# Nuclear Structure based on Correlated Realistic NN-Interactions

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# Overview

- Motivation
- Correlations in Nuclei
- Unitary Correlation Operator Method (UCOM)
- UCOM-Hartree-Fock
- Fermionic Molecular Dynamics

# Two Problems in Nuclear Structure

consider the nucleus as a
non-relativistic microscopic
many-nucleon system

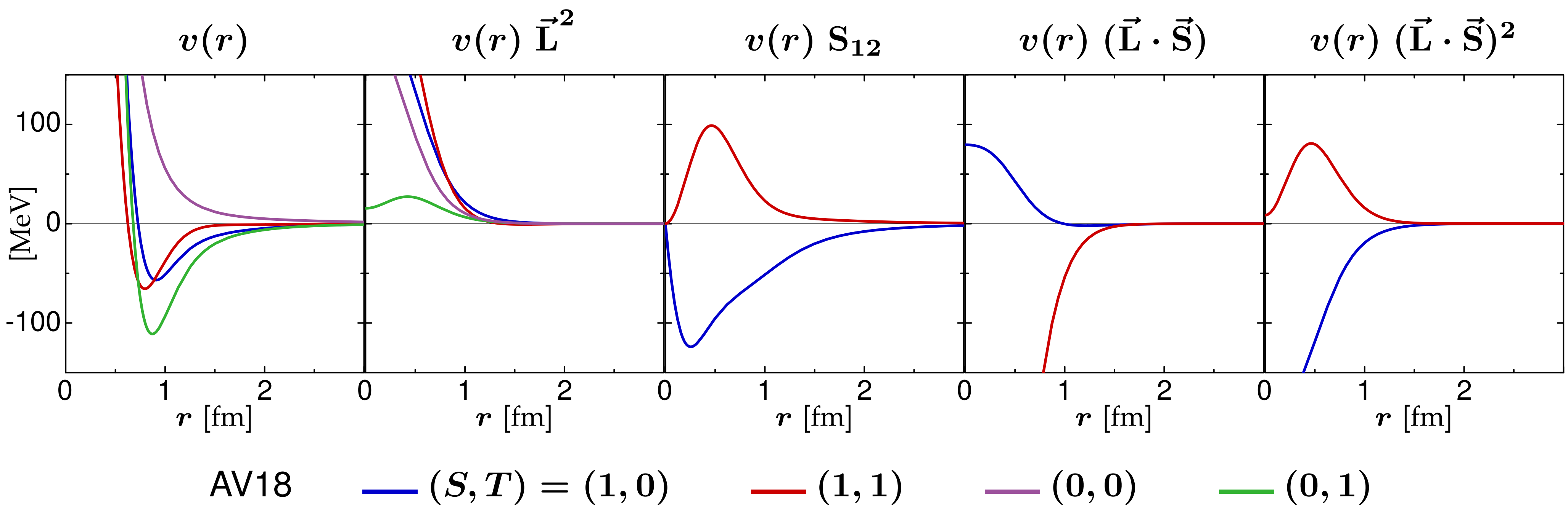
**What is the interaction between the nucleons?**

**How to solve the quantum many-body problem?**

significant progress over the past decade....

# Realistic Potentials

- several realistic NN-potentials are available
  - Argonne V18, CD Bonn, Nijmegen,...
  - reproduce experimental scattering data and deuteron properties with high accuracy

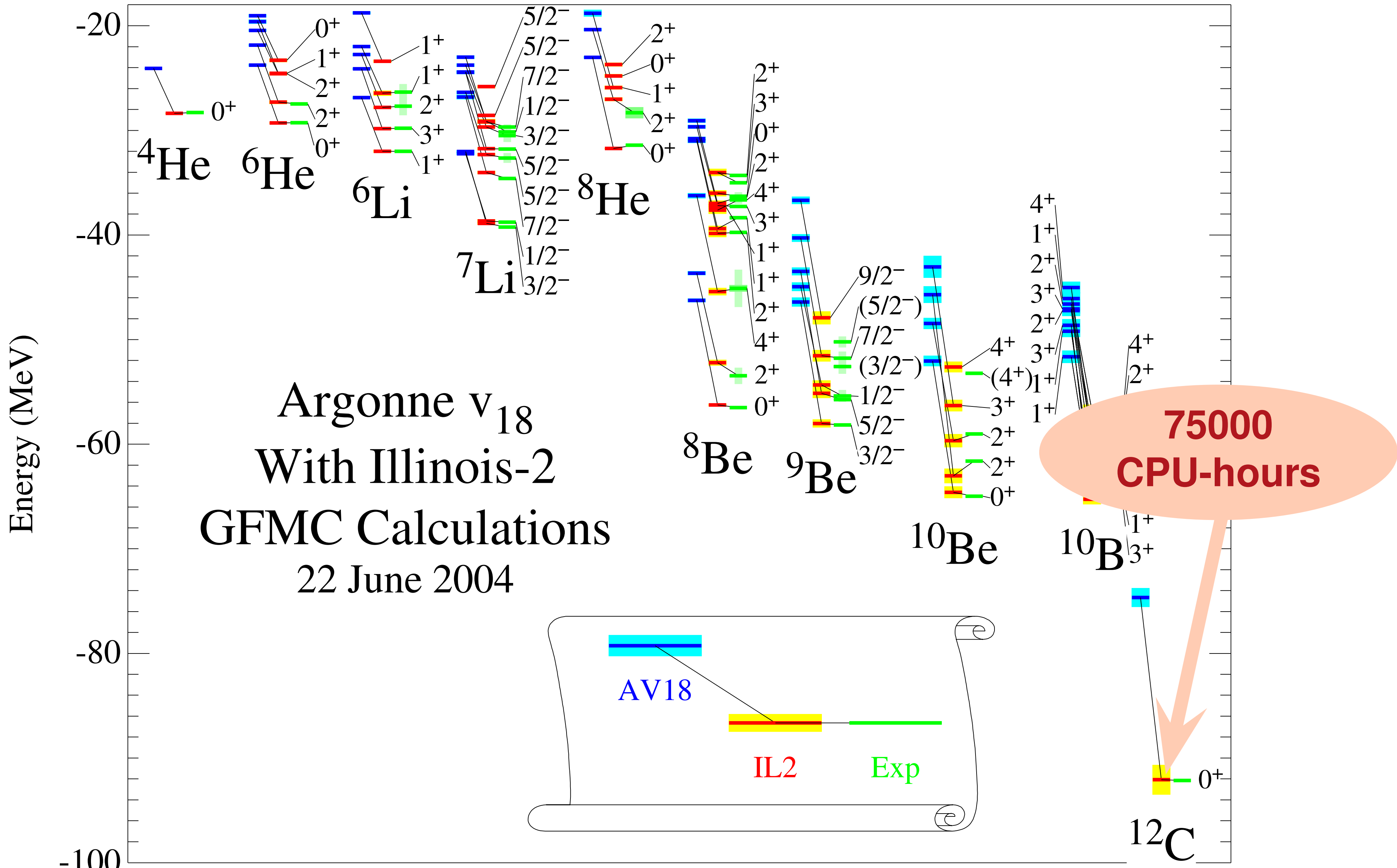


# Realistic Potentials

- several realistic NN-potentials are available
  - Argonne V18, CD Bonn, Nijmegen,...
  - reproduce experimental scattering data and deuteron properties with high accuracy

- need to be supplemented by a three-nucleon potential
  - NNN-potential depends on NN-potential
  - present NNN-potentials are purely phenomenological
  - very promising developments in chiral effective field theories towards a consistent NN + NNN-potential

# Ab initio Calculations




[S. Pieper, private comm.]

$^{12}$C results are preliminary.

# 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**

# Correlations in Nuclei

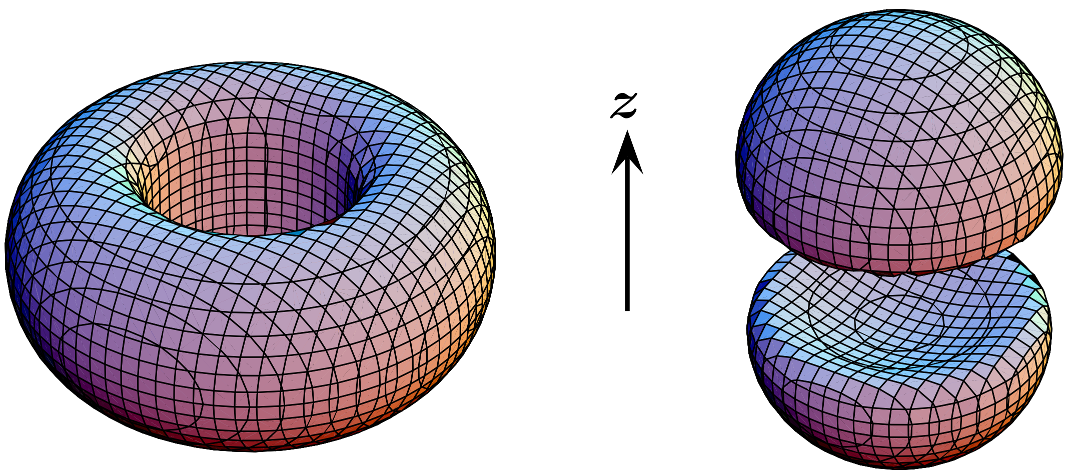
# Deuteron: Manifestation of Correlations

$M_S = 0$

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

$M_S = \pm 1$

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




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

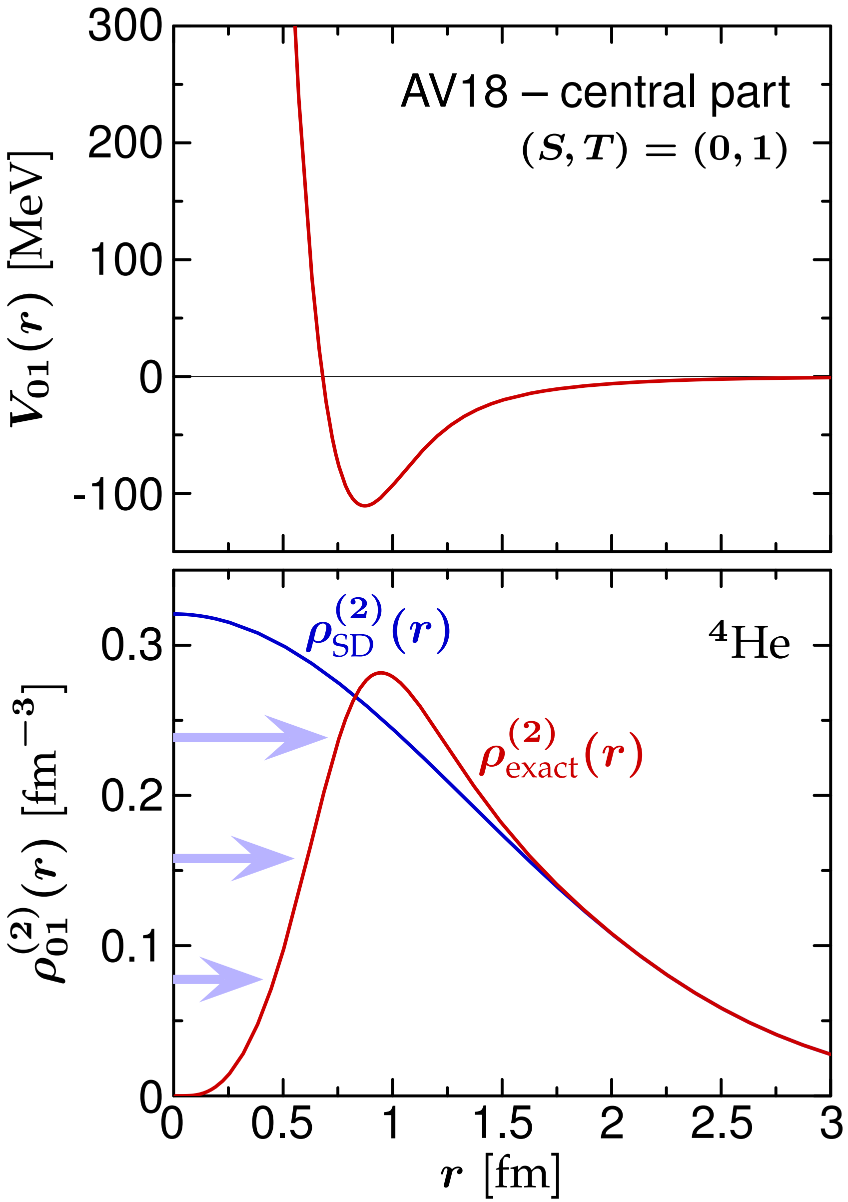
two-body density fully suppressed at small particle distances $|\vec{r}|$

**central correlations**

angular distribution depends strongly on relative spin orientation

**tensor correlations**

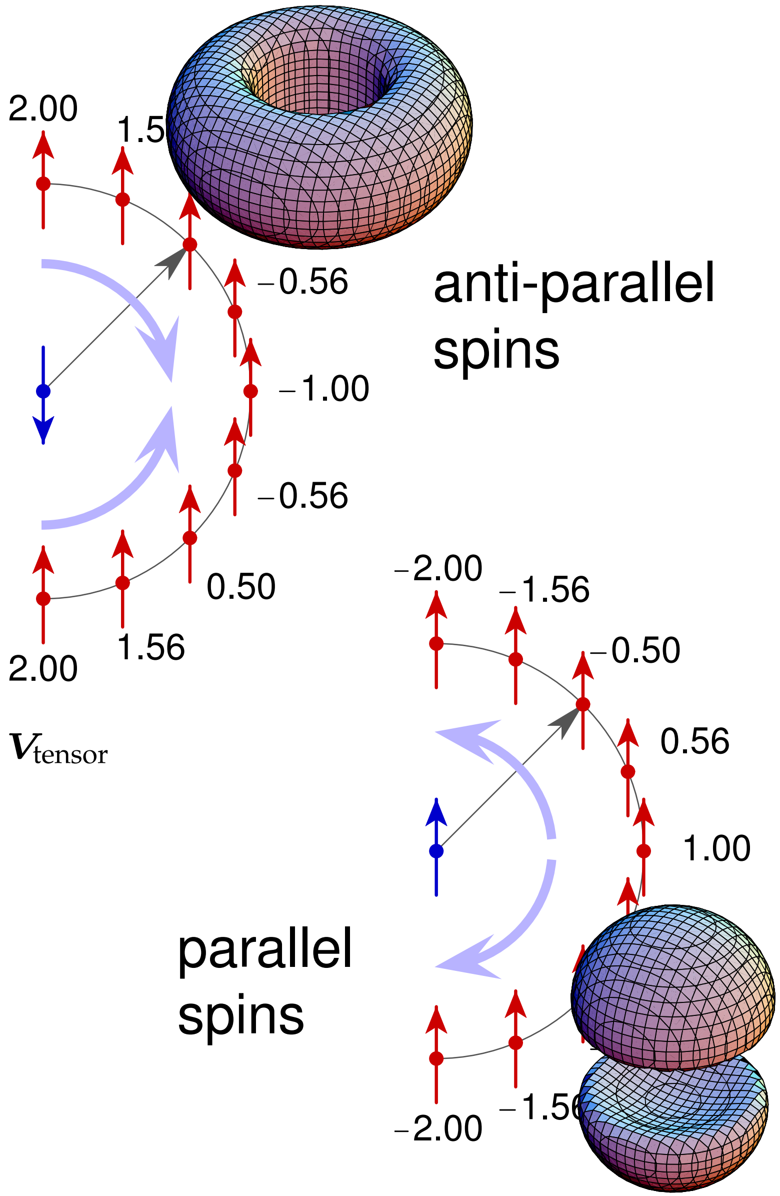
# Central Correlations




- strong repulsive core in central part of realistic interactions
- suppression of the probability density for finding two nucleons within the core region ➔ **central correlations**
- cannot be described by single or superpos. of few Slater determinants

**“shift the nucleons out of the core region”**

# Tensor Correlations




- analogy with dipole-dipole interaction

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

- couples the relative spatial orientation of two nucleons with their spin orientation ➔ **tensor correlations**

- cannot be described by single or superpos. of few Slater determinants

**“rotate nucleons towards poles or equator depending on spin orientation”**

# Unitary Correlation Operator Method (UCOM)

# Unitary Correlation Operator Method

## Correlation Operator

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

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

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

$$\mathrm{G}^\dagger = \mathrm{G}$$
$$\mathrm{C}^\dagger\mathrm{C} = 1$$

**Correlated Operators**

$$\widehat{\mathrm{O}} = \mathrm{C}^\dagger\ \mathrm{O}\ \mathrm{C}$$

**Correlated States**

$$\big|\widehat{\psi}\big\rangle = \mathrm{C}\ \big|\psi\big\rangle$$

$$\big\langle\psi\big|\,\widehat{\mathrm{O}}\,\big|\psi'\big\rangle = \big\langle\psi\big|\,\mathrm{C}^\dagger\ \mathrm{O}\ \mathrm{C}\,\big|\psi'\big\rangle = \big\langle\widehat{\psi}\big|\,\mathrm{O}\,\big|\widehat{\psi}'\big\rangle$$

# Central and Tensor Correlators

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

## Central Correlator $\mathrm{C}_r$

- 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 $\mathrm{C}_\Omega$

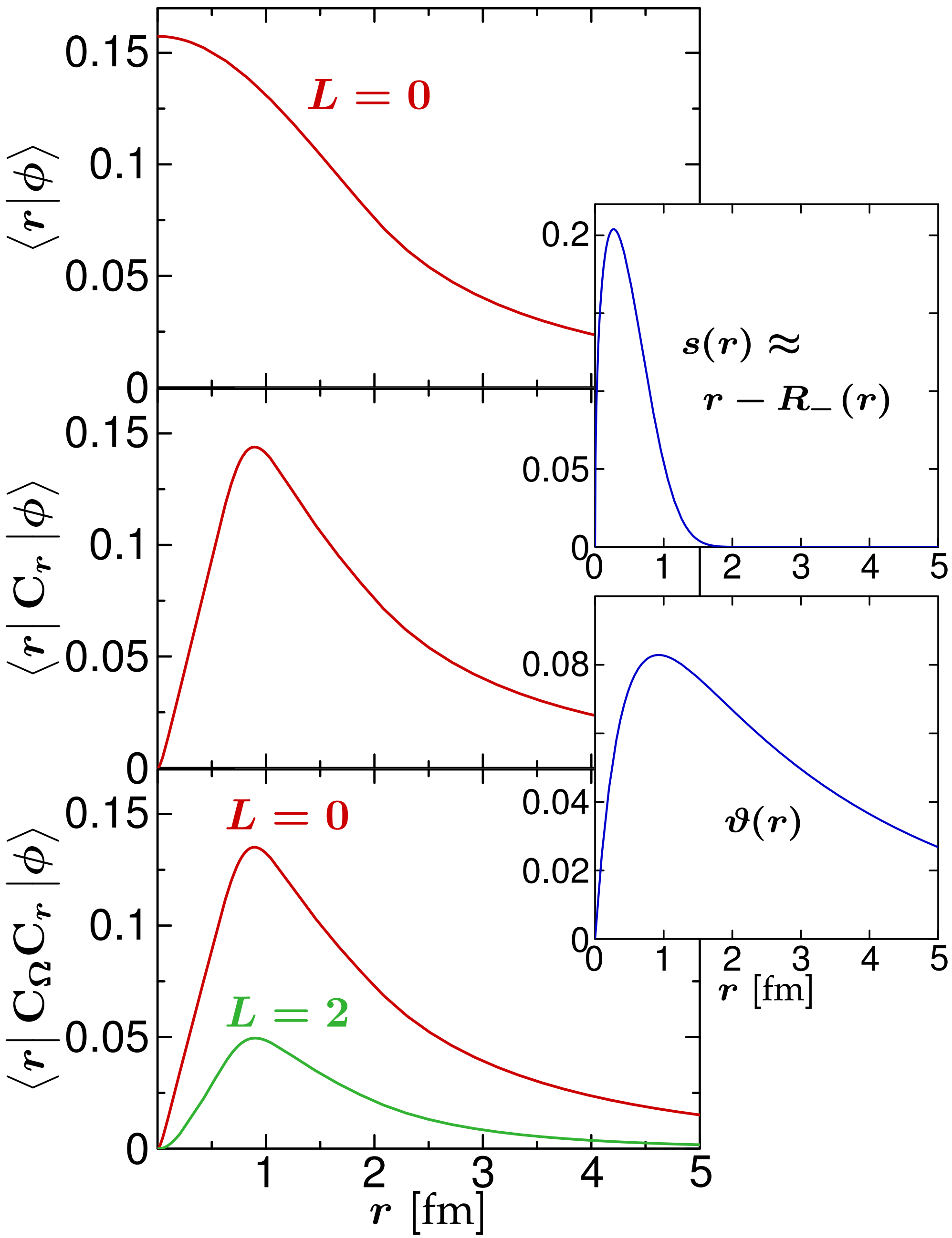
- angular shift depending on the orientation of spin and relative coordinate of a nucleon pair

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

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

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

# Correlated States




## Central Correlations

$$\langle \vec{r} | \, \mathrm{C}_r \, | \phi; (01)1 \rangle =$$

$$= \sqrt{R'_-(r)} \, \frac{R_-(r)}{r} \, \langle R_-(r) \tfrac{\vec{r}}{r} | \phi; (01)1 \rangle$$

## Tensor Correlations

$$\langle \vec{r} | \, \mathrm{C}_\Omega \, | \phi; (01)1 \rangle =$$

$$= \cos(3\sqrt{2} \, \vartheta(r)) \, \langle \vec{r} | \phi; (01)1 \rangle$$

$$+ \sin(3\sqrt{2} \, \vartheta(r)) \, \langle \vec{r} | \phi; (21)1 \rangle$$

# Correlated Operators

**Cluster Expansion**

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

**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.**

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

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

# Correlated NN-Potential — $V_{\mathrm{UCOM}}$

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

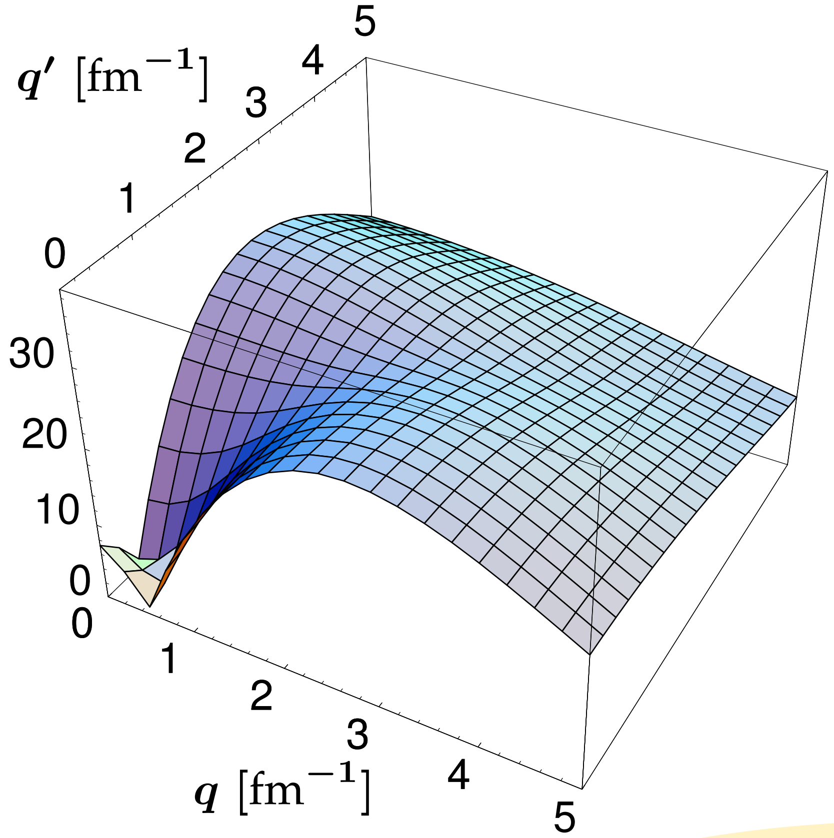
- **closed operator expression** for the correlated interaction $\mathbf{V}_{\mathrm{UCOM}}$ in two-body approximation
- correlated interaction and original NN-potential are **phase shift equivalent** by construction
- **central correlator**: removes the repulsive core and generates additional momentum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

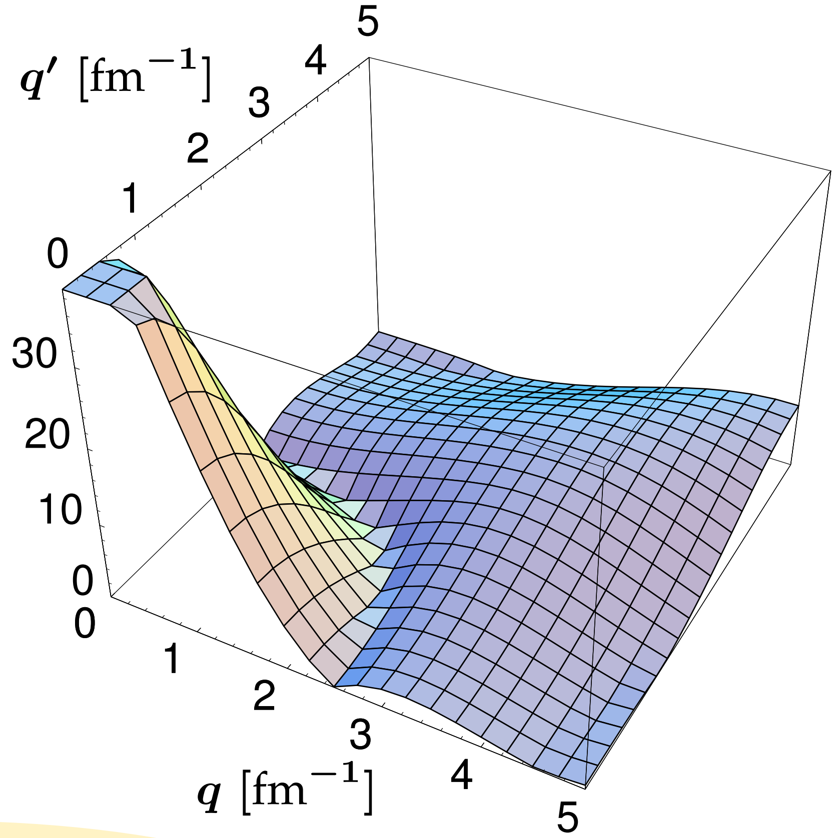
# Momentum-Space Matrix Elements

$|\langle q|\ \mathrm{V}\ |q'\rangle|$

$^3S_1$

$|\langle q|\ \mathrm{V}_{\mathrm{UCOM}}\ |q'\rangle|$

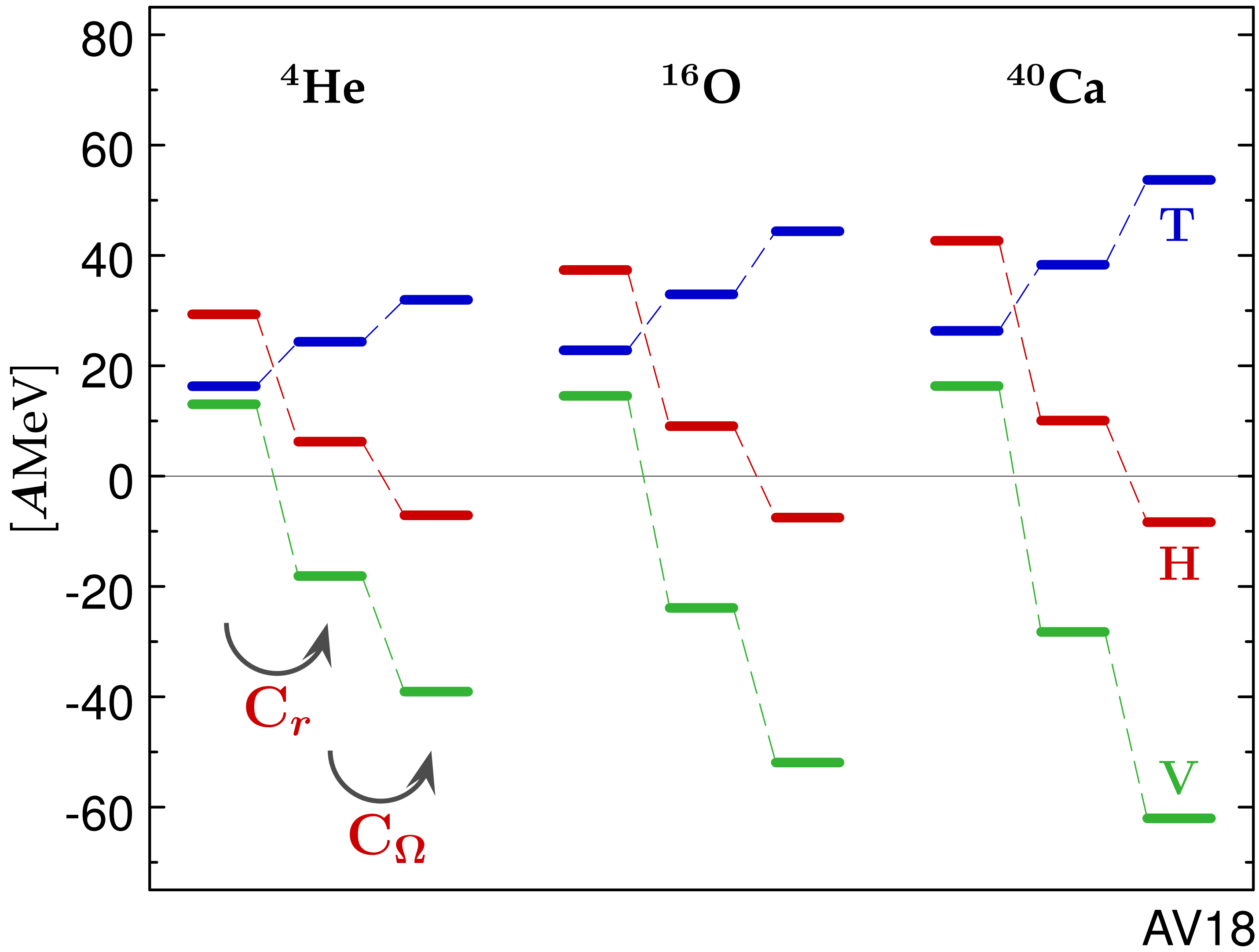



**pre-diagonalisation of Hamiltonian**

AV18

# 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 Hartree-Fock

# UCOM-HF Scheme

**"Standard" Hartree-Fock**

**+**

**Matrix Elements of Correlated Realistic NN-Interaction $\mathrm{V}_{\mathrm{UCOM}}$**

- single-particle states expanded in a spherical oscillator basis
- truncation in $n$, $l$, and/or $N = 2n + l$ (typically $N_{\mathrm{max}} = 6 \ldots 10$)
- Coulomb interaction included exactly
- formulated with intrinsic kinetic energy $\mathrm{T}_{\mathrm{int}} = \mathrm{T} - \mathrm{T}_{\mathrm{cm}}$ to eliminate centre of mass contributions

# Correlated Oscillator Matrix Elements

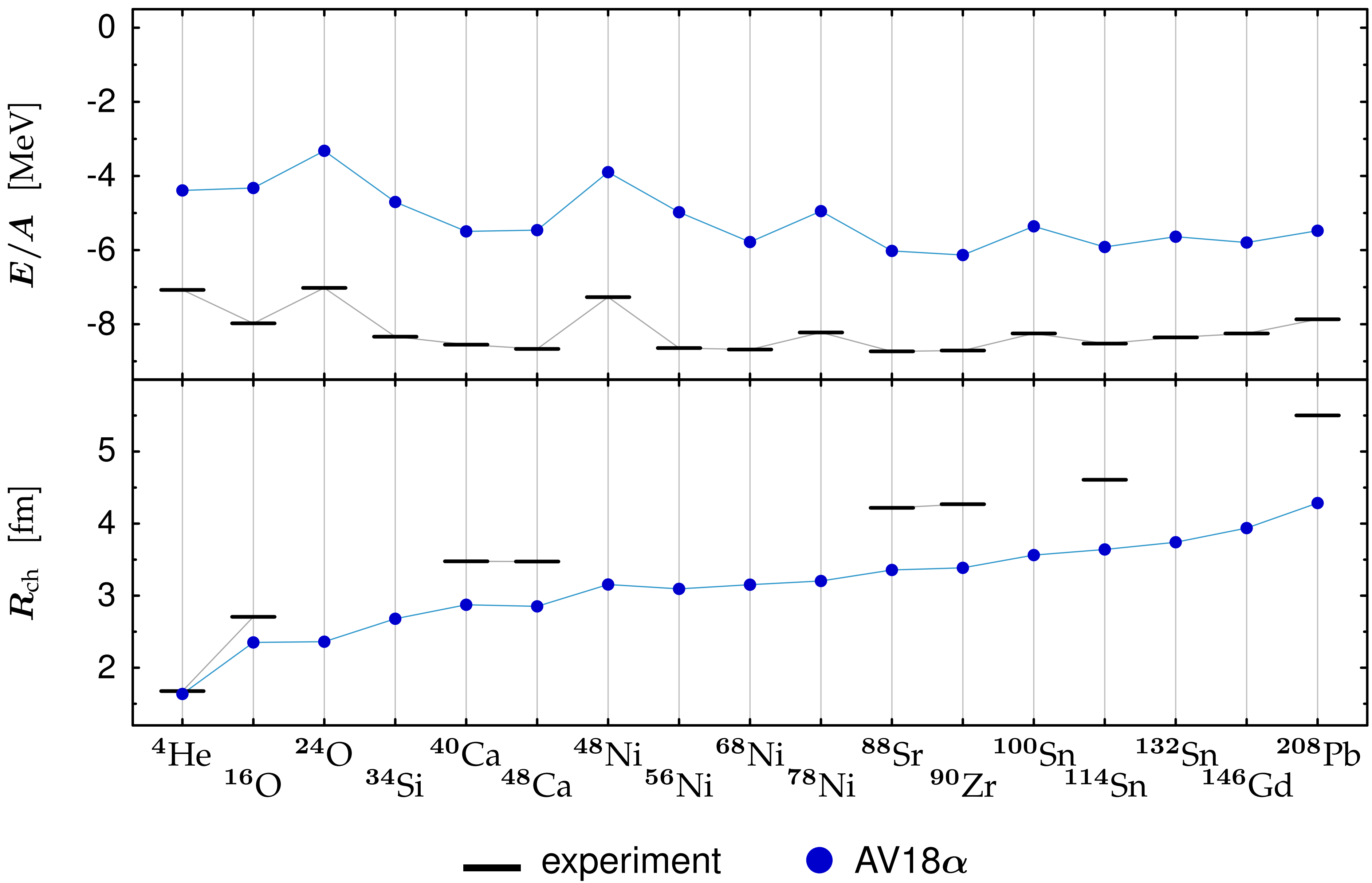
$$\langle n(LS)JT | \mathrm{C}_r^\dagger \mathrm{C}_\Omega^\dagger \, \mathrm{H} \, \mathrm{C}_\Omega \mathrm{C}_r | n'(L'S)JT \rangle$$
$$= \langle n(LS)JT | \mathrm{T} + \mathrm{V}_{\mathrm{UCOM}} | n'(L'S)JT \rangle$$

calculate using uncorrelated states and operator form of $\mathrm{V}_{\mathrm{UCOM}}$

map correlator onto states and use bare interaction (avoids BCH expansion)

- Talmi-Moshinsky transformation & recoupling to obtain $jj$-coupled matrix elements
- input for all kinds of many-body methods (HF, NCSM, CC,...)

# Correlated Argonne V18



# Missing Pieces

**long-range correlations**

**genuine three-body forces**

**three-body cluster contributions**

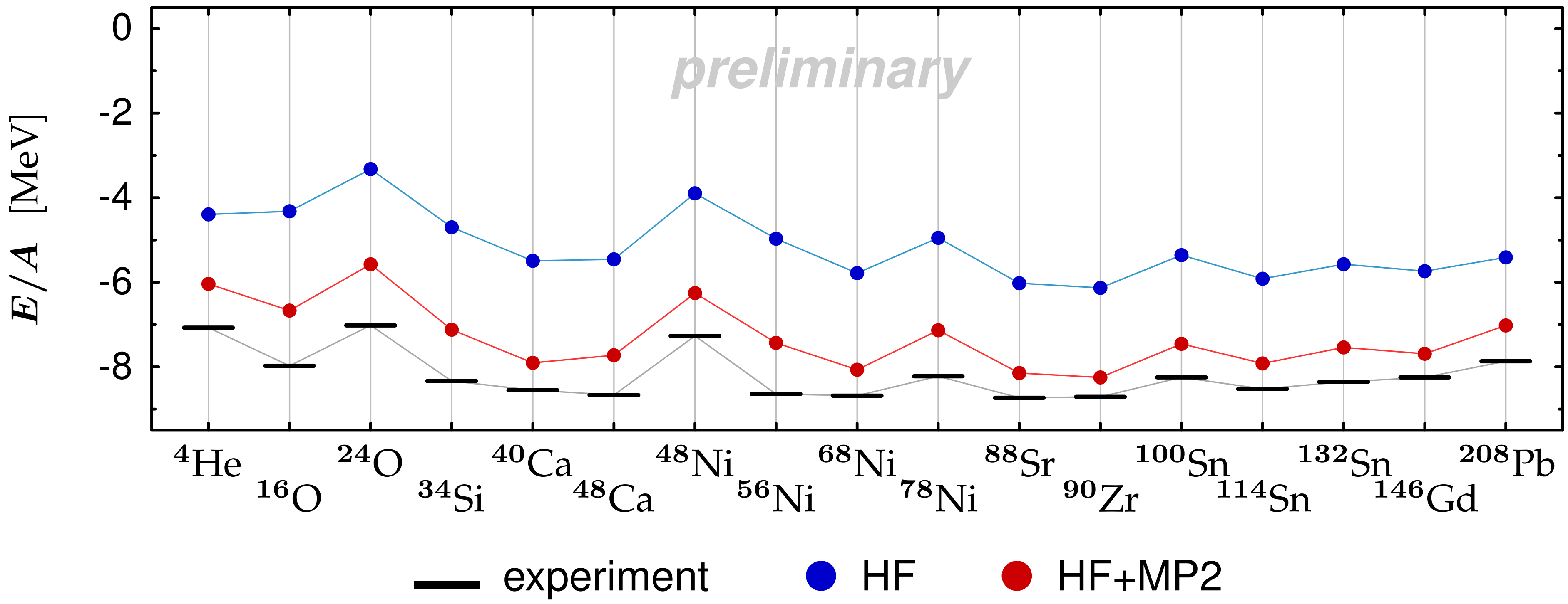
## Improvements

- improved many-body state: RPA, CI, CC, NCSM,...
- include genuine three-body forces & three-body clusters
- construct phenomenological three-body force

# Long-Range Correlations

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

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



# Missing Pieces

long-range correlations

genuine three-body forces

three-body cluster contributions

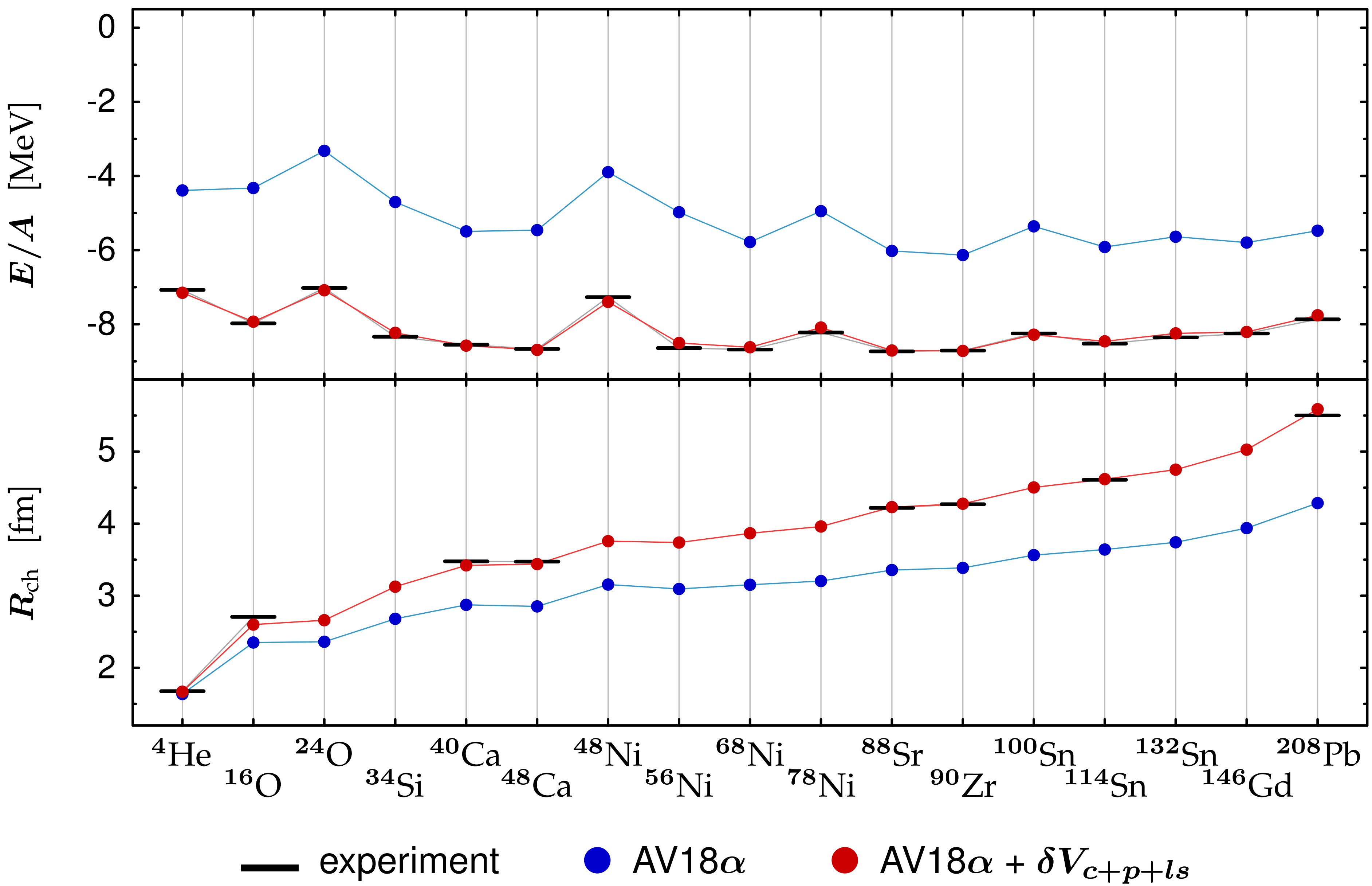
## Pragmatic Approach

- phenomenological two-body correction

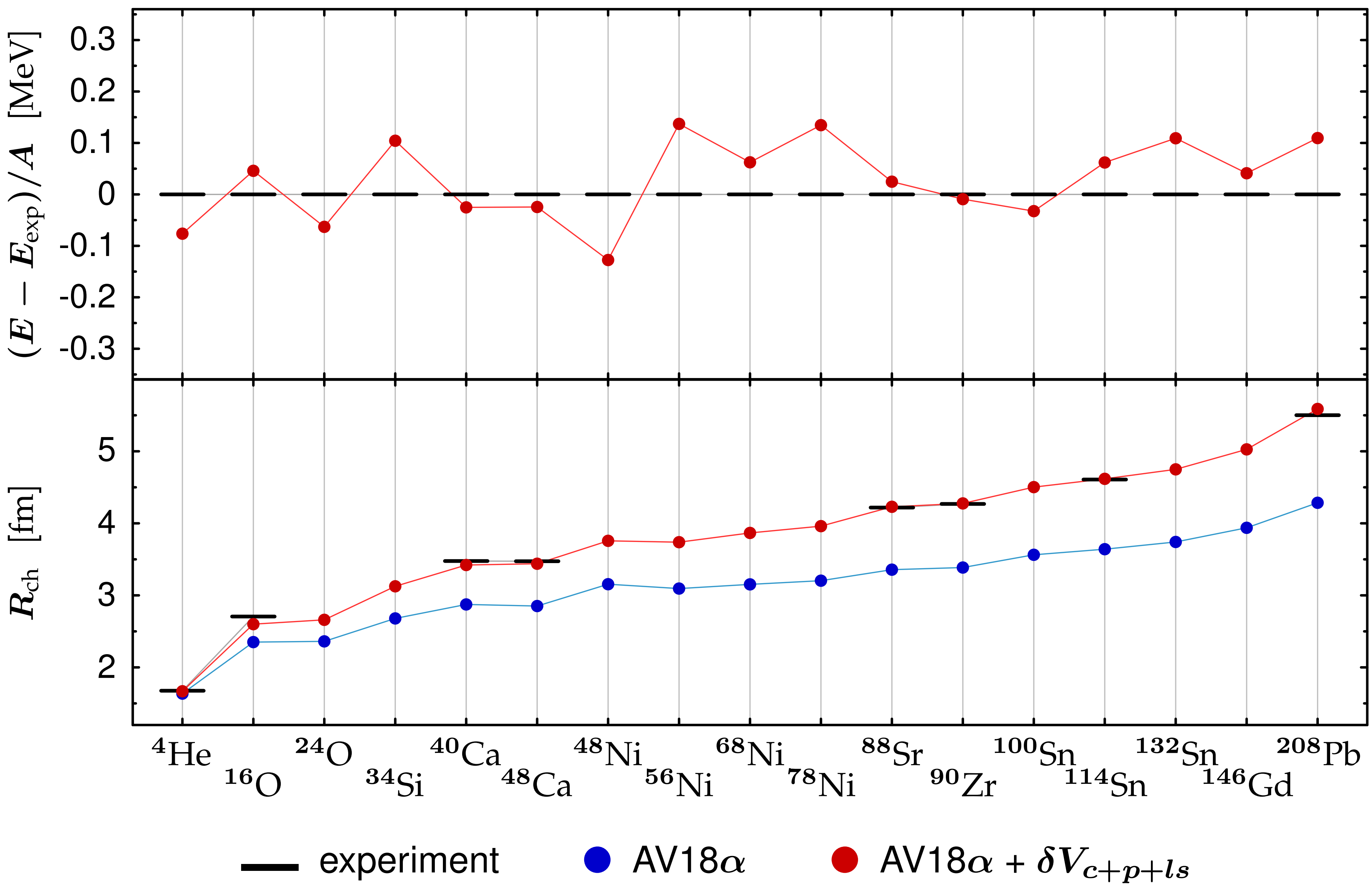
$$\delta \mathrm{V}_{c+p+ls} = v_1(\mathrm{r}) + \vec{\mathrm{q}}\, v_{qq}(\mathrm{r})\, \vec{\mathrm{q}} + v_{LS}(\mathrm{r})\, \vec{\mathrm{L}} \cdot \vec{\mathrm{S}}$$

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

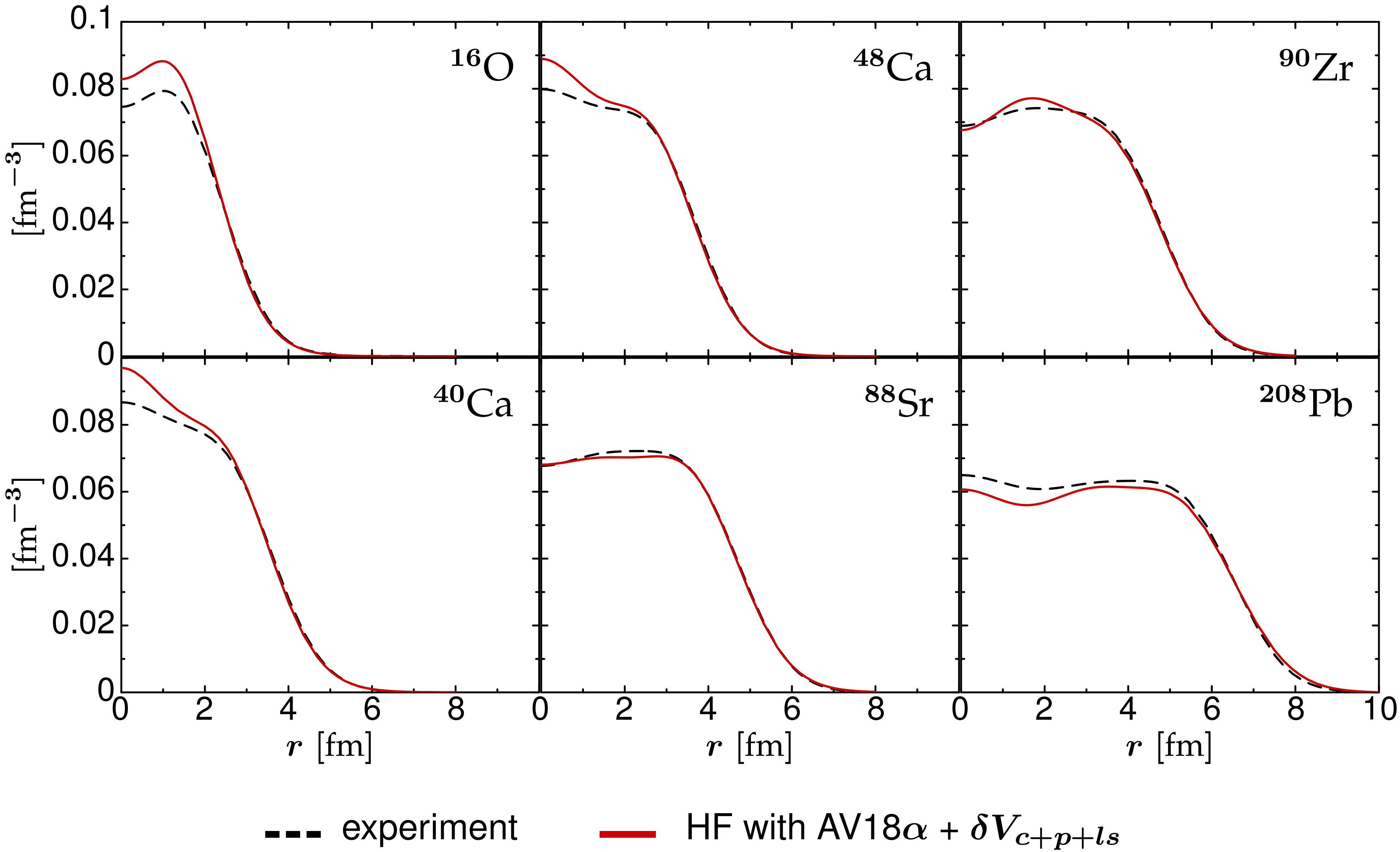
# Correlated Argonne V18 + Correction



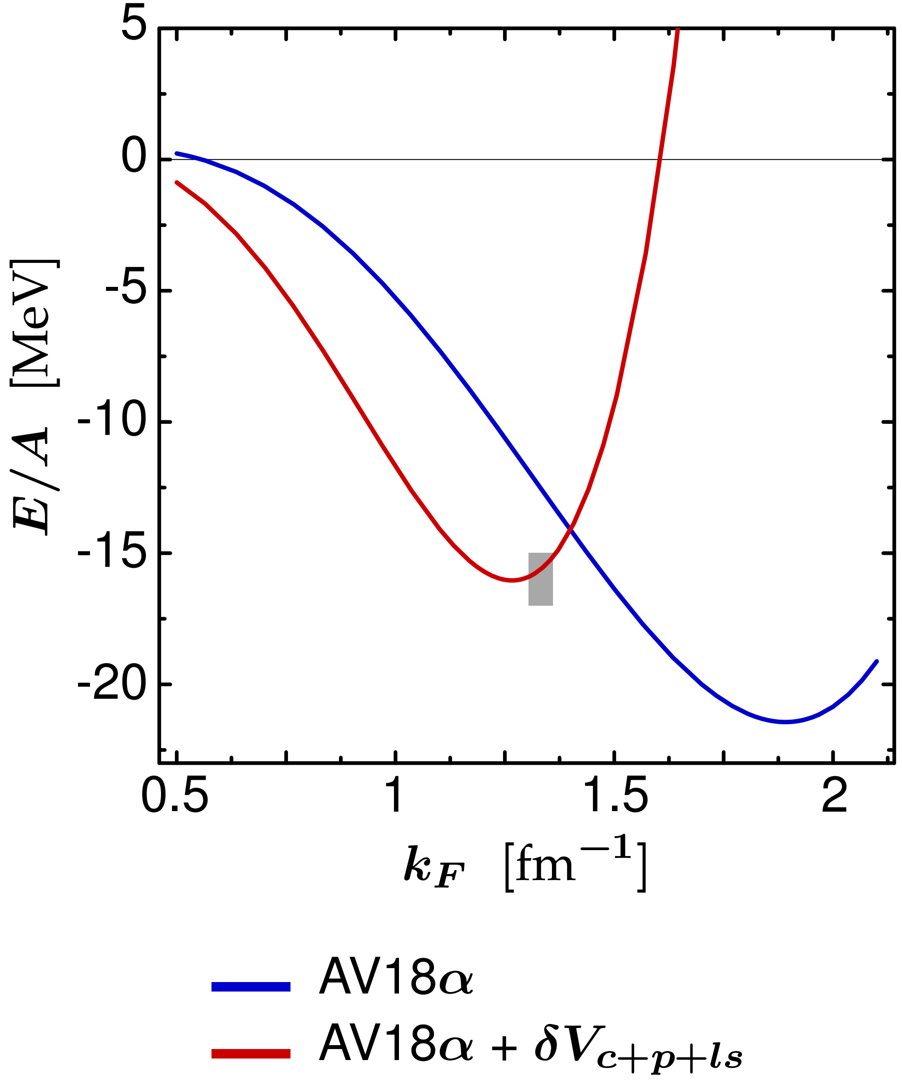
# Correlated Argonne V18 + Correction



# Charge Distributions



# Nuclear Matter: Equation of State




- symmetric nuclear matter
- Slater determinant of plane-wave states $|\vec{k}| \leq k_F$
- correlated momentum space matrix elements
- saturation point:

$$(E/A)_0 \approx -16.0\,\text{MeV}$$
$$\rho_0 \approx 0.14\,\text{fm}^{-3}$$
$$K_0 \approx 280\,\text{MeV}$$

- HvH theorem fulfilled

# Fermionic Molecular Dynamics (FMD)

# FMD Trial States

## Gaussian Single-Particle States

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

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

$a_\nu$ : complex width

$\chi_\nu$ : 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

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

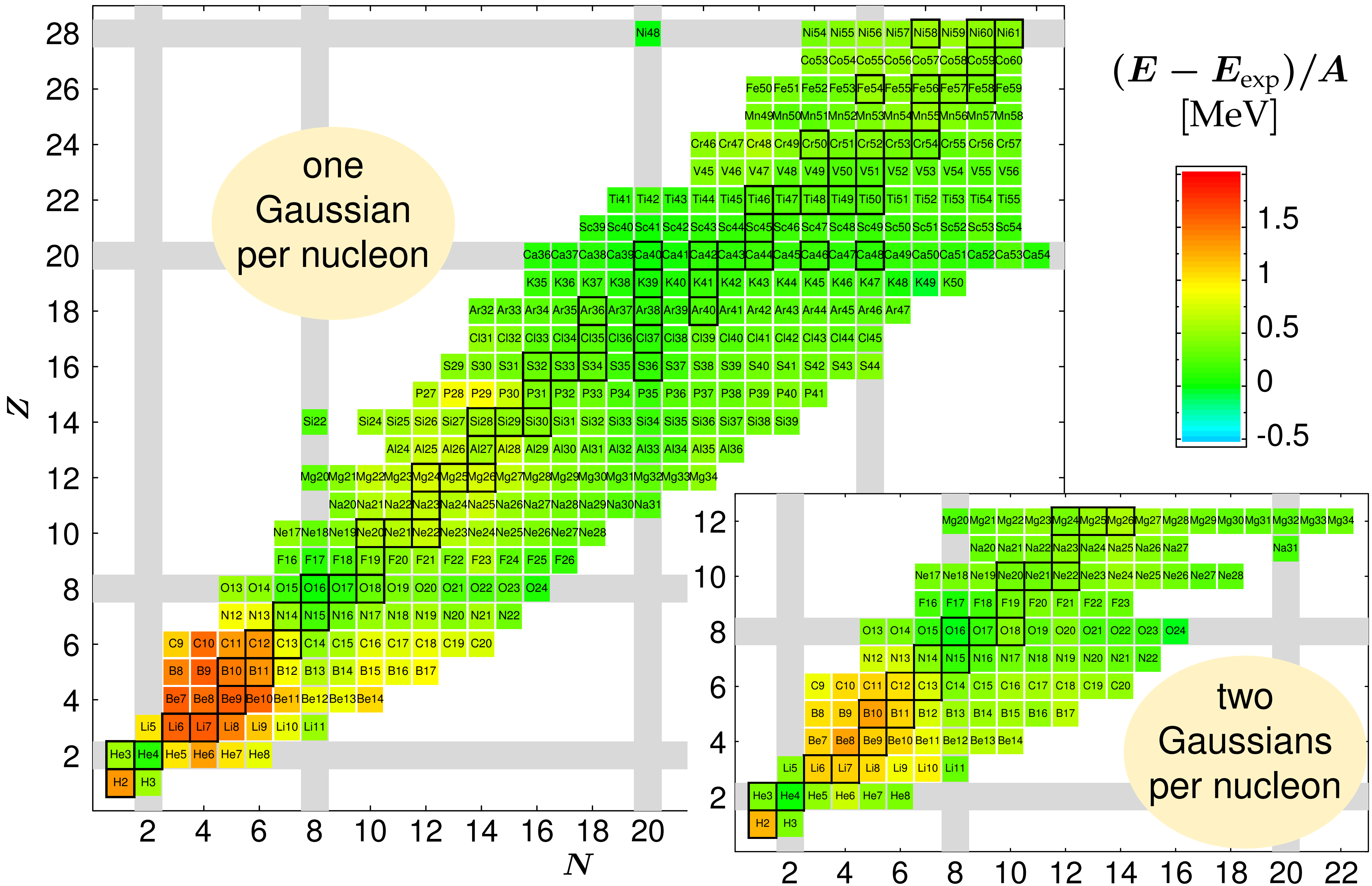
**Variation**

$$\frac{\langle Q | \widehat{\mathrm{H}}^{C2} | Q \rangle}{\langle Q | Q \rangle} \longrightarrow \min$$

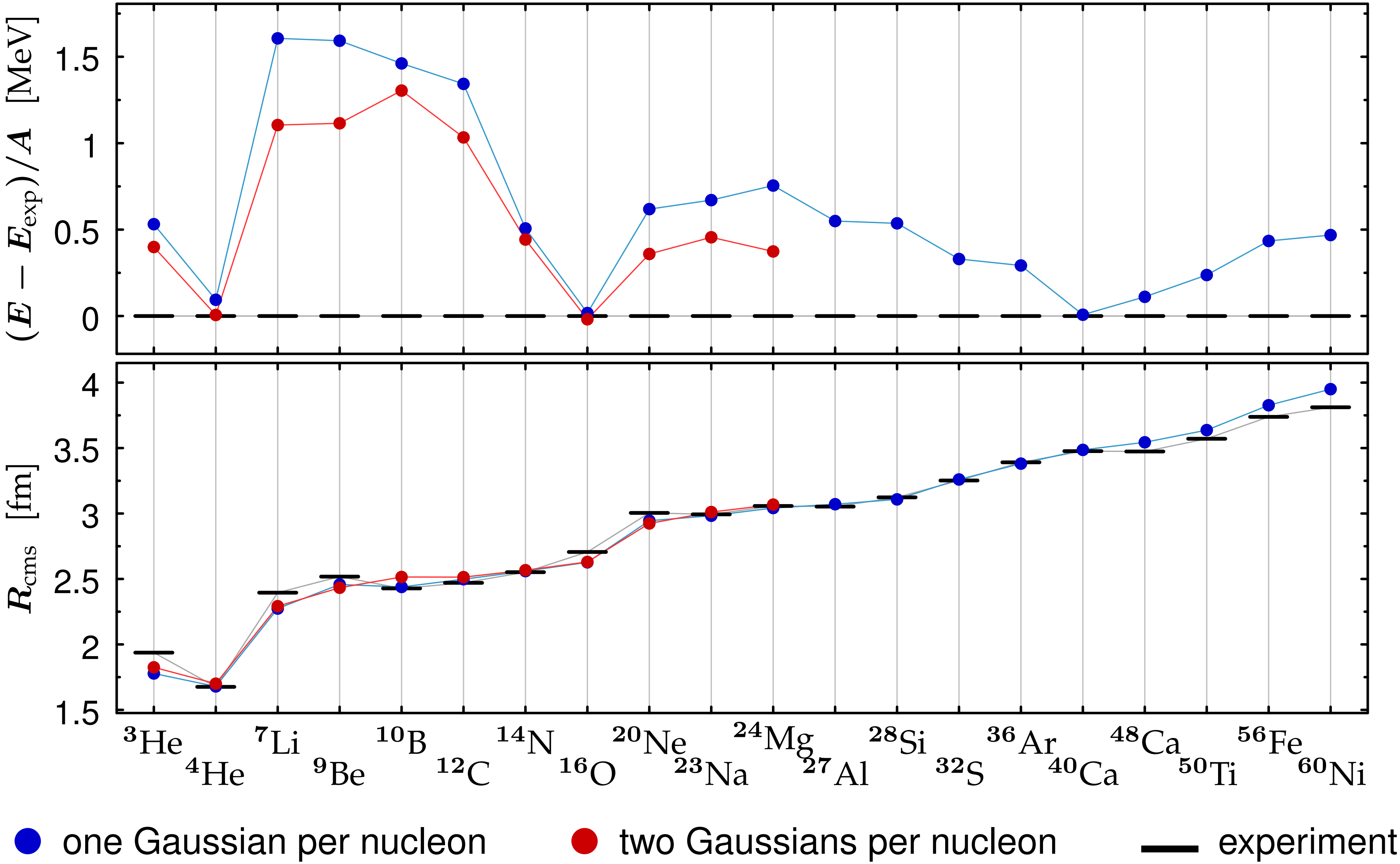
**Diagonalisation**

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

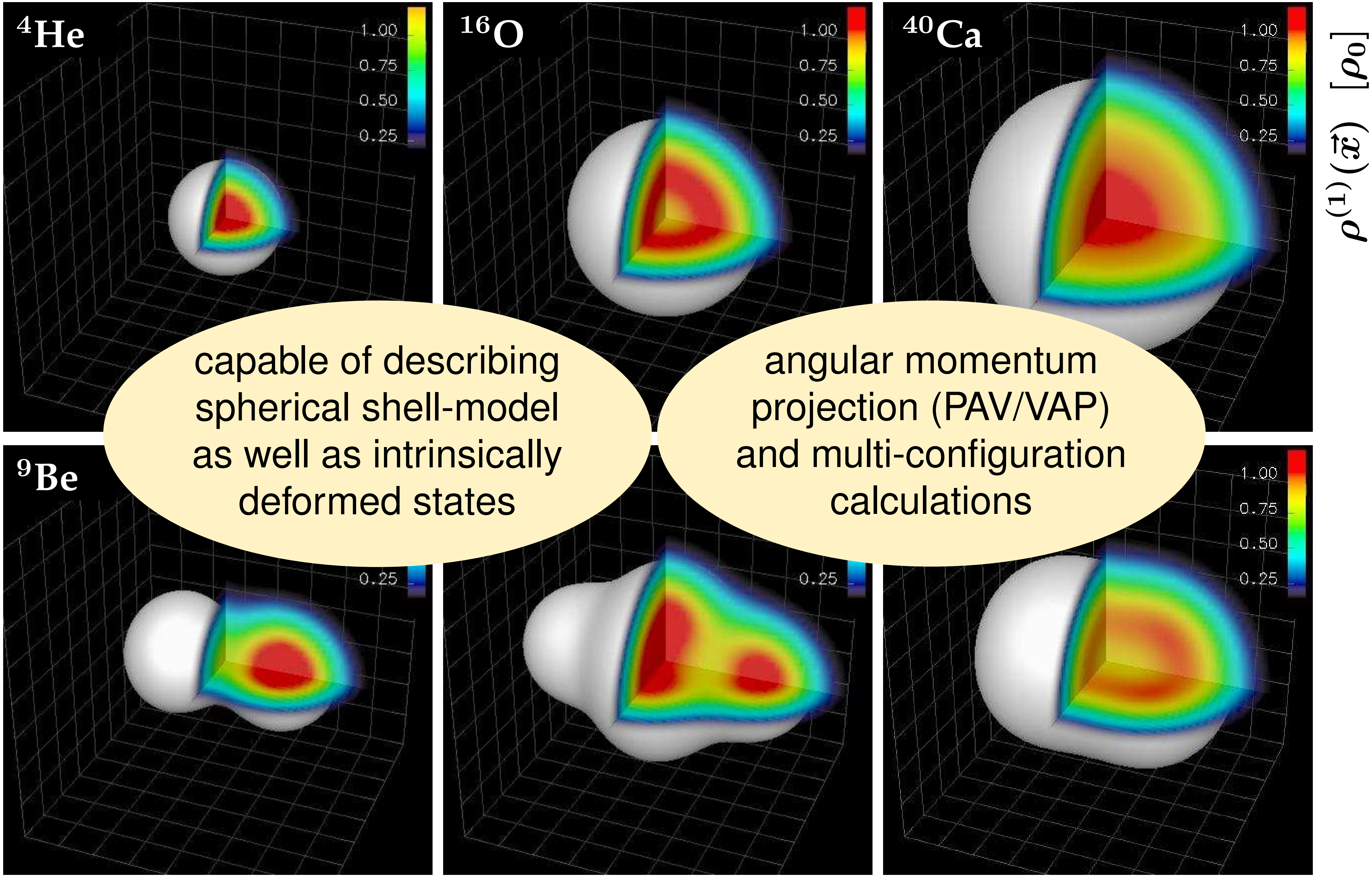
# Chart of Nuclei



# Selected Stable Nuclei



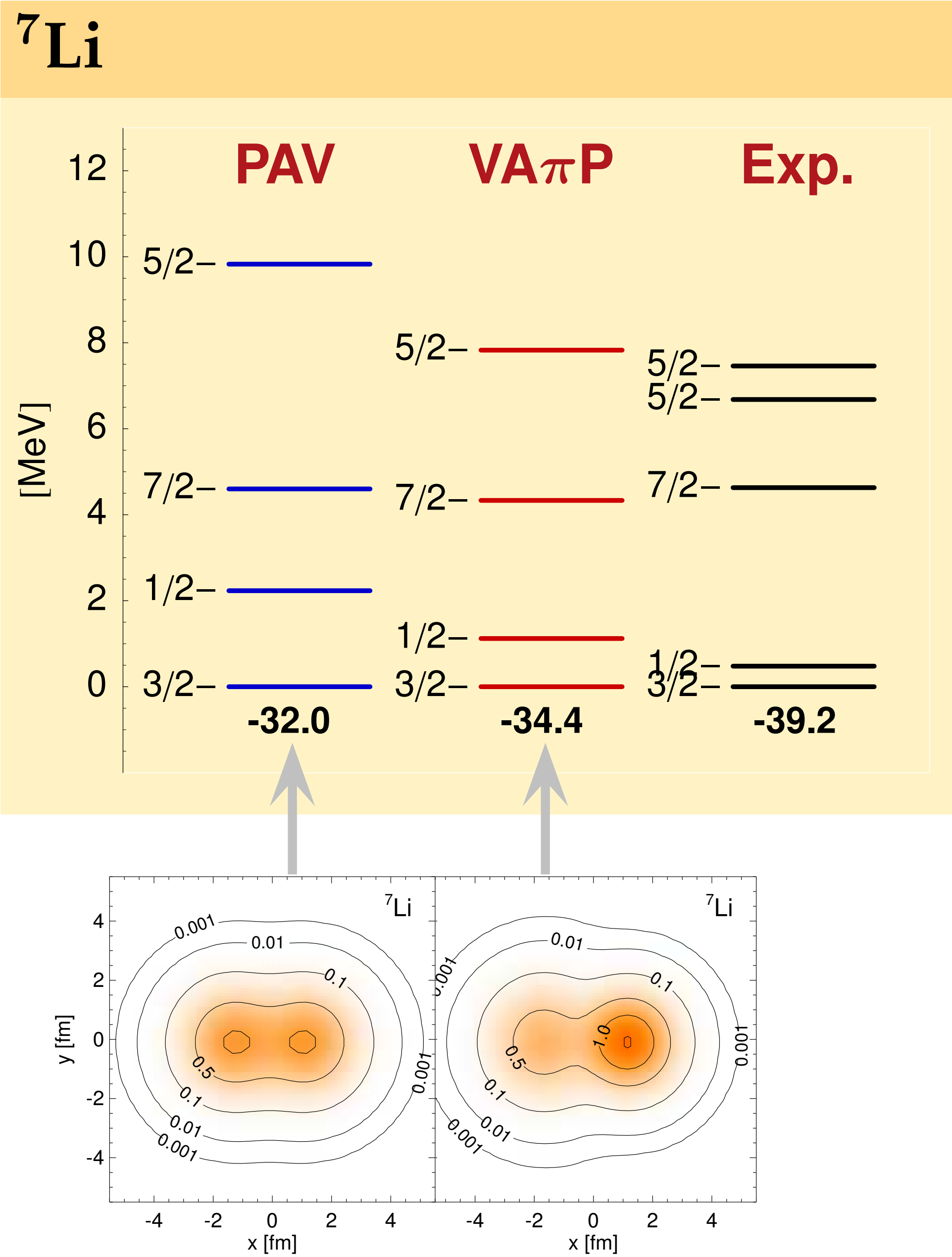
# Intrinsic One-Body Density Distributions

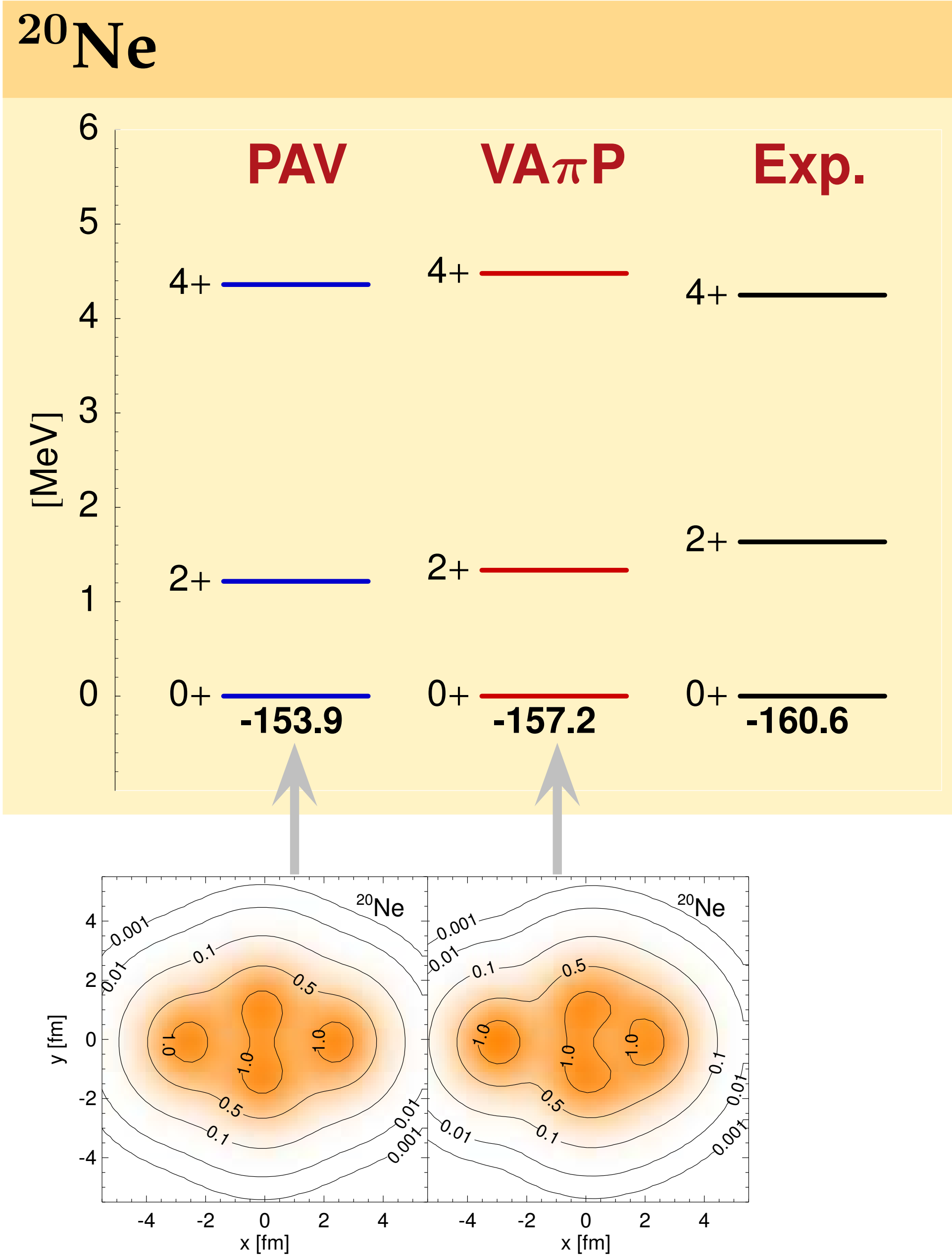



capable of describing spherical shell-model as well as intrinsically deformed states

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

# Parity and Angular Momentum Projection



# Conclusions

- **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 $V_{\mathrm{UCOM}}$**
  - low-momentum / phase-shift equivalent / operator representation
  - robust starting point for all kinds of many-body calculations

# Conclusions

- **UCOM Hartree-Fock**
  - closed shell nuclei across the whole nuclear chart
  - basis for improved many-body calculations (RPA, HFB,...)
- **UCOM + Fermionic Molecular Dynamics**
  - strong intrinsic deformation and clustering for $A \lesssim 60$
  - PAV, VAP, and multi-configuration calculations