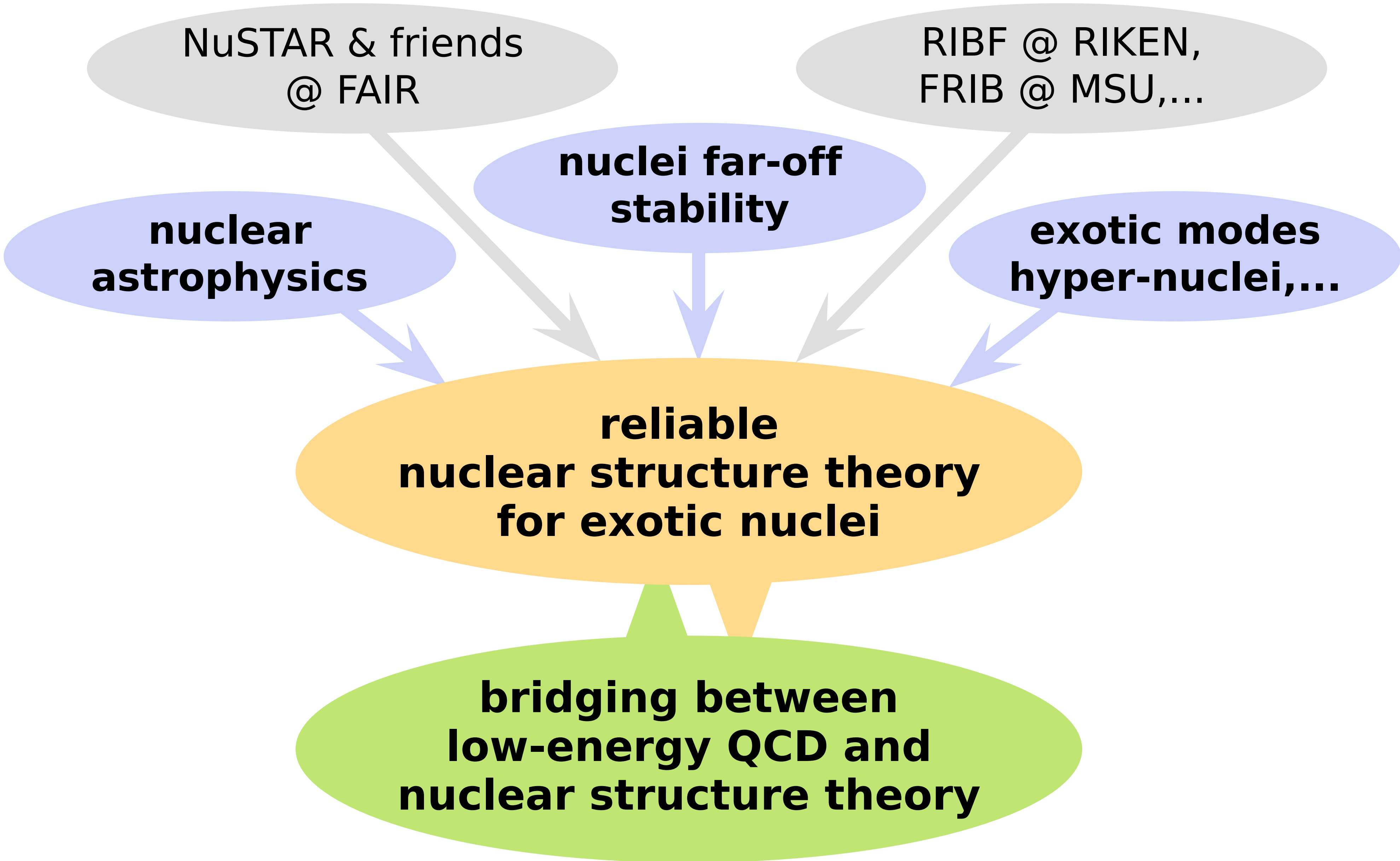
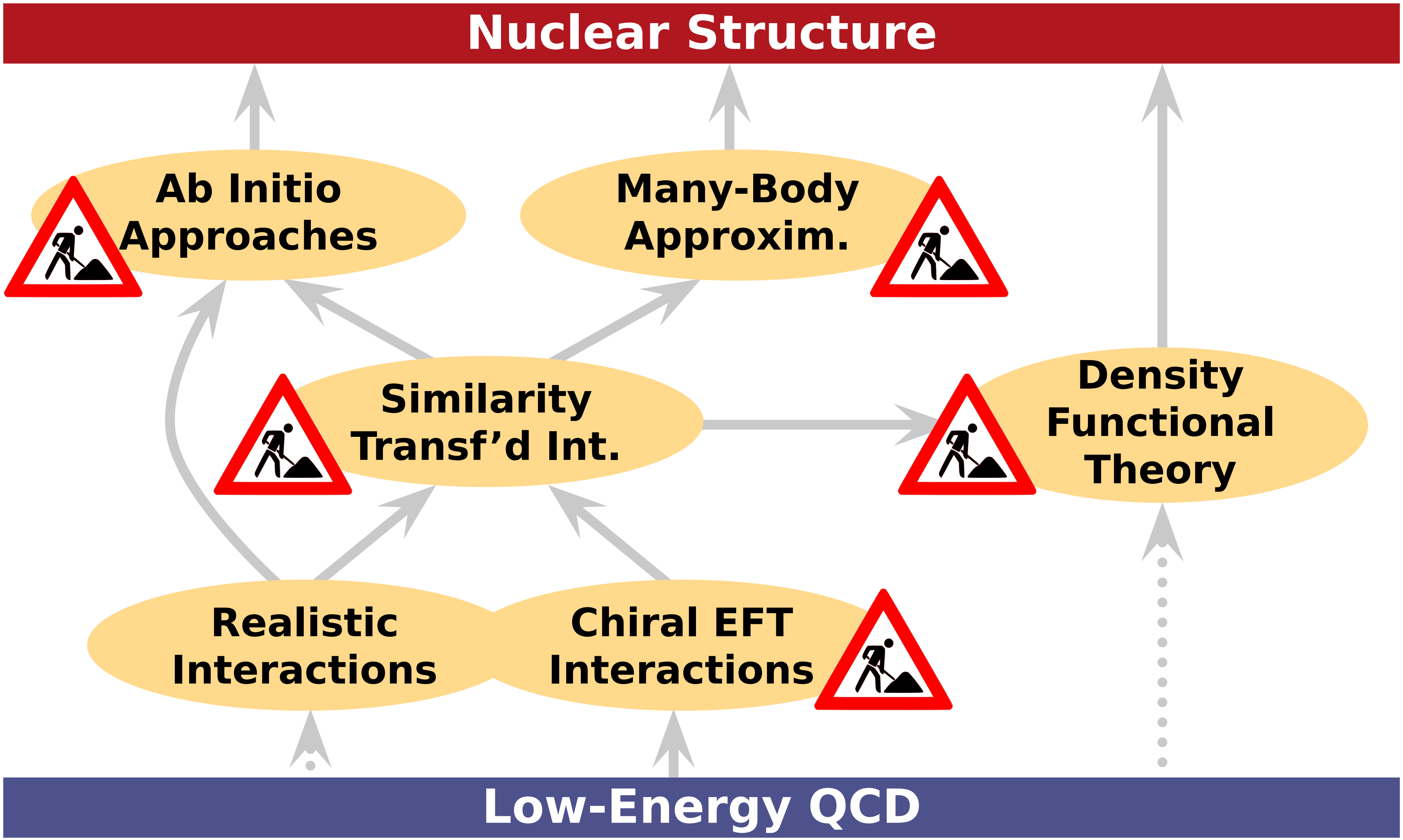
Frontiers in Nuclear Structure Theory from a FAIR Perspective

Robert Roth
Institut für Kernphysik
TECHNISCHE UNIVERSITÄT DARMSTADT

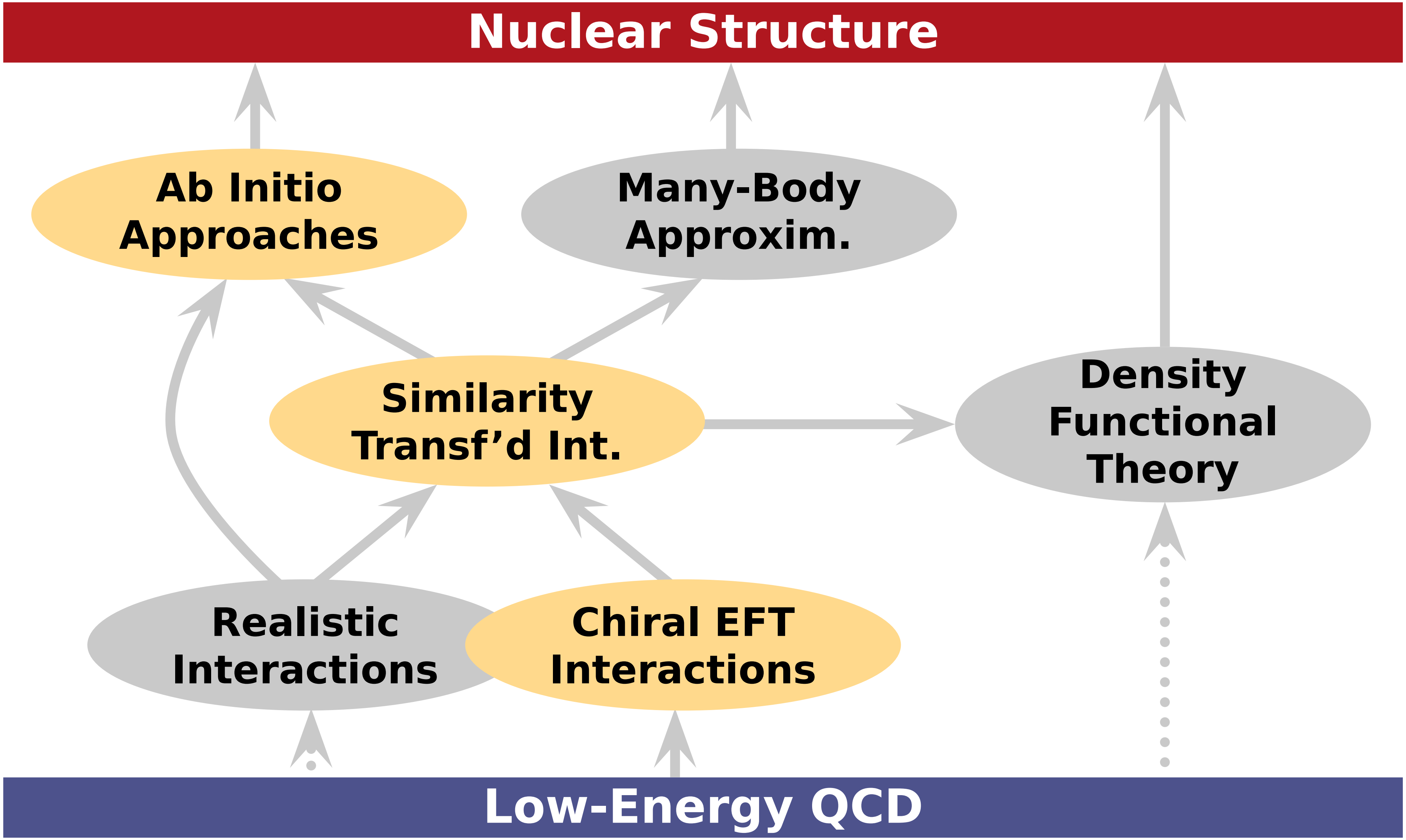
Nuclear Structure from a FAIR Perspective



Modern Nuclear Structure Theory



Modern Nuclear Structure Theory



Nuclear Interactions from QCD

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

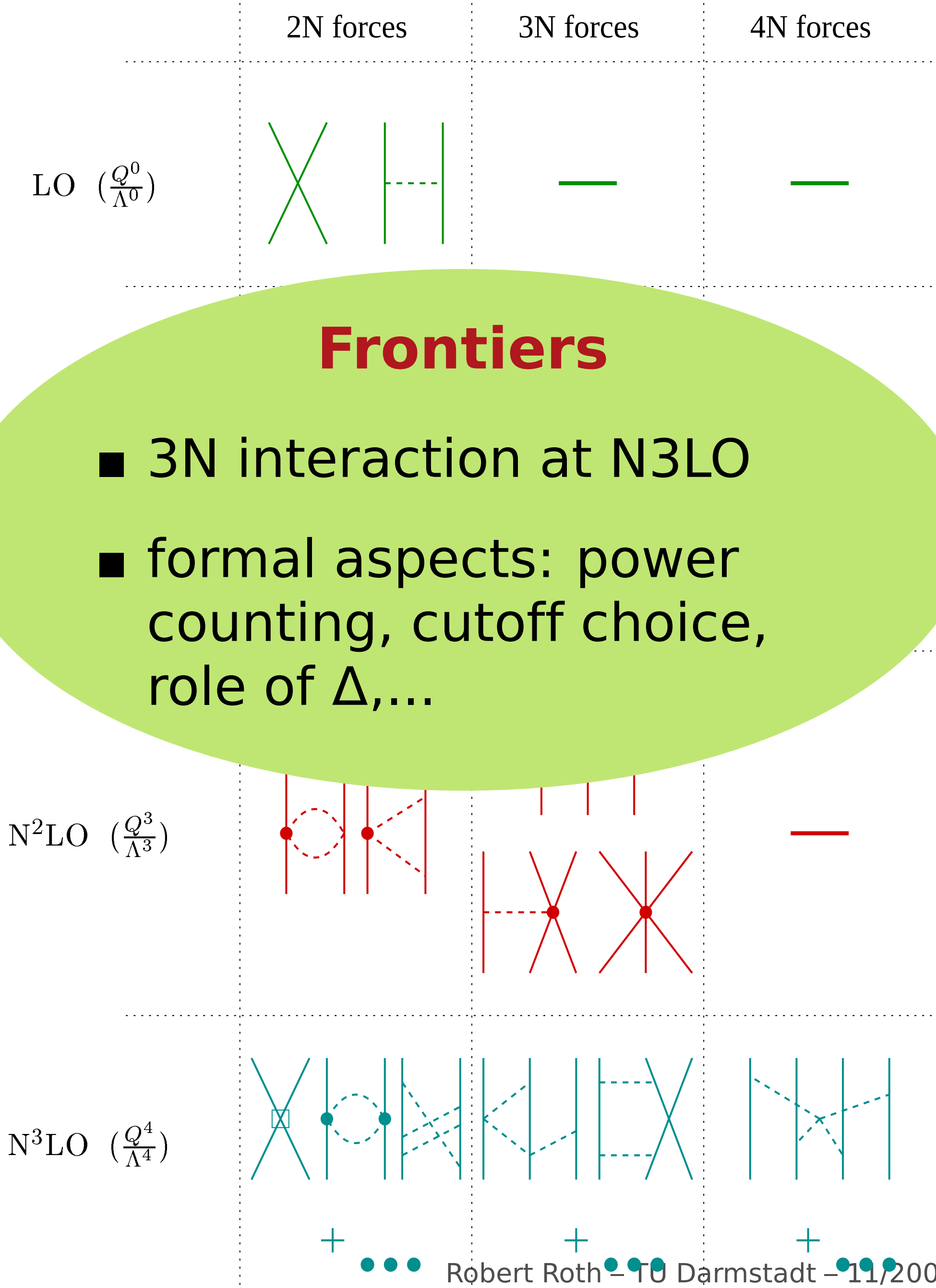
Chiral N3LO

Argonne V18 + **Illinois 2**

Chiral N3LO + **N2LO**

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)



Frontiers

- 3N interaction at N3LO
- formal aspects: power counting, cutoff choice, role of Δ,...

Meißner, NPA 751 (2005) 149c

Similarity Transformed Interactions

Why Transformed Interactions?

Realistic Interactions

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

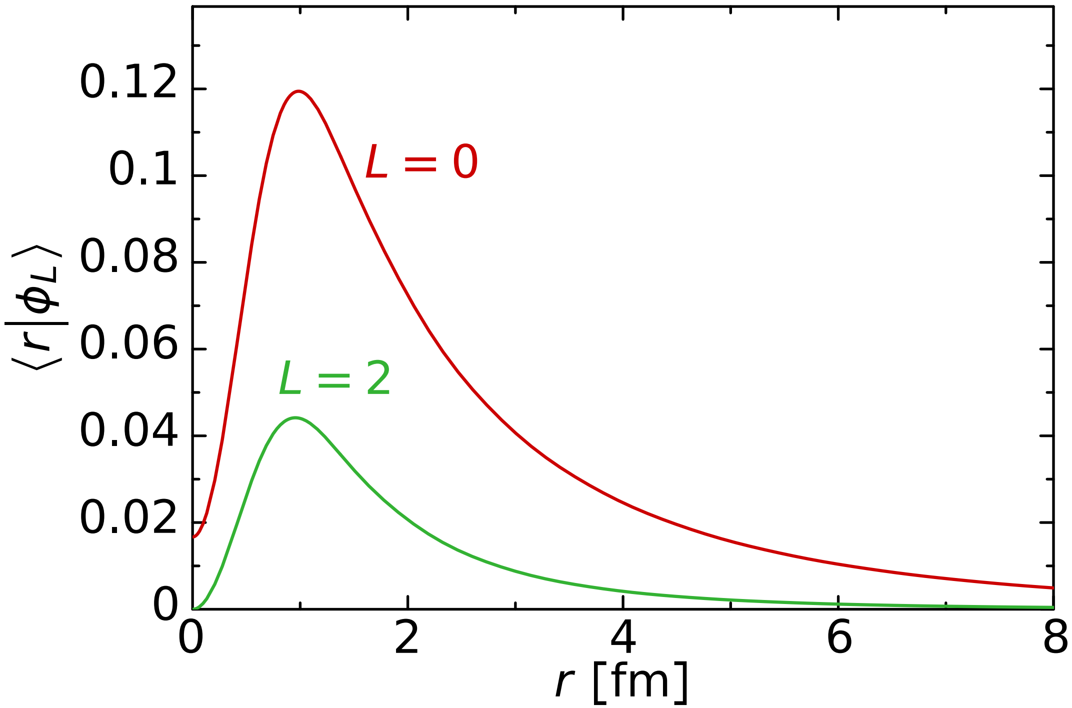
Similarity Transformation

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

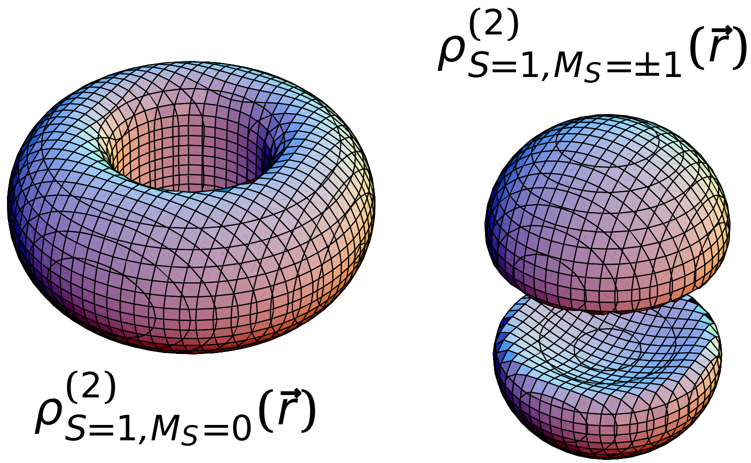
Many-Body Methods

- 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

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

Correlated States

imprint short-range correlations onto uncorrelated many-body states

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

Correlated Operators

adapt Hamiltonian to uncorrelated states (pre-diagonalization)

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

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

Unitary Correlation Operator Method

explicit ansatz for 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

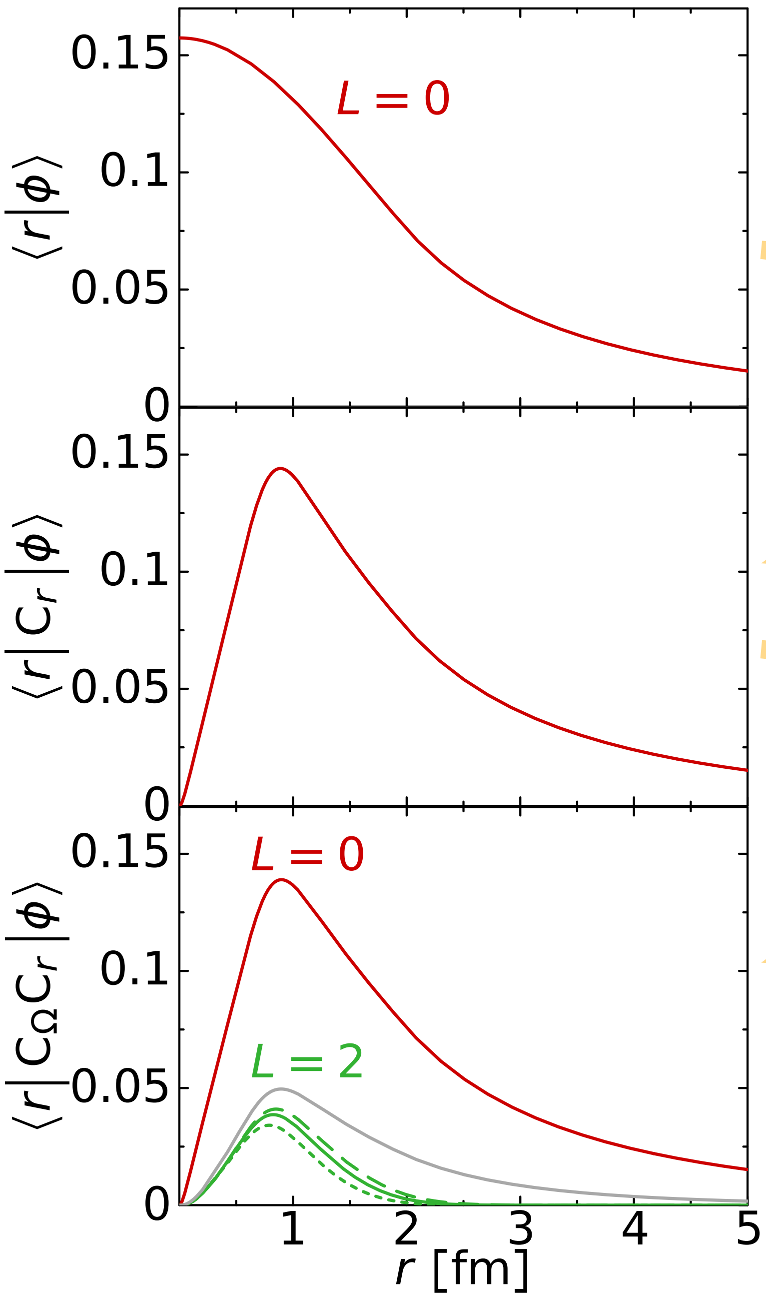
$$g_\Omega = \frac{3}{2}\vartheta(r)\big[(\vec{\sigma}_1\cdot\vec{q}_\Omega)(\vec{\sigma}_2\cdot\vec{r}) + (\vec{r}\leftrightarrow\vec{q}_\Omega)\big]$$

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

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

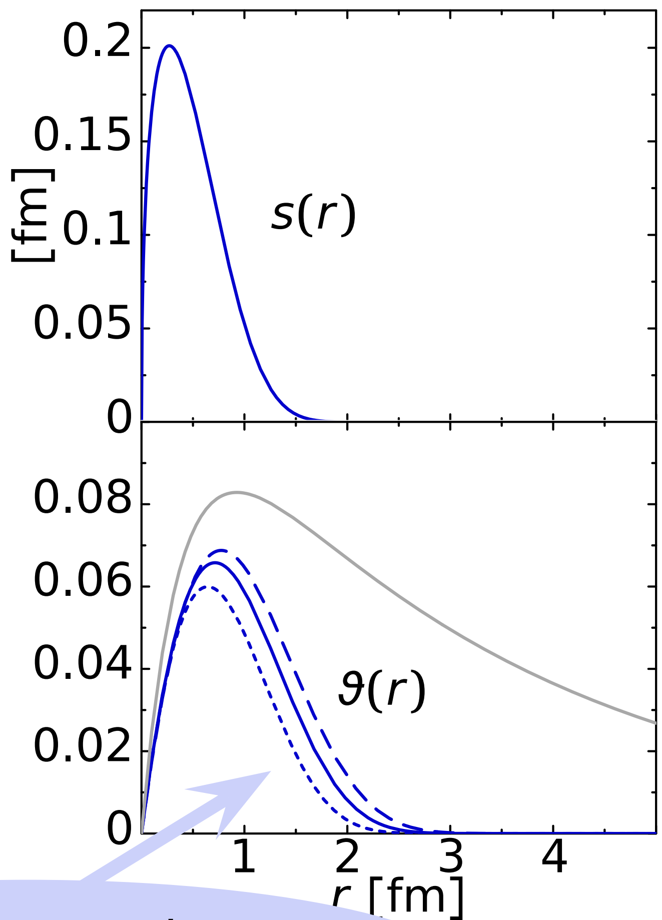
- $s(r)$ and $\vartheta(r)$ are optimized for the initial potential

Correlated States: The Deuteron



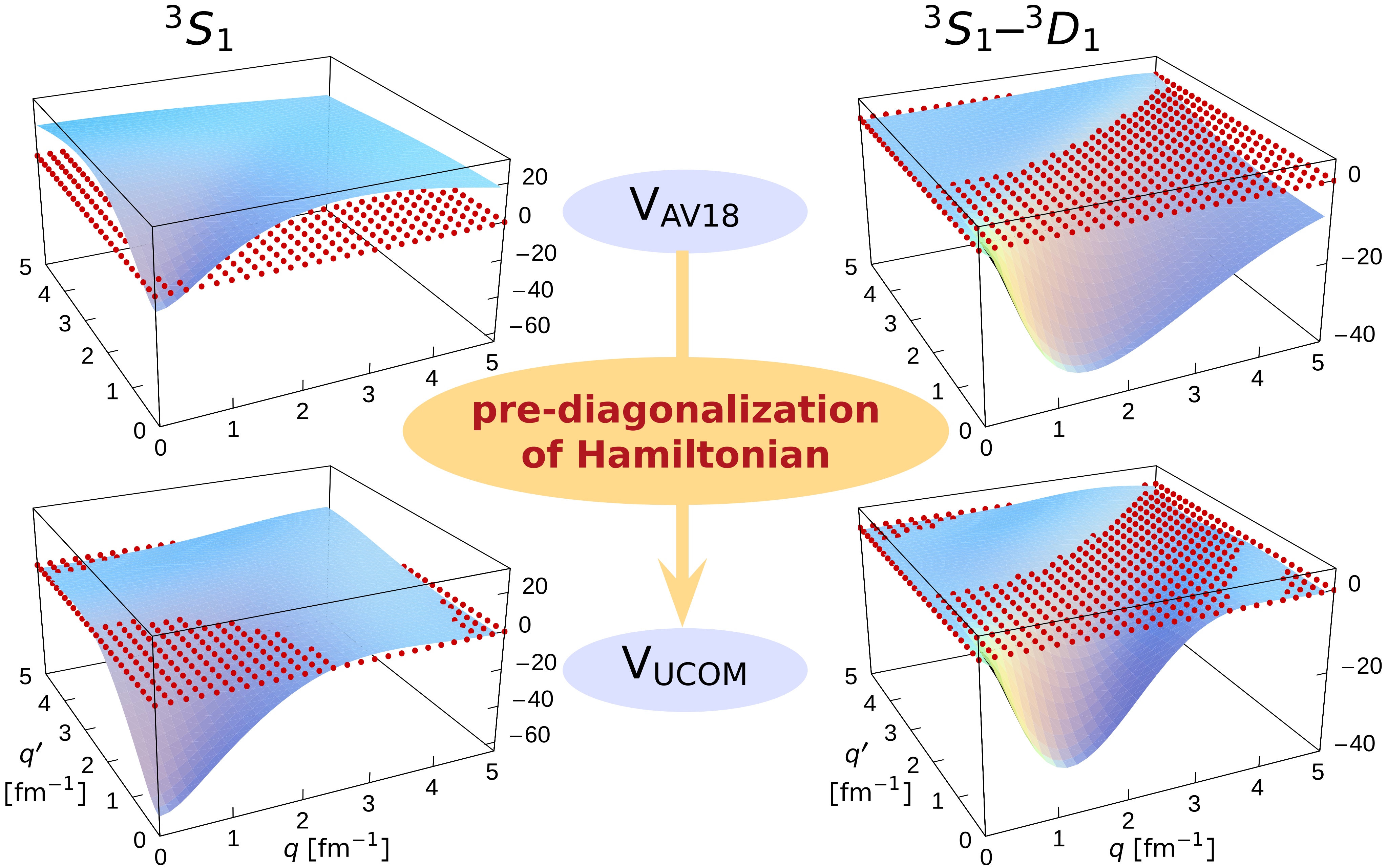
central correlations

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

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

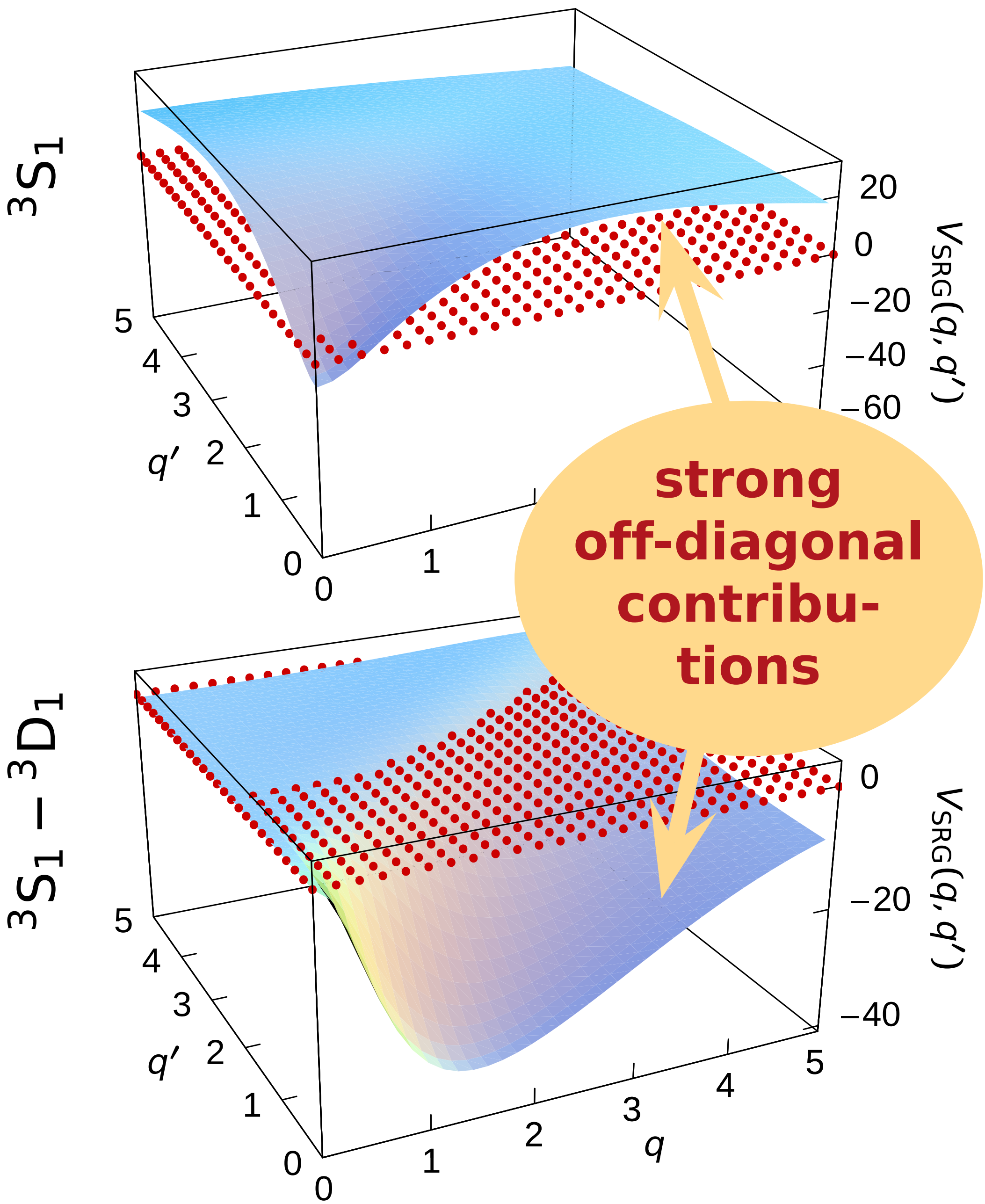
- dynamical generator defined as commutator with the operator in whose eigenbasis H shall be diagonalized

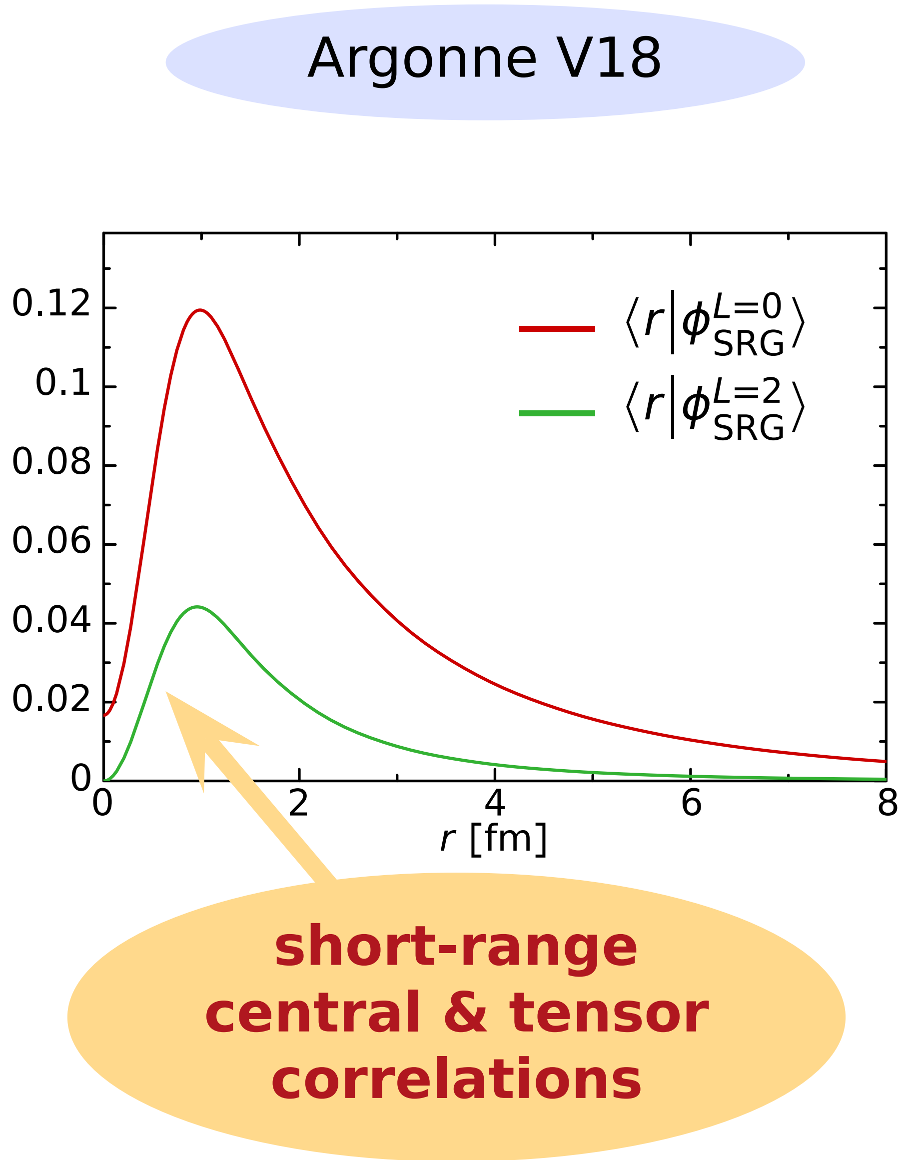
$$\eta(\alpha) \stackrel{2B}{=} \frac{1}{2\mu}\left[\vec{q}^{\,2}, \widetilde{H}(\alpha)\right]$$

UCOM vs. SRG

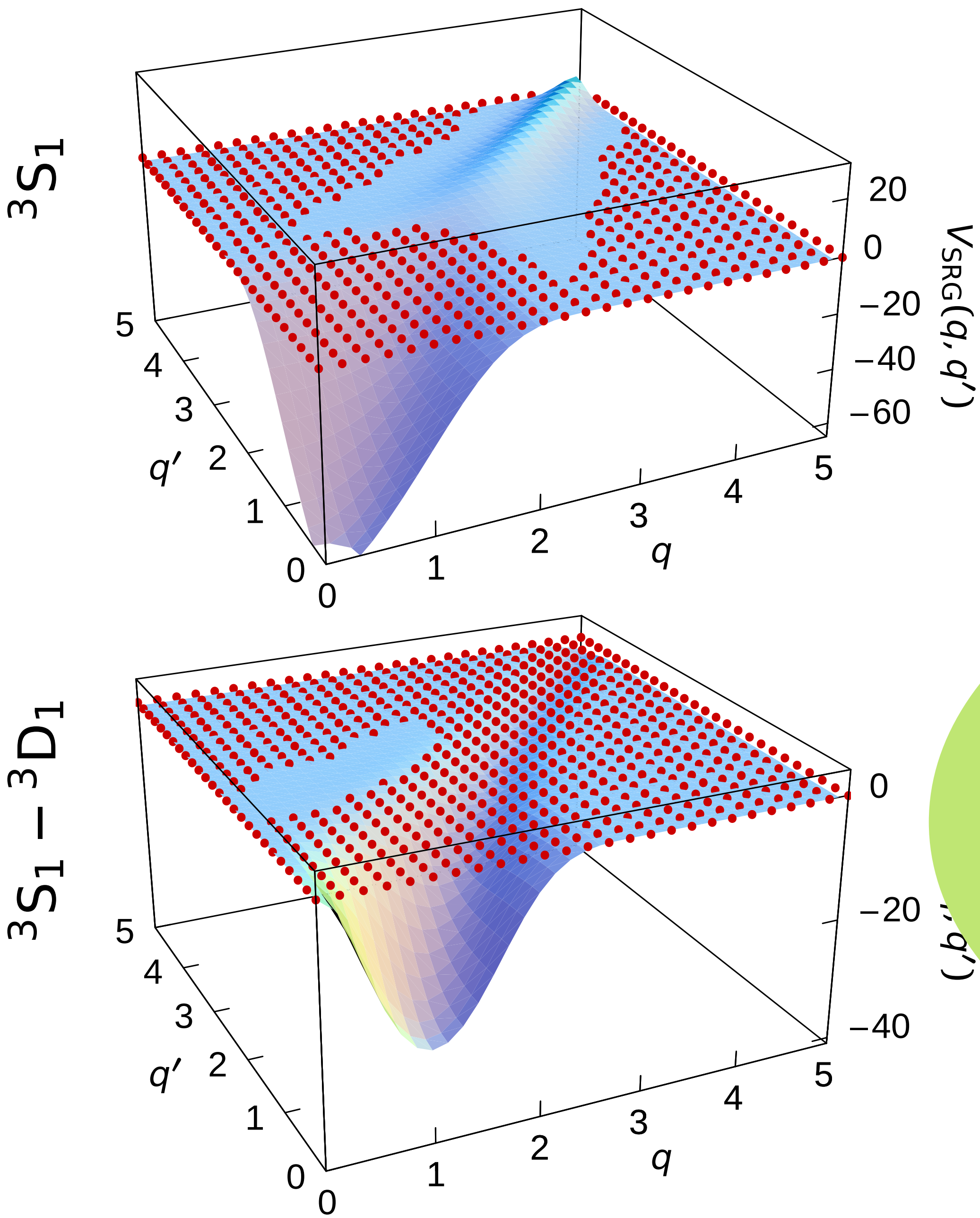
$\eta(0)$ has the same structure as UCOM generators g_r & g_Ω

SRG Evolution: The Deuteron

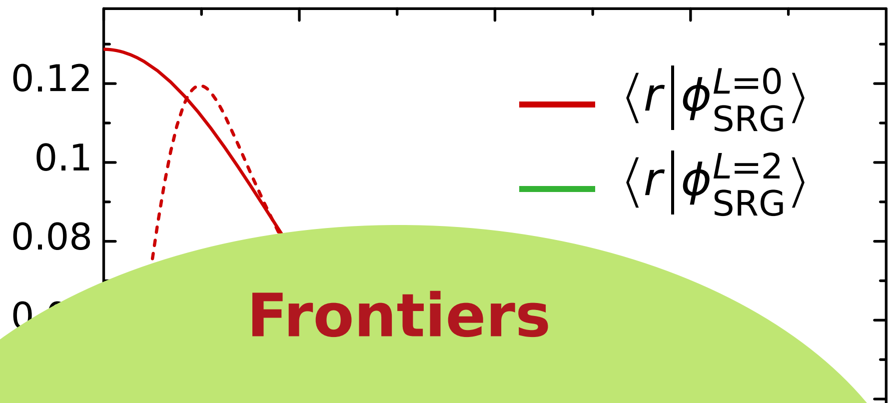




SRG Evolution: The Deuteron



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



Frontiers

- consistent transformation of NN+3N Hamiltonian
- transformed observables
- alternative SRG & UCOM generators

Ab Initio Approaches

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

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

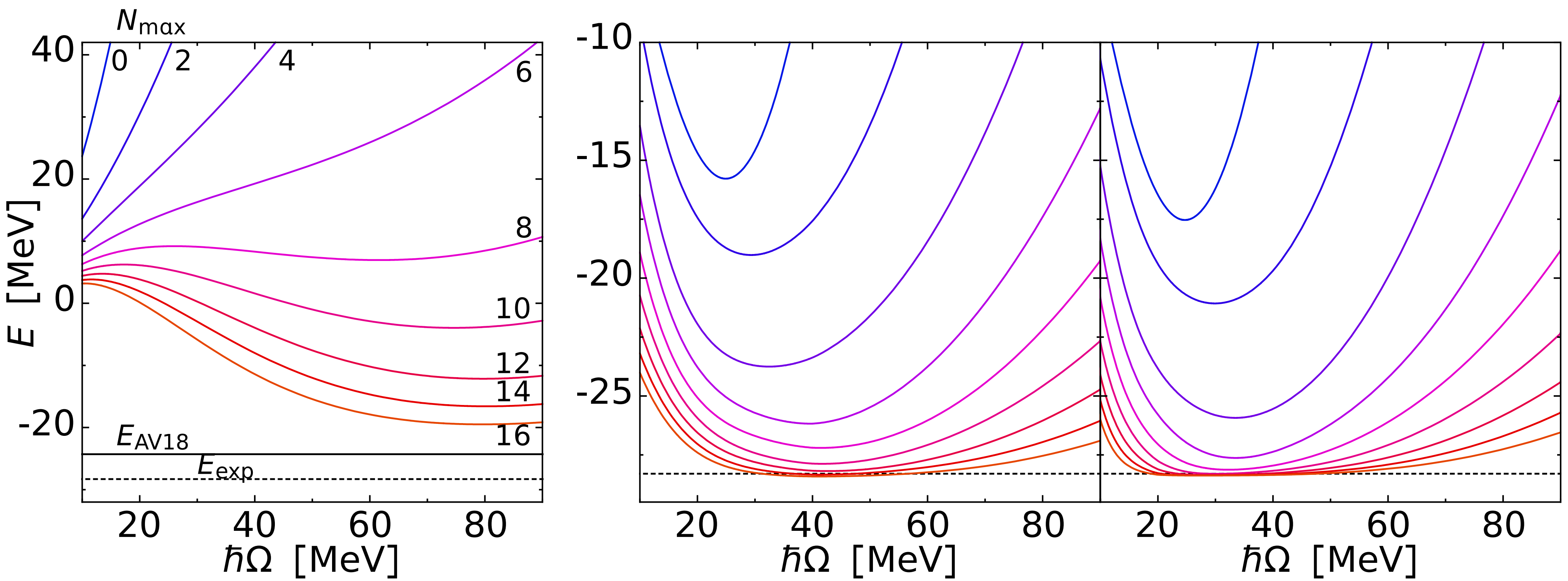
- **model space**: spanned by basis states $|\Phi_\nu\rangle$ with unperturbed excitation energies of up to $N_{\max}\hbar\Omega$
  - ► **exact factorization** of intrinsic and CM component is possible
- numerical solution of **eigenvalue problem** for H_{int} within $N_{\max}\hbar\Omega$ model space 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}

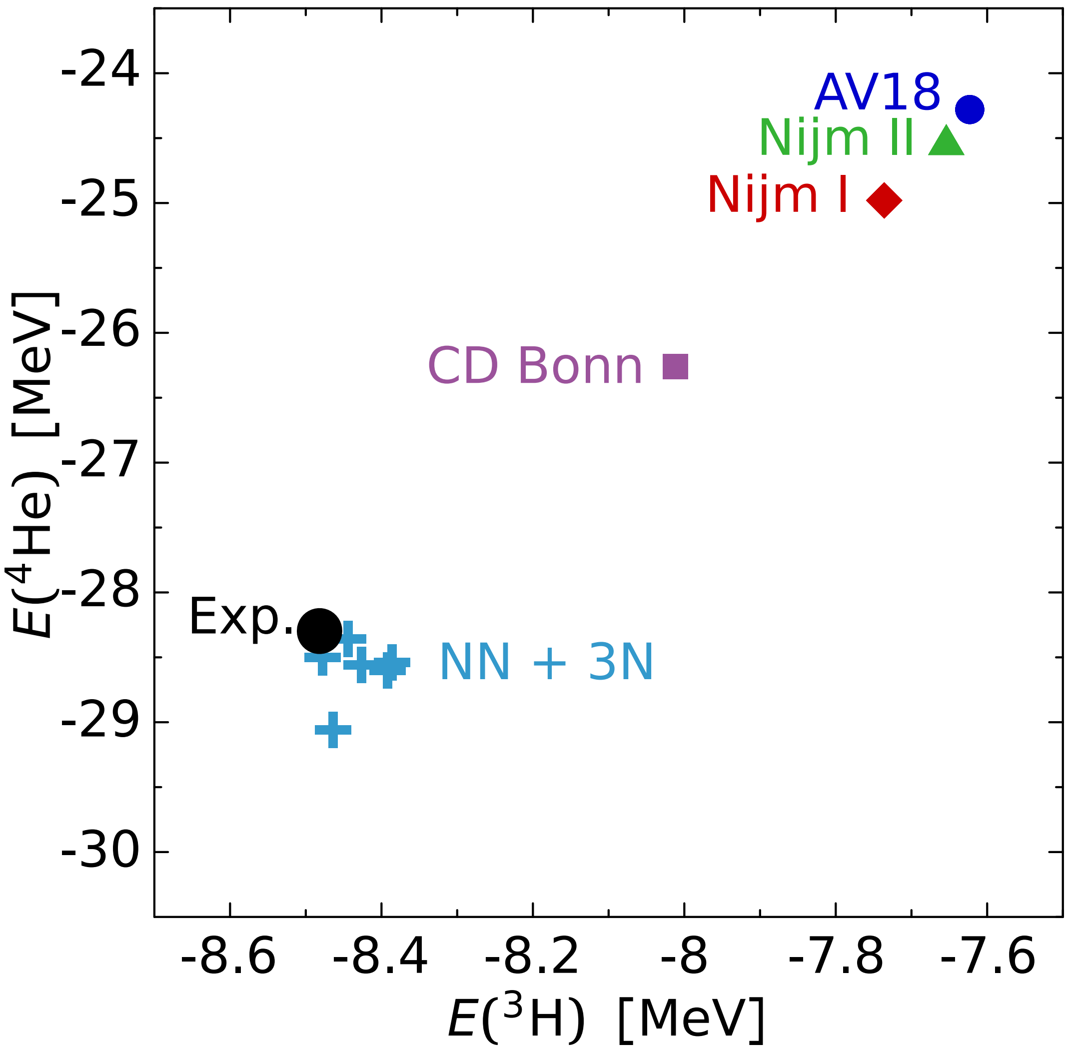
V_{UCOM}
MIN, $I_\vartheta = 0.09\,\mathrm{fm}^3$

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



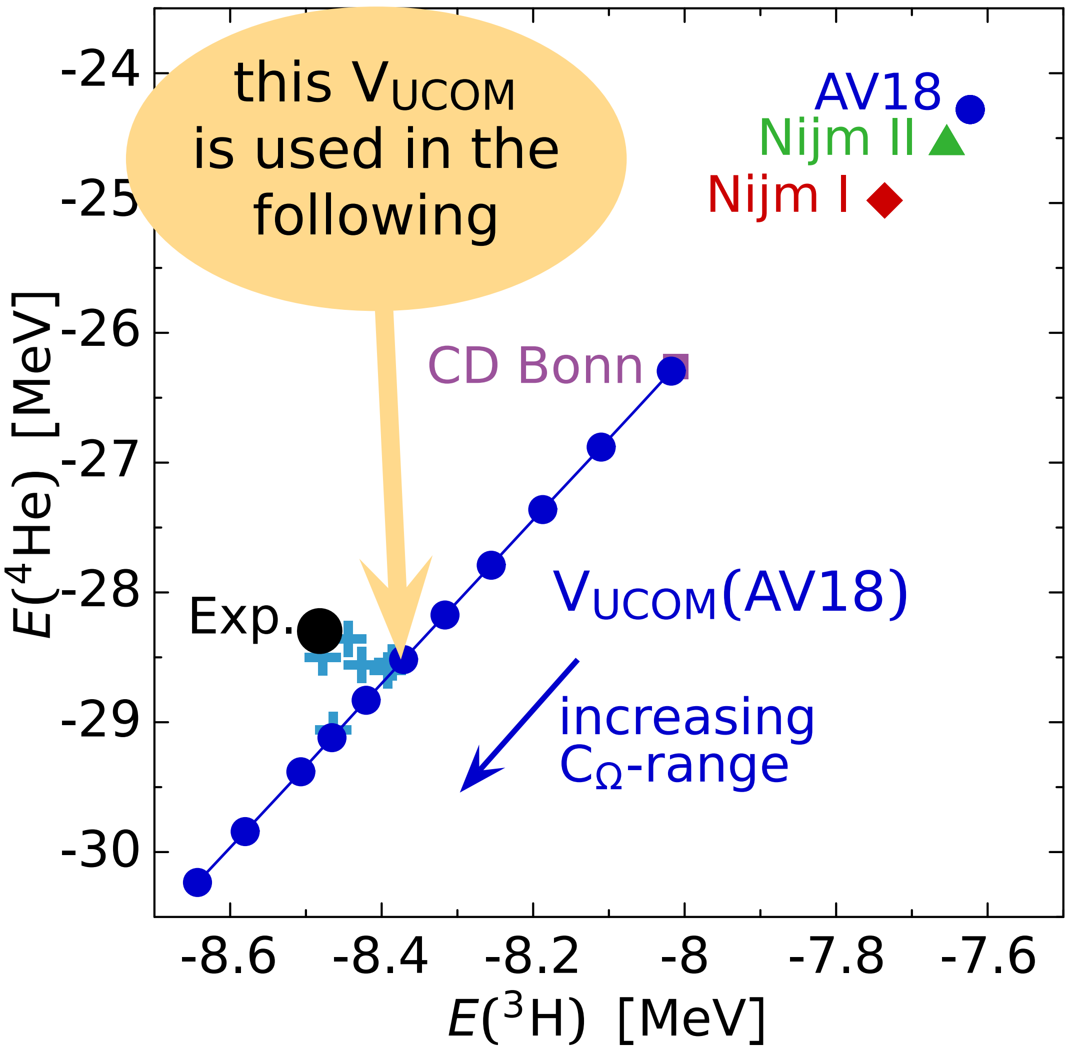
- I_ϑ or $\bar{\alpha}$ adjusted such that ^{4}He binding energy is reproduced

Tjon-Line and 3N Interactions



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

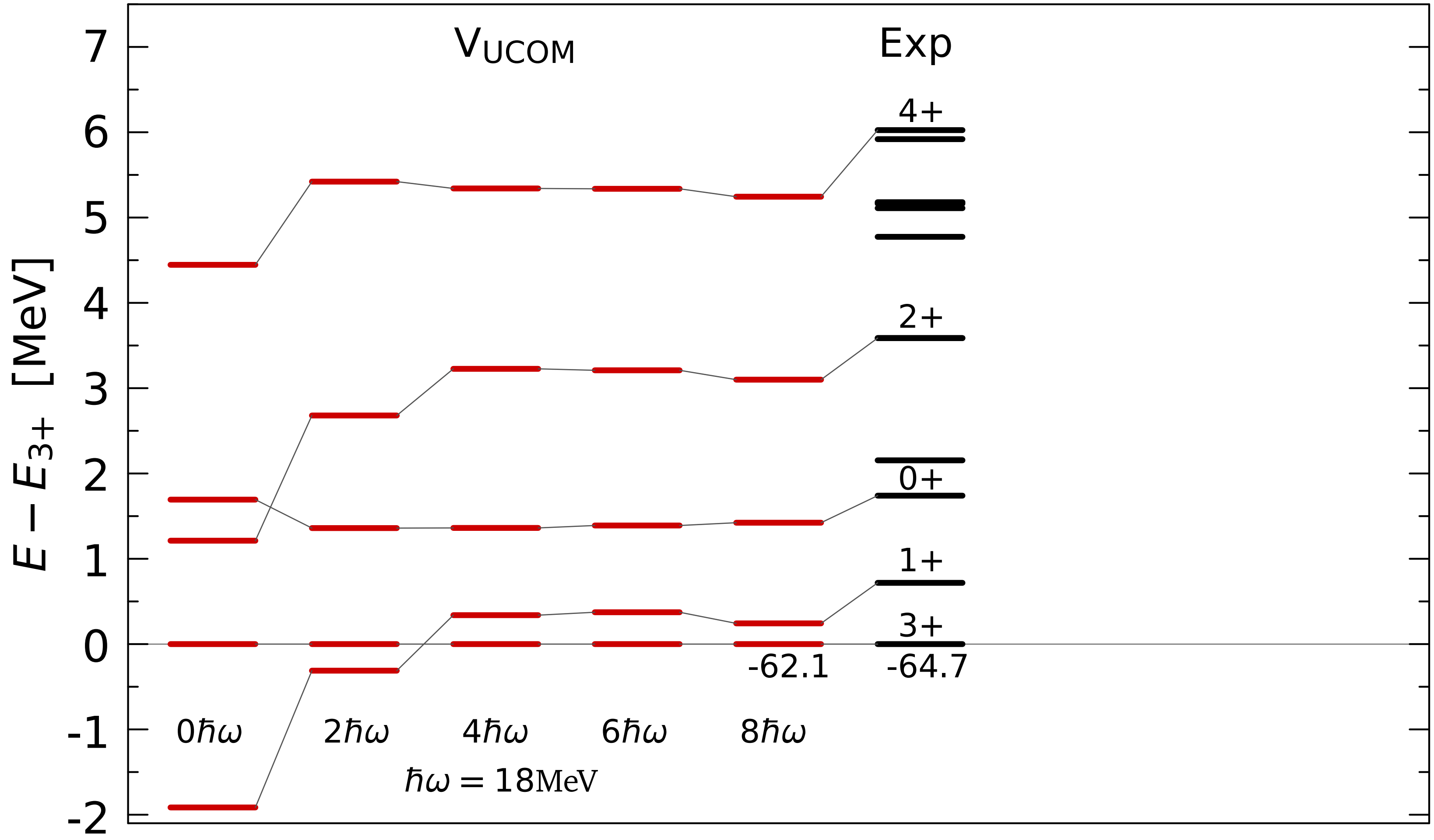
Tjon-Line and 3N Interactions



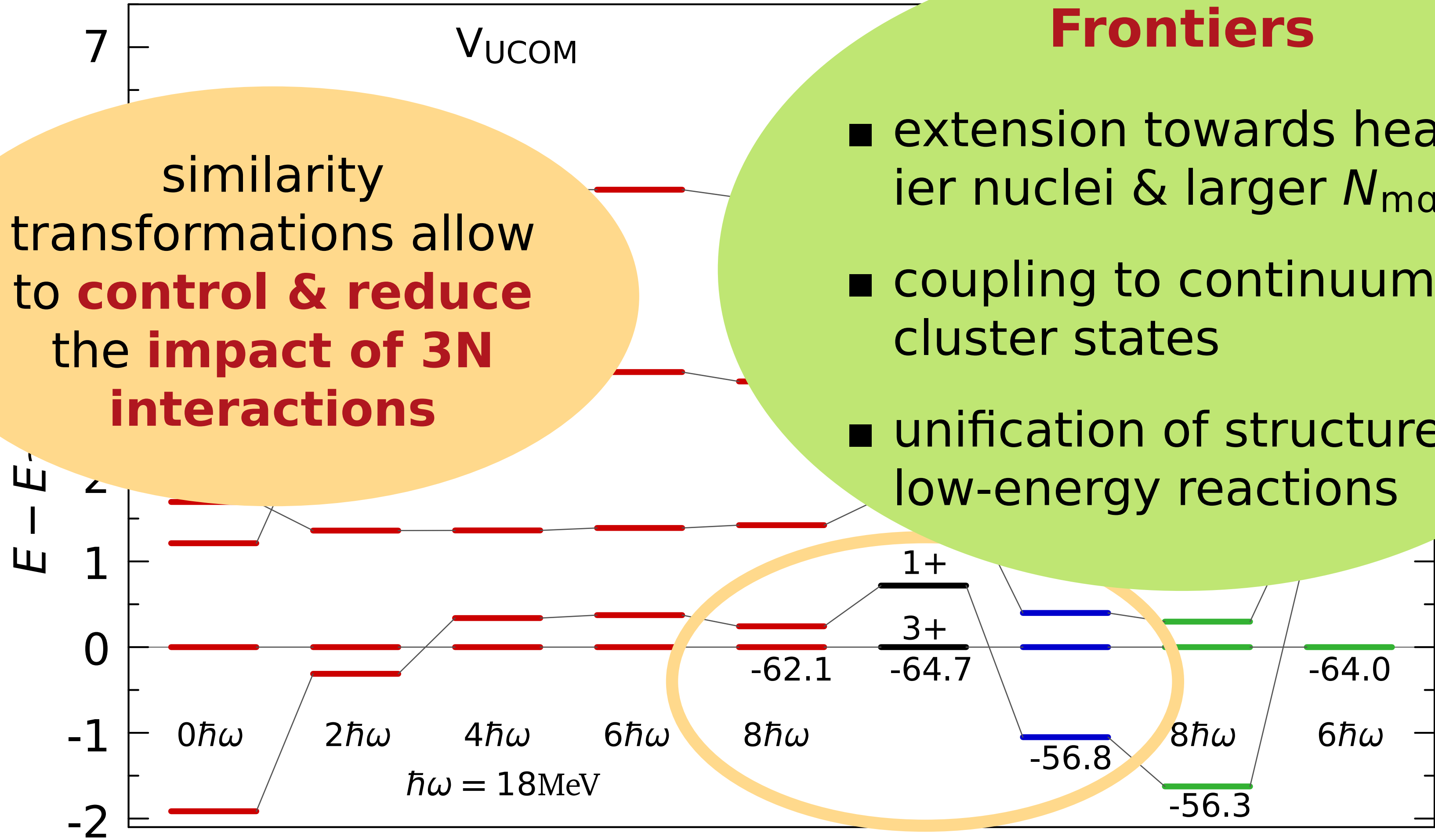
- **Tjon-line**: $E(^4\text{He})$ vs. $E(^3\text{H})$ for phase-shift equivalent NN-interactions
- change of C_{Ω}-correlator range results in shift along Tjon-line

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?



similarity transformations allow to **control & reduce** the **impact of 3N interactions**

Frontiers

- extension towards heavier nuclei & larger N_{max}
- coupling to continuum & cluster states
- unification of structure & low-energy reactions

Ab Initio Approaches

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 restricted to p-s
- full 10 o
for ^{16}O r
(basis din

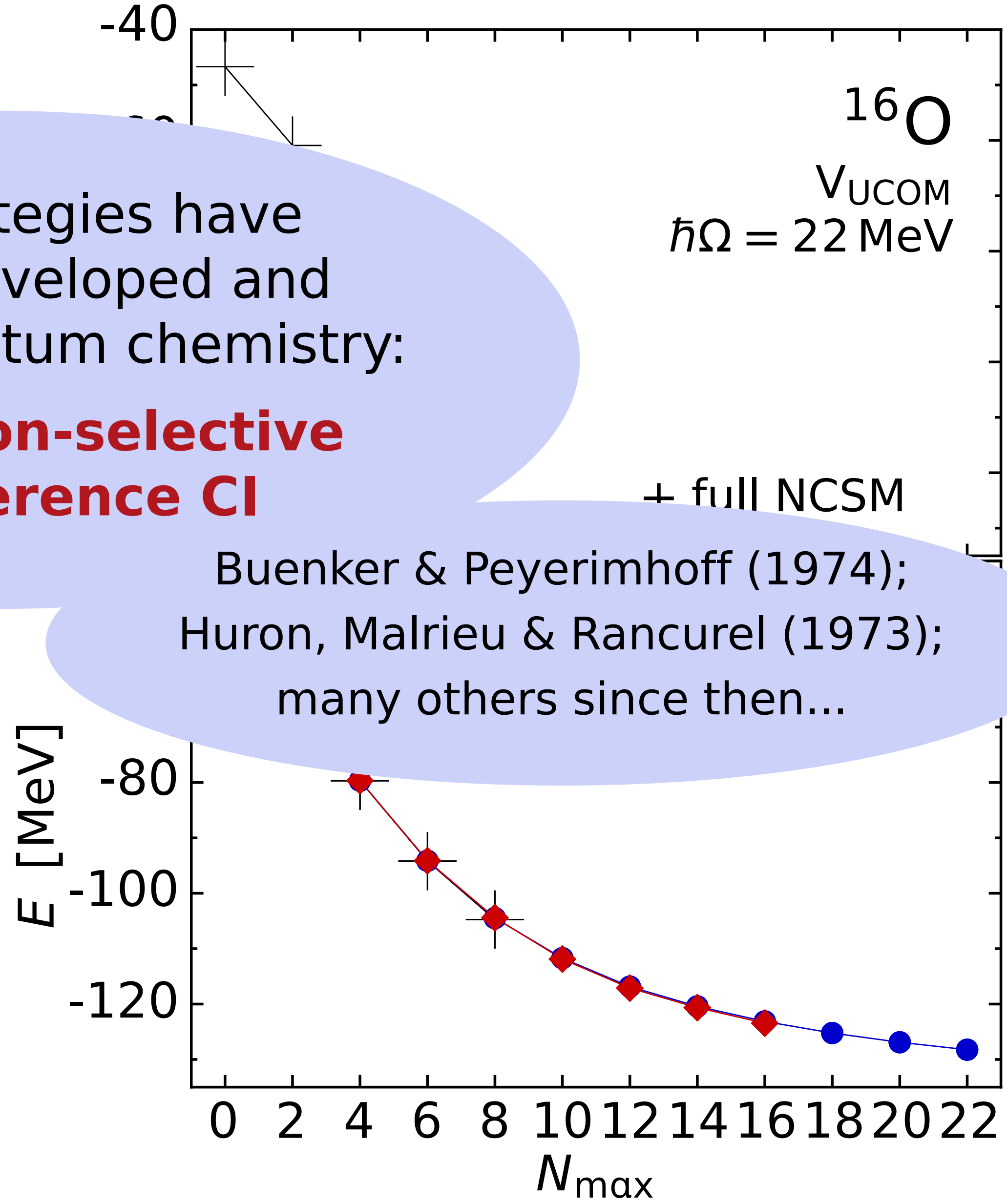
similar strategies have first been developed and applied in quantum chemistry:

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**

- **measure the importance** of individual basis state $|\Phi_\nu\rangle$ via first-order multiconfigurational perturbation theory

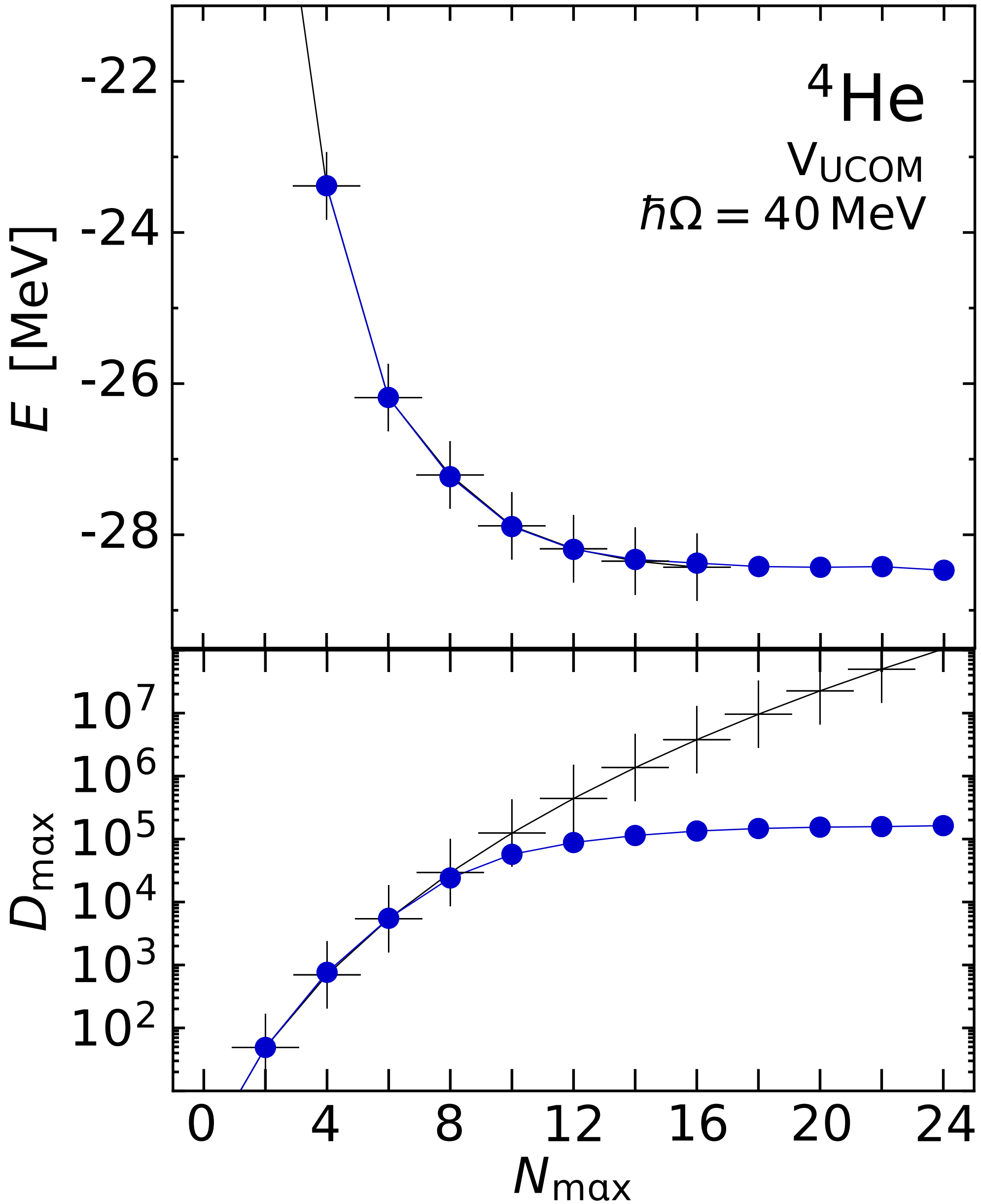
$$\kappa_\nu = -\frac{\langle \Phi_\nu | H | \Psi_{\text{ref}} \rangle}{\epsilon_\nu - \epsilon_{\text{ref}}}$$

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

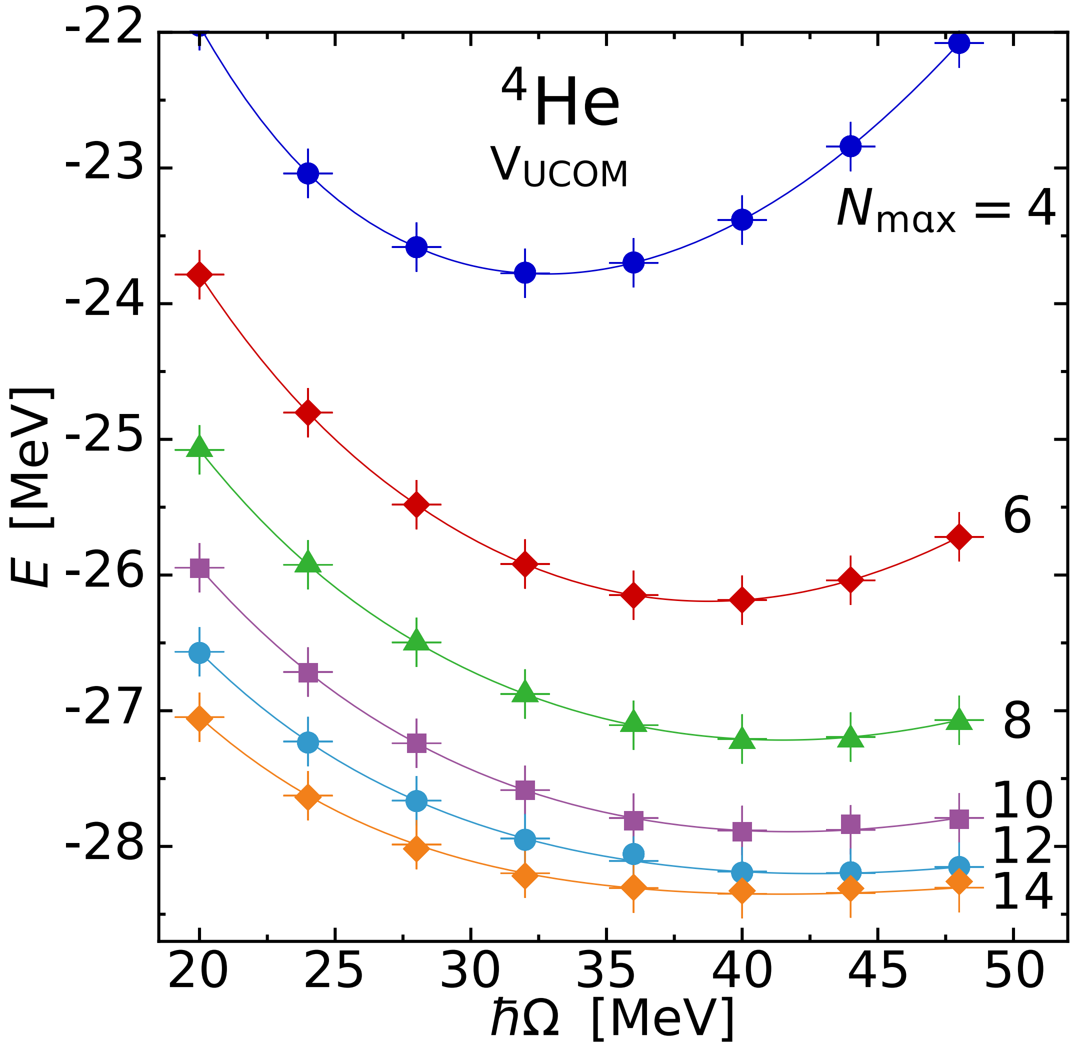
^{4}He: Importance-Truncated NCSM



- **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)

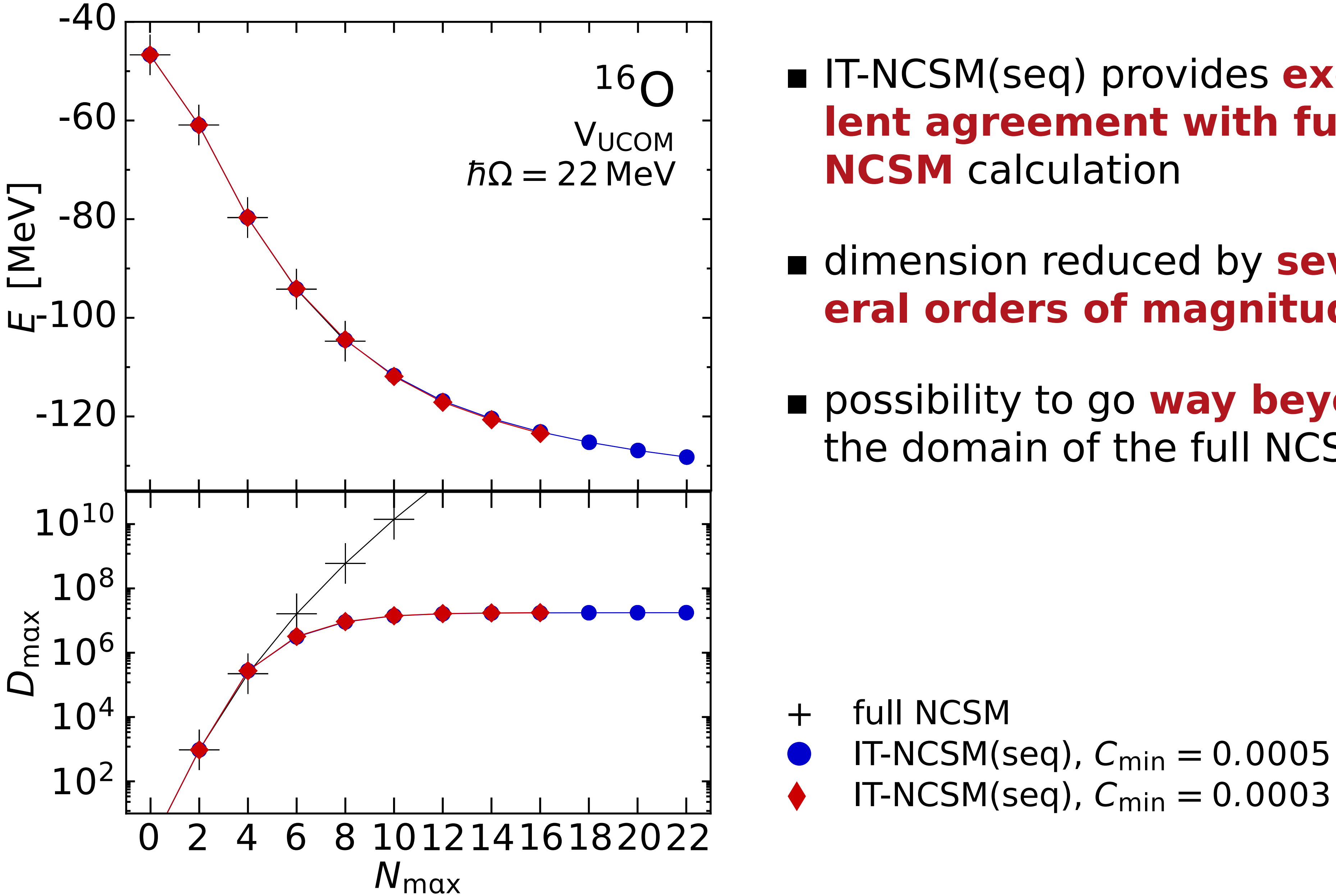
^{4}He: Importance-Truncated NCSM



- **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 $\hbar\Omega$

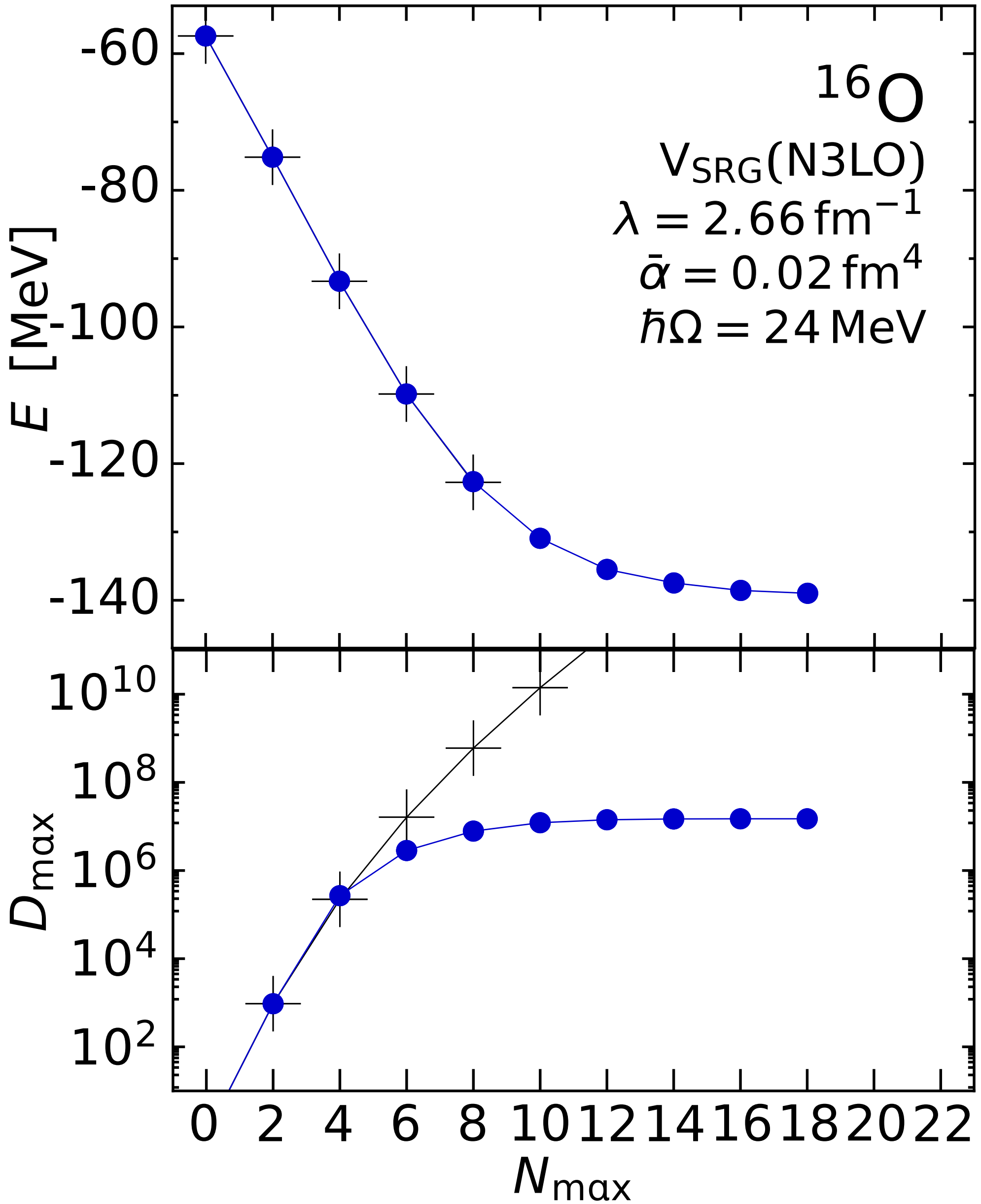
+ full NCSM
● IT-NCSM(seq)

^{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

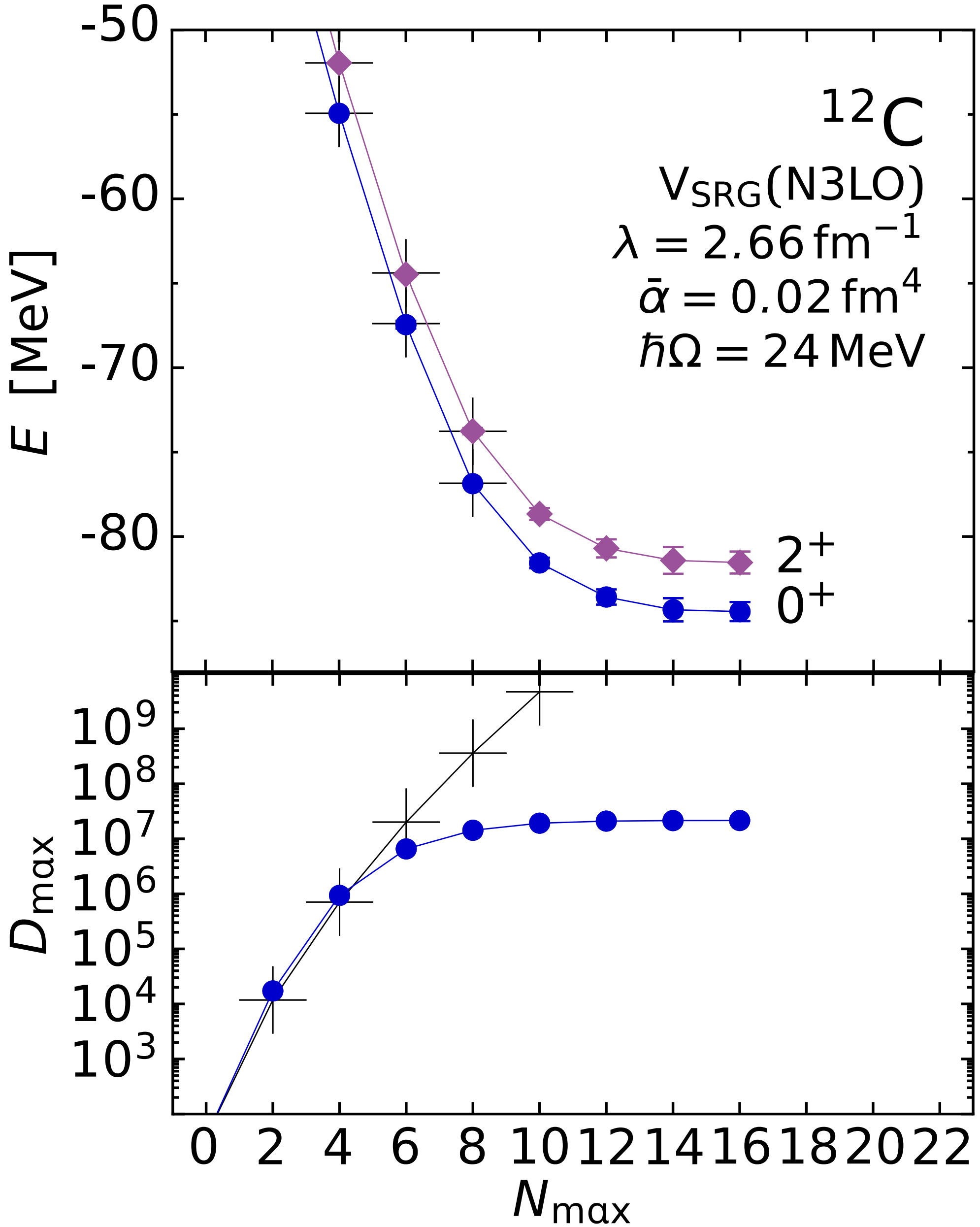
^{16}O: Importance-Truncated NCSM



- **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

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

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

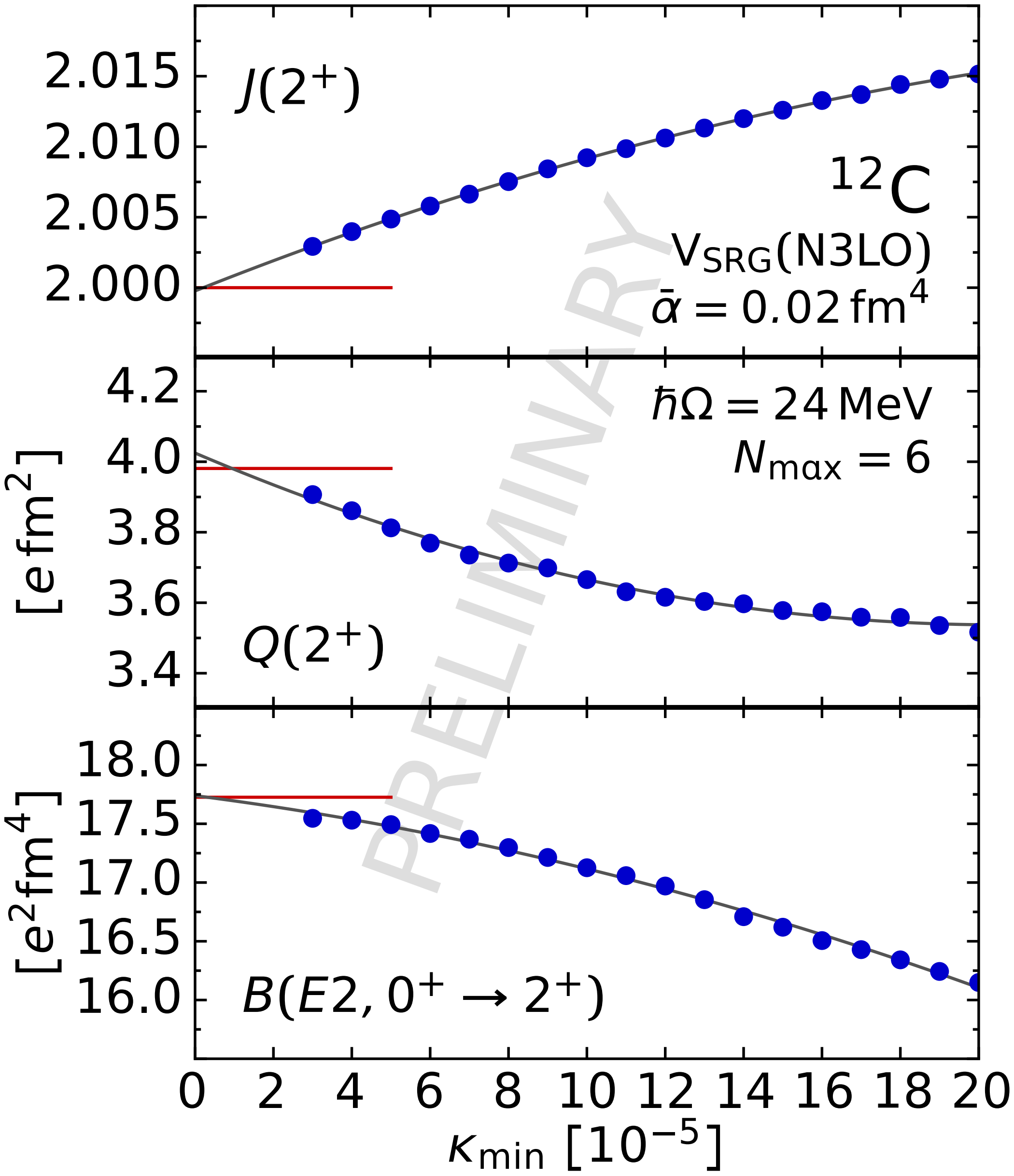


- **target ground & excited states** simultaneously
  - ► separate importance measure $\kappa_\nu^{(n)}$ for each target state
  - ► basis state is included if $|\kappa_\nu^{(n)}| \geq \kappa_{min}$ for any n
- dimension of importance truncated space **grows linearly** with # of target states

+ full NCSM

●♦ IT-NCSM(seq), $C_{min} = 0.0005$

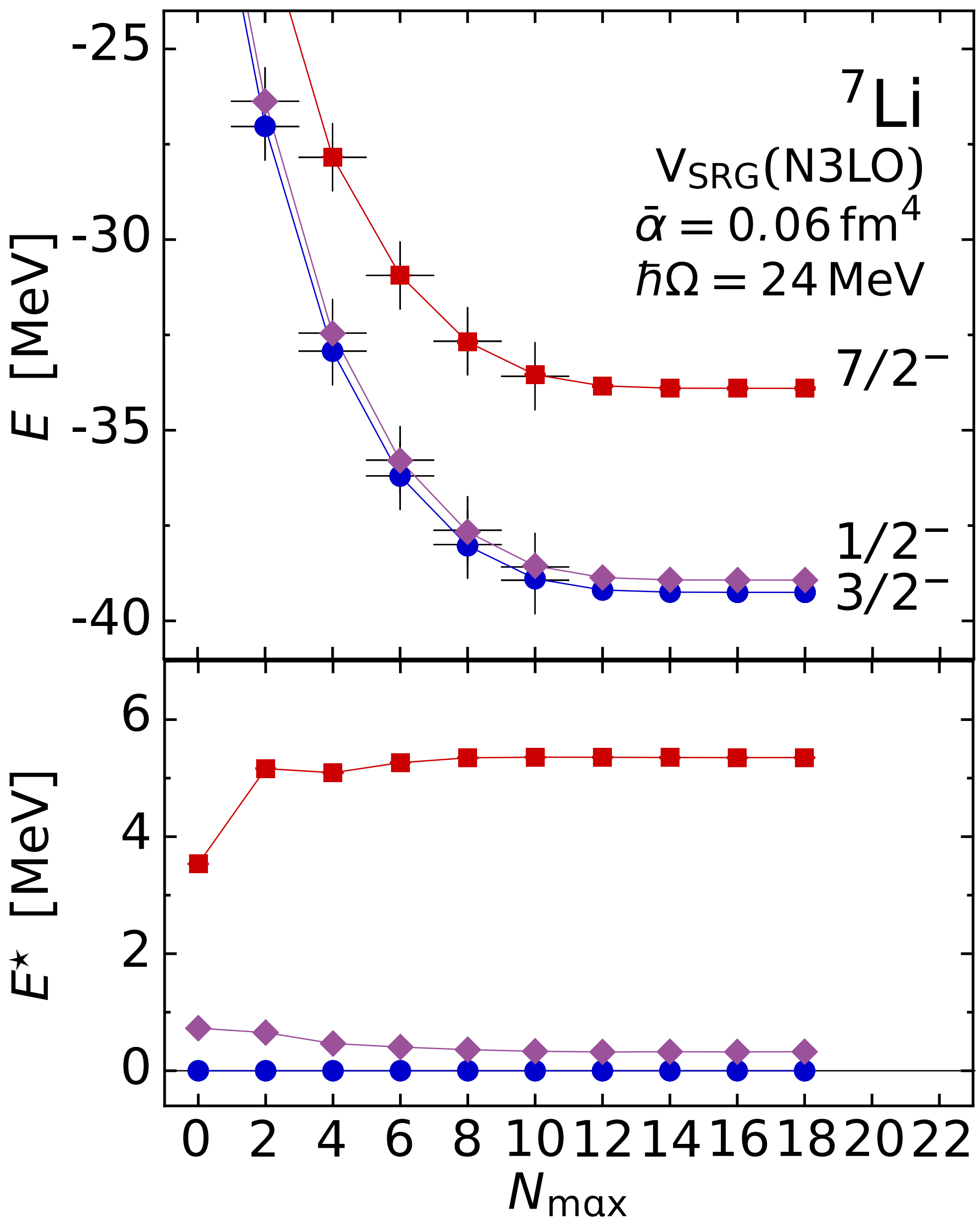
^{12}C: IT-NCSM for Spectroscopy



- access to **spectroscopic observables** via eigenstates
- multipole moments, transition strengths, transition form-factors, 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



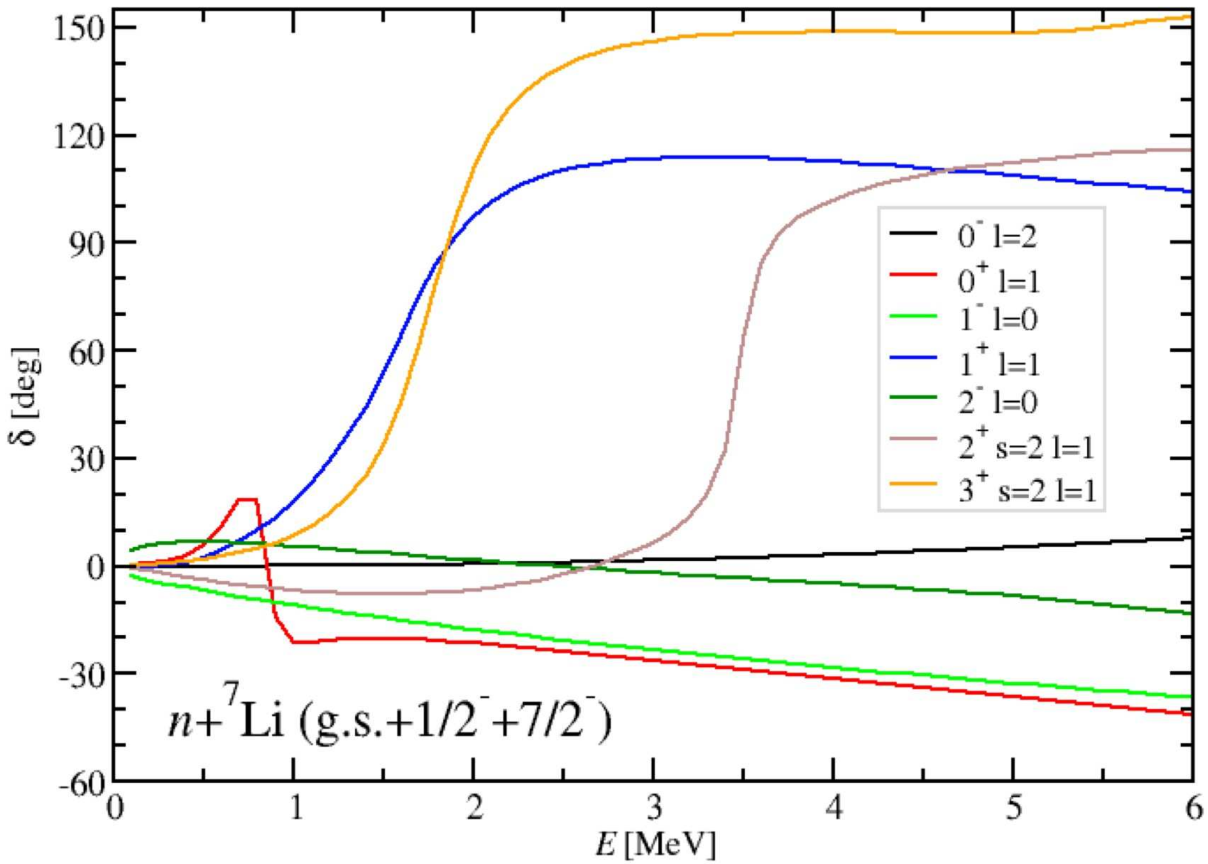
- IT-NCSM(seq) treats a ground state & low-lying excited states for open- and closed-shell nuclei **on the same footing**
- **excellent agreement with full NCSM** calculations in all cases

+ 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

Many-Body Approximations

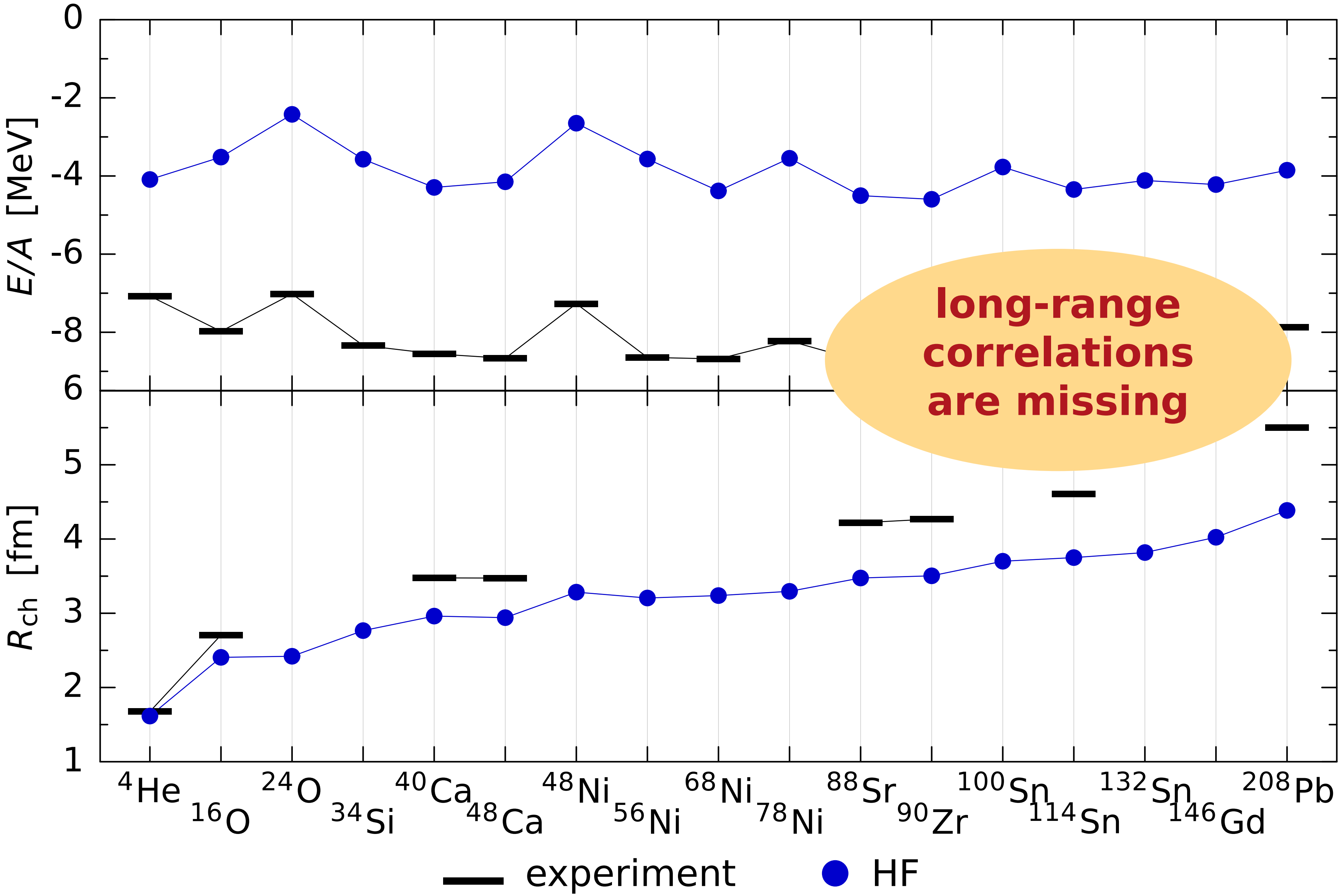
Other Options...

Other Options...

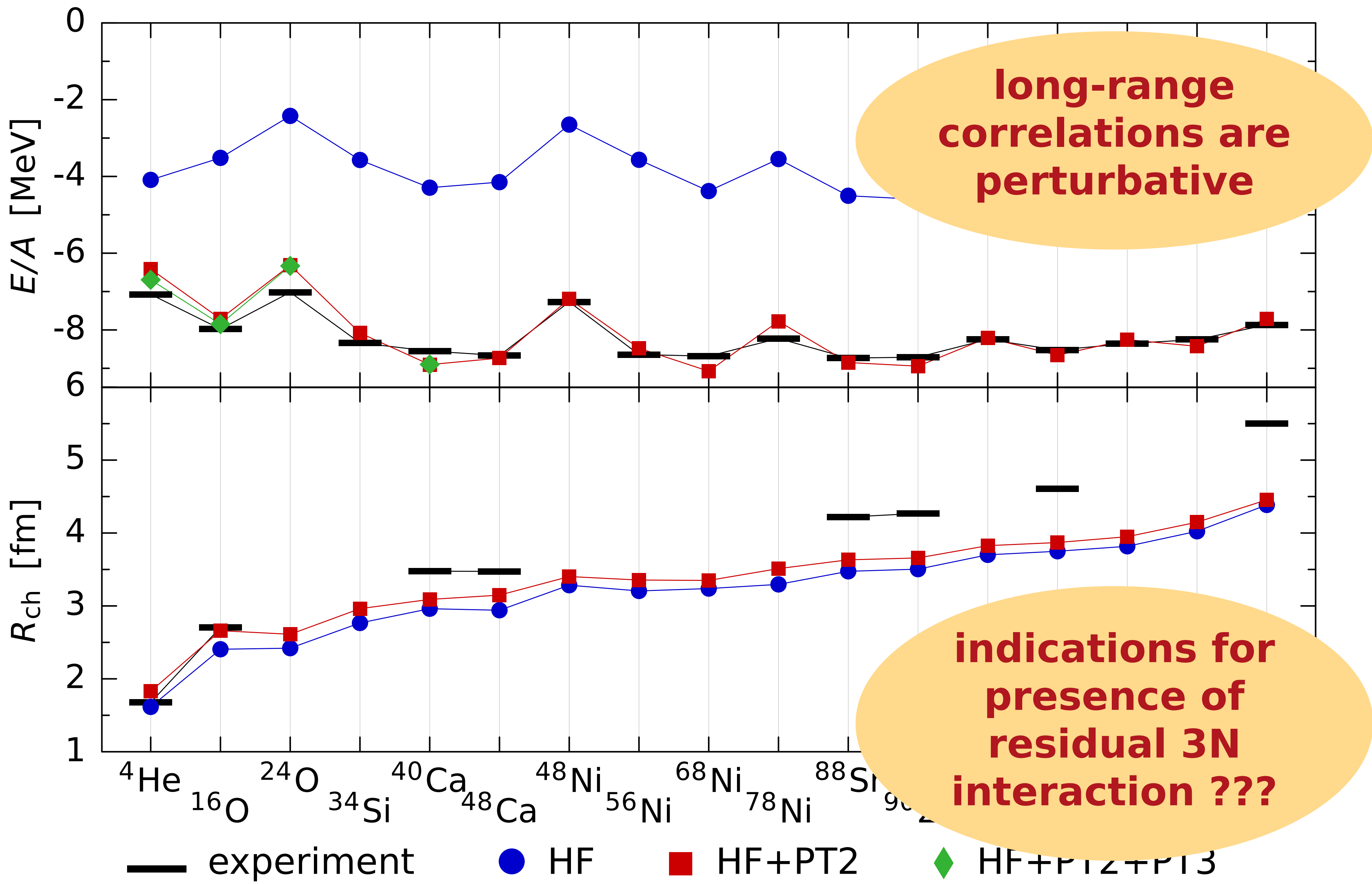
similarity transformed interactions (e.g. V_{UCOM}, V_{SRG}) provide universal input for various many-body methods

- coupled-cluster method
- Hartree-Fock & many-body perturbation theory
- Hartree-Fock-Bogoliubov & particle-number projection
- RPA & Second-RPA
- FMD with projection & configuration mixing

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,...)
  - exact & approximate 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

thanks to my group & my collaborators

- S. Binder, A. Calci, B. Erler, A. Günther, M. Hild, H. Krutsch, J. Langhammer, P. Papakonstantinou, S. Reinhardt, F. Schmitt
  Institut für Kernphysik, TU Darmstadt
- P. Navrátil, S. Quaglioni
  Lawrence Livermore National Laboratory, USA
- H. Hergert, P. Piecuch, J. Gour
  Michigan State University, USA
- C. Forssén
  Chalmers University of Technology, Sweden
- H. Feldmeier, T. Neff,...
  Gesellschaft für Schwerionenforschung (GSI)

Deutsche Forschungsgemeinschaft DFG

SFB 634

HIC for FAIR

LOEWE – Landes-Offensive zur Entwicklung Wissenschaftlich-ökonomischer Exzellenz