Nuclear Structure & Reactions with Correlated Realistic NN-Potentials

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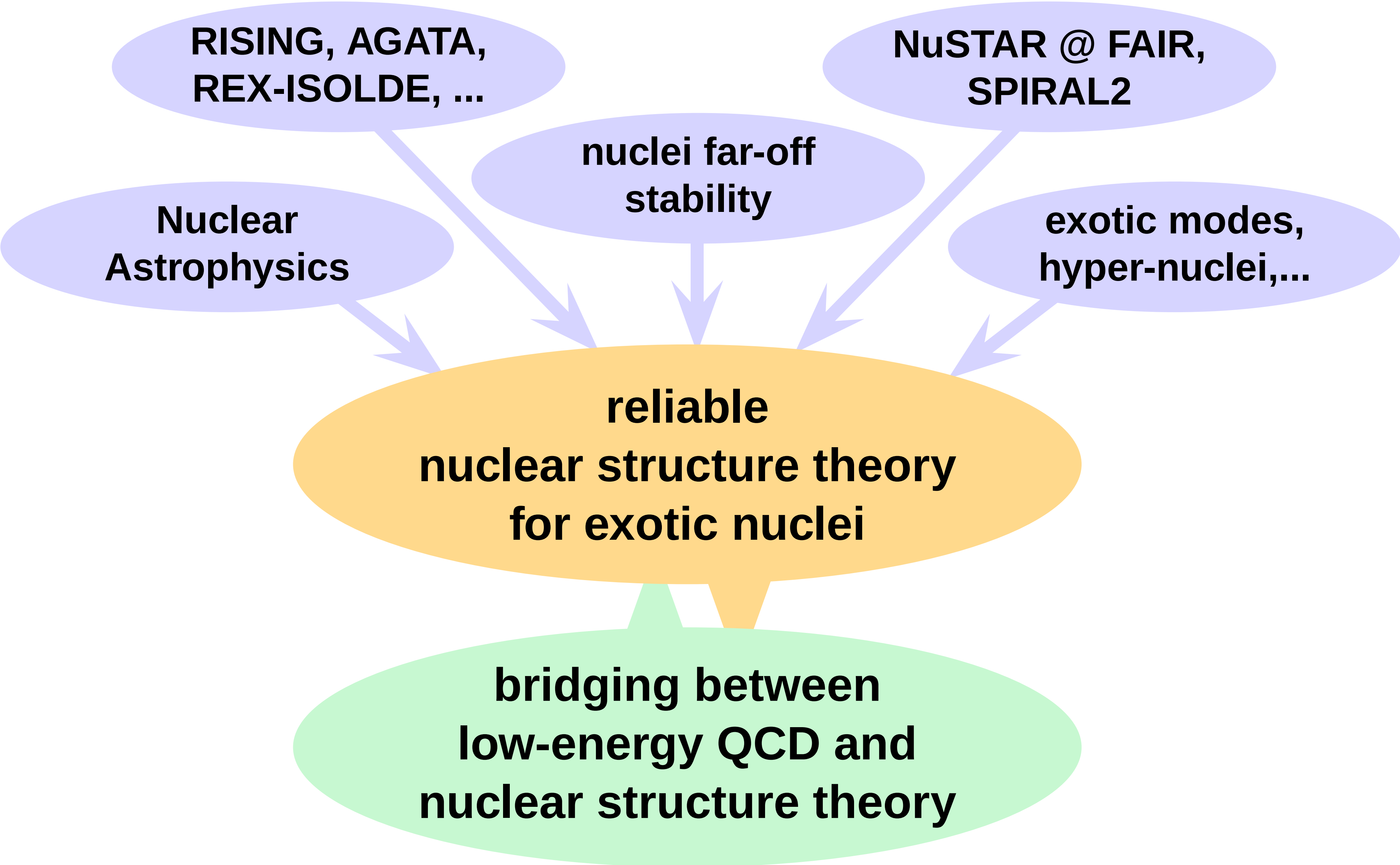
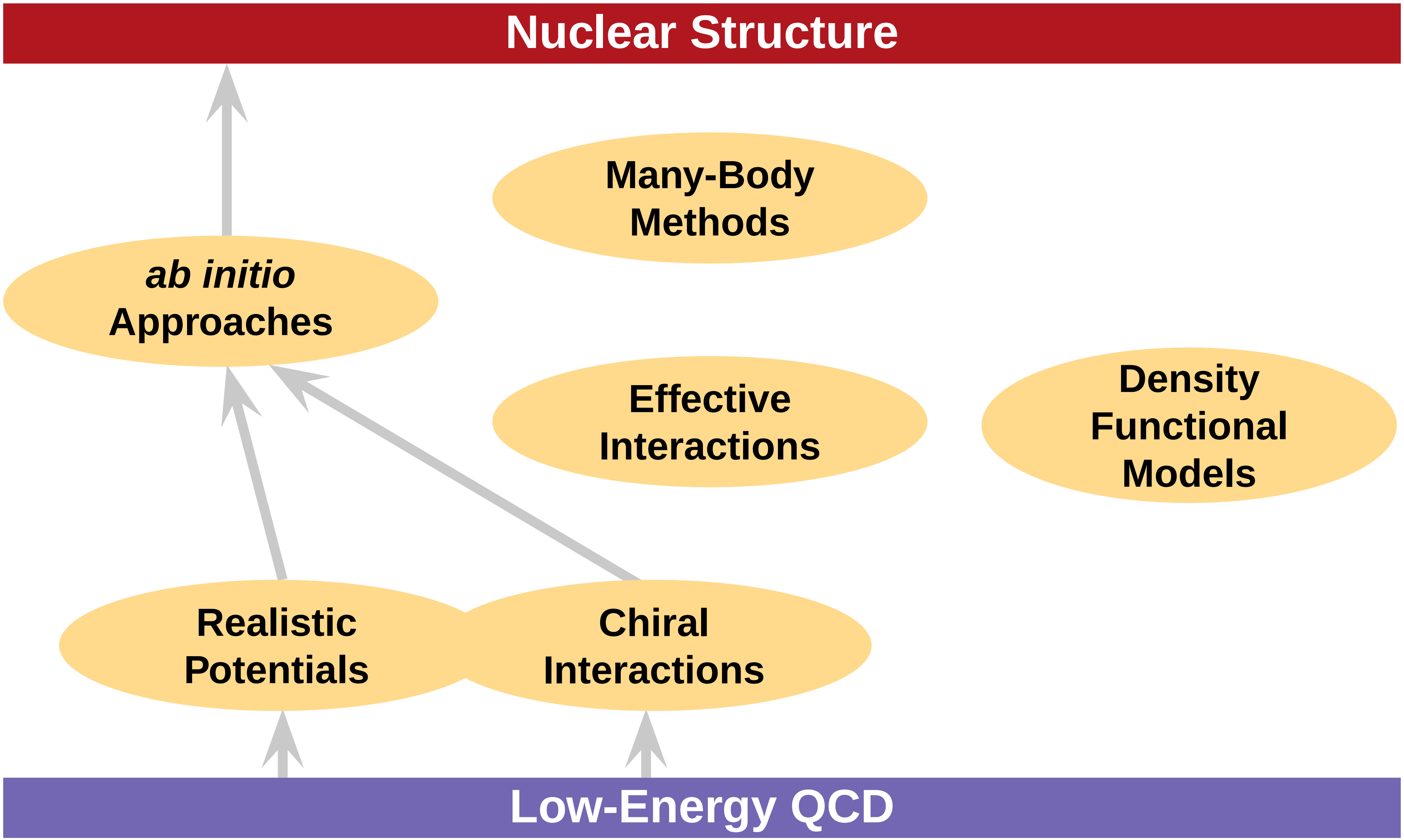
Overview

- Motivation
- Correlated Realistic NN-Potentials
  - 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

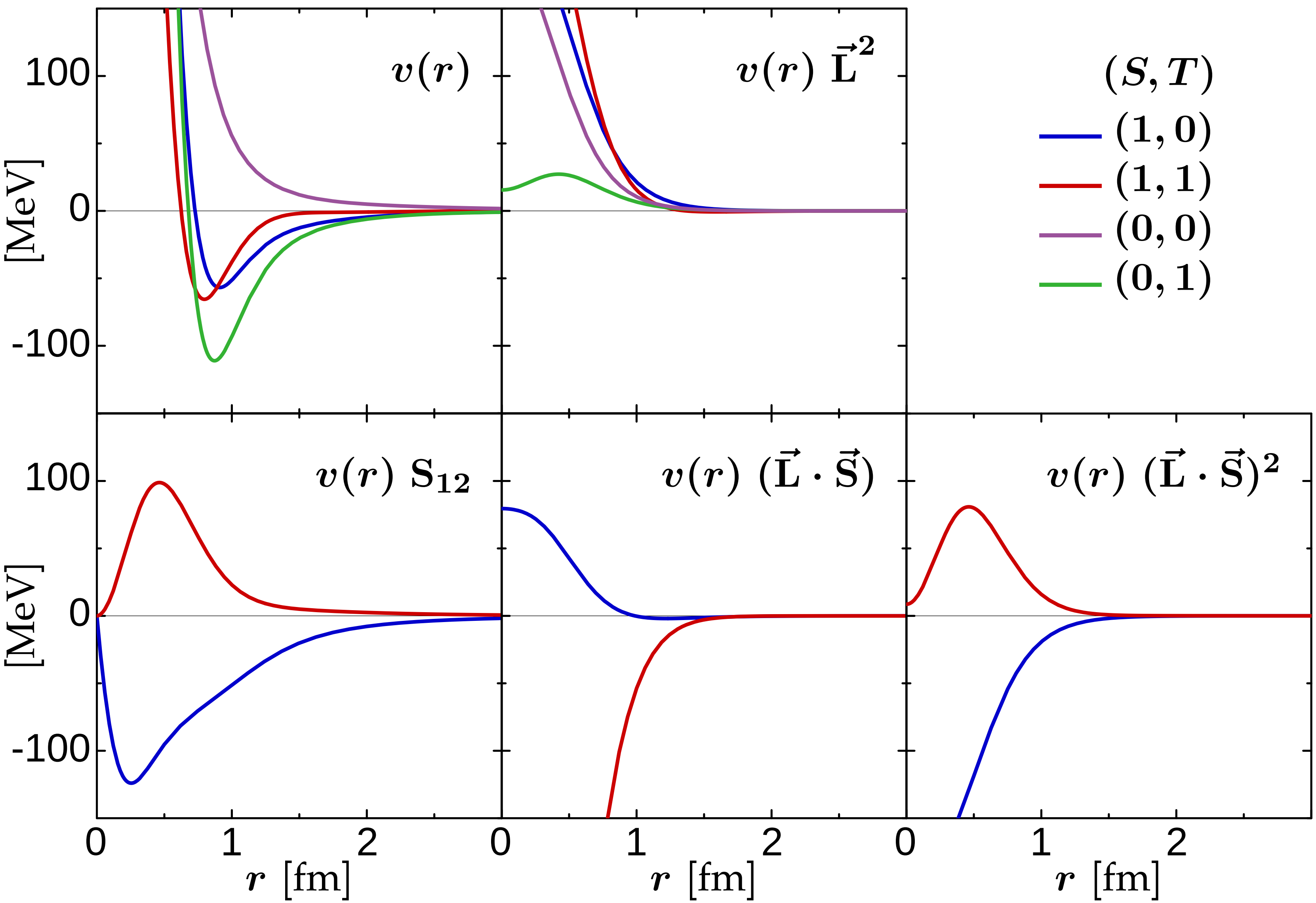
Nijmegen I/II

Chiral N3LO

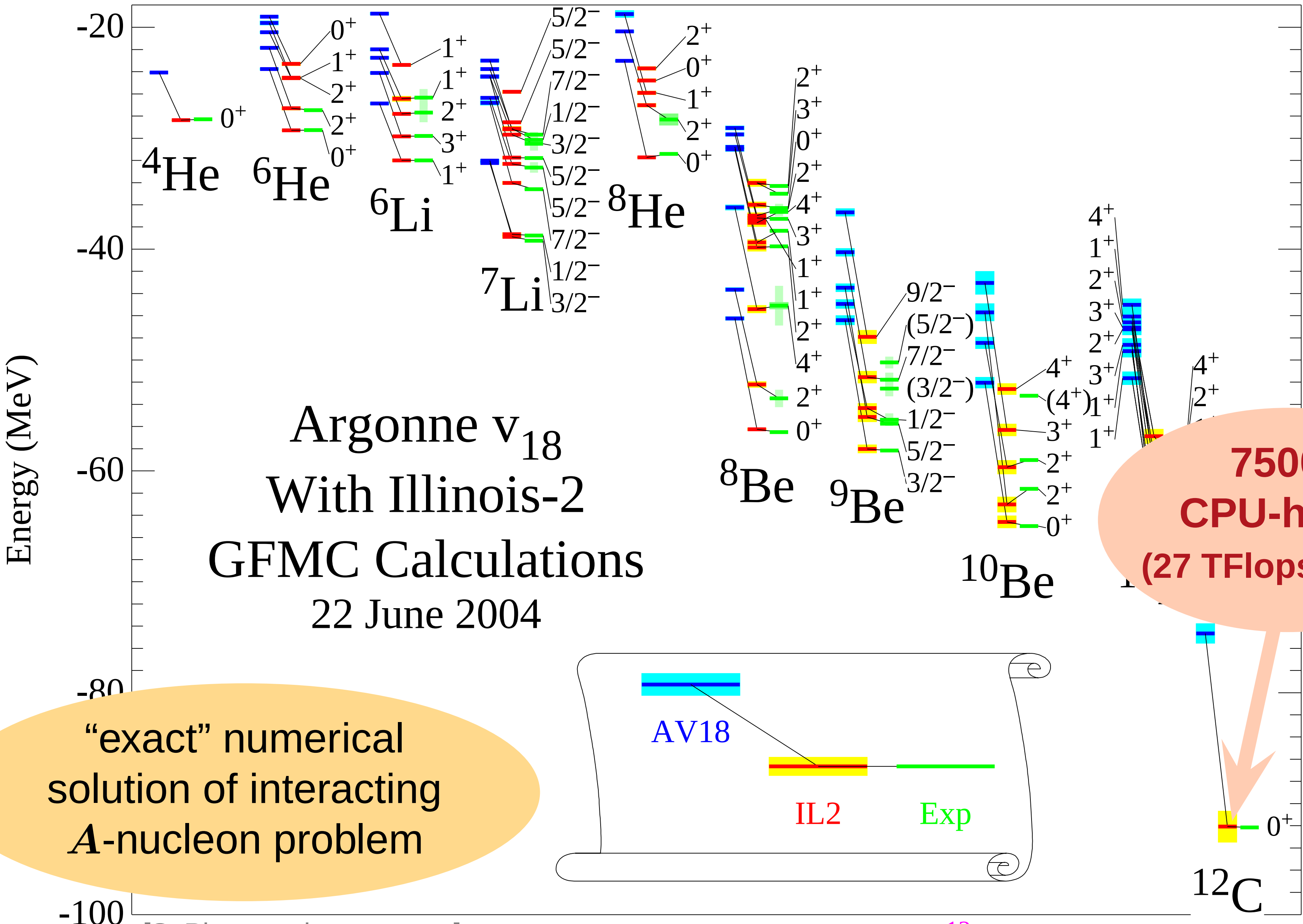
Argonne V18 + **Illinois 2**

Chiral N3LO + **N2LO**

Argonne V18 Potential



Ab initio Methods: GFMC



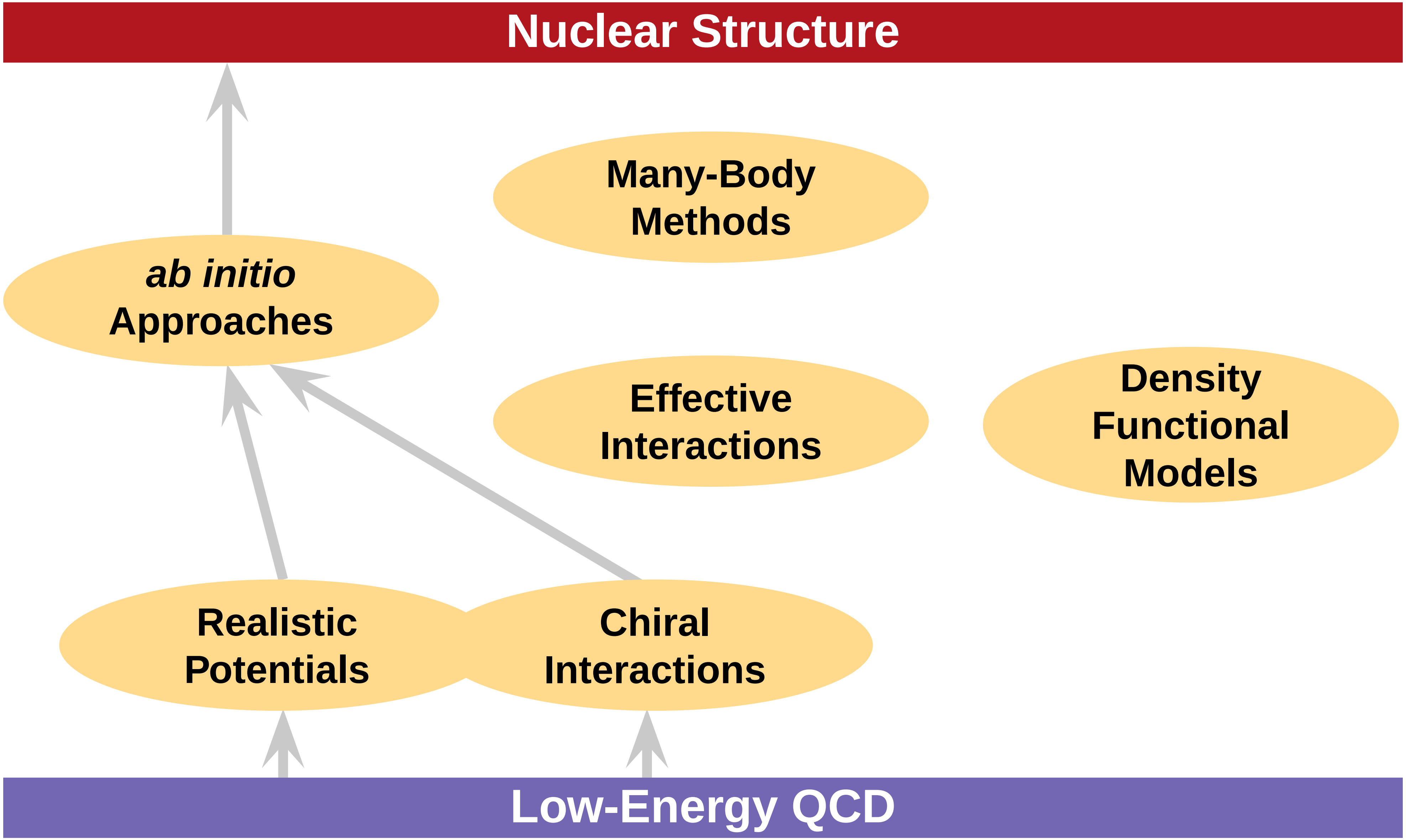
[S. Pieper, private comm.]

12C results are preliminary.

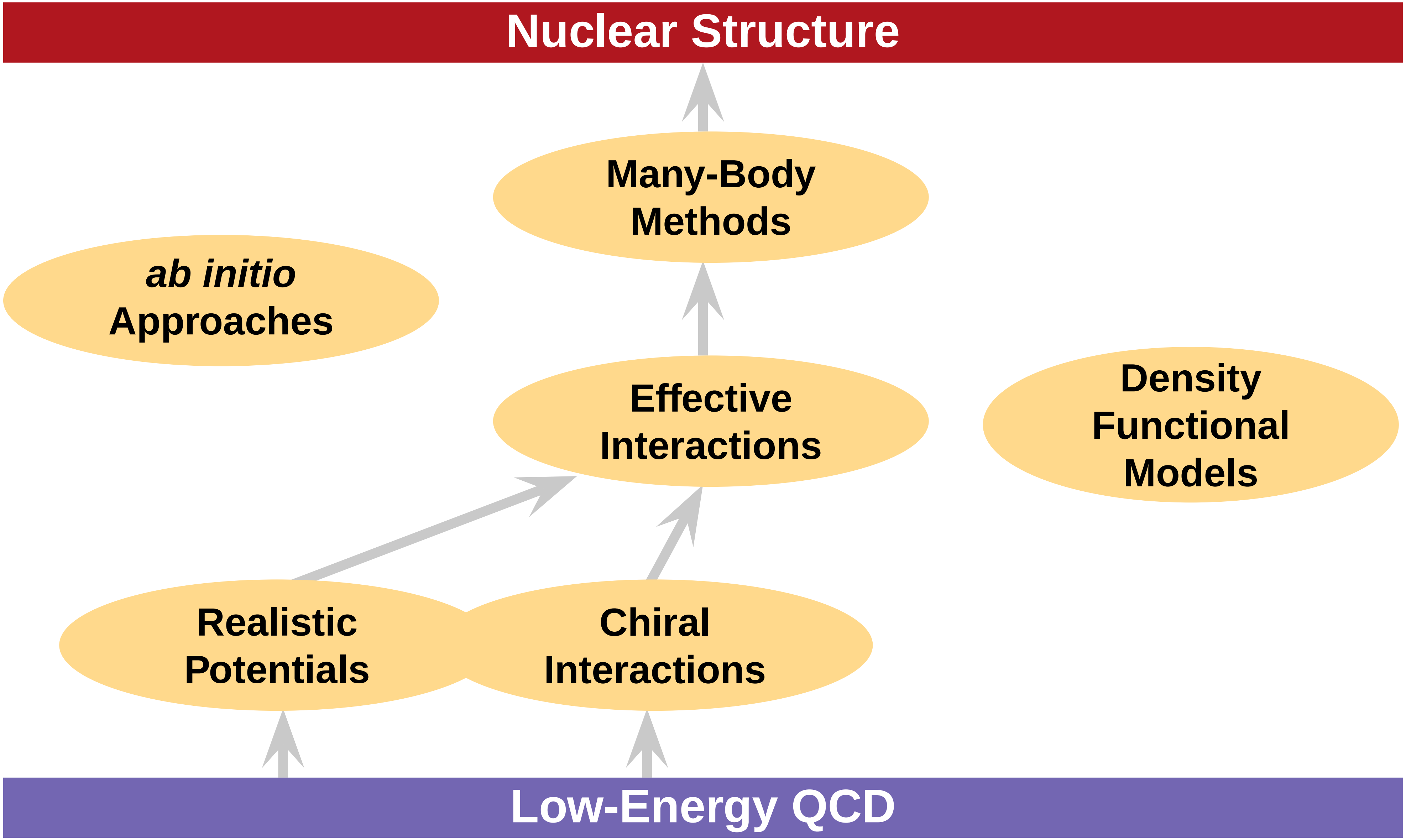
“exact” numerical solution of interacting *A*-nucleon problem

75000 CPU-hours (27 TFlops-hours)

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

Many-Body Methods

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

Modern Effective Interactions

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

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

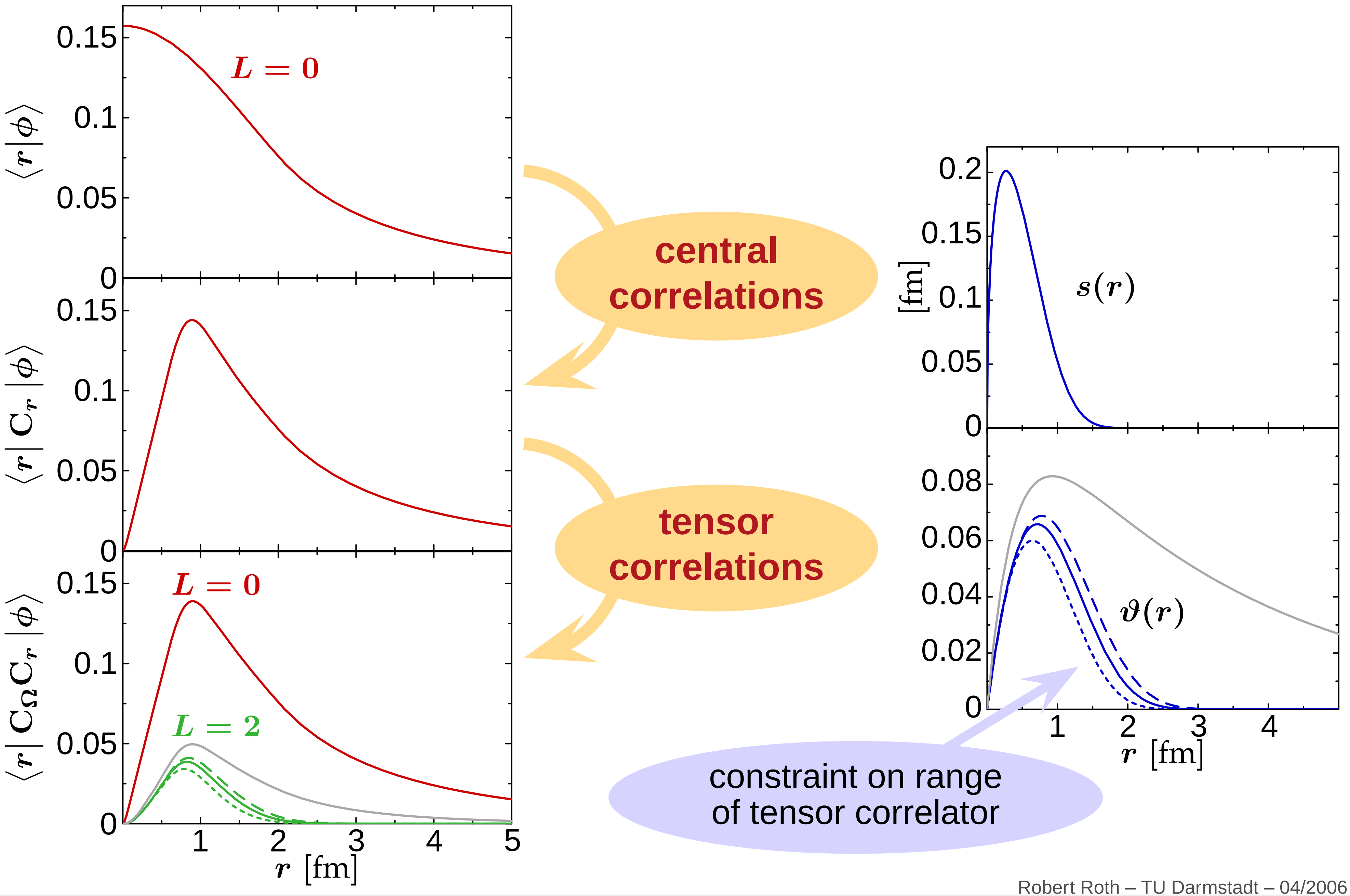
- angular shift depending on the orientation of spin and relative coordinate of a nucleon pair

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

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

$s(r)$ and $\vartheta(r)$
for given potential determined
in the two-body system

Correlated States: The Deuteron



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

Application I

No-Core Shell Model

UCOM + NCSM

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

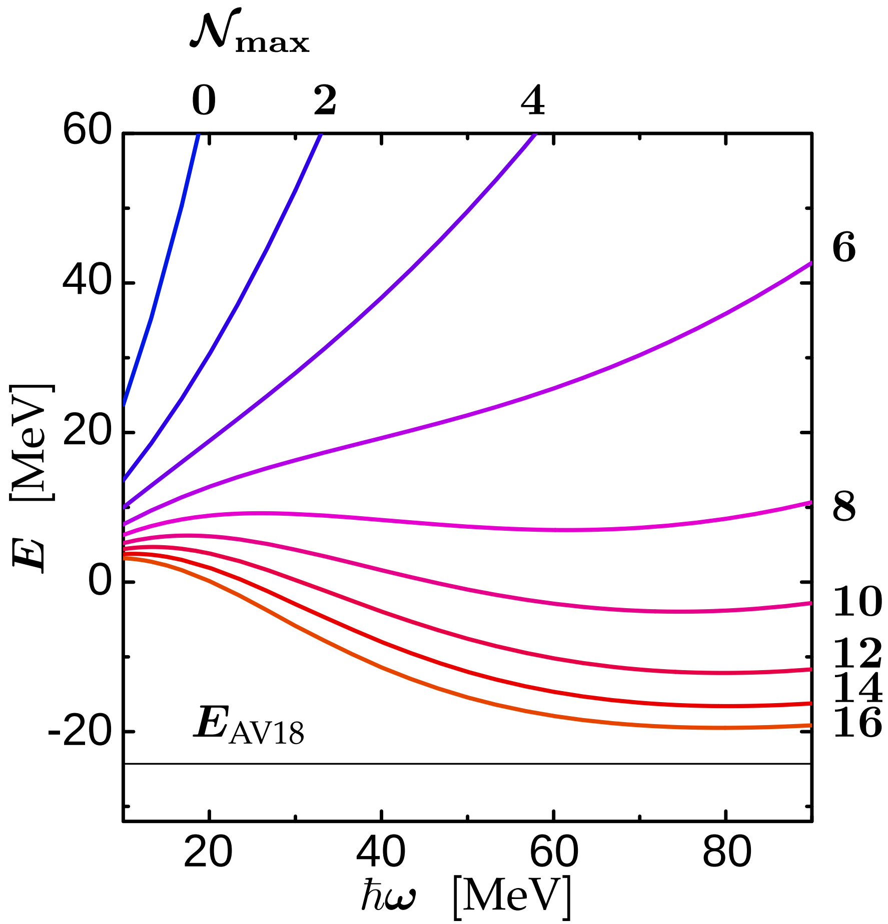
- many-body state is expanded in Slater determinants of harmonic oscillator single-particle states
- large scale diagonalisation of Hamiltonian within a truncated model space ($\mathcal{N}\hbar\omega$ truncation)
- assessment of short- and long-range correlations

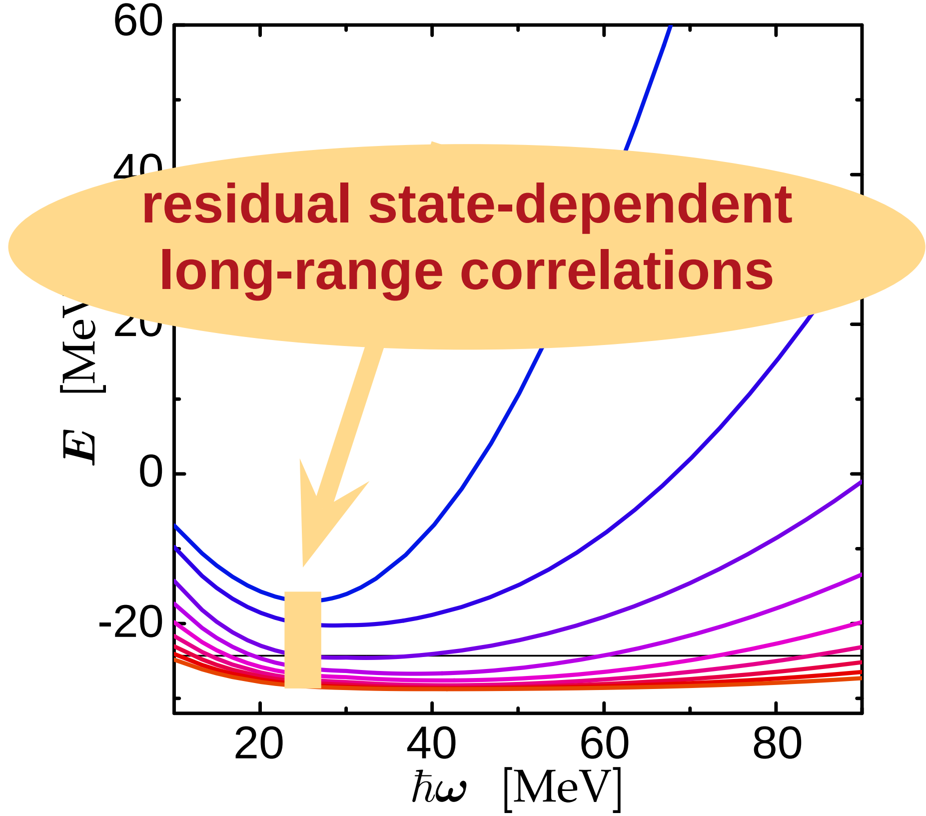
NCSM code by Petr Navrátil [PRC 61, 044001 (2000)]

^{4}He: Convergence

V_{AV18}

V_{UCOM}





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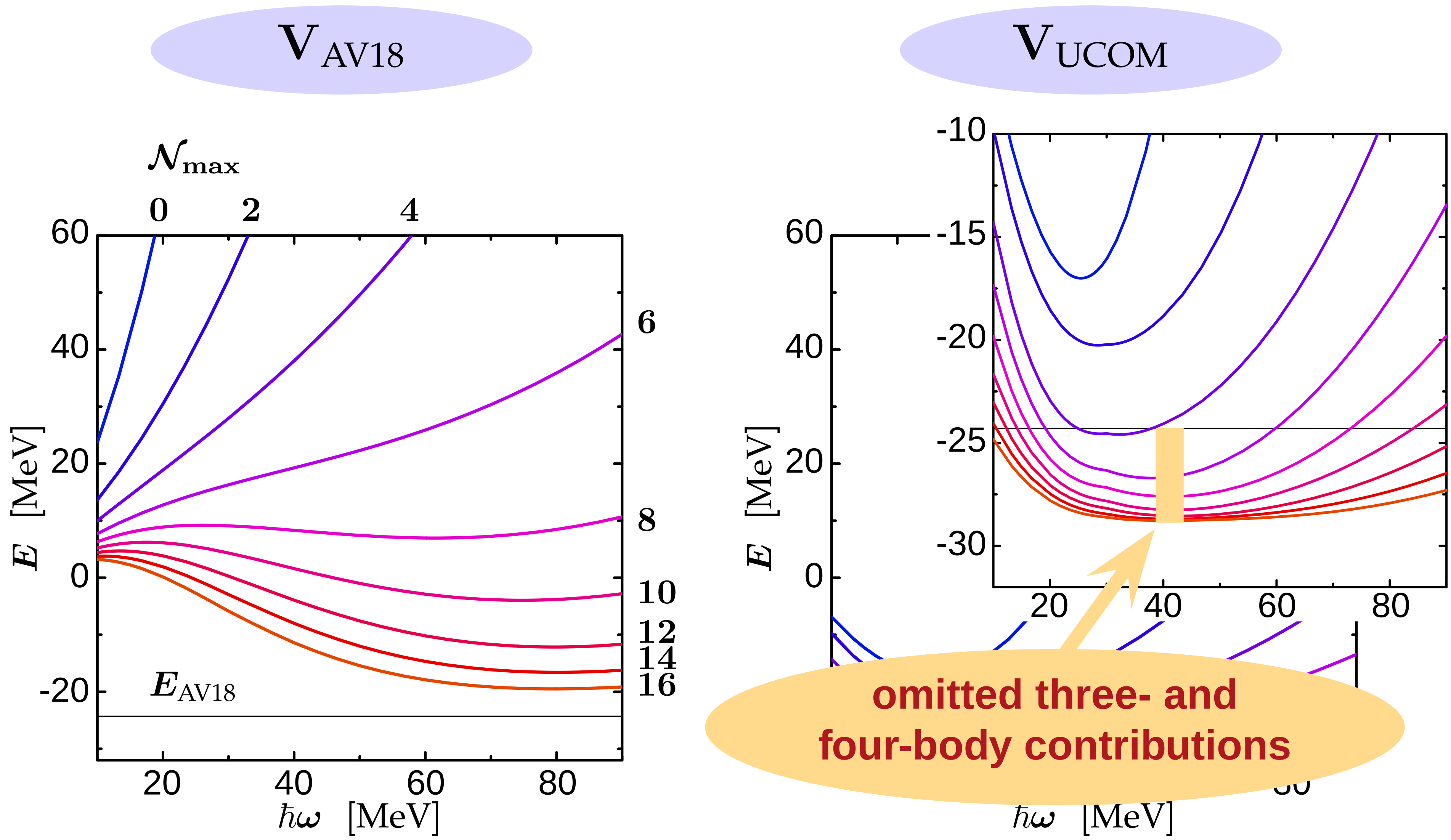
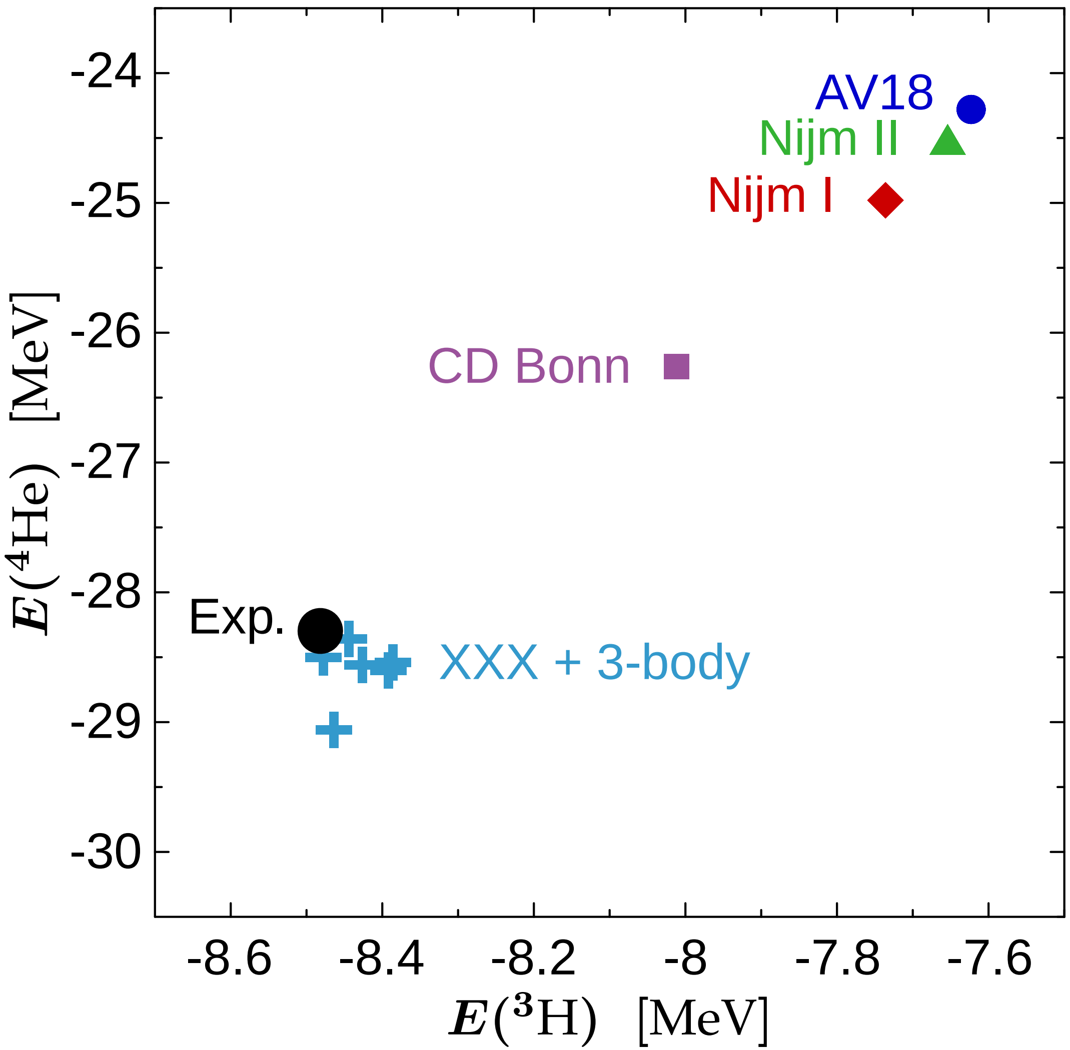
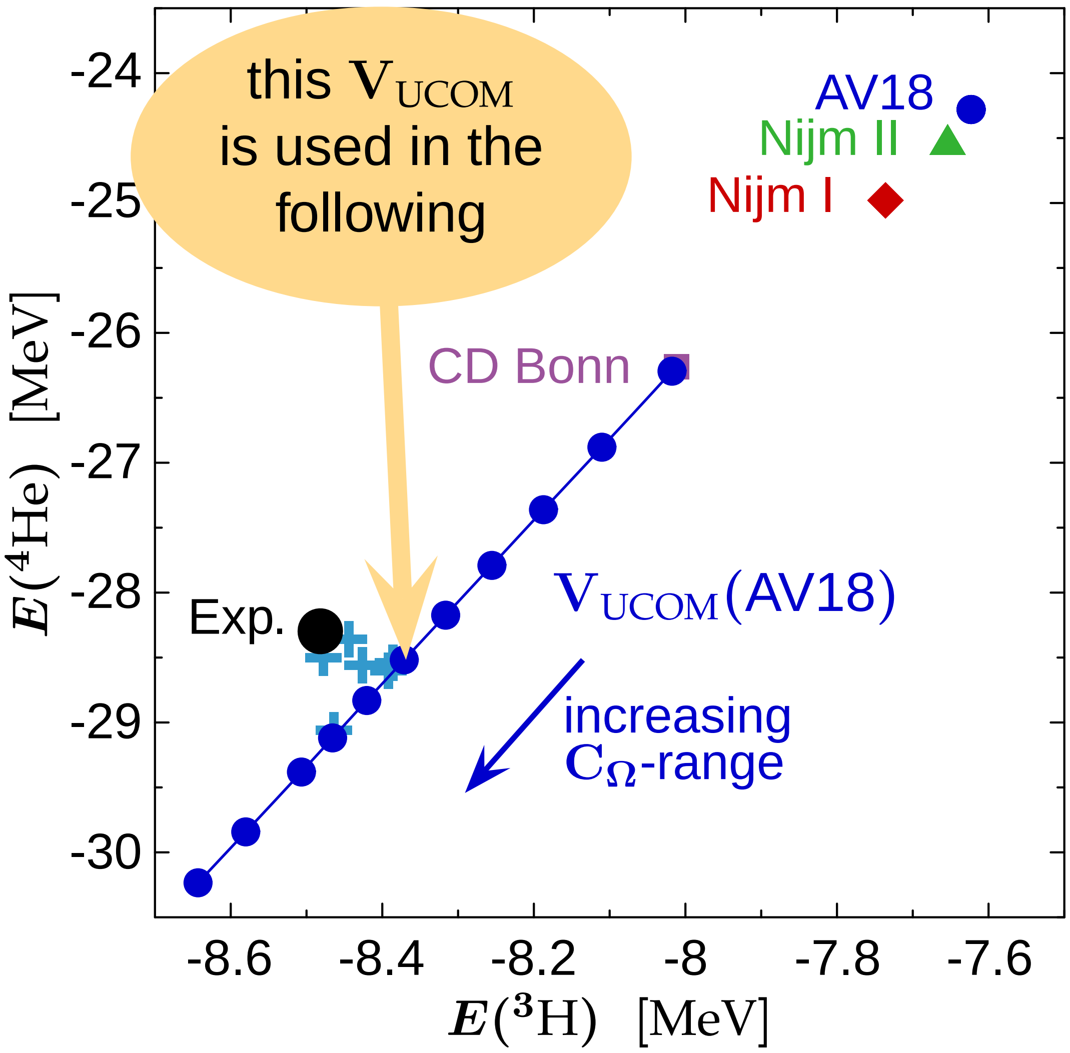


Tjon-Line and Correlator Range



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

Tjon-Line and Correlator Range



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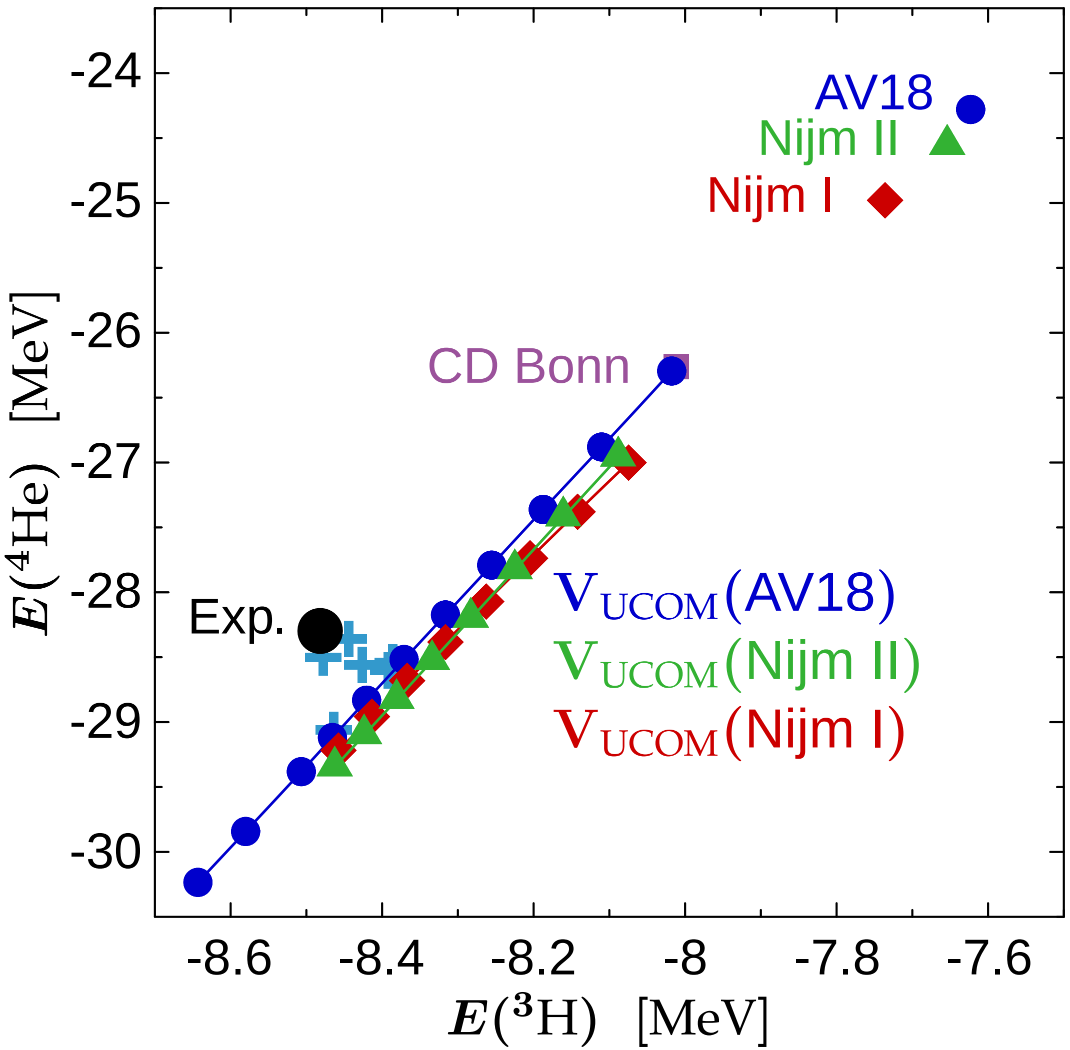
- change of C_Ω-correlator range results in shift along Tjon-line

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

Tjon-Line and Correlator Range



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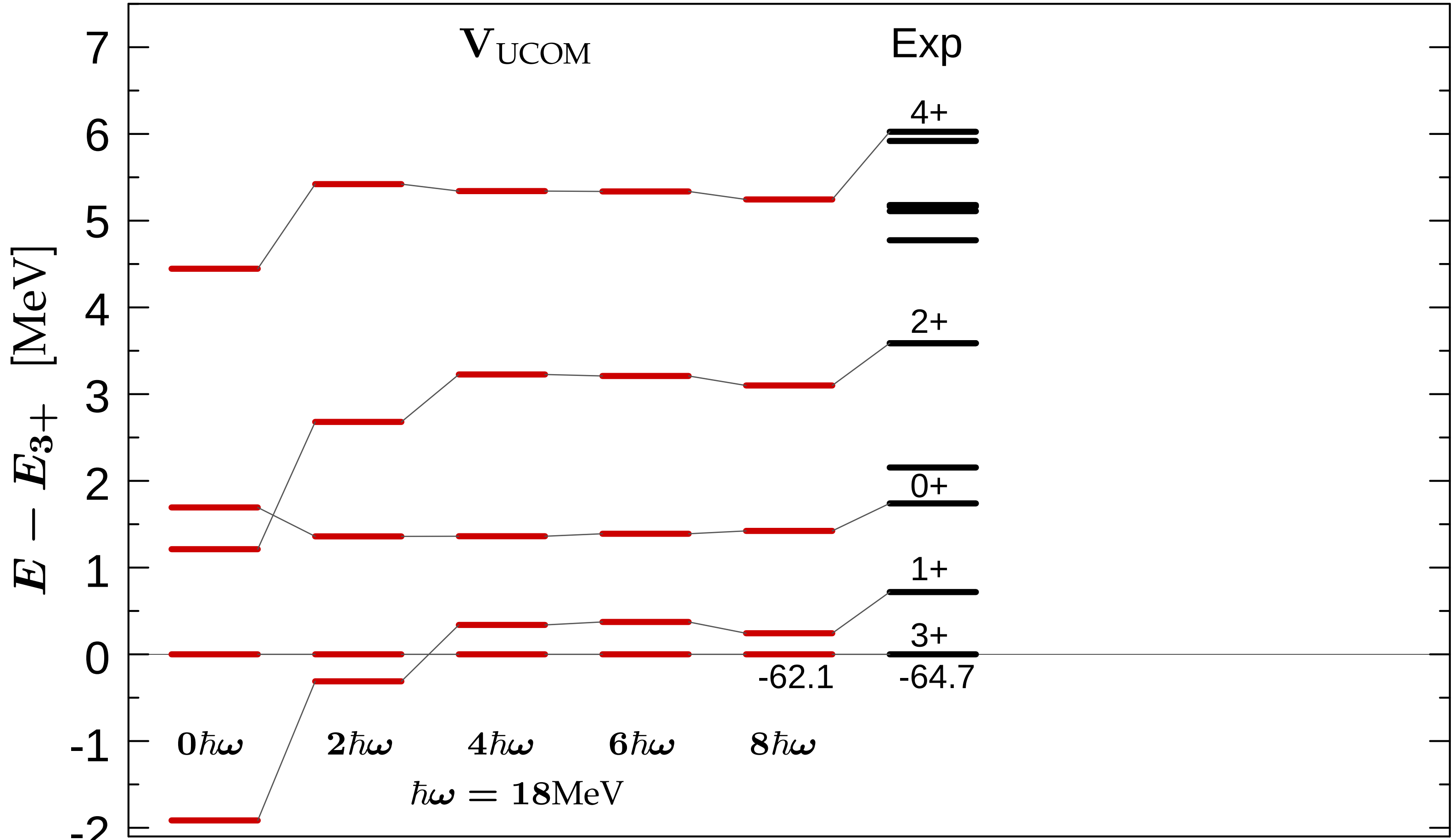
^{10}B: Benchmarking V_{UCOM}

- large-scale NCSM calculations troughout the p-shell in progress (with and w/o Lee-Suzuki transformation)



calculations by Petr Navrátil – preliminary

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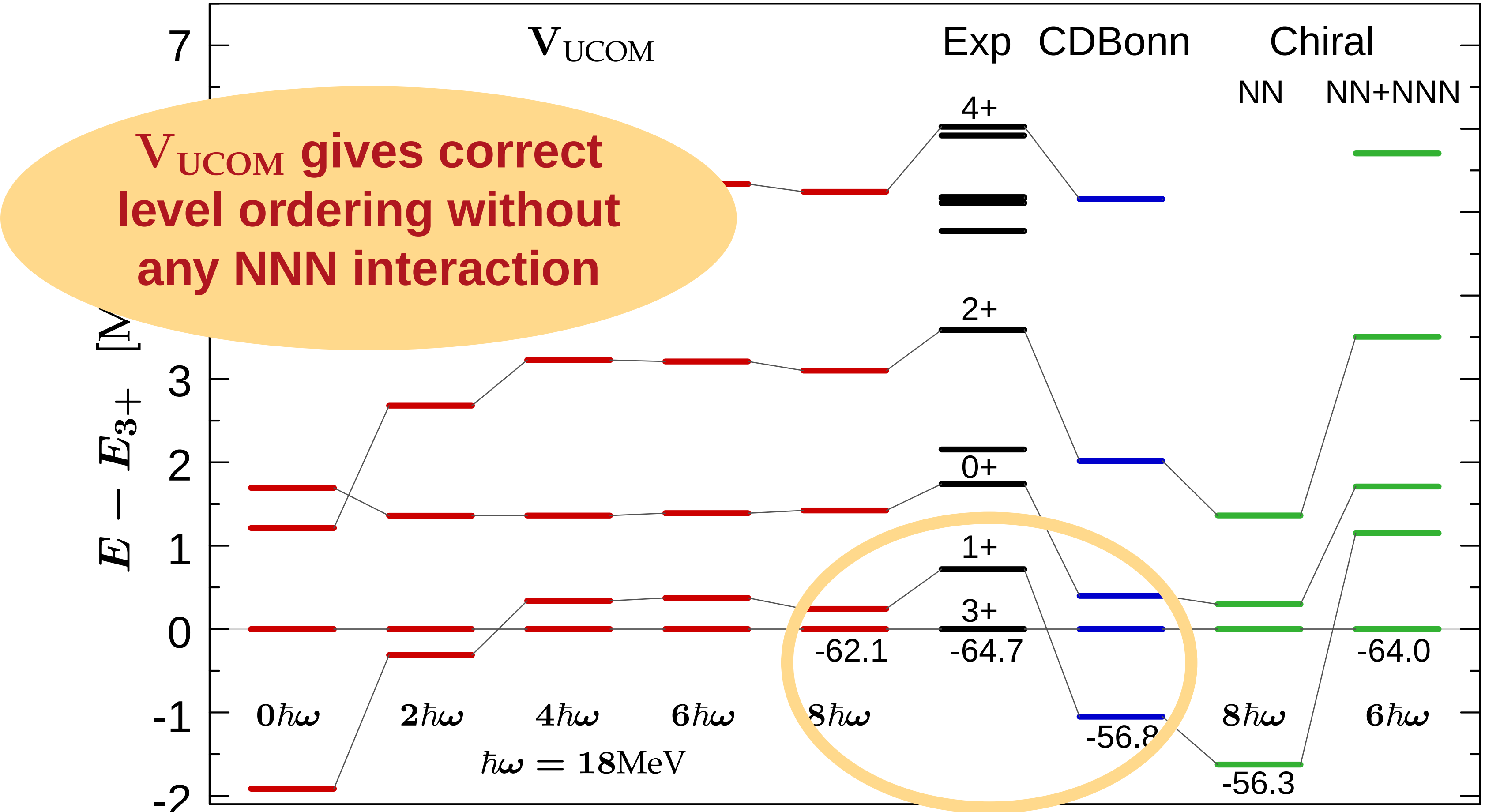


calculations by Petr Navrátil – preliminary

Application II:

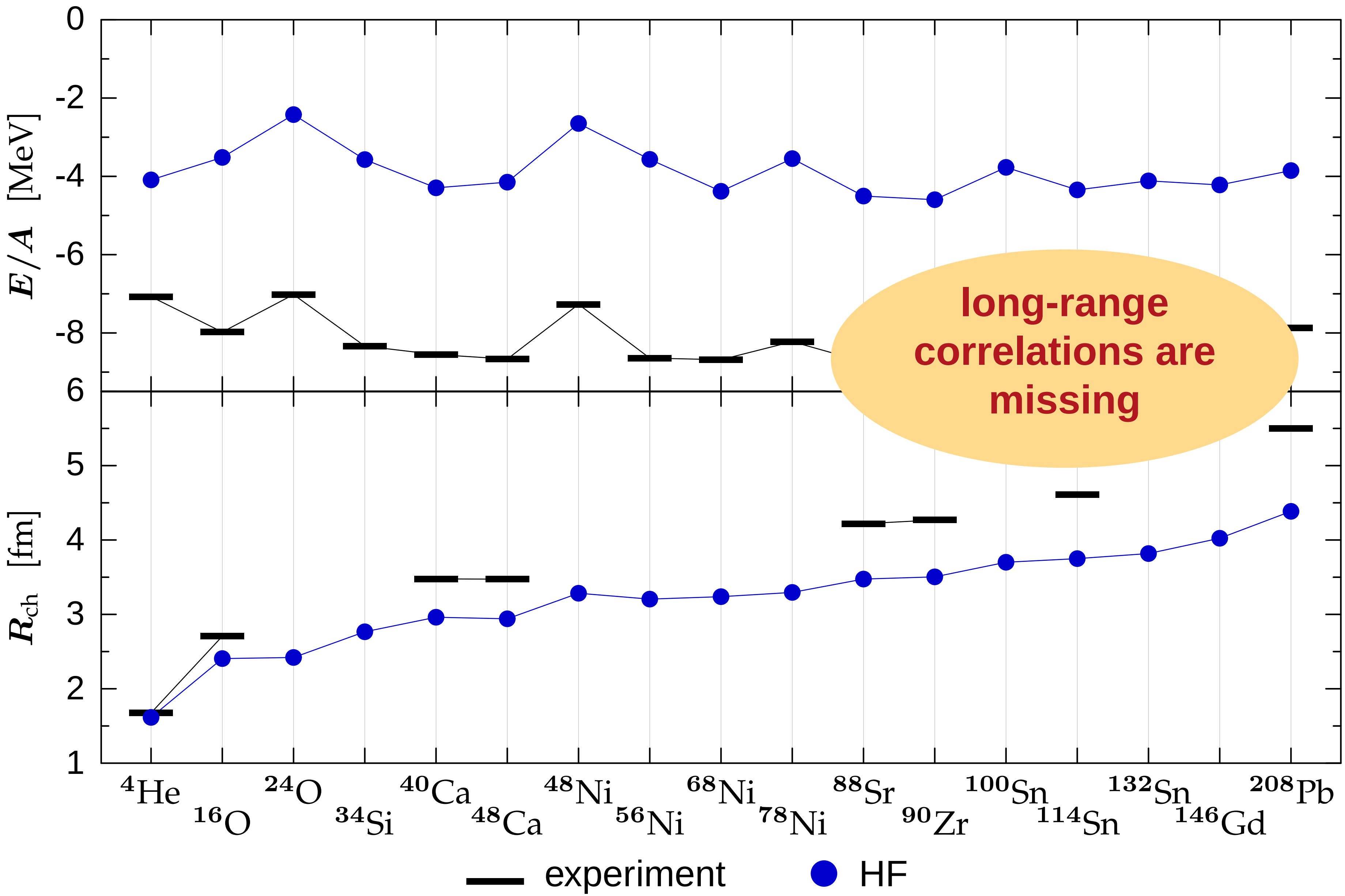
Hartree-Fock & Beyond

UCOM + HF

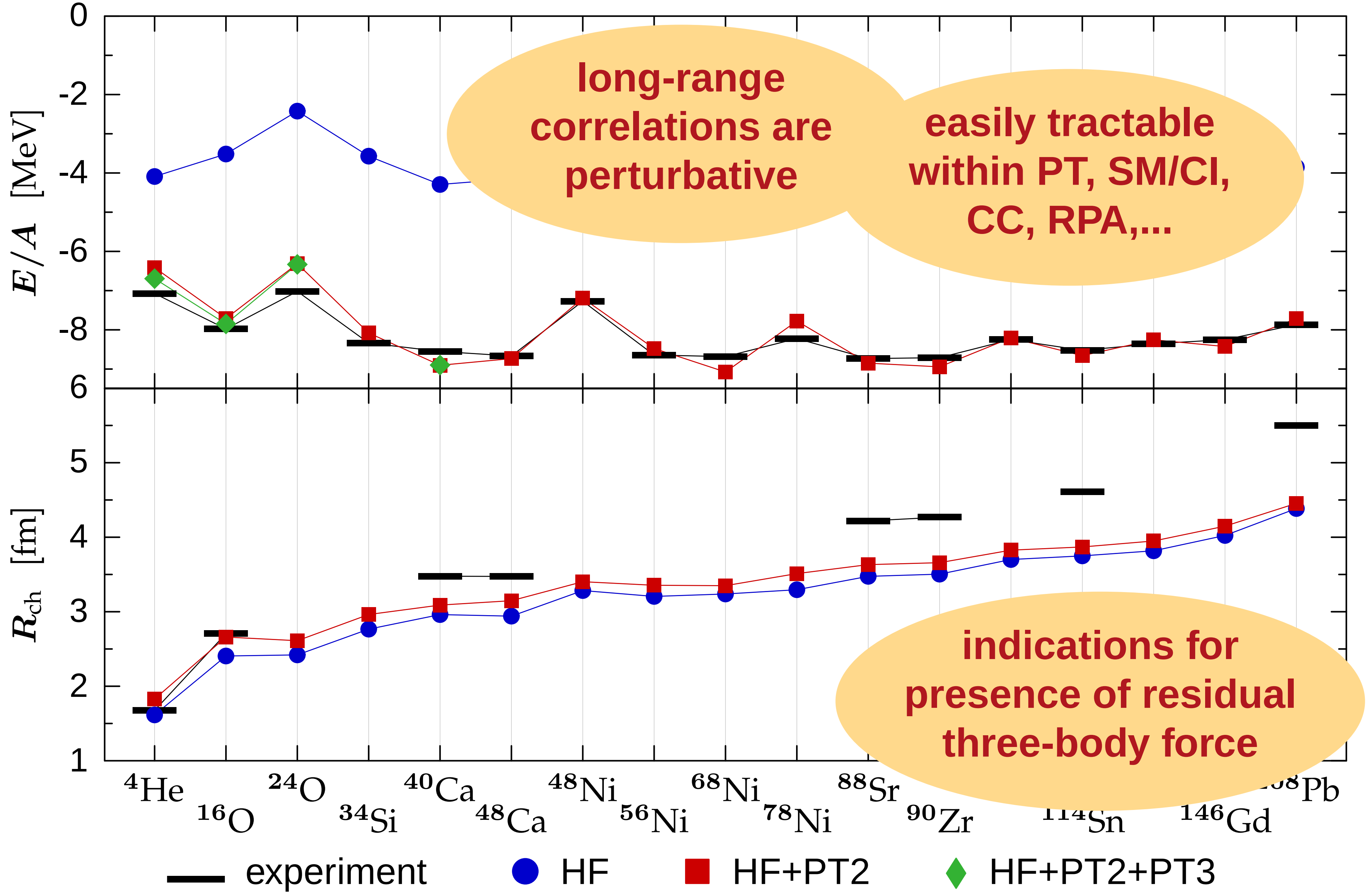
Standard Hartree-Fock
+
Matrix Elements of Correlated Realistic NN-Interaction V_{UCOM}

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

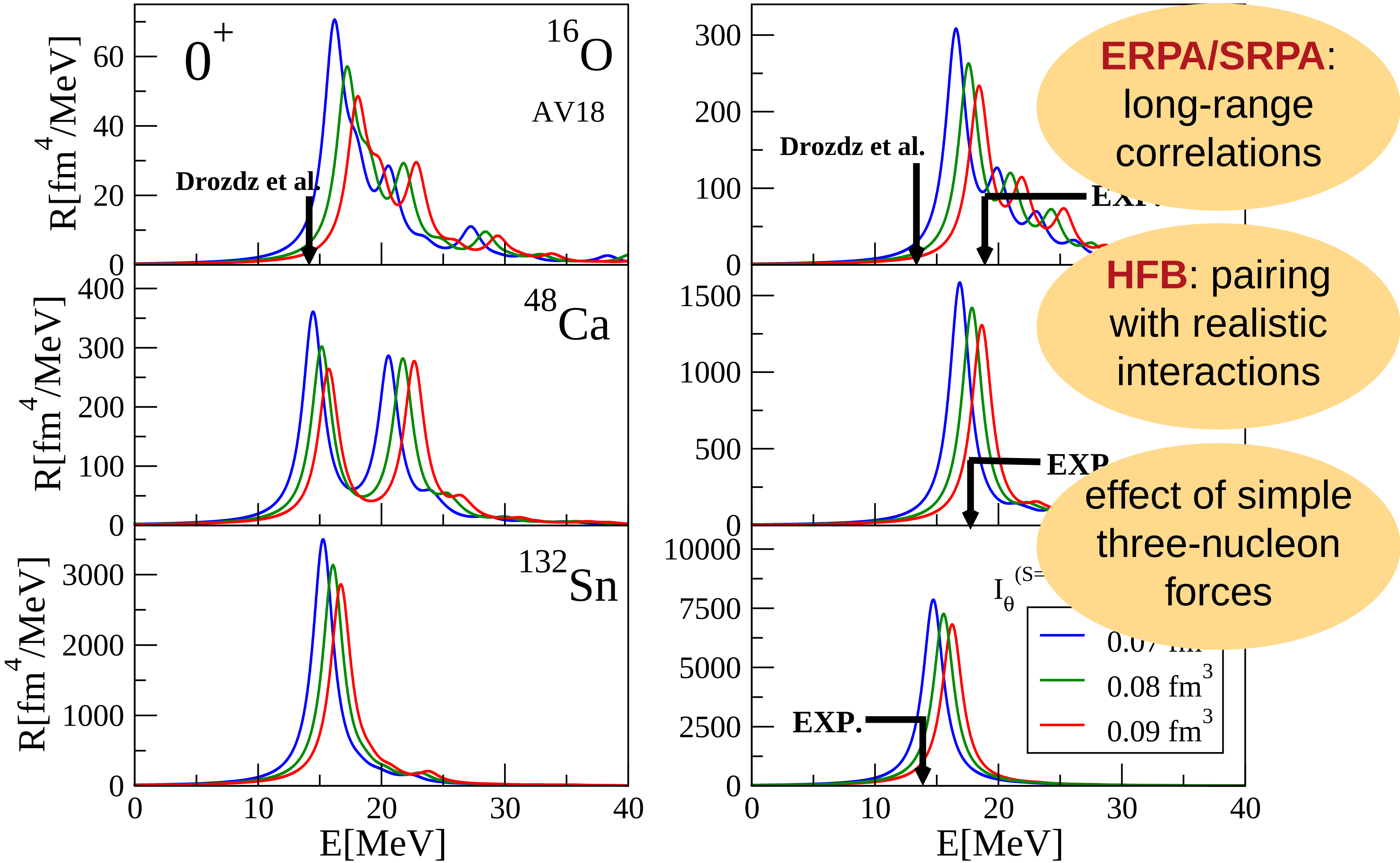
Hartree-Fock with V_{UCOM}



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

$\vec{b}_\nu$: 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

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

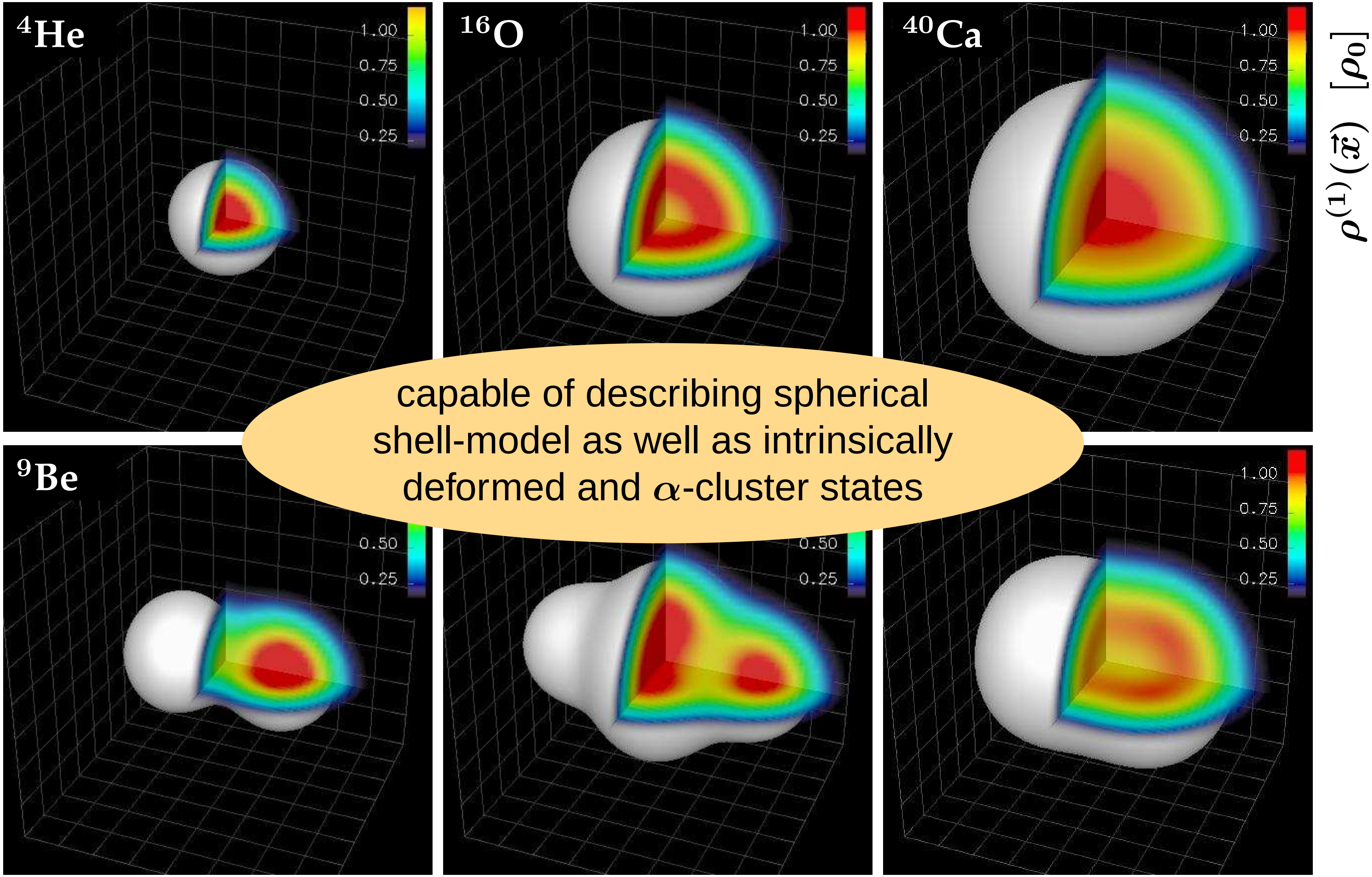
Projection

restoration of rotational and inversion symmetry (PAV / VAP)

Multi-Configuration

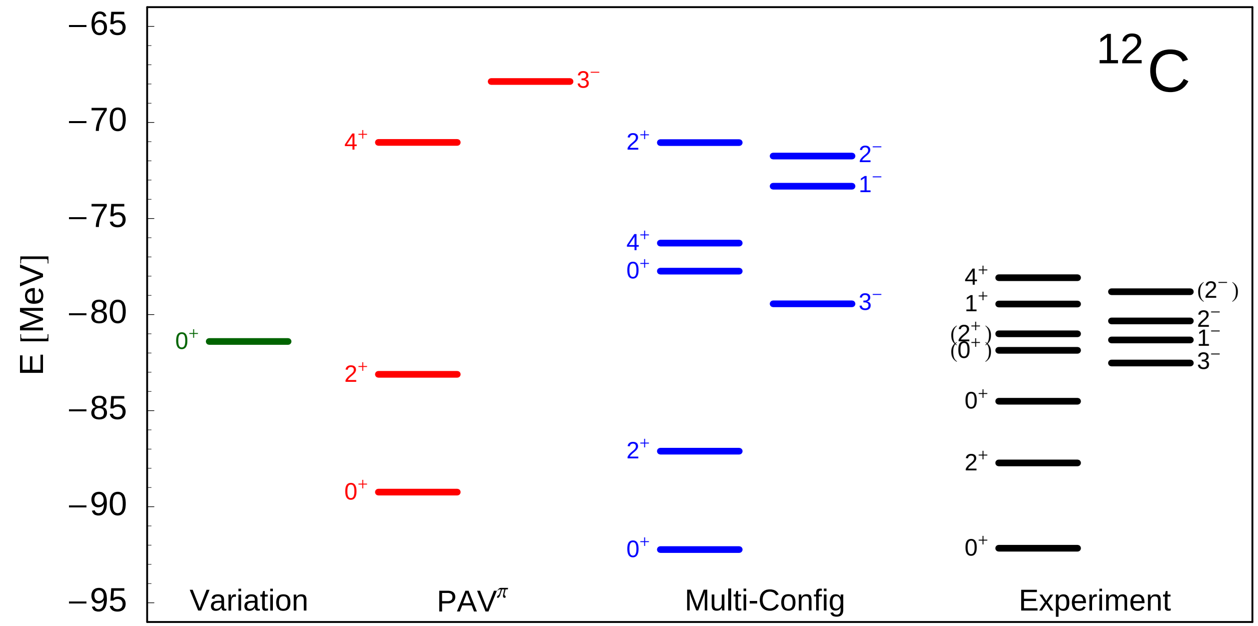
mixing of several intrinsic configurations (GCM)

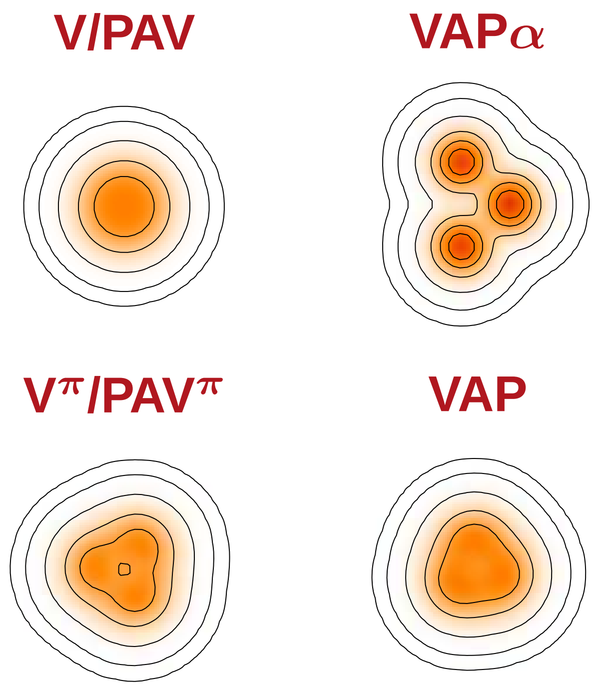
Intrinsic One-Body Density Distributions



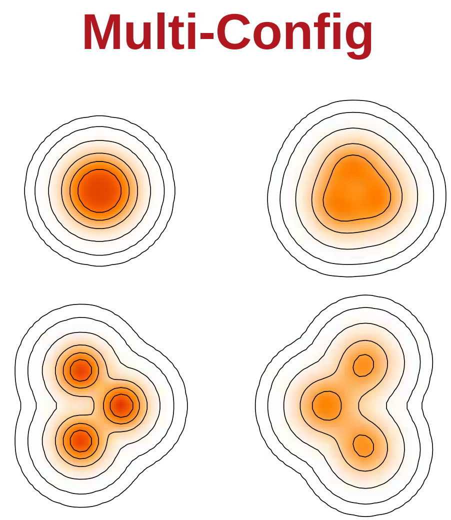
capable of describing spherical shell-model as well as intrinsically deformed and α-cluster states

Structure of ^{12}C

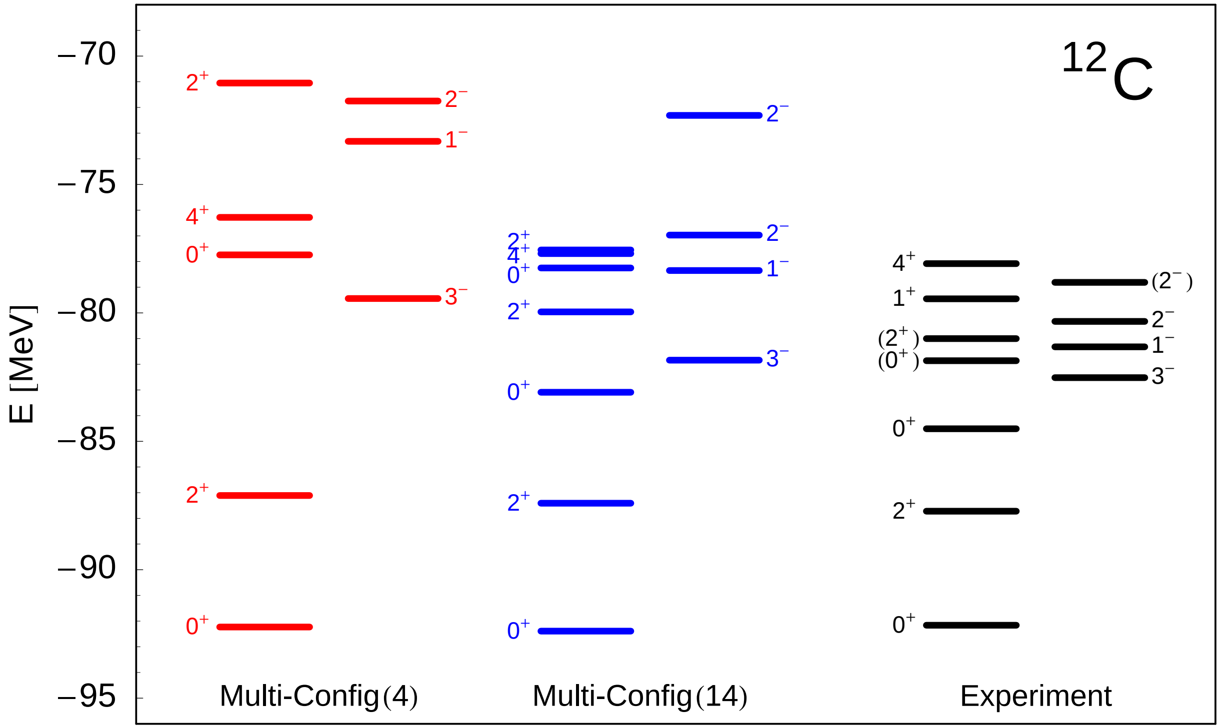




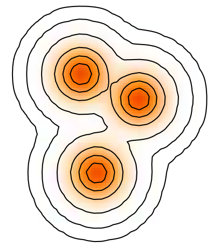
	E [MeV]	R_{ch} [fm]	$B(E2)$ [e^2 fm^4]
V/PAV	81.4	2.36	-
VAP α-cluster	79.1	2.70	76.9
PAV$^\pi$	88.5	2.51	36.3
VAP	89.2	2.42	26.8
Multi-Config	92.2	2.52	42.8
Experiment	92.2	2.47	39.7 ± 3.3

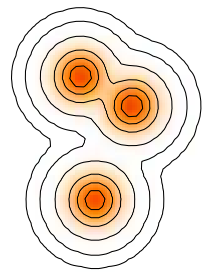


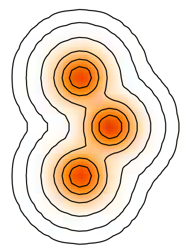
Structure of ^{12}C — Hoyle State



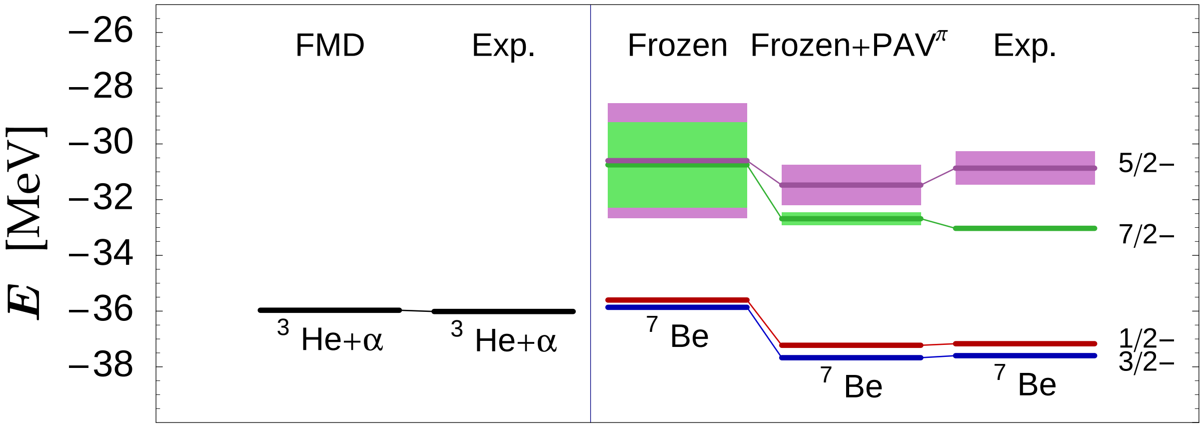
	Multi-Config	Experiment
E [MeV]	92.4	92.2
R_{ch} [fm]	2.52	2.47
$B(E2, 0_1^+ \to 2_1^+)$ [e^2 fm^4]	42.9	39.7 ± 3.3
$M(E0, 0_1^+ \to 0_2^+)$ [fm^2]	5.67	5.5 ± 0.2

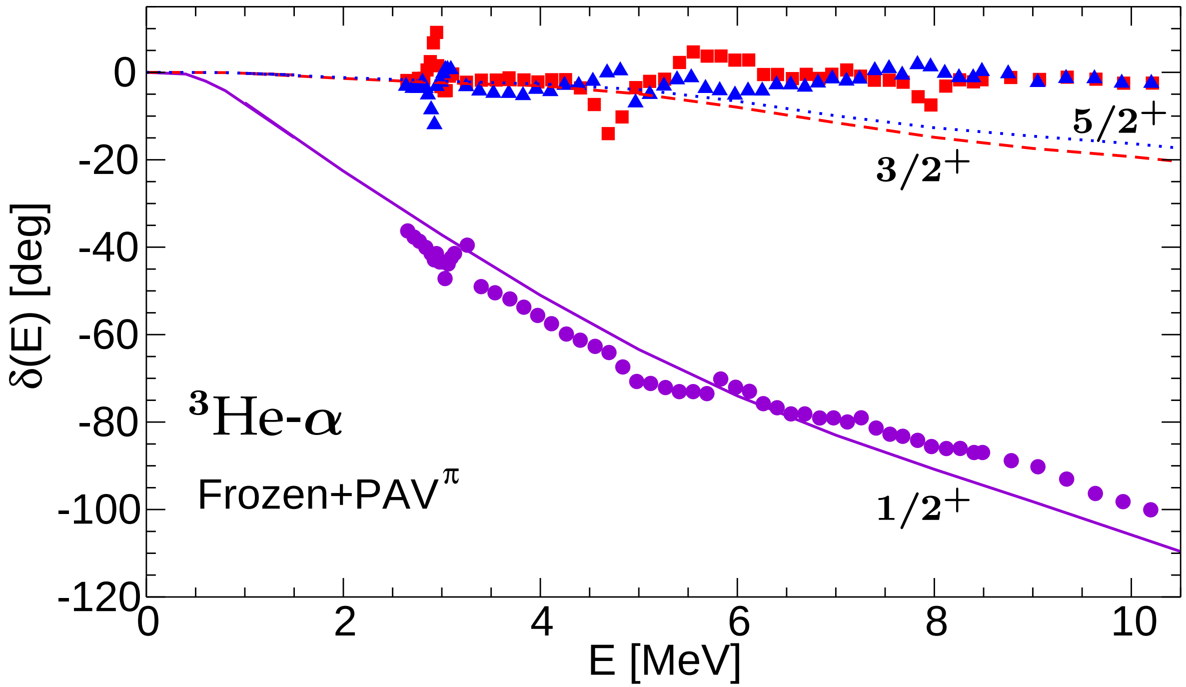
$|\langle$  $|0_2^+\rangle| = 0.76$

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

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

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**
  - P. Hedfeld, H. Hergert, N. Paar, P. Papakonstantinou, A. Zapp

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  - T. Neff

    NSCL, Michigan State University
  - H. Feldmeier, K. Langanke

    Gesellschaft für Schwerionenforschung (GSI)

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