Correlated Realistic NN-Interactions

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Our Aim

nuclear structure calculations across the whole nuclear chart based on realistic NN-potentials

stay as close as possible to an **ab initio** treatment

bound to **simple Hilbert spaces** for large particle numbers

need to deal with **strong interaction-induced correlations**

Overview

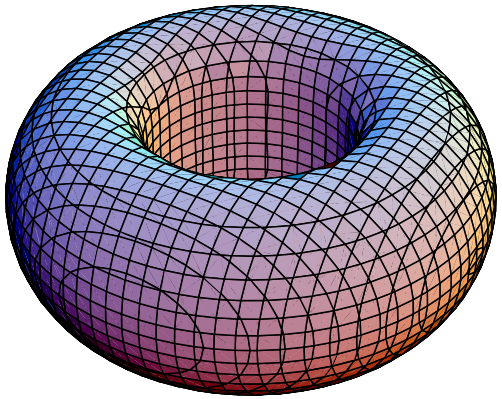
- Correlations in Nuclei
- Unitary Correlation Operator Method (UCOM)
- UCOM + No-Core Shell Model
- UCOM + Hartree-Fock

Correlations in Nuclei

Deuteron: Manifestation of Correlations

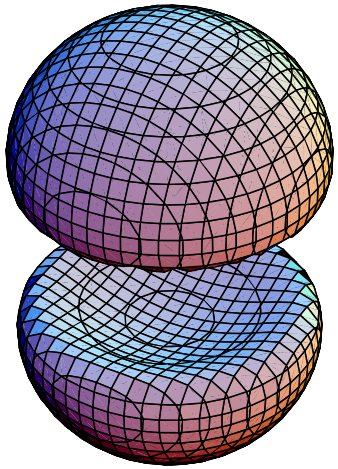
$M_S = 0$

$\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$



$M_S = \pm 1$

$|\uparrow\uparrow\rangle, |\downarrow\downarrow\rangle$



spin-projected two-body density $\rho^{(2)}_{1,M_S}(\vec{r})$ of the deuteron for AV18 potential

two-body density fully suppressed at small particle distances $|\vec{r}|$

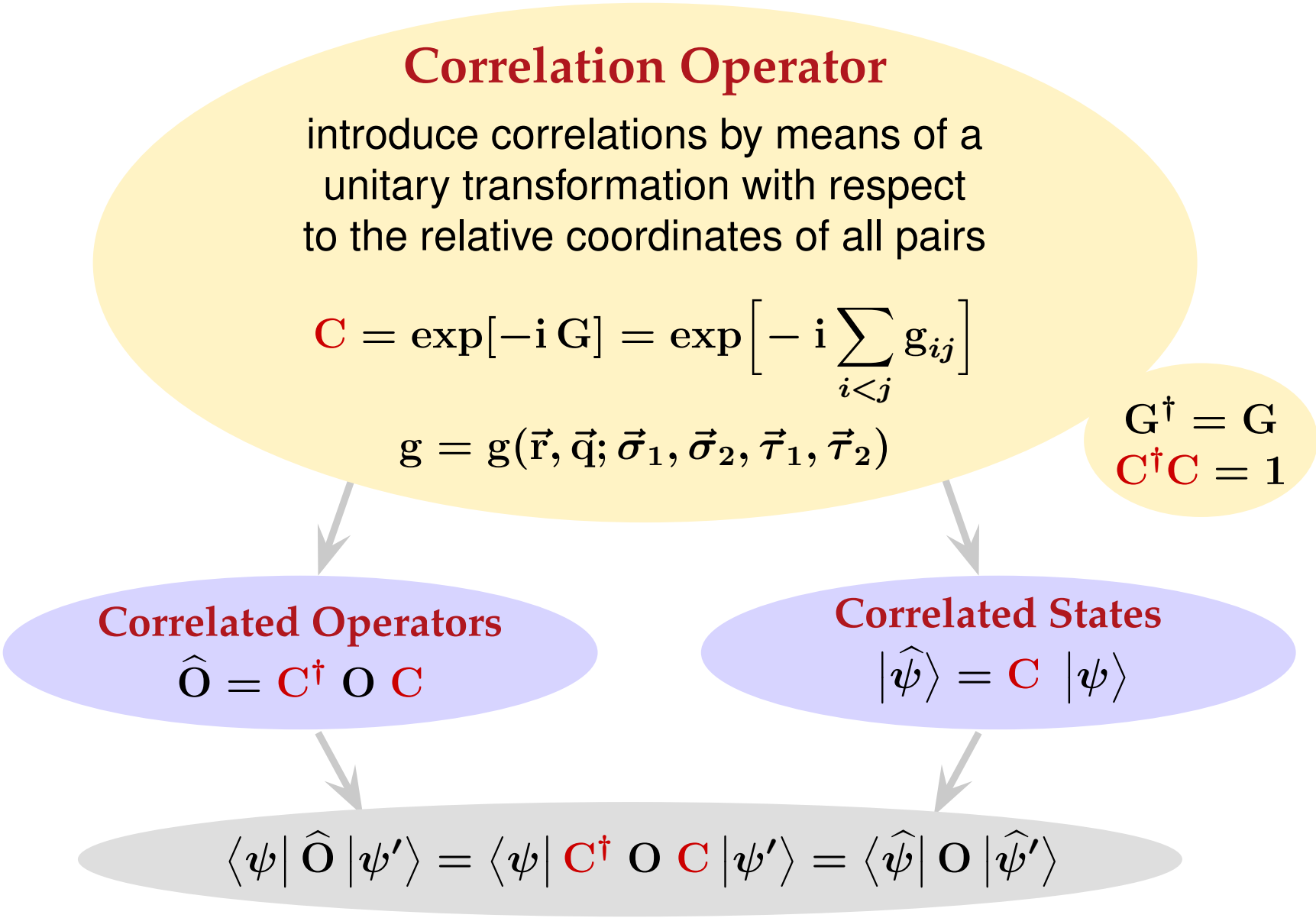
central correlations

angular distribution depends strongly on relative spin orientation

tensor correlations

Unitary Correlation Operator Method (UCOM)

Unitary Correlation Operator Method



Central and Tensor Correlators

$$\mathrm{C} = \mathrm{C}_\Omega \mathrm{C}_r$$

Central Correlator C_r

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

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

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

Tensor Correlator C_Ω

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

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

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

$s(r)$ and $\vartheta(r)$ describe the distance dependence of the transformations

Correlated Operators

Cluster Expansion

$$\hat{O} = C^\dagger O C = \hat{O}^{[1]} + \hat{O}^{[2]} + \hat{O}^{[3]} + \cdots$$

Cluster Decomposition Principle

if the correlation range is small compared to the mean particle distance, then higher orders are negligible

restrict range of the correlators in order to minimise higher order contributions

Two-Body Approx.

$$\hat{O}^{C2} = \hat{O}^{[1]} + \hat{O}^{[2]}$$

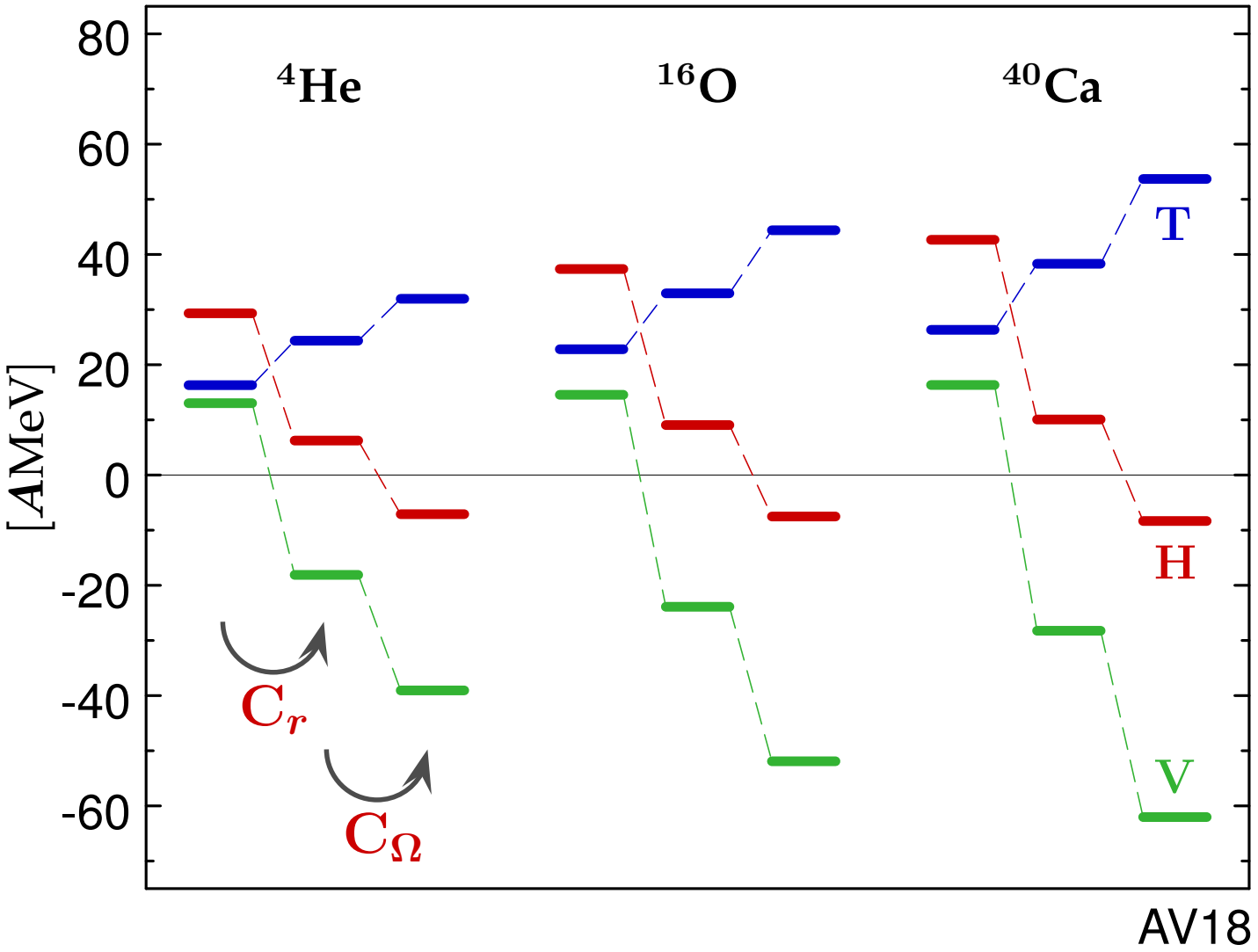
operators for all observables can be and have to be correlated consistently

Correlated NN-Potential — V_{UCOM}

$$\hat{\mathbf{H}}^{C2} = \hat{\mathbf{T}}^{[1]} + \hat{\mathbf{T}}^{[2]} + \hat{\mathbf{V}}^{[2]} = \mathbf{T} + \mathbf{V}_{\mathrm{UCOM}}$$

- **closed operator expression** for the correlated interaction $\mathbf{V}_{\mathrm{UCOM}}$ in two-body approximation
- correlated interaction and original NN-potential are **phase shift equivalent** by construction
- **central correlator**: removes the repulsive core and generates additional momentum dependence
- **tensor correlator**: "rotates" part of tensor force into other operator channels (central, spin-orbit,...)
- momentum-space matrix elements of correlated interaction are **similar to** $V_{\mathrm{low}-k}$

Effect of Unitary Transformation



- expectation values for harmonic osc. Slater determinant
- nuclei unbound without inclusion of correlations
- central and tensor correlations essential to obtain bound system

UCOM +
No-Core Shell Model

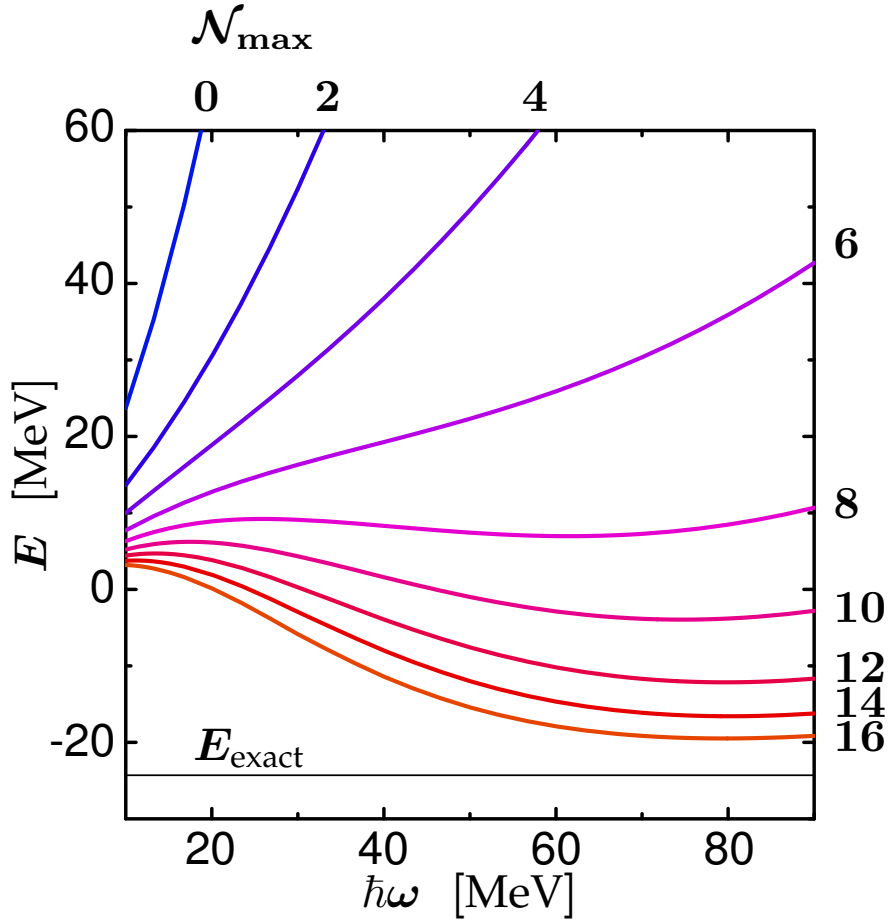
UCOM + NCSM

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

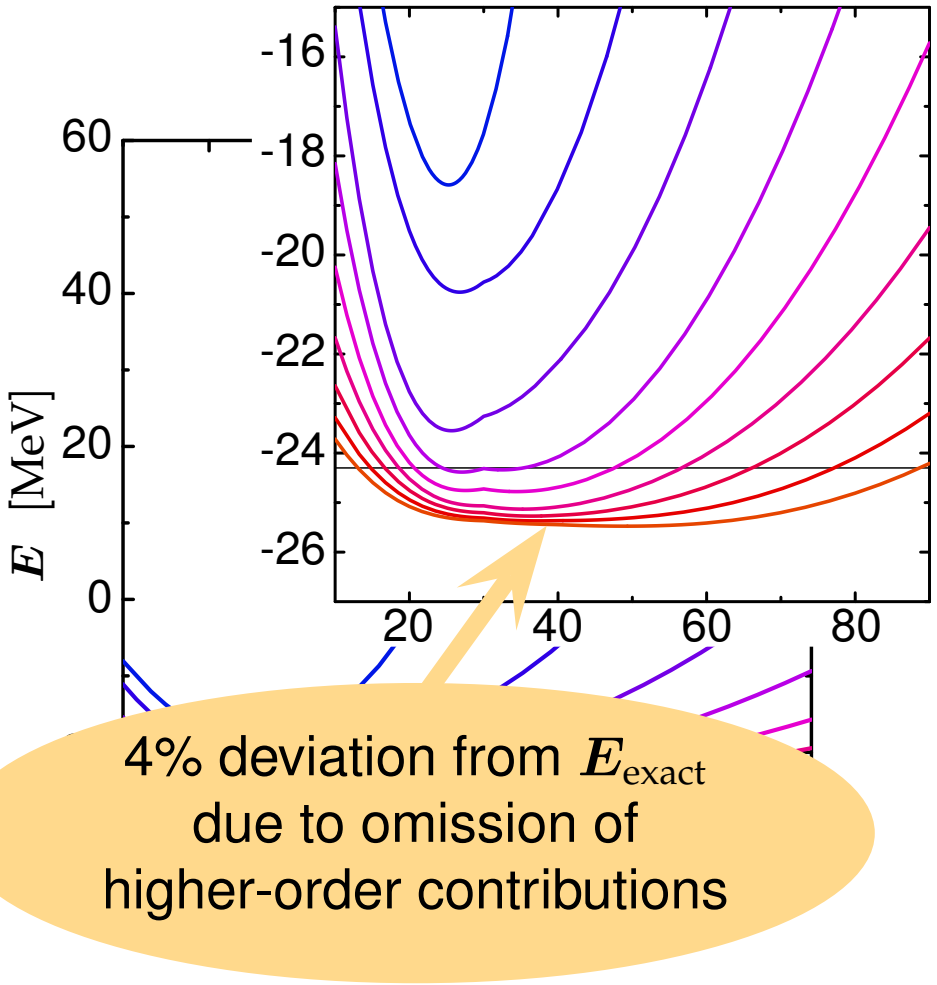
- convergence dramatically improved compared to bare interaction
- direct evaluation of omitted higher-order contributions
- tool to determine optimal correlation functions
- NCSM code by Petr Navratil [PRC 61, 044001 (2000)]

^{4}He: Convergence

V_{bare}



V_{UCOM}



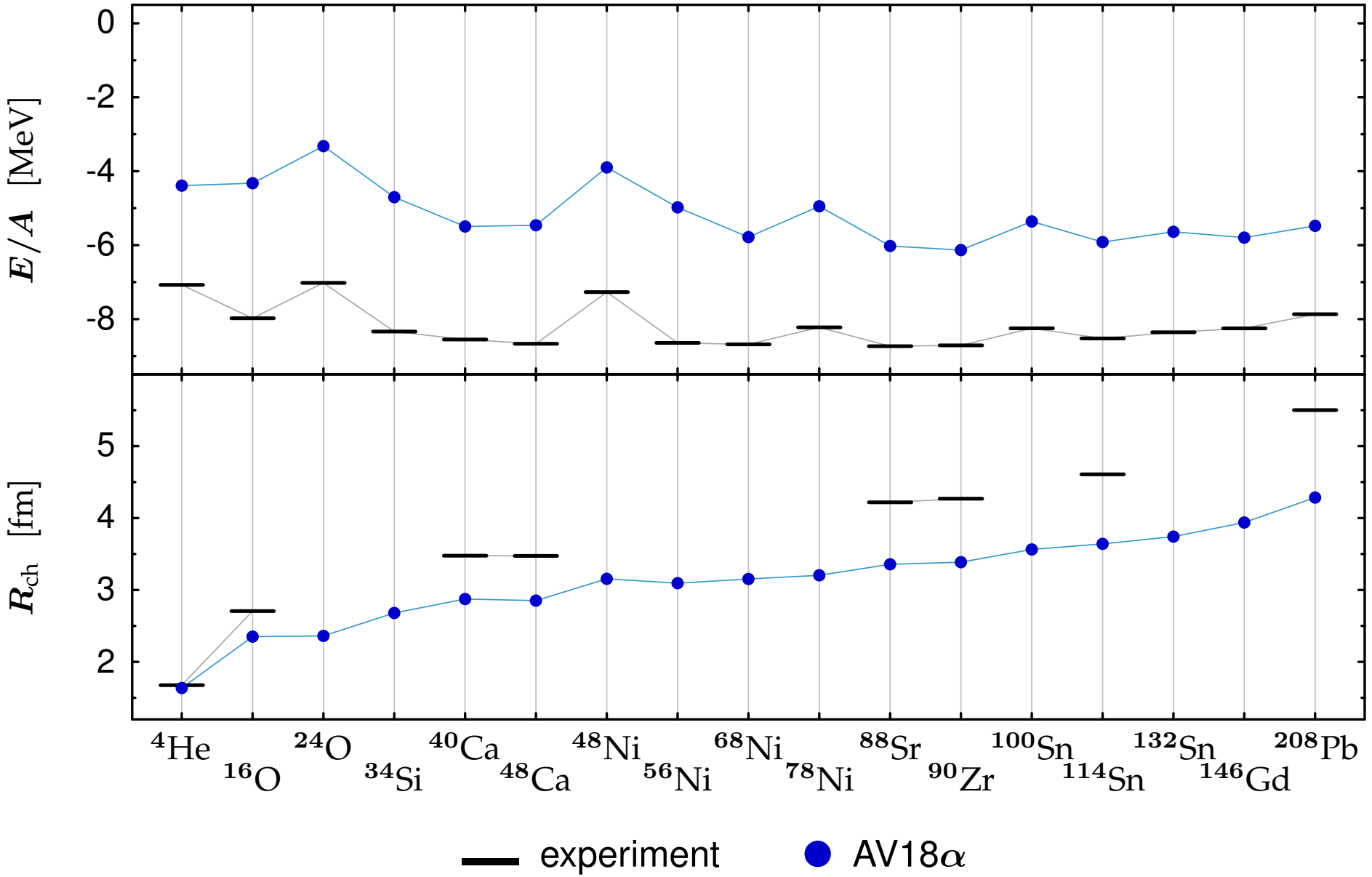
UCOM + Hartree-Fock

UCOM + HF

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

- single-particle states expanded in a spherical oscillator basis
- truncation in n, l, and/or $N = 2n + l$ (typically $N_{max} = 6...12$)
- Coulomb interaction included exactly
- formulated with intrinsic kinetic energy $T_{int} = T - T_{cm}$ to eliminate centre of mass contributions

Correlated Argonne V18



Missing Pieces

long-range correlations

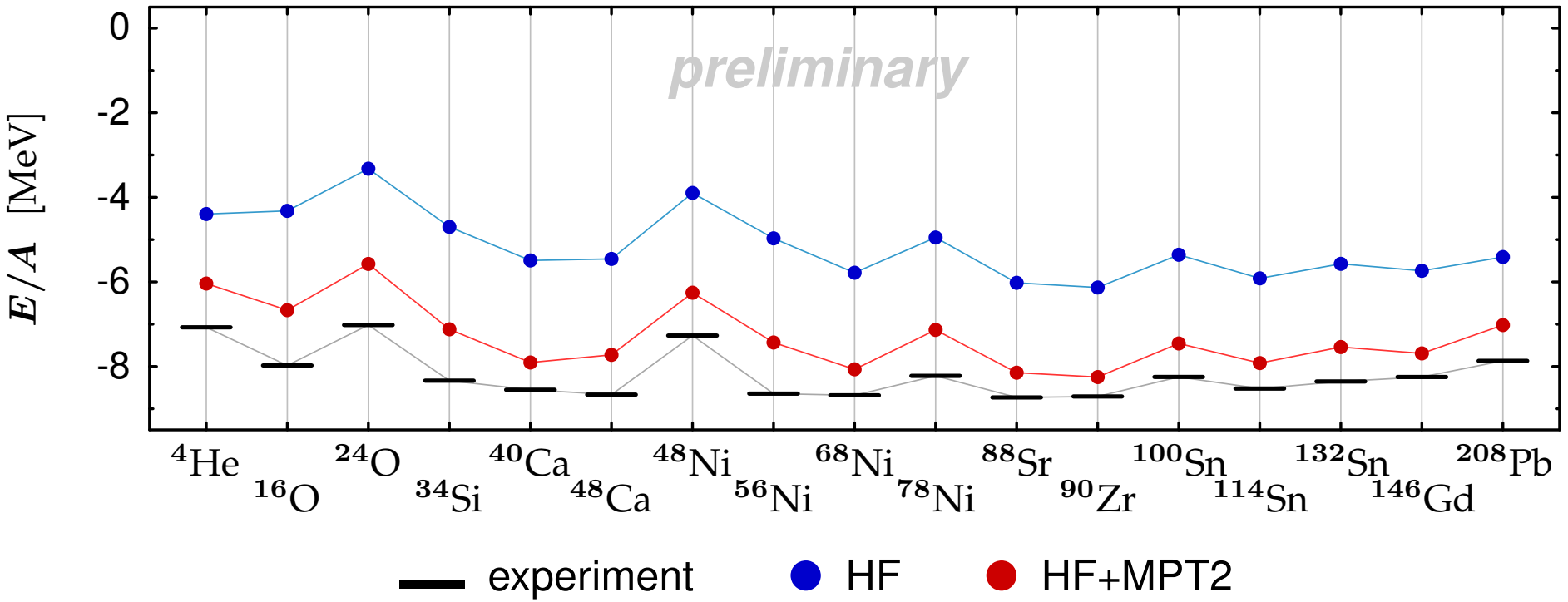
Ab Initio Strategy

- improve many-body states such that long-range correlations are included
- MPT, RPA, CC,...

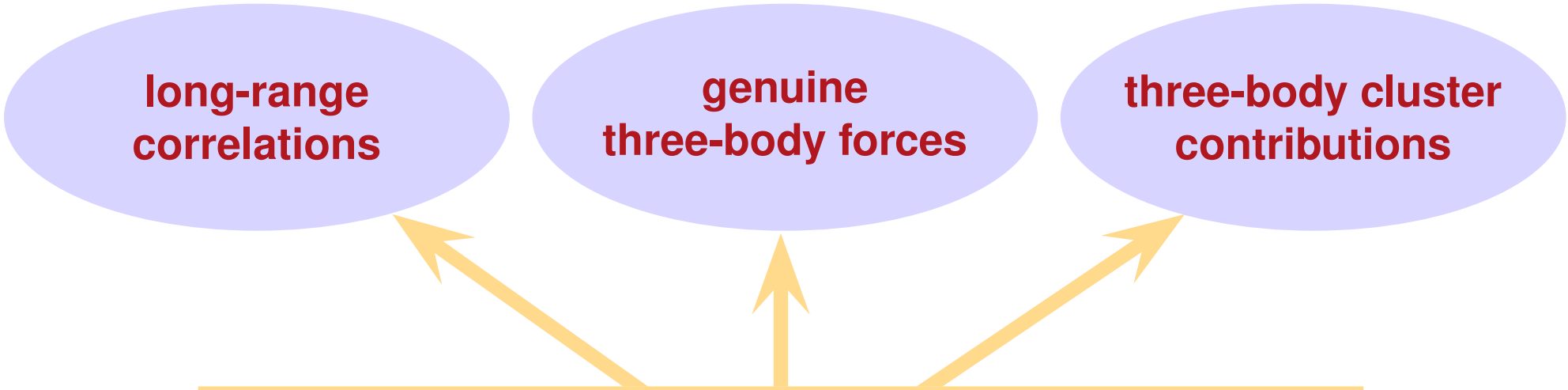
Long-Range Correlations

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

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



Missing Pieces



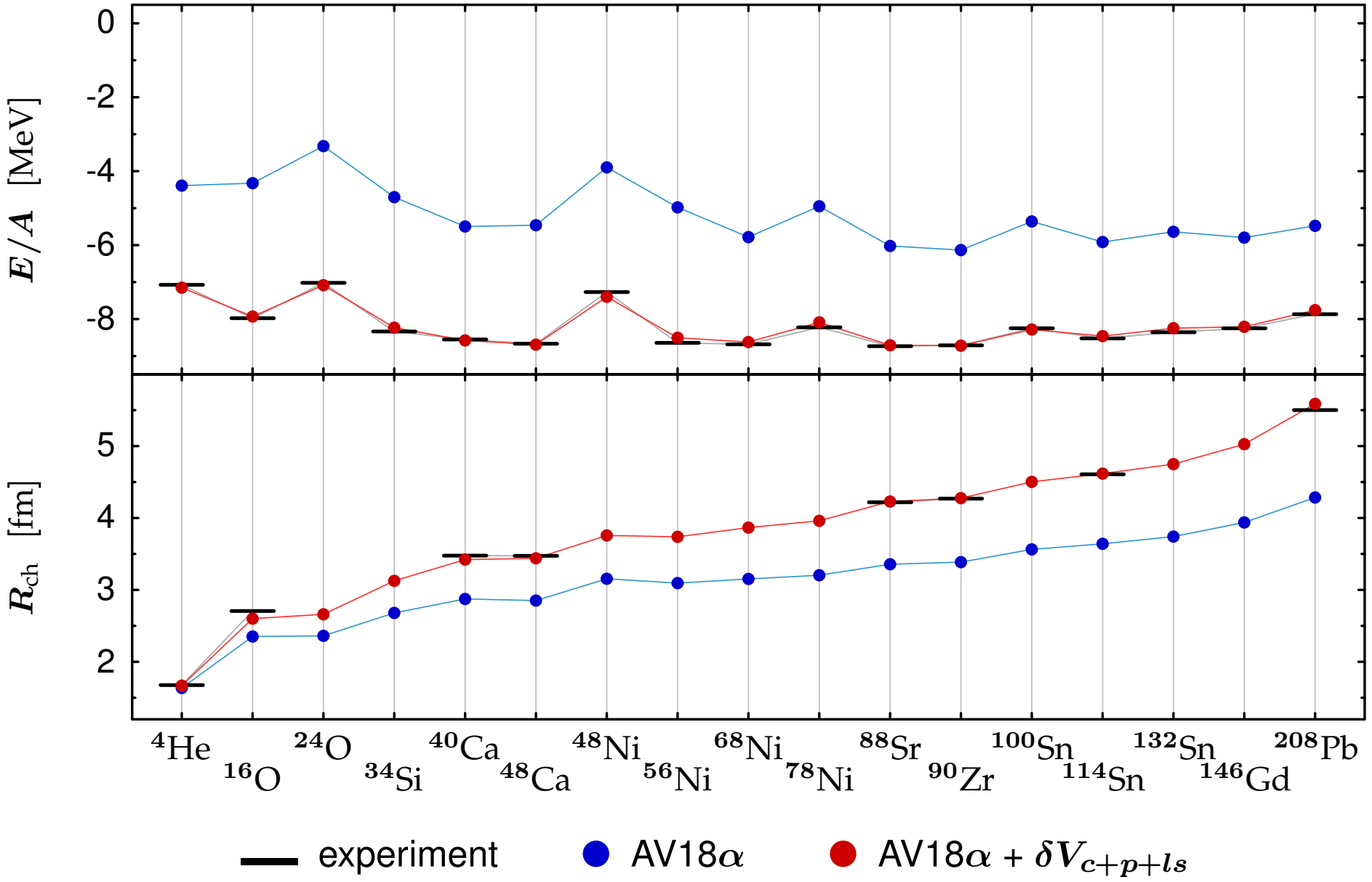
Pragmatic Approach

- phenomenological two-body correction

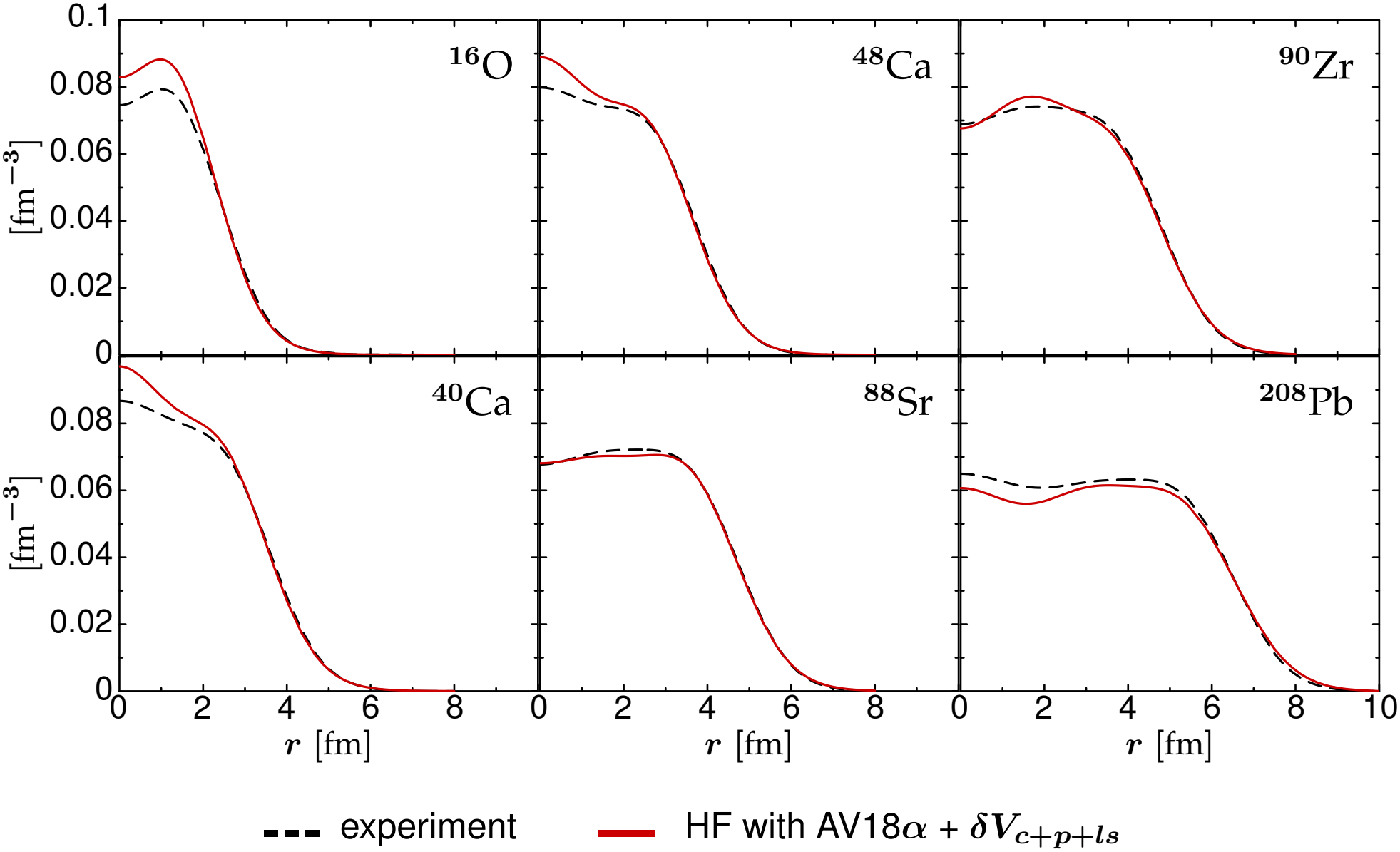
$$\delta \mathrm{V}_{c+p+ls} = v_1(\mathrm{r}) + \vec{\mathrm{q}}\, v_{qq}(\mathrm{r})\, \vec{\mathrm{q}} + v_{LS}(\mathrm{r})\, \vec{\mathrm{L}} \cdot \vec{\mathrm{S}}$$

- Gaussian radial dependencies with fixed ranges
- strengths used as fit parameters (3 parameters)

Correlated Argonne V18 + Correction



Charge Distributions



Summary

- **Unitary Correlation Operator Method (UCOM)**
  - short-range central and tensor correlations treated explicitly
  - long-range correlations have to be accounted for by model space

- **Correlated Realistic NN-Potential V_{UCOM}**
  - low-momentum / phase-shift equivalent / operator representation
  - robust starting point for all kinds of many-body calculations

Summary

- **UCOM + No-Core Shell Model**
  - dramatically improved convergence
  - tool to assess higher-order contributions
- **UCOM + Hartree-Fock**
  - closed shell nuclei across the whole nuclear chart
  - basis for improved many-body calculations (MPT, RPA, CC,...)
- **UCOM + Fermionic Molecular Dynamics**
  - talk by T. Neff