Towards *ab initio* Nuclear Structure Calculations

A Tale of Short-Range & Long-Range Correlations

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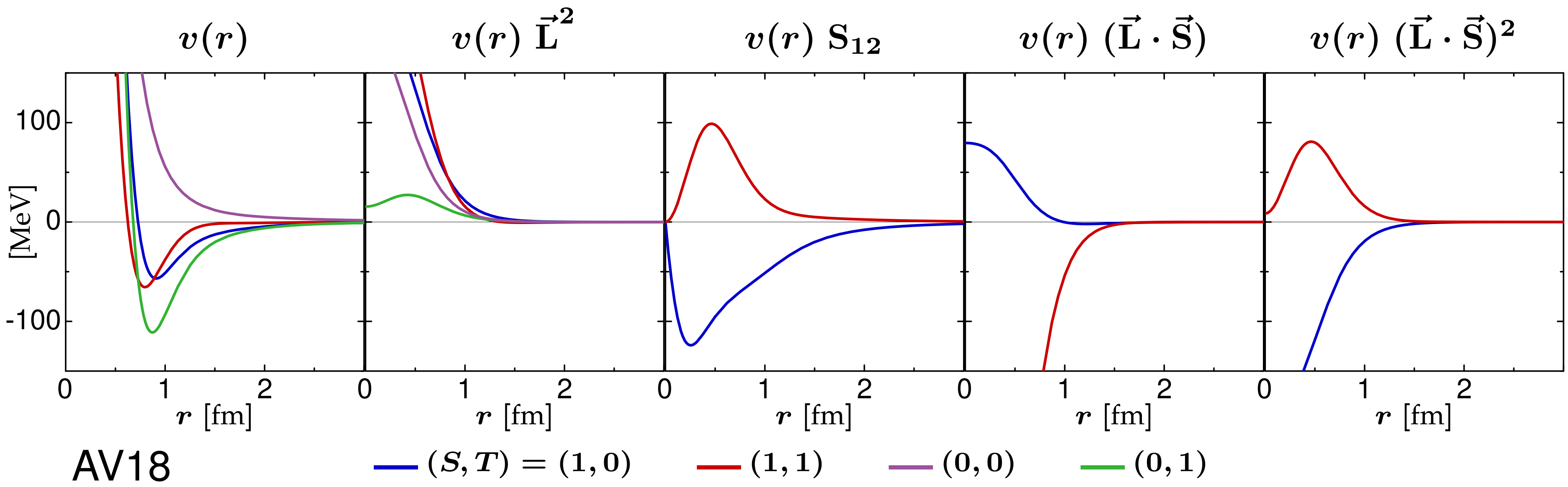
GSI

What are *ab initio* Calculations?

- **Realistic Nucleon-Nucleon Interactions**
  - QCD inspired: meson-exchange, chiral perturbation theory
  - reproduce experimental two-body data (phase-shifts and deuteron properties) with high accuracy
  - Argonne V18, CD Bonn, Nijmegen,...



What are *ab initio* Calculations?

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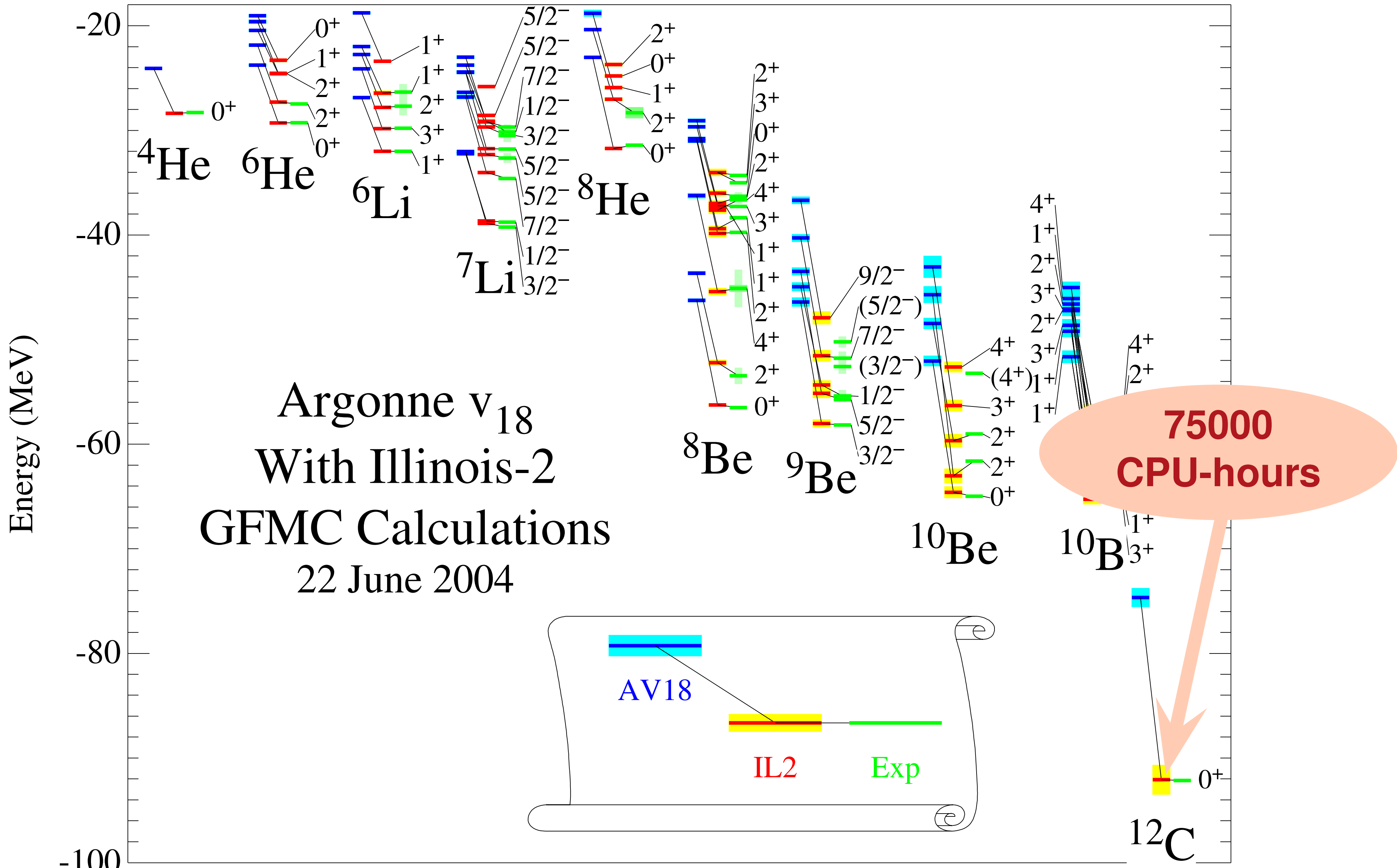
  - Argonne V18, CD Bonn, Nijmegen,...

- **“Exact” Solution of Quantum Many-Body Problem**
  - Green’s Function Monte Carlo, No-Core Shell Model,...
  - computationally extremely elaborate and costly

Green's Function Monte Carlo



[S. Pieper, private comm.]

12C results are preliminary.

Our Aim

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

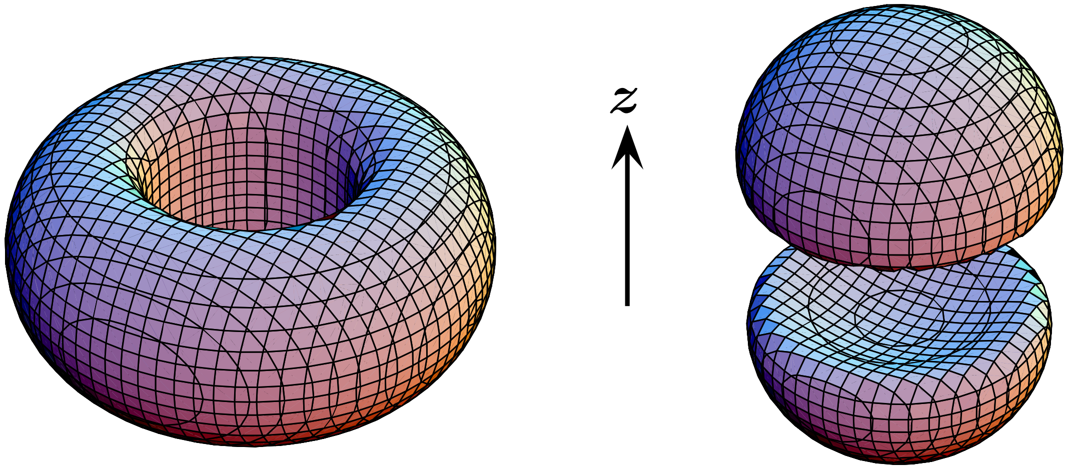
- UCOM + No-Core Shell Model
- UCOM + Hartree-Fock
- UCOM + Fermionic Molecular Dynamics

Correlations in Nuclei

Deuteron: Manifestation of Correlations

$M_S = 0$ $\qquad$ $M_S = \pm 1$

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



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

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 States

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

Correlated Operators

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

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

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

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

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

Tensor Correlator C_Ω

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

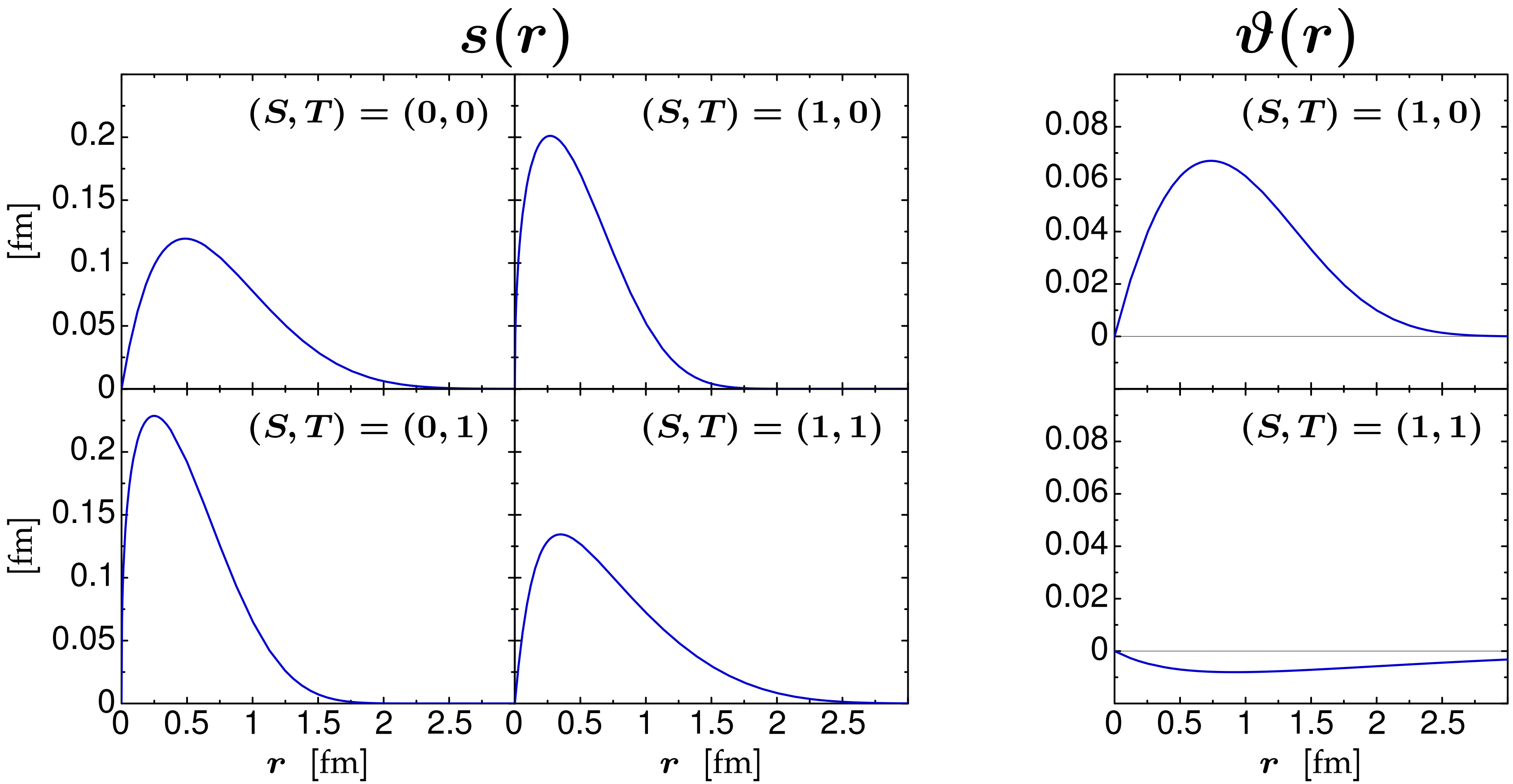
$$\mathrm{g}_\Omega = \frac{3}{2}\vartheta(\mathrm{r})\big[(\vec{\sigma}_1 \cdot \vec{\mathrm{q}}_\Omega)(\vec{\sigma}_2 \cdot \vec{\mathrm{r}}) + (\vec{\mathrm{r}} \leftrightarrow \vec{\mathrm{q}}_\Omega)\big]$$

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

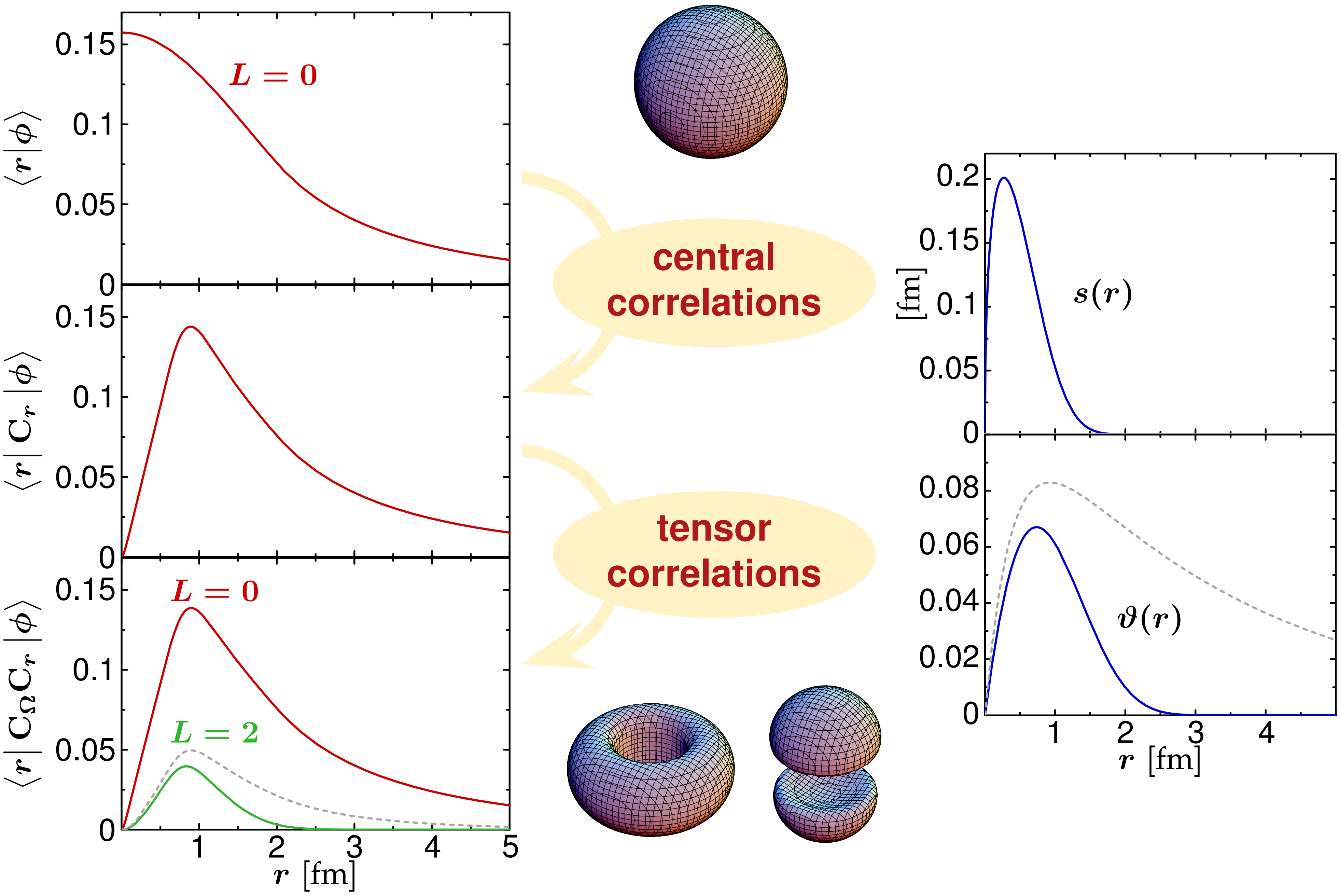
$s(r)$ and $\vartheta(r)$
encapsulate the physics of
short-range correlations

Optimal Correlation Functions

- $s(r)$ and $\vartheta(r)$ determined by two-body **energy minimization**
- constraint on range of the tensor correlators $\vartheta(r)$ to isolate state independent **short-range correlations**



Correlated States



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 small

Two-Body Approx.

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

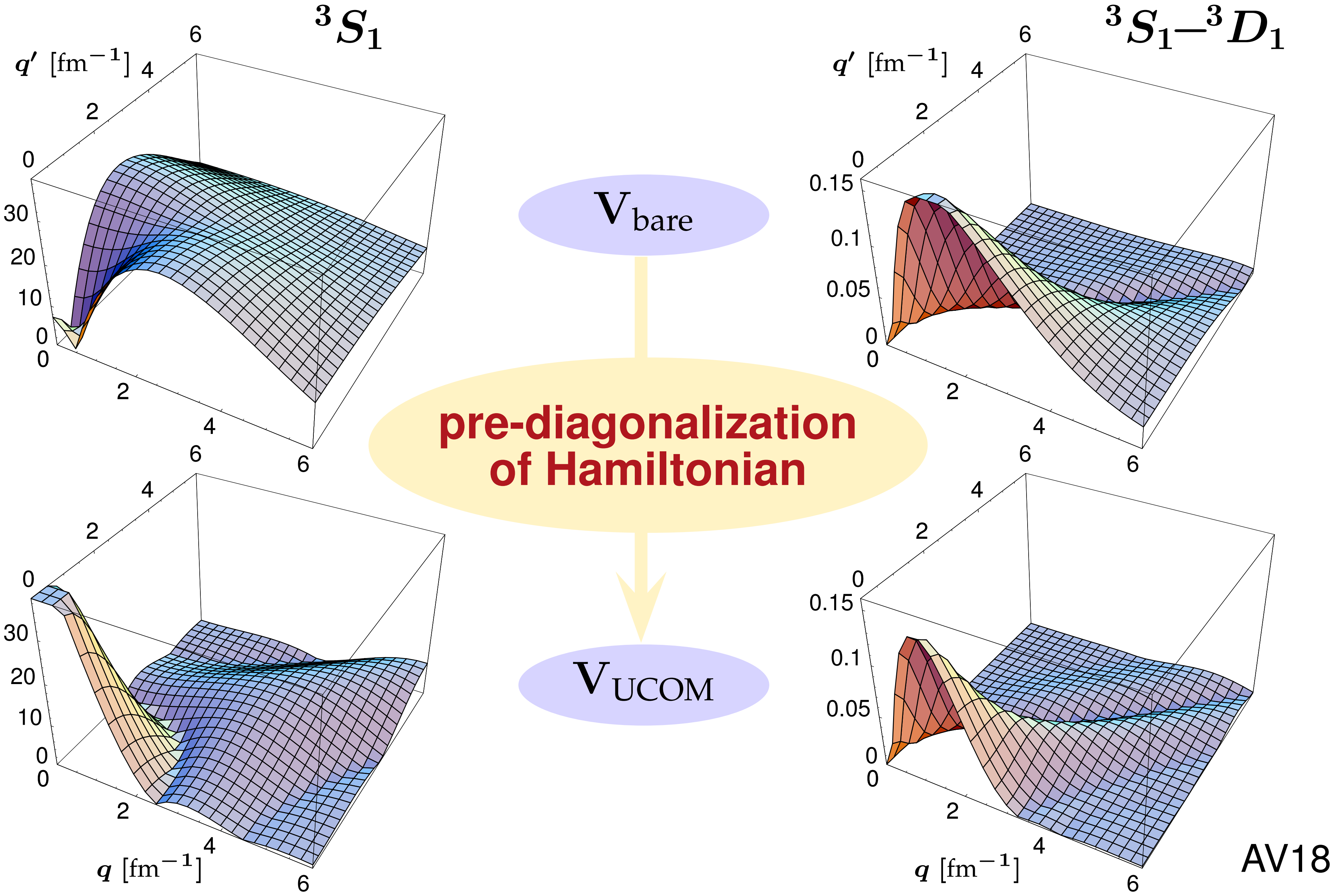
operators of all observables can be and have to be correlated consistently

Correlated NN-Potential — V_{UCOM}

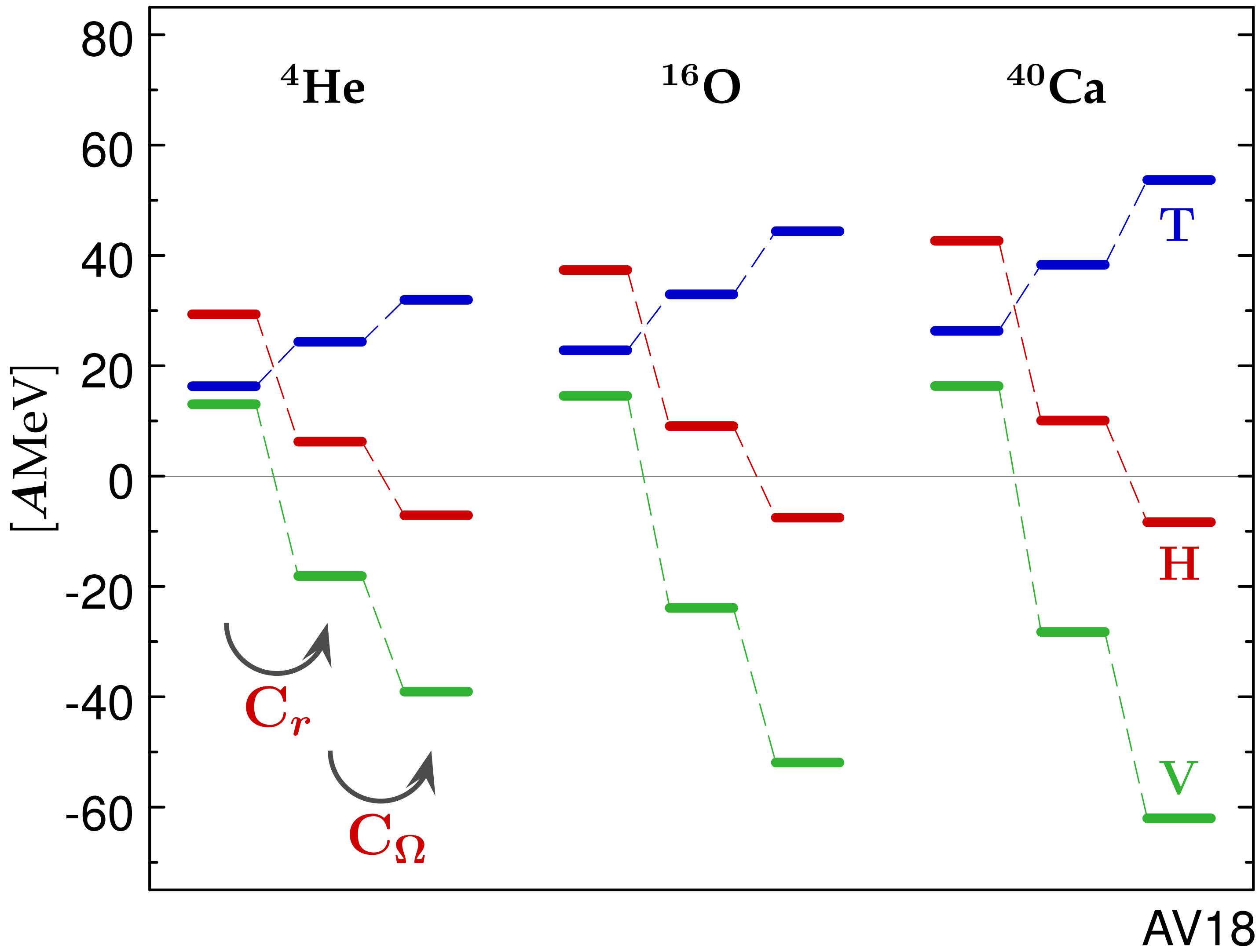
$$\widehat{\mathbf{H}}^{C2} = \widehat{\mathbf{T}}^{[1]} + \widehat{\mathbf{T}}^{[2]} + \widehat{\mathbf{V}}^{[2]} = \mathbf{T} + \mathbf{V}_{\mathrm{UCOM}}$$

- **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
- unitary transformation results in a **pre-diagonalization** of Hamiltonian
- momentum-space matrix elements of correlated interaction are **similar to $V_{\mathrm{low}-k}$**

Momentum-Space Matrix Elements



Simplistic "Shell-Model" Calculation



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

Application I

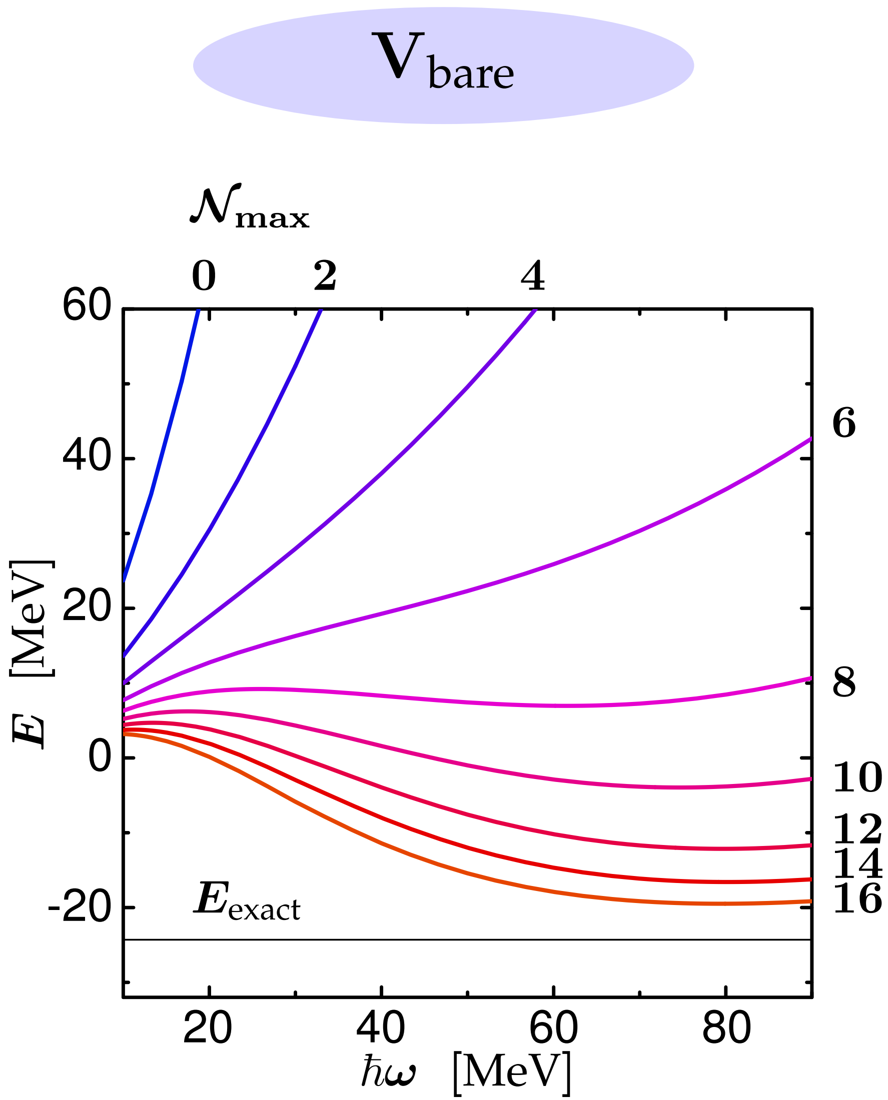
No-Core Shell Model

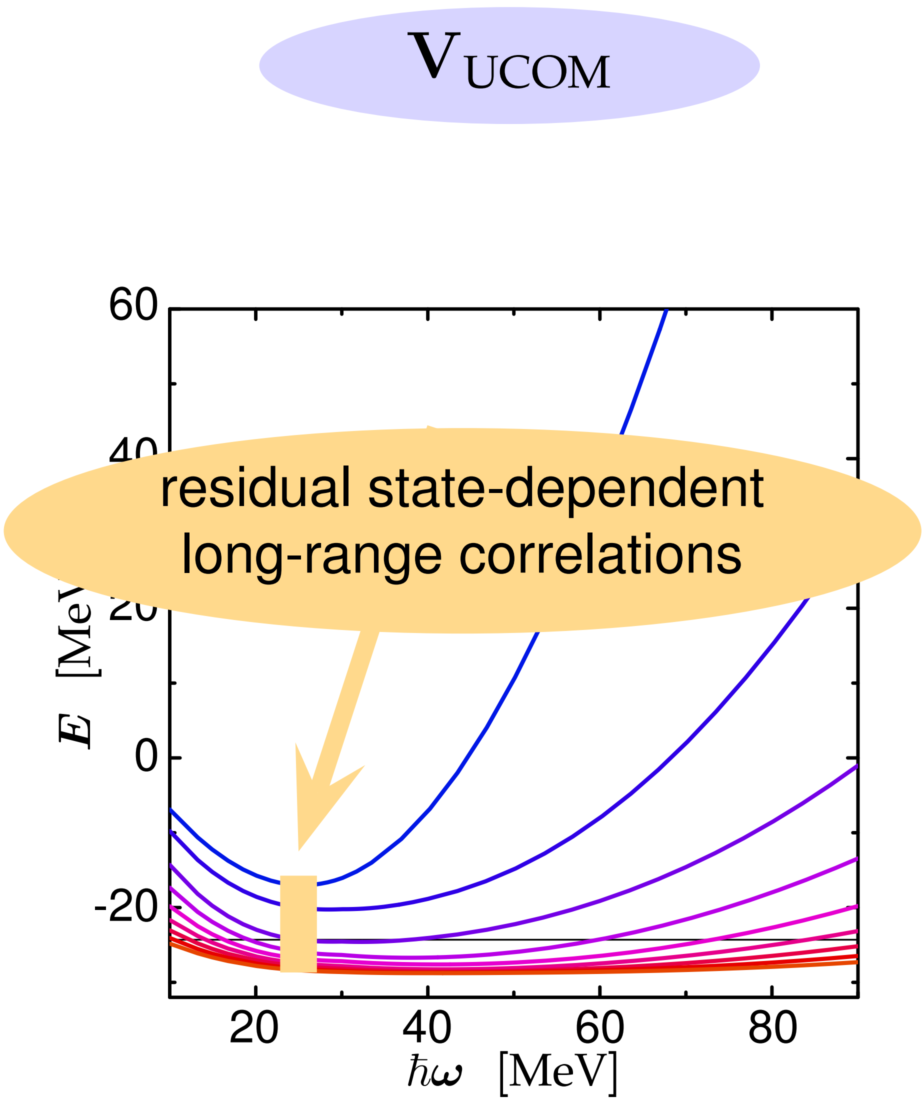
UCOM + NCSM

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

- convergence dramatically improved compared to bare interaction
- assessment of the importance of long-range correlations
- direct evaluation of omitted higher-order contributions
- NCSM code by Petr Navratil [PRC 61, 044001 (2000)]

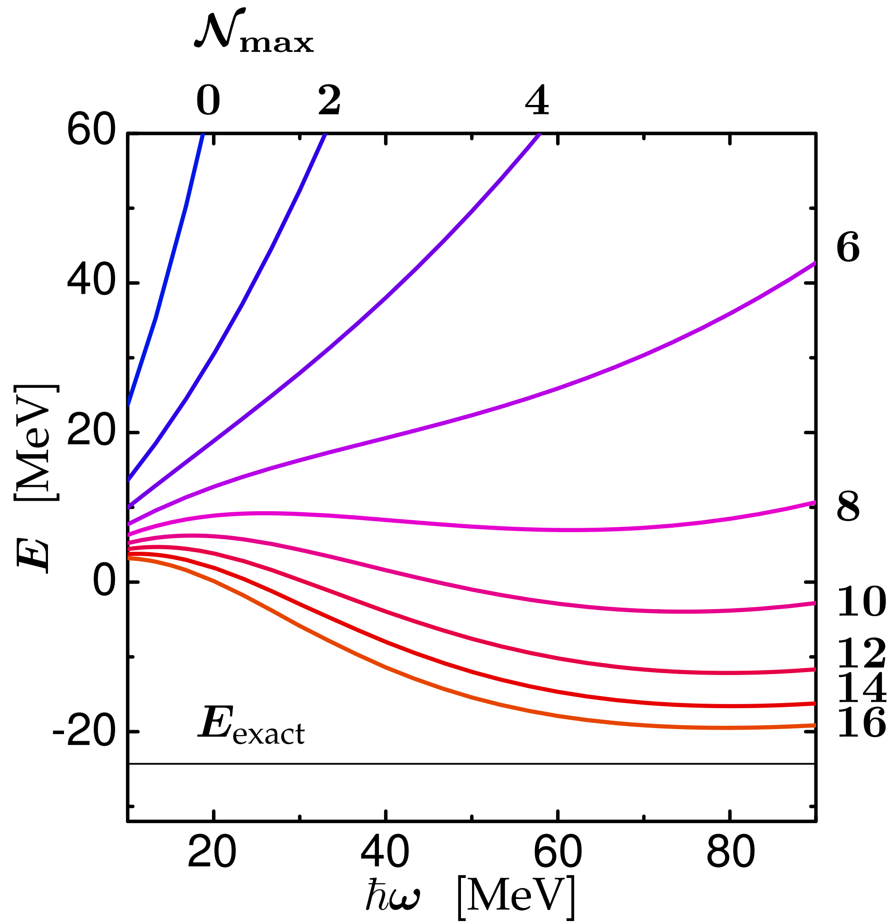
^{4}He: Convergence



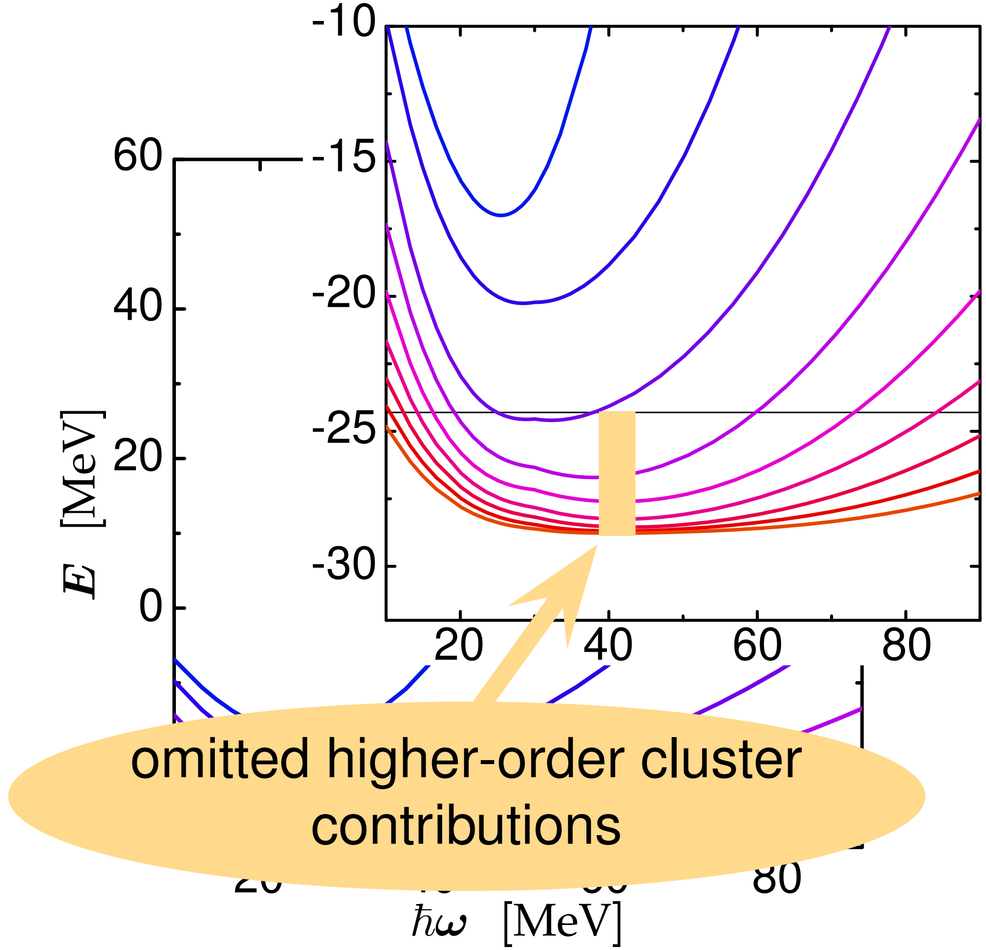


^{4}He: Convergence

V_{bare}



V_{UCOM}



Application II

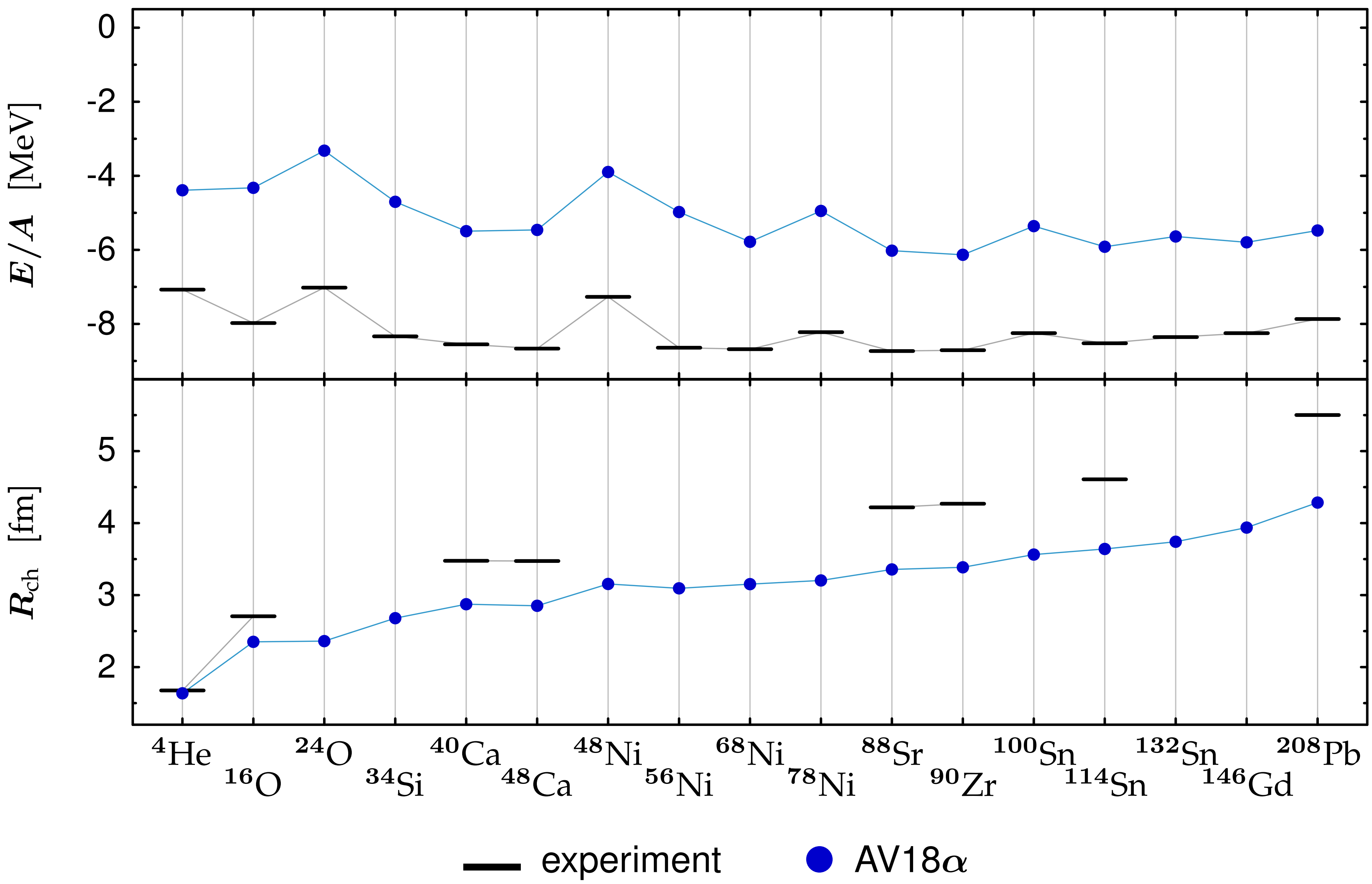
Hartree-Fock

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 center of mass contributions

Correlated Argonne V18



Missing Pieces

long-range correlations

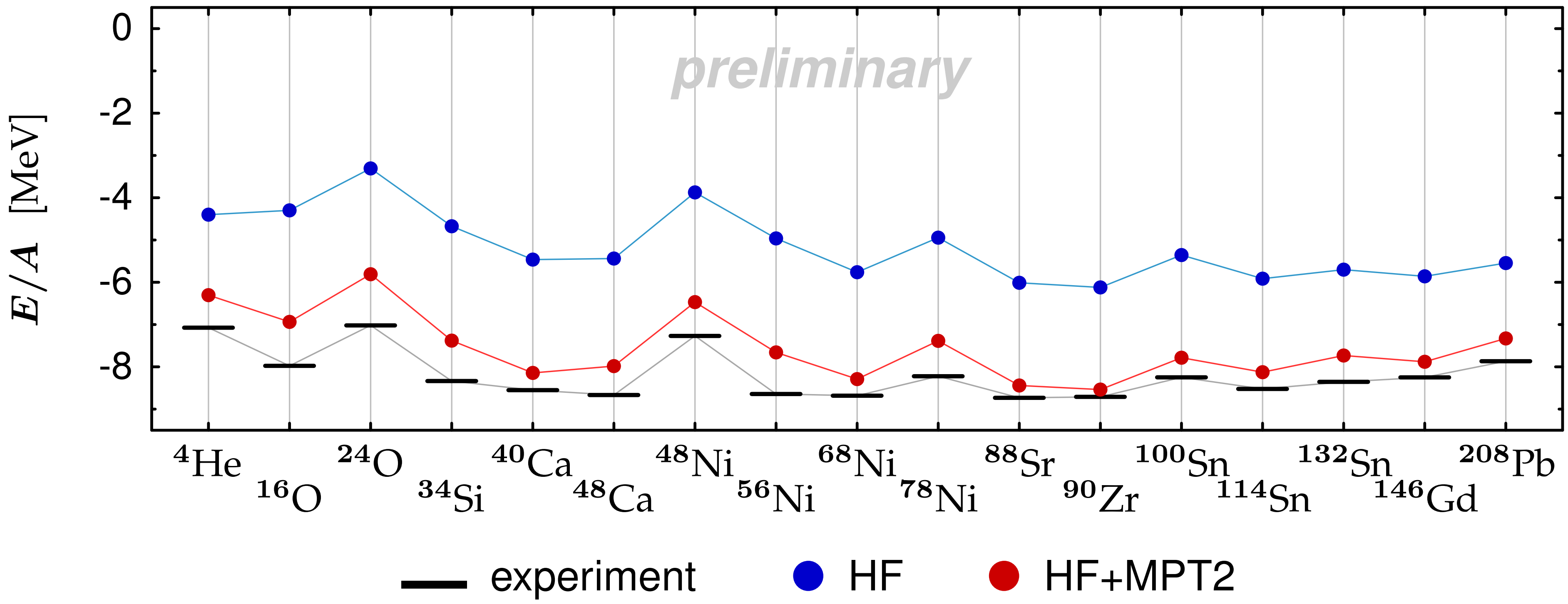
Ab Initio Strategy

- improve many-body states such that long-range correlations are included
- many-body perturbation theory (MPT), configuration interaction (CI), coupled-cluster (CC),...

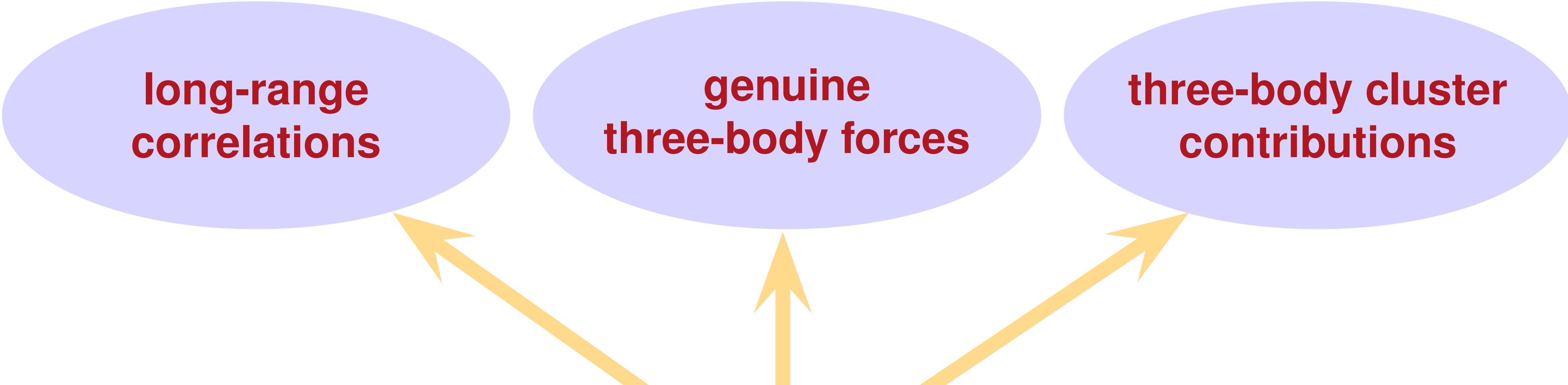
Long-Range Correlations

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

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



Missing Pieces



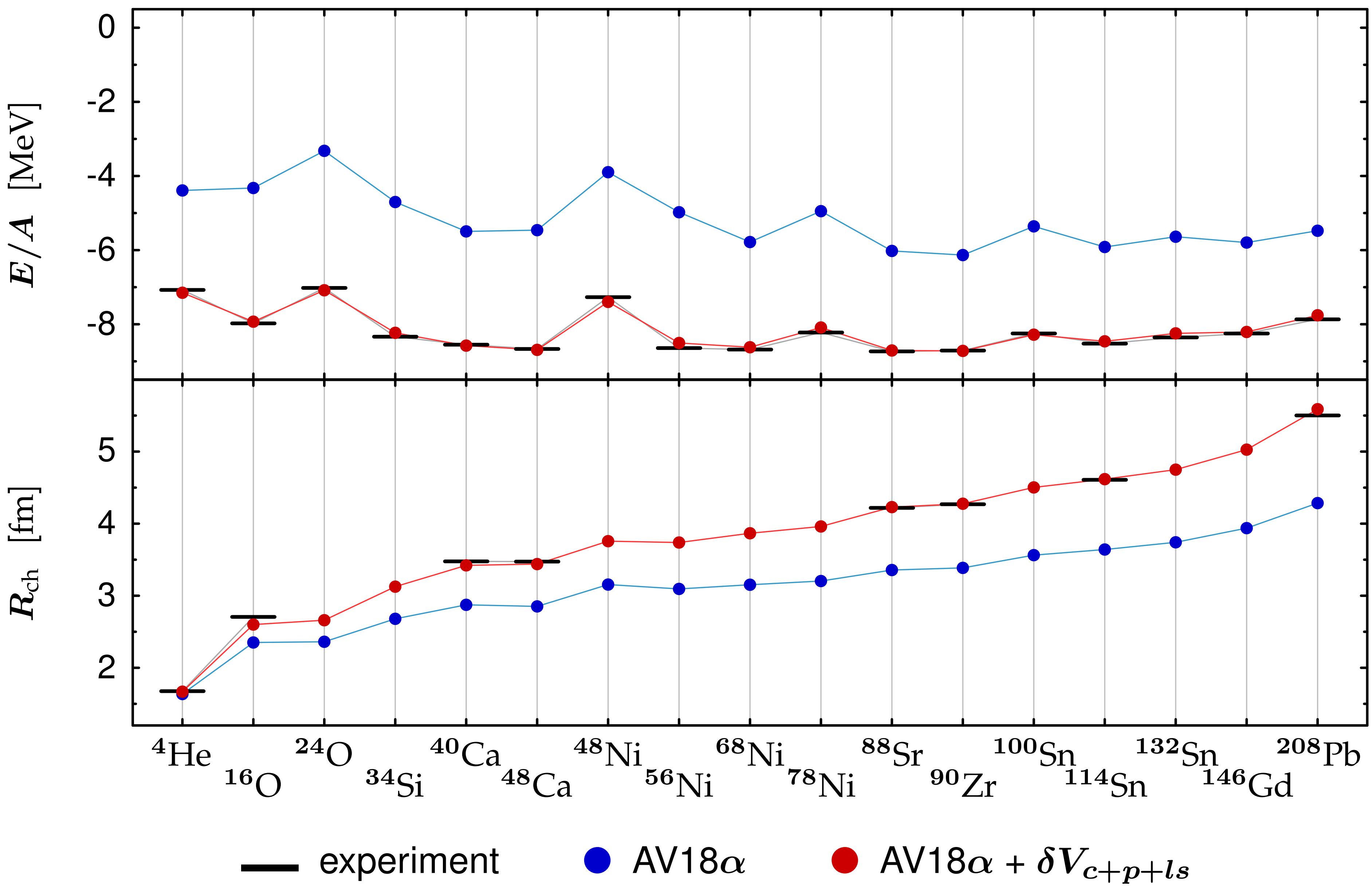
Pragmatic Approach

- phenomenological two-body correction

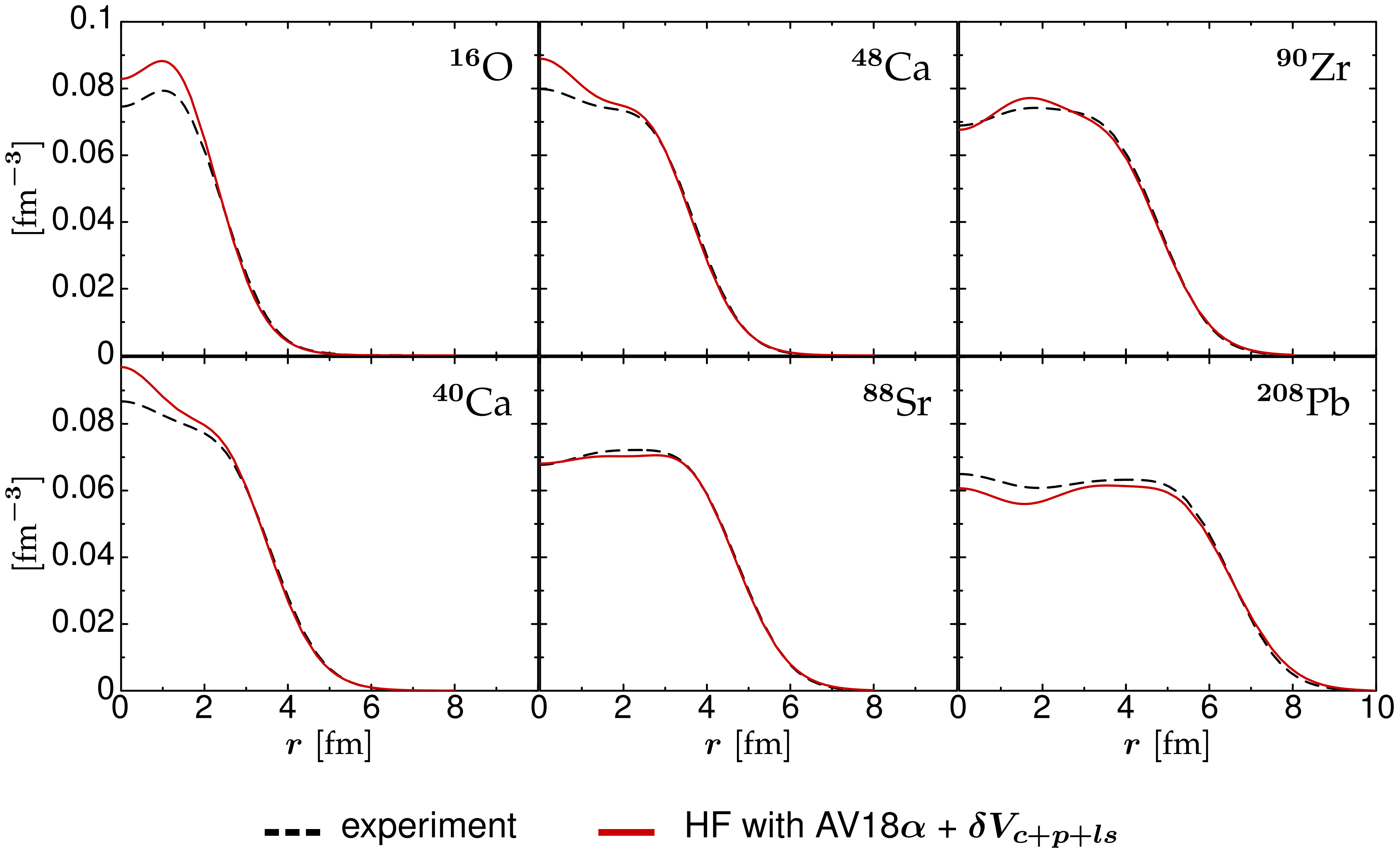
$$\delta \mathrm{V}_{c+p+ls} = v_1(\mathrm{r}) + \vec{\mathrm{q}}\, v_{qq}(\mathrm{r})\, \vec{\mathrm{q}} + v_{LS}(\mathrm{r})\, \vec{\mathrm{L}} \cdot \vec{\mathrm{S}}$$

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

Correlated Argonne V18 + Correction



Charge Distributions



Application III

Fermionic Molecular Dynamics (FMD)

FMD Approach

Gaussian Single-Particle States

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

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

a_ν : complex width

χ_ν : spin orientation

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

Slater Determinant

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

Correlated Hamiltonian

$$\widehat{\mathrm{H}} = \mathrm{T} + \mathrm{V}_{\mathrm{UCOM}} \; [+\delta \mathrm{V}_{c+p+ls}]$$

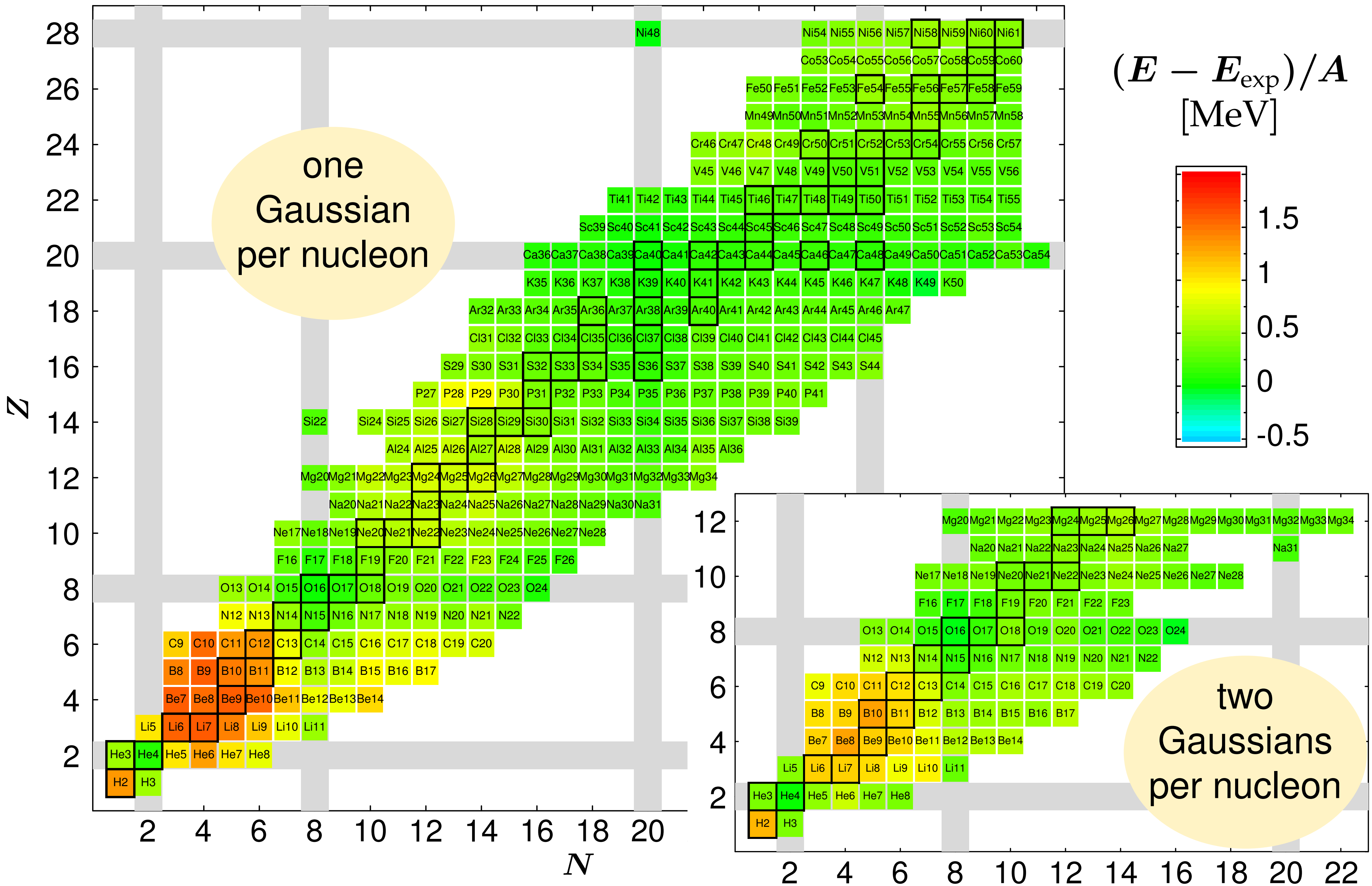
Variation

$$\frac{\langle Q | \, \widehat{\mathrm{H}} - \mathrm{T}_{\mathrm{cm}} \, | Q \rangle}{\langle Q | Q \rangle} \longrightarrow \min$$

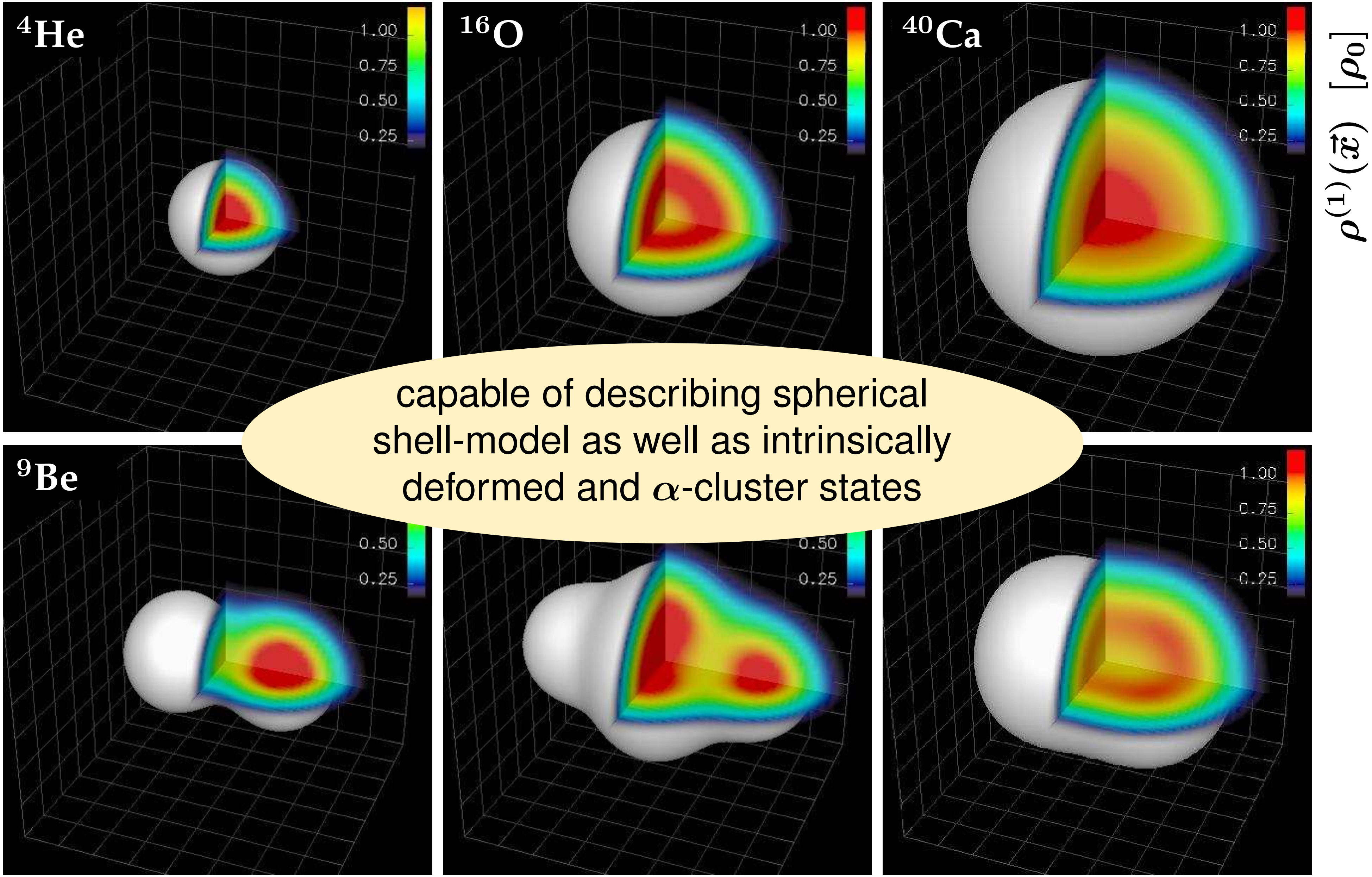
Diagonalization

in sub-space spanned by several non-orthogonal Slater determinants $|Q_i\rangle$

Variation: Chart of Nuclei



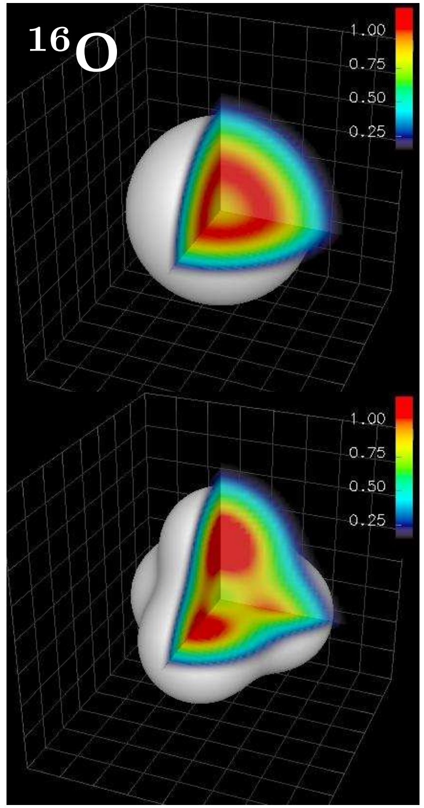
Intrinsic One-Body Density Distributions



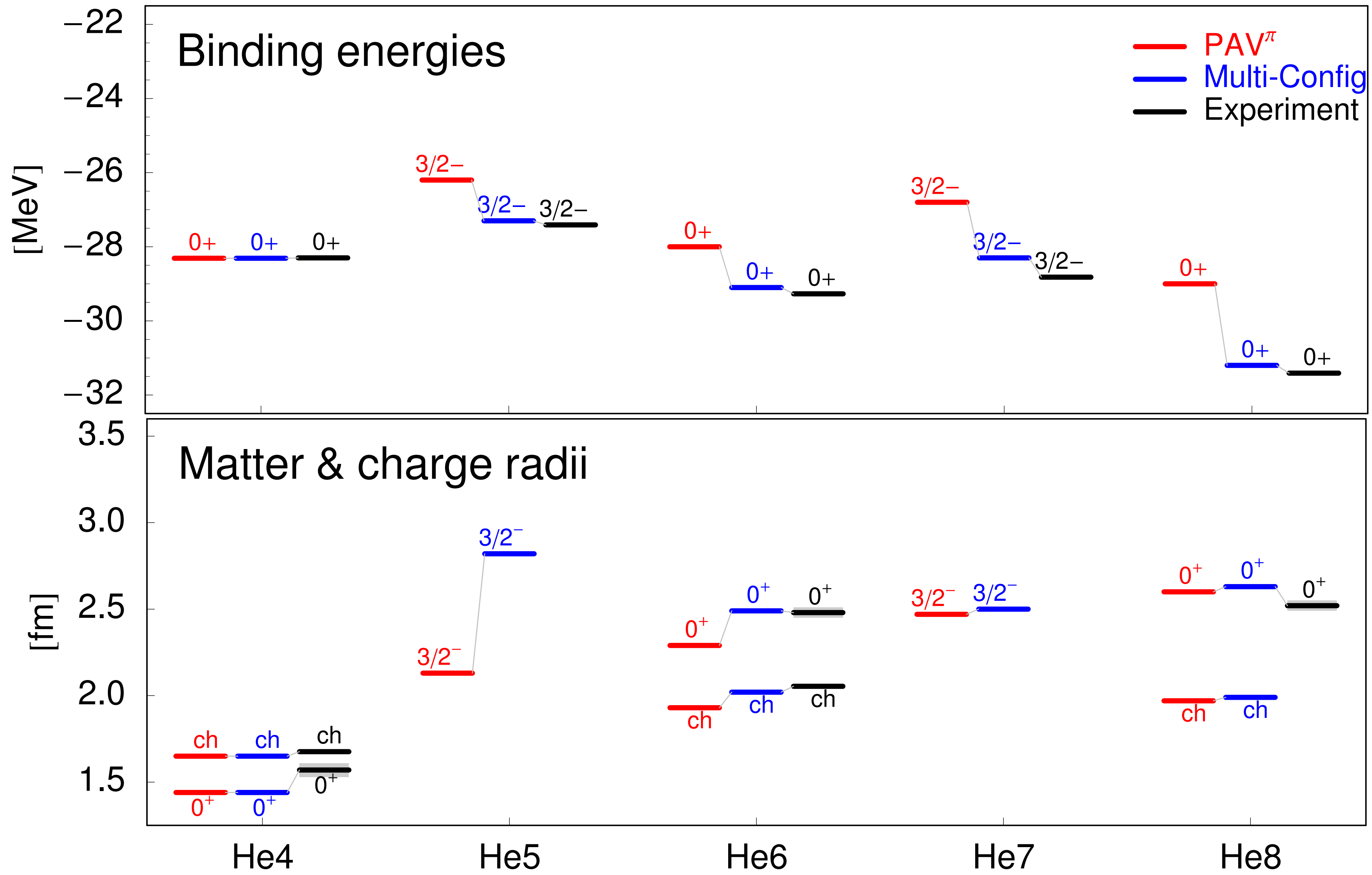
capable of describing spherical shell-model as well as intrinsically deformed and α-cluster states

Beyond Simple Variation

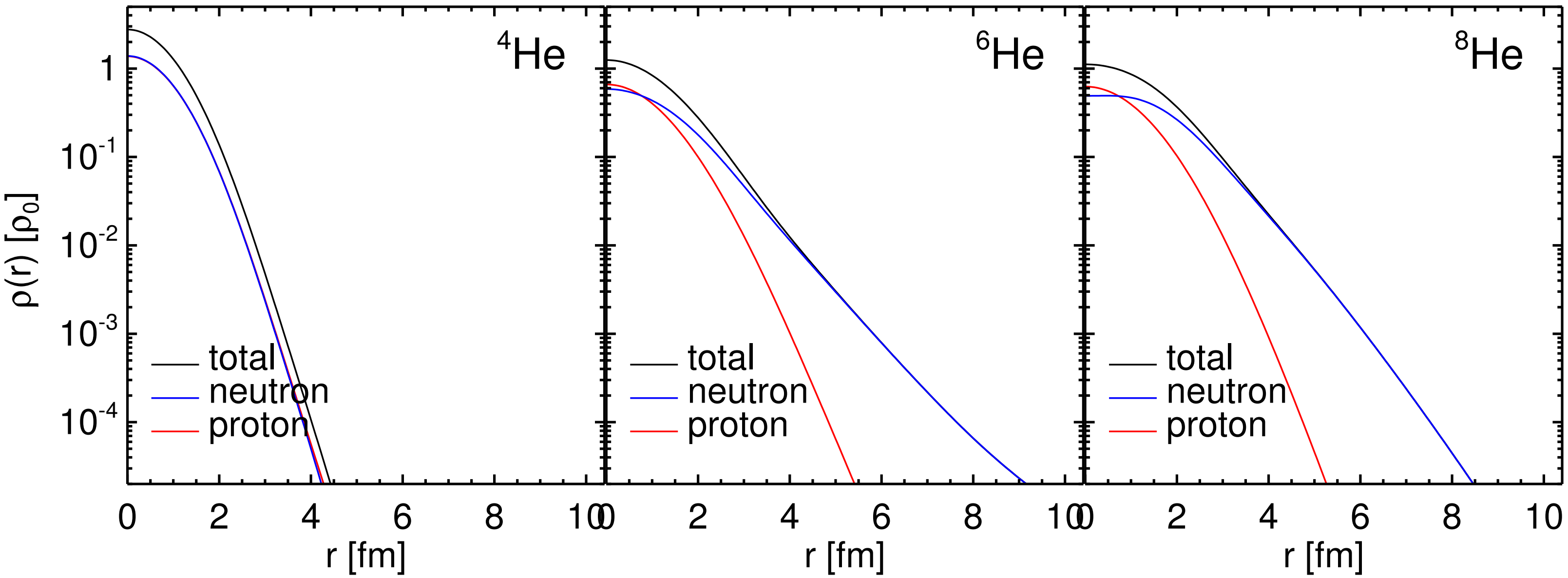
- **Projection after Variation (PAV)**
  - restore inversion and rotational symmetry by angular momentum projection
- **Variation after Projection (VAP)**
  - find energy minimum within parameter space of parity and angular momentum projected states
  - implementation via generator coordinate method (constraints on multipole moments)
- **Multi-Configuration**
  - diagonalization within a set of different Slater determinants



Helium Isotopes: Energies & Radii

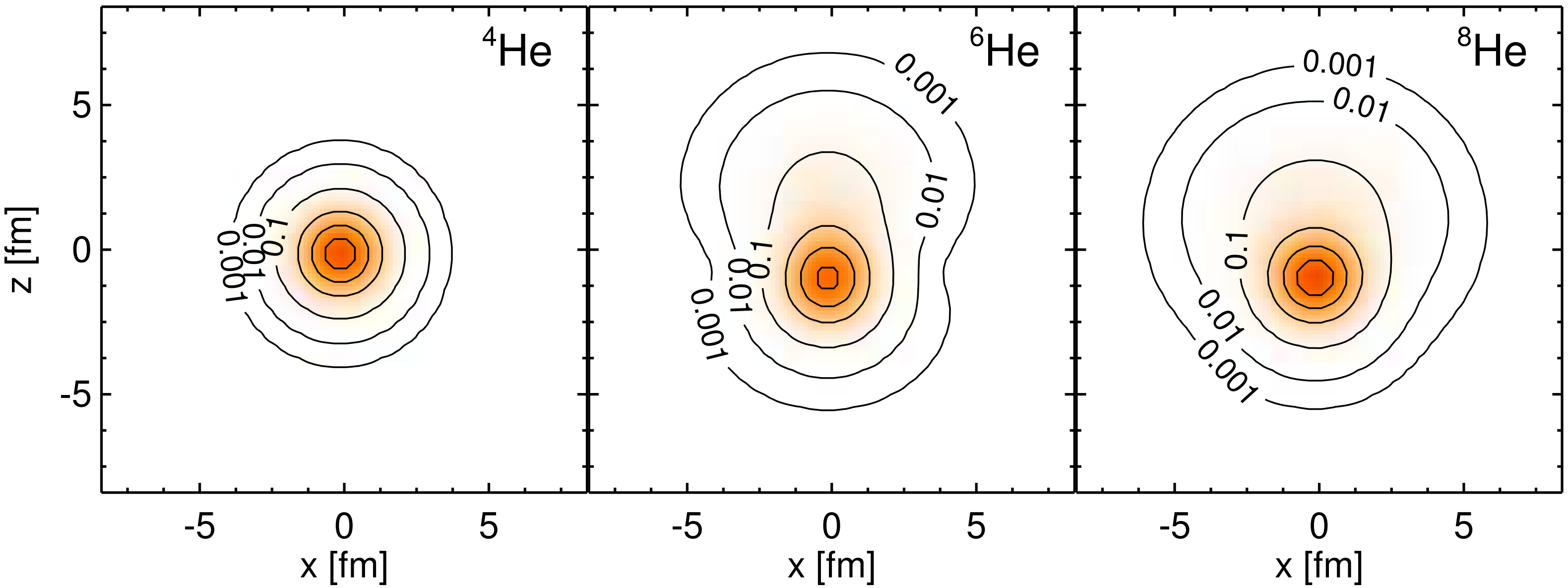


Helium Isotopes: Densities



Multi-Config

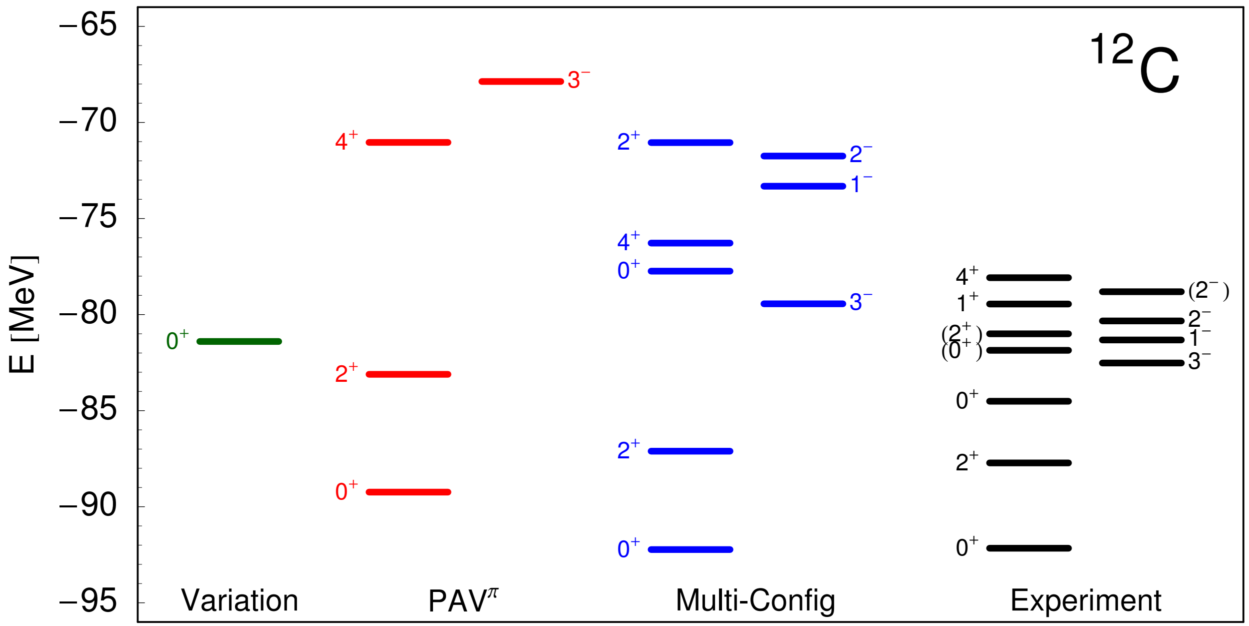
radial density profiles

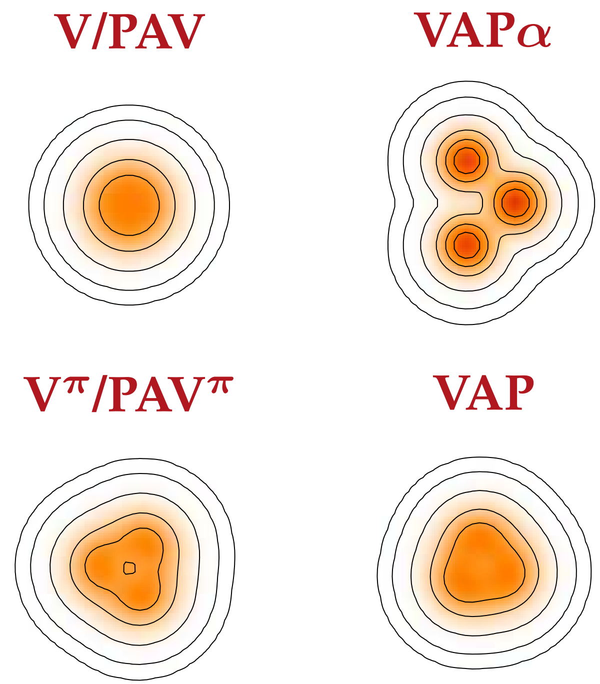


PAV$^{\pi}$

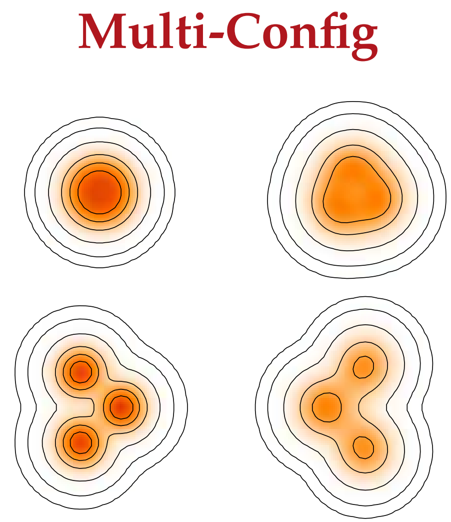
intrinsic densities

Structure of ^{12}C

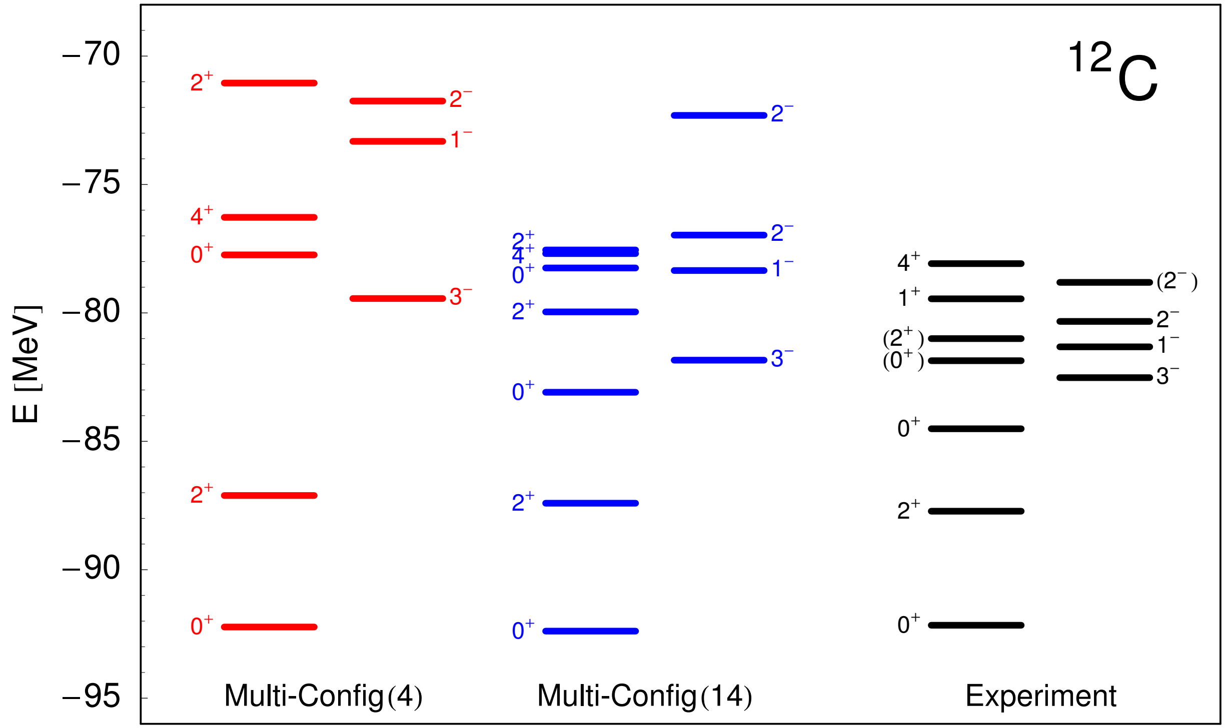


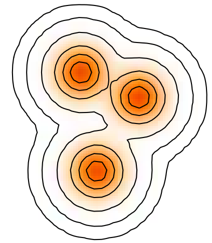


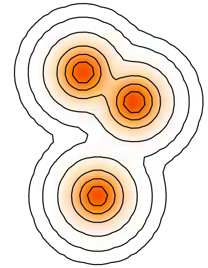
	E [MeV]	R_{ch} [fm]	$B(E2)$ [e^2 fm^4]
V/PAV	81.4	2.36	-
VAP α-cluster	79.1	2.70	76.9
PAV$^{\pi}$	88.5	2.51	36.3
VAP	89.2	2.42	26.8
Multi-Config	92.2	2.52	42.8
Experiment	92.2	2.47	39.7 ± 3.3

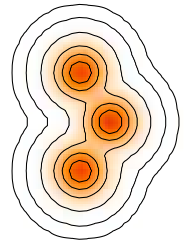


Structure of ^{12}C — Hoyle State



$|\langle$  $|0_2^+\rangle| = \mathbf{0.76}$

$|\langle$  $|0_2^+\rangle| = \mathbf{0.71}$

$|\langle$  $|0_2^+\rangle| = \mathbf{0.50}$

	Multi-Config	Experiment
E [MeV]	92.4	92.2
R_{ch} [fm]	2.52	2.47
$B(E2, 0_1^+ \to 2_1^+)$ [e^2 fm^4]	42.9	39.7 ± 3.3
$M(E0, 0_1^+ \to 0_2^+)$ [fm^2]	5.67	5.5 ± 0.2

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 long-range correlations & higher-order contributions
- **UCOM + Hartree-Fock**
  - closed shell nuclei across the whole nuclear chart
  - basis for improved many-body calculations
- **UCOM + Fermionic Molecular Dynamics**
  - clustering and intrinsic deformations in p- and sd-shell
  - projection / multi-config provide detailed structure information

Outlook

- **residual “long-range” correlations**
  - many-body perturbation theory
  - configuration interaction & coupled-cluster calculations
  - pairing correlations, Hartree-Fock-Bogoliubov
- **collective excitations**
  - random phase approximation (RPA, SRPA, QRPA)
- **make contact to experiment!!!**