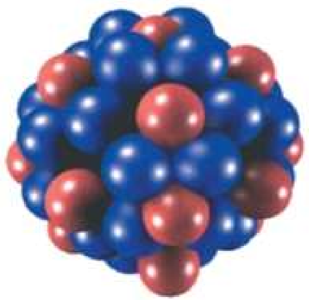


Theoretical Context

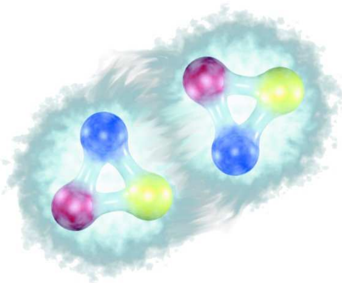
better resolution / more fundamental

Quantum Chromo Dynamics

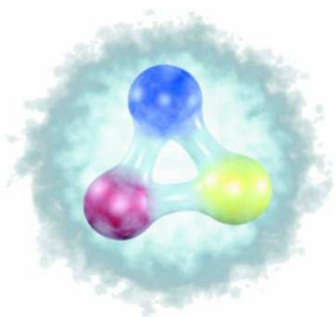
Nuclear Structure



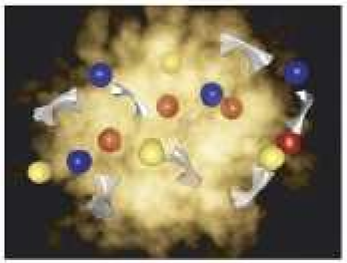
- finite nuclei



- few-nucleon systems
- nucleon-nucleon interaction

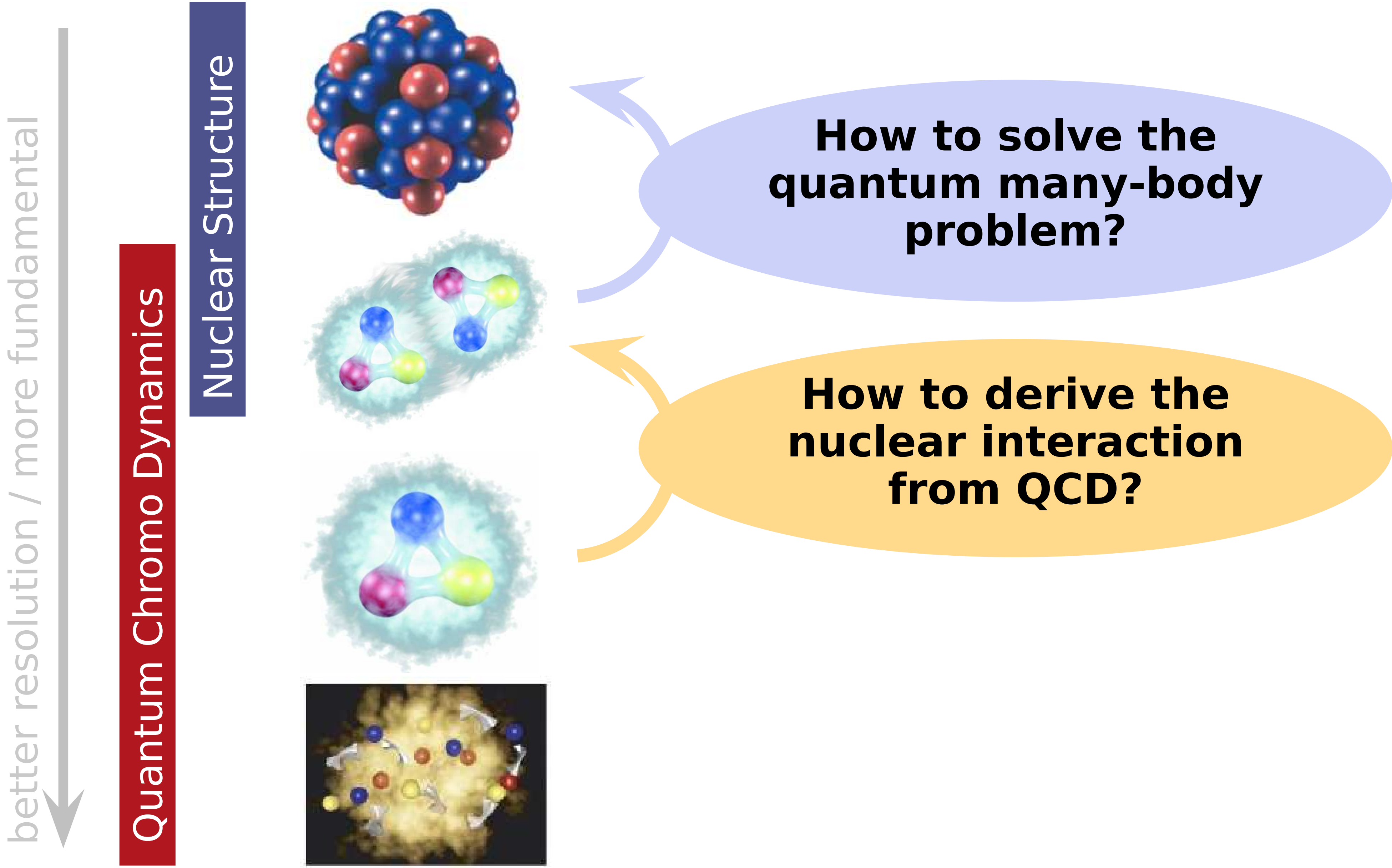


- hadron structure



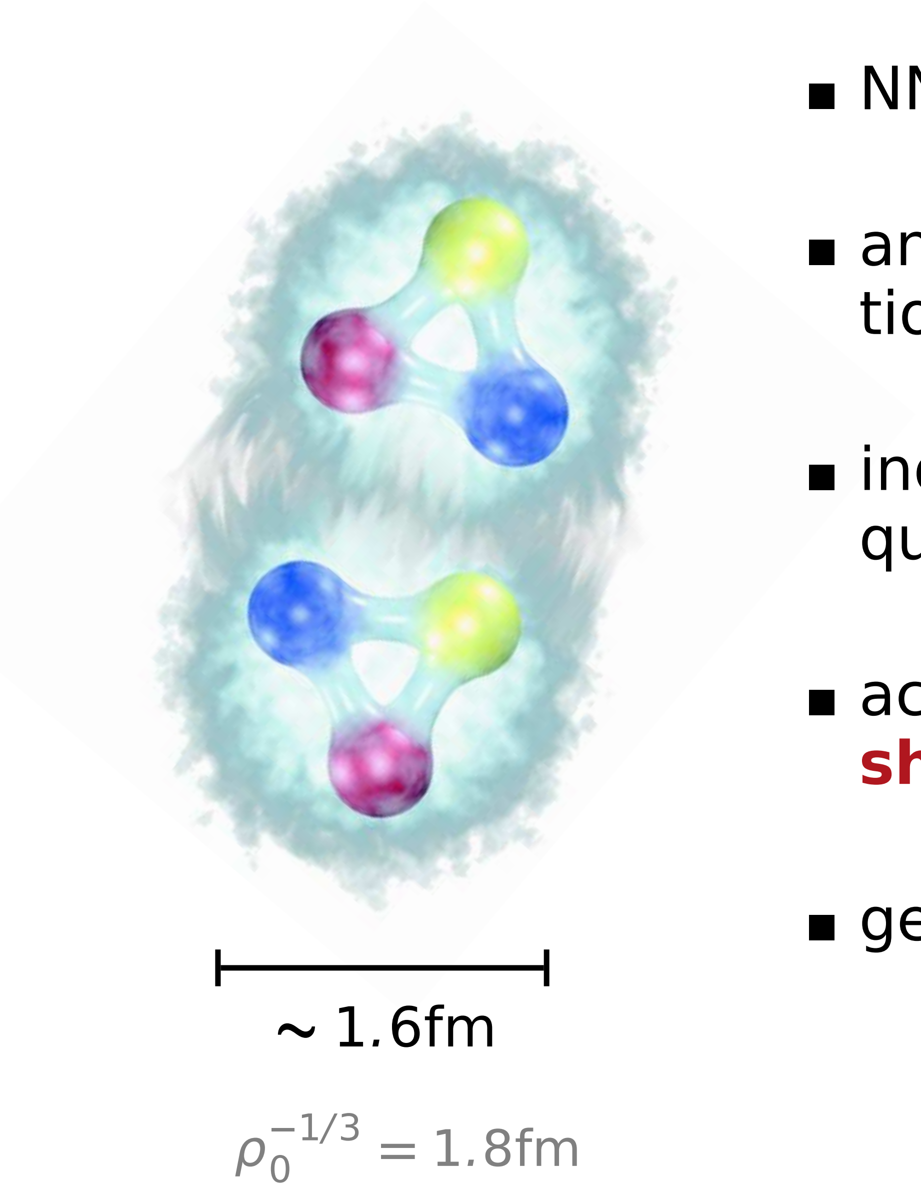
- quarks & gluons
- deconfinement

Theoretical Context



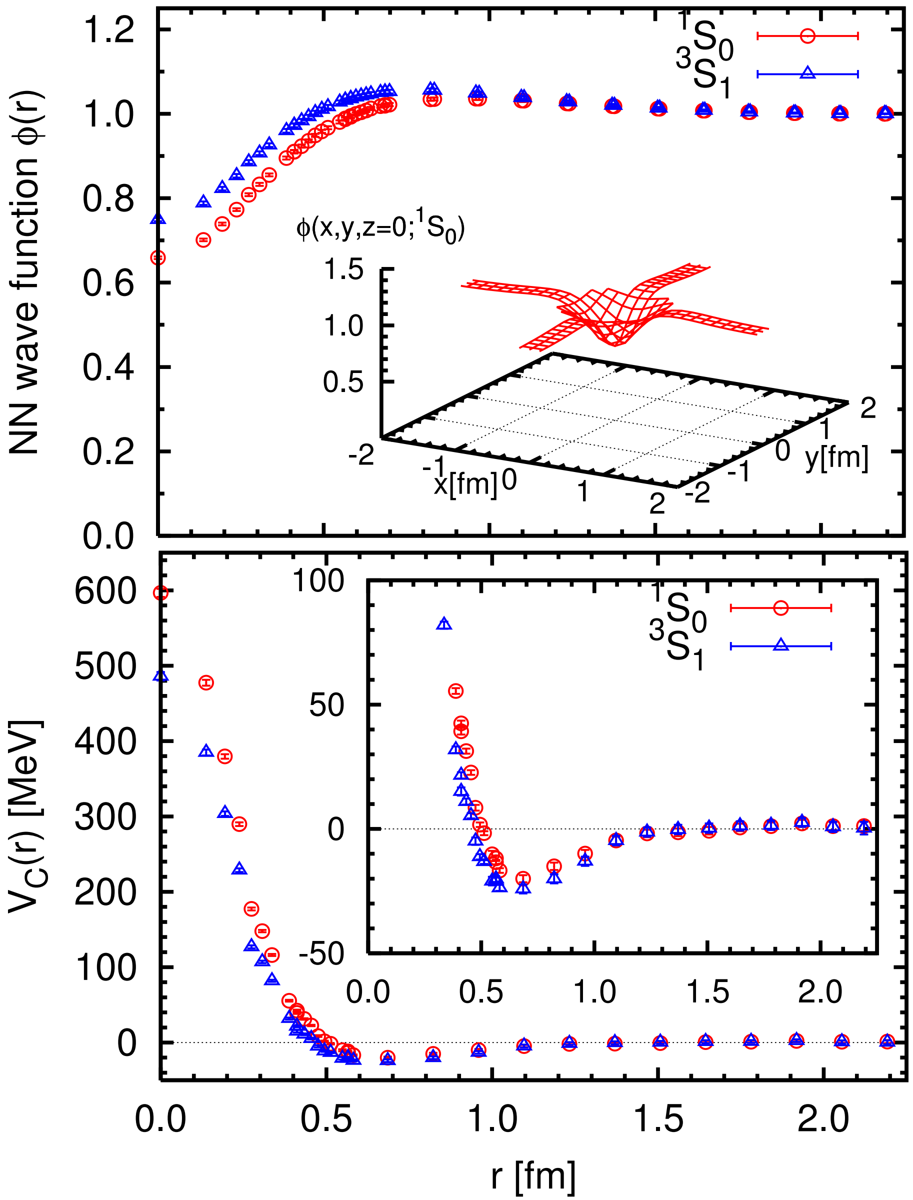
Nuclear Interactions from QCD

Nature of the Nuclear Interaction



- 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

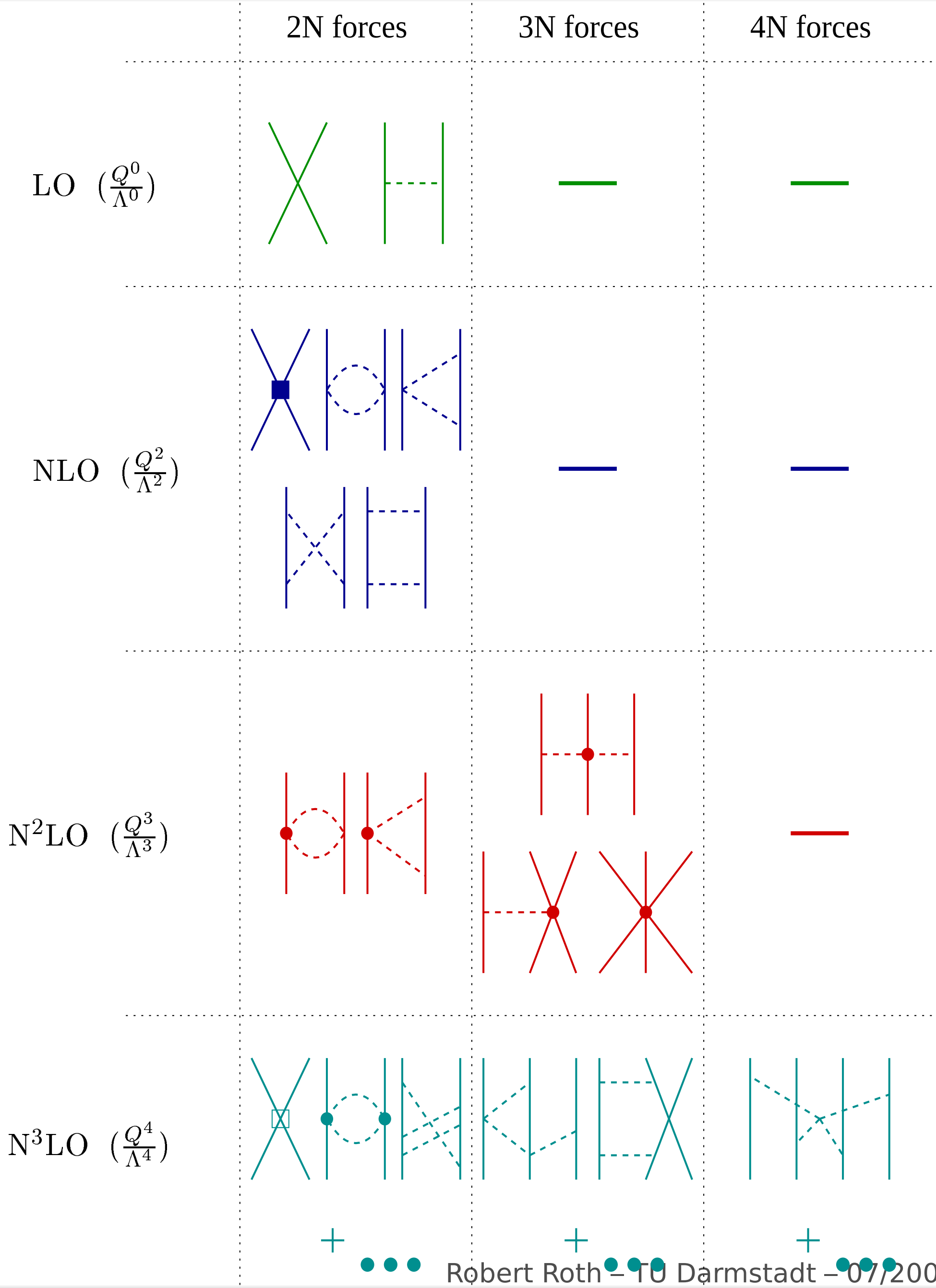


N. Ishii et al., PRL 99, 022001 (2007)

- 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 NN-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

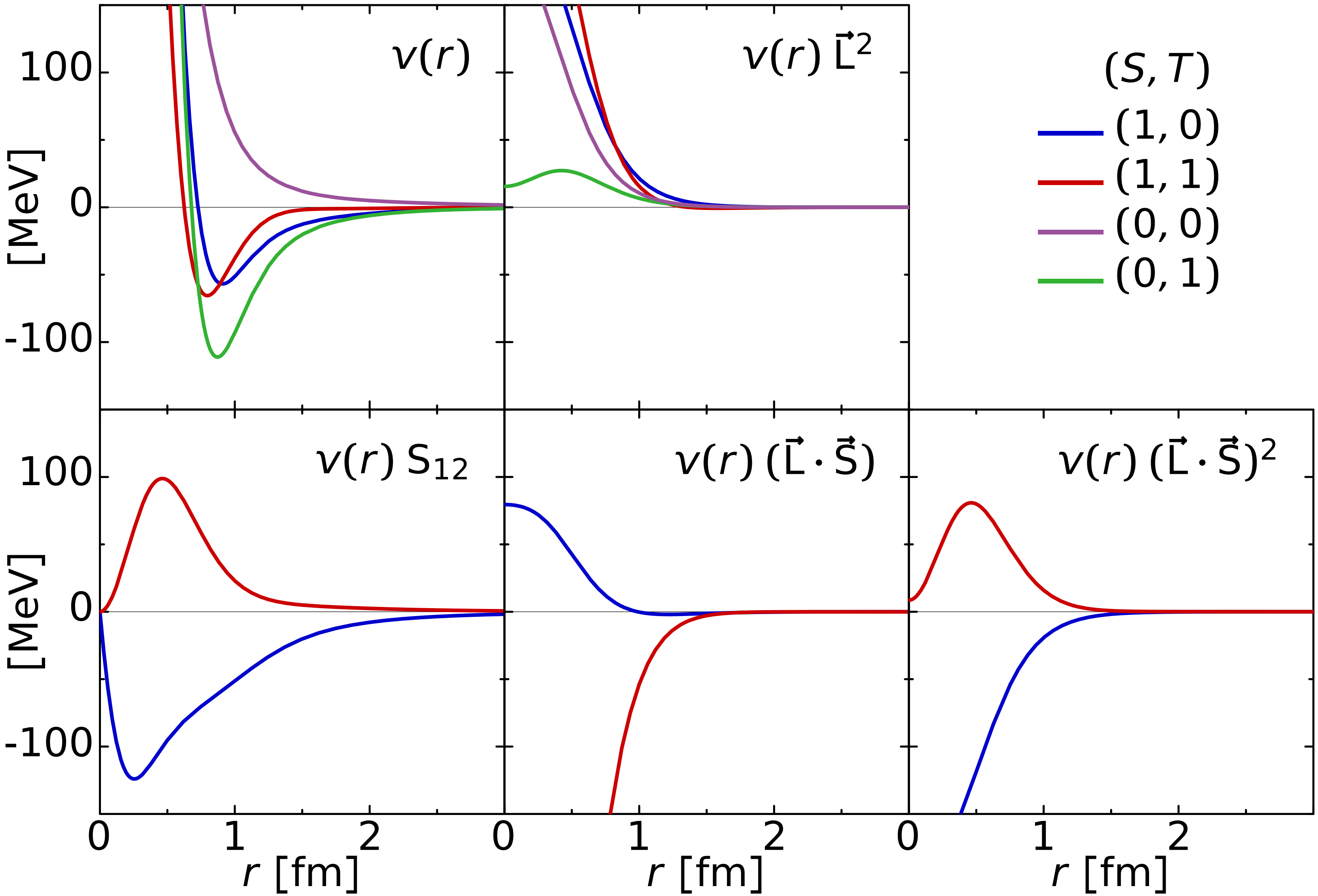
Nijmegen I/II

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

What are Correlations?

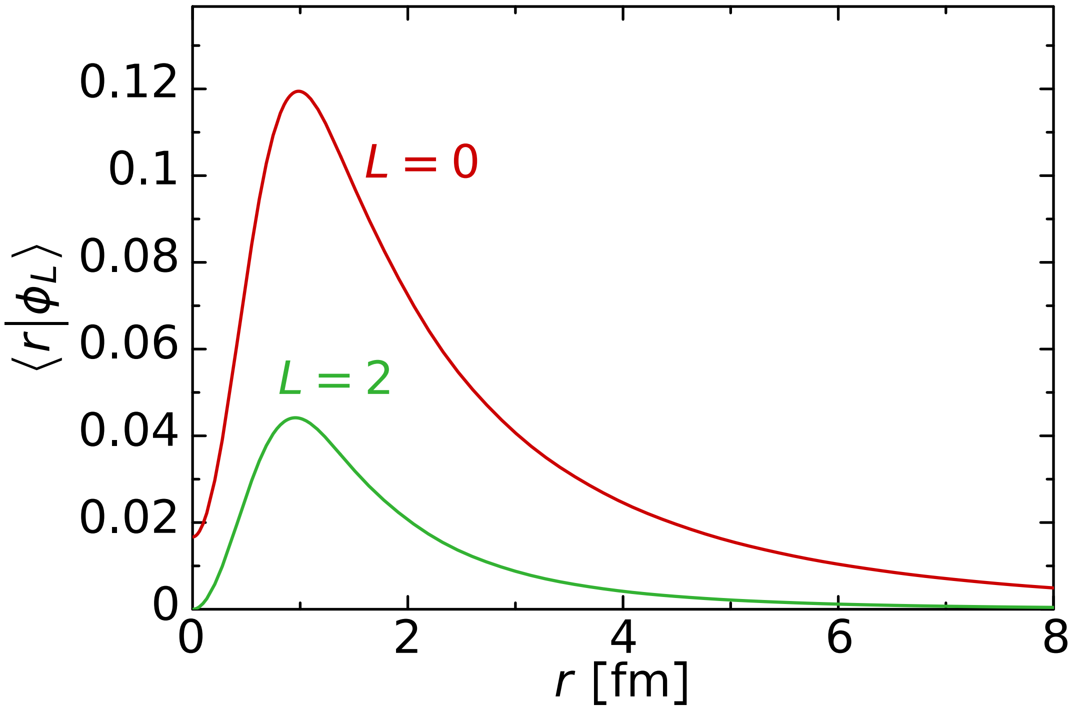
correlations:
everything beyond the
independent-particle picture

- the quantum state of A independent (non-interacting) fermions is a **Slater determinant**

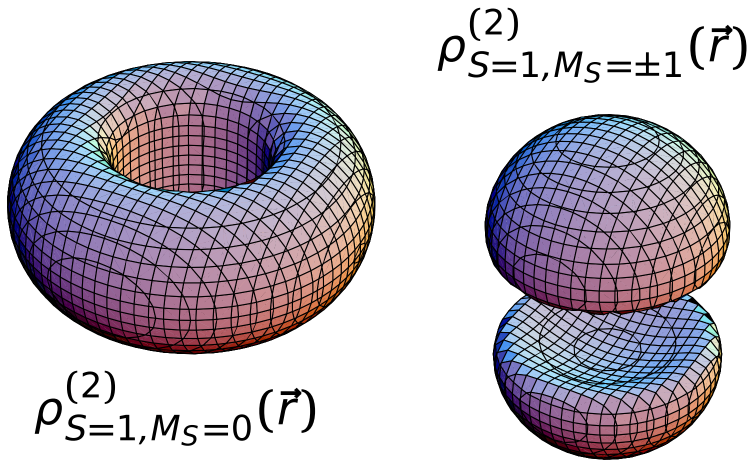
$$\left|\psi\right\rangle = \mathcal{A}\ \left(\left|\phi_1\right\rangle \otimes \left|\phi_2\right\rangle \otimes \cdots \otimes \left|\phi_A\right\rangle\right)$$

- **any two-body interaction induces correlations** which cannot be described by a 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

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

Correlated States

imprint short-range cor-
relations onto uncorre-
lated 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

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

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

Tensor Correlator C_Ω

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

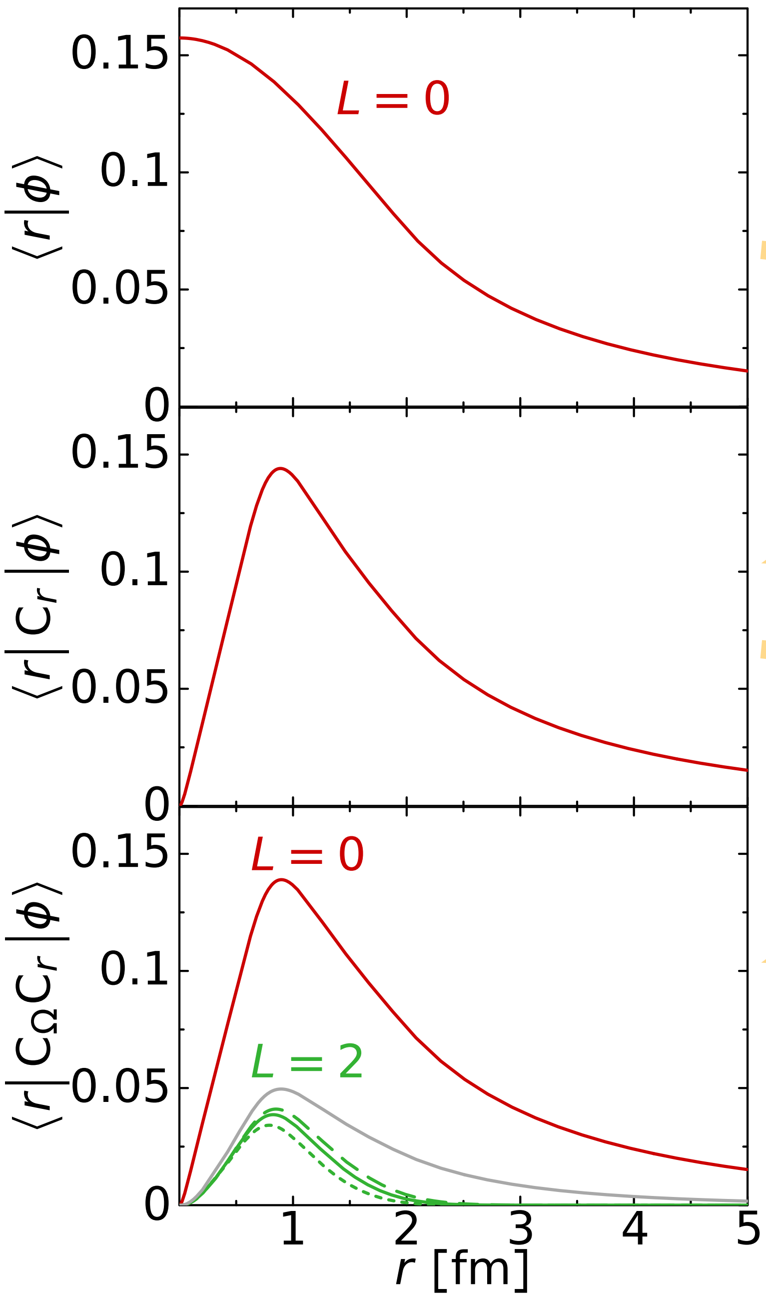
$$g_\Omega = \frac{3}{2}\vartheta(r)\left[(\vec{\sigma}_1\cdot\vec{q}_\Omega)(\vec{\sigma}_2\cdot\vec{r}) + (\vec{r}\leftrightarrow\vec{q}_\Omega)\right]$$

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

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

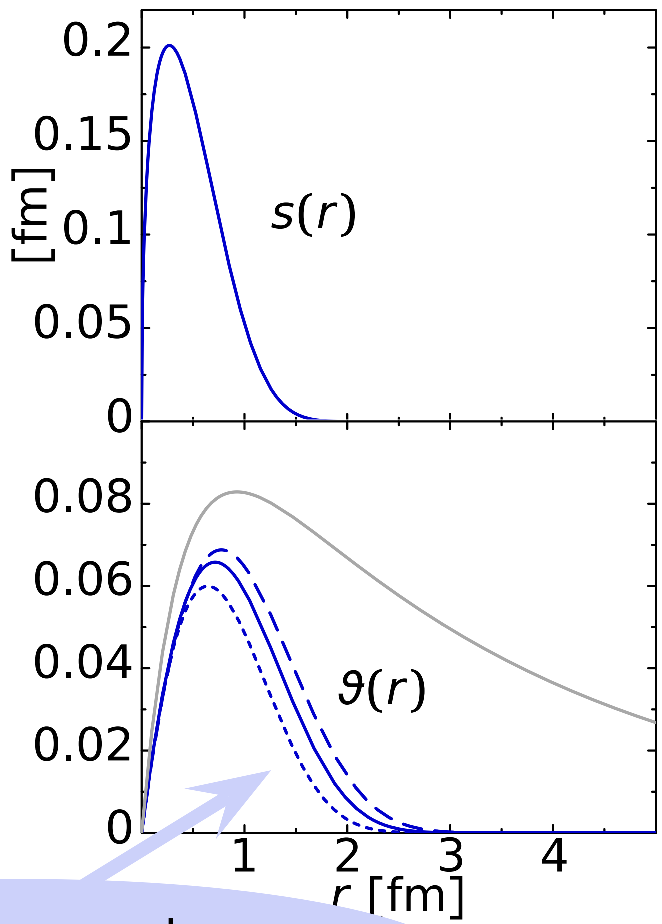
- $s(r)$ and $\vartheta(r)$ are optimized for the initial potential

Correlated States: The Deuteron



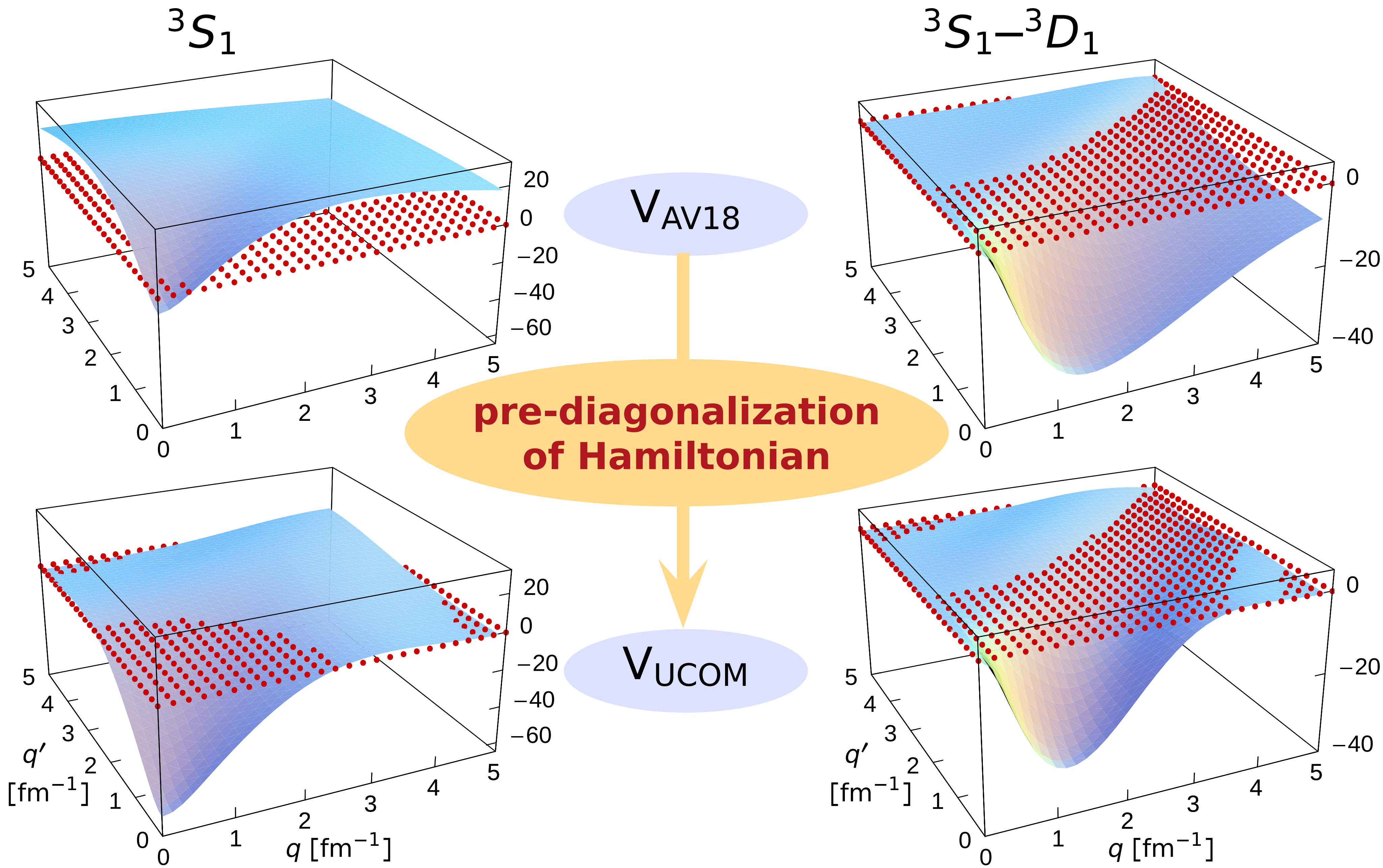
central correlations

tensor correlations



only short-range tensor correlations treated by C_Ω

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

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

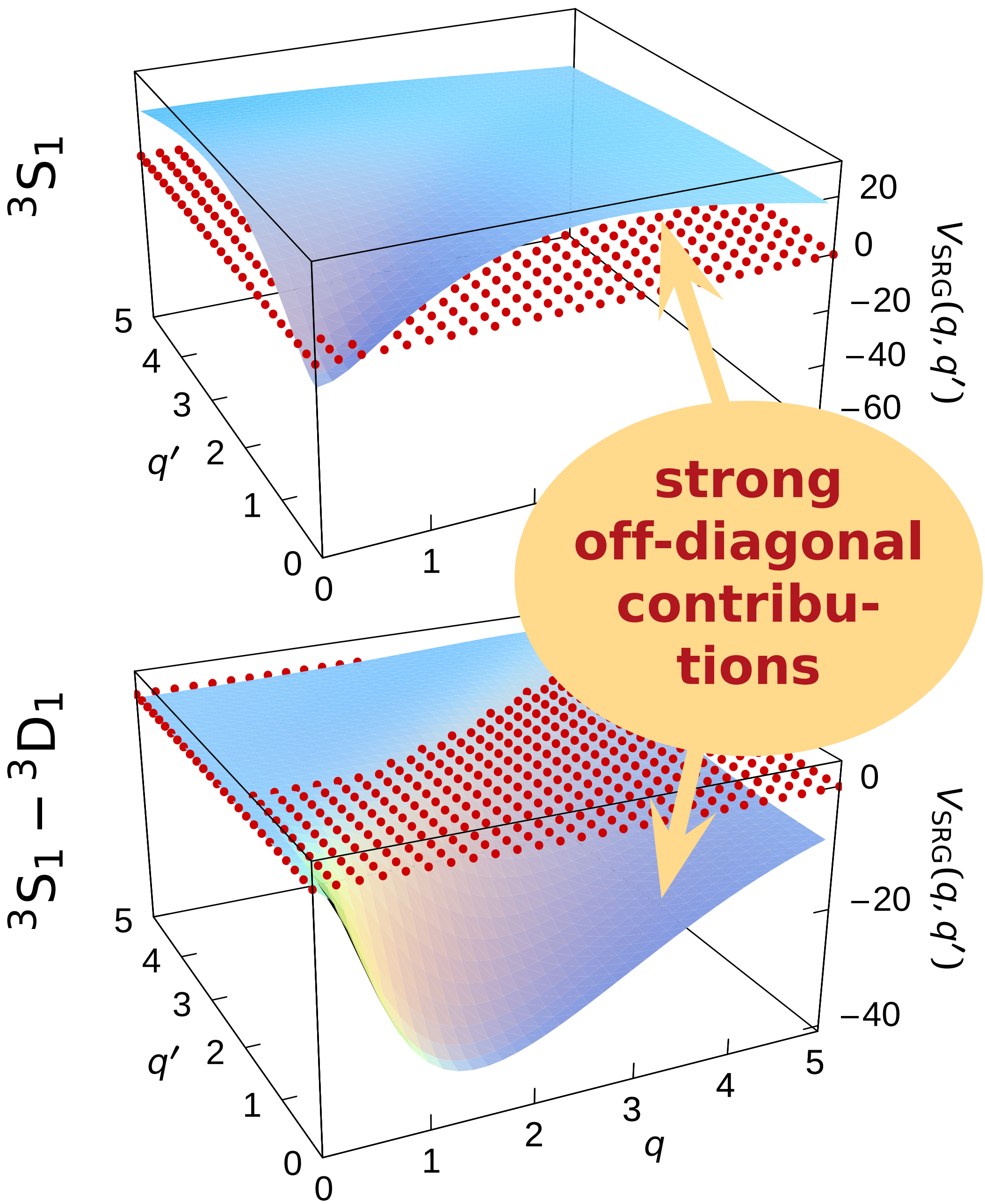
- dynamical generator defined as commutator with the operator in whose eigenbasis H shall be diagonalized

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

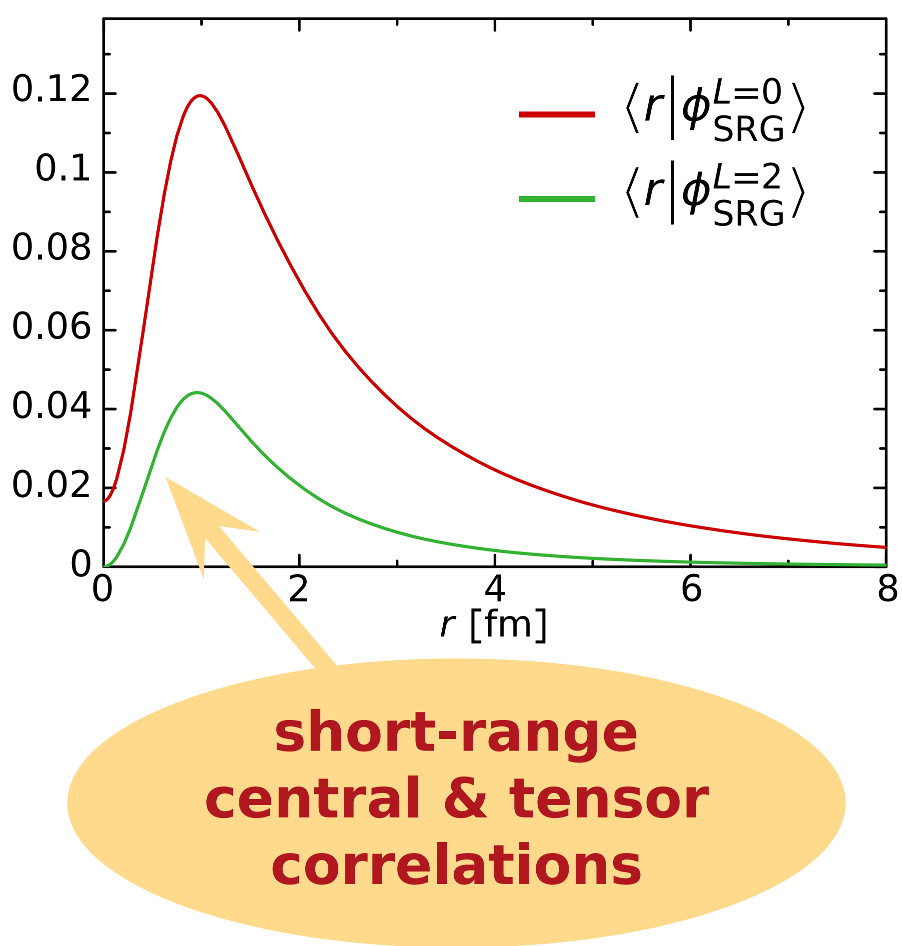
UCOM vs. SRG

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

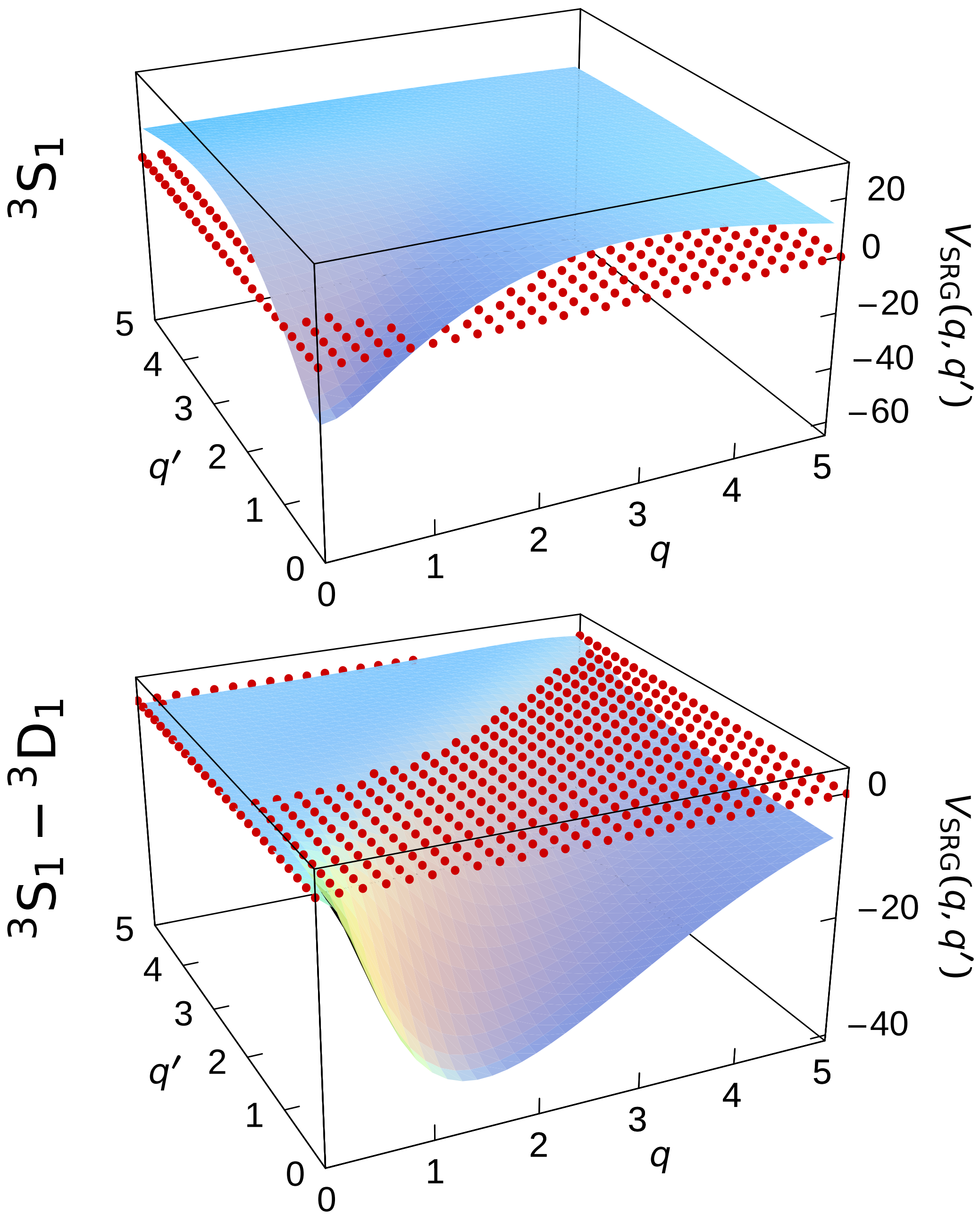
SRG Evolution: The Deuteron



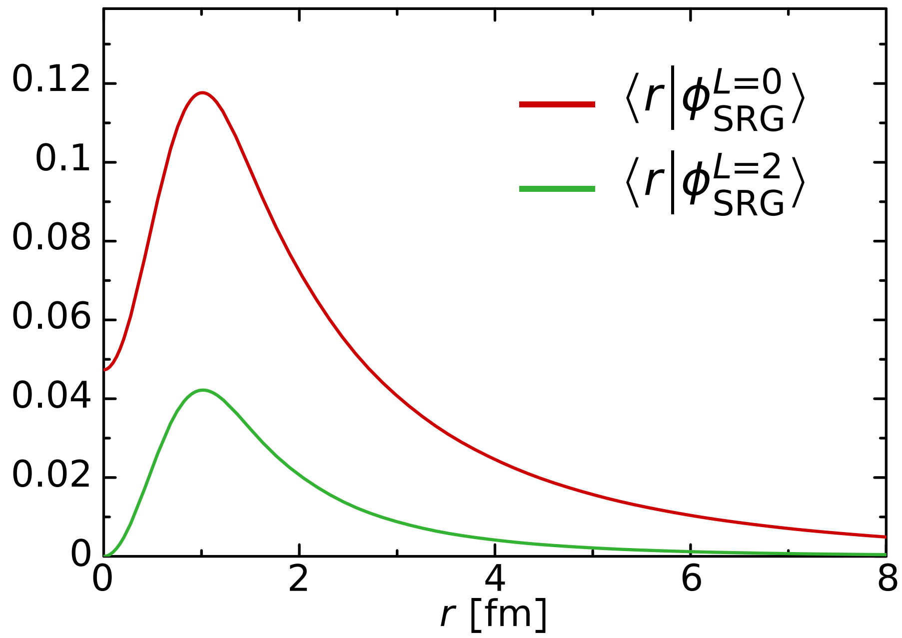
Argonne V18



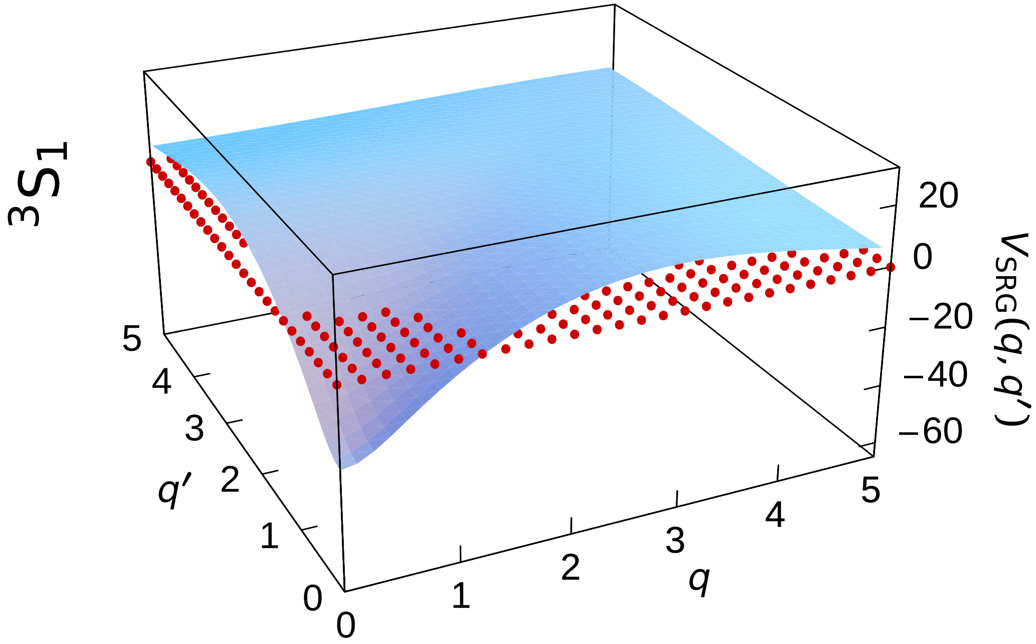
SRG Evolution: The Deuteron

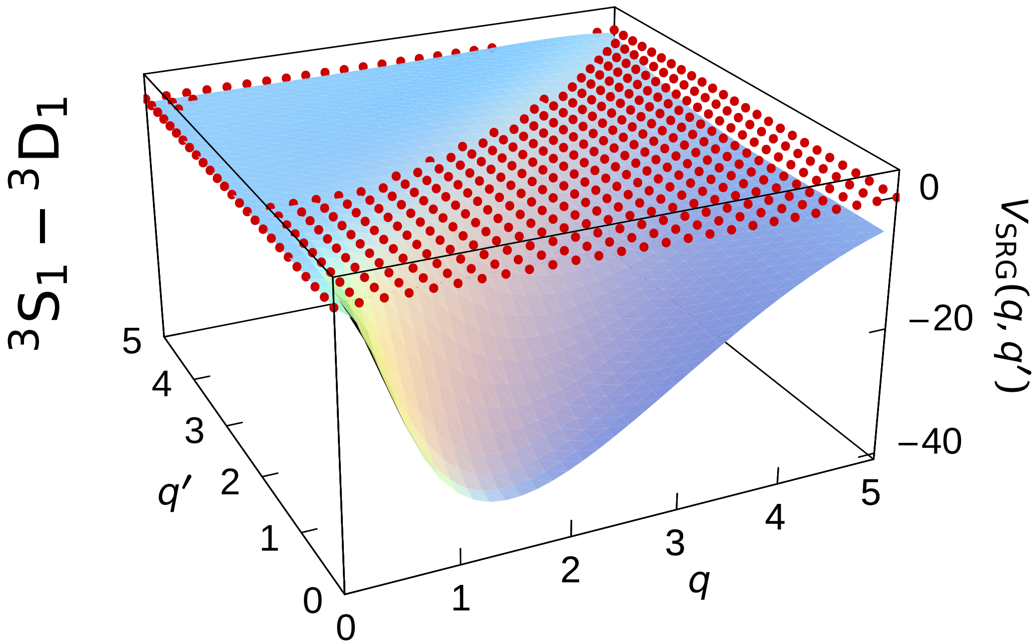


$\alpha = 0.0004\,\text{fm}^4$



SRG Evolution: The Deuteron





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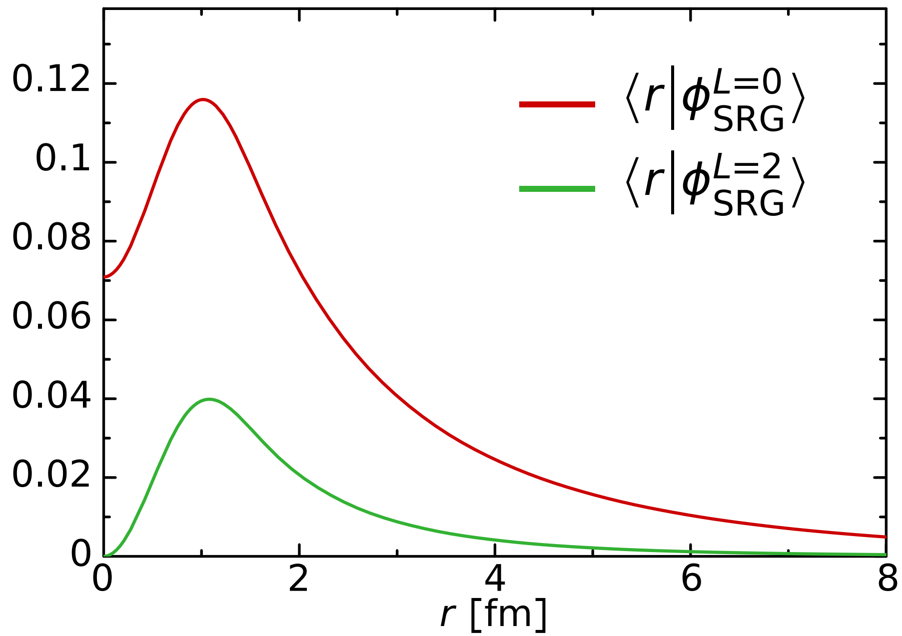
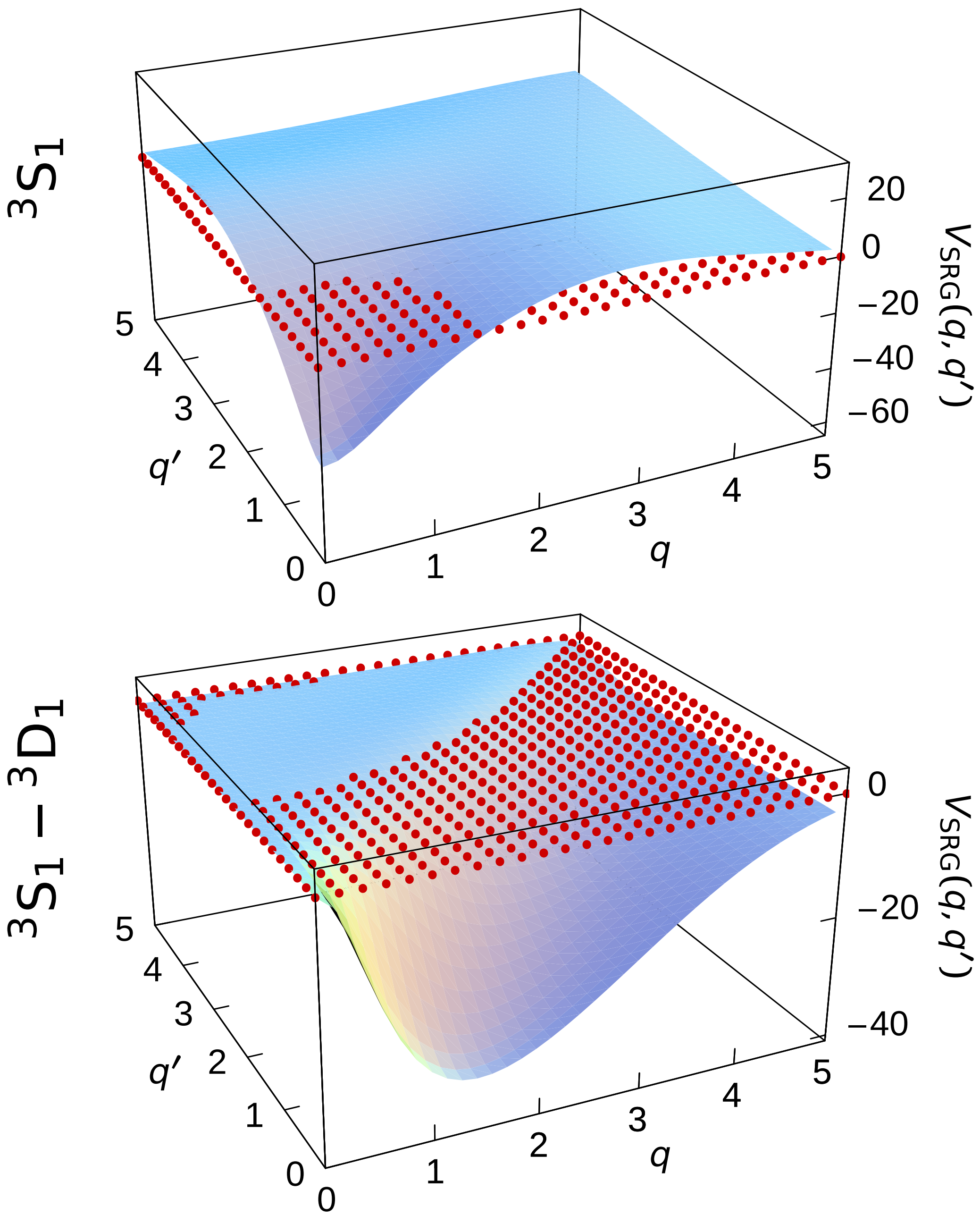


SRG Evolution: The Deuteron



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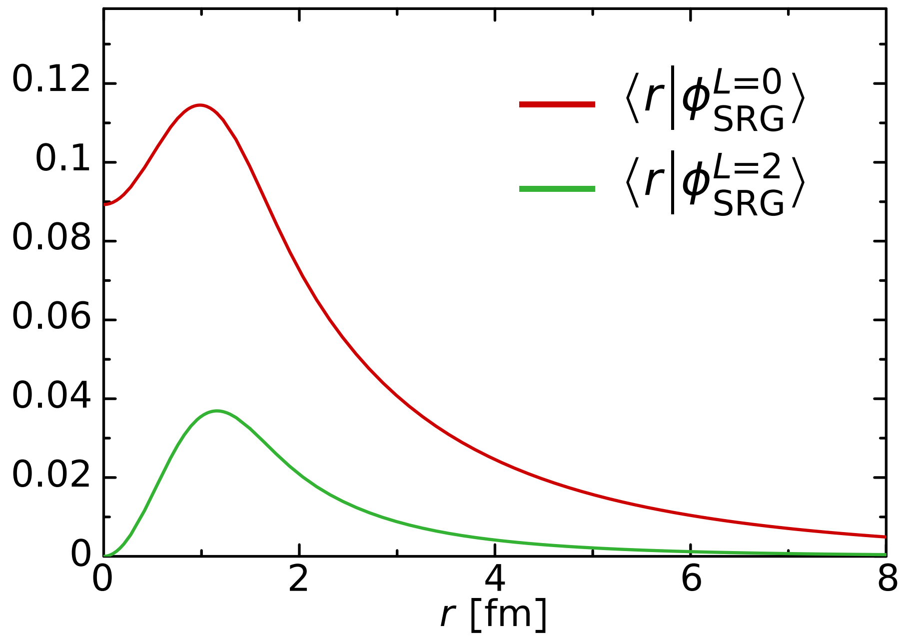
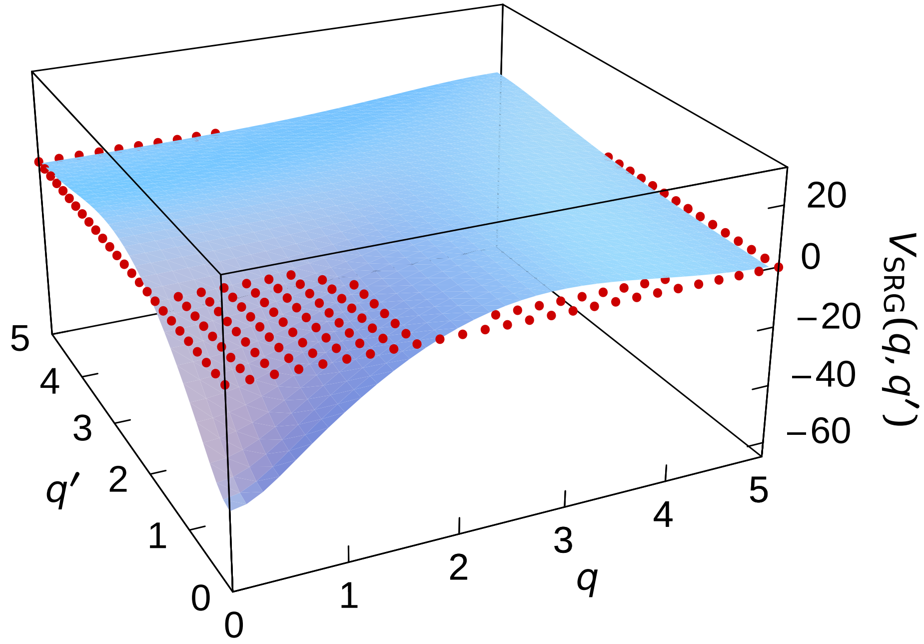
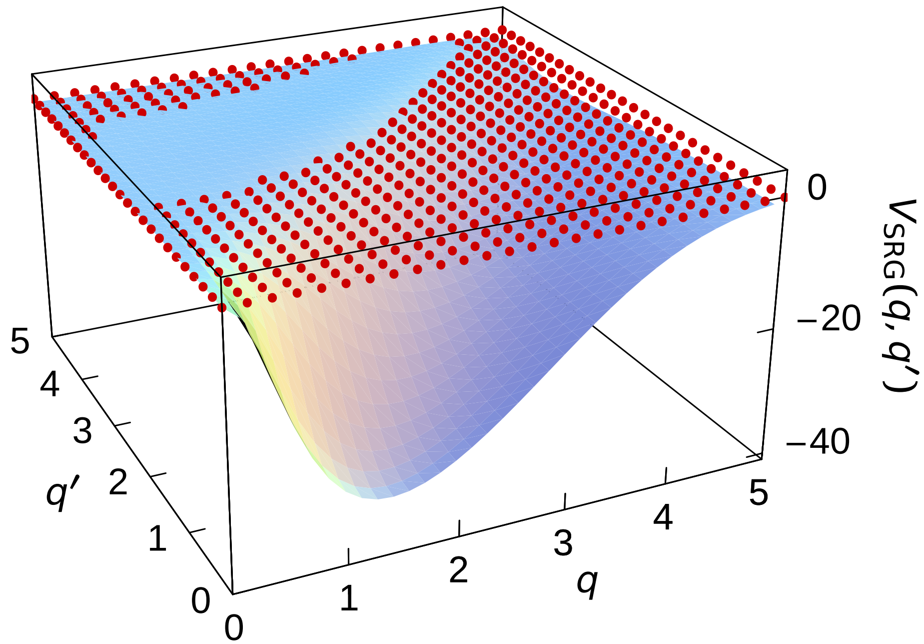


SRG Evolution: The Deuteron

$^3S_1$



$^3S_1 - {}^3D_1$



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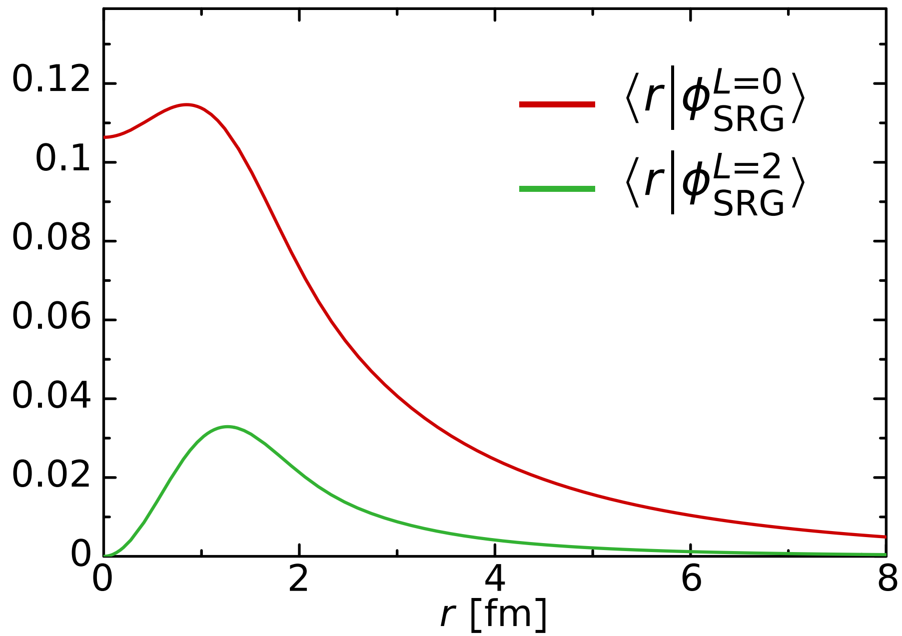
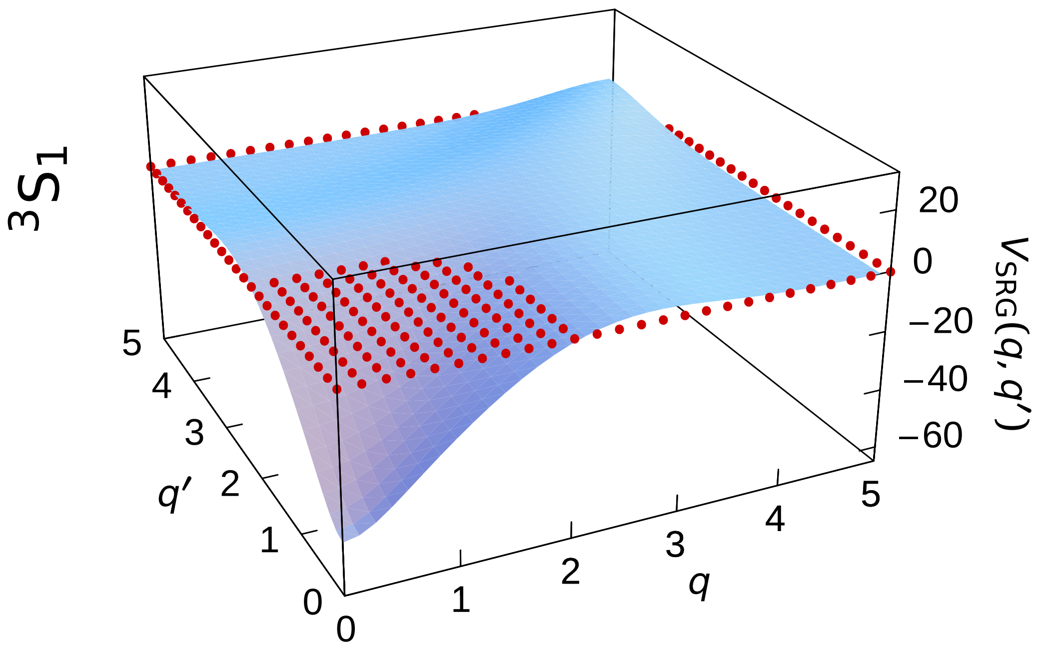
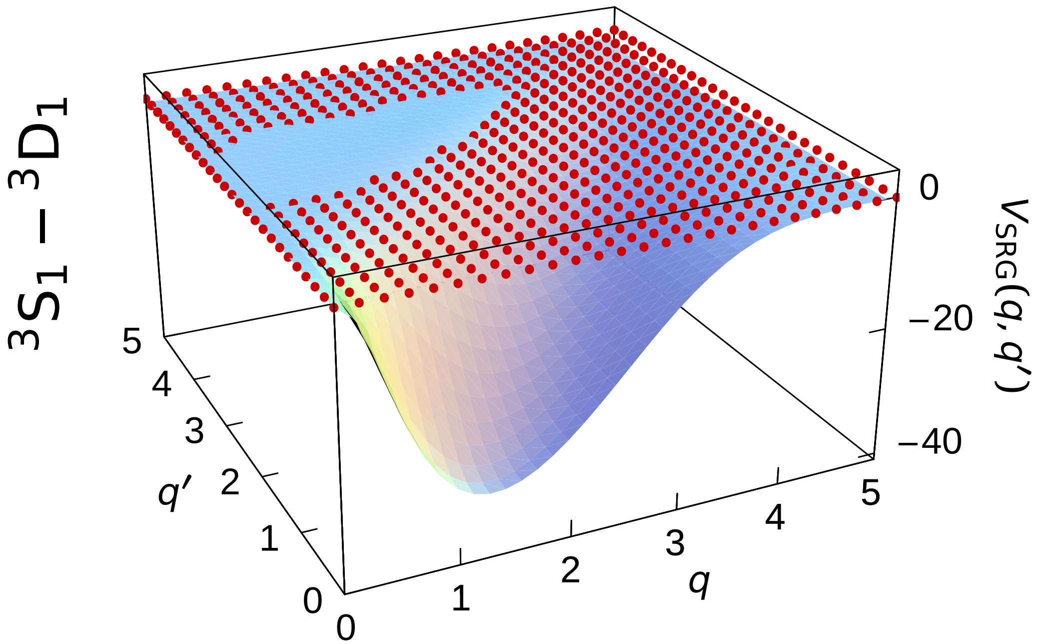


SRG Evolution: The Deuteron





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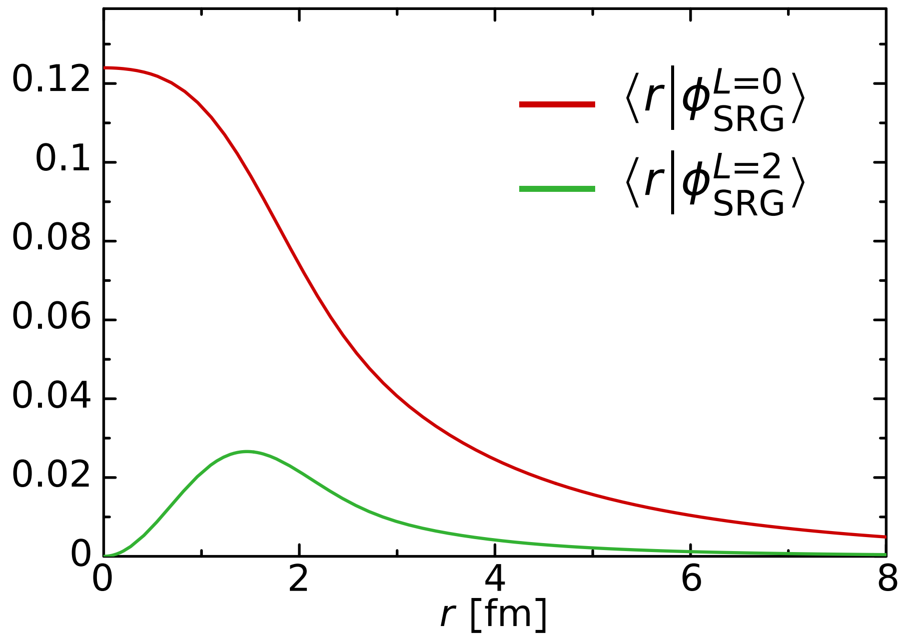
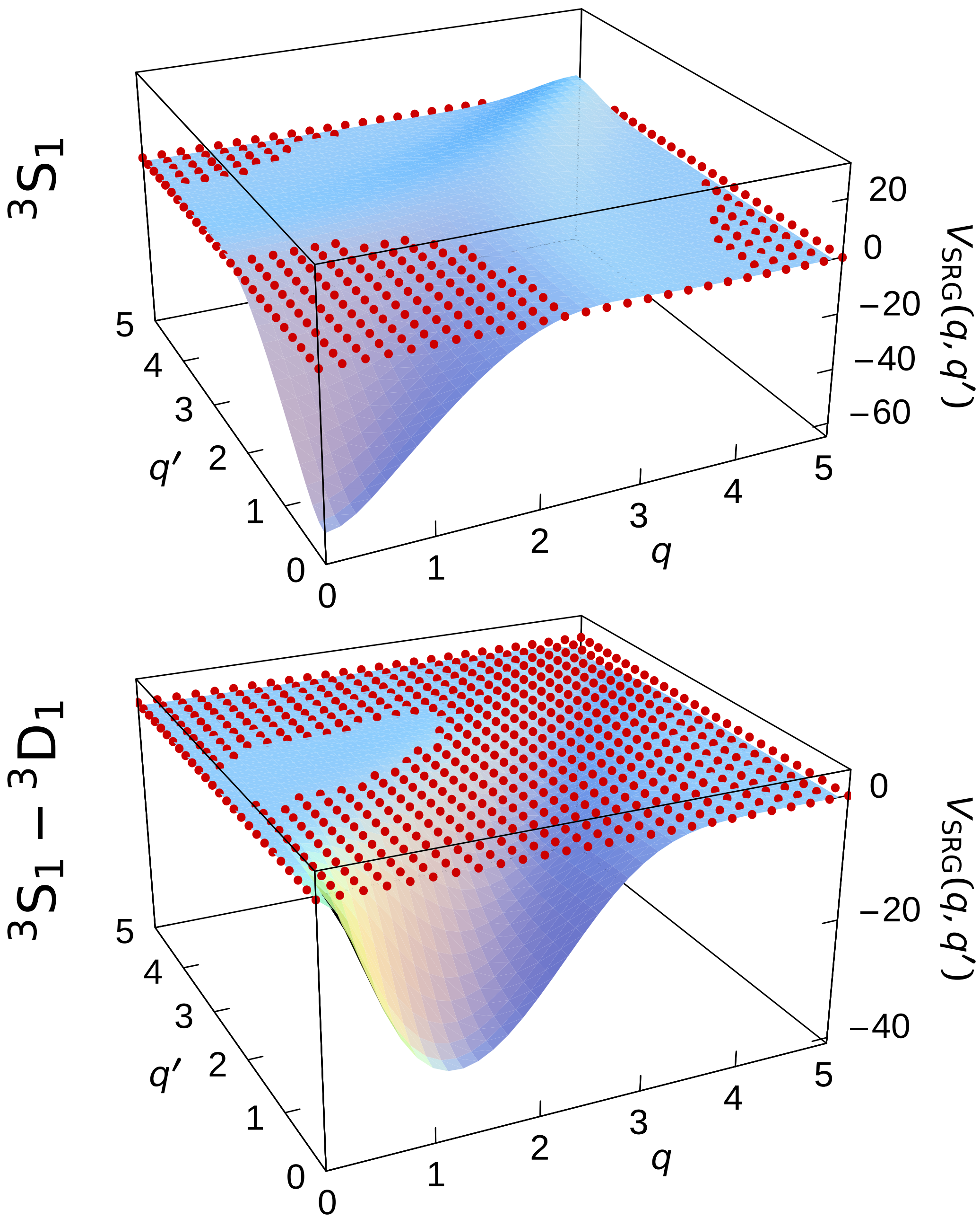


SRG Evolution: The Deuteron



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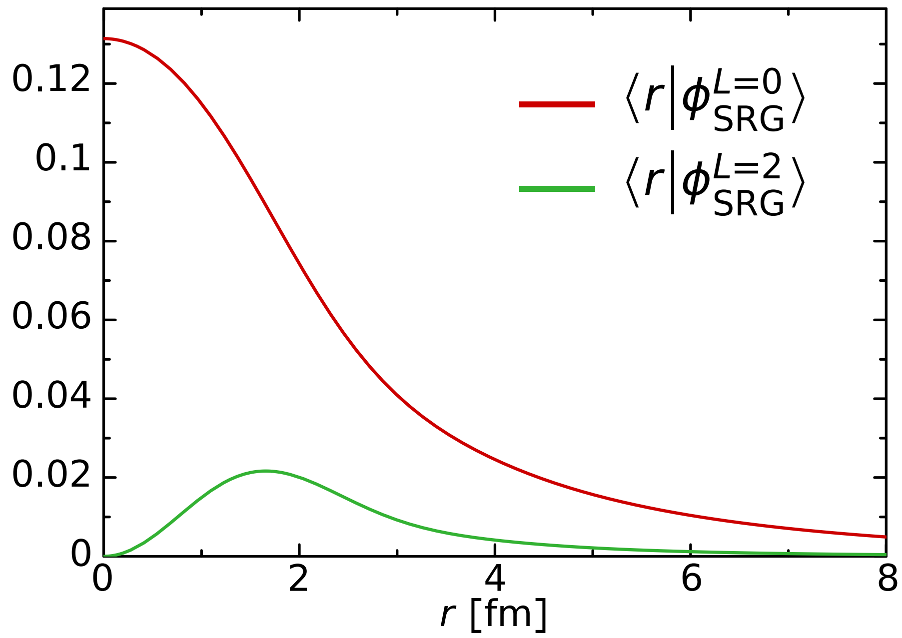
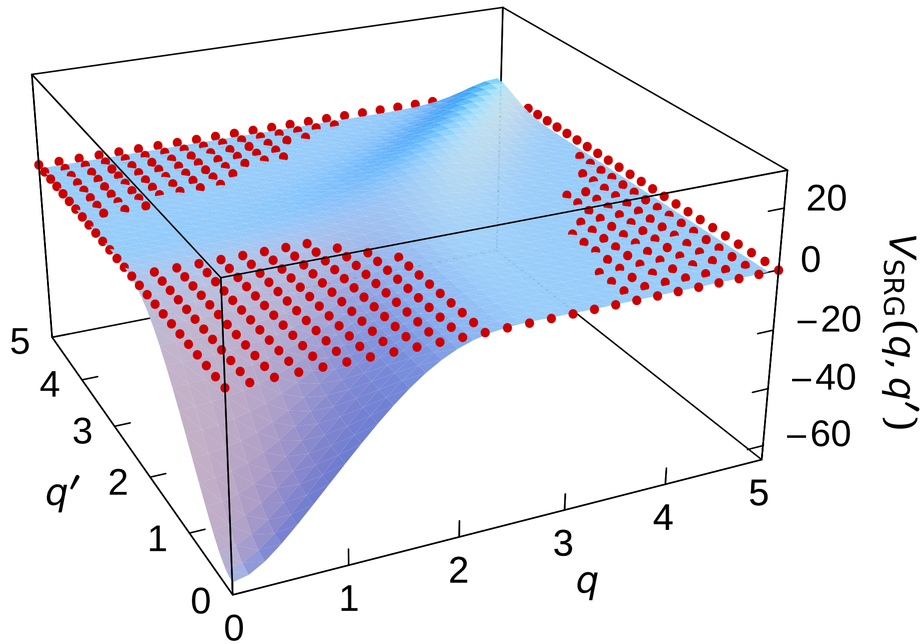
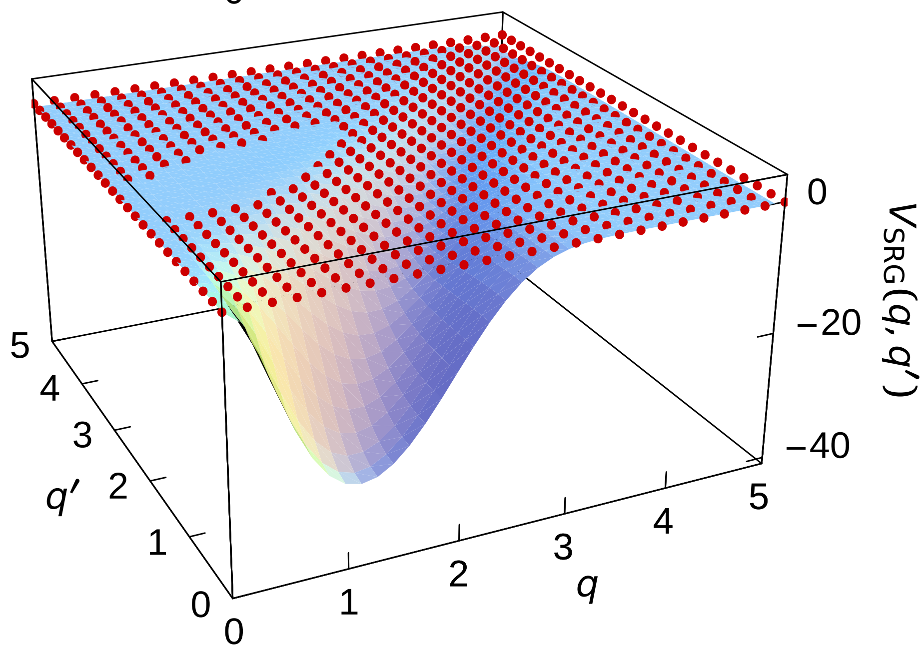


SRG Evolution: The Deuteron

$^3S_1$



$^3S_1 - {}^3D_1$



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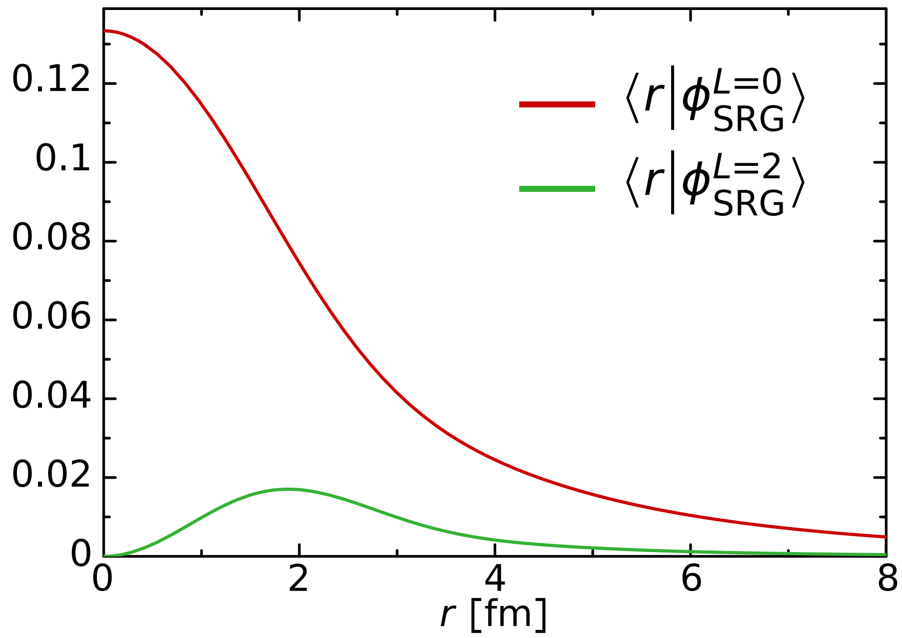
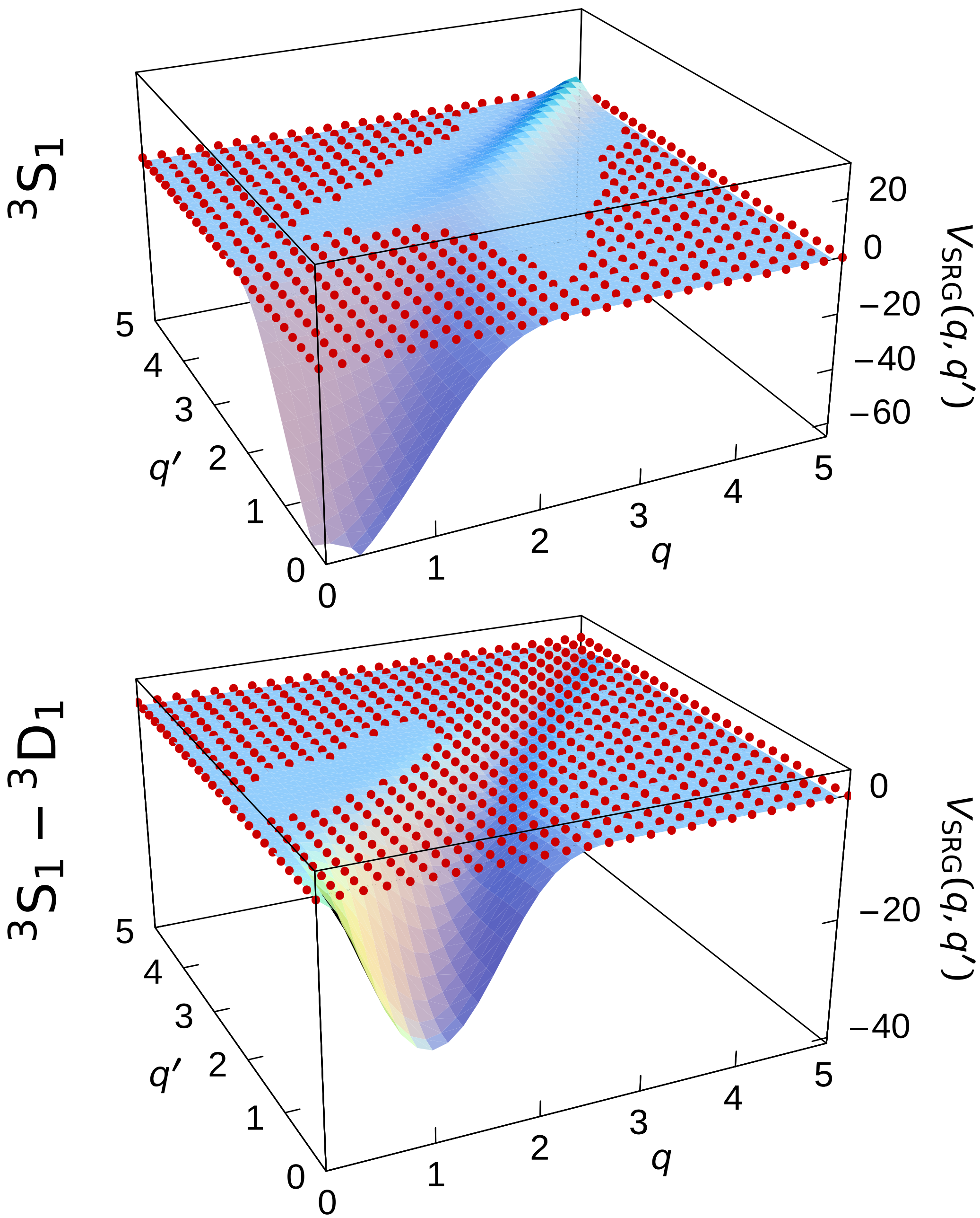


SRG Evolution: The Deuteron



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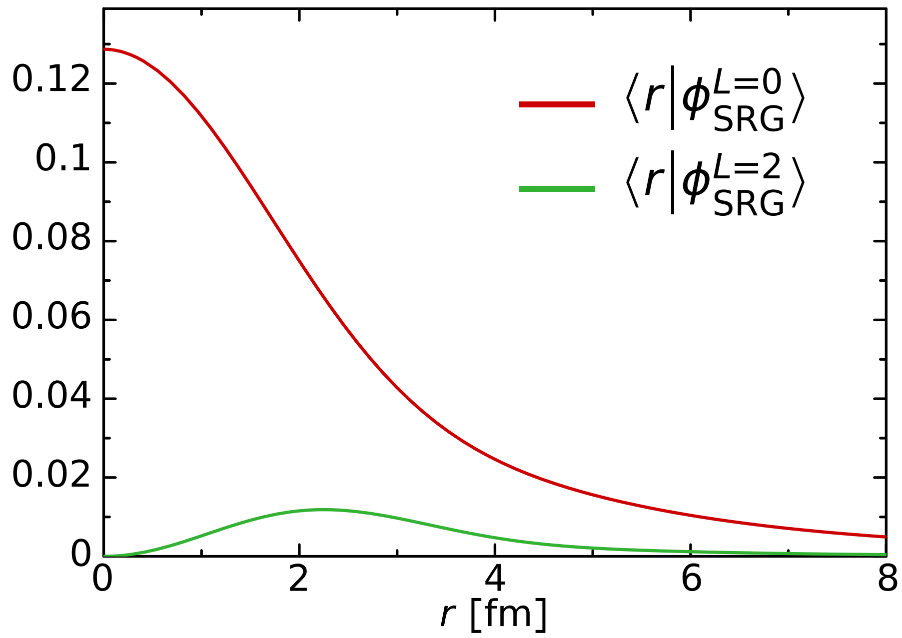
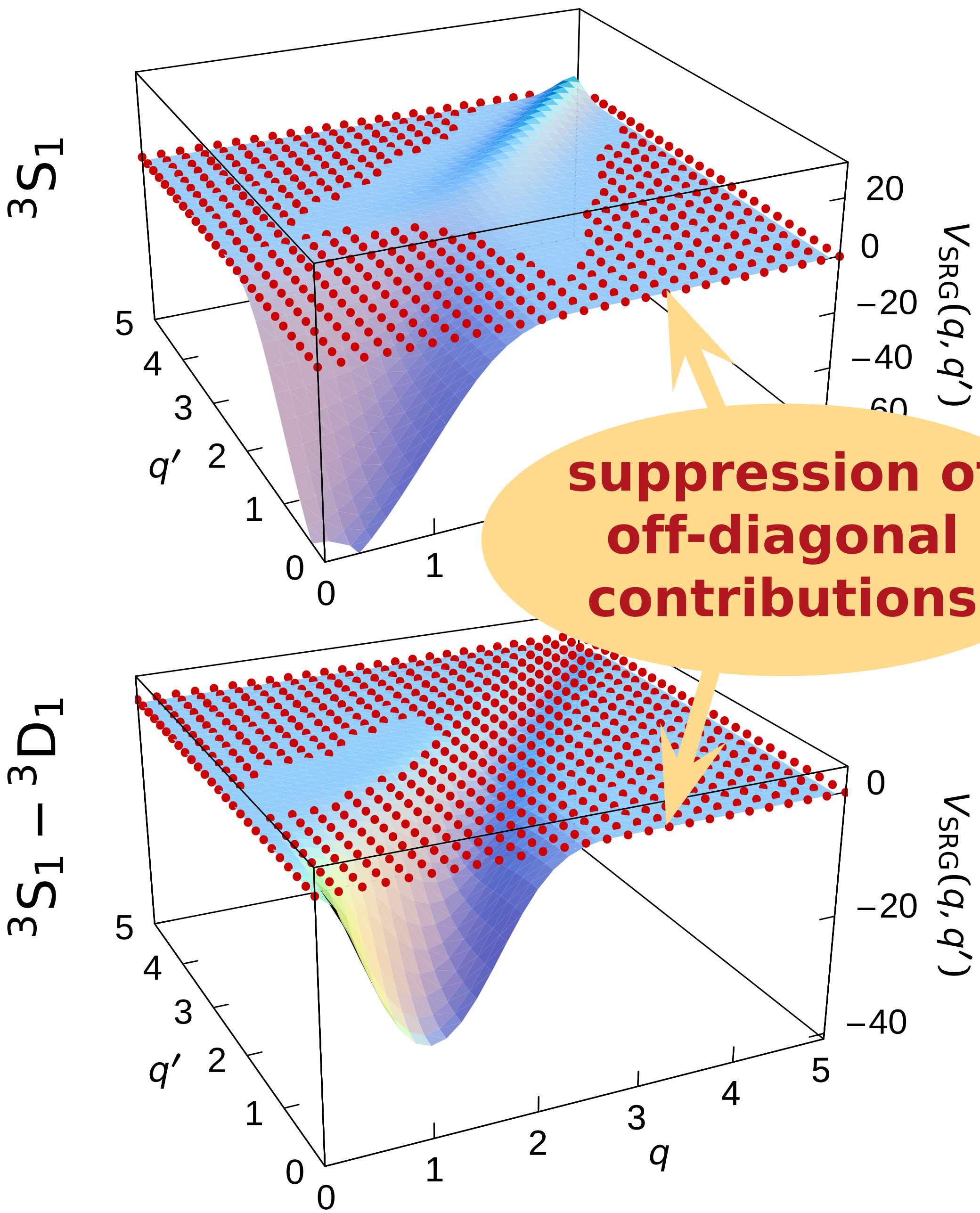


SRG Evolution: The Deuteron



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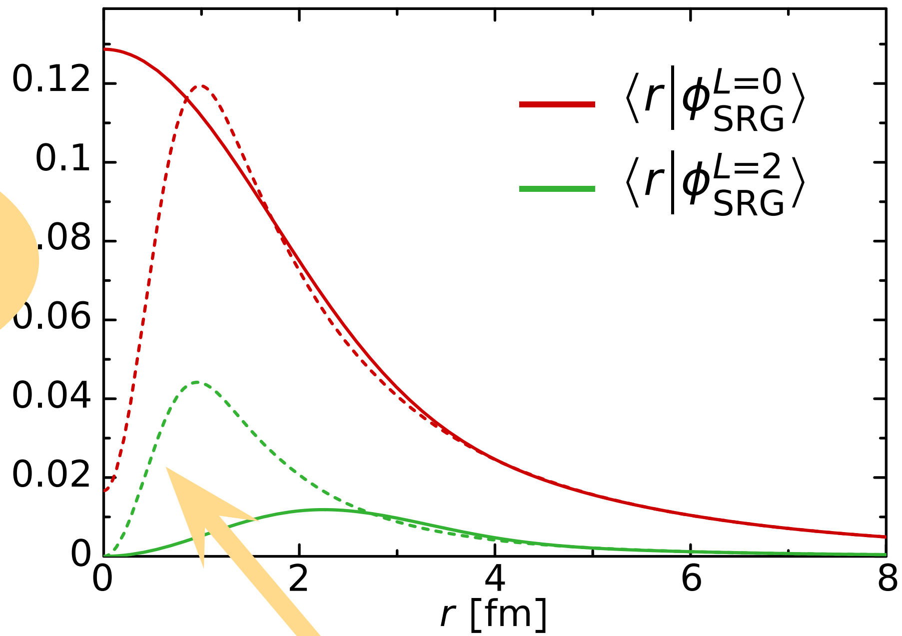
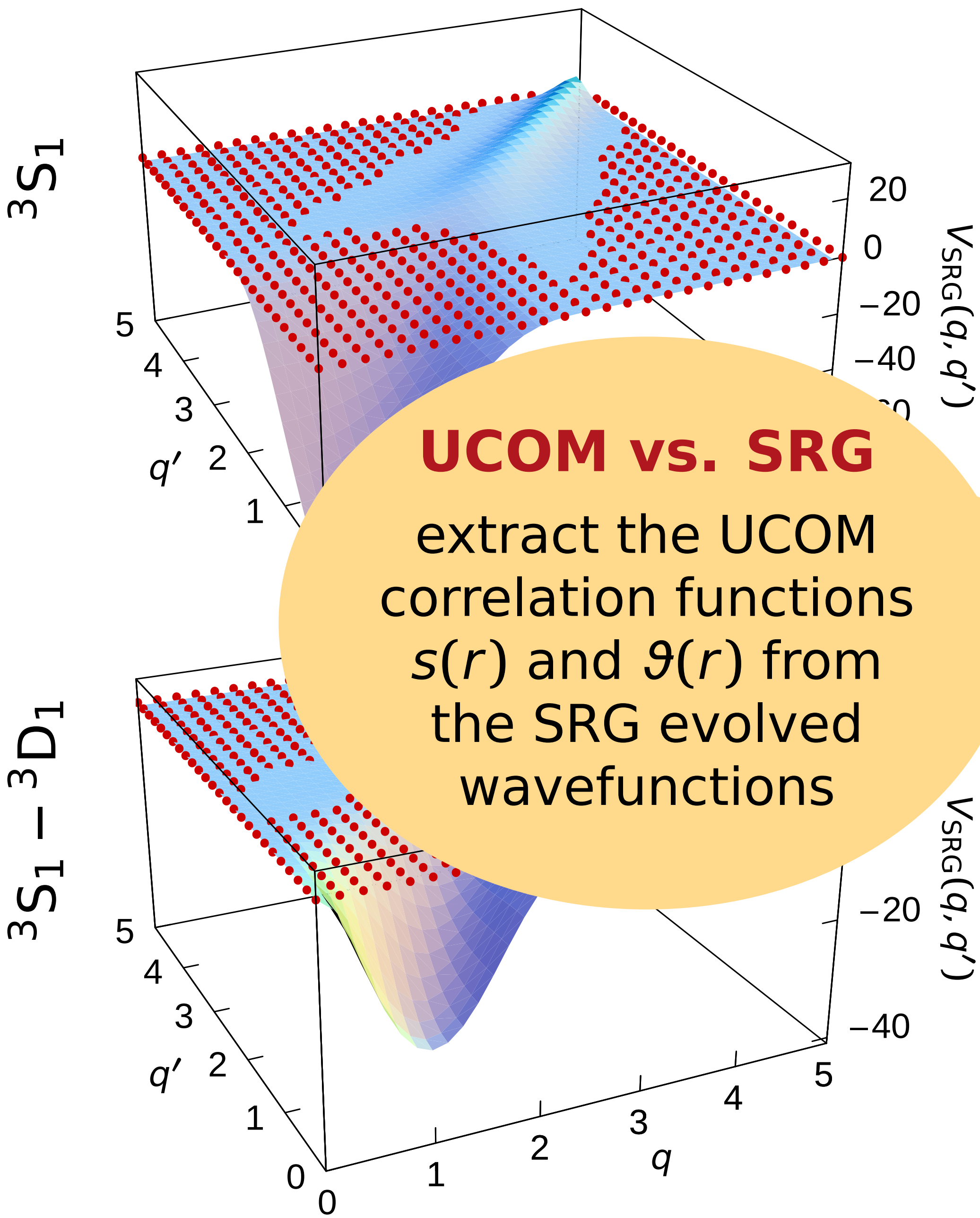


suppression of off-diagonal contributions

elimination of short- range correlations

SRG Evolution: The Deuteron



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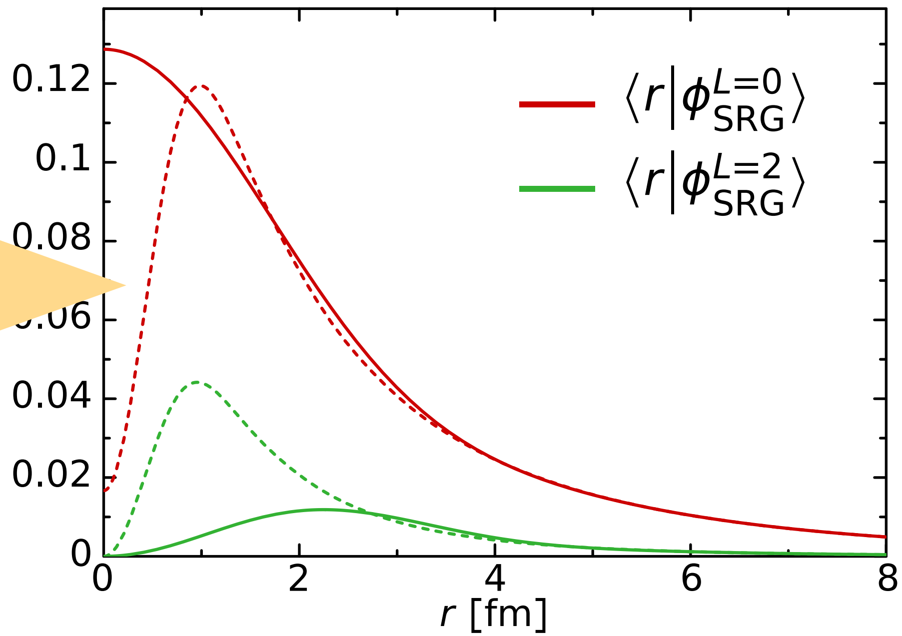


UCOM vs. SRG

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

Basics of the No-Core Shell Model

- **many-body basis**: Slater determinants $|\Phi_\nu\rangle$ composed of harmonic oscillator single-particle states

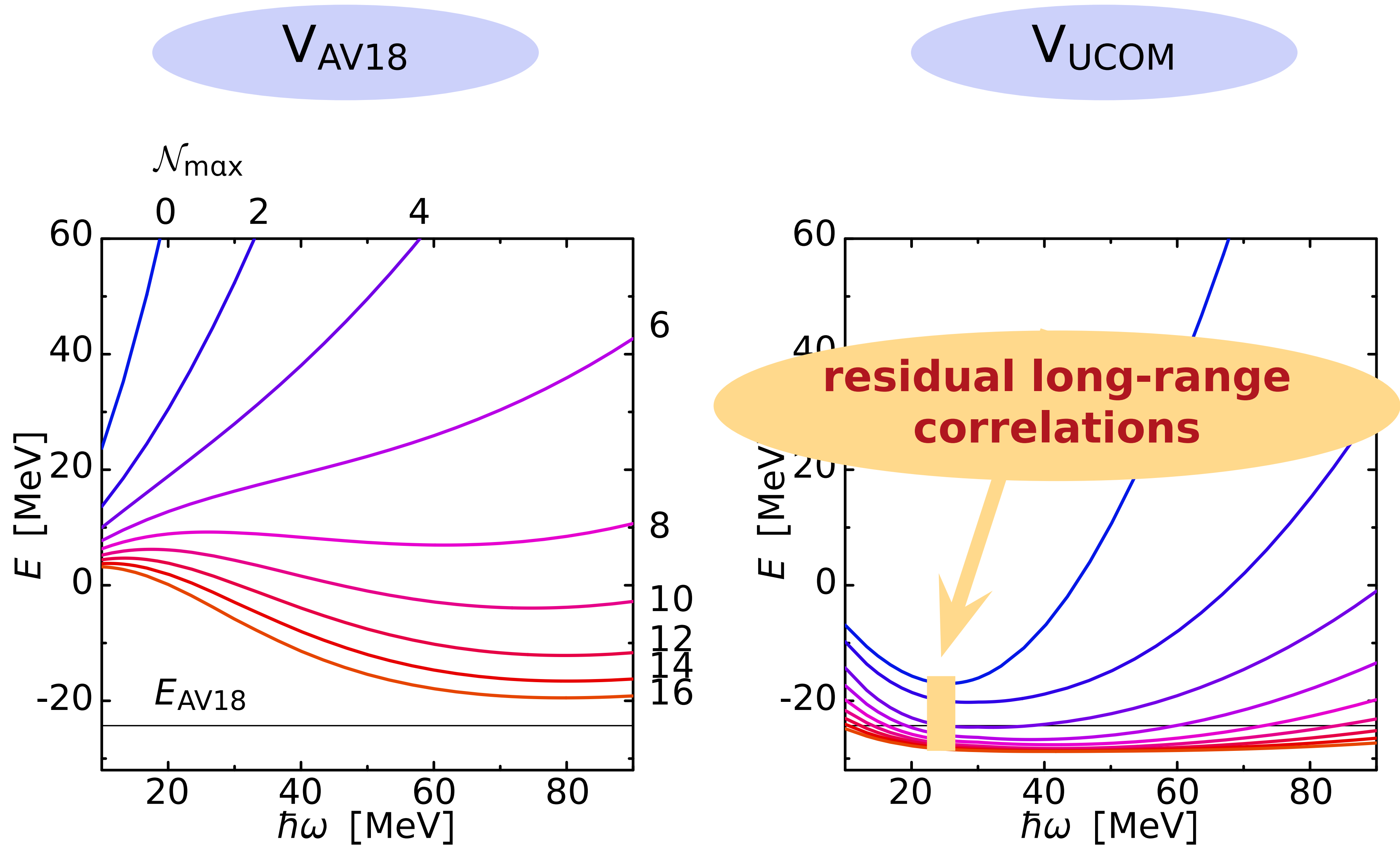
$$|\Psi\rangle = \sum_\nu C_\nu |\Phi_\nu\rangle$$

- **model space**: spanned by basis states $|\Phi_\nu\rangle$ with unperturbed excitation energies of up to $\mathcal{N}_{\text{max}}\hbar\omega$

with increasing model space size more and more **correlations can be described** by the model space

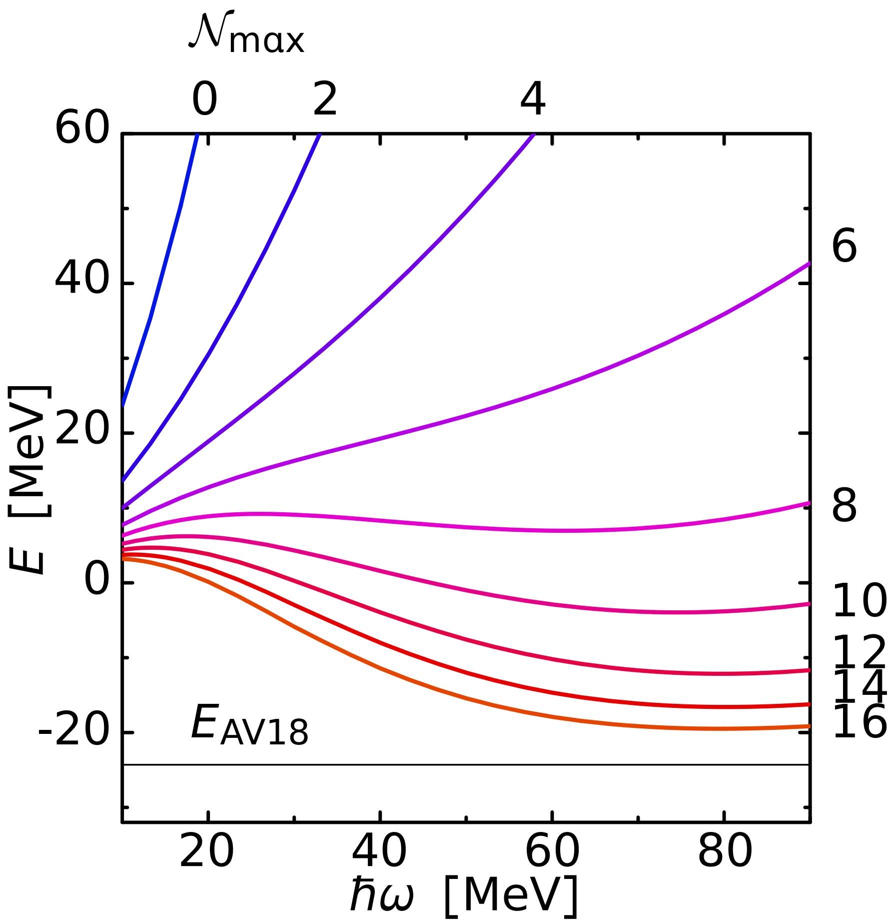
facilitates systematic study of short- and long-range correlations

^{4}He: Convergence

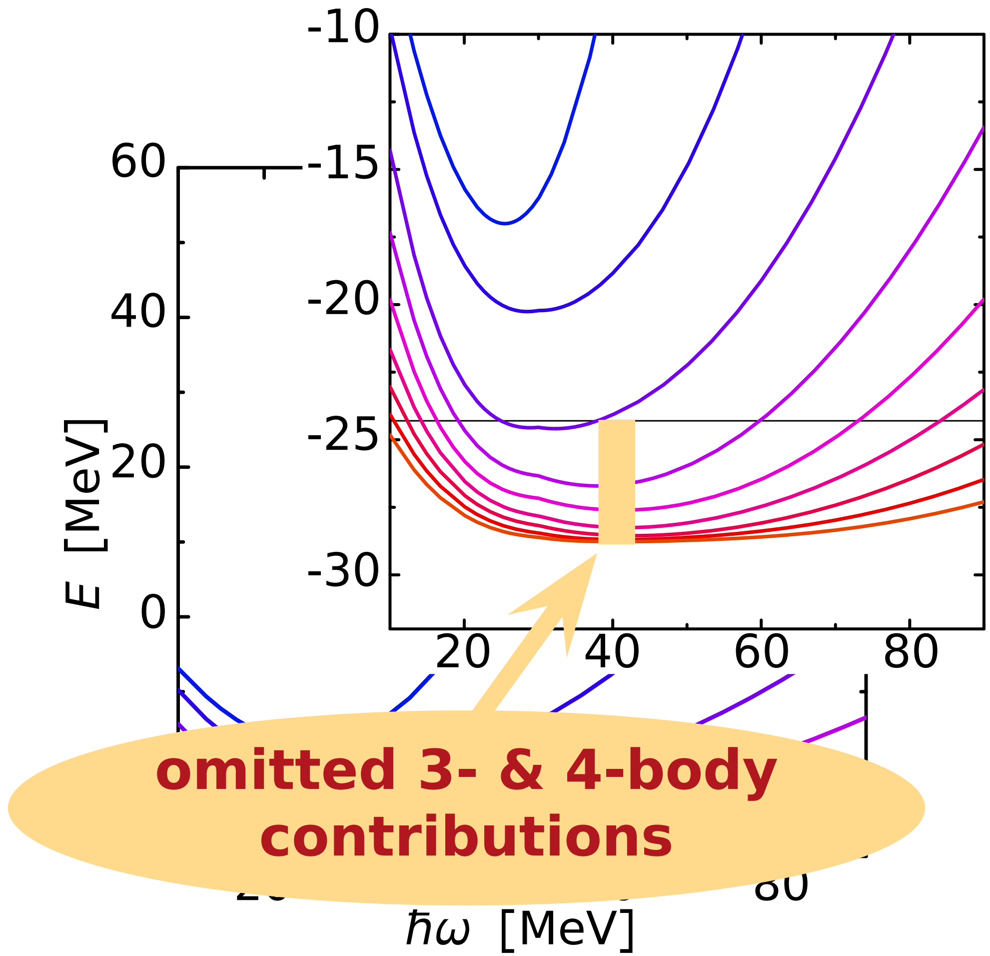


^{4}He: Convergence

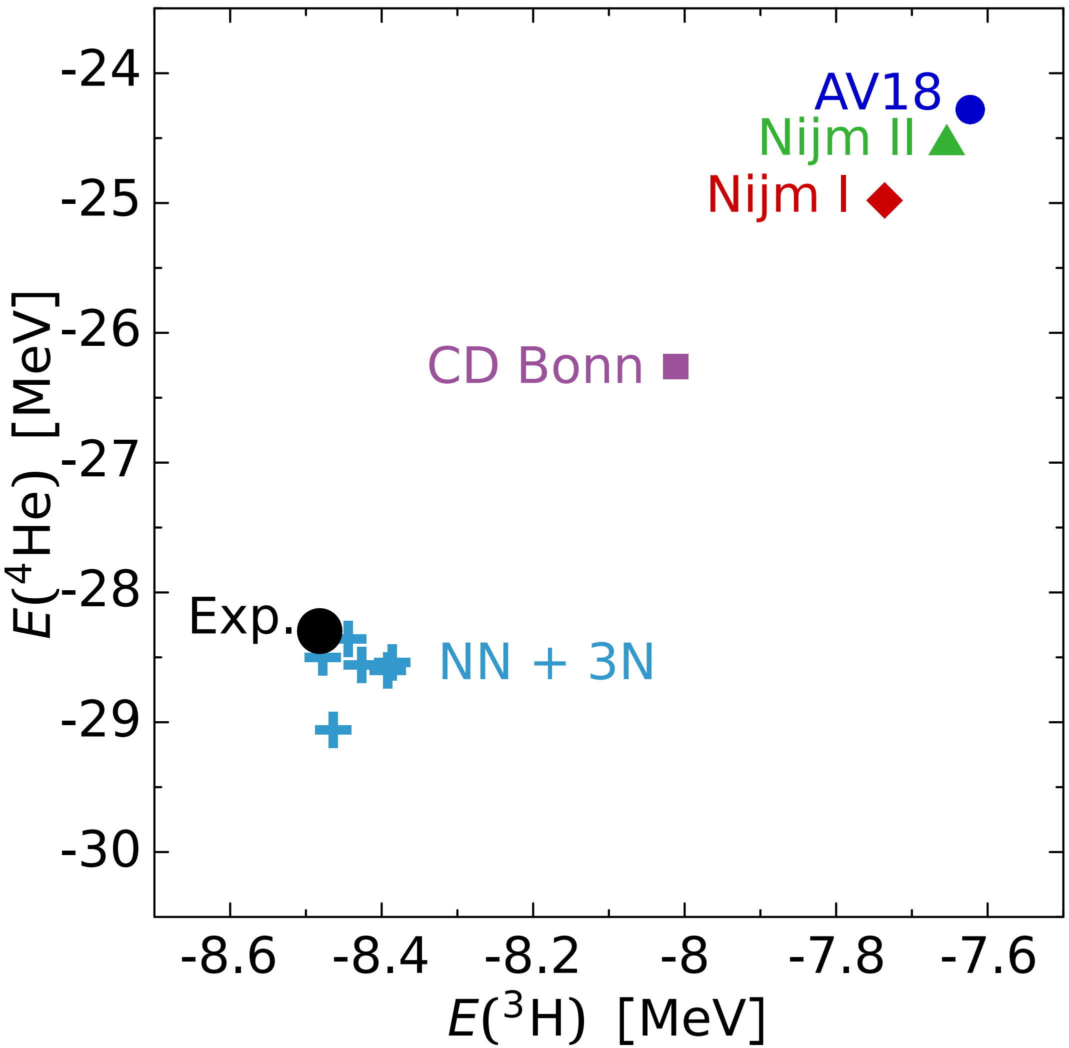
V_{AV18}



V_{UCOM}

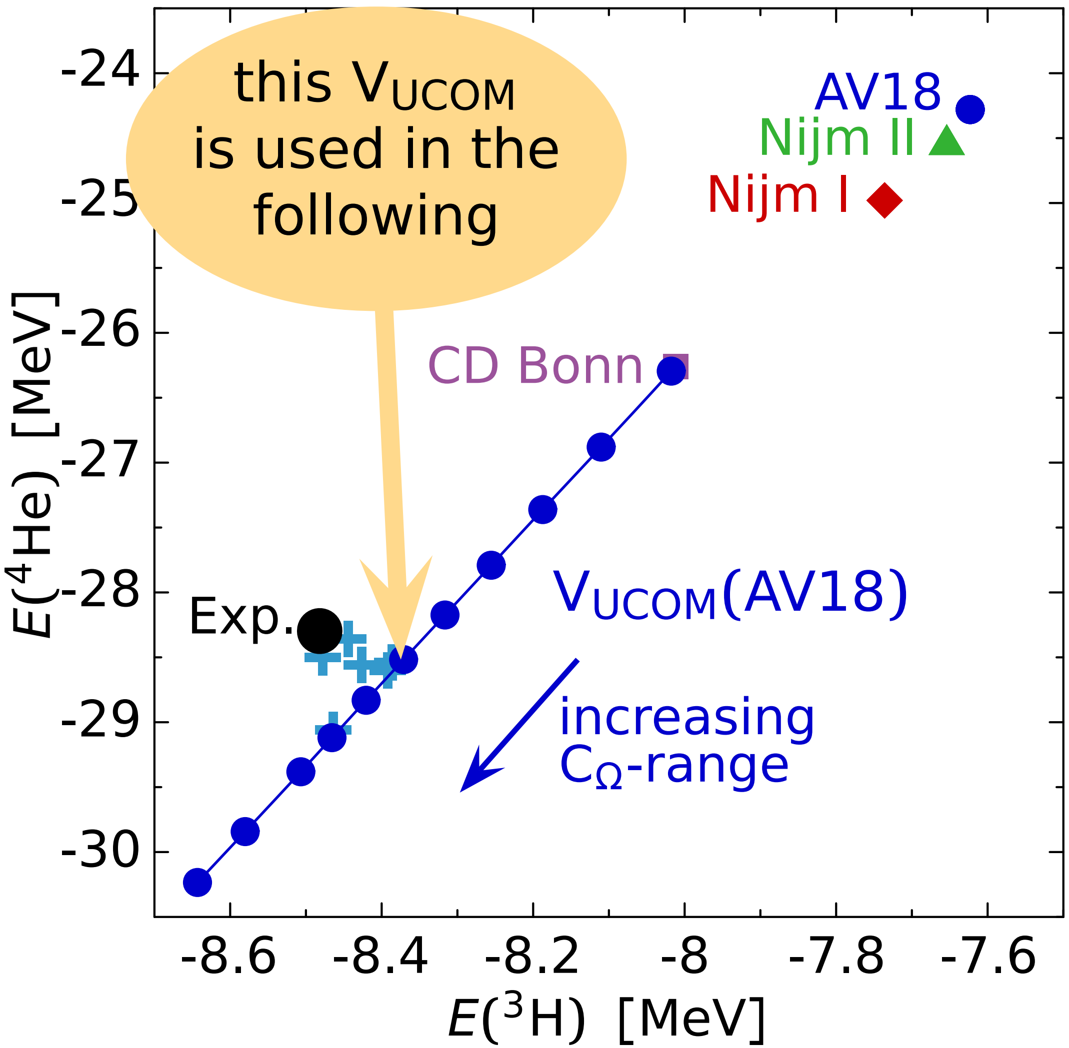


Tjon-Line and Correlator Range



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

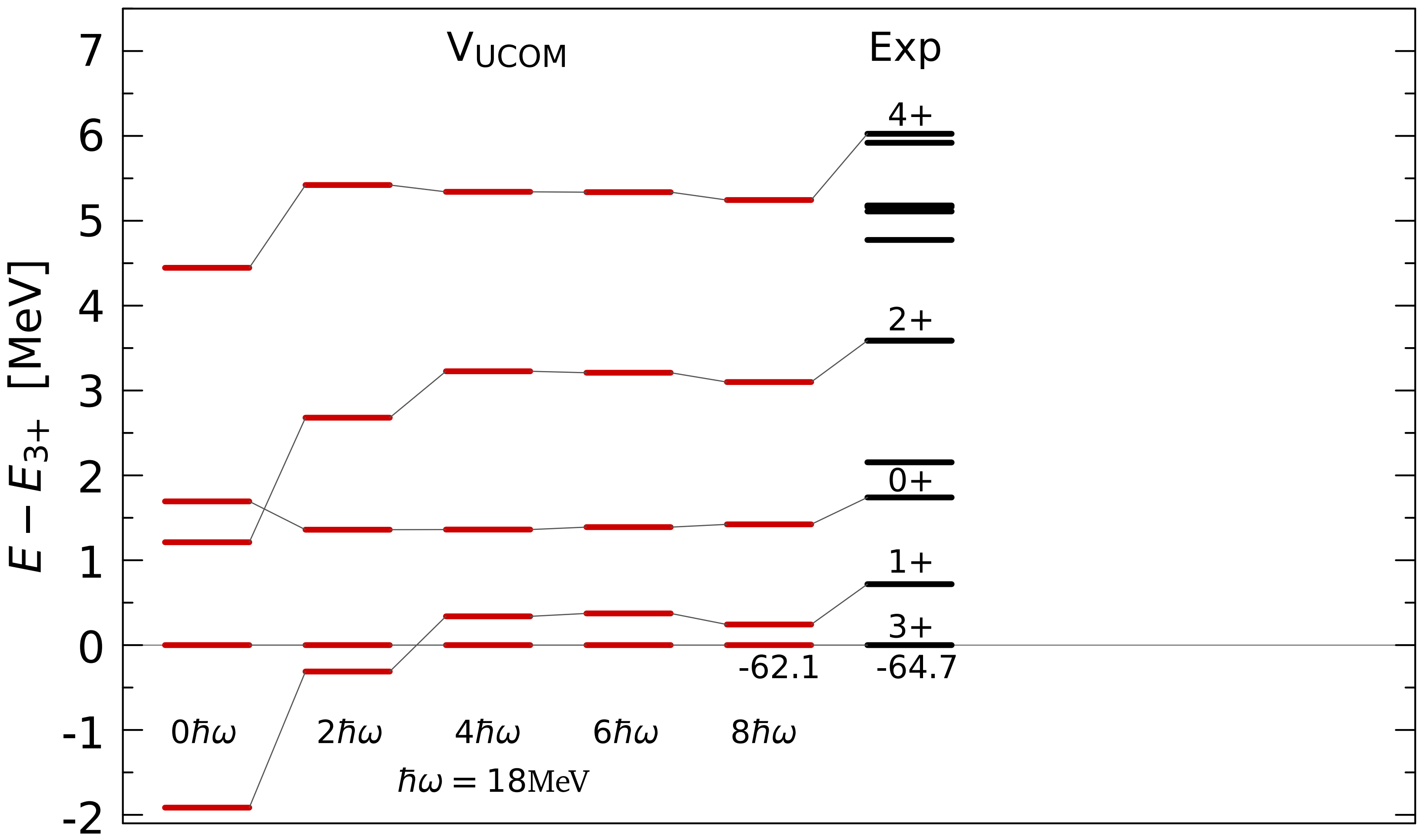
Tjon-Line and Correlator Range



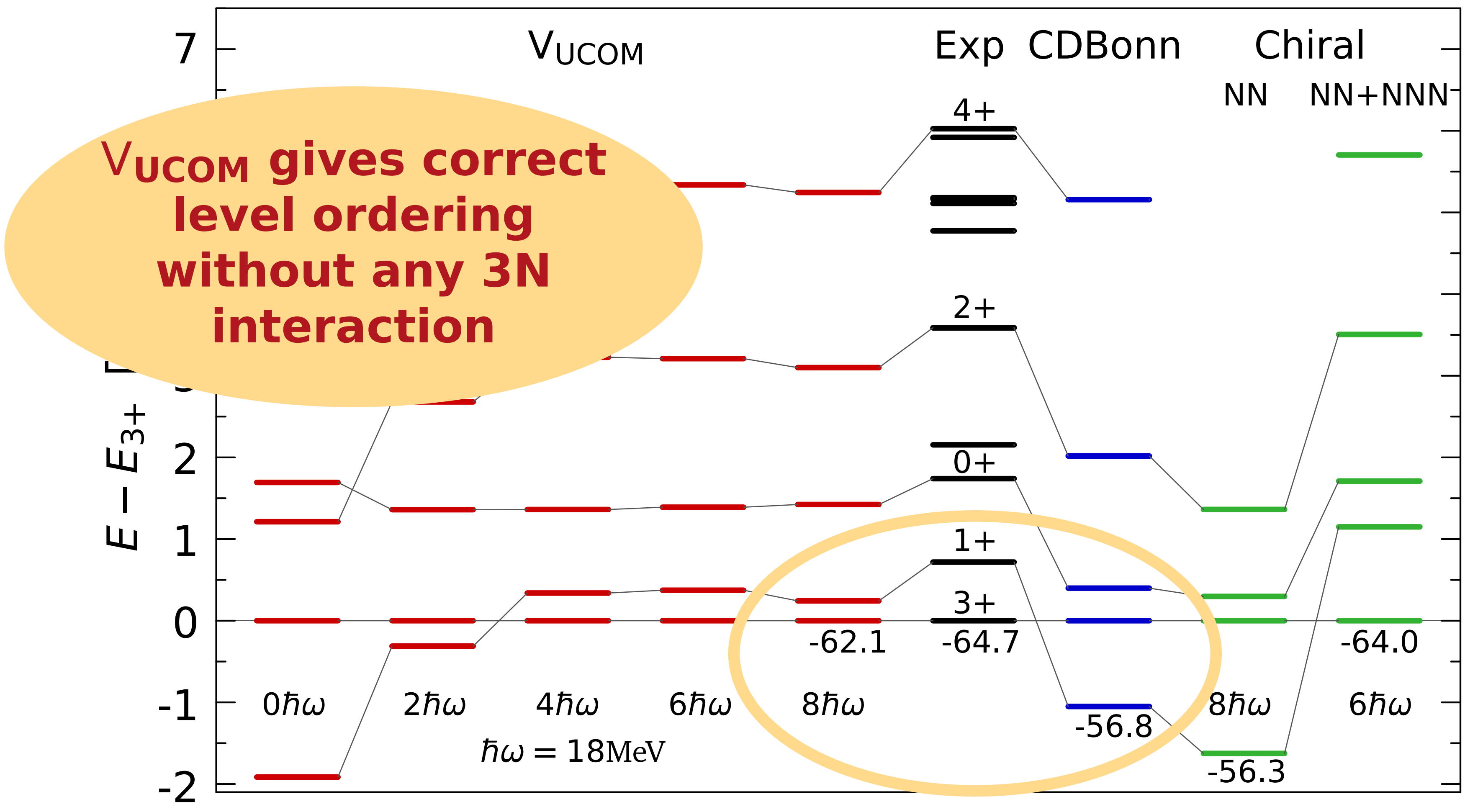
- **Tjon-line**: $E(^4\text{He})$ vs. $E(^3\text{H})$ for phase-shift equivalent NN-interactions
- change of C_Ω-correlator range results in shift along Tjon-line

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?



Computational Many-Body Methods

Importance Truncated No-Core Shell Model

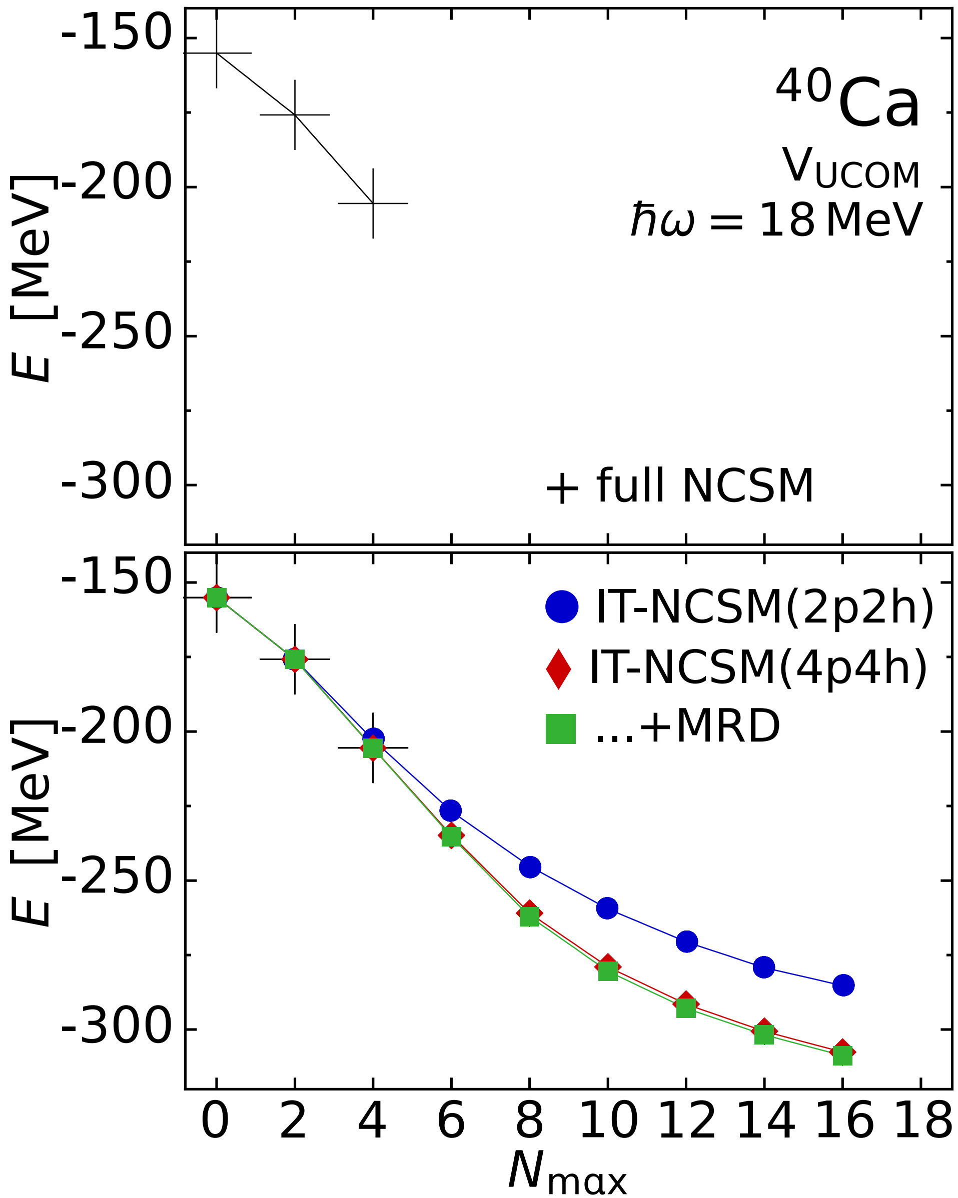
Roth & Navrátil — Phys. Rev. Lett. 99, 092501 (2007)
Roth, Piecuch, Gour — arXiv: 0806.0333
Roth — in preparation

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 $\sim 10^{10}$)

Importance Truncation

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



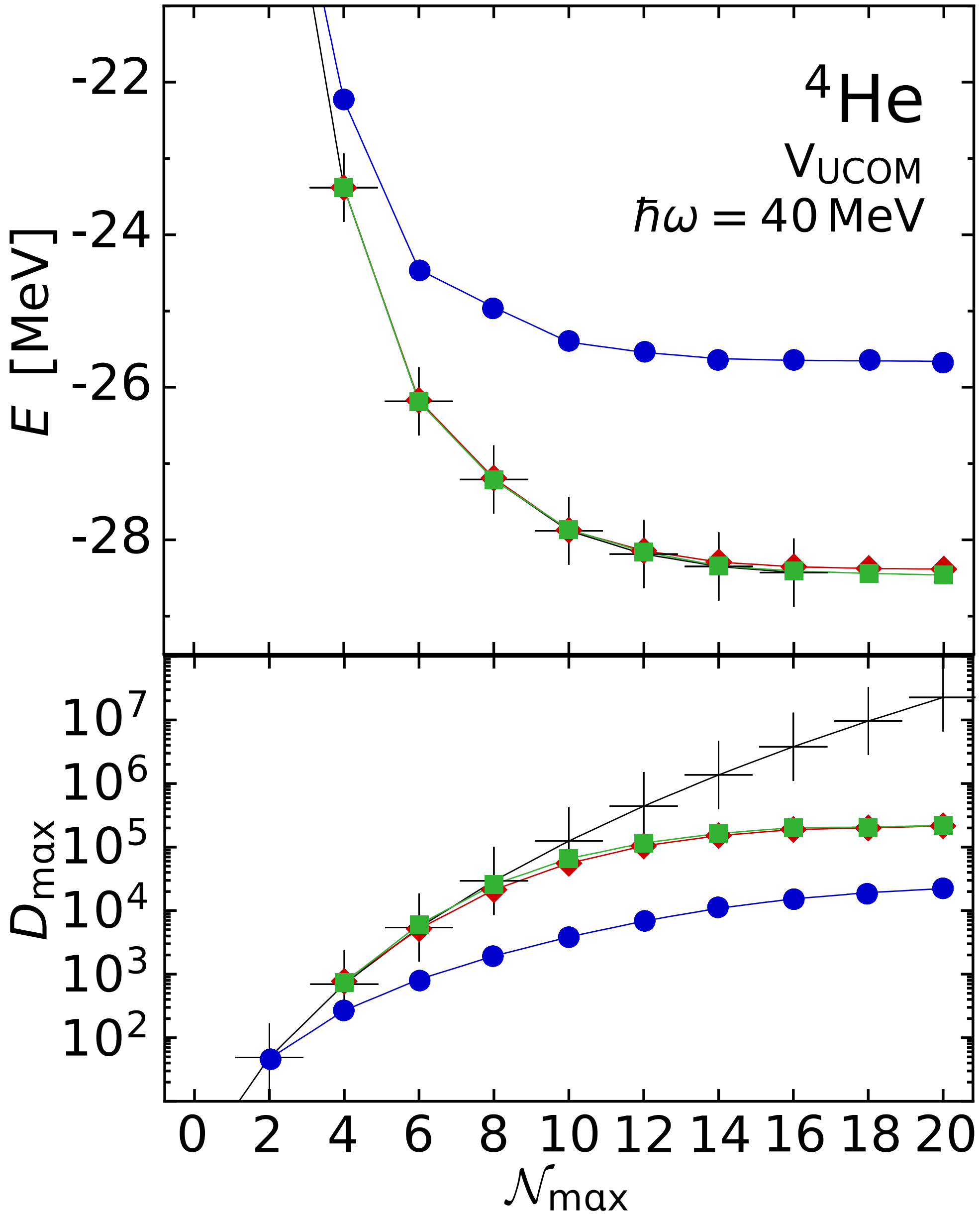
Importance Truncation: General Idea

- given an initial approximation $|\Psi_{\text{ref}}\rangle$ for the **target state**
- **measure the importance** of individual basis state $|\Phi_\nu\rangle$ 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** spanned by basis states with $|\kappa_\nu| \geq \kappa_{\min}$ and solve eigenvalue problem
- **iterative scheme**: repeat construction of importance truncated model space using eigenstate as improved reference $|\Psi_{\text{ref}}\rangle$
- **threshold extrapolations** and **perturbative corrections** can be used to account for discarded basis states

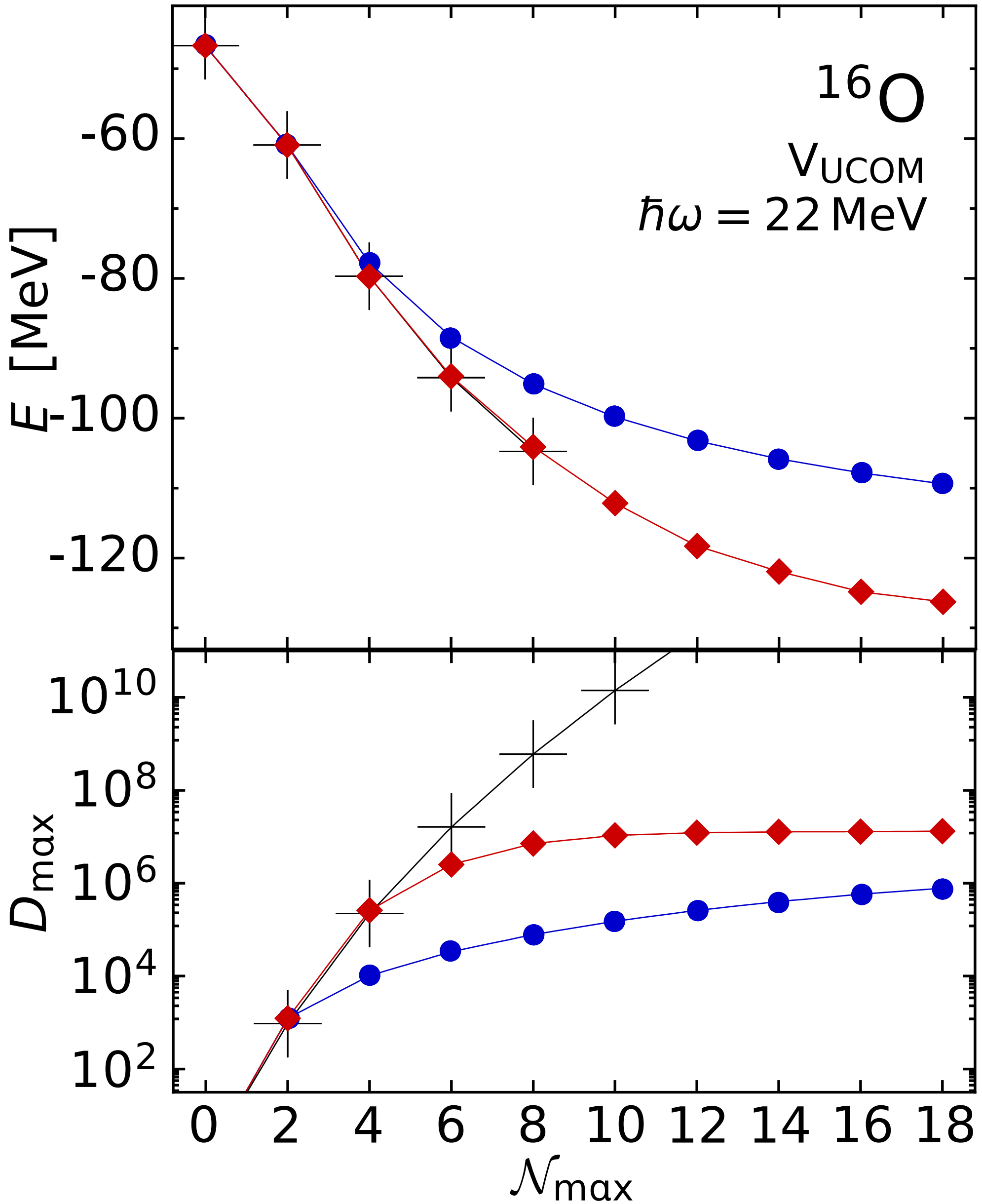
^{4}He: Importance Truncated NCSM



- **reproduces exact NCSM result** for all $\hbar\omega$ and $\mathcal{N}_{max}$
- iterations converge very fast
- reduction of basis by more than two orders of magnitude w/o loss of precision
- saturation of IT-NCSM dimension indicates convergence

+ full NCSM
● IT-NCSM(1 iter, 2p2h)
♦ IT-NCSM(2 iter, 4p4h)
■ IT-NCSM(3 iter, 4p4h)

^{16}O: Importance Truncated NCSM

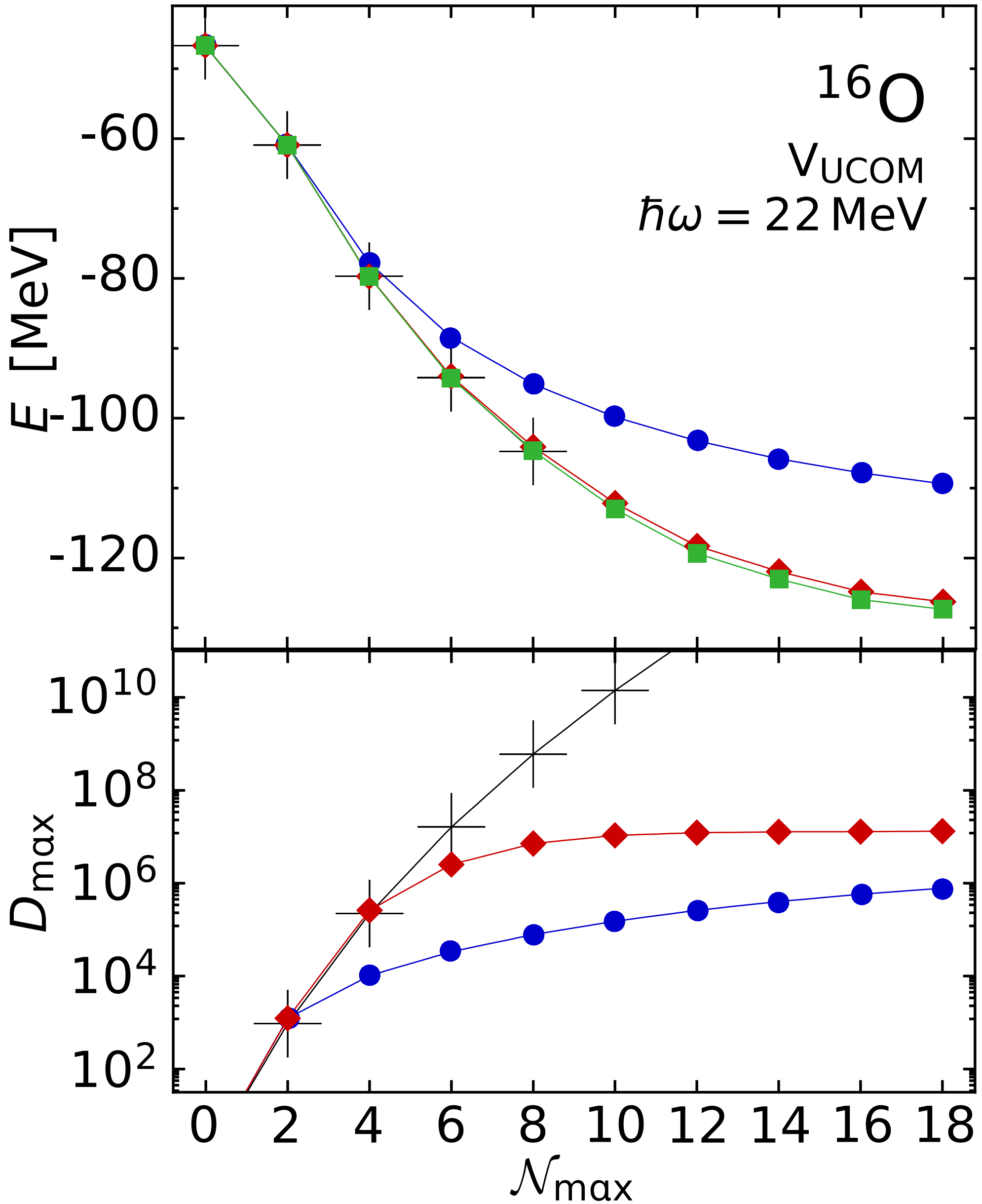


- **excellent agreement with full NCSM** calculation although configurations beyond 4p4h are not included

- dimension reduced by **several orders of magnitude**; possibility to go way beyond the domain of the full NCSM

+ full NCSM
● IT-NCSM(1 iter, 2p2h)
♦ IT-NCSM(2 iter, 4p4h)

^{16}O: Importance Truncated NCSM



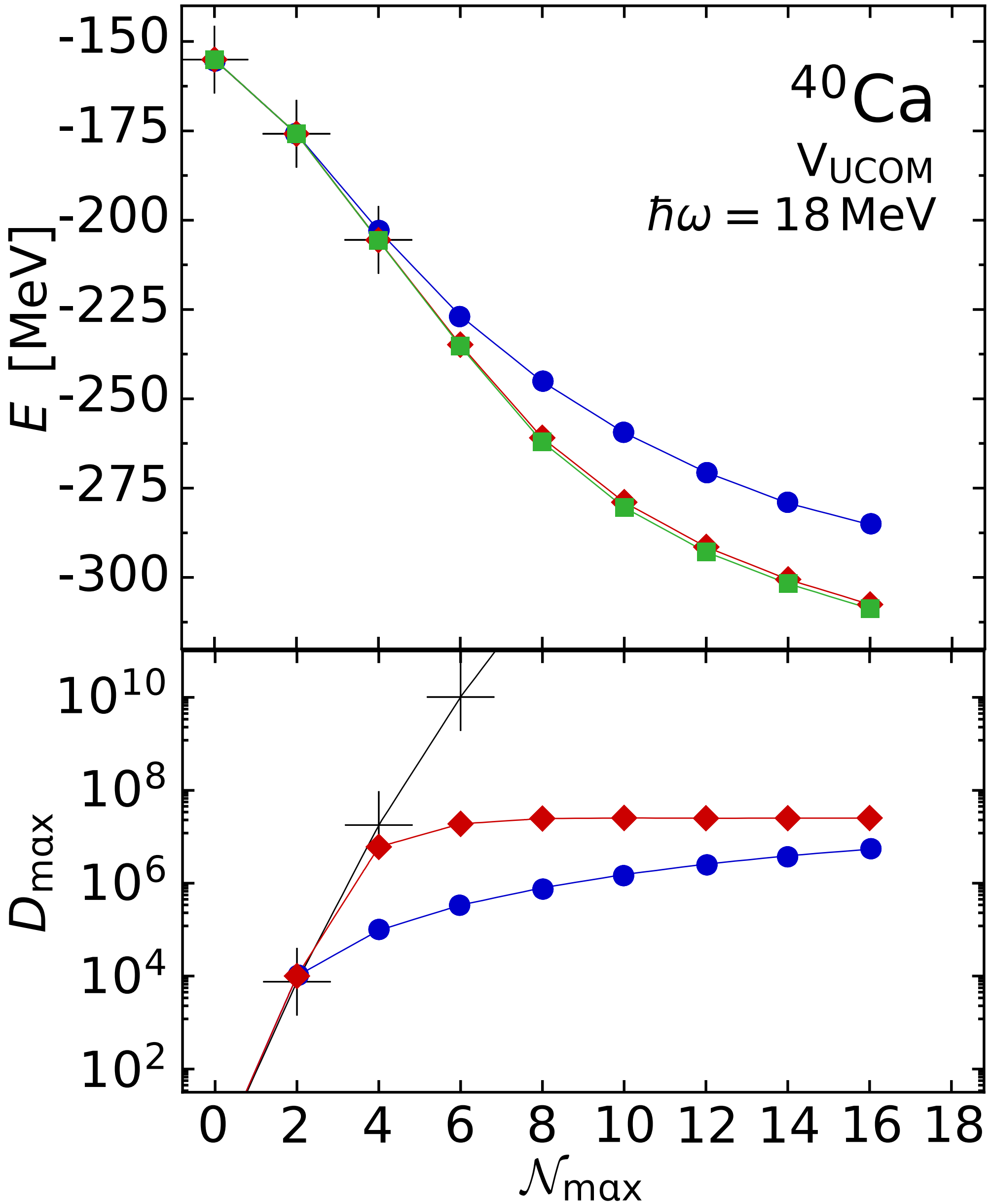
- extrapolation to $\mathcal{N}_{max} \to \infty$

$$E_{\text{IT-NCSM(2 iter)}} \approx -129 \pm 1\,\text{MeV}$$
$$E_{\text{IT-NCSM(2 iter)+MRD}} \approx -130 \pm 1\,\text{MeV}$$
$$E_{\text{exp}} = -127.6\,\text{MeV}$$

- V_{UCOM} predicts **reasonable binding energies** also for heavier nuclei

+ full NCSM
● IT-NCSM(1 iter, 2p2h)
♦ IT-NCSM(2 iter, 4p4h)
■ IT-NCSM(2 iter, 4p4h) + MRD

^{40}Ca: Importance Truncated NCSM



- **16ℏω and more are feasible** for ^{40}Ca in IT-NCSM(2 iter)
- dramatic reduction of basis dimension
- rough extrapolation $\mathcal{N}_{max} \to \infty$ is consistent with experimental binding energy

+ full NCSM
● IT-NCSM(1 iter, 2p2h)
♦ IT-NCSM(2 iter, 4p4h)
■ IT-NCSM(2 iter, 4p4h) + MRD

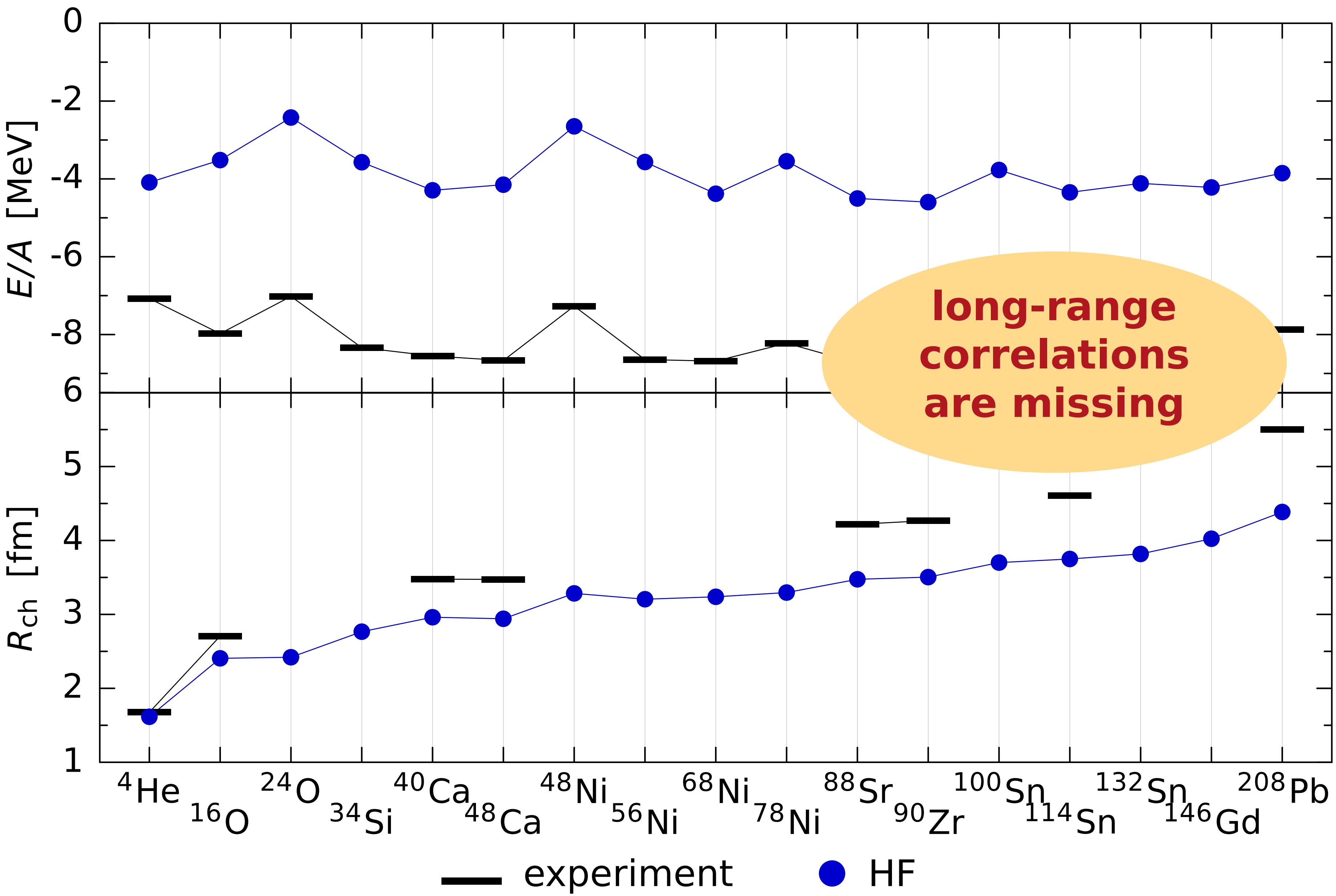
Other Options...

Other Options...

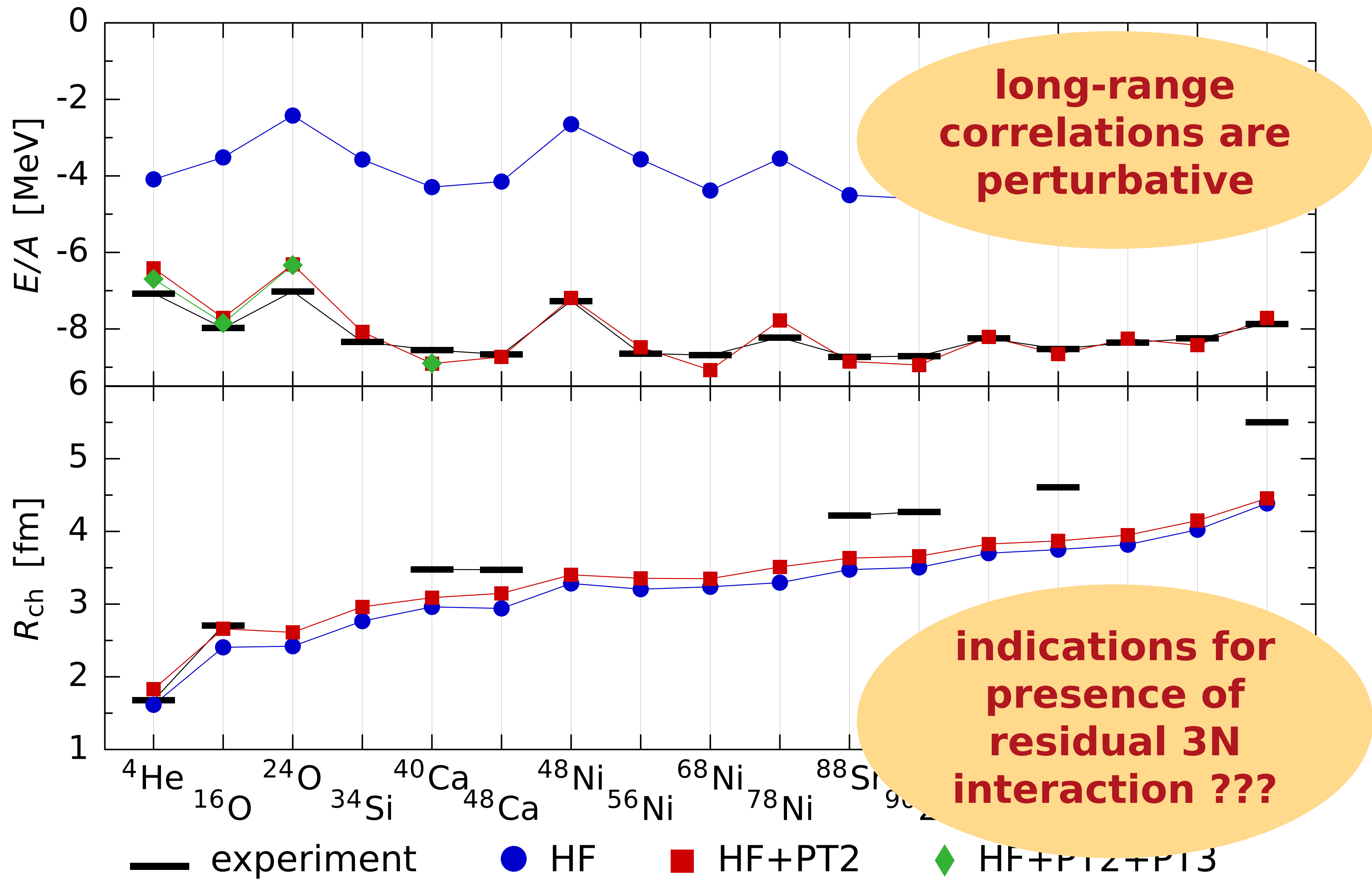
similarity transformed interactions (e.g. V_{UCOM}) provide universal input for various many-body methods

- 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
- 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

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