Nuclear Structure in the UCOM Framework: UCOM-Hartree-Fock

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Overview

- UCOM Basics
  - Central and Tensor Correlations
  - Momentum Space Matrix Elements
  - Tjon-Line
- UCOM-Hartree-Fock
- Summary and Outlook

Central and Tensor Correlators

Central Correlator C_r

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

$$\mathrm{C}_r = \exp(-i \sum_{i,j}^{A} \mathrm{g}_{r,ij})$$

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

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

Tensor Correlator C_Ω

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

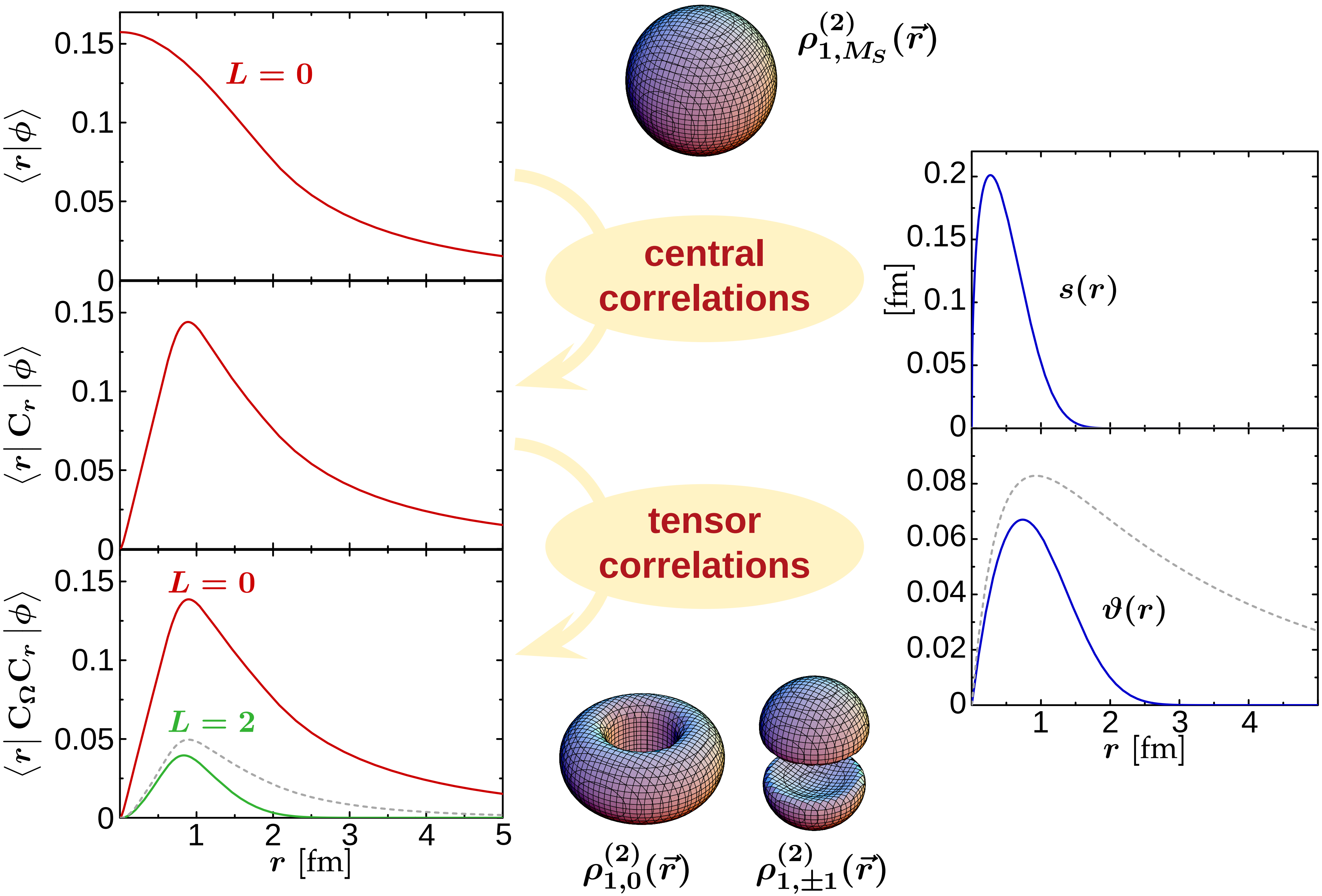
$$\mathrm{C}_\Omega = \exp(-i \sum_{i,j}^{A} \mathrm{g}_{\Omega,ij})$$

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

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

$s(r)$ and $\vartheta(r)$
encapsulate the physics of
short-range correlations.

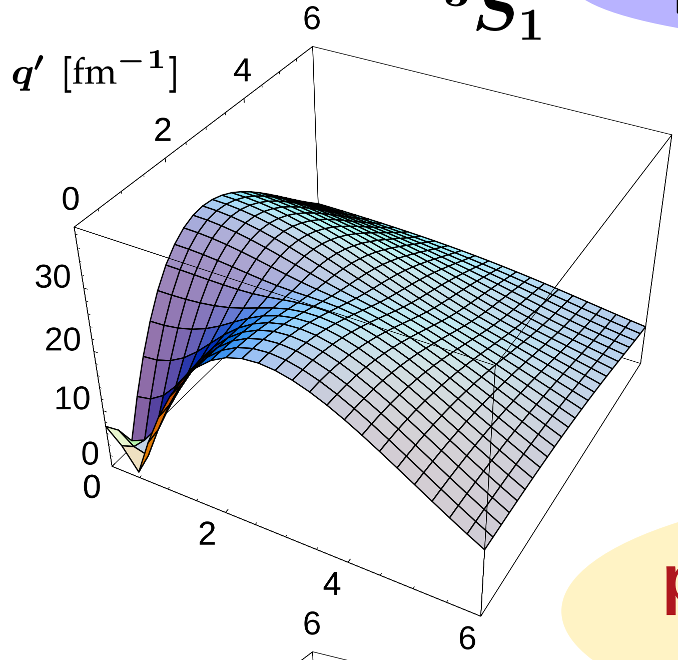
Correlated States



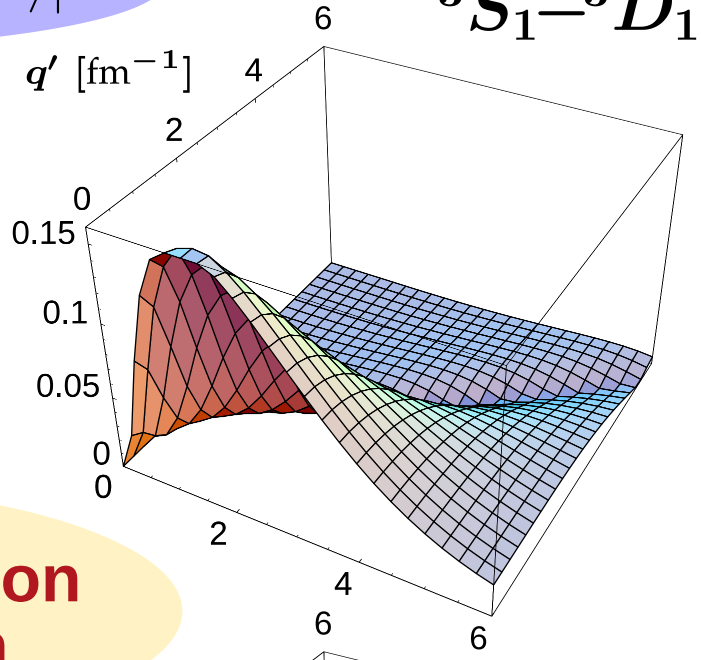
Momentum-Space Matrix Elements

$$\left|\langle q(LS)J \right| \mathrm{V} \left| q'(L'S)J \rangle\right|$$

$^3S_1$



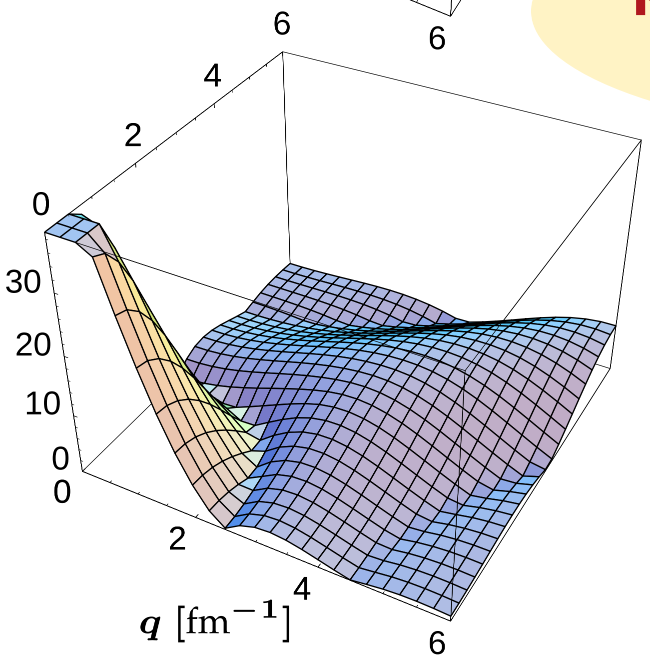
$^3S_1$—$^3D_1$

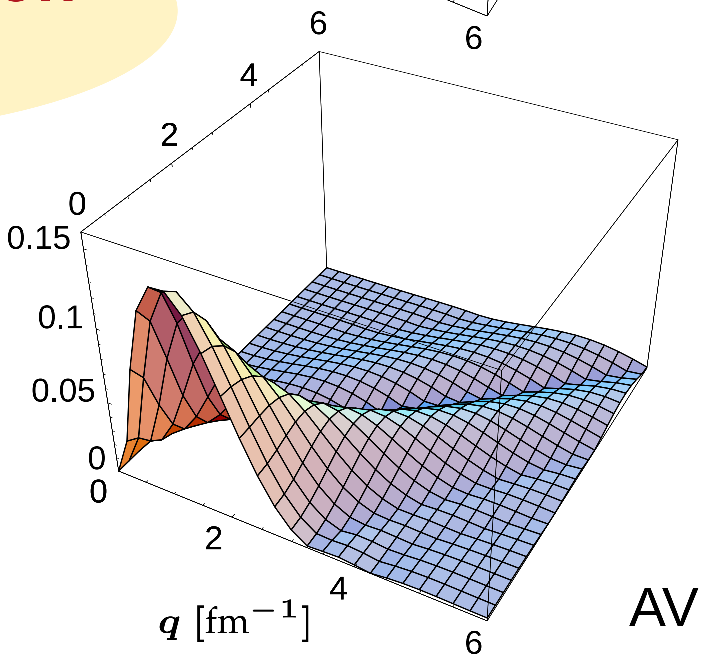


$\mathrm{V}_{\mathrm{bare}}$

pre-diagonalization of Hamiltonian

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

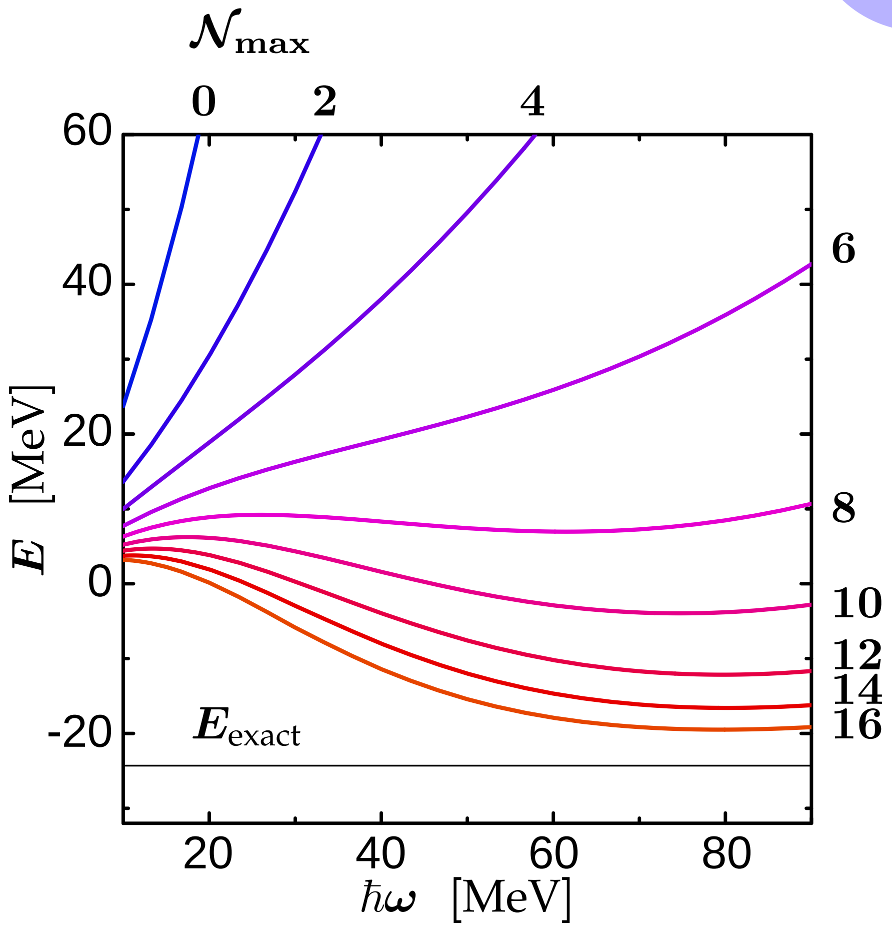


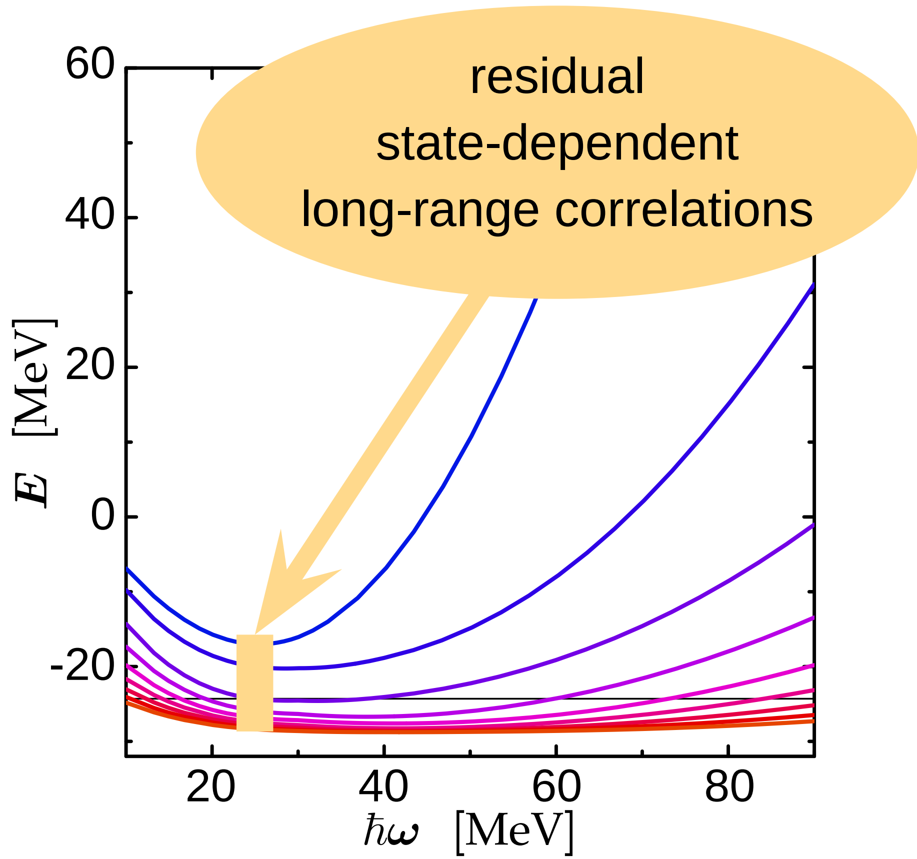


AV18

Short- and Long-Range Correlations

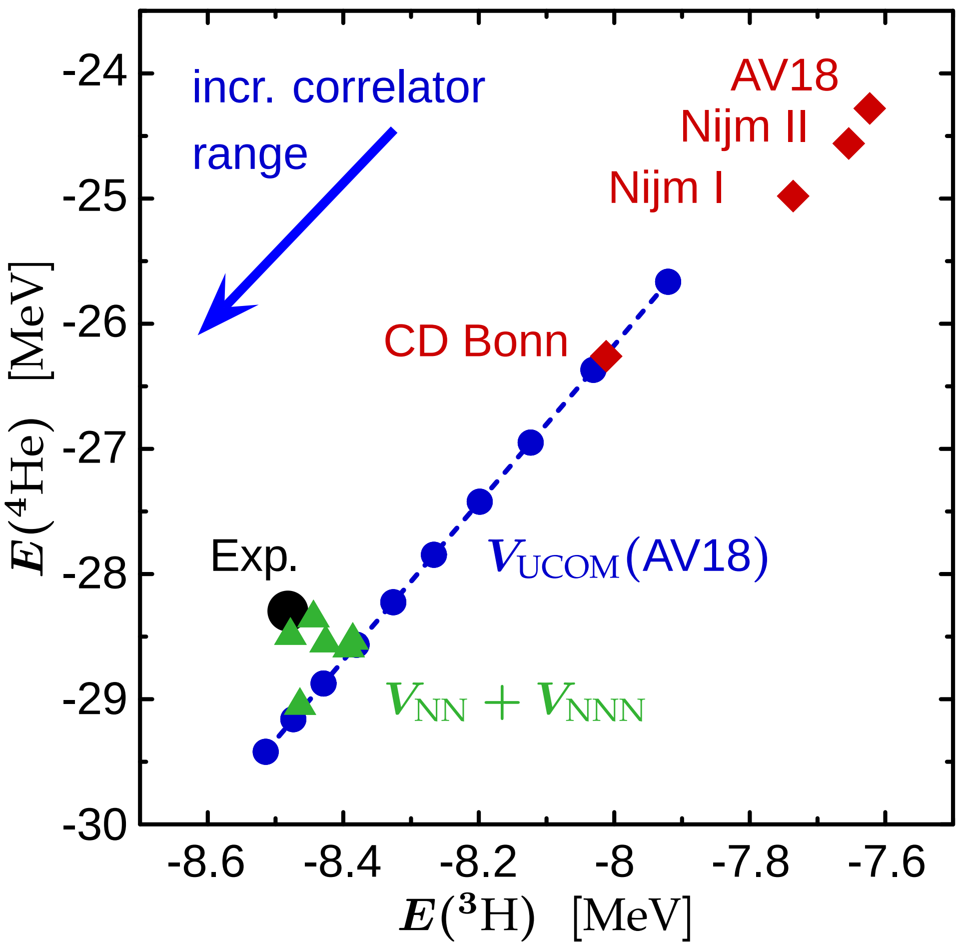
V_{bare} | ^4He | V_{UCOM}





NCSM code by P. Navrátil [PRC 61, 044001 (2000)]

Tjon-Line and Correlator Range



- **Tjon-line**: $E(^4\mathrm{He})$ vs. $E(^3\mathrm{H})$ for phase-shift equivalent NN-interactions
- change in correlator range results in shift along Tjon-line
- choose correlator with energies close to experimental value, i.e. **minimize three-body force**

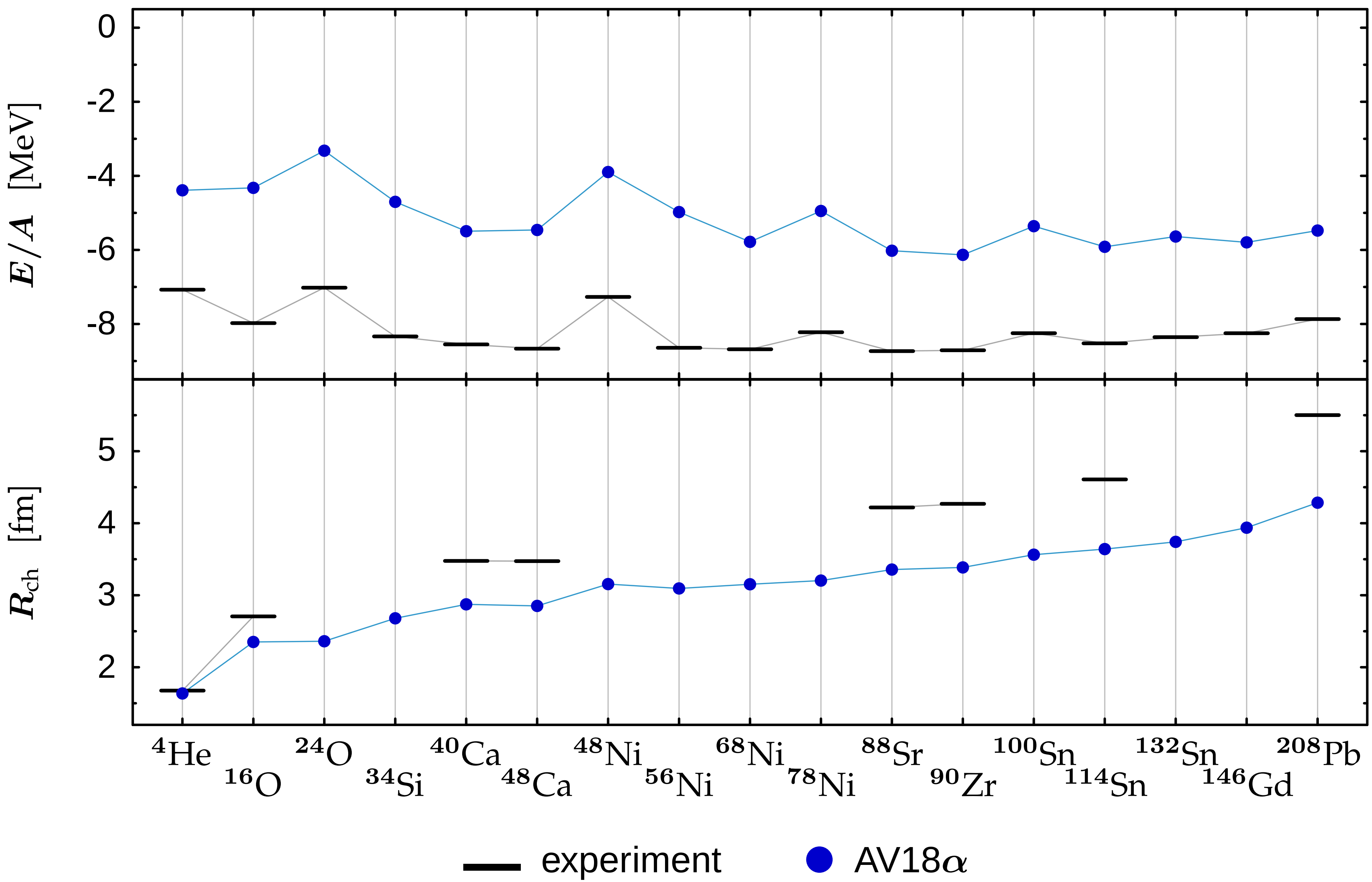
Data points: A. Nogga et al., Phys. Rev. Lett. **85**, 944 (2000)

UCOM-Hartree-Fock

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

- single-particle states are expanded in a spherical harmonic oscillator basis
- HF is formulated with the intrinsic kinetic energy $\mathbf{T}_{\text{int}} = \mathbf{T} - \mathbf{T}_{\text{cm}}$ to eliminate centner of mass contributions
- Coulomb interaction is included exactly

Correlated Argonne V18



Missing Pieces

long-range correlations

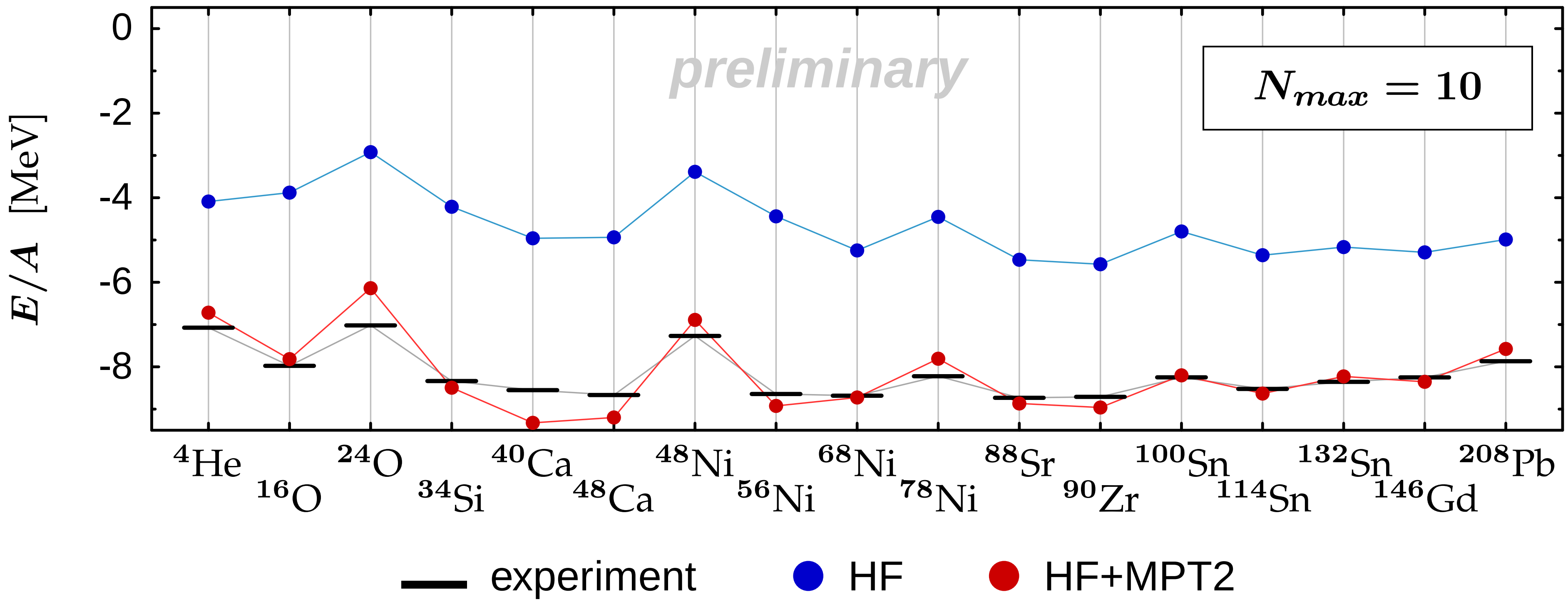
Ab Initio Strategy

- improve many-body states to include long-range correlations
- many-body perturbation theory (MPT), Coupled-Cluster (CC),...

Long-Range Correlations

- **many-body perturbation theory**: second-order energy shift gives estimate for influence of long-range correlations

$$\Delta E^{(2)} = -\frac{1}{4} \sum_{i,j}^{\text{occu.}} \sum_{a,b}^{\text{unoccu.}} \frac{\left|\langle \phi_a \phi_b \right| \mathrm{V}_{\mathrm{UCOM}} \left| \phi_i \phi_j \rangle\right|^2}{\epsilon_a + \epsilon_b - \epsilon_i - \epsilon_j}$$



Missing Pieces

- long-range correlations
- genuine three-body forces
- three-body cluster contributions

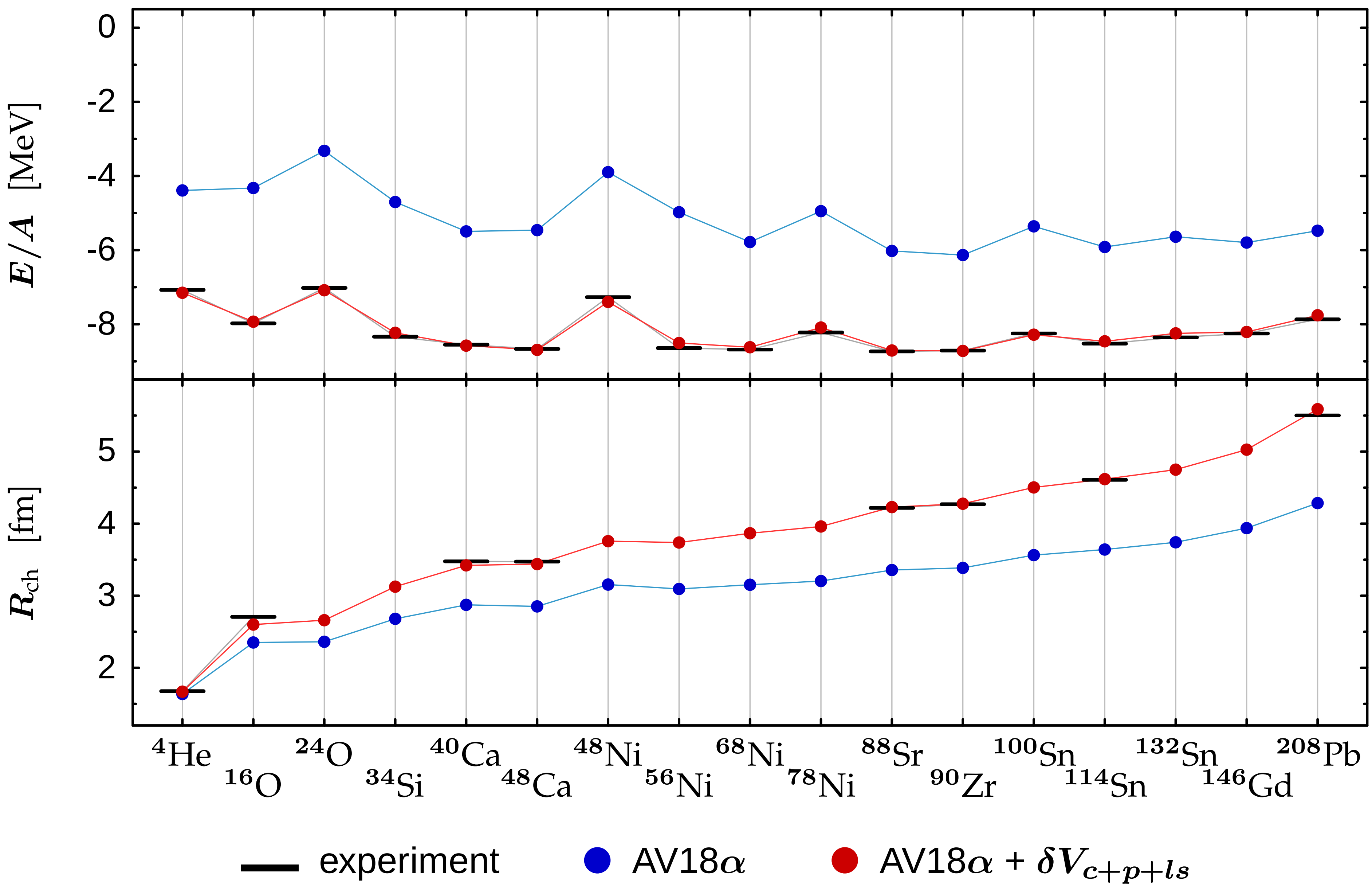
Pragmatic Approach

- phenomenological two-body correction

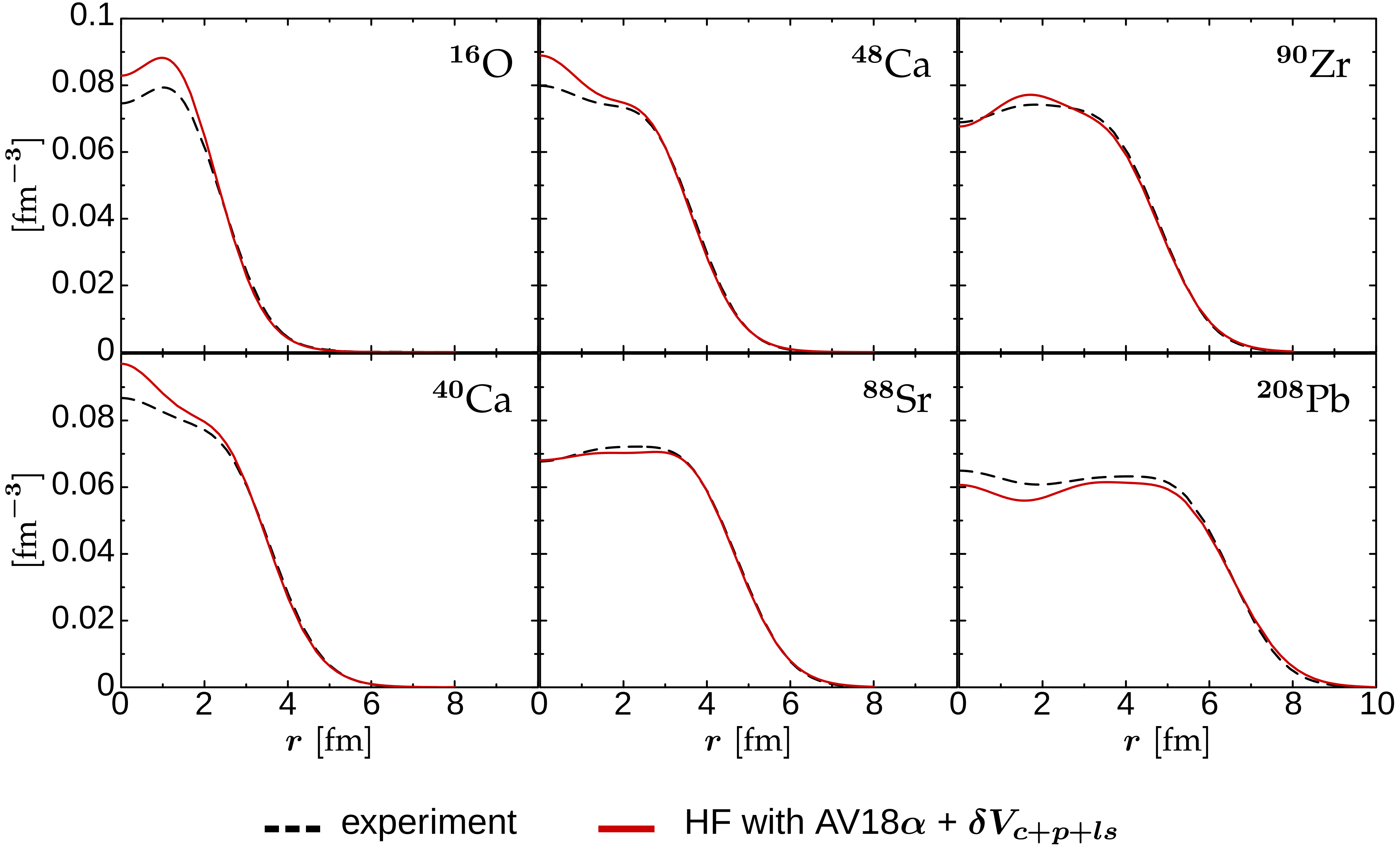
$$\delta \mathrm{V}_{c+p+ls} = v_1(\mathrm{r}) + \vec{\mathrm{q}}\, v_{qq}(\mathrm{r})\, \vec{\mathrm{q}} + v_{LS}(\mathrm{r})\, \vec{\mathrm{L}} \cdot \vec{\mathrm{S}}$$

- $v_i(\mathrm{r})$: Gaussian radial dependencies with fixed ranges
- 3 strengths used as parameters to fit E/A of $^{16}\mathrm{O}$, $^{24}\mathrm{O}$, $^{40}\mathrm{Ca}$, $^{48}\mathrm{Ca}$, $^{48}\mathrm{Ni}$, and $^{90}\mathrm{Zr}$

Correlated Argonne V18 + Correction



Charge Distributions



Summary

- UCOM enables the use of **realistic NN-interactions** in computationally affordable Hilbert spaces and calculation schemes.
- UCOM-Hartree-Fock calculations yield finite, converged results.
- Results including perturbation theory or a phenomenological correction are in good agreement with experiment.

Outlook

- Further improvement of the many-body model space: Coupled-Cluster Method, ...
- Pairing effects: Hartree-Fock-Bogoliubov theory
- UCOM-RPA ($\longrightarrow$ N. Paar, HK 27.4)
- Reduction (or replacement) of the phenomenological correction by implementation of three-body forces

References

- H. Feldmeier, T. Neff, R. Roth, and J. Schnack, Nucl. Phys. **A632**, 61 (1998)
- T. Neff, and H. Feldmeier, Nucl. Phys. **A713**, 311 (2003)
- R. Roth, T. Neff, H. Hergert, and H. Feldmeier, Nucl. Phys. **A745**, 3 (2004)
- http://crunch.ikp.physik.tu-darmstadt.de/tnp/

UCOM / Lee-Suzuki / $V_{\mathrm{low}k}$

Lee-Suzuki

- decoupling of P and Q space by similarity transformation
- same representation as used in many-body method
- (state dependent)

$V_{\mathrm{low}k}$

- decimation to low-momentum P space; Q space discarded
- uses momentum representation
- state independent
- phase-shift equivalent

UCOM

- pre-diagonalization with respect to short-range correlations
- no specific model-space or representation
- state independent
- phase-shift equivalent

Momentum-Space Matrix Elements