New Frontiers in Nuclear Structure Theory

From Realistic Interactions to the Nuclear Chart

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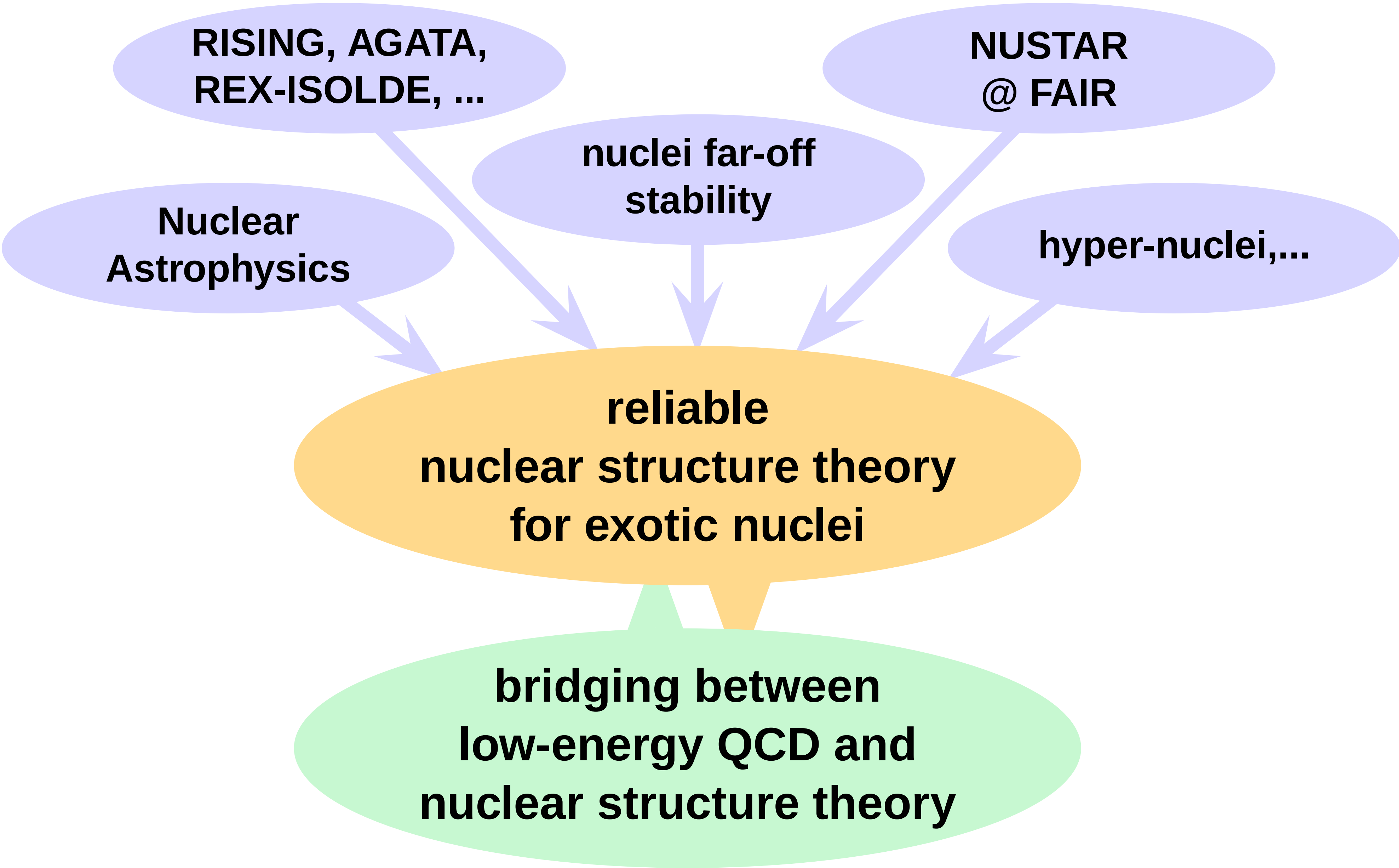
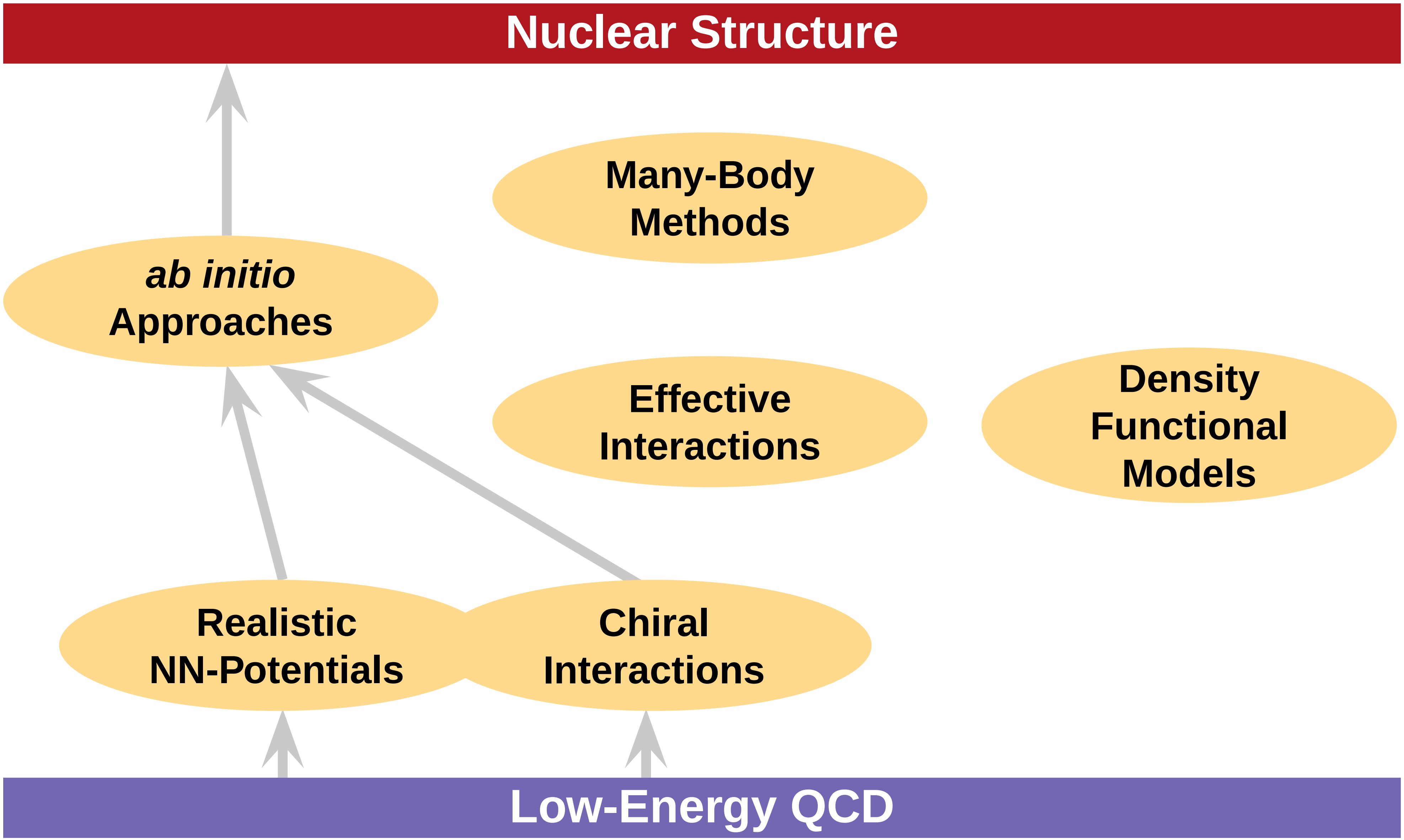
Overview

- Motivation
- Modern Effective Interactions
  - Correlations & Unitary Correlation Operator Method
- Applications
  - No Core Shell Model
  - Hartree-Fock & Beyond
  - Fermionic Molecular Dynamics

Nuclear Structure in the 21st Century



Modern Nuclear Structure Theory



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

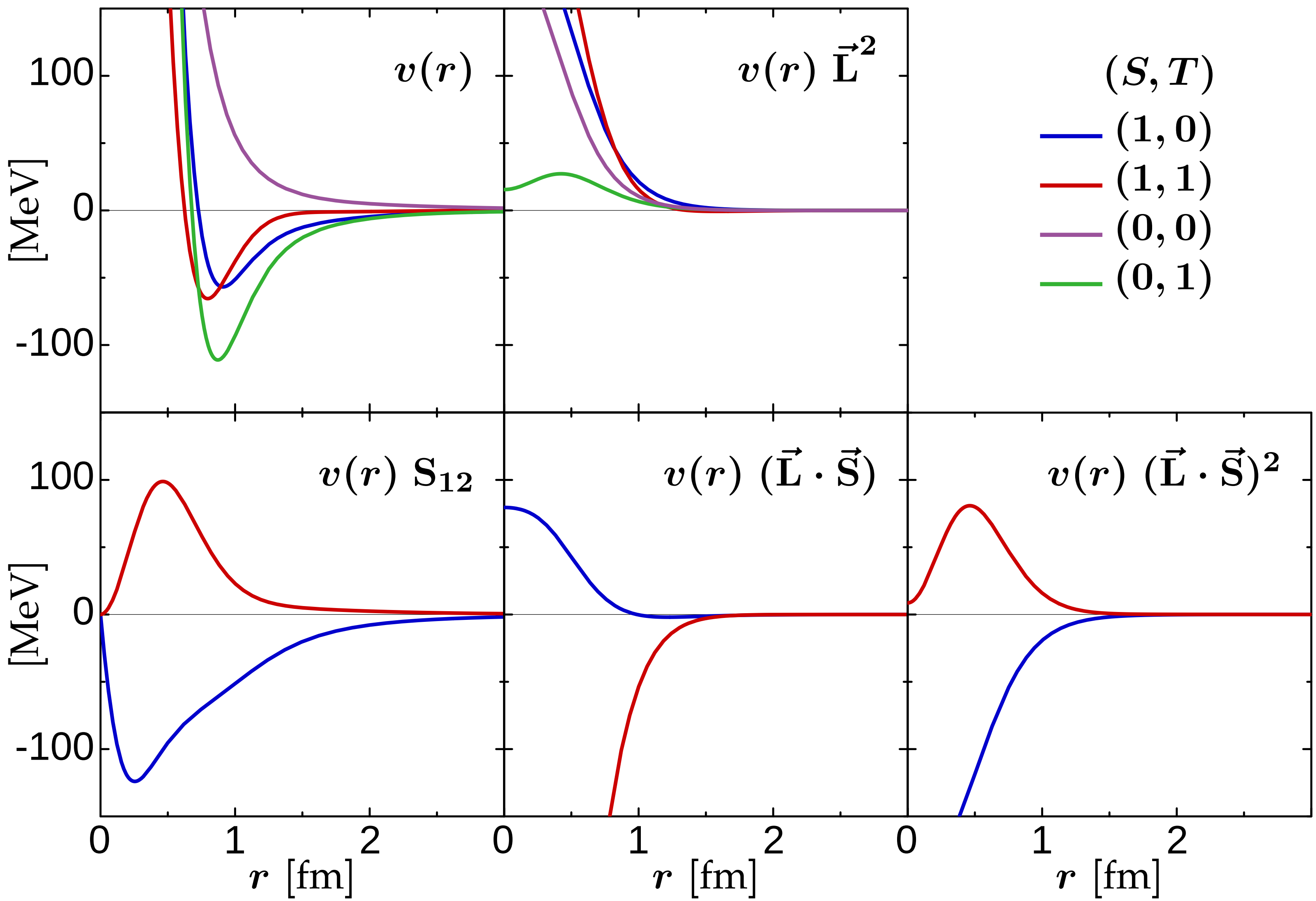
Nijmegen I/II

Chiral N3LO

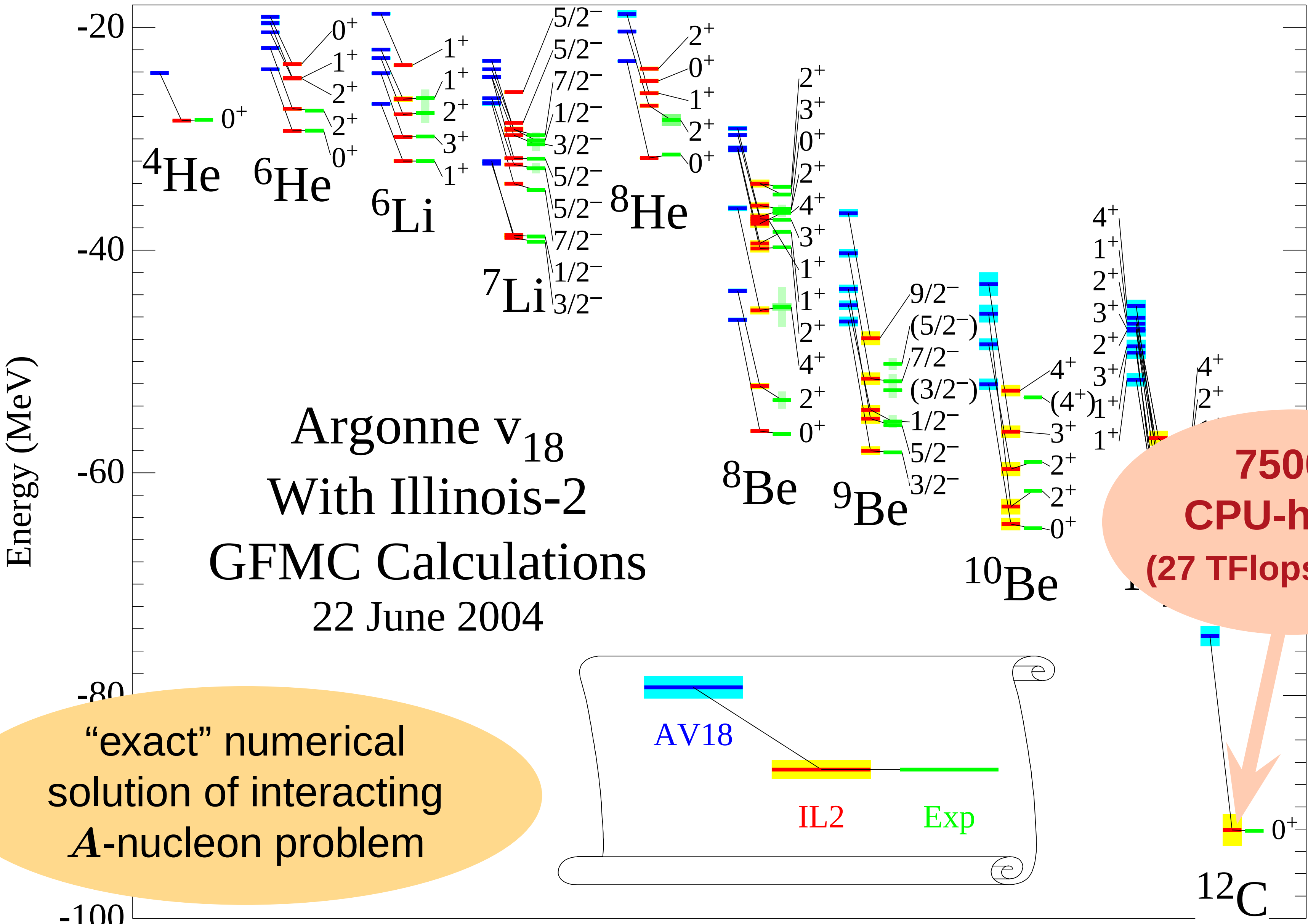
Argonne V18 +
Illinois 2

Chiral N3LO +
N2LO

Argonne V18 Potential



Ab initio Methods: GFMC



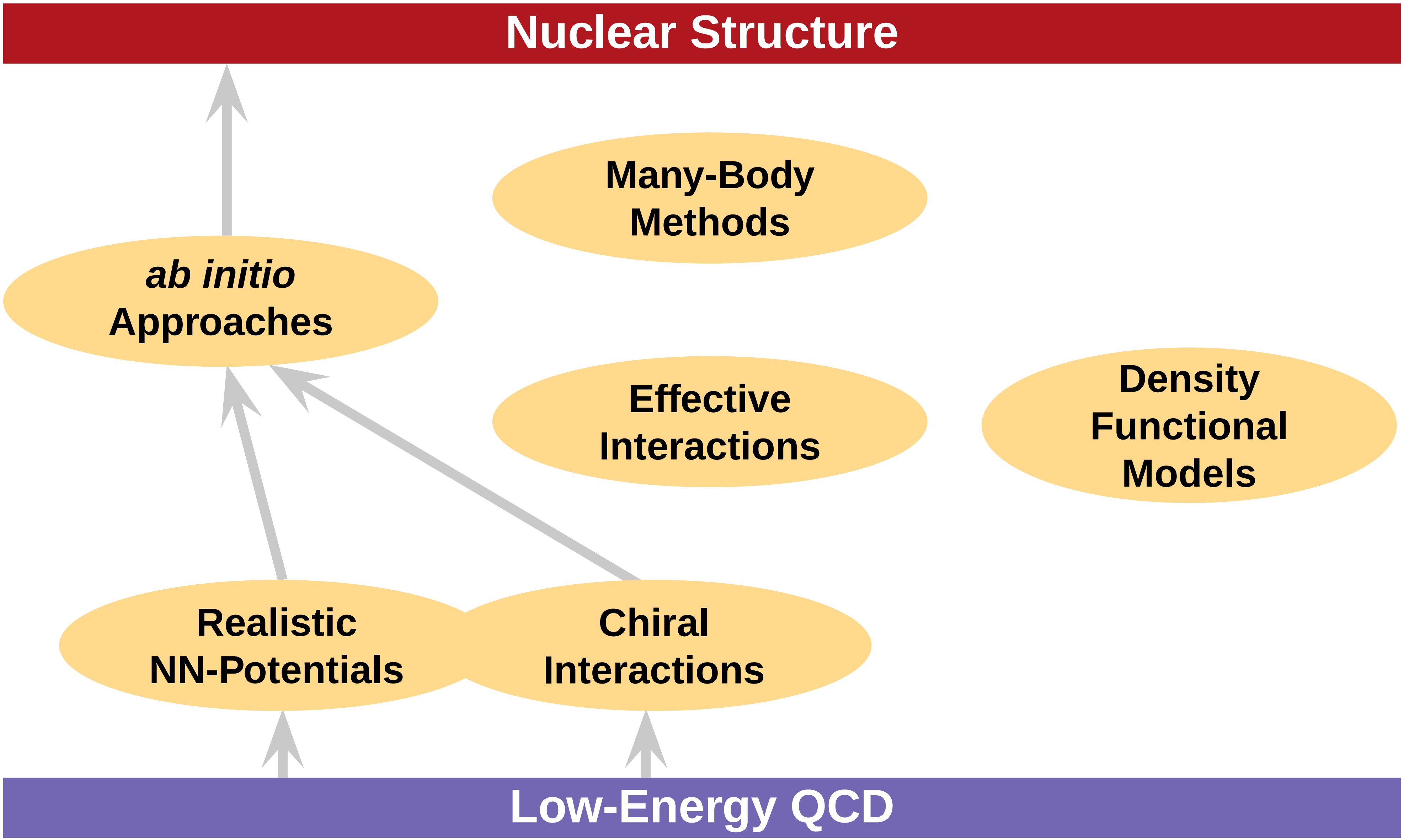
"exact" numerical solution of interacting *A*-nucleon problem

75000 CPU-hours (27 TFlops-hours)

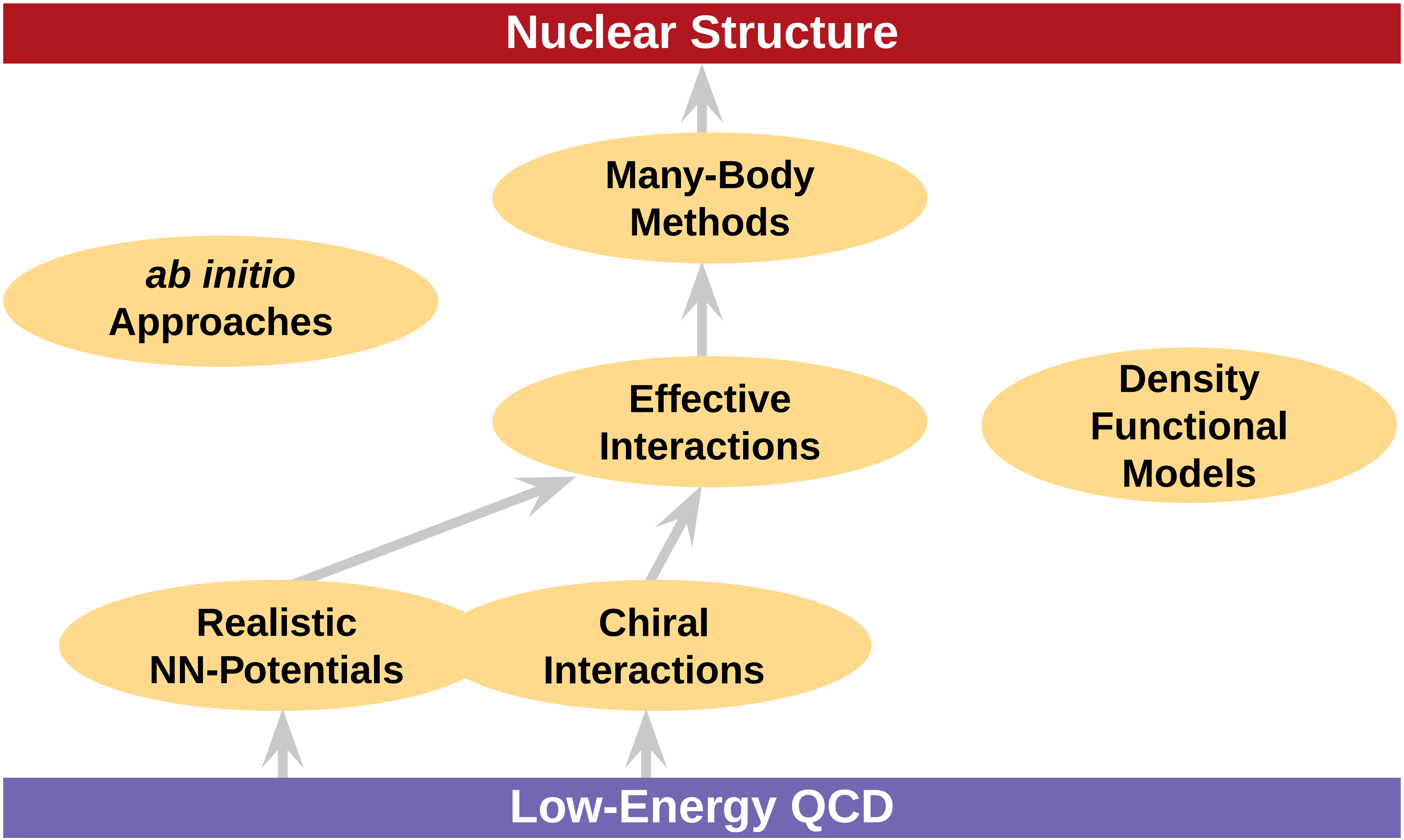
[S. Pieper, private comm.]

^{12}C results are preliminary.

Modern Nuclear Structure Theory



Modern Nuclear Structure Theory



Why Effective Interactions?

Realistic Potentials

- generate strong correlations in many-body states
- short-range central & tensor correlations most important

Modern Effective Interactions

- adapt realistic potential to the available model space
- conserve experimentally constrained properties (phase shifts)

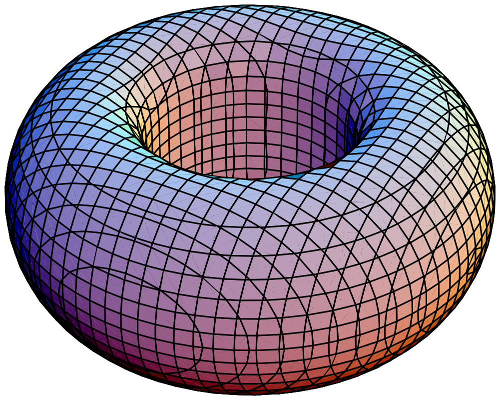
Many-Body Methods

- rely on truncated many-nucleon Hilbert spaces for $A > 12$
- not capable of describing short-range correlations
- extreme: Hartree-Fock based on single Slater determinant

Deuteron: Manifestation of Correlations

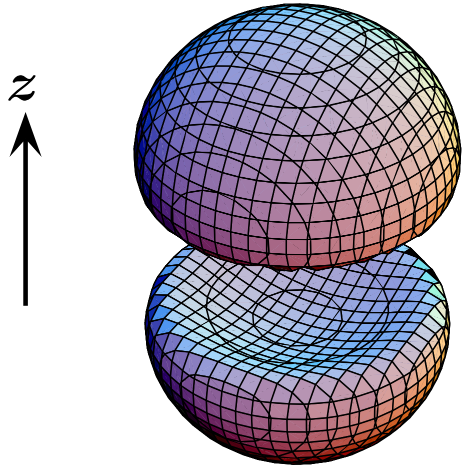
$M_S = 0$

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



$M_S = \pm 1$

$|\uparrow\uparrow\rangle, \ |\downarrow\downarrow\rangle$



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

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

$$\mathrm{G}^\dagger = \mathrm{G}$$
$$\mathrm{C}^\dagger\mathrm{C} = 1$$

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 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

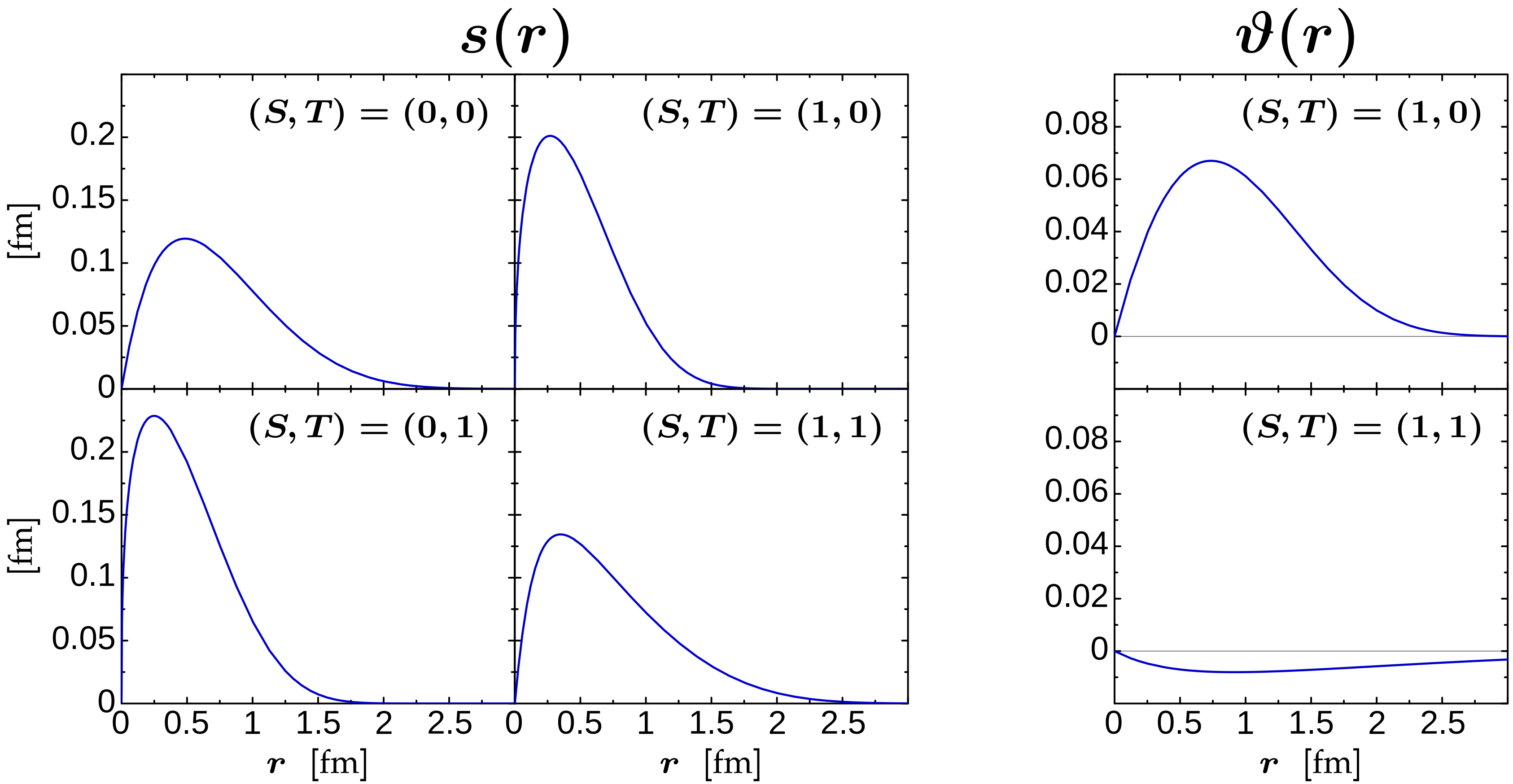
$$\mathrm{g}_\Omega = \frac{3}{2}\vartheta(\mathrm{r})\big[(\vec{\sigma}_1 \cdot \vec{\mathrm{q}}_\Omega)(\vec{\sigma}_2 \cdot \vec{\mathrm{r}}) + (\vec{\mathrm{r}} \leftrightarrow \vec{\mathrm{q}}_\Omega)\big]$$

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

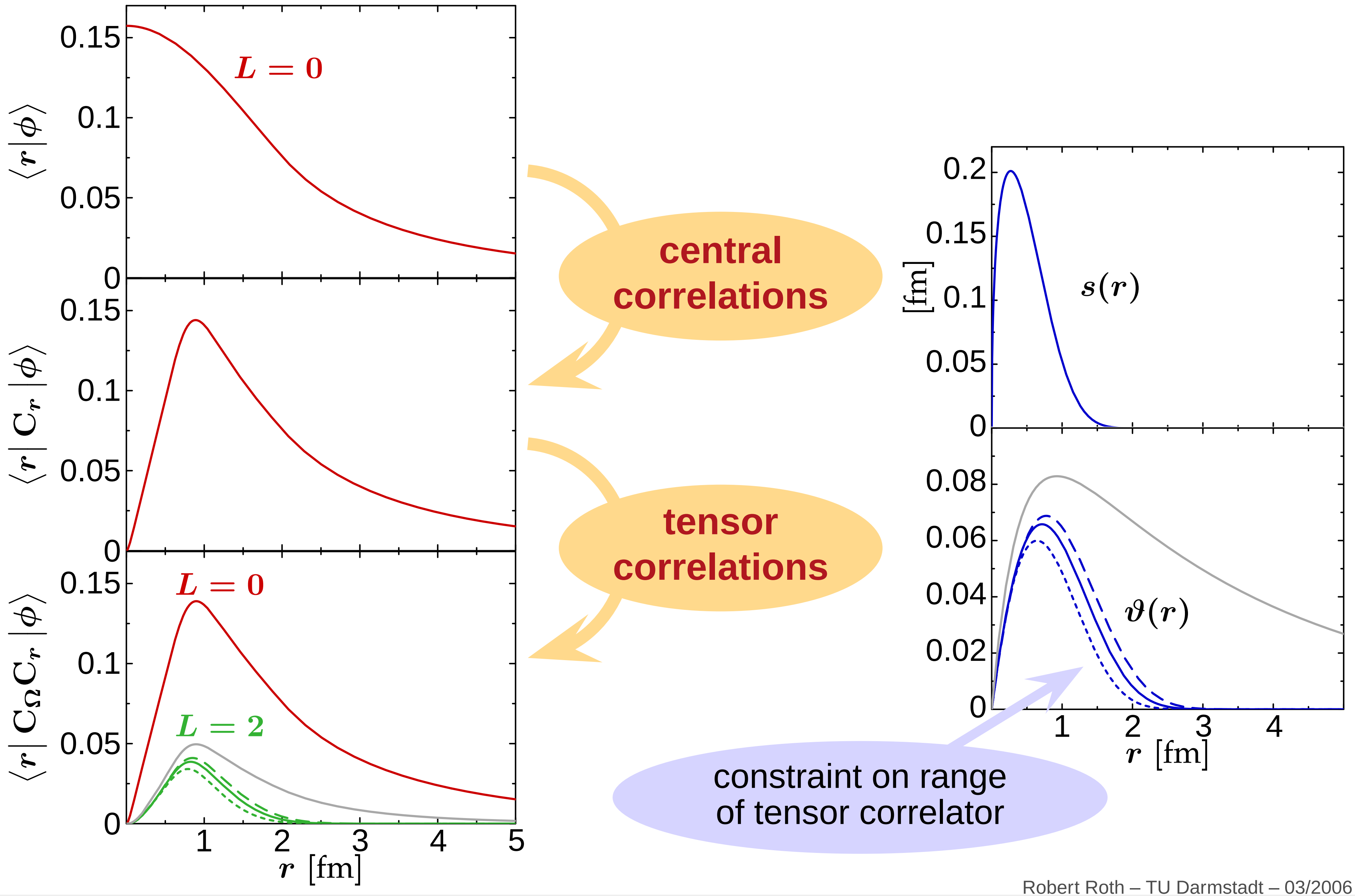
$s(r)$ and $\vartheta(r)$
describe the physics of
short-range correlations

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}

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

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

Correlated Interaction — V_{UCOM}

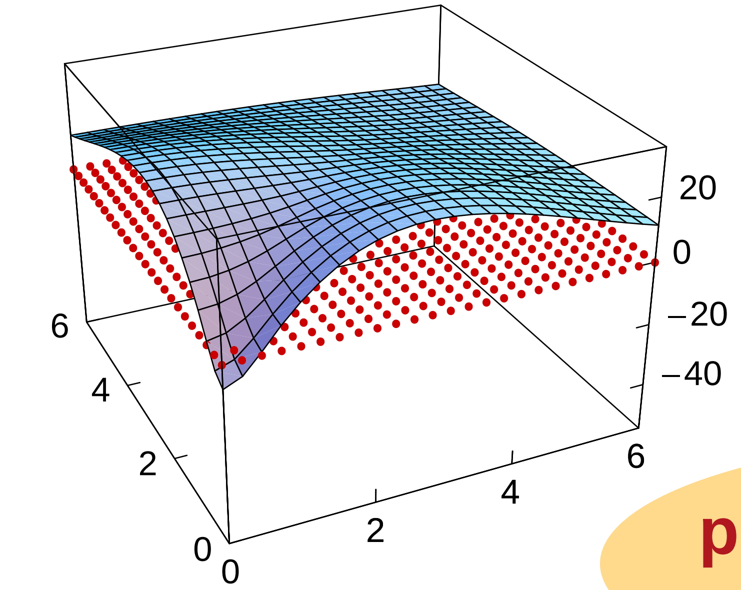
$$\mathrm{V}_{\mathrm{UCOM}} = \sum_{p} \tfrac{1}{2}\big[\widetilde{v}_p(\mathrm{r})\ \mathrm{O}_p + \mathrm{O}_p\ \widetilde{v}_p(\mathrm{r})\big]$$

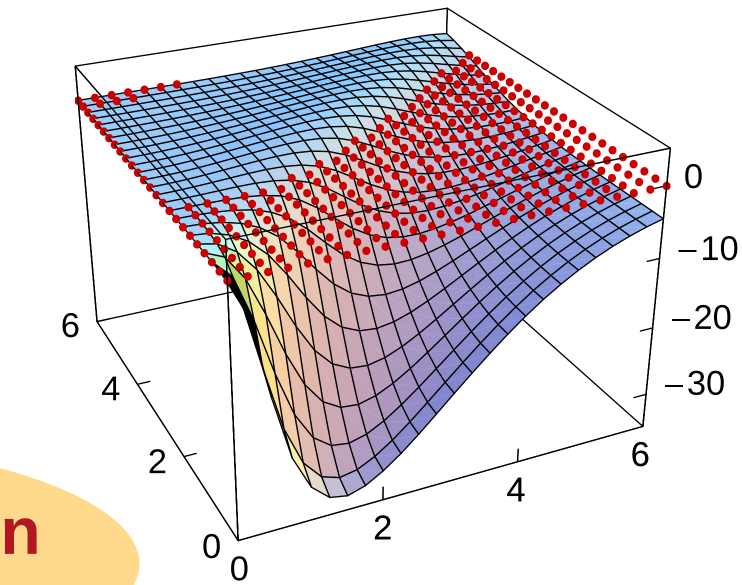
$$\begin{aligned}\mathrm{O} = \{1,\ & (\vec{\sigma}_1\cdot\vec{\sigma}_2),\ \vec{\mathrm{q}}^2,\ \vec{\mathrm{q}}^2(\vec{\sigma}_1\cdot\vec{\sigma}_2),\ \vec{\mathrm{L}}^2,\ \vec{\mathrm{L}}^2(\vec{\sigma}_1\cdot\vec{\sigma}_2),\\ & (\vec{\mathrm{L}}\cdot\vec{\mathrm{S}}),\ \mathrm{S}_{12}(\vec{\mathrm{r}},\vec{\mathrm{r}}),\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

- 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

$^3S_1$ | $^3S_1$—$^3D_1$

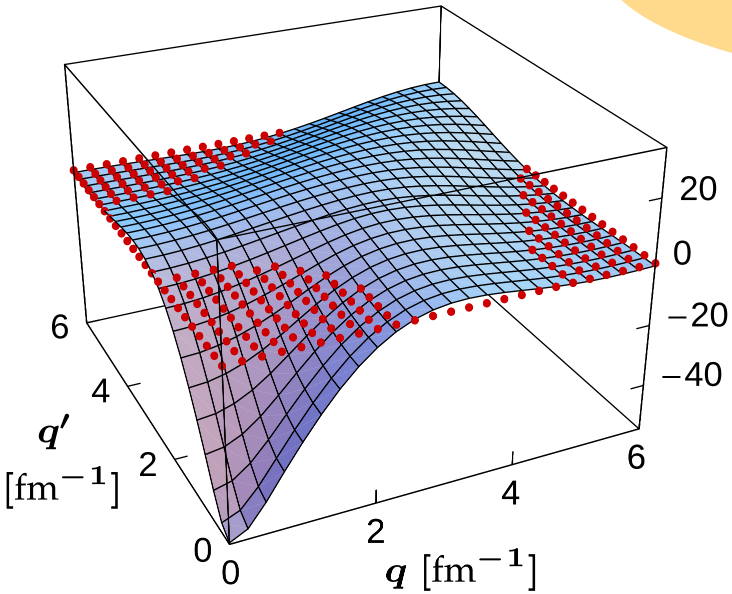


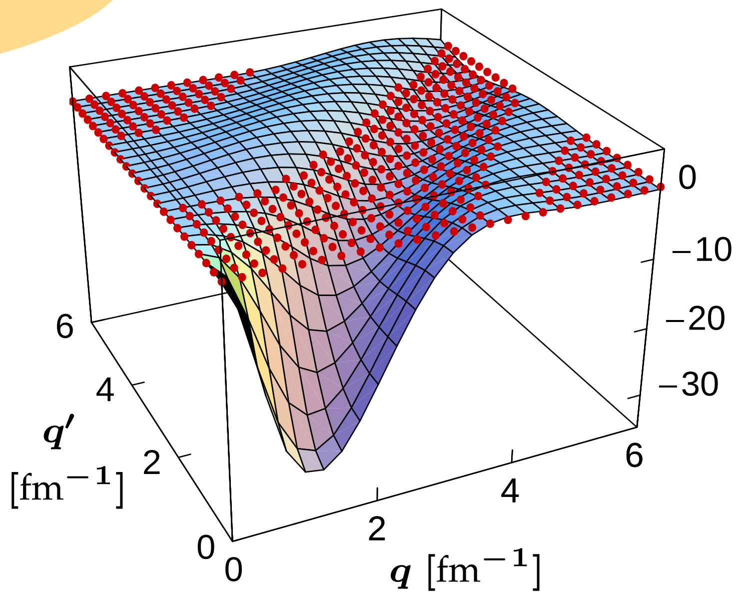


V_{AV18}

pre-diagonalisation of Hamiltonian

V_{UCOM}

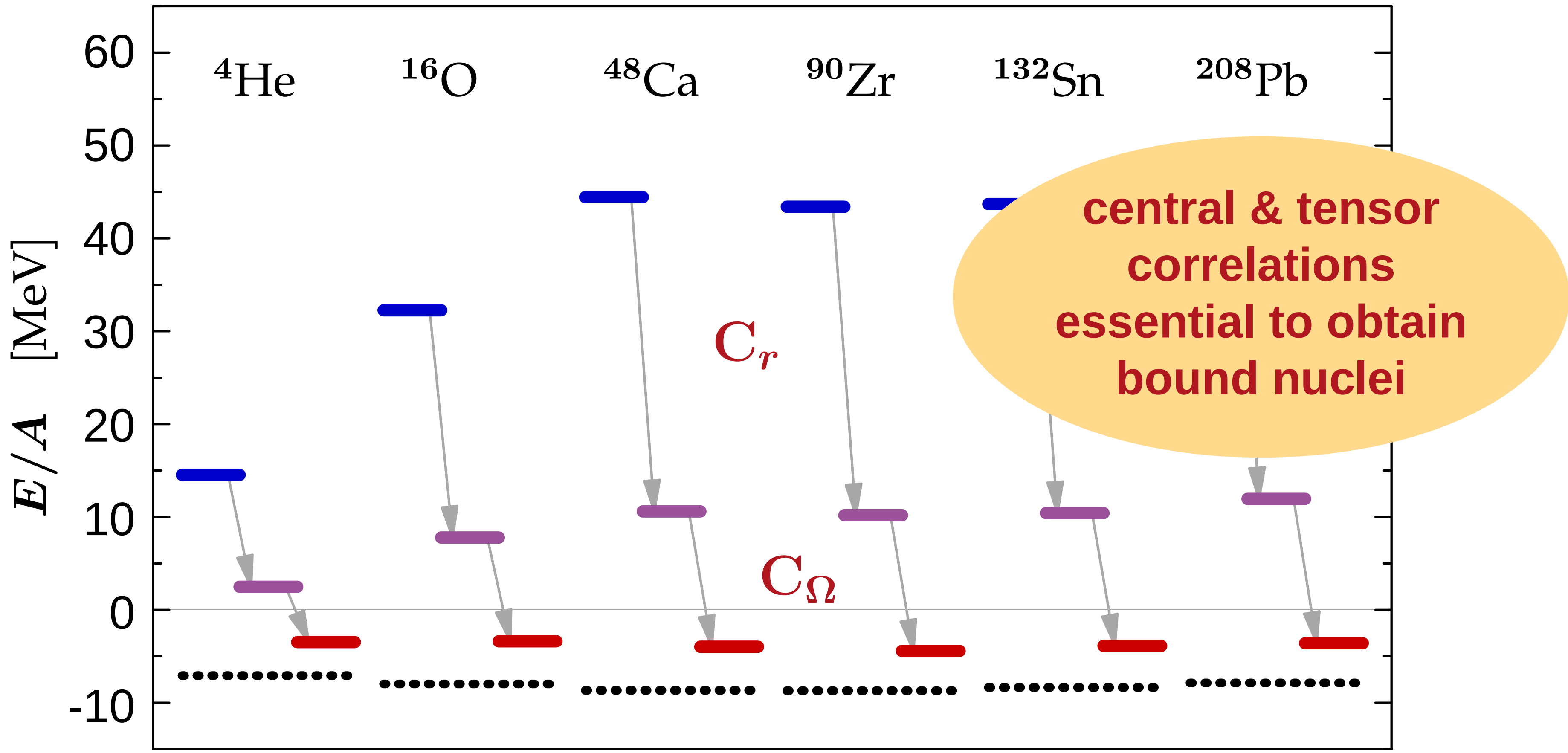




AV18

Simplistic "Shell-Model" Calculation

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



Application I

No-Core Shell Model

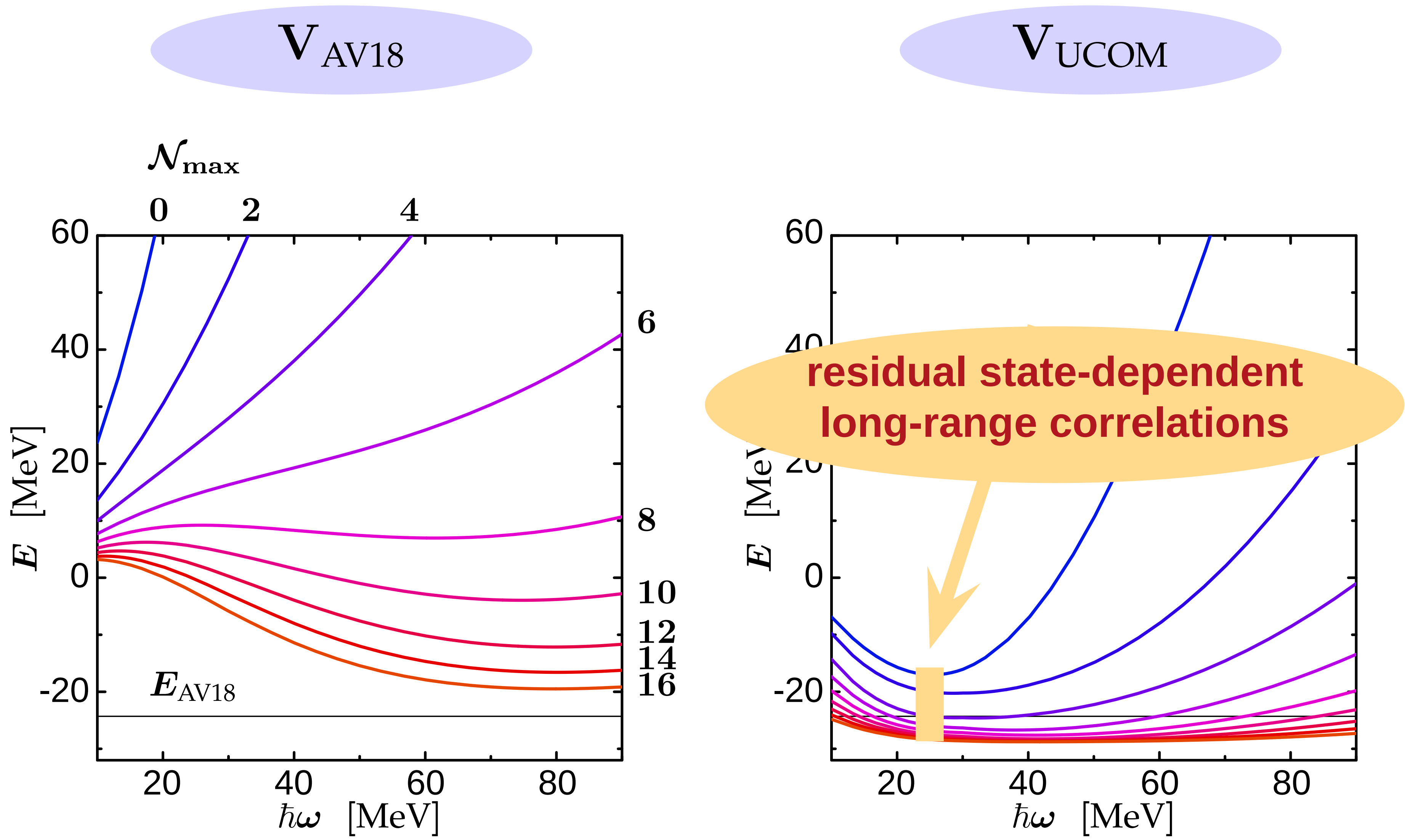
UCOM + NCSM

No-Core Shell Model
+
Matrix Elements of Correlated Realistic NN-Interaction $\mathrm{V}_{\mathrm{UCOM}}$

- 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

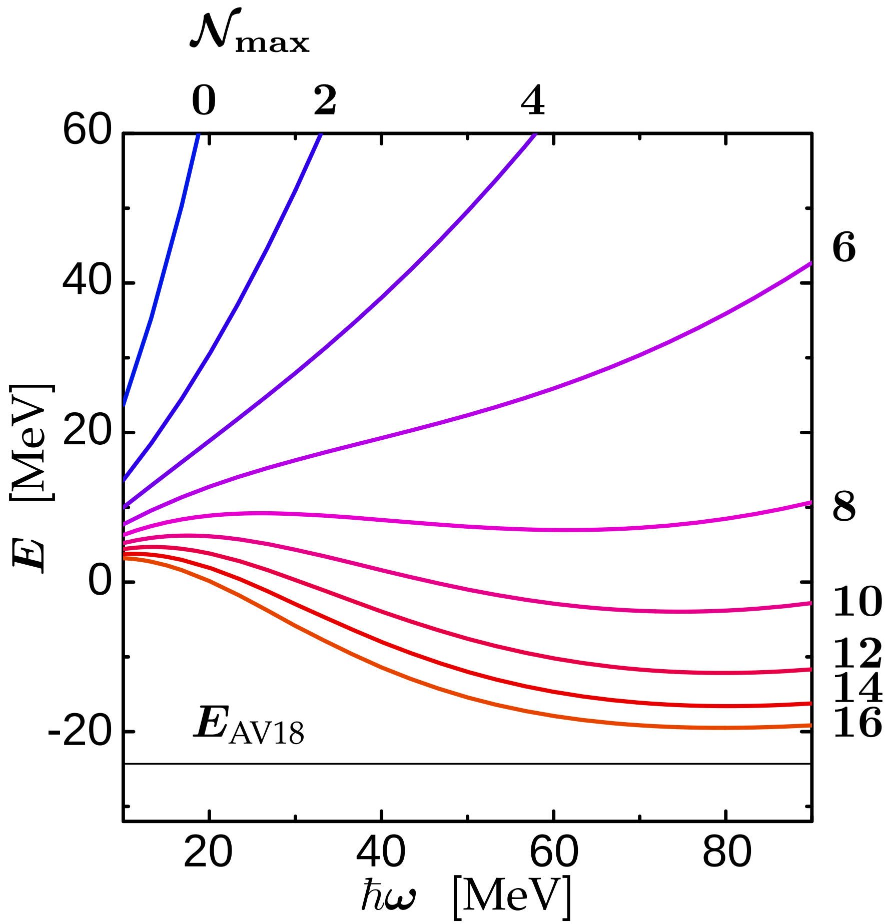
NCSM code by Petr Navrátil [PRC 61, 044001 (2000)]

^{4}He: Convergence

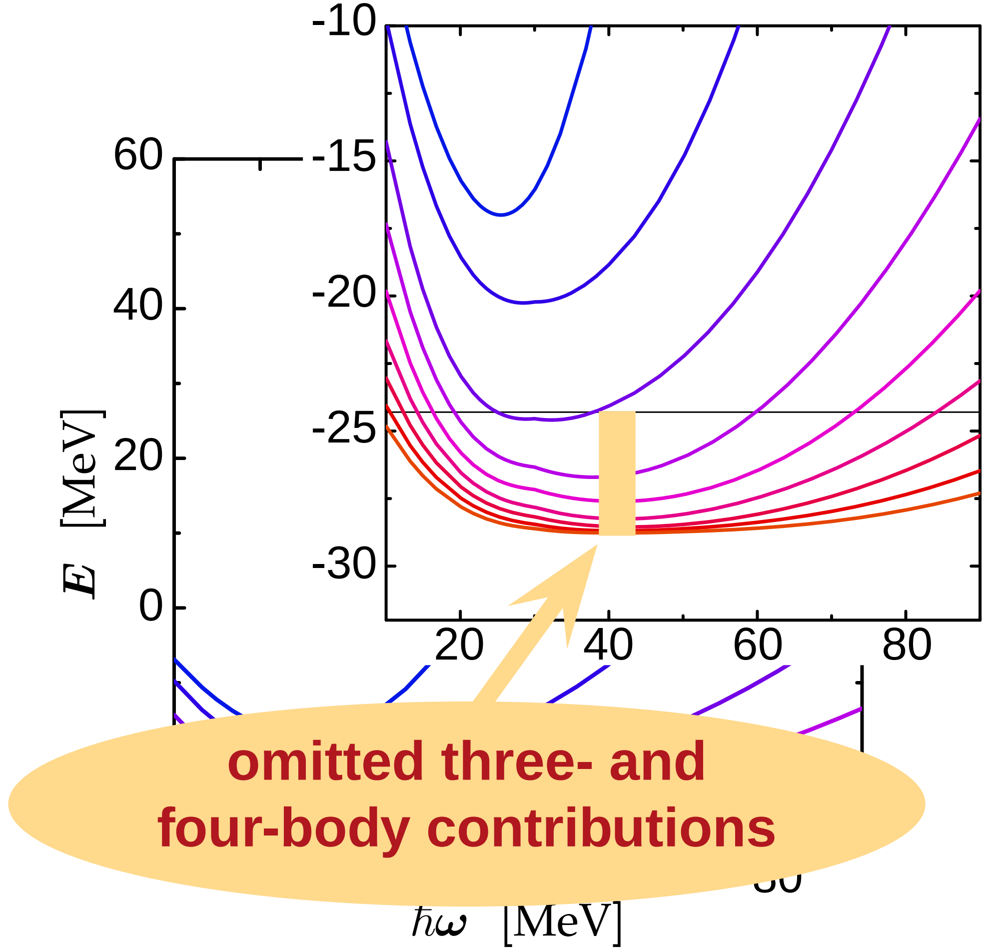


^{4}He: Convergence

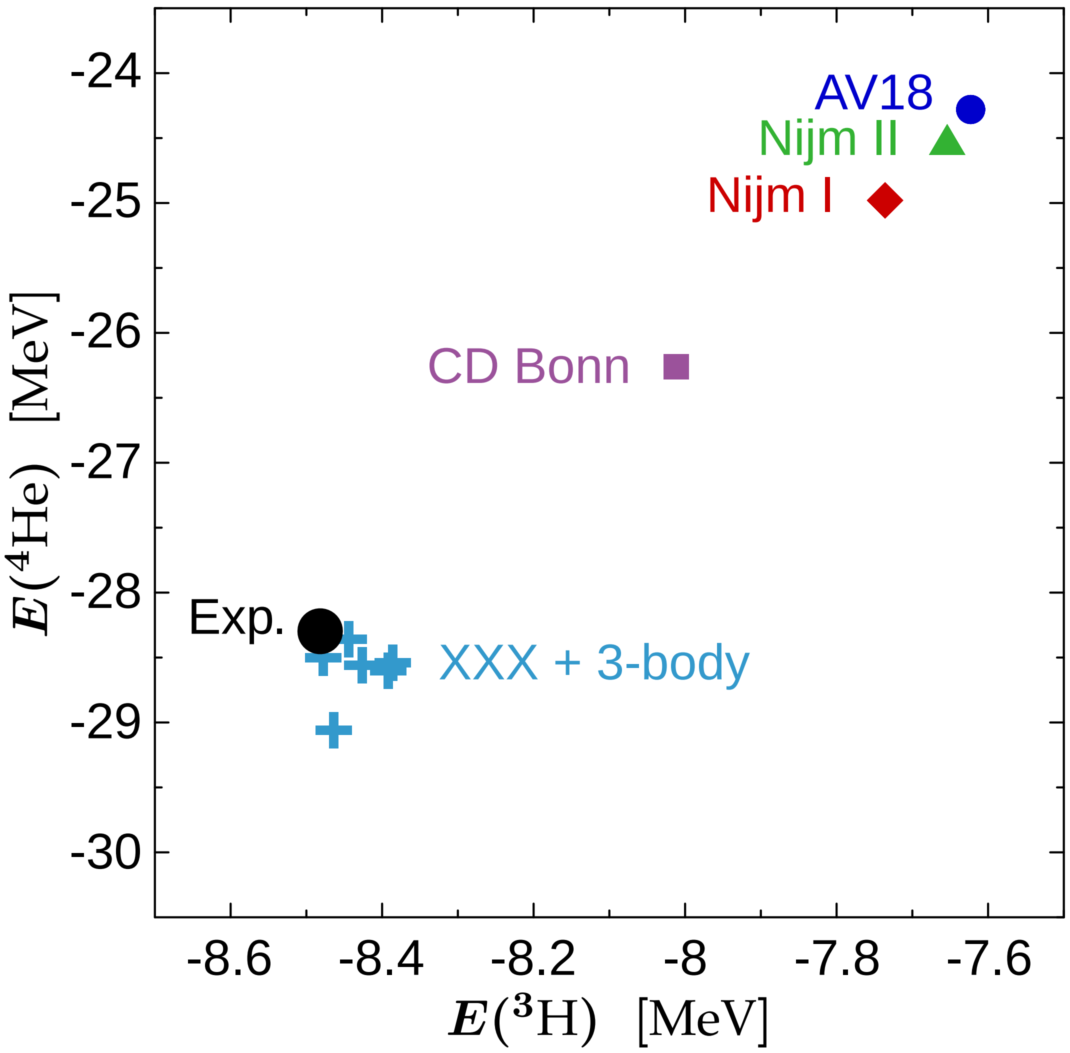
V_{AV18}



V_{UCOM}

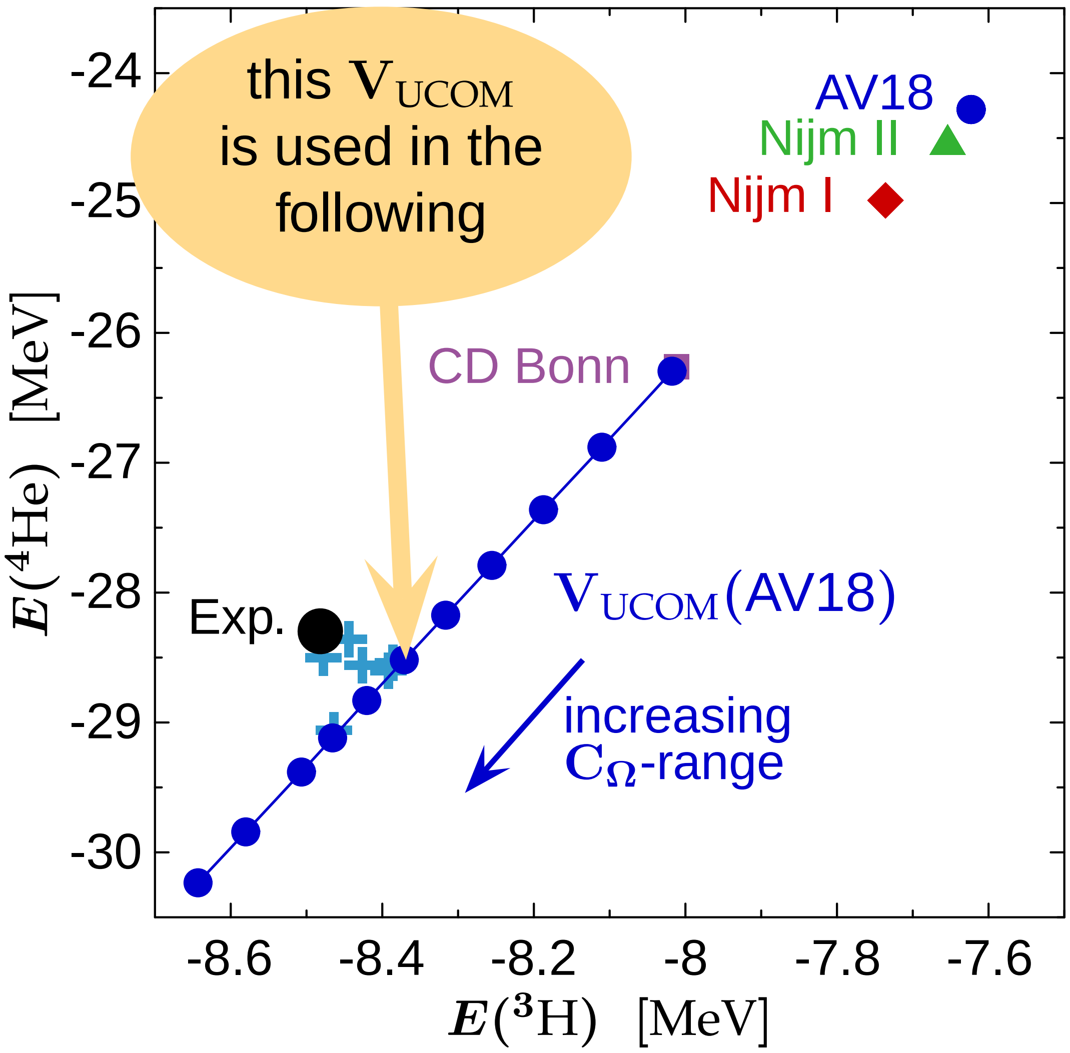


Tjon-Line and Correlator Range



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

Tjon-Line and Correlator Range



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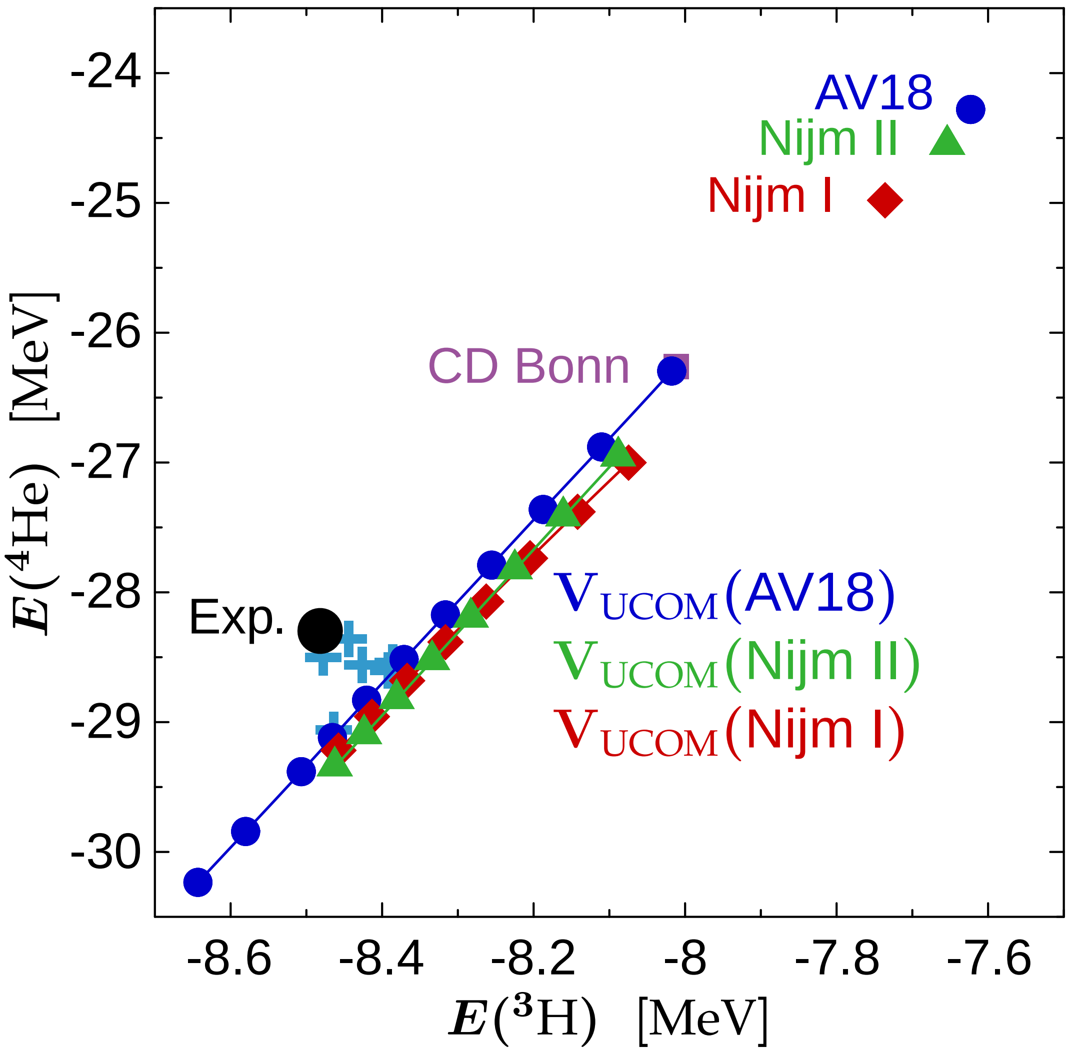
- change of C_{Ω}-correlator range results in shift along Tjon-line

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

Tjon-Line and Correlator Range



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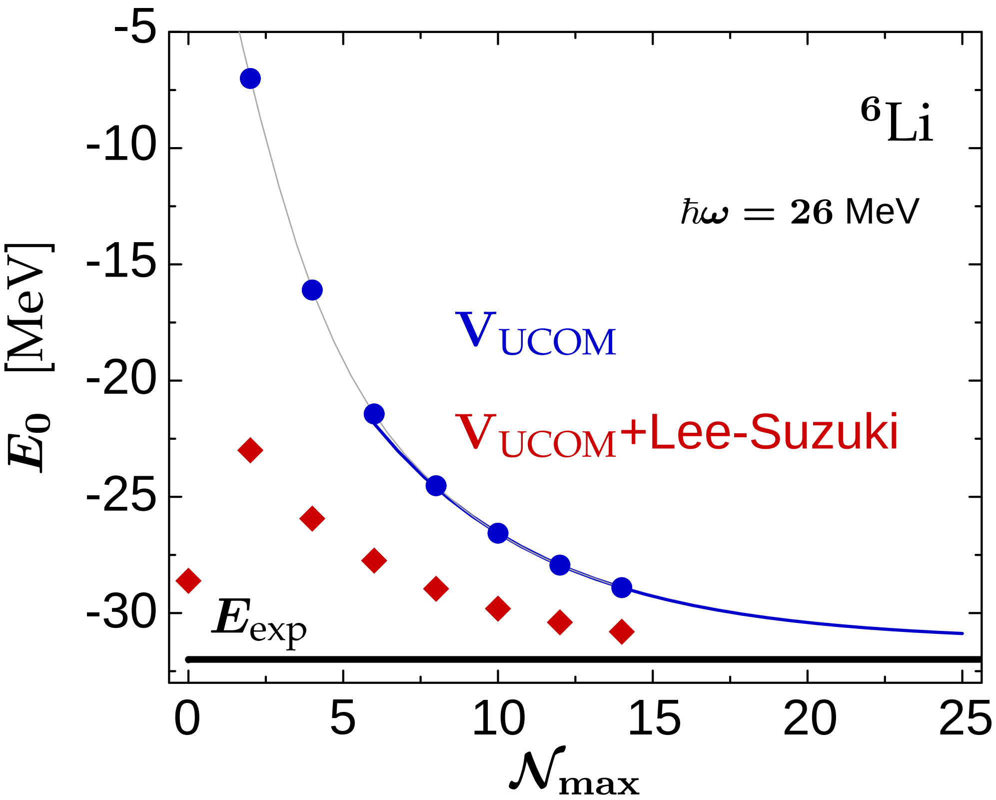
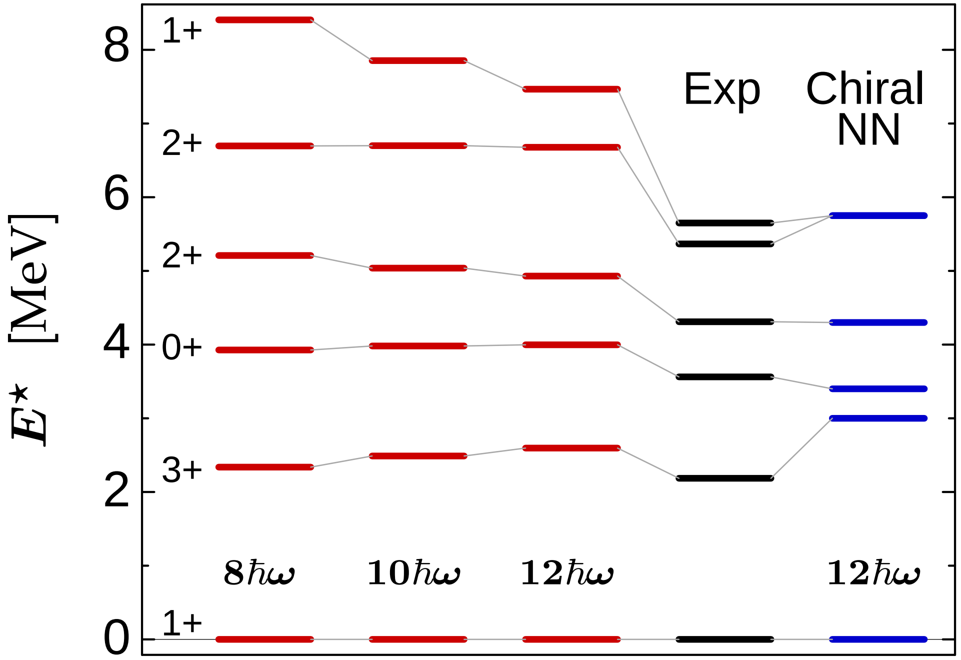
minimise net three-body force
by choosing correlator with energies close to experimental value

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

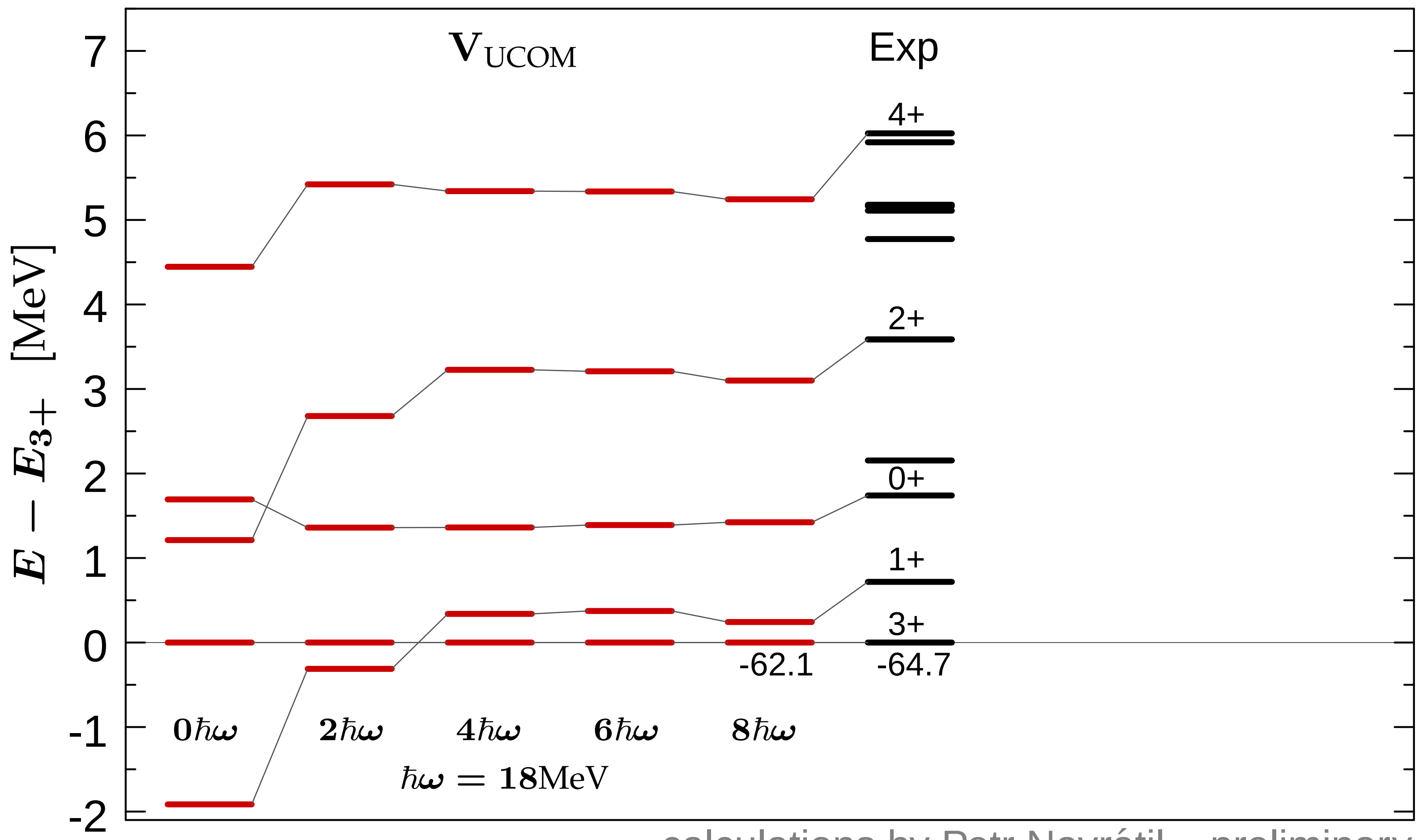
- systematic NCSM calculations throughout p-shell in progress (with and without Lee-Suzuki transformation)





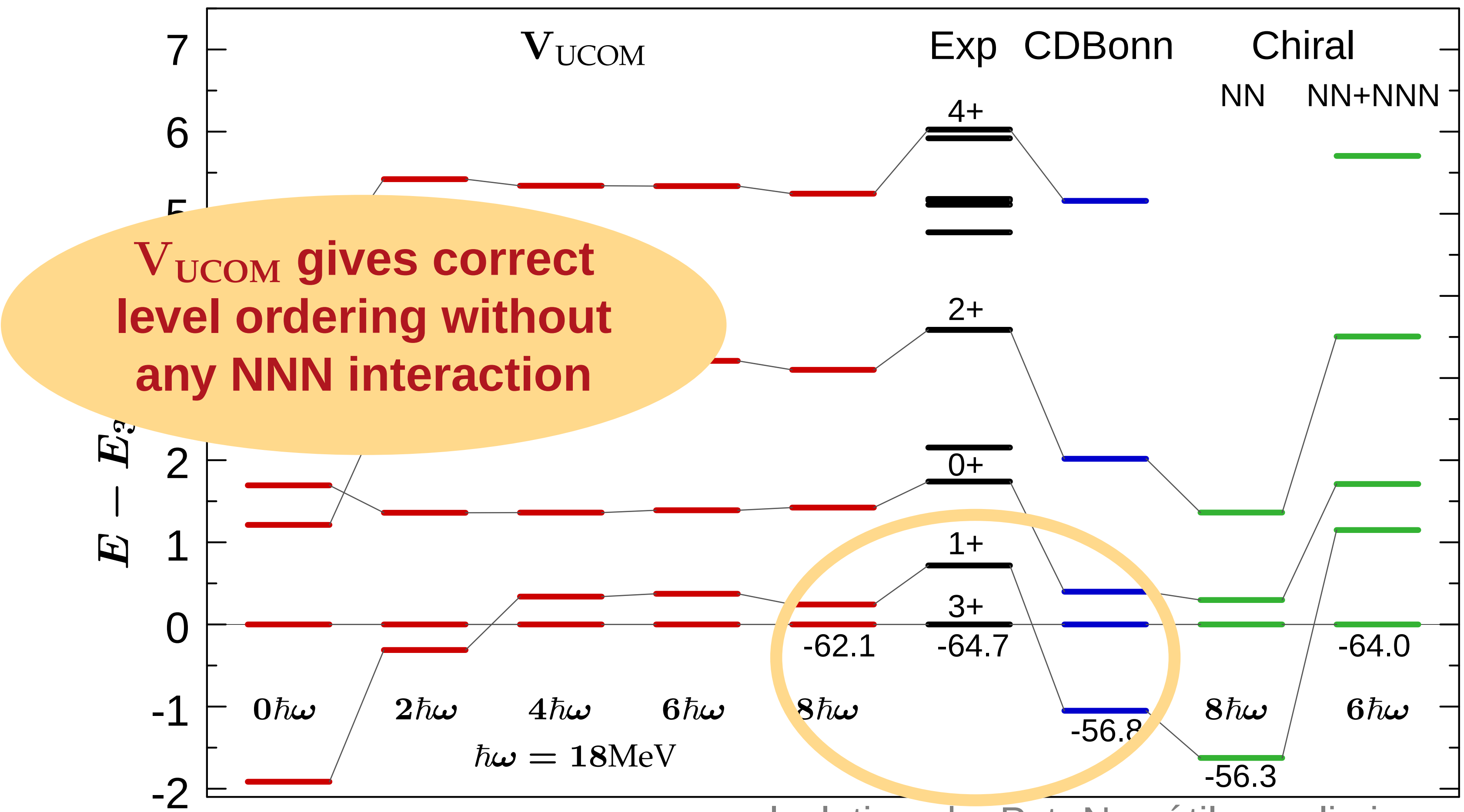
calculations by Petr Navrátil – preliminary

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



calculations by Petr Navrátil – preliminary

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



calculations by Petr Navrátil – preliminary

Application II:

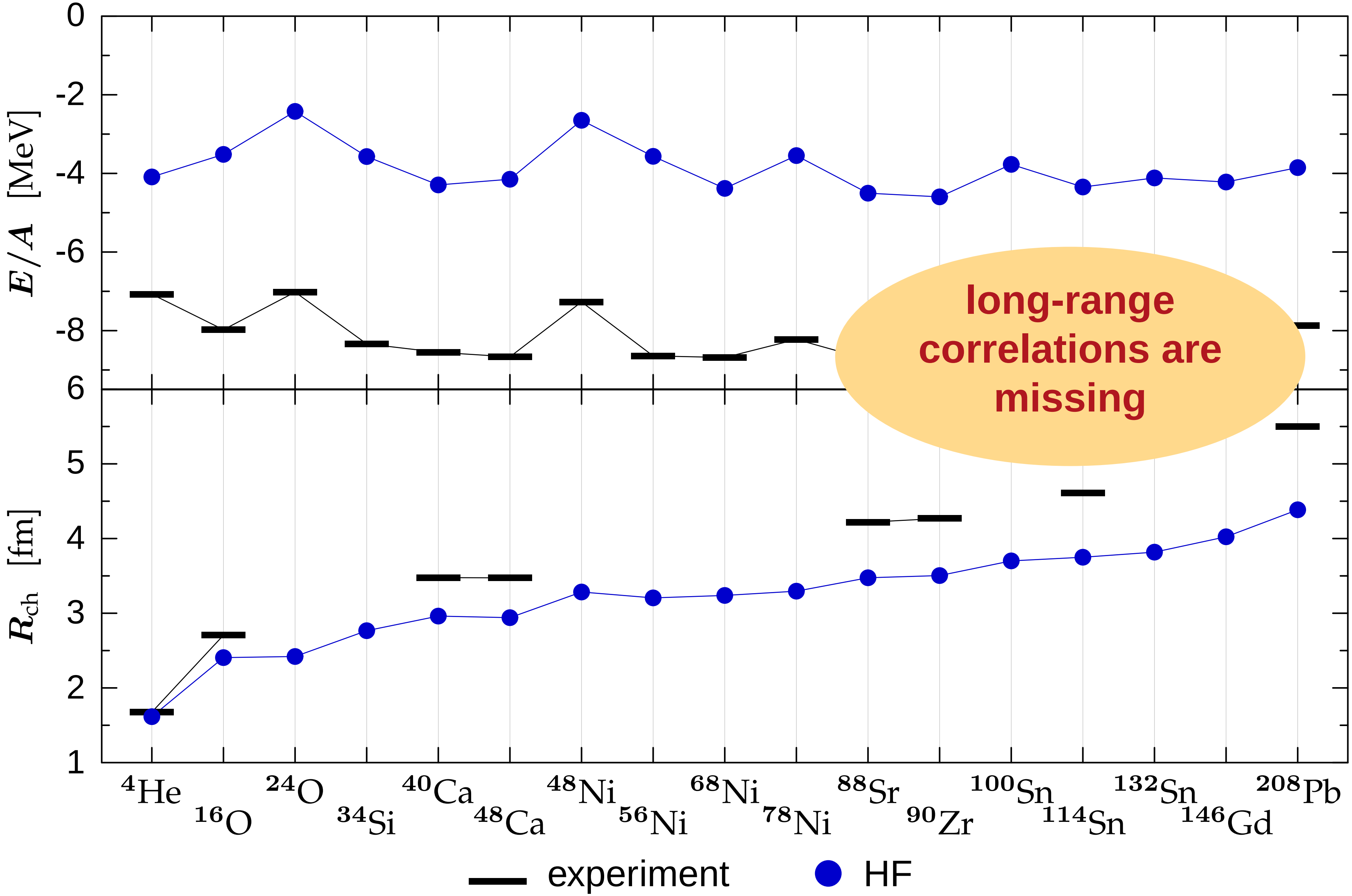
Hartree-Fock & Beyond

UCOM + HF

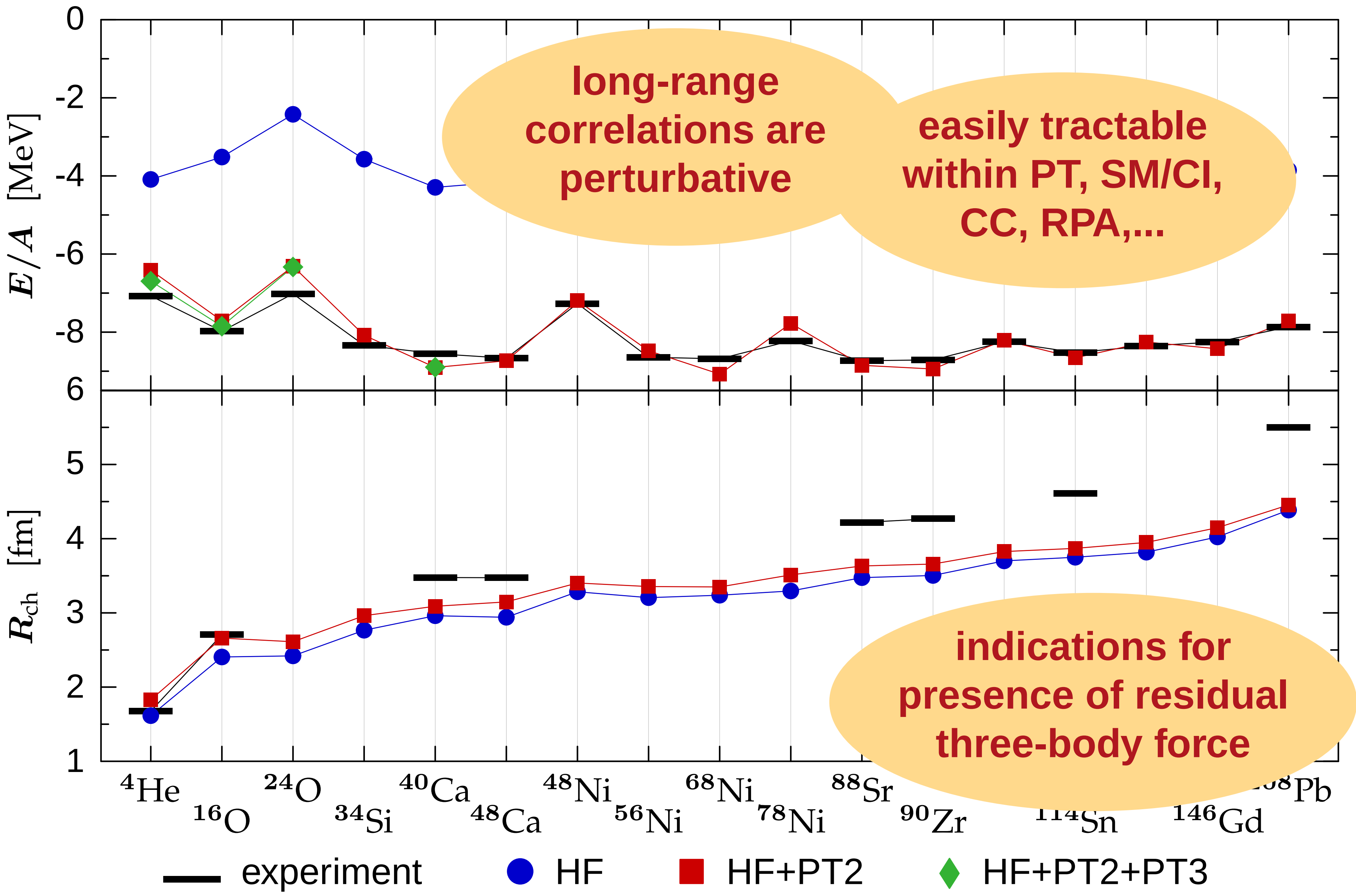
Standard Hartree-Fock
+
Matrix Elements of Correlated Realistic NN-Interaction $\mathrm{V}_{\mathrm{UCOM}}$

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

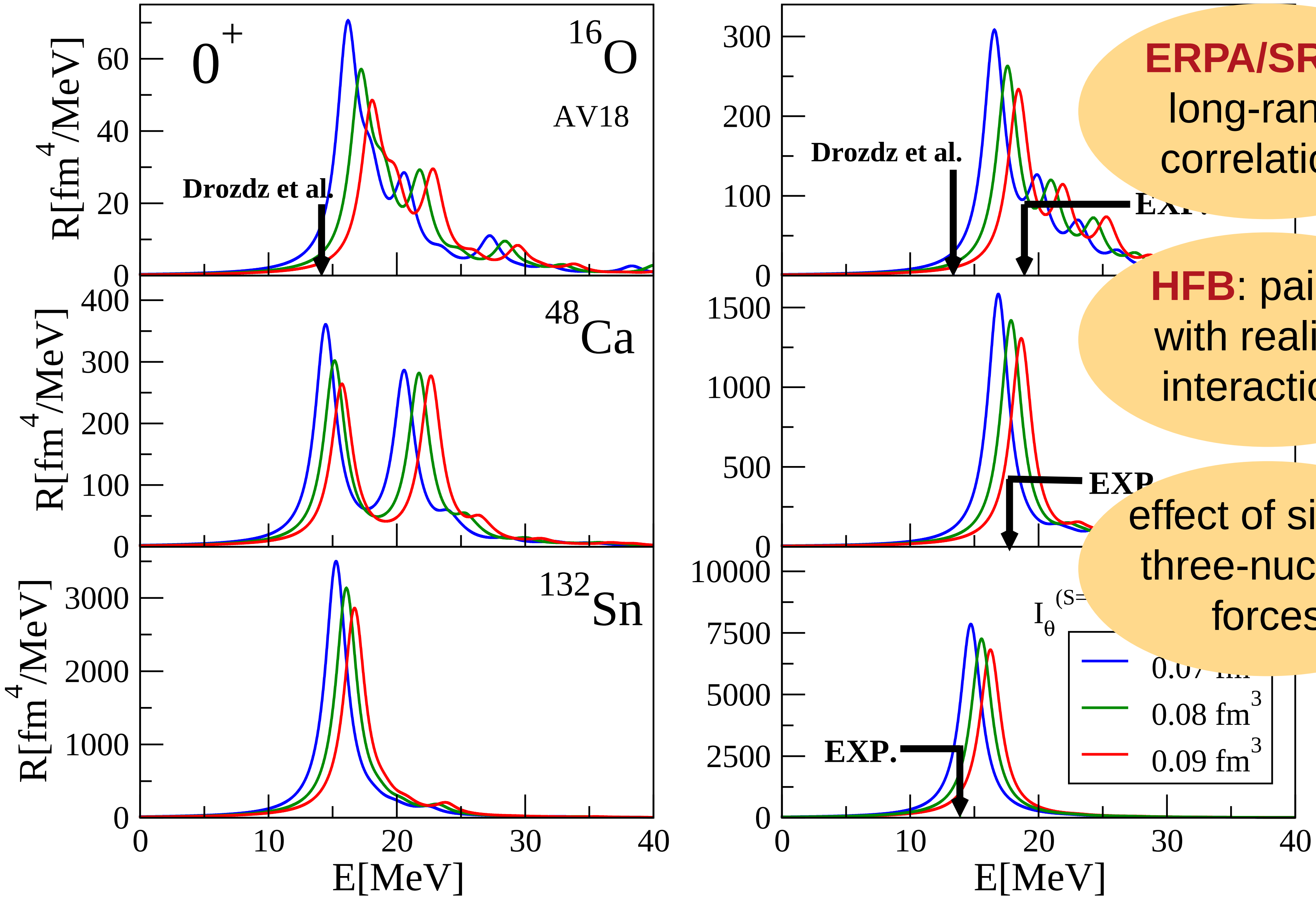
Hartree-Fock with V_{UCOM}



Perturbation Theory with V_{UCOM}



Outlook: UCOM + RPA



ERPA/SRPA: long-range correlations

HFB: pairing with realistic interactions

effect of simple three-nucleon forces

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

$\vec{b}_\nu$: 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

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

Projection

restoration of rotational and inversion symmetry

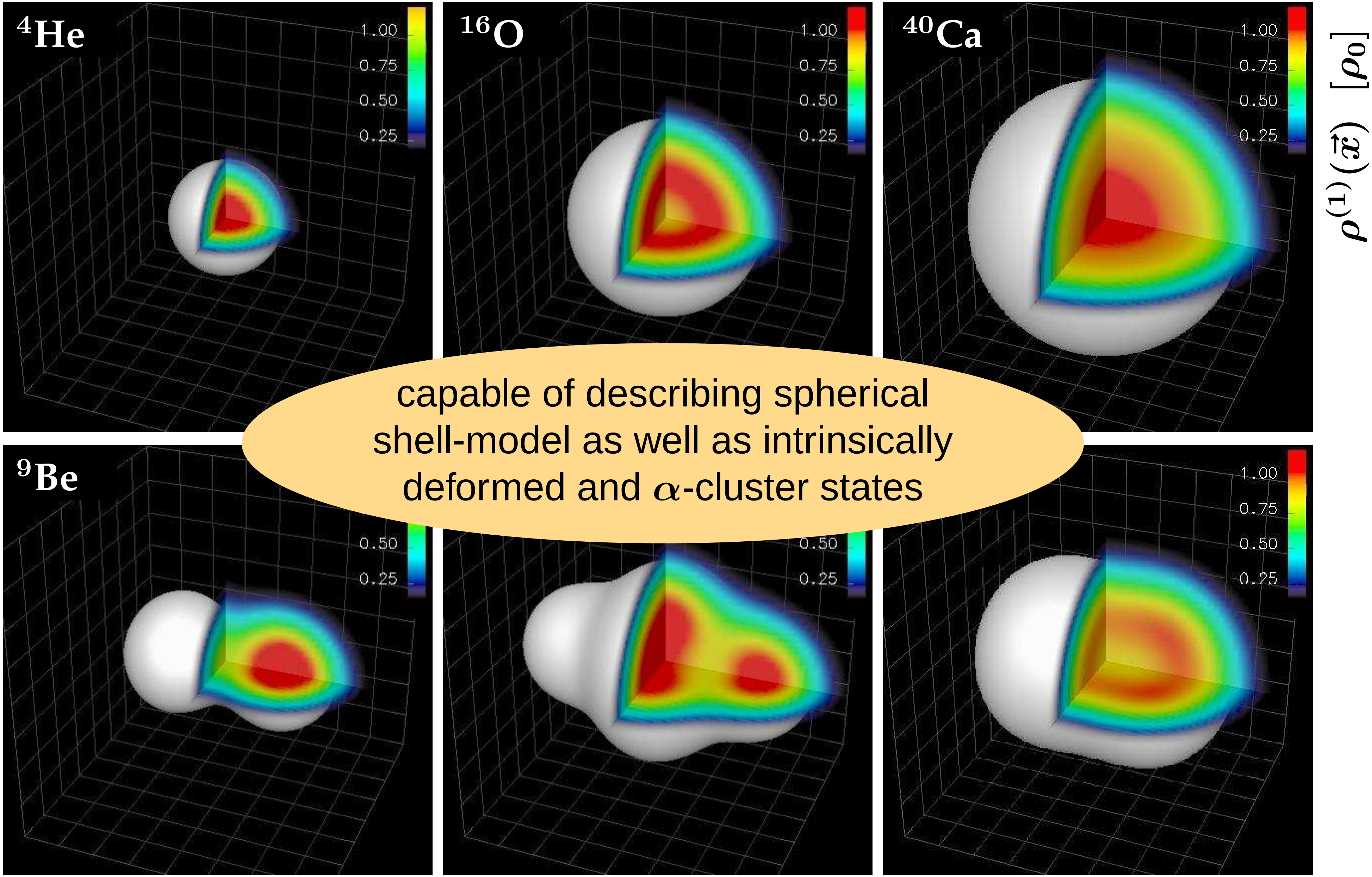
PAV / VAP

Multi-Configuration

mixing of several intrinsic configurations

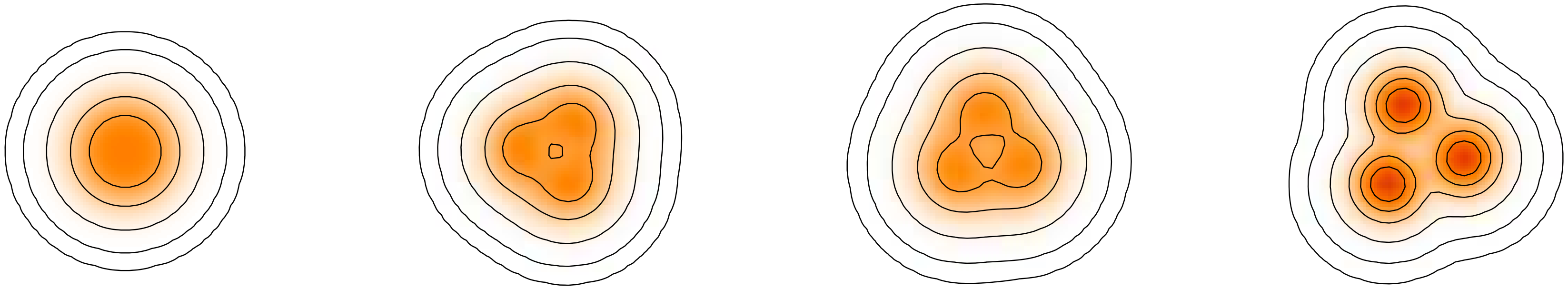
GCM

Intrinsic One-Body Density Distributions



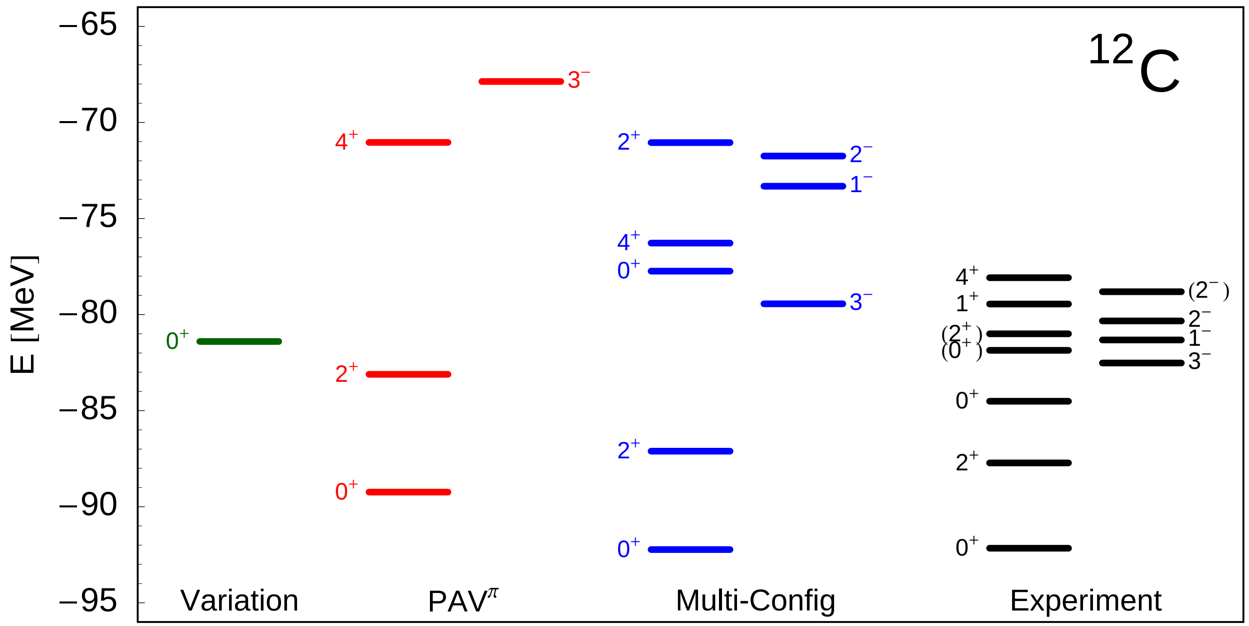
capable of describing spherical shell-model as well as intrinsically deformed and α-cluster states

Intrinsic Shapes of ^{12}C



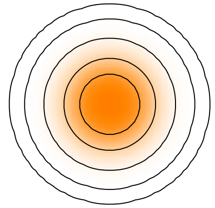
	intrinsic	projected	intrinsic	projected	intrinsic	projected	intrinsic	projected
$\langle \mathbf{H} \rangle$	-81.4	**-81.5**	-77.0	**-88.5**	-74.1	**-85.5**	-57.0	**-75.9**
$\langle \mathbf{T} \rangle$	212.1	212.1	189.2	186.1	182.8	179.0	213.9	201.4
$\langle \mathbf{V}_{ls} \rangle$	-39.8	-40.2	-12.0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

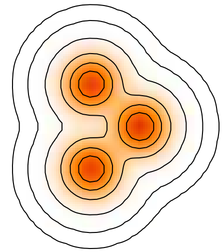


	E [MeV]	R_{ch} [fm]	$B(E2)$ [e^2 fm^4]
V/PAV	81.4	2.36	-
VAP α-cluster	79.1	2.70	76.9
PAV$^\pi$	88.5	2.51	36.3
VAP	89.2	2.42	26.8
Multi-Config	92.2	2.52	42.8
Experiment	92.2	2.47	39.7 ± 3.3

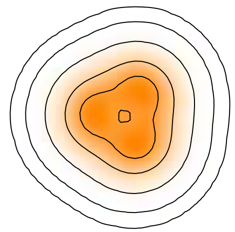
V/PAV



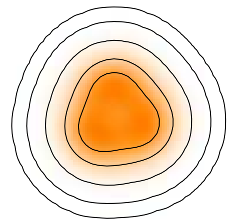
VAPα



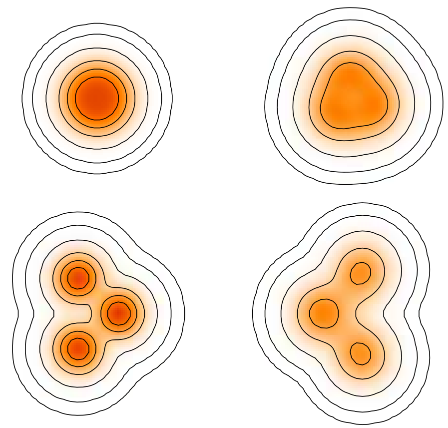
V$^\pi$/PAV$^\pi$



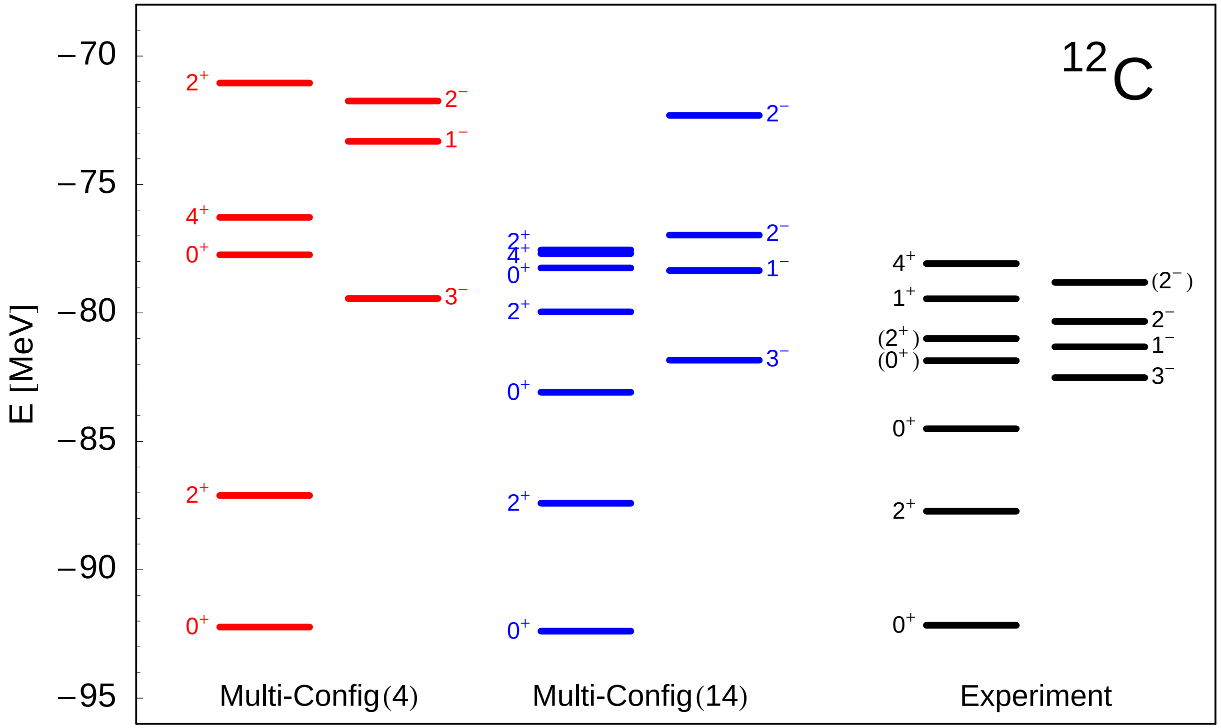
VAP



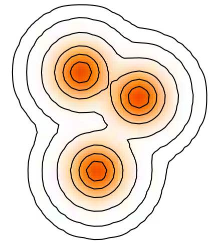
Multi-Config

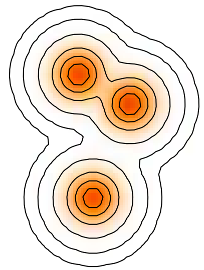


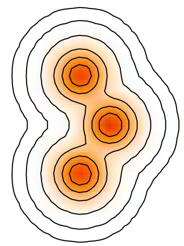
Structure of ^{12}C — Hoyle State



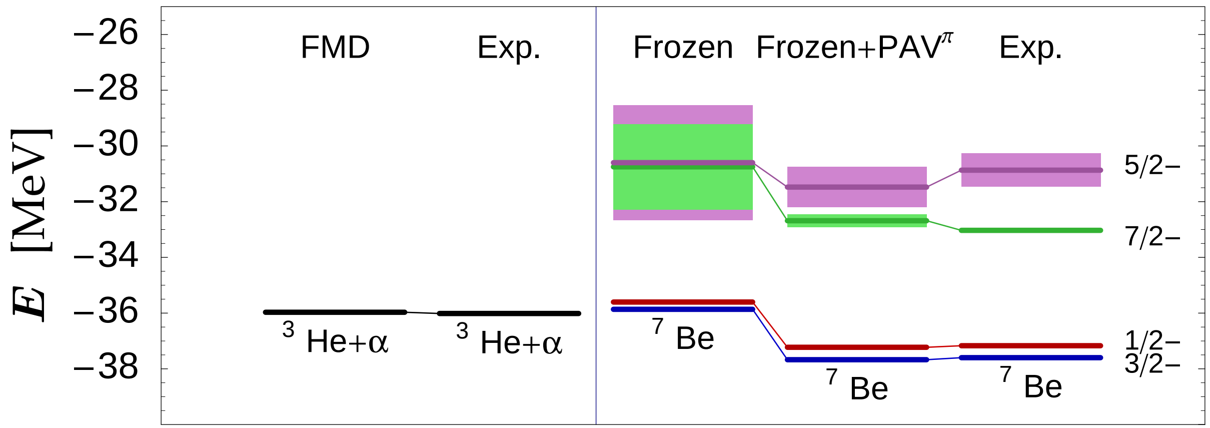
	Multi-Config	Experiment
E [MeV]	92.4	92.2
R_{ch} [fm]	2.52	2.47
$B(E2, 0_1^+ \to 2_1^+)$ [e^2 fm^4]	42.9	39.7 $\pm$ 3.3
$M(E0, 0_1^+ \to 0_2^+)$ [fm^2]	5.67	5.5 $\pm$ 0.2

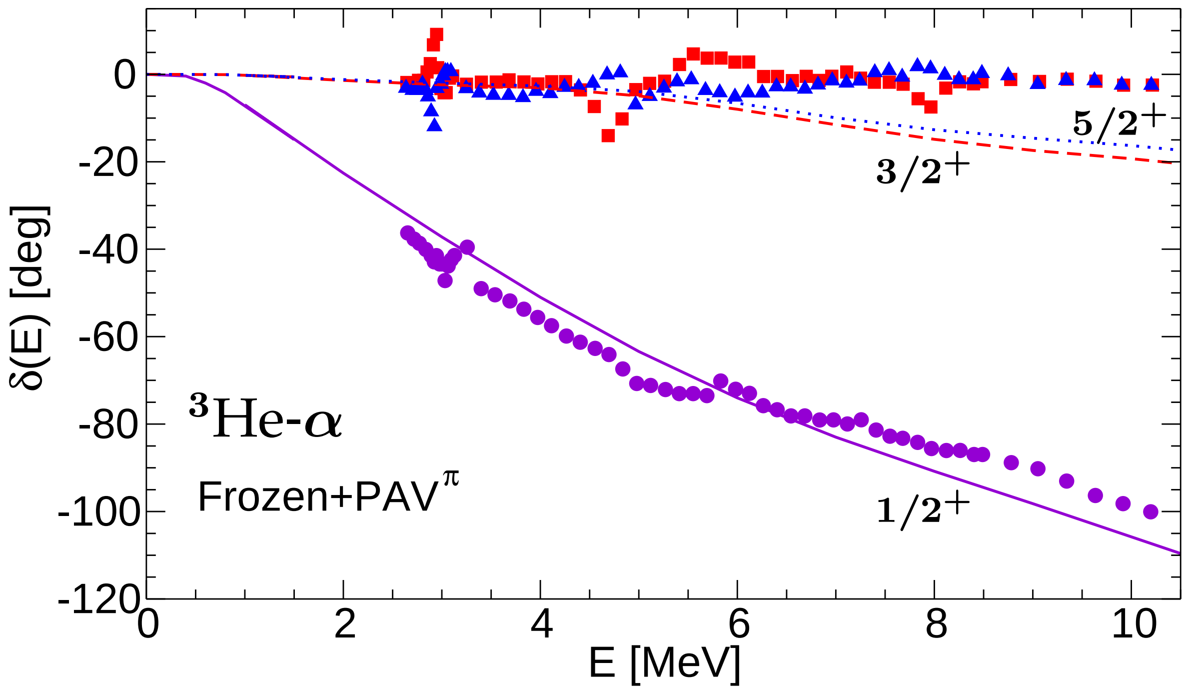
$|\langle$  $|0_2^+\rangle| = 0.76$

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

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

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 $\mathbf{V}_{\mathrm{UCOM}}$
- **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

Epilogue

- **thanks to my group & my collaborators**
  - H. Hergert, N. Paar, P. Papakonstantinou, A. Zapp

    Institut für Kernphysik, TU Darmstadt
  - T. Neff

    NSCL, Michigan State University
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