Nuclear Structure from Fermionic Molecular Dynamics

Robert Roth

Institut für Kernphysik, TU Darmstadt

International Summer School
“Nuclear Theory & Astrophysical Applications”
JINR Dubna, 2005

From Realistic NN-Interactions to Cluster Structures

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Correlations in Nuclei

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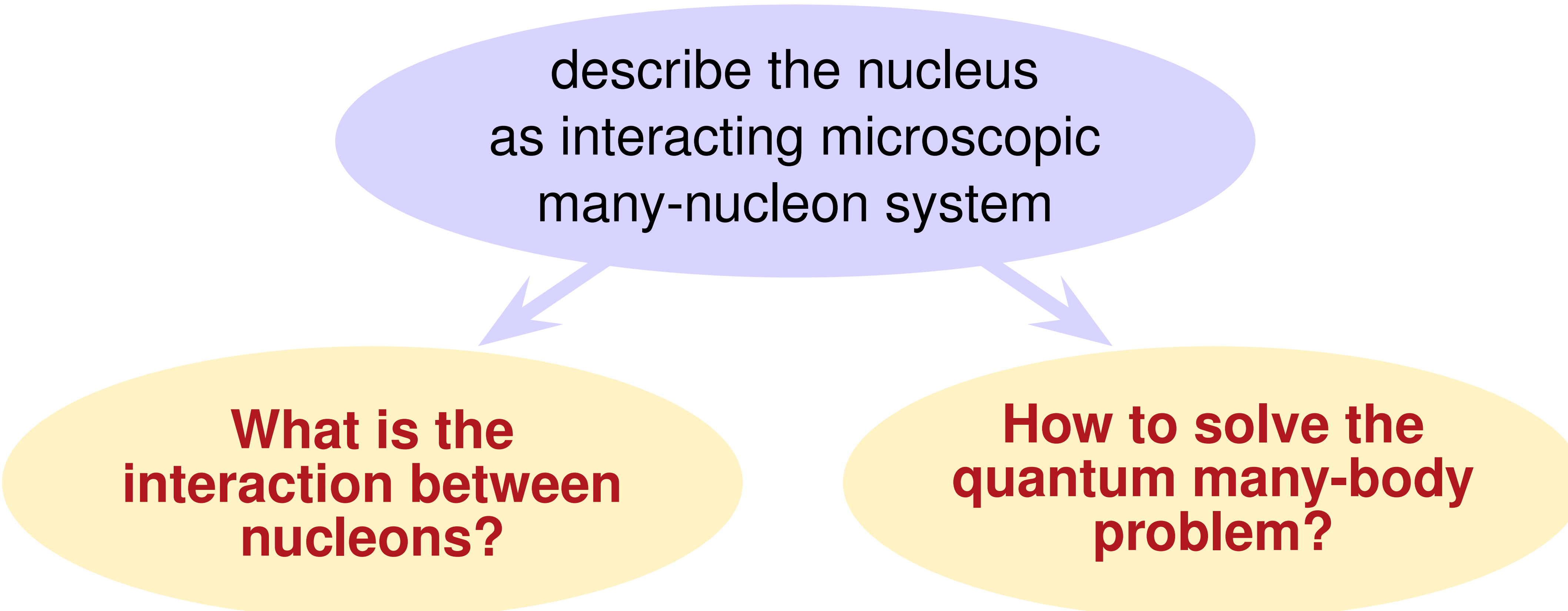
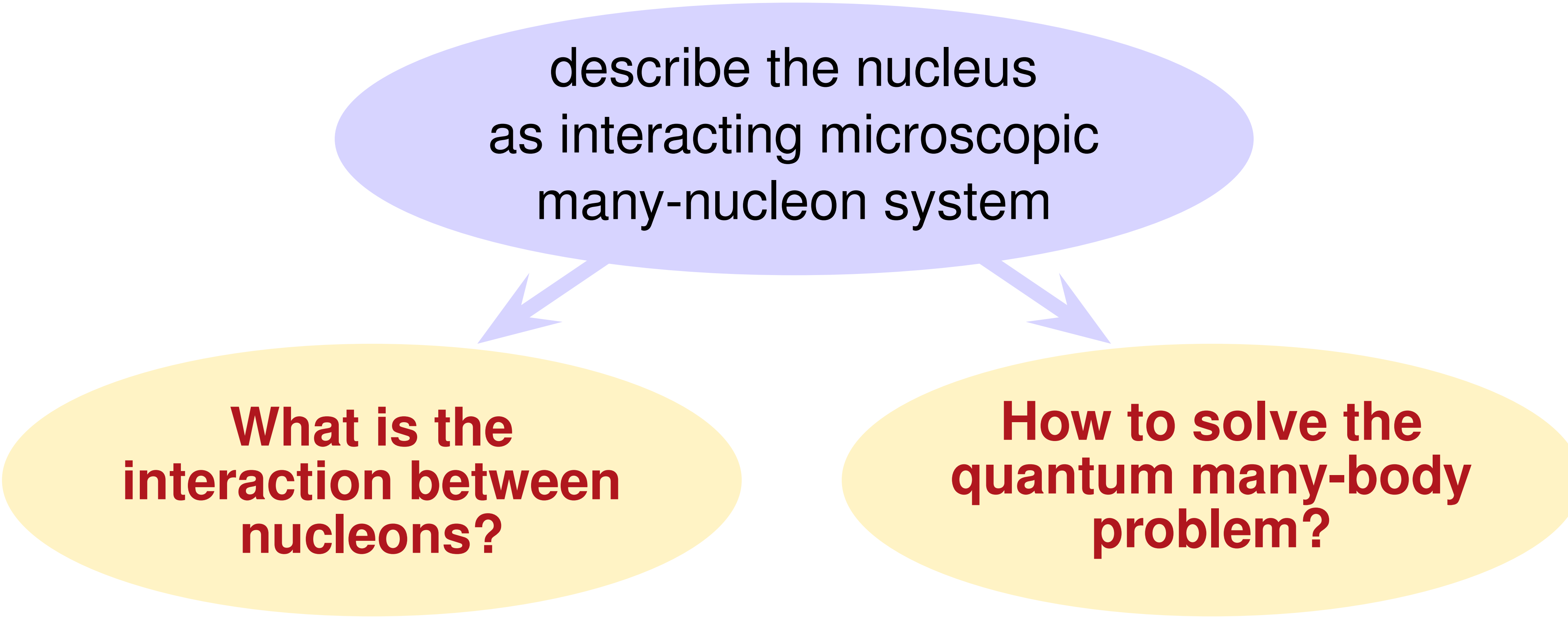
Two Problems of Nuclear Structure

describe the nucleus
as interacting microscopic
many-nucleon system

Two Problems of Nuclear Structure



Two Problems of Nuclear Structure



significant progress over the past decade....

Realistic NN-Potentials

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

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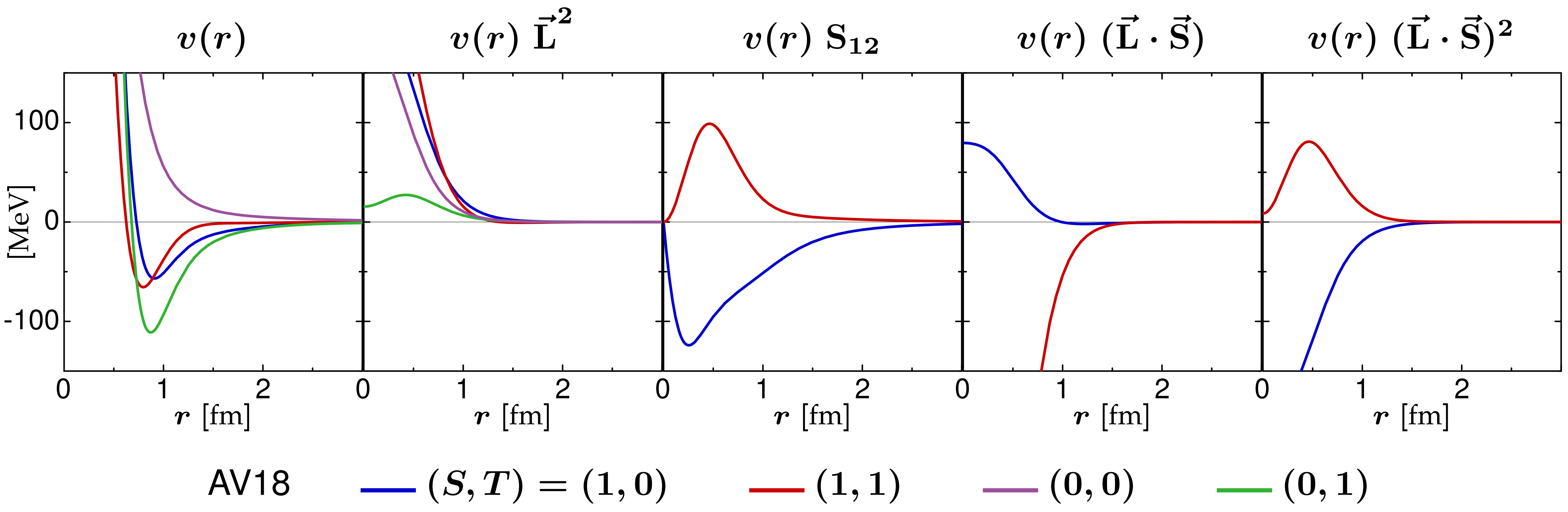


Realistic NN-Potentials

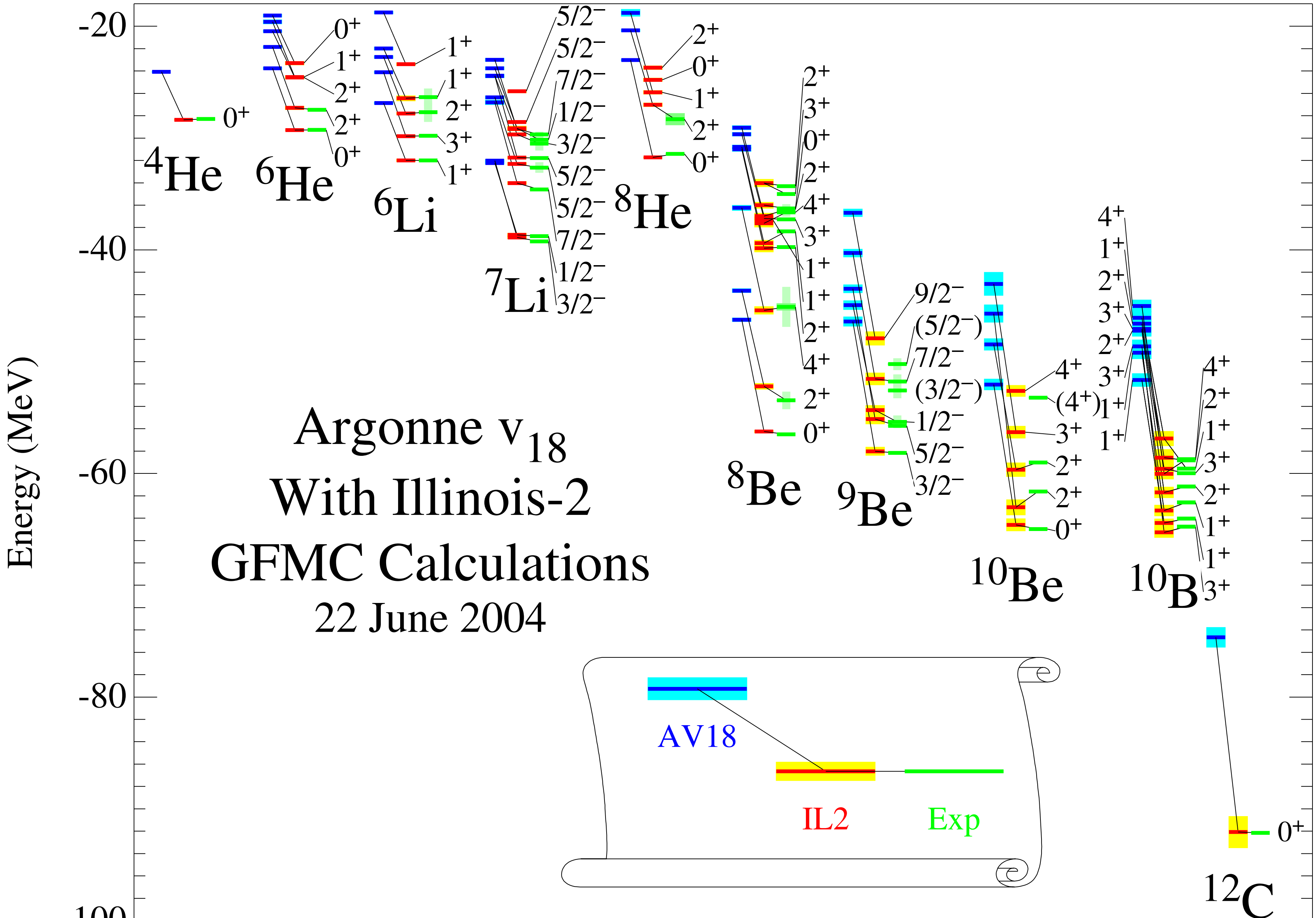
- several realistic NN-potentials are available
  - Argonne V18, CD Bonn, Nijmegen,...
  - reproduce experimental scattering data and deuteron properties with high accuracy
- need to be supplemented by a three-nucleon potential
  - NNN-potential depends on NN-potential
  - present NNN-potentials are purely phenomenological
  - very promising developments in chiral effective field theories towards a consistent NN + NNN-potential

Microscopic *ab initio* Calculations

solve the quantum many-body problem for A nucleons interacting via a realistic NN-potential

- exact numerical solution possible for small systems at an enormous computational cost
- **Green's Function Monte Carlo**: Monte Carlo sampling of the A-body wave function in coordinate space; imaginary time cooling
- **No-Core Shell Model**: large-scale diagonalization of the Hamiltonian in a harmonic oscillator basis

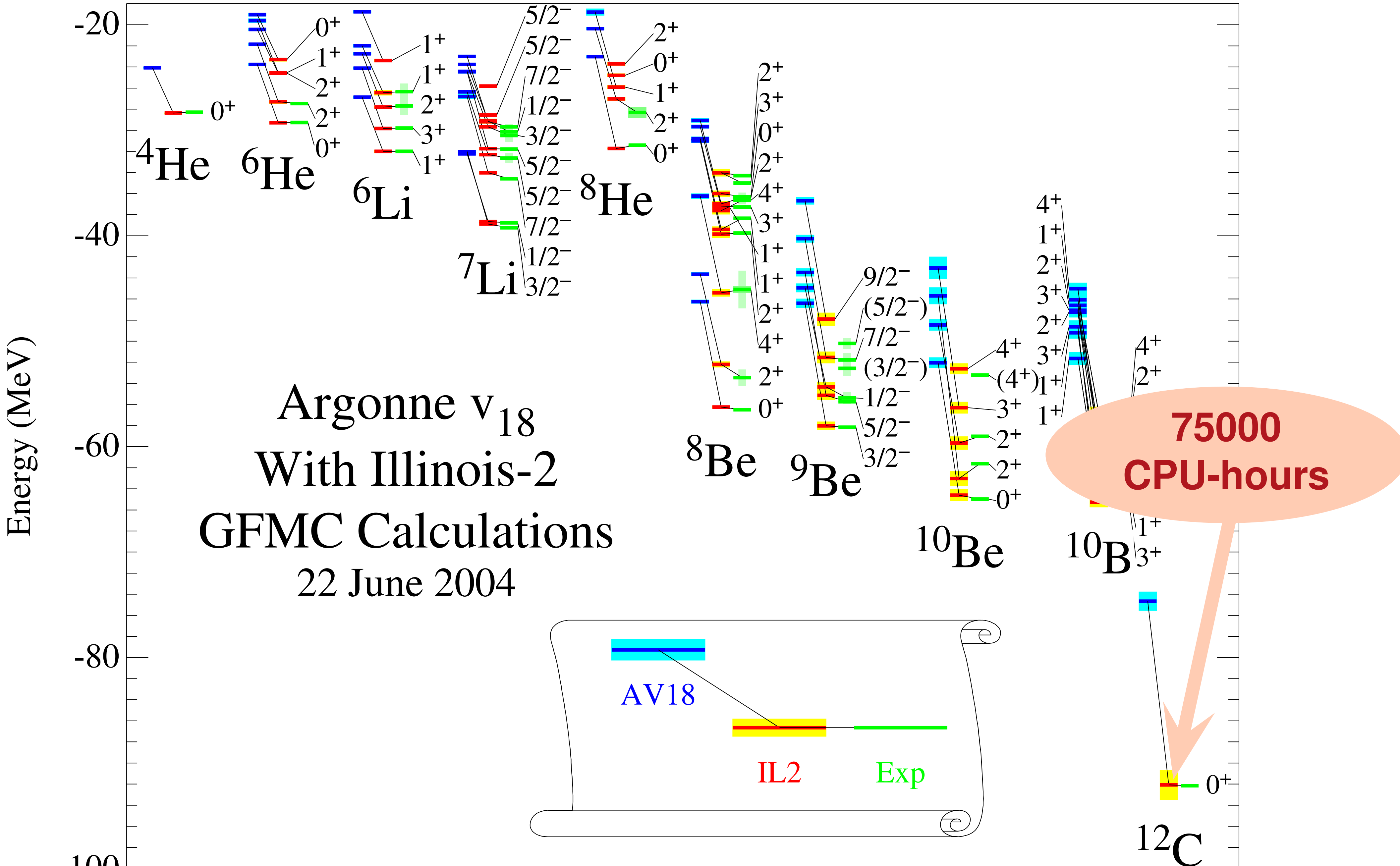
Green's Function Monte Carlo



[S. Pieper, private comm.]

^{12}C results are preliminary.

Green's Function Monte Carlo



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Our Aim

nuclear structure calculations
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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

What are Correlations?

Correlations

everything beyond the
independent particle picture

- quantum state of A independent (non-interacting) fermions is a **Slater determinant**

$$|\psi\rangle = \mathcal{A}(\,|\phi_1\rangle \otimes |\phi_2\rangle \otimes \cdots \otimes |\phi_A\rangle)$$

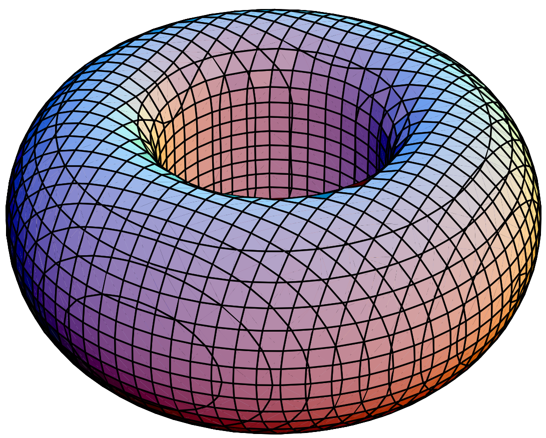
- Slater determinants **cannot describe correlations** by definition

- simple many-body approximations (e.g. Hartree-Fock) cannot handle correlations

Deuteron: Manifestation of Correlations

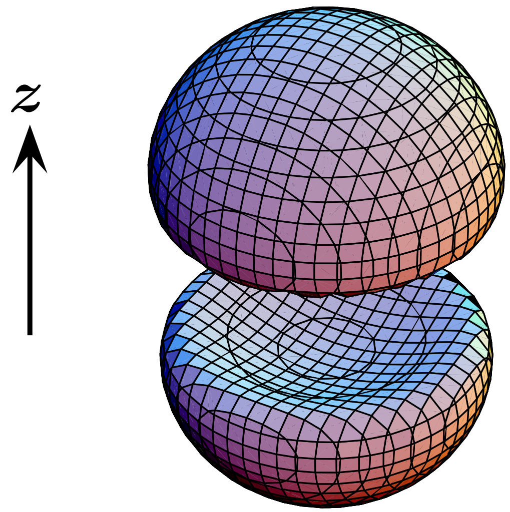
$M_S = 0$

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



$M_S = \pm 1$

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



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

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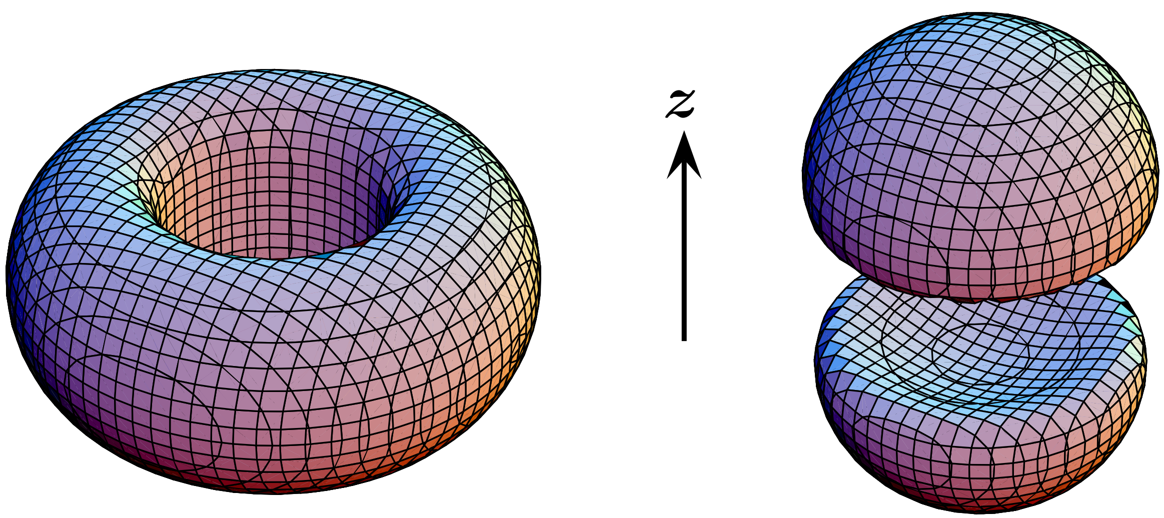


- spin-projected two-body density $\rho^{(2)}_{1,M_S}(\vec{r})$
- **exact deuteron solution** for Argonne V18 potential

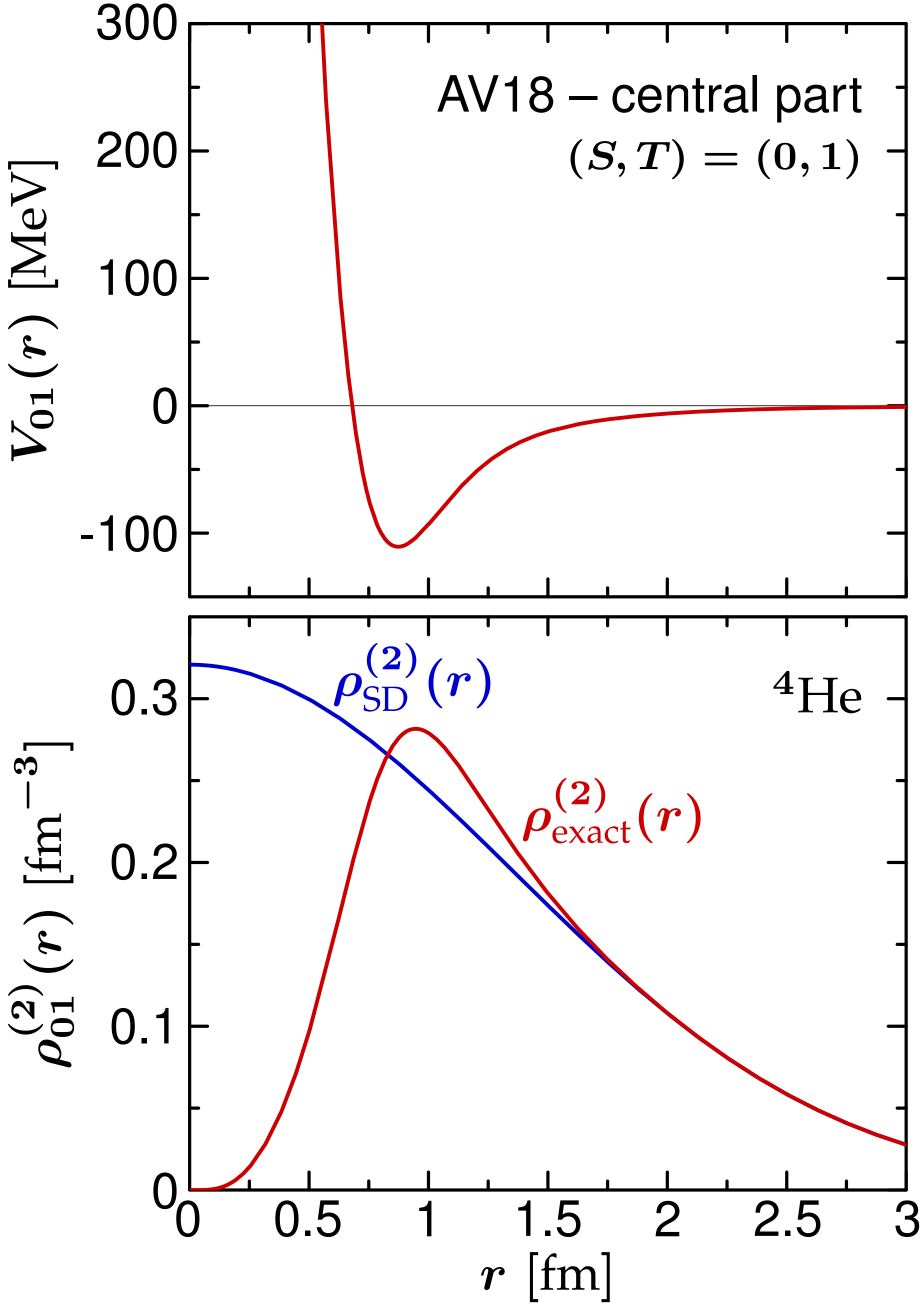
two-body density fully suppressed at small particle distances $|\vec{r}|$

central correlations

angular distribution depends strongly on relative spin orientation

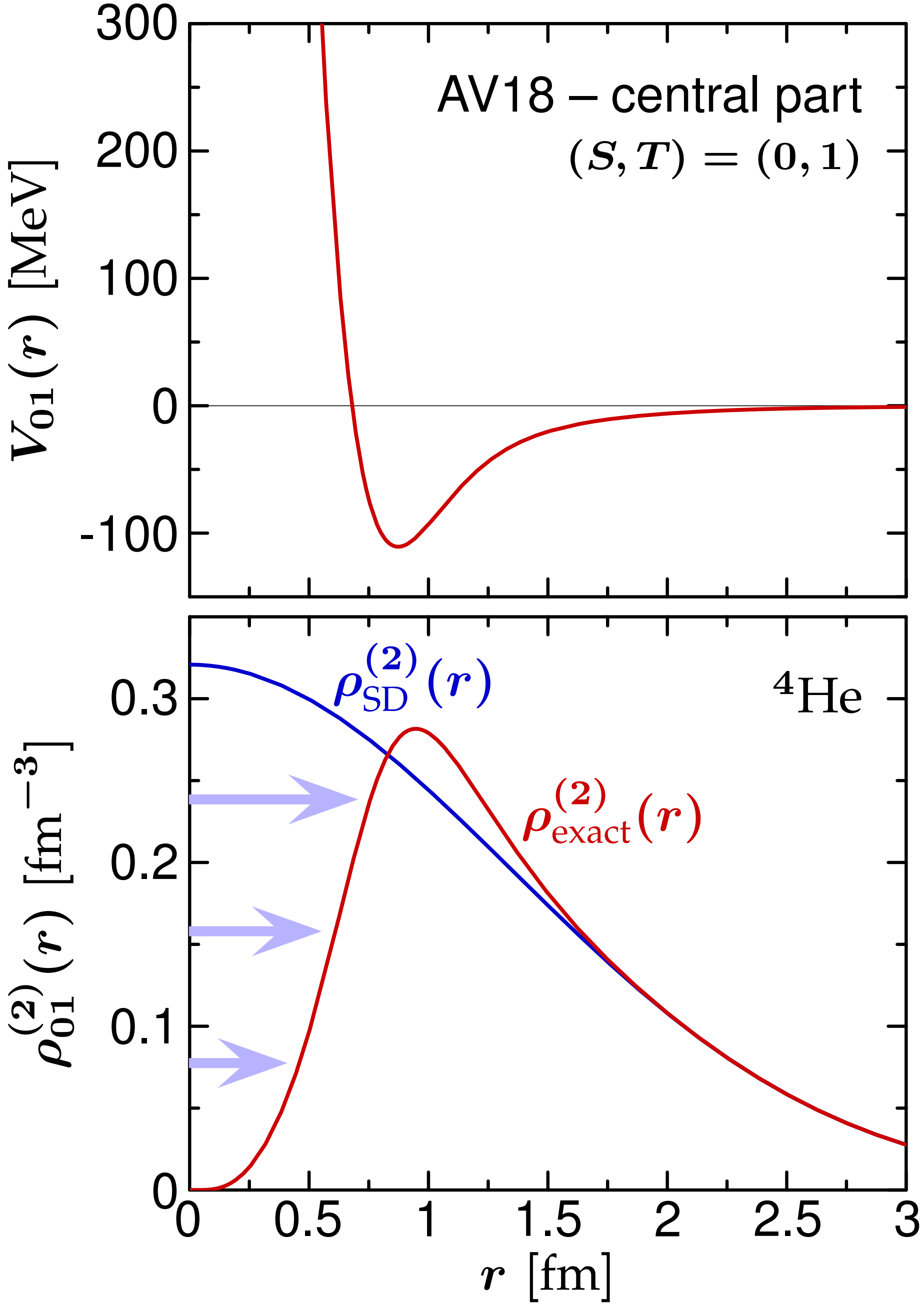
tensor correlations

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

Central Correlations



- strong repulsive core in central part of realistic interactions
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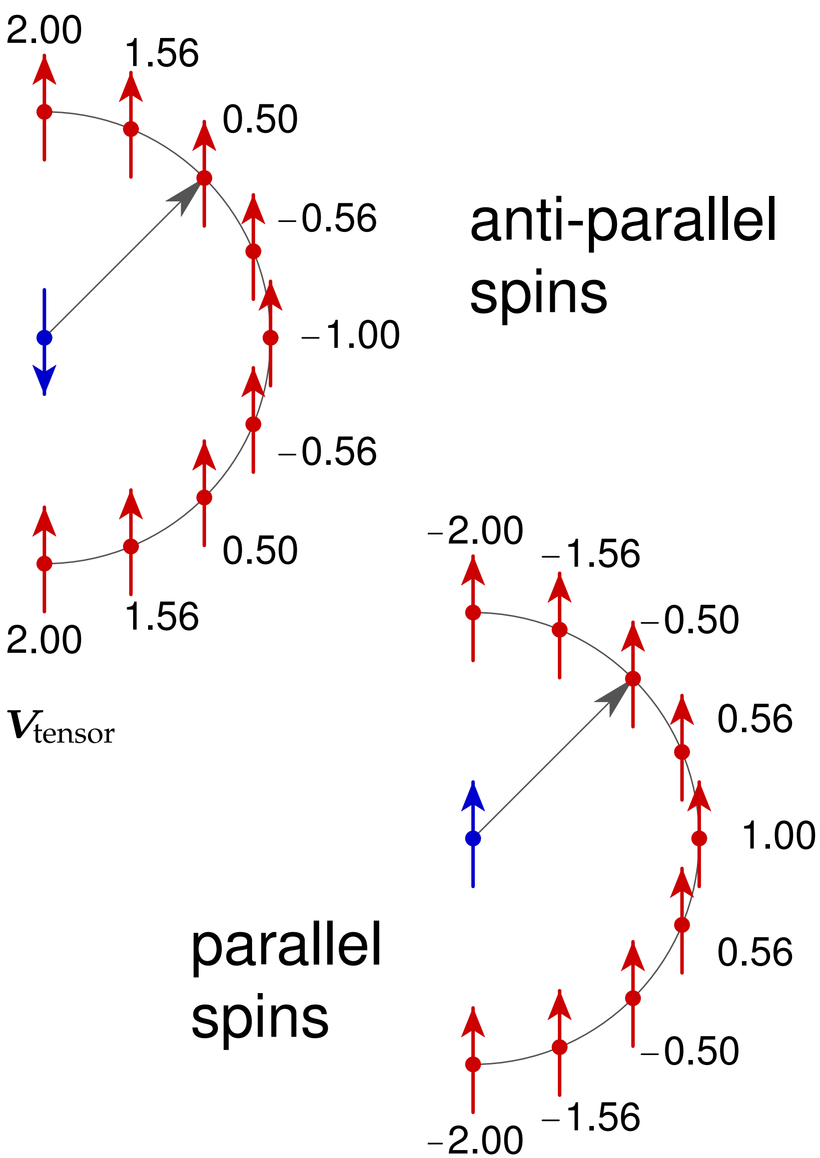
"shift the nucleons out of the core region"

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**

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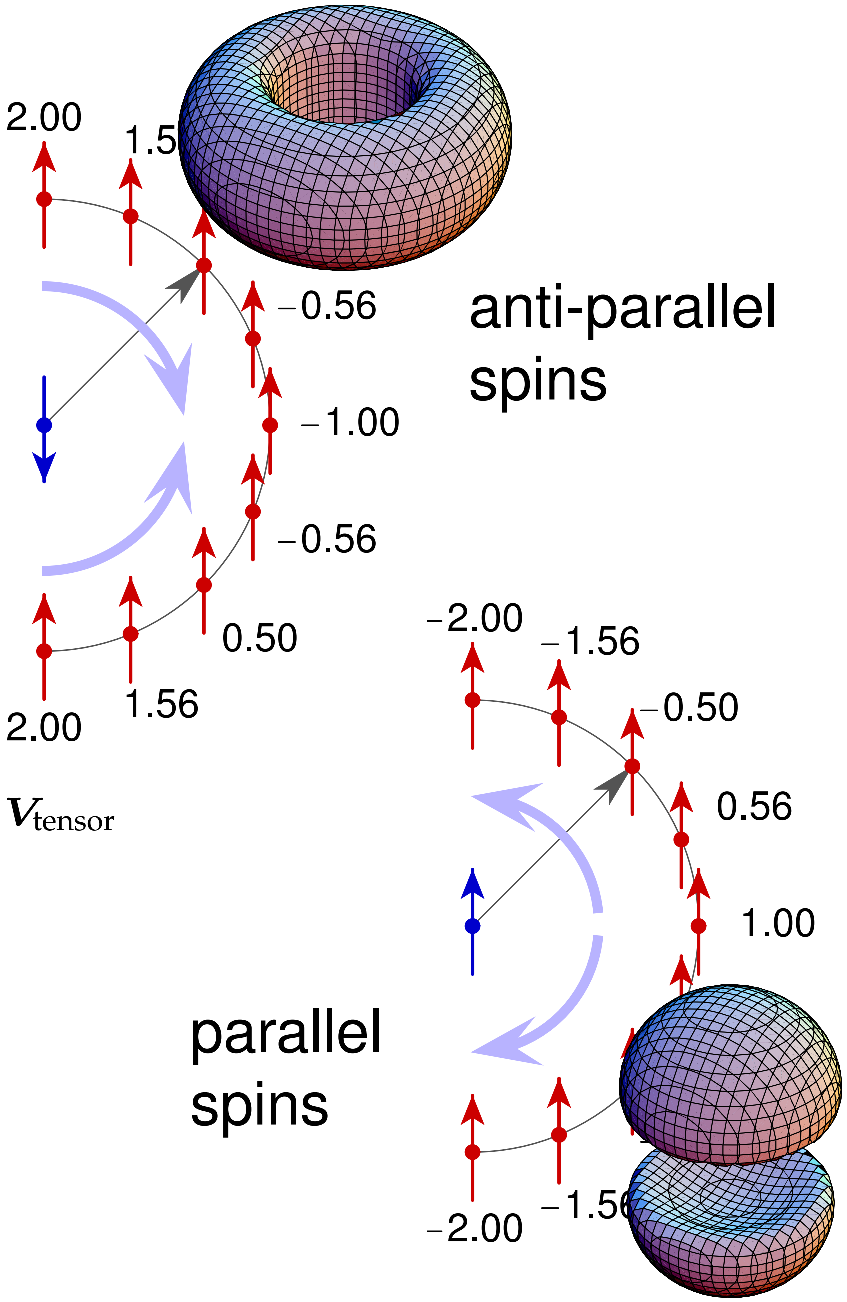
Tensor Correlations



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“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

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

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

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

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

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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 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

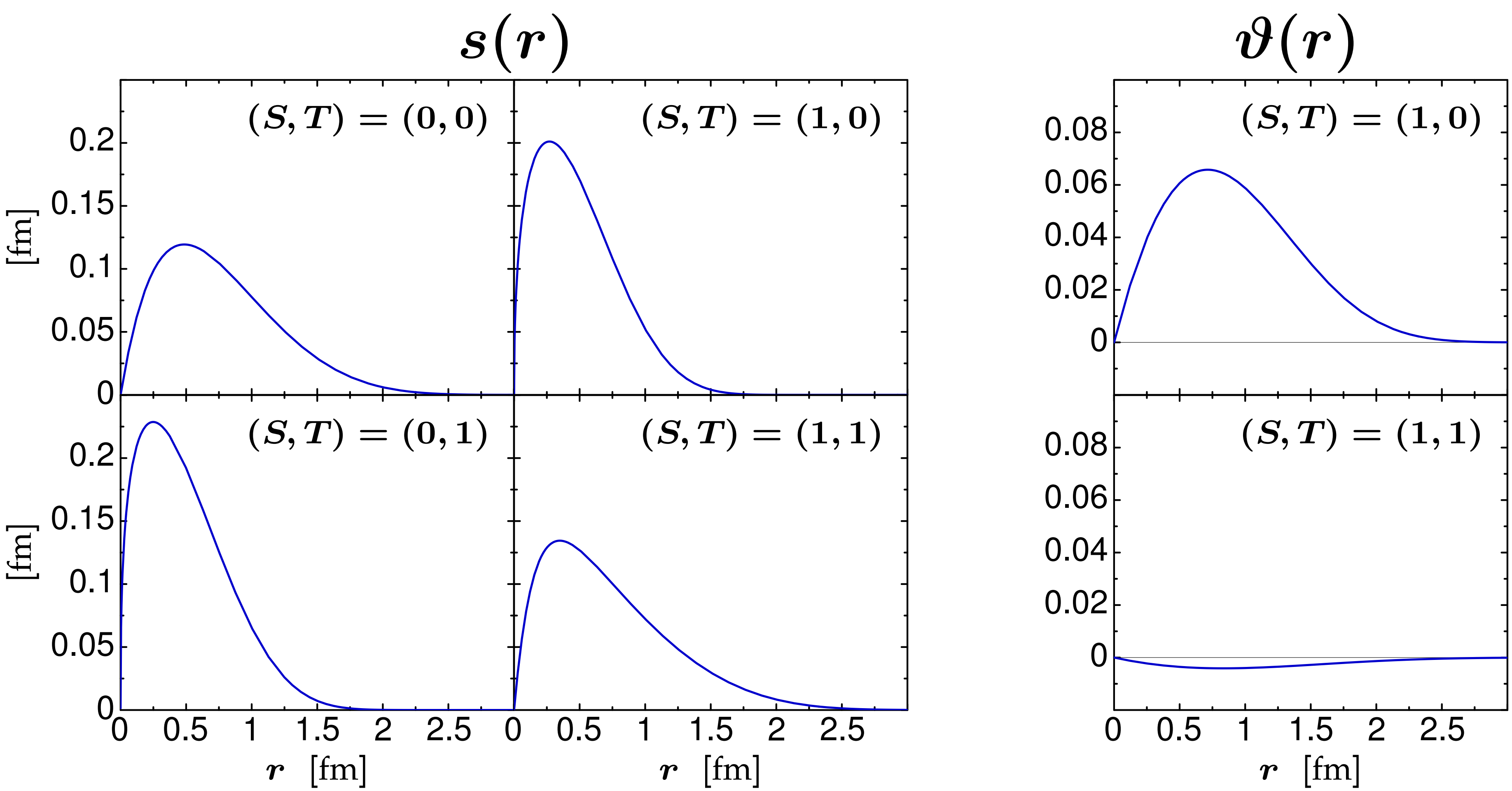
$$\mathrm{g}_\Omega = \frac{3}{2}\vartheta(\mathrm{r})\big[(\vec{\sigma}_1 \cdot \vec{\mathrm{q}}_\Omega)(\vec{\sigma}_2 \cdot \vec{\mathrm{r}}) + (\vec{\mathrm{r}} \leftrightarrow \vec{\mathrm{q}}_\Omega)\big]$$

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

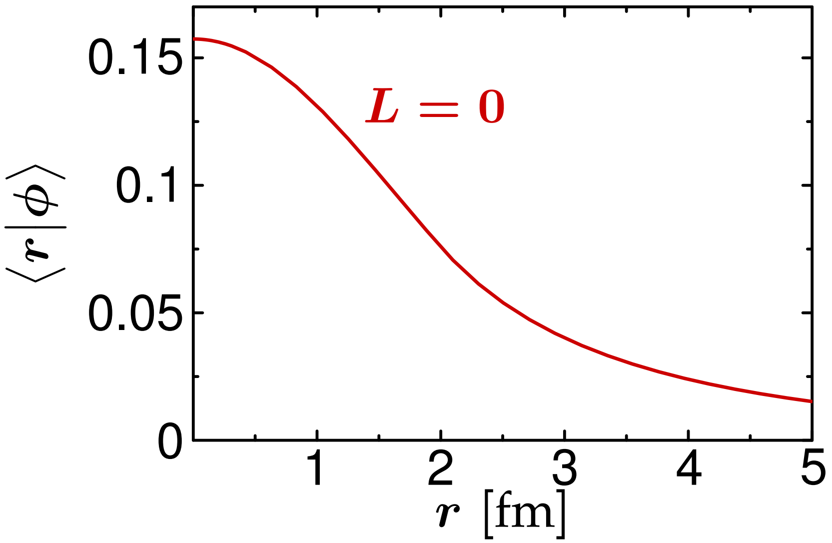
$s(r)$ and $\vartheta(r)$
encapsulate the physics of
short-range correlations

Optimal Correlation Functions

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



Correlated States



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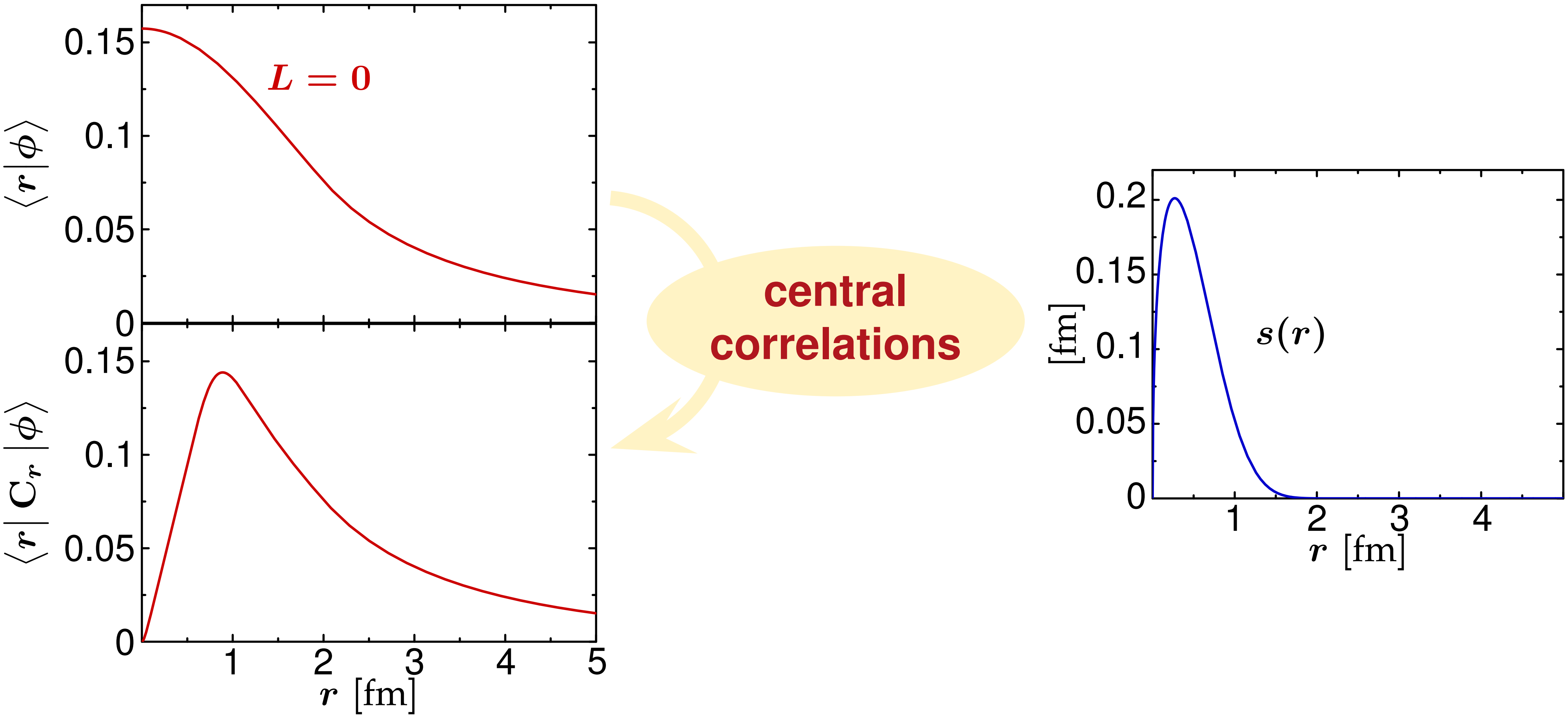

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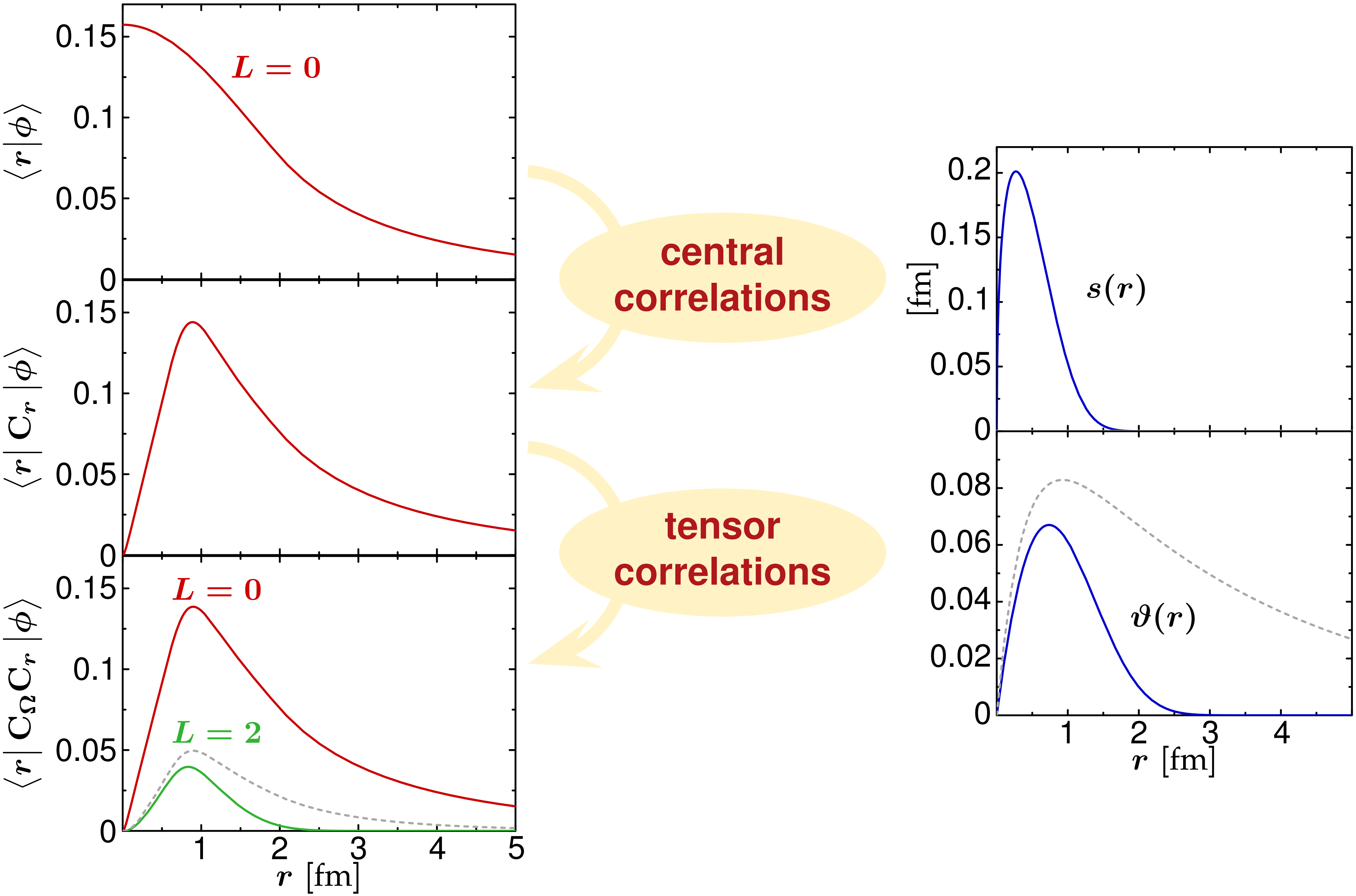

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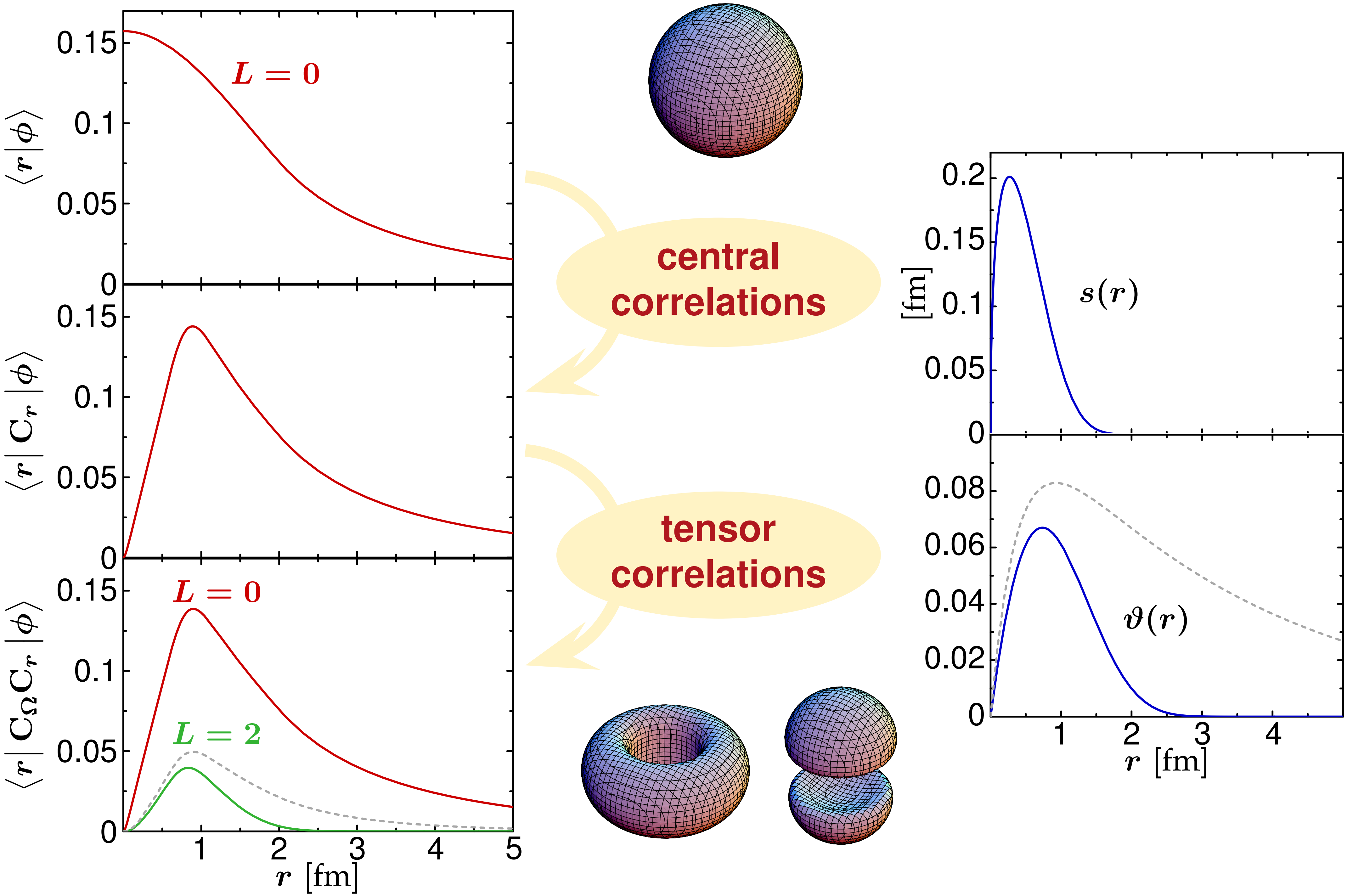

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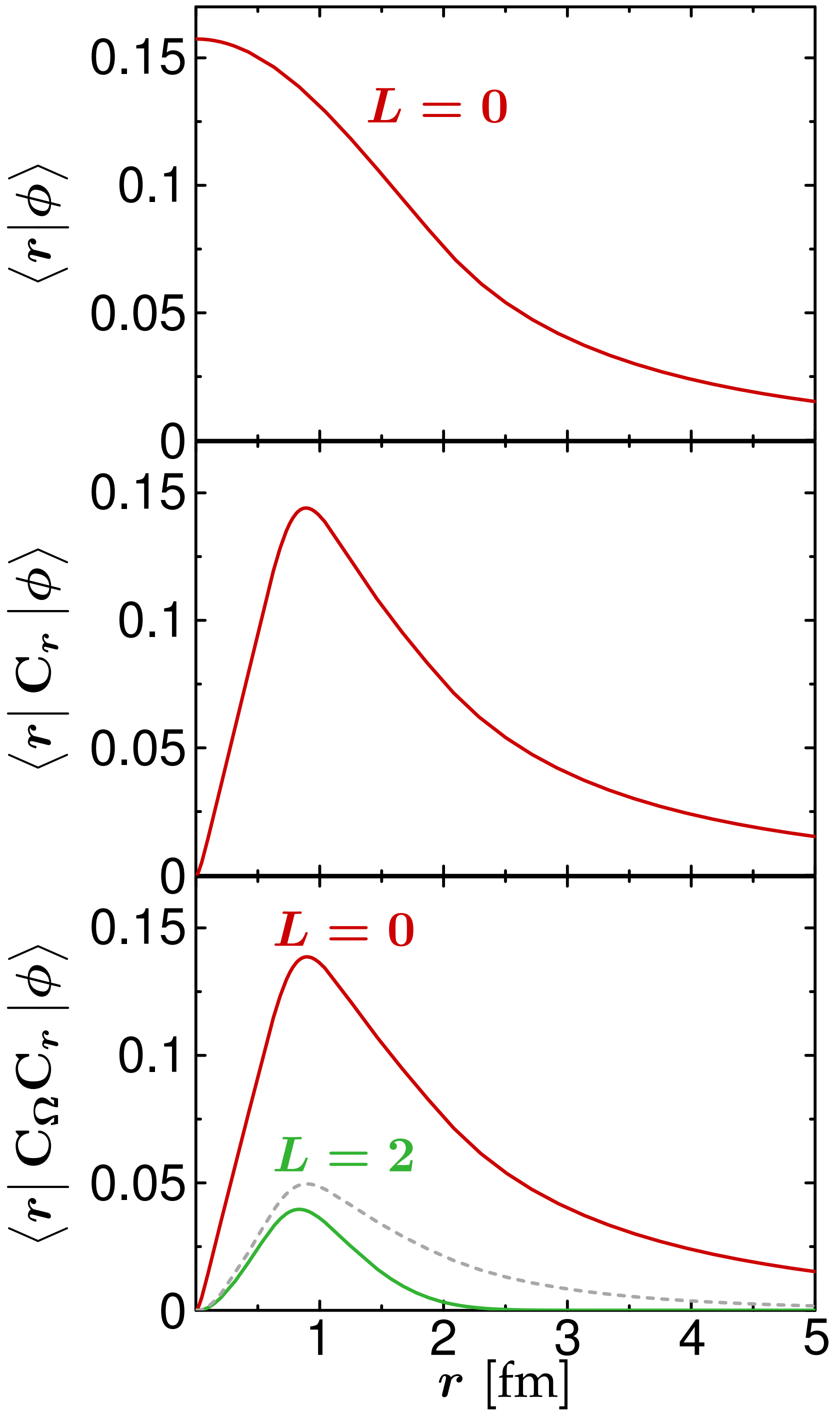

central correlations

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

$$R_\pm(r) \approx r \pm s(r)$$

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

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

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Cluster Decomposition Principle

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

Two-Body Approx.

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

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

Correlated NN-Potential — V_{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 $V_{\mathrm{low}-k}$**

Correlated NN-Potential — V_{UCOM}

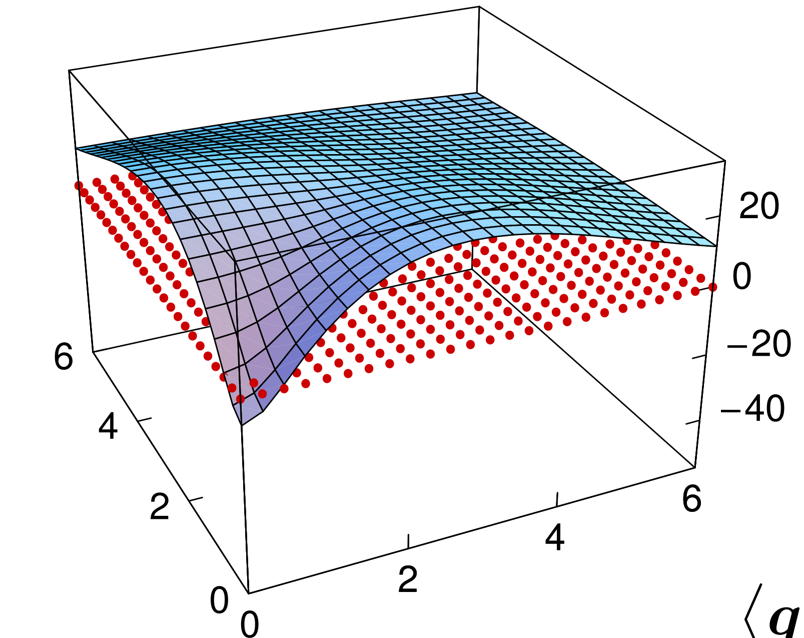
$$\mathrm{V}_{\mathrm{UCOM}} = \sum_{p} \tfrac{1}{2}\big[\widetilde{v}_p(\mathrm{r})\ \mathrm{O}_p + \mathrm{O}_p\ \widetilde{v}_p(\mathrm{r})\big]$$

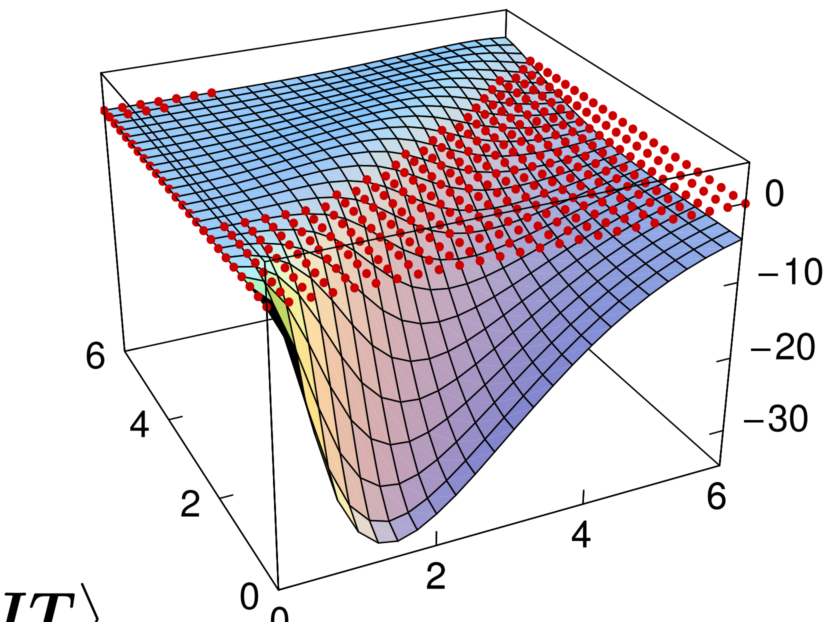
$$\begin{aligned}\mathrm{O} = \{&1,\ \ (\vec{\sigma}_1\cdot\vec{\sigma}_2),\ \ \vec{\mathrm{q}}^2,\ \ \vec{\mathrm{q}}^2(\vec{\sigma}_1\cdot\vec{\sigma}_2),\ \ \vec{\mathrm{L}}^2,\ \ \vec{\mathrm{L}}^2(\vec{\sigma}_1\cdot\vec{\sigma}_2),\\ &(\vec{\mathrm{L}}\cdot\vec{\mathrm{S}}),\ \ \mathrm{S}_{12}(\vec{\mathrm{r}},\vec{\mathrm{r}}),\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

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

Momentum-Space Matrix Elements

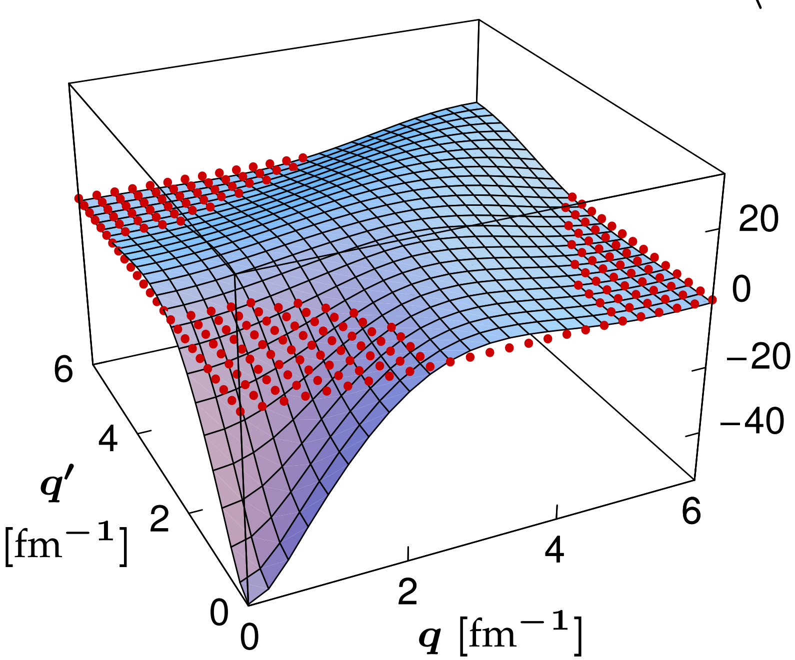
$^3S_1$ | $^3S_1$–$^3D_1$

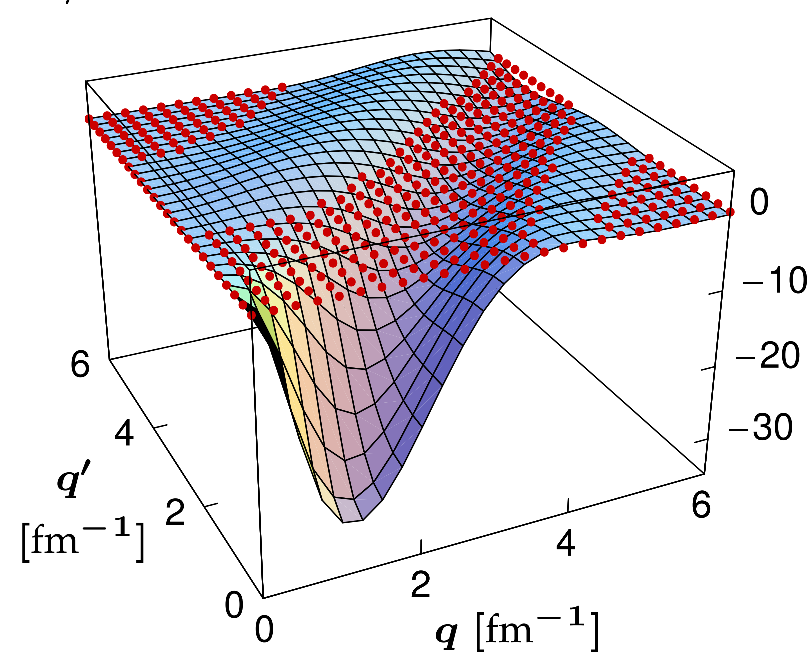




$\mathrm{V}_{\mathrm{bare}}$

$$\left\langle q(LS)JT \right| \circ \left| q'(L'S)JT \right\rangle$$

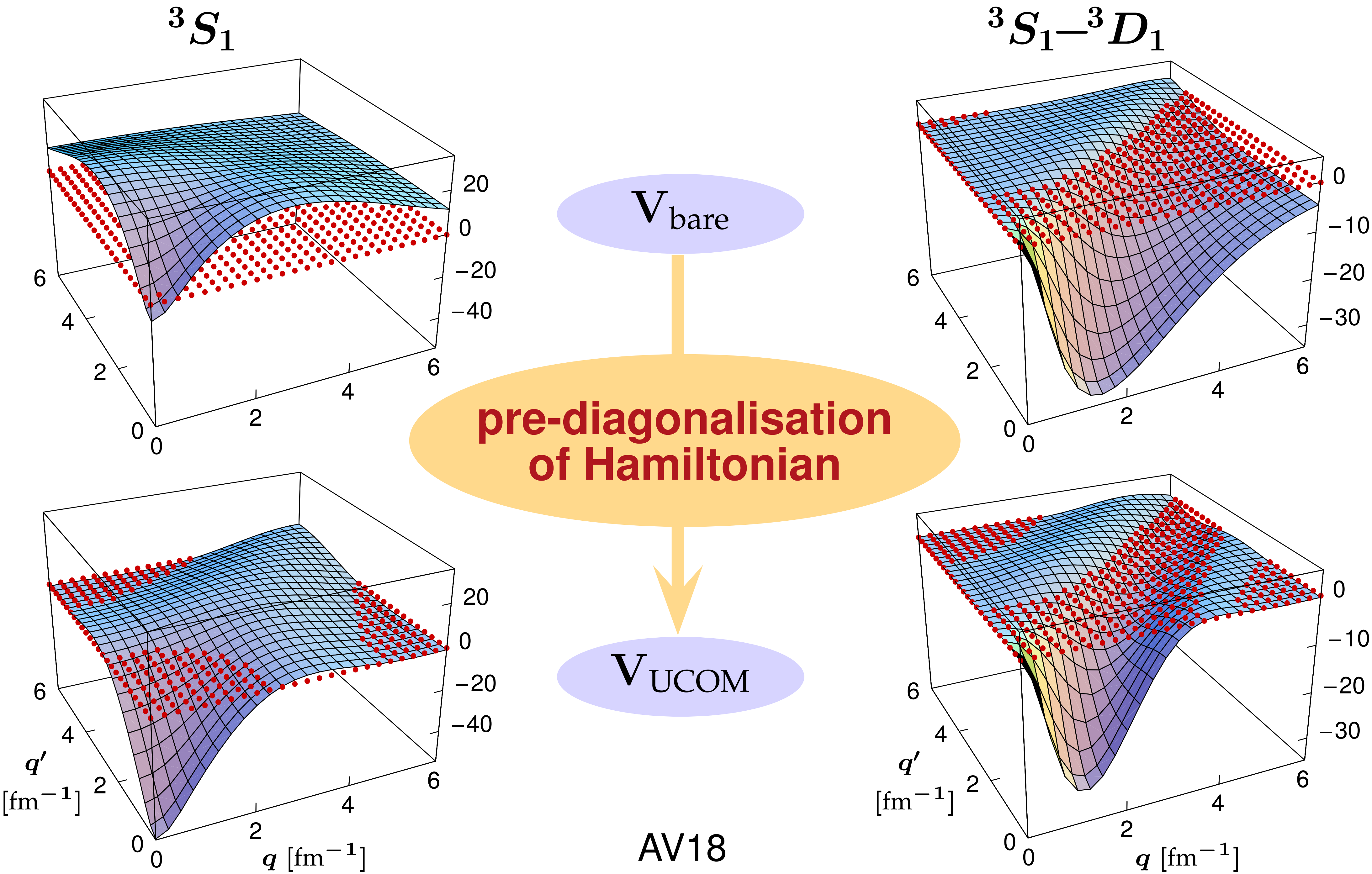




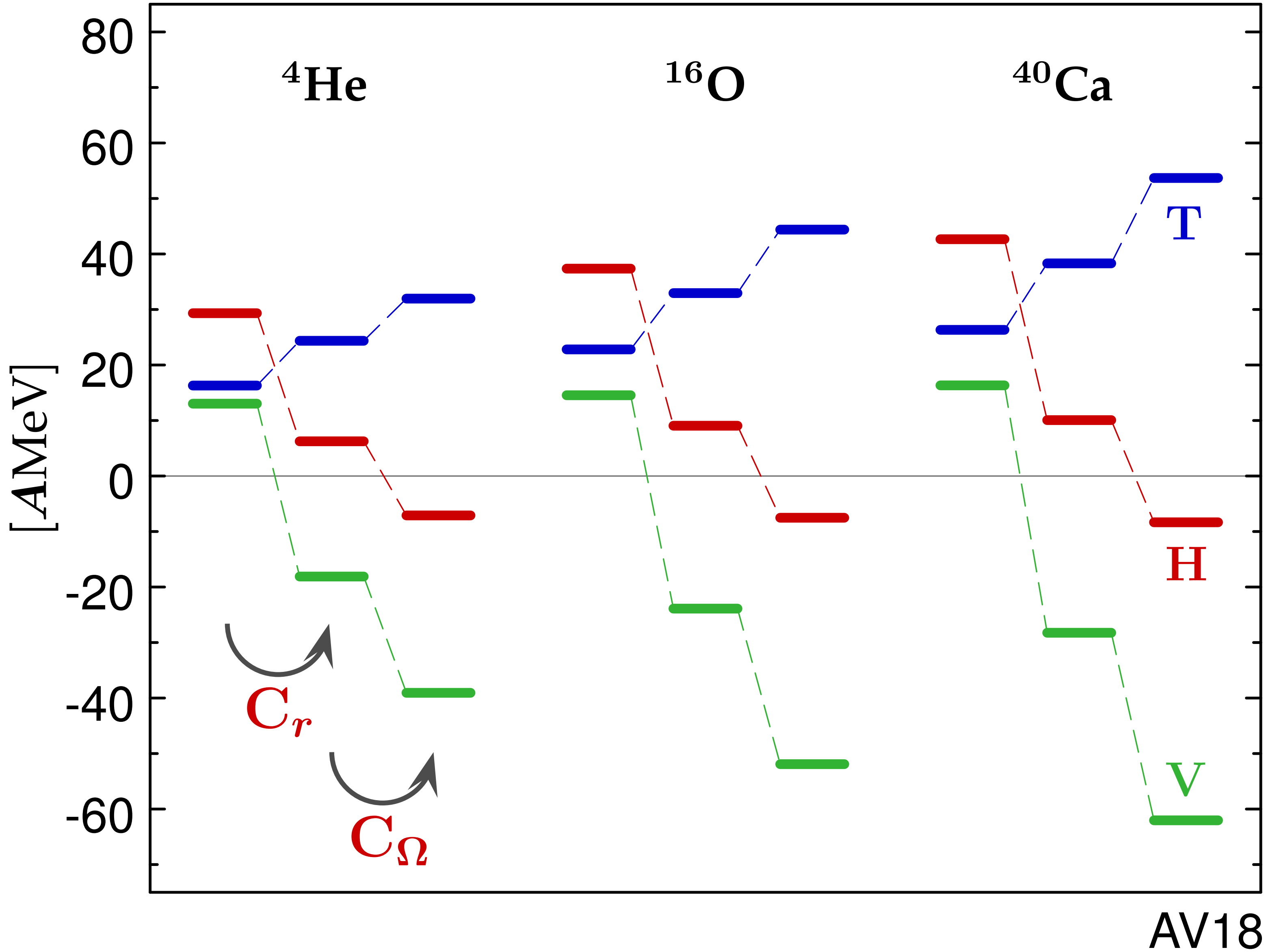
$\mathrm{V}_{\mathrm{UCOM}}$

AV18

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

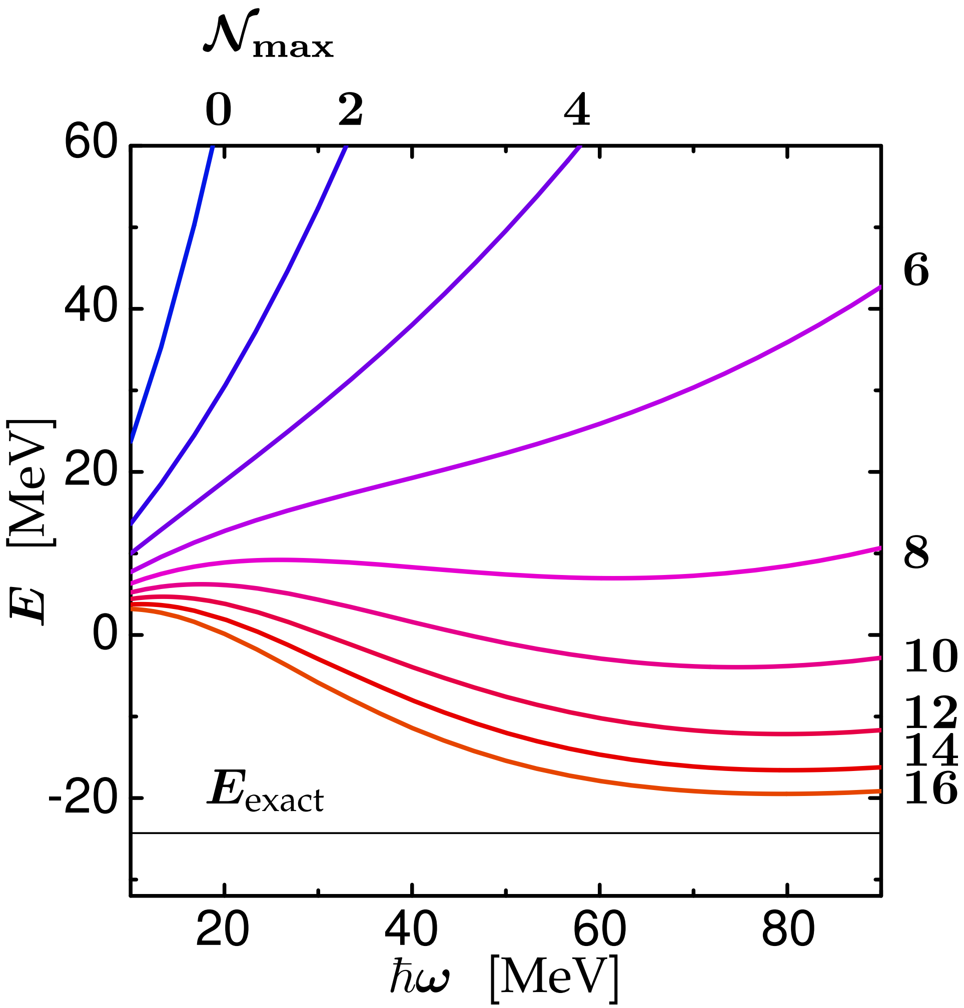
UCOM + NCSM

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

V_{bare}



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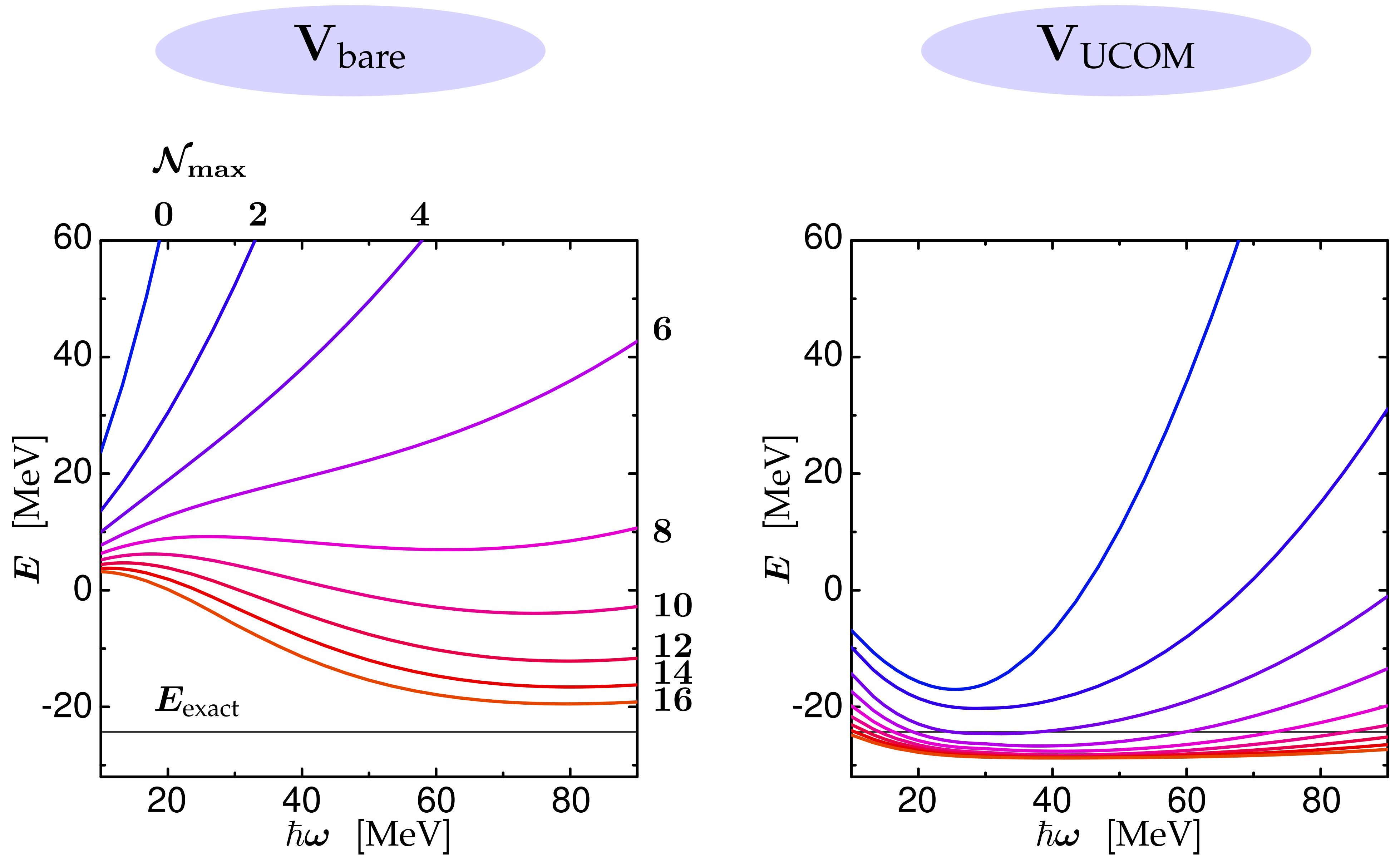

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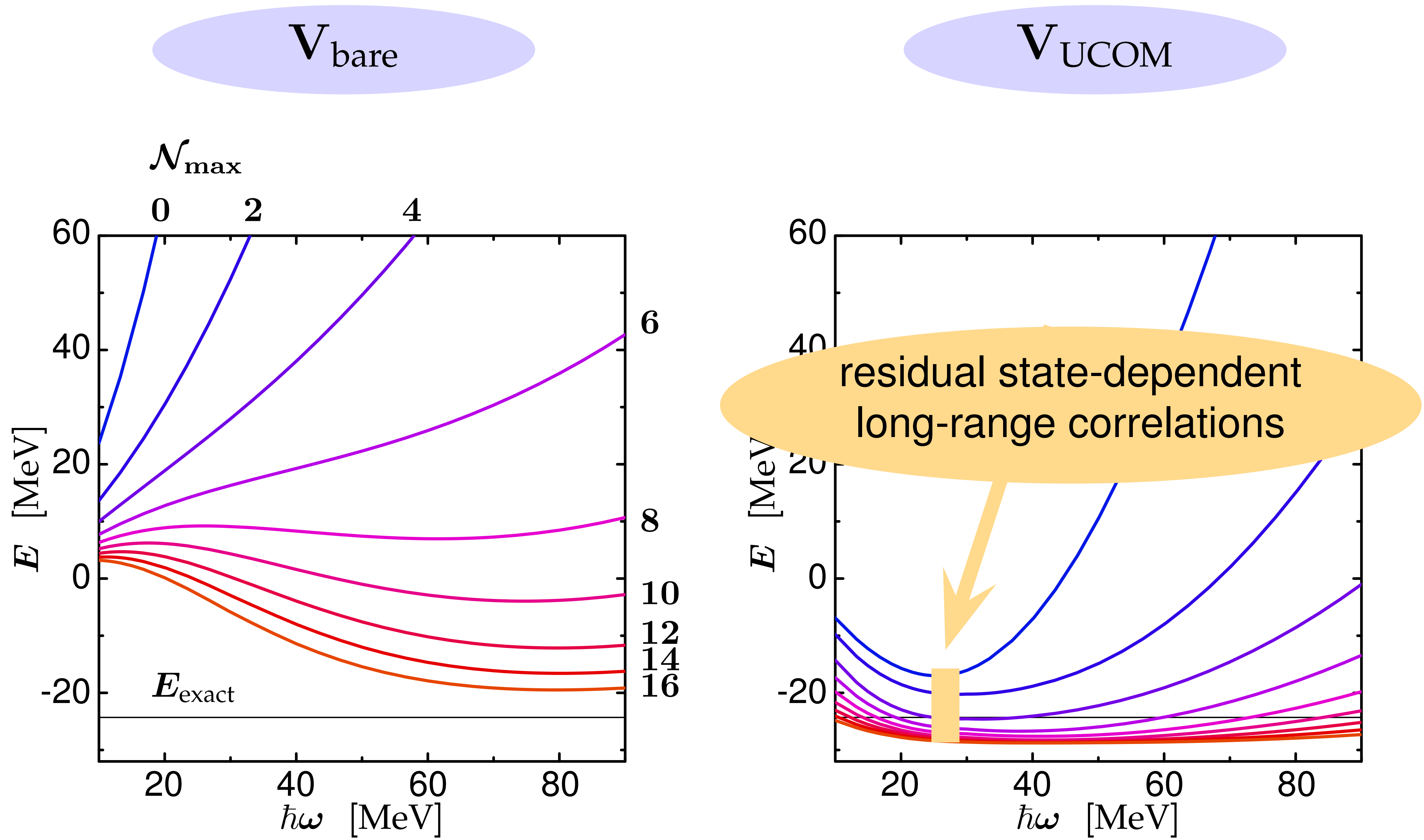

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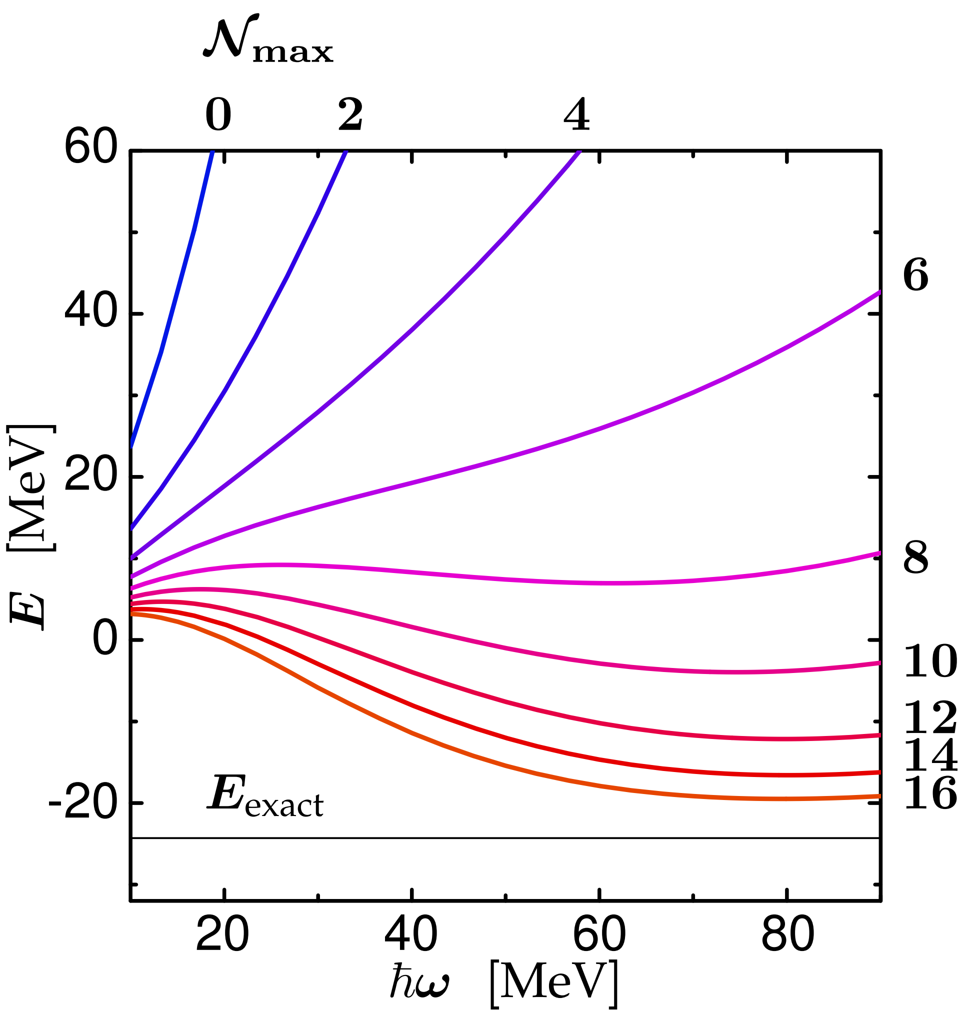
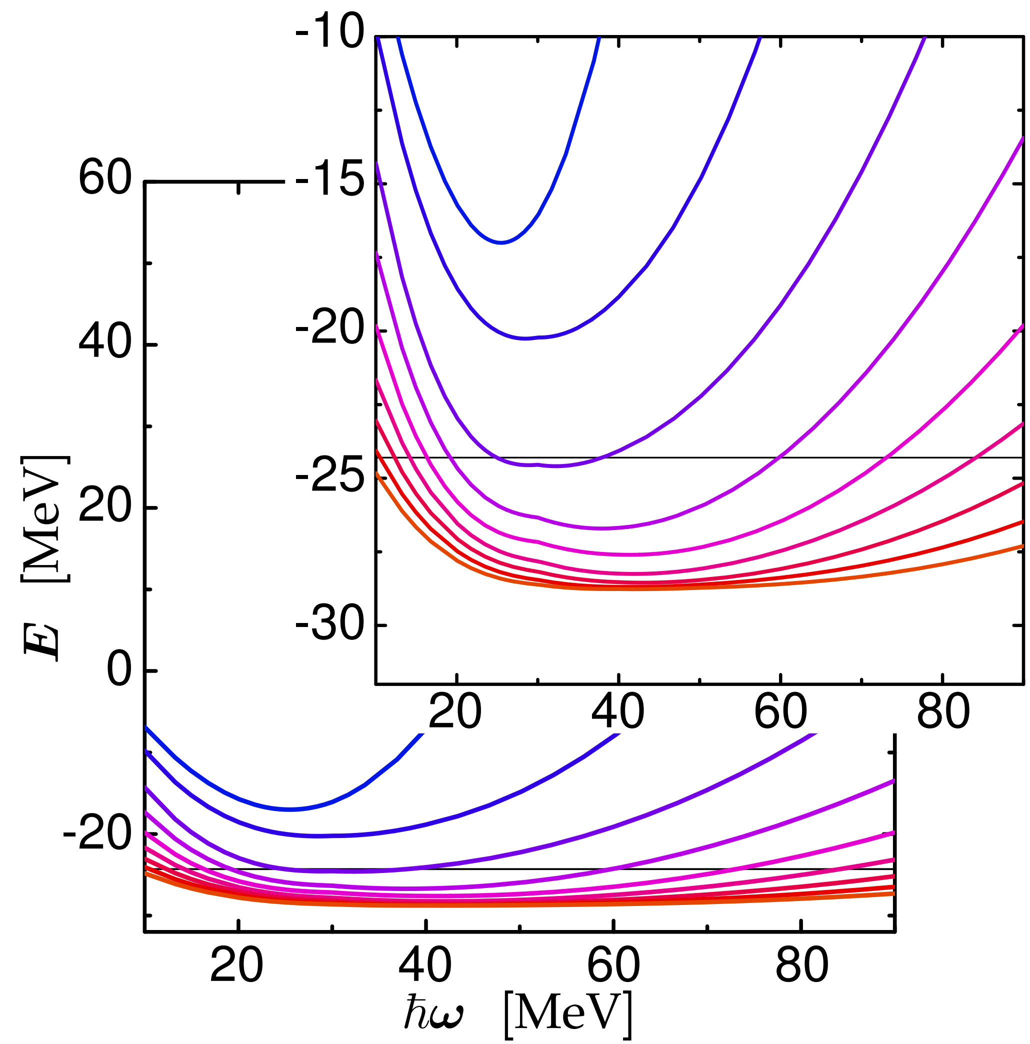


V_{UCOM}



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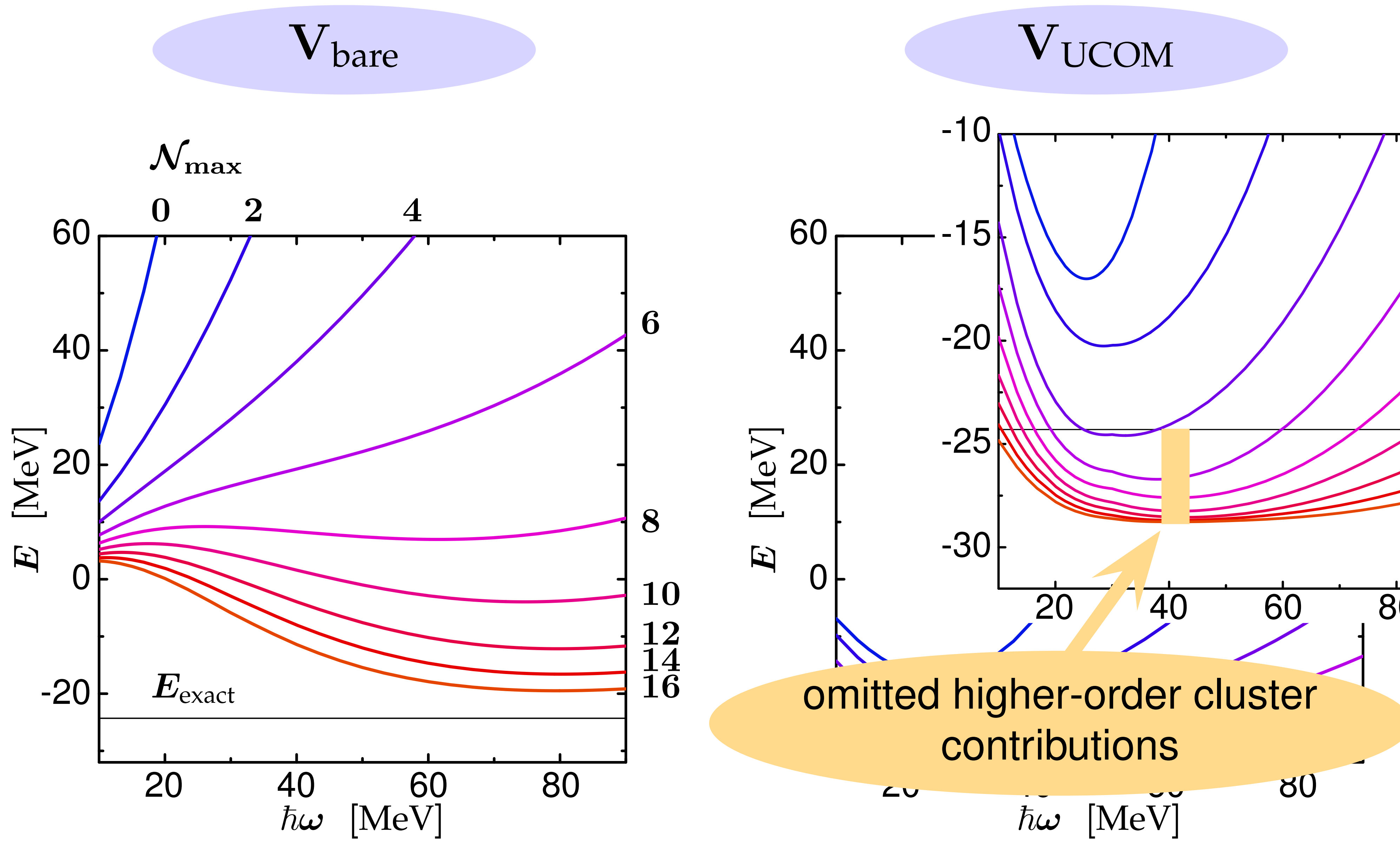
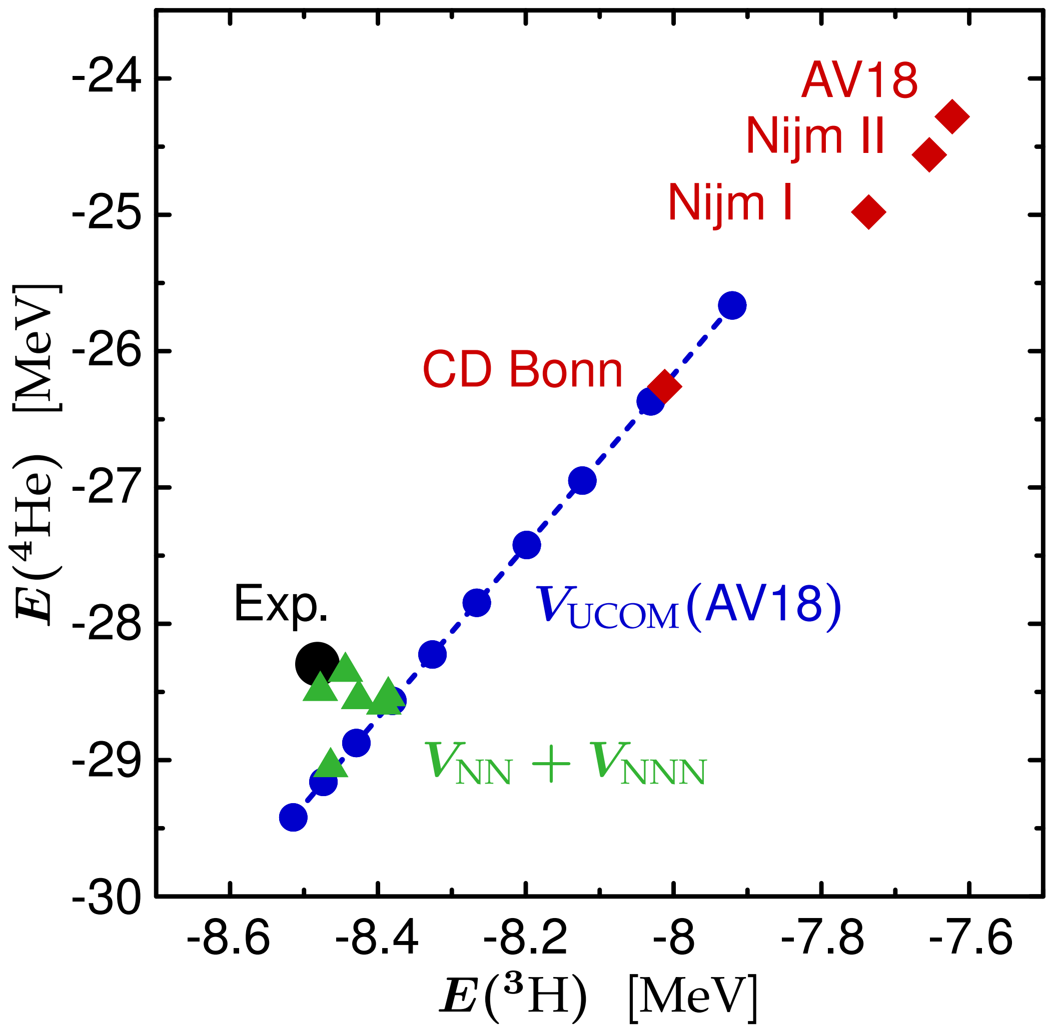
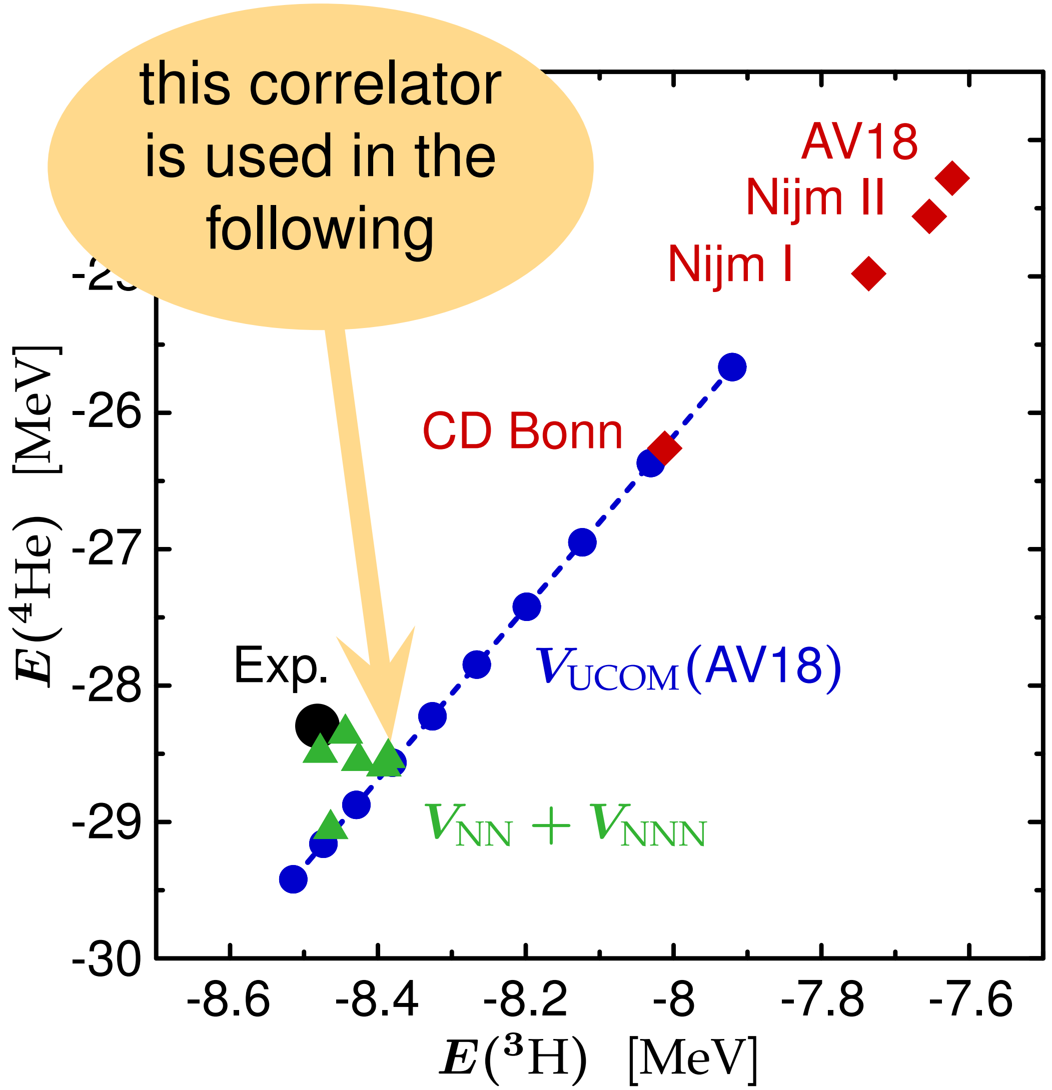


Tjon-Line and Correlator Range



- **Tjon-line**: $E(^4\text{He})$ vs. $E(^3\text{H})$ 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 three-body force**

Tjon-Line and Correlator Range



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Application II

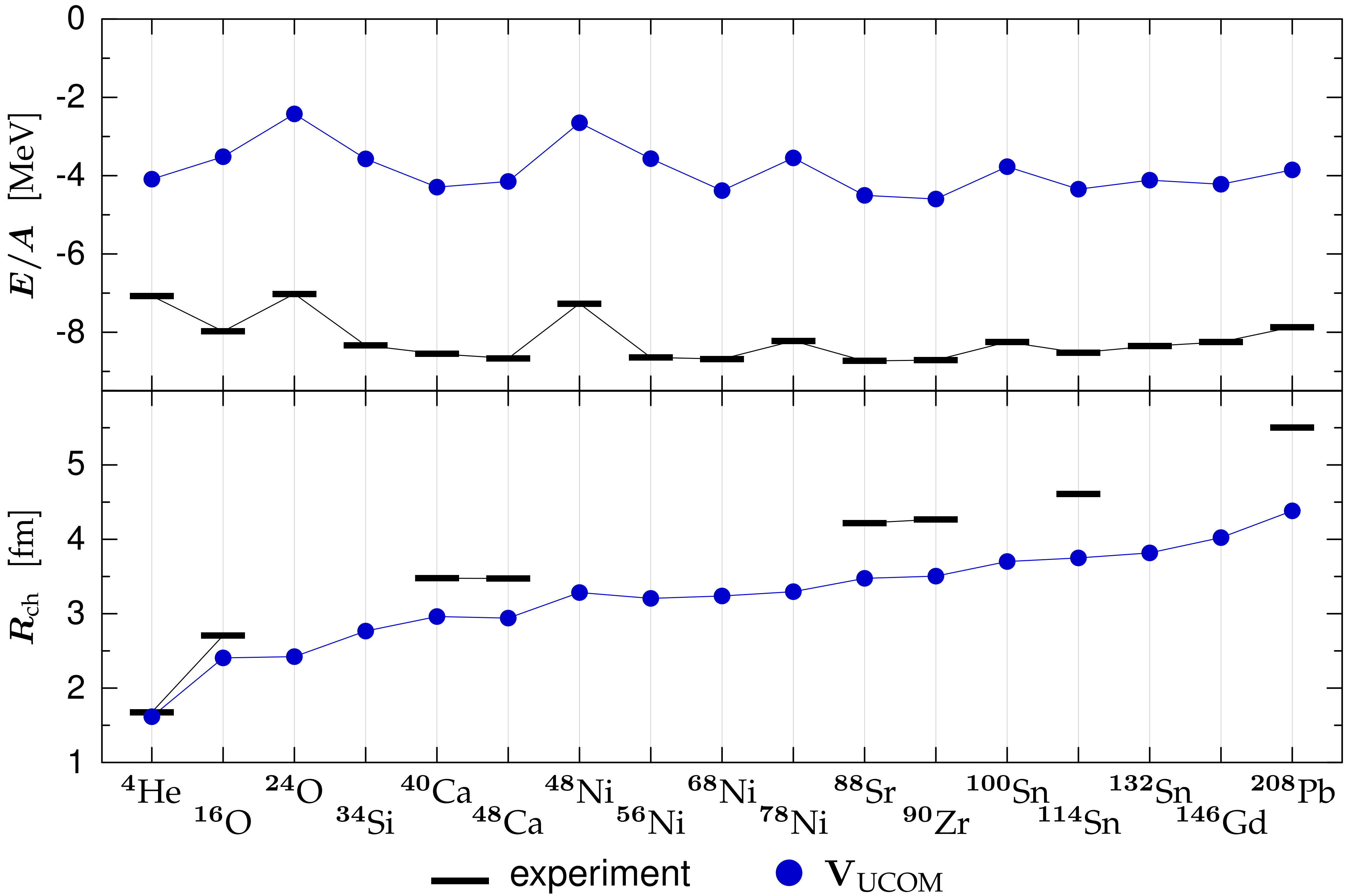
Hartree-Fock

UCOM + HF

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 $N_{\max} = 8 \ldots 14$)
- 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 Argonne V18



Missing Pieces

long-range correlations

Missing Pieces

long-range correlations

Ab Initio Strategy

- 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

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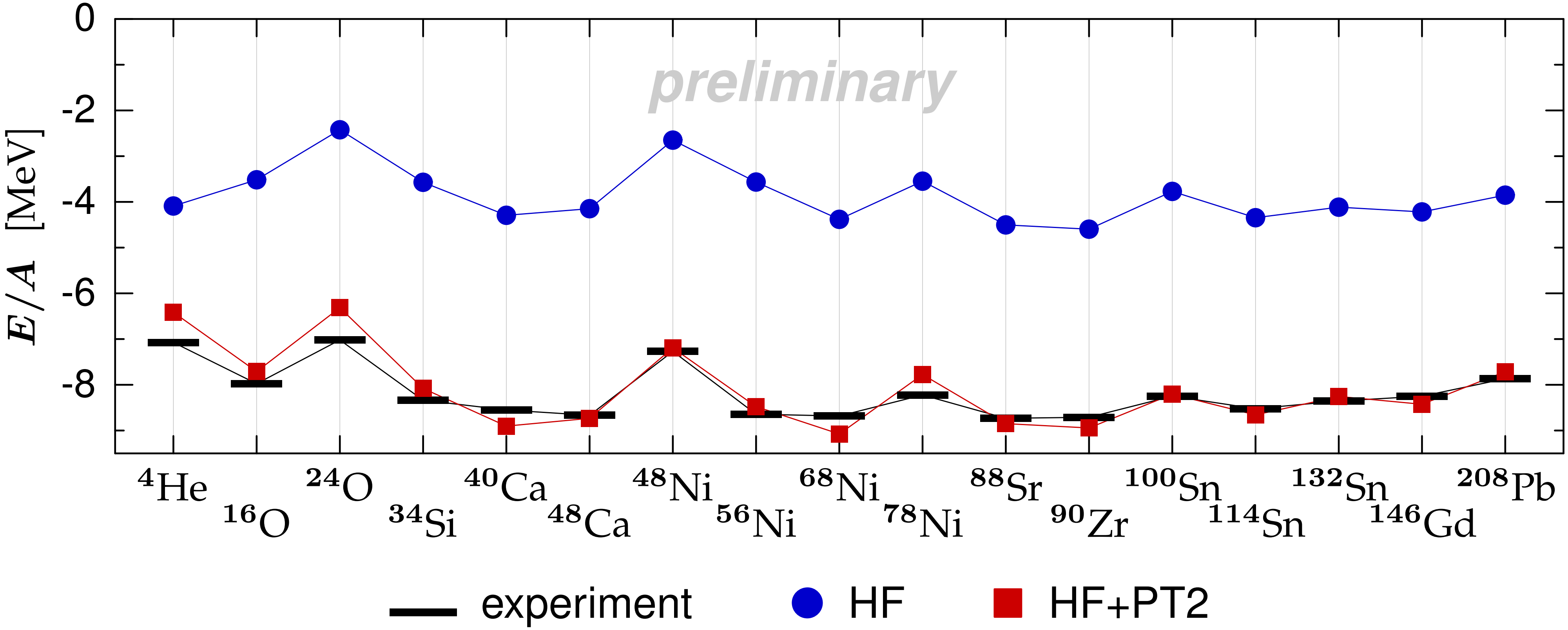
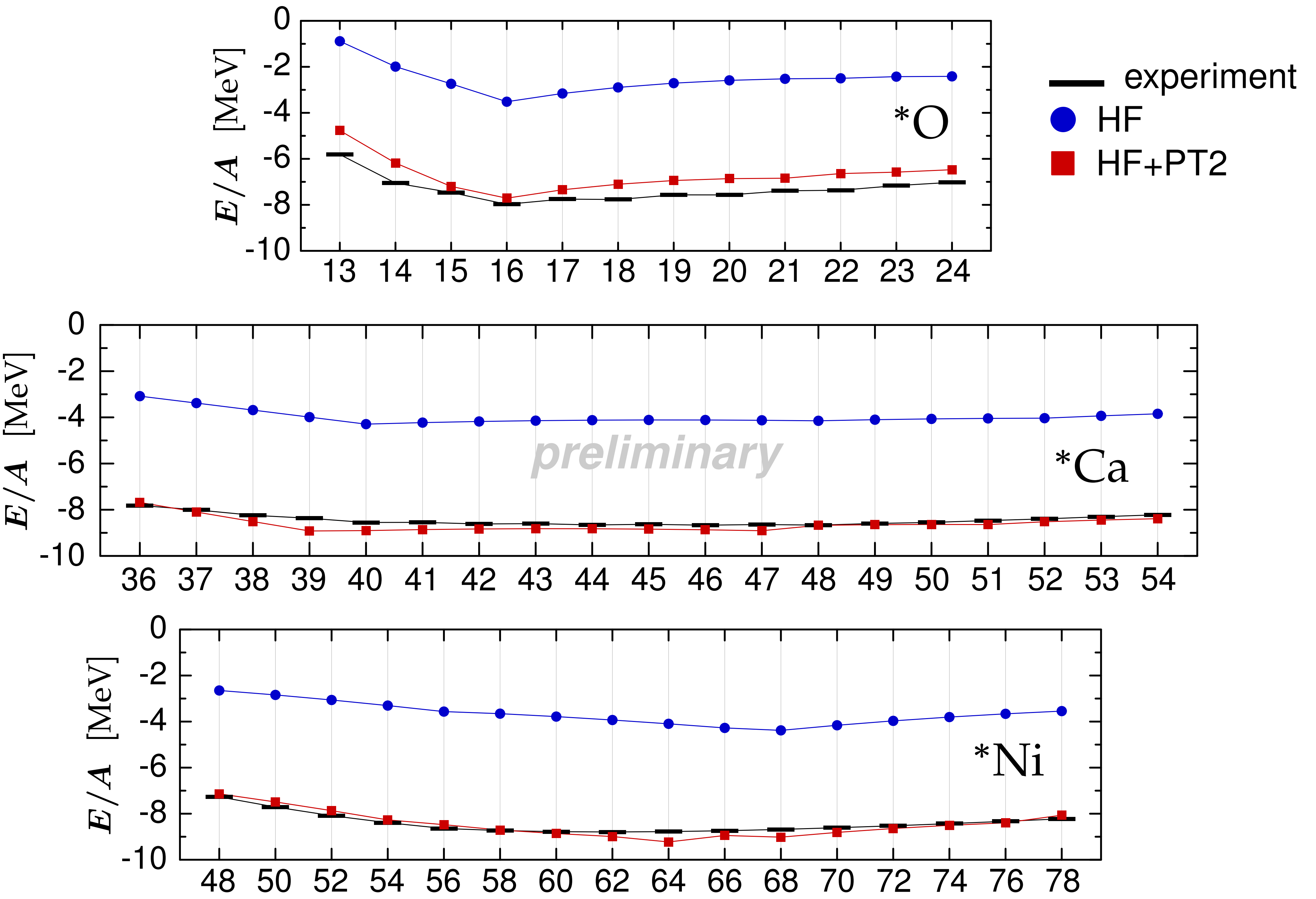
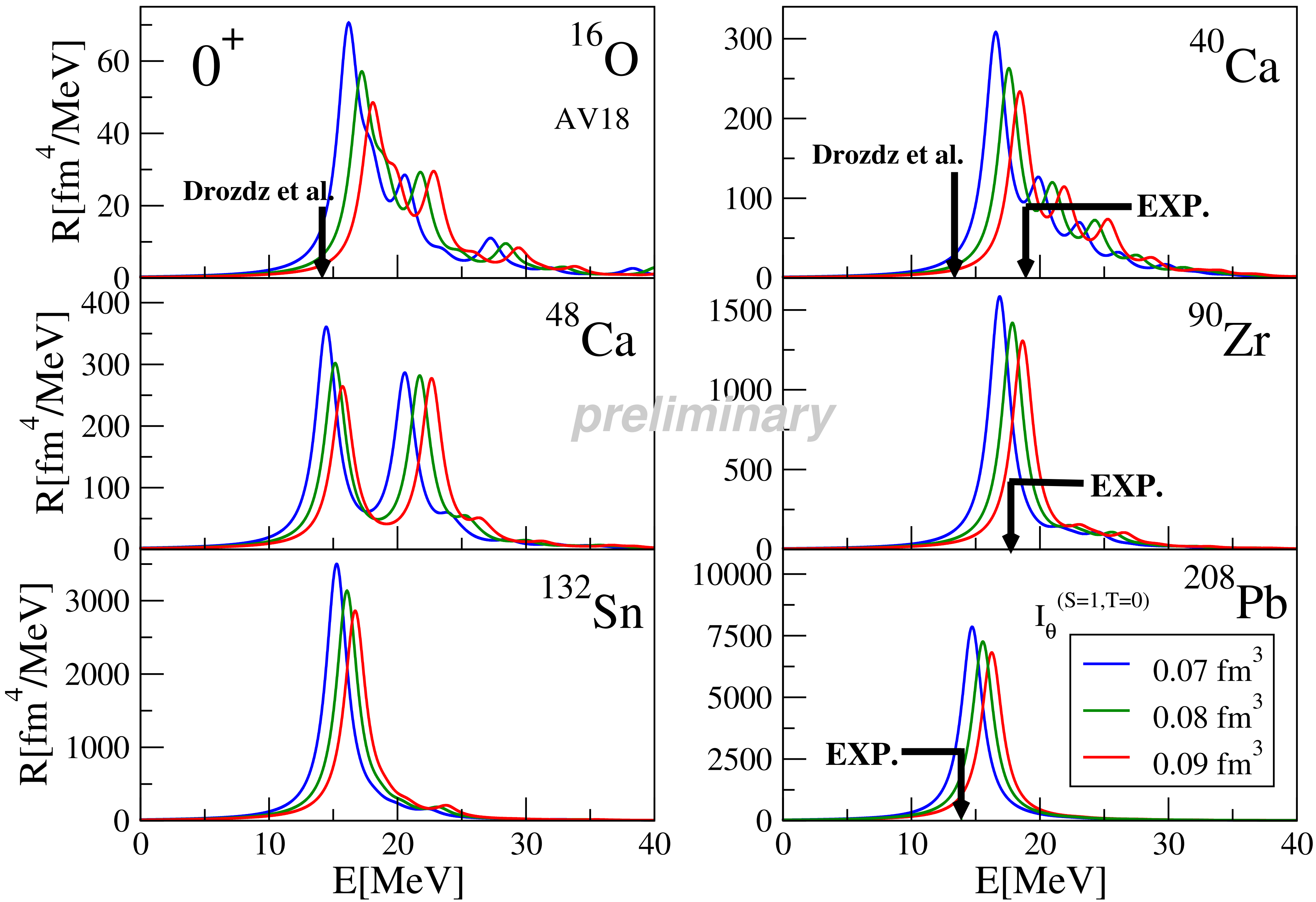
$$\Delta E^{(2)} = -\frac{1}{4} \sum_{i,j}^{\text{occu.}} \sum_{a,b}^{\text{unoccu.}} \frac{|\langle \phi_a \phi_b | \mathbf{T}_{\text{int}} + \mathbf{V}_{\text{UCOM}} | \phi_i \phi_j \rangle|^2}{\epsilon_a + \epsilon_b - \epsilon_i - \epsilon_j}$$



Long-Range Correlations: MBPT



Outlook: UCOM + RPA



Missing Pieces

long-range
correlations

genuine
three-body forces

three-body cluster
contributions

Missing Pieces

long-range correlations

genuine three-body forces

three-body cluster contributions

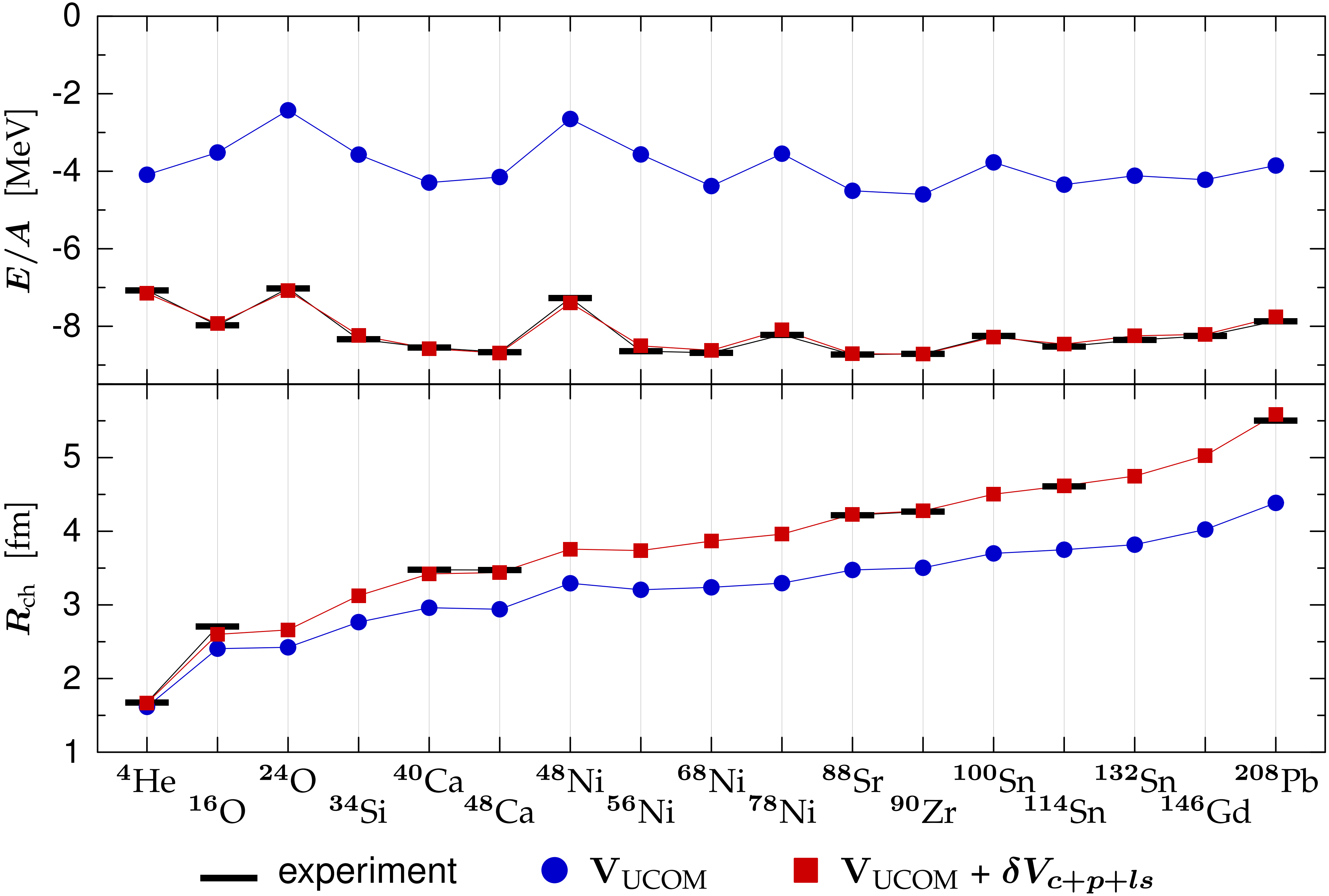
Pragmatic Approach

- phenomenological two-body correction

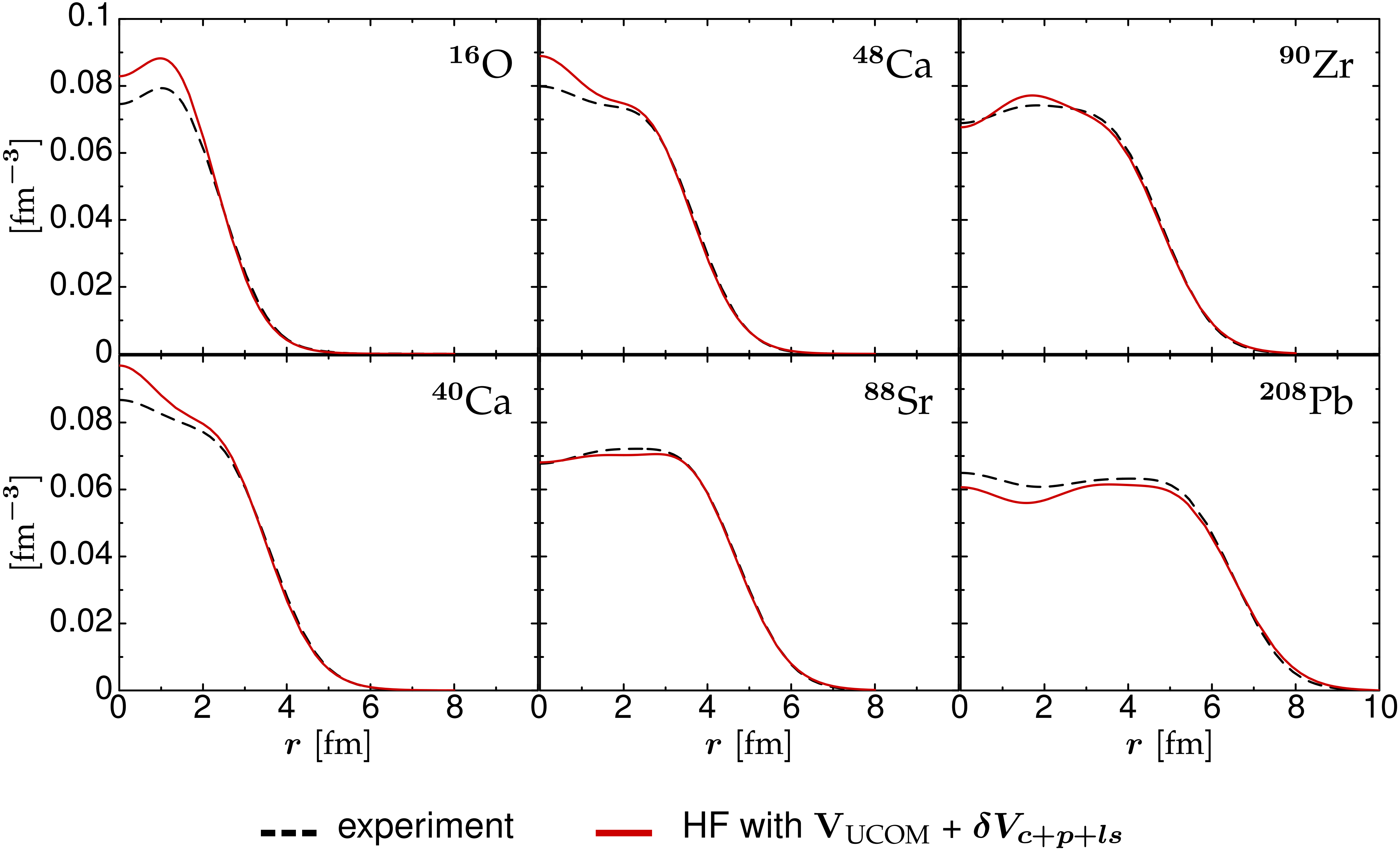
$$\delta \mathrm{V}_{c+p+ls} = v_1(\mathrm{r}) + \vec{\mathrm{q}}\, v_{qq}(\mathrm{r})\, \vec{\mathrm{q}} + v_{LS}(\mathrm{r})\, \vec{\mathrm{L}} \cdot \vec{\mathrm{S}}$$

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

Correlated Argonne V18 + Correction



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_ν : complex width

χ_ν : 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

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

FMD Approach

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

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

Diagonalisation

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

FMD Matrix Elements

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

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

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

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

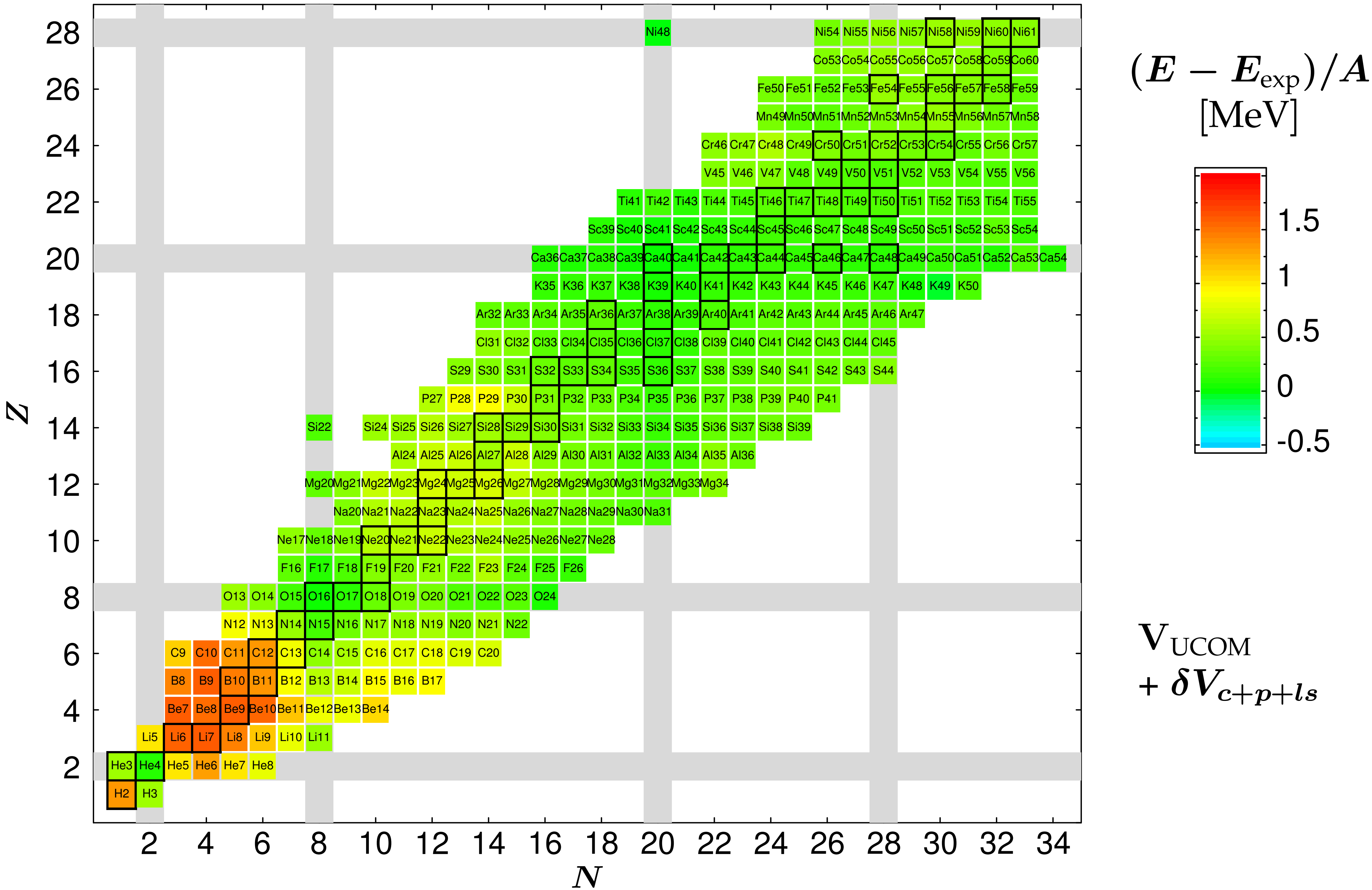
$$\left. \frac{5}{2}\gamma_{klmn}\beta_{klmn}\vec{\rho}_{klmn}^{\,2} + 4\gamma_{klmn}^2(\vec{\pi}_{klmn} \cdot \vec{\rho}_{klmn})\vec{\rho}_{klmn}^{\,2}\right) +$$

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

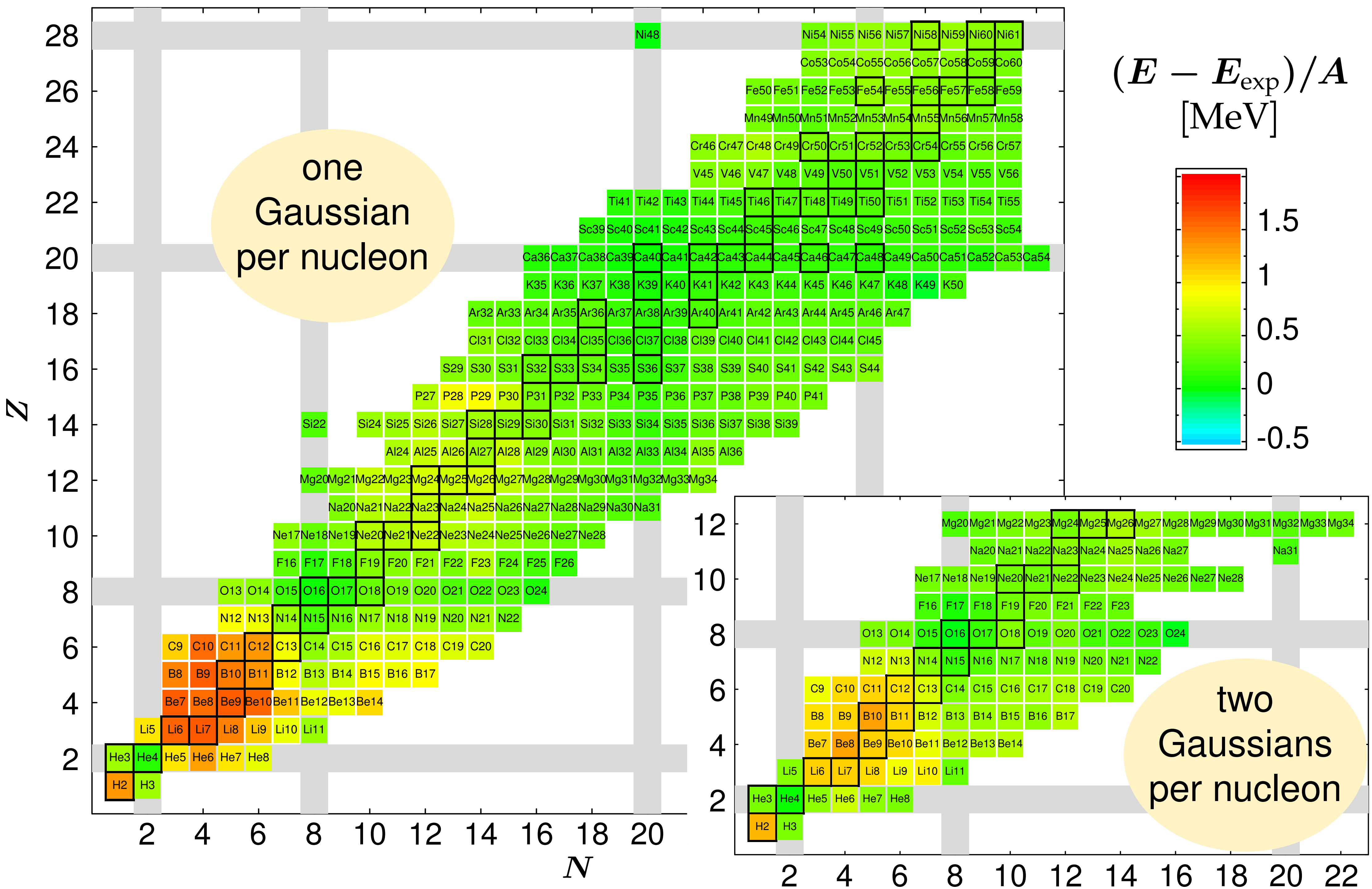
$$2\gamma_{klmn}^2(\vec{\pi}_{klmn} \cdot \vec{\rho}_{klmn})^2 + 4\gamma_{klmn}\beta_{klmn}(\vec{\pi}_{klmn} \cdot \vec{\rho}_{klmn}) -$$

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

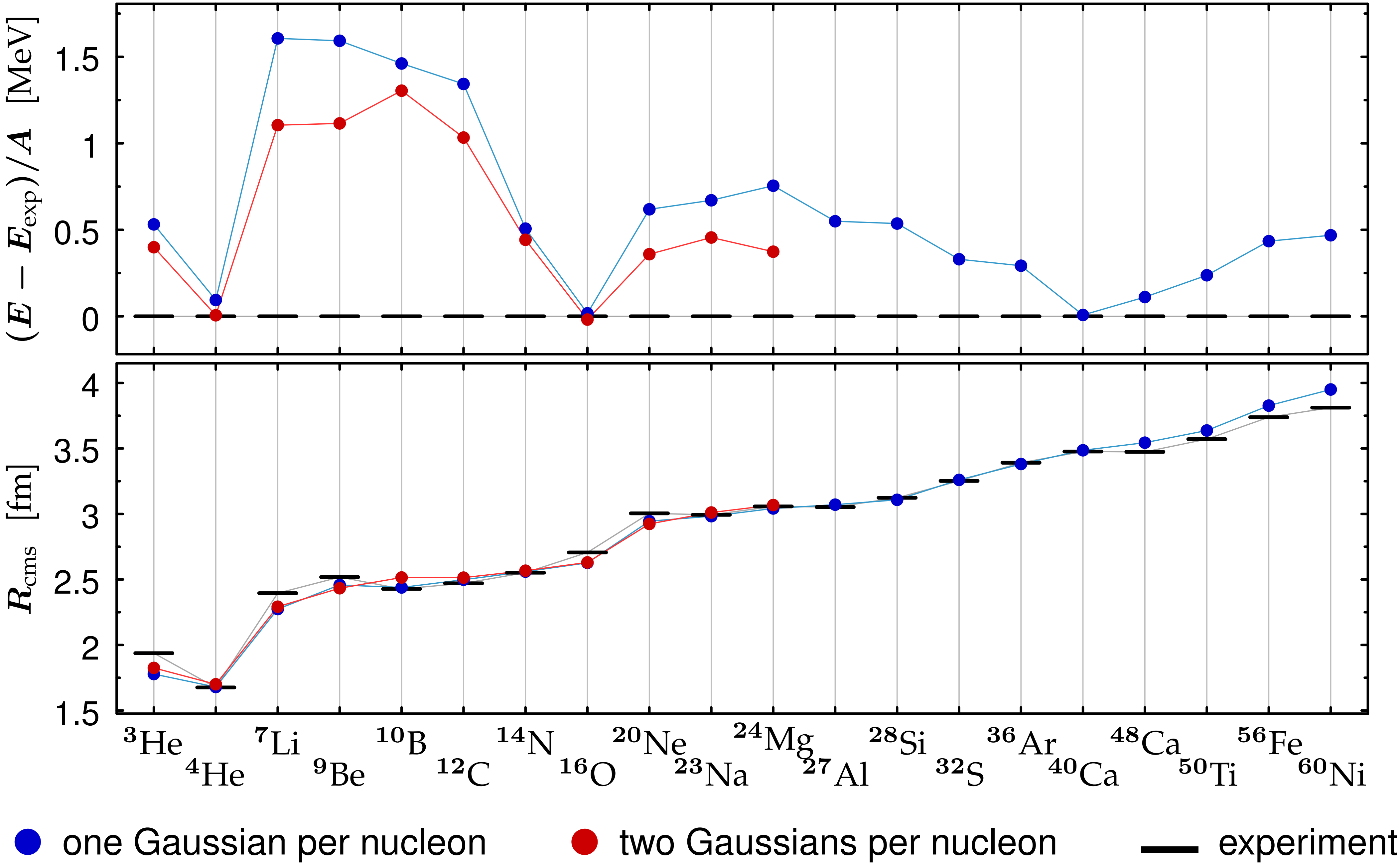
Variation: Chart of Nuclei



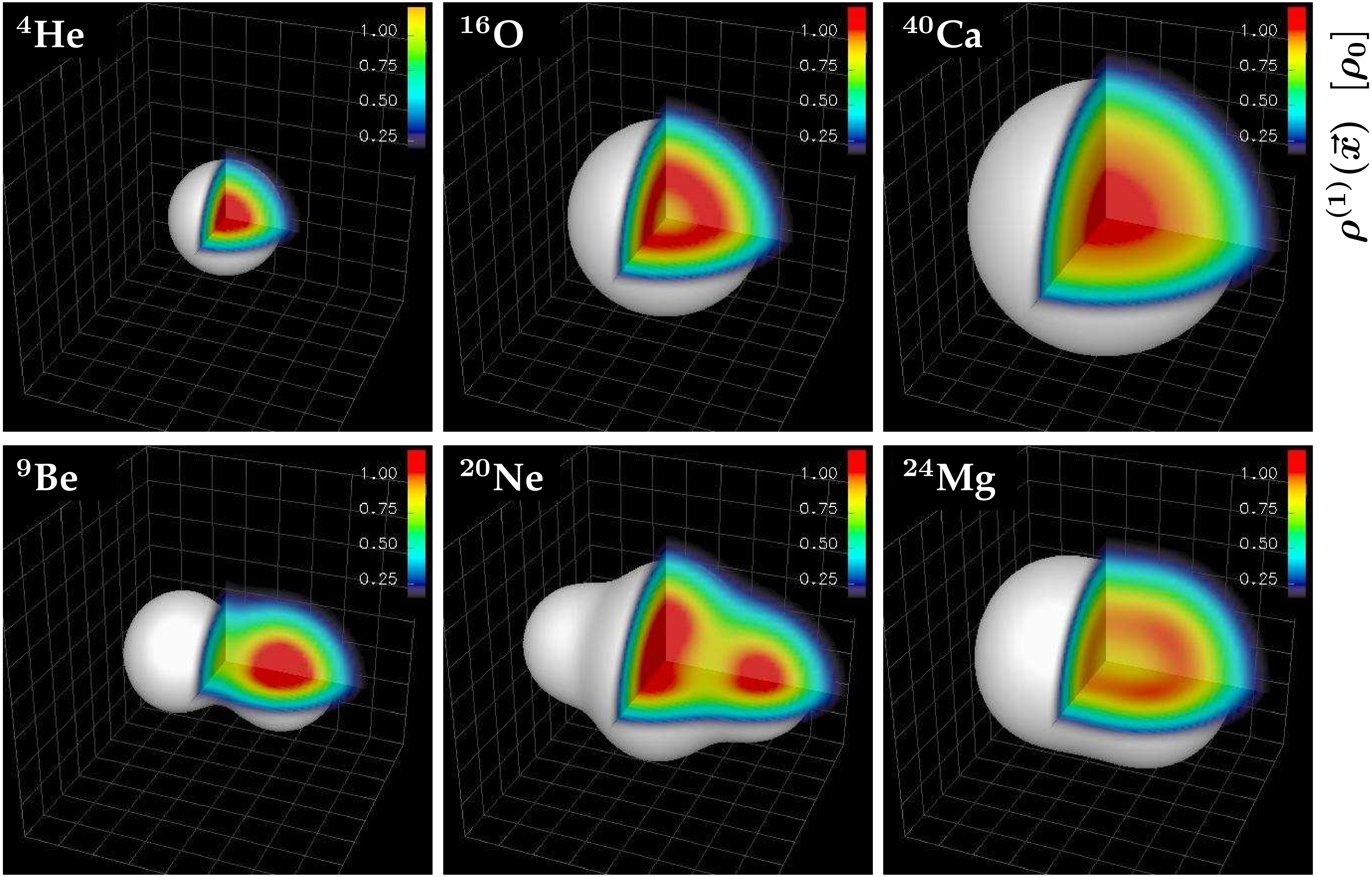
Variation: Chart of Nuclei



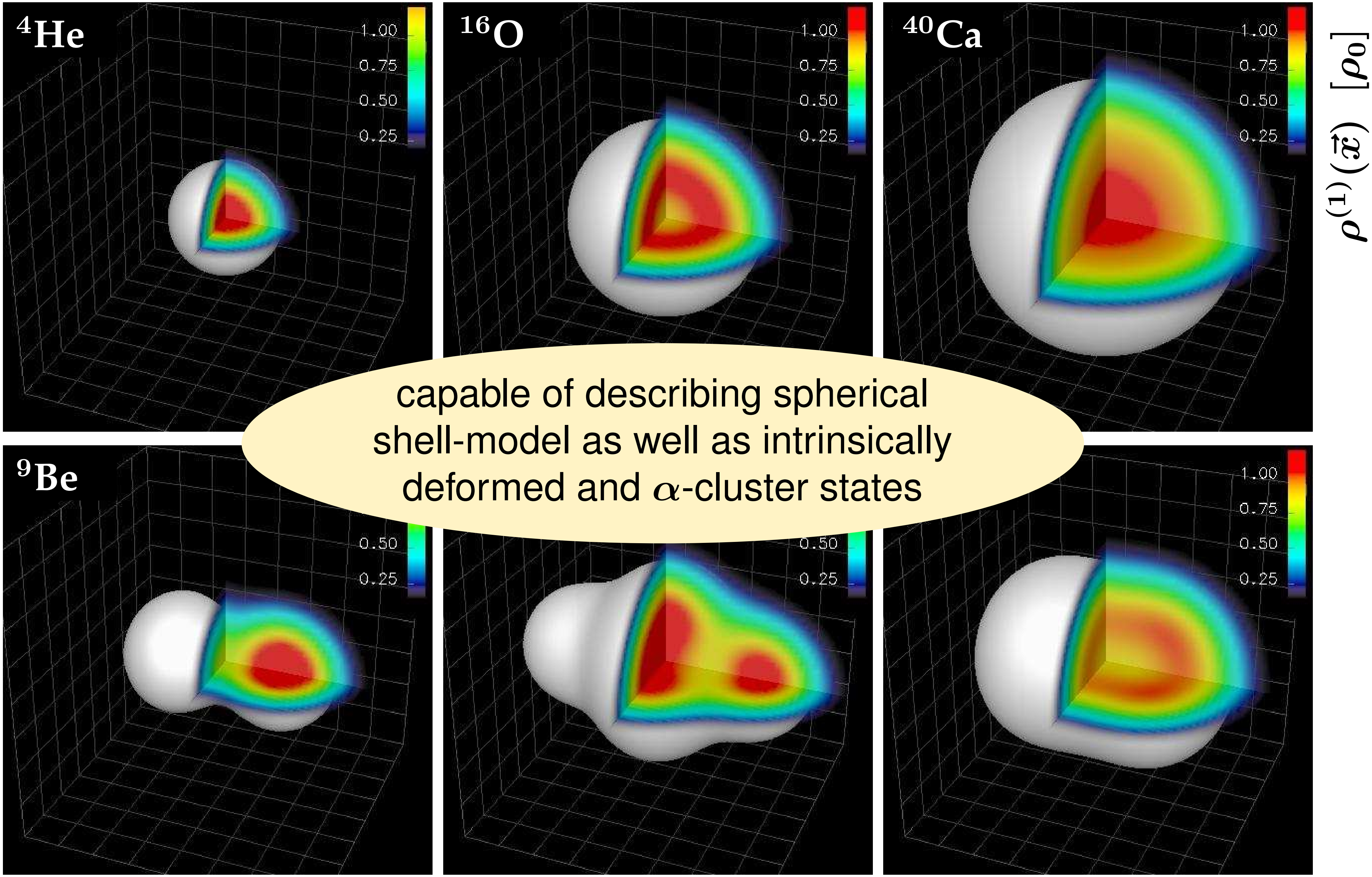
Selected Stable Nuclei



Intrinsic One-Body Density Distributions



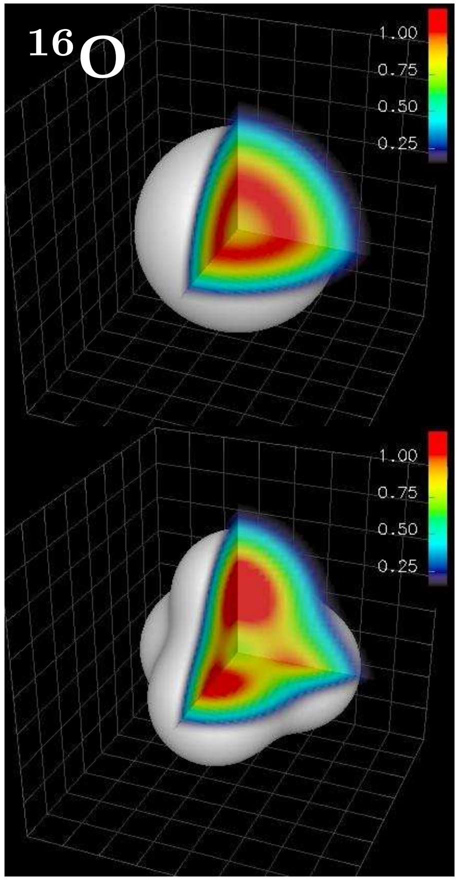
Intrinsic One-Body Density Distributions



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**
  - diagonalisation within a set of different Slater determinants



Angular Momentum Projection

- project intrinsically deformed many-body state $|Q\rangle$ onto **angular momentum eigenstate** $|\Psi_{JM}\rangle$

$$|\Psi_{JM}\rangle = \sum_K g_K^J \, \mathrm{P}_{MK}^J \, |Q\rangle$$

$$\mathrm{P}_{MK}^J = \frac{2J+1}{8\pi^2} \int \mathrm{d}^3\omega \; D_{MK}^{J\star}(\vec{\omega}) \; \mathrm{R}(\vec{\omega})$$

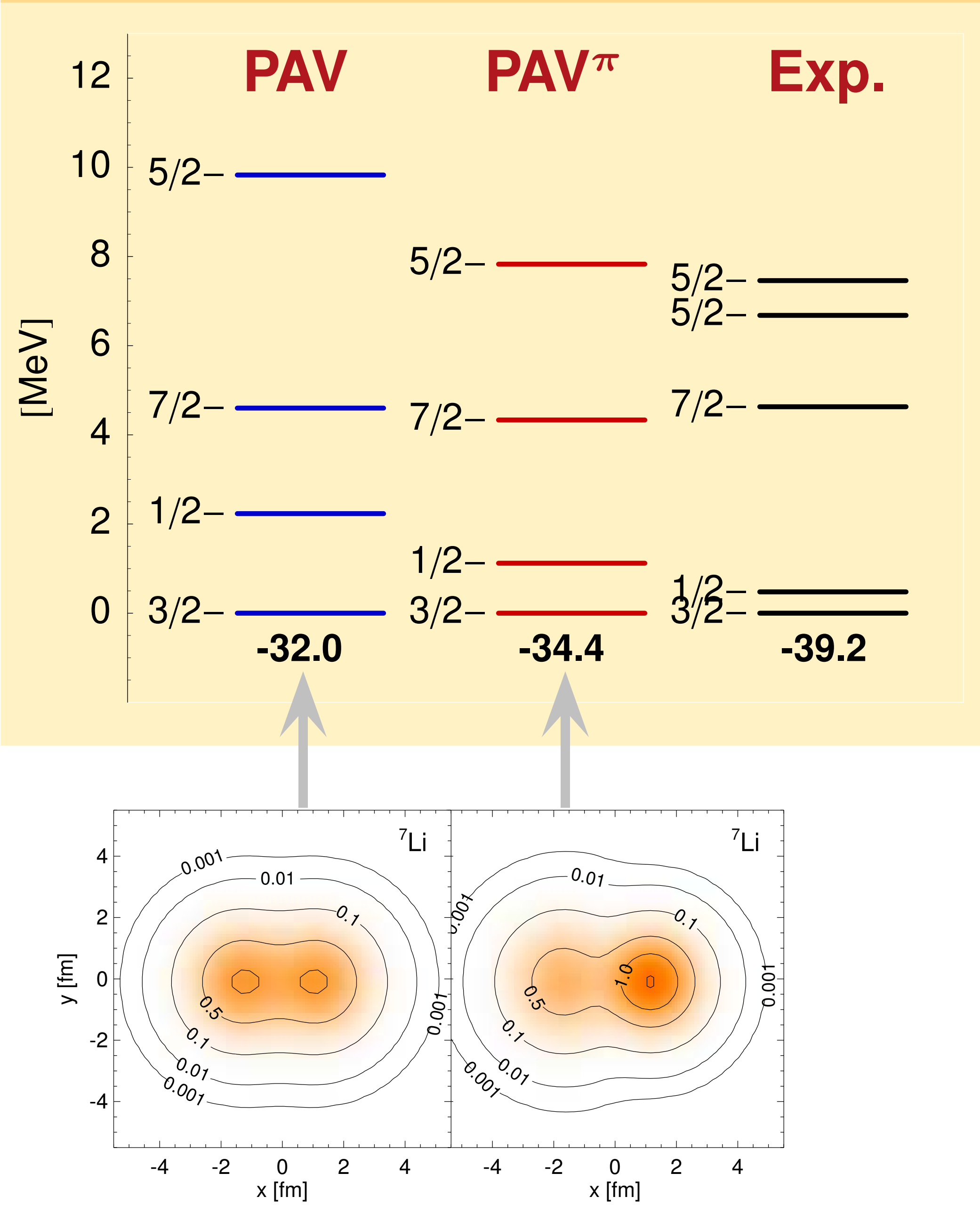
- energy of angular momentum projected states

$$E_J = \frac{\langle \Psi_{JM} | \widetilde{\mathrm{H}}_{\text{int}} | \Psi_{JM} \rangle}{\langle \Psi_{JM} | \Psi_{JM} \rangle}$$

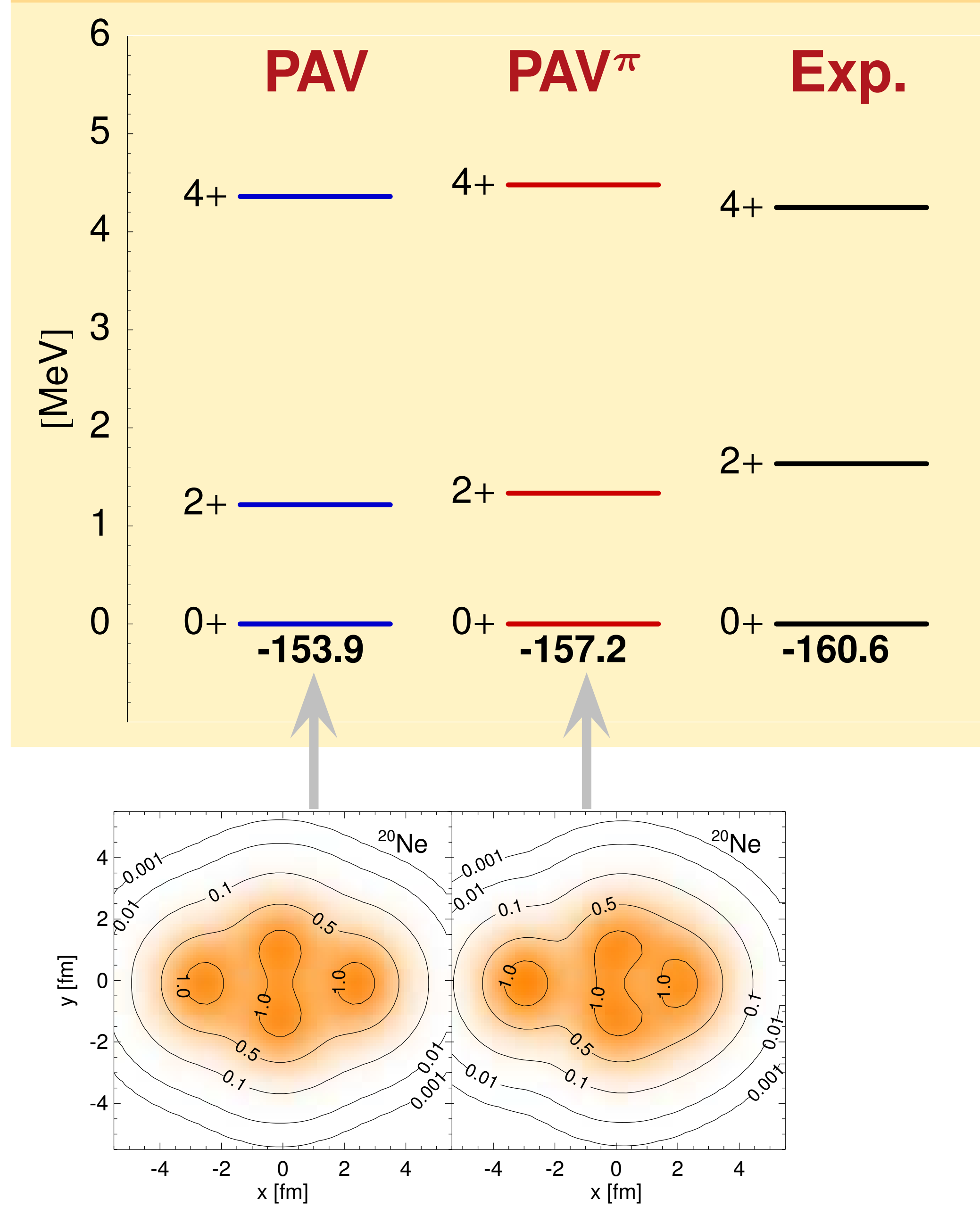
- **PAV**: calculate E_J for $|Q\rangle$ obtained by minimisation of unprojected energy
- **VAP**: determine parameters of $|Q\rangle$ through minimisation of E_J

Angular Momentum Projection – Example

^{7}Li

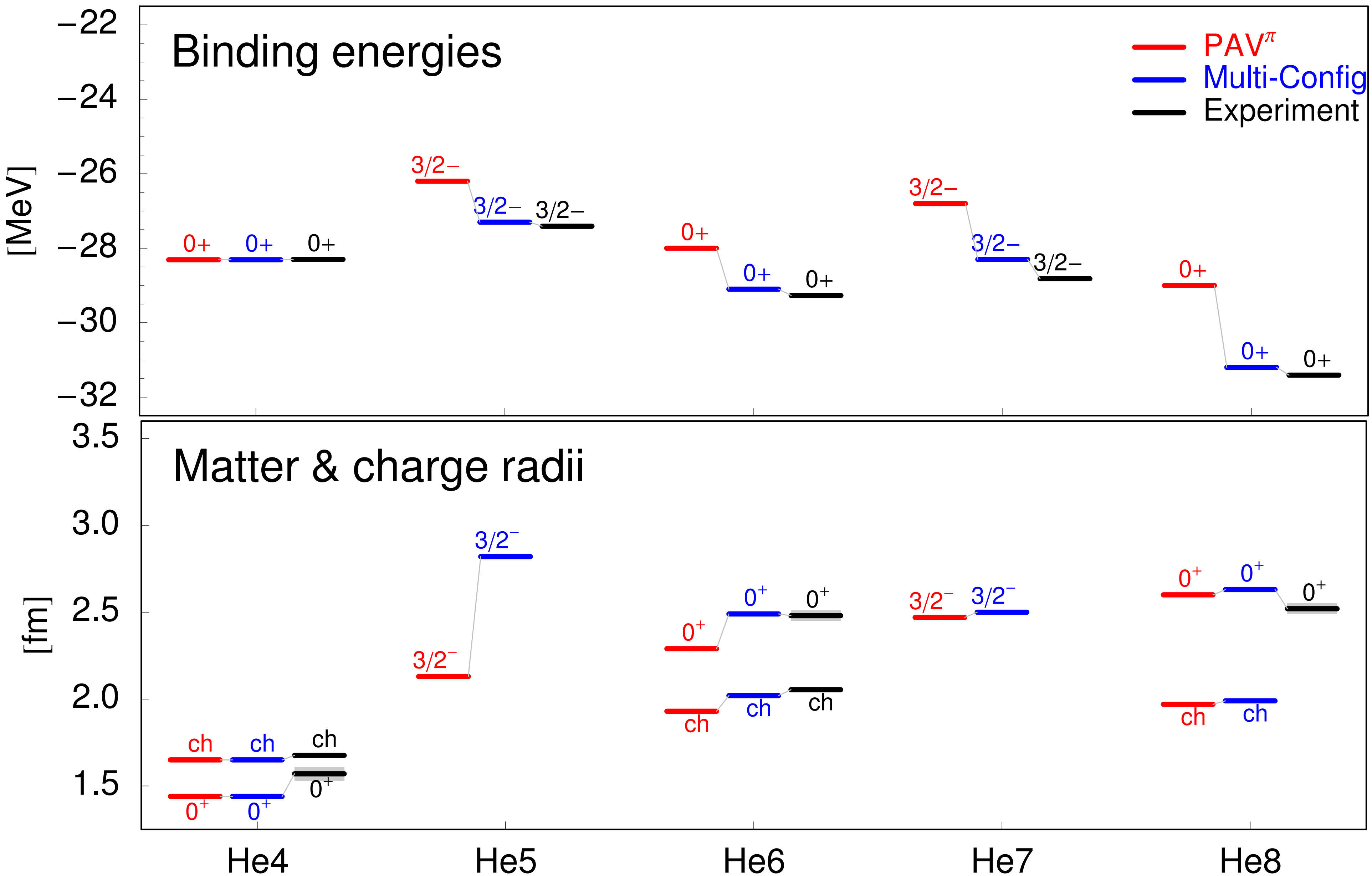


^{20}Ne



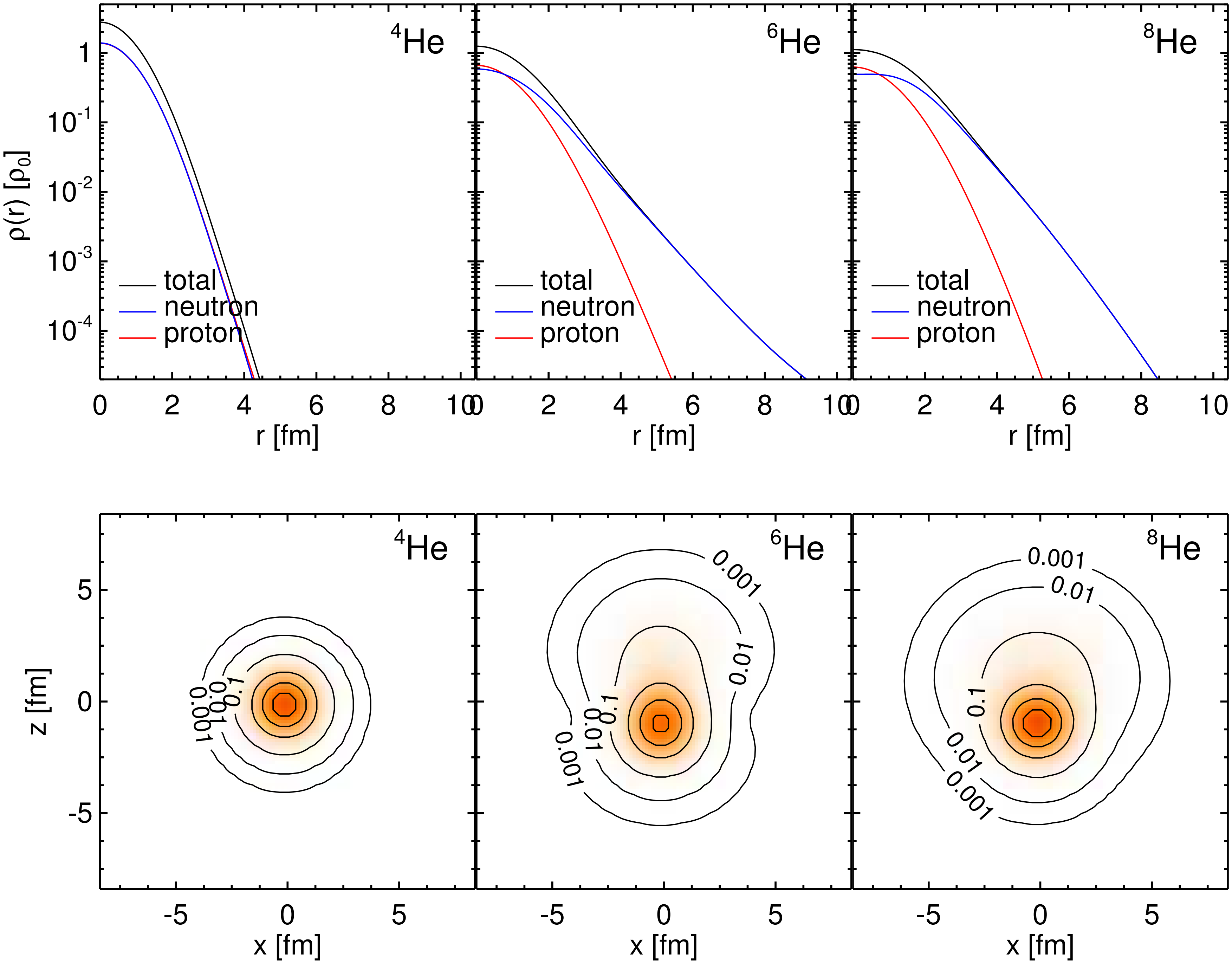
Results for p-Shell Nuclei

Helium Isotopes: Energies & Radii



[figures provided by T. Neff]

Helium Isotopes: Densities



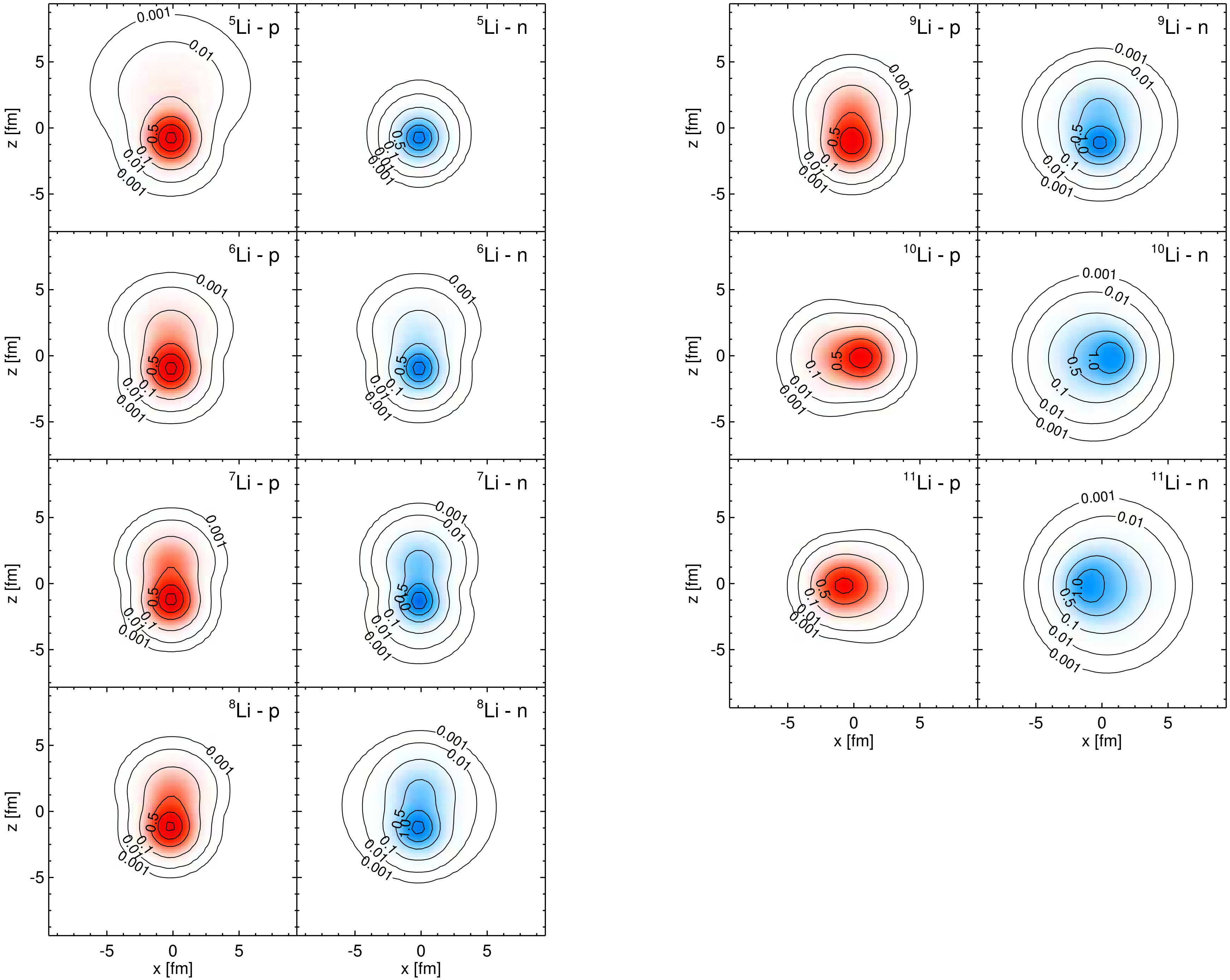
Multi-Config

radial density profiles

PAV$^{\pi}$

intrinsic densities

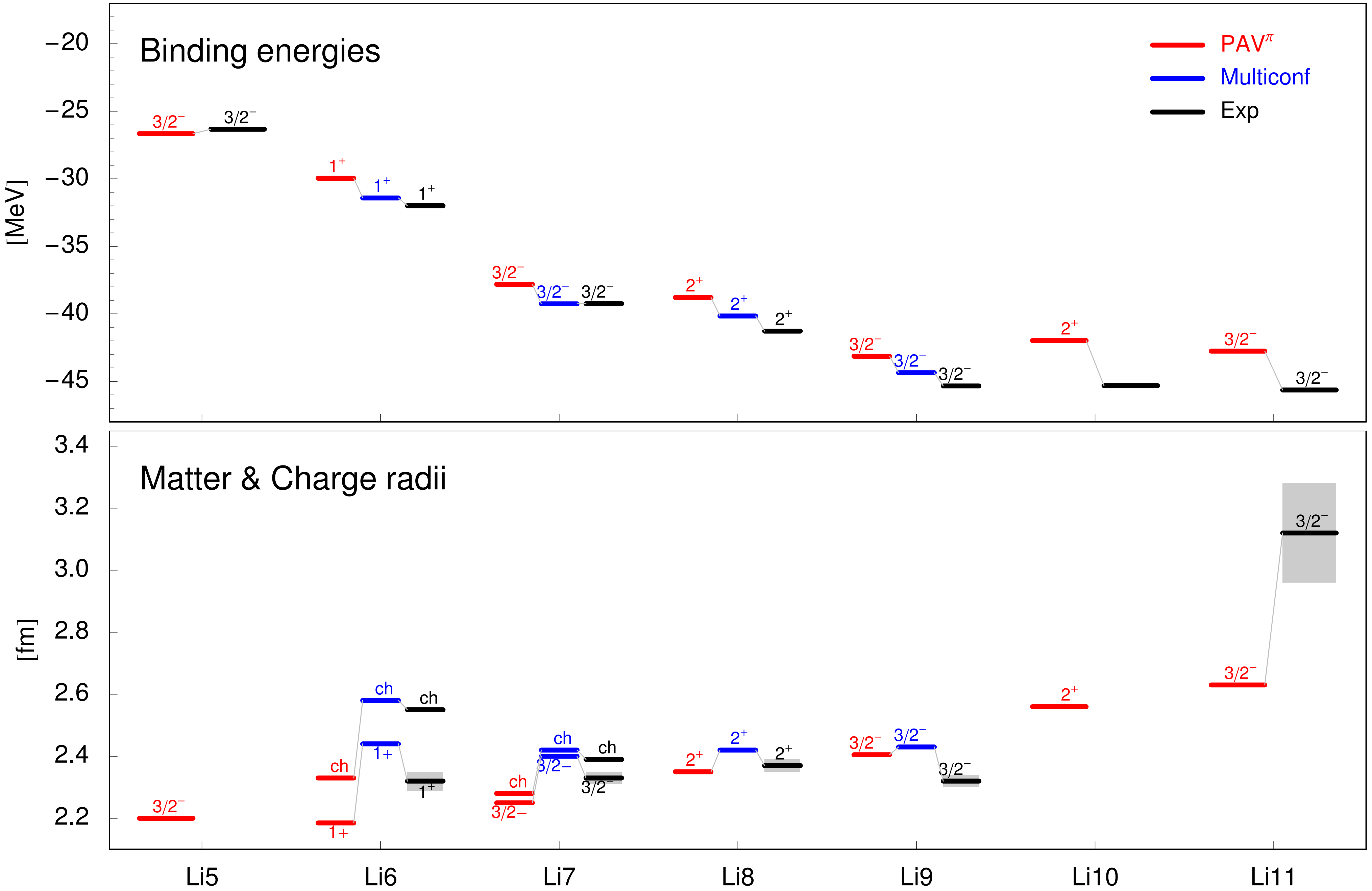
Lithium Isotopes: Intrinsic Densities



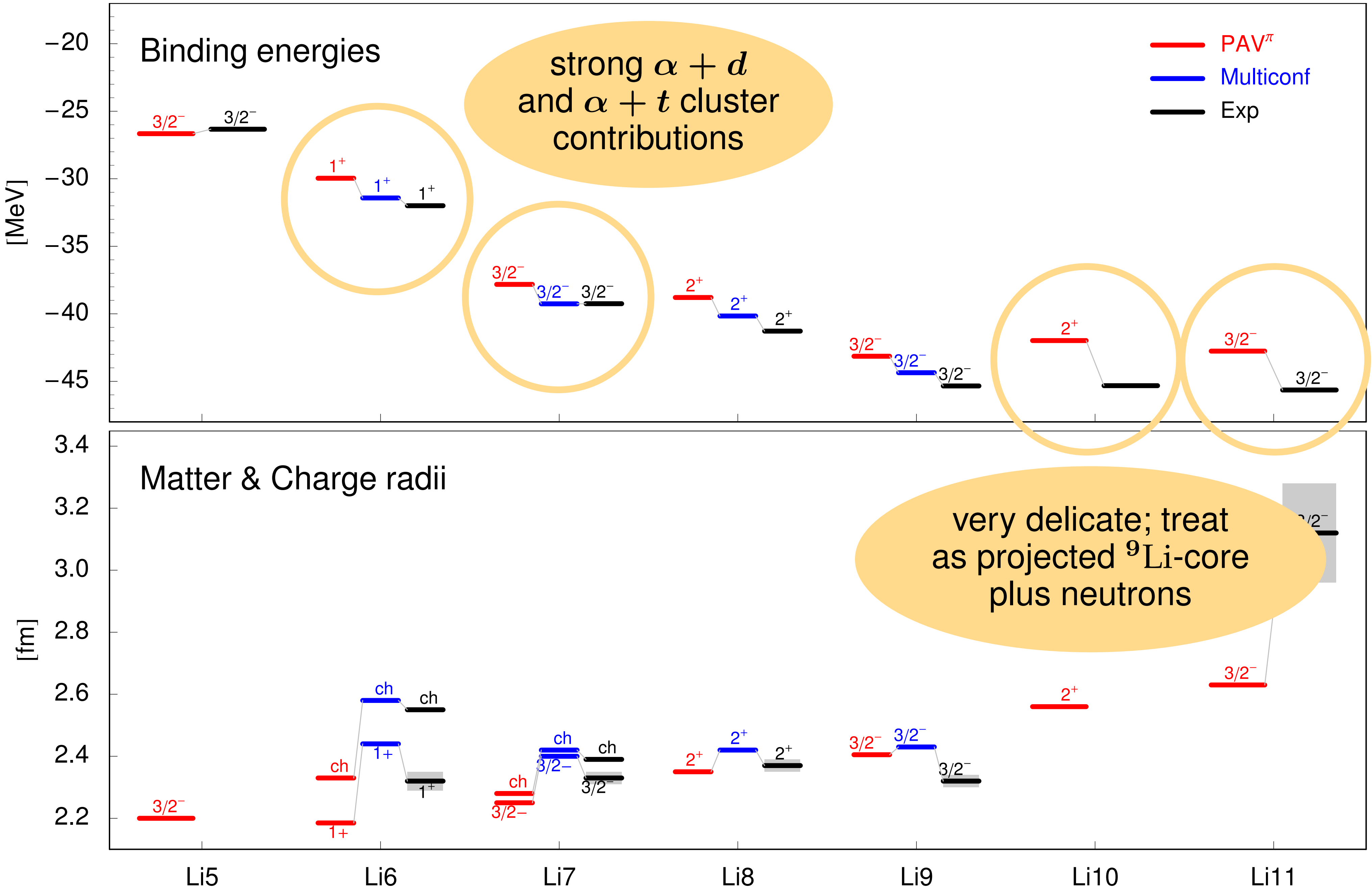
PAV$^{\pi}$

intrinsic densities

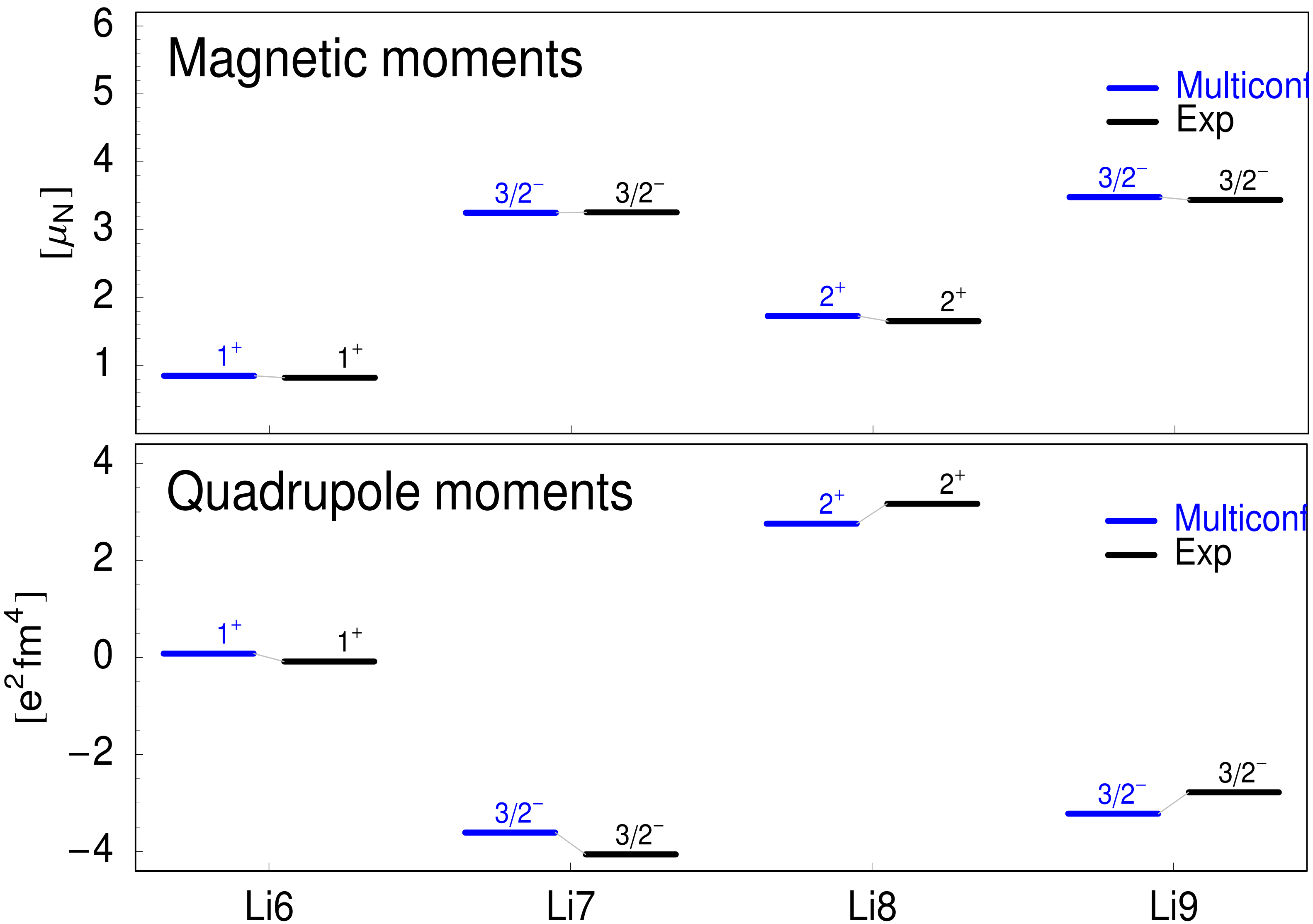
Lithium Isotopes: Energies & Radii



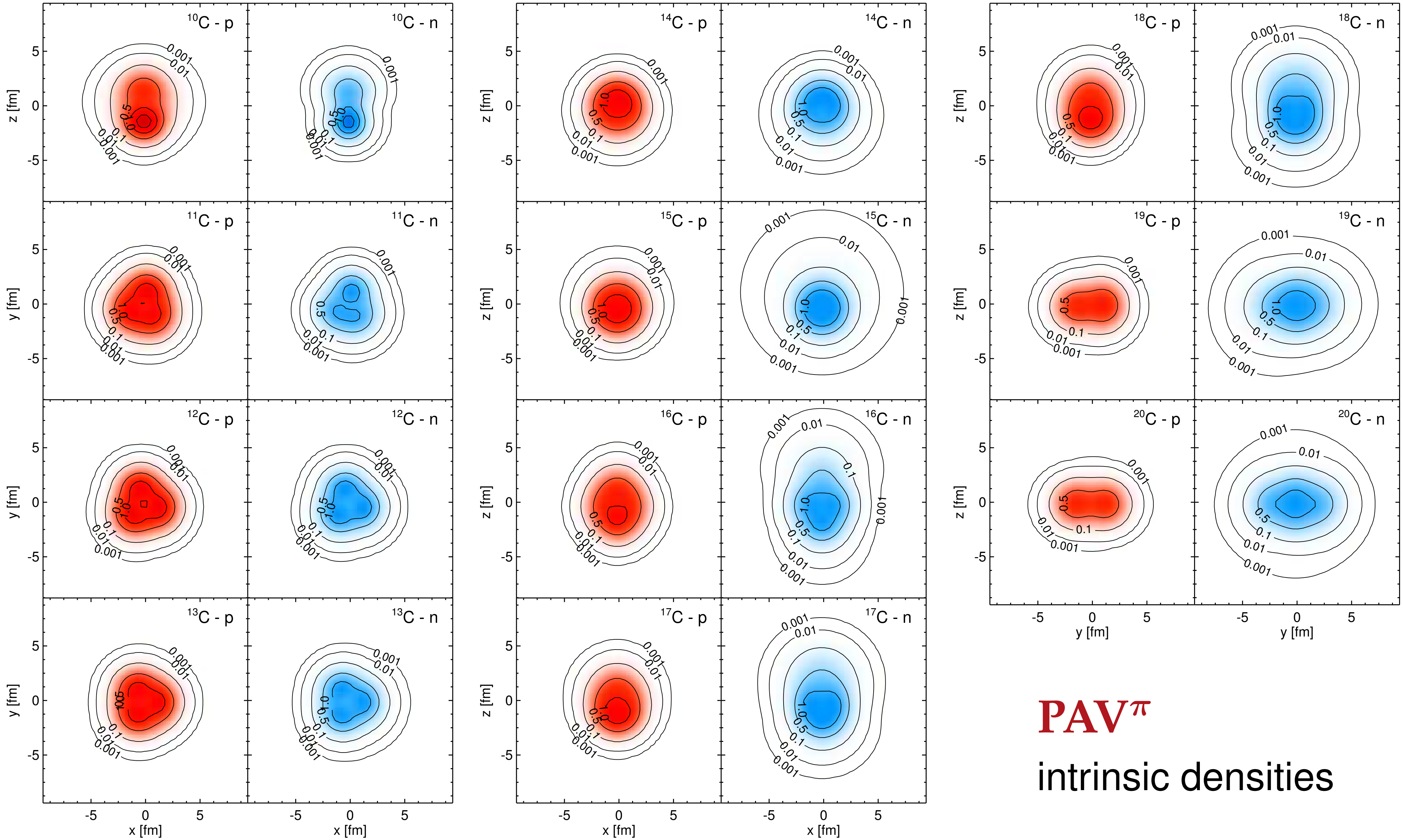
Lithium Isotopes: Energies & Radii



Lithium Isotopes: Moments



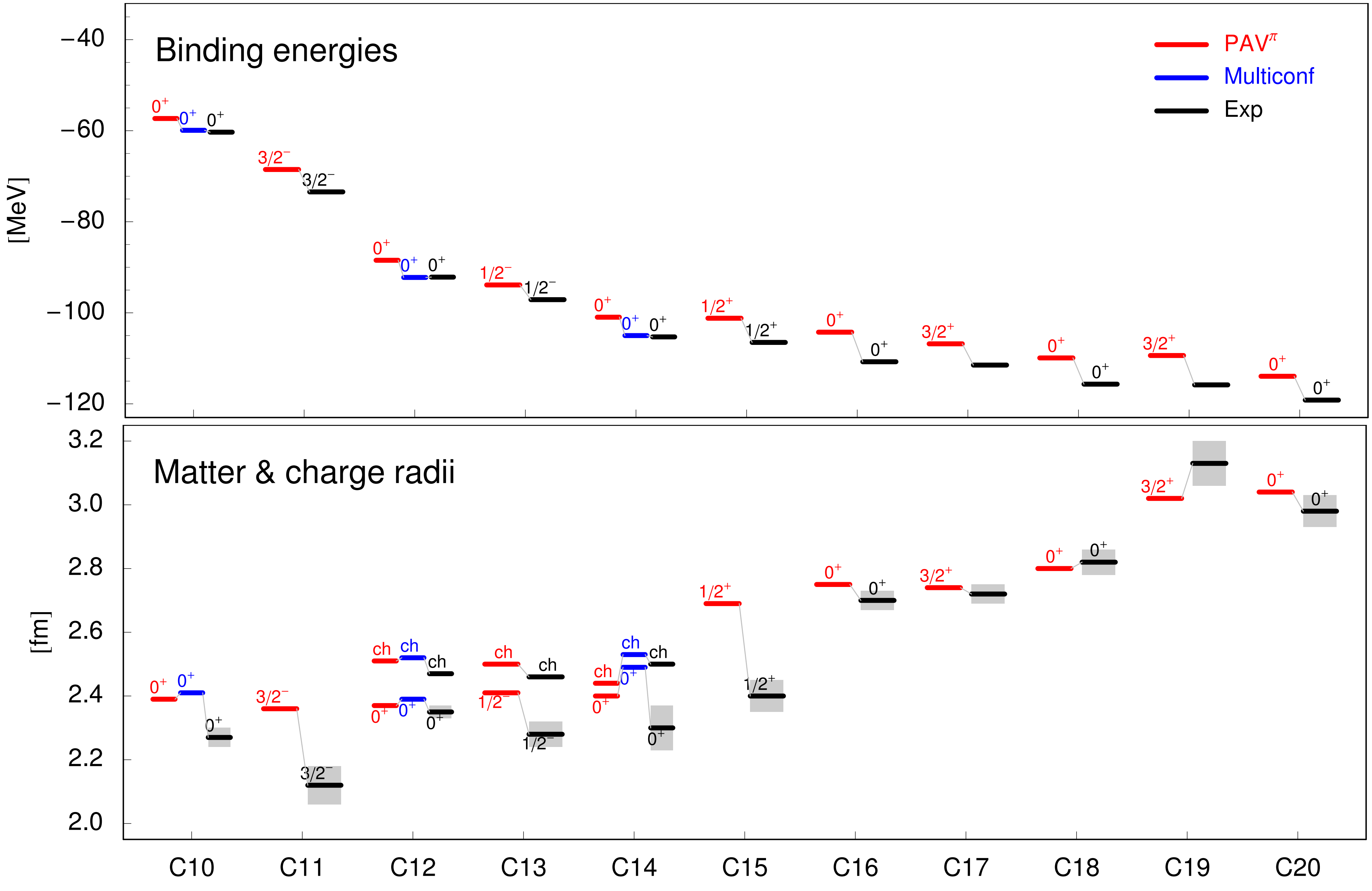
Carbon Isotopes: Intrinsic Densities



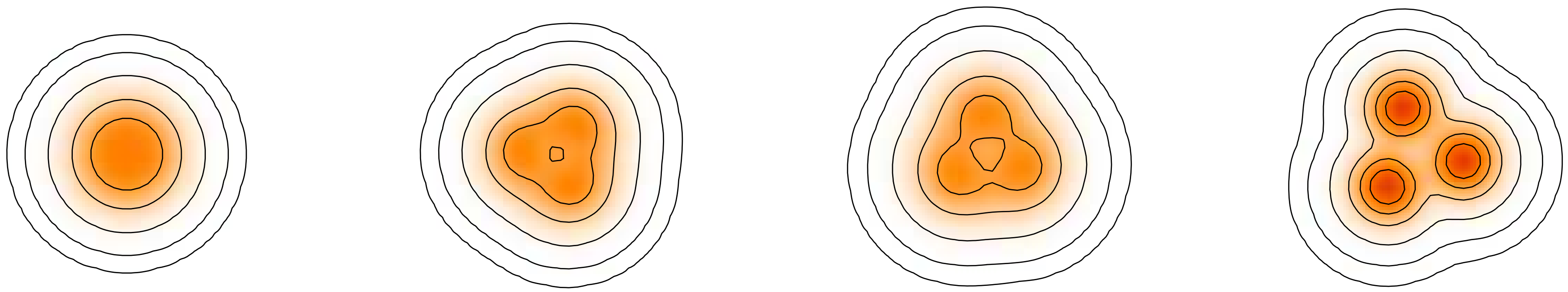
PAV$^{\pi}$

intrinsic densities

Carbon Isotopes: Energies & Radii

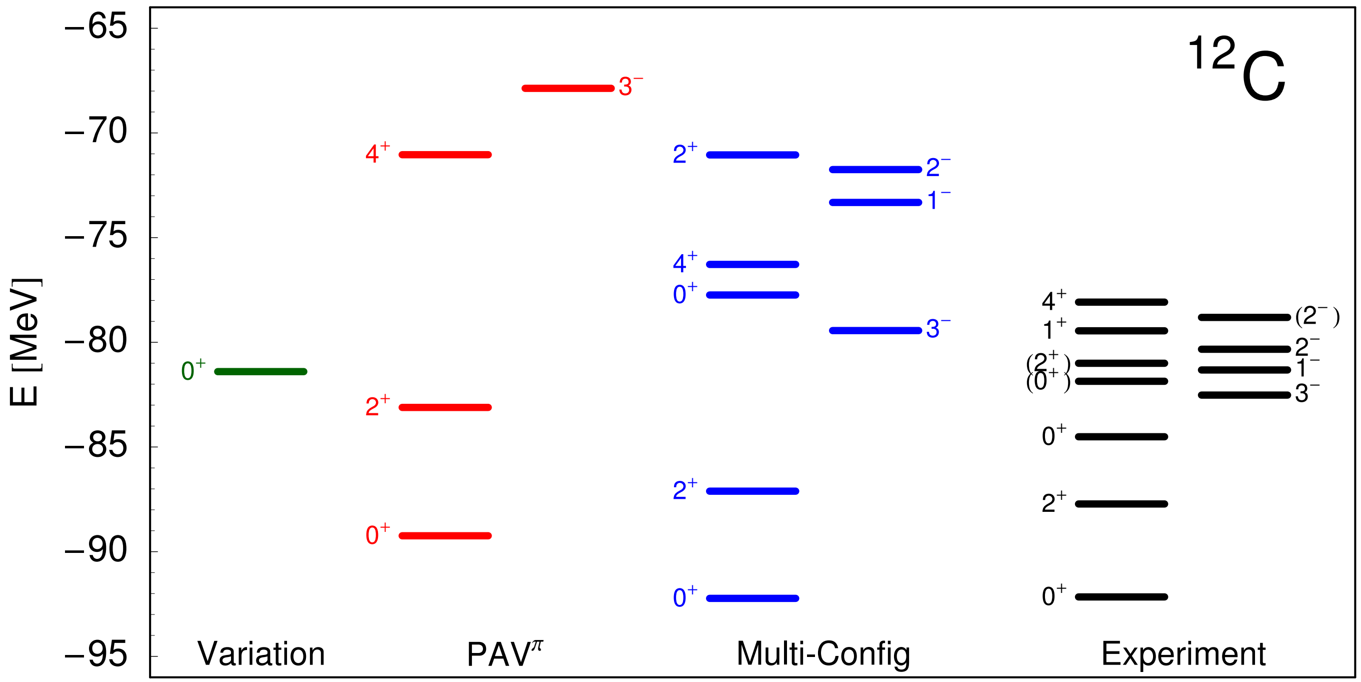


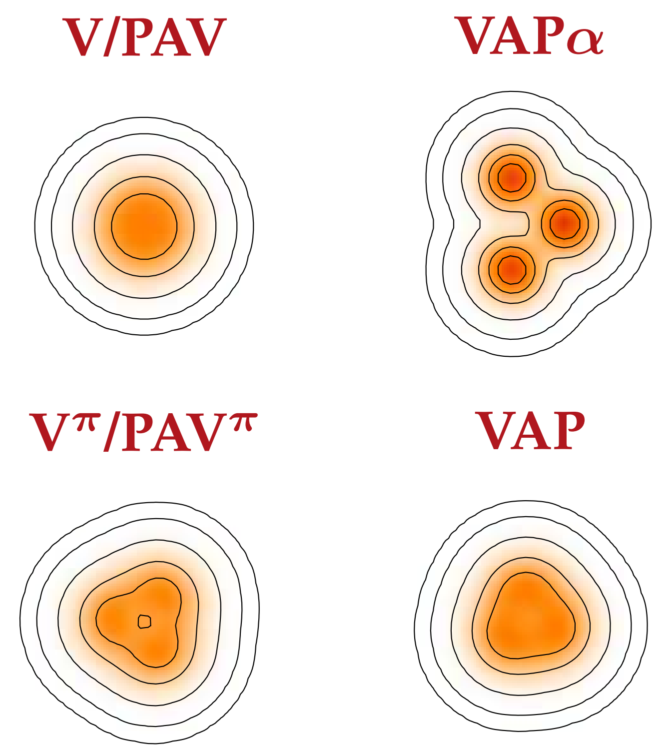
Intrinsic Shapes of ^{12}C



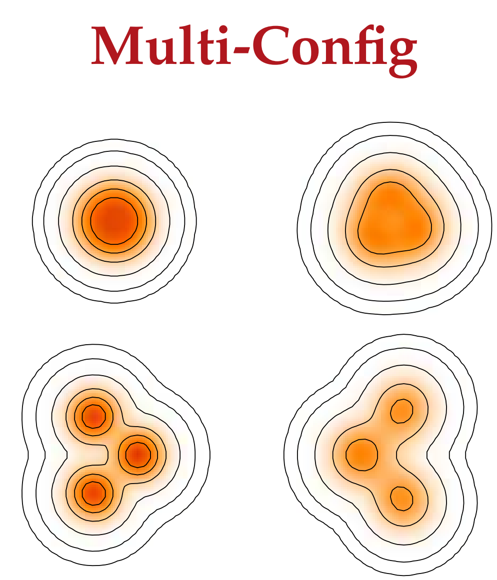
	intrinsic	projected	intrinsic	projected	intrinsic	projected	intrinsic	projected
$\langle \mathbf{H} \rangle$	-81.4	**-81.5**	-77.0	**-88.5**	-74.1	**-85.5**	-57.0	**-75.9**
$\langle \mathbf{T} \rangle$	212.1	212.1	189.2	186.1	182.8	179.0	213.9	201.4
$\langle \mathbf{V}_{ls} \rangle$	-39.8	-40.2	-12.0	-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

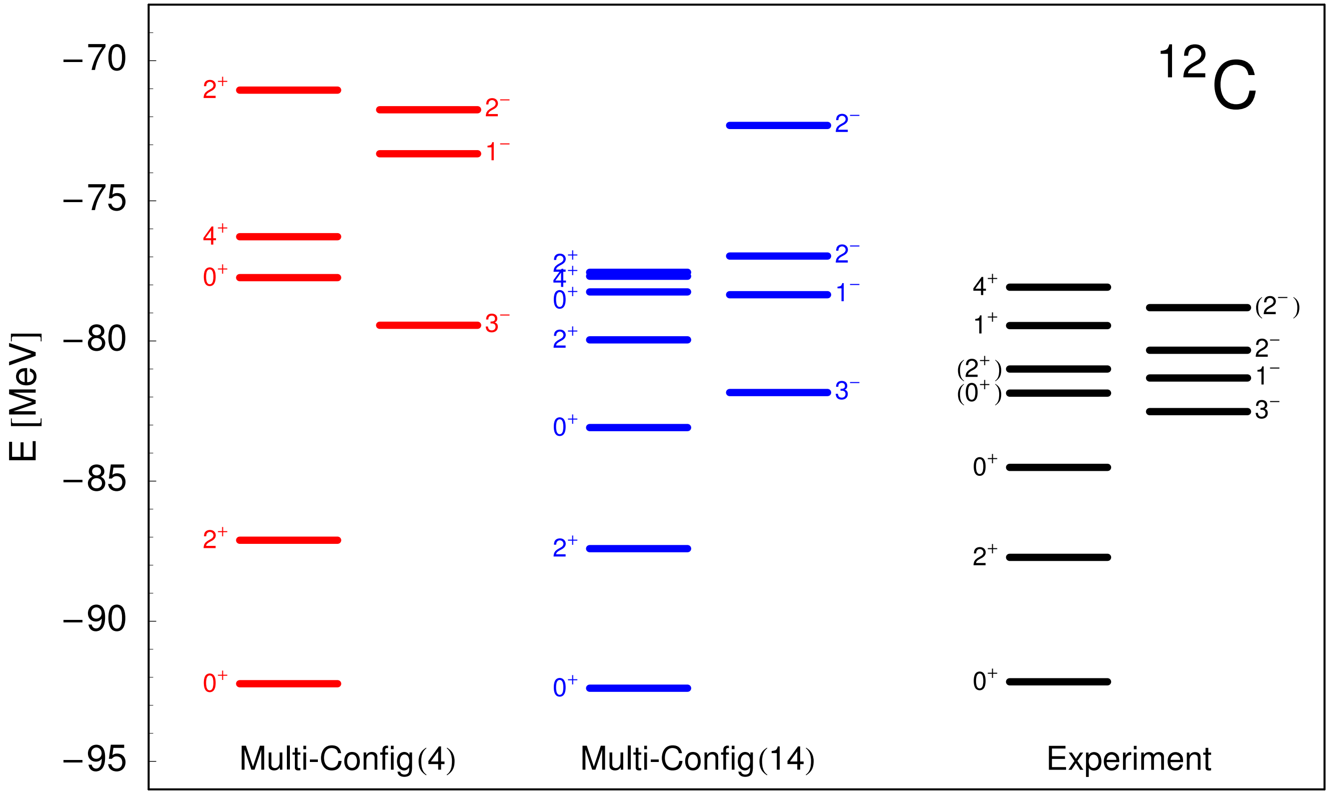




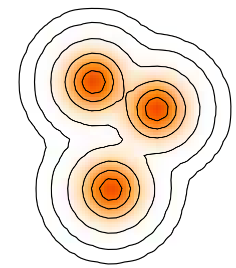
	E [MeV]	R_{ch} [fm]	$B(E2)$ [e^2 fm^4]
V/PAV	81.4	2.36	-
VAP α-cluster	79.1	2.70	76.9
PAV$^\pi$	88.5	2.51	36.3
VAP	89.2	2.42	26.8
Multi-Config	92.2	2.52	42.8
Experiment	92.2	2.47	39.7 $\pm$ 3.3

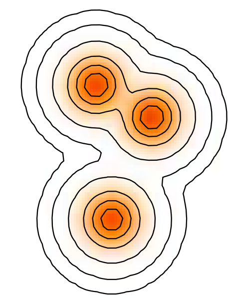


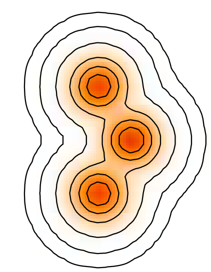
Structure of ^{12}C — Hoyle State



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

$|\langle$  $|0_2^+\rangle| = 0.76$

$|\langle$  $|0_2^+\rangle| = 0.71$

$|\langle$  $|0_2^+\rangle| = 0.50$

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**
  - 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)

supported by the DFG through SFB 634
“Nuclear Structure, Nuclear Astrophysics and
Fundamental Experiments...”

Supplements

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

Lee-Suzuki

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

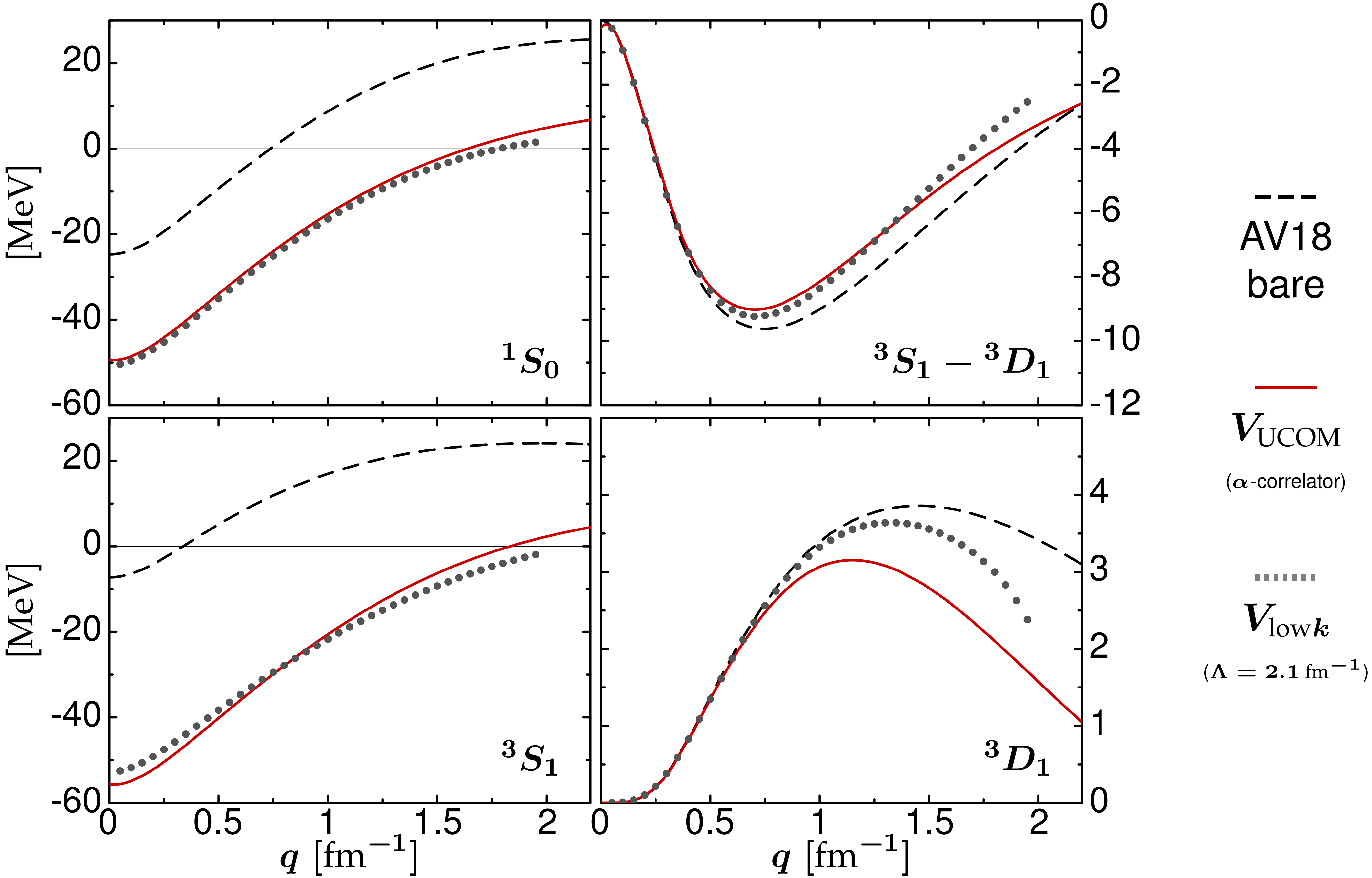
$V_{\mathrm{low}k}$

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

UCOM

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

Momentum-Space Matrix Elements



Correlated Oscillator Matrix Elements

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

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

Correlated Oscillator Matrix Elements

$$\langle n(LS)JT | \mathrm{C}_r^\dagger \mathrm{C}_\Omega^\dagger \, \mathrm{H} \, \mathrm{C}_\Omega \mathrm{C}_r | n'(L'S)JT \rangle$$
$$= \langle n(LS)JT | \mathrm{T} + \mathrm{V}_{\mathrm{UCOM}} | n'(L'S)JT \rangle$$

calculate using uncorrelated states and operator form of $\mathrm{V}_{\mathrm{UCOM}}$

map correlator onto states and use bare interaction (avoids BCH expansion)

Correlated Oscillator Matrix Elements

$$\langle n(LS)JT| \, \mathrm{C}_r^\dagger \mathrm{C}_\Omega^\dagger \, \mathrm{H} \, \mathrm{C}_\Omega \mathrm{C}_r \, |n'(L'S)JT\rangle$$
$$= \langle n(LS)JT| \, \mathrm{T} + \mathrm{V}_{\mathrm{UCOM}} \, |n'(L'S)JT\rangle$$

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,...)

Reminder: Hartree-Fock Approximation

- ground state approximated by a **single Slater-determinant**

$$\left|\mathrm{HF}\right\rangle = \left|\phi_1, \phi_2, \ldots, \phi_A\right\rangle_a = \mathcal{A}\left(\left|\phi_1\right\rangle \otimes \left|\phi_2\right\rangle \otimes \cdots \otimes \left|\phi_A\right\rangle\right)$$

Reminder: Hartree-Fock Approximation

- ground state approximated by a **single Slater-determinant**

$$\left|\mathrm{HF}\right\rangle = \left|\phi_1, \phi_2, \ldots, \phi_A\right\rangle_a = \mathcal{A}\left(\left|\phi_1\right\rangle \otimes \left|\phi_2\right\rangle \otimes \cdots \otimes \left|\phi_A\right\rangle\right)$$

- **single-particle states** $\left|\phi_i\right\rangle$ determined by minimising the energy expectation value

$$E_{\mathrm{HF}} = \left\langle\mathrm{HF}\right| \widetilde{\mathrm{H}}_{\mathrm{int}} \left|\mathrm{HF}\right\rangle = \frac{1}{2}\sum_{i,j=1}^{A} {}_a\left\langle\phi_i\phi_j\right| \mathrm{T}_{\mathrm{int}} + \mathrm{V}_{\mathrm{UCOM}} \left|\phi_i\phi_j\right\rangle_a$$

Reminder: Hartree-Fock Approximation

- ground state approximated by a **single Slater-determinant**

$$\left|\mathrm{HF}\right\rangle = \left|\phi_1, \phi_2, \ldots, \phi_A\right\rangle_a = \mathcal{A}\left(\left|\phi_1\right\rangle \otimes \left|\phi_2\right\rangle \otimes \cdots \otimes \left|\phi_A\right\rangle\right)$$

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$$E_{\mathrm{HF}} = \left\langle\mathrm{HF}\right| \widetilde{\mathrm{H}}_{\mathrm{int}} \left|\mathrm{HF}\right\rangle = \frac{1}{2} \sum_{i,j=1}^{A} {}_a\!\left\langle\phi_i\phi_j\right| \mathrm{T}_{\mathrm{int}} + \mathrm{V}_{\mathrm{UCOM}} \left|\phi_i\phi_j\right\rangle_a$$

- expand single-particle states in a complete basis, e.g., a harmonic oscillator basis

$$\left|\phi_i\right\rangle = \sum_{\alpha} D_{\alpha}^{(i)} \left|\alpha\right\rangle \quad , \qquad \left|\alpha\right\rangle = \left|n, (l\tfrac{1}{2})jm, \tfrac{1}{2}m_t\right\rangle$$

Reminder: Hartree-Fock Approximation

- variational principle leads to a nonlinear eigenvalue equation for the expansion coefficients

$$\sum_{\bar{\alpha}} h_{\alpha\bar{\alpha}}[D]\; D_{\bar{\alpha}}^{(k)} = \epsilon_k\; D_{\alpha}^{(k)} \qquad\qquad k = 1, 2, \ldots$$

- $h_{\alpha\bar{\alpha}}$ is the single-particle **Hartree-Fock Hamiltonian**

$$h_{\alpha\bar{\alpha}}[D] = \sum_{\alpha',\bar{\alpha}'} \sum_{i=1}^{A} D_{\alpha'}^{(i)\star} D_{\bar{\alpha}'}^{(i)} \;\; {}_a\langle \alpha\alpha' \big| \, \mathrm{T}_{\text{int}} + \mathrm{V}_{\text{UCOM}} \, \big| \bar{\alpha}\bar{\alpha}' \rangle_a$$

Reminder: Hartree-Fock Approximation

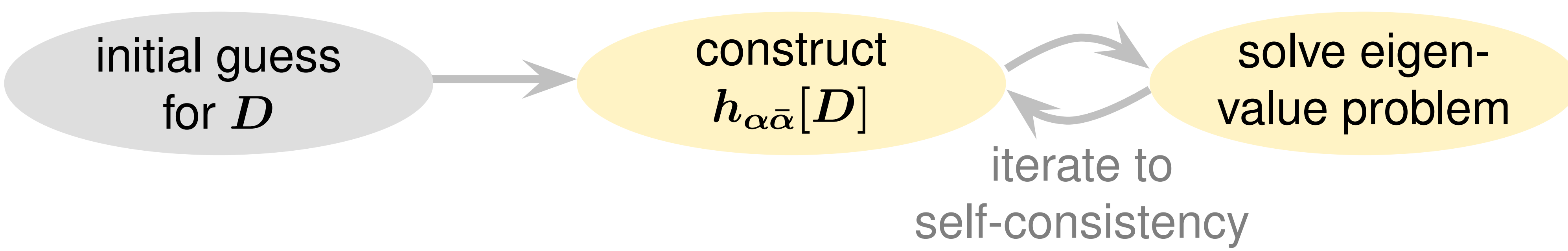
- variational principle leads to a nonlinear eigenvalue equation for the expansion coefficients

$$\sum_{\bar{\alpha}} h_{\alpha\bar{\alpha}}[D]\; D^{(k)}_{\bar{\alpha}} = \epsilon_k \; D^{(k)}_{\alpha} \qquad\qquad k = 1, 2, \ldots$$

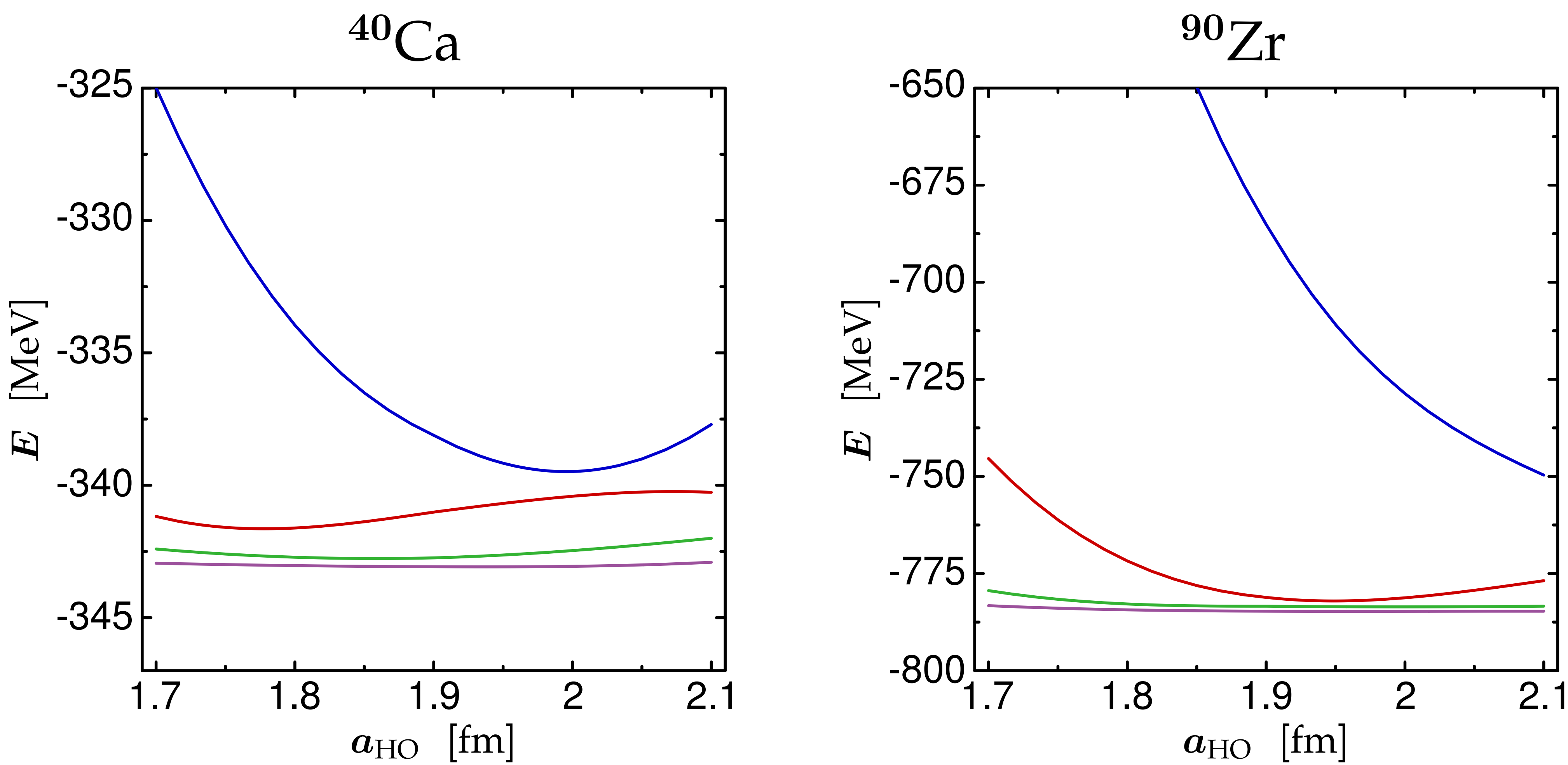
- $h_{\alpha\bar{\alpha}}$ is the single-particle **Hartree-Fock Hamiltonian**

$$h_{\alpha\bar{\alpha}}[D] = \sum_{\alpha',\bar{\alpha}'} \sum_{i=1}^{A} D^{(i)\star}_{\alpha'} D^{(i)}_{\bar{\alpha}'} \;\; {}_a\langle \alpha\alpha' | \, \mathrm{T}_{\text{int}} + \mathrm{V}_{\text{UCOM}} \, | \bar{\alpha}\bar{\alpha}' \rangle_a$$

- **iterative solution** of nonlinear eigenvalue problem:

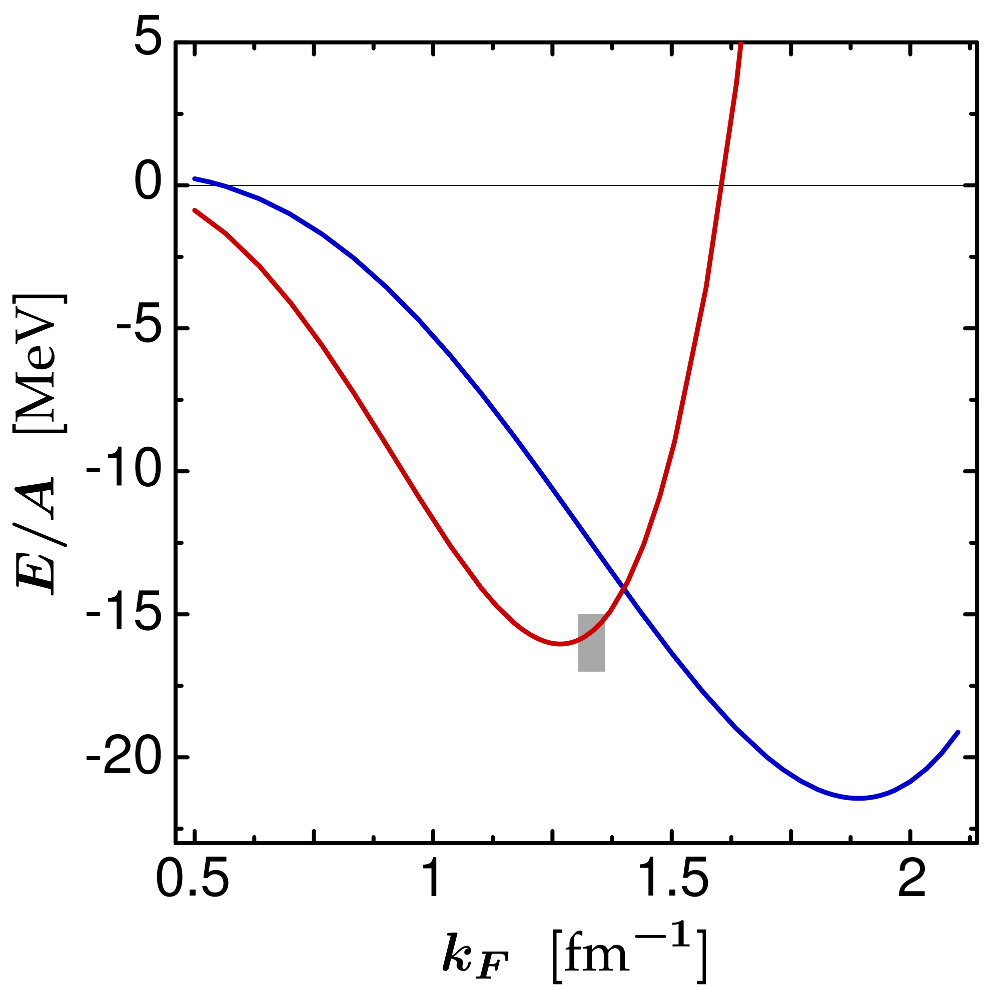


Basis Truncation & Convergence



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

Nuclear Matter: Equation of State

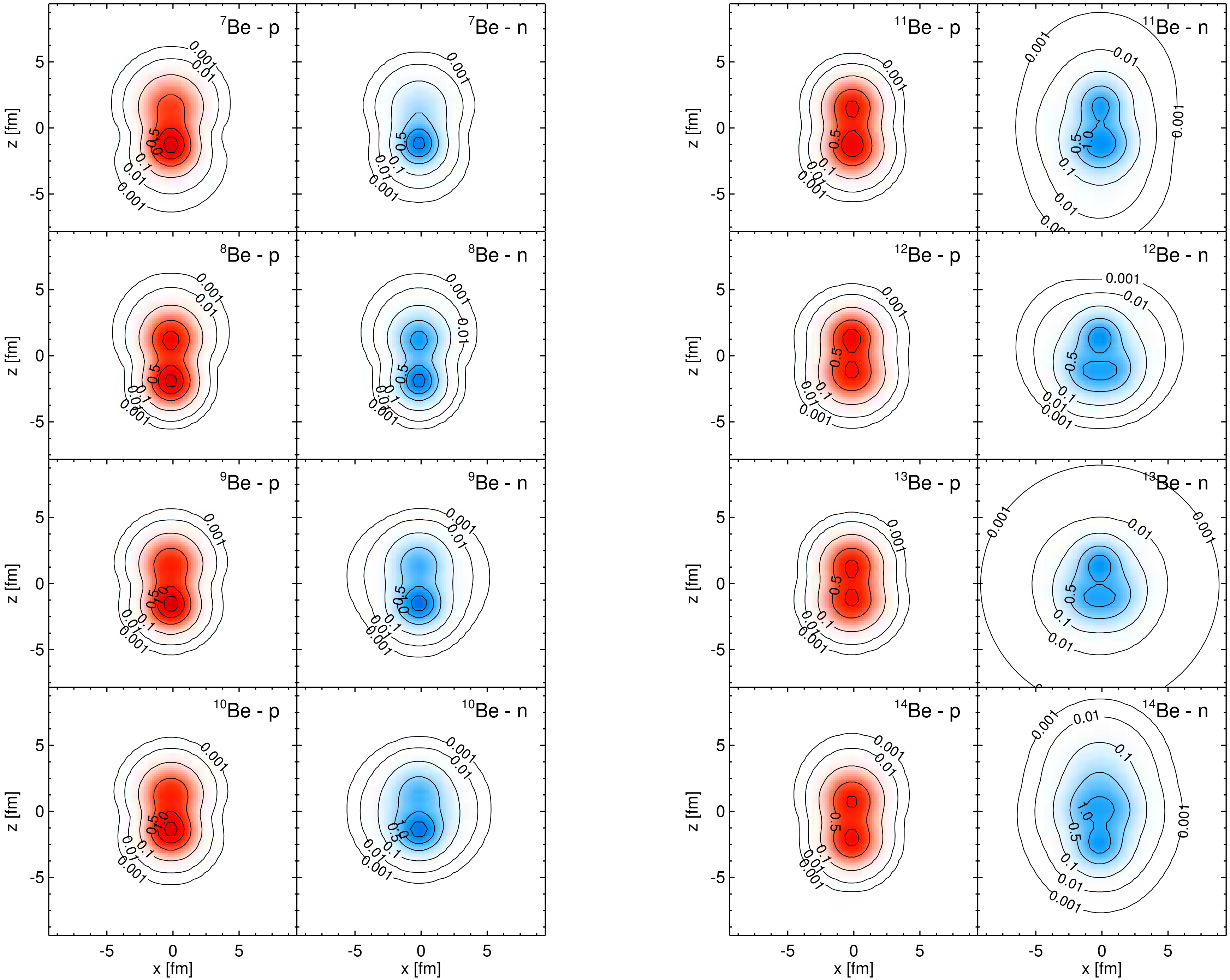


- symmetric nuclear matter
- Slater determinant of plane-wave states $|\vec{k}| \leq k_F$
- correlated momentum space matrix elements
- saturation point:

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

- HvH theorem fulfilled

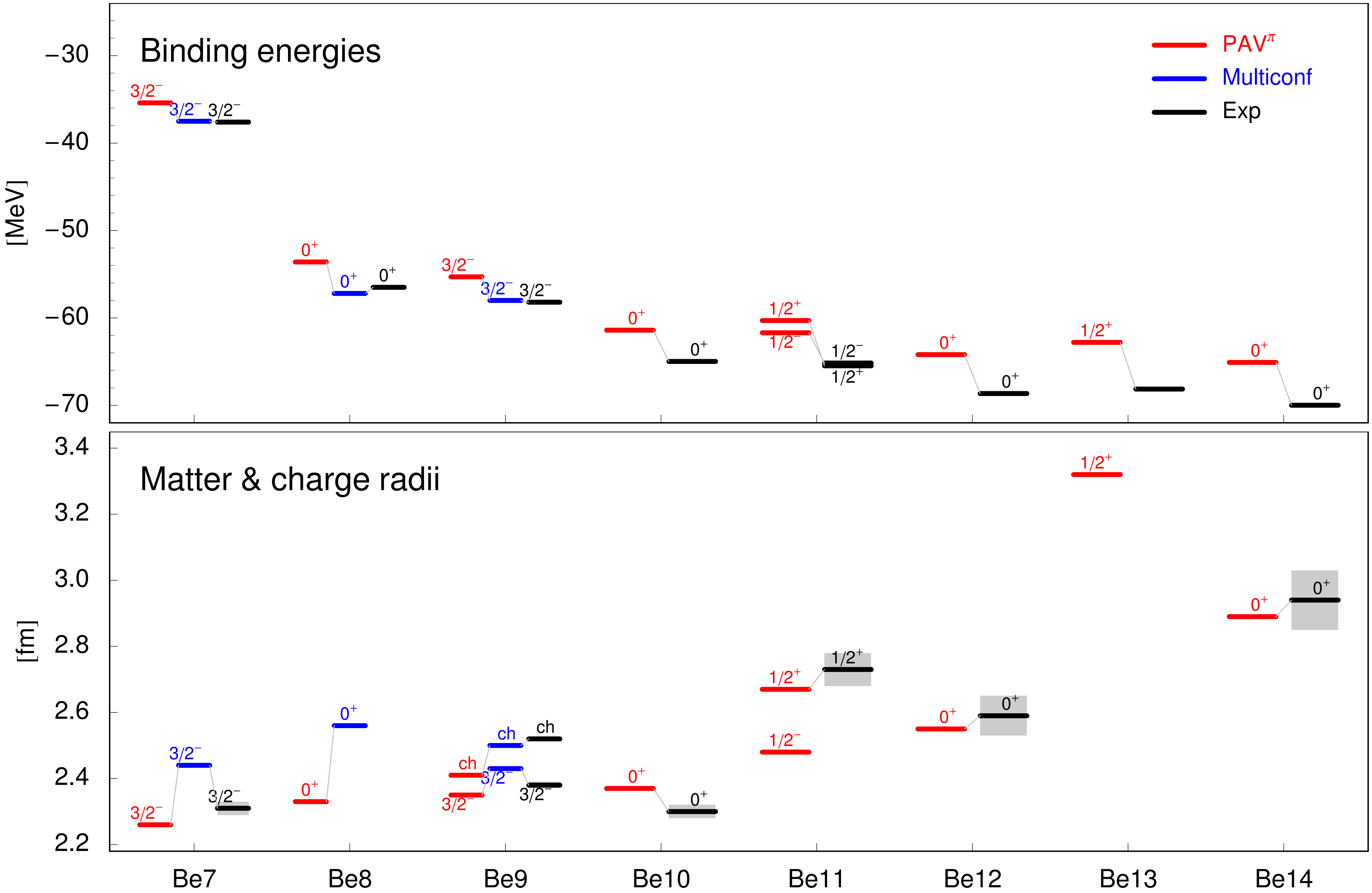
Beryllium Isotopes: Intrinsic Densities



PAV$^{\pi}$

intrinsic densities

Beryllium Isotopes: Energies & Radii



Beryllium Isotopes: Energies & Radii