Towards Ab Initio Nuclear Structure Calculations

R. Roth, H. Hergert
Institut für Kernphysik, TU Darmstadt

T. Neff, H. Feldmeier
Gesellschaft für Schwerionenforschung

supported by DFG
through the SFB 634

Overview

- Central- and Tensor Correlations
- Unitary Correlation Operator Method
- Correlated Realistic NN-Potentials and Phenomenological Corrections
- Variational Ground State Calculations
- Outlook

Objective

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**

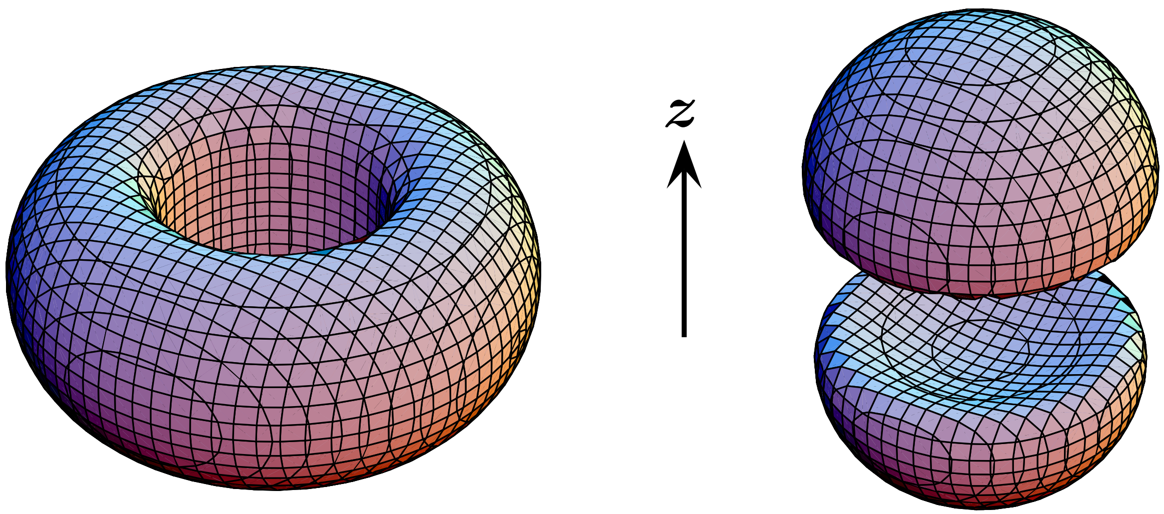
Deuteron: Manifestation of Correlations

$M_S = 0$

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

$M_S = \pm 1$

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



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

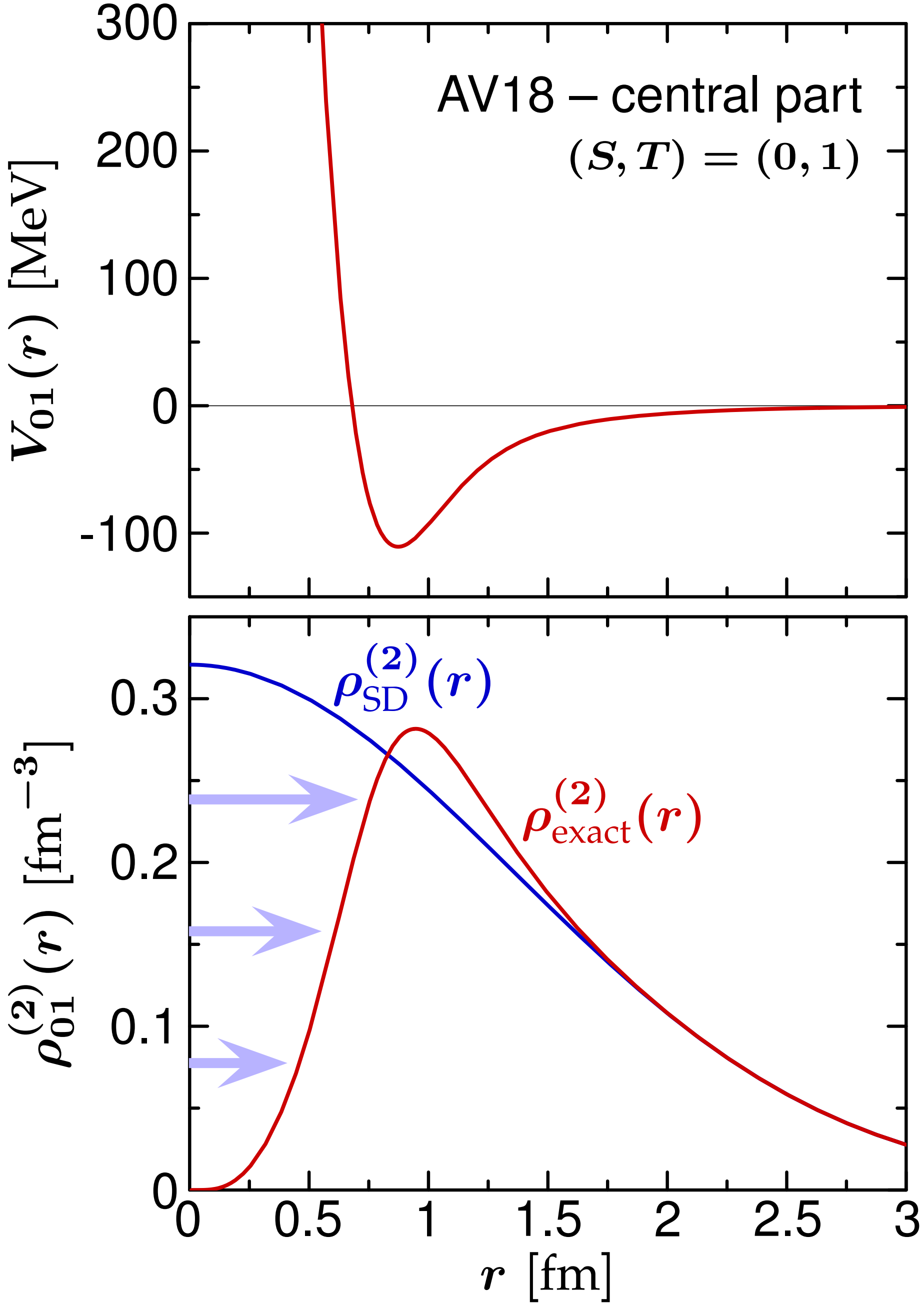
two-body density fully suppressed at small particle distances $|\vec{r}|$

central correlations

angular distribution depends strongly on relative spin orientation

tensor correlations

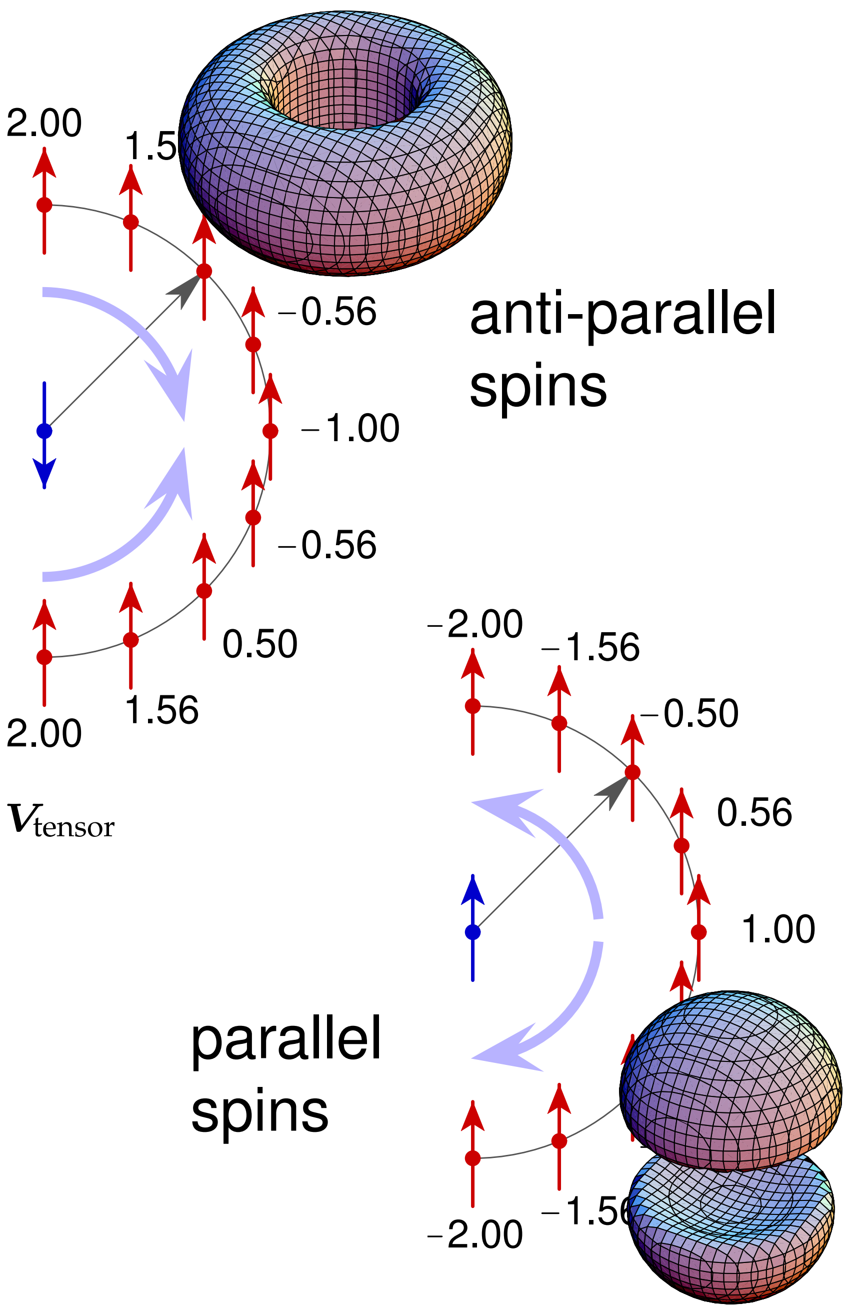
Central Correlations



- two-body density distribution of ^{4}He in the $(S,T) = (0,1)$ channel
- strong repulsive core in the central part of realistic interactions
- suppression of the probability density for finding two nucleons within the core region ➔ **correlation hole**
- short-range central correlations cannot be described by single or a superposition of few Slater determinants

"shift the nucleons out of the core region"

Tensor Correlations



- analogy with classical dipole-dipole interaction

$$V_{\text{tensor}} \sim -\left(3\,\frac{(\vec{\sigma}_1\vec{r})(\vec{\sigma}_2\vec{r})}{r^2} - \vec{\sigma}_1\vec{\sigma}_2\right)$$

- tensor interaction couples the relative spatial orientation of two nucleons with their spin orientation

- **tensor correlations** cannot be described by a single or a superposition of few Slater determinants

"rotate nucleons towards poles or equator depending on spin orientation"

Unitary Correlation Operator Method

Unitary Correlation Operator Method

Correlation Operator

introduce correlations by means of a unitary transformation with respect to the relative coordinates of all pairs

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

$$\mathbf{g} = \mathbf{g}(\vec{\mathbf{r}}, \vec{\mathbf{q}}; \vec{\boldsymbol{\sigma}}_1, \vec{\boldsymbol{\sigma}}_2, \vec{\boldsymbol{\tau}}_1, \vec{\boldsymbol{\tau}}_2)$$

$$\mathbf{G}^\dagger = \mathbf{G}$$

$$\mathbf{C}^\dagger\mathbf{C} = 1$$

Correlated Operators

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

Correlated States

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

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

Central and Tensor Correlators

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

Central Correlator C_r

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

$$\mathbf{g}_r = \frac{1}{2}\Big[s(\mathbf{r})\ (\tfrac{\vec{\mathbf{r}}}{\mathbf{r}} \cdot \vec{\mathbf{q}}) + (\vec{\mathbf{q}} \cdot \tfrac{\vec{\mathbf{r}}}{\mathbf{r}})\ s(\mathbf{r})\Big]$$

$$\vec{\mathbf{q}} = \tfrac{1}{2}(\vec{\mathbf{p}}_1 - \vec{\mathbf{p}}_2)$$

Tensor Correlator C_Ω

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

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

$$\vec{\mathbf{q}}_\Omega = \tfrac{1}{2\mathbf{r}}\big(\vec{\mathbf{l}} \times \tfrac{\vec{\mathbf{r}}}{\mathbf{r}} - \tfrac{\vec{\mathbf{r}}}{\mathbf{r}} \times \vec{\mathbf{l}}\big) = \vec{\mathbf{q}} - \tfrac{\vec{\mathbf{r}}}{\mathbf{r}}(\tfrac{\vec{\mathbf{r}}}{\mathbf{r}} \cdot \vec{\mathbf{q}})$$

$s(r)$ and $\vartheta(r)$ determined once for each (S,T)-channel of the potential

Central Correlations

- correlated two-body wave function

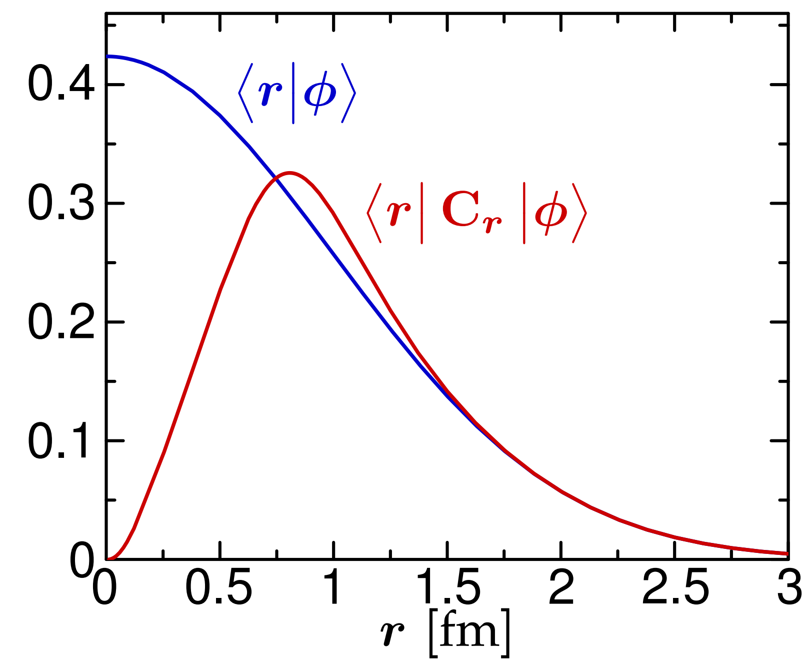
$$\langle \vec{r}, \vec{X} | \begin{matrix} \mathrm{C}_r^\dagger \\ \mathrm{C}_r \end{matrix} |\psi\rangle = \sqrt{R'_\pm(r)}\, \frac{R_\pm(r)}{r} \langle R_\pm(\vec{r})\tfrac{\vec{r}}{r}, \vec{X} | \psi \rangle$$

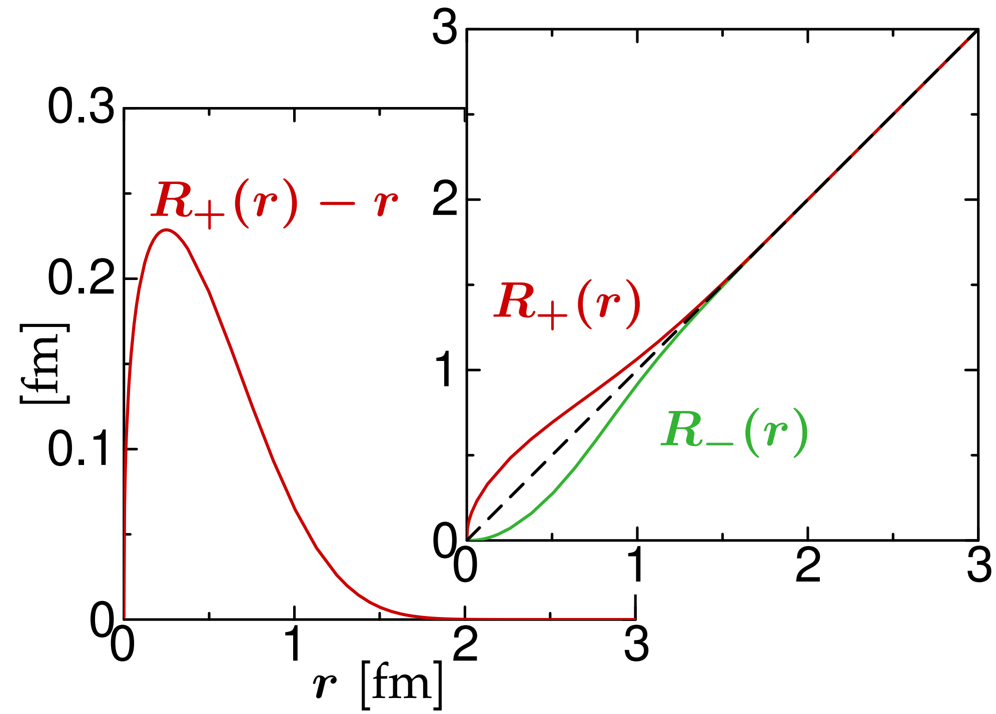
- correlation $\hat{=}$ norm conserving coordinate transformation

$$\vec{r} \quad \mapsto \quad R_\pm(r)\, \frac{\vec{r}}{r}$$

- correlation functions $R_\pm(r)$ are connected to $s(r)$

$$\pm 1 = \int_r^{R_\pm(r)} \frac{d\xi}{s(\xi)}\;, \qquad R_\pm(r) \approx r \pm s(r)$$





Tensor Correlations

- tensor correlated $^3S_1$ two-body state

$$\mathbf{C}_{\Omega} \left| \phi_S, {}^3S_1 \right\rangle = \left| \widetilde{\phi}_S, {}^3S_1 \right\rangle + \left| \widetilde{\phi}_D, {}^3D_1 \right\rangle$$

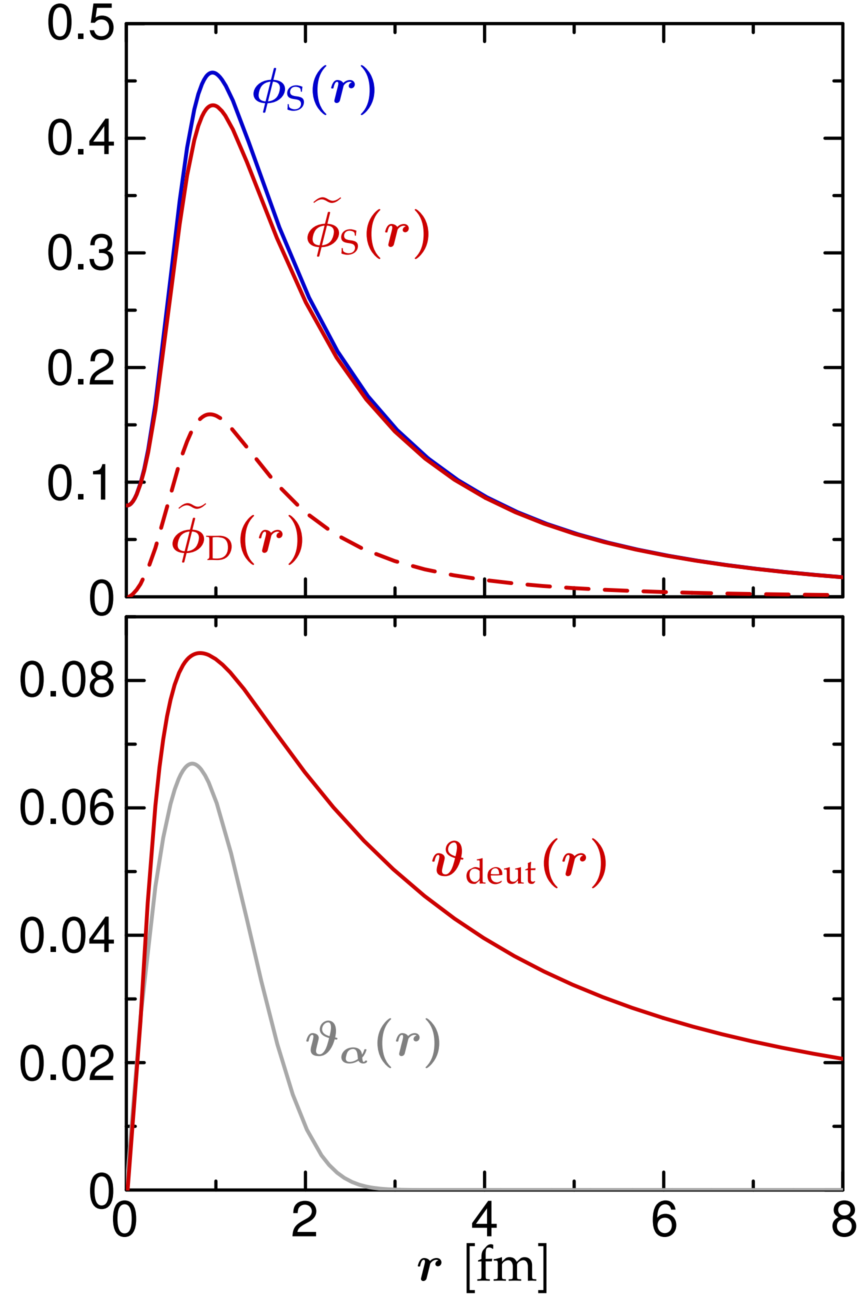
$$\langle \boldsymbol{r} | \widetilde{\phi}_S \rangle = \cos[3\sqrt{2}\, \vartheta(\boldsymbol{r})]\ \langle \boldsymbol{r} | \phi_S \rangle$$

$$\langle \boldsymbol{r} | \widetilde{\phi}_D \rangle = \sin[3\sqrt{2}\, \vartheta(\boldsymbol{r})]\ \langle \boldsymbol{r} | \phi_S \rangle$$

- tensor force admixes higher orbital angular momenta — and so does the tensor correlator

- tensor correlator for the deuteron

$$\vartheta_{\text{deut}}(\boldsymbol{r}) = \frac{1}{3\sqrt{2}} \arctan \frac{\langle \boldsymbol{r} | \widetilde{\phi}_D^{\text{deut}} \rangle}{\langle \boldsymbol{r} | \widetilde{\phi}_S^{\text{deut}} \rangle}$$



Correlated Operators

Cluster Expansion

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

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.

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

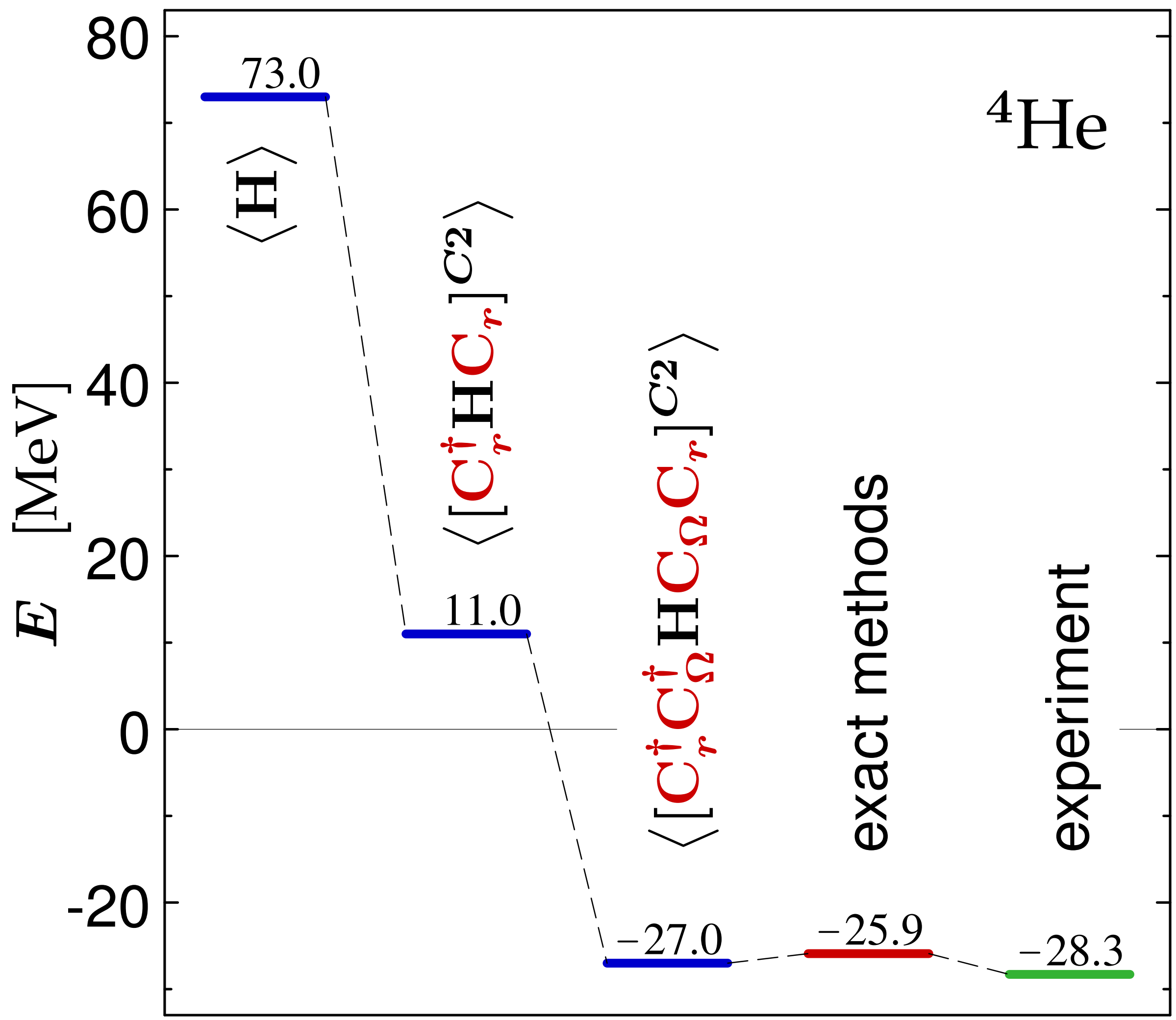
operators for all observables can be and have to be correlated consistently

Correlated Realistic NN-Potential

$$\widetilde{\mathbf{H}}^{C2} = \widetilde{\mathbf{T}}^{[1]} + \widetilde{\mathbf{T}}^{[2]} + \widetilde{\mathbf{V}}^{[2]} = \mathbf{T} + \mathbf{V}_{\text{corr}}$$

- **closed analytic expression** for the correlated interaction $\mathbf{V}_{\text{corr}}$ 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 **identical to $V_{\text{low}-k}$**

UCOM in Action



- shell-model-like Slater determinant for ^{4}He with fixed width
- expectation value for uncorrelated and correlated AV8' potential
- energy is difference of two large numbers

$$\langle \mathbf{T} \rangle \approx +102 \text{ MeV}$$
$$\langle \mathbf{V} \rangle \approx -128 \text{ MeV}$$

- tensor interaction provides large contribution

$$\langle \mathbf{V}_{\text{central}} \rangle \approx -55 \text{ MeV}$$
$$\langle \mathbf{V}_{\text{tensor}} \rangle \approx -69 \text{ MeV}$$

Ground State Structure of Finite Nuclei

Many-Body Problem

Single-Particle States

$$\left|q\right\rangle = \sum_{\nu=1}^{n} c_\nu \; \left|g_\nu\right\rangle \otimes \left|\chi_\nu\right\rangle \otimes \left|m_t\right\rangle$$

$$\left\langle \vec{x} \middle| g_\nu \right\rangle = \exp\Big(- \frac{(\vec{x} - \vec{\xi}_\nu)^2}{2\,\alpha_\nu} - \mathrm{i}\, \vec{\pi}_\nu \vec{x} \Big)$$

$\vec{\xi}_\nu$: mean position

$\vec{\pi}_\nu$: mean momentum

α_ν : complex width

χ_ν : spin angle

Slater Determinant

$$\left|Q\right\rangle = \mathcal{A}\left(\left|q_1\right\rangle \otimes \left|q_2\right\rangle \otimes \cdots \otimes \left|q_A\right\rangle \right)$$

Correlated Hamiltonian

$$\widetilde{\mathrm{H}}^{C2} = [\mathrm{C}_r^\dagger \mathrm{C}_\Omega^\dagger \mathrm{H} \mathrm{C}_\Omega \mathrm{C}_r]^{C2} = \mathrm{T} + \mathrm{V}^{\mathrm{eff}}$$

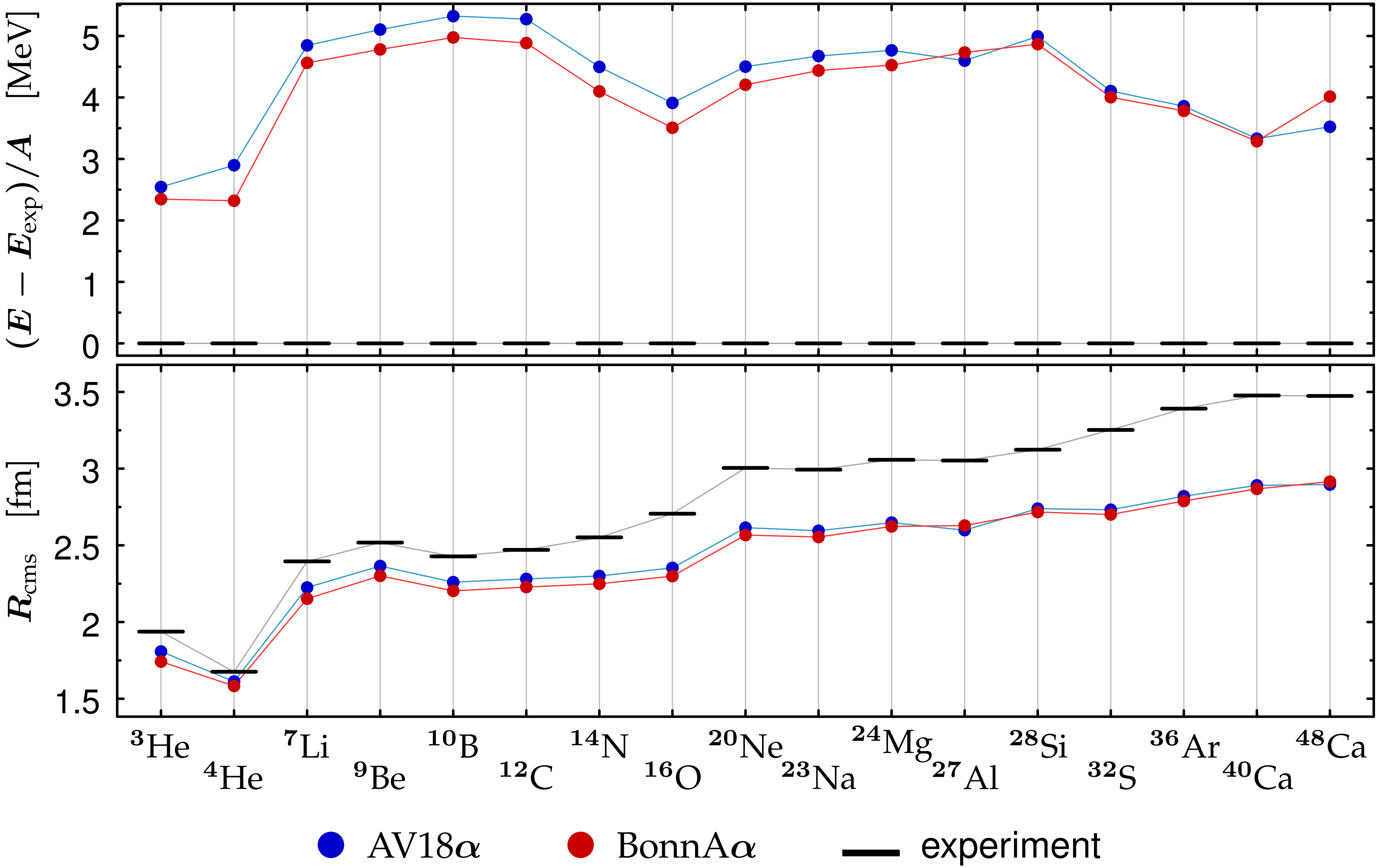
Variation

$$\frac{\left\langle Q \right| \widetilde{\mathrm{H}}^{C2} \left| Q \right\rangle}{\left\langle Q \middle| Q \right\rangle} \longrightarrow \min$$

Diagonalisation

in sub-space spanned by several (suitably chosen) Slater determinants $\left|Q_i\right\rangle$

Variational Energies & Charge Radii



Missing Pieces

"Physical" Points

- genuine three-body forces
- genuine many-body correlations

"Technical" Points

- residual three-body contributions of cluster expansion
- imperfect two-body correlations

Pragmatic Approach

simulate these by a phenomenological correction to the correlated two-body potential

Phenomenological Corrections

Central Correction

- Wigner-type local and momentum-dependent Gaussian potentials

$$\mathrm{V_C} = v_1(\mathrm{r}) + \vec{\mathrm{q}}\, v_{qq}(\mathrm{r})\, \vec{\mathrm{q}}$$

- parameters fixed (2-4) to reproduce binding energies and cms-radii of ^{4}He, ^{16}O, and ^{40}Ca

Spin-Orbit Correction

- isospin-independent attractive $\vec{\mathrm{L}}\cdot\vec{\mathrm{S}}$-potential

$$\mathrm{V_{LS}} = v_{LS}(\mathrm{r})\, \vec{\mathrm{L}}\cdot\vec{\mathrm{S}}$$

- parameters (1-2) fixed to binding energy of ^{24}O and ^{48}Ca

$\sim 15\%$ of potential energy generated by correction

additional $\vec{\mathrm{L}}\cdot\vec{\mathrm{S}}$-term of similar size as original $\vec{\mathrm{L}}\cdot\vec{\mathrm{S}}$

Effect of the Phenomenological Correction

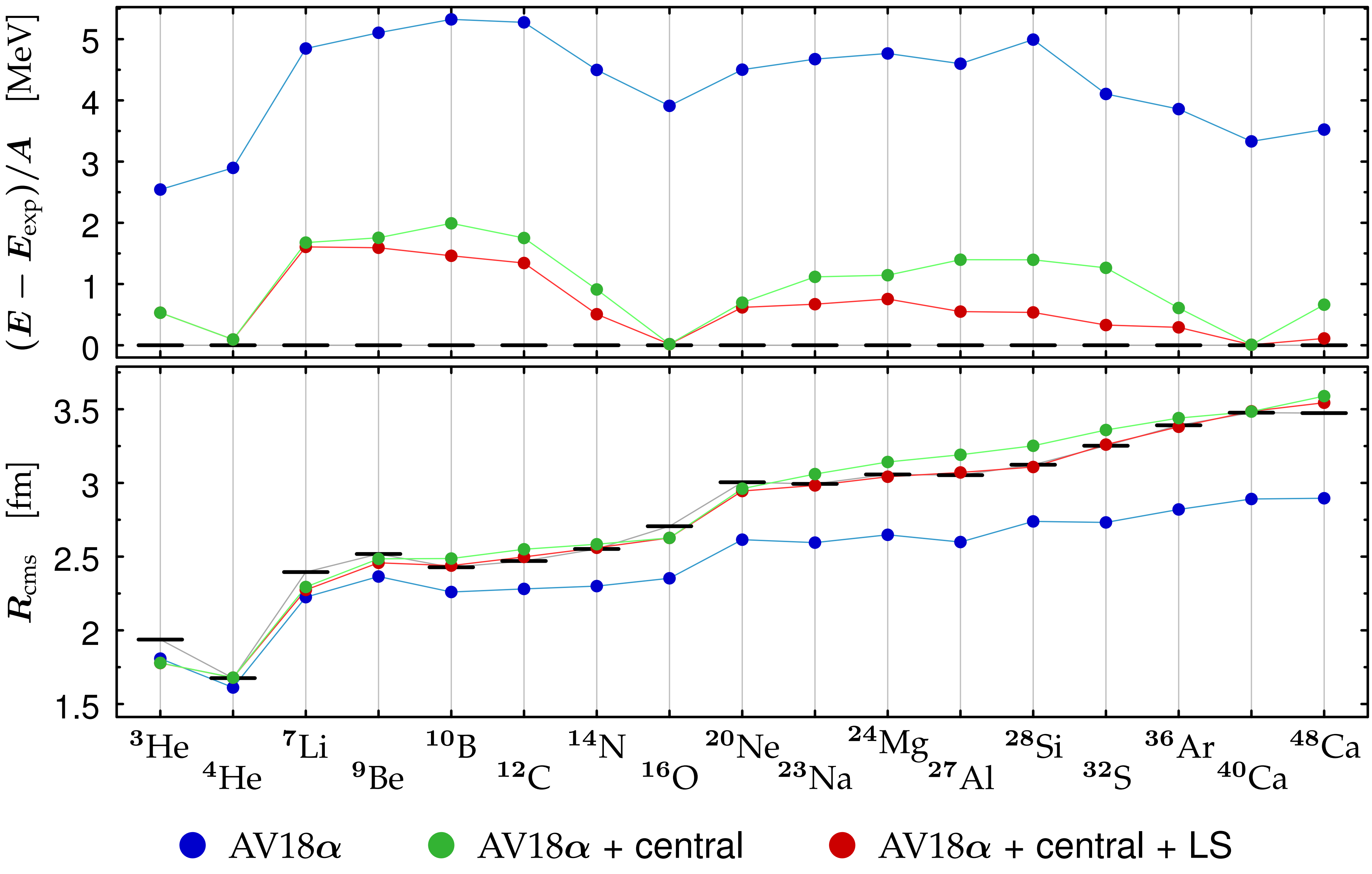
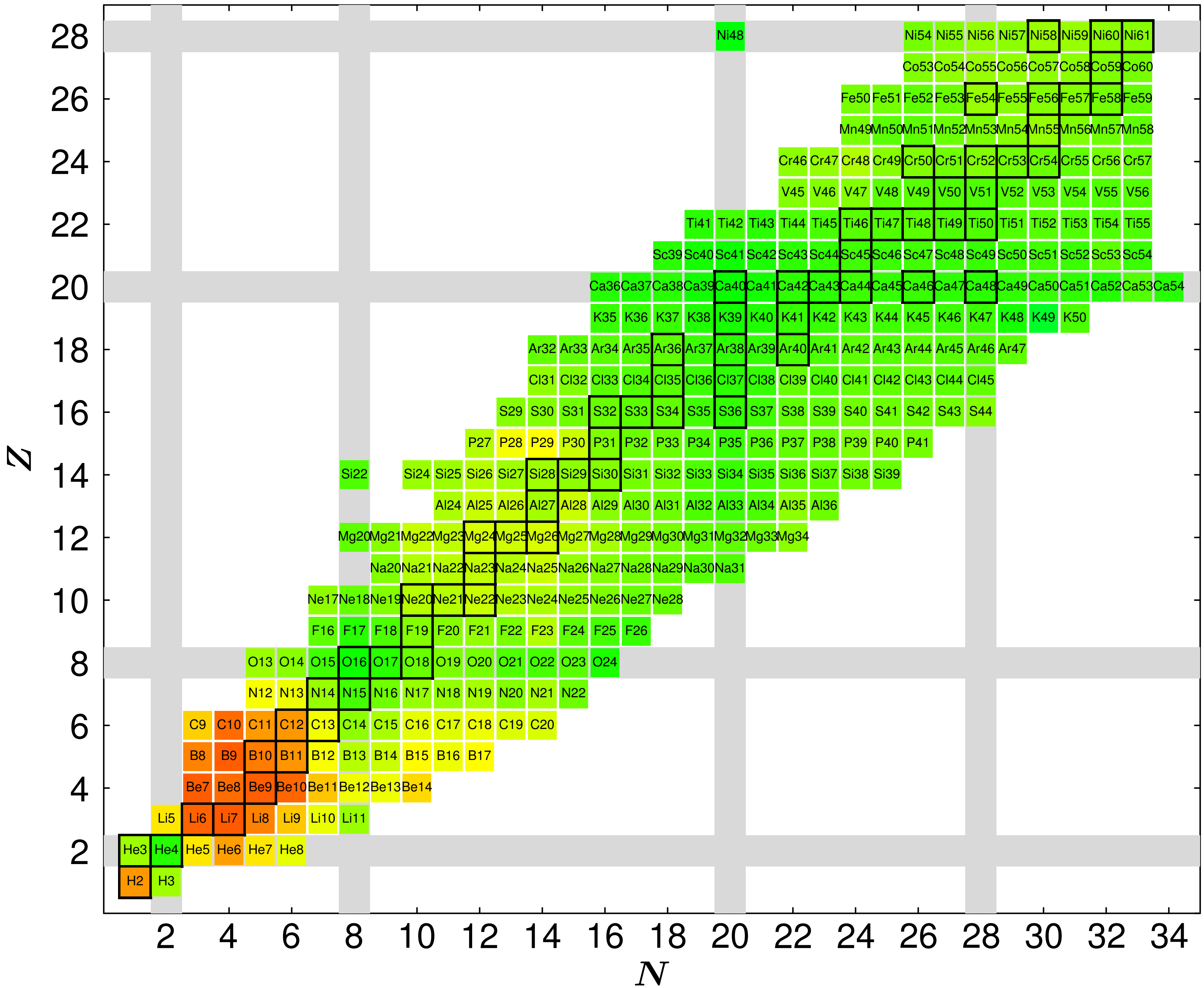
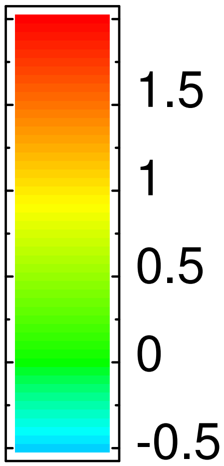


Chart of Nuclei



$(\boldsymbol{E} - \boldsymbol{E}_{\mathrm{exp}})/\boldsymbol{A}$
[MeV]

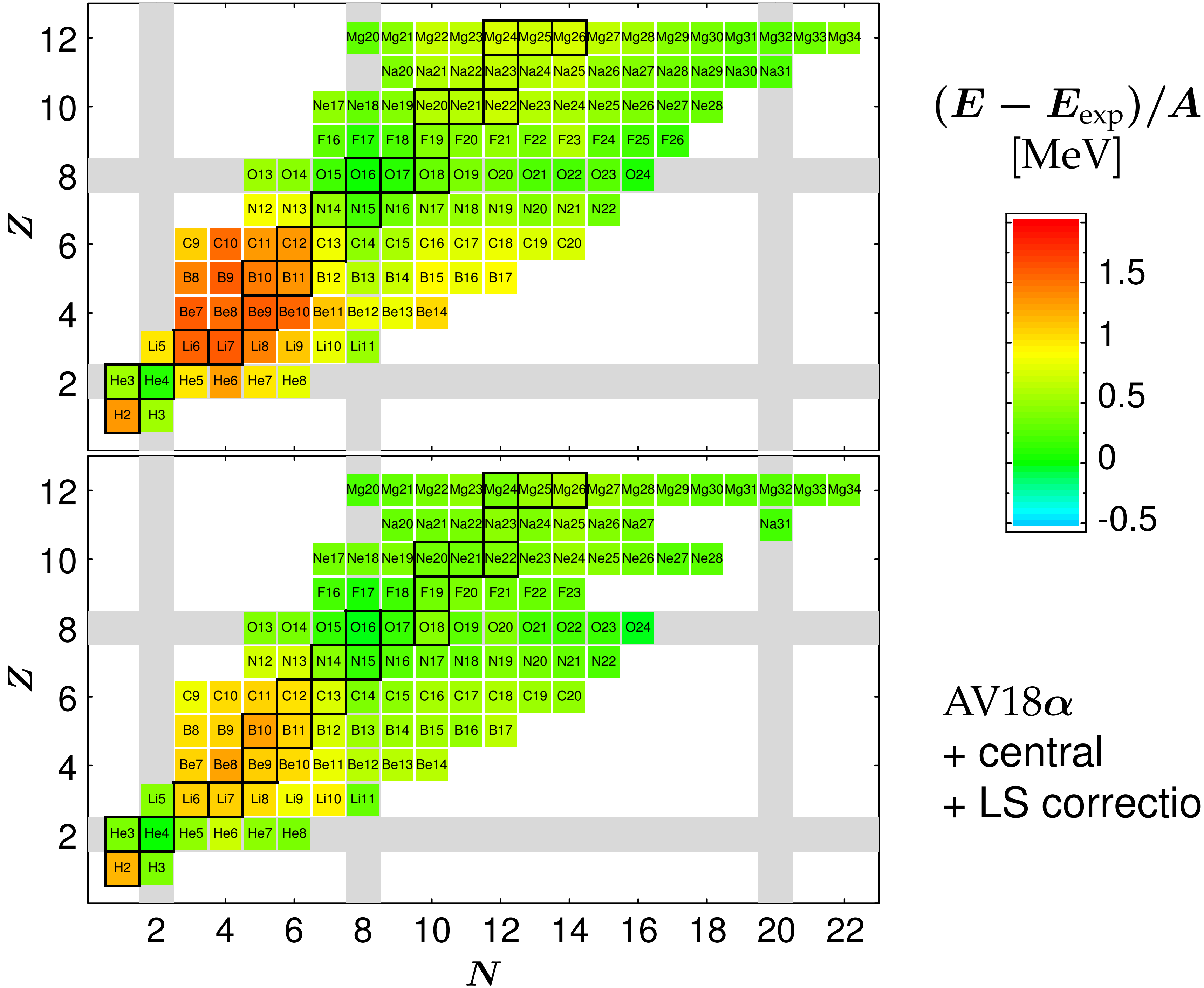


AV18α
+ central
+ LS correction

Chart of Nuclei II

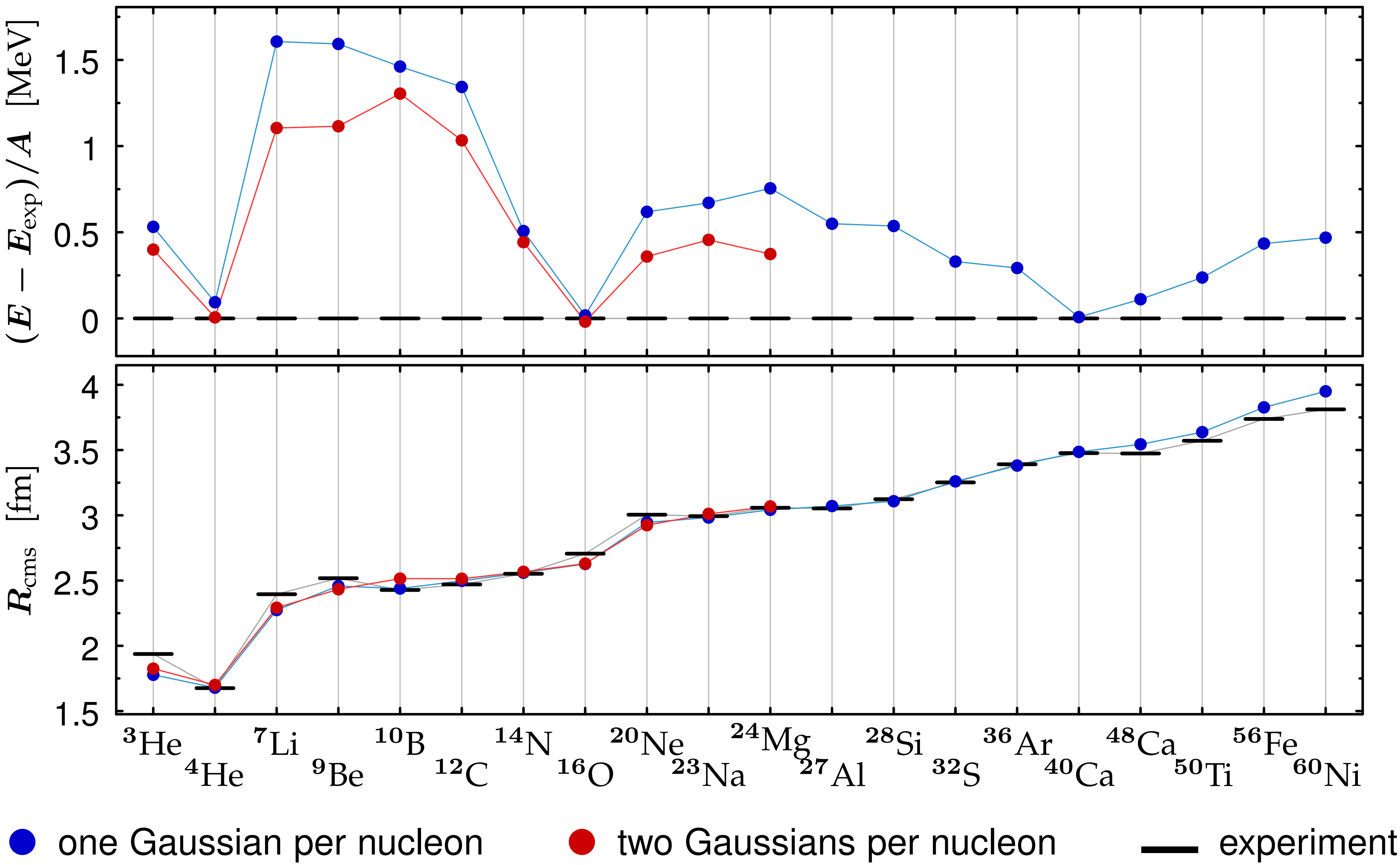
one Gaussian per nucleon

two Gaussians per nucleon

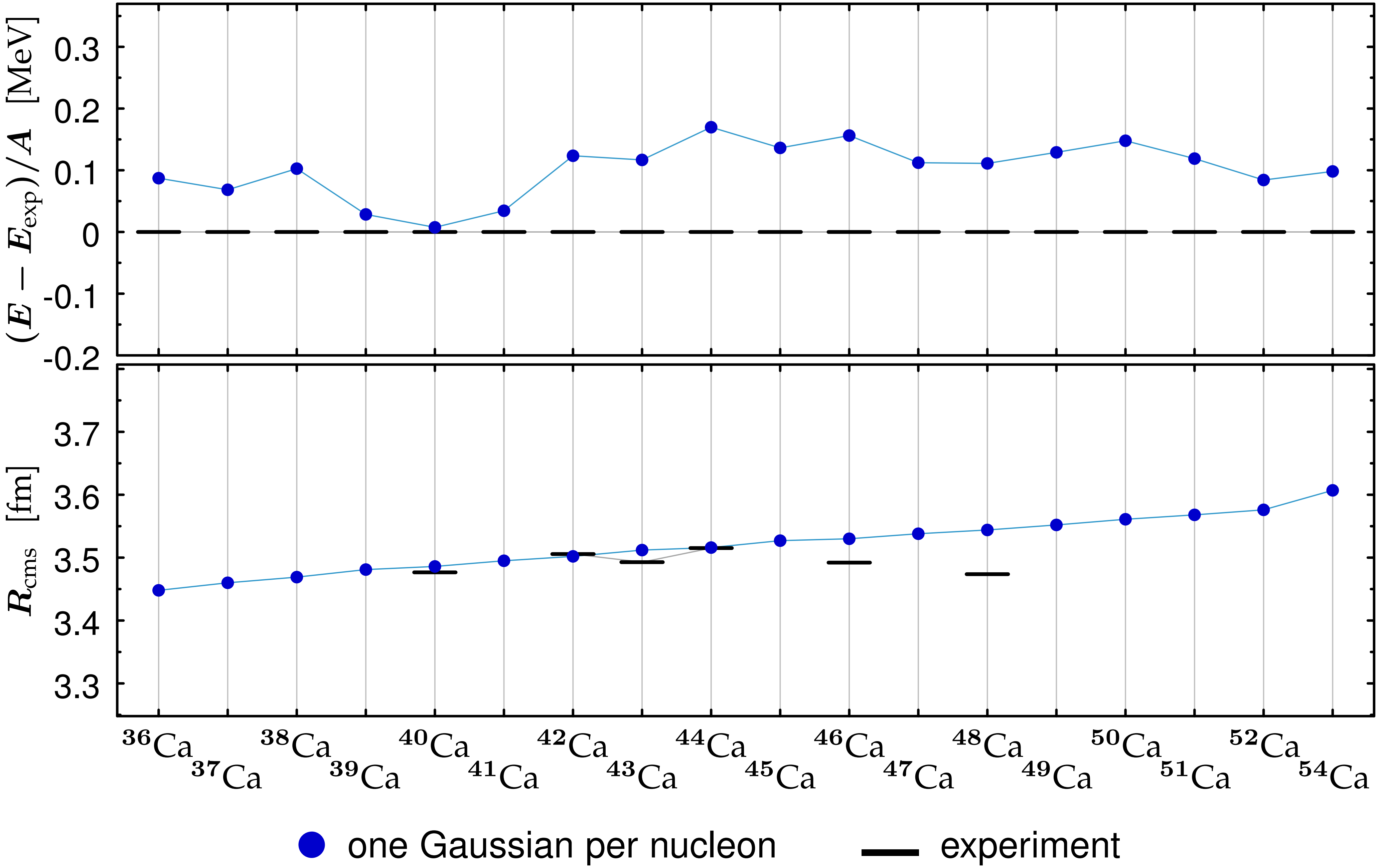


AV18α
+ central
+ LS correction

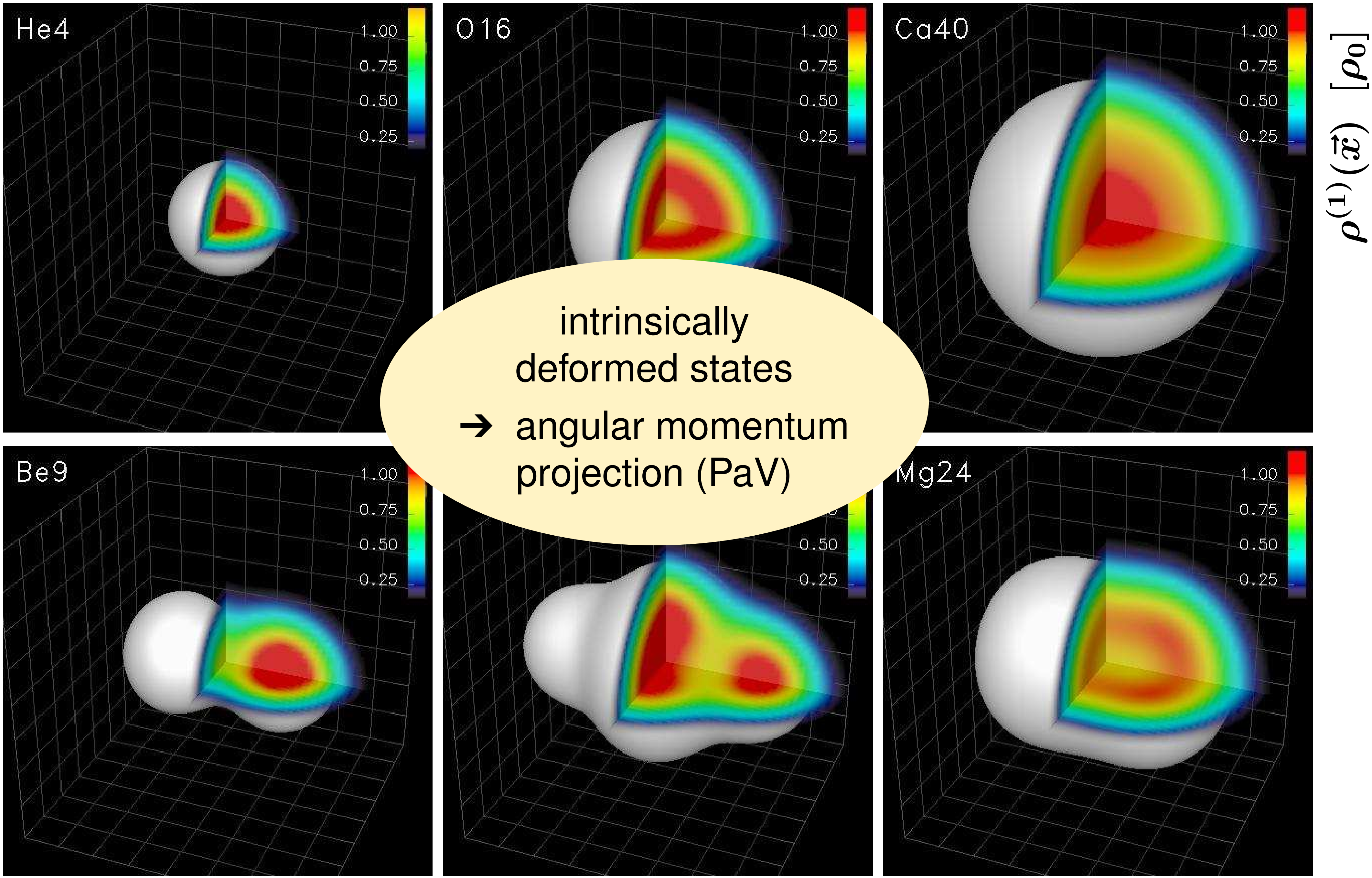
Selected Stable Nuclei



Calcium Isotopes



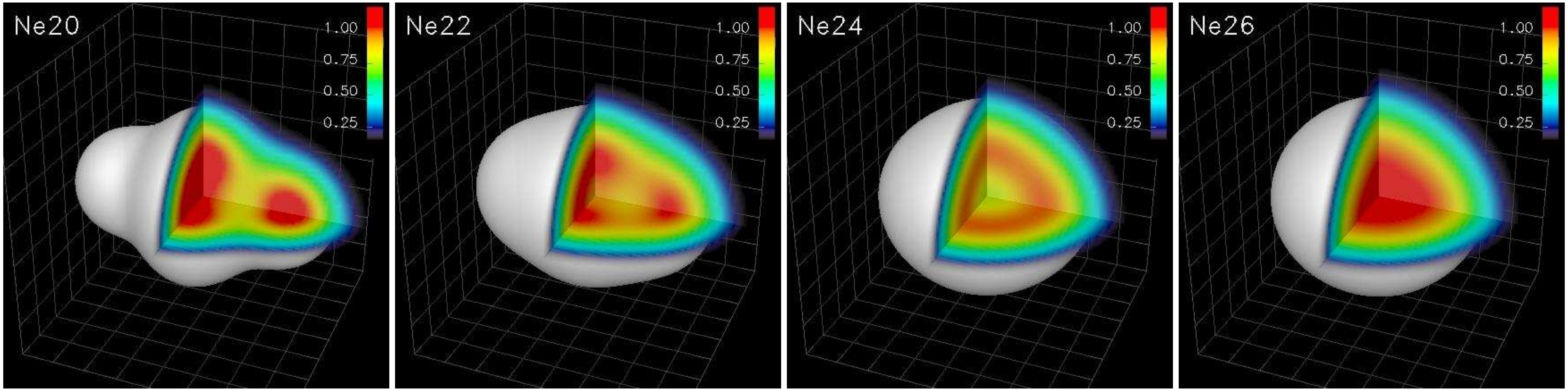
Intrinsic One-Body Density Distributions

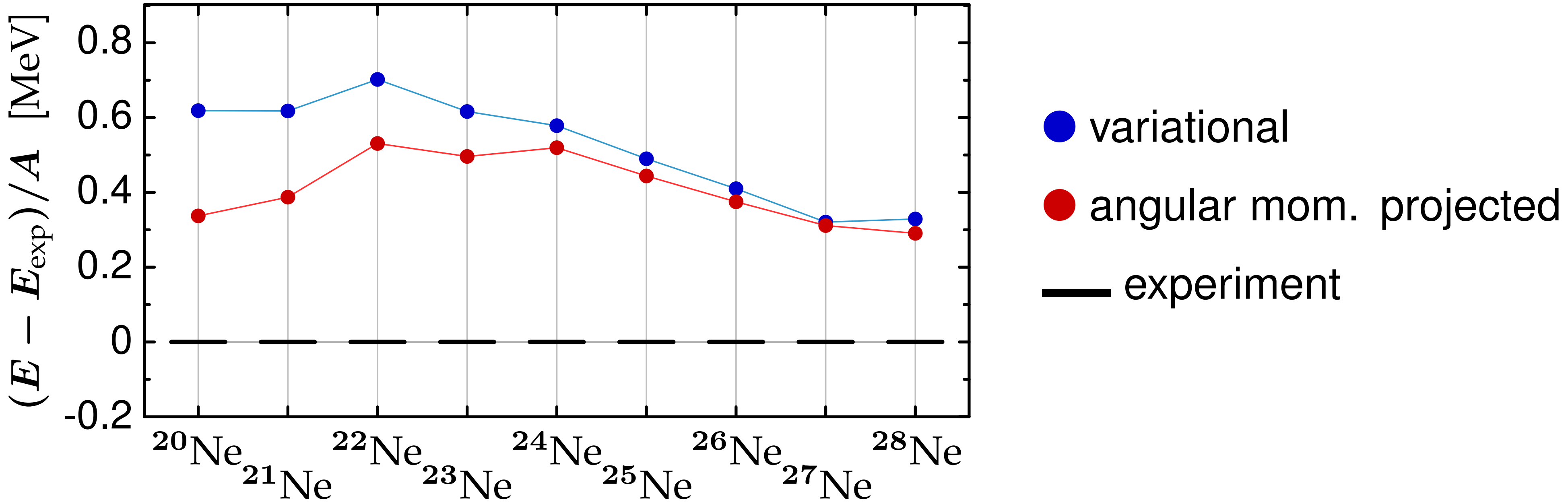


intrinsically deformed states

➔ angular momentum projection (PaV)

Neon Isotopes





Summary

- **Unitary Correlation Operator Method** for the treatment of dominant short-range central and tensor correlations
- **correlated realistic NN-potentials** (AV18, BonnA) for use with simple many-body spaces
- momentum and spin-orbit-dependent **two-body correction** to simulate effect of three-body terms (pragmatic approach)
- **variational ground state calculations** for $A \lesssim 60$ in good agreement with experiment

Outlook

- correlated realistic NN-interaction provides **robust starting point for all kinds of many-body models**
- **PaV, VaP, and multi-configuration** calculations for light nuclei within the Gaussian basis ➔ talk by T. Neff
- **Hartree-Fock** calculations for larger nuclei based on correlated realistic interaction
- implementation of **effective three-body forces** instead of phenomenological two-body corrections