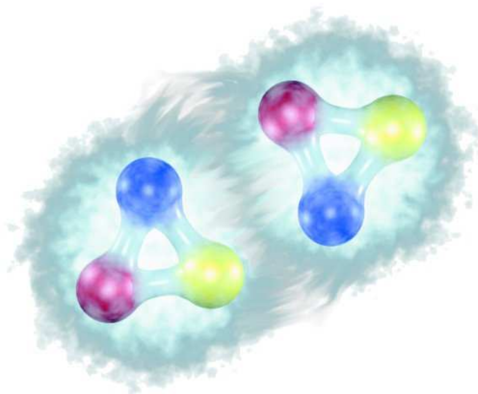
# New Frontiers in Nuclear Structure Theory

## From Realistic Interactions to the Nuclear Chart

Robert Roth

Institut für Kernphysik
Technical University Darmstadt



# Overview

- Motivation
- Nucleon-Nucleon Interactions
- Solving the Many-Body Problem
- Correlations & Unitary Correlation Operator Method
- Applications

# Nuclear Structure in the 21$^{st}$ Century

**new frontiers in nuclear structure physics**

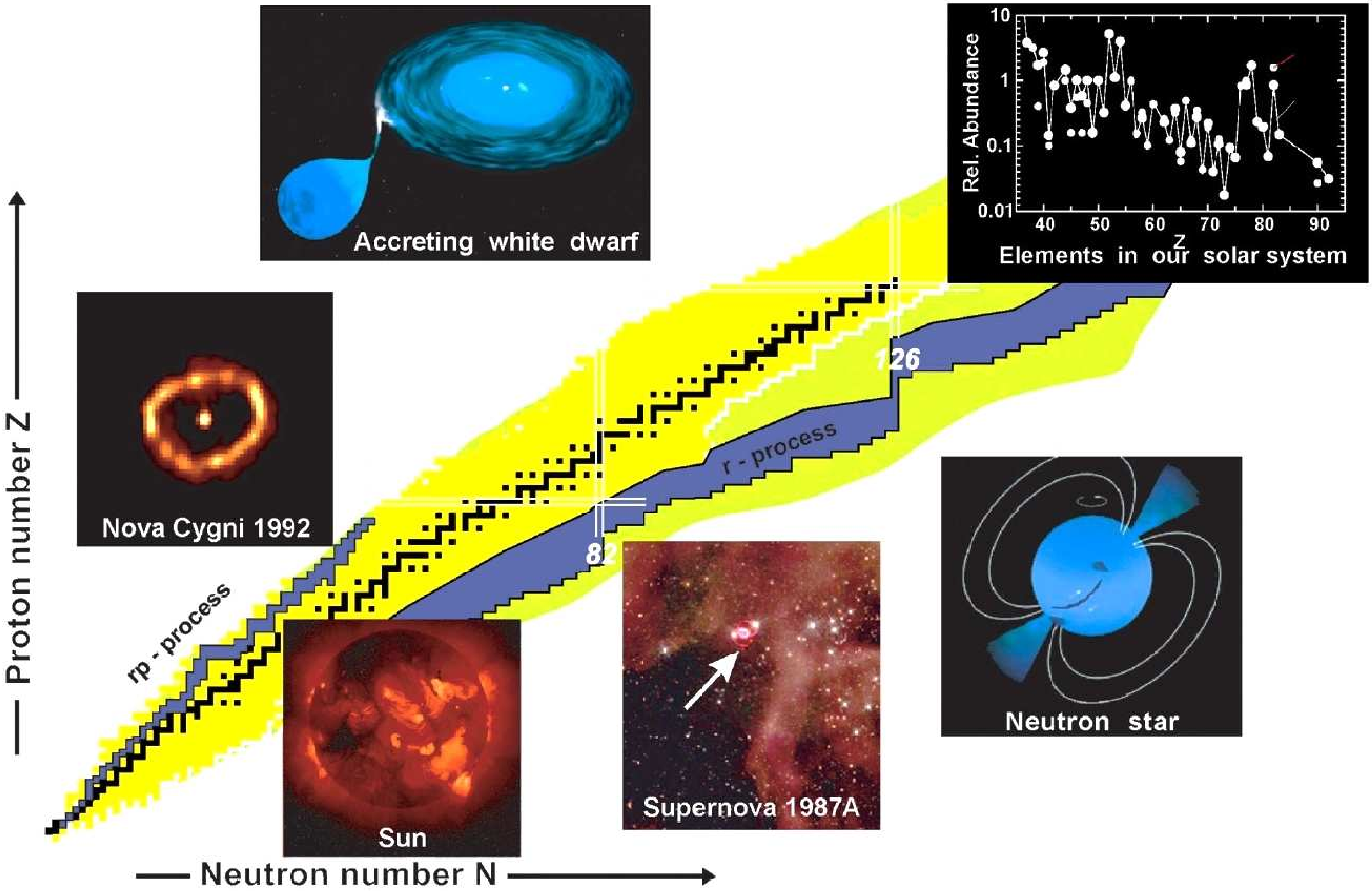
## Experiment

- fundamental astrophysical questions need nuclear input
- possibilities to investigate nuclei far off stability
- new nuclear structure facilities: RIA, FAIR@GSI,...

## Theory

- improved understanding of fundamental degrees of freedom / QCD
- high-precision realistic nucleon-nucleon potentials
- *ab initio* treatment of the many-body problem

# Astrophysical Challenges

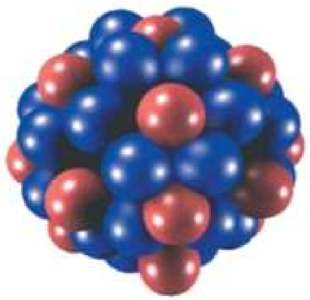


# Theoretical Context

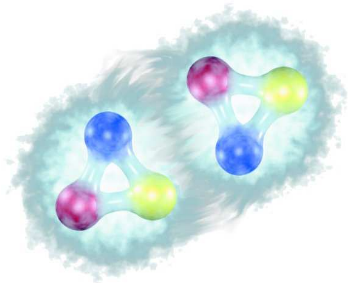
better resolution / more fundamental

Quantum Chromo Dynamics

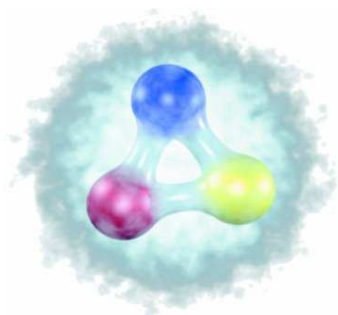
Nuclear Structure



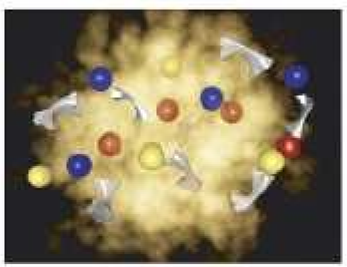
- finite nuclei



- few-nucleon systems
- nucleon-nucleon interaction



- hadron structure



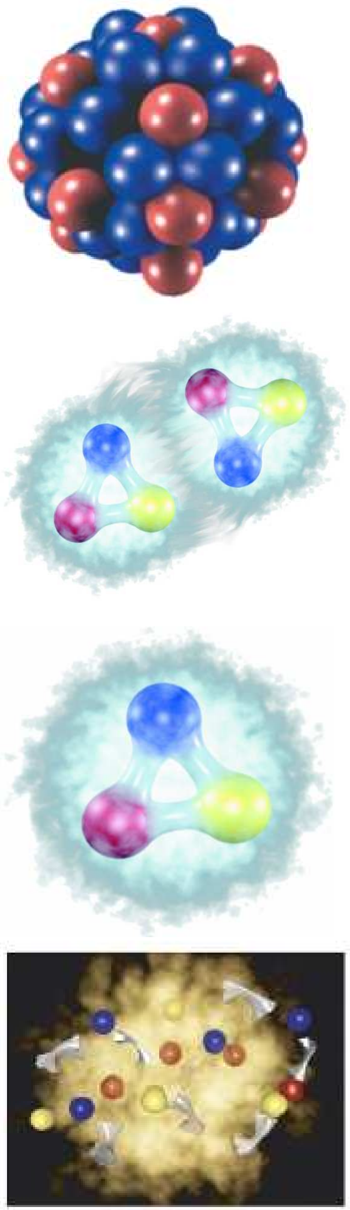
- quarks & gluons
- deconfinement

# Theoretical Context

better resolution / more fundamental

Quantum Chromo Dynamics

Nuclear Structure

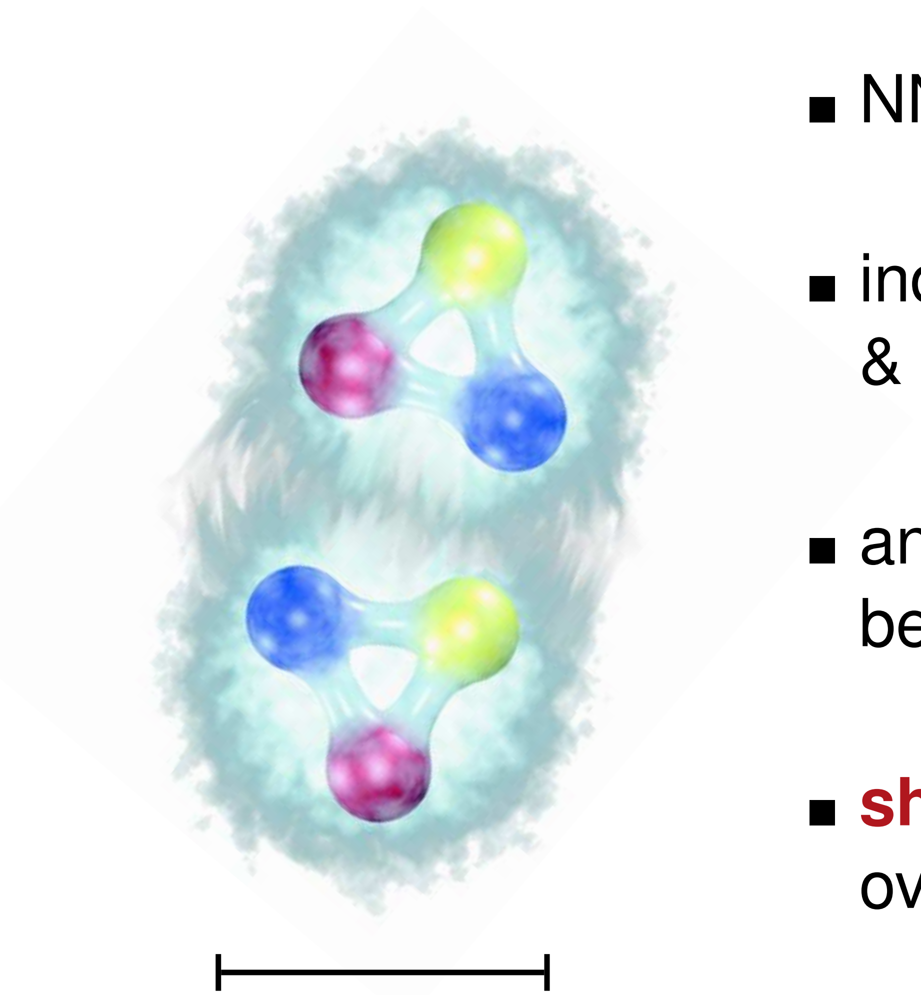


"solve" the quantum many-body problem with this interaction

"derive" a realistic nucleon-nucleon interaction from QCD

# Realistic Nucleon-Nucleon Potentials

# Nature of the NN-Interaction



$\sim 1.6\text{fm}$

$\rho_0^{-1/3} = 1.8\text{fm}$

- NN-interaction is **not fundamental**
- induced via mutual **polarization** of quark & gluon distributions
- analogous to **van der Waals** interaction between neutral atoms
- **short-ranged**: acts only if the nucleons overlap
- genuine **NNN-interaction** is important

# How to Construct the NN-Potential?

- **QCD input**
  - symmetries
  - meson-exchange picture
  - chiral perturbation theory
- **short-range phenomenology**
  - ansatz for short-range behavior
- **experimental two-body data**
  - scattering phase-shifts & deuteron properties
  - reproduced with $\chi^2/\mathrm{datum} \approx 1$

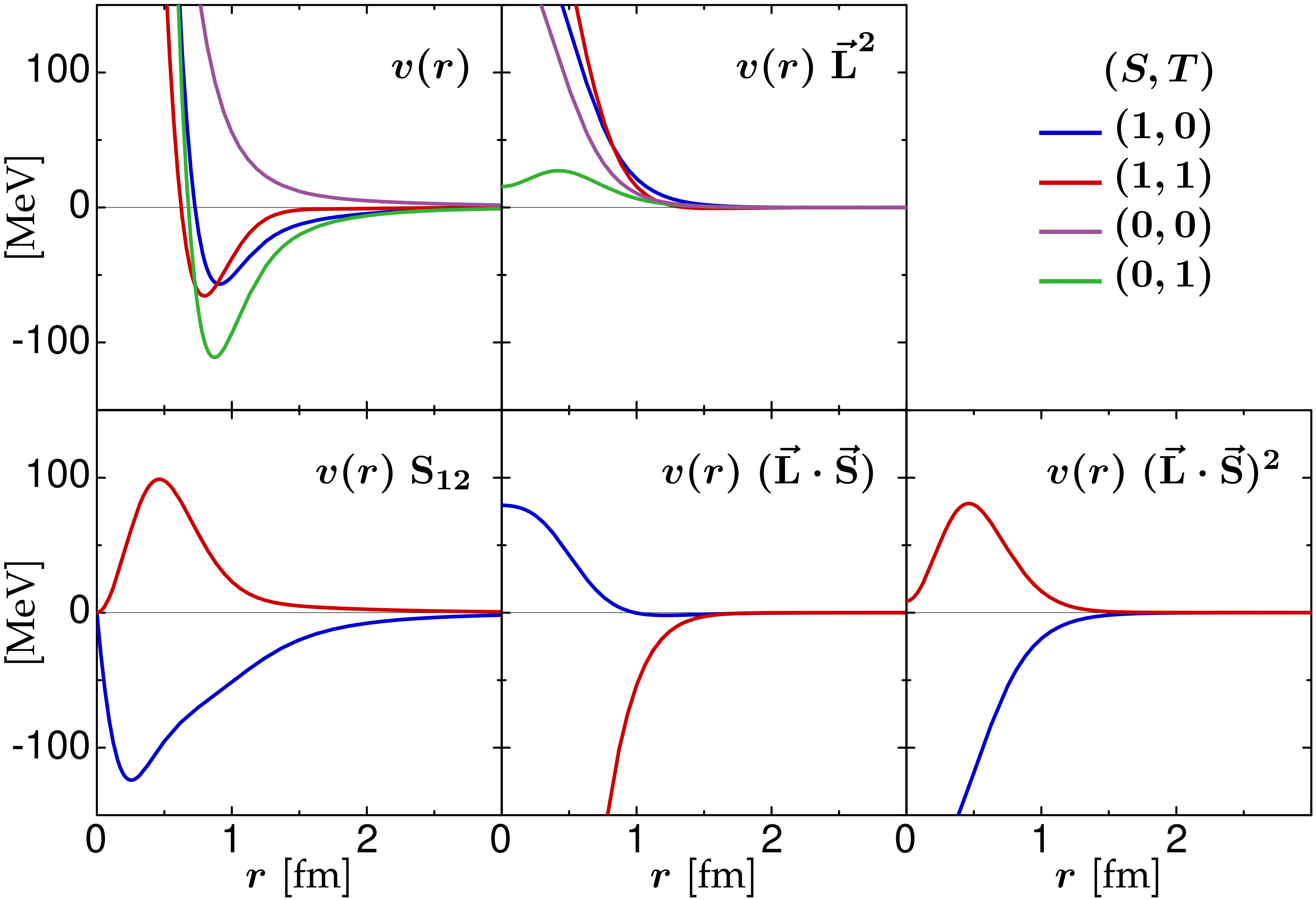
**Argonne V18**

**CD Bonn**

**Nijmegen I/II**

**Chiral...**

# Argonne V18 Potential



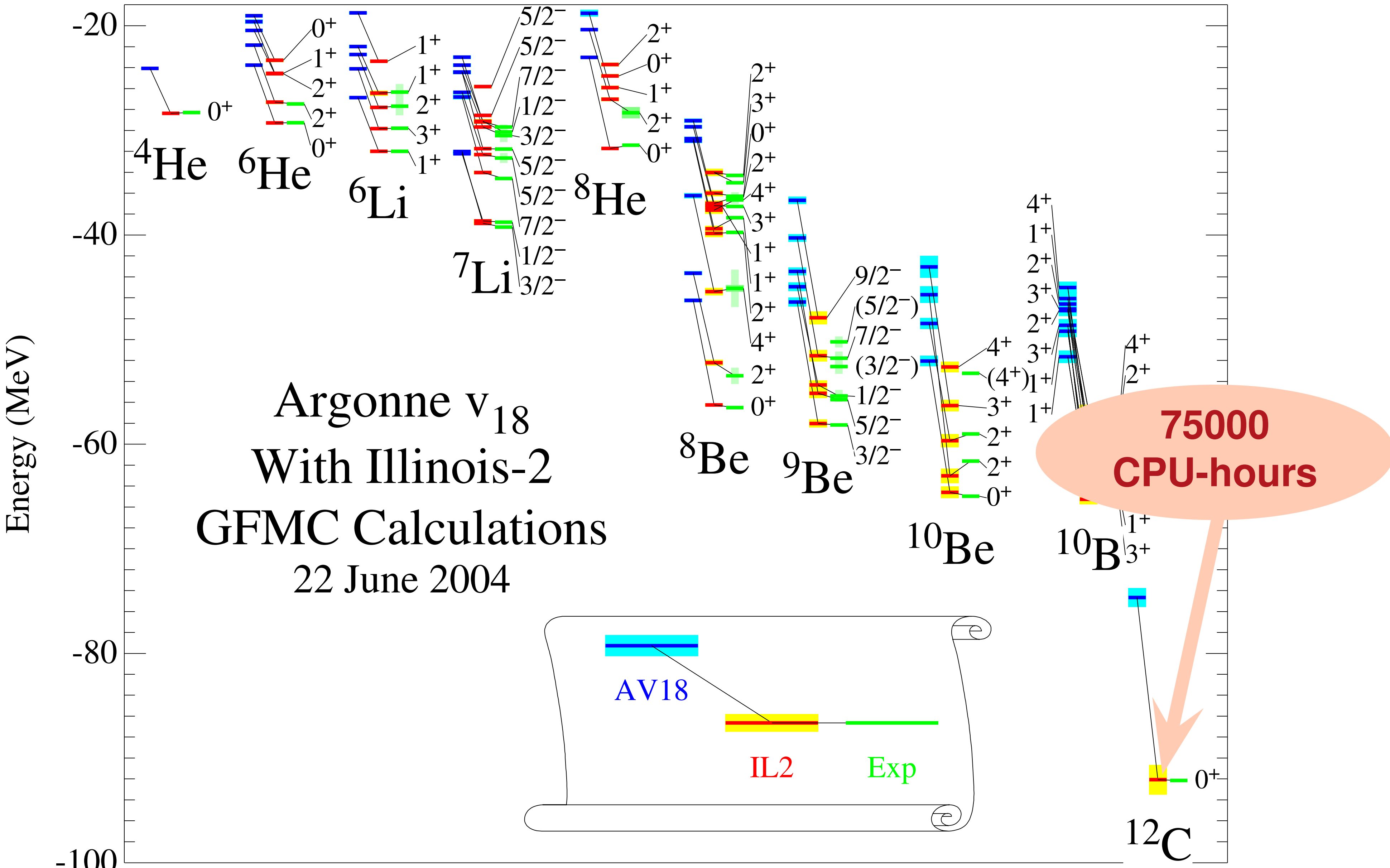
# Nuclear
# Many-Body Problem

# *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 $\boldsymbol{A}$-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.

# Our Goal

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

bound to **simple Hilbert spaces** for large particle numbers

need to deal with strong **interaction-induced correlations**

# Correlations in Nuclei

# What are Correlations?

**correlations**

**=**

everything beyond the independent particle picture

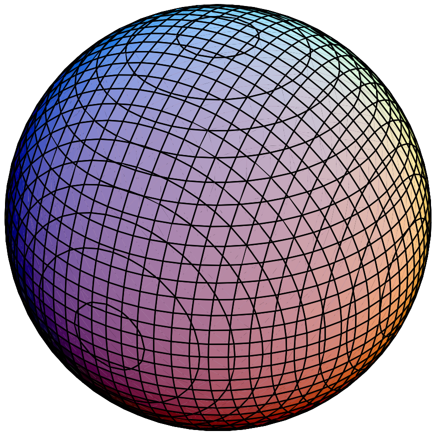
- the quantum state of $A$ independent (non-interacting) fermions is a **Slater determinant**

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

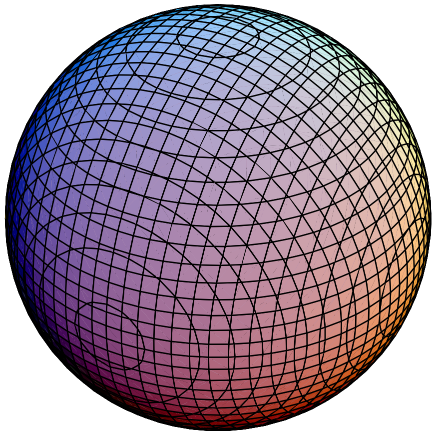
- Slater determinants **cannot describe correlations** by definition

# Deuteron: Manifestation of Correlations

$$\boldsymbol{M_S = 0}$$
$$\tfrac{1}{\sqrt{2}}(\,|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$$



$$\boldsymbol{M_S = \pm 1}$$
$$|\uparrow\uparrow\rangle,\ |\downarrow\downarrow\rangle$$

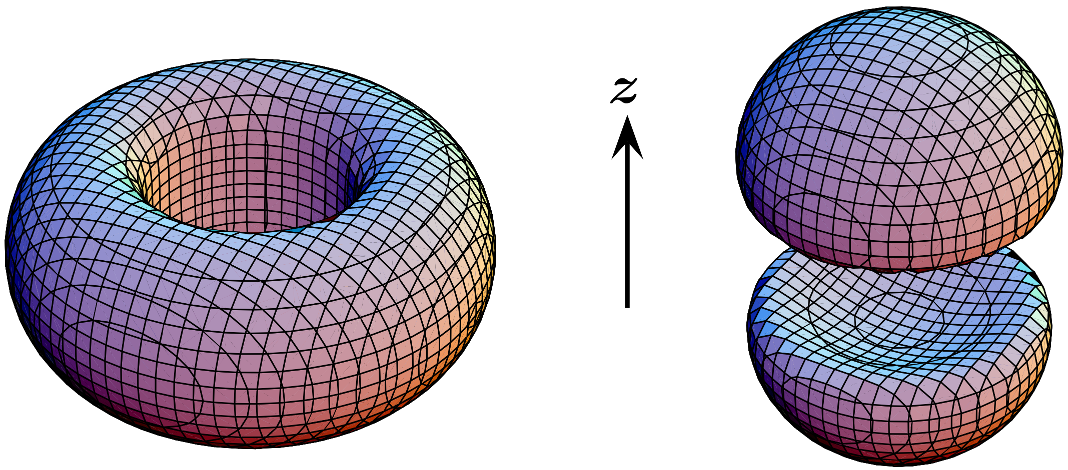


- spin-projected two-body density $\rho^{(2)}_{1,M_S}(\vec{r})$
- **uncorrelated** two-body state

# Deuteron: Manifestation of Correlations

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

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




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

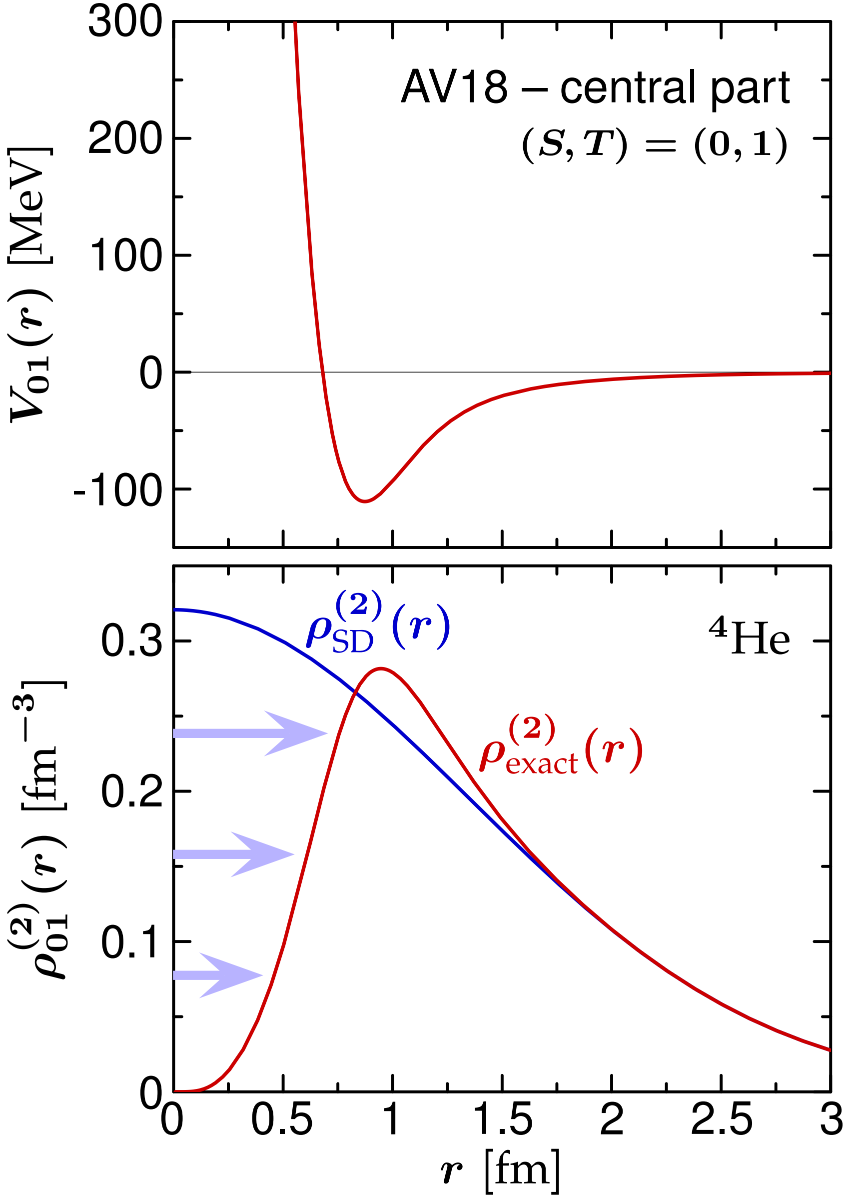
two-body density fully suppressed at small particle distances $|\vec{r}|$

**central correlations**

angular distribution depends strongly on relative spin orientation

**tensor correlations**

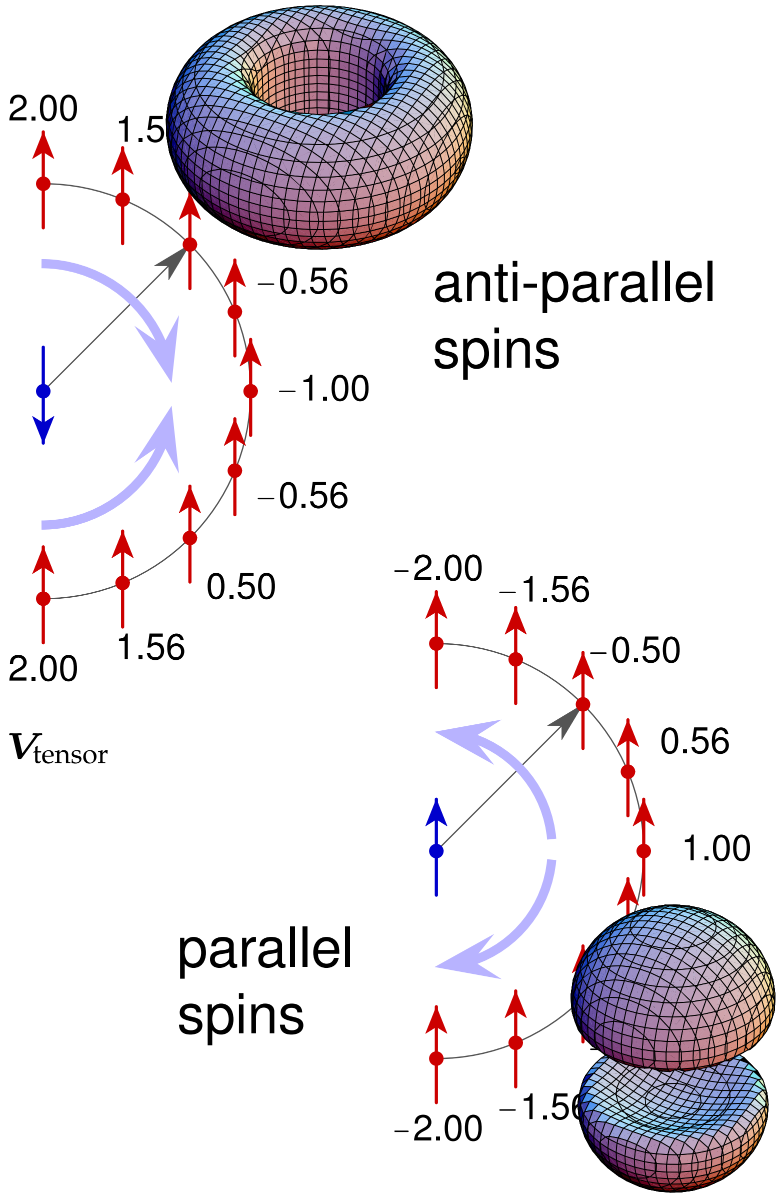
# Central Correlations




- strong repulsive core in central part of realistic interactions
- suppression of the probability density for finding two nucleons within the core region ➔ **central correlations**

can be described by **"shifting" 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**

can be described by
**“rotating” nucleons towards pole or equator depending on spin**

# 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

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

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

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

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

## Correlated States

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

## Correlated Operators

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

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

# Central and Tensor Correlators

$$\mathrm{C} = \mathrm{C}_{\Omega}\mathrm{C}_{r}$$

## Central Correlator $\mathrm{C}_r$

- 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 $\mathrm{C}_\Omega$

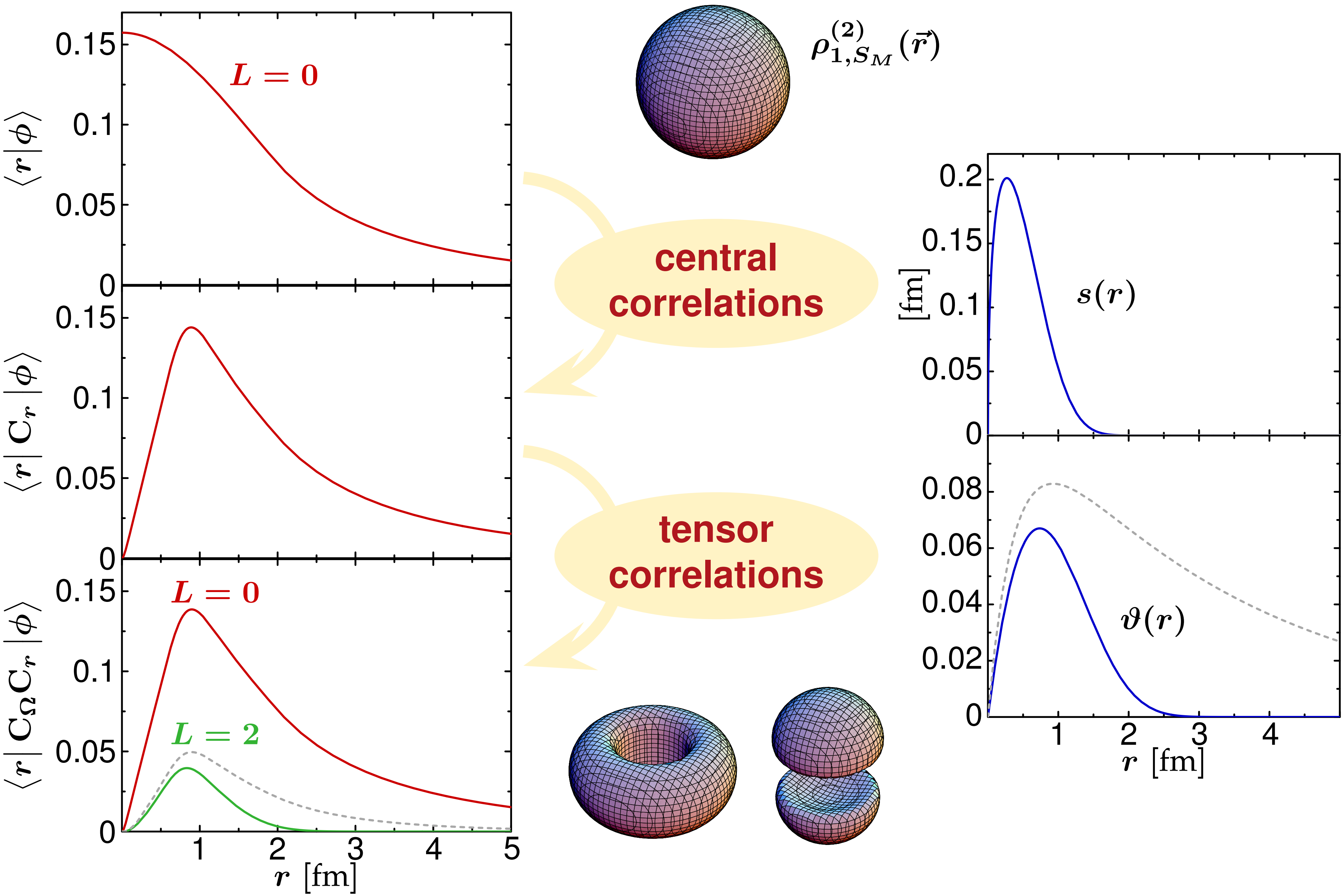
- angular shift depending on the orientation of spin and relative coordinate of a nucleon pair

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

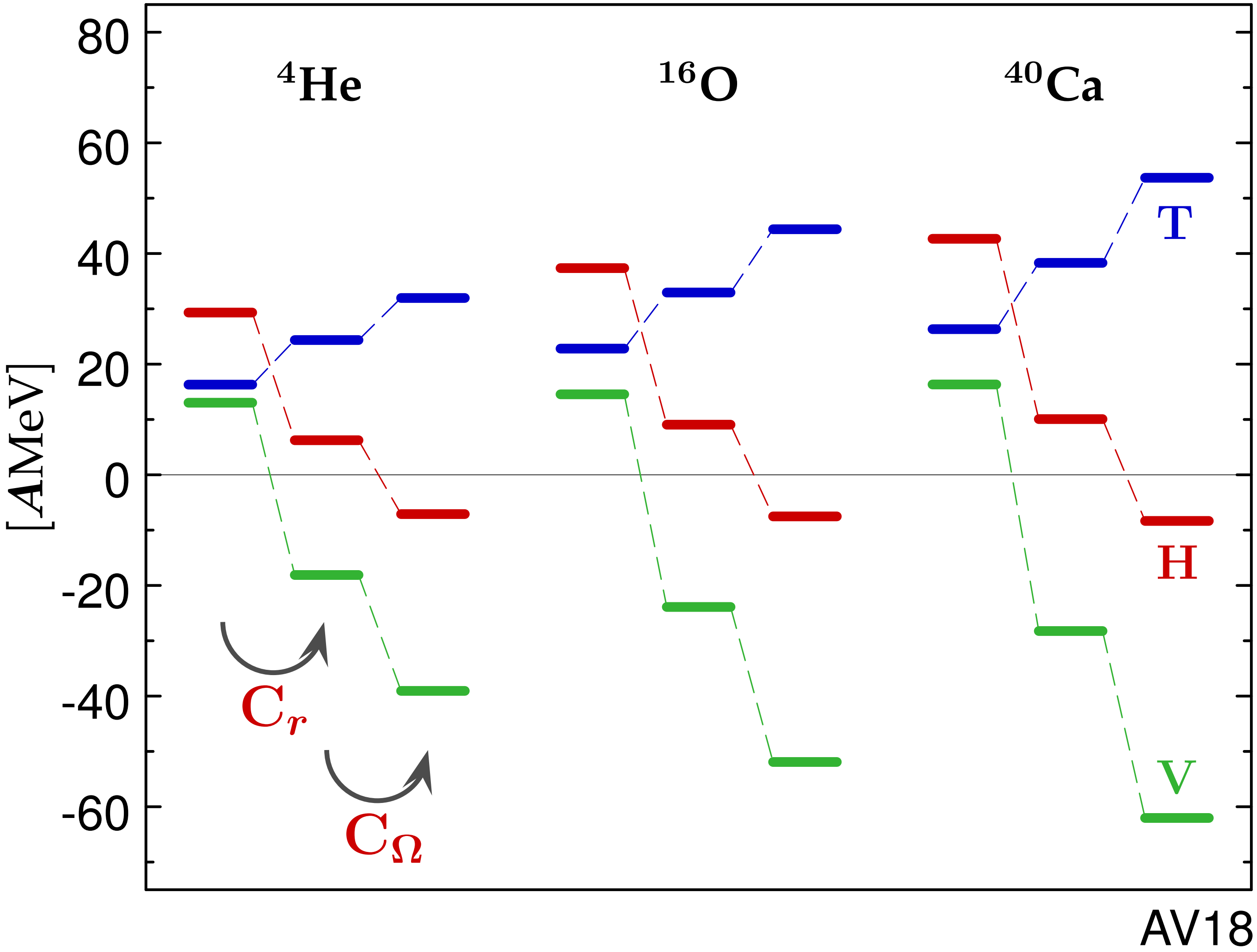
$$\vec{\mathrm{q}}_\Omega = \vec{\mathrm{q}} - \tfrac{\vec{\mathrm{r}}}{\mathrm{r}}\ \mathrm{q}_r$$

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

# Correlated States



# 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:

# Hartree-Fock Calculations

# UCOM-Hartree-Fock Approach

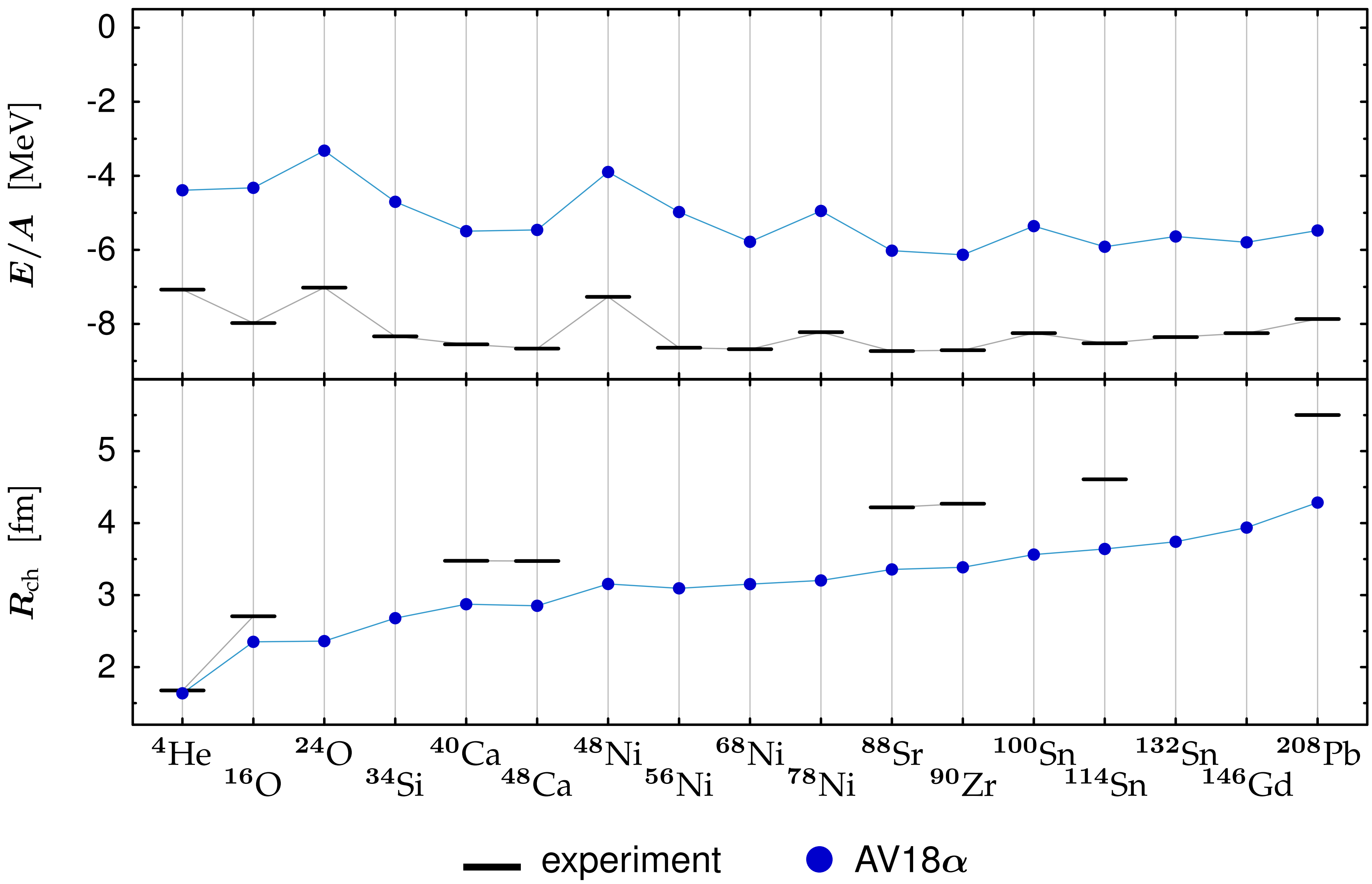
**Standard Hartree-Fock**

**+**

**Matrix Elements of Correlated Realistic NN-Interaction $V_{UCOM}$**

- many-body state is a **Slater determinant** of single-particle states obtained by energy minimization
- **correlations cannot be described** by Hartree-Fock states
- bare realistic NN-potential leads to **unbound nuclei**

# Correlated Argonne V18



# Missing Pieces

**long-range correlations**

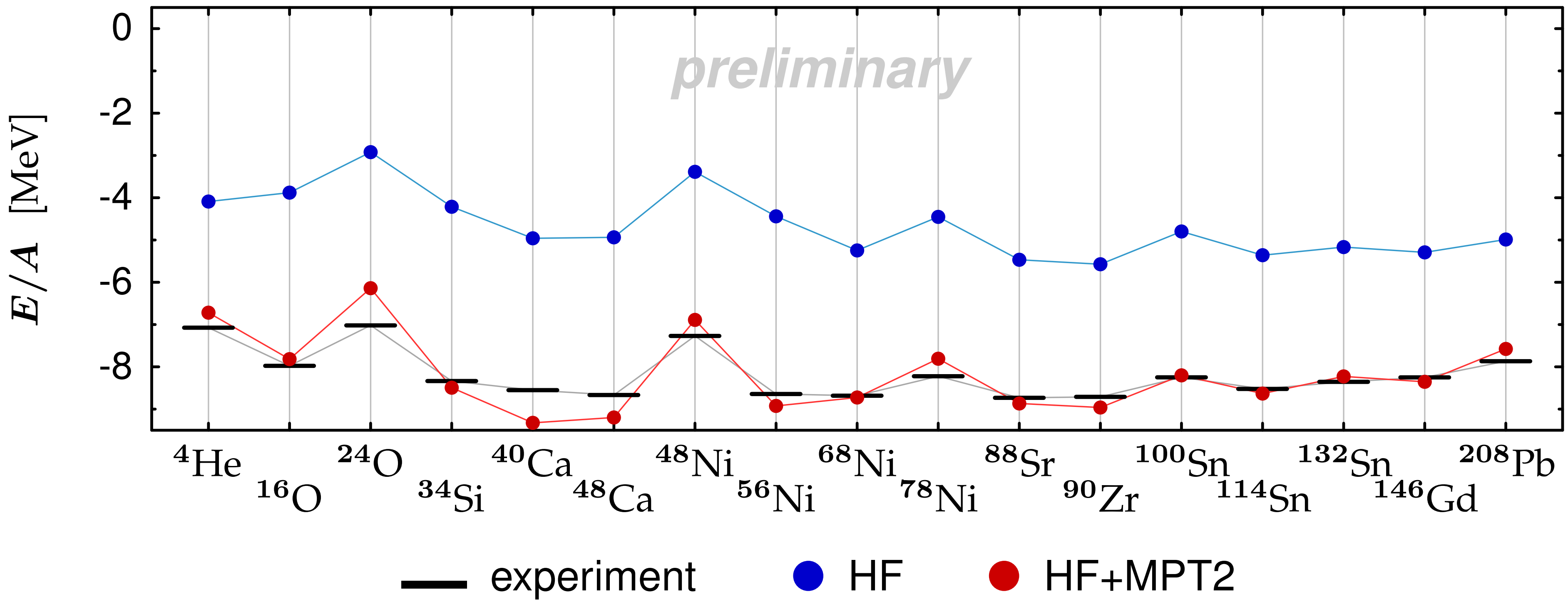
## Ab Initio Strategy

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

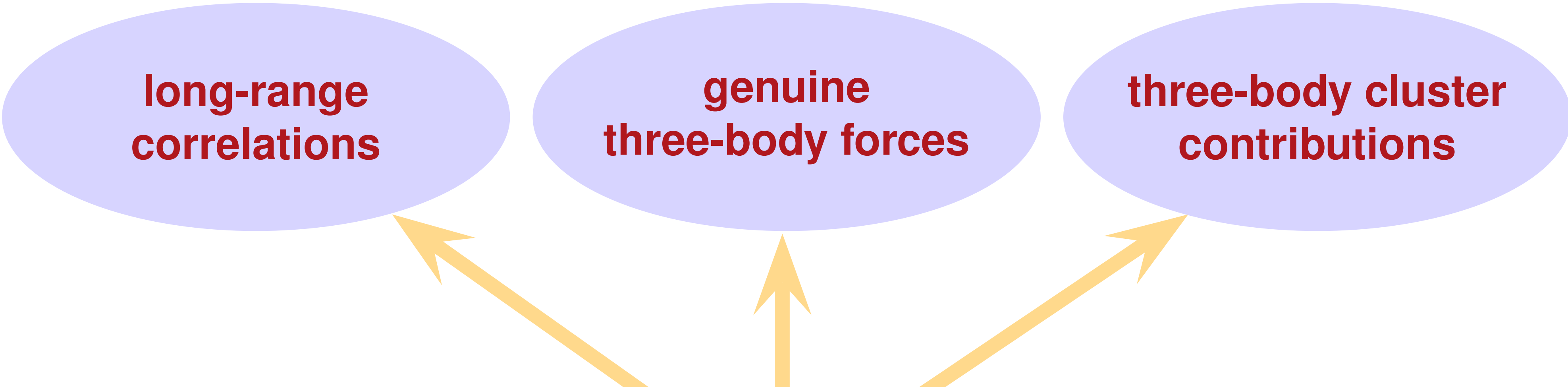
# Long-Range Correlations

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

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



# Missing Pieces



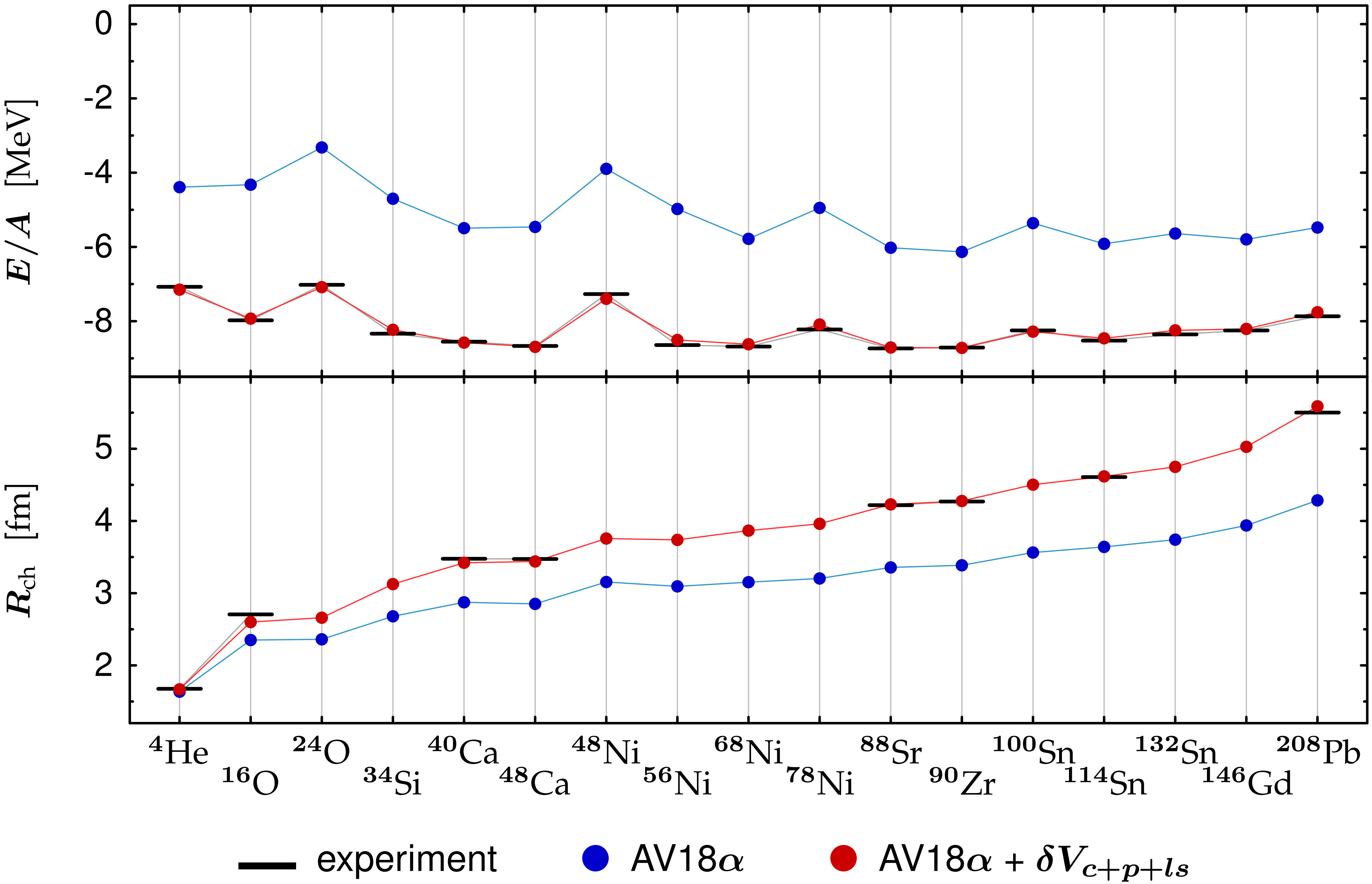

## Pragmatic Approach

- phenomenological two-body correction

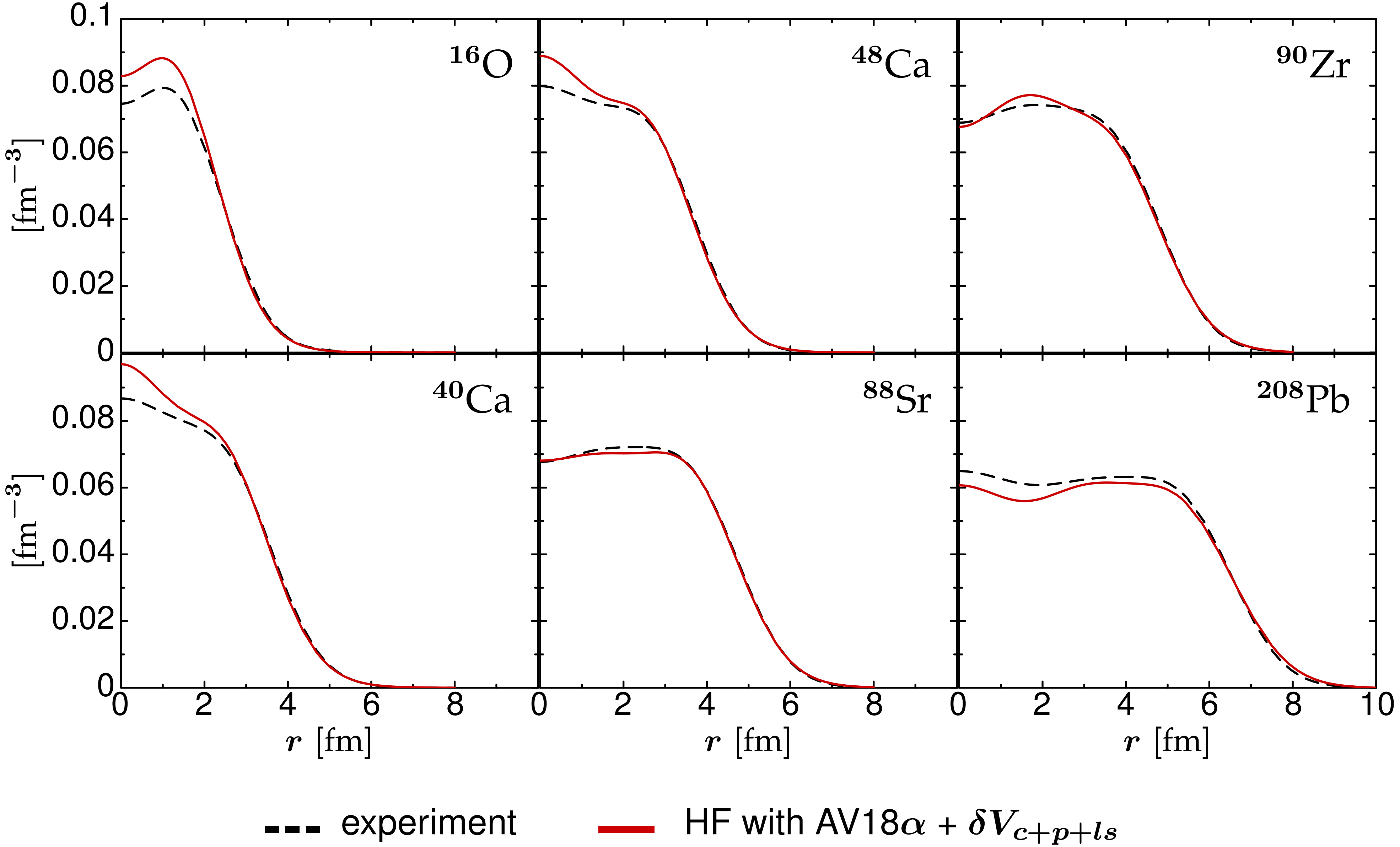
$$\delta \mathrm{V}_{c+p+ls} = v_1(\mathbf{r}) + \vec{\mathbf{q}}\, v_{qq}(\mathbf{r})\, \vec{\mathbf{q}} + v_{LS}(\mathbf{r})\, \vec{\mathbf{L}} \cdot \vec{\mathbf{S}}$$

- Gaussian radial dependencies with fixed ranges
- strengths used as fit parameters
  (fitted to $^{4}\mathrm{He}$, $^{16}\mathrm{O}$, $^{24}\mathrm{O}$, $^{40}\mathrm{Ca}$, $^{48}\mathrm{Ca}$, $^{48}\mathrm{Ni}$, $^{90}\mathrm{Zr}$)

# Correlated Argonne V18 + Correction



# Charge Distributions



Application II

# Fermionic Molecular Dynamics (FMD)

# UCOM-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

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

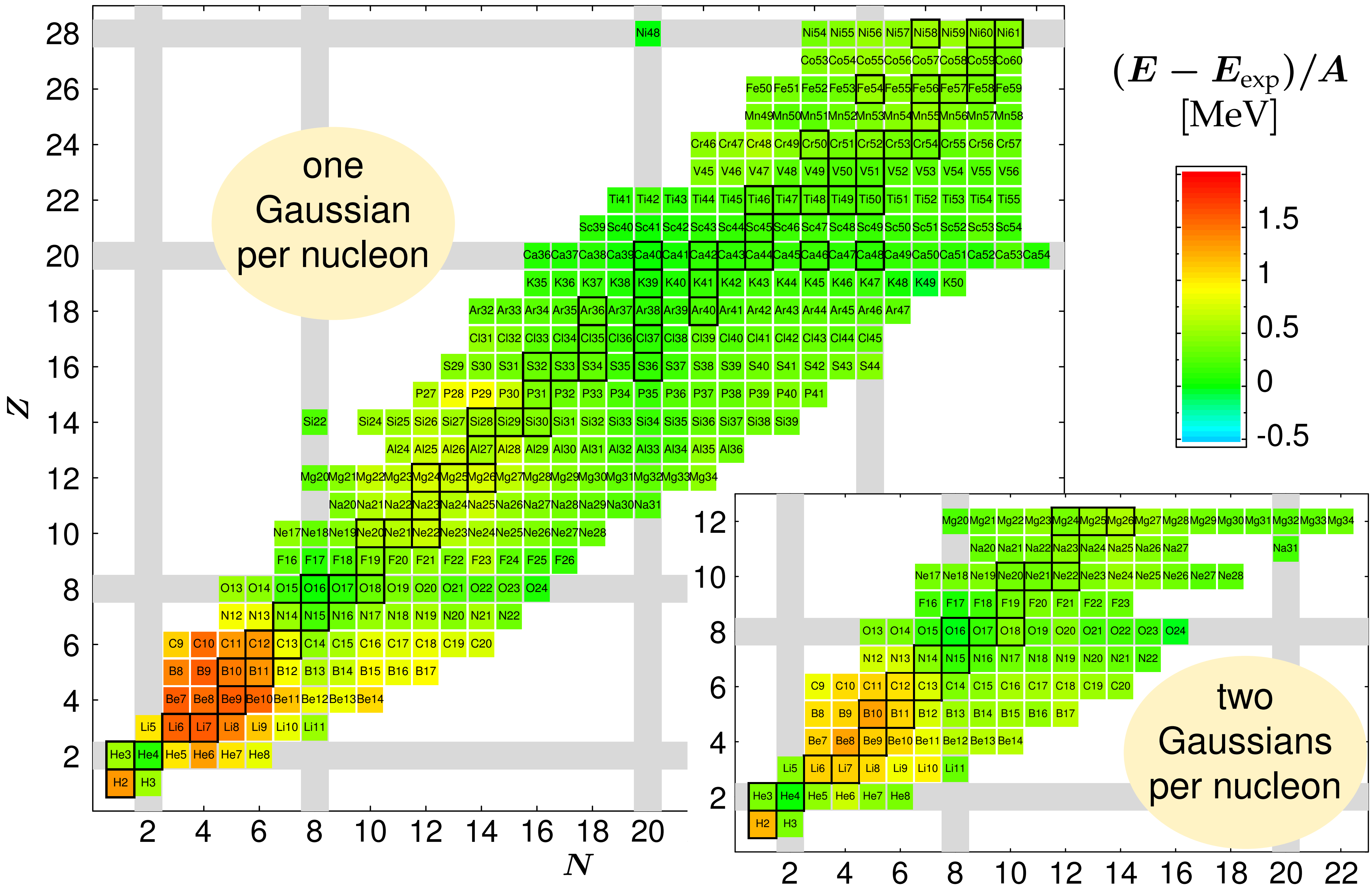
## Variation

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

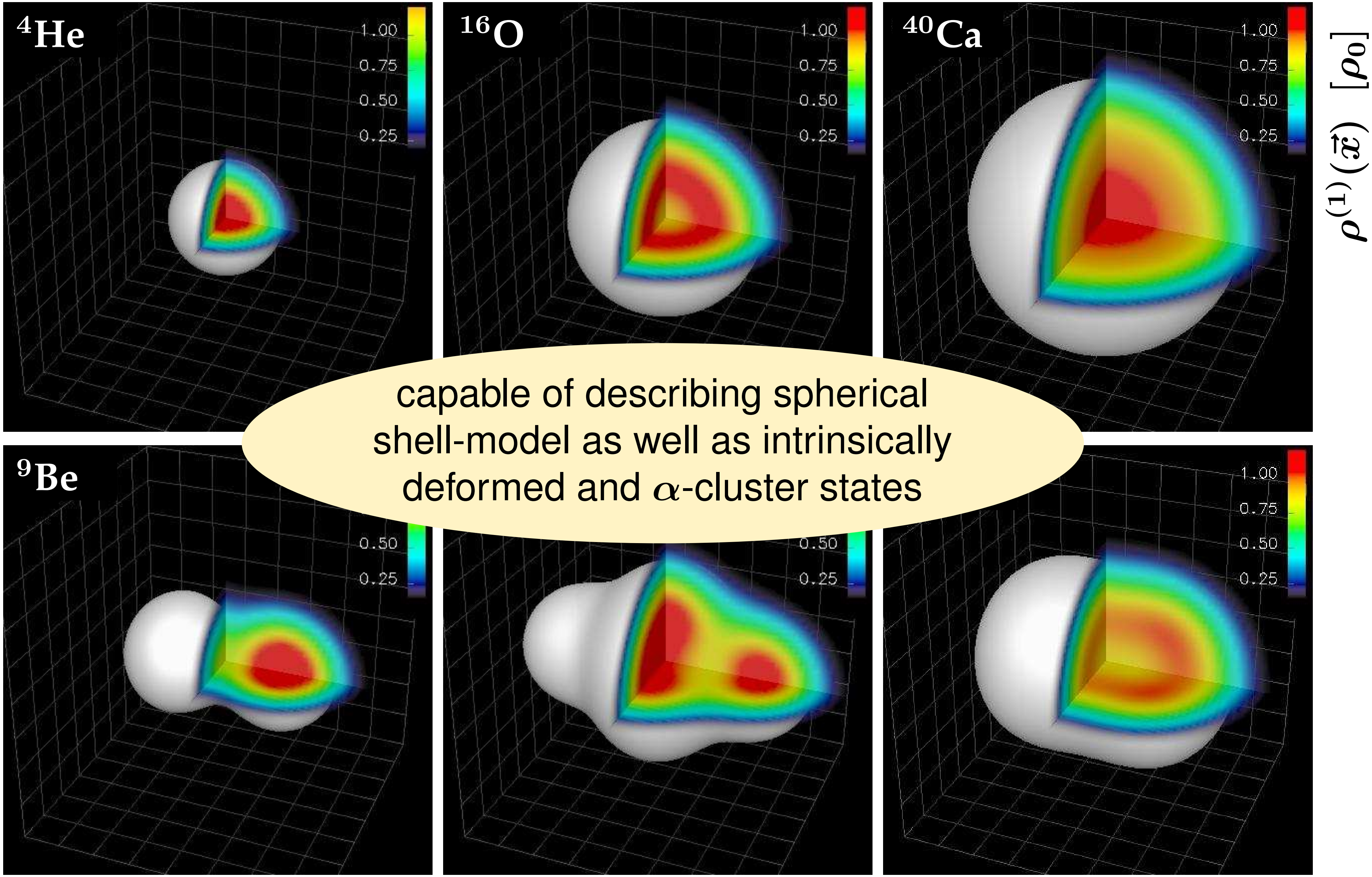
## Diagonalization

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

# Variation: Chart of Nuclei



# Intrinsic One-Body Density Distributions

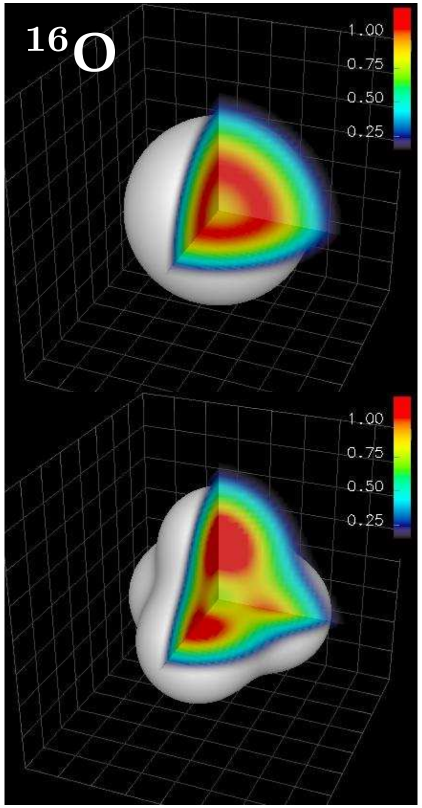



capable of describing spherical shell-model as well as intrinsically deformed and $\alpha$-cluster states

# Beyond Simple Variation

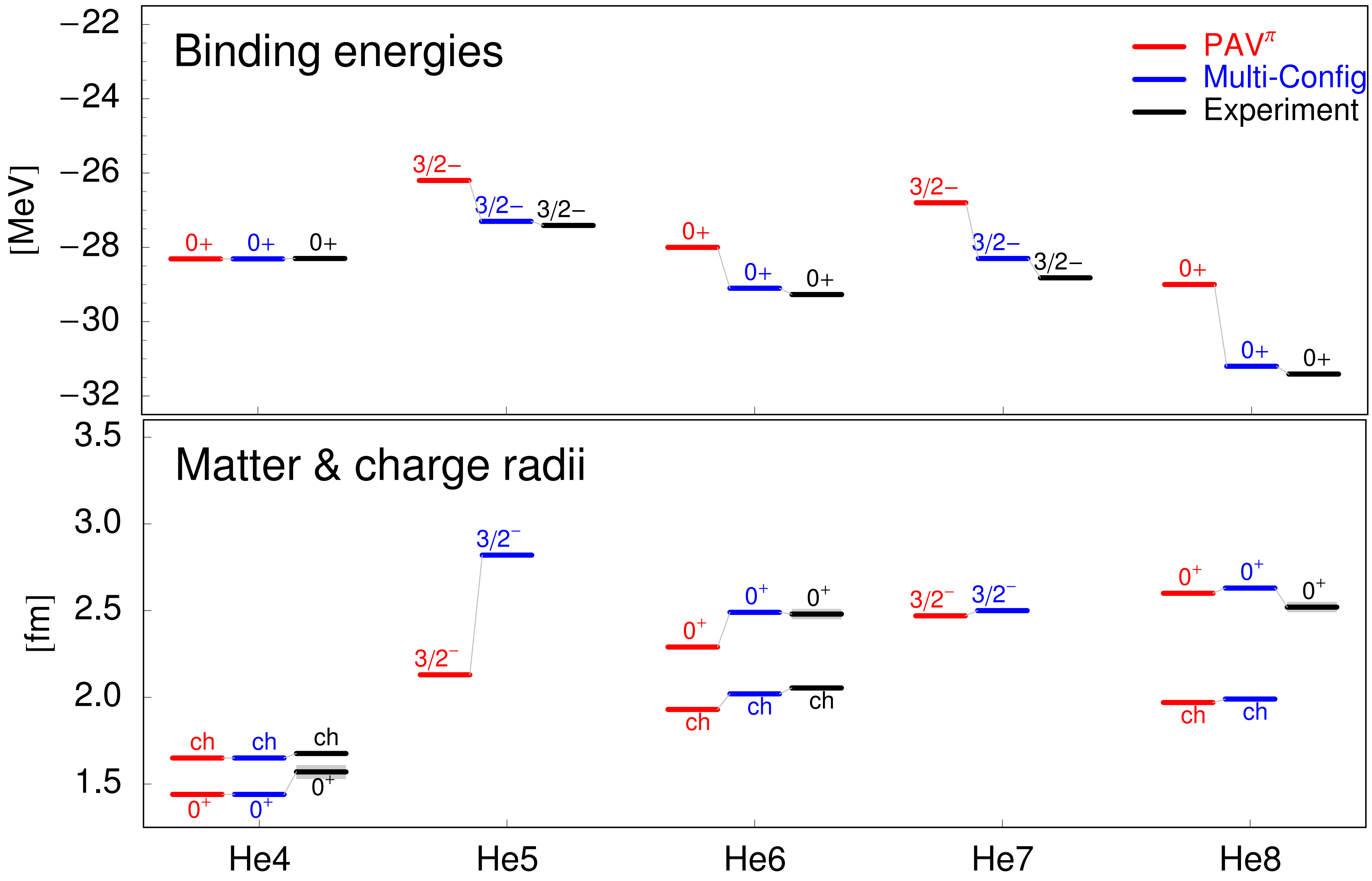
- **Projection after Variation (PAV)**
  - restore inversion and rotational symmetry by angular momentum projection

- **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)

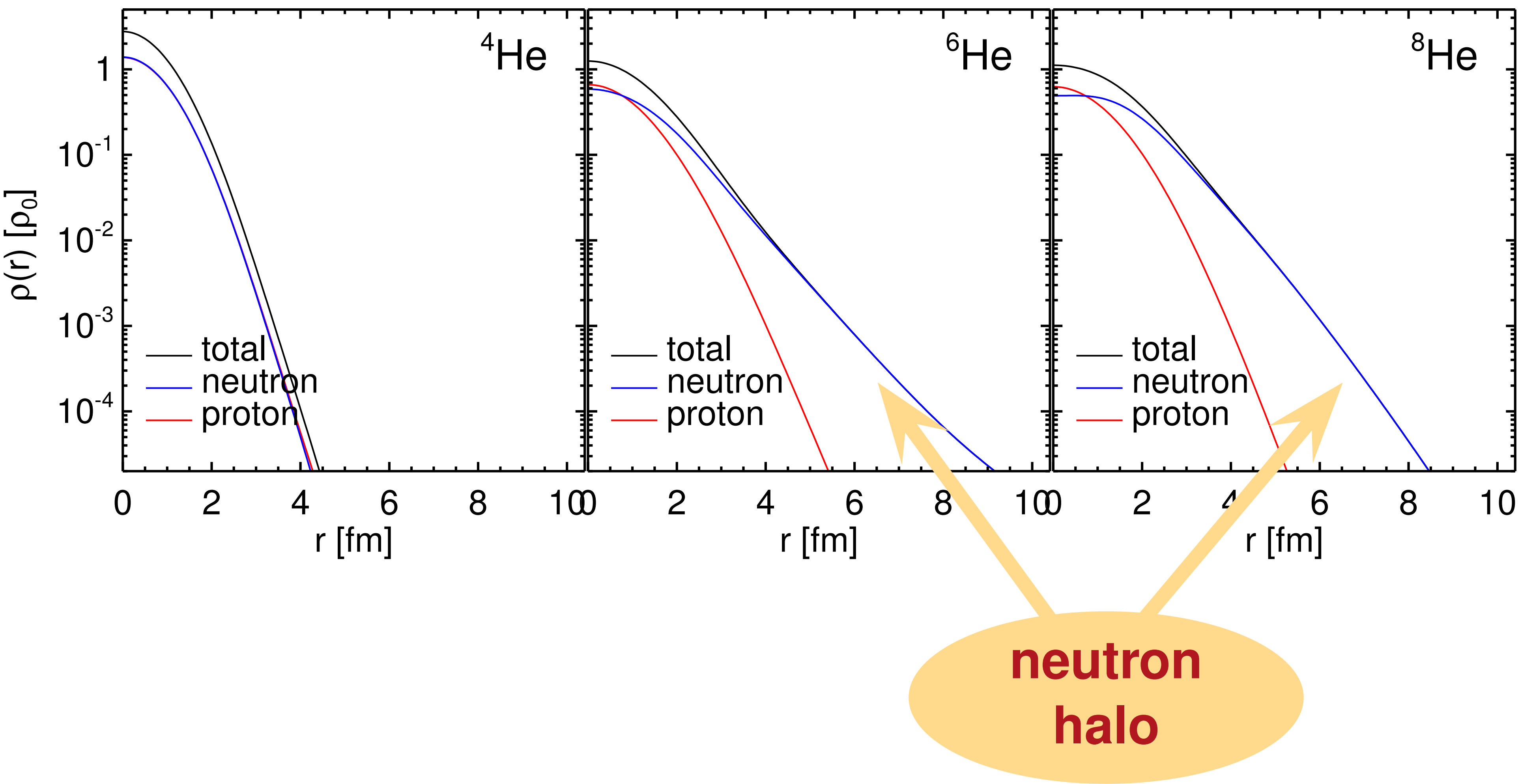



- **Multi-Configuration**
  - diagonalization within a set of different Slater determinants

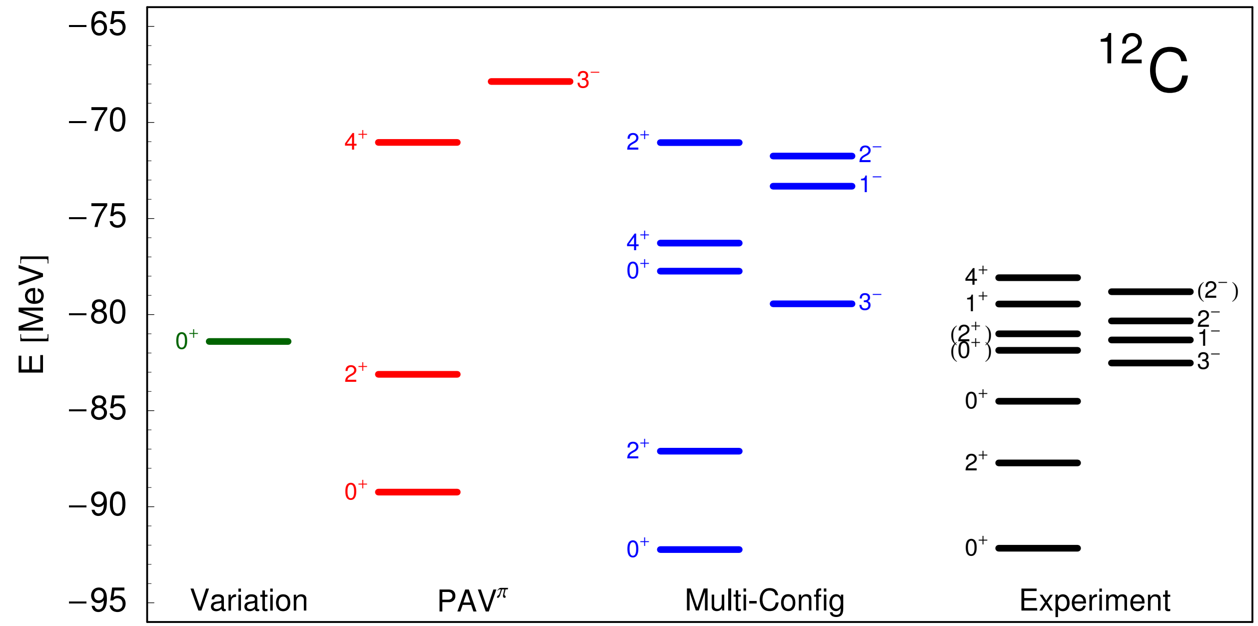
# Helium Isotopes: Energies & Radii

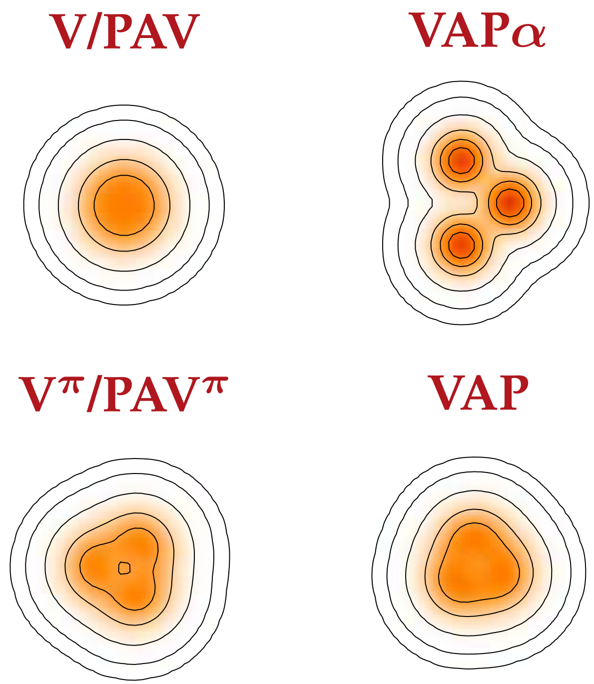


# Helium Isotopes: Density Profiles

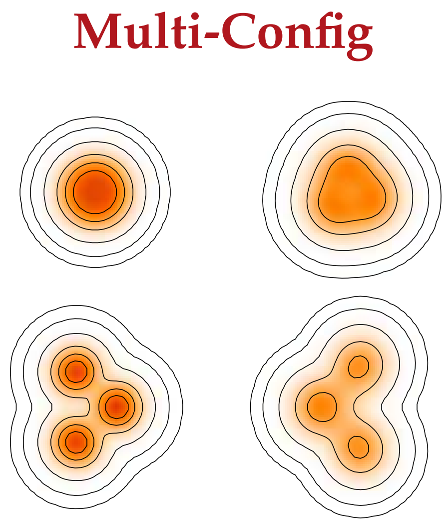


# Structure of $^{12}$C

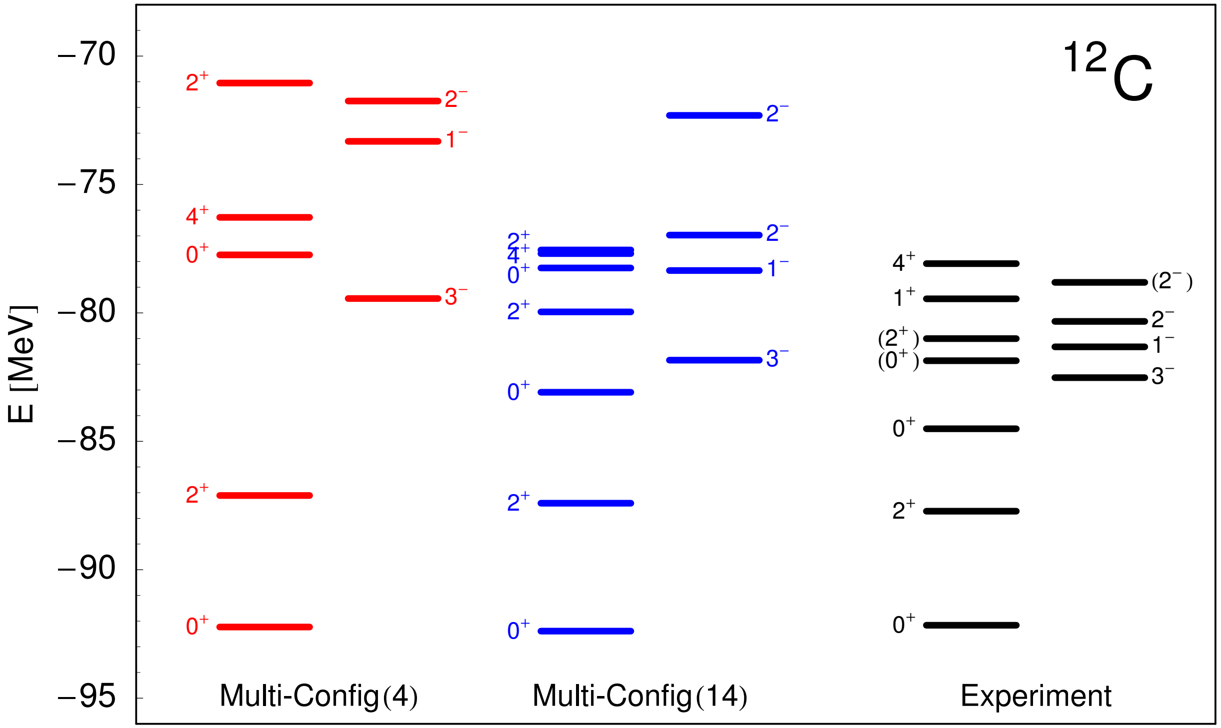


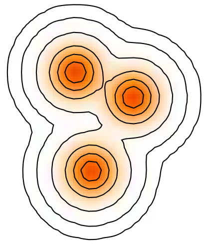



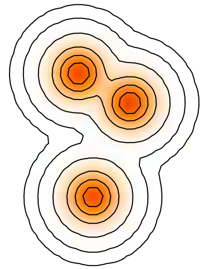

| | $E$ [MeV] | $R_{ch}$ [fm] | $B(E2)$ [$e^2$ fm$^4$] |
|---|---|---|---|
| V/PAV | 81.4 | 2.36 | - |
| VAP $\alpha$-cluster | 79.1 | 2.70 | 76.9 |
| PAV$^{\pi}$ | 88.5 | 2.51 | 36.3 |
| VAP | 89.2 | 2.42 | 26.8 |
| Multi-Config | 92.2 | 2.52 | 42.8 |
| Experiment | 92.2 | 2.47 | $39.7 \pm 3.3$ |

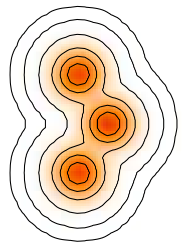


# Structure of $^{12}$C — Hoyle State




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

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

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

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

# Conclusions

- exciting times for nuclear structure physics!
- realistic NN-potentials & *ab initio* calculations
- systematic schemes to derive effective (correlated / low-momentum) interactions
- innovative ways to treat the many-body problem

**unified description of nuclear structure across the whole nuclear chart is within reach**

# Epilogue

- **thanks to my group & my collaborators**
  - A. Ehrlich, H. Hergert, N. Paar, P. Papakonstantinou,
    Technical University Darmstadt
  - H. Feldmeier, T. Neff
    Gesellschaft für Schwerionenforschung (GSI)

SFB 634

supported by DFG through SFB 634
“Nuclear Structure and Nuclear Astrophysics...”