

Correlated Realistic Interactions for Nuclear Structure & Reactions



Robert Roth

Institut für Kernphysik
Technische Universität Darmstadt

■ Motivation

- Nucleon-Nucleon Interaction
- Solving the Many-Body Problem

■ Correlations & Unitary Correlation Operator Method

- Correlated Realistic Interaction V_{UCOM}

■ 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: NuSTAR @ FAIR,...

Theory

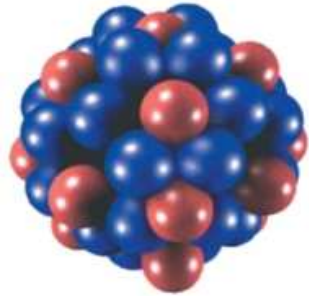
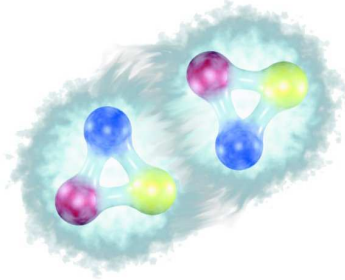
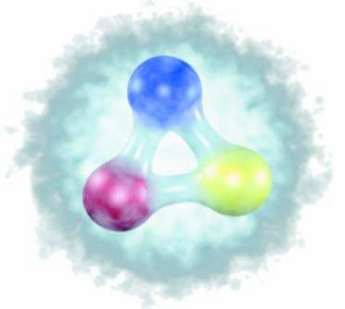
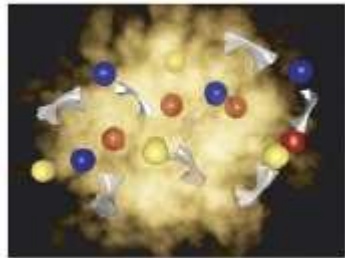
- improved understanding of fundamental degrees of freedom / QCD
- high-precision realistic nucleon-nucleon potentials
- *ab initio* treatment of the many-body problem

From QCD to Nuclear Structure

better resolution / more fundamental

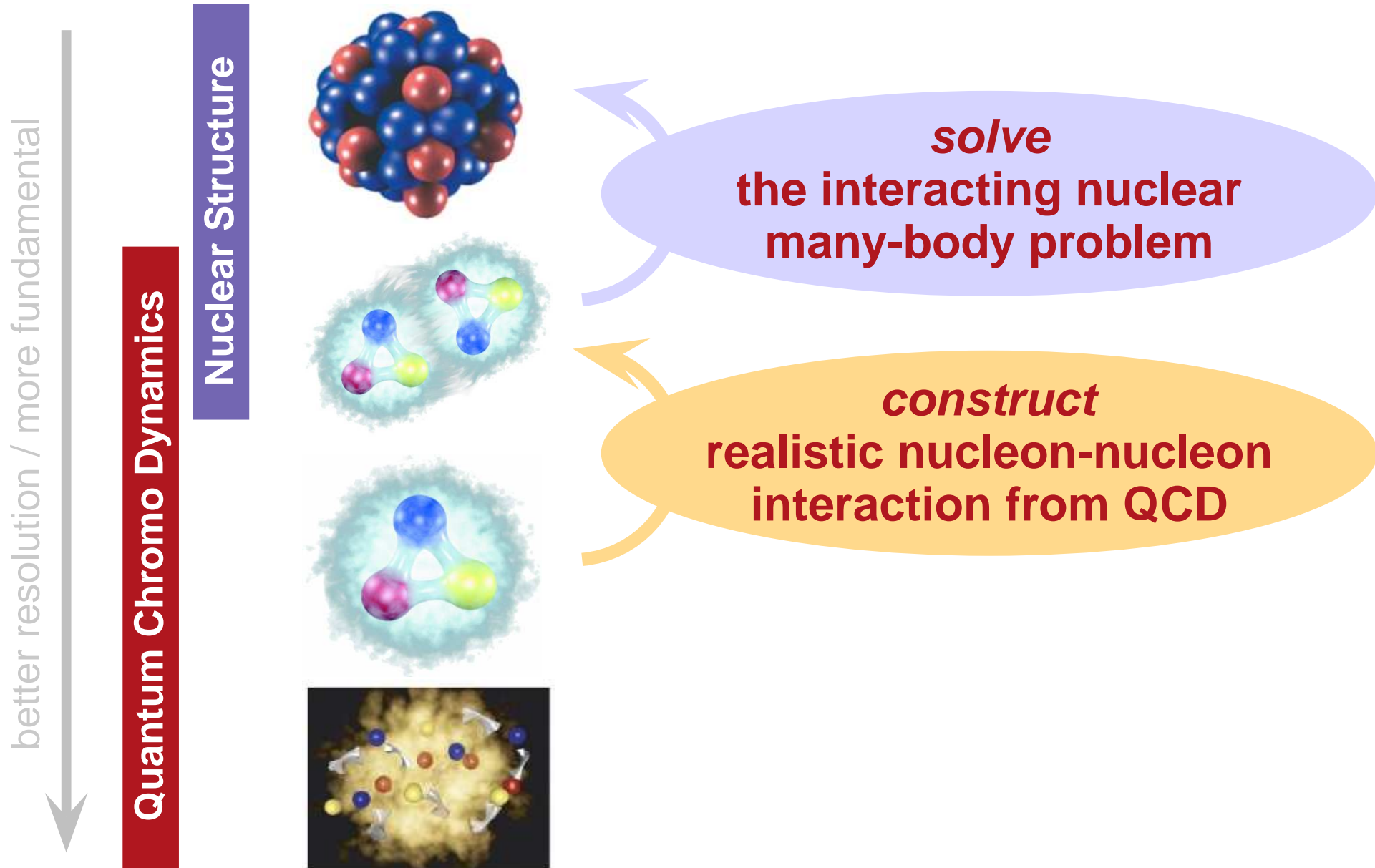
Quantum Chromo Dynamics

Nuclear Structure



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

From QCD to Nuclear Structure



Realistic Nucleon-Nucleon Potentials

Realistic NN-Potentials

■ QCD motivated

- symmetries, meson-exchange picture
- chiral effective field theory

■ short-range phenomenology

- short-range parametrisation or contact terms

■ experimental two-body data

- scattering phase-shifts & deuteron properties reproduced with high precision

■ supplementary three-nucleon force

- adjusted to spectra of light nuclei

Argonne V18

CD Bonn

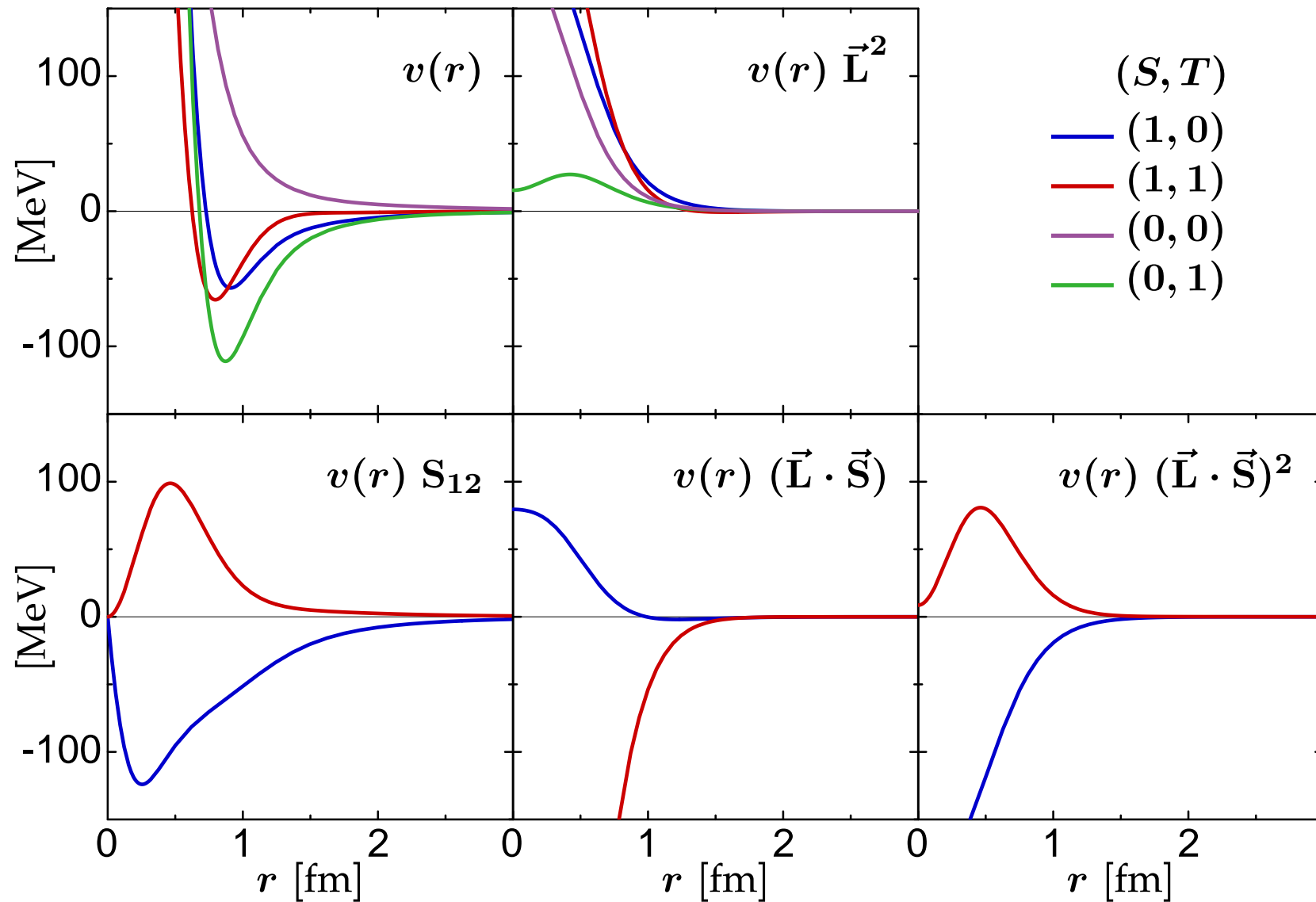
Nijmegen I/II

Chiral N3LO

Argonne V18 +
Illinois 2

Chiral N3LO +
N2LO

Argonne V18 Potential

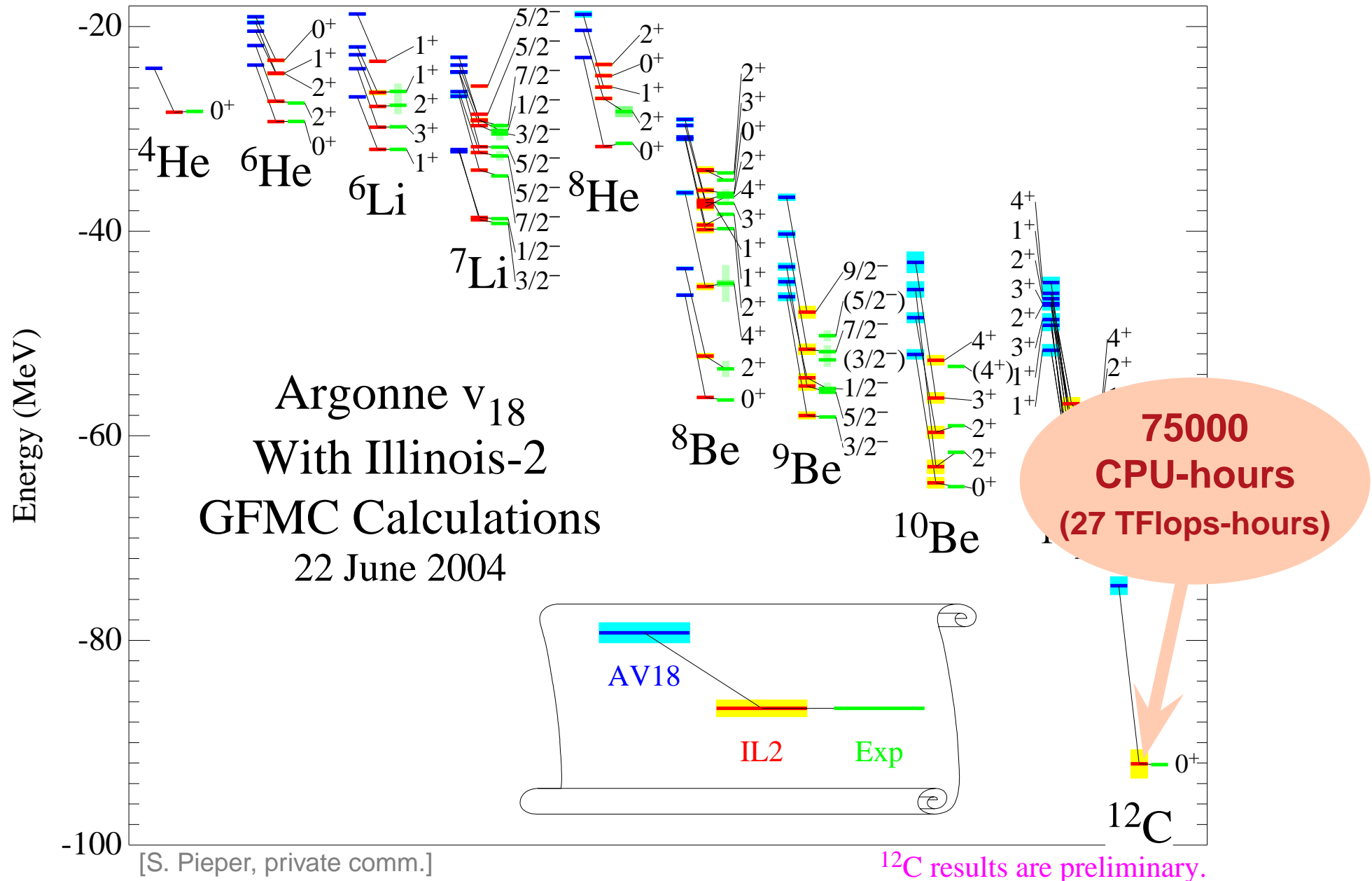


Nuclear Many-Body Problem

**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

Ab initio Methods: GFMC



Our Goal

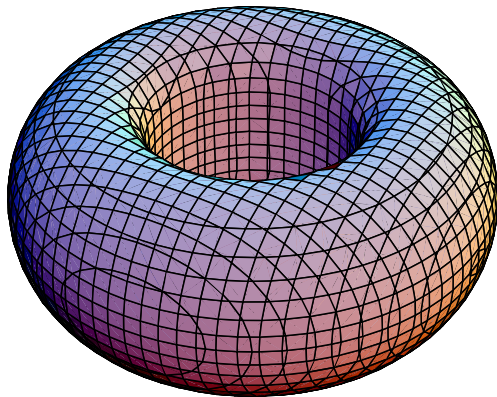
nuclear structure calculations
across the **whole nuclear chart**
based on **realistic NN-potentials**
and as close as possible to
an **ab initio** treatment

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

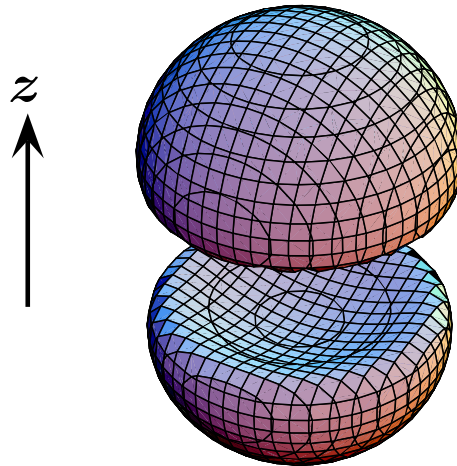
need to deal with
strong **interaction-**
induced correlations

Deuteron: Manifestation of Correlations

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



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



- spin-projected two-body density $\rho_{1,M_S}^{(2)}(\vec{r})$
- **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 short-range correlations by means of a unitary transformation with respect to the relative coordinates of all pairs

$$\mathbf{C} = \exp[-i \mathbf{G}] = \exp\left[-i \sum_{i < j} g_{ij}\right]$$

$$\begin{aligned} \mathbf{G}^\dagger &= \mathbf{G} \\ \mathbf{C}^\dagger \mathbf{C} &= \mathbf{1} \end{aligned}$$

Correlated States

$$|\tilde{\psi}\rangle = \mathbf{C} |\psi\rangle$$

Correlated Operators

$$\tilde{\mathbf{O}} = \mathbf{C}^\dagger \mathbf{O} \mathbf{C}$$

$$\langle \tilde{\psi} | \mathbf{O} | \tilde{\psi}' \rangle = \langle \psi | \mathbf{C}^\dagger \mathbf{O} \mathbf{C} | \psi' \rangle = \langle \psi | \tilde{\mathbf{O}} | \psi' \rangle$$

Central and Tensor Correlators

$$C = C_{\Omega} C_r$$

Central Correlator C_r

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

$$g_r = \frac{1}{2} [s(r) q_r + q_r s(r)]$$

$$q_r = \frac{1}{2} \left[\frac{\vec{r}}{r} \cdot \vec{q} + \vec{q} \cdot \frac{\vec{r}}{r} \right]$$

Tensor Correlator C_{Ω}

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

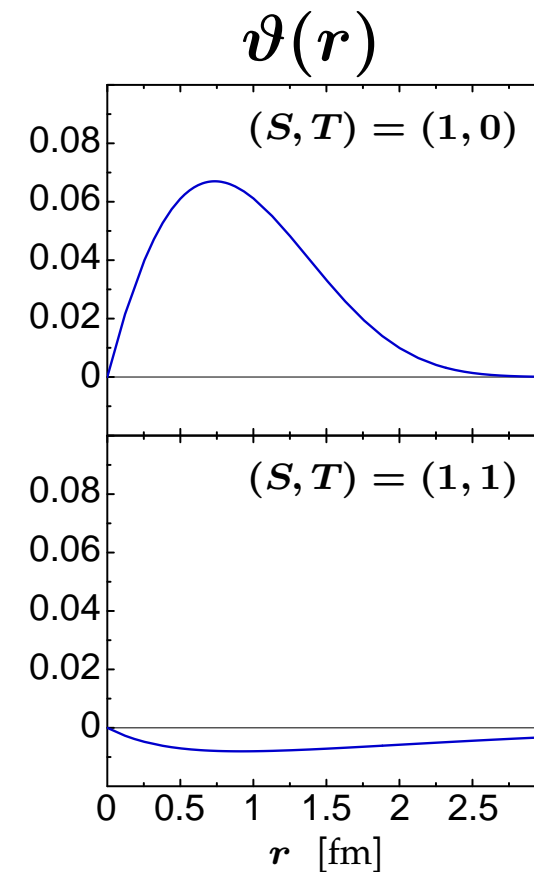
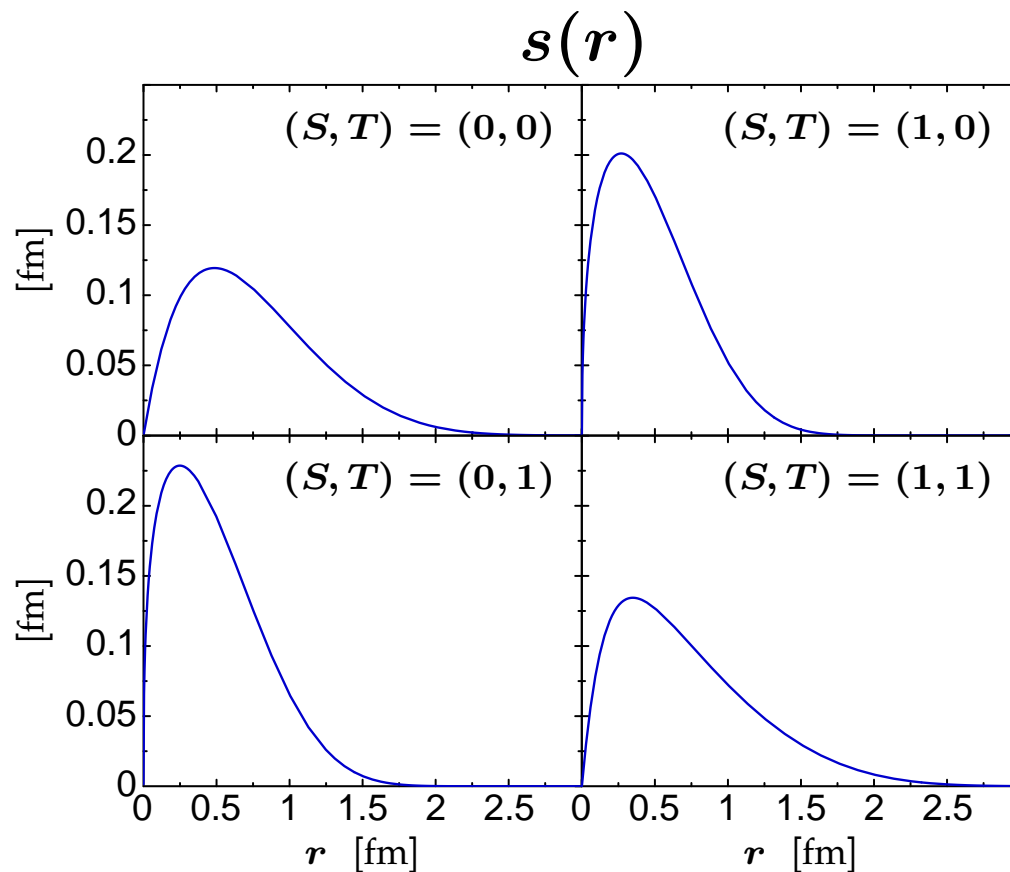
$$g_{\Omega} = \frac{3}{2} \vartheta(r) [(\vec{\sigma}_1 \cdot \vec{q}_{\Omega})(\vec{\sigma}_2 \cdot \vec{r}) + (\vec{r} \leftrightarrow \vec{q}_{\Omega})]$$

$$\vec{q}_{\Omega} = \vec{q} - \frac{\vec{r}}{r} q_r$$

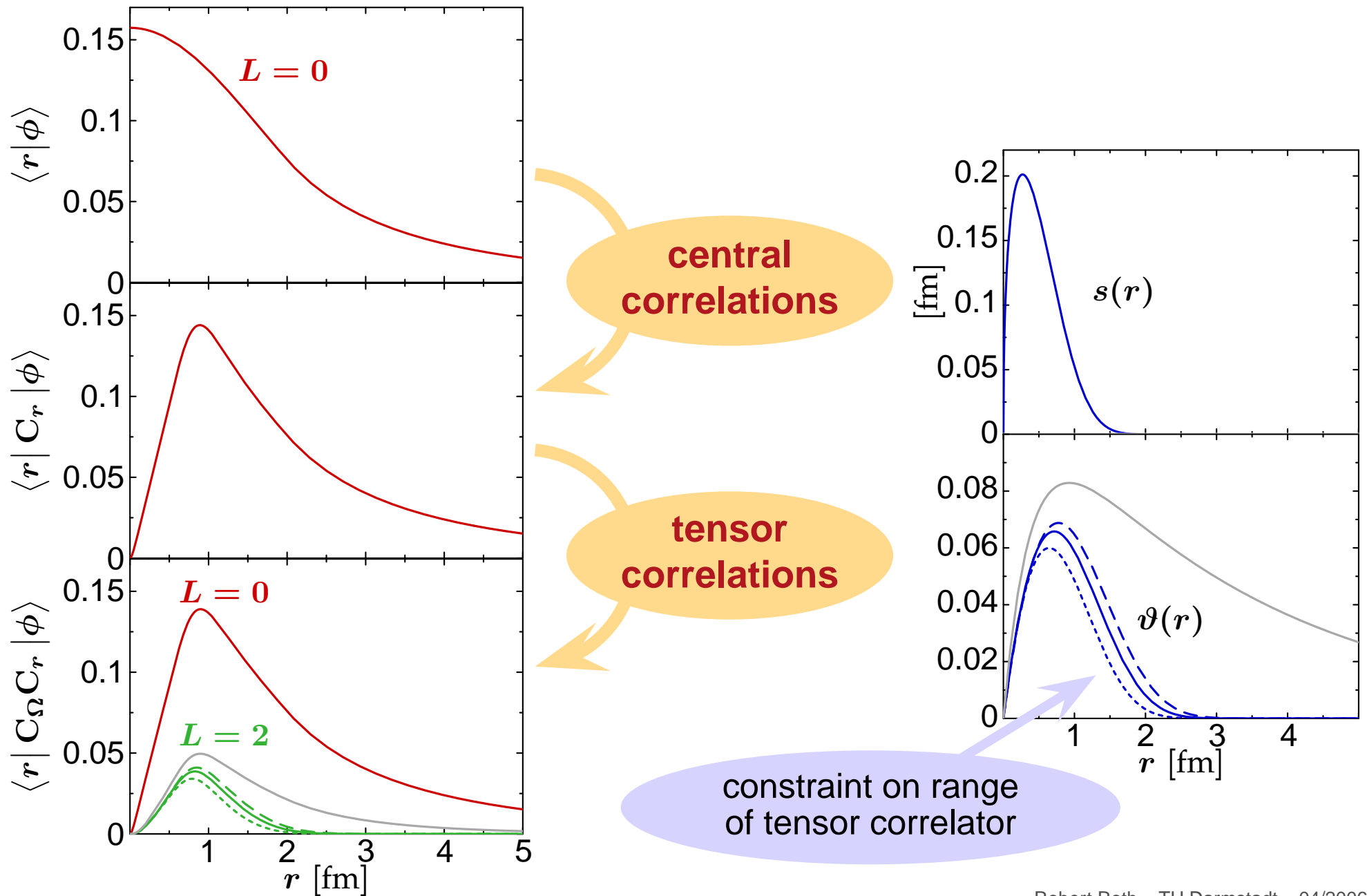
$s(r)$ and $\vartheta(r)$
describe the physics of
short-range correlations

Optimal Correlation Functions (AV18)

- $s(r)$ 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: The Deuteron



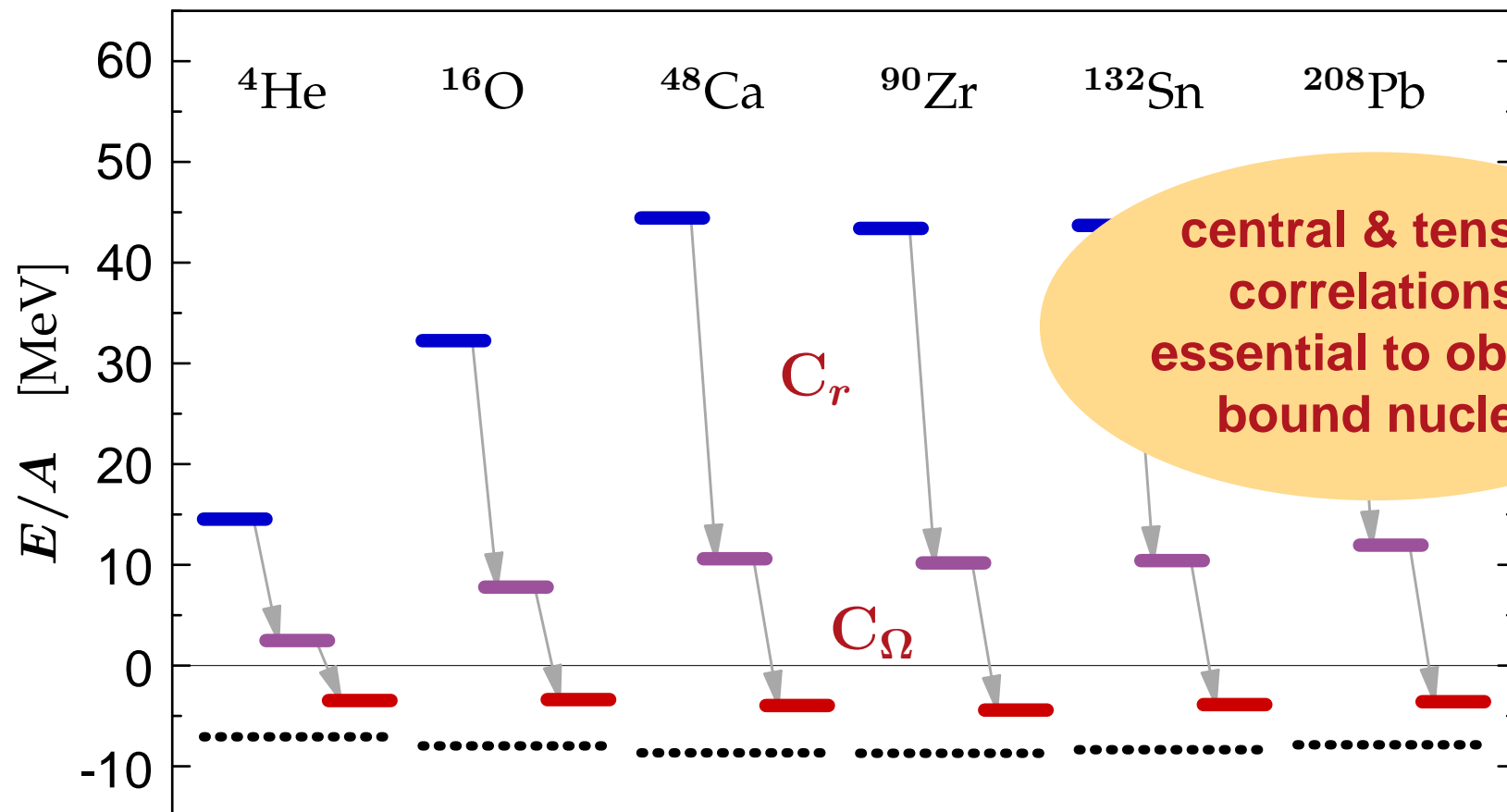
Correlated Interaction — V_{UCOM}

$$\tilde{H} = T + V_{\text{UCOM}} + V_{\text{UCOM}}^{[3]} + \dots$$

- **closed operator expression** for the correlated interaction V_{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** $V_{\text{low-}k}$

Simplistic “Shell-Model” Calculation

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



Application I

No-Core Shell Model

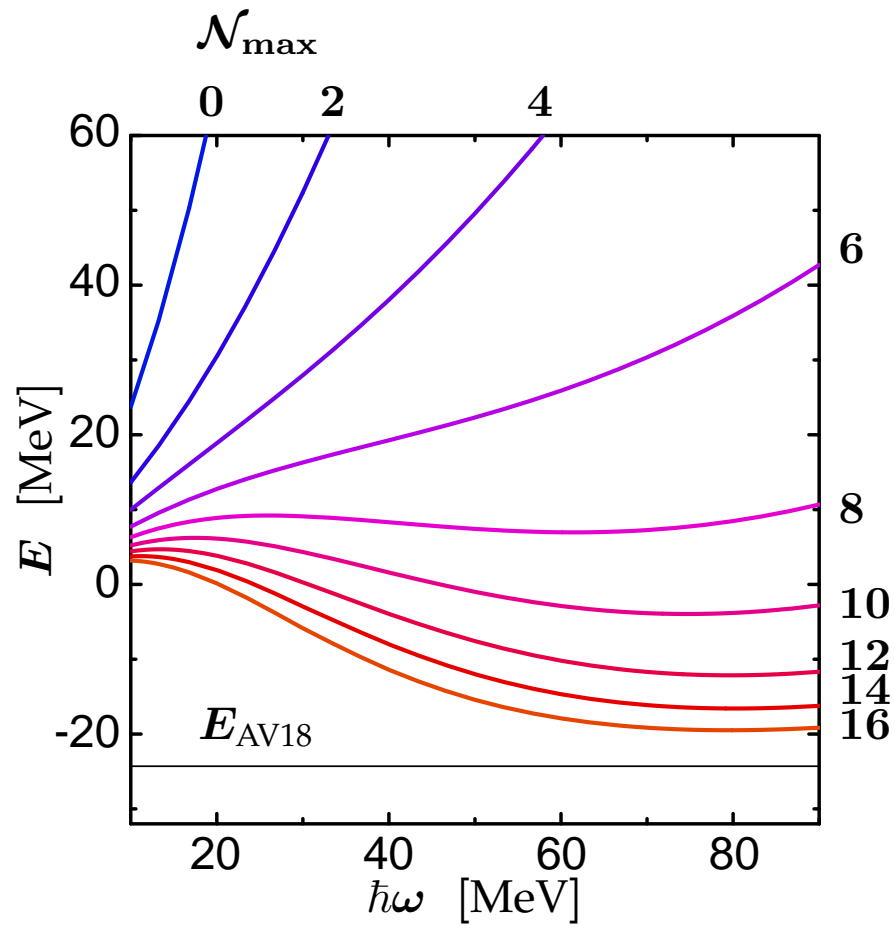
No-Core Shell Model
+
**Matrix Elements of Correlated
Realistic NN-Interaction V_{UCOM}**

- 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

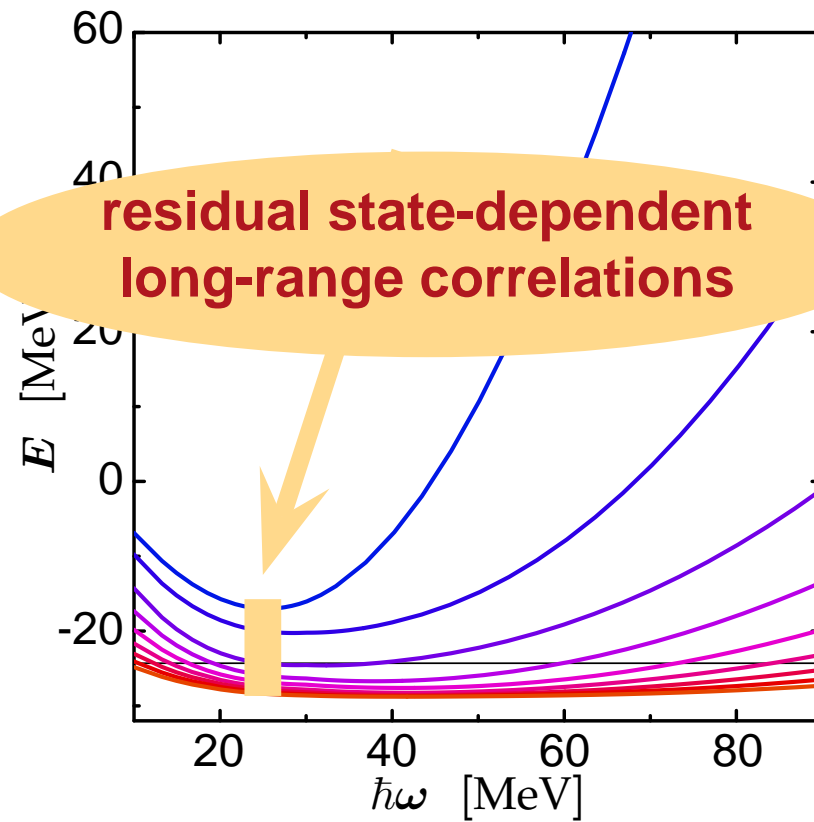
NCSM code by Petr Navrátil [PRC 61, 044001 (2000)]

^4He : Convergence

V_{AV18}

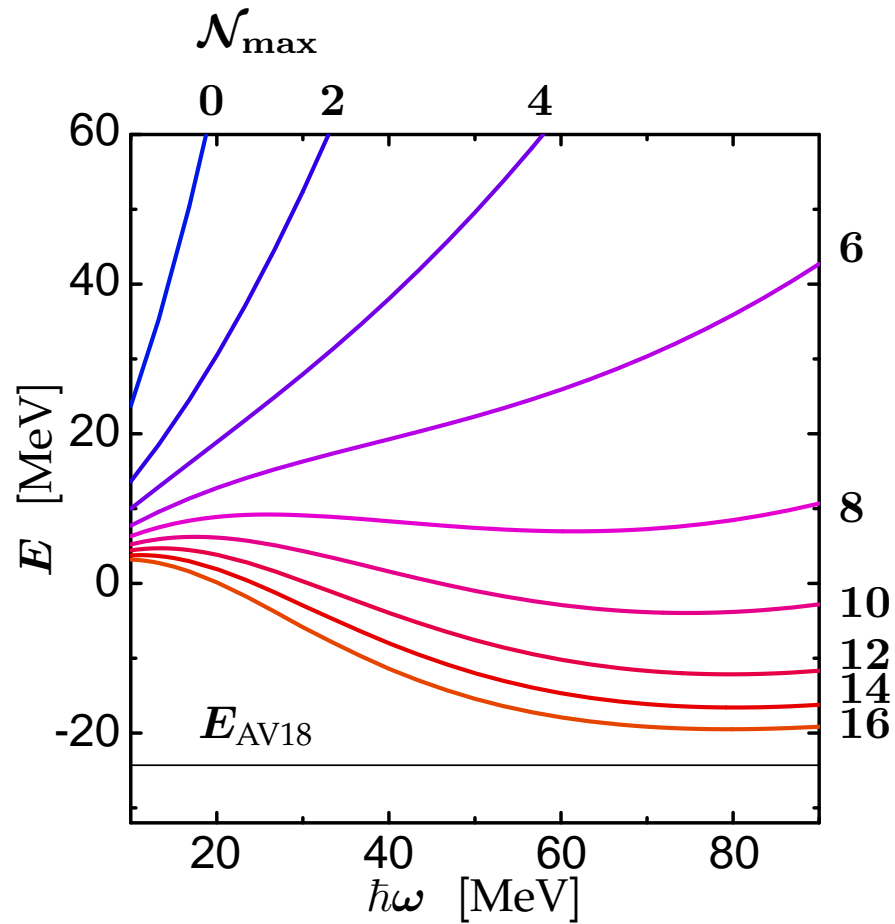


V_{UCOM}

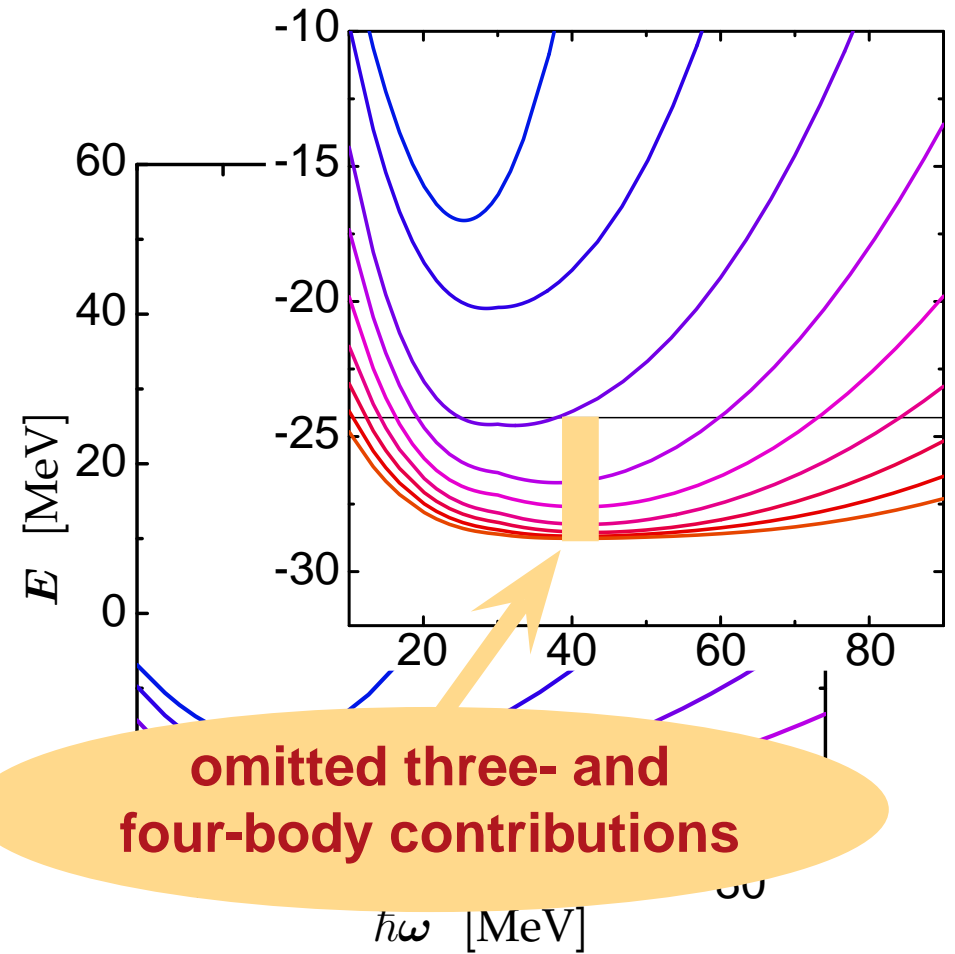


^4He : Convergence

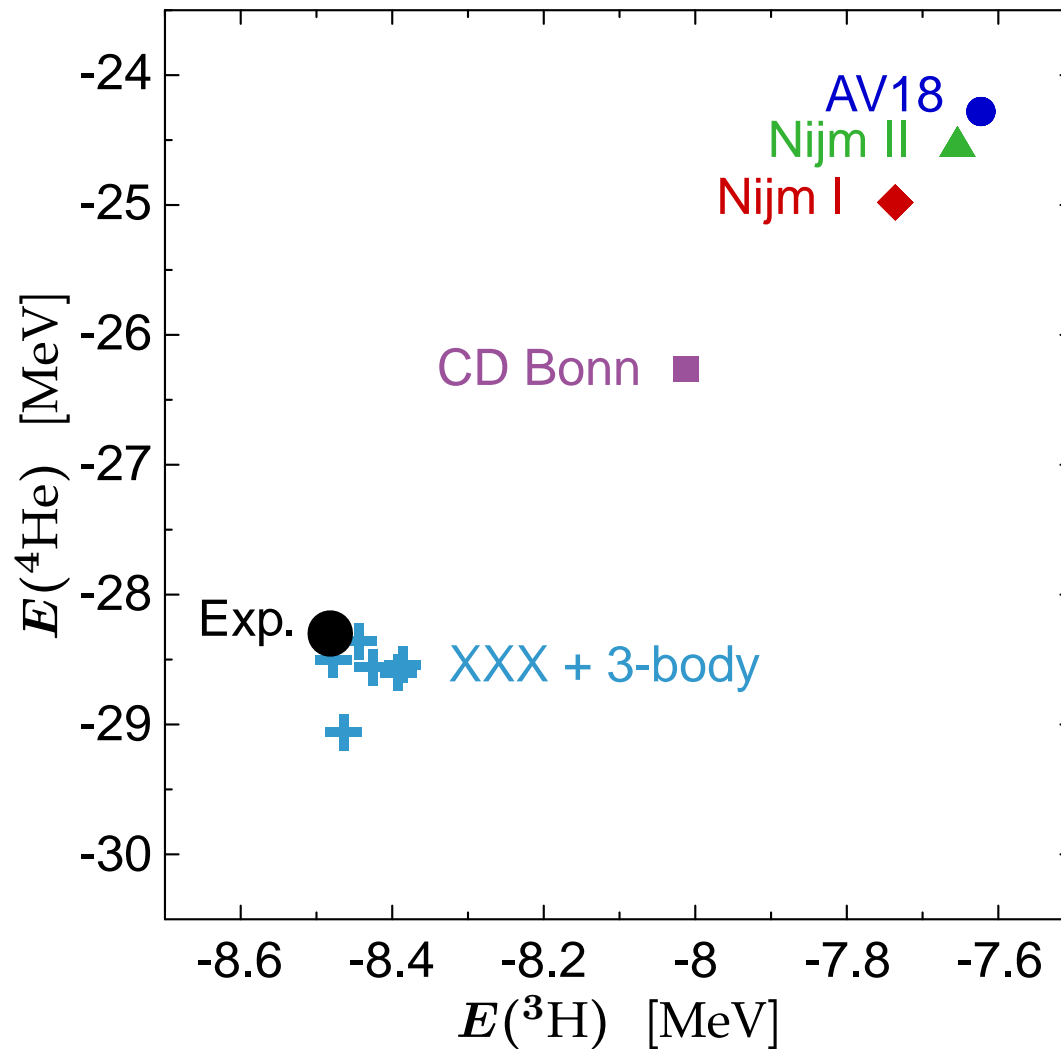
V_{AV18}



V_{UCOM}

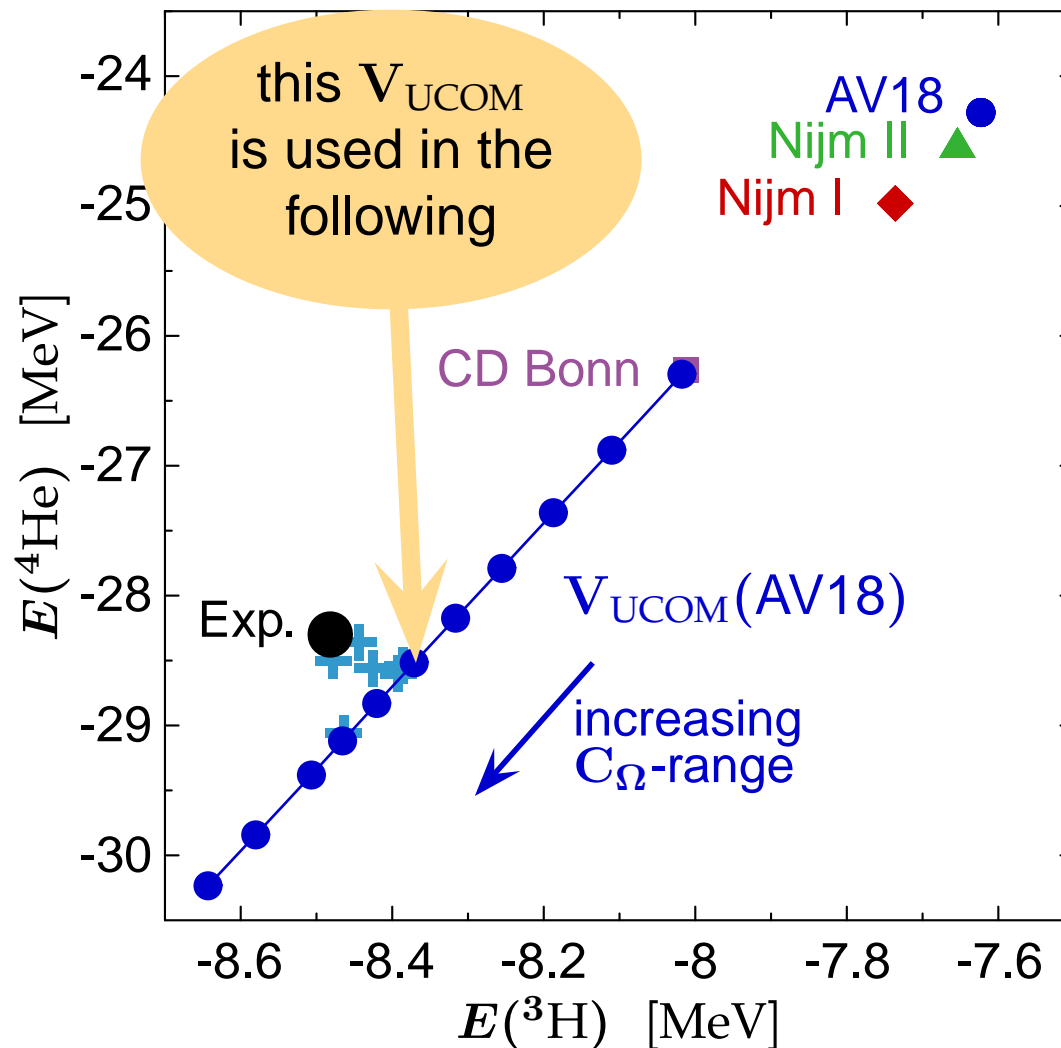


Tjon-Line and Correlator Range



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

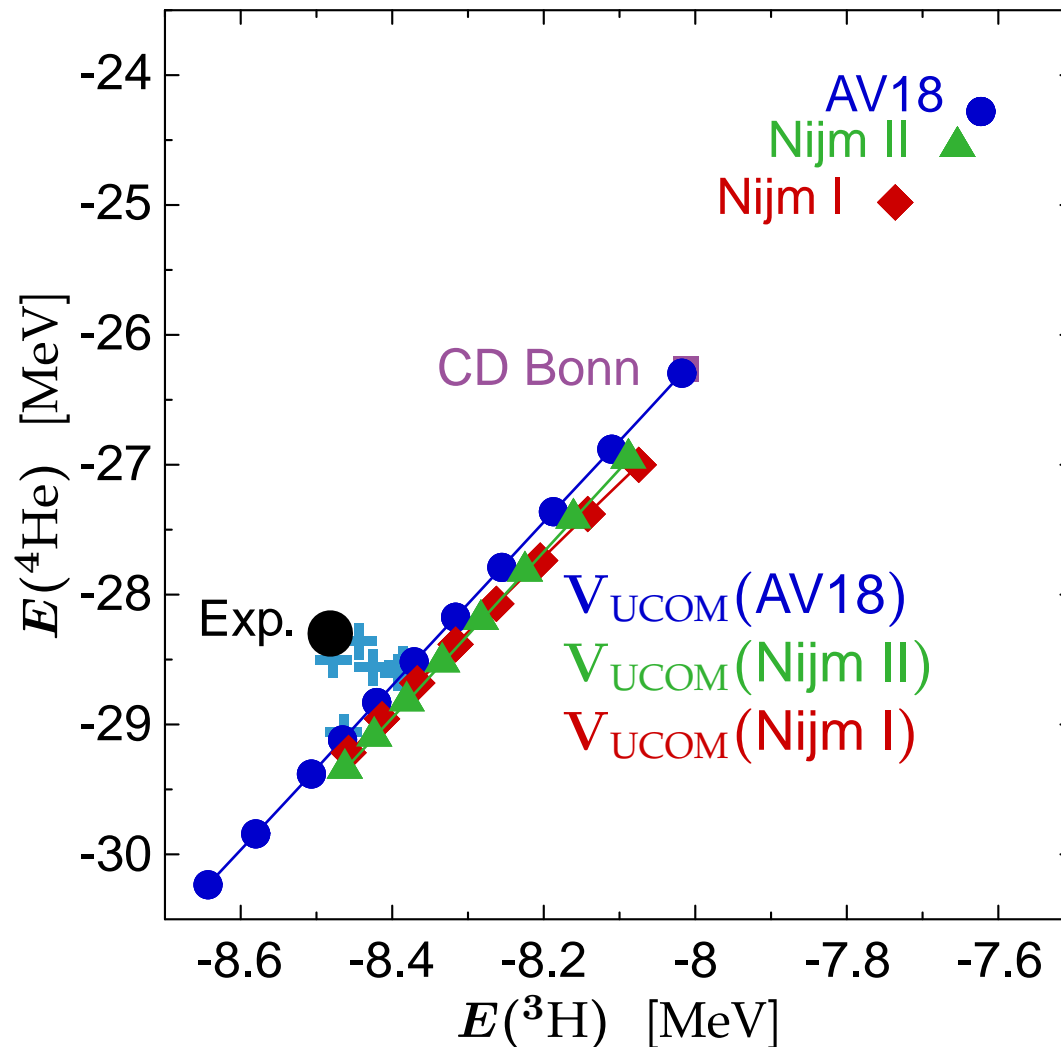
Tjon-Line and Correlator Range



- **Tjon-line:** $E(^4\text{He})$ vs. $E(^3\text{H})$ for phase-shift equivalent NN-interactions
- change of C_{Ω} -correlator range results in shift along Tjon-line

minimise net three-body force by choosing correlator with energies close to experimental value

Tjon-Line and Correlator Range

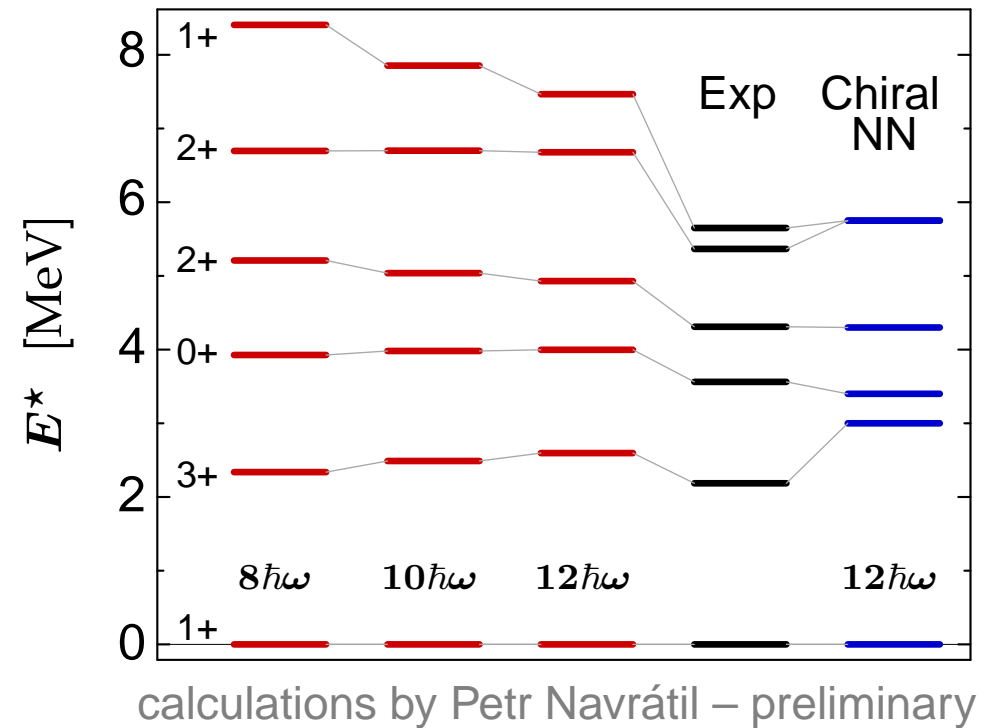
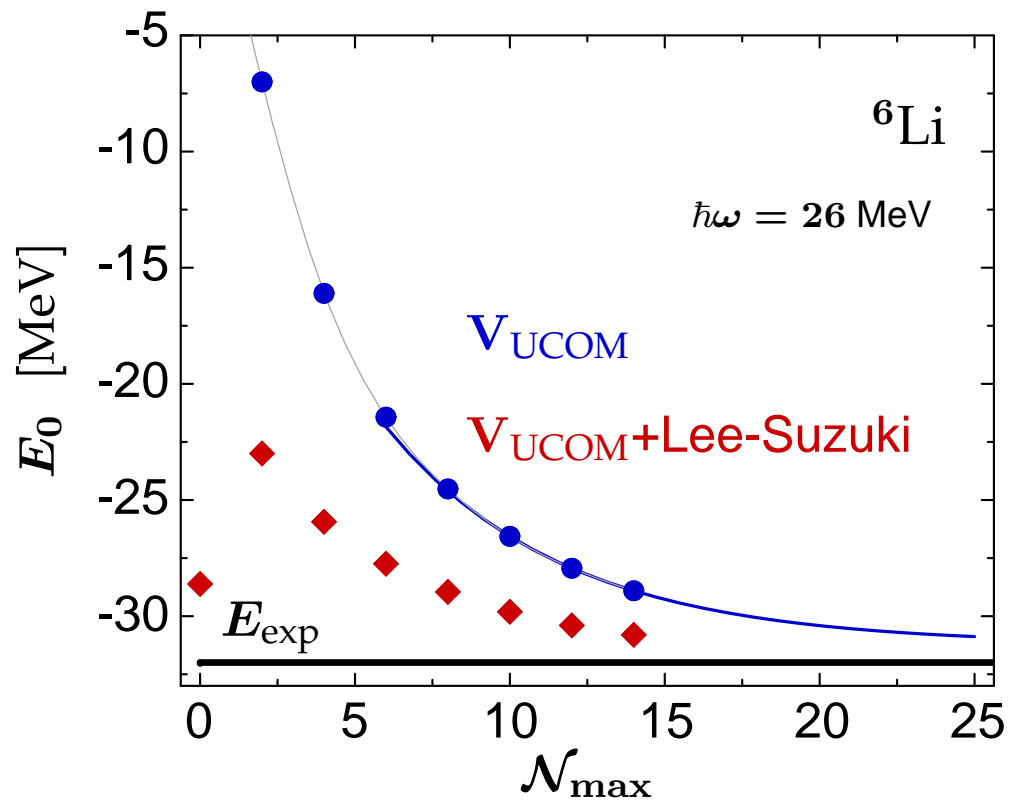


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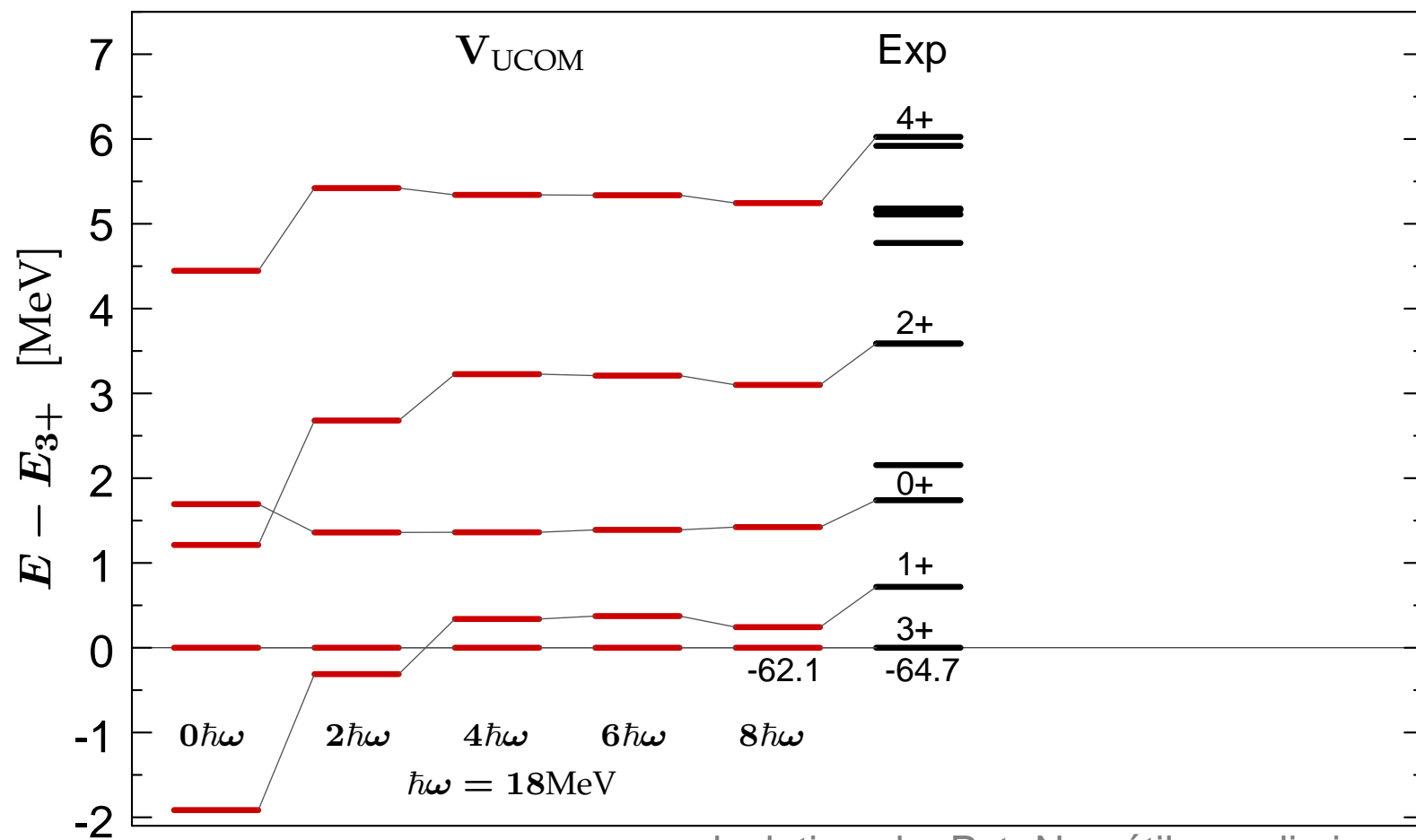
**minimise net
three-body force**
by choosing correlator
with energies close to
experimental value

${}^6\text{Li}$: NCSM for p-Shell Nuclei

- systematic NCSM calculations throughout p-shell in progress (with and without Lee-Suzuki transformation)

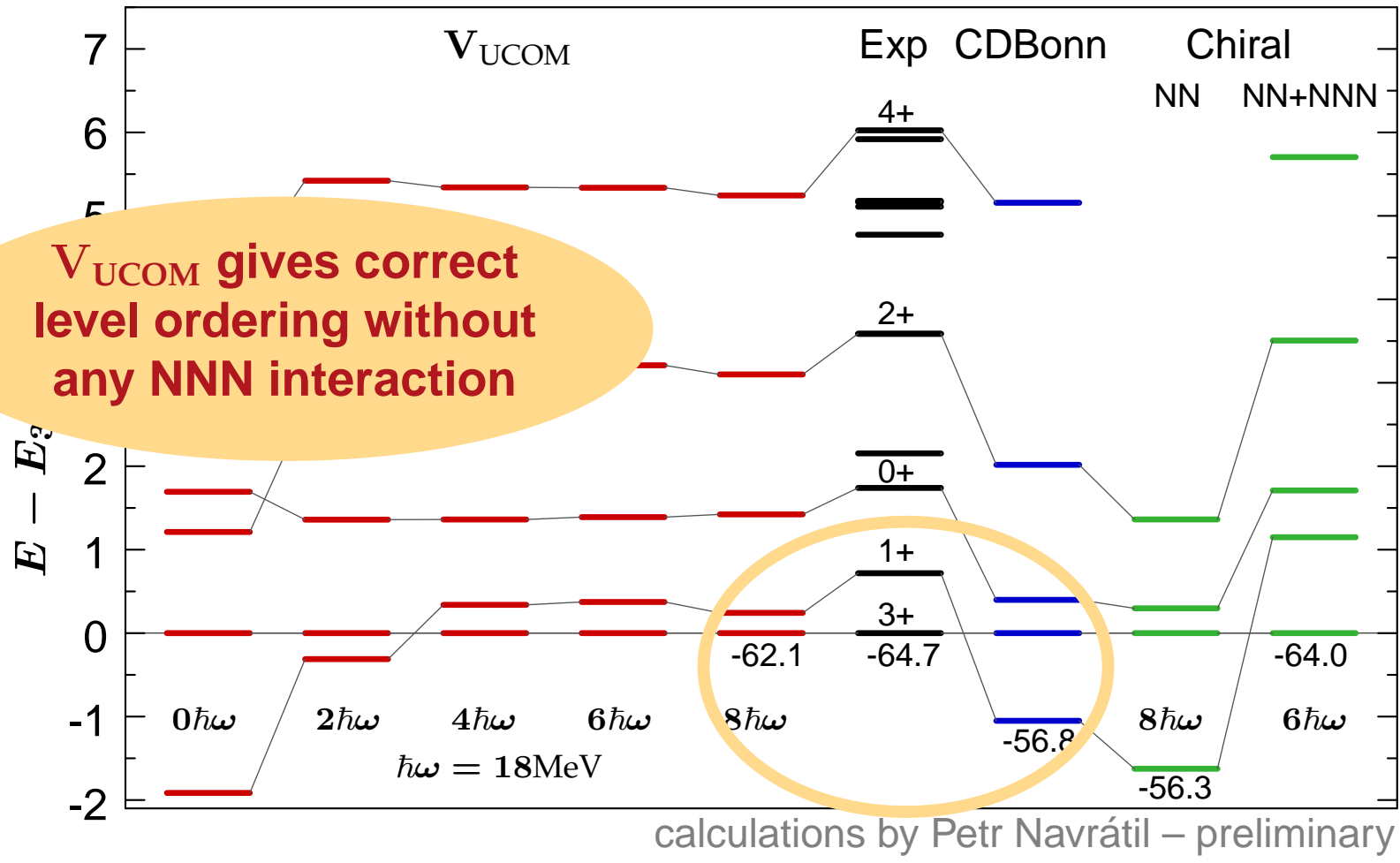


^{10}B : Benchmark for V_{UCOM}



calculations by Petr Navrátil – preliminary

^{10}B : Benchmark for V_{UCOM}



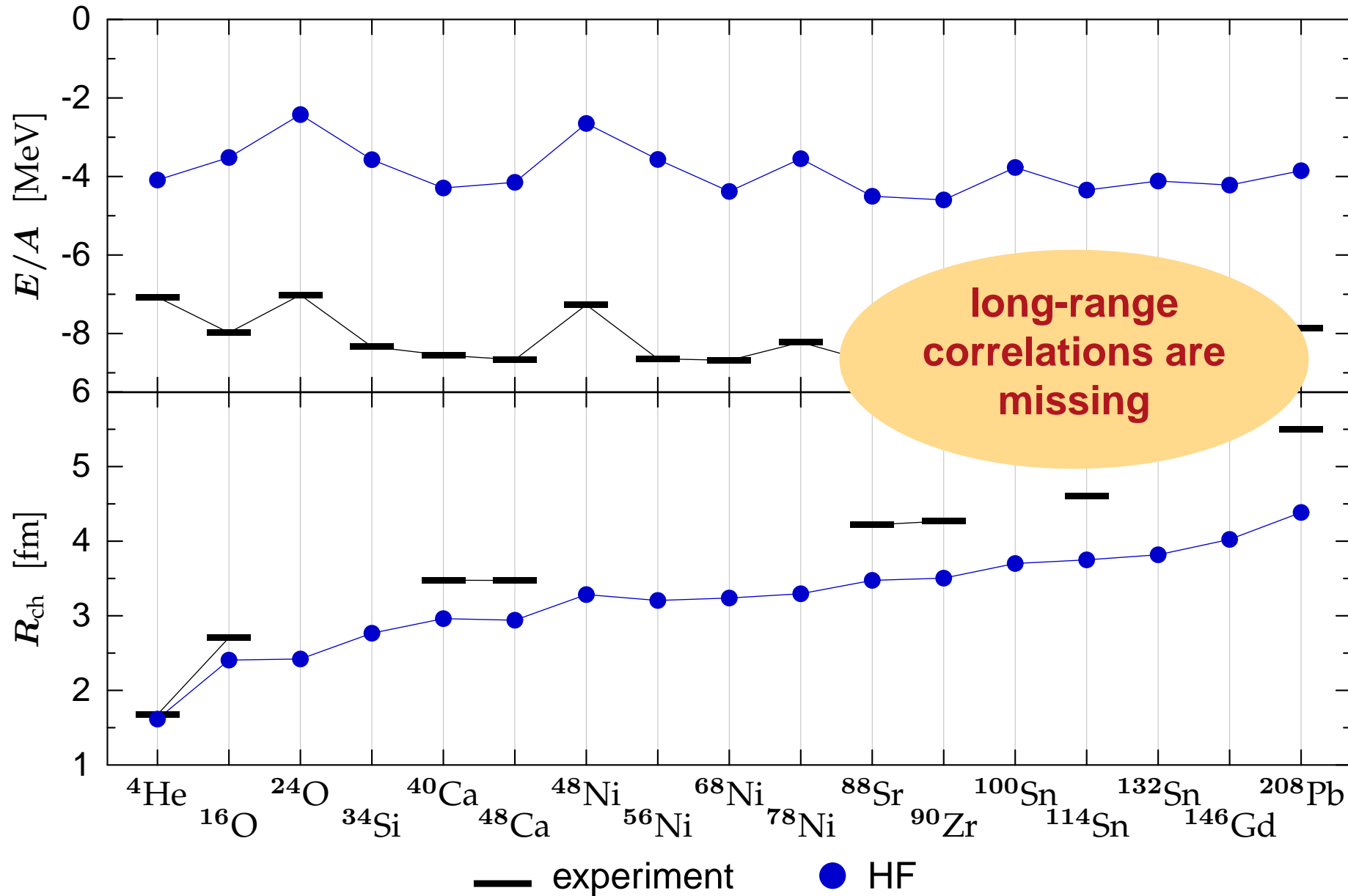
Application II:

Hartree-Fock & Beyond

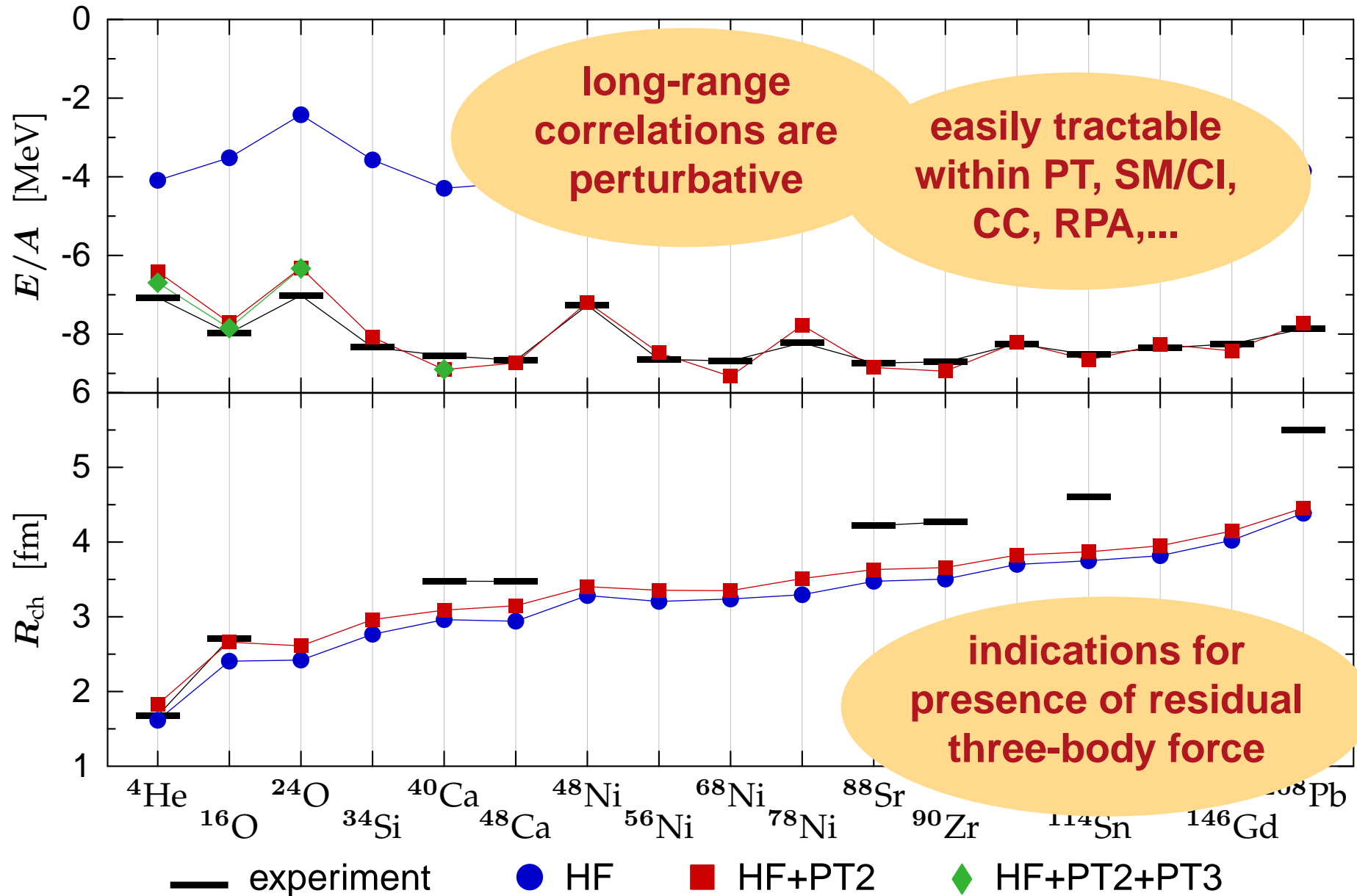
**Standard Hartree-Fock
+
Matrix Elements of Correlated
Realistic NN-Interaction V_{UCOM}**

- many-body state is a **Slater determinant** of single-particle states expanded in oscillator basis (~ 12 major shells)
- **correlations cannot be described** by Hartree-Fock states
- starting point for **improved many-body calculations**: MBPT, RPA, SM/CI, CC,...

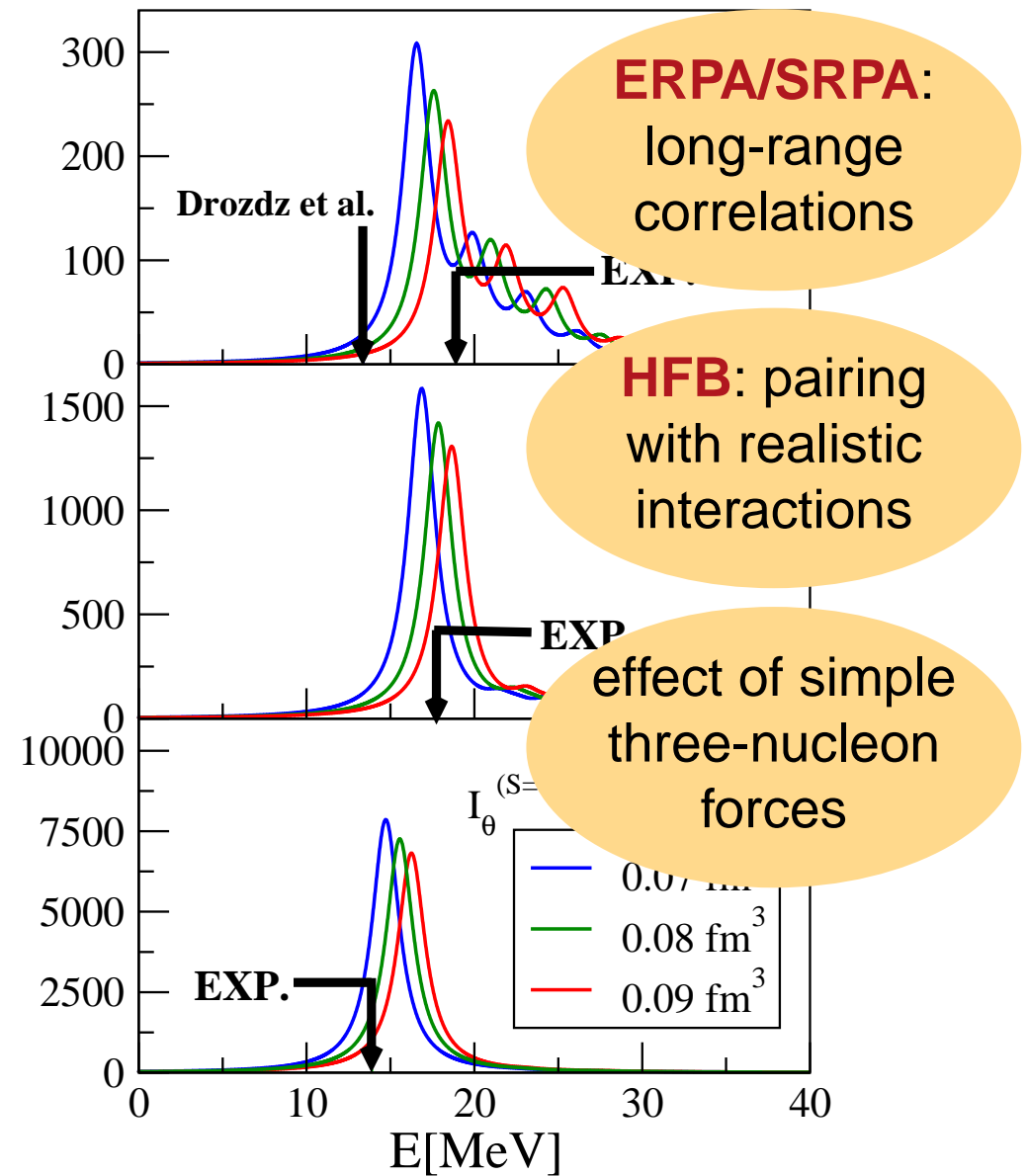
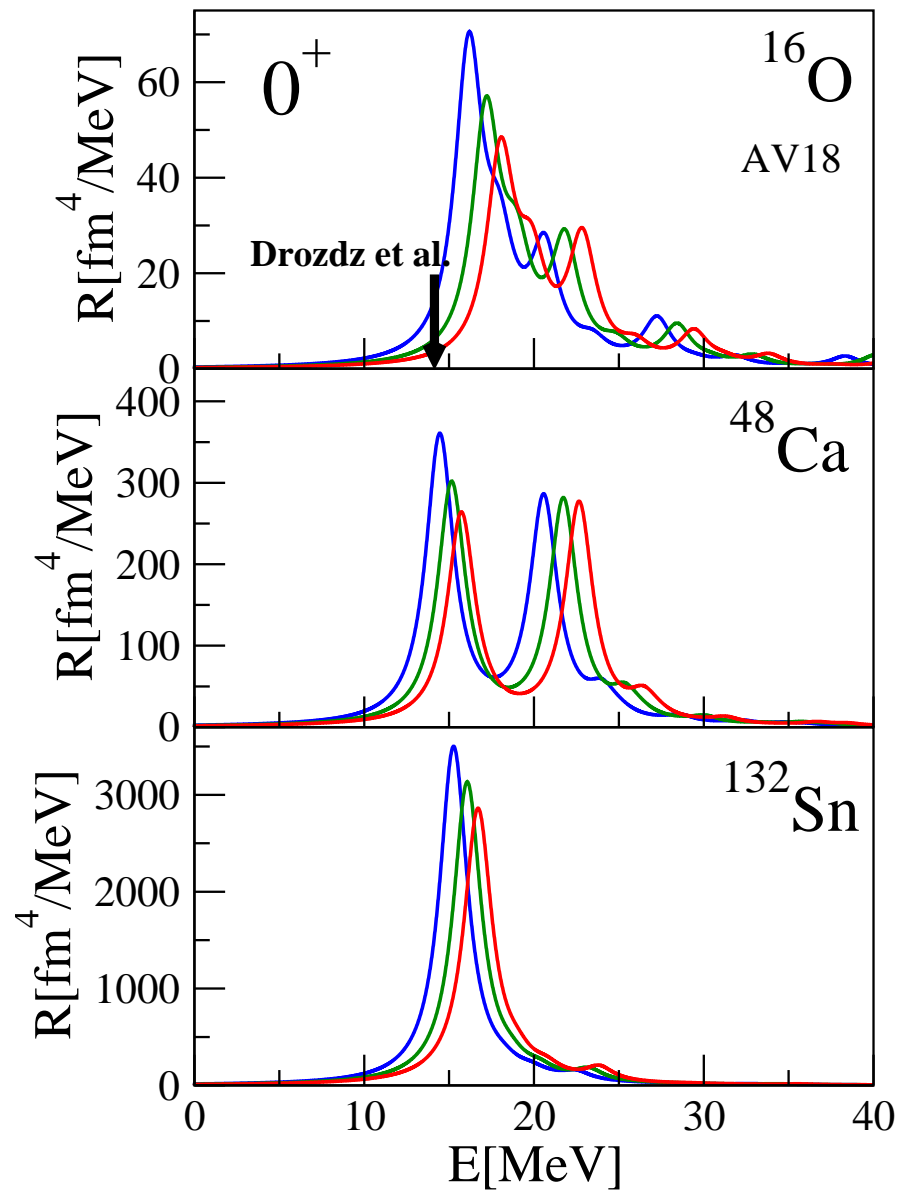
Hartree-Fock with V_{UCOM}



Perturbation Theory with V_{UCOM}



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_{ν} : complex width

χ_{ν} : spin orientation

\vec{b}_{ν} : mean position & momentum

Slater Determinant

$$|Q\rangle = \mathcal{A} (|q_1\rangle \otimes |q_2\rangle \otimes \cdots \otimes |q_A\rangle)$$

Correlated Hamiltonian

$$\tilde{H} = T + V_{\text{UCOM}} + \delta V_{c+p+ls}$$

Variation

$$\frac{\langle Q | \tilde{H} - T_{\text{cm}} | Q \rangle}{\langle Q | Q \rangle} \rightarrow \min$$

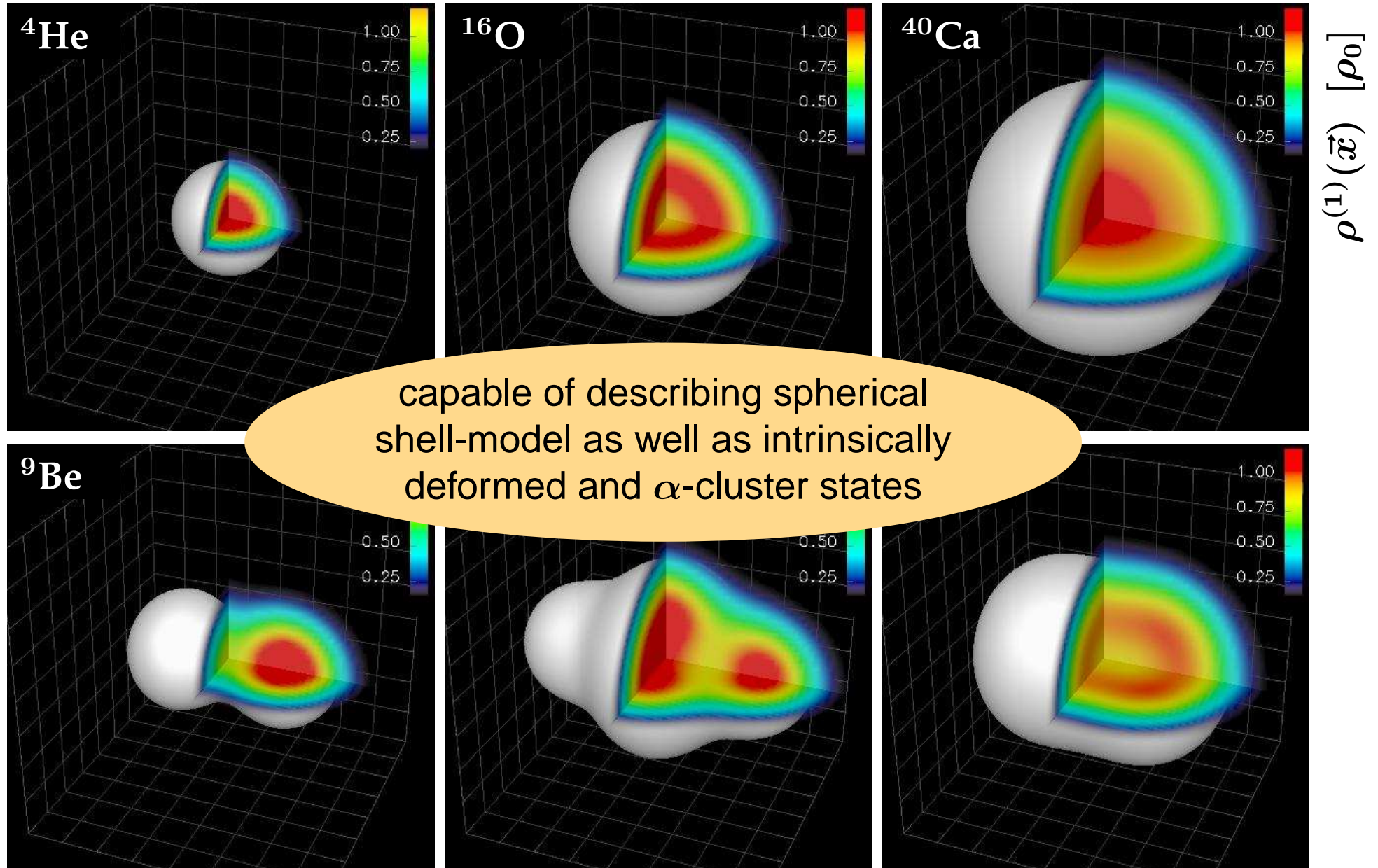
Projection

restoration of rotational
and inversion symmetry
PAV / VAP

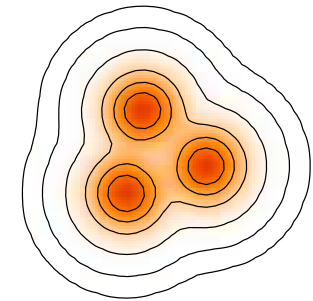
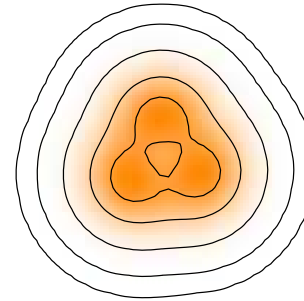
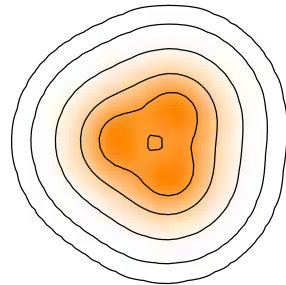
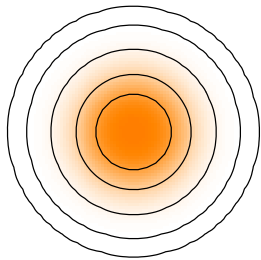
Multi- Configuration

mixing of several
intrinsic configurations
GCM

Intrinsic One-Body Density Distributions

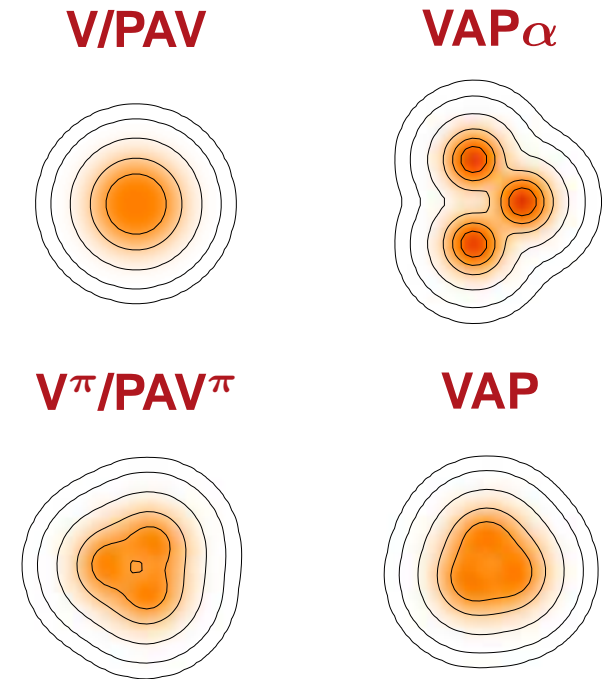
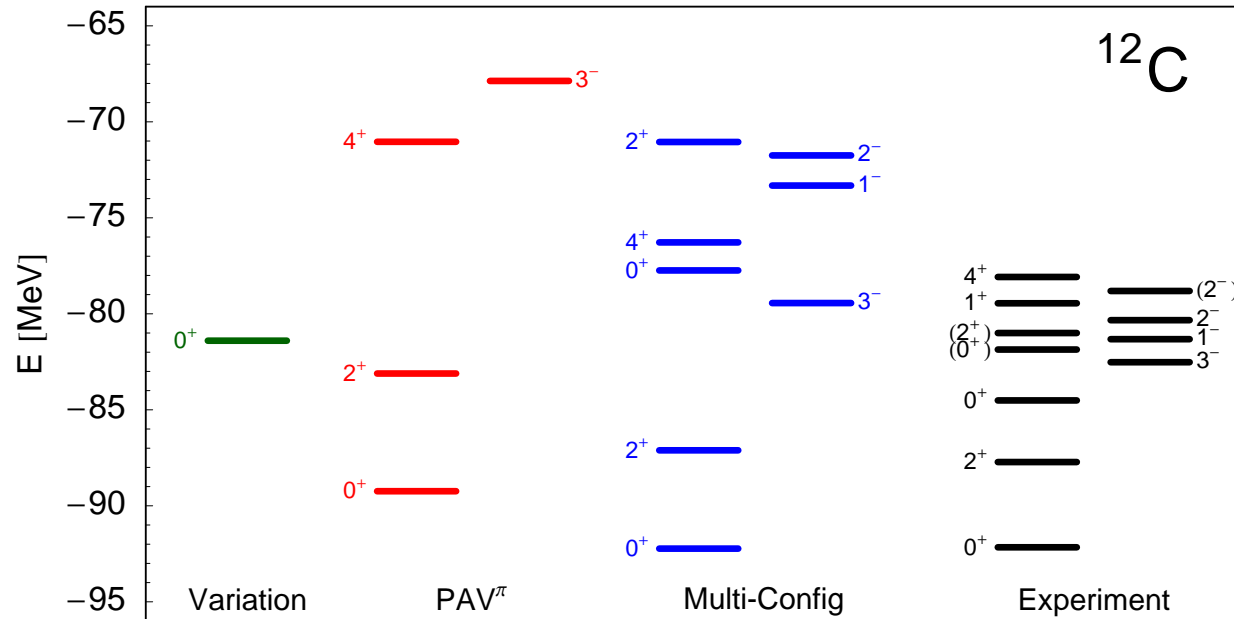


Intrinsic Shapes of ^{12}C



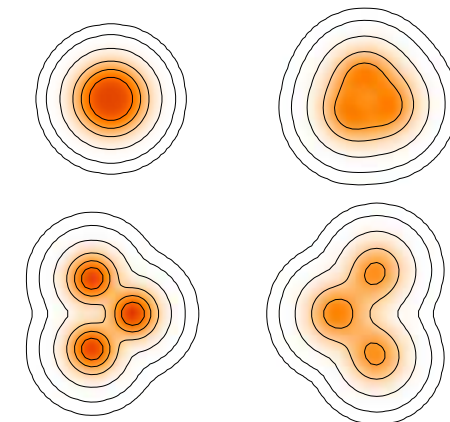
	intrinsic	projected	intrinsic	projected	intrinsic	projected	intrinsic	projected
$\langle \mathbf{H} \rangle$	-81.4	-81.5	-77.0	-88.5	-74.1	-85.5	-57.0	-75.9
$\langle \mathbf{T} \rangle$	212.1	212.1	189.2	186.1	182.8	179.0	213.9	201.4
$\langle \mathbf{V}_{ls} \rangle$	-39.8	-40.2	-12.0	-17.1	-5.8	-8.0	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

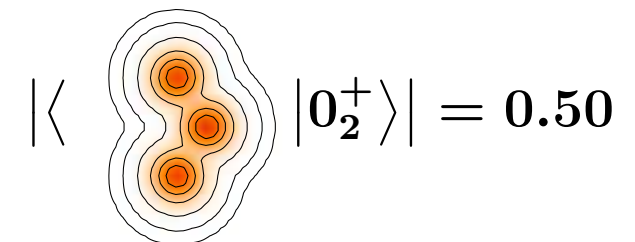
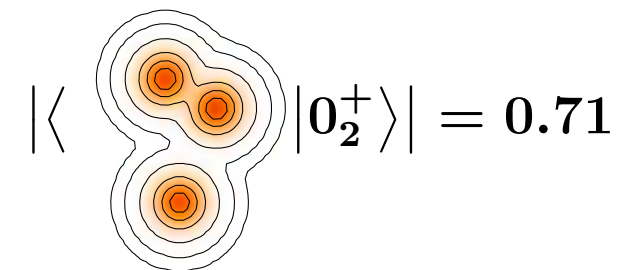
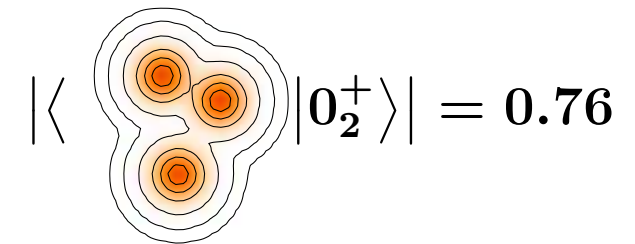
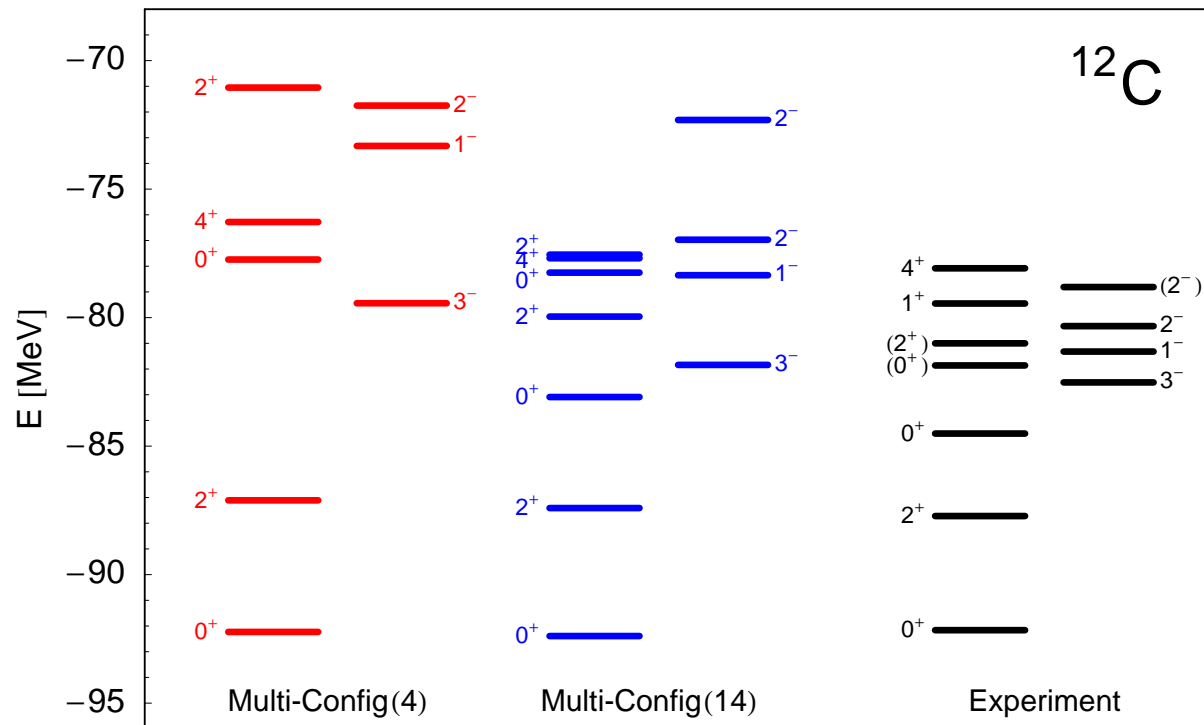


	E [MeV]	R_{ch} [fm]	$B(E2)$ [$e^2 \text{fm}^4$]
V/PAV	81.4	2.36	-
VAP α -cluster	79.1	2.70	76.9
PAV $^\pi$	88.5	2.51	36.3
VAP	89.2	2.42	26.8
Multi-Config	92.2	2.52	42.8
Experiment	92.2	2.47	39.7 ± 3.3

Multi-Config

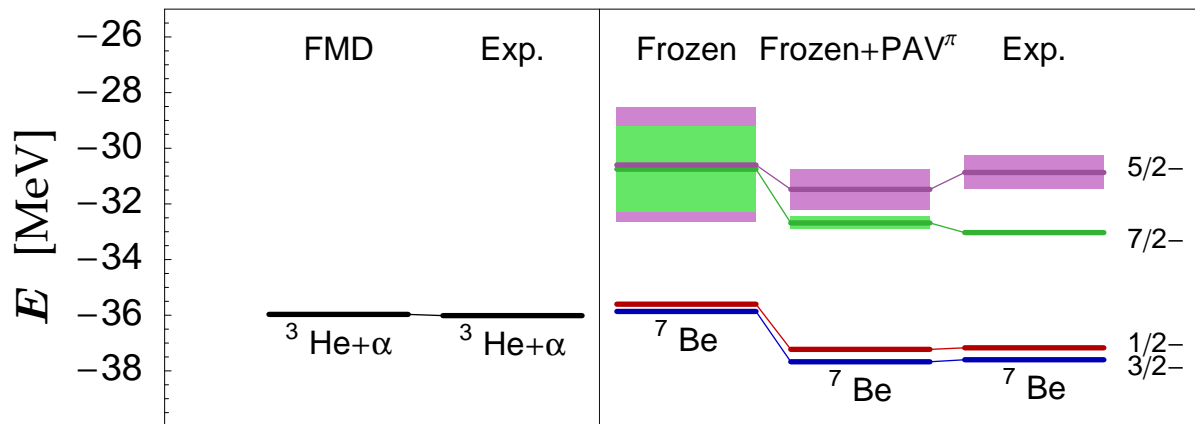


Structure of ^{12}C — Hoyle State

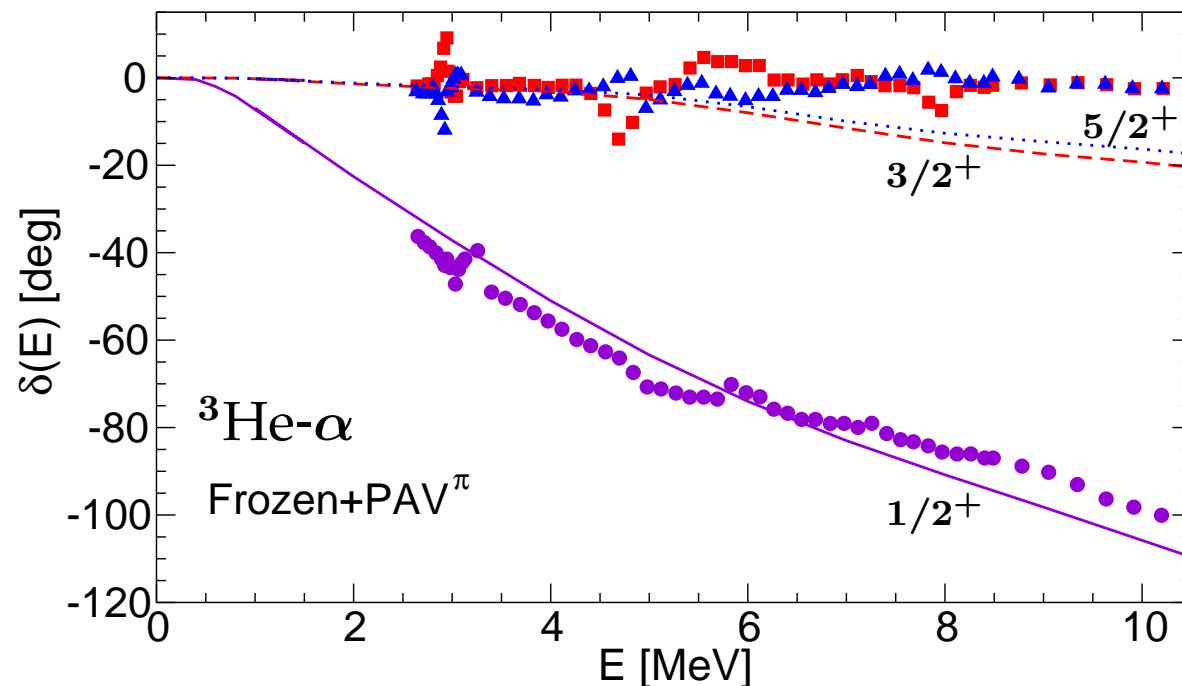


	Multi-Config	Experiment
E [MeV]	92.4	92.2
R_{ch} [fm]	2.52	2.47
$B(E2, 0_1^+ \rightarrow 2_1^+)$ [$e^2 \text{ fm}^4$]	42.9	39.7 ± 3.3
$M(E0, 0_1^+ \rightarrow 0_2^+)$ [fm^2]	5.67	5.5 ± 0.2

Outlook: Resonances & Scattering in FMD



- collective coordinate representation as tool for the description of continuum states in FMD



first steps towards fully microscopic and consistent description of **structure and reactions**

Conclusions

■ Unitary Correlation Operator Method (UCOM)

- explicit description of short-range central and tensor correlations
- universal phase-shift equivalent correlated interaction V_{UCOM}

■ Innovative Many-Body Methods

- No-Core Shell Model
- Hartree-Fock, MBPT, SM/CI, CC, RPA, ERPA, SRPA,...
- Fermionic Molecular Dynamics

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

■ thanks to my group & my collaborators

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Fundamental Experiments...”