# Nuclear Structure based on Correlated Realistic NN-Interactions

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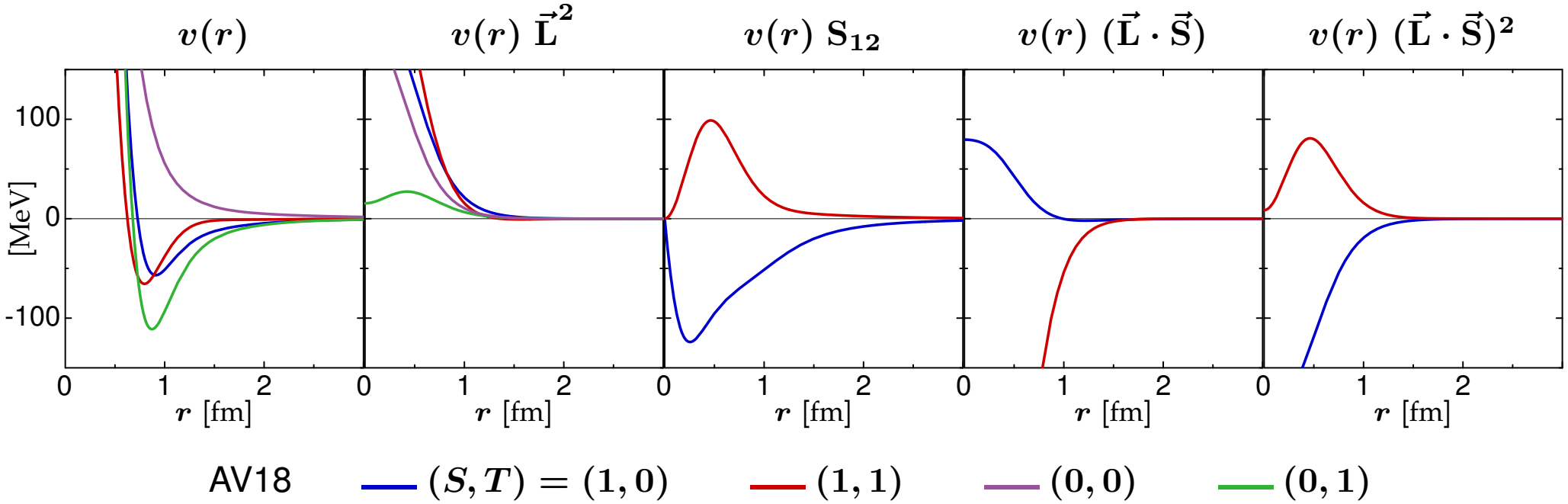
# Our Aim

nuclear structure calculations
across the **whole nuclear chart**
based on **realistic NN-potentials**
and as close as possible to
an **ab initio** treatment

# Realistic NN-Potentials

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

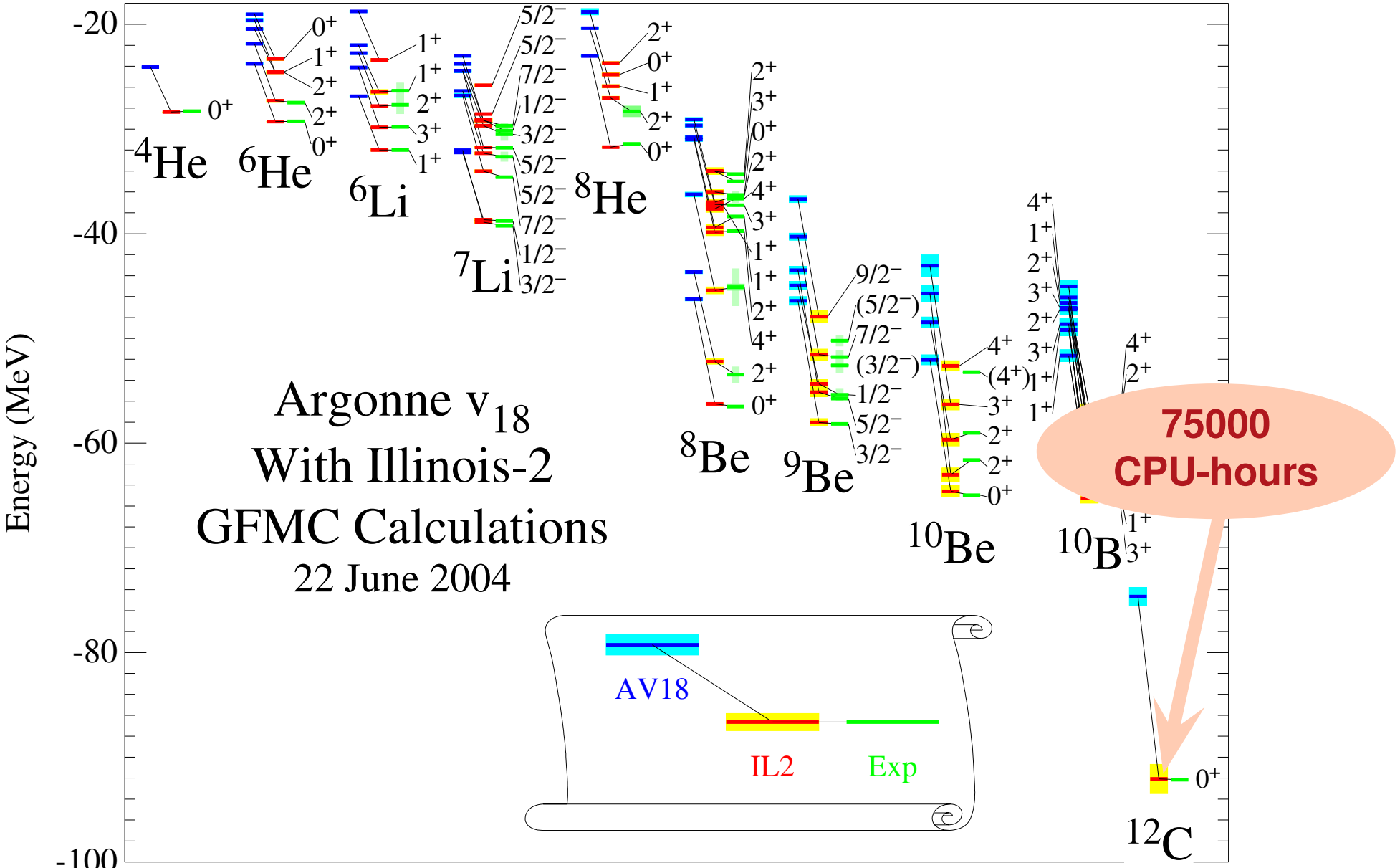


# Realistic NN-Potentials

- 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* Many-Body 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**
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

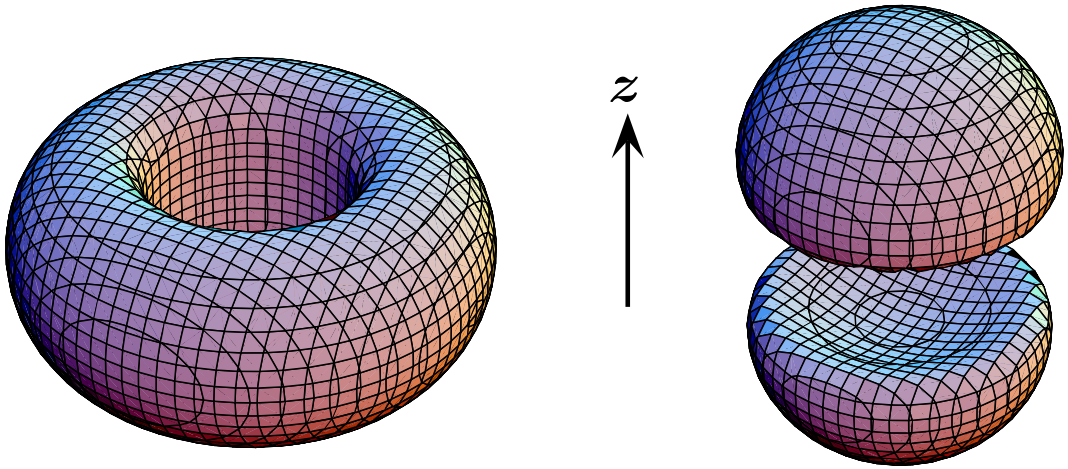
# Deuteron: Manifestation of Correlations

$M_S = 0$

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

$M_S = \pm 1$

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




- spin-projected two-body density $\rho^{(2)}_{1,M_S}(\vec{r})$
- **exact deuteron solution** for Argonne V18 potential

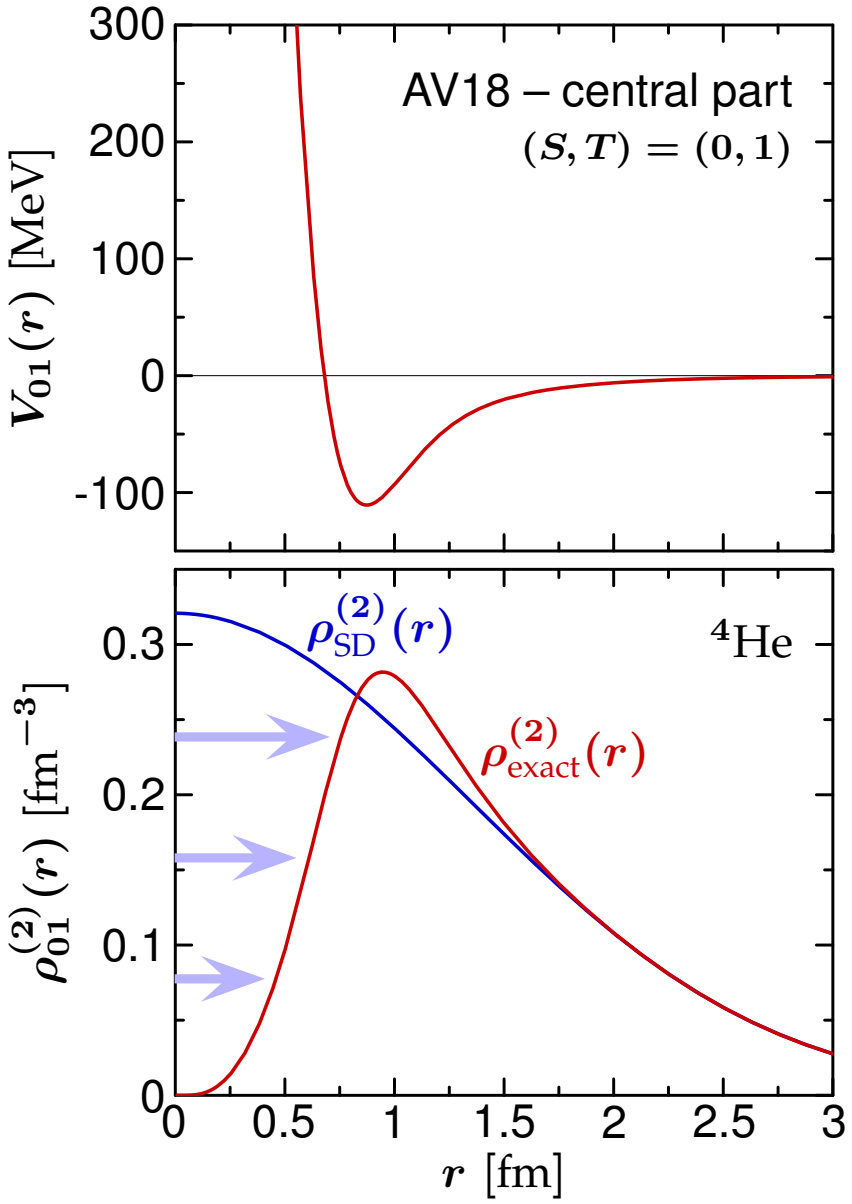
two-body density fully suppressed at small particle distances $|\vec{r}|$

**central correlations**

angular distribution depends strongly on relative spin orientation

**tensor correlations**

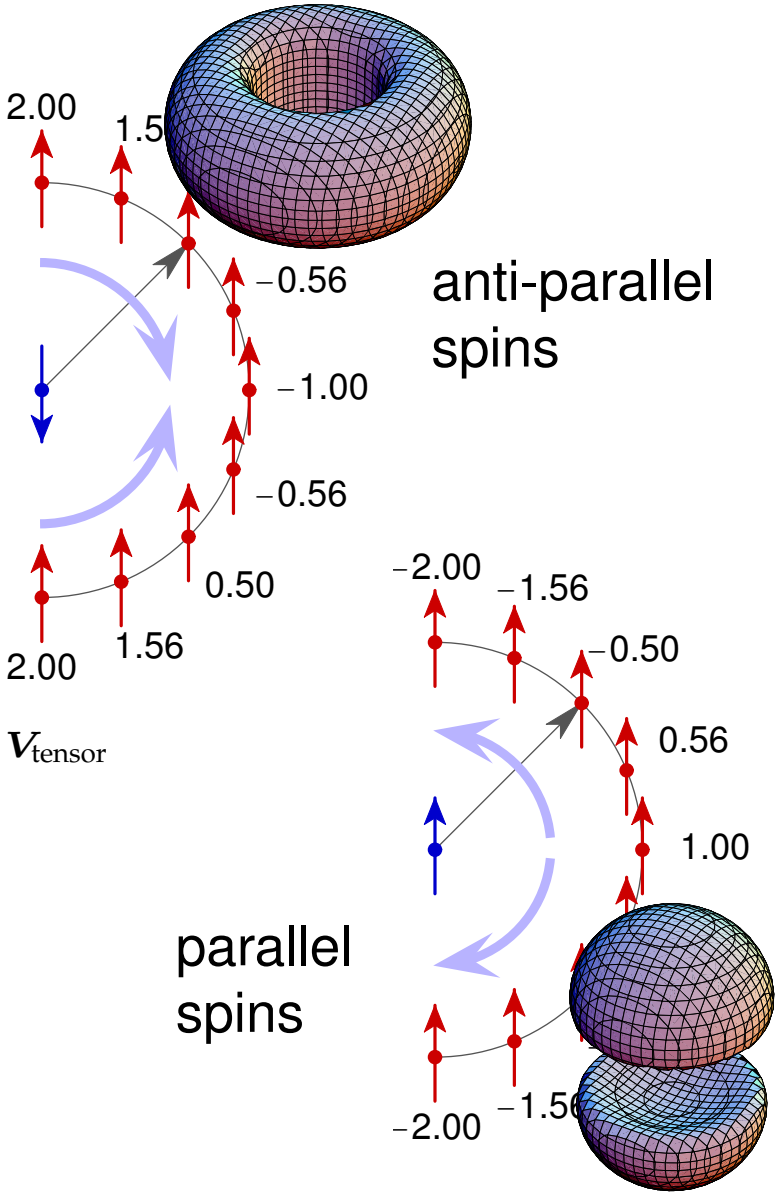
# Central Correlations




- 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 an 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 States

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

## Correlated Operators

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

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

# 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

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

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

## Tensor Correlator $\mathrm{C}_\Omega$

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

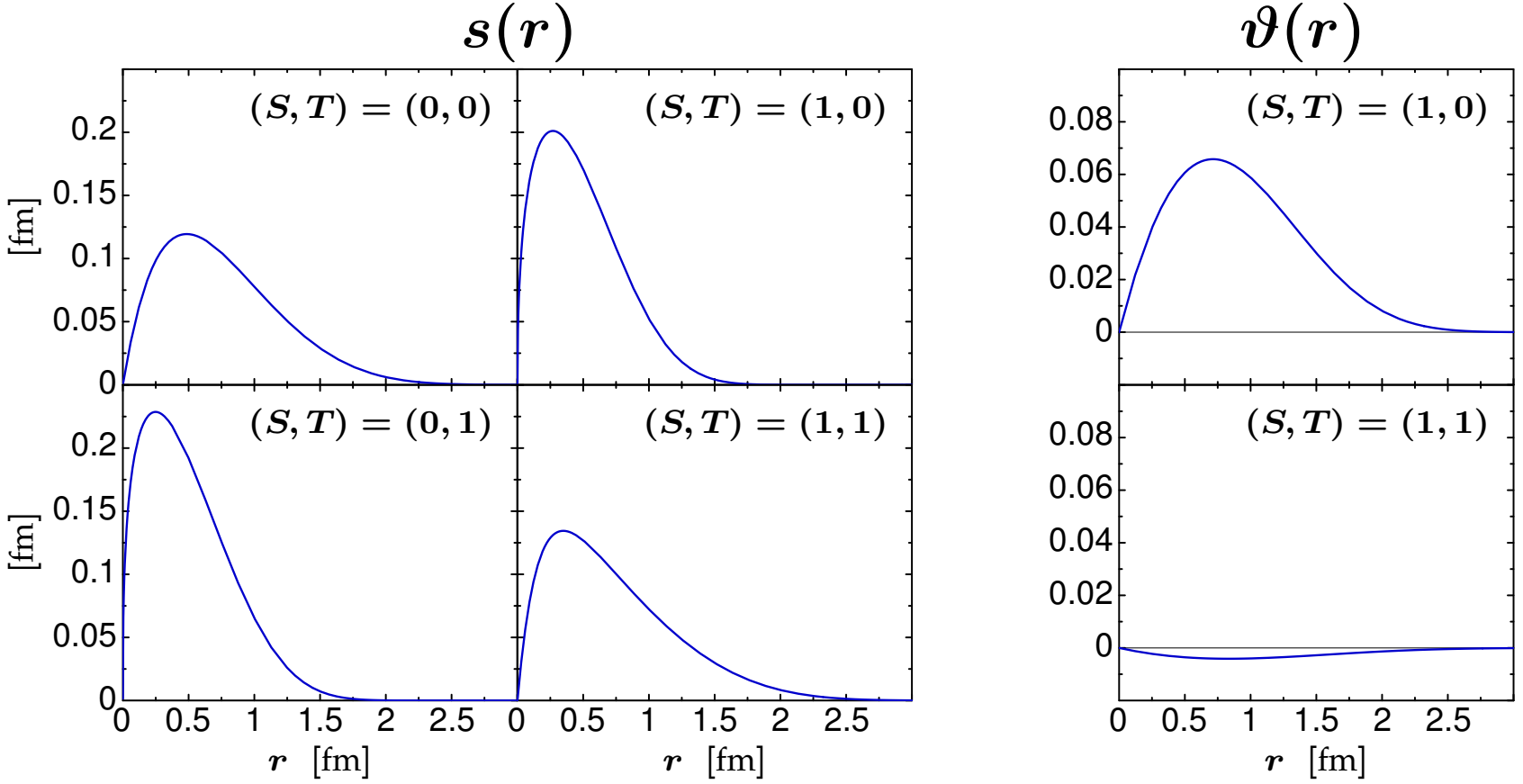
$$\mathrm{g}_\Omega = \frac{3}{2}\vartheta(\mathrm{r})\left[(\vec{\sigma}_1 \cdot \vec{\mathrm{q}}_\Omega)(\vec{\sigma}_2 \cdot \vec{\mathrm{r}}) + (\vec{\mathrm{r}} \leftrightarrow \vec{\mathrm{q}}_\Omega)\right]$$

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

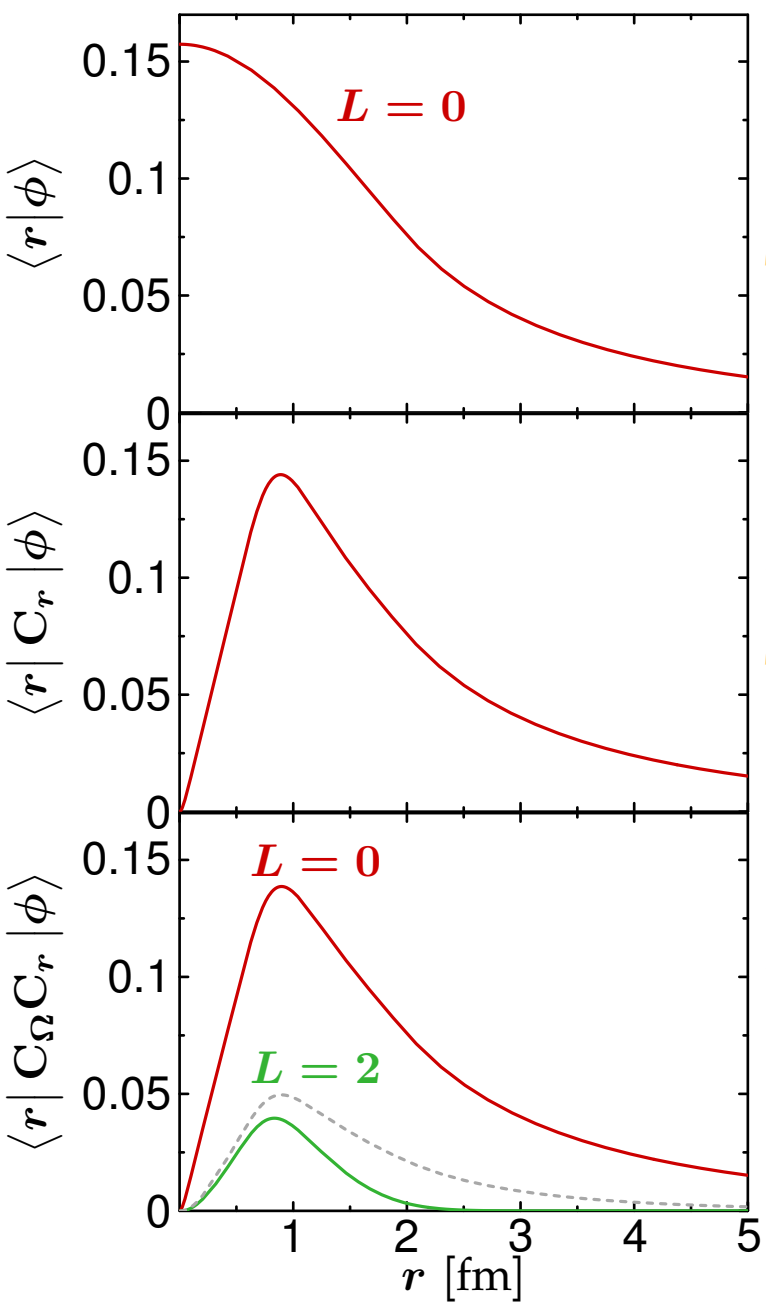
$s(r)$ and $\vartheta(r)$
encapsulate the physics of
short-range correlations

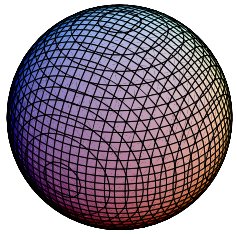
# Optimal Correlation Functions

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



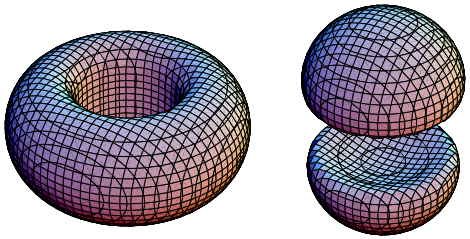
# Correlated States

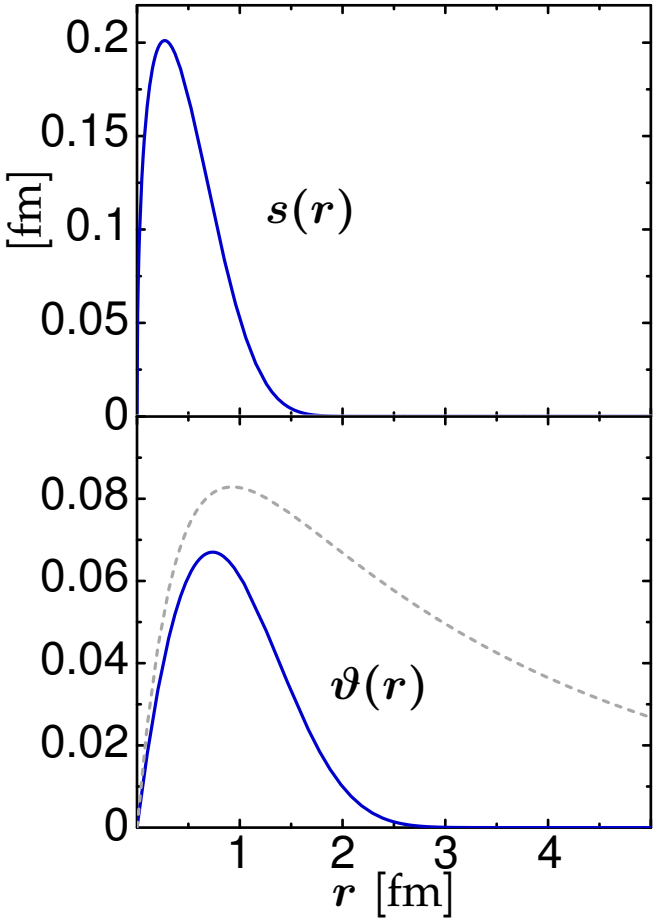


central correlations

tensor correlations





# Correlated Operators

**Cluster Expansion**

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

**Cluster Decomposition Principle**

if the correlation range is small compared to the mean particle distance, then higher orders are small

**Two-Body Approx.**

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

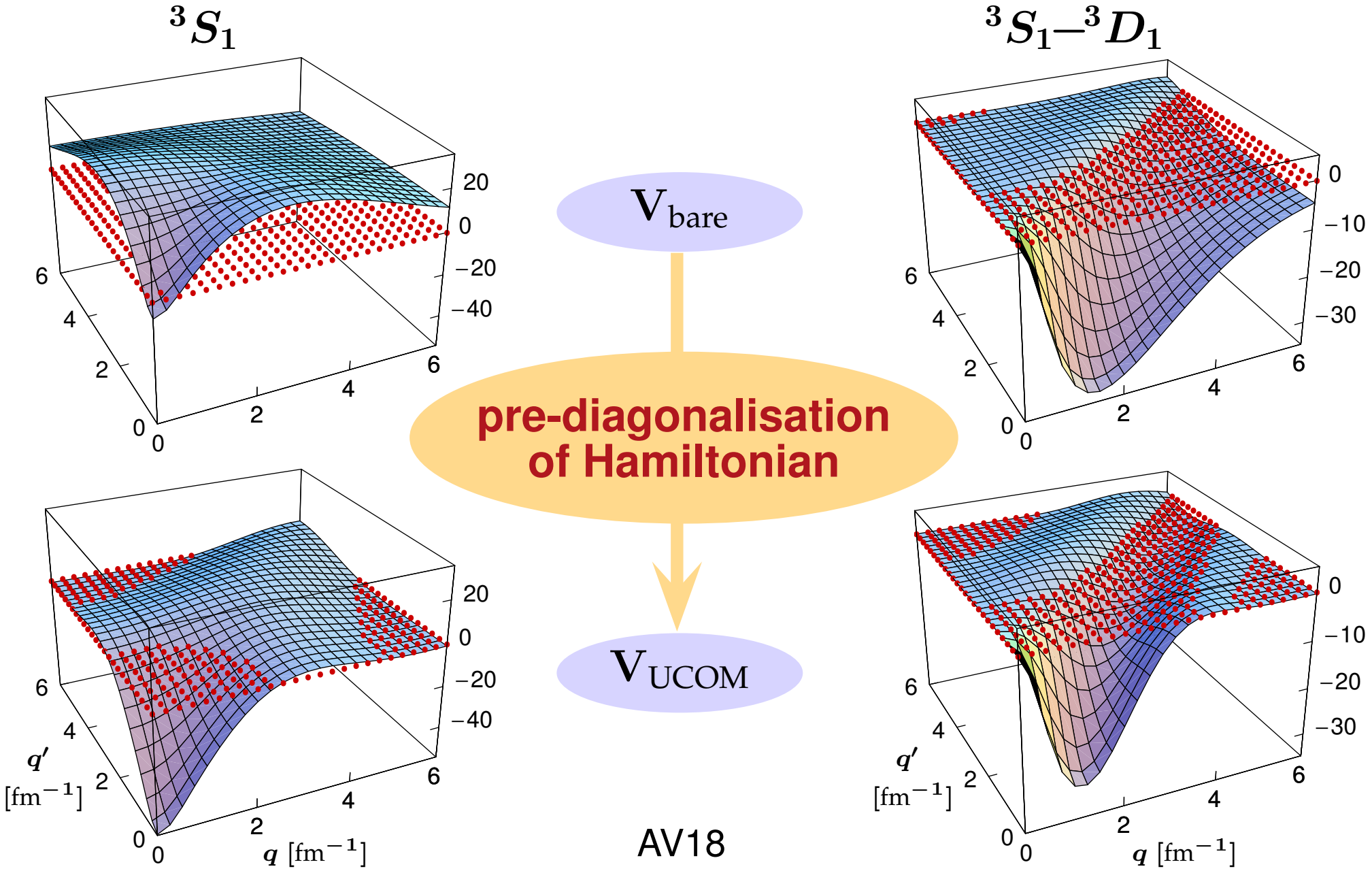
**operators of all observables can be and have to be correlated consistently**

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

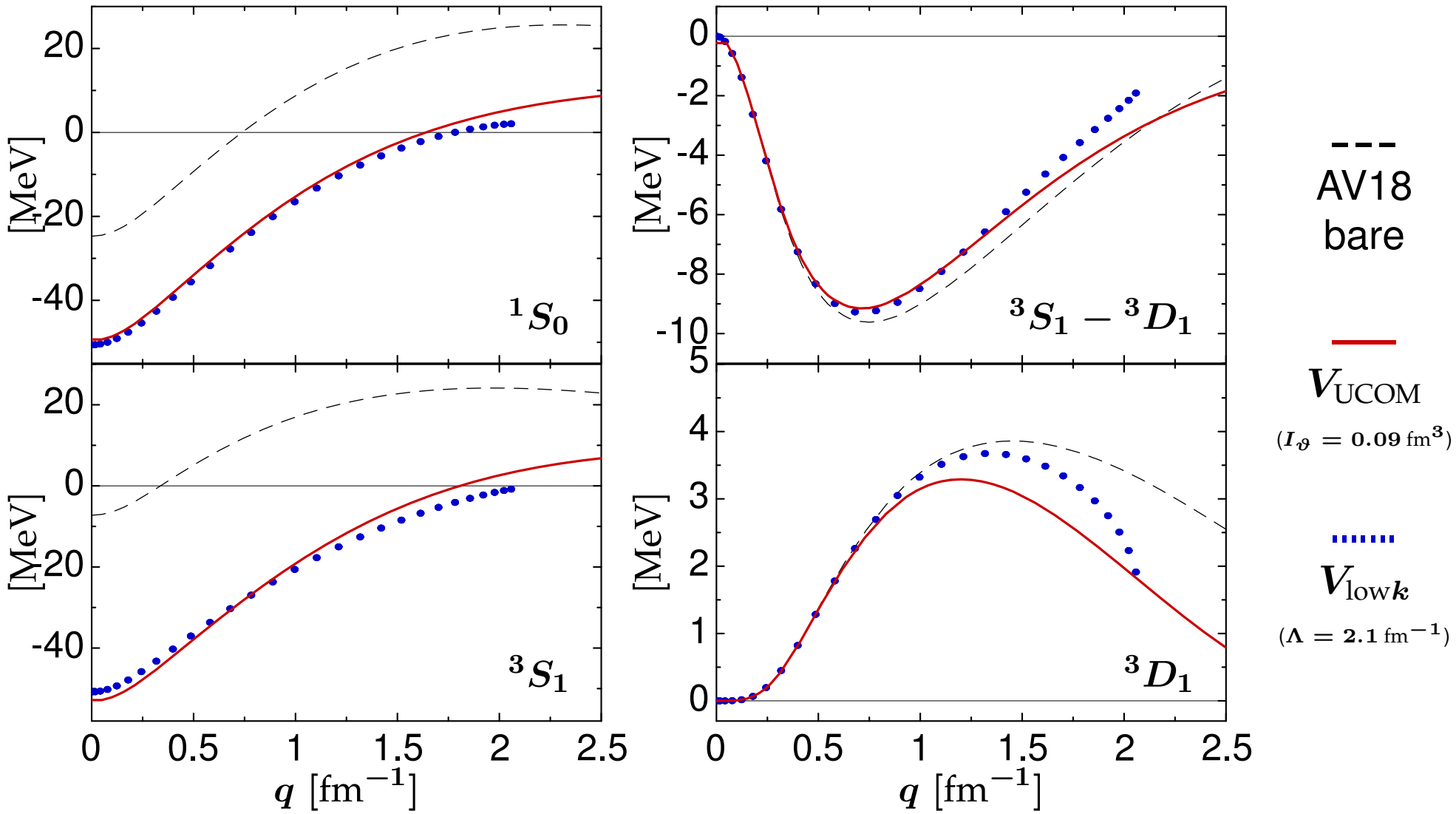
$$\widetilde{\mathbf{H}}^{C2} = \widetilde{\mathbf{T}}^{[1]} + \widetilde{\mathbf{T}}^{[2]} + \widetilde{\mathbf{V}}^{[2]} = \mathbf{T} + \mathbf{V}_{\mathrm{UCOM}}$$

- **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-diagonalisation** of Hamiltonian
- momentum-space matrix elements of correlated interaction are **similar to** $V_{\mathrm{low}-k}$

# Momentum-Space Matrix Elements

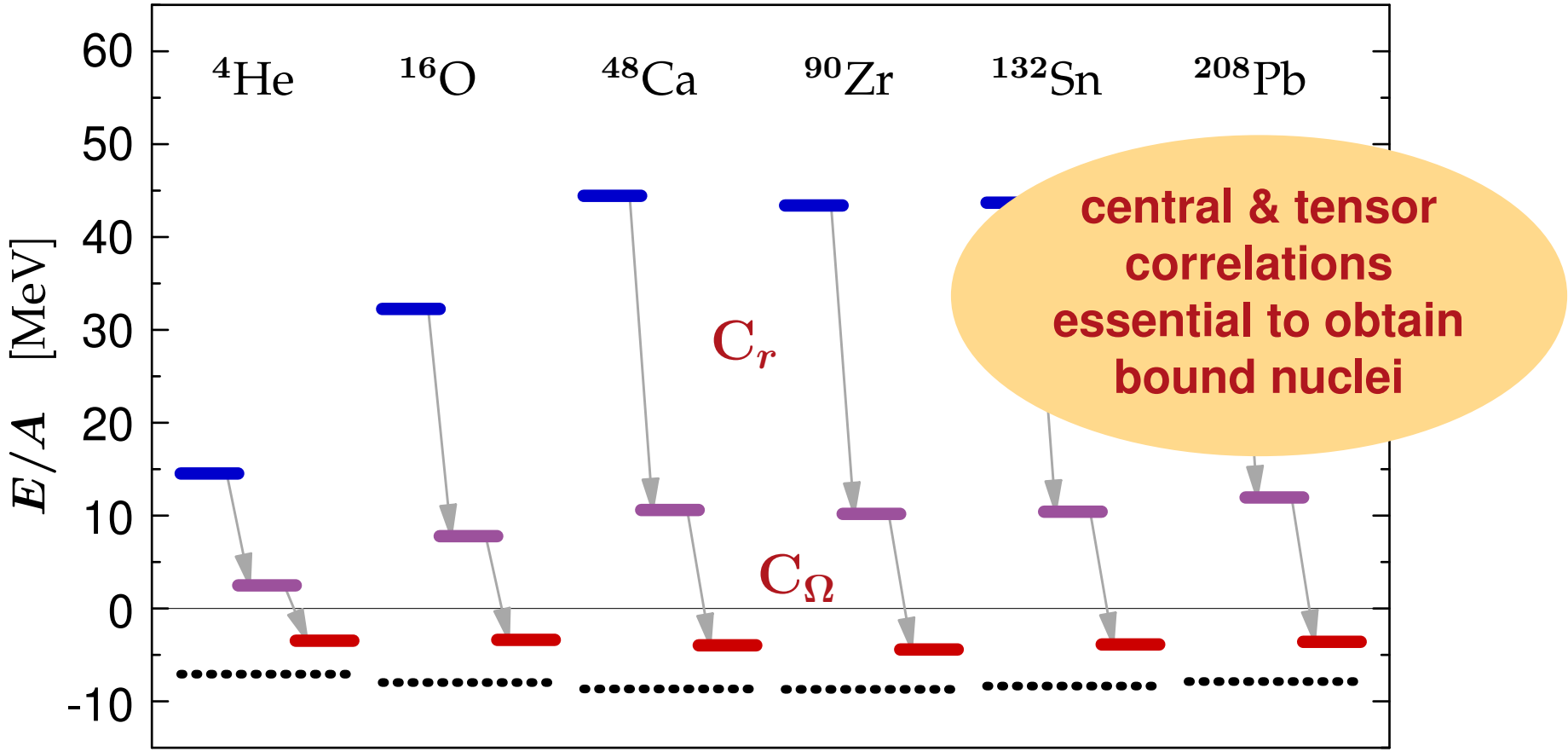


# Comparison with $V_{\mathrm{low}k}$



# Simplistic "Shell-Model" Calculation

- expectation value of Hamiltonian (with AV18) for Slater determinant of harmonic oscillator states



Application I

# No-Core Shell Model

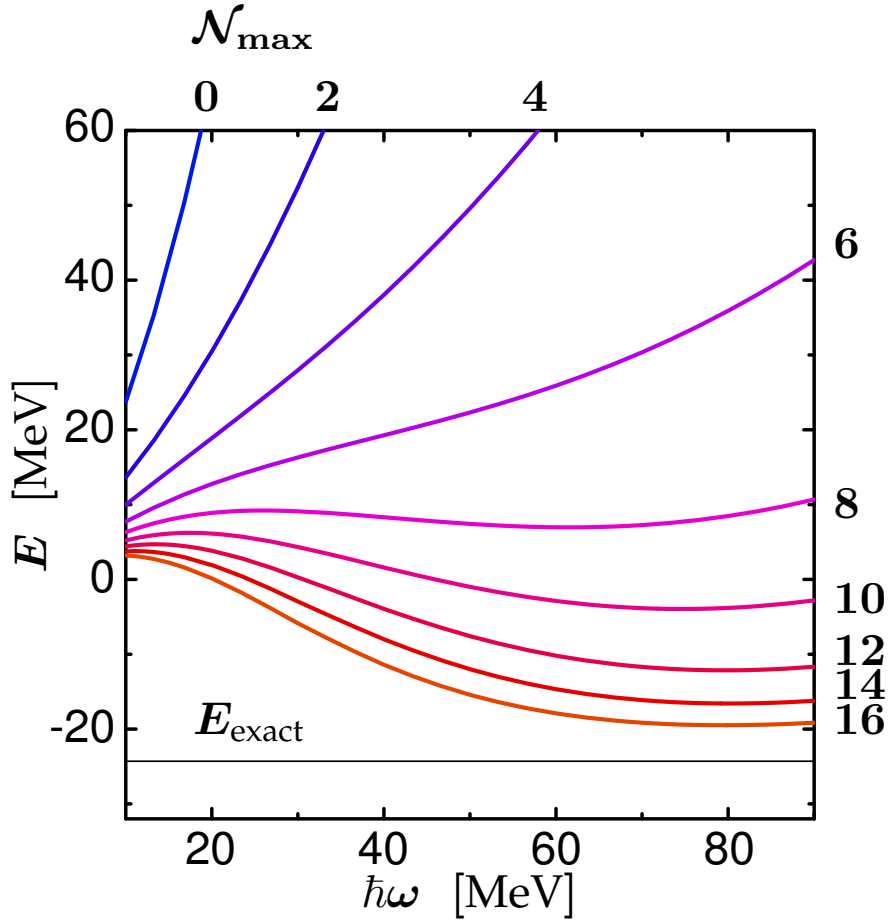
# UCOM + NCSM

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

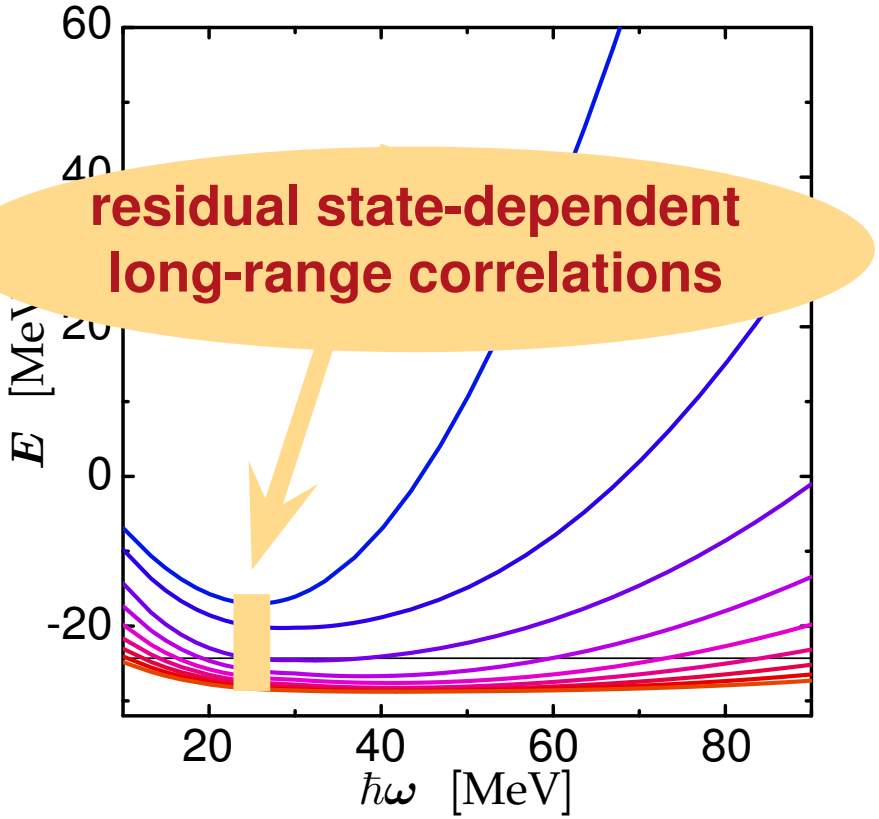
- convergence dramatically improved compared to bare interaction
- assessment of the importance of long-range correlations
- direct evaluation of omitted higher-order contributions
- Jacobi-NCSM code by Petr Navrátil without Lee-Suzuki
  [PRC 61, 044001 (2000)]

# $^4$He: Convergence

$\mathbf{V}_{\text{bare}}$

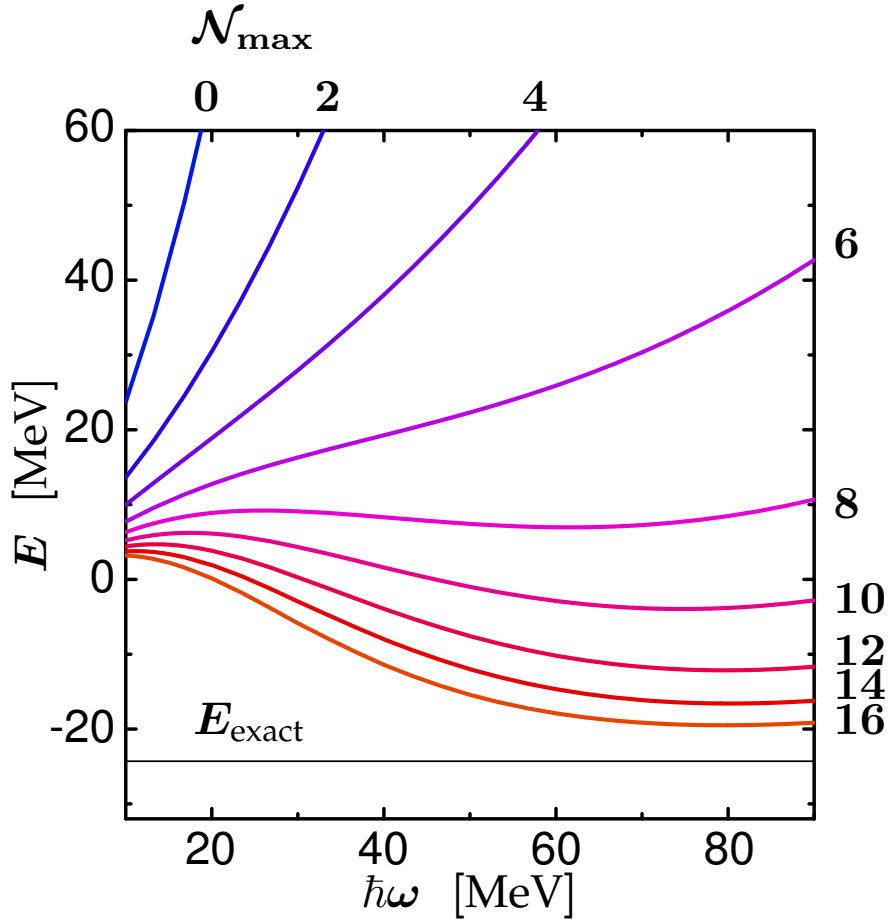



$\mathbf{V}_{\text{UCOM}}$

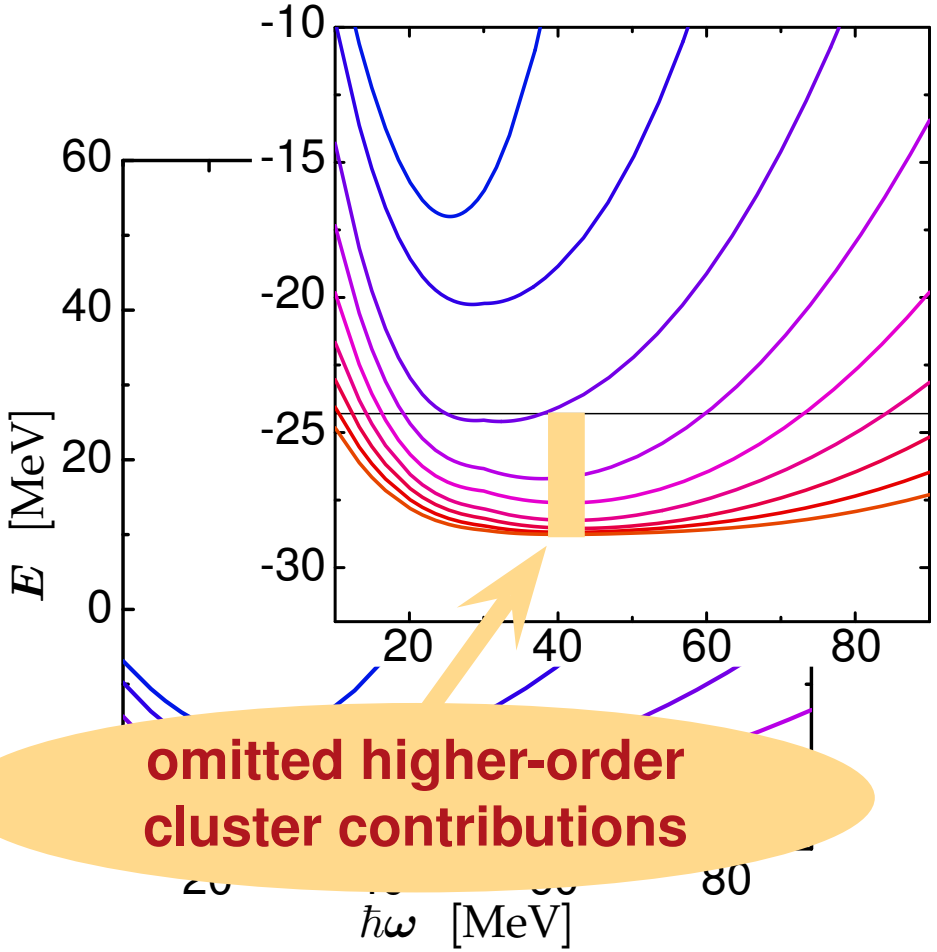


# $^4$He: Convergence

$V_{bare}$

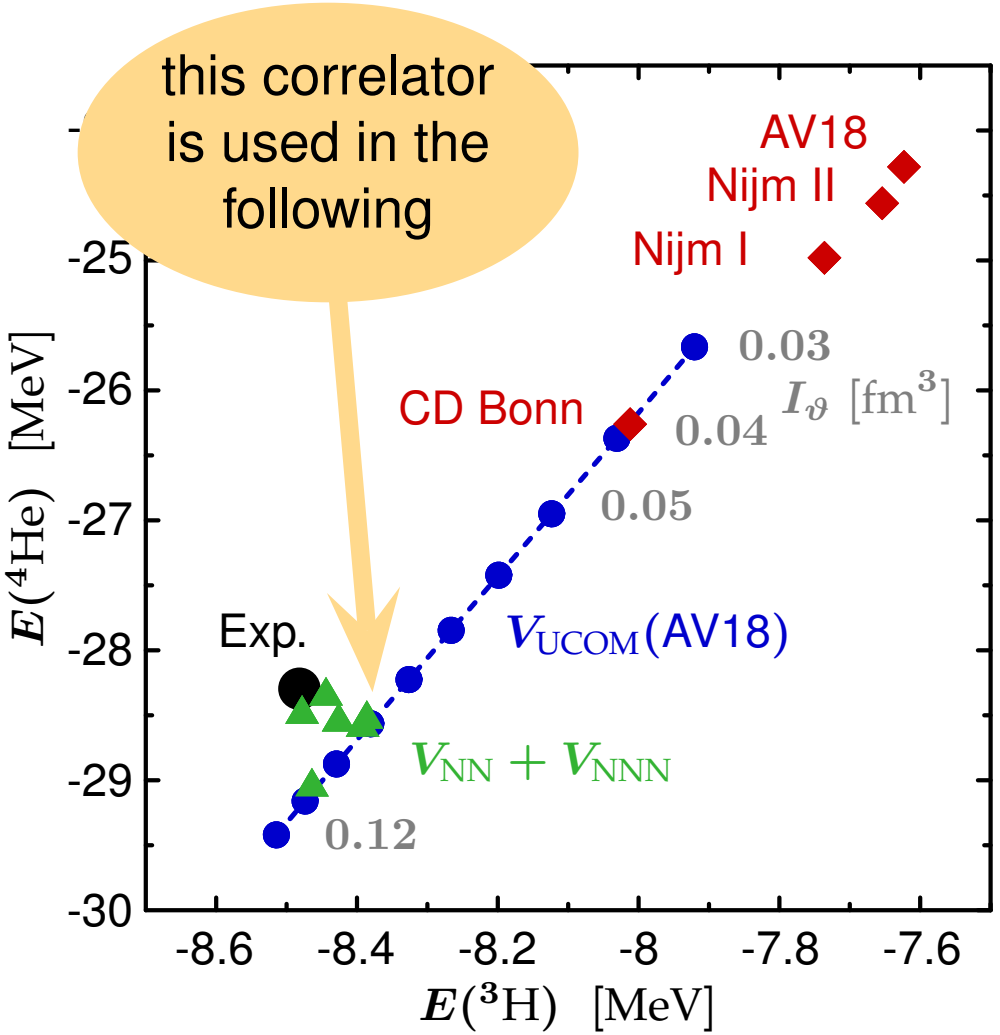



$V_{UCOM}$




**omitted higher-order cluster contributions**

# Tjon-Line and Correlator Range




- **Tjon-line**: $E(^4\mathrm{He})$ vs. $E(^3\mathrm{H})$ for phase-shift equivalent NN-interactions
- change in correlator range results in shift along Tjon-line

choose correlator with energies close to experimental value, i.e., **minimise net three-body force**

Application II

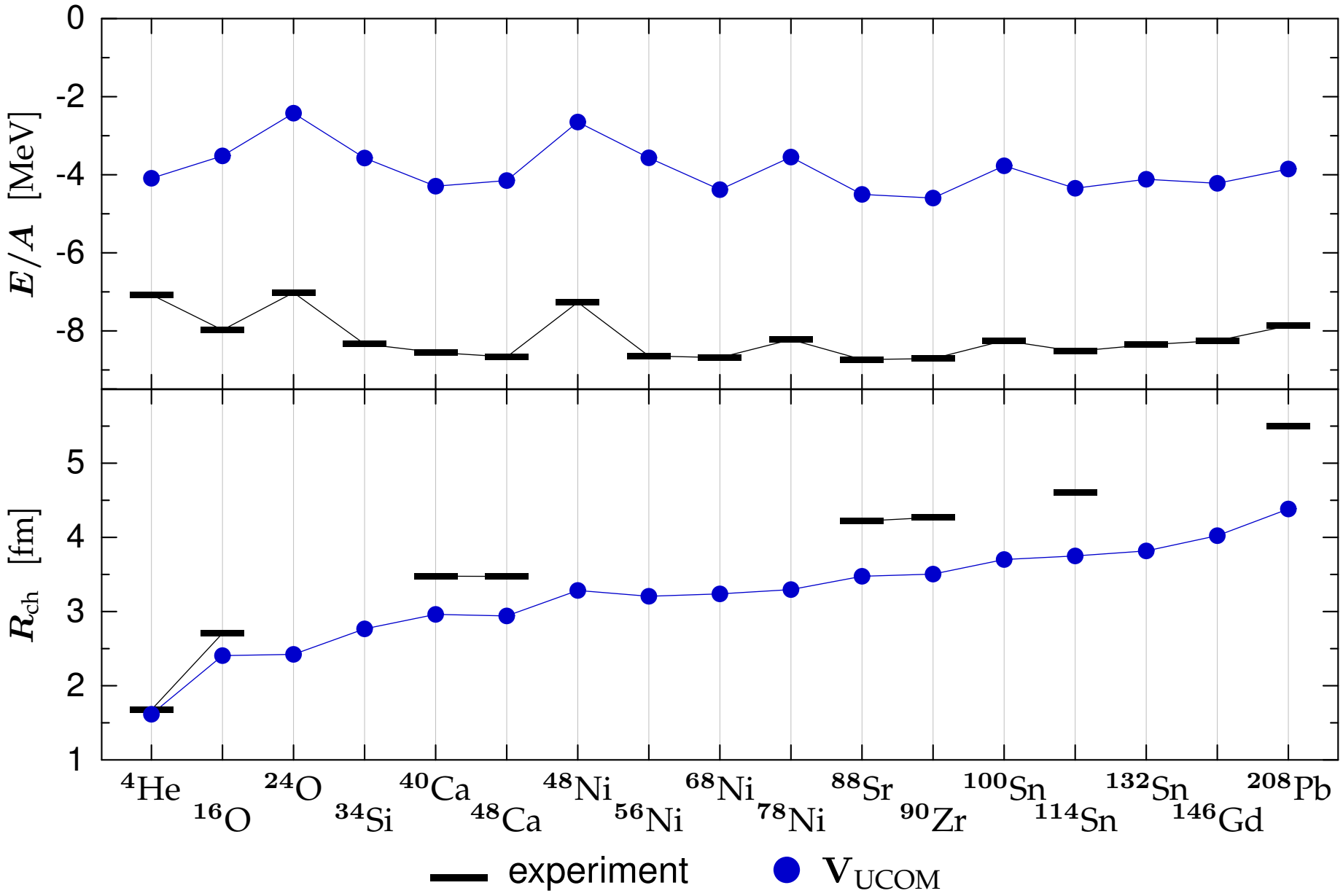
# Hartree-Fock

# 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 $N_{max} = 8...14$)
- 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

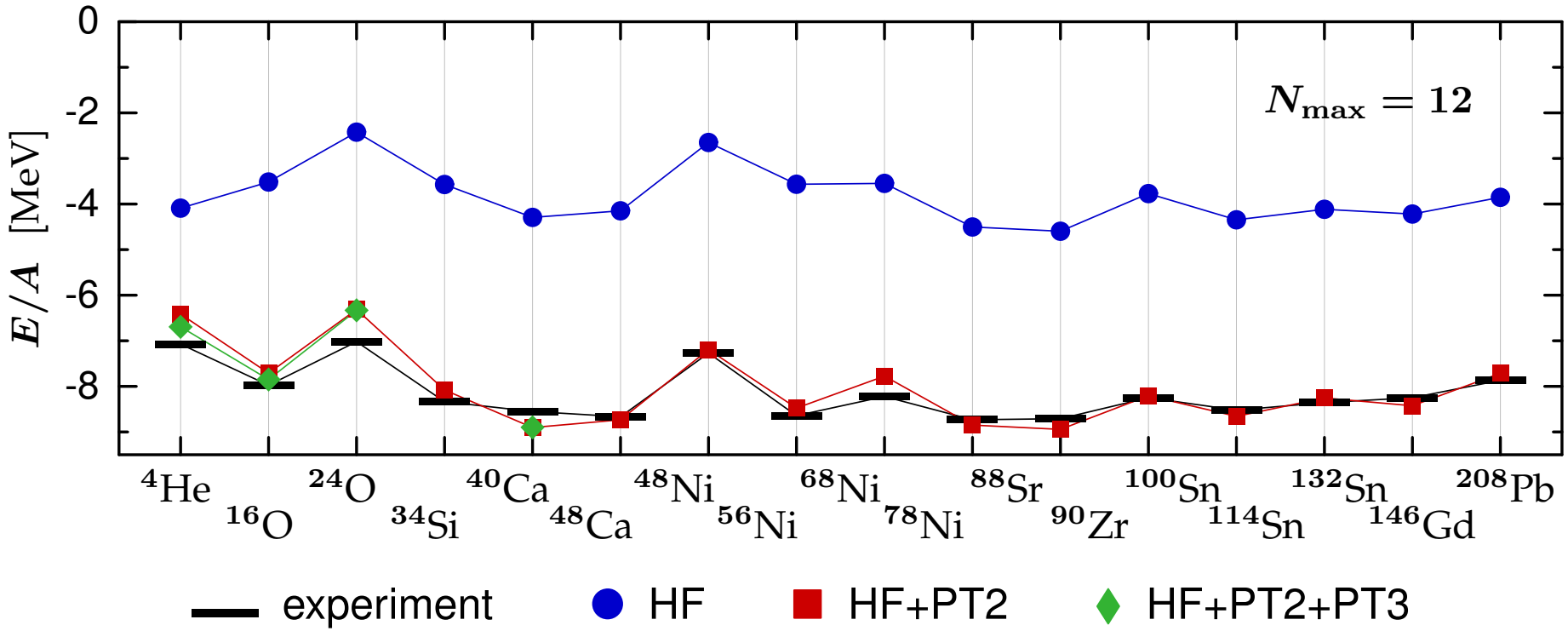

## Beyond Hartree-Fock

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

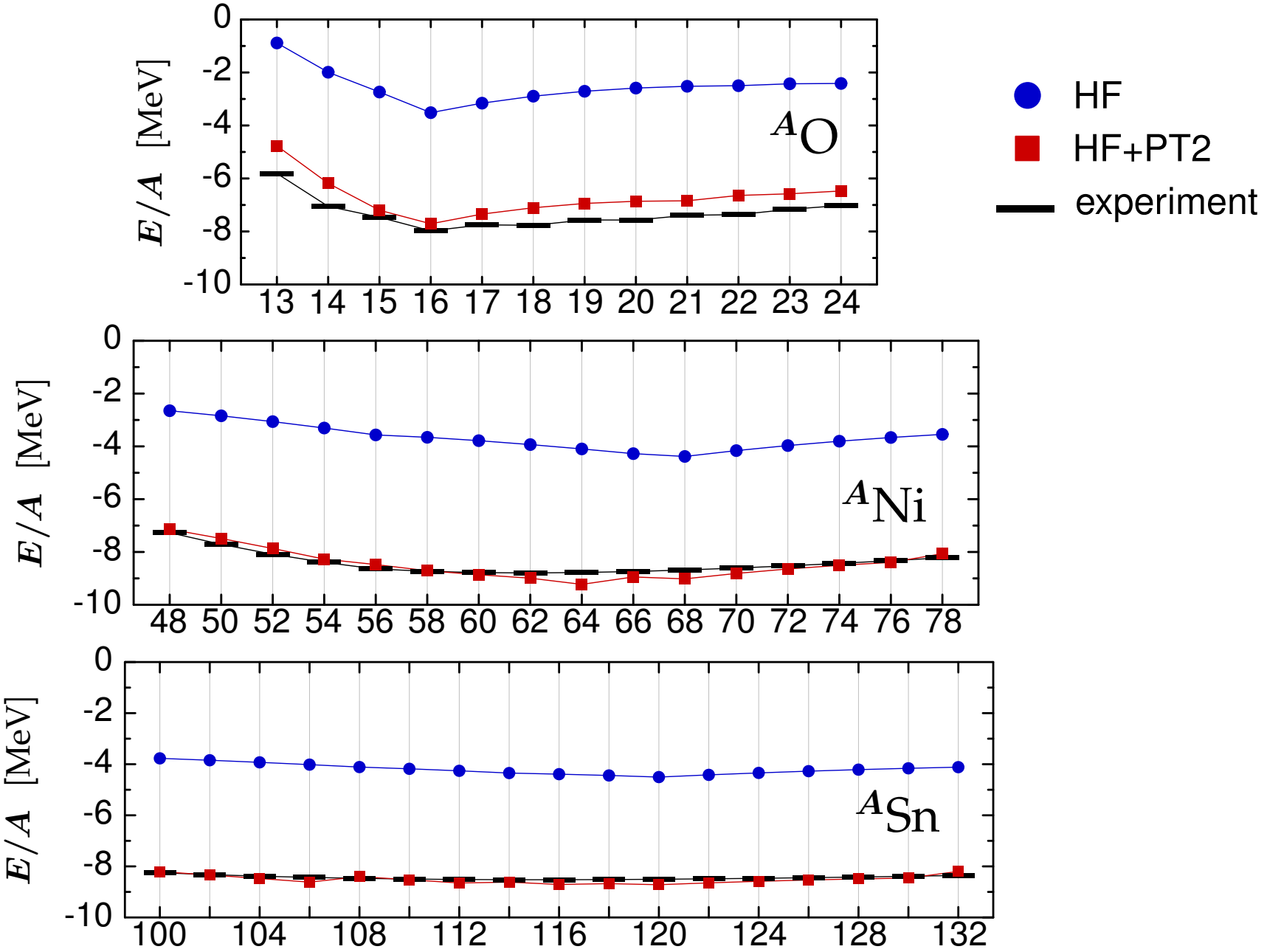
# Long-Range Correlations: MBPT

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

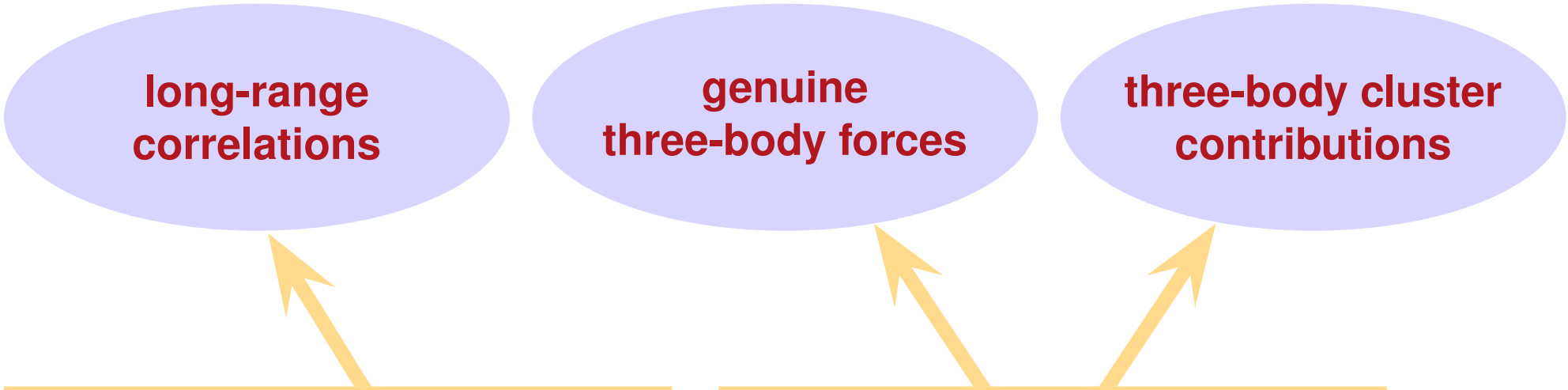
$$\Delta E^{(2)} = -\frac{1}{4} \sum_{i,j}^{\text{occu.}} \sum_{a,b}^{\text{unoccu.}} \frac{\left| \left\langle \phi_a \phi_b \right| \mathbf{T}_{\text{int}} + \mathbf{V}_{\text{UCOM}} \left| \phi_i \phi_j \right\rangle \right|^2}{\epsilon_a + \epsilon_b - \epsilon_i - \epsilon_j}$$



# Long-Range Correlations: MBPT



# Missing Pieces



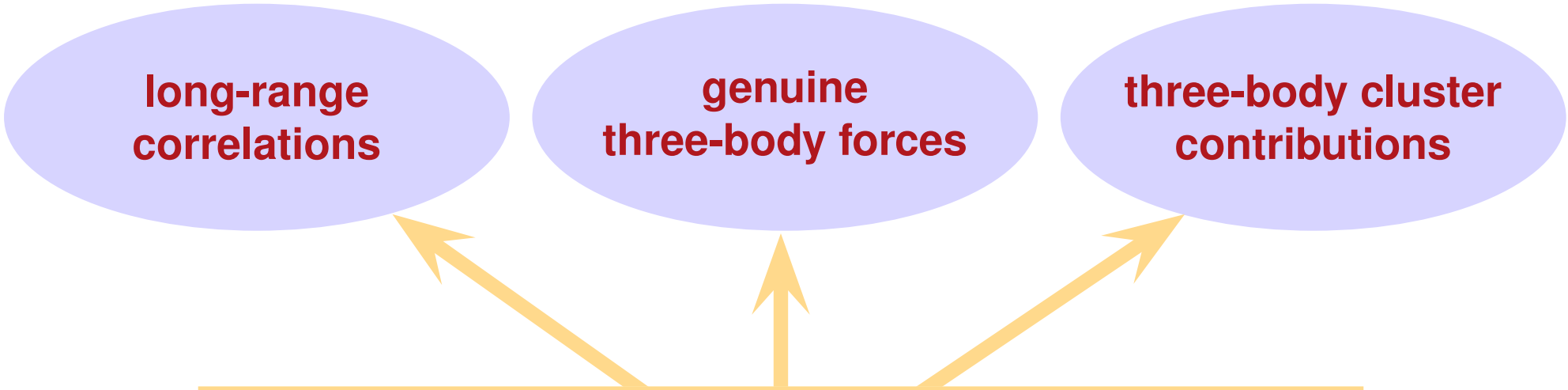

## Beyond Hartree-Fock

- residual long-range correlations are **perturbative**
- mostly long-range **tensor correlations**
- easily tractable within MBPT, CI, CC,...

## Net Three-Body Force

- small effect on binding energies for all masses
- cancellation does not work for all observables
- construct simple effective three-body force

# Missing Pieces



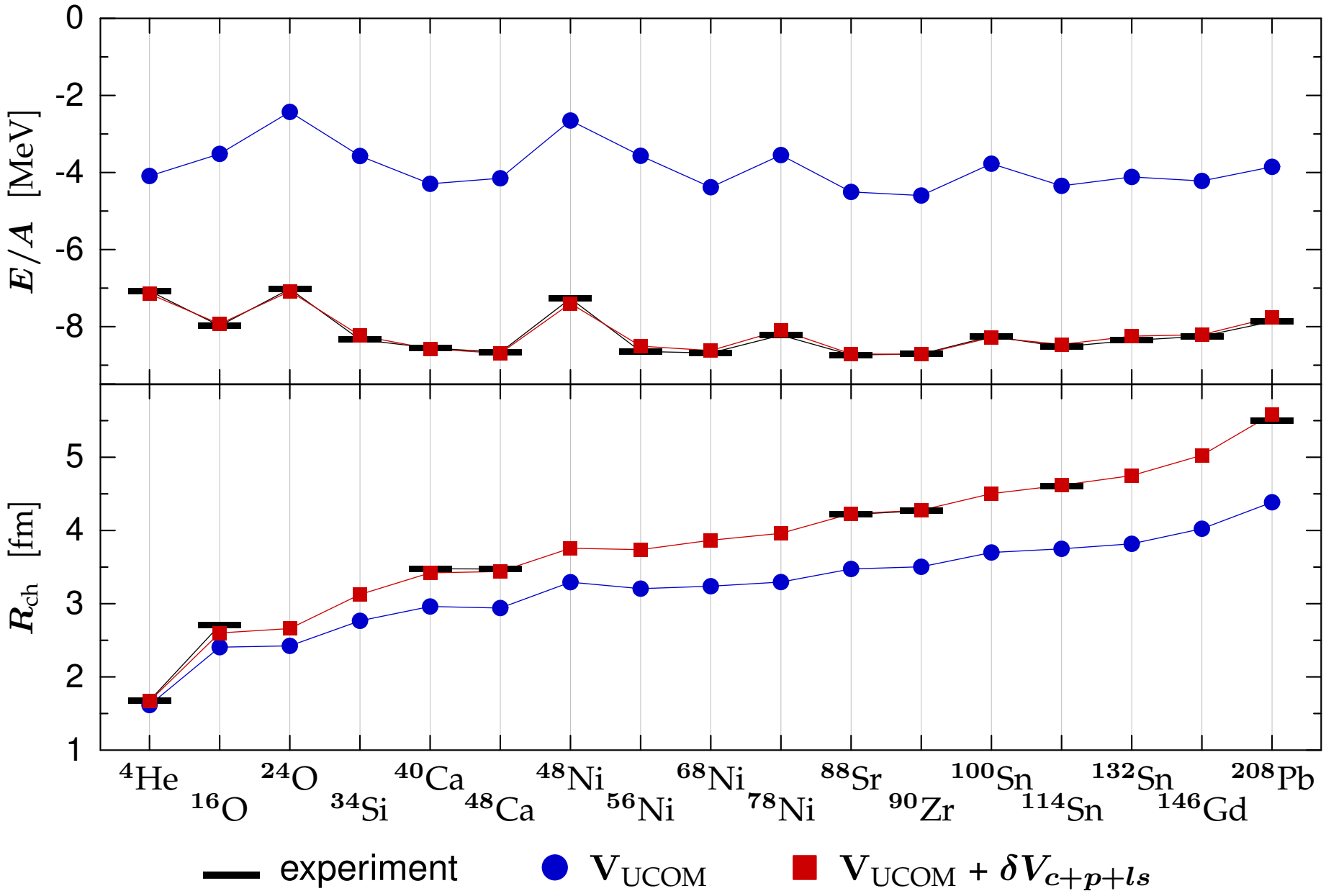

## Pragmatic Approach

- phenomenological two-body correction

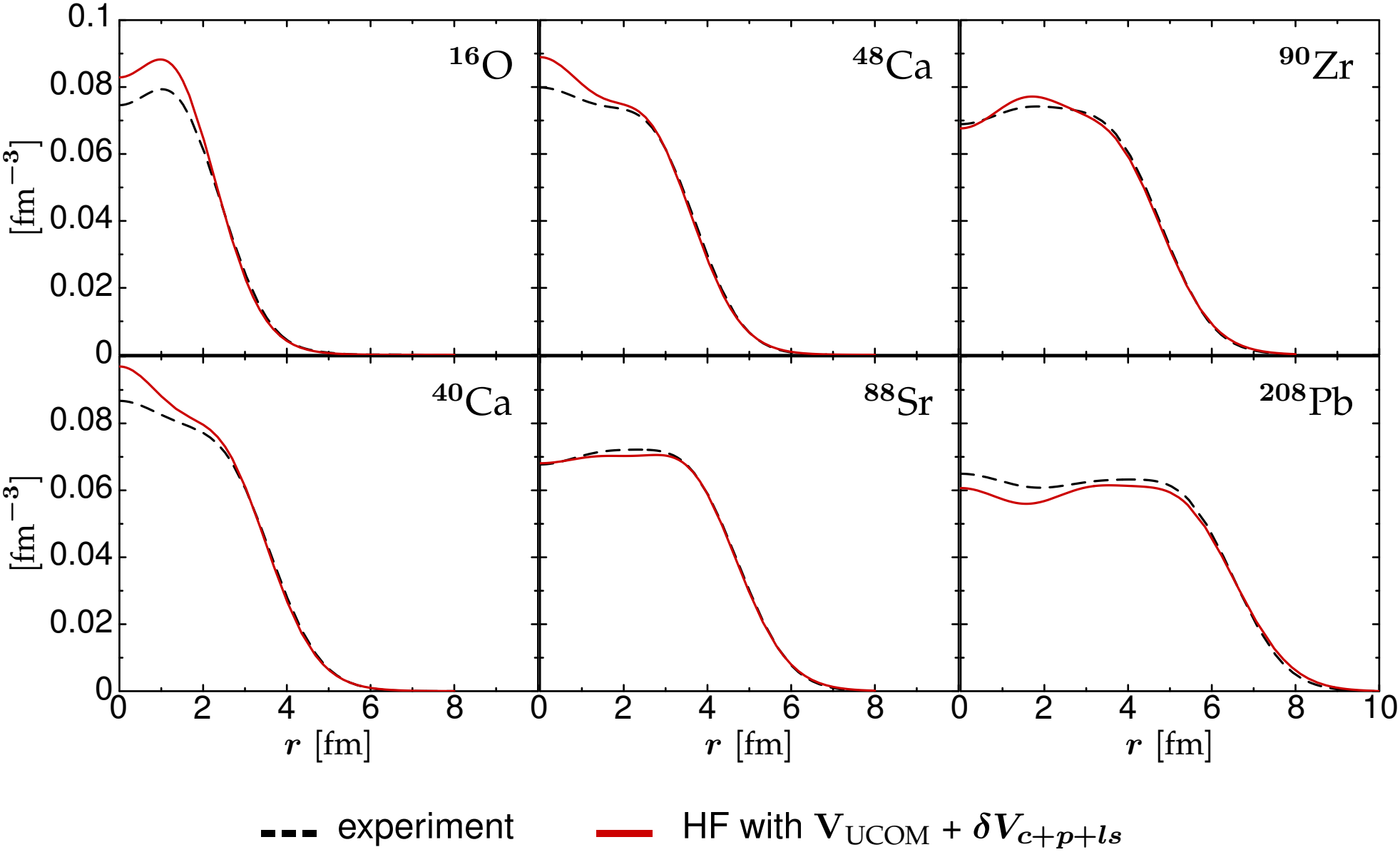
$$\delta \mathrm{V}_{c+p+ls} = v_1(\mathrm{r}) + \vec{\mathrm{q}}\, v_{qq}(\mathrm{r})\, \vec{\mathrm{q}} + v_{LS}(\mathrm{r})\, \vec{\mathrm{L}} \cdot \vec{\mathrm{S}}$$

- 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

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

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

$a_\nu$ : 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

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

## Variation

$$\frac{\langle Q | \widetilde{\mathrm{H}}_{\mathrm{int}} | Q \rangle}{\langle Q | Q \rangle} \rightarrow \min$$

## Diagonalisation

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

# FMD Matrix Elements

$$\left\langle q_k, q_l \right| G(\mathrm{r}) \mathrm{S}_{12}(\vec{\mathrm{q}}_\Omega, \vec{\mathrm{q}}_\Omega) \left| q_m, q_n \right\rangle = \gamma_{klmn}^2 R_{km} R_{ln} G_{klmn} \Bigg\{$$

$$s_{12}(\vec{\rho}_{klmn} \times \vec{\pi}_{klmn}, \vec{\rho}_{klmn} \times \vec{\pi}_{klmn}) \left(5\alpha_{klmn} + \gamma_{klmn}\vec{\rho}_{klmn}^2\right) +$$

$$s_{12}(\vec{\pi}_{klmn}, \vec{\pi}_{klmn}) \left(9\alpha_{klmn}^2 + 13\alpha_{klmn}\gamma_{klmn}\vec{\rho}_{klmn}^2 + 2\gamma_{klmn}^2\vec{\rho}_{klmn}^4\right) -$$

$$s_{12}(\vec{\pi}_{klmn}, \vec{\rho}_{klmn}) \Bigg( \frac{9}{2}\alpha_{klmn}\beta_{klmn} + 16\alpha_{klmn}\gamma_{klmn}(\vec{\pi}_{klmn} \cdot \vec{\rho}_{klmn}) +$$

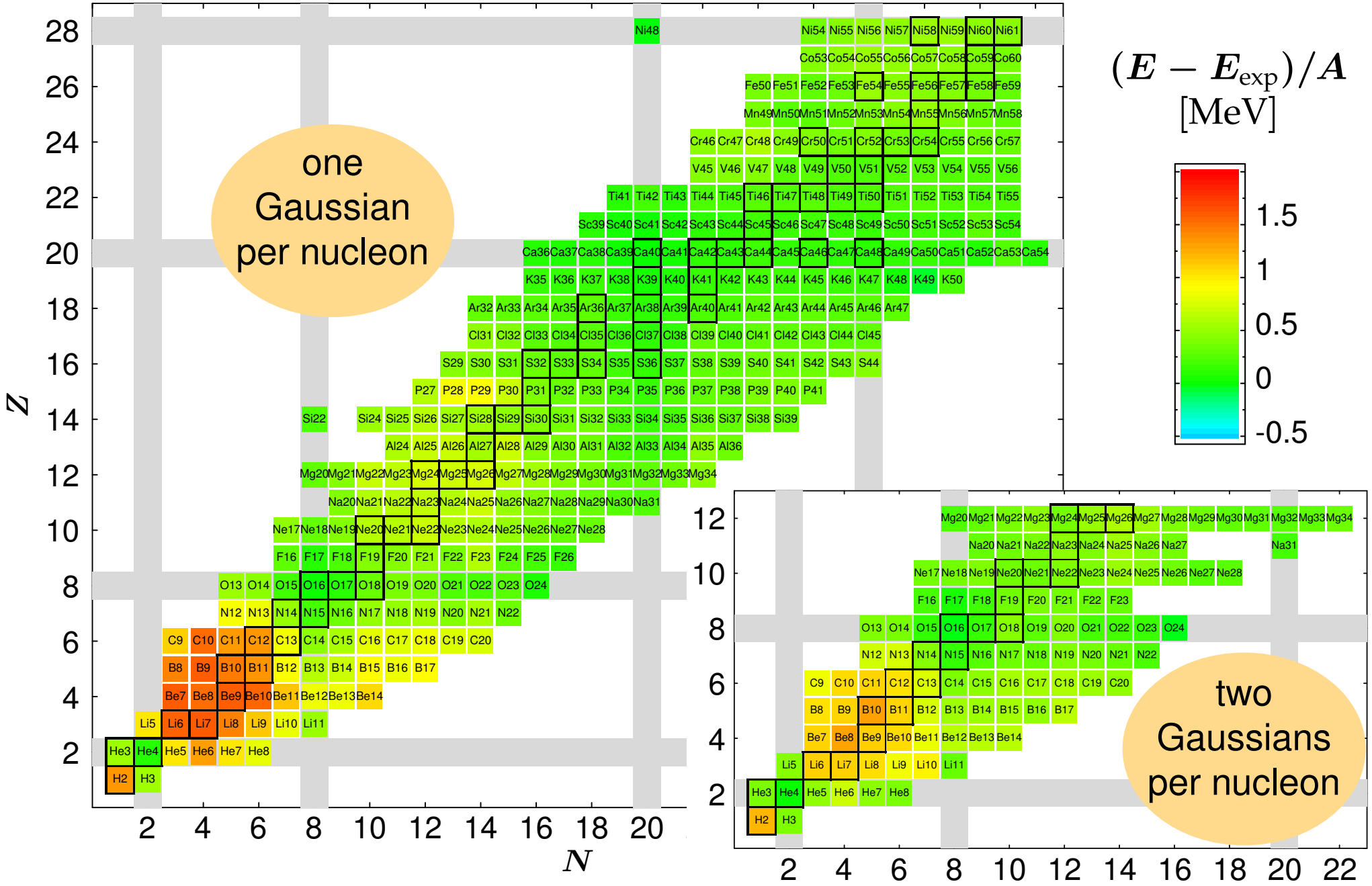
$$\frac{5}{2}\gamma_{klmn}\beta_{klmn}\vec{\rho}_{klmn}^2 + 4\gamma_{klmn}^2(\vec{\pi}_{klmn} \cdot \vec{\rho}_{klmn})\vec{\rho}_{klmn}^2 \Bigg) +$$

$$s_{12}(\vec{\rho}_{klmn}, \vec{\rho}_{klmn}) \Bigg( \frac{21}{4}\gamma_{klmn}(\theta_{klmn} - \alpha_{klmn}\lambda_{klmn}) + \frac{9}{4}\theta_{klmn} - \frac{9}{2} +$$

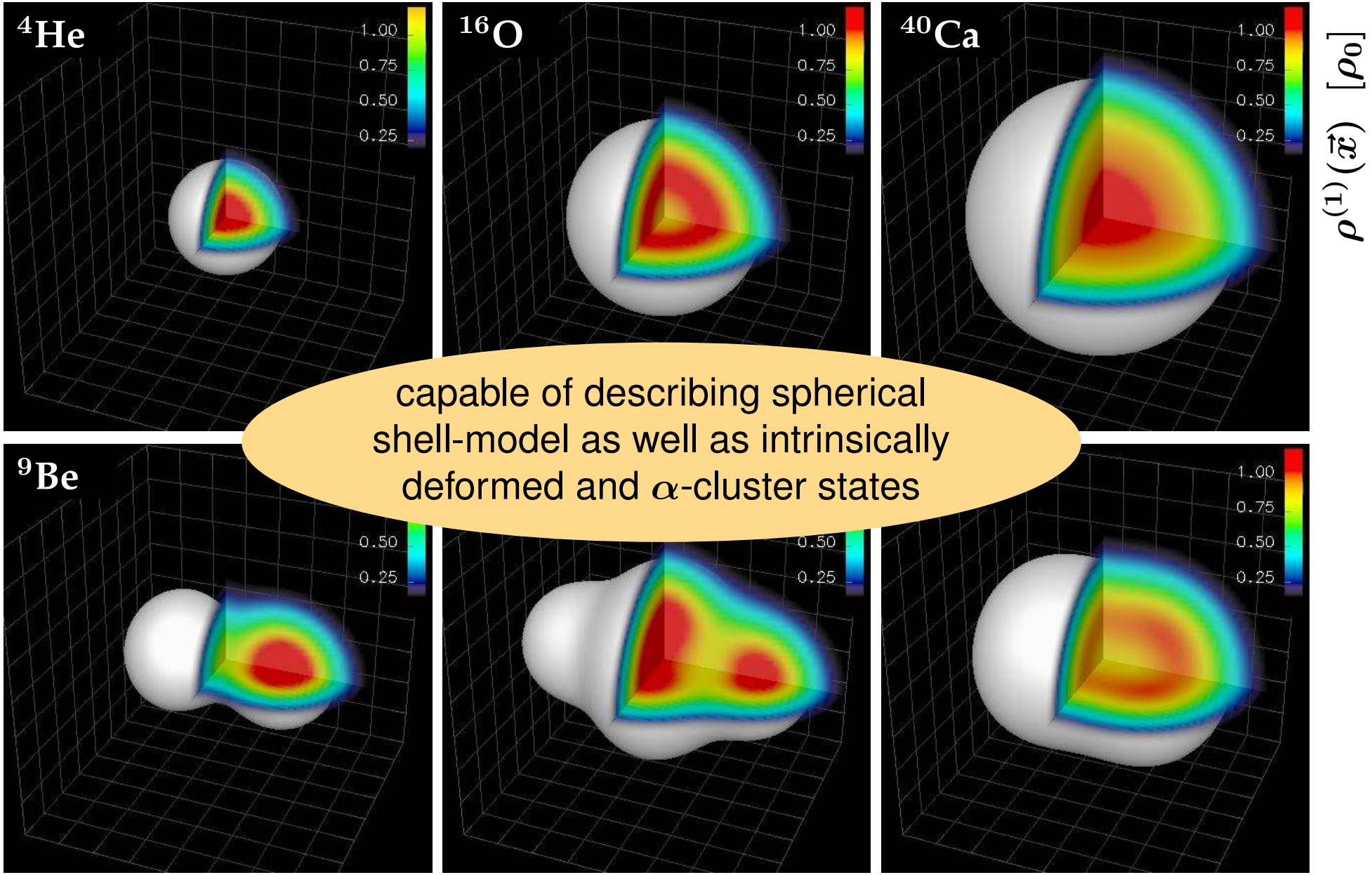
$$2\gamma_{klmn}^2(\vec{\pi}_{klmn} \cdot \vec{\rho}_{klmn})^2 + 4\gamma_{klmn}\beta_{klmn}(\vec{\pi}_{klmn} \cdot \vec{\rho}_{klmn}) -$$

$$\frac{3}{4}\gamma_{klmn}\left(\frac{\theta_{klmn}}{\alpha_{klmn} + \kappa} + \gamma_{klmn}\lambda_{klmn}\right)\vec{\rho}_{klmn}^2 \Bigg) \Bigg\}$$

# Variation: Chart of Nuclei



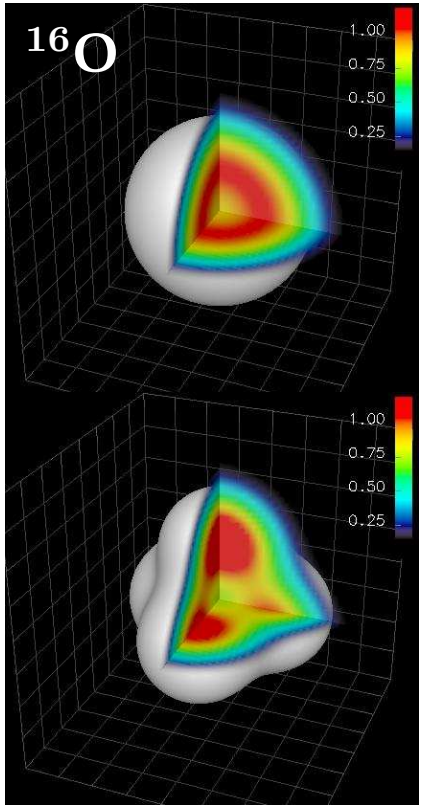
# Intrinsic One-Body Density Distributions




capable of describing spherical shell-model as well as intrinsically deformed and $\alpha$-cluster states

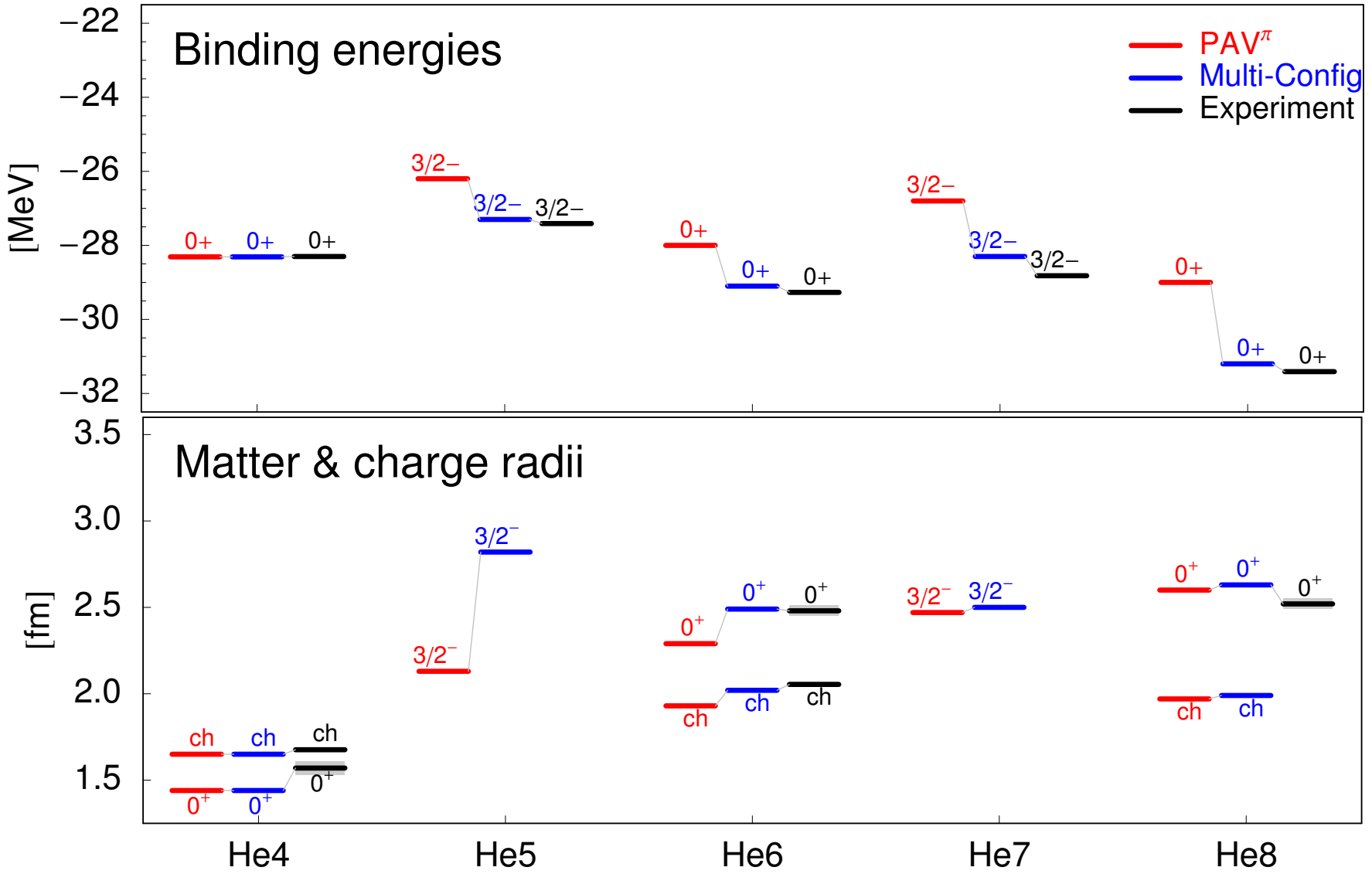
# Beyond Simple Variation

- **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**
  - diagonalisation within a set of different Slater determinants



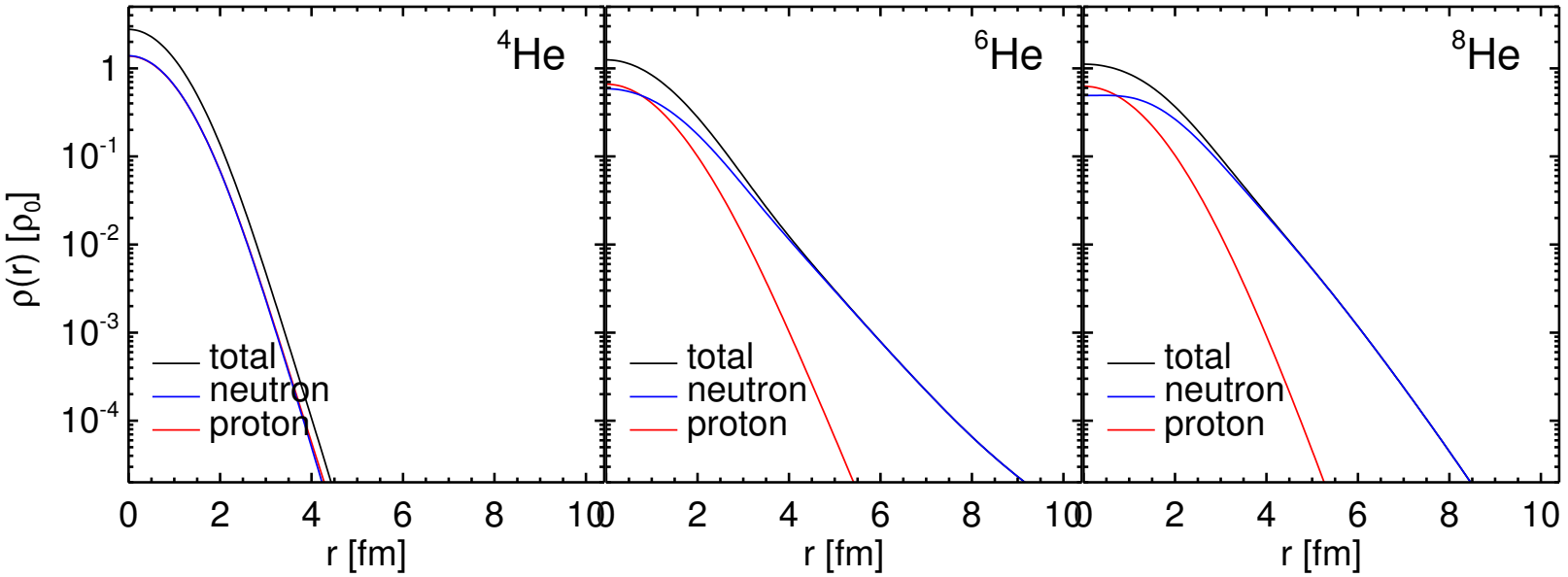
# Results for p-Shell Nuclei

# Helium Isotopes: Energies & Radii



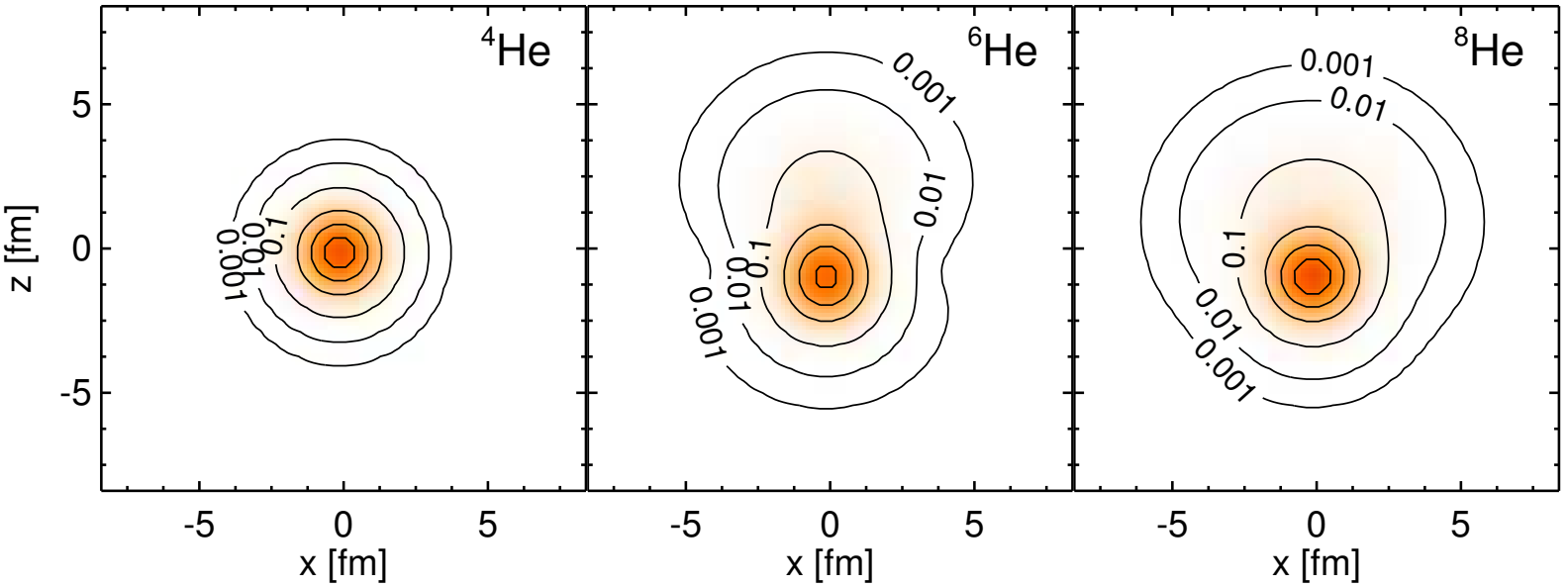

[figures provided by T. Neff]

# Helium Isotopes: Densities




**Multi-Config**

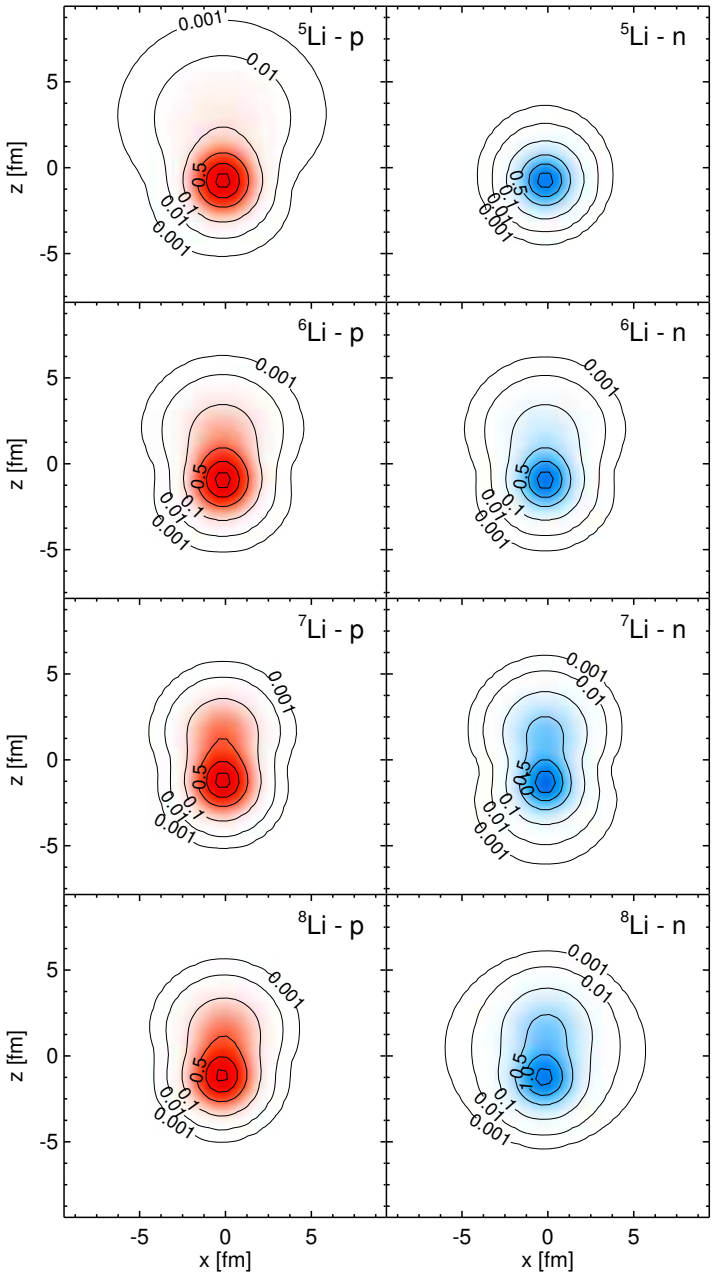
radial density profiles

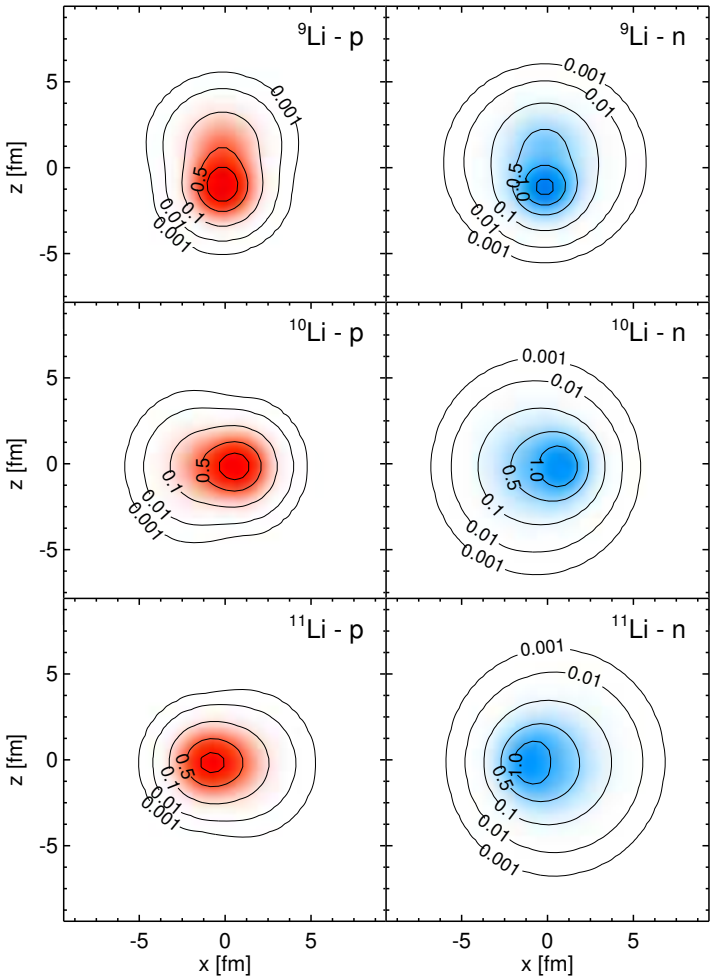



**PAV$^\pi$**

intrinsic densities

# Lithium Isotopes: Intrinsic Densities

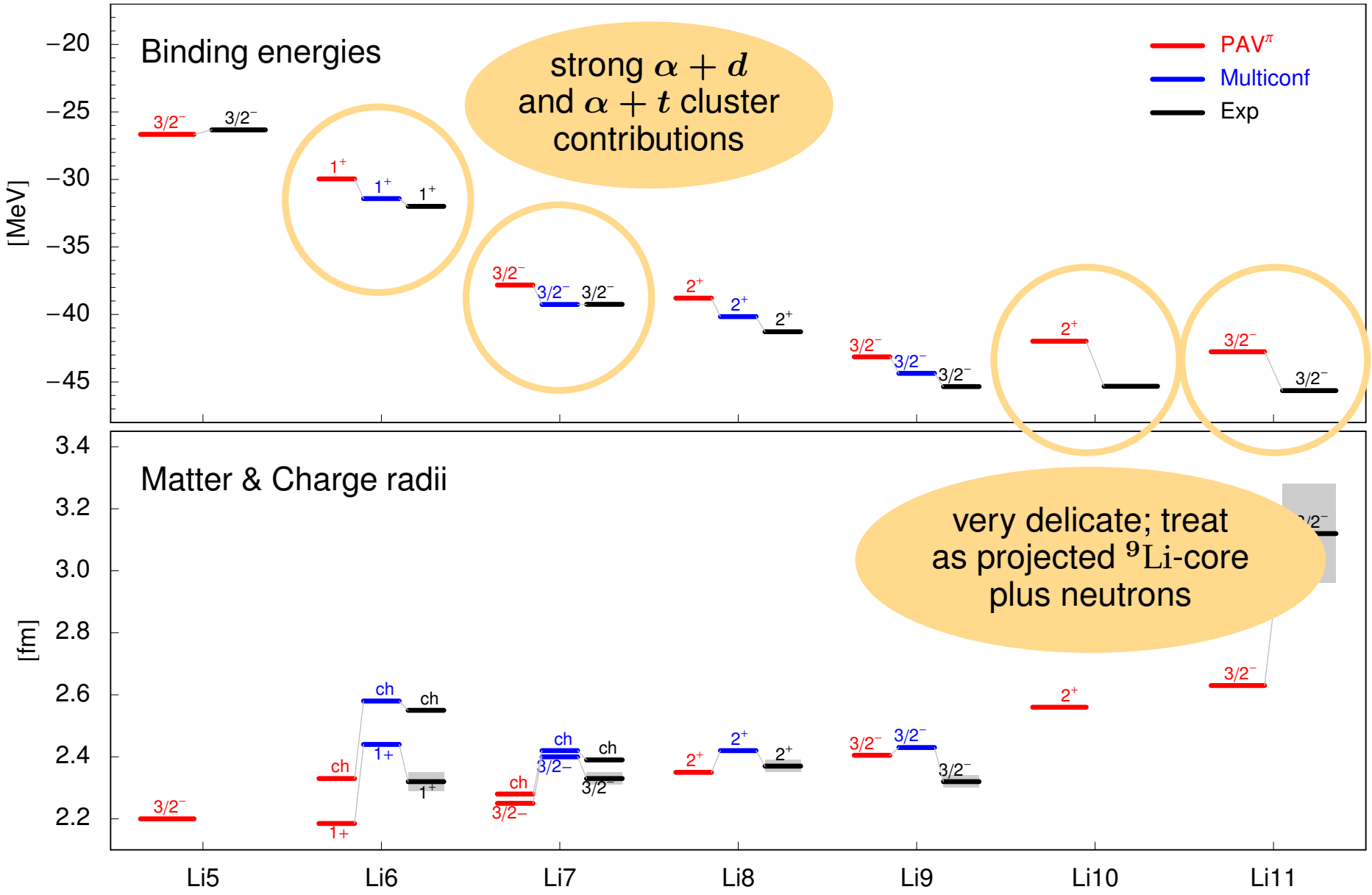


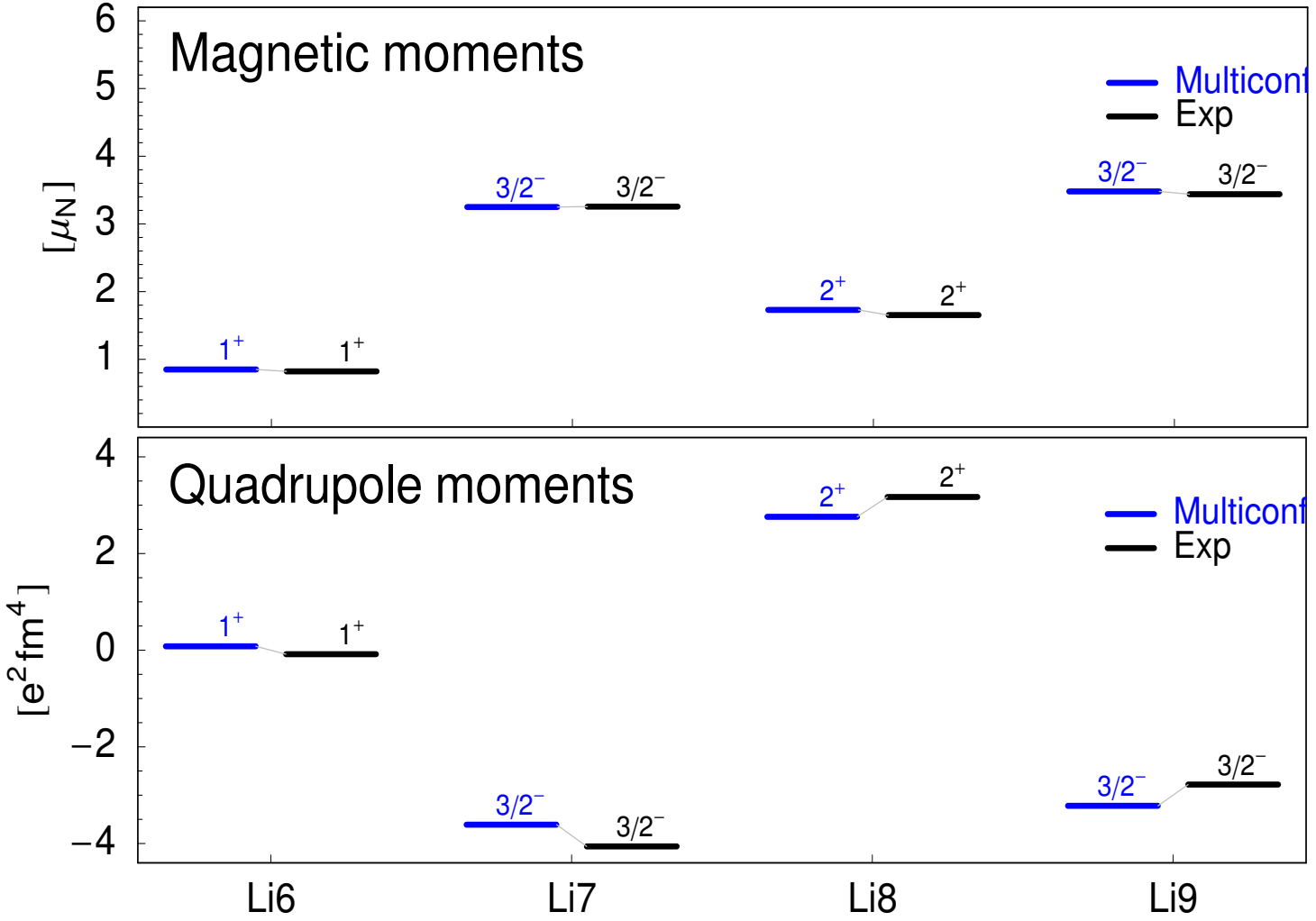

**PAV$^{\pi}$**

intrinsic densities

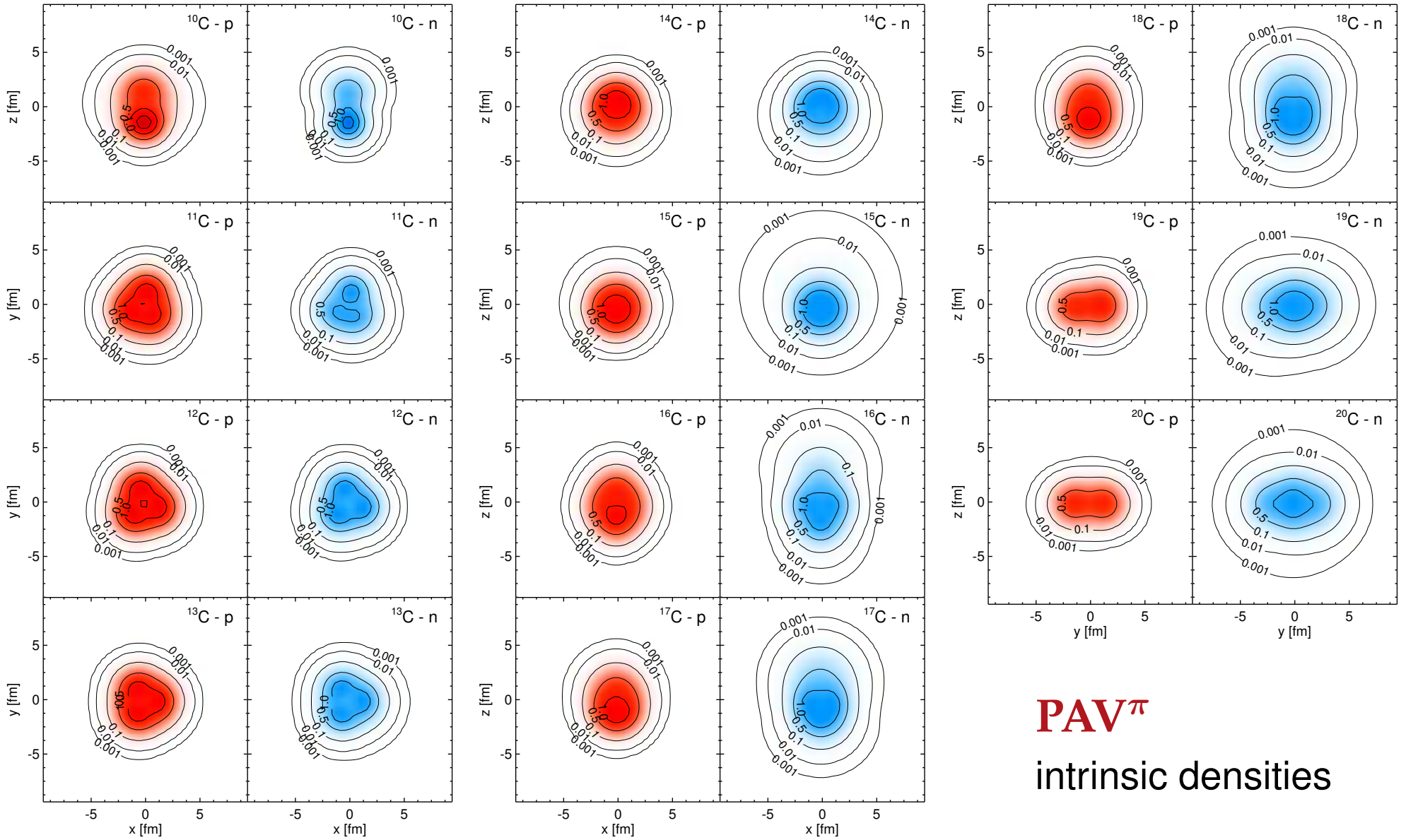
# Lithium Isotopes: Energies & Radii



# Lithium Isotopes: Moments



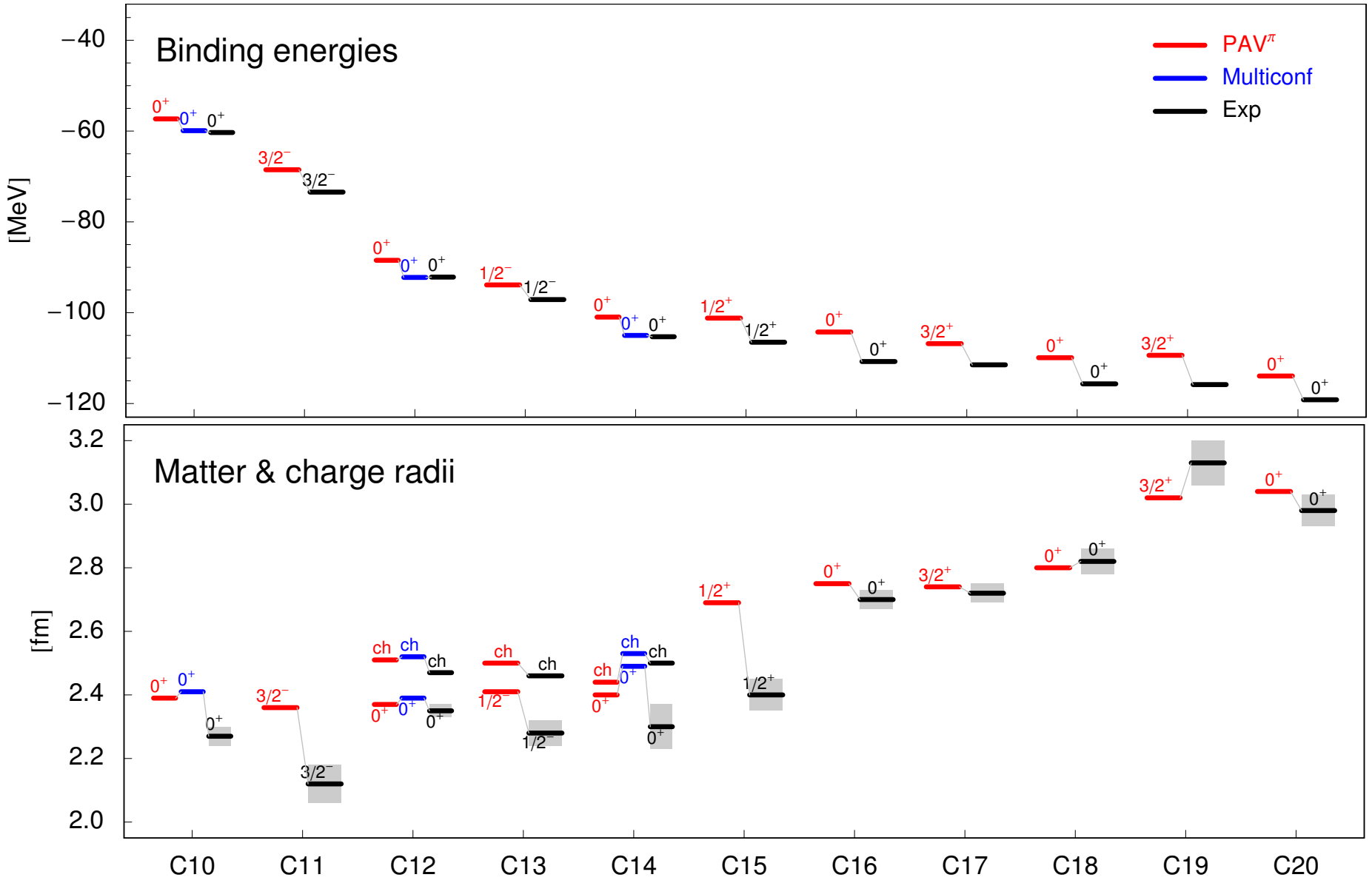
# Carbon Isotopes: Intrinsic Densities



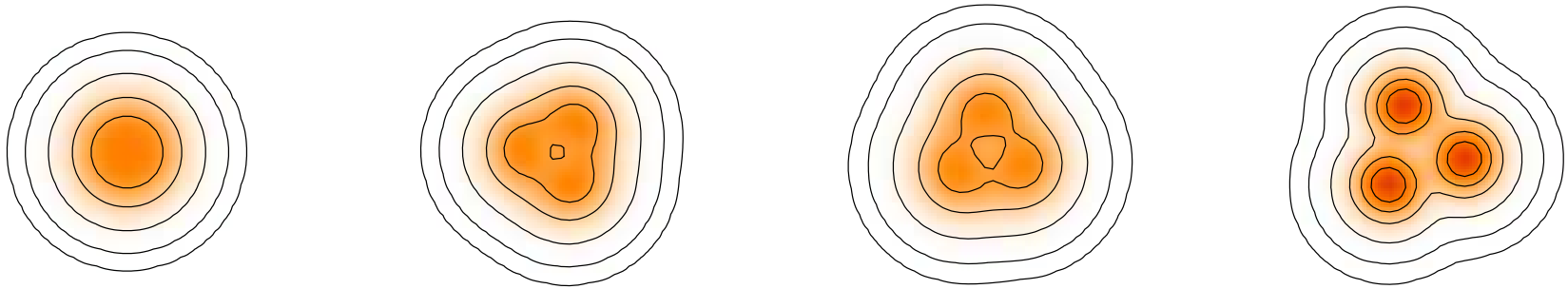

**PAV$^{\pi}$**

intrinsic densities

# Carbon Isotopes: Energies & Radii

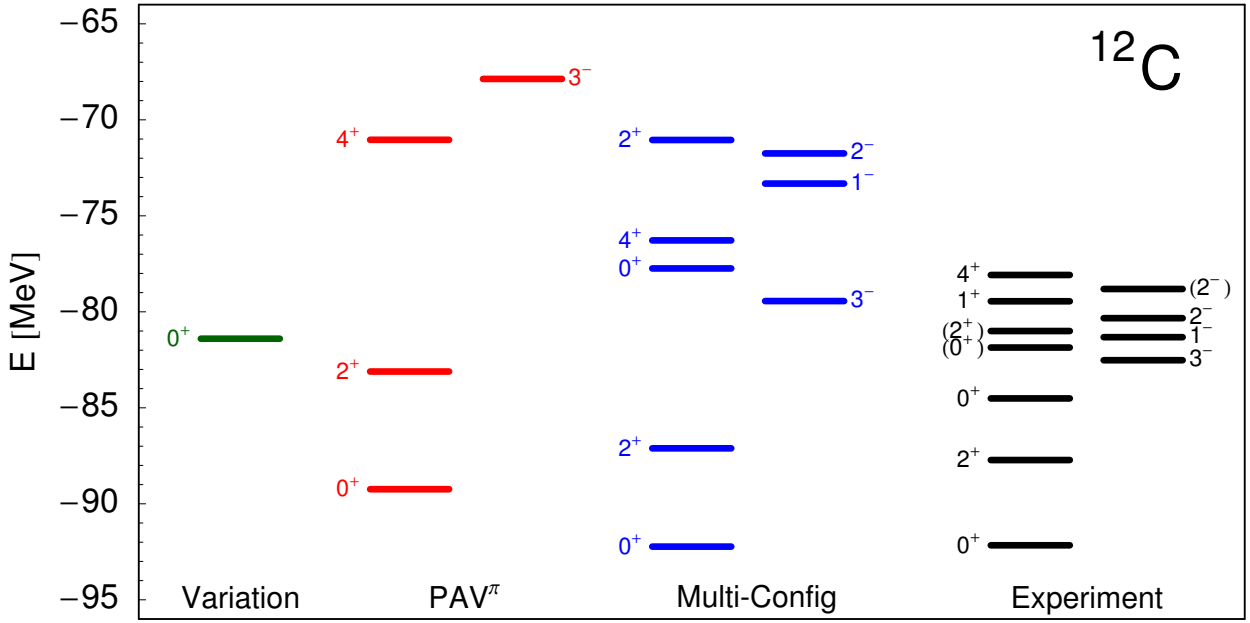


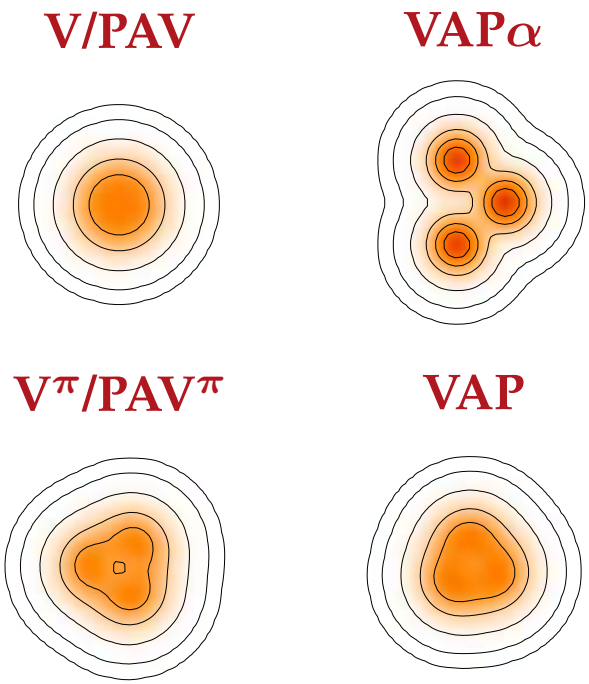
# Intrinsic Shapes of $^{12}C$



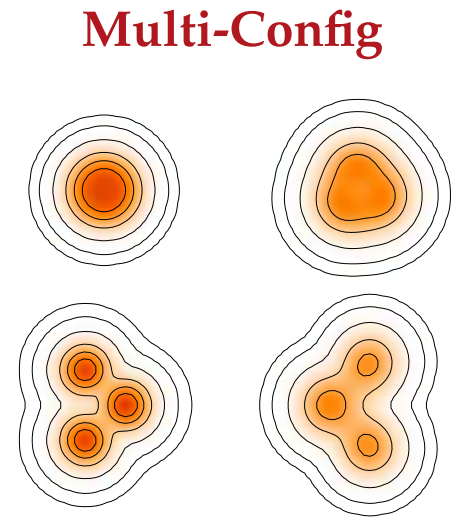
| | intrinsic | projected | intrinsic | projected | intrinsic | projected | intrinsic | projected |
|---|---|---|---|---|---|---|---|---|
| $\langle \mathbf{H} \rangle$ | -81.4 | **-81.5** | -77.0 | **-88.5** | -74.1 | **-85.5** | -57.0 | **-75.9** |
| $\langle \mathbf{T} \rangle$ | 212.1 | 212.1 | 189.2 | 186.1 | 182.8 | 179.0 | 213.9 | 201.4 |
| $\langle \mathbf{V}_{ls} \rangle$ | -39.8 | -40.2 | -12.0 | -17.1 | -5.8 | -8.0 | 0.0 | 0.0 |
| $\sqrt{\langle \mathbf{r^2} \rangle}$ | 2.22 | 2.22 | 2.40 | 2.37 | 2.45 | 2.42 | 2.44 | 2.42 |

# Structure of $^{12}C$

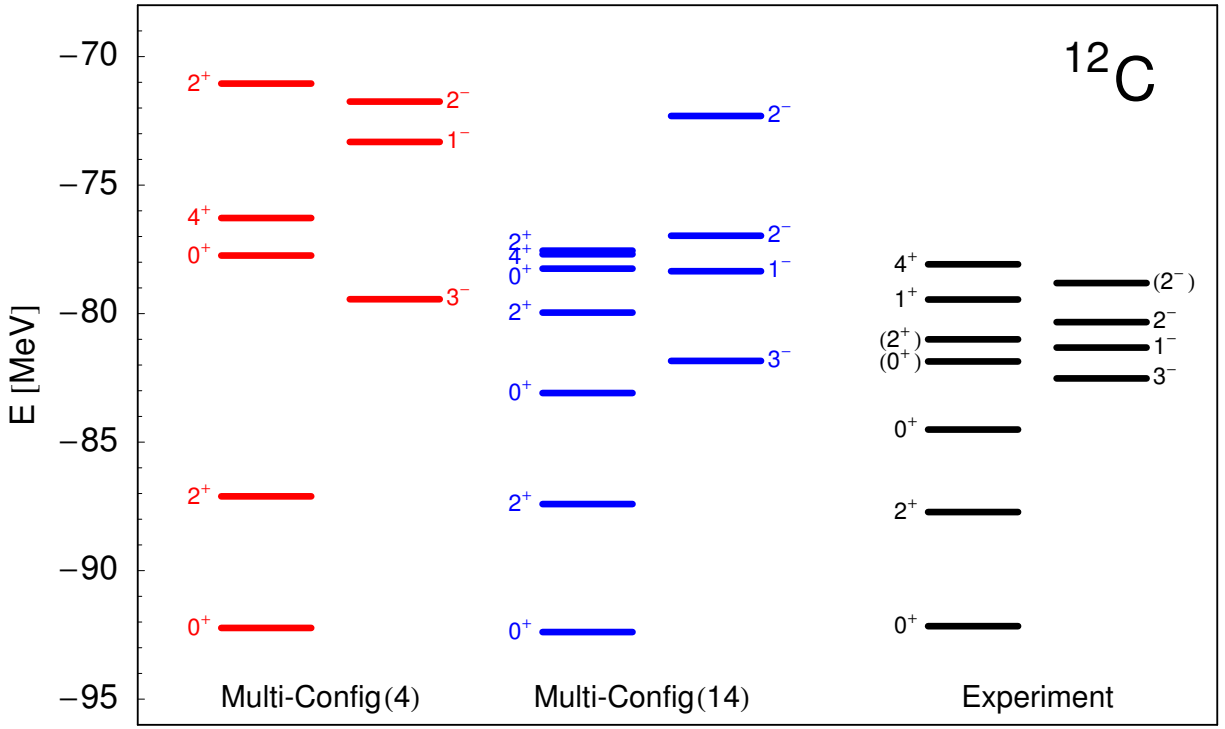


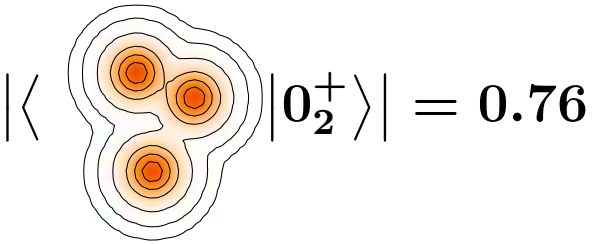



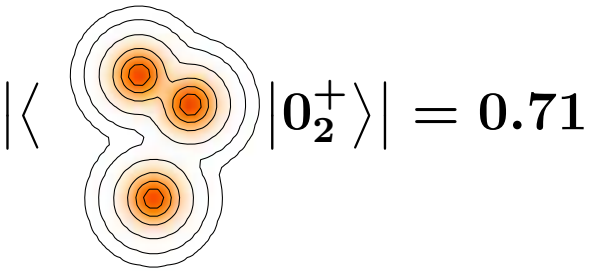

| | $E$ [MeV] | $R_{ch}$ [fm] | $B(E2)$ [$e^2$ fm$^4$] |
|---|---|---|---|
| V/PAV | 81.4 | 2.36 | - |
| VAP $\alpha$-cluster | 79.1 | 2.70 | 76.9 |
| PAV$^\pi$ | 88.5 | 2.51 | 36.3 |
| VAP | 89.2 | 2.42 | 26.8 |
| Multi-Config | 92.2 | 2.52 | 42.8 |
| Experiment | 92.2 | 2.47 | 39.7 $\pm$ 3.3 |

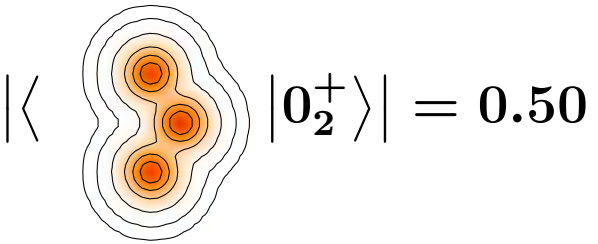


# Structure of $^{12}$C — Hoyle State




| | Multi-Config | Experiment |
|---|---|---|
| $E$ [MeV] | 92.4 | 92.2 |
| $R_{\mathrm{ch}}$ [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 $V_{\mathrm{UCOM}}$**
  - 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**
  - access to nuclei across the whole nuclear chart
  - basis for improved many-body calculations: MBPT, CI, CC, RPA,...
- **UCOM + Fermionic Molecular Dynamics**
  - clustering and intrinsic deformations in p- and sd-shell
  - projection / multi-config provide detailed structure information

# Epilogue

- **thanks to my group & my collaborators**

  - H. Hergert, N. Paar, P. Papakonstantinou

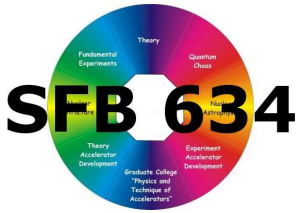
    Institut für Kernphysik, TU Darmstadt

  - T. Neff

    NSCL, Michigan State University

  - H. Feldmeier

    Gesellschaft für Schwerionenforschung (GSI)

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