Towards Ab Initio Nuclear Structure Calculations

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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**

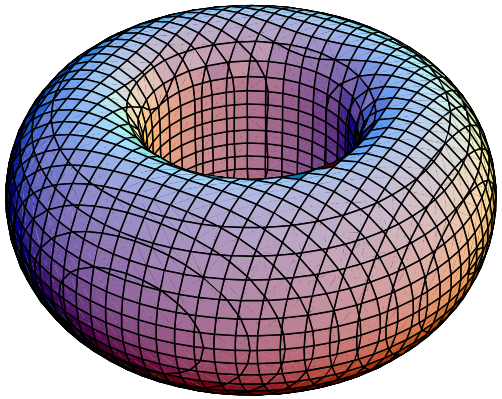
Overview

- Central and Tensor Correlations
- Unitary Correlation Operator Method
- Correlated Realistic NN-Potentials
- Variational Ground State Calculations for $A \lesssim 60$
- Angular Momentum Projection and Multi-Configuration
- Outlook

Deuteron: Manifestation of Correlations

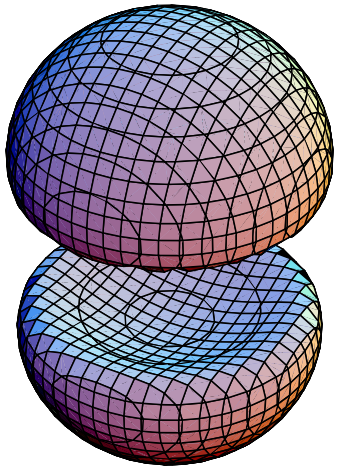
$M_S = 0$

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



$M_S = \pm 1$

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



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

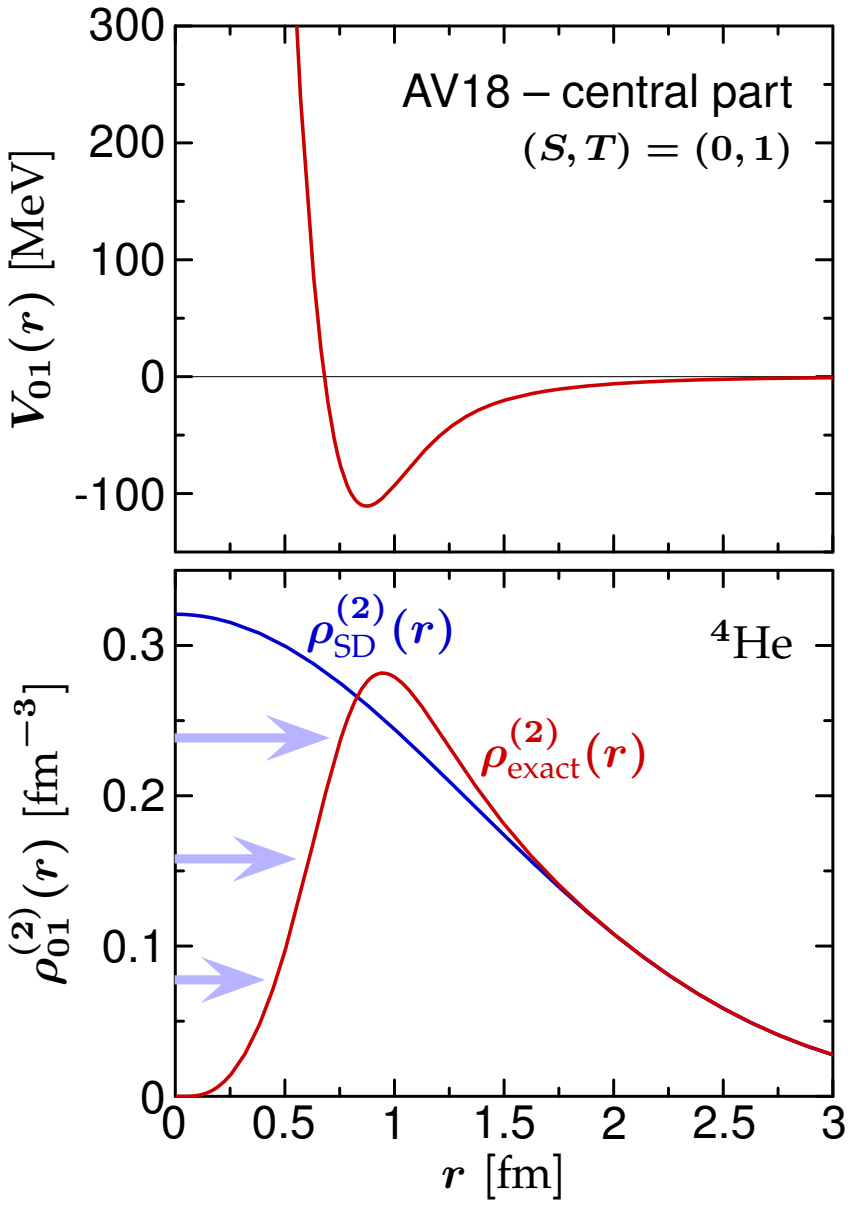
two-body density fully suppressed at small particle distances $|\vec{r}|$

central correlations

angular distribution depends strongly on relative spin orientation

tensor correlations

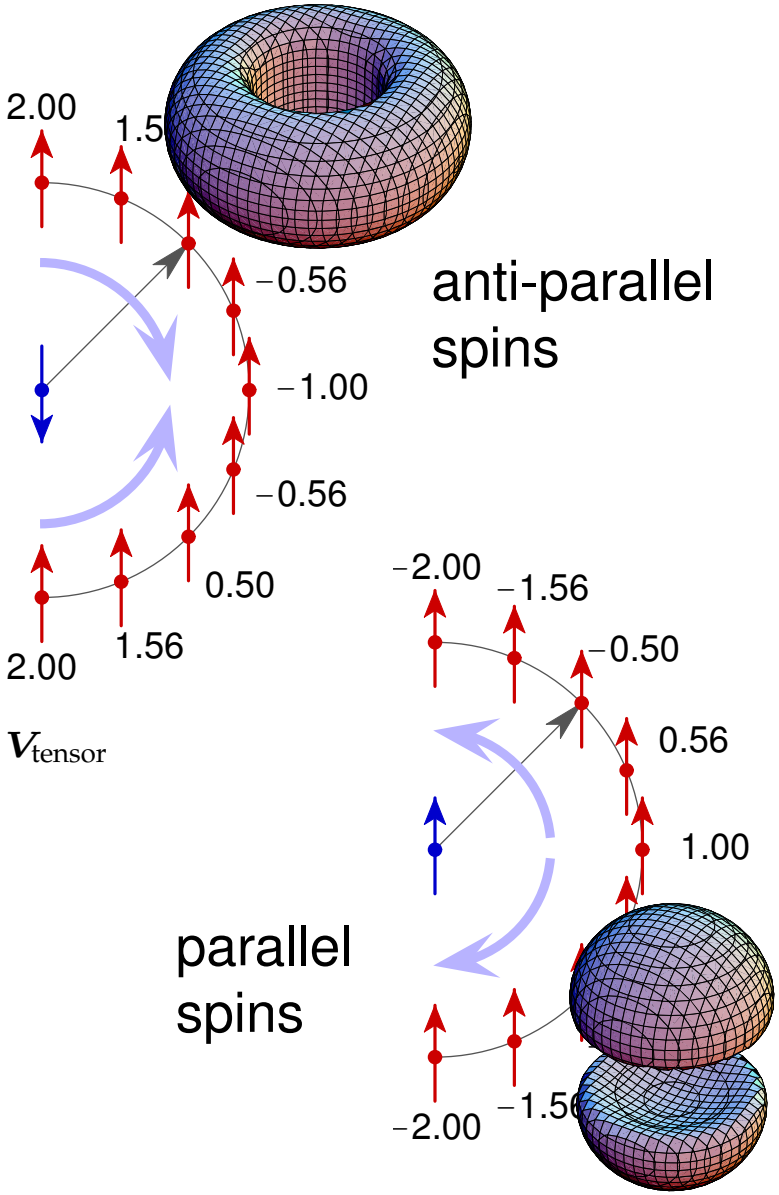
Central Correlations



- 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 superpositions of few Slater determinants

"shift the nucleons out of the core region"

Tensor Correlations



- analogy with classical dipole-dipole interaction

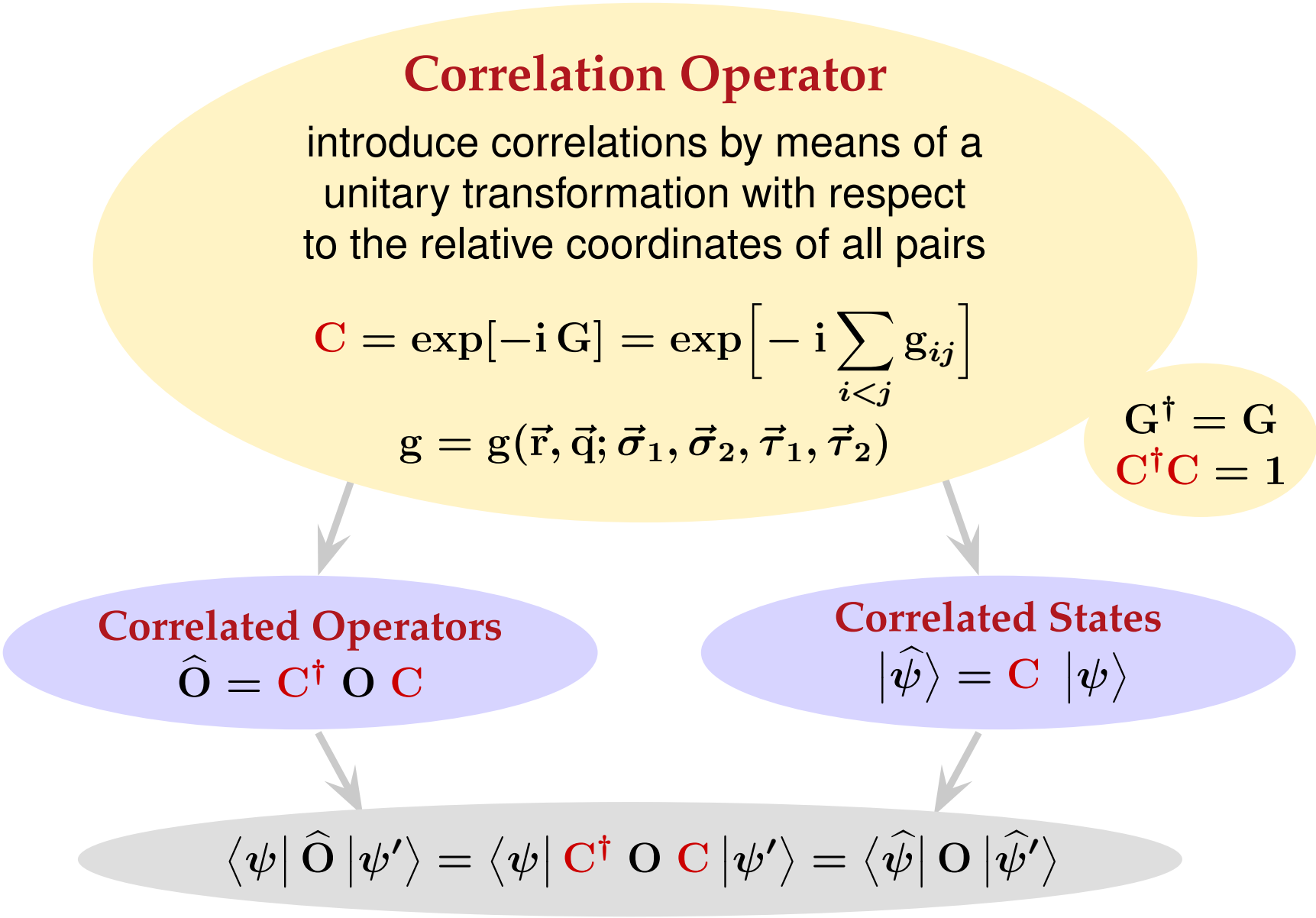
$$V_{\text{tensor}} \sim -\left(3\,\frac{(\vec{\sigma}_1\vec{r})(\vec{\sigma}_2\vec{r})}{r^2} - \vec{\sigma}_1\vec{\sigma}_2\right)$$

- tensor interaction couples the relative spatial orientation of two nucleons with their spin orientation
- **tensor correlations** cannot be described by single or superpositions of few Slater determinants

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

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.

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

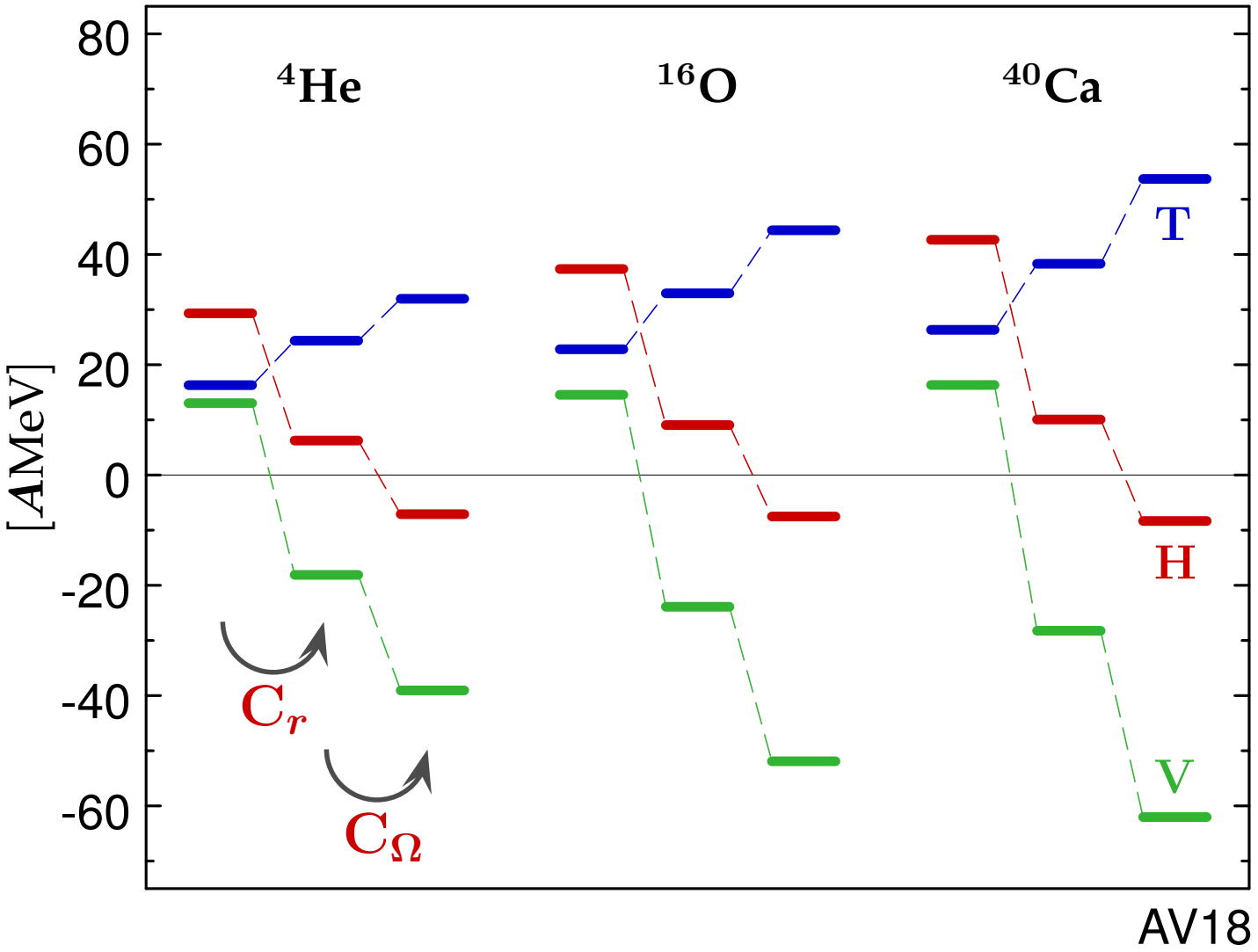
operators for all observables can be and have to be correlated consistently

Correlated Realistic NN-Potential

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

- **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 **identical to** $V_{\mathrm{low}-k}$

Effect of Unitary Transformation



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

Ground State Structure of Finite Nuclei

Many-Body Problem (FMD)

Gaussian Single-Particle States

$$|q\rangle = \sum_{\nu=1}^{n} c_\nu \; |a_\nu, \vec{b}_\nu\rangle \otimes |\chi_\nu\rangle \otimes |m_t\rangle$$

$$\langle \vec{x} | a_\nu, \vec{b}_\nu \rangle = \exp\left[- \frac{(\vec{x} - \vec{b}_\nu)^2}{2\, a_\nu} \right]$$

a_ν : complex width

χ_ν : spin orientation

$\vec{b}_\nu$: mean position & momentum

Slater Determinant

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

Correlated Hamiltonian

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

Variation

$$\frac{\langle Q | \hat{\mathrm{H}}^{C2} | Q \rangle}{\langle Q | Q \rangle} \rightarrow \min$$

Diagonalisation

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

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 to reproduce binding energies and cms-radii of $^4\mathrm{He}$, $^{16}\mathrm{O}$, and $^{40}\mathrm{Ca}$

Spin-Orbit Correction

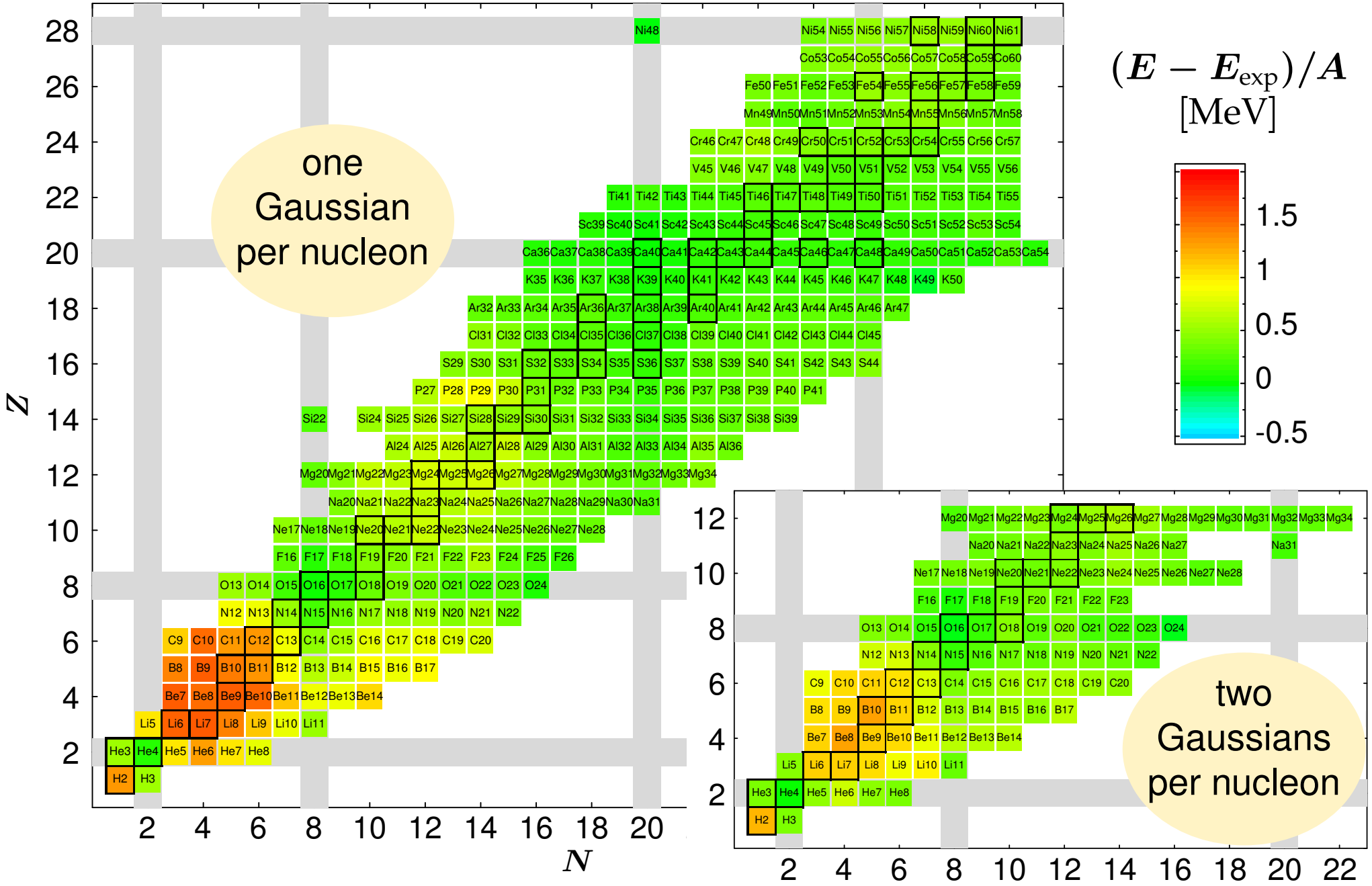
- isospin-independent attractive $\vec{\mathrm{L}} \cdot \vec{\mathrm{S}}$-potential

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

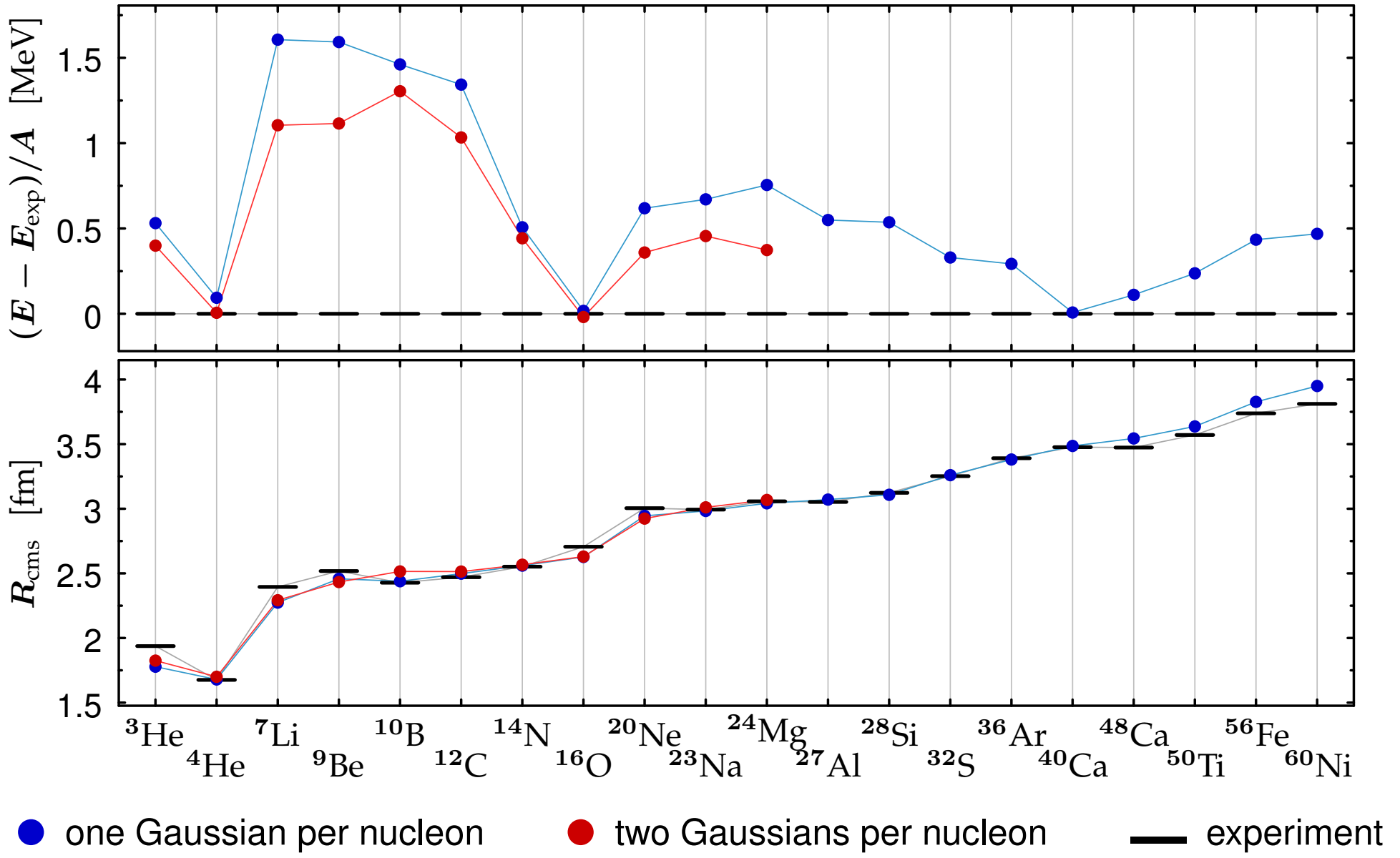
- parameters adjusted to binding energy of $^{24}\mathrm{O}$ and $^{48}\mathrm{Ca}$

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

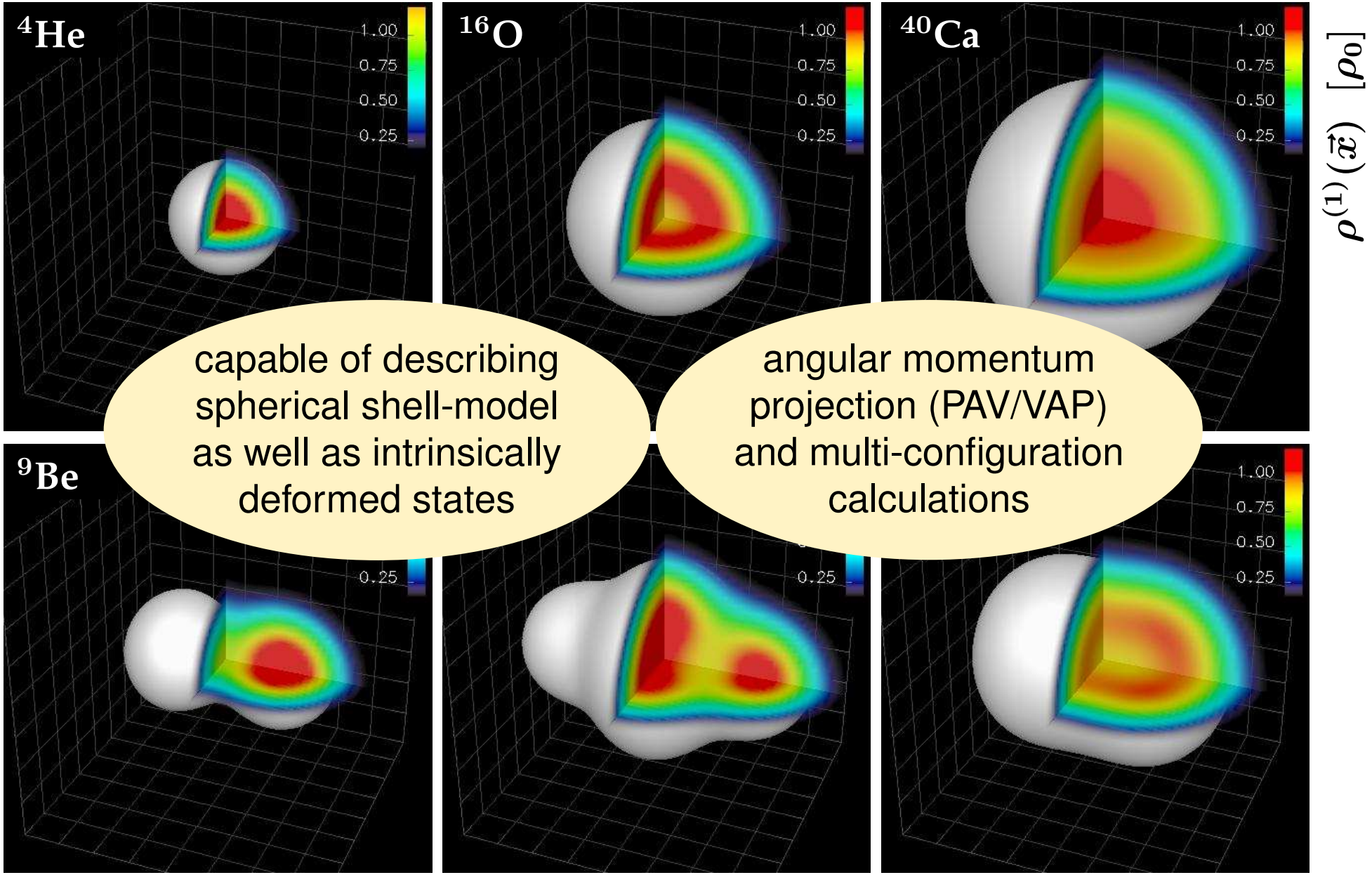
Chart of Nuclei



Selected Stable Nuclei



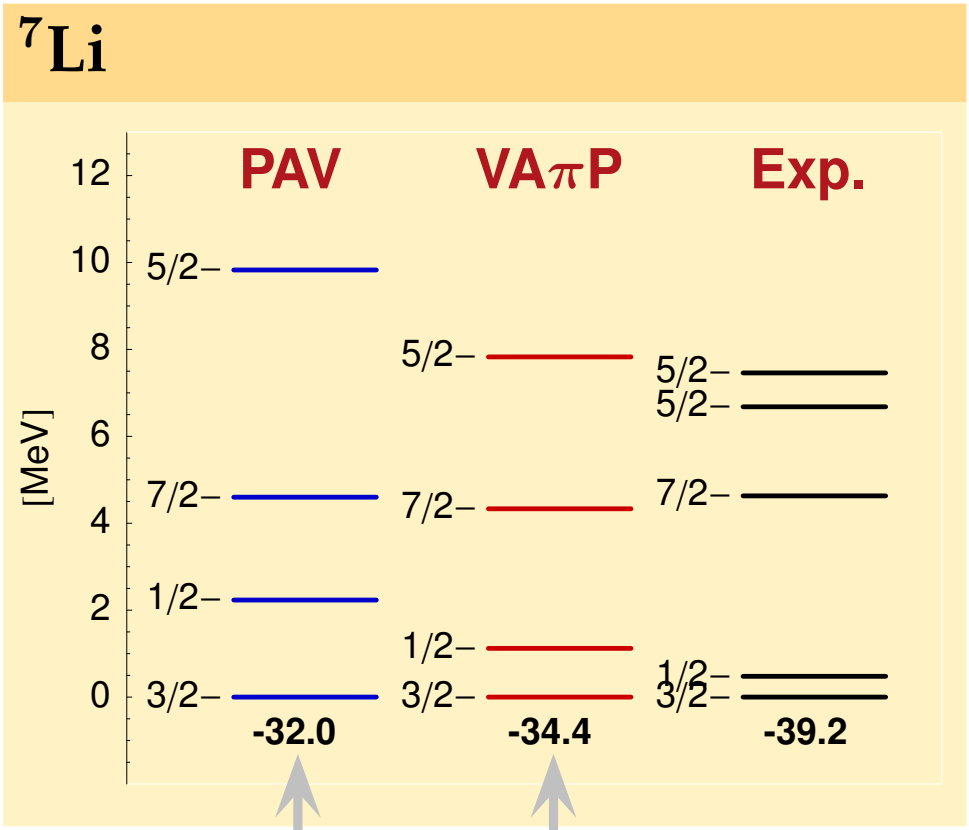
Intrinsic One-Body Density Distributions

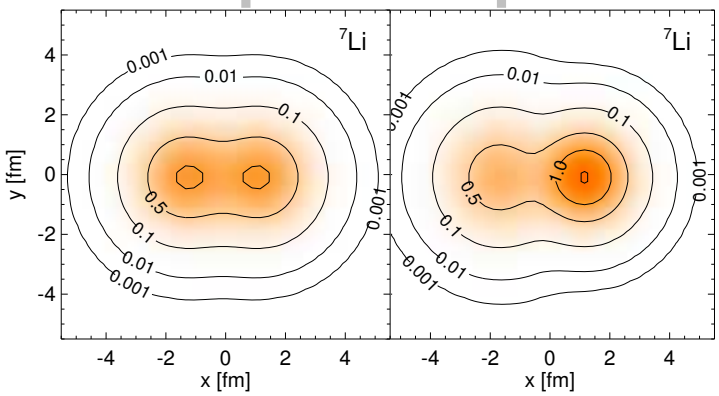


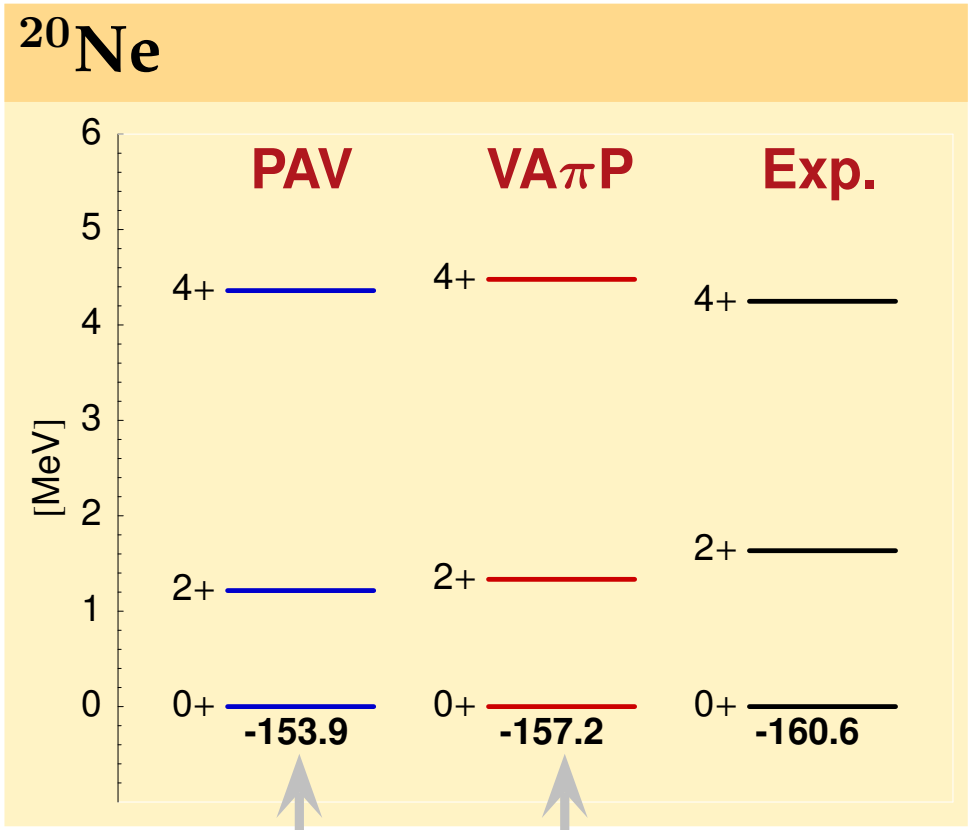
capable of describing spherical shell-model as well as intrinsically deformed states

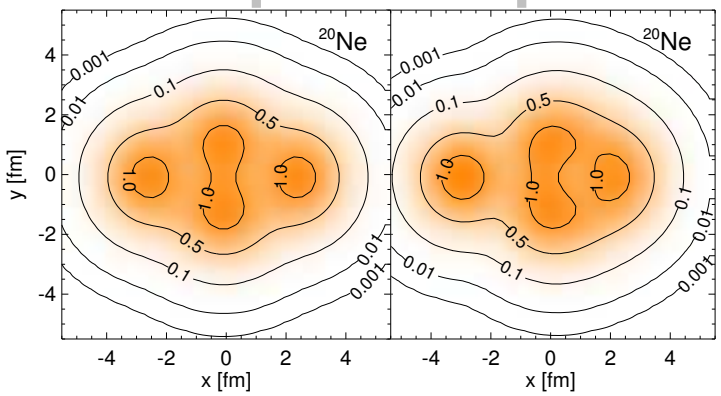
angular momentum projection (PAV/VAP) and multi-configuration calculations

Parity and Angular Momentum Projection

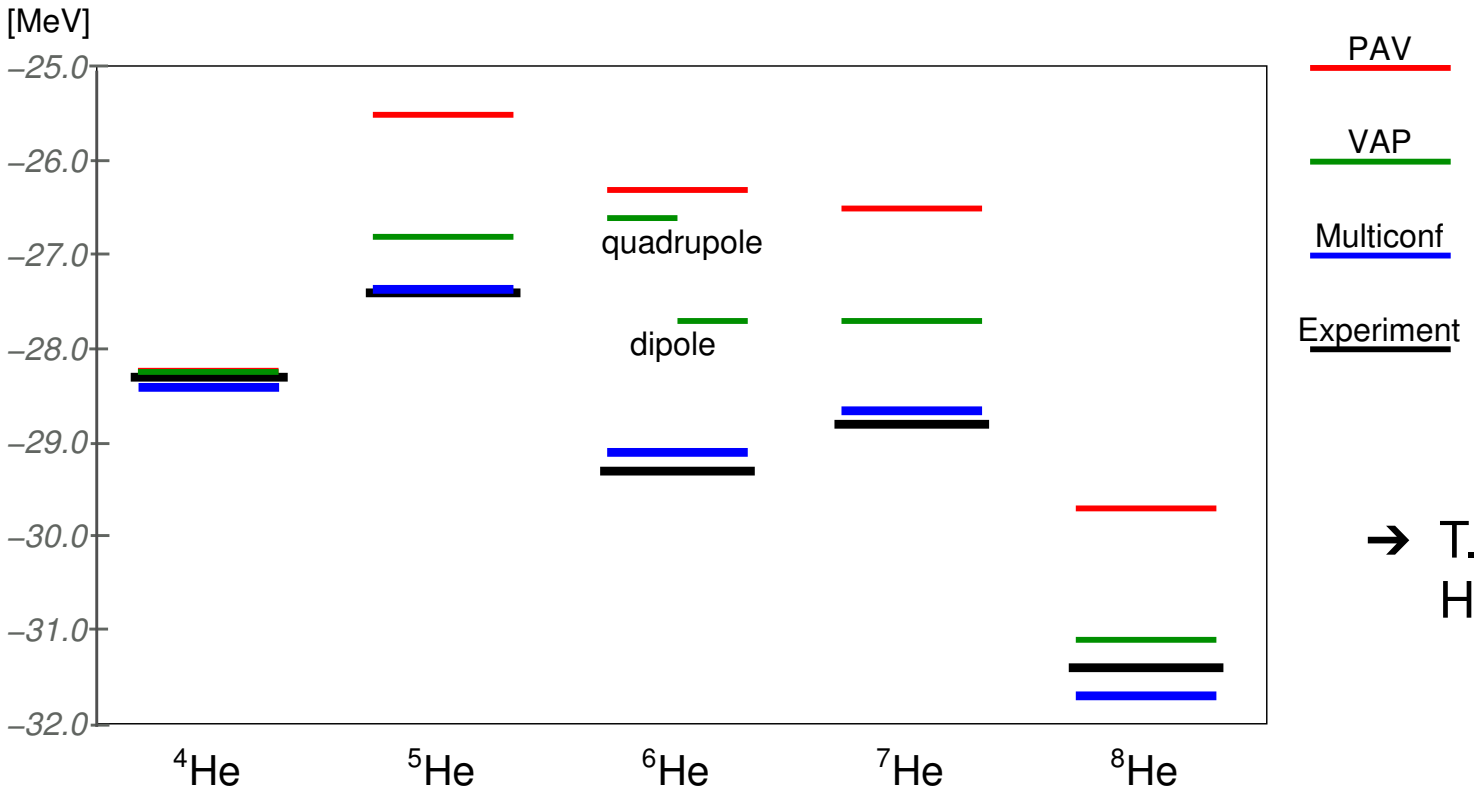




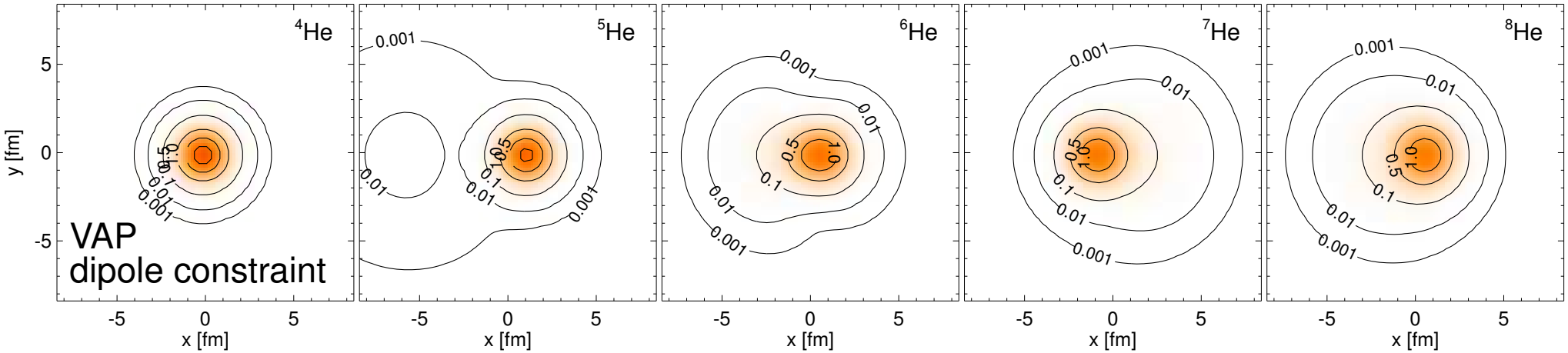




Helium Isotopes: VAP / Multi-Configuration



➔ T. Neff
HK 6.8



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
- first **PAV, VAP, and multi-configuration** calculations for light nuclei look very promising ➔ T. Neff, HK 6.8

Outlook

- correlated realistic NN-interaction provides **robust starting point for all kinds of many-body models**
- **Hartree-Fock** calculations for larger nuclei based on correlated realistic interaction
- systematic study of **excitation spectra**, transition strengths, spectroscopic factors,...
- implementation of **effective three-body forces** instead of phenomenological two-body corrections