Nuclear Structure in the UCOM Framework:

Formalism and Few-Body Systems

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Overview

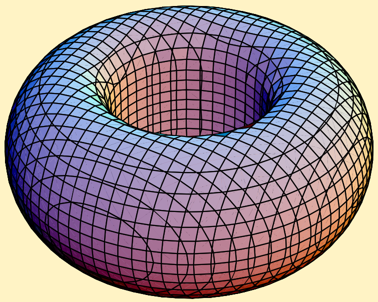
- UCOM Concepts and Formalism
- Few-Body Calculations
  - No-Core Shell Model (NCSM)
  - Fermionic Molecular Dynamics (FMD)
- Summary

Motivation

Argonne V18 Deuteron Solution

$$M_S = 0$$

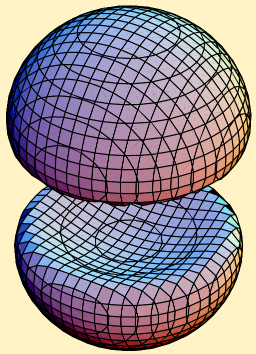
$$\frac{1}{\sqrt{2}}\left(\left|\uparrow\downarrow\right\rangle + \left|\downarrow\uparrow\right\rangle \right)$$



$$\rho^{(2)}_{1,M_S}(\vec{r})$$

$$M_S = \pm 1$$

$$\left|\uparrow\uparrow\right\rangle,\ \left|\downarrow\downarrow\right\rangle$$

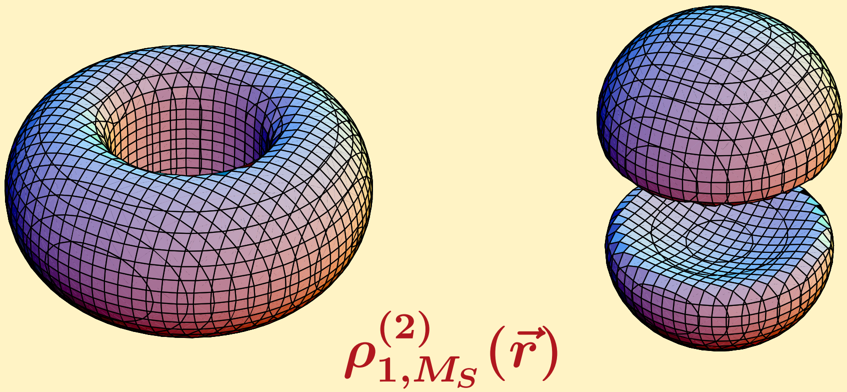


Motivation

Argonne V18 Deuteron Solution

$M_S = 0$ — $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$

$M_S = \pm 1$ — $|\uparrow\uparrow\rangle, |\downarrow\downarrow\rangle$



- **central correlations:**
  two-body density is suppressed at low distances

Motivation

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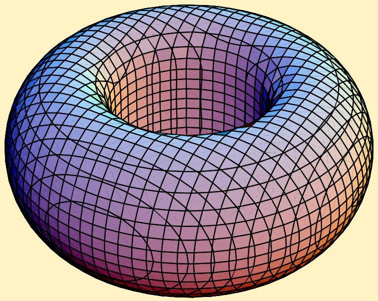

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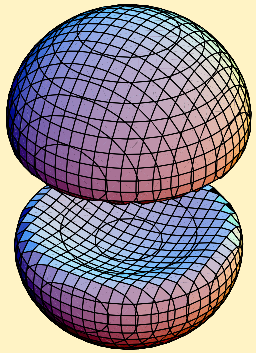

$\rho^{(2)}_{1,M_S}(\vec{r})$

- **central correlations:**
  two-body density is suppressed at low distances

- **tensor correlations:**
  angular distribution depends on the relative spin alignments

Motivation

Argonne V18 Deuteron Solution

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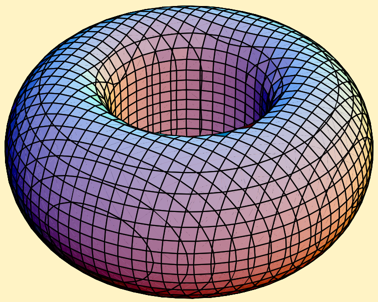

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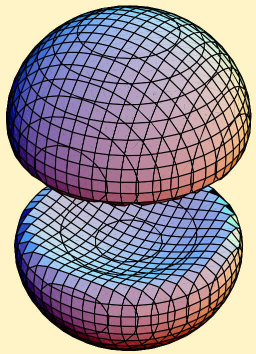

$\rho^{(2)}_{1,M_S}(\vec{r})$

- **central correlations:** two-body density is suppressed at low distances
- **tensor correlations:** angular distribution depends on the relative spin alignments

use very large many-body Hilbert spaces

$\Rightarrow$ **high computational effort**

Motivation

Argonne V18 Deuteron Solution

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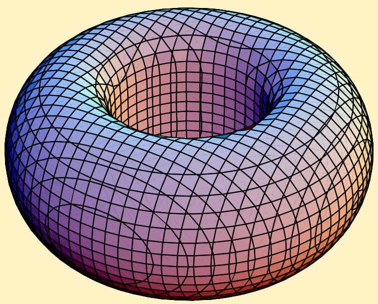

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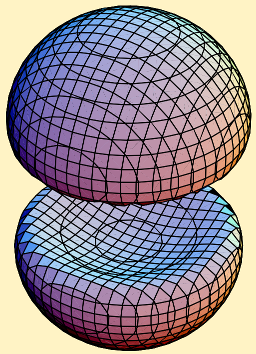


$\rho^{(2)}_{1,M_S}(\vec{r})$

- **central correlations:** two-body density is suppressed at low distances
- **tensor correlations:** angular distribution depends on the relative spin alignments

use very large many-body Hilbert spaces
$\Rightarrow$ **high computational effort**

or

use numerically affordable Hilbert spaces and **treat strong correlations explicitly**

Central and Tensor Correlators

Central Correlator C_r

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

$$\mathrm{C}_r = \exp\Big(-i \sum_{i,j}^{A} \mathrm{g}_{r,ij}\Big)$$

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

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

Tensor Correlator C_Ω

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

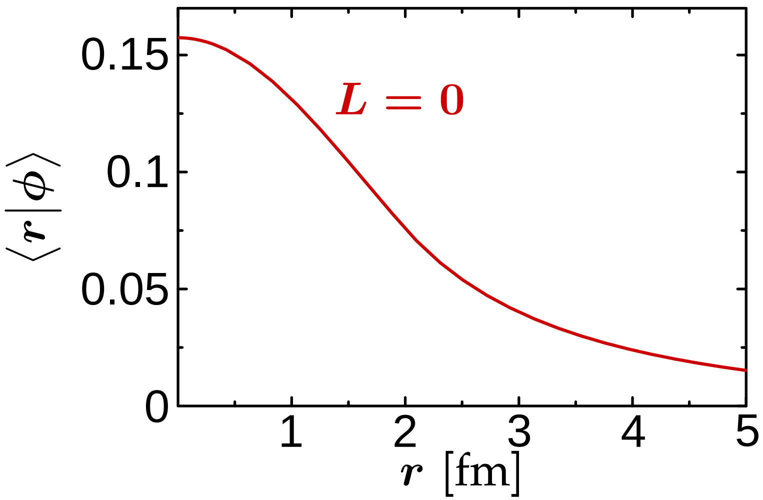
$$\mathrm{C}_\Omega = \exp\Big(-i \sum_{i,j}^{A} \mathrm{g}_{\Omega,ij}\Big)$$

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

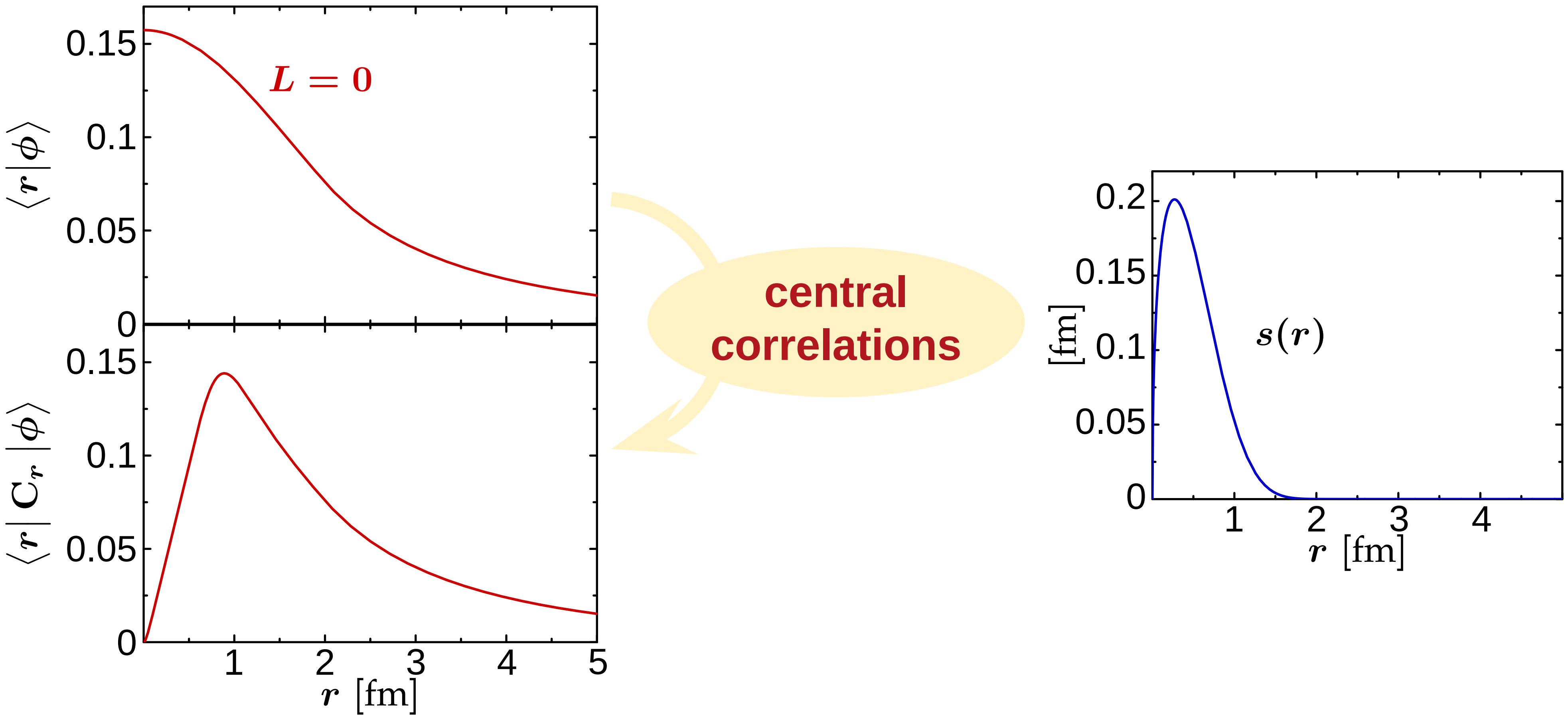
$$\vec{\mathrm{q}}_\Omega = \vec{\mathrm{q}} - \tfrac{\vec{\mathrm{r}}}{\mathrm{r}}\ \mathrm{q}_r$$

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

Correlated States



Correlated States



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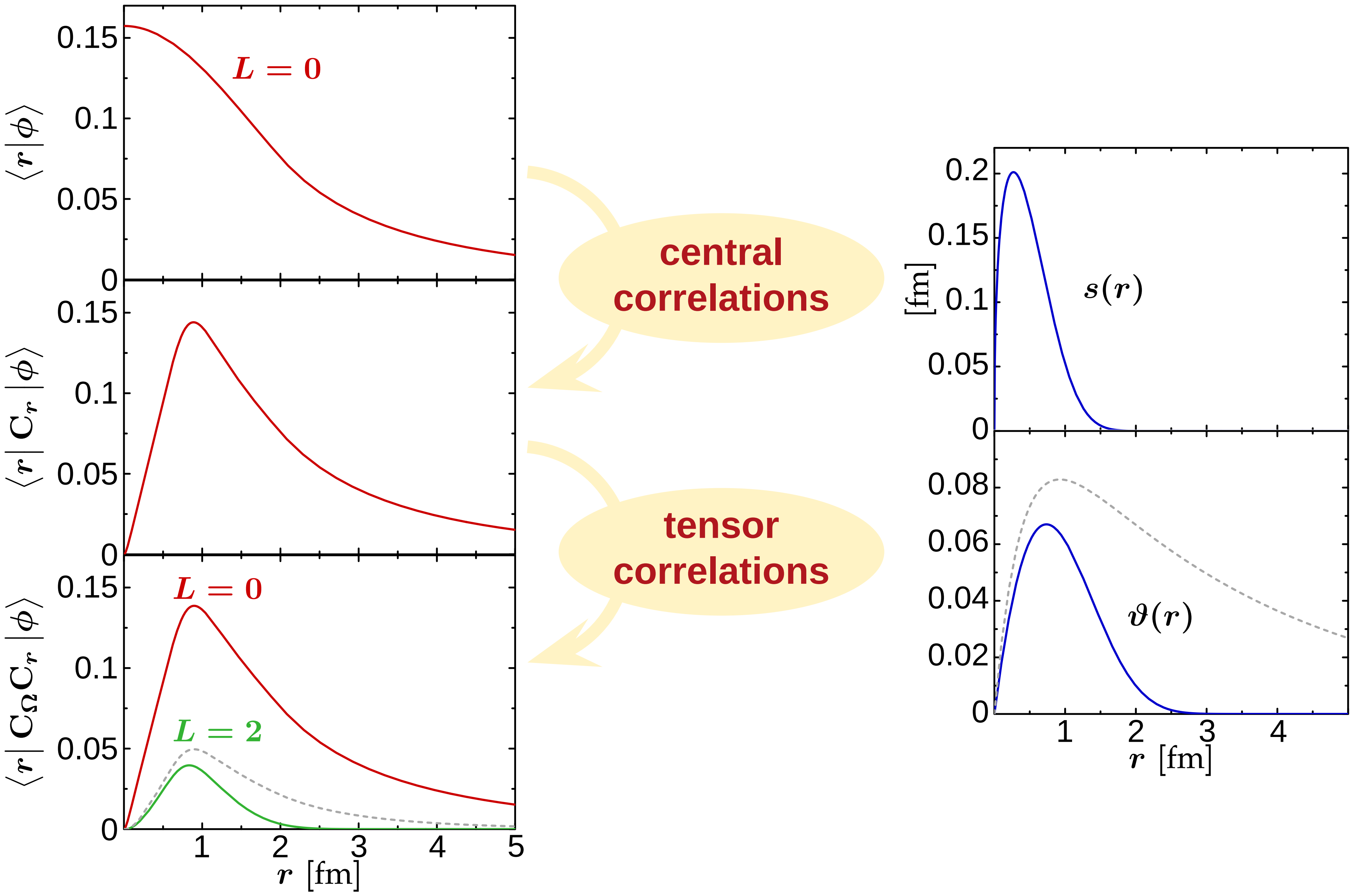

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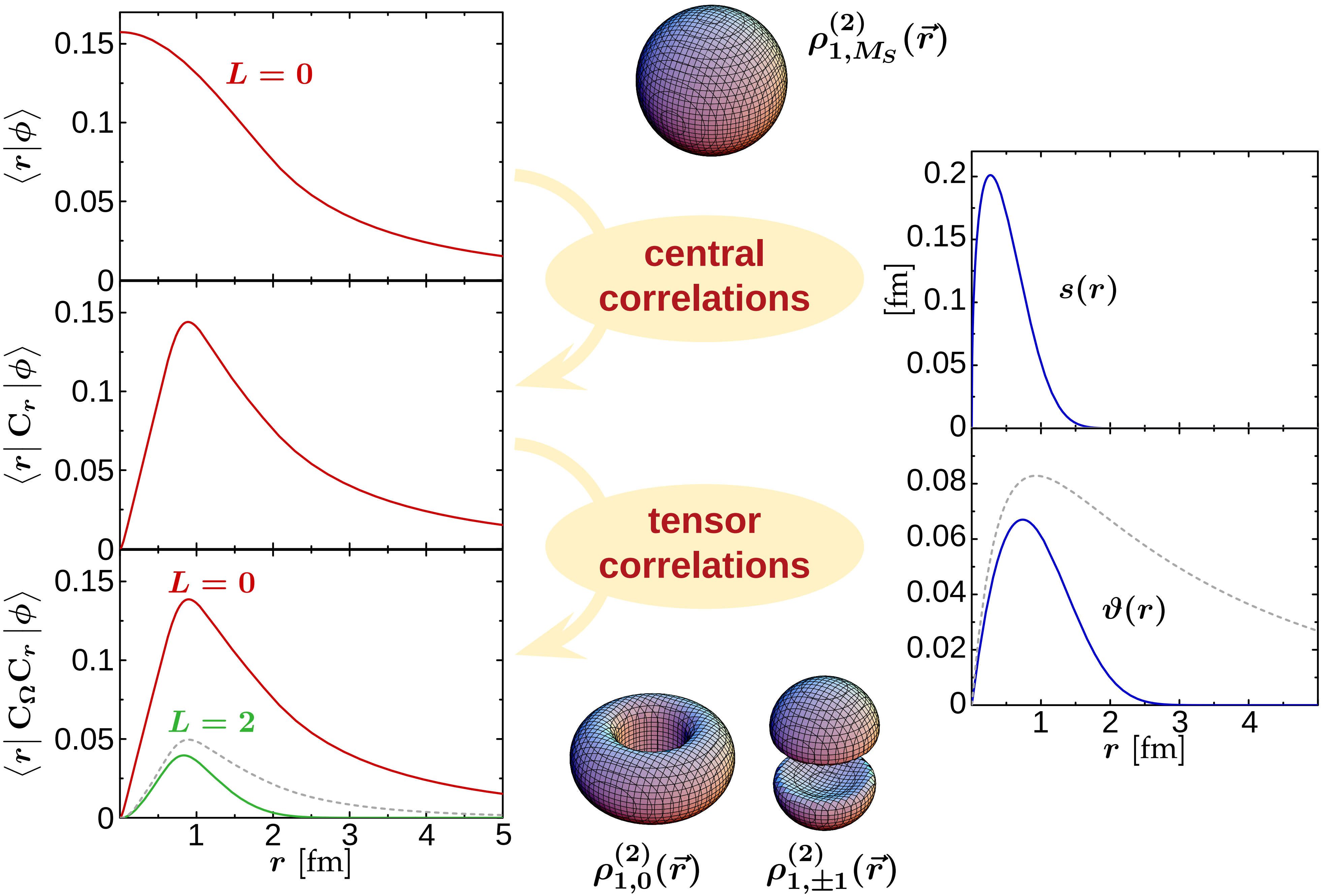
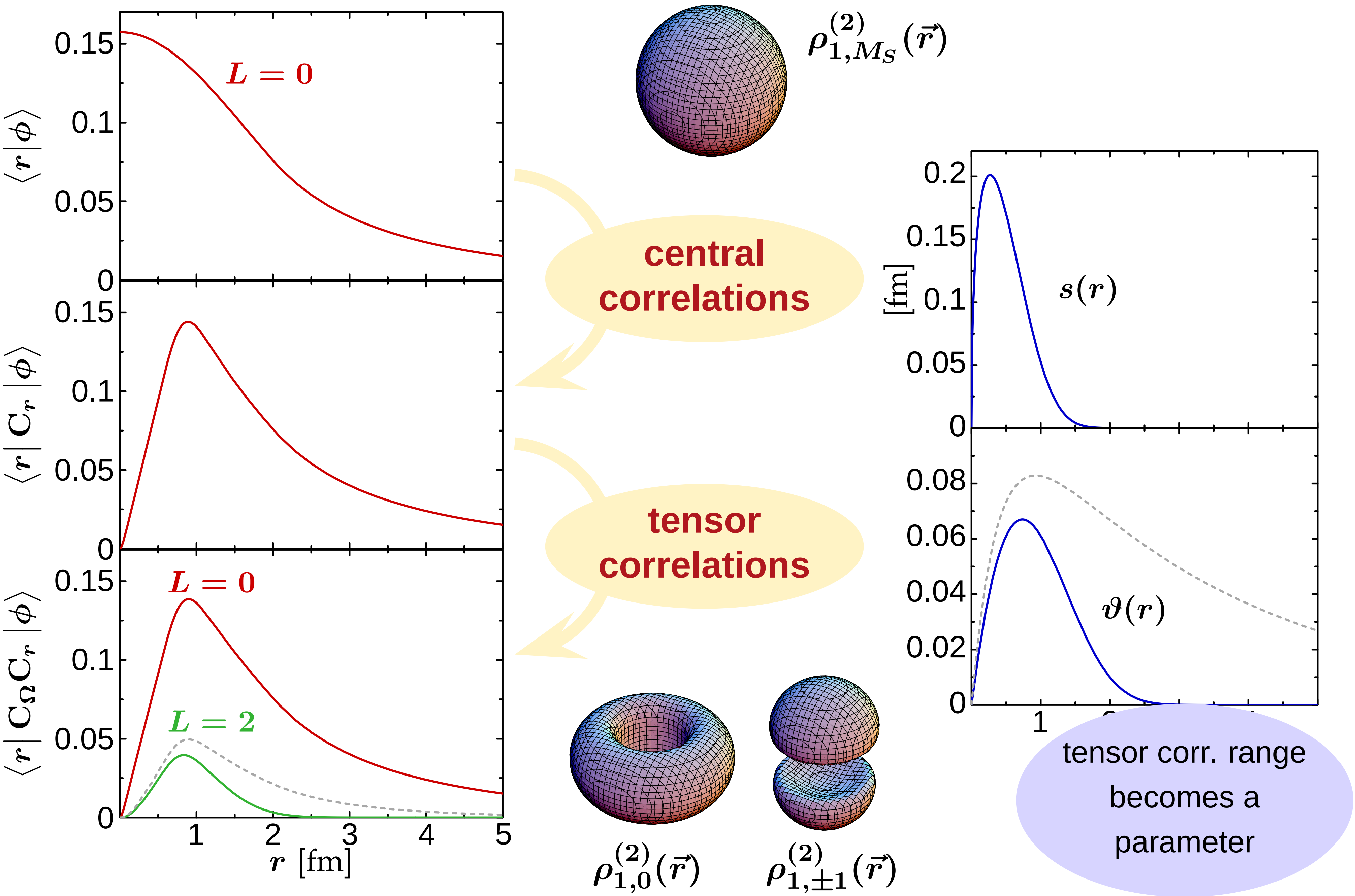


Correlated States



Correlated Operators

- application of $\mathrm{C}_r \mathrm{C}_\Omega$ is a **unitary transformation**:

$$\left\langle \widetilde{\Psi} \right| \mathrm{O} \left| \widetilde{\Psi} \right\rangle = \left\langle \Psi \right| \mathrm{C}_\Omega^\dagger \mathrm{C}_r^\dagger \mathrm{O} \mathrm{C}_r \mathrm{C}_\Omega \left| \Psi \right\rangle = \left\langle \Psi \right| \widetilde{\mathrm{O}} \left| \Psi \right\rangle$$

- **all observables need to be correlated consistently**

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Correlated Hamiltonian

$$\mathbf{C}_\Omega^\dagger \mathbf{C}_r^\dagger \mathbf{H} \mathbf{C}_r \mathbf{C}_\Omega = \mathbf{T}^{[1]} + \widetilde{\mathbf{T}}^{[2]} + \widetilde{\mathbf{V}}^{[2]} + \widetilde{\mathbf{T}}^{[3]} + \widetilde{\mathbf{V}}^{[3]} + \ldots$$

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Correlated Hamiltonian

$$\mathrm{C}_{\boldsymbol{\Omega}}^{\dagger}\mathrm{C}_{\boldsymbol{r}}^{\dagger}\mathrm{H}\mathrm{C}_{\boldsymbol{r}}\mathrm{C}_{\boldsymbol{\Omega}} = \mathrm{T}^{[1]} + \mathrm{V}_{\mathrm{UCOM}} + \mathrm{V}_{\mathrm{UCOM}}^{[3]} + \dots$$

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Correlated Hamiltonian

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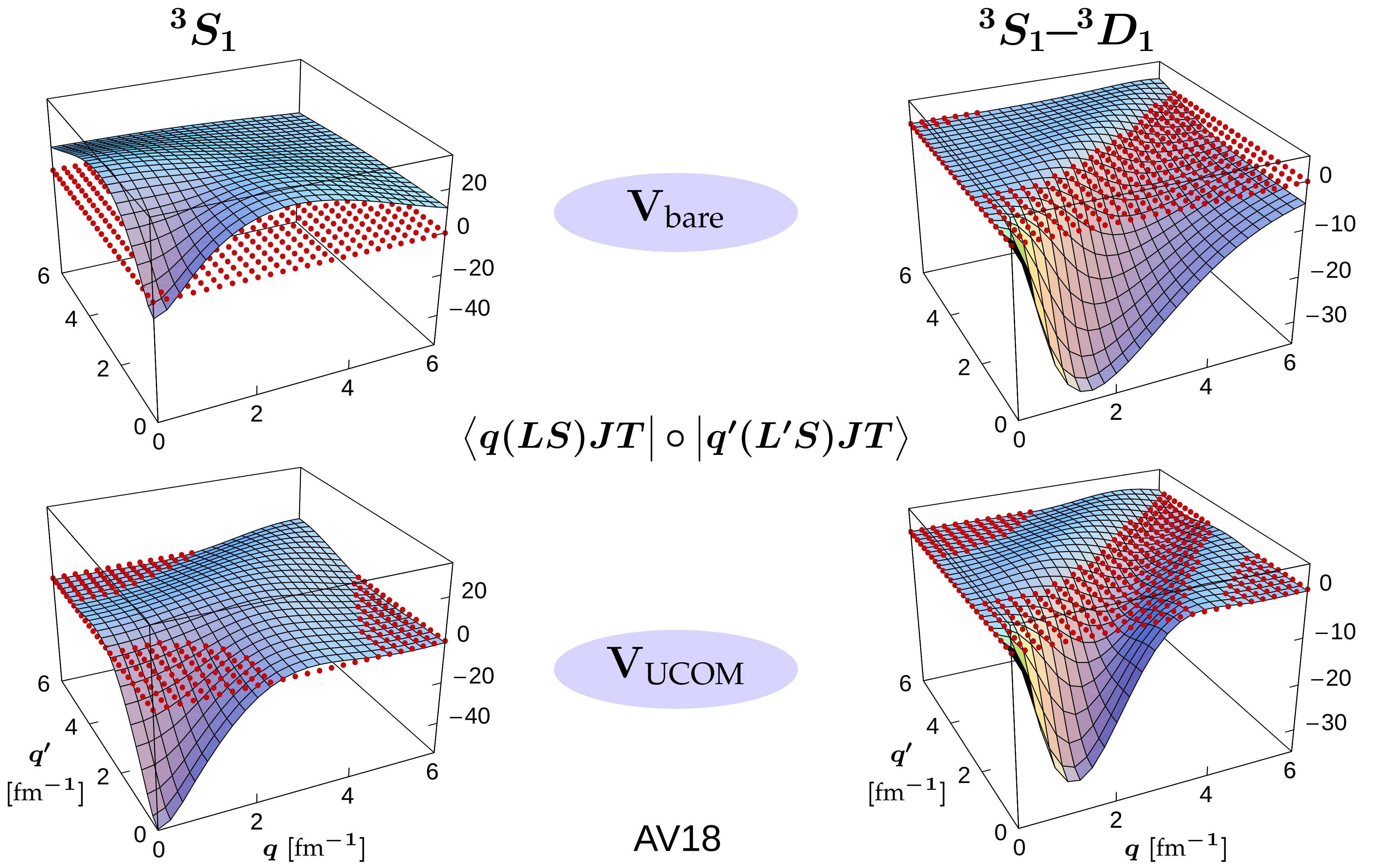
$\mathrm{V}_{\mathrm{UCOM}}$

$$\mathrm{V}_{\mathrm{UCOM}} = \sum_{i,S,T} \frac{1}{2}\left(\tilde{v}_{ST}^{i}(\mathrm{r})\mathrm{O}_i + \mathrm{O}_i\tilde{v}_{ST}^{i}(\mathrm{r})\right)\Pi_{ST}$$

$$\mathrm{O}_i \in \{\mathbb{1},\ \mathrm{q}_r^2,\ \vec{\mathrm{l}}^2,\ \vec{\mathrm{l}}\cdot\vec{\mathrm{s}},\ \mathrm{s}_{12}(\vec{\mathrm{r}},\vec{\mathrm{r}}),\ \vec{\mathrm{l}}^2\vec{\mathrm{l}}\cdot\vec{\mathrm{s}},\ \mathrm{s}_{12}(\vec{\mathrm{l}},\vec{\mathrm{l}}),\ \bar{\mathrm{s}}_{12}(\vec{\mathrm{q}}_\Omega,\vec{\mathrm{q}}_\Omega),\ \{\vec{\mathrm{l}}^2\bar{\mathrm{s}}_{12}(\vec{\mathrm{q}}_\Omega,\vec{\mathrm{q}}_\Omega)\}_H,\ \mathrm{q}_r\mathrm{s}_{12}(\vec{\mathrm{r}},\vec{\mathrm{q}}_\Omega),\ \ldots\}$$

Momentum-Space Matrix Elements



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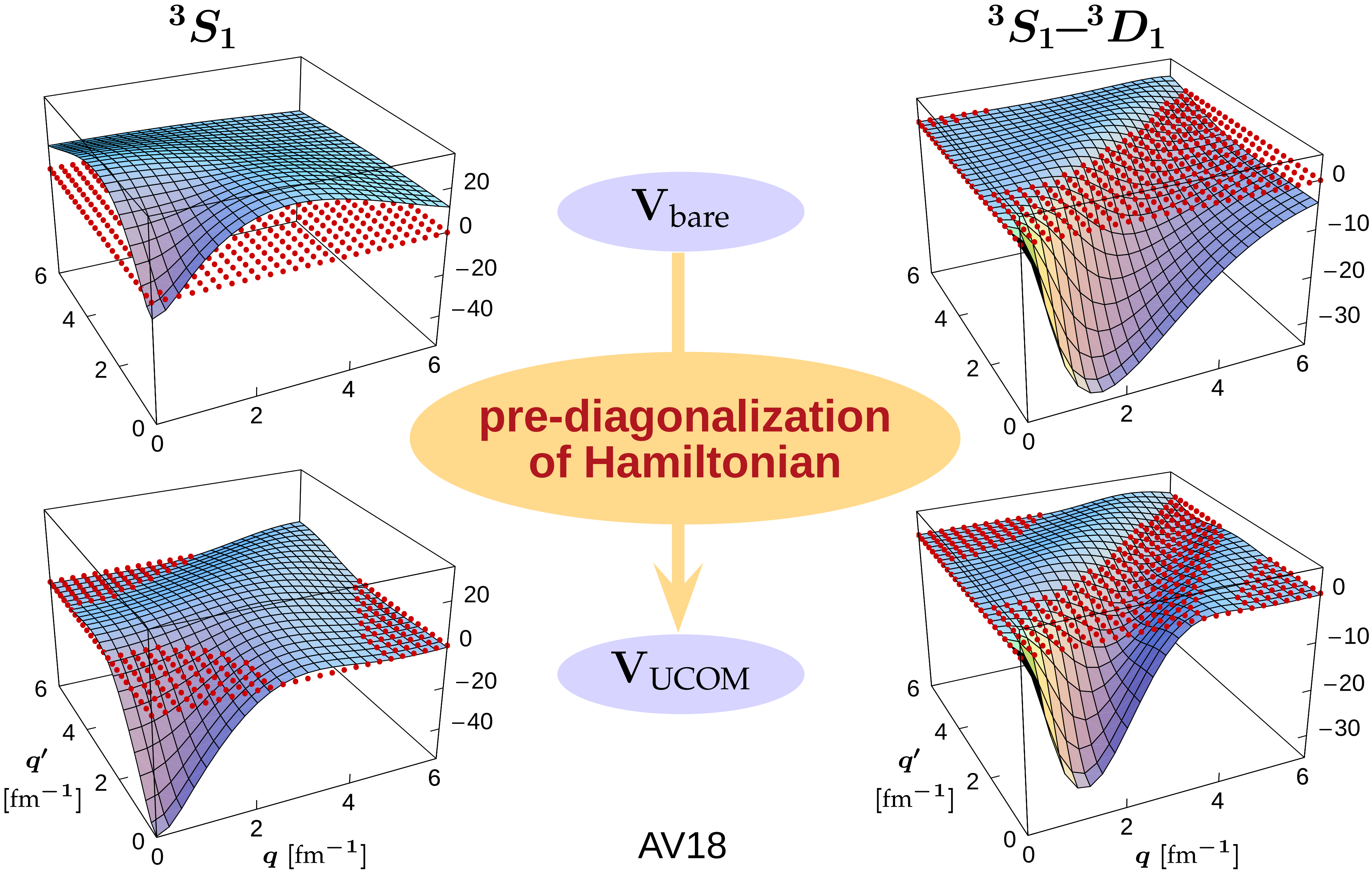
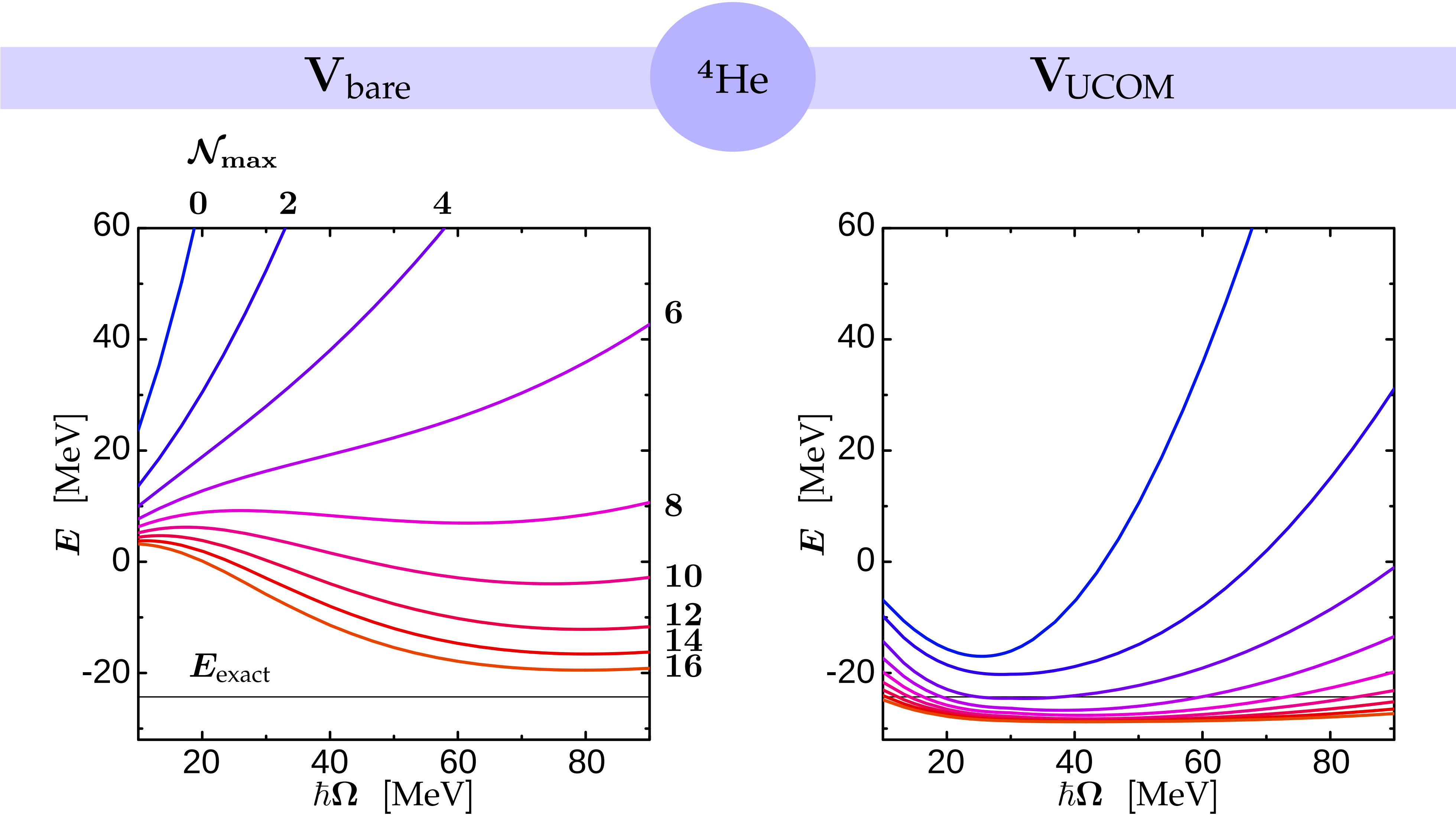


Few-Body Calculations:

No-Core Shell Model (NCSM)

^{4}He: Convergence



NCSM code by P. Navrátil [PRC 61, 044001 (2000)]

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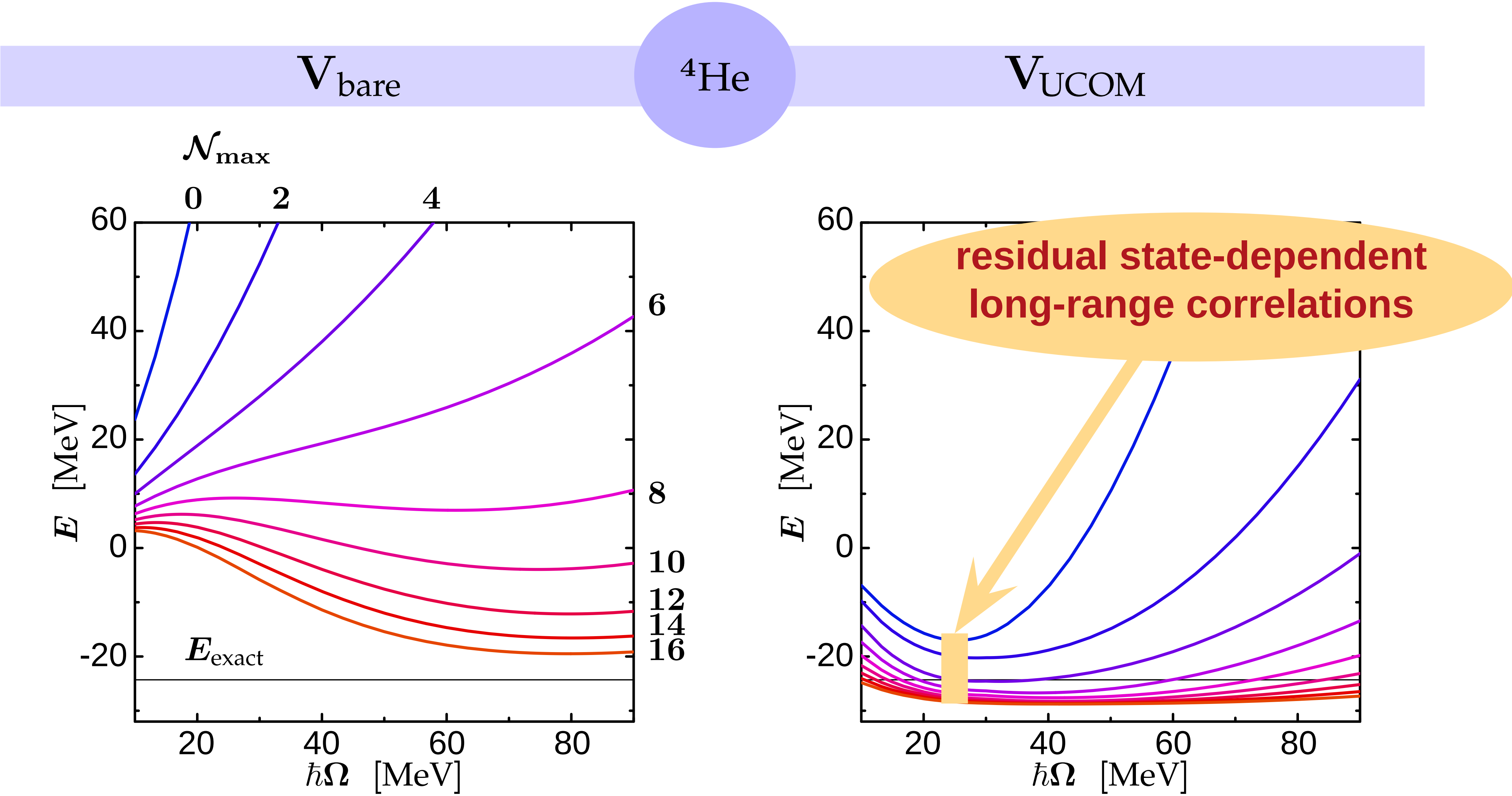

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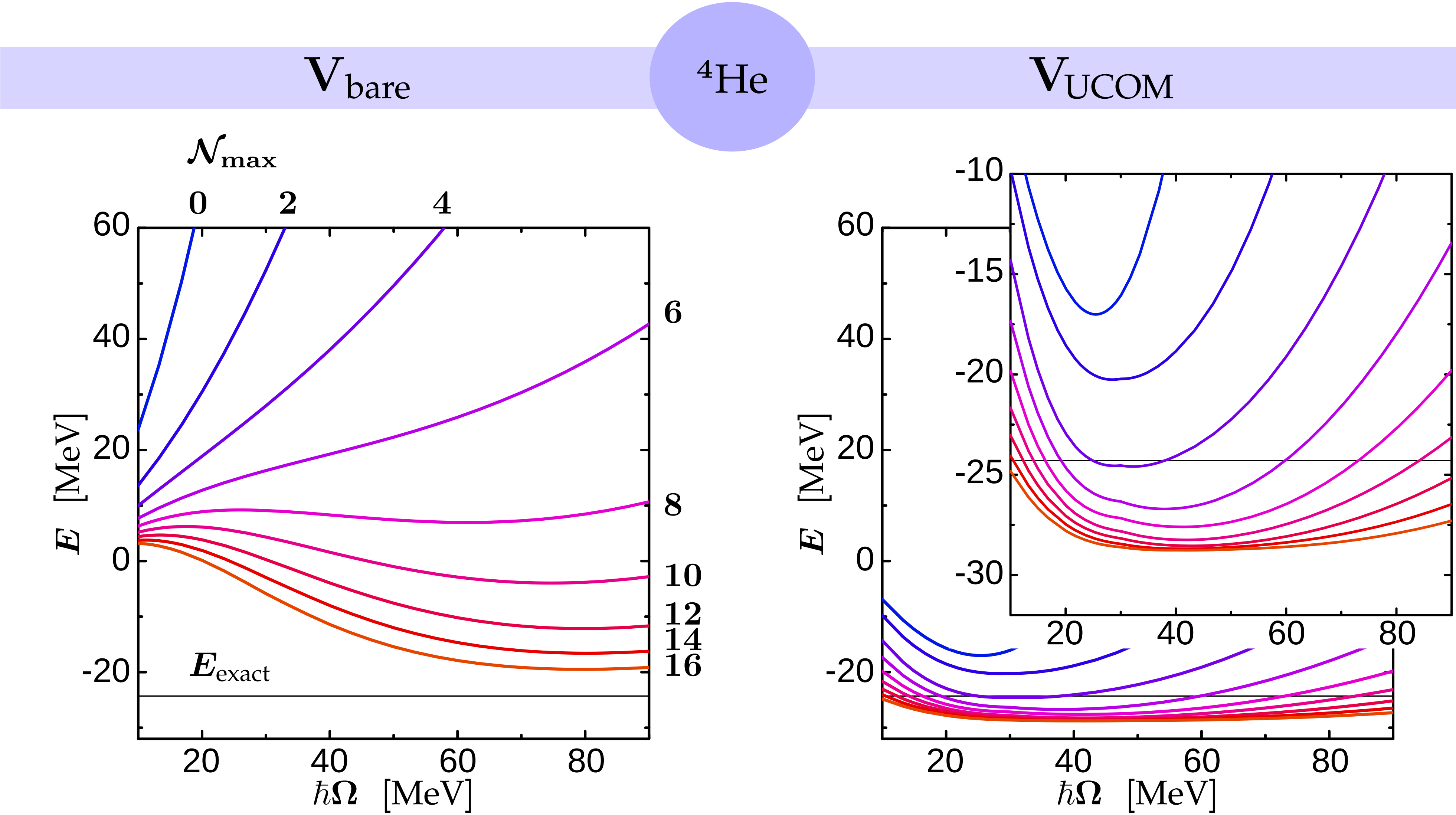

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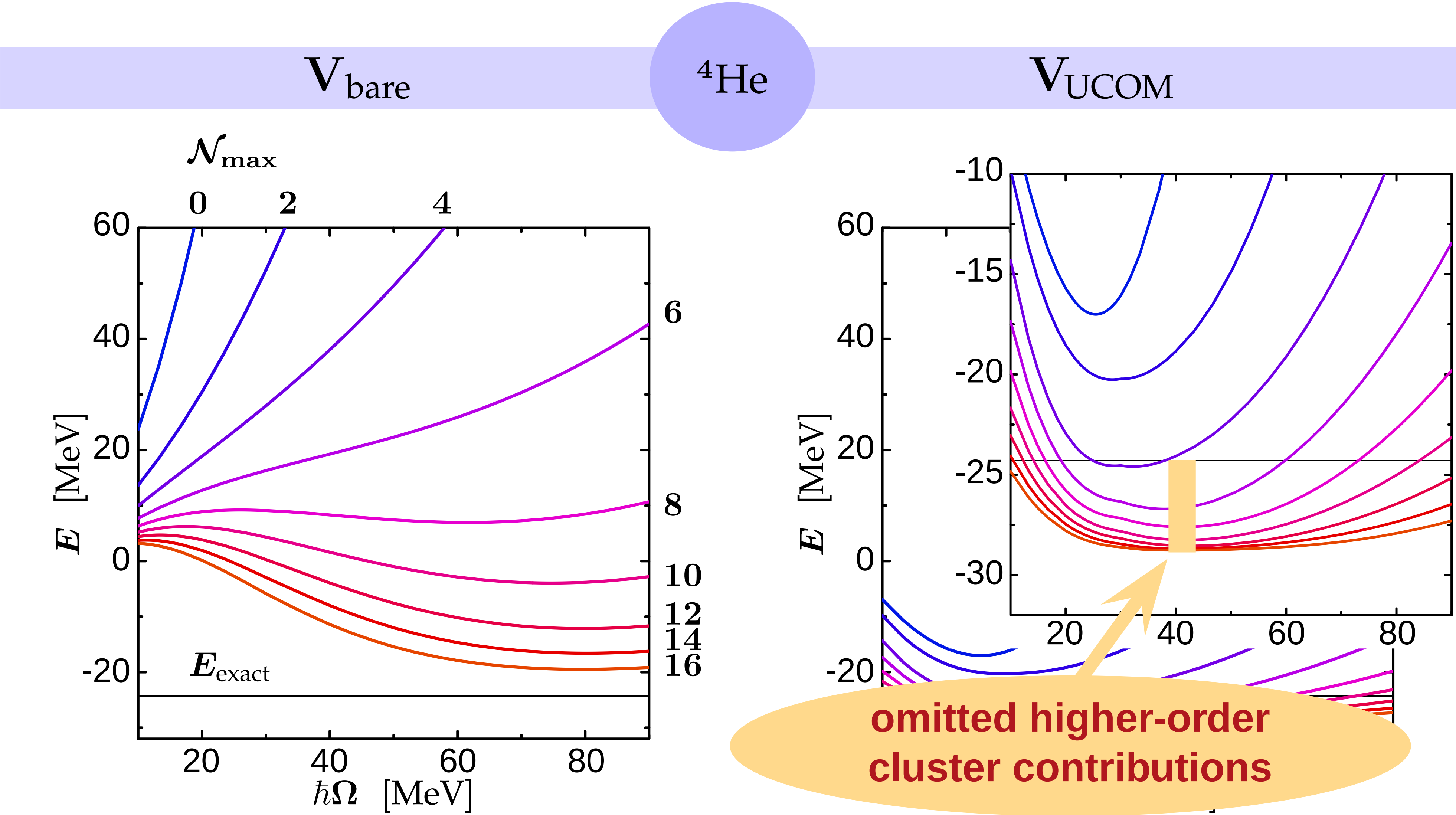

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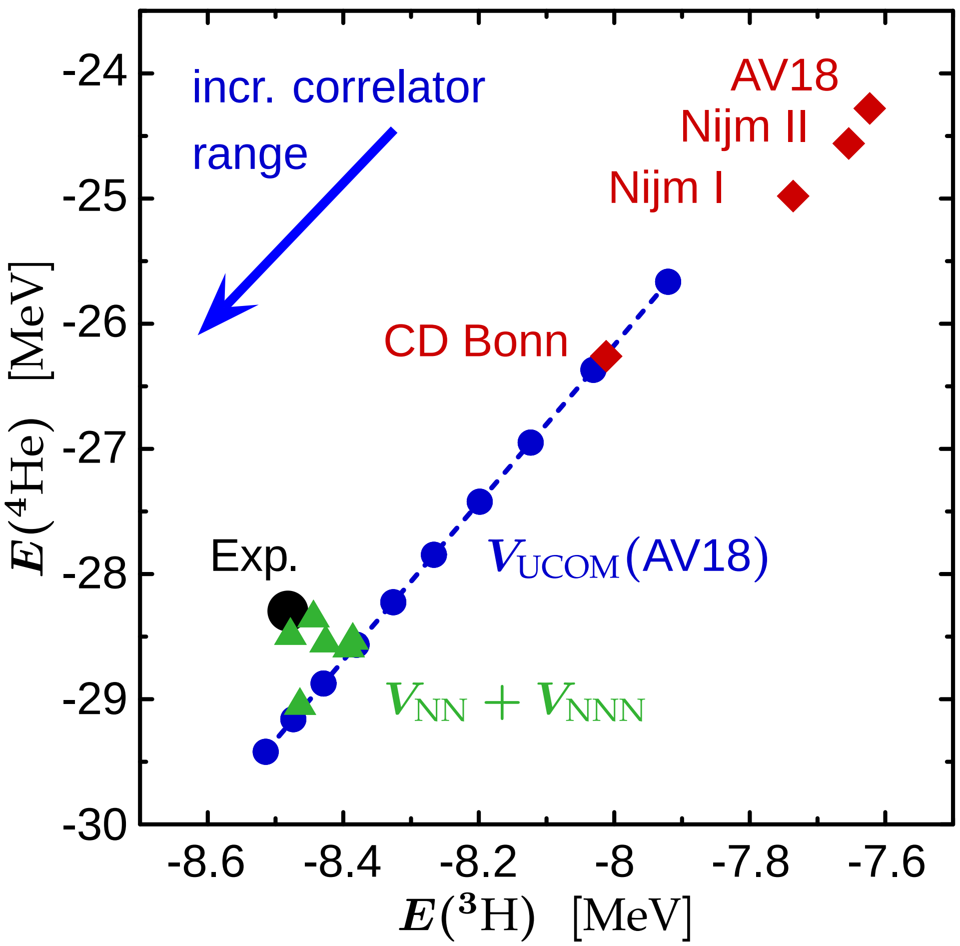
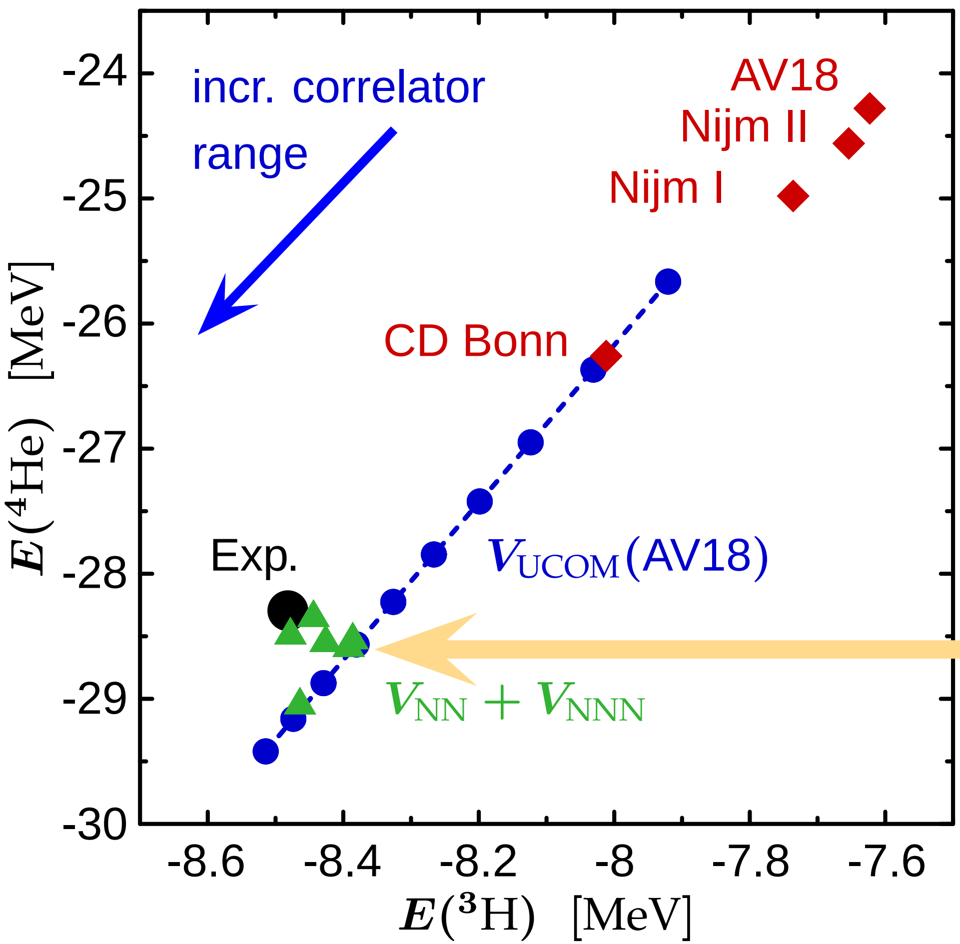
Tjon-Line and Correlator Range



- **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

Data points: A. Nogga et al., Phys. Rev. Lett. **85**, 944 (2000)

Tjon-Line and Correlator Range



- **Tjon-line**: $E(^4\mathrm{He})$ vs. $E(^3\mathrm{H})$ for phase-shift equivalent NN-interactions
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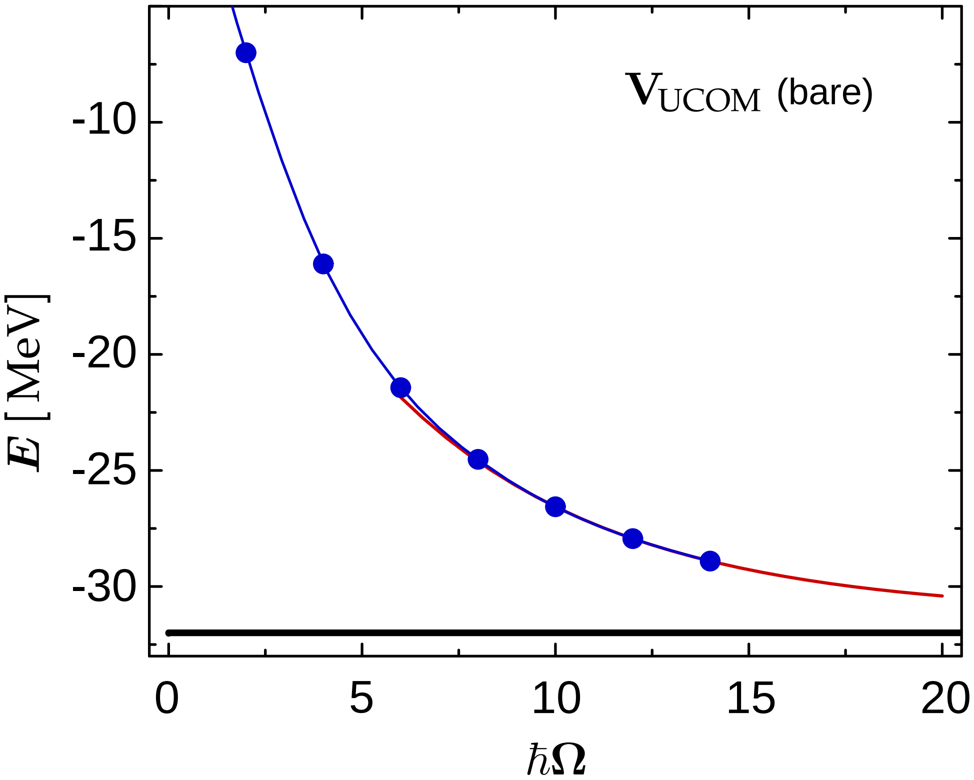
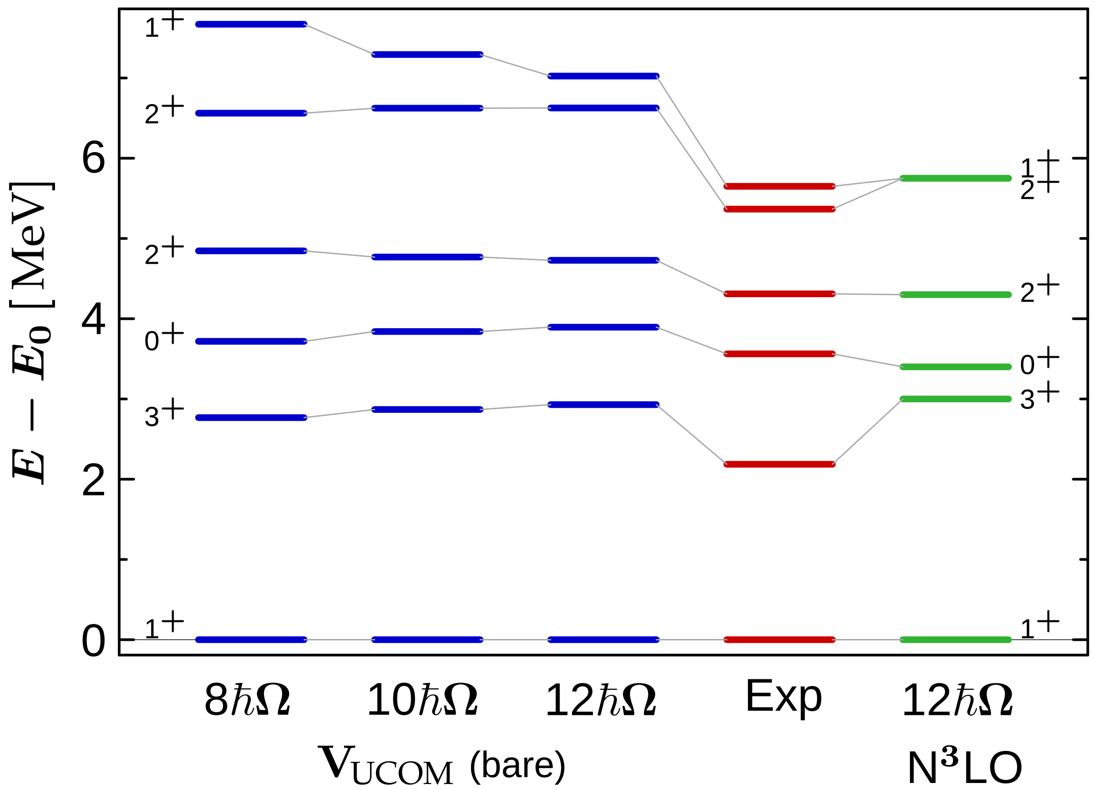
choose correlator with energies close to experimental value, i.e., **minimize net three-body force**

Data points: A. Nogga et al., Phys. Rev. Lett. **85**, 944 (2000)

^{6}Li — Work in Progress





$\hbar\Omega$	8	10	12	14
E [MeV]	-24.522	-26.564	-27.938	-28.906

E [MeV] (extrapolation)	-31.226
E [MeV] (experiment)	-31.995

NCSM calculations @ LLNL by P. Navratíl

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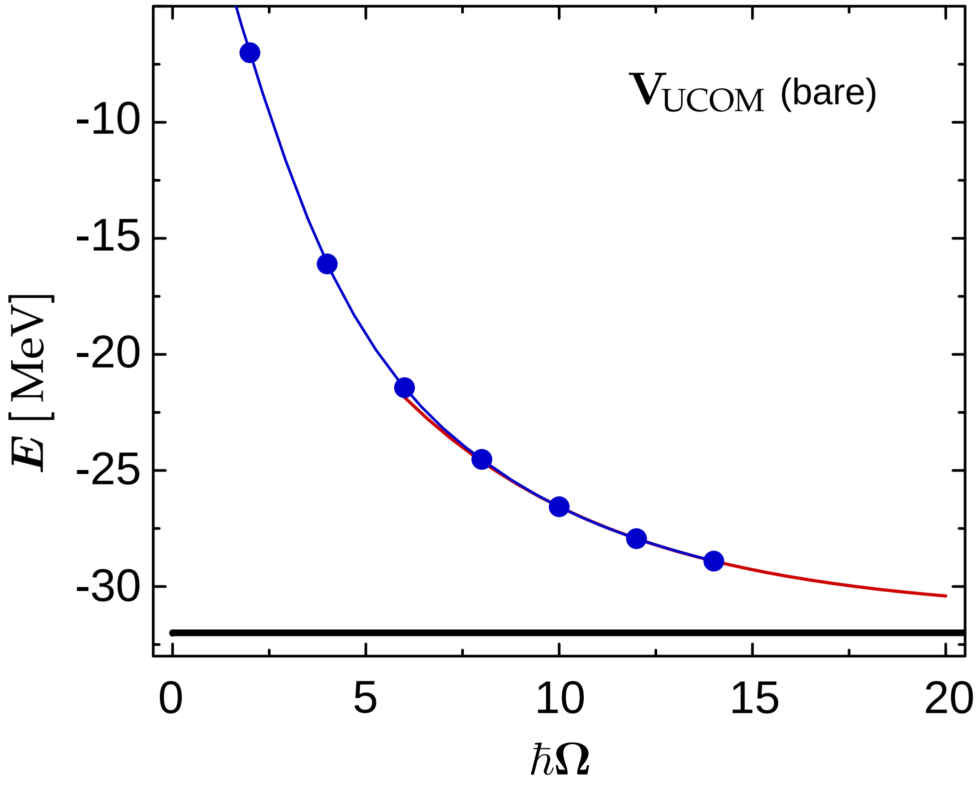

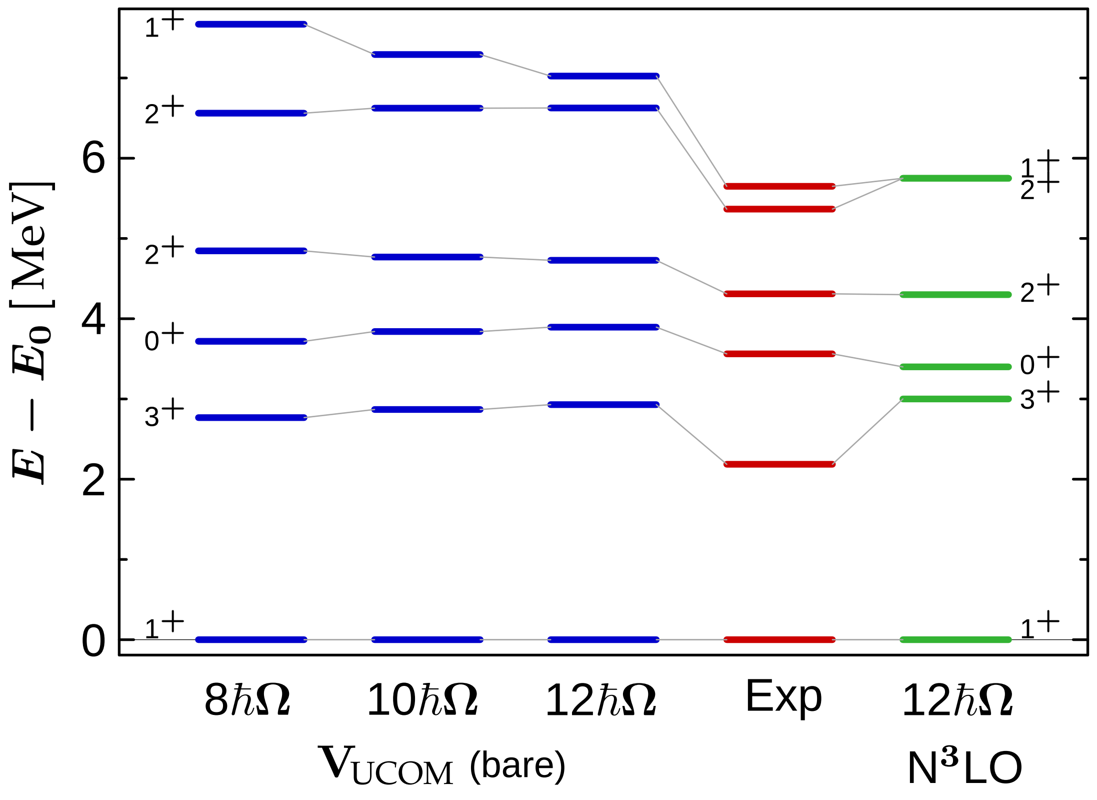

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V_{UCOM}+Lee-Suzuki and more p-shell nuclei in progress...

NCSM calculations @ LLNL by P. Navratíl

Few-Body Calculations:

Fermionic Molecular Dynamics (FMD)

FMD Trial State

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

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

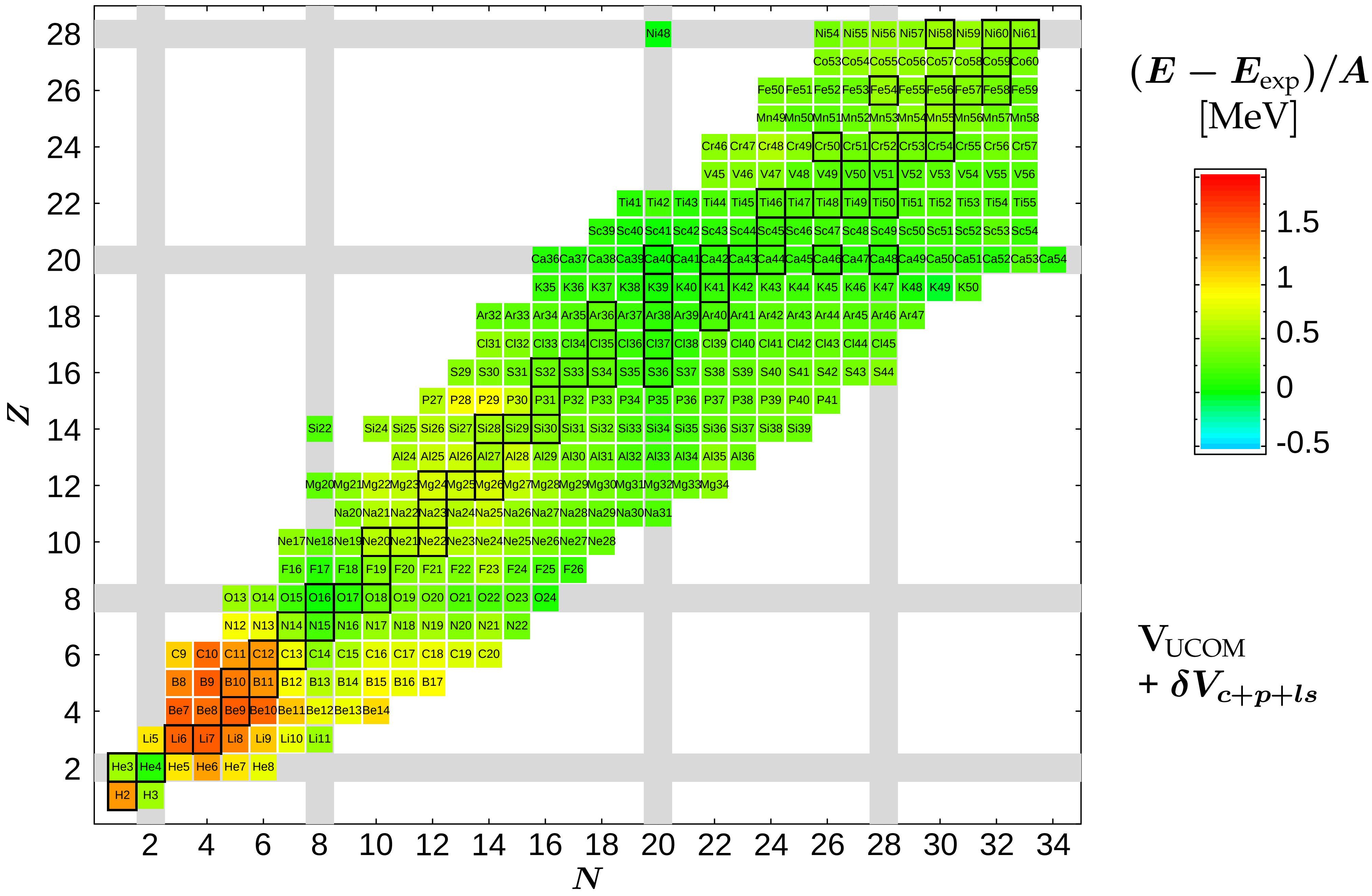
Variation

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

Diagonalization

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

Variation: Chart of Nuclei



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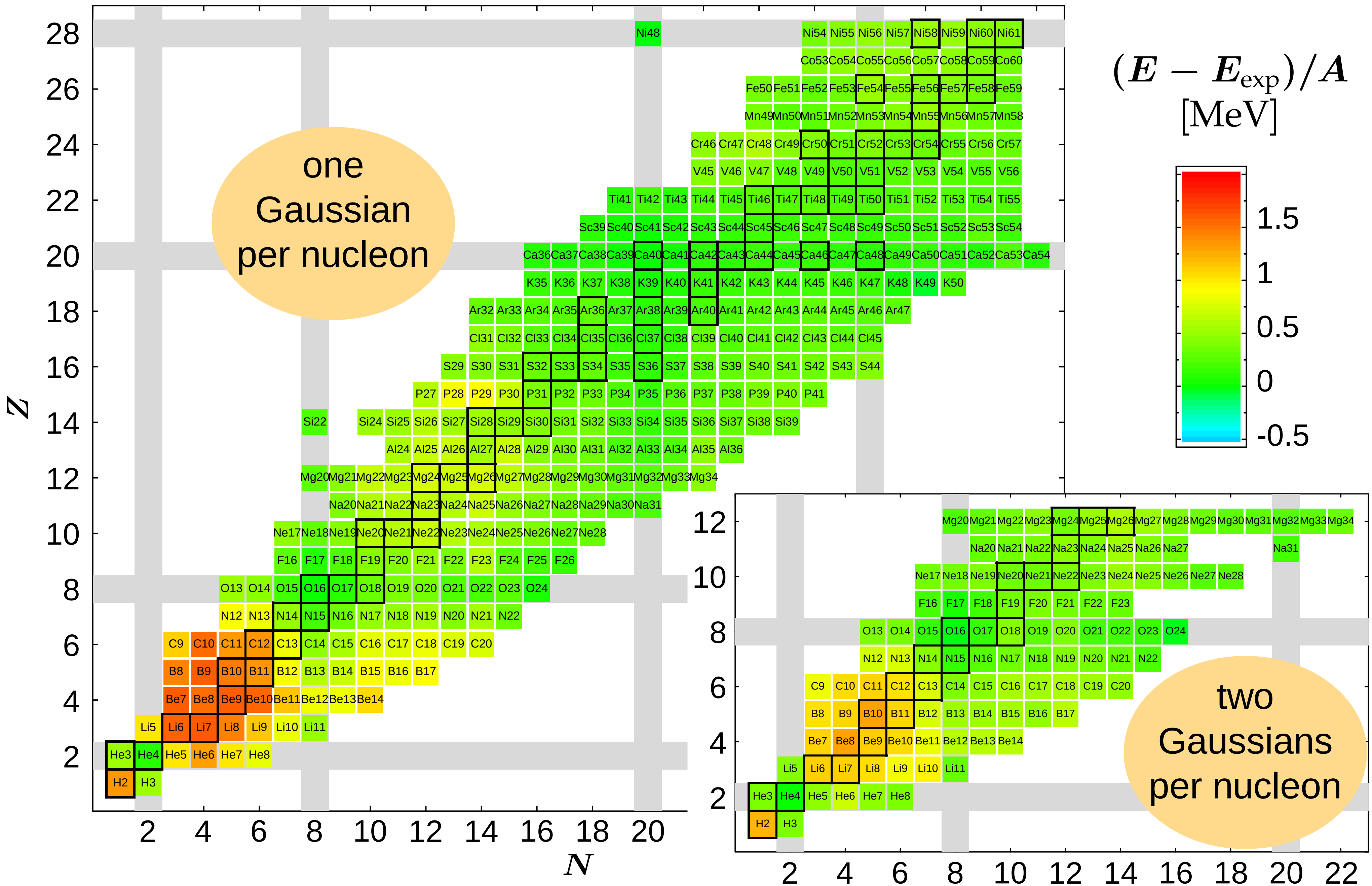
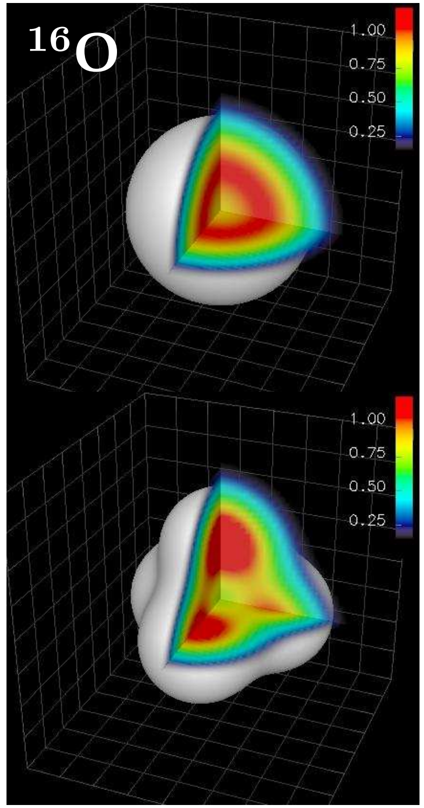


Beyond Simple Variation

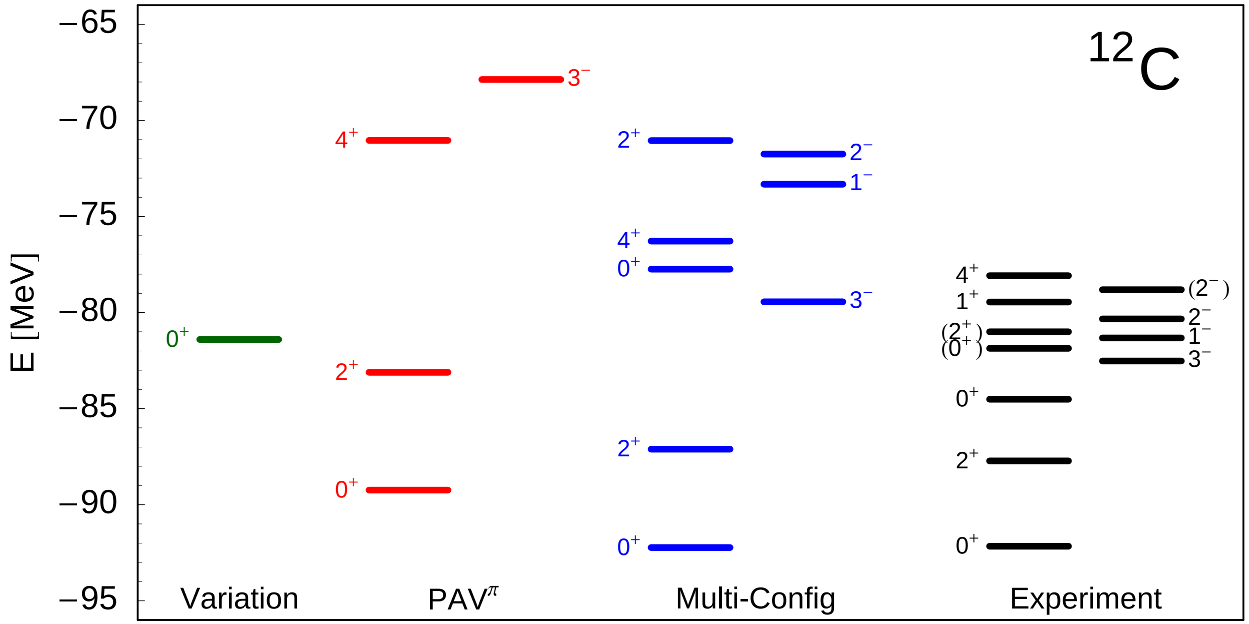
- **Projection after Variation (PAV)**
  - restore parity and rotational symmetry by angular momentum projection

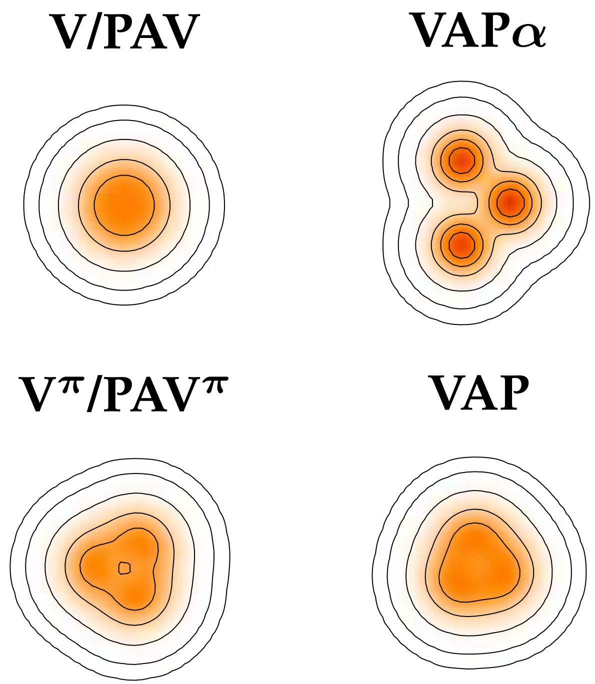


- **Variation after Projection (VAP)**
  - find energy minimum within parameter space of parity and angular momentum projected states
  - implementation via generator coordinate method (constraints on multipole moments)

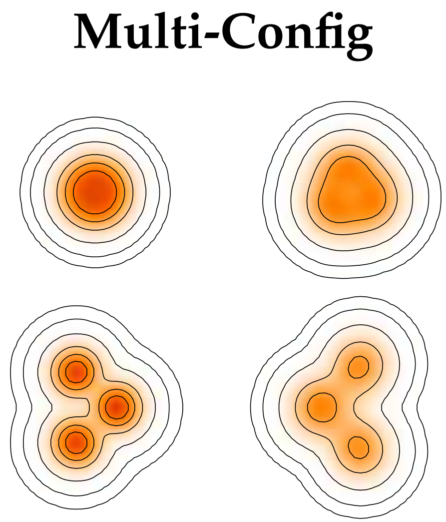
- **Multi-Configuration**
  - diagonalization within a set of different Slater determinants

Structure of ^{12}C

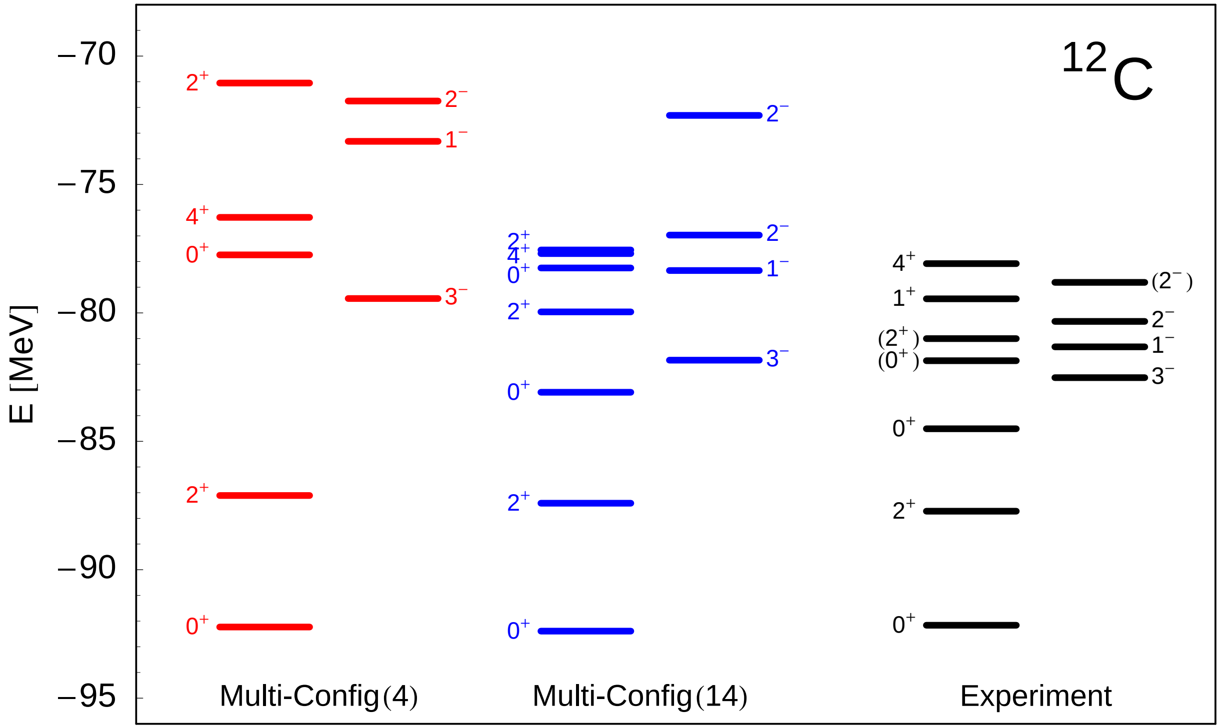


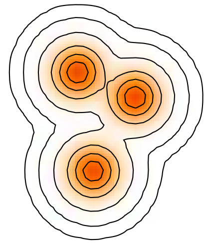


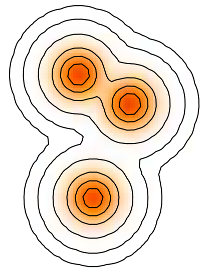
	E [MeV]	R_{ch} [fm]	$B(E2)$ [e^2 fm^4]
V/PAV	81.4	2.36	-
VAP α-cluster	79.1	2.70	76.9
PAV$^\pi$	88.5	2.51	36.3
VAP	89.2	2.42	26.8
Multi-Config	92.2	2.52	42.8
Experiment	92.2	2.47	39.7 ± 3.3

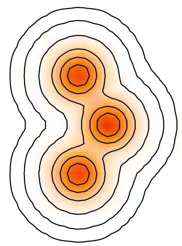


Structure of ^{12}C — Hoyle State



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

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

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

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

Summary

- UCOM enables the use of **realistic NN-interactions** in computationally affordable Hilbert spaces
- UCOM **improves convergence behavior** by pre-diagonalizing the Hamiltonian
- input from **few-body calculations** (NCSM) can be used to **constrain and optimize** the correlated NN-interaction $\mathbf{V}_{\text{UCOM}}$
- calculations using $\mathbf{V}_{\text{UCOM}}$ in a wide range of methods yield encouraging results