# New Frontiers in Nuclear Structure Theory

## From Realistic Interactions to the Nuclear Chart

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# Overview

- Motivation
  - Nucleon-Nucleon Interactions
  - Solving the Many-Body Problem
- Correlations & Unitary Correlation Operator Method
- Applications
  - No Core Shell Model
  - Hartree-Fock and beyond
  - Fermionic Molecular Dynamics

# Nuclear Structure in the 21st Century

**new frontiers in nuclear structure physics**

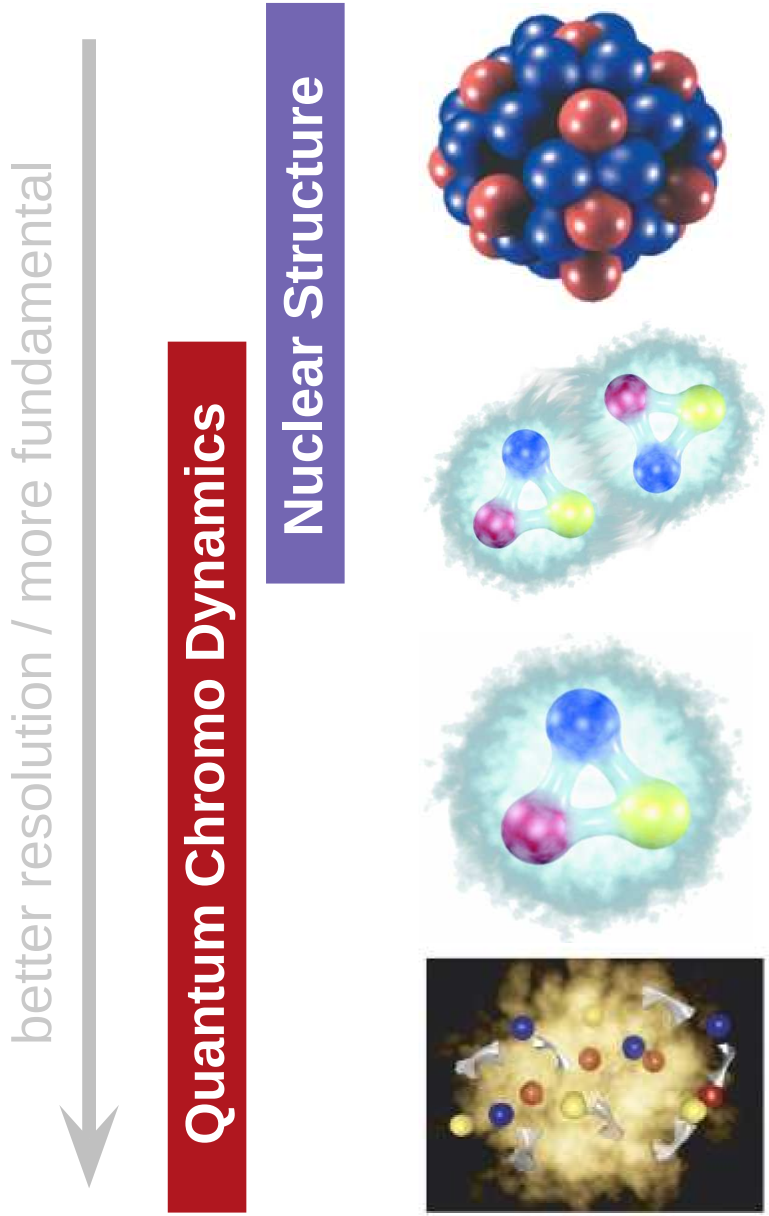
## Experiment

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

## Theory

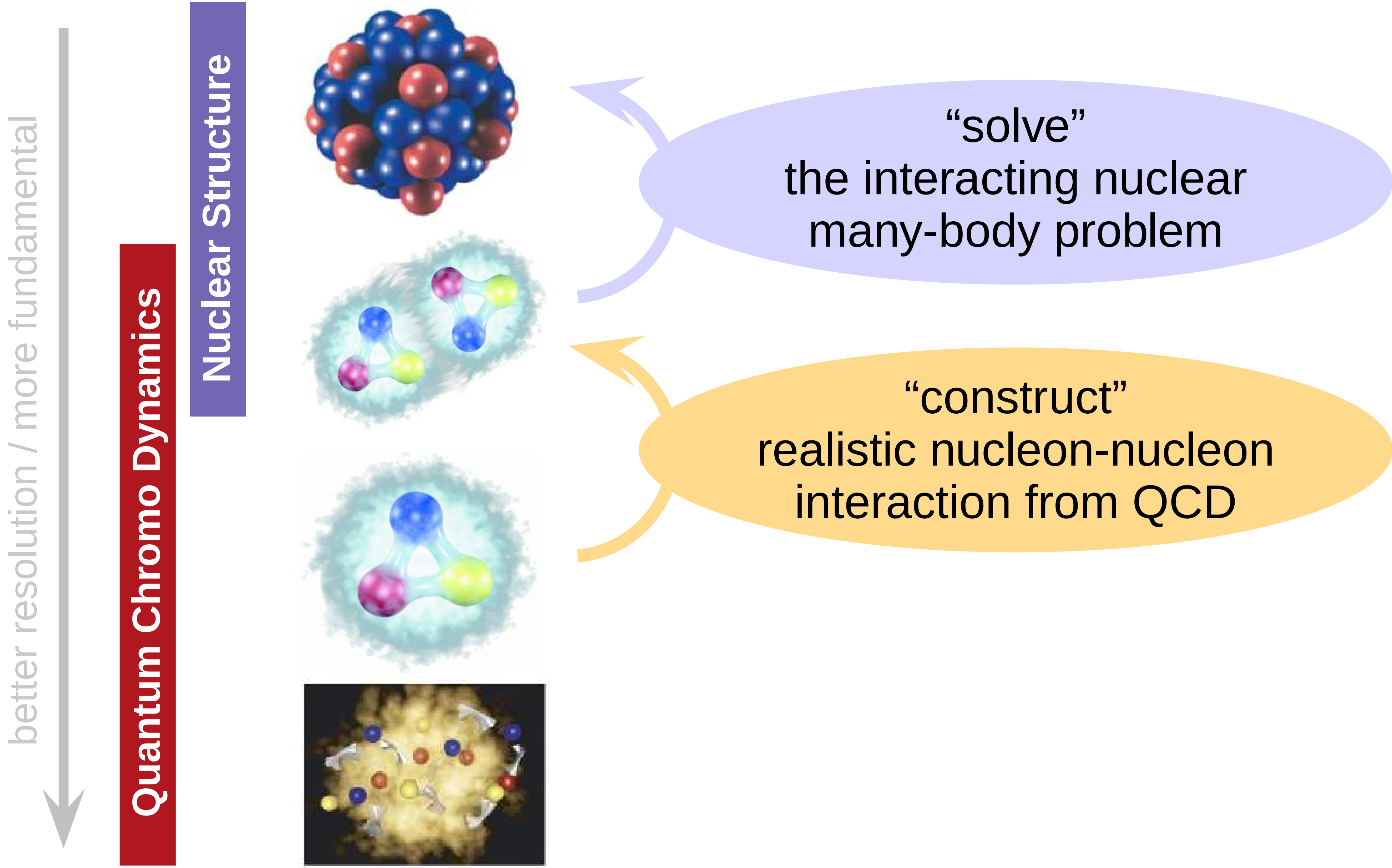
- improved understanding of fundamental degrees of freedom / QCD
- high-precision realistic nucleon-nucleon potentials
- *ab initio* treatment of the many-body problem

# Theoretical Context




- finite nuclei
- few-nucleon systems
- nucleon-nucleon interaction
- hadron structure
- quarks & gluons
- deconfinement

# Theoretical Context



# Realistic
# Nucleon-Nucleon Potentials

# How to Construct the NN-Potential?

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

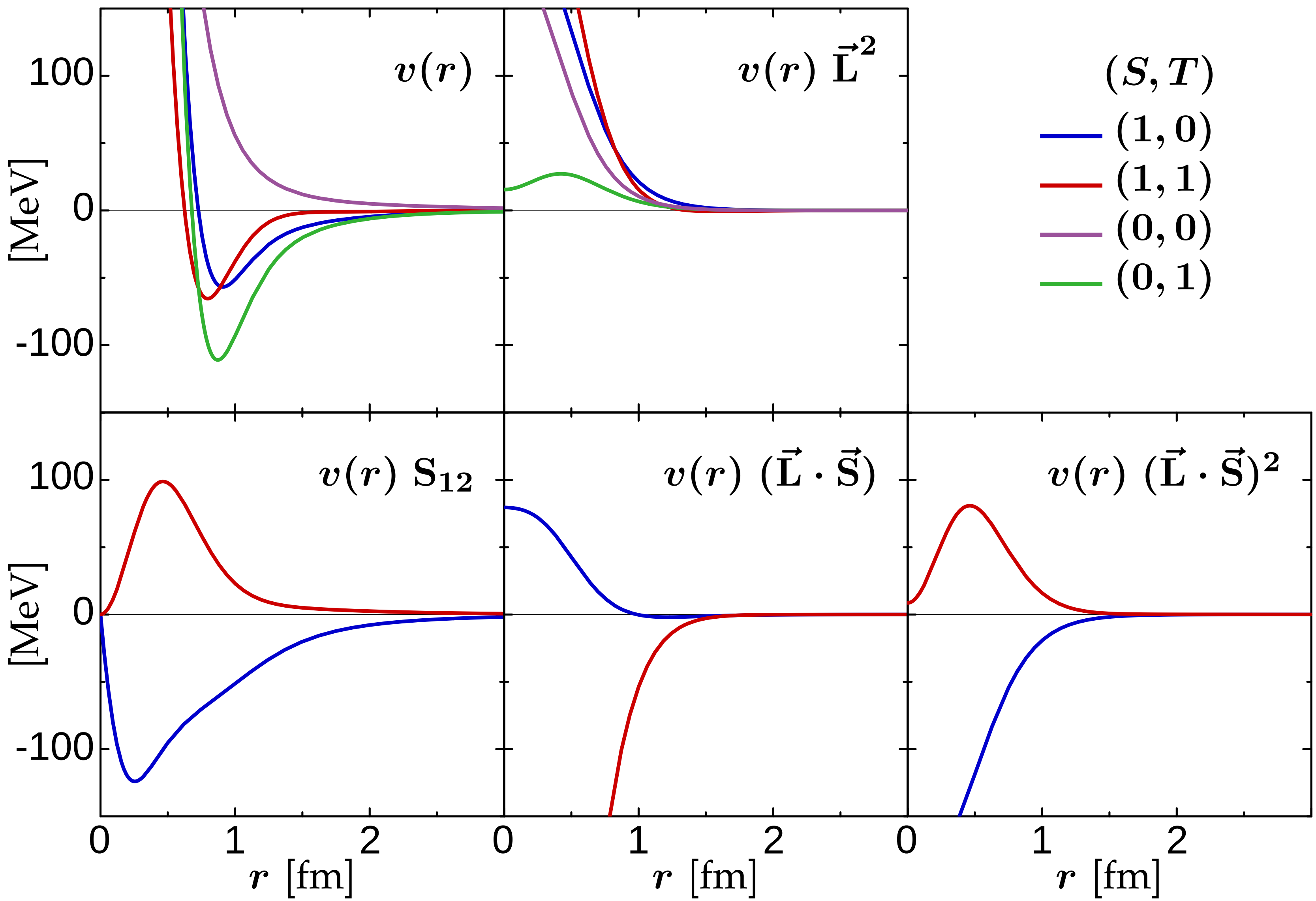
**Argonne V18**

**CD Bonn**

**Nijmegen I/II**

**Chiral...**

# Argonne V18 Potential



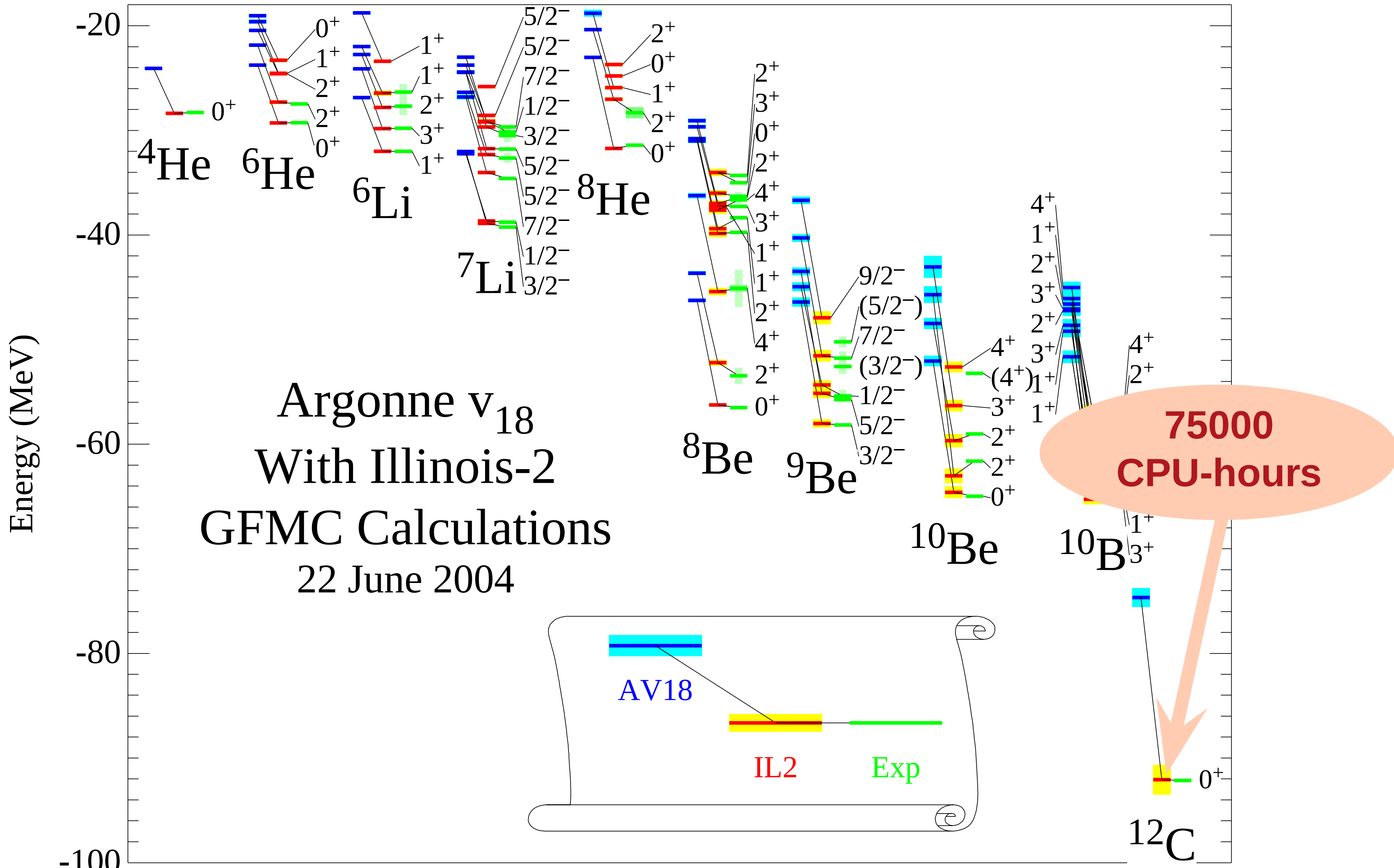
# Nuclear
# Many-Body Problem

# *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 $A$-body wave function in coordinate space; imaginary time cooling
- **No-Core Shell Model**: large-scale diagonalisation 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**
and as close as possible to
an **ab initio** treatment

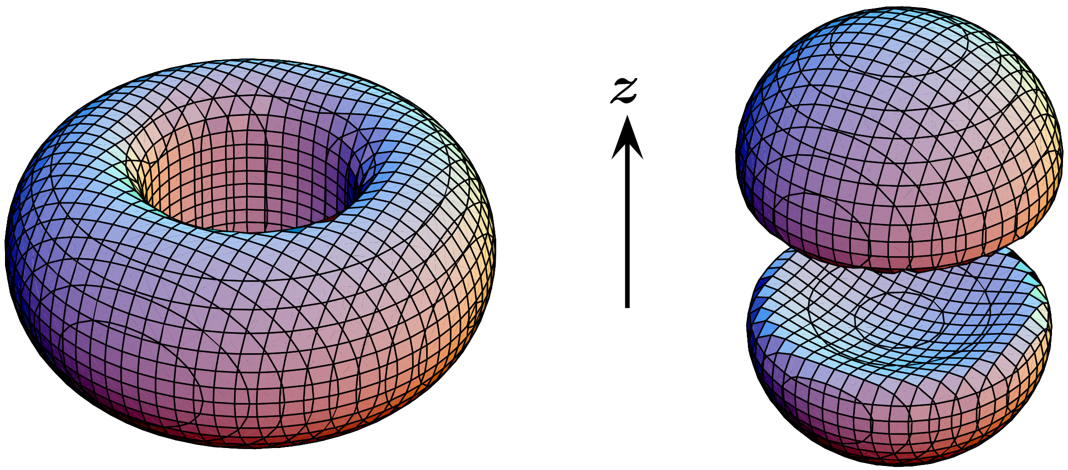
bound to **simple Hilbert spaces** for large particle numbers

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

# Deuteron: Manifestation of Correlations

$\boldsymbol{M_S = 0}$ $\qquad\qquad$ $\boldsymbol{M_S = \pm 1}$

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




- 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**

# 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

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

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

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

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

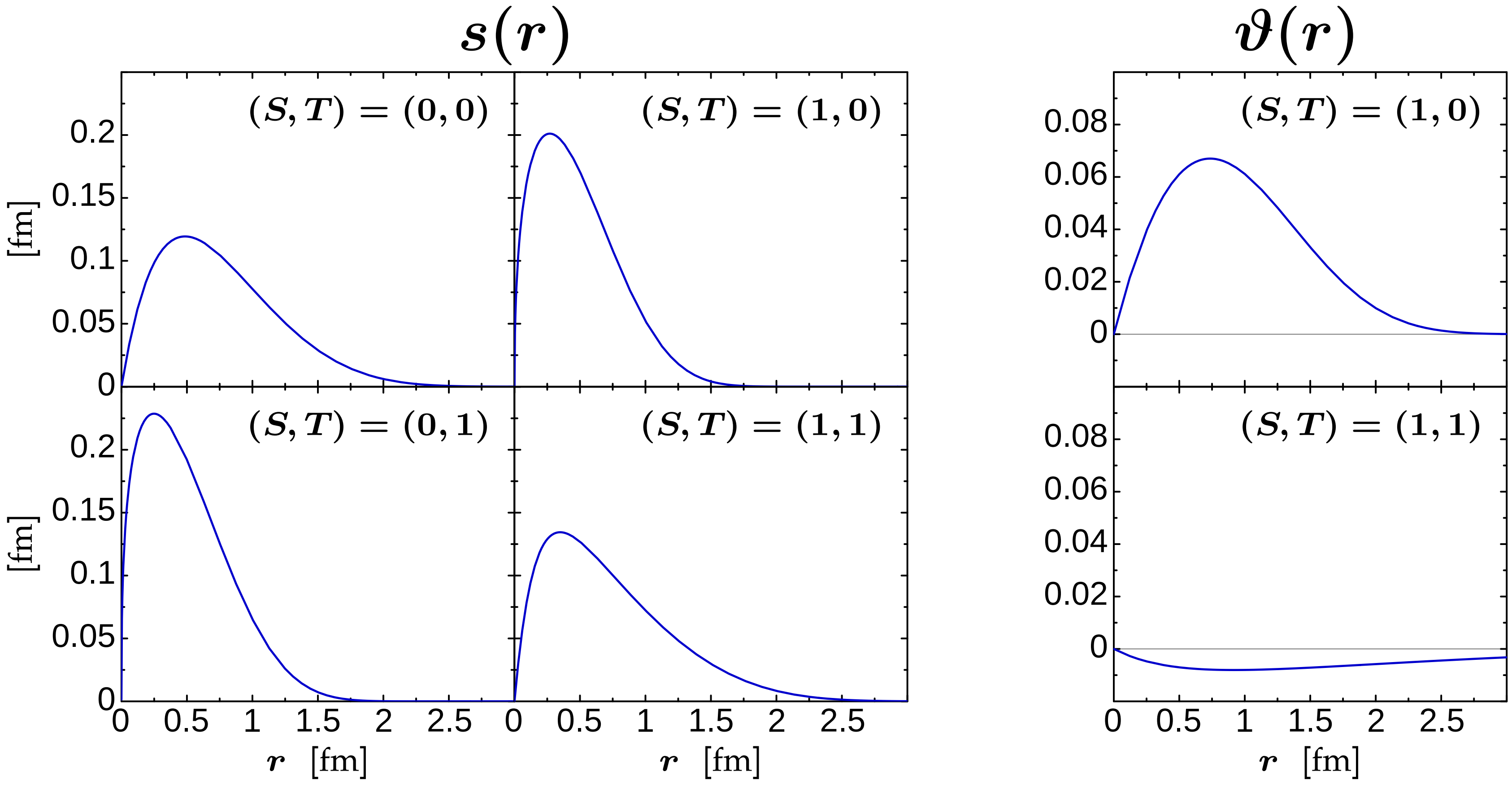
$$\mathrm{g}_\Omega = \frac{3}{2}\vartheta(\mathrm{r})\big[(\vec{\sigma}_1 \cdot \vec{\mathrm{q}}_\Omega)(\vec{\sigma}_2 \cdot \vec{\mathrm{r}}) + (\vec{\mathrm{r}} \leftrightarrow \vec{\mathrm{q}}_\Omega)\big]$$

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

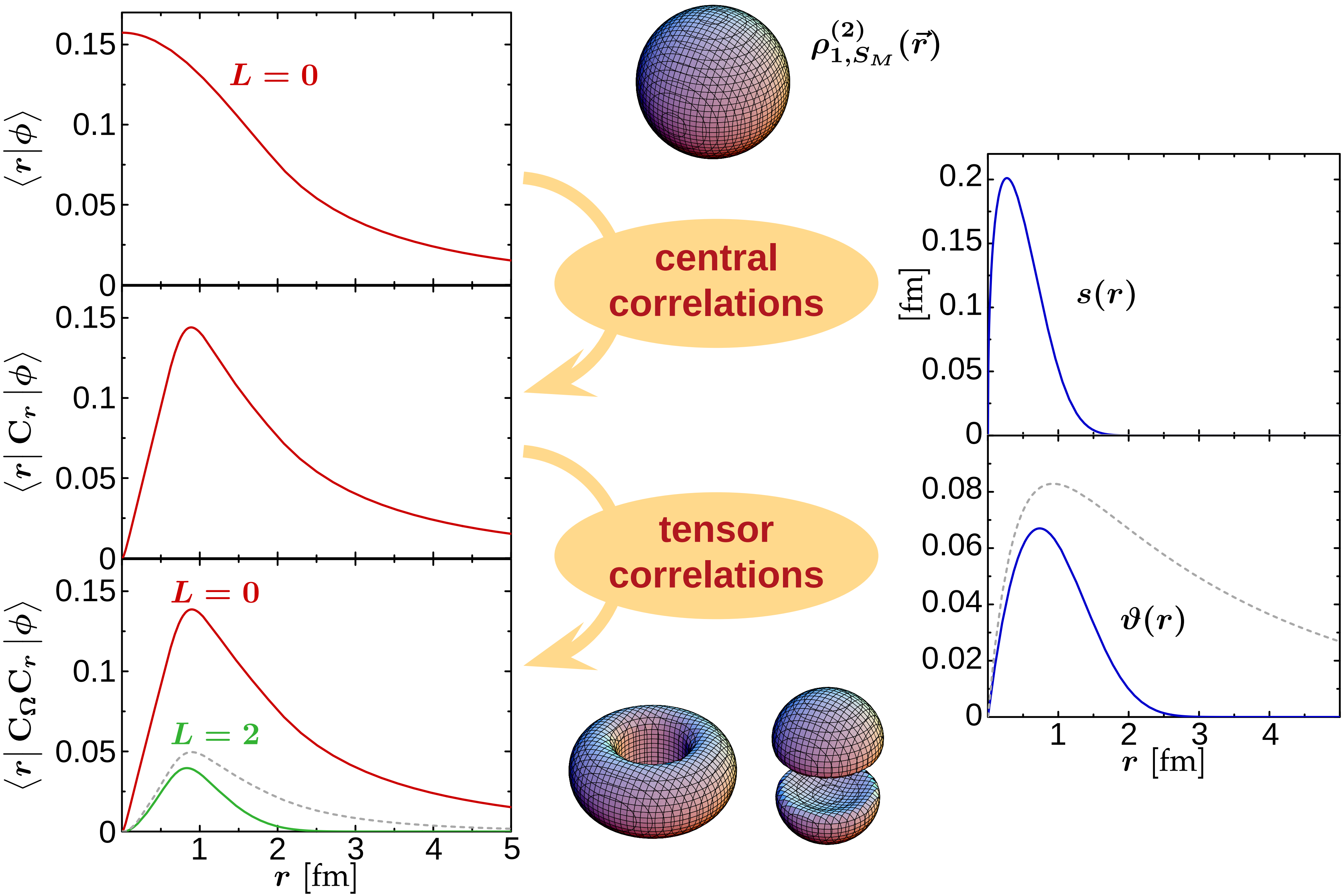
$s(r)$ and $\vartheta(r)$
encapsulate the physics of
**short-range correlations**

# 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



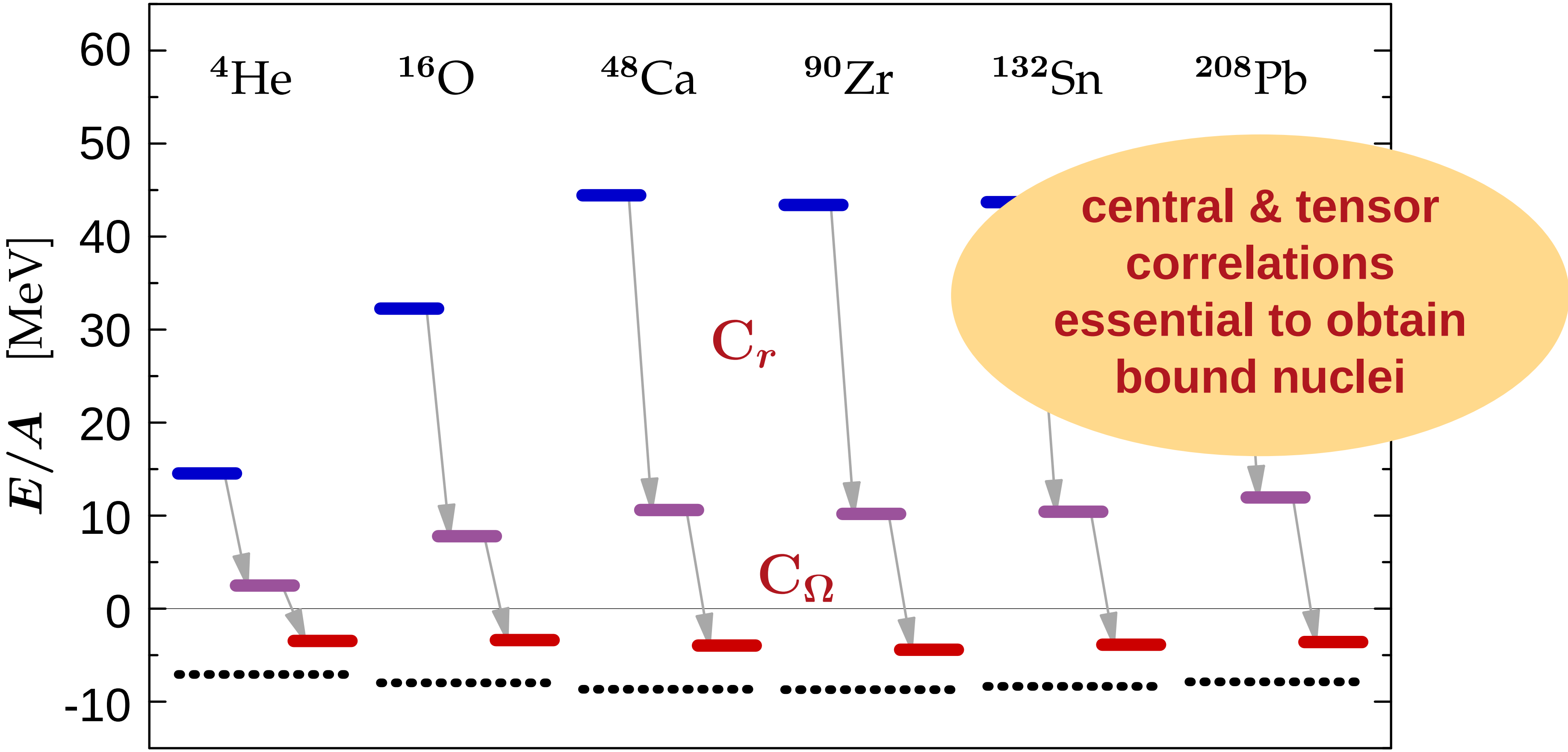
# Correlated NN-Potential — $V_{\mathrm{UCOM}}$

$$\widetilde{\mathbf{H}} = \mathbf{T} + \mathbf{V}_{\mathrm{UCOM}} + \mathbf{V}_{\mathrm{UCOM}}^{[3]} + \cdots$$

- **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 $V_{\mathrm{low}-k}$**

# Simplistic "Shell-Model" Calculation

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



Application I

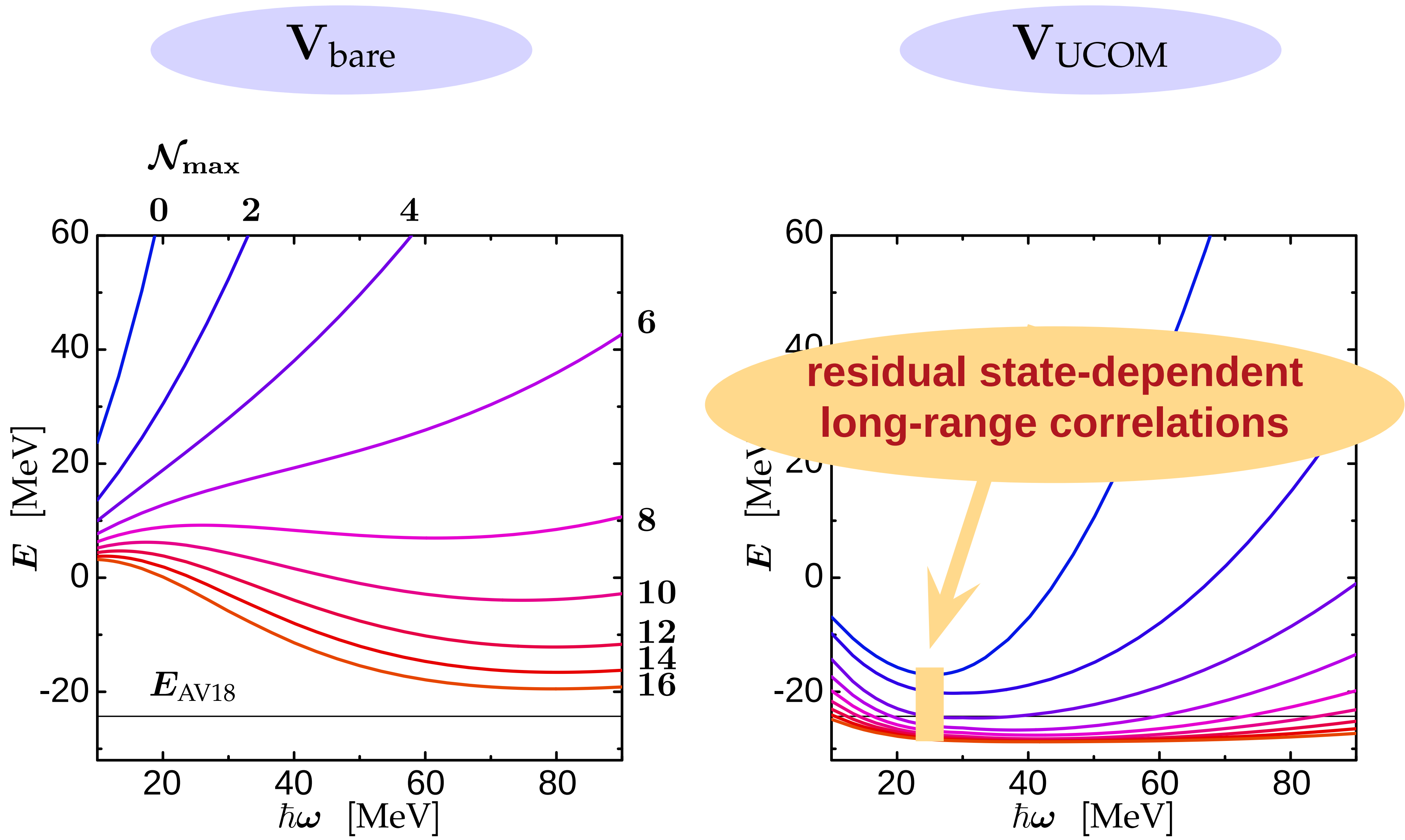
# No-Core Shell Model

# UCOM + NCSM

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

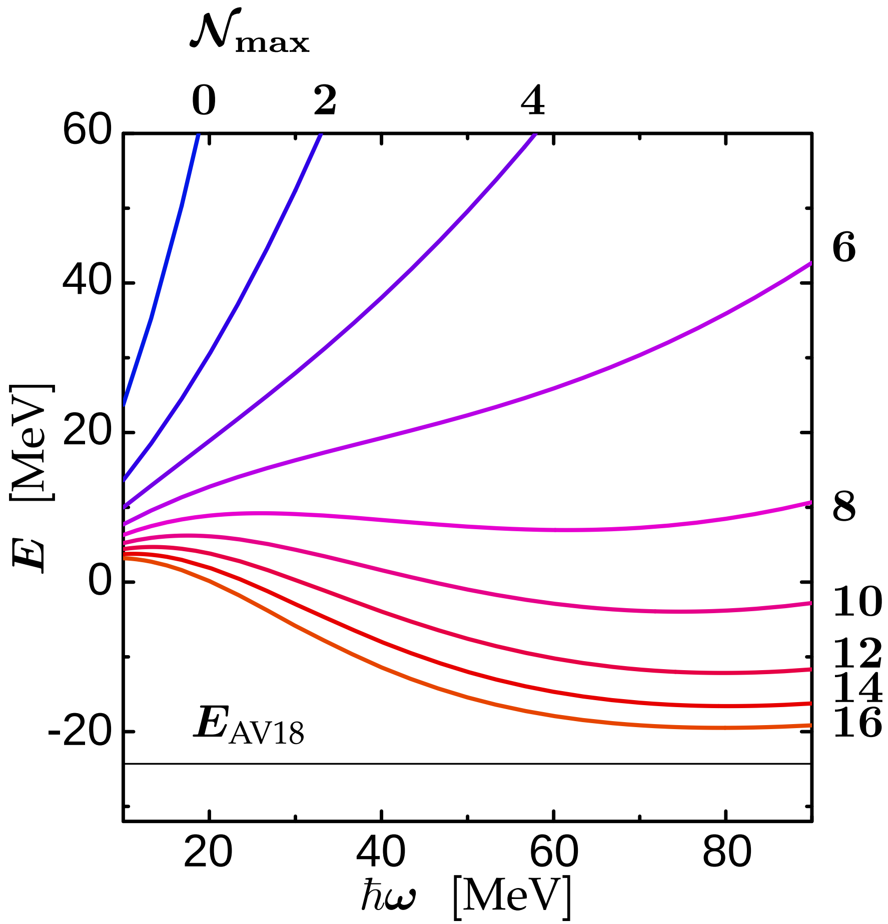
- many-body state is expanded in Slater determinants of harmonic oscillator single-particle states
- large scale diagonalisation of Hamiltonian within a truncated model space ($\mathcal{N}\hbar\omega$ truncation)
- assessment of short- and long-range correlations
- NCSM code by Petr Navrátil [PRC 61, 044001 (2000)]

# $^4$He: Convergence

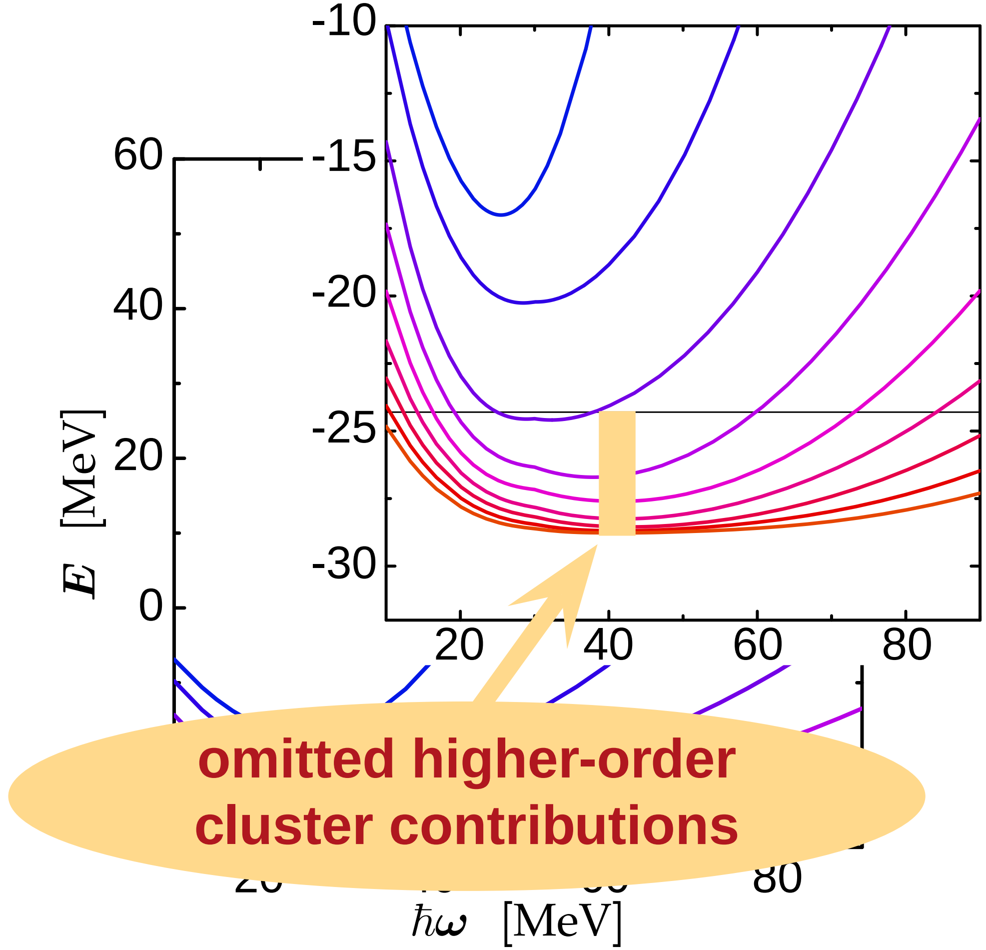


# $^4$He: Convergence

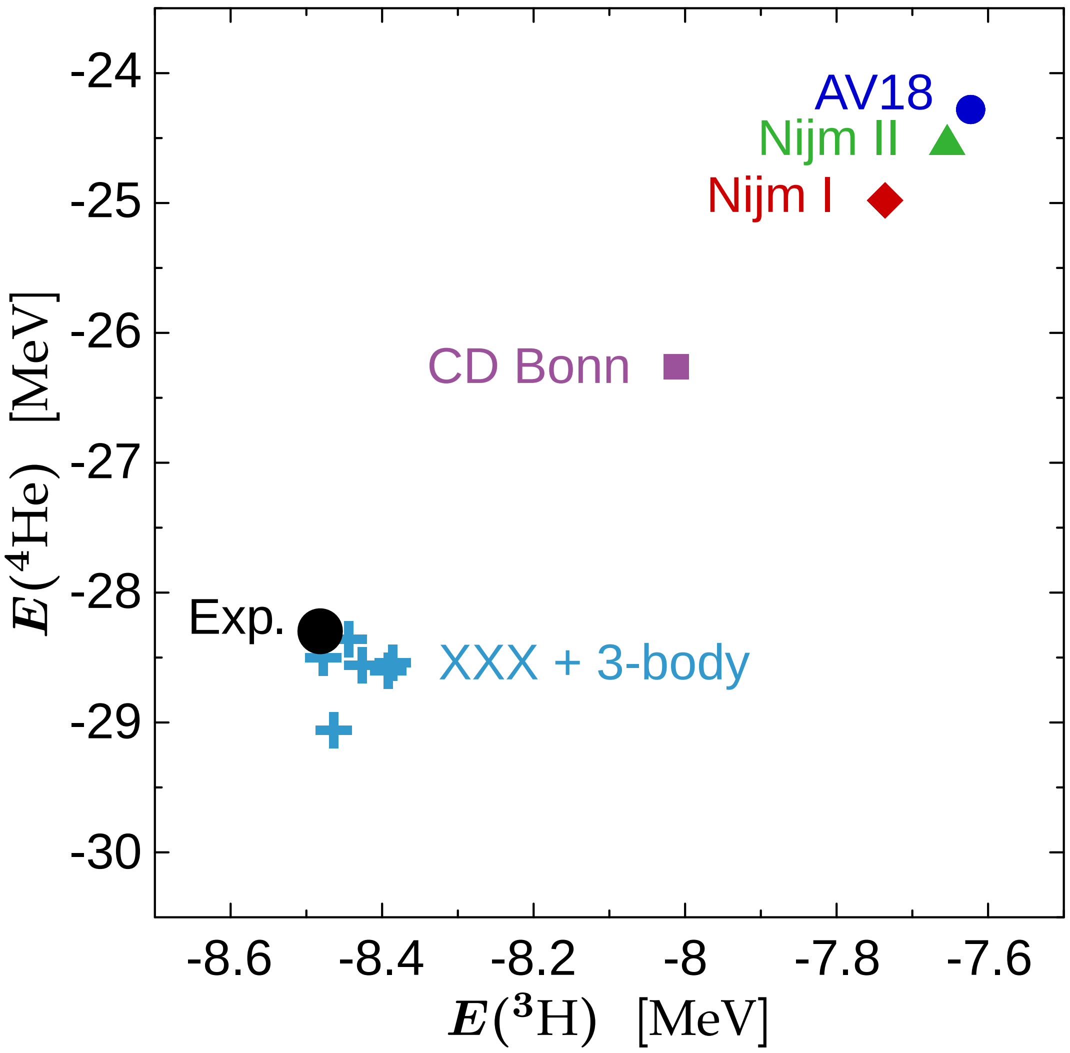
$V_{bare}$




$V_{UCOM}$

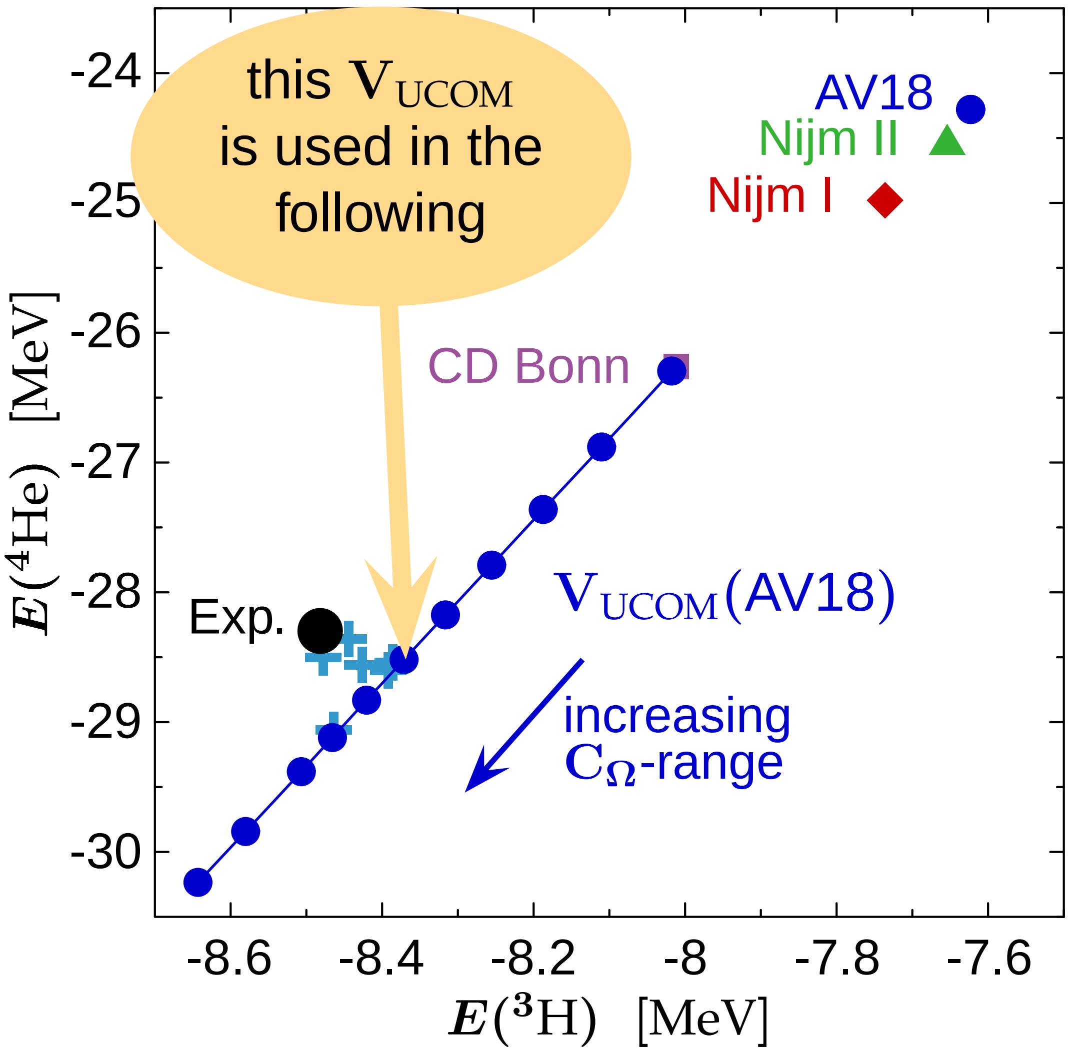


# Tjon-Line and Correlator Range




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

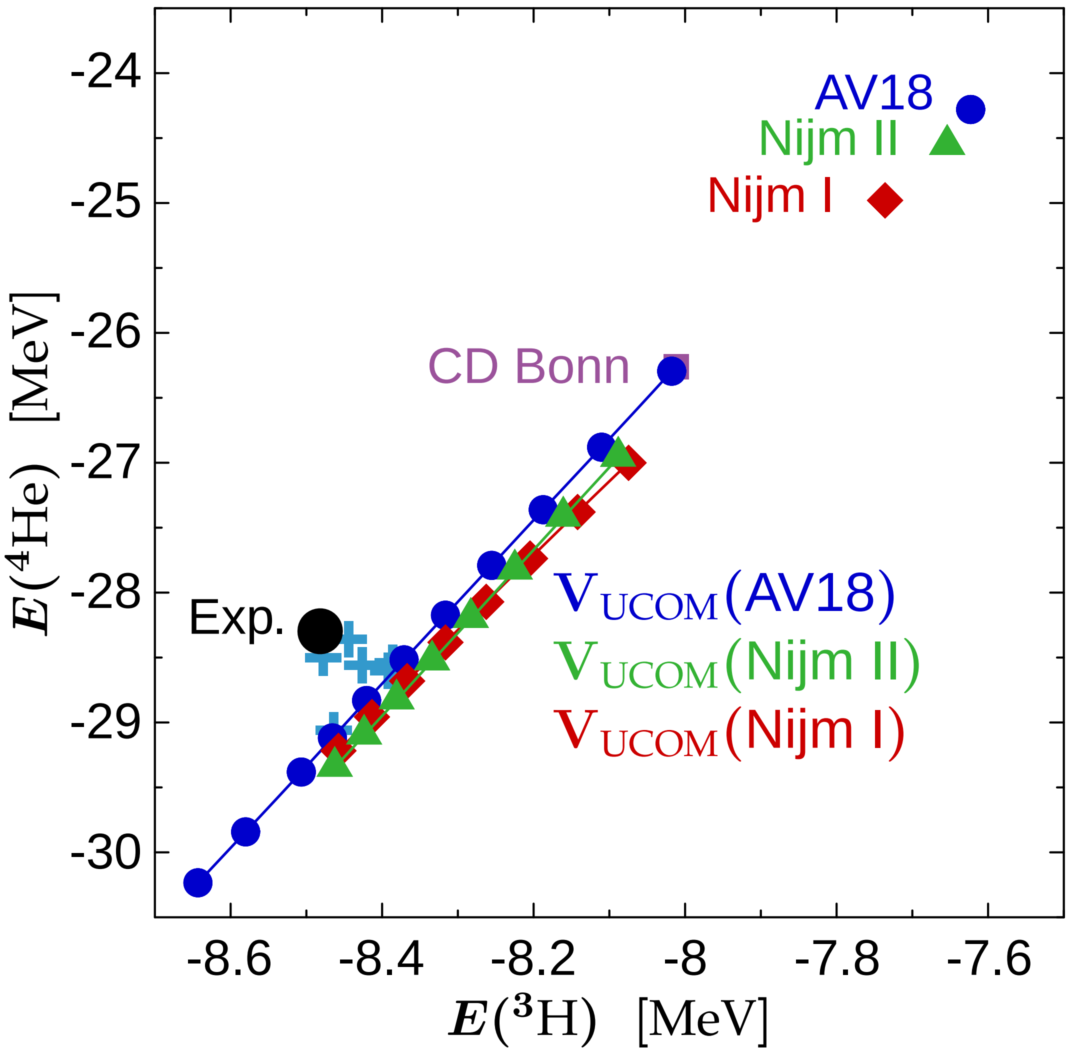
# Tjon-Line and Correlator Range




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

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

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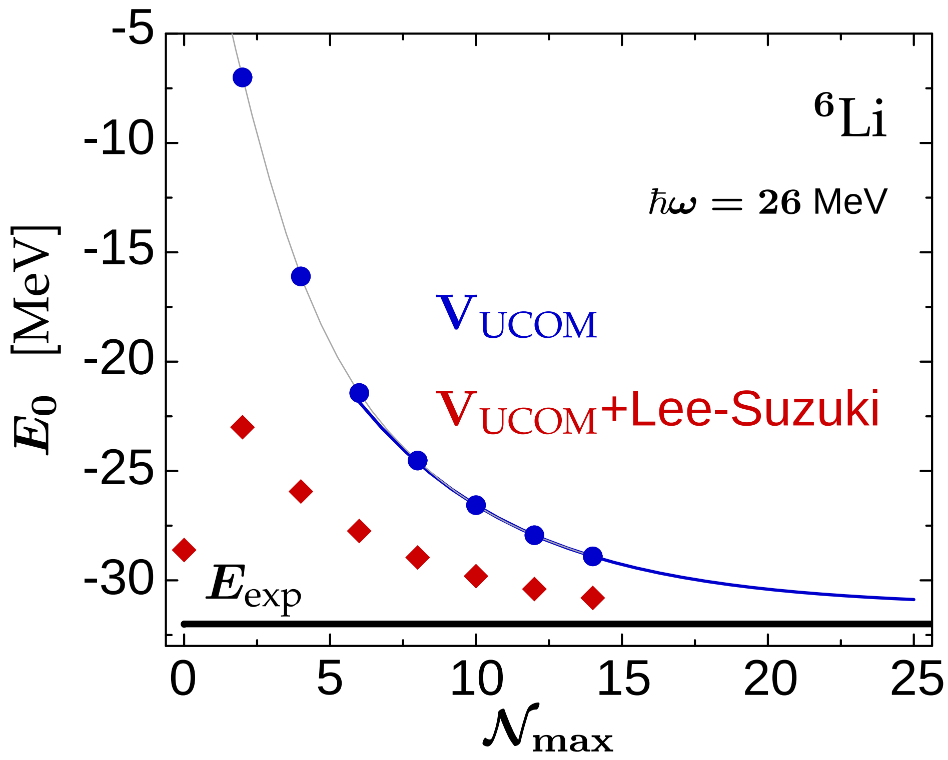
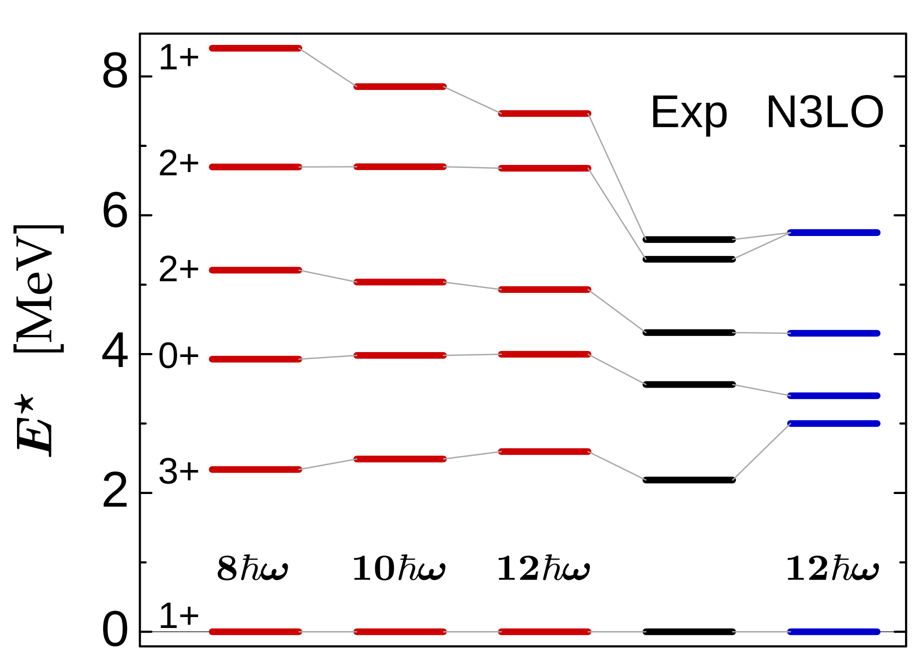
choose correlator with energies close to experimental value, i.e., **minimise net three-body force**

# $^6$Li: NCSM for p-Shell Nuclei

systematic NCSM
study throughout p-shell
in progress




calculations by Petr Navratil

Application II:

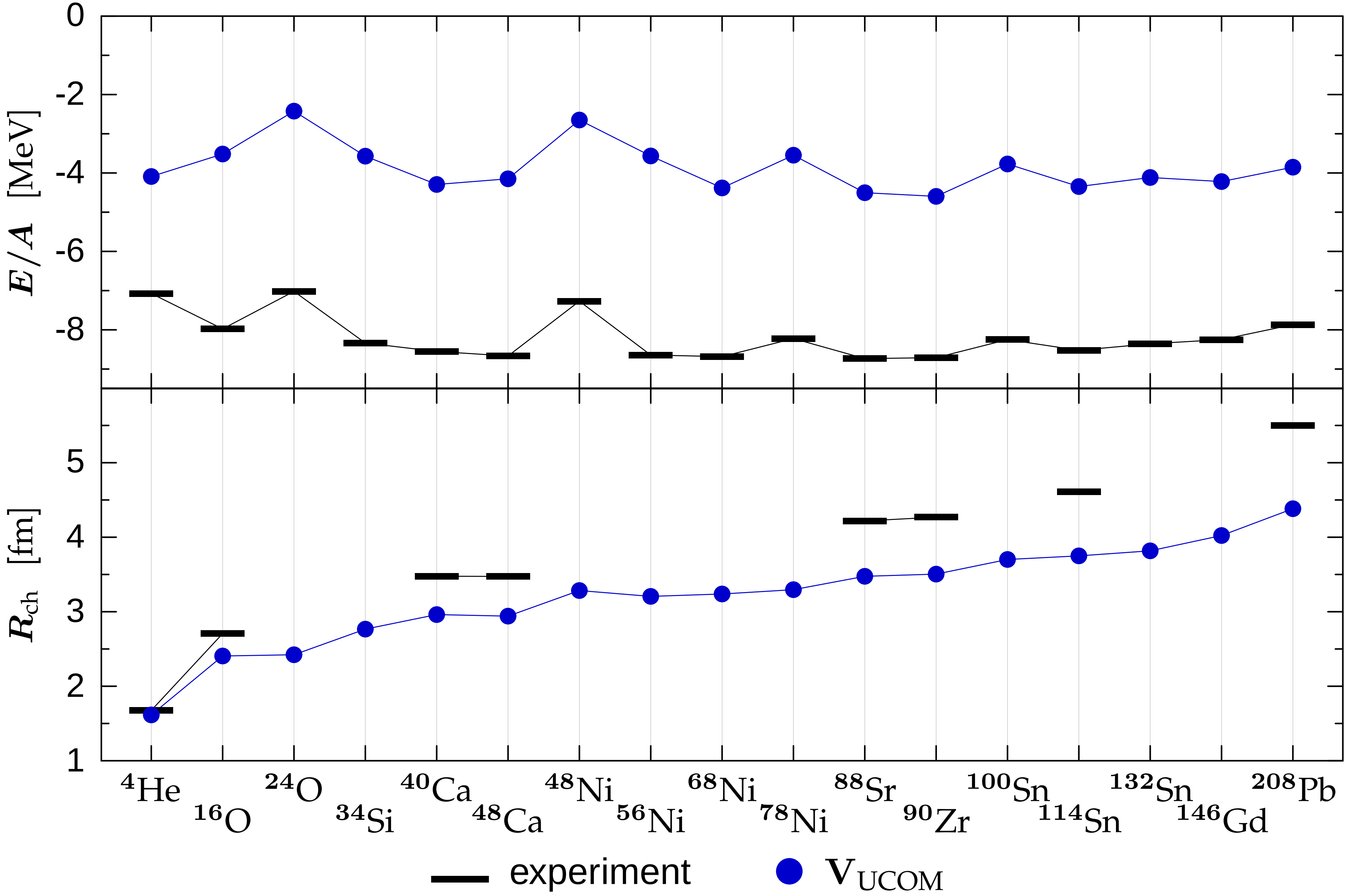
# Hartree-Fock Calculations

# 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 expanded in oscillator basis
- **correlations cannot be described** by Hartree-Fock states
- bare realistic NN-potential leads to **unbound nuclei**

# Hartree-Fock with Correlated AV18



# Missing Pieces

**long-range correlations**

**genuine three-body forces**

**three-body cluster contributions**

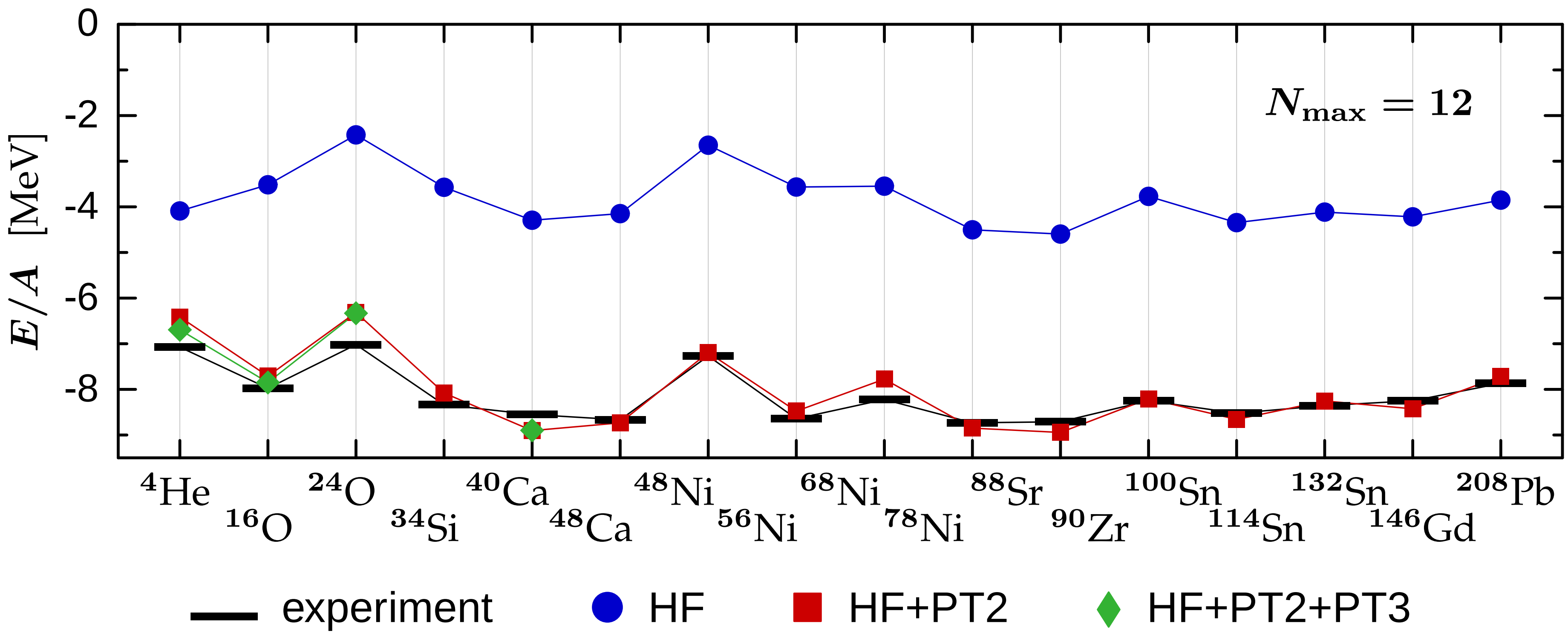
**Beyond Hartree-Fock**

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

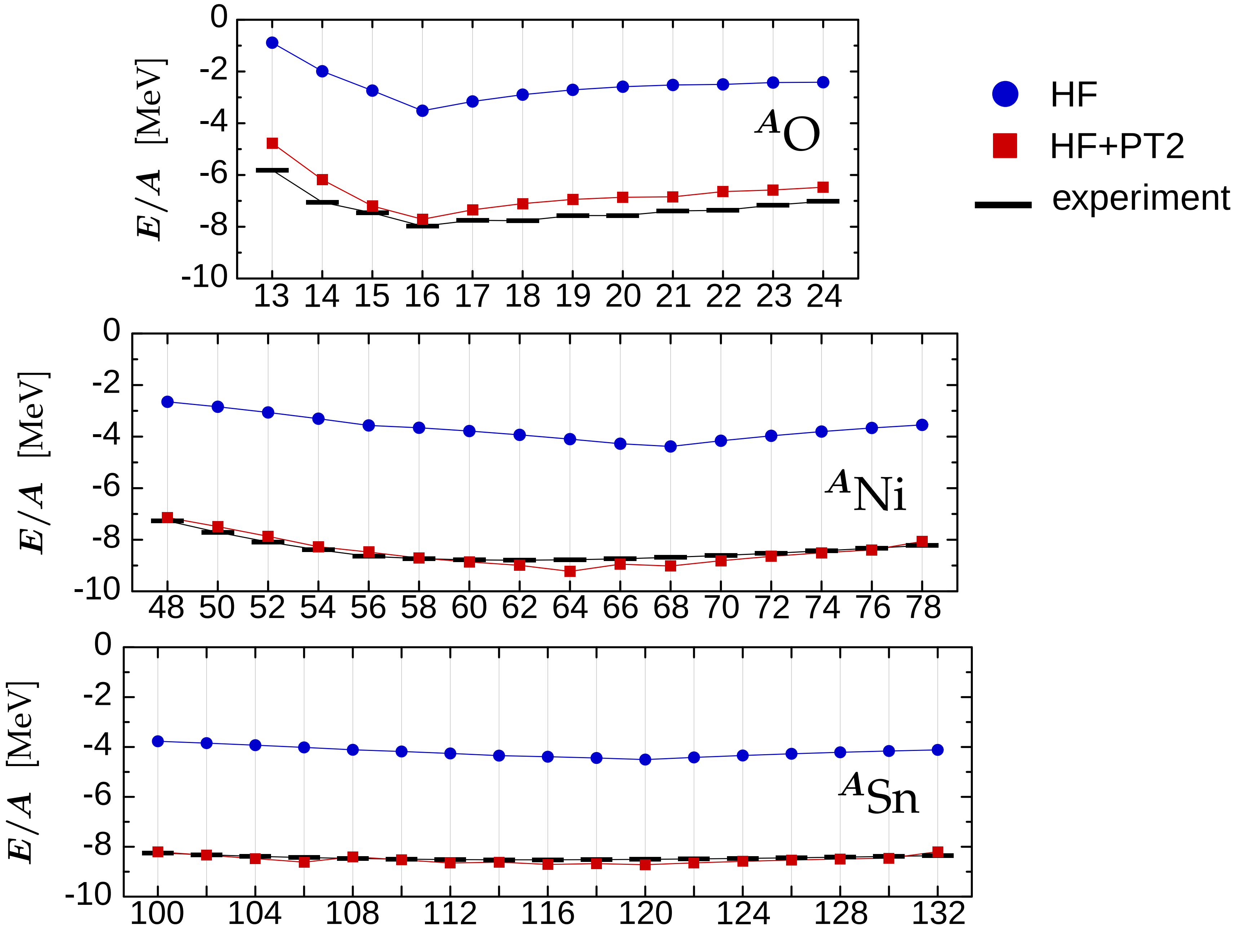
# Long-Range Correlations: MBPT

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

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



# Long-Range Correlations: MBPT



# Missing Pieces

**long-range correlations**

**genuine three-body forces**

**three-body cluster contributions**

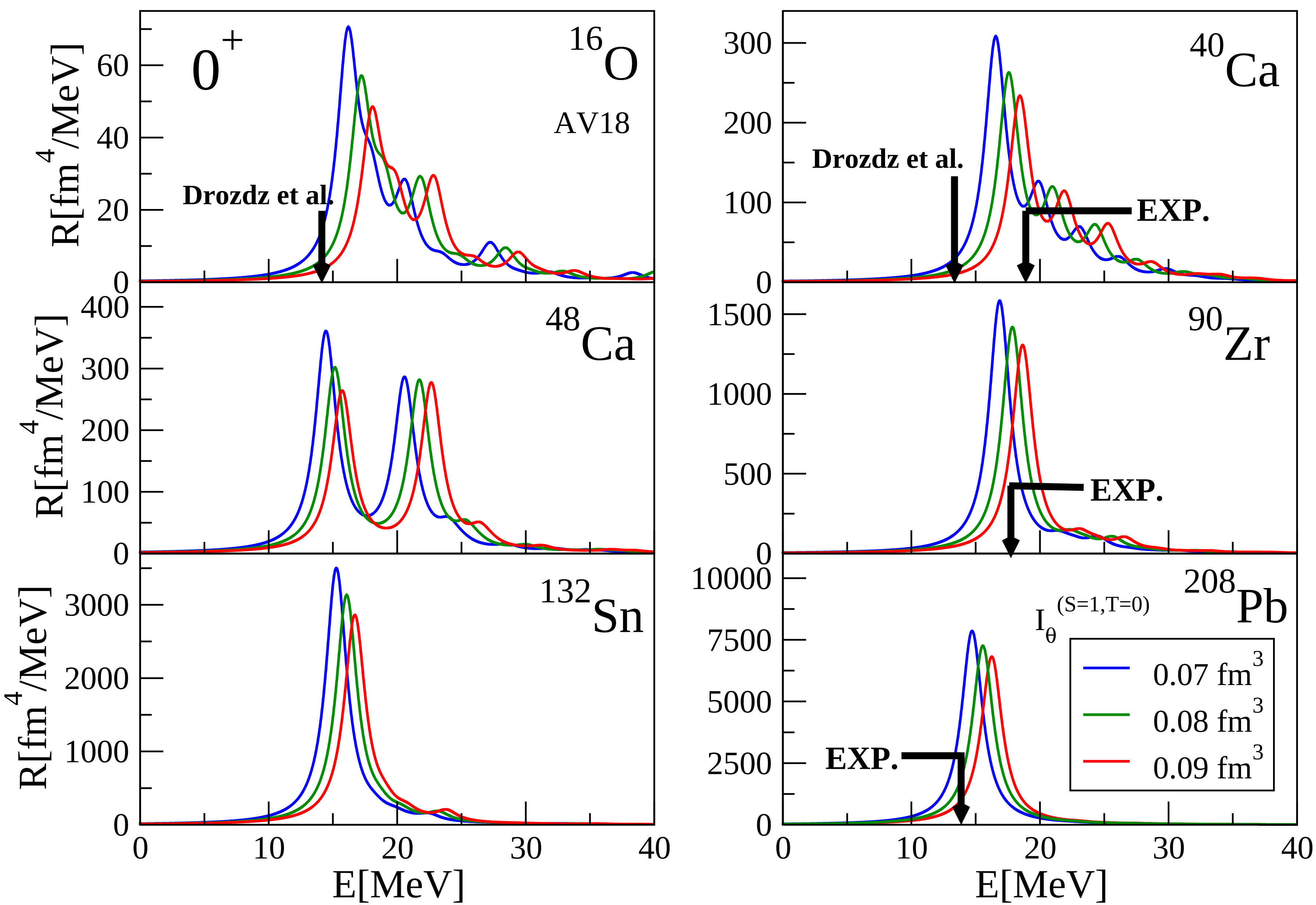
## Beyond Hartree-Fock

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

## Residual Three-Body Force

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

# Outlook: UCOM + RPA



Application III

# 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

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

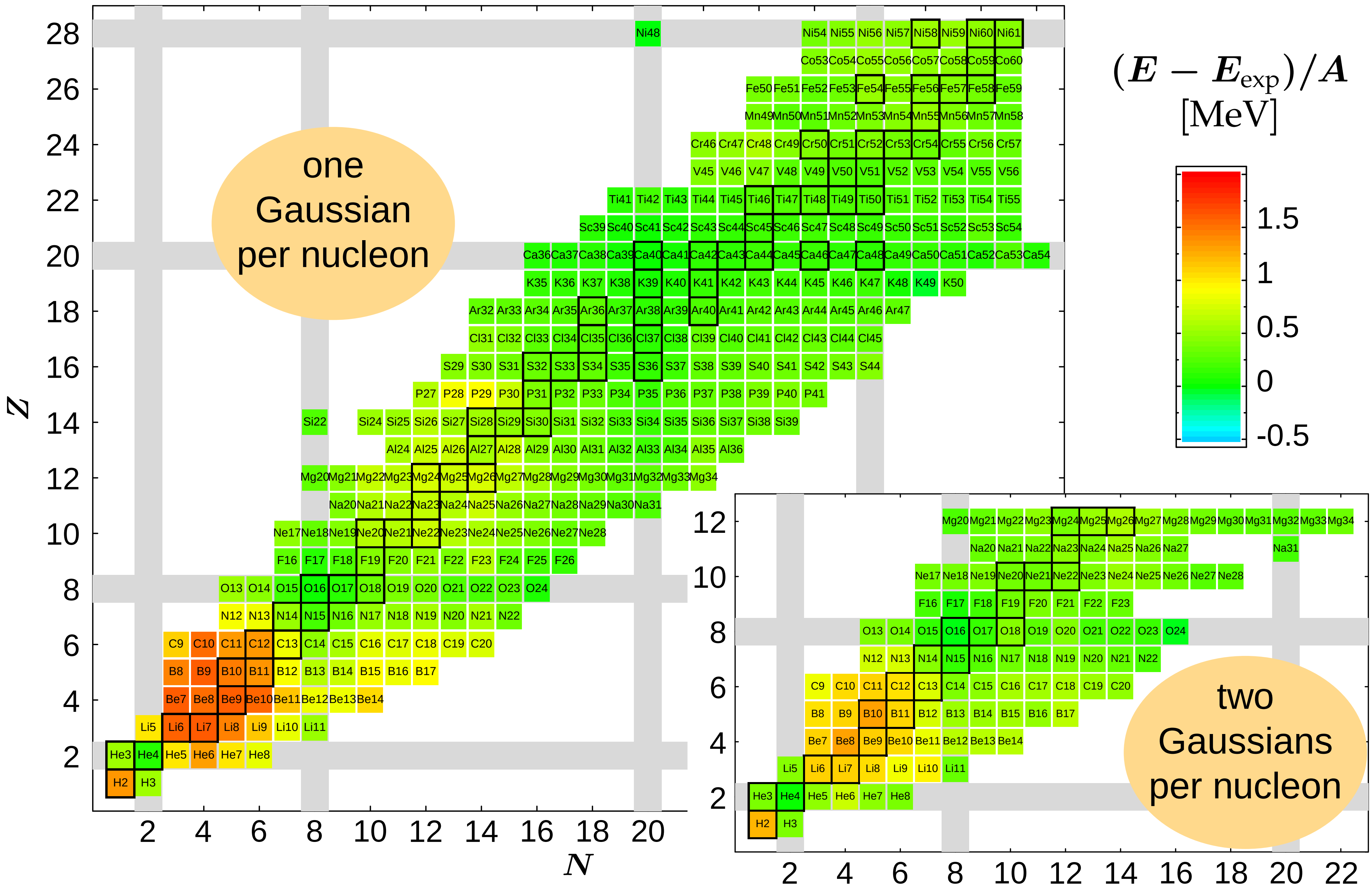
## Variation

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

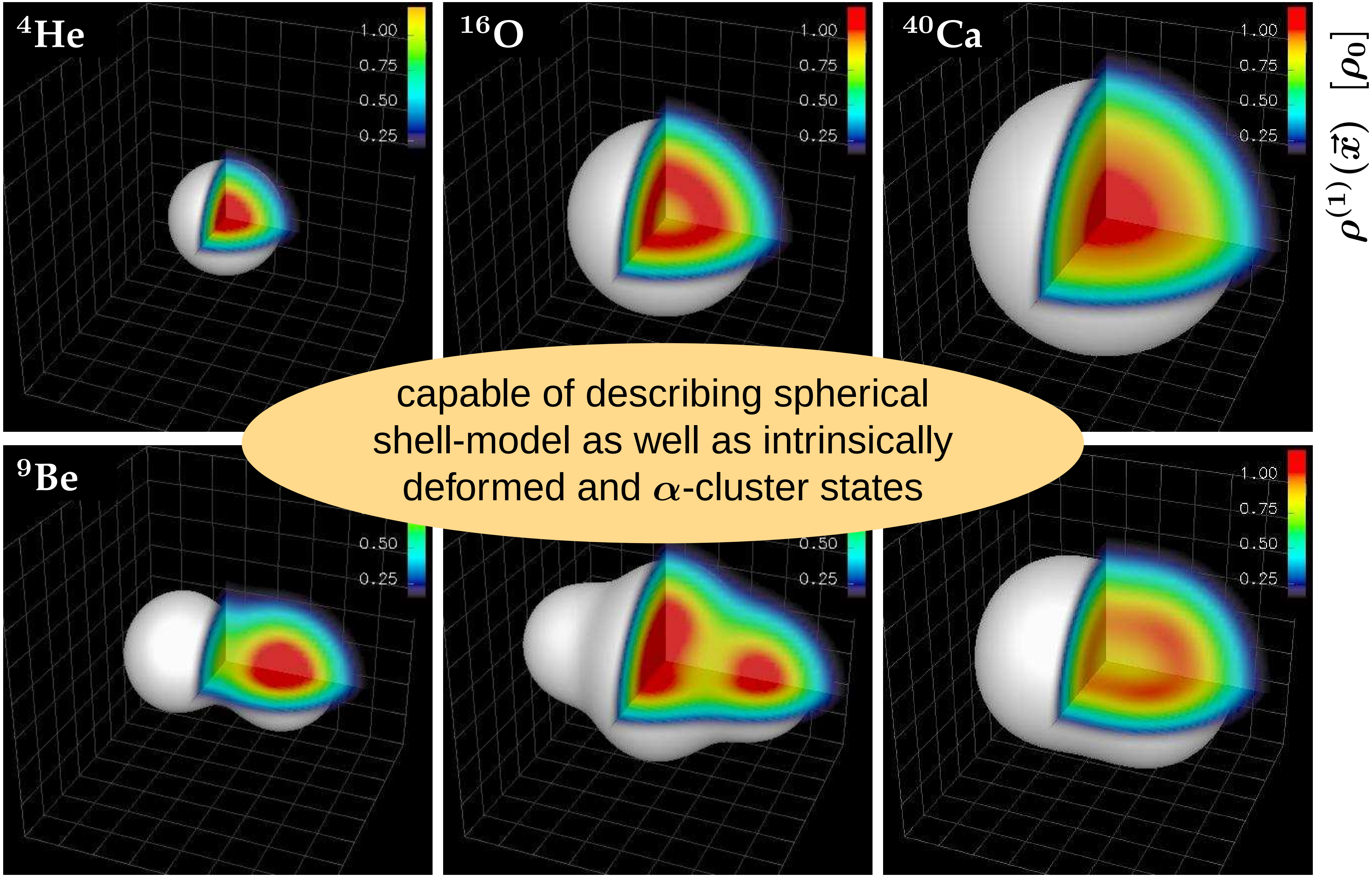
## Diagonalisation

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

# Variation: Chart of Nuclei



# Intrinsic One-Body Density Distributions

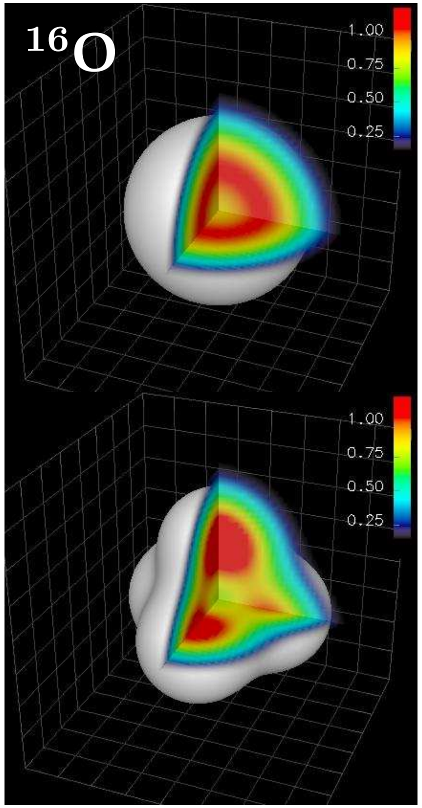



capable of describing spherical shell-model as well as intrinsically deformed and $\alpha$-cluster states

# Beyond Simple Variation

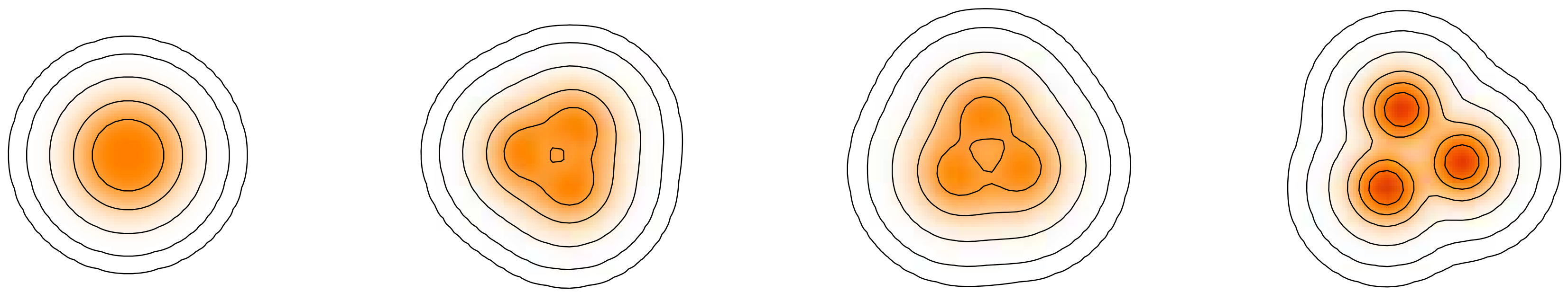
- **Projection after Variation (PAV)**
  - restore inversion and rotational symmetry by angular momentum projection

- **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)



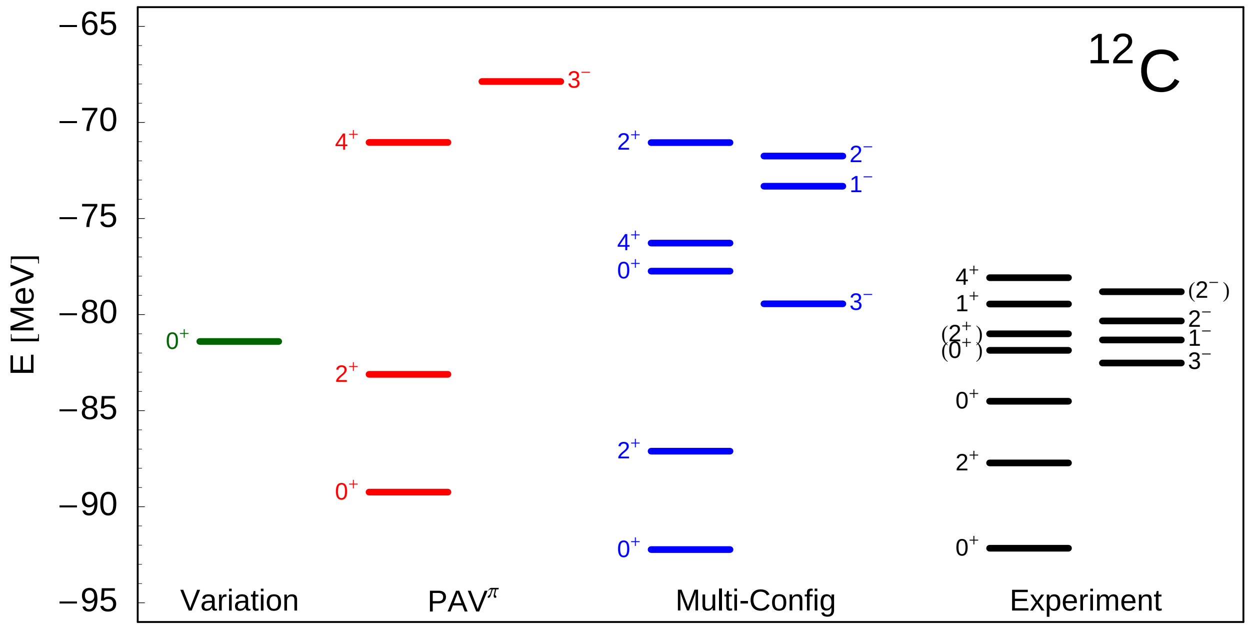

- **Multi-Configuration**
  - diagonalisation within a set of different Slater determinants

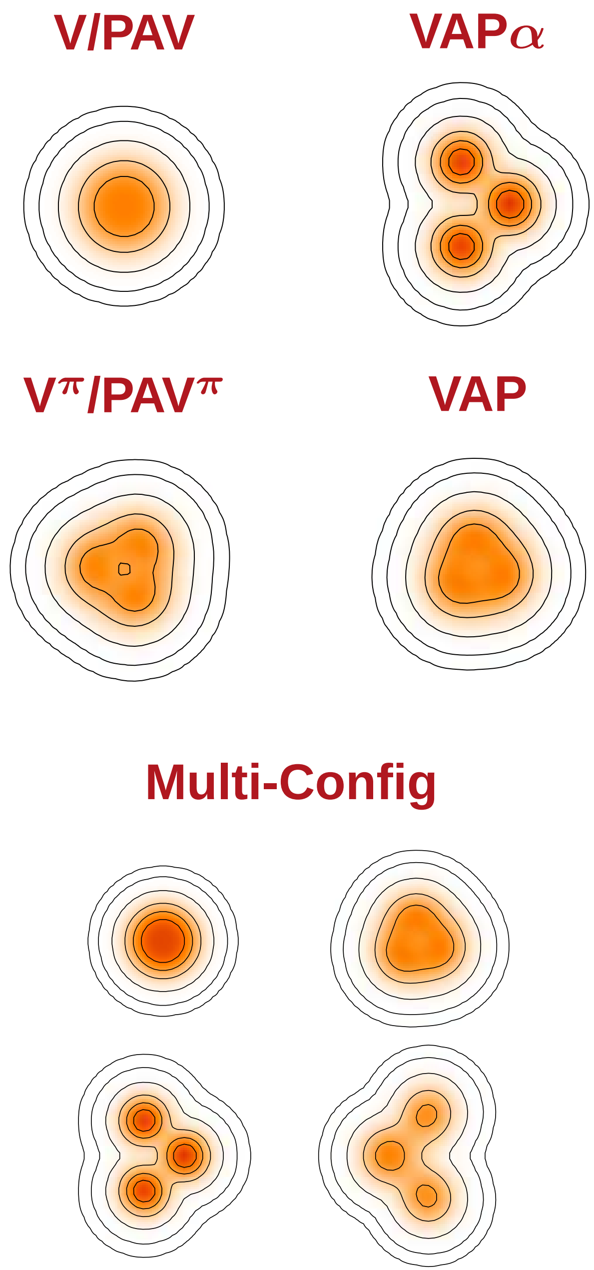
# Intrinsic Shapes of $^{12}C$



| | 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 |

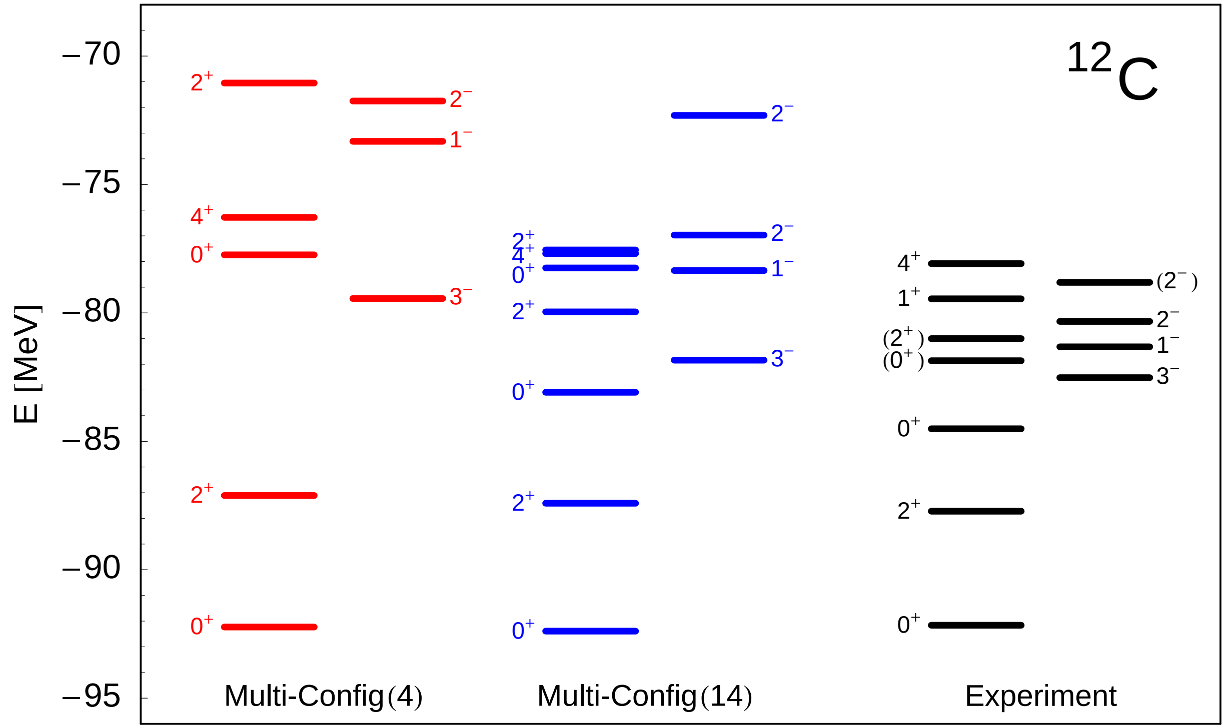
# Structure of $^{12}C$



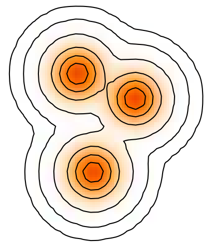



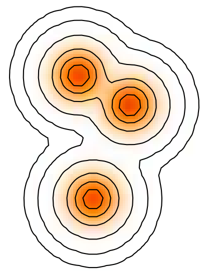

| | $E$ [MeV] | $R_{ch}$ [fm] | $B(E2)$ [$e^2$ fm$^4$] |
|---|---|---|---|
| V/PAV | 81.4 | 2.36 | - |
| VAP $\alpha$-cluster | 79.1 | 2.70 | 76.9 |
| $PAV^{\pi}$ | 88.5 | 2.51 | 36.3 |
| VAP | 89.2 | 2.42 | 26.8 |
| Multi-Config | 92.2 | 2.52 | 42.8 |
| Experiment | 92.2 | 2.47 | 39.7 $\pm$ 3.3 |

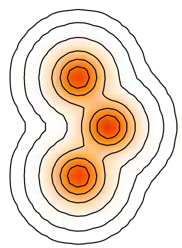
# Structure of $^{12}C$ — Hoyle State




| | Multi-Config | Experiment |
|---|---|---|
| $\boldsymbol{E}$ [MeV] | 92.4 | 92.2 |
| $\boldsymbol{R}_{\text{ch}}$ [fm] | 2.52 | 2.47 |
| $\boldsymbol{B(E2, 0_1^+ \rightarrow 2_1^+)}$ [$e^2$ fm$^4$] | 42.9 | 39.7 ± 3.3 |
| $\boldsymbol{M(E0, 0_1^+ \rightarrow 0_2^+)}$ [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 $V_{\mathrm{UCOM}}$**
  - 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 / RPA**
  - ground states & excitations across the whole nuclear chart
  - basis for improved many-body calculations: MBPT, SM/CI, CC,...
- **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**
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