SFB 634 — Project D1:

Towards *ab initio* Nuclear Structure

- R. Roth
  The Unitary Correlation Operator Method
- H. Hergert
  Structure of p and sd-Shell Nuclei
- R. Roth
  Towards Heavier Nuclei: UCOM-Hartree-Fock

The Unitary Correlation Operator Method

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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**

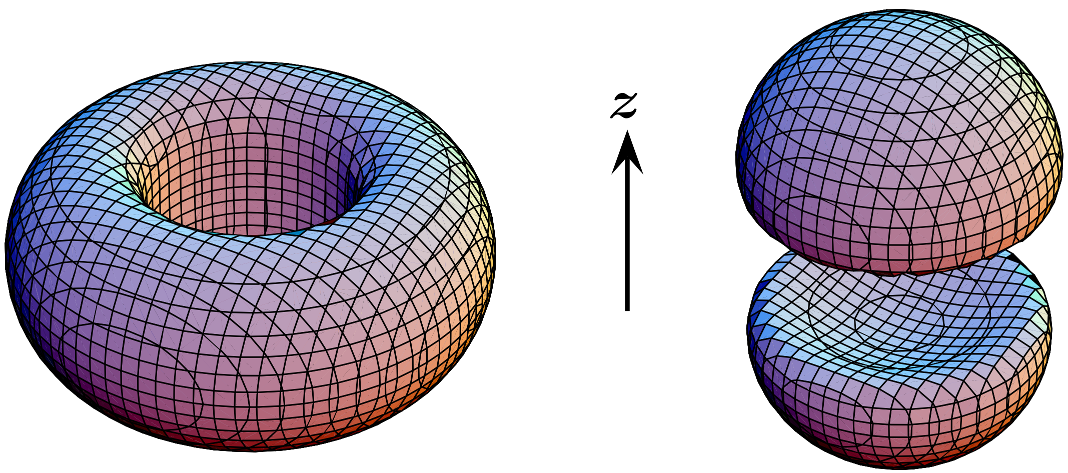
Overview

- Correlations in Nuclei
- Central and Tensor Correlations
- Unitary Correlation Operator Method
- Correlated Realistic NN-Potentials

Deuteron: Manifestation of Correlations

$M_S = 0$ $\quad$ $M_S = \pm 1$

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



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

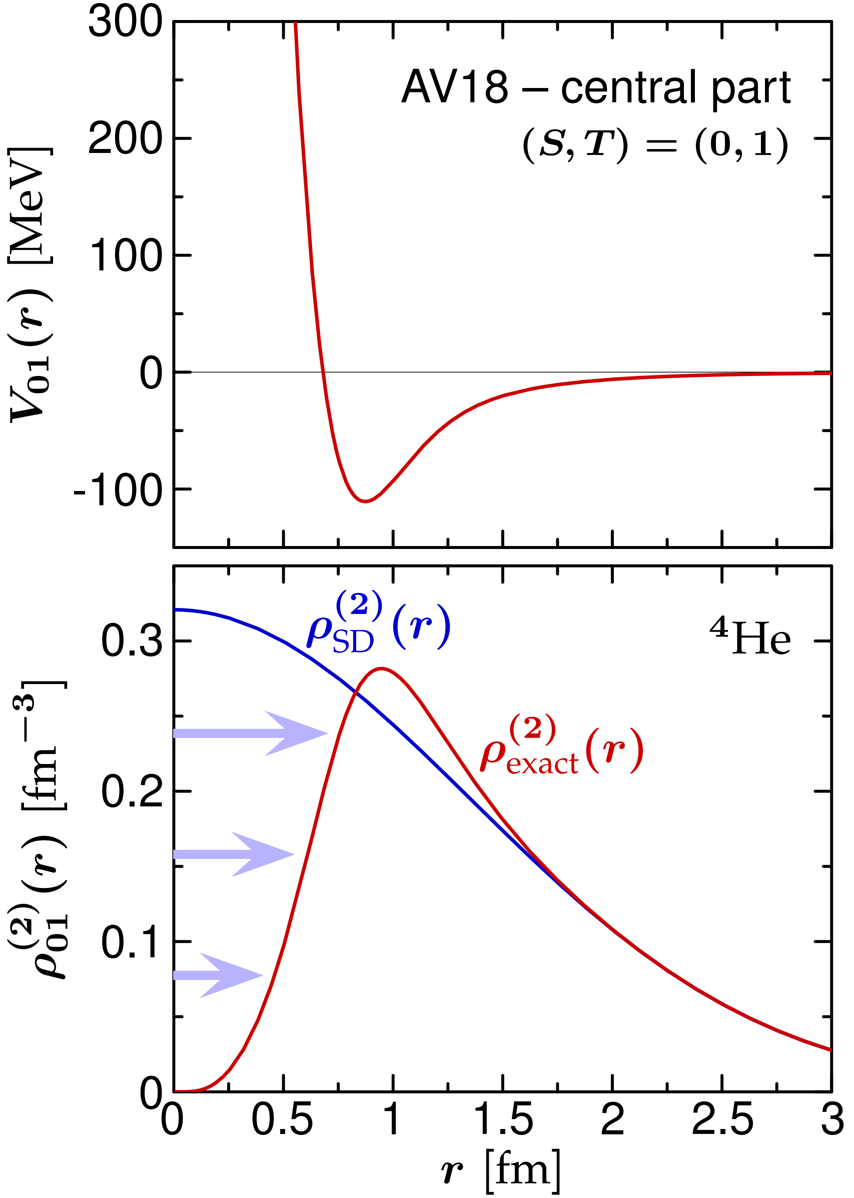
two-body density fully suppressed at small particle distances $|\vec{r}|$

central correlations

angular distribution depends strongly on relative spin orientation

tensor correlations

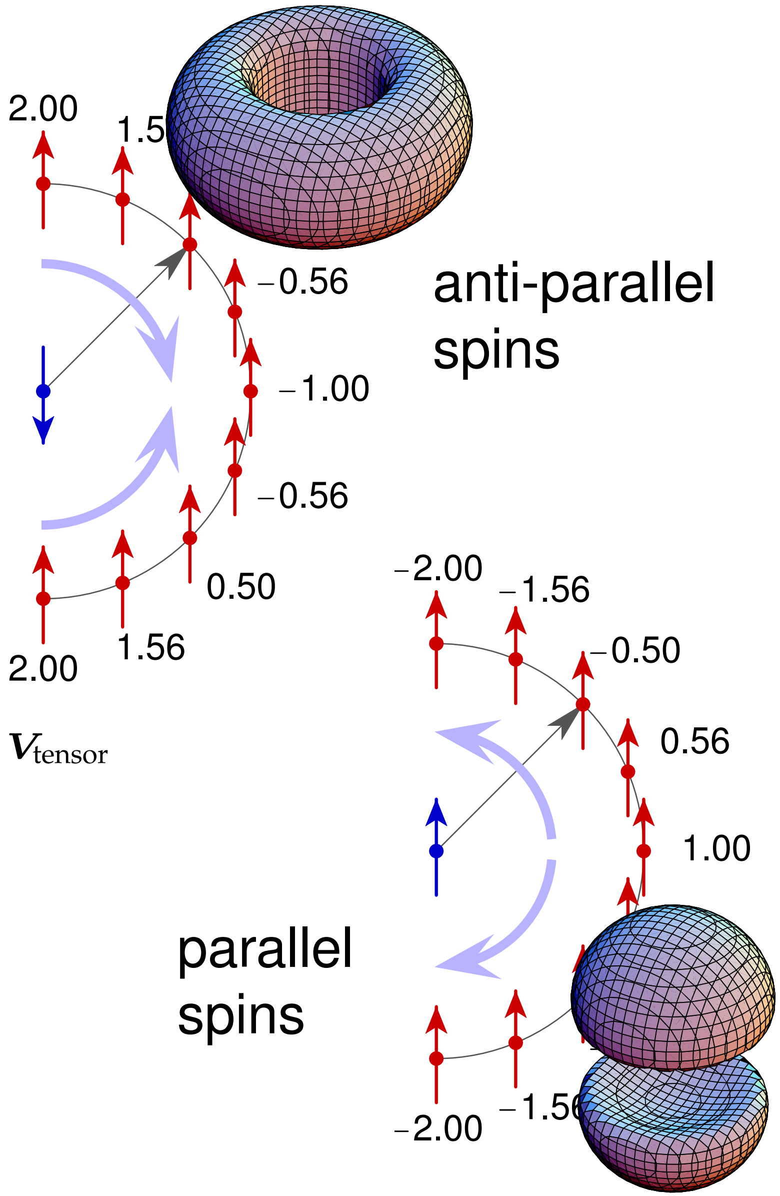
Central Correlations



- 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

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

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

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

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

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

Central Correlator $\mathbf{C}_r$

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

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

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

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

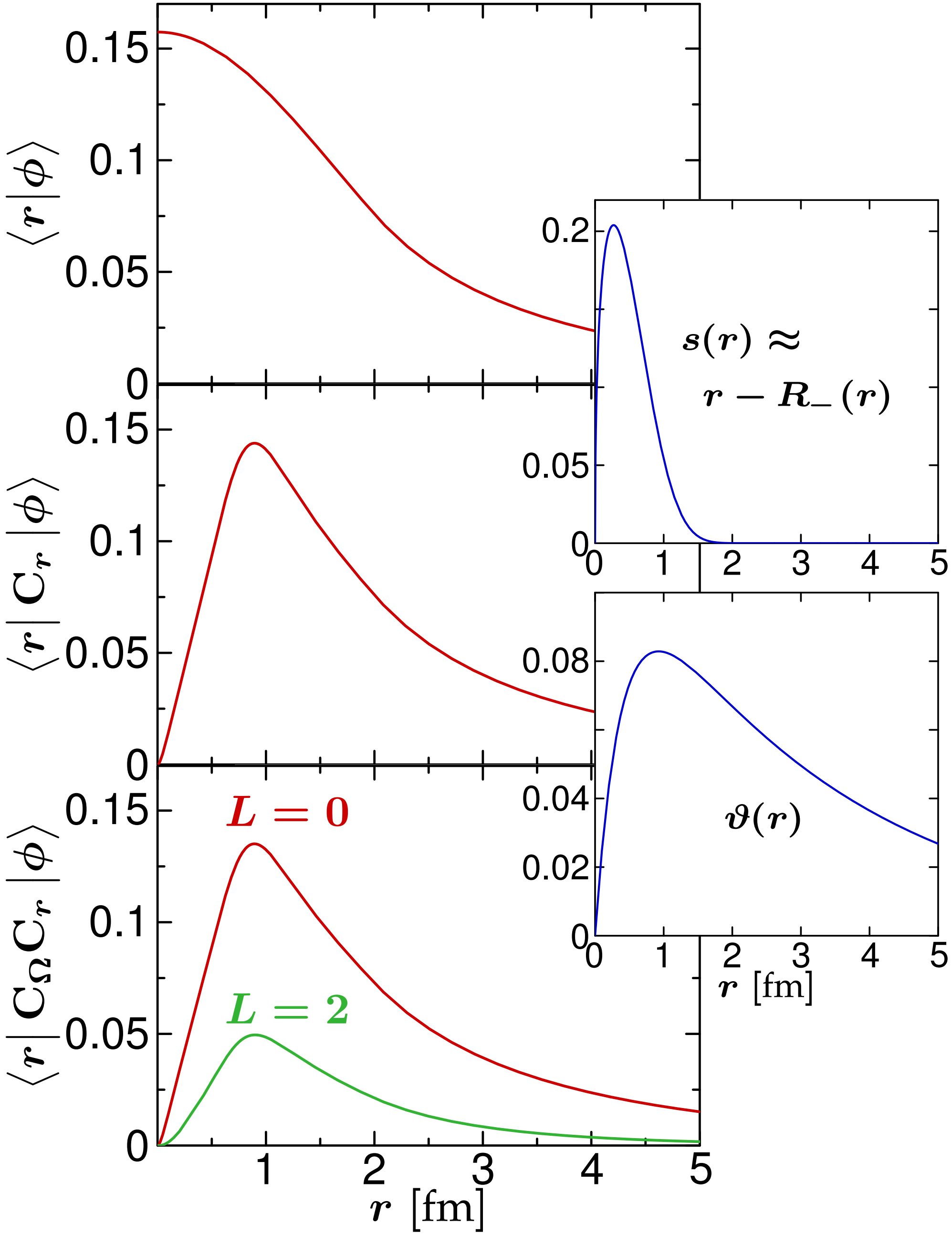
- angular shift depending on the orientation of spin and relative coordinate of a nucleon pair

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

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

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

Correlated States



Central Correlations

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

Tensor Correlations

$$\langle \vec{r} | \, C_\Omega \, | \phi; (01)1 \rangle = \\ = \cos(3\sqrt{2} \, \vartheta(r)) \, \langle \vec{r} | \phi; (01)1 \rangle \\ + \sin(3\sqrt{2} \, \vartheta(r)) \, \langle \vec{r} | \phi; (21)1 \rangle$$

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.

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

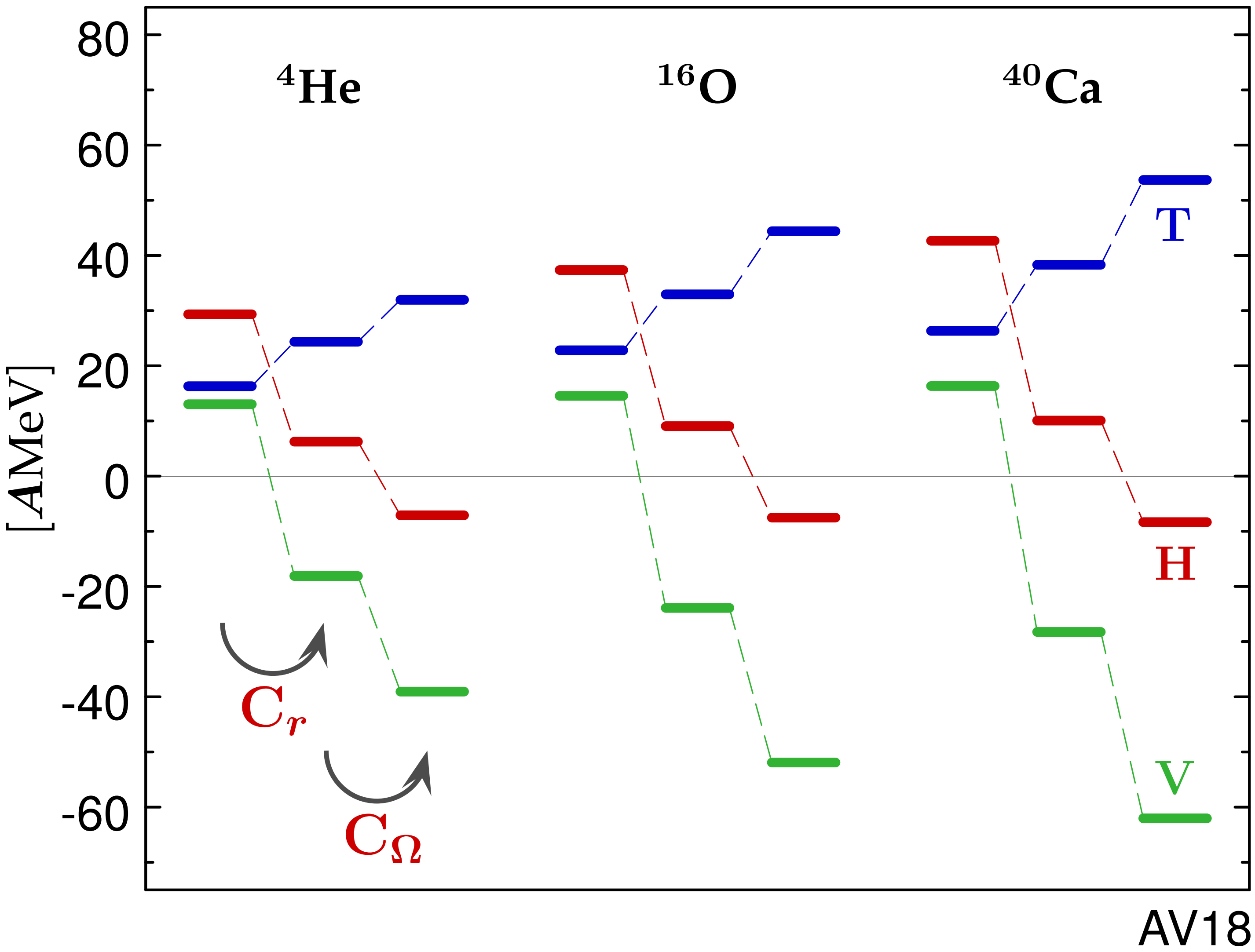
operators for all observables can be and have to be correlated consistently

Correlated 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

Summary

- **Unitary Correlation Operator Method (UCOM)**
  - imprint short-range central and tensor correlations explicitly by an unitary transformation
  - correlated states and correlated operators

- **Correlated Realistic NN-Potentials**
  - correlated / low-momentum interaction in closed operator representation
  - phase shift equivalent to original potential
  - robust starting point for all kinds of many-body models: Hartree-Fock, shell model,...

Supplements

Correlated States — Central Correlations

- correlated two-body wave function

$$\langle \vec{r}, \vec{X} | \begin{matrix} \mathrm{C}_r^\dagger \\ \mathrm{C}_r \end{matrix} | \psi \rangle$$

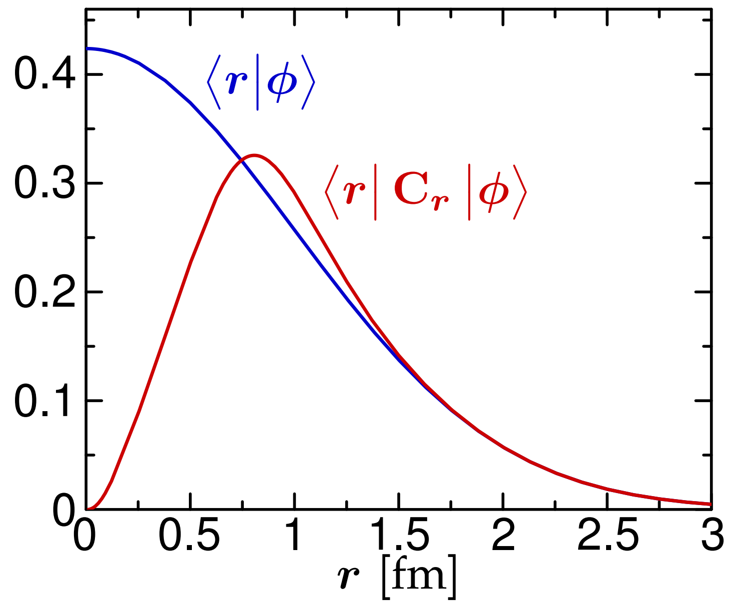
$$= \sqrt{R'_\pm(r)} \, \frac{R_\pm(r)}{r} \, \langle R_\pm(\vec{r}) \tfrac{\vec{r}}{r}, \vec{X} | \psi \rangle$$

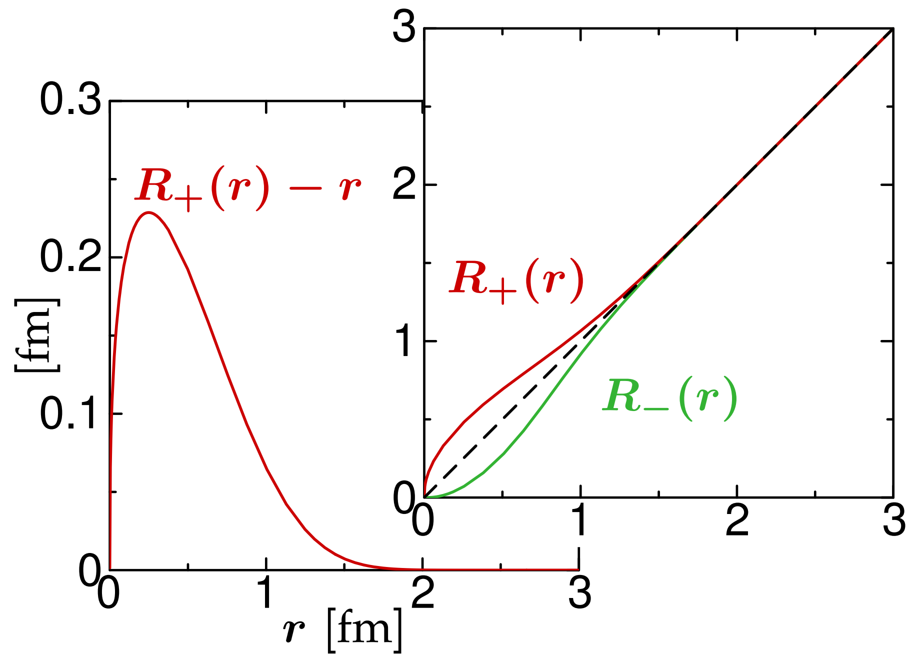
- correlation $\hat{=}$ norm conserving coordinate transformation

$$\vec{r} \quad \longmapsto \quad R_\pm(r) \, \frac{\vec{r}}{r}$$

- correlation functions $R_\pm(r)$ are connected to $s(r)$

$$\pm 1 = \int_r^{R_\pm(r)} \frac{\mathrm{d}\xi}{s(\xi)} \, , \qquad R_\pm(r) \approx r \pm s(r)$$





Correlated States — Tensor Correlations

- tensor correlated $^3S_1$ two-body state

$$\mathbf{C}_\Omega \, |\phi_S, {}^3S_1\rangle = |\widehat{\phi}_S, {}^3S_1\rangle + |\widehat{\phi}_D, {}^3D_1\rangle$$

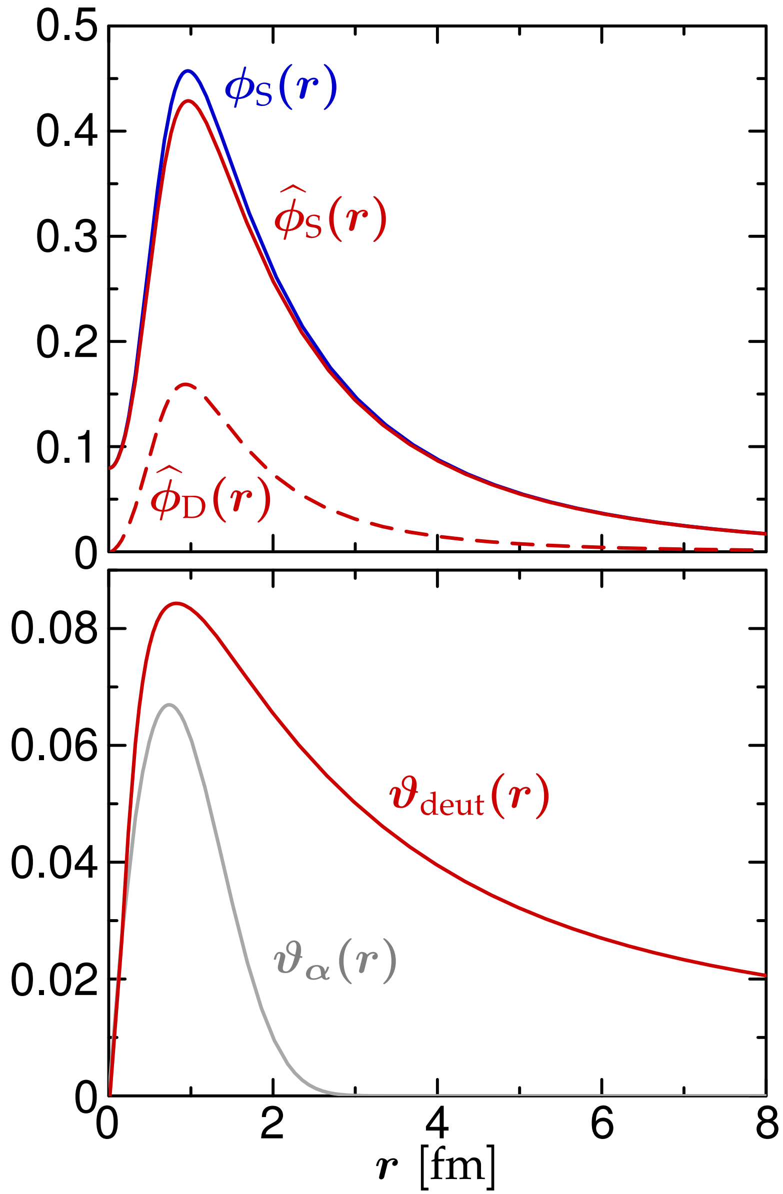
$$\langle \boldsymbol{r}|\widehat{\phi}_S\rangle = \cos[3\sqrt{2}\,\vartheta(r)]\;\langle \boldsymbol{r}|\phi_S\rangle$$

$$\langle \boldsymbol{r}|\widehat{\phi}_D\rangle = \sin[3\sqrt{2}\,\vartheta(r)]\;\langle \boldsymbol{r}|\phi_S\rangle$$

- tensor force admixes higher orbital angular momenta — and so does the tensor correlator

- tensor correlator for the deuteron

$$\vartheta_{\text{deut}}(r) = \frac{1}{3\sqrt{2}} \arctan \frac{\langle r|\widehat{\phi}_D^{\text{deut}}\rangle}{\langle r|\widehat{\phi}_S^{\text{deut}}\rangle}$$



Momentum-Space Matrix Elements

$$\left\langle \boldsymbol{k}(\boldsymbol{LS})\boldsymbol{JT} \right| \mathrm{V}_{\mathrm{UCOM}} \left| \boldsymbol{k'}(\boldsymbol{L'S})\boldsymbol{JT} \right\rangle$$