New Horizons in Nuclear Structure Theory

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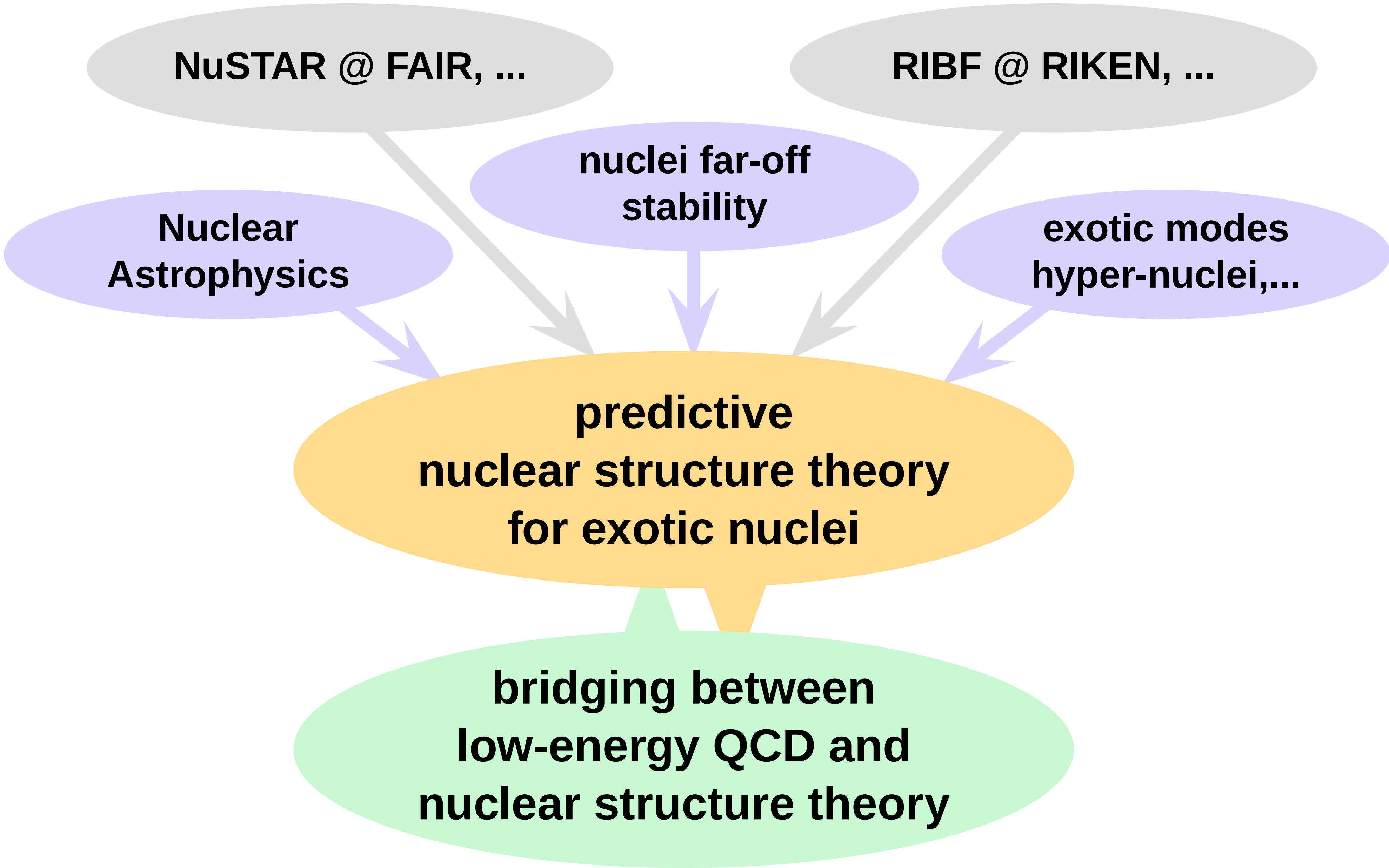
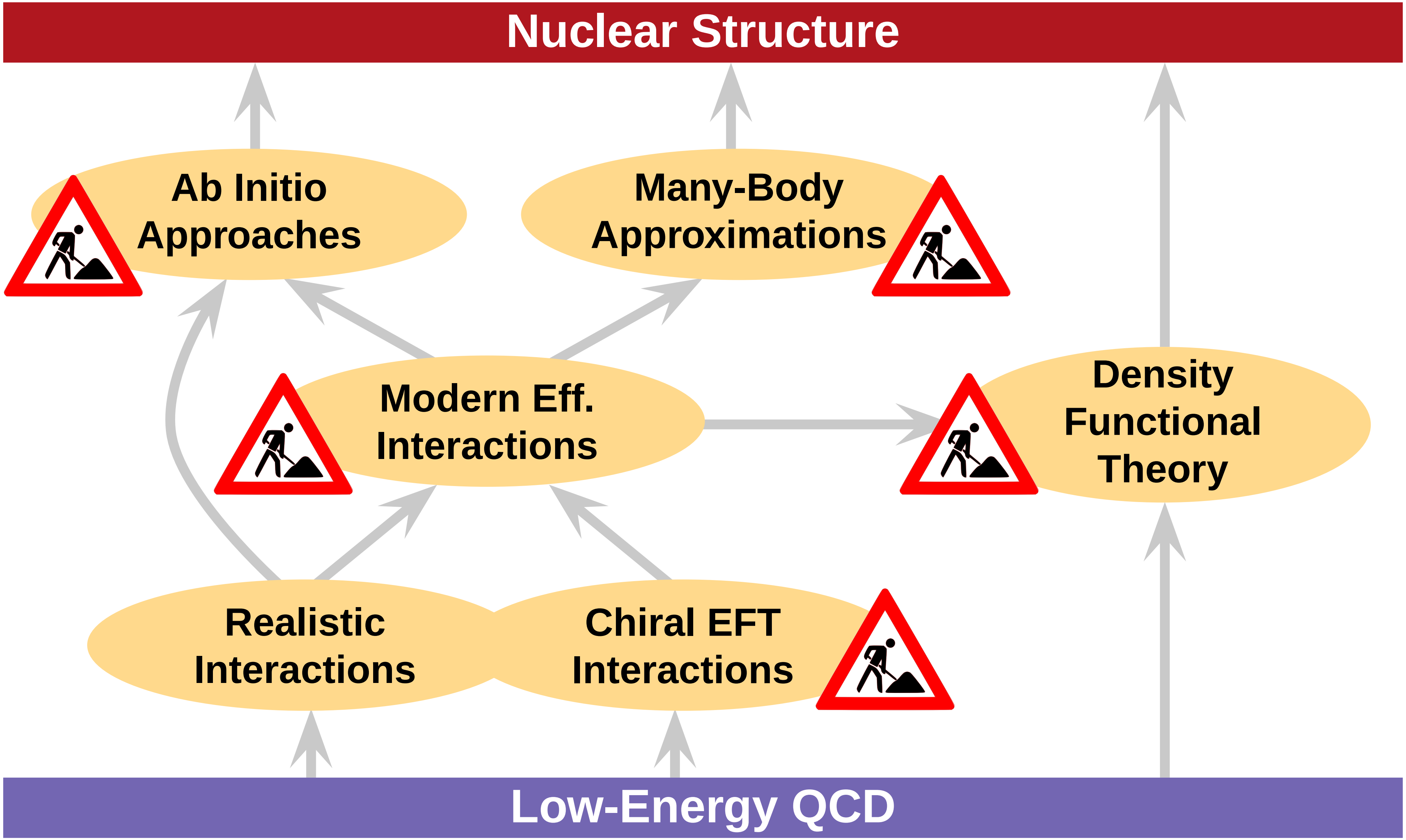
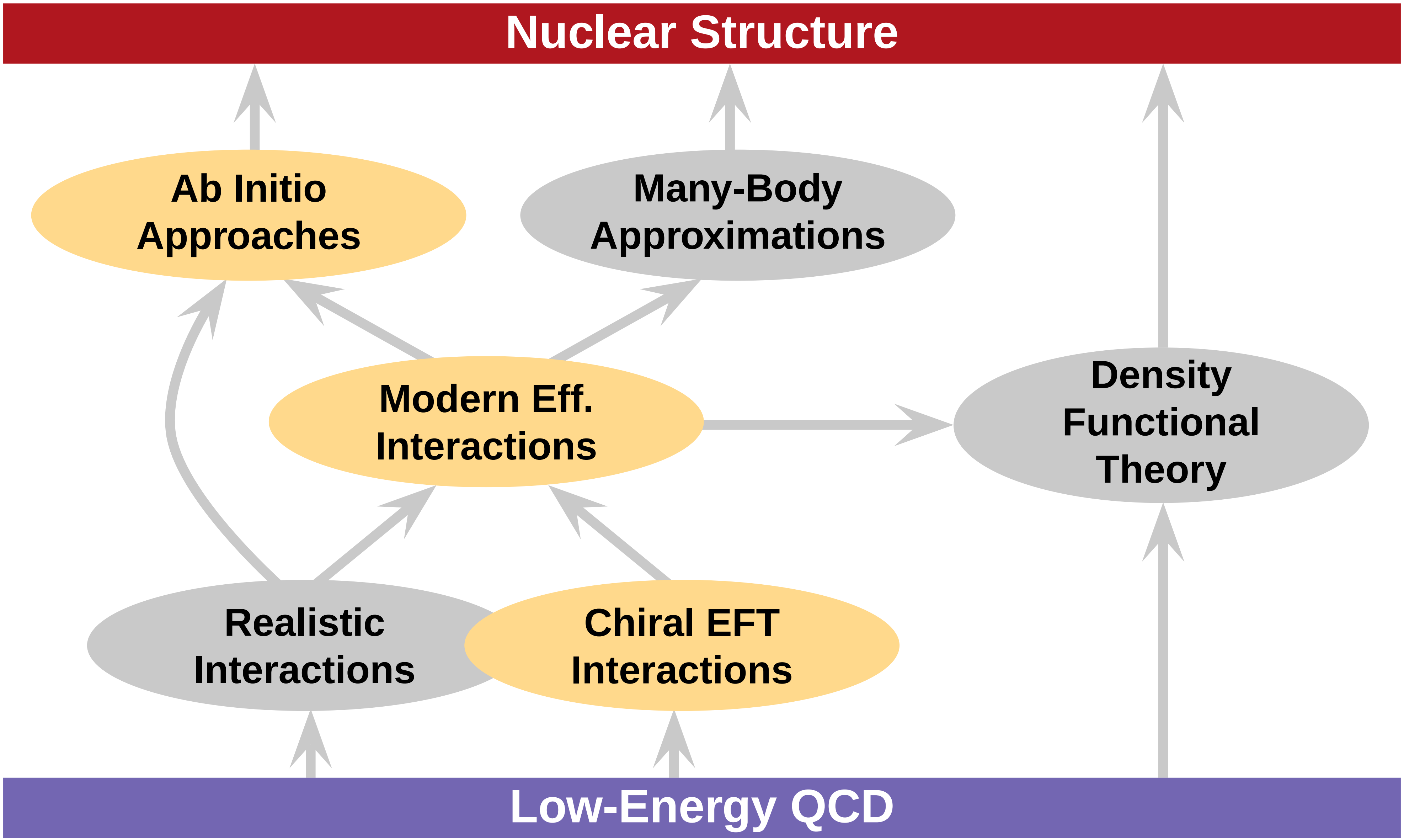
Nuclear Structure in the 21st Century



Modern Nuclear Structure Theory

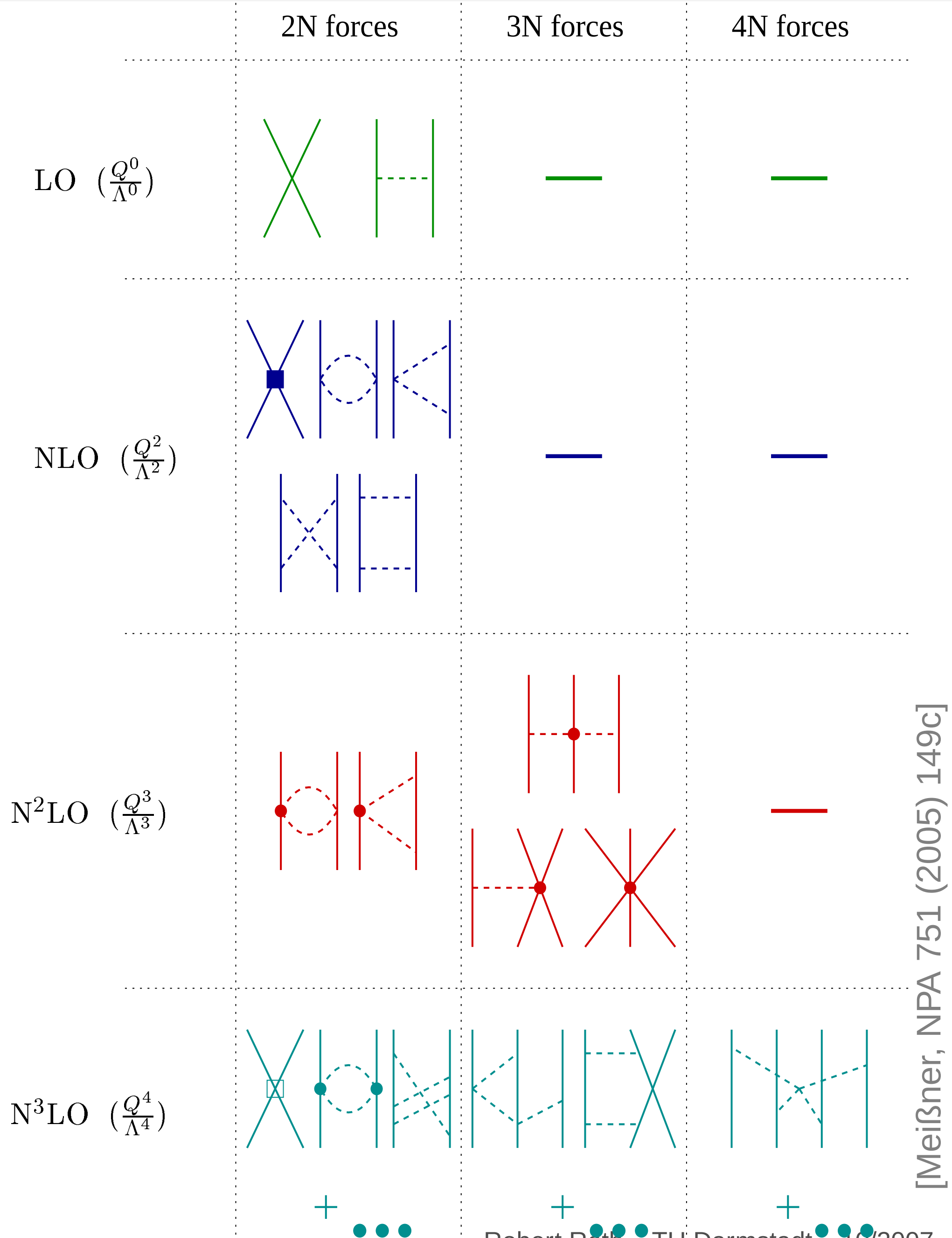


Modern Nuclear Structure Theory



Chiral EFT Interactions

- EFT for relevant degrees of freedom (π,N) based on symmetries of QCD (chiral symmetry)
- long-range pion dynamics treated explicitly
- unresolved short-range physics absorbed in contact terms
- low-energy constants fitted to experimental data (NN, πN)
- hierarchy of consistent NN & 3N (& 4N) interactions (including current operators)



Why Effective Interactions?

Realistic Potentials

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

Modern Effective Interactions

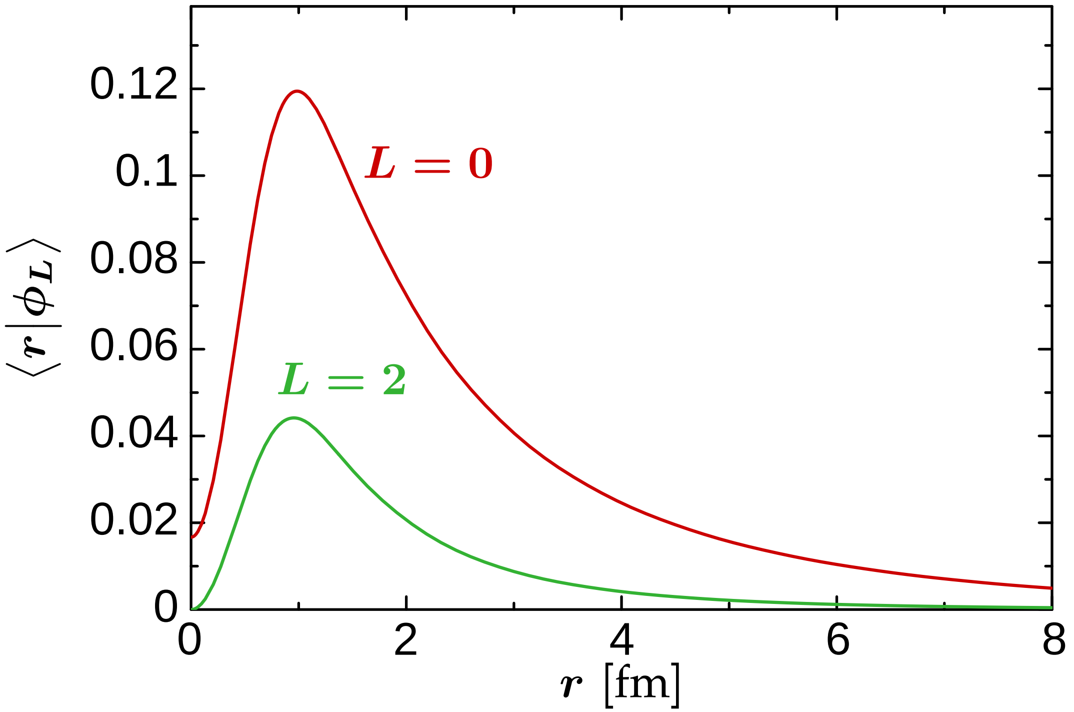
- adapt realistic potential to the available model space
  - tame short-range correlations
  - improve convergence behavior
- conserve experimentally constrained properties (phase shifts)

can be viewed as realistic interactions

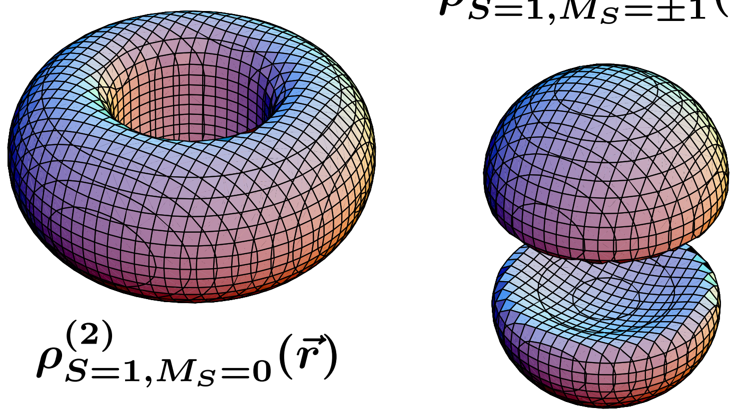
Many-Body Approximations

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

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 D-wave admixture in the ground state

tensor correlations

Modern Effective 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 an unitary operator $\mathbf{C}$ to describe the effect of short-range correlations

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

Correlated States

imprint short-range correlations onto uncorrelated many-body states

$$|\widetilde{\psi}\rangle = \mathbf{C}\;|\psi\rangle$$

Correlated Operators

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

$$\widetilde{\mathbf{O}} = \mathbf{C}^{\dagger}\;\mathbf{O}\;\mathbf{C}$$

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

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

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

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

Tensor Correlator C_Ω

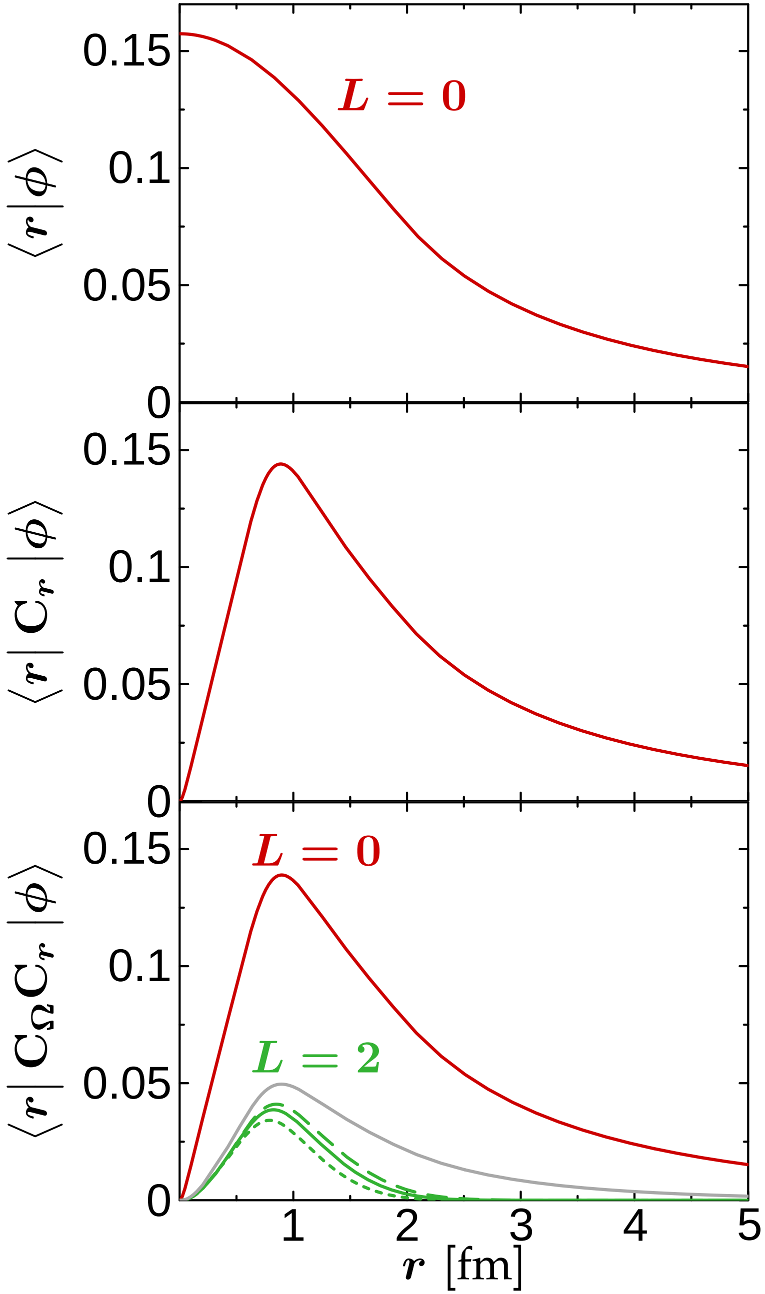
- angular shift depending on the orientation of spin and relative coordinate of a nucleon pair

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

$$\vec{\mathrm{q}}_\Omega = \vec{\mathrm{q}} - \tfrac{\vec{\mathrm{r}}}{\mathrm{r}}\ \mathrm{q}_r$$

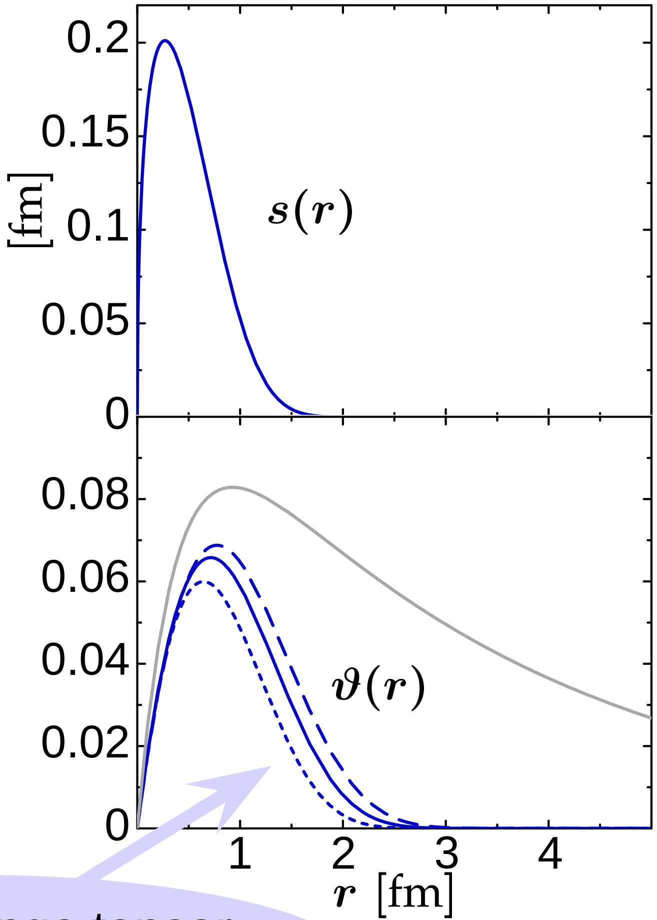
- $s(r)$ and $\vartheta(r)$ for given potential determined by energy minimization in the two-body system (for each S, T)

Correlated States: The Deuteron



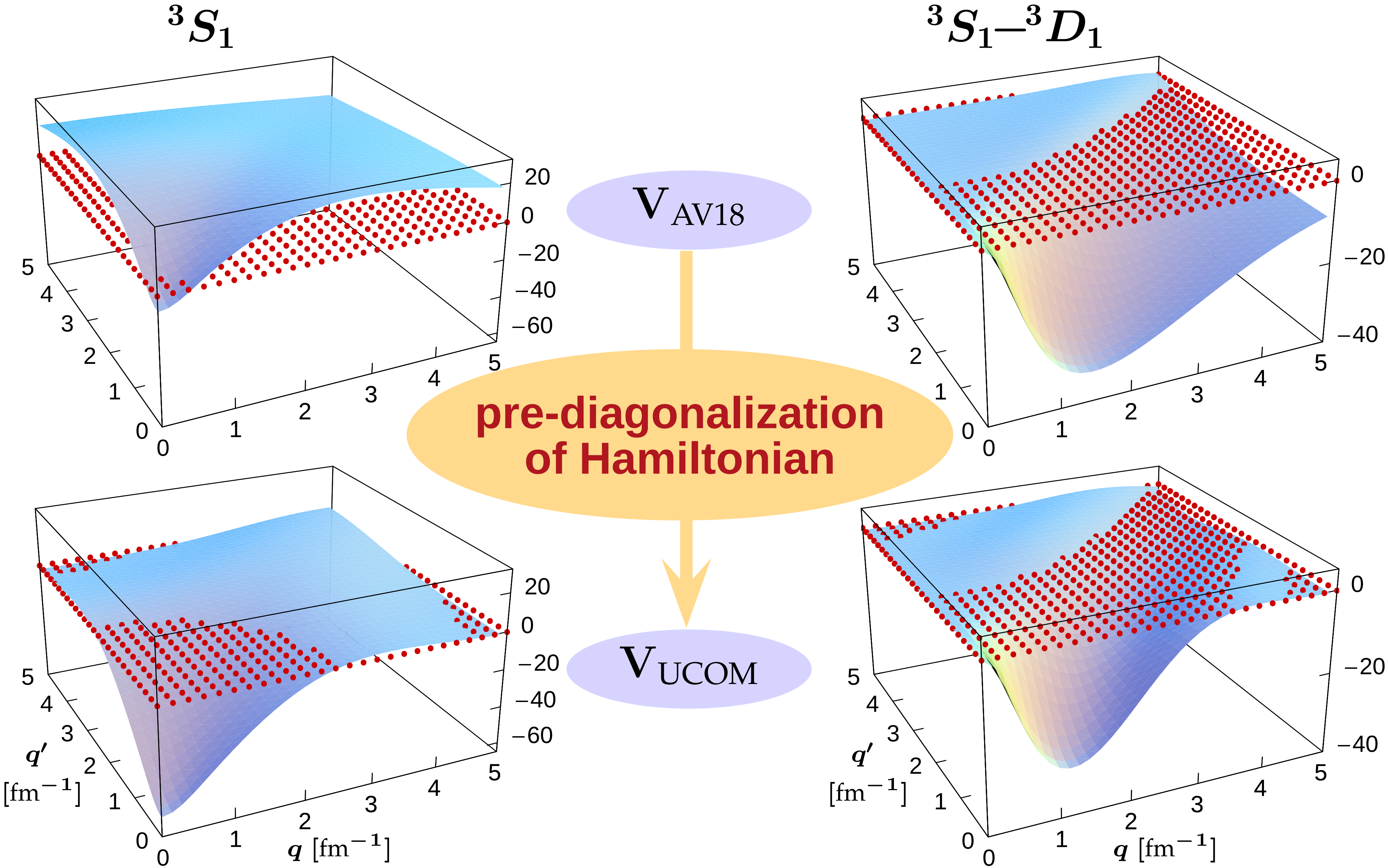
central correlations

tensor correlations



only short-range tensor correlations treated by $\mathbf{C}_\Omega$

Correlated Interaction: V_{UCOM}



Modern Effective Interactions

Similarity Renormalization Group (SRG)

Hergert & Roth — Phys. Rev. C 75, 051001(R) (2007)
Bogner et al. — Phys. Rev. C 75, 061001(R) (2007)

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

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

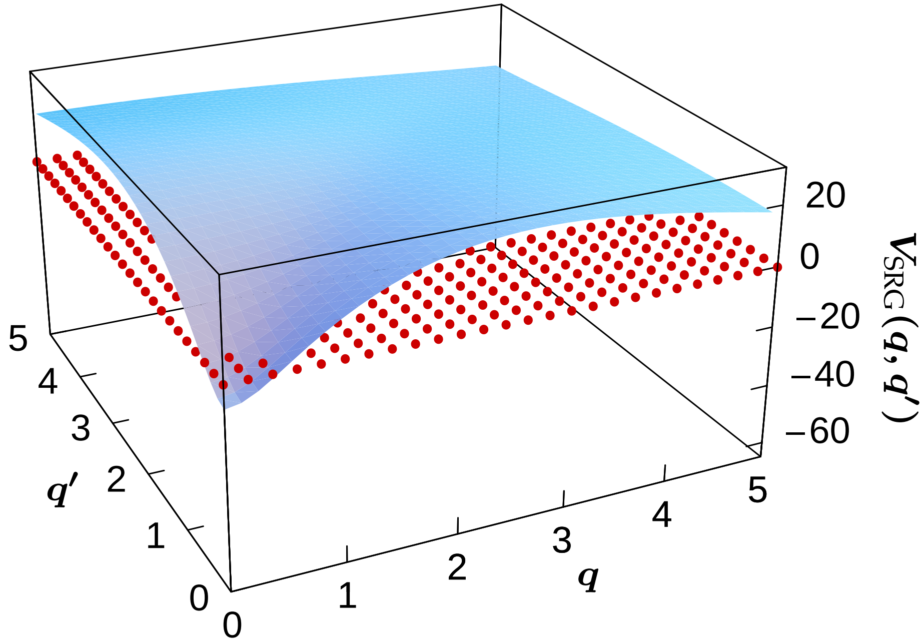
- dynamical generator defined as commutator with the operator in whose eigenbasis H shall be diagonalized

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

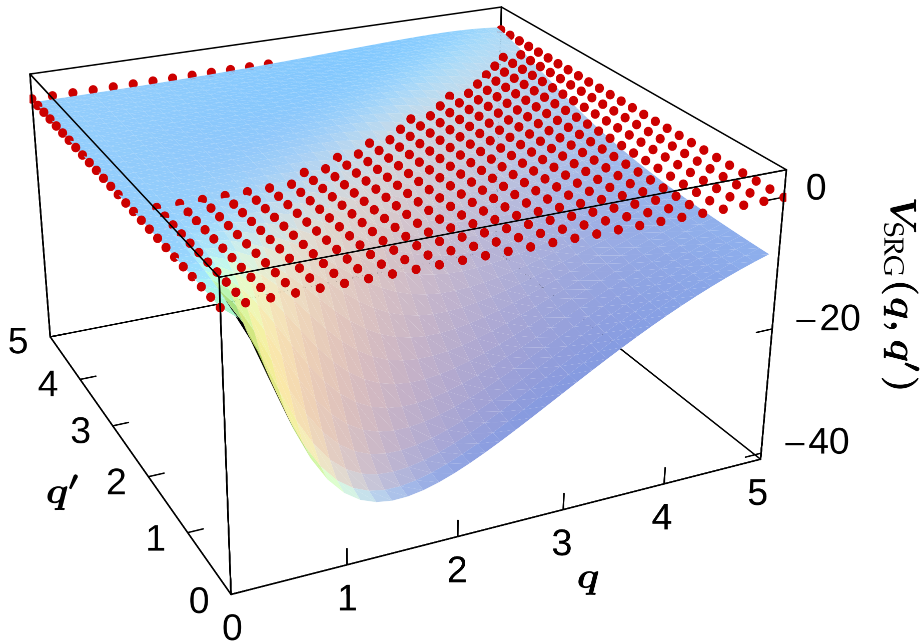
- $\eta(0)$ has the same structure as the UCOM generators g_r and g_Ω

SRG Evolution: The Deuteron

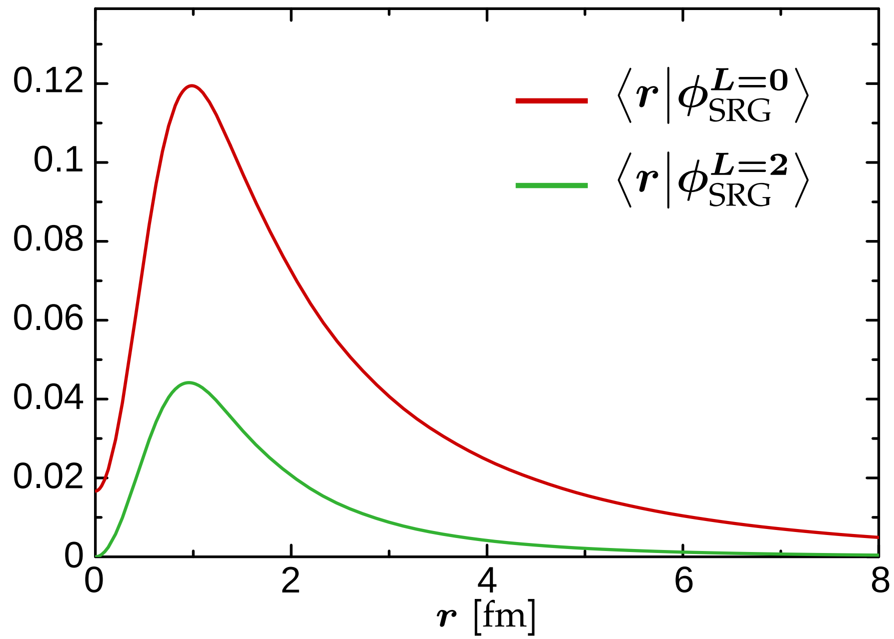
$^3S_1$



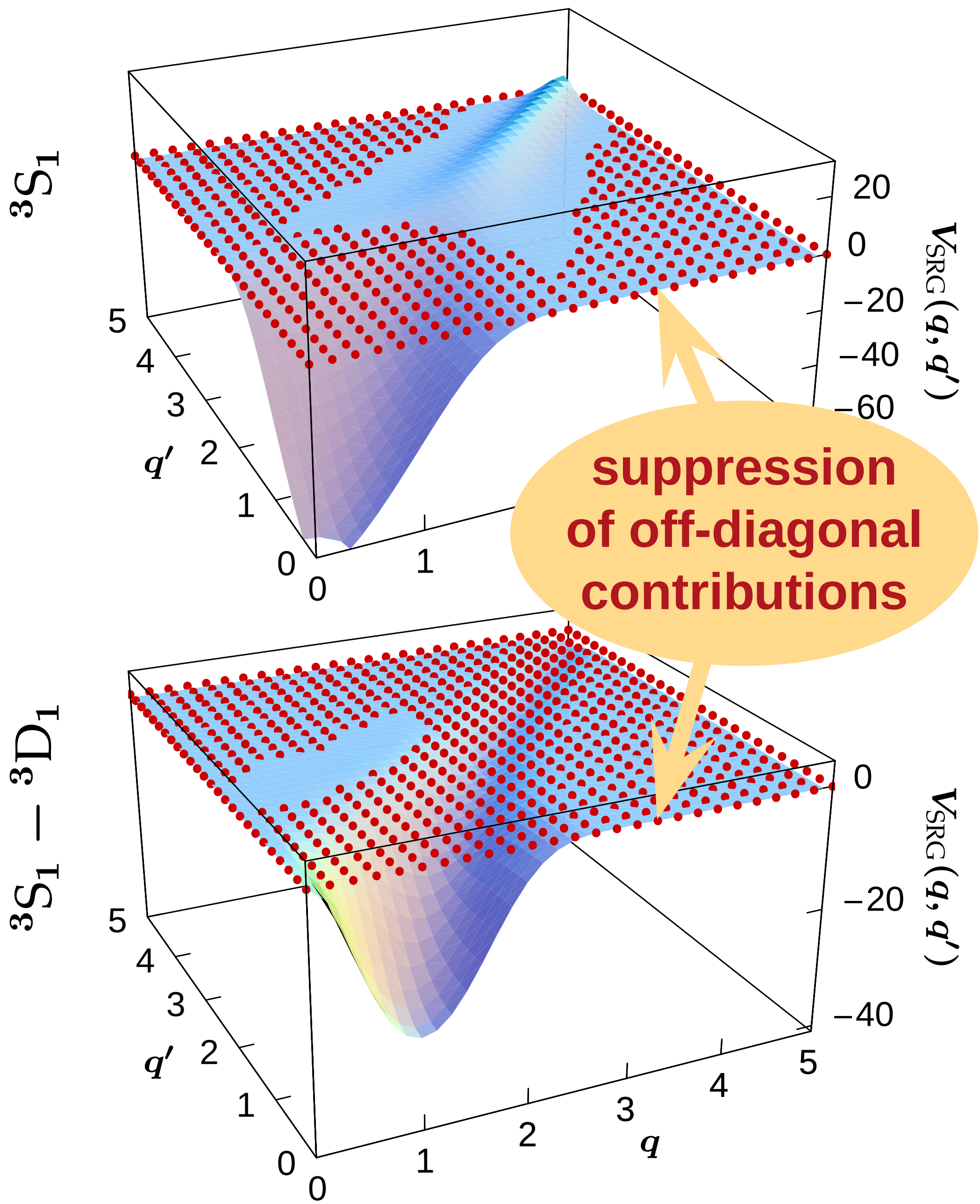
$^3S_1 - {}^3D_1$



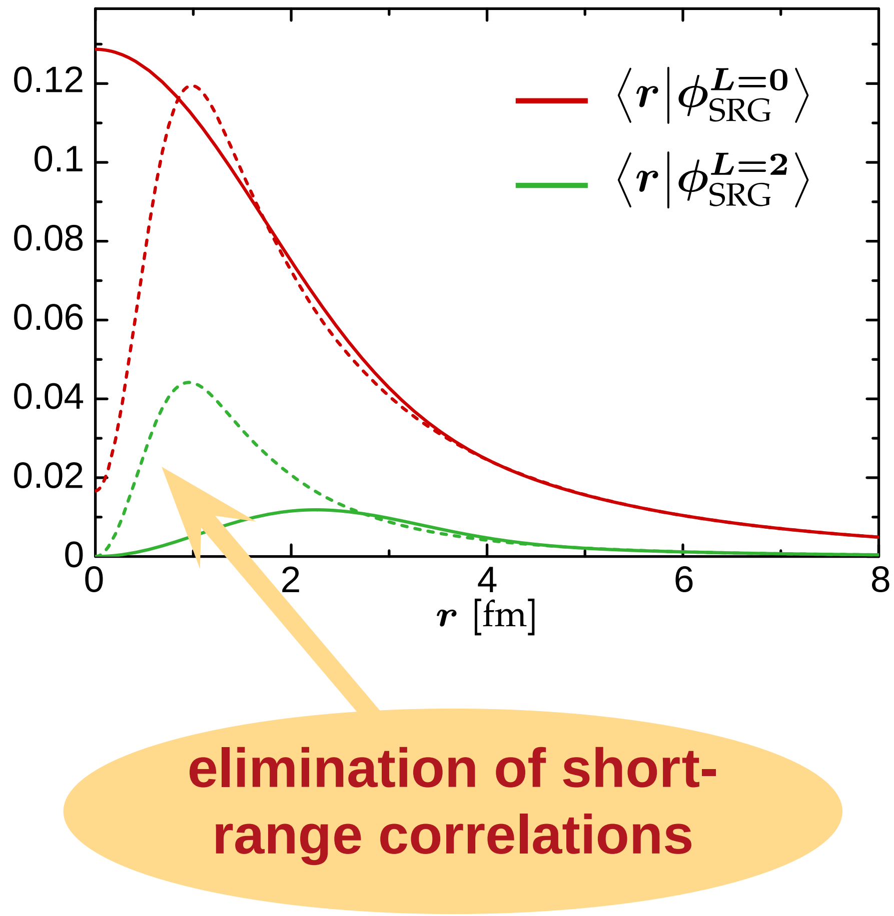
Argonne V18



SRG Evolution: The Deuteron



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



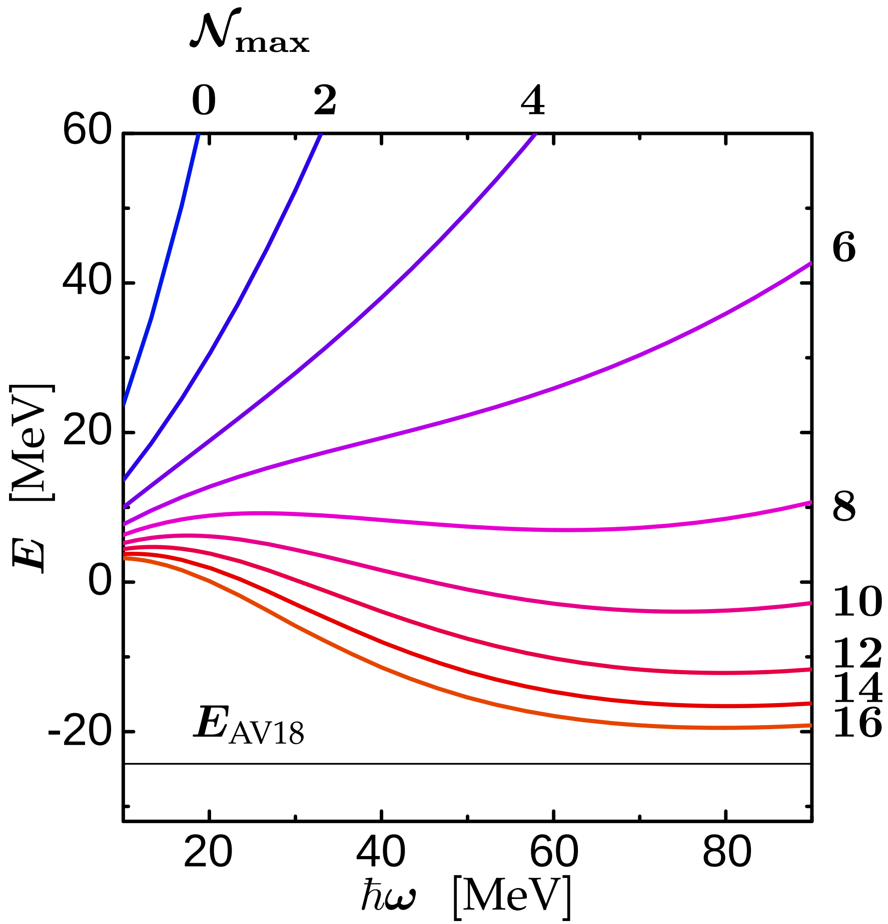
Ab Initio Approaches

No-Core Shell Model

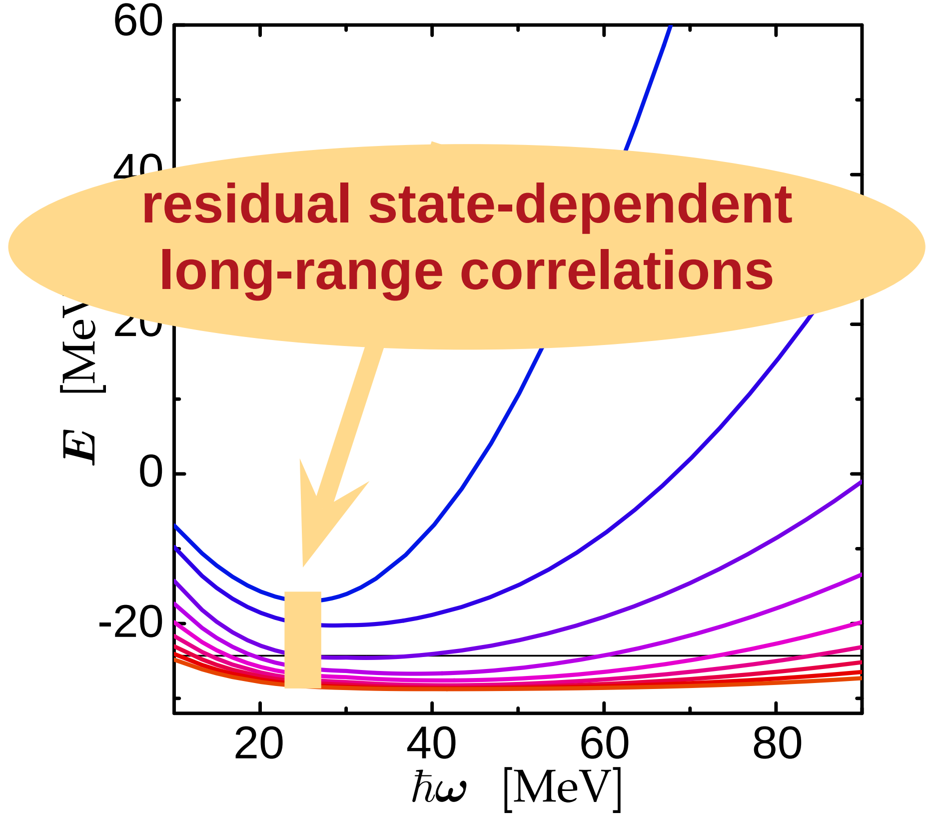
Roth et al. — Phys. Rev. C 72, 034002 (2005)
Roth & Navrátil — in preparation

^{4}He: Convergence

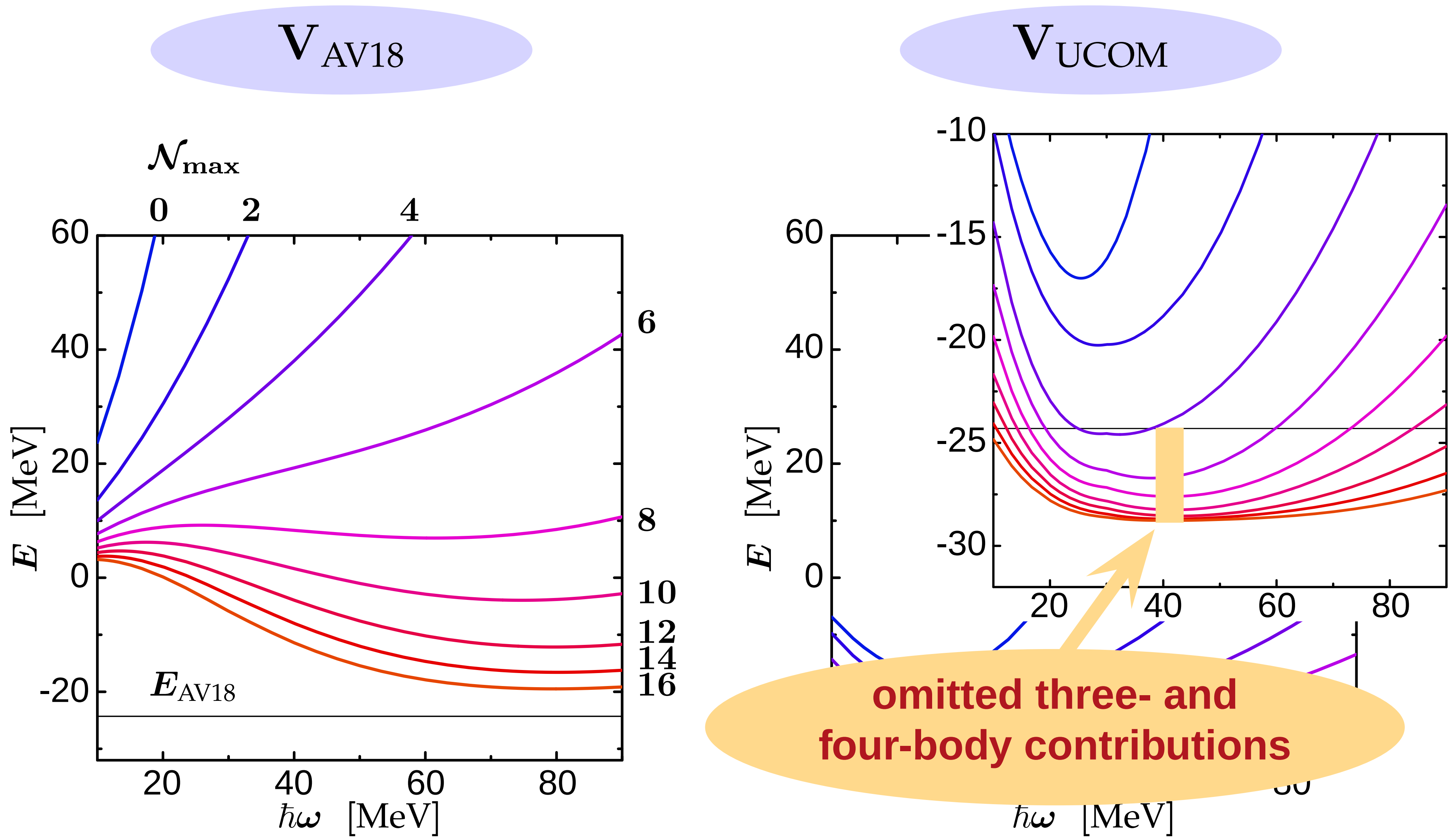
V_{AV18}



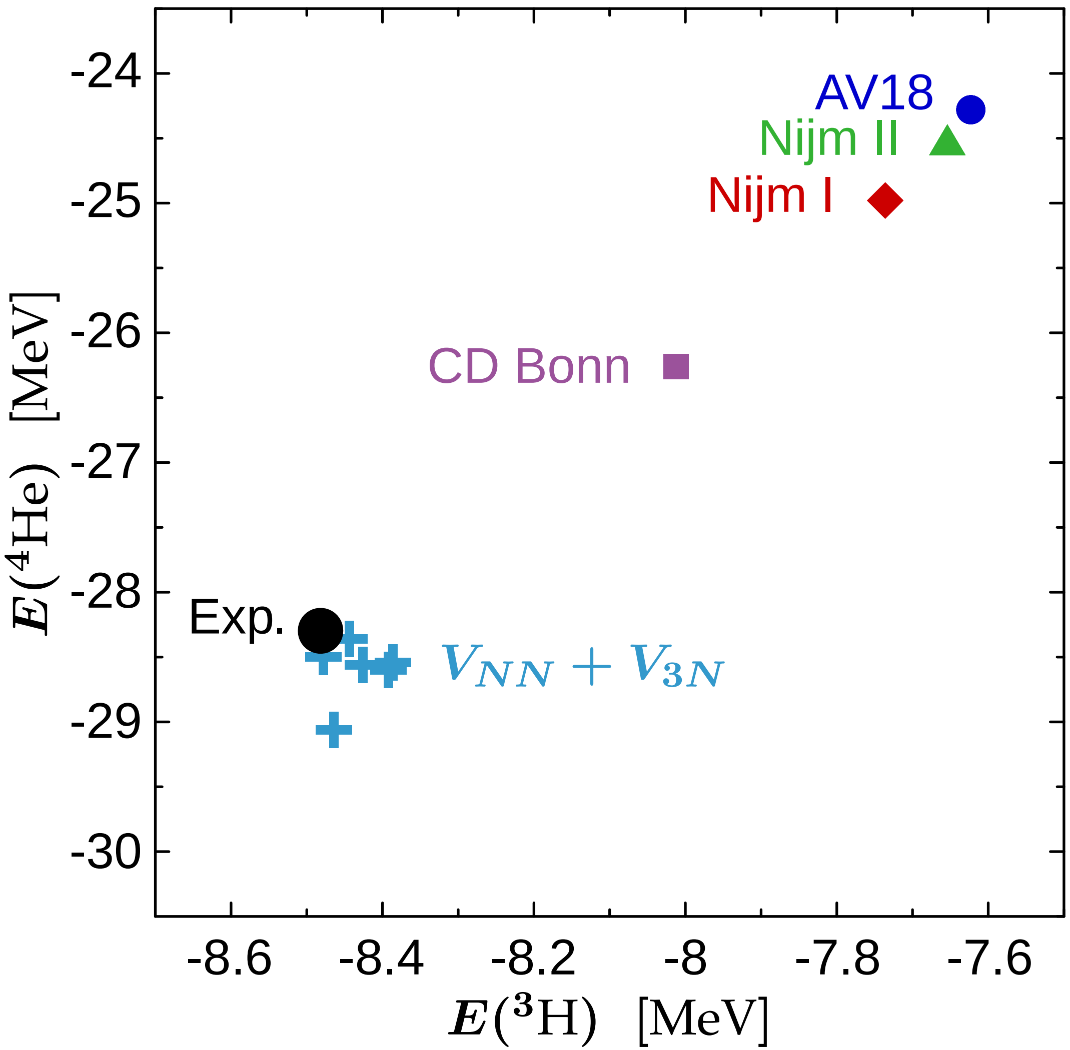
V_{UCOM}



^{4}He: Convergence

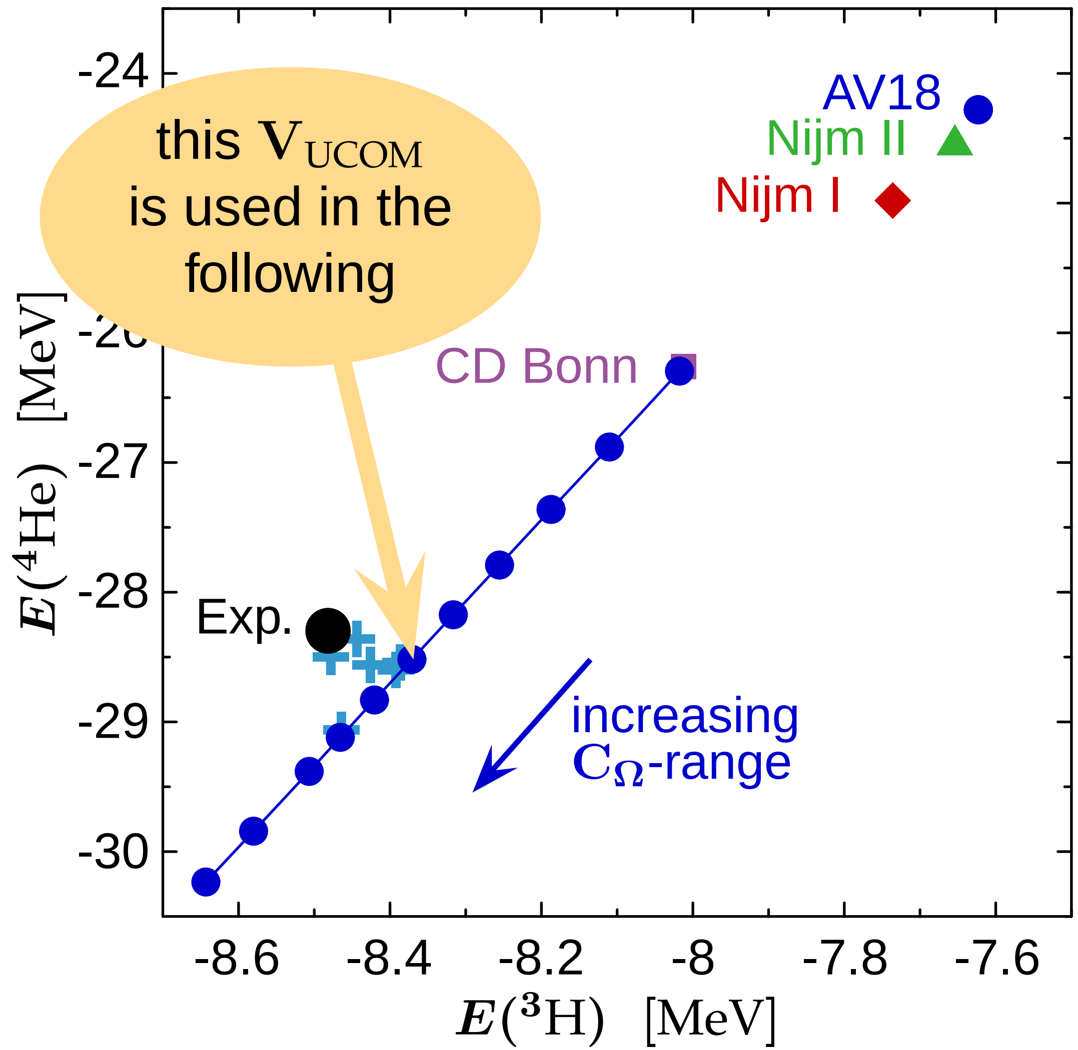


Three-Body Interactions — Tjon Line



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

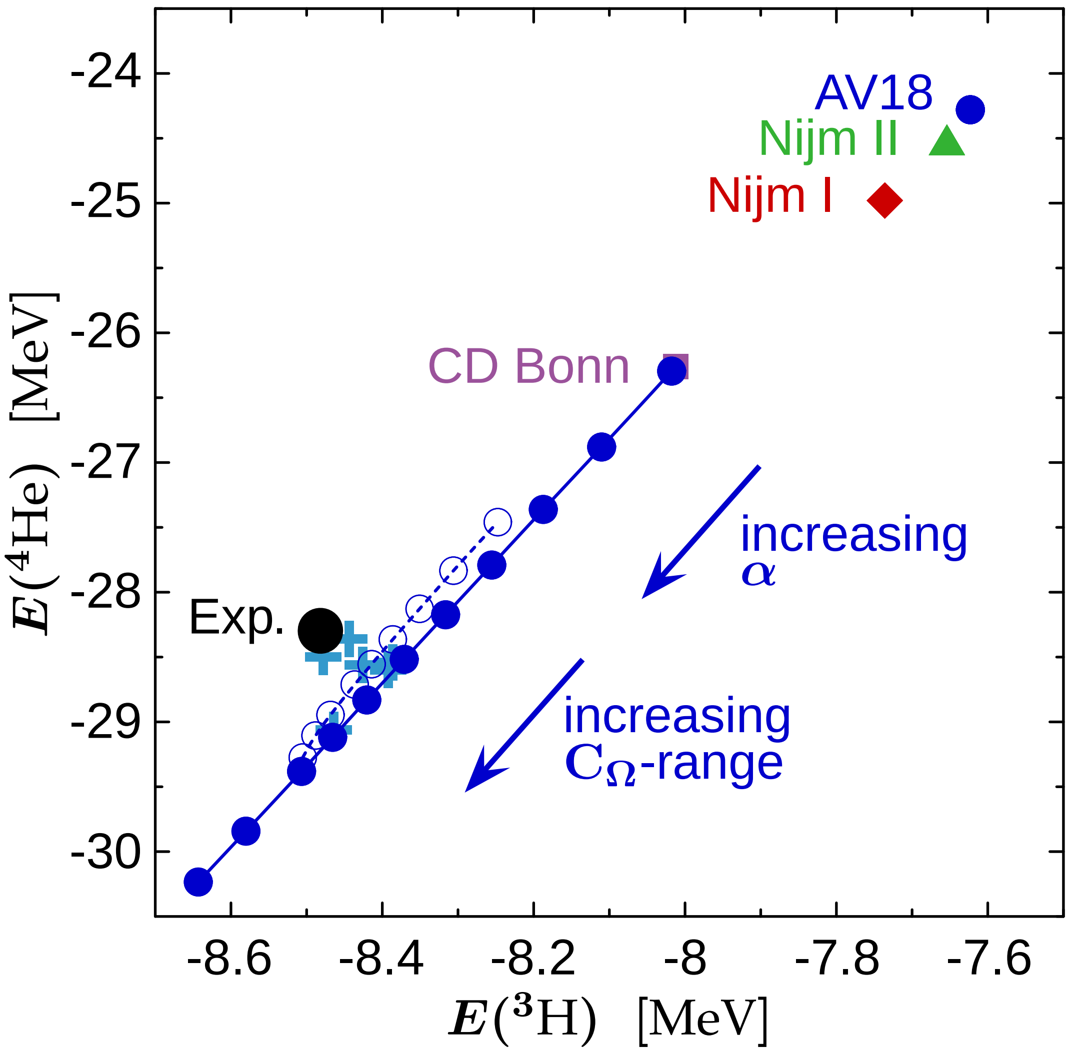
Three-Body Interactions — Tjon Line



- **Tjon-line**: $E(^4\text{He})$ 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 three-body force by choosing correlator with energies close to experimental value

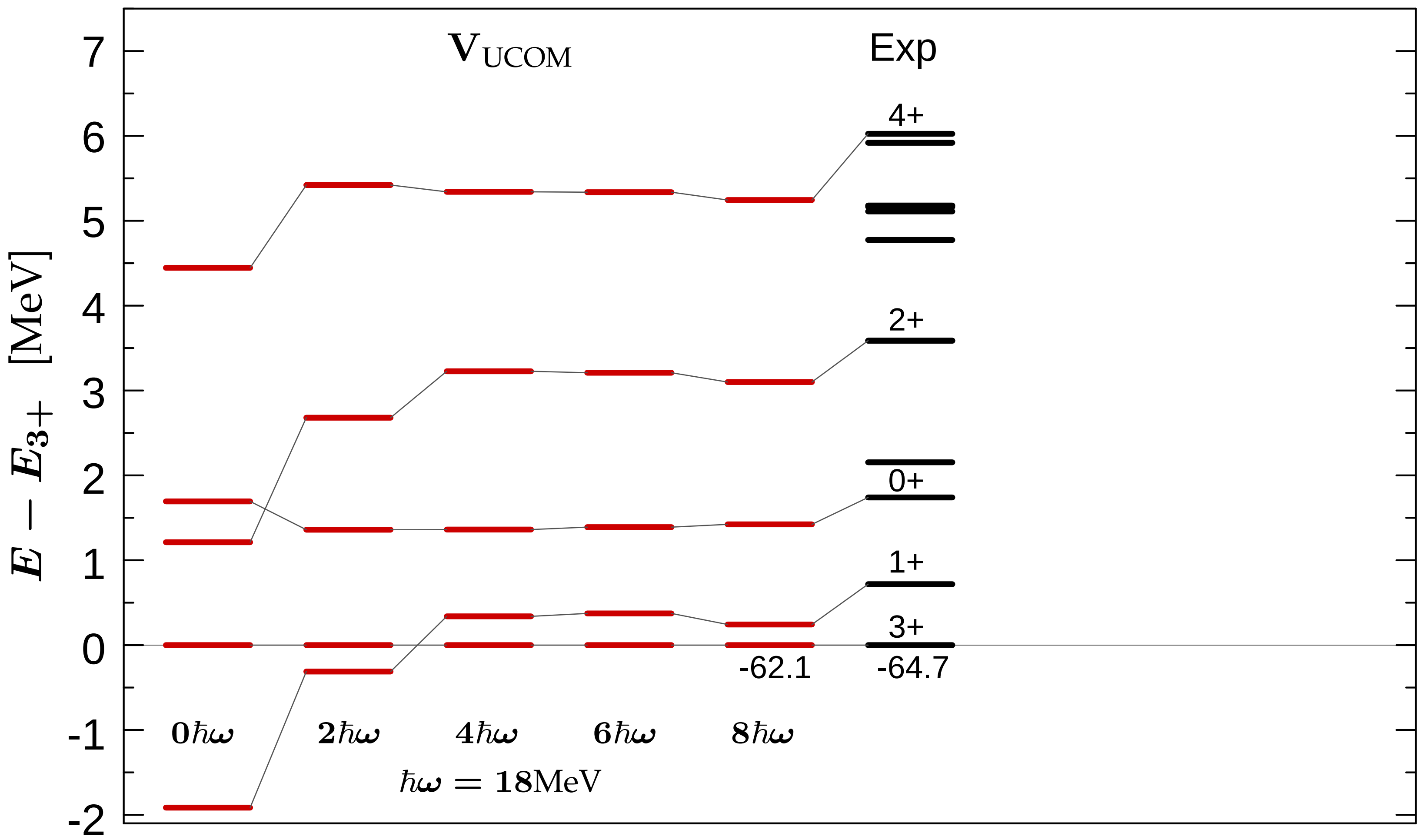
Three-Body Interactions — Tjon Line



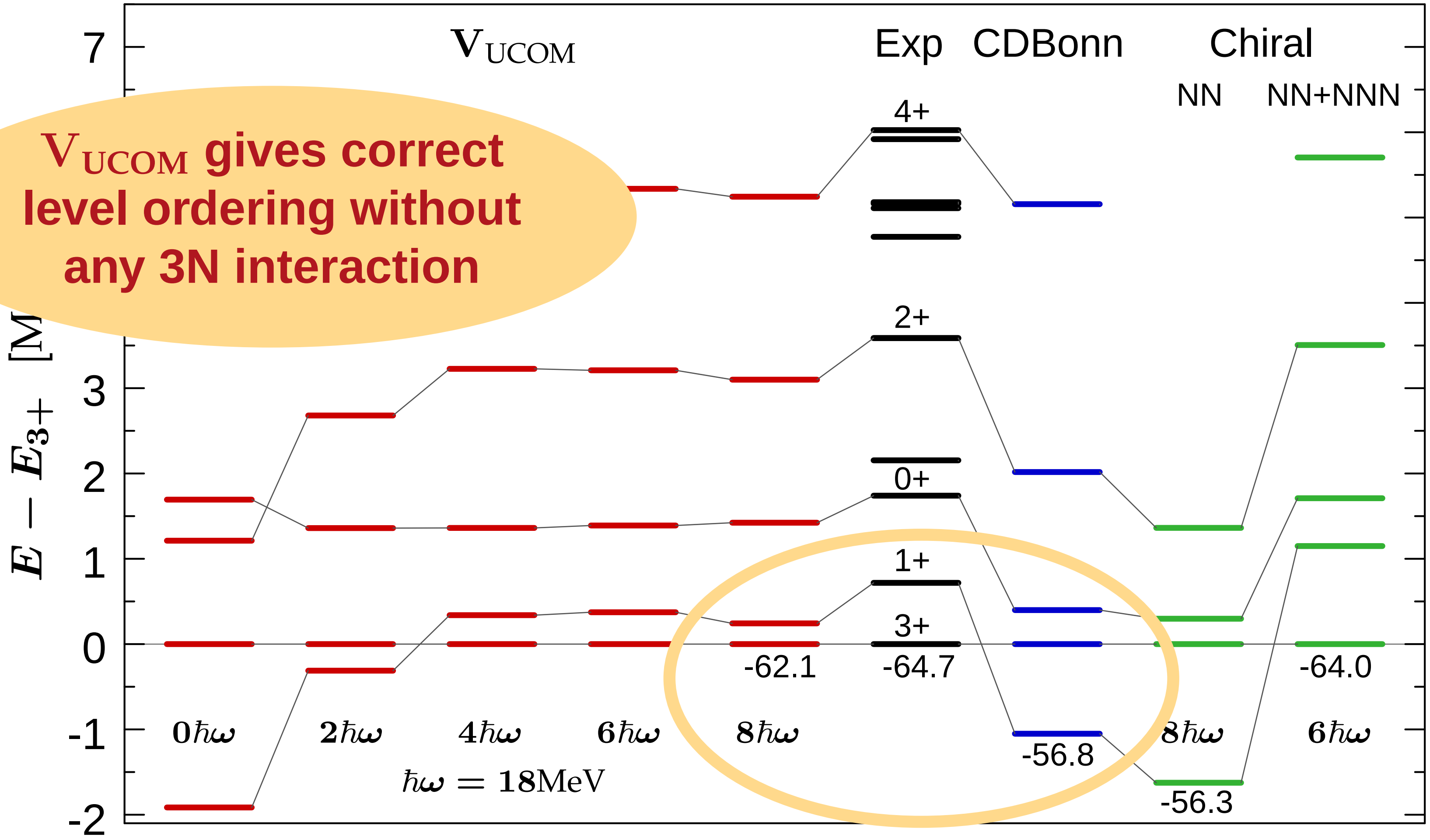
- **Tjon-line**: $E(^4\mathrm{He})$ vs. $E(^3\mathrm{H})$ for phase-shift equivalent NN-interactions
- same behavior for the SRG interaction as function of α

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

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



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



V_{UCOM} gives correct level ordering without any 3N interaction

Ab Initio Approaches

Importance Truncated No-Core Shell Model

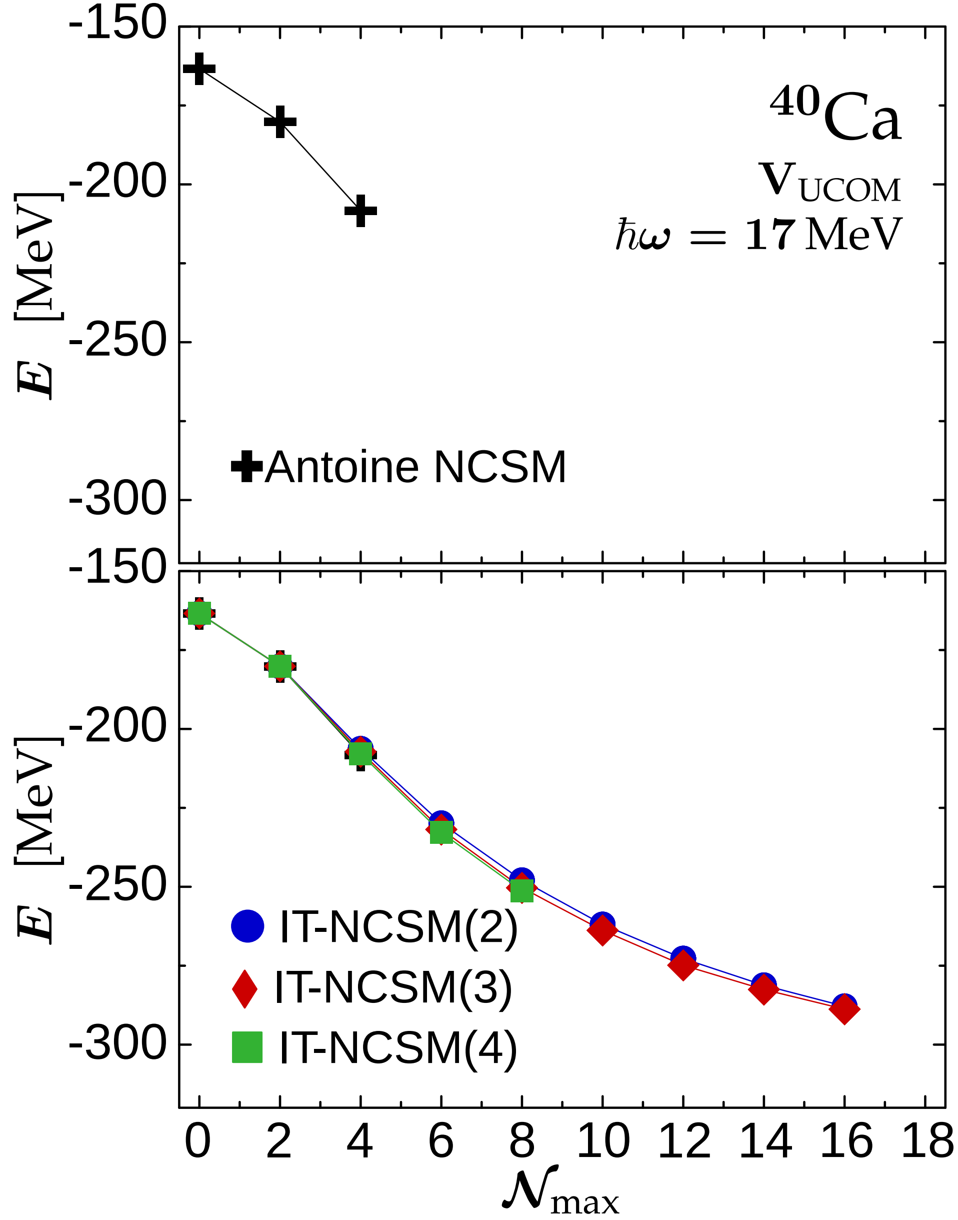
Roth & Navrátil — Phys. Rev. Lett. 99, 092501 (2007)
Roth — in preparation

Importance Truncated NCSM

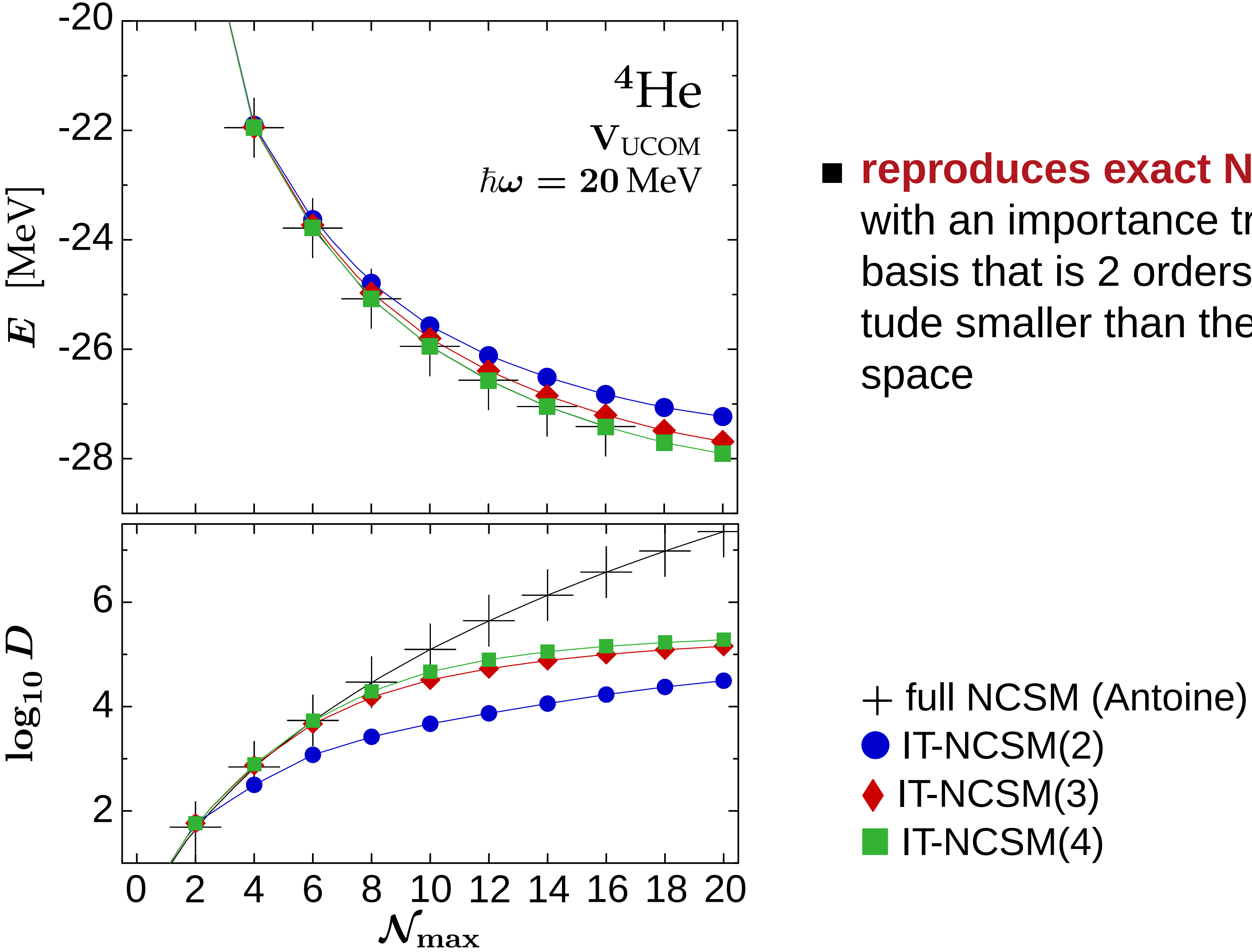
- converged NCSM calculations essentially restricted to p-shell
- full $6\hbar\omega$ calculation for ^{40}Ca presently not feasible (basis dimension $\sim 10^{10}$)

Importance Truncation

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

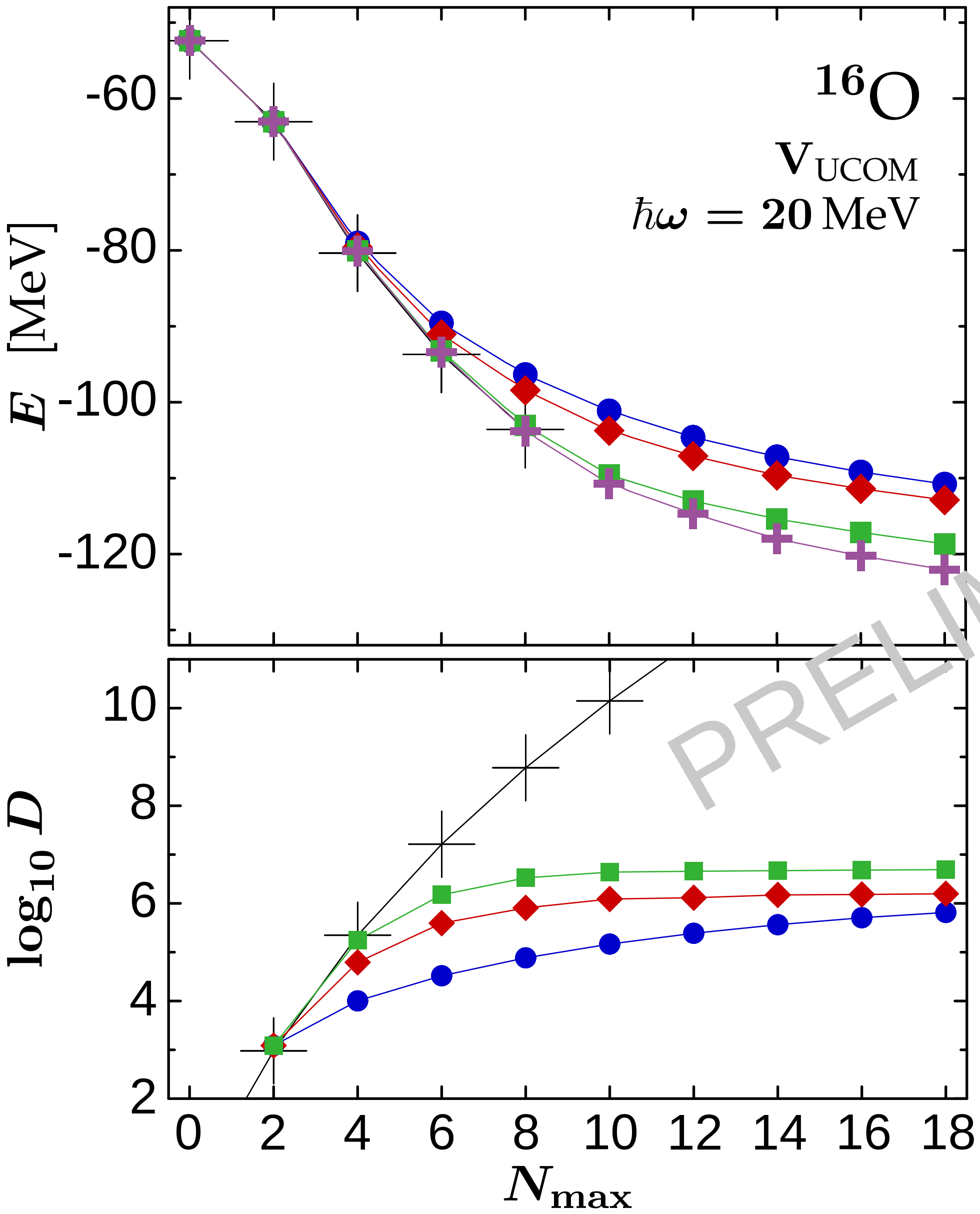


^{4}He: Importance Truncated NCSM



- **reproduces exact NCSM result** with an importance truncated basis that is 2 orders of magnitude smaller than the full $\mathcal{N}_{\max}\hbar\omega$ space

^{16}O: Importance Truncated NCSM



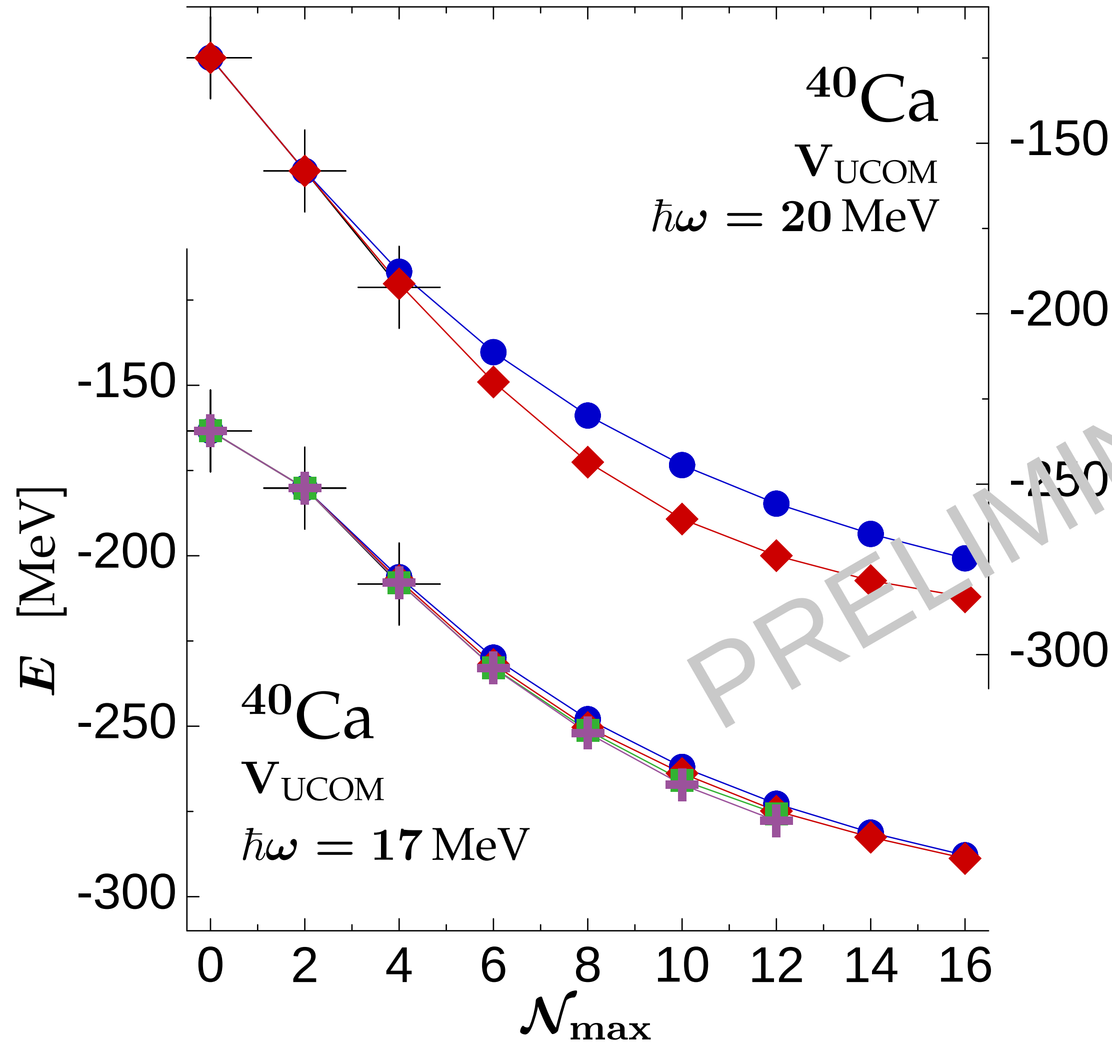
- **excellent agreement with full NCSM** calculation although dimension reduced by several orders of magnitude

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

$$E_{\text{IT-NCSM(4)D}} = -127.9 \pm 2\,\text{MeV}$$
$$E_{\text{exp}} = -127.6\,\text{MeV}$$

+ full NCSM (Antoine)
● IT-NCSM(2)
♦ IT-NCSM(3)
■ IT-NCSM(4)
✚ IT-NCSM(4) + Davidson

^{40}Ca: Importance Truncated NCSM

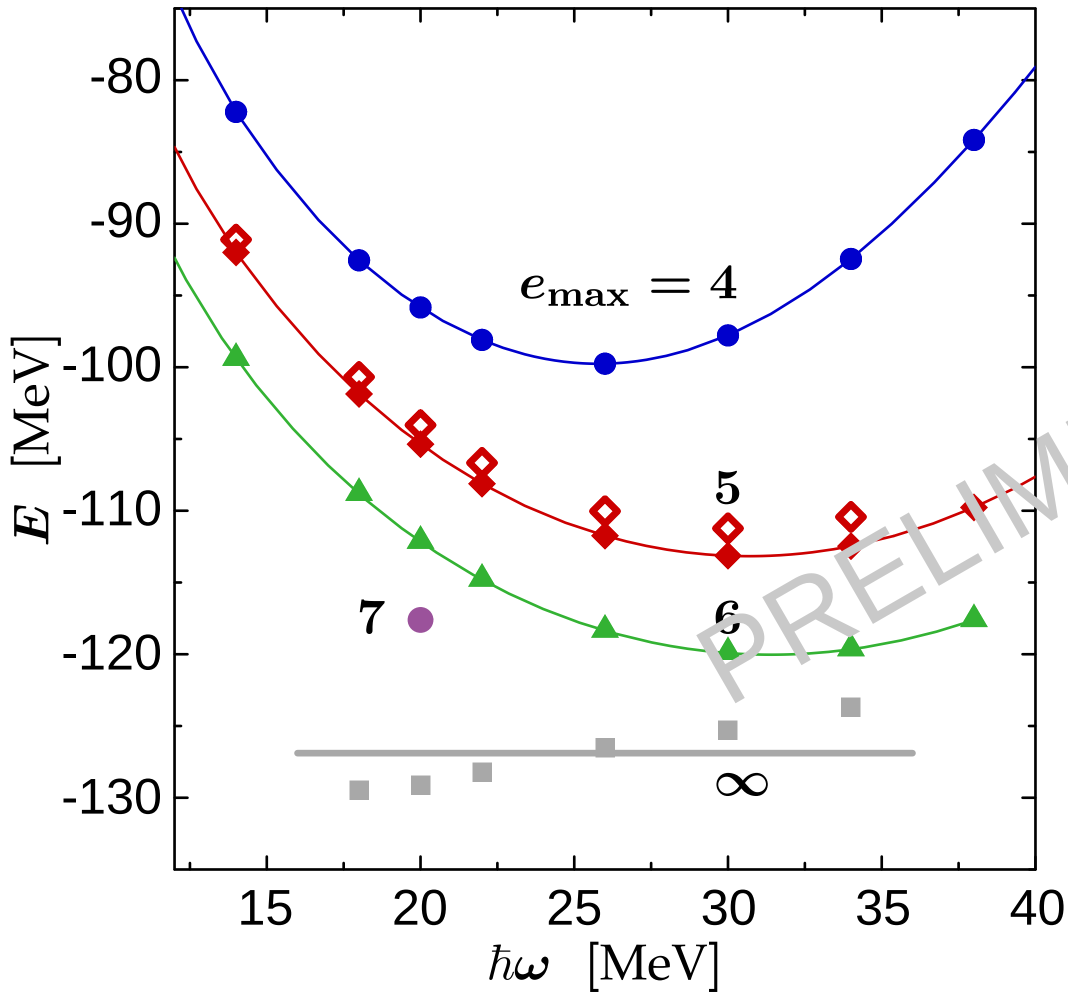


- **$16\hbar\omega$ and more are feasible** for ^{40}Ca in IT-NCSM(4)D
- size of individual npnh-contributions depends on oscillator frequency
- result consistent with experimental binding energy

+ full NCSM (Antoine)
● IT-NCSM(2)
◆ IT-NCSM(3)
■ IT-NCSM(4)
✚ IT-NCSM(4) + Davidson

^{16}O: Coupled Cluster Method

CR-CC(2,3)



calculations by J. Gour & P. Piecuch

- coupled-cluster calculation for ^{16}O with $\mathbf{V}_{\text{UCOM}}$
- including non-perturbative triples correction (completely renormalized CC)
- extrapolated ground-state energies

$$E_{\text{CR-CC(2,3)}} = -126.9 \pm 5\,\text{MeV}$$
$$E_{\text{IT-NCSM(4)D}} = -127.9 \pm 2\,\text{MeV}$$
$$E_{\text{exp}} = -127.6\,\text{MeV}$$

Perspectives

- **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, Coupled Cluster,...
  - Hartree-Fock plus MBPT, Padé Resummed MBPT, RPA,...
  - Fermionic Molecular Dynamics,...

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

Epilogue

- **thanks to my group & my collaborators**
  - S. Binder, P. Hedfeld, H. Hergert, M. Hild, P. Papakonstantinou, A. Popa, S. Reinhardt, F. Schmitt, I. Türschmann, A. Zapp

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  - P. Navrátil

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

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

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