The Unitary Correlation Operator Method:

Towards ab initio Nuclear Structure

R. Roth

Institut für Kernphysik, TU Darmstadt

in Collaboration with

H. Hergert, N. Paar,
P. Papakonstantinou,
T. Neff, H. Feldmeier

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GSI

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**

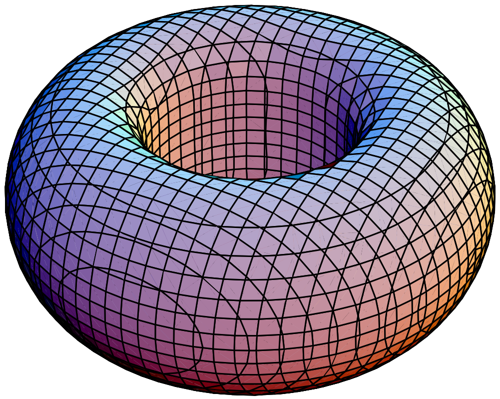
Overview

- Correlations in Nuclei
- Unitary Correlation Operator Method (UCOM)
- Correlated Realistic NN-Potentials
- UCOM-Hartree-Fock
- Fermionic Molecular Dynamics

Deuteron: Manifestation of Correlations

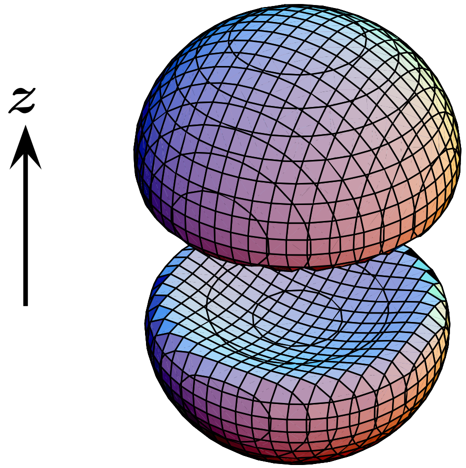
$M_S = 0$

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



$M_S = \pm 1$

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



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

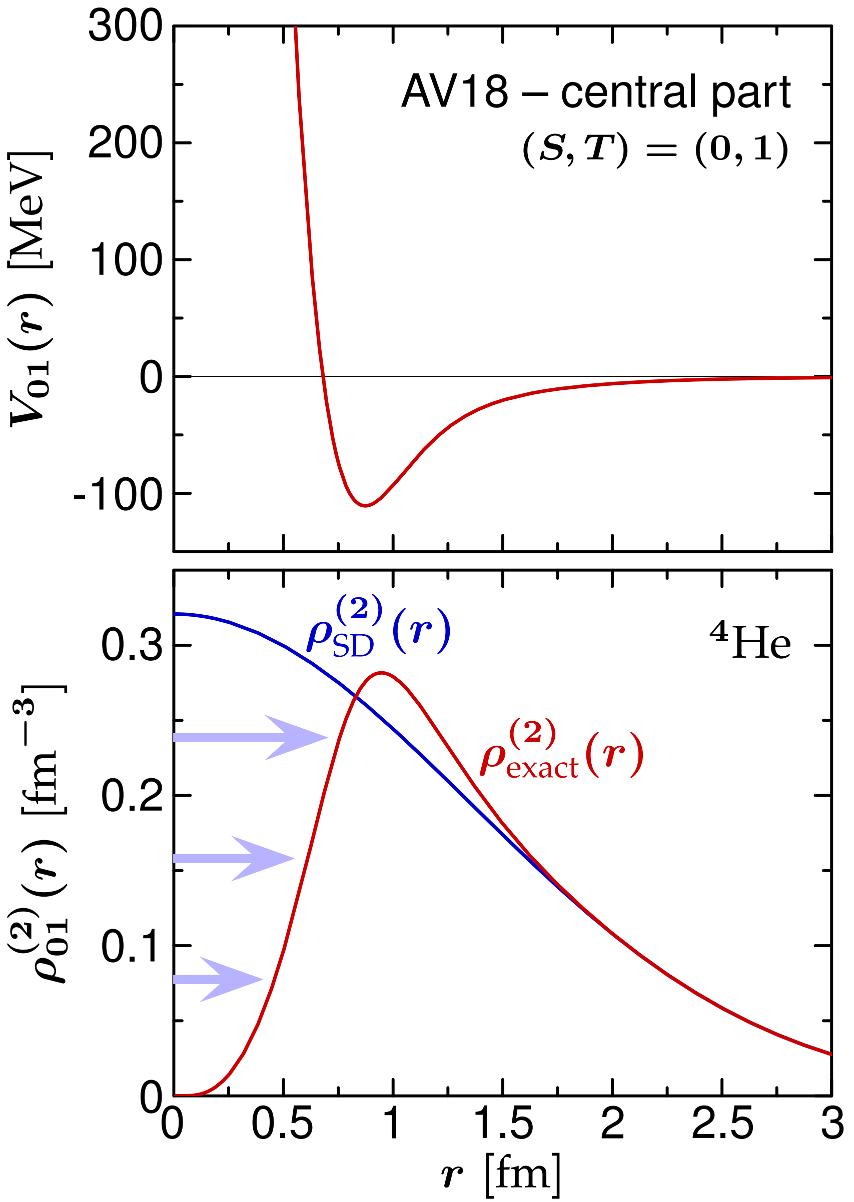
two-body density fully suppressed at small particle distances $|\vec{r}|$

central correlations

angular distribution depends strongly on relative spin orientation

tensor correlations

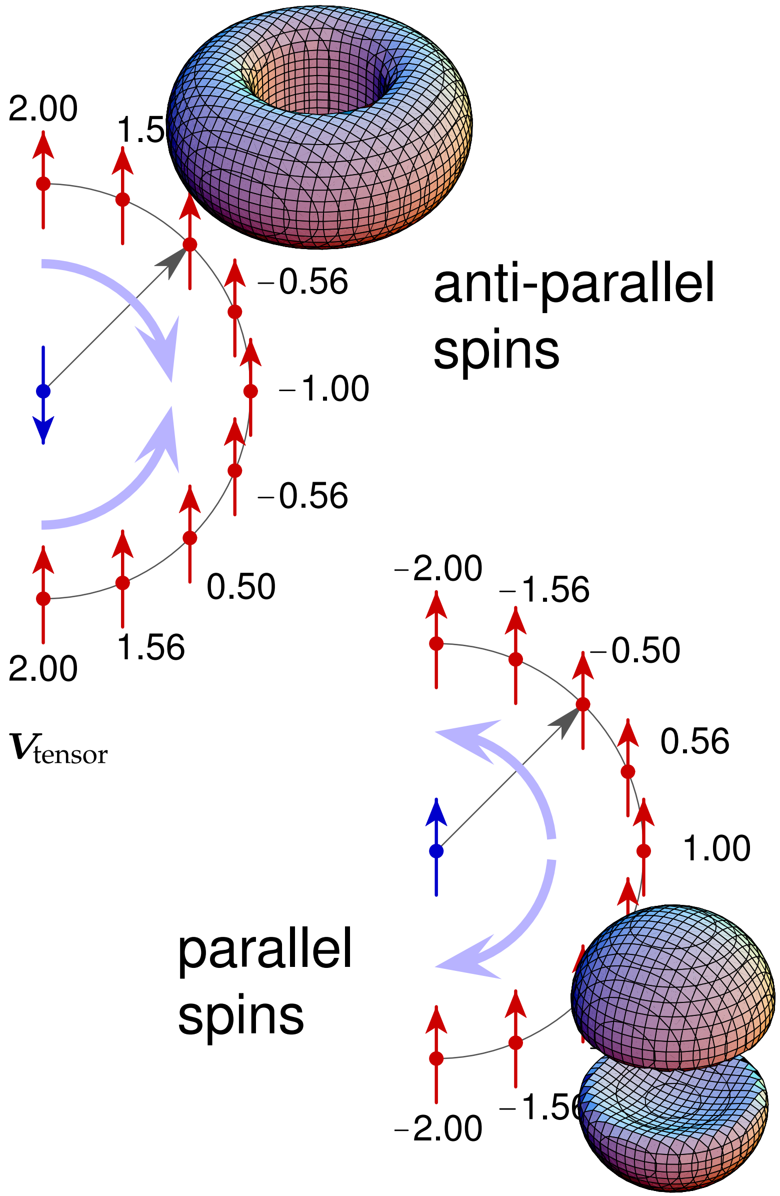
Central Correlations



- two-body density distribution of ^{4}He for $(S,T) = (0,1)$
- strong repulsive core in the 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

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

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

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

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

Correlated Operators

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

Correlated States

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

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

Central and Tensor Correlators

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

Central Correlator $\mathbf{C}_r$

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

$$\mathbf{g}_r = \frac{1}{2}\big[s(\mathbf{r})\ \mathbf{q}_r + \mathbf{q}_r\ s(\mathbf{r})\big]$$

$$\mathbf{q}_r = \tfrac{1}{2}\big[\tfrac{\vec{\mathbf{r}}}{\mathbf{r}} \cdot \vec{\mathbf{q}} + \vec{\mathbf{q}} \cdot \tfrac{\vec{\mathbf{r}}}{\mathbf{r}}\big]$$

Tensor Correlator $\mathbf{C}_\Omega$

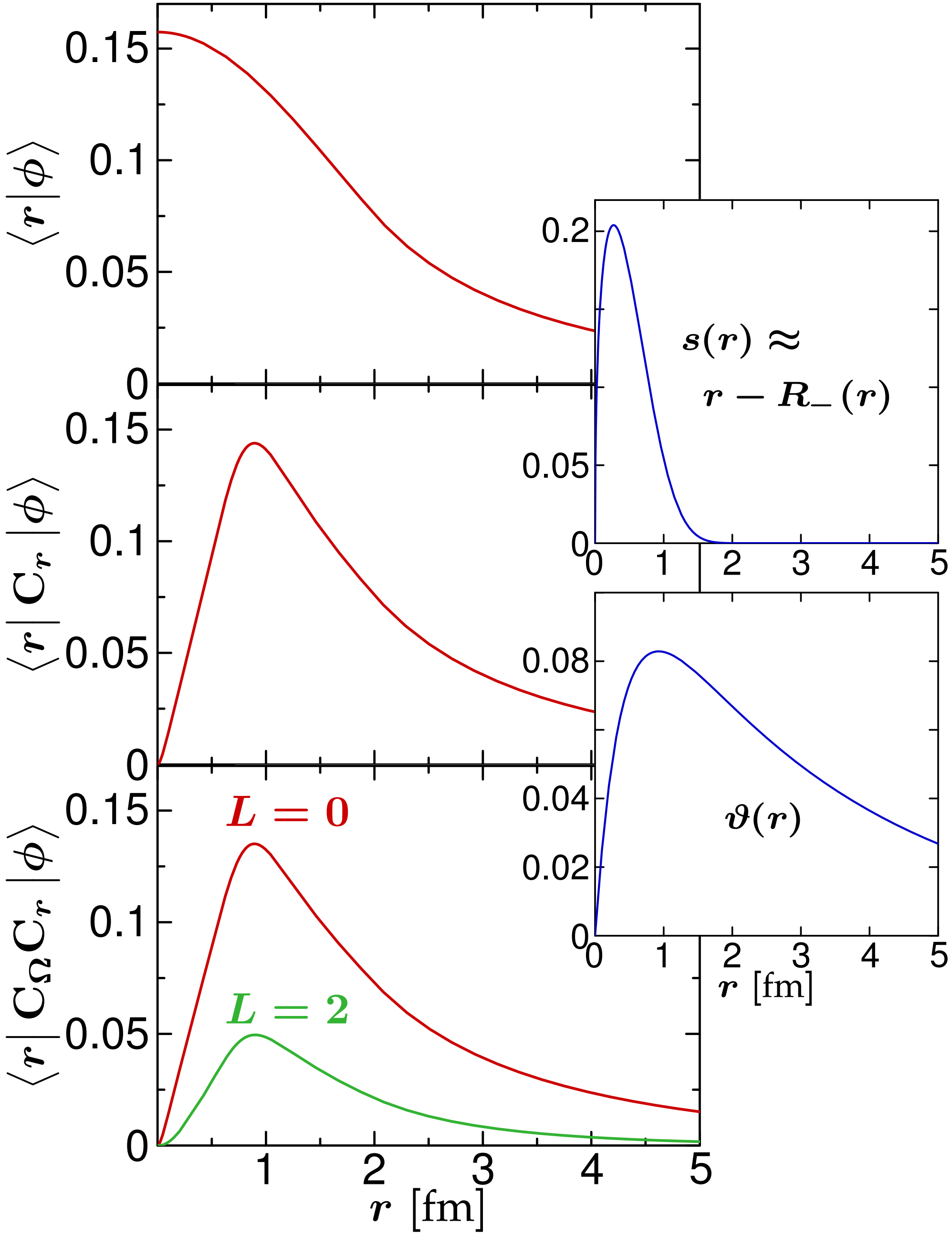
- angular shift depending on the orientation of spin and relative coordinate of a nucleon pair

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

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

$s(r)$ 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_{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 $V_{\mathrm{low}-k}$**

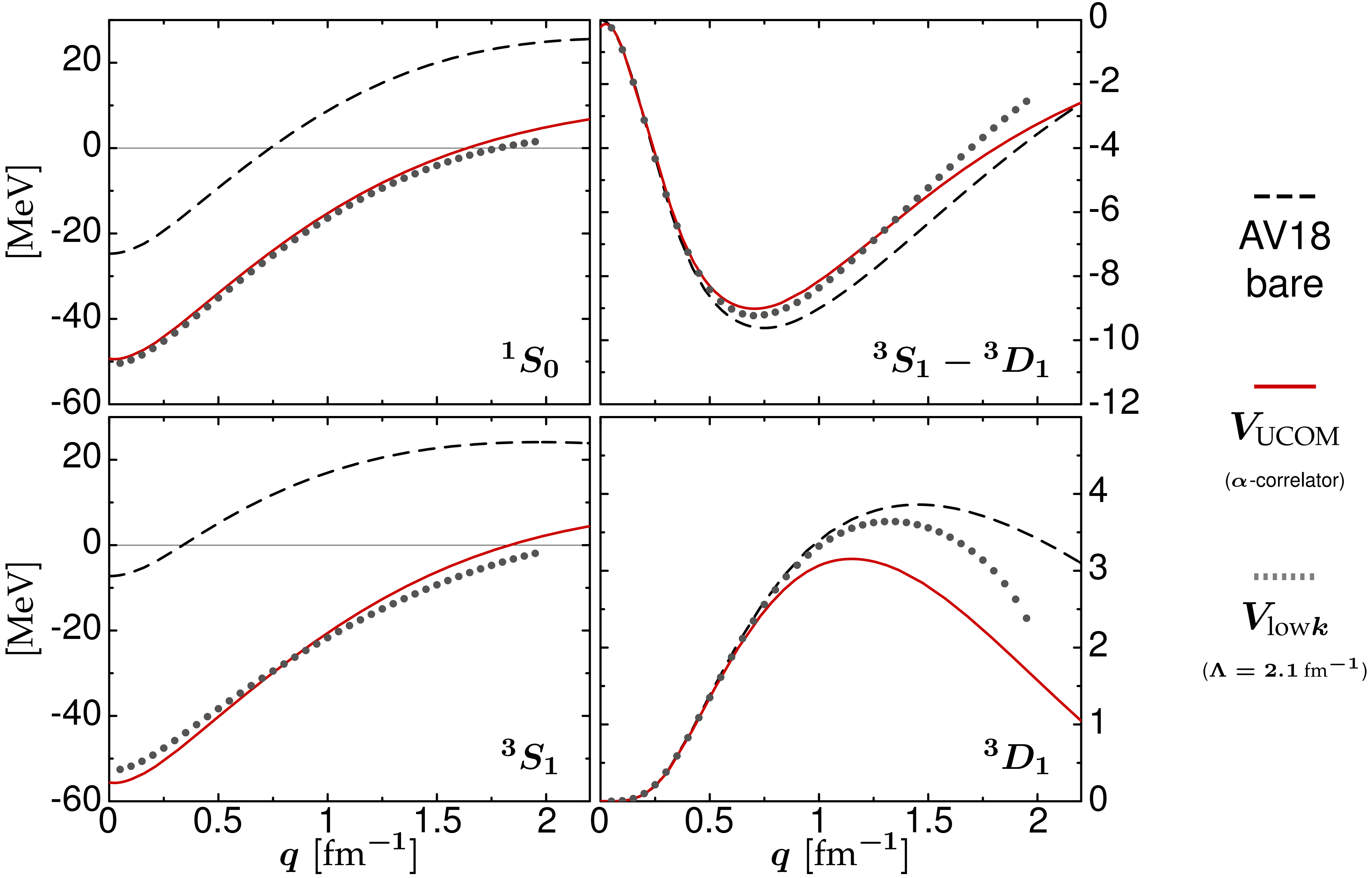
Correlated NN-Potential — V_{UCOM}

$$\mathrm{V}_{\mathrm{UCOM}} = \sum_p \tfrac{1}{2}\big[\widehat{v}_p(\mathbf{r})\ \mathrm{O}_p + \mathrm{O}_p\ \widehat{v}_p(\mathbf{r})\big]$$

$$\begin{aligned}\mathrm{O} = \{1,\ (\vec{\sigma}_1\cdot\vec{\sigma}_2),\ \vec{\mathrm{q}}^2,\ \vec{\mathrm{q}}^2(\vec{\sigma}_1\cdot\vec{\sigma}_2),\ \vec{\mathrm{L}}^2,\ \vec{\mathrm{L}}^2(\vec{\sigma}_1\cdot\vec{\sigma}_2),\\ (\vec{\mathrm{L}}\cdot\vec{\mathrm{S}}),\ \mathrm{S}_{12}(\vec{\mathrm{r}},\vec{\mathrm{r}}),\ \mathrm{S}_{12}(\vec{\mathrm{L}},\vec{\mathrm{L}}),\\ \bar{\mathrm{S}}_{12}(\vec{\mathrm{q}}_\Omega,\vec{\mathrm{q}}_\Omega),\ \mathrm{q}_r\,\mathrm{S}_{12}(\vec{\mathrm{r}},\vec{\mathrm{q}}_\Omega),\ \vec{\mathrm{L}}^2(\vec{\mathrm{L}}\cdot\vec{\mathrm{S}}),\\ \vec{\mathrm{L}}^2\bar{\mathrm{S}}_{12}(\vec{\mathrm{q}}_\Omega,\vec{\mathrm{q}}_\Omega),\ \ldots\} \otimes \{1,\ (\vec{\tau}_1\cdot\vec{\tau}_2)\}\end{aligned}$$

- C_r-transformation evaluated directly
- C_Ω-transformation through Baker-Campell-Hausdorff expansion
- $\widehat{v}_p(r)$ uniquely determined by bare potential and correlation functions

Momentum-Space Matrix Elements



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

Lee-Suzuki

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

$V_{\text{low}k}$

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

UCOM

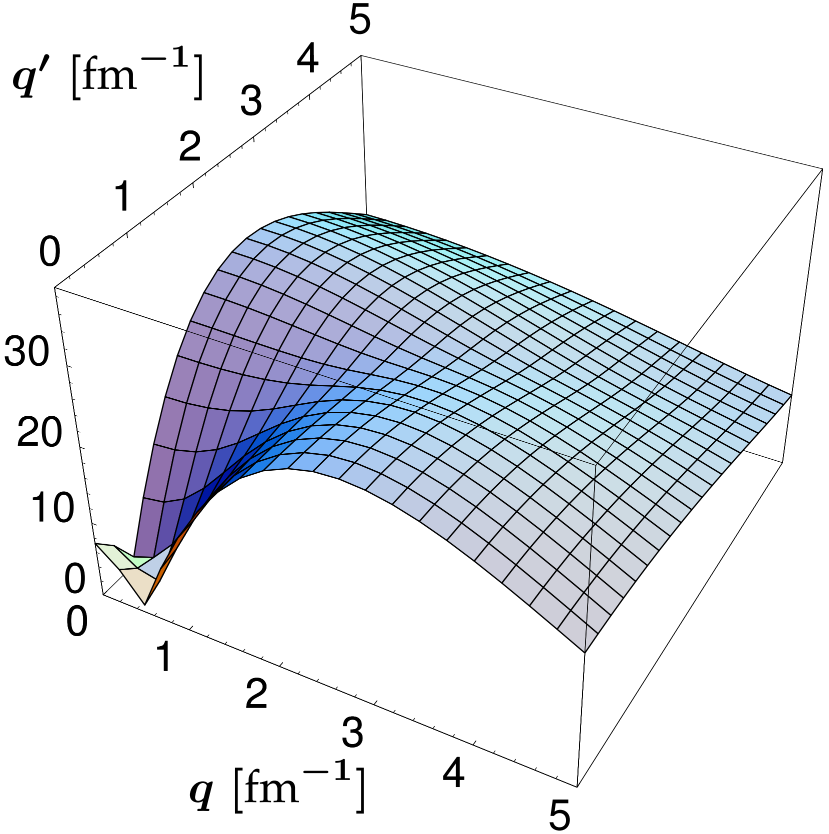
- pre-diagonalization with respect to short-range correlations
- no specific model-space or representation
- state independent
- phase-shift equivalent

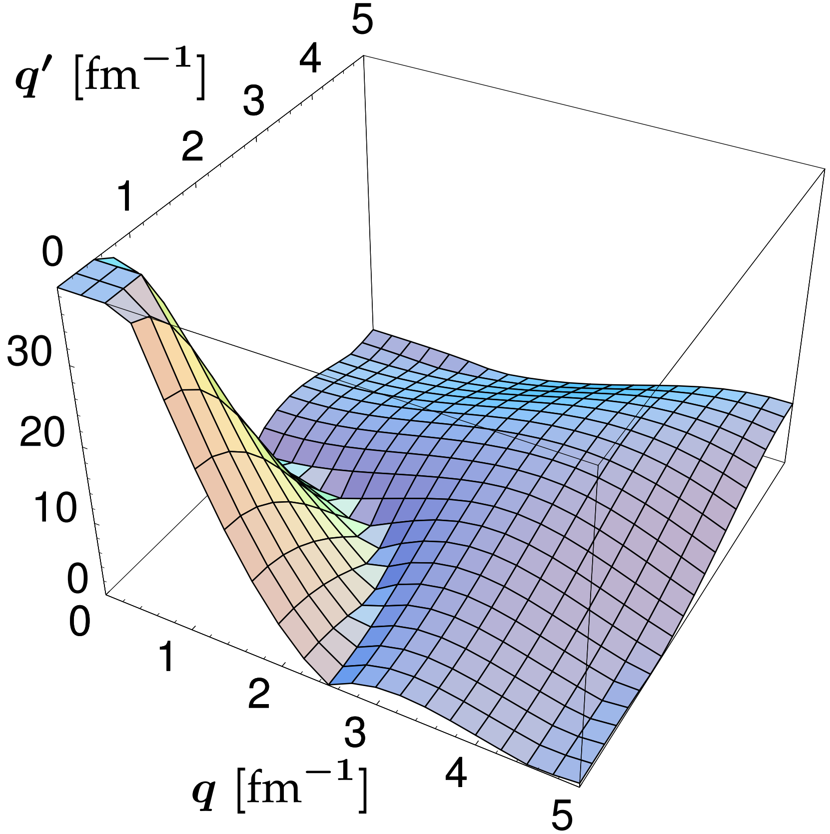
Pre-Diagonalization in Momentum Space

$|\langle \boldsymbol{q}|\,\mathbf{V}\,|\boldsymbol{q}'\rangle|$

$^3S_1$

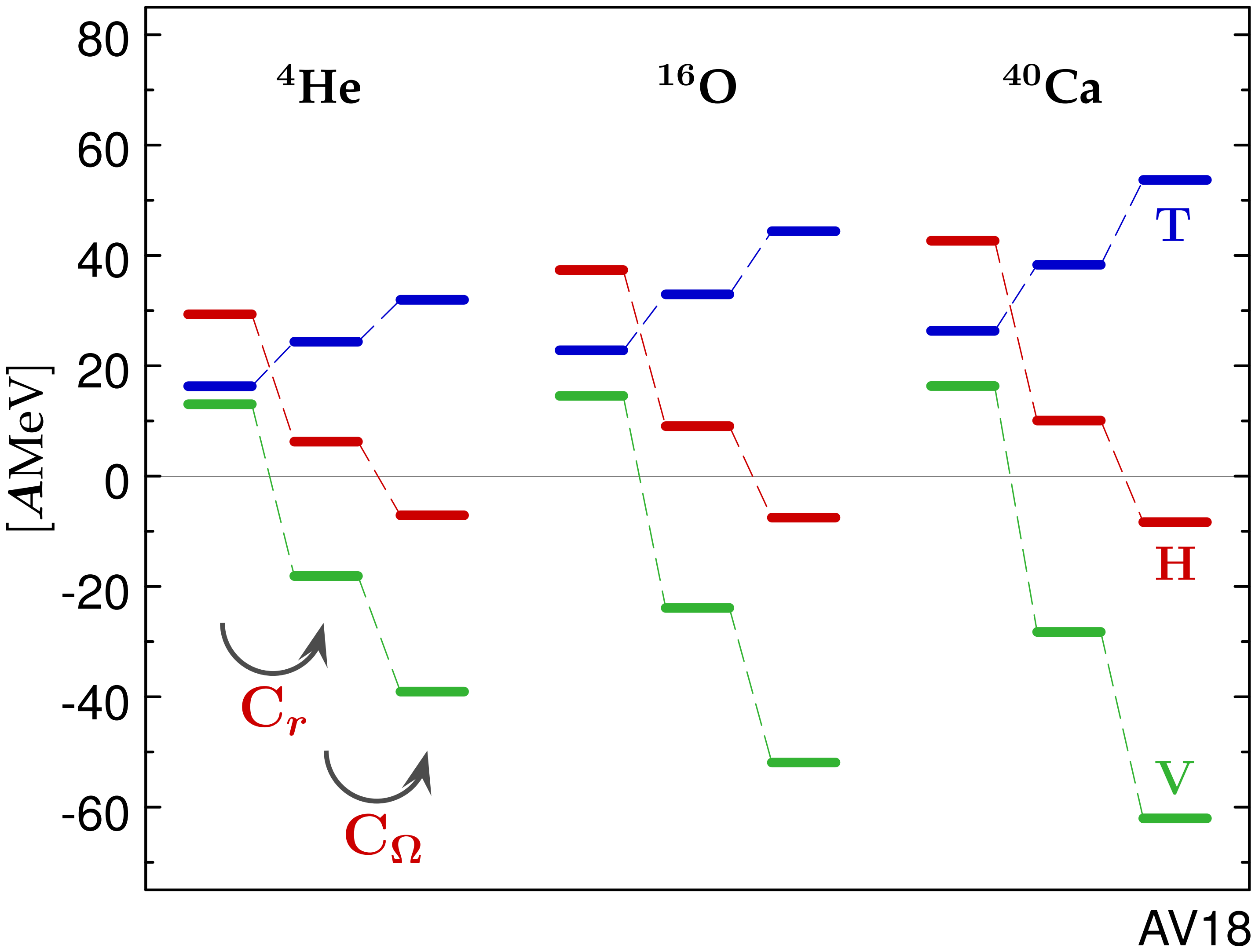
$|\langle \boldsymbol{q}|\,\mathbf{V}_{\mathrm{UCOM}}\,|\boldsymbol{q}'\rangle|$





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 $N_{\max} = 6...10$)
- Coulomb interaction included exactly
- formulated with intrinsic kinetic energy $\mathrm{T}_{\mathrm{int}} = \mathrm{T} - \mathrm{T}_{\mathrm{cm}}$ to eliminate center of mass contributions

Correlated Oscillator Matrix Elements

$$\left\langle n(LS)JT \right| \mathrm{C}_r^\dagger \mathrm{C}_\Omega^\dagger \, \mathrm{H} \, \mathrm{C}_\Omega \mathrm{C}_r \left| n'(L'S)JT \right\rangle$$

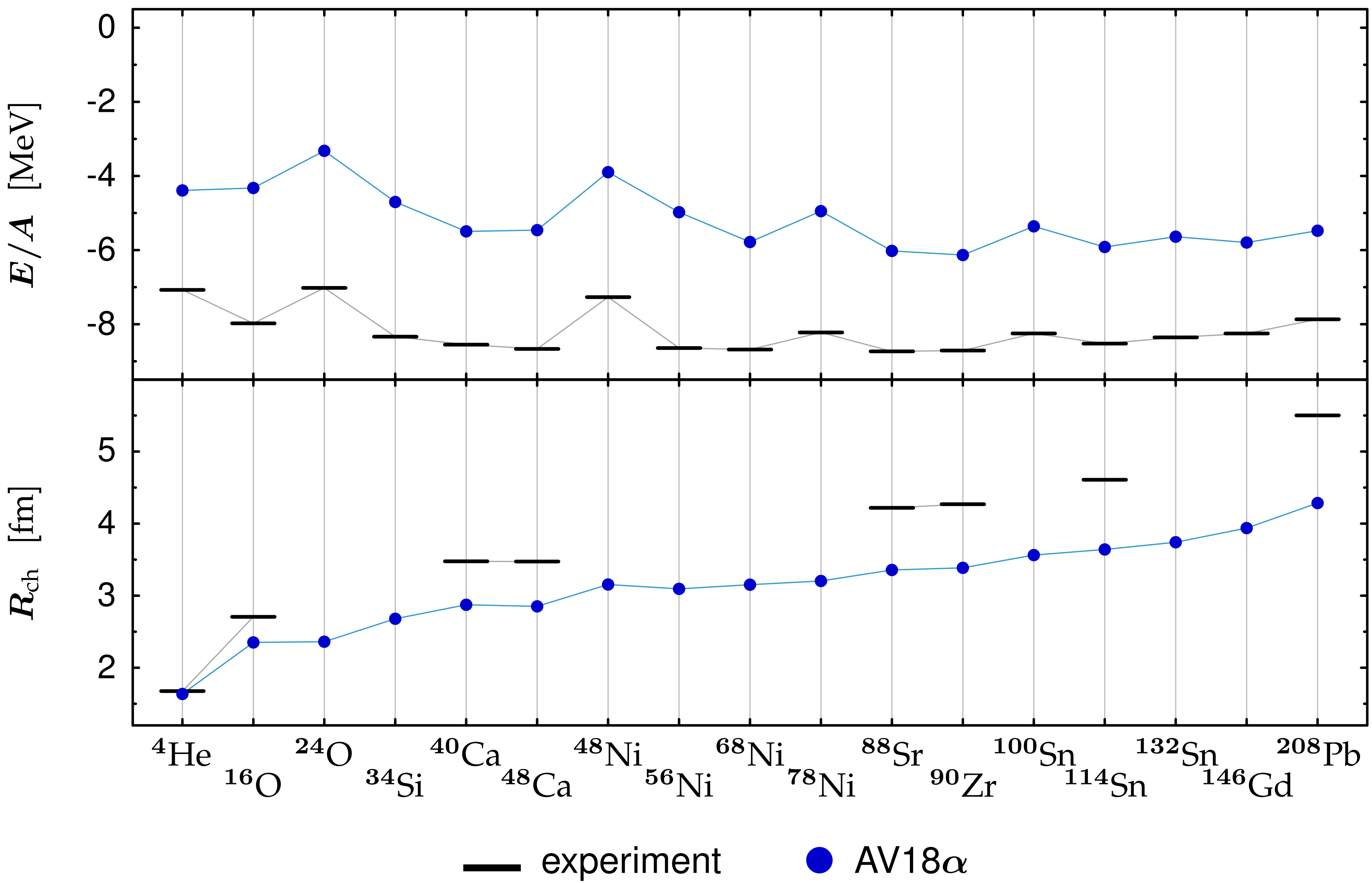
$$= \left\langle n(LS)JT \right| \mathrm{T} + \mathrm{V}_{\mathrm{UCOM}} \left| n'(L'S)JT \right\rangle$$

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

- include genuine three-body forces & three-body clusters
  ➔ hardly possible for heavier systems
- construct phenomenological three-body force
  ➔ will be considered
- improved many-body state: RPA, CI, CC, NCSM,...
  ➔ in progress

Missing Pieces

long-range correlations

genuine three-body forces

three-body cluster contributions

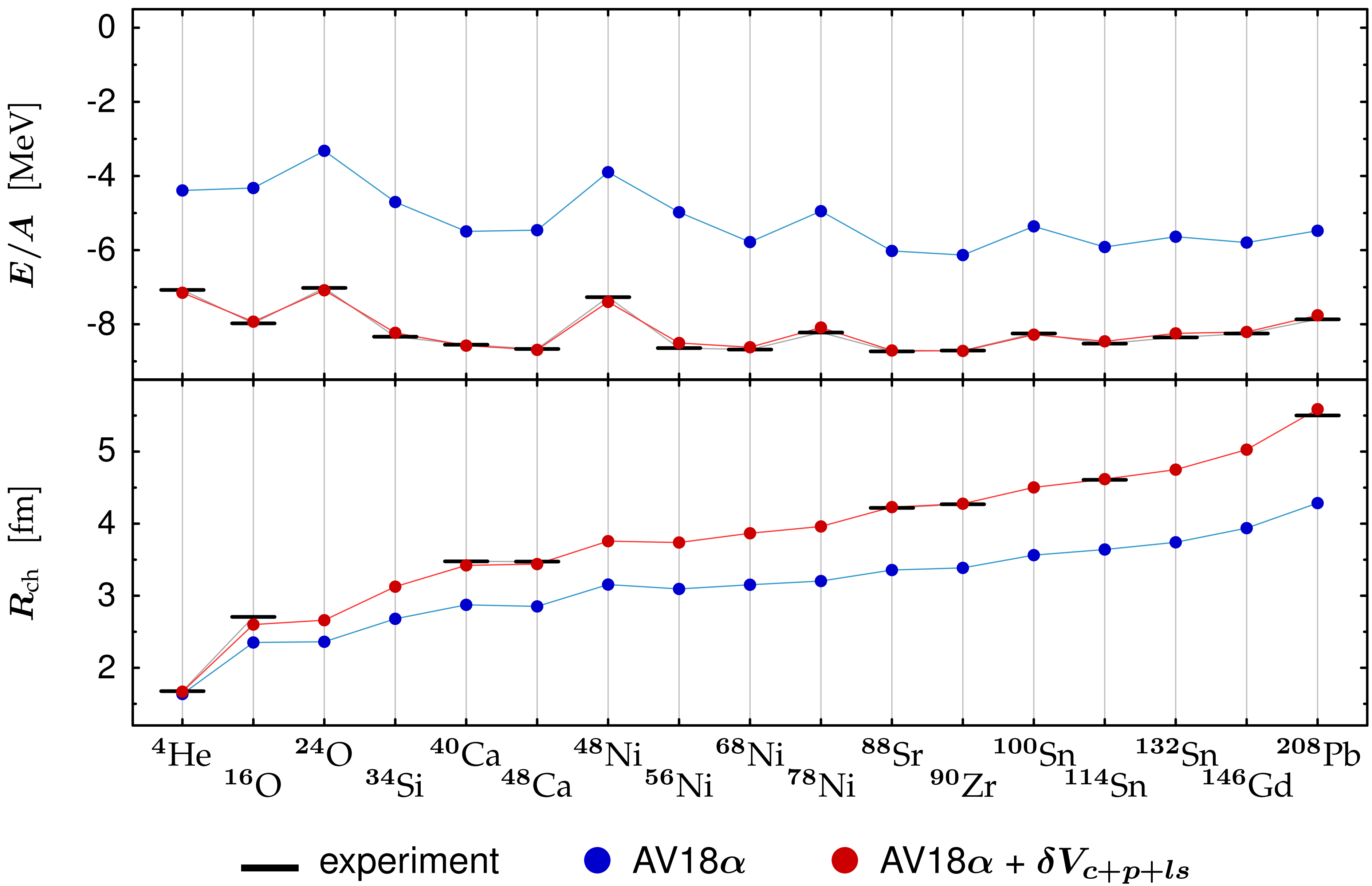
Pragmatic Approach

- phenomenological two-body correction

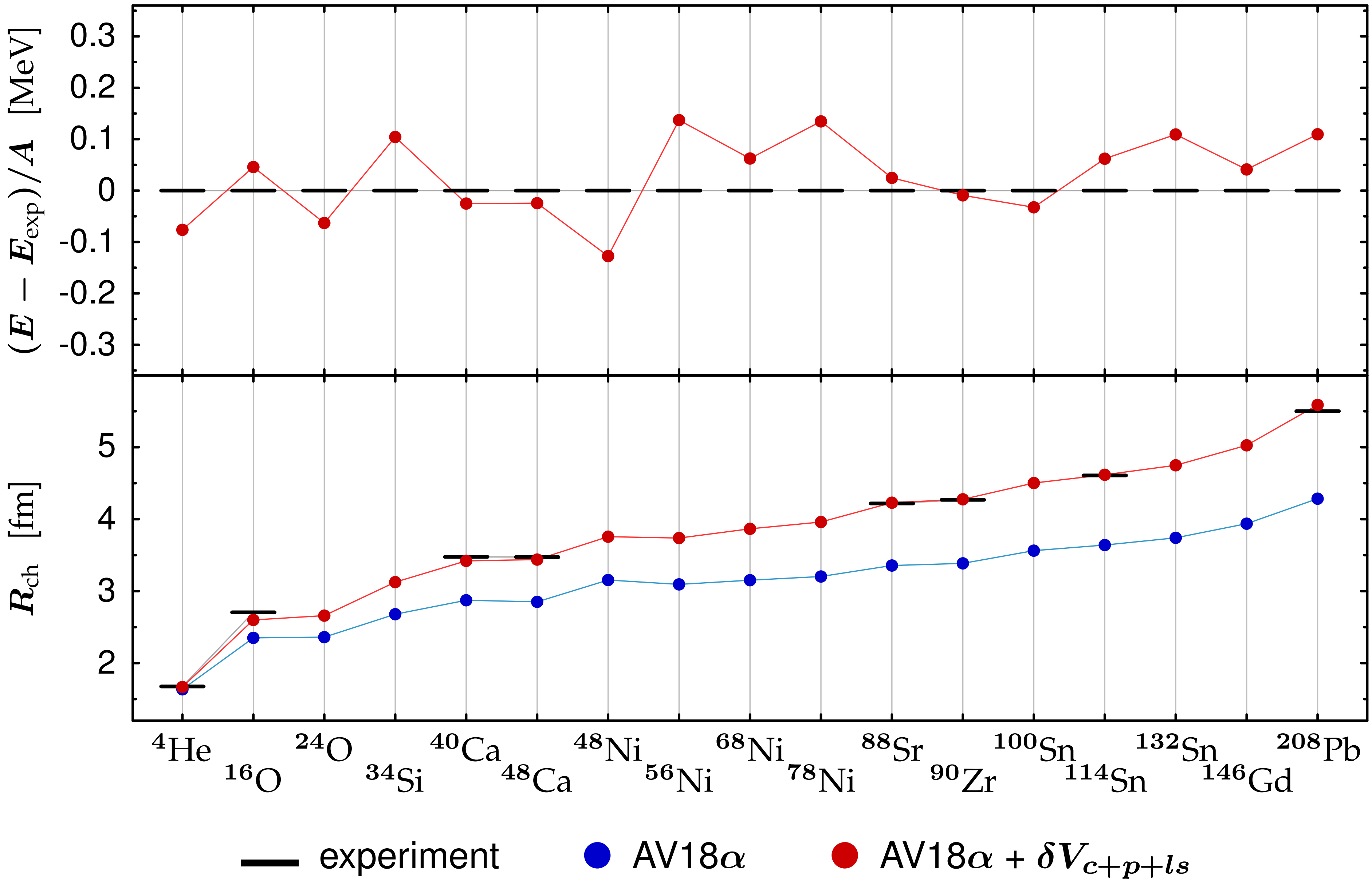
$$\delta \mathrm{V}_{c+p+ls} = v_1(\mathrm{r}) + \vec{\mathrm{q}}\, v_{qq}(\mathrm{r})\, \vec{\mathrm{q}} + v_{LS}(\mathrm{r})\, \vec{\mathrm{L}} \cdot \vec{\mathrm{S}}$$

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

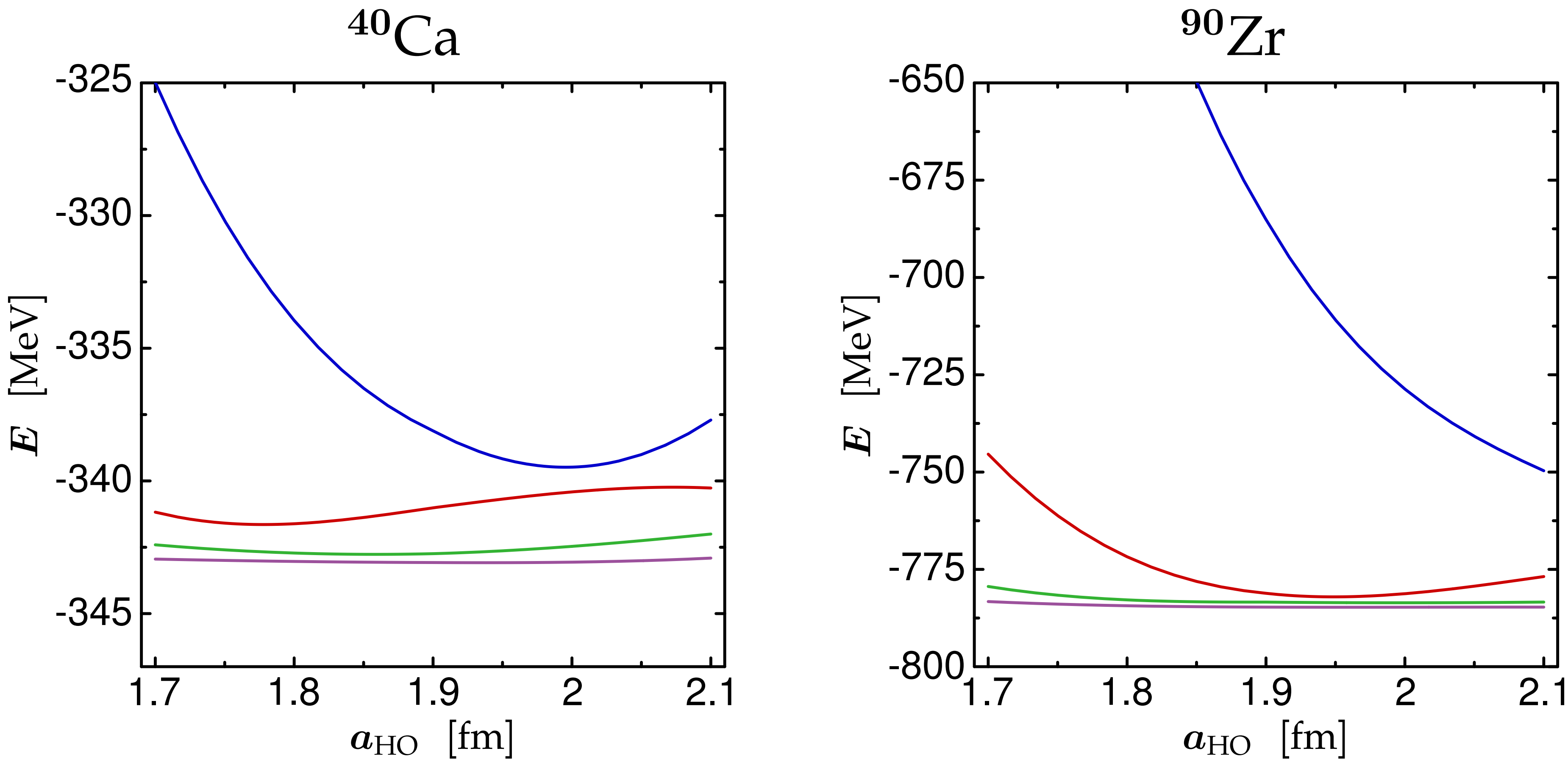
Correlated Argonne V18 + Correction



Correlated Argonne V18 + Correction

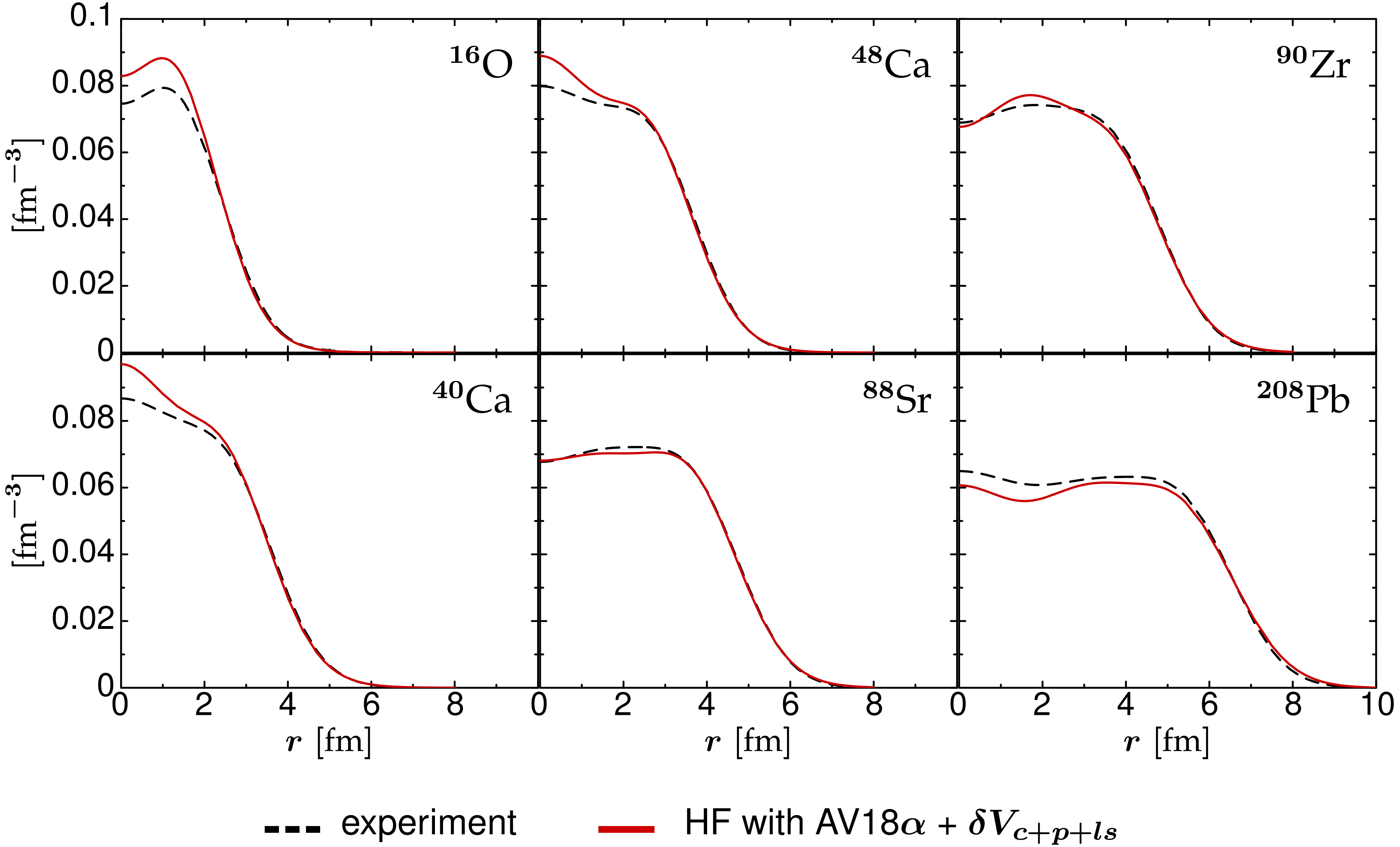


Basis Truncation & Convergence

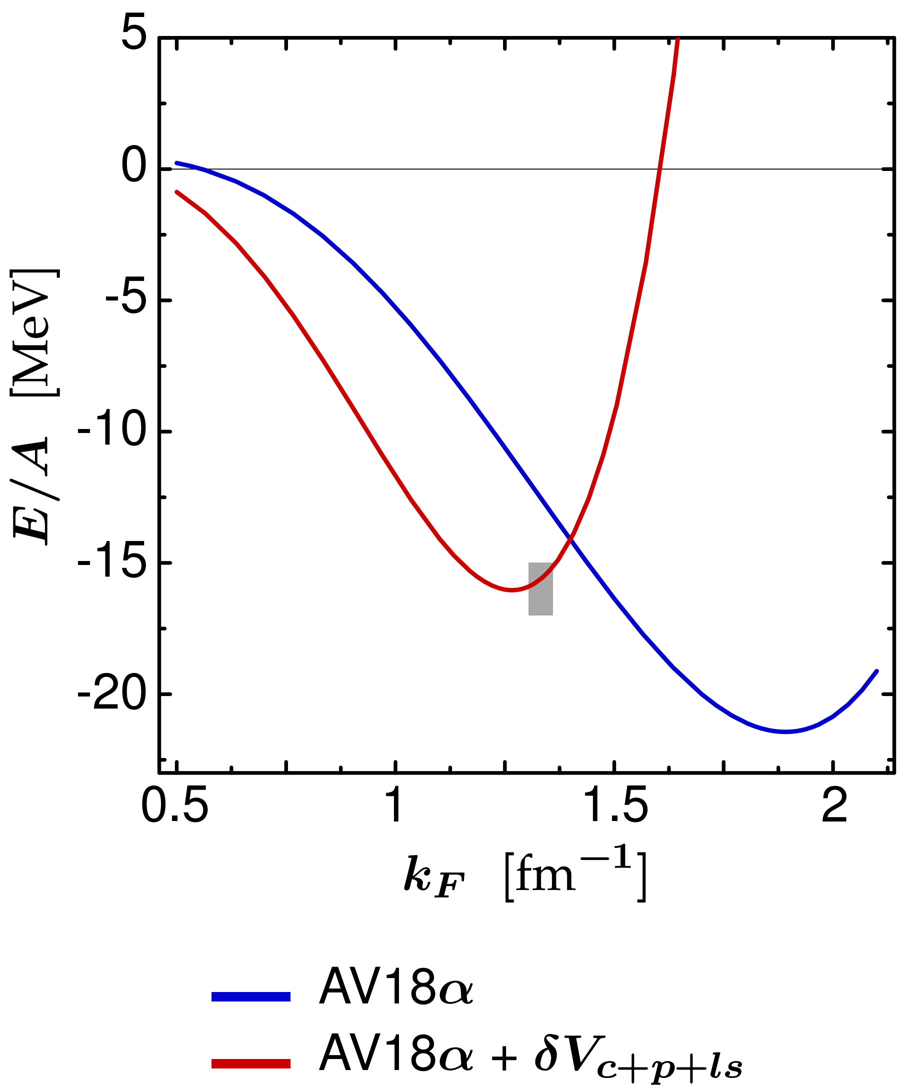


$n_{\max} = 1$ (——), 2 (——), 3 (——), 4 (——)

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:

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

- HvH theorem fulfilled

Fermionic Molecular Dynamics (FMD)

FMD Trial States

Gaussian Single-Particle States

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

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

a_ν : complex width

χ_ν : spin orientation

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

Slater Determinant

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

Correlated Hamiltonian

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

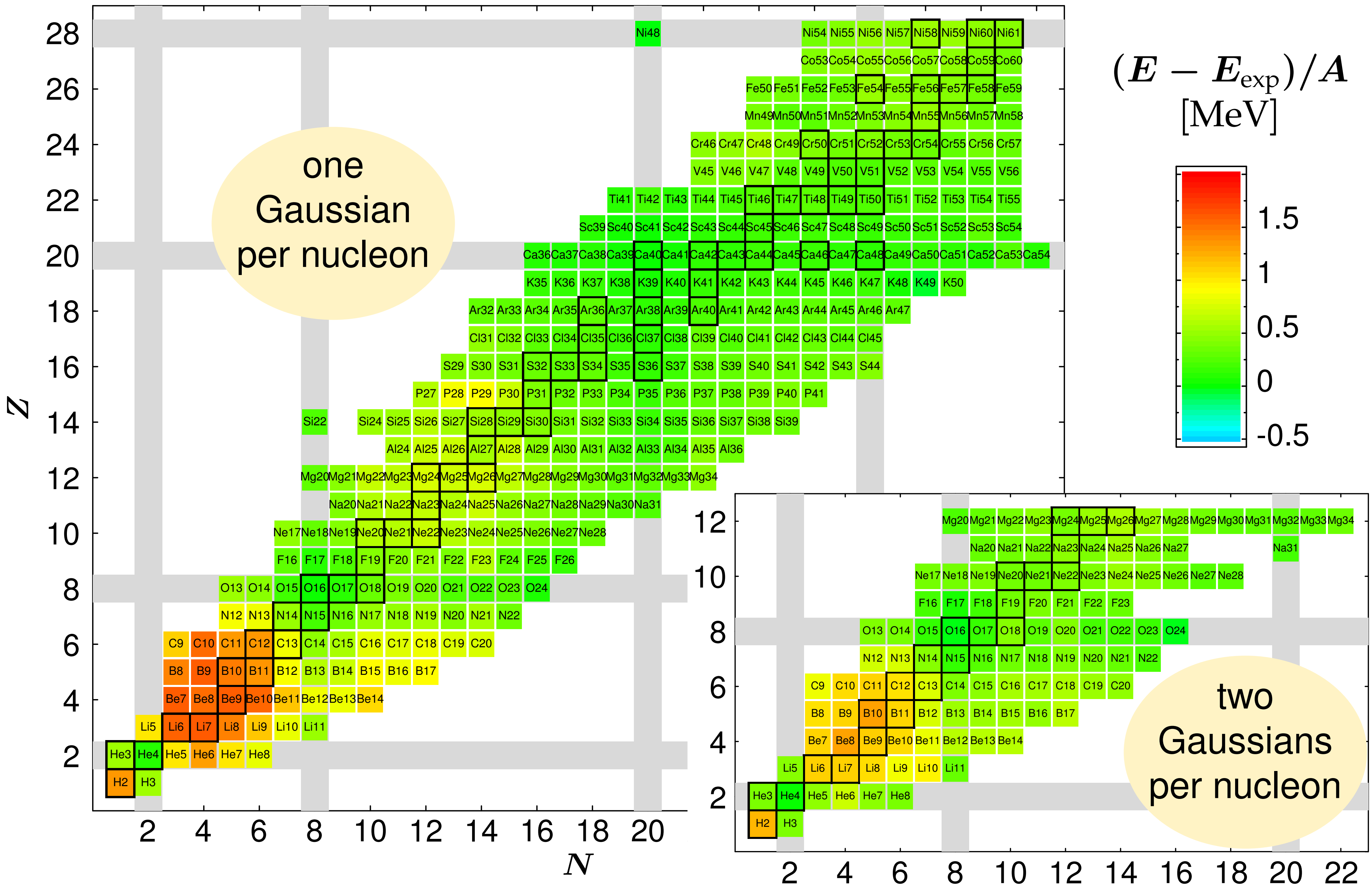
Variation

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

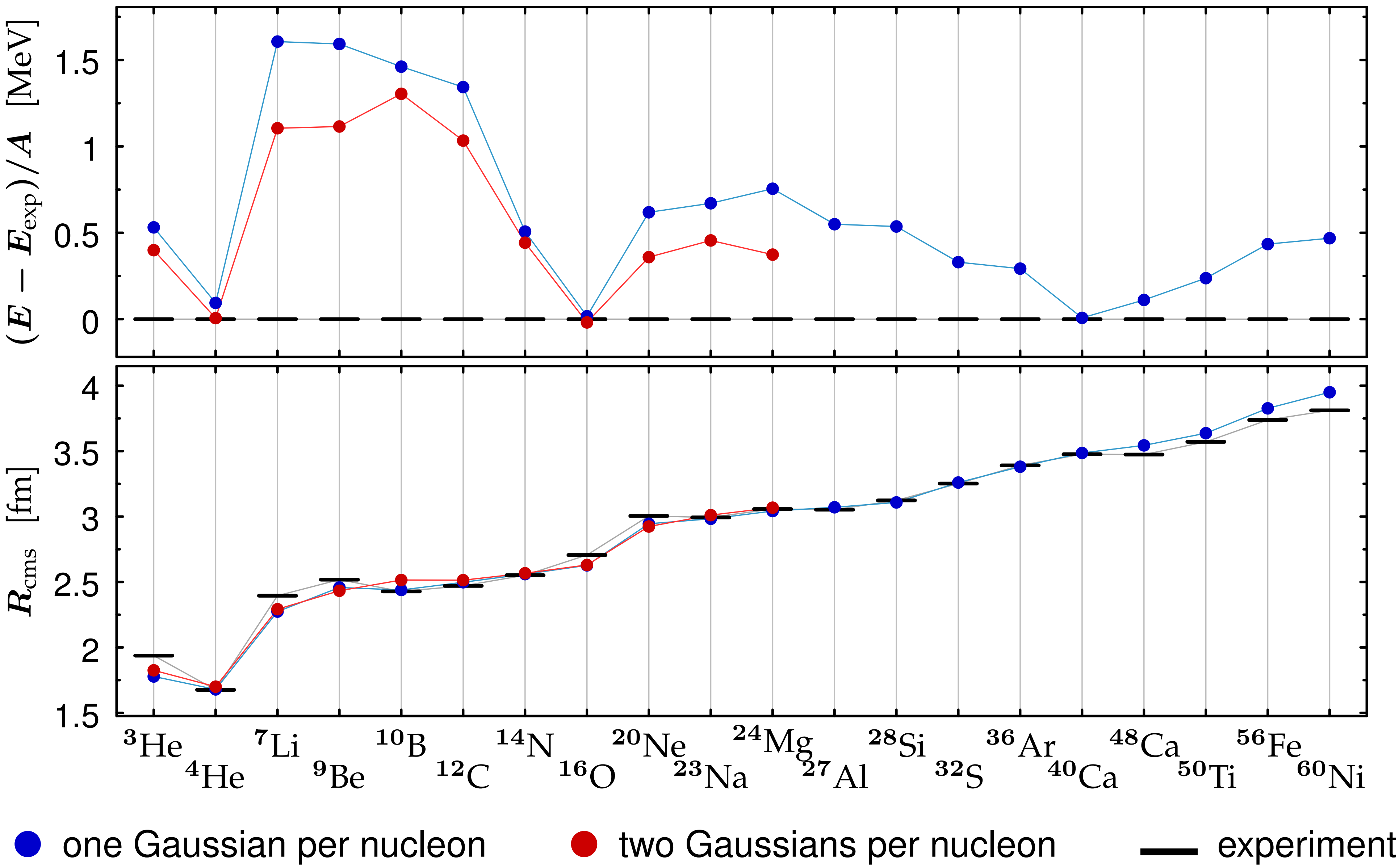
Diagonalization

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

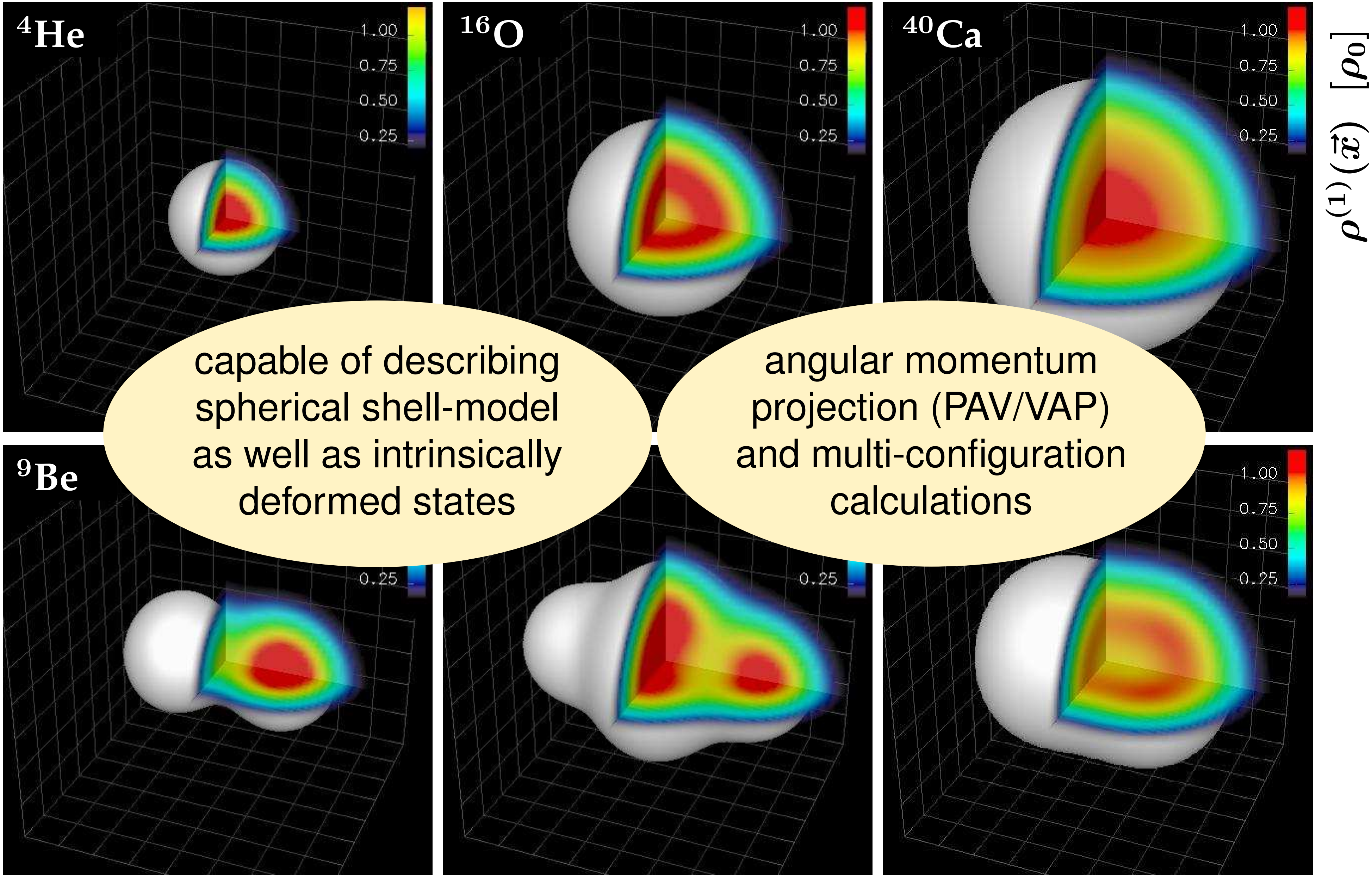
Chart of Nuclei



Selected Stable Nuclei



Intrinsic One-Body Density Distributions

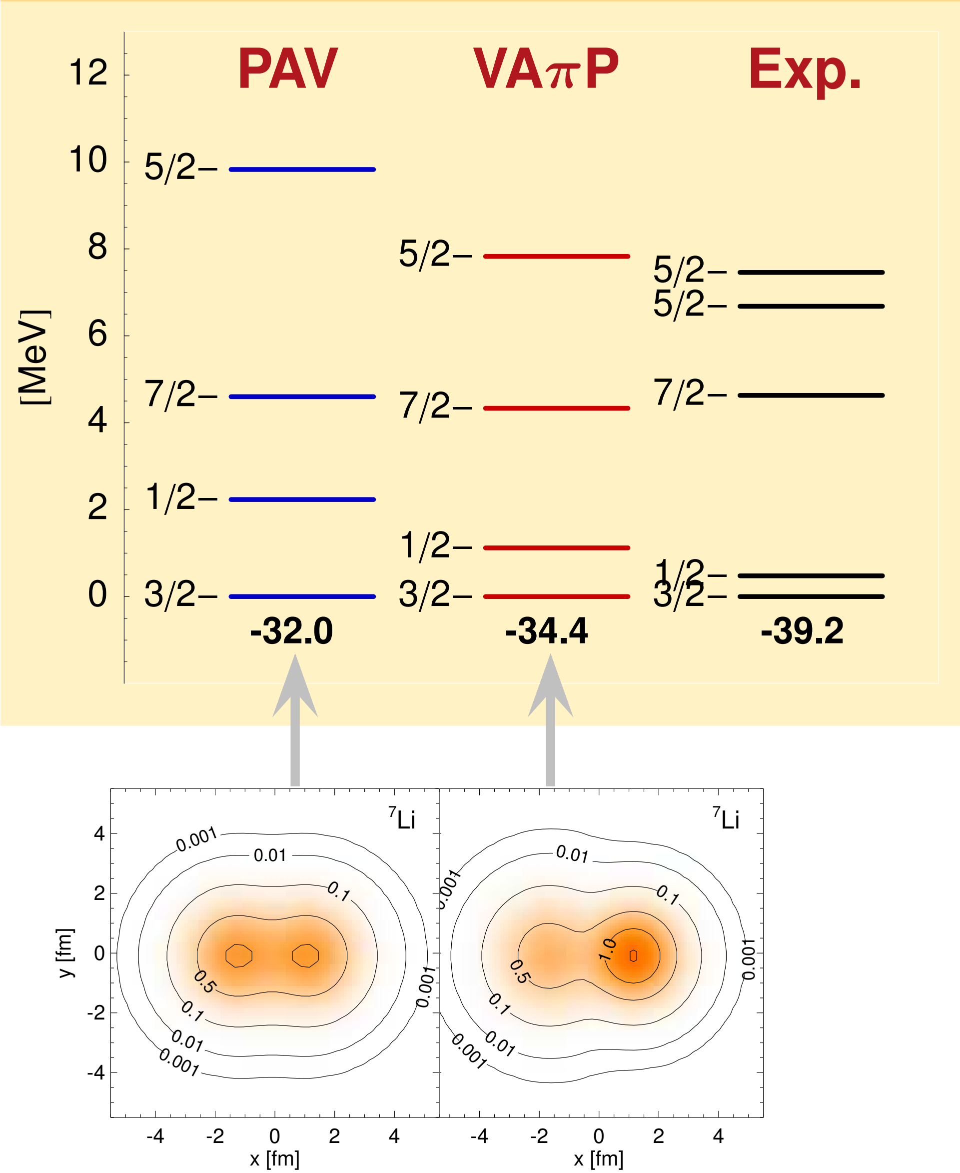


capable of describing spherical shell-model as well as intrinsically deformed states

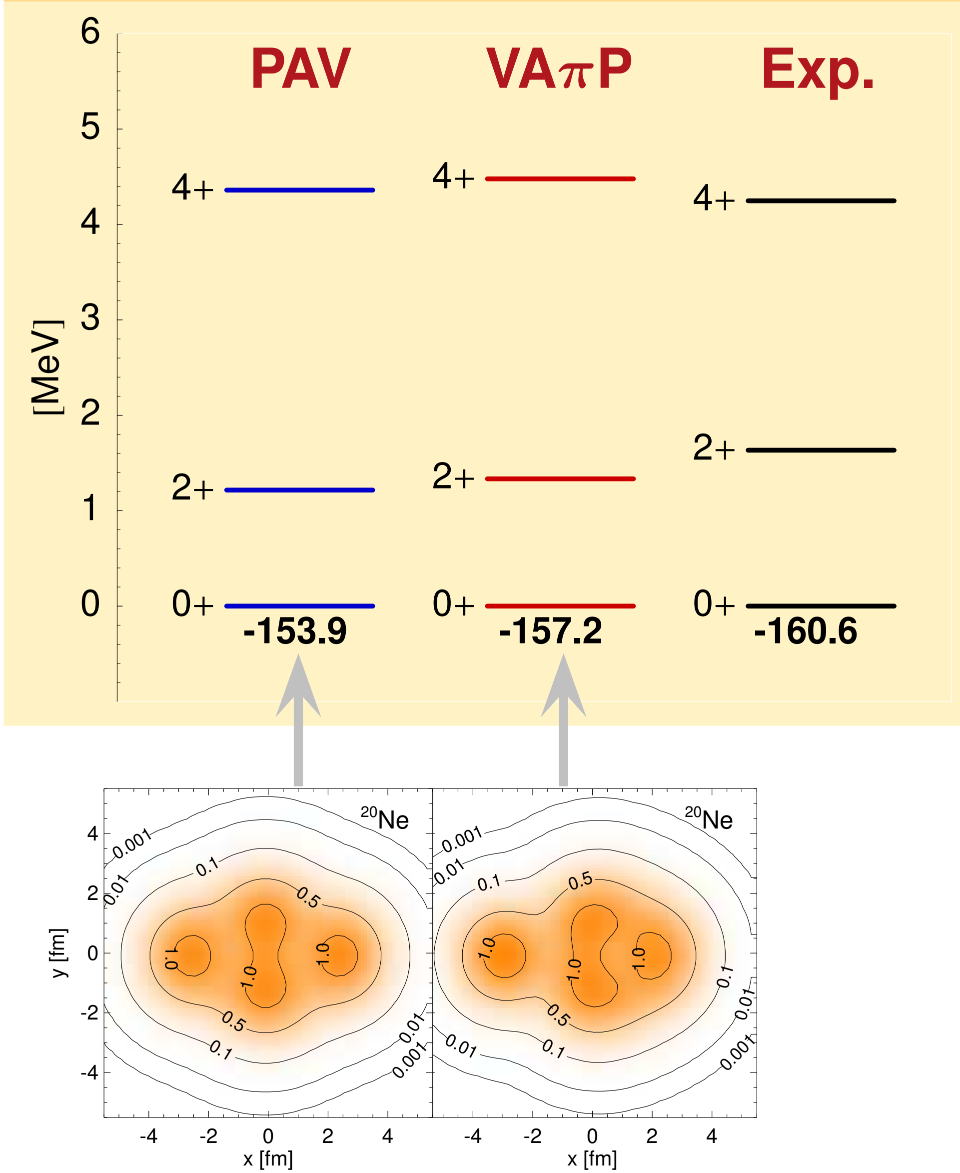
angular momentum projection (PAV/VAP) and multi-configuration calculations

Parity and Angular Momentum Projection

^{7}Li



^{20}Ne



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_{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