# Nuclear Structure for Exotic Nuclei based on $V_{\mathrm{UCOM}}$

Robert Roth

Institut für Kernphysik
Technische Universität Darmstadt

# Overview

- Motivation
- Correlated Realistic NN-Potentials
  - Correlations & Unitary Correlation Operator Method
- Applications
  - No Core Shell Model
  - Hartree-Fock & Beyond
  - Random Phase Approximation

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

RISING, AGATA,
REX-ISOLDE, ...

NuSTAR @ FAIR,
SPIRAL2, ...

nuclei far-off
stability

nuclear
astrophysics

exotic modes,
hyper-nuclei,...

**reliable**
**nuclear structure theory**
**for exotic nuclei**

**bridging between**
**low-energy QCD and**
**nuclear structure theory**

# Modern Nuclear Structure Theory

**Nuclear Structure**

**Many-Body Approximations**

***ab initio*** **Approaches (GFMC,NCSM,...)**

**Effective Interactions**

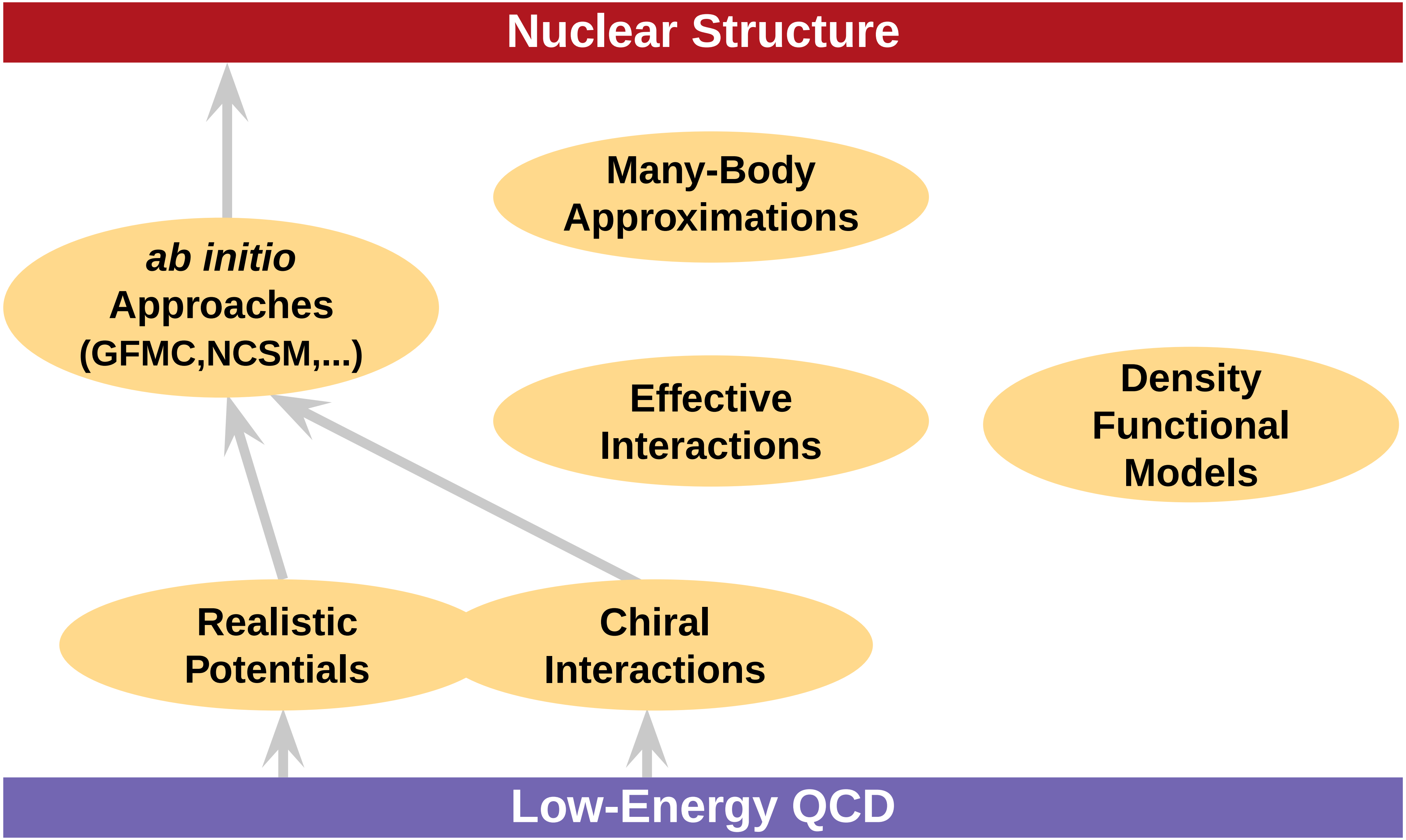
**Density Functional Models**

**Realistic Potentials**

**Chiral Interactions**

**Low-Energy QCD**

# Modern Nuclear Structure Theory



# Realistic NN-Potentials

- **QCD motivated**
  - symmetries, meson-exchange picture
  - chiral effective field theory
- **short-range phenomenology**
  - short-range parametrization 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**

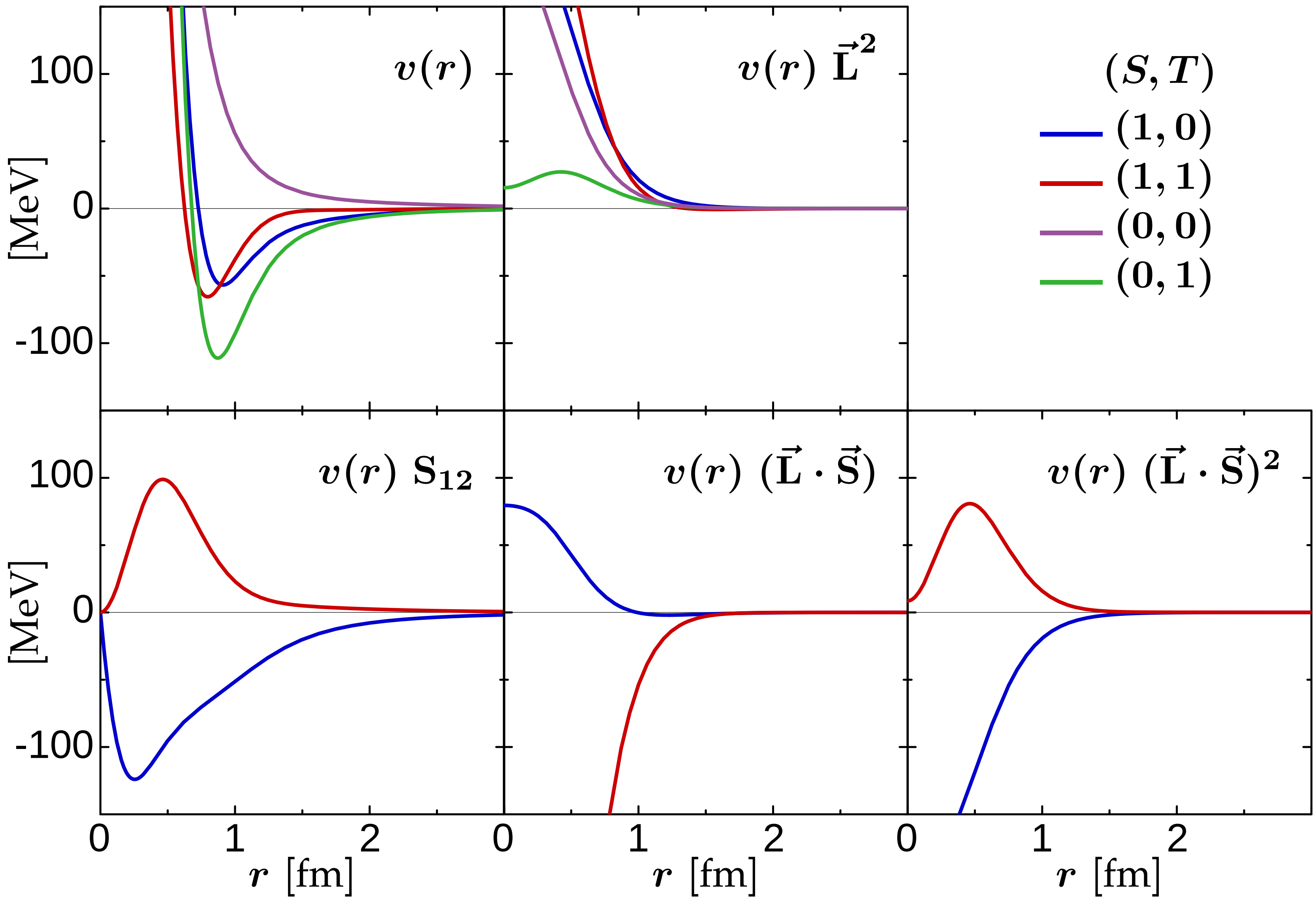
**Nijmegen I/II**

**Chiral N3LO**

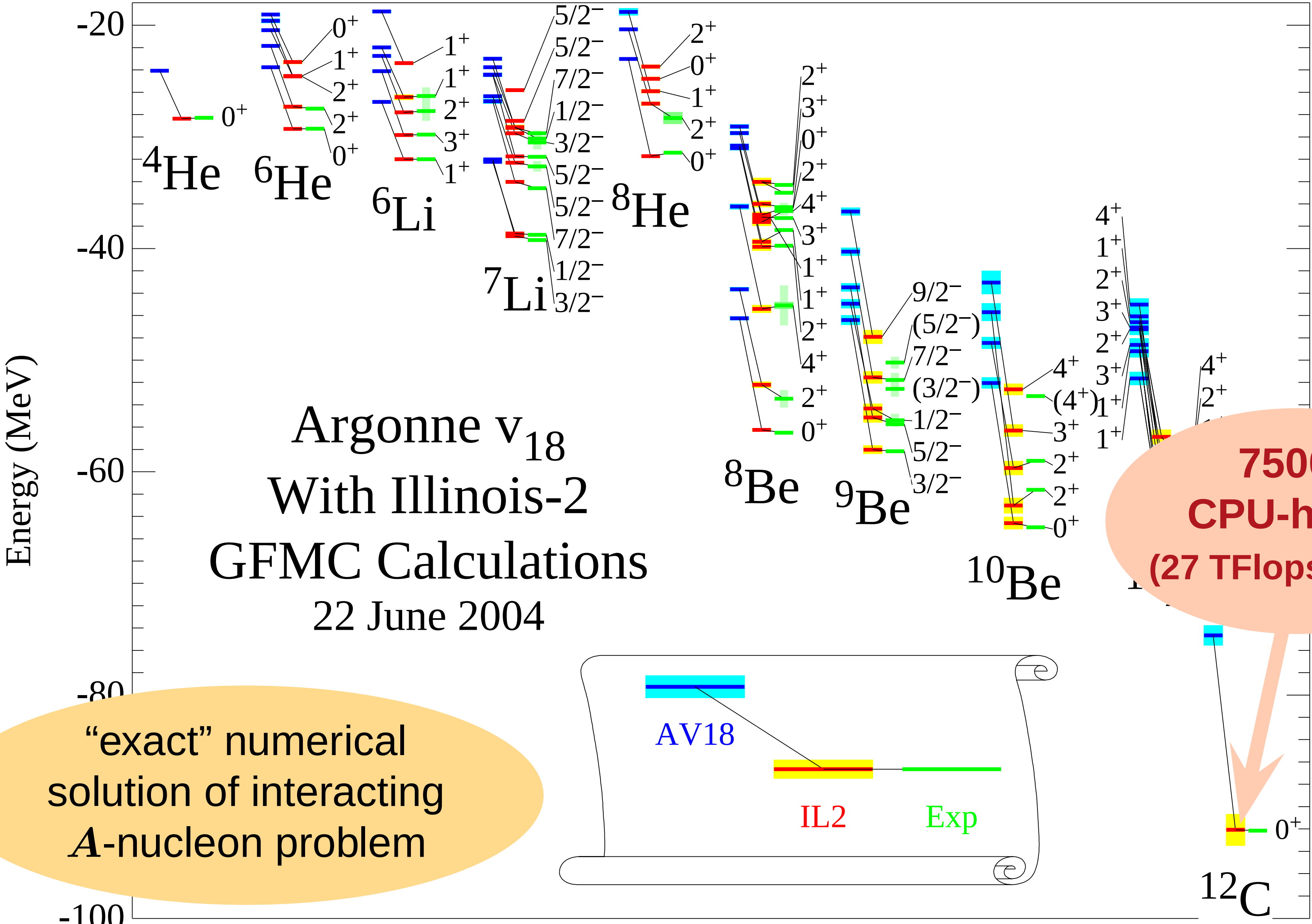
Argonne V18 +
**Illinois 2**

Chiral N3LO +
**N2LO**

# Argonne V18 Potential



# *Ab initio* Methods: GFMC



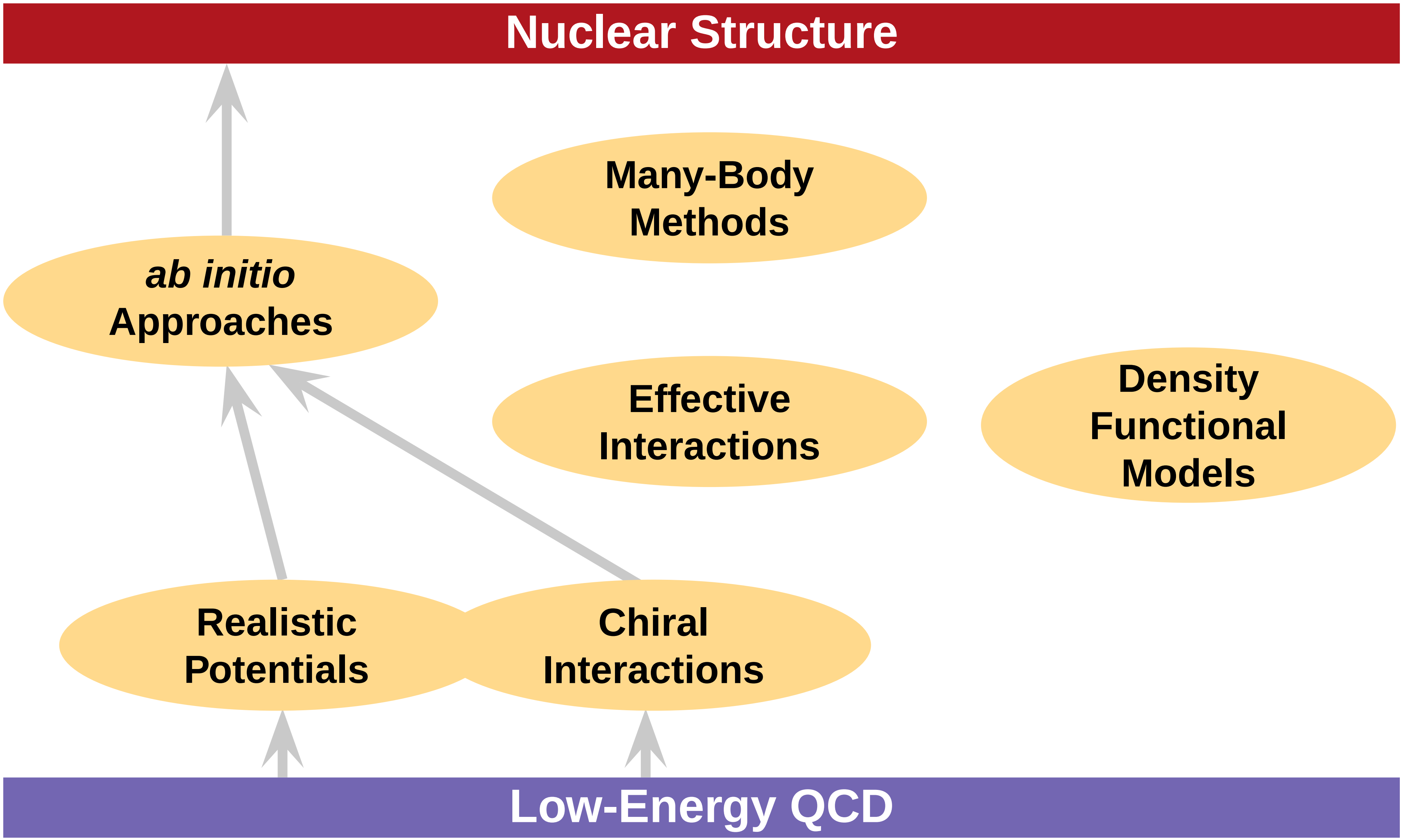

"exact" numerical solution of interacting *A*-nucleon problem

**75000 CPU-hours (27 TFlops-hours)**

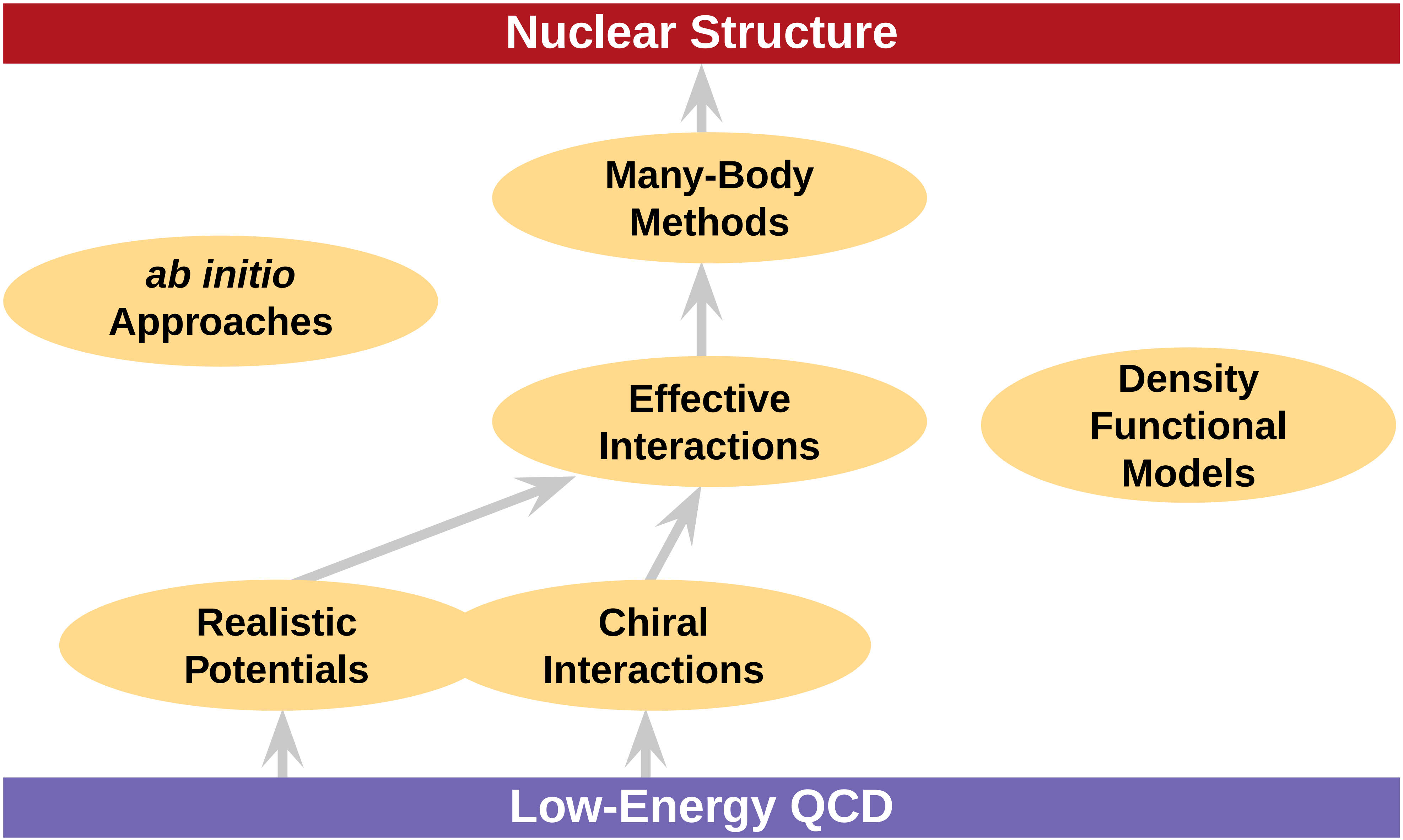
[S. Pieper, private comm.]

$^{12}$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 spaces
- conserve experimentally constrained properties (phase shifts)

## Many-Body Approximations

- 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

# 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

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

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

## Correlated States

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

## Correlated Operators

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

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

# Central and Tensor Correlators

$$\mathbf{C} = \mathbf{C}_\Omega \mathbf{C}_r$$

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

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

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

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

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

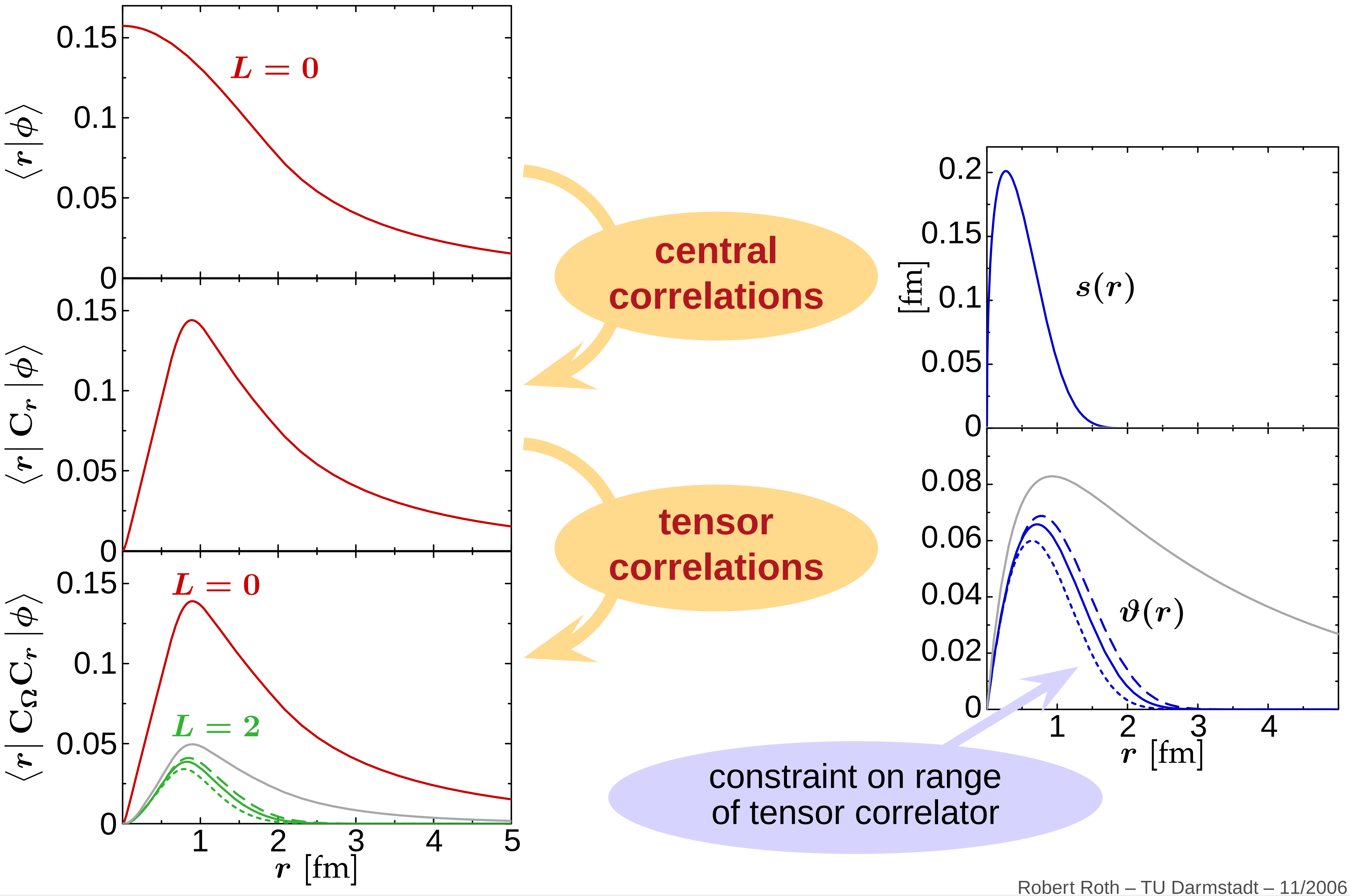
- angular shift depending on the orientation of spin and relative coordinate of a nucleon pair

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

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

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

# Correlated States: The Deuteron



# Correlated Interaction: $V_{\text{UCOM}}$

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

- **closed operator expression** for the correlated interaction $\mathbf{V}_{\text{UCOM}}$ in two-body approximation
- correlated interaction and original NN-potential are **phase shift equivalent** by construction
- momentum-space matrix elements of correlated interaction are **similar to $V_{\text{low}-k}$**
- consistent **correlated operators** for other observables (transitions, densities,...) available

Application I

# No-Core Shell Model

in collaboration with

Petr Navrátil (LLNL)

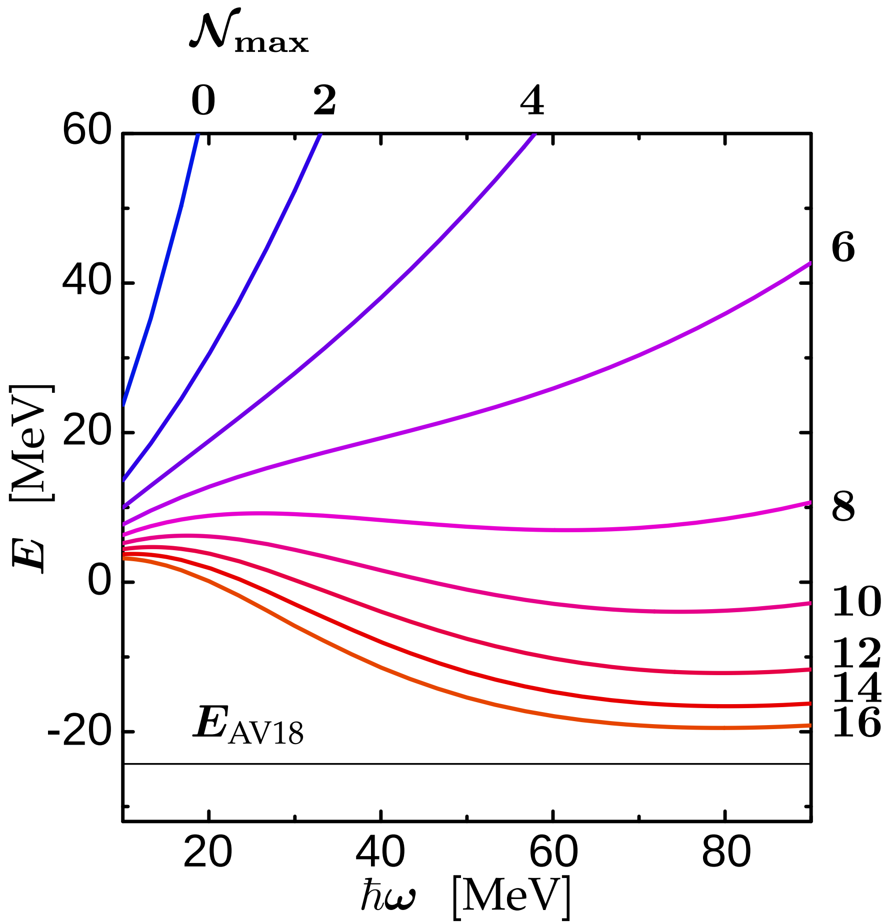
# UCOM + NCSM

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

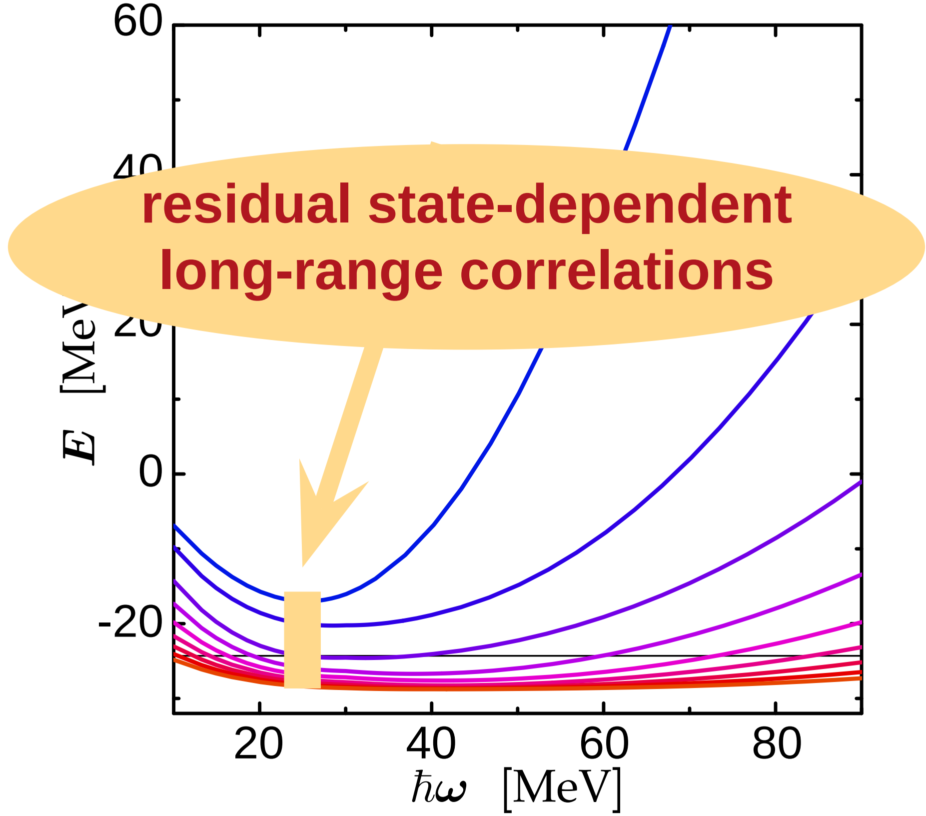
- many-body state is **expanded in Slater determinants** of harmonic oscillator single-particle states
- **large scale diagonalization** of Hamiltonian within a truncated model space ($\mathcal{N}\hbar\omega$ truncation)
- assessment of **short and long-range correlations**

# $^4$He: Convergence

$\mathbf{V}_{\text{AV18}}$




$\mathbf{V}_{\text{UCOM}}$



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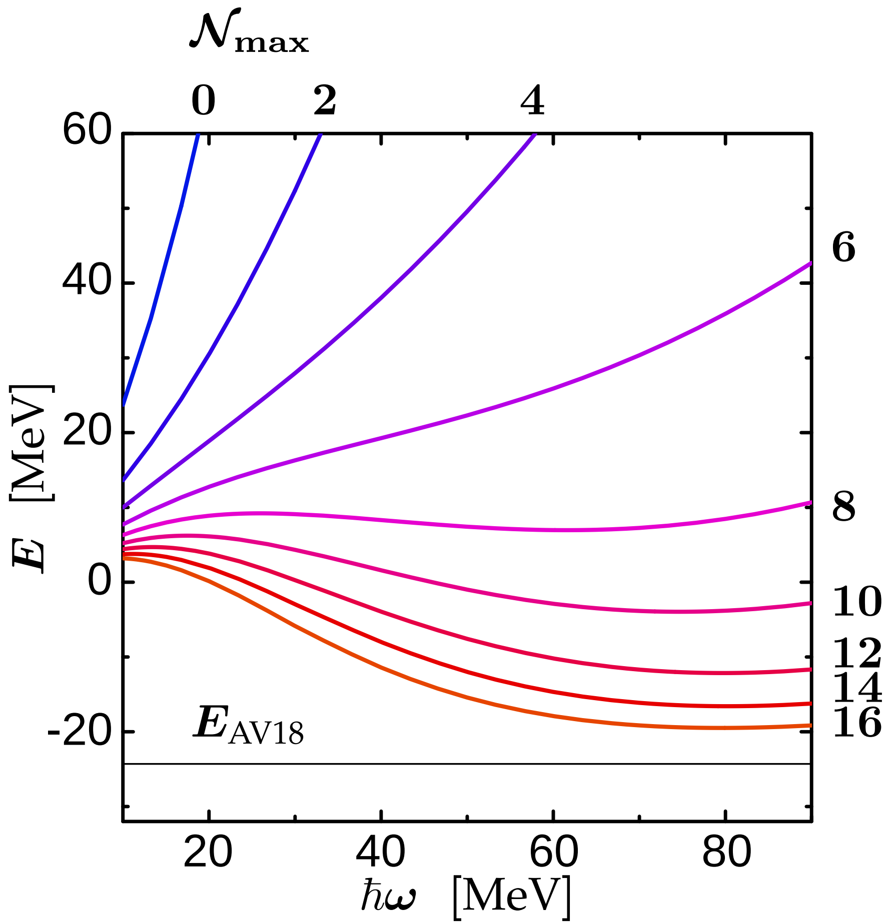
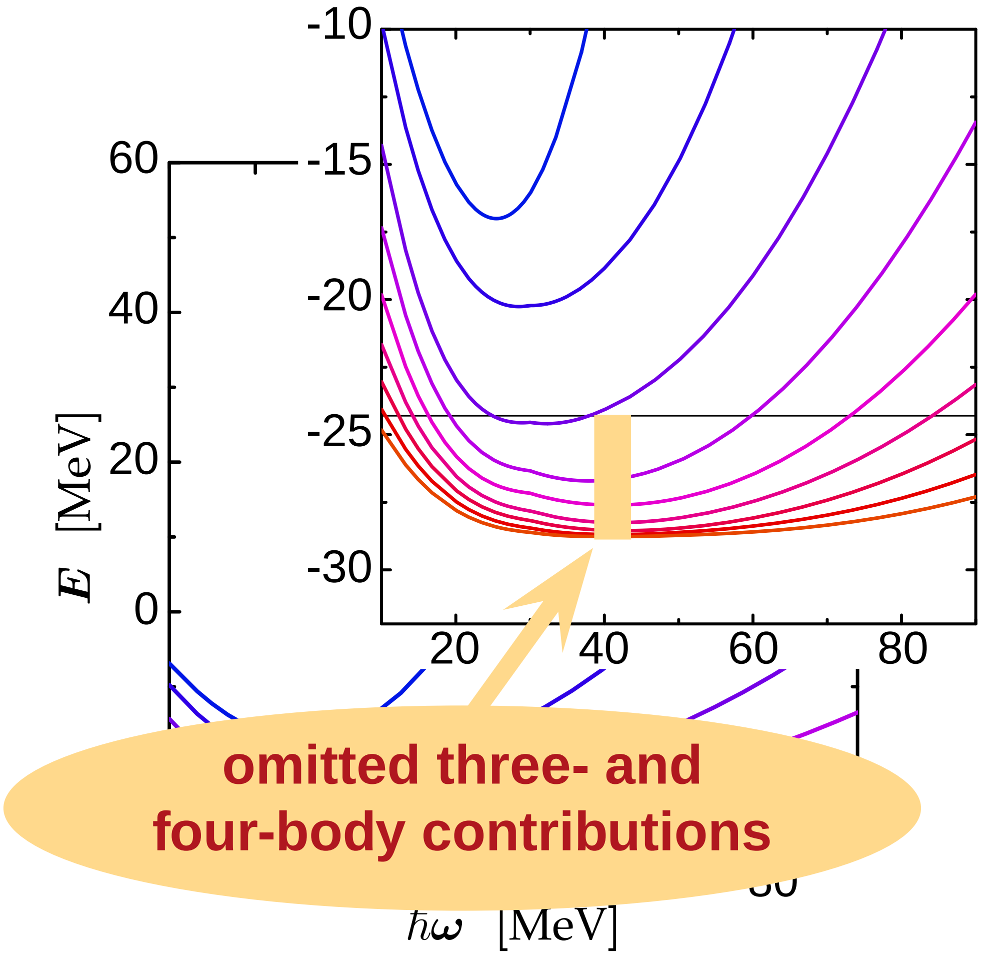
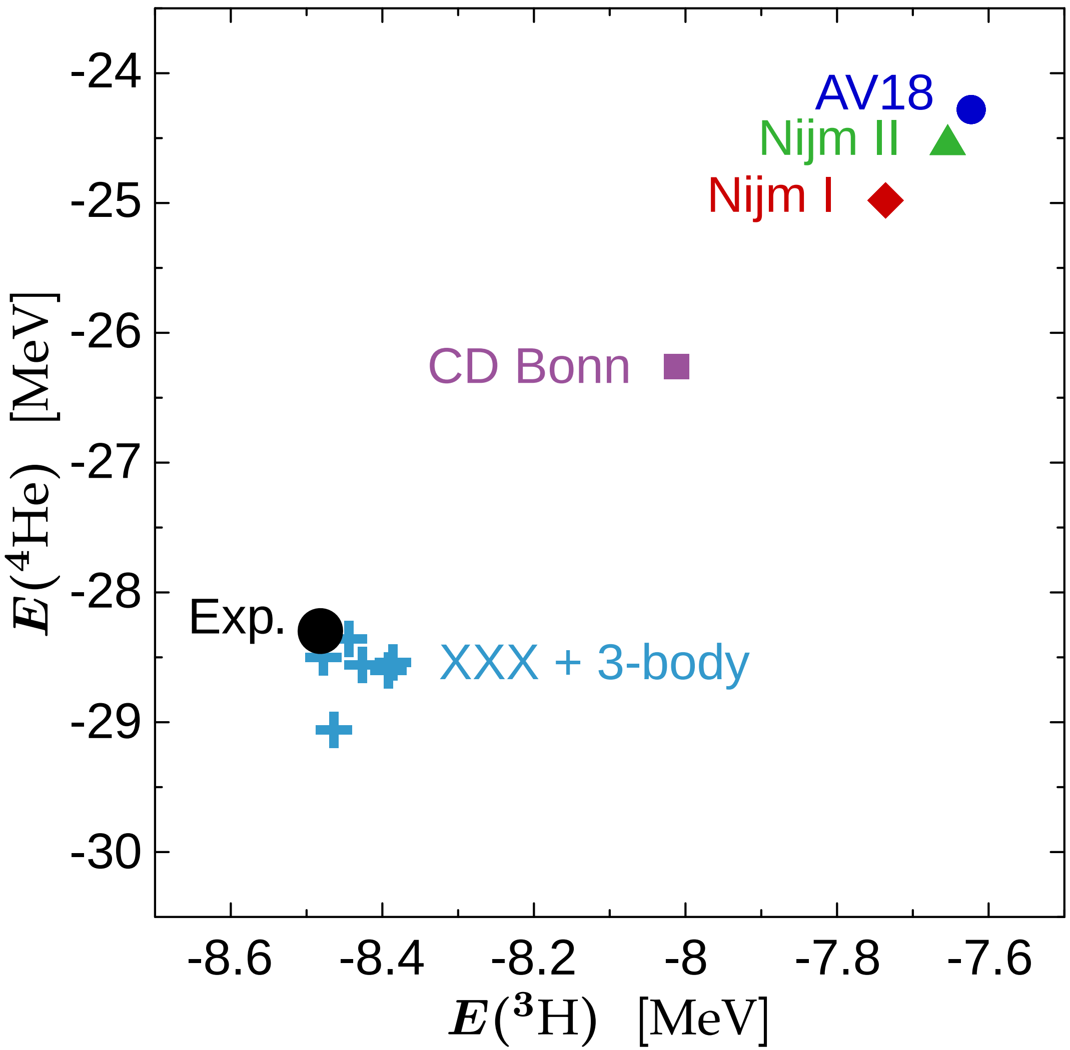



$\mathbf{V}_{\mathrm{UCOM}}$



# 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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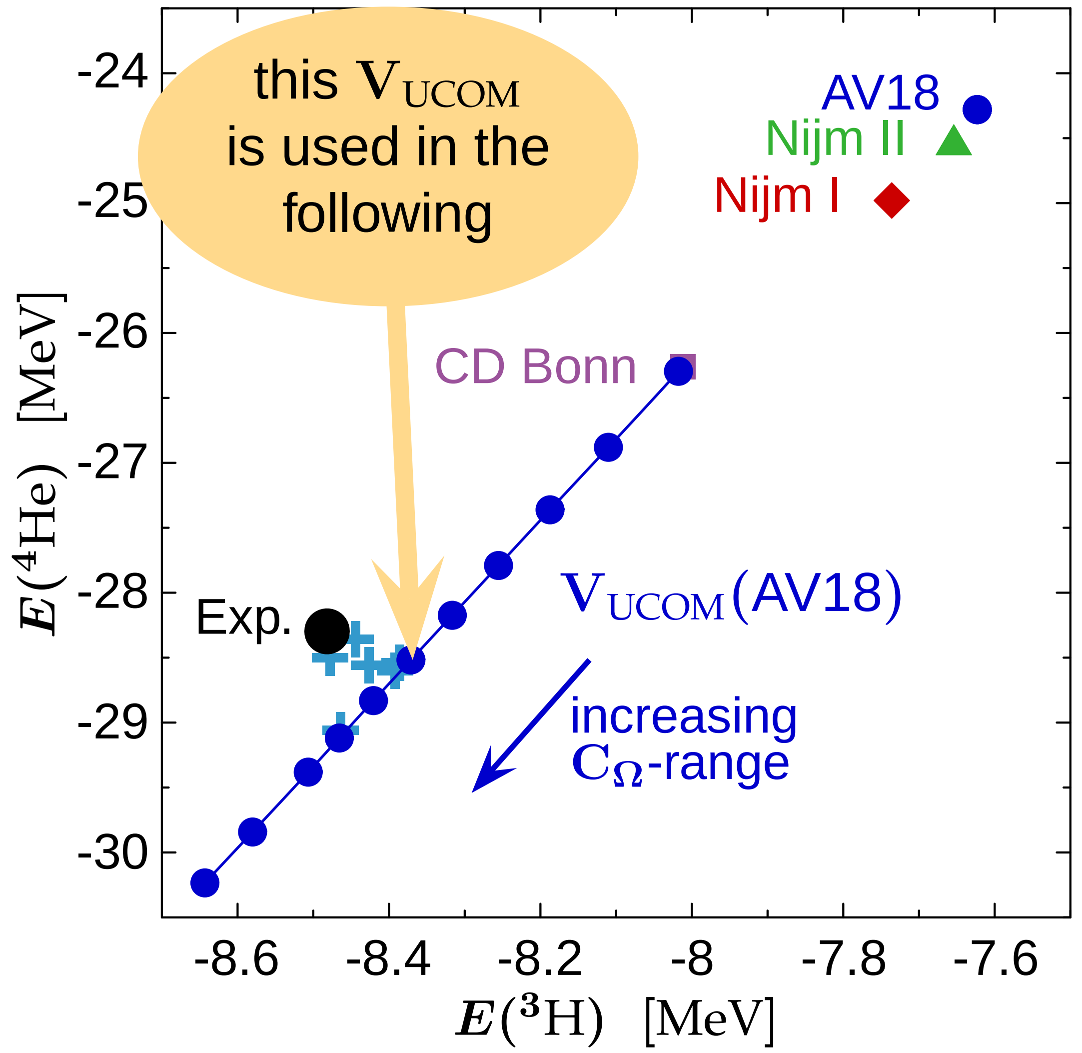


- **Tjon-line**: $E(^4\mathrm{He})$ vs. $E(^3\mathrm{H})$ for phase-shift equivalent NN-interactions
- change of $\mathrm{C}_\Omega$-correlator range results in shift along Tjon-line

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

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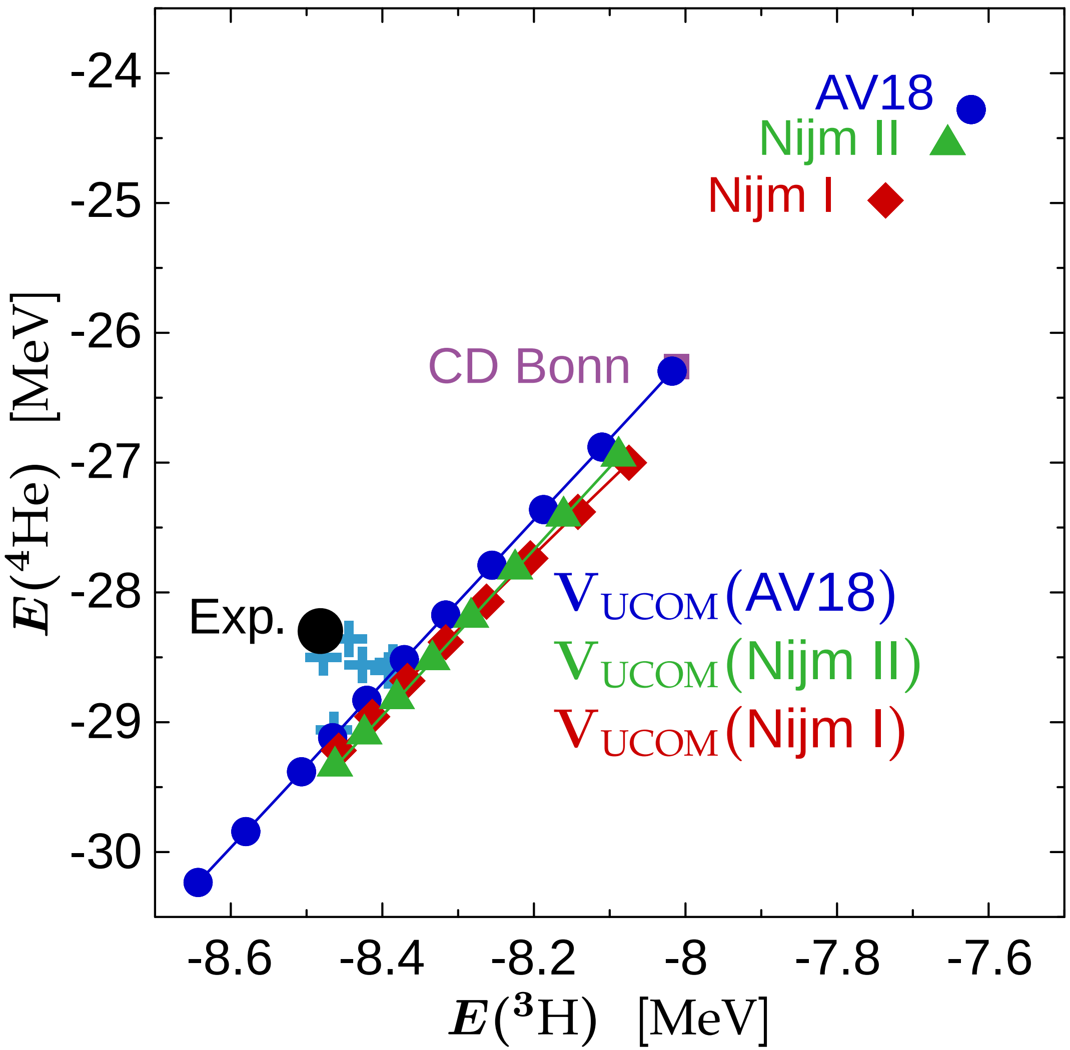


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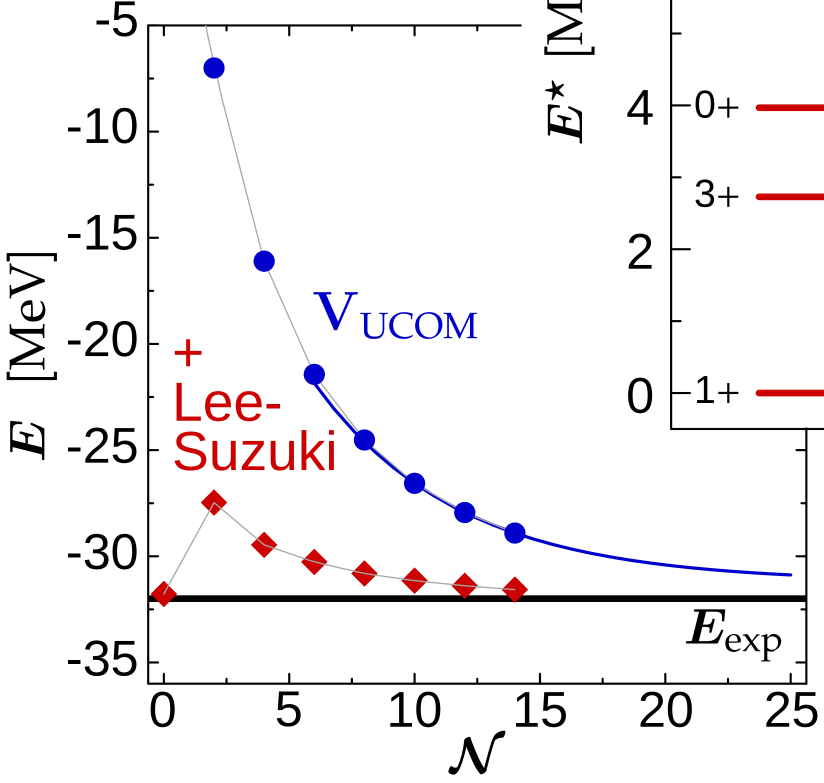
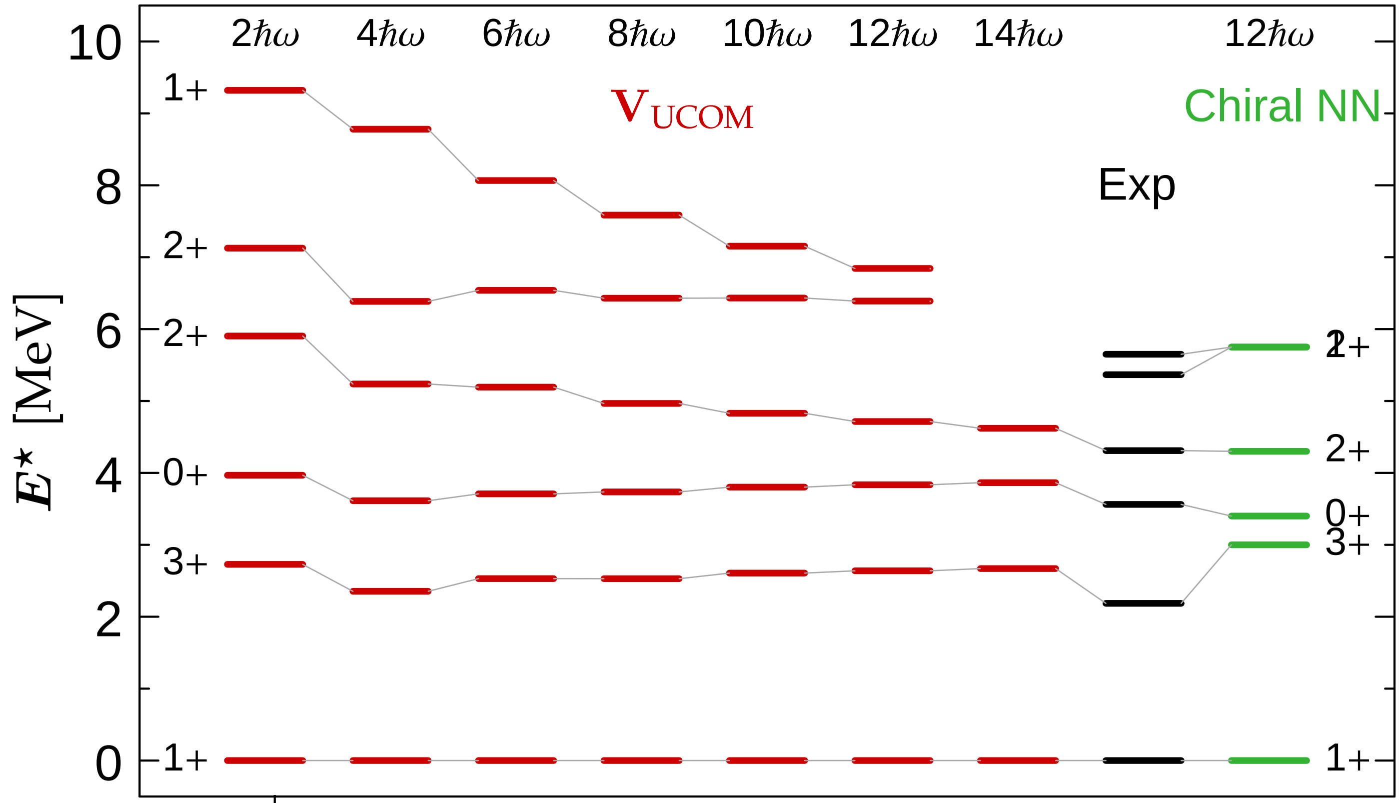
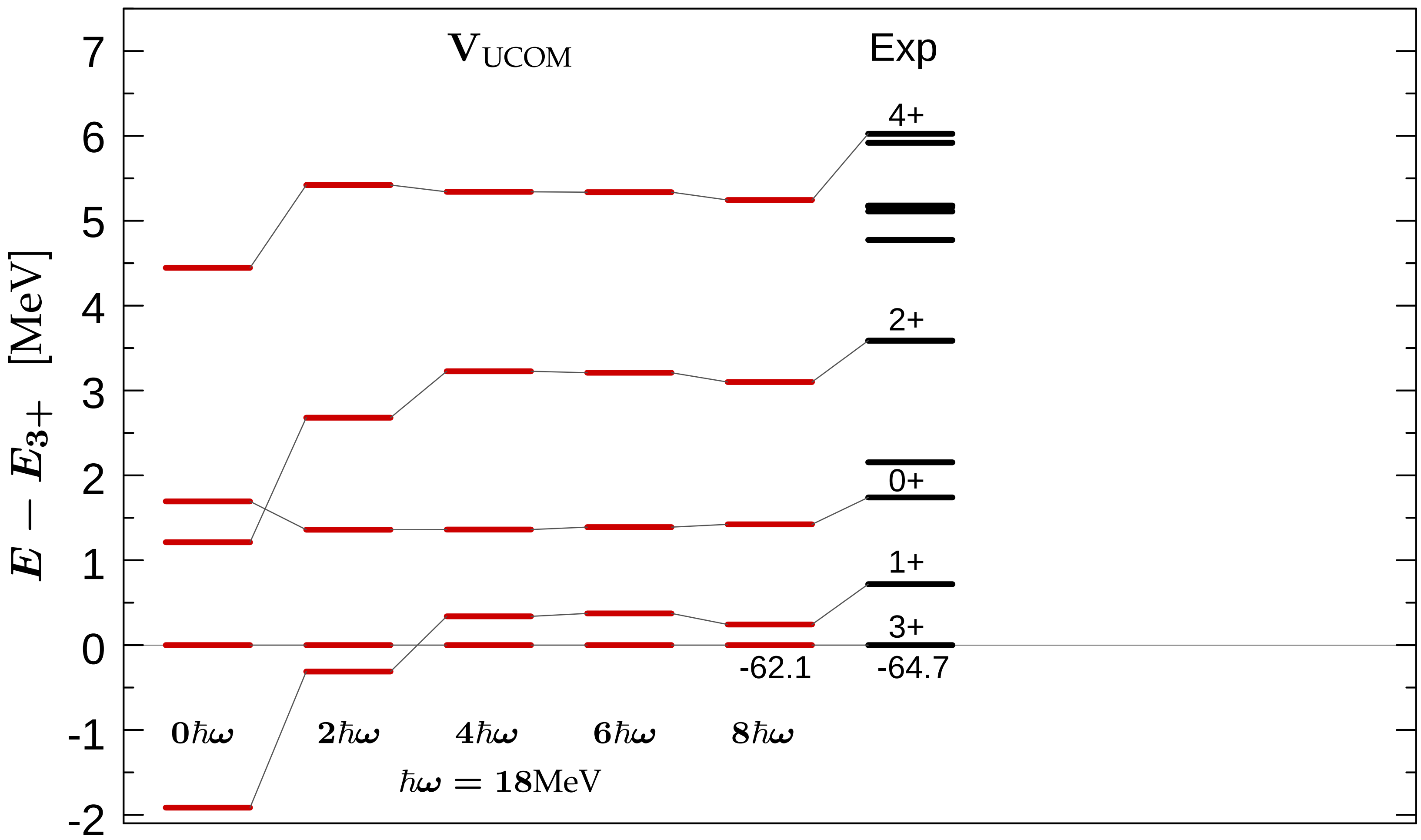
# $^6$Li: NCSM throughout the p-Shell




systematic NCSM studies throughout p-shell with V$_{\text{UCOM}}$ (+ Lee-Suzuki transformation)

# $^{10}$B: Hallmark of a 3N Interaction?



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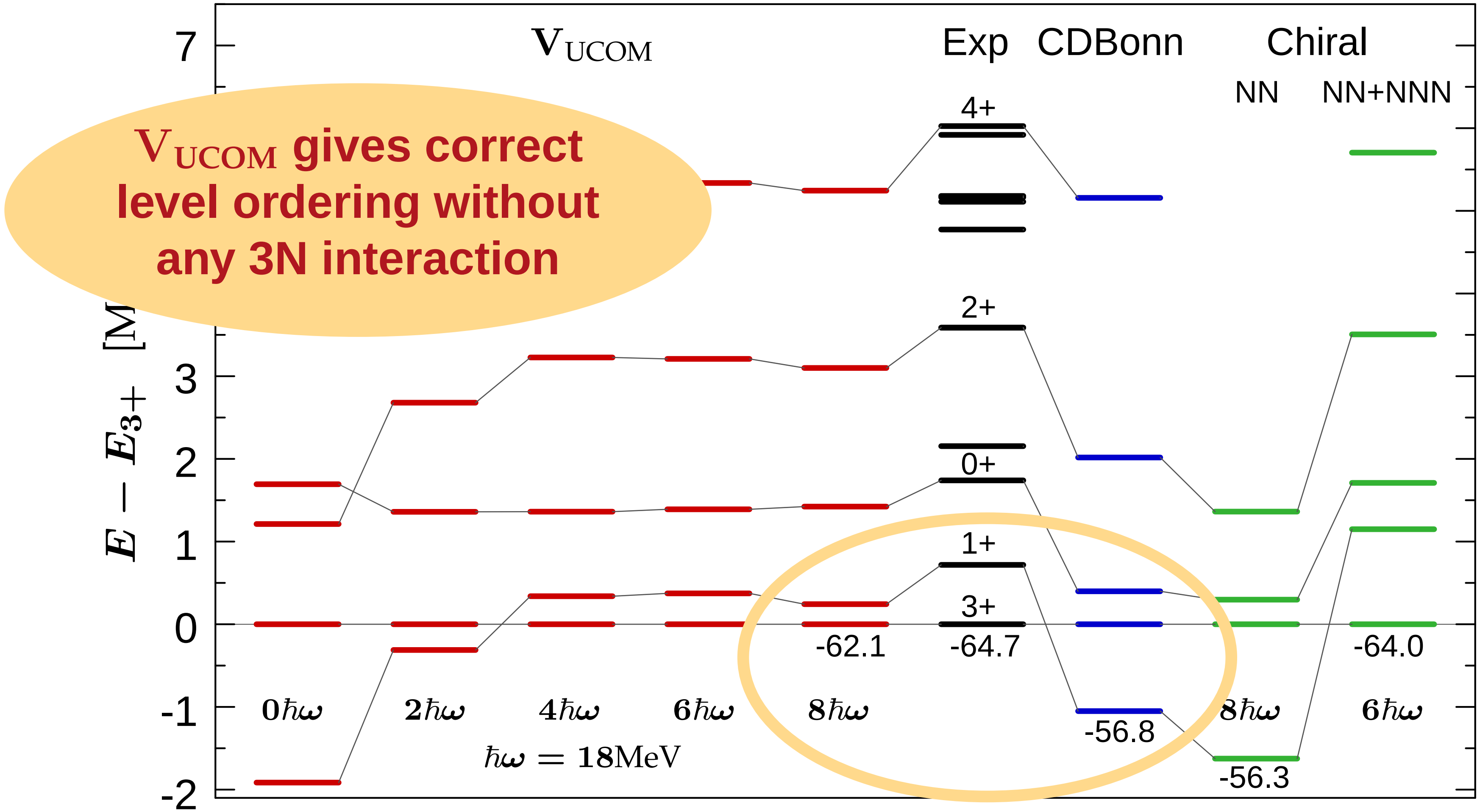


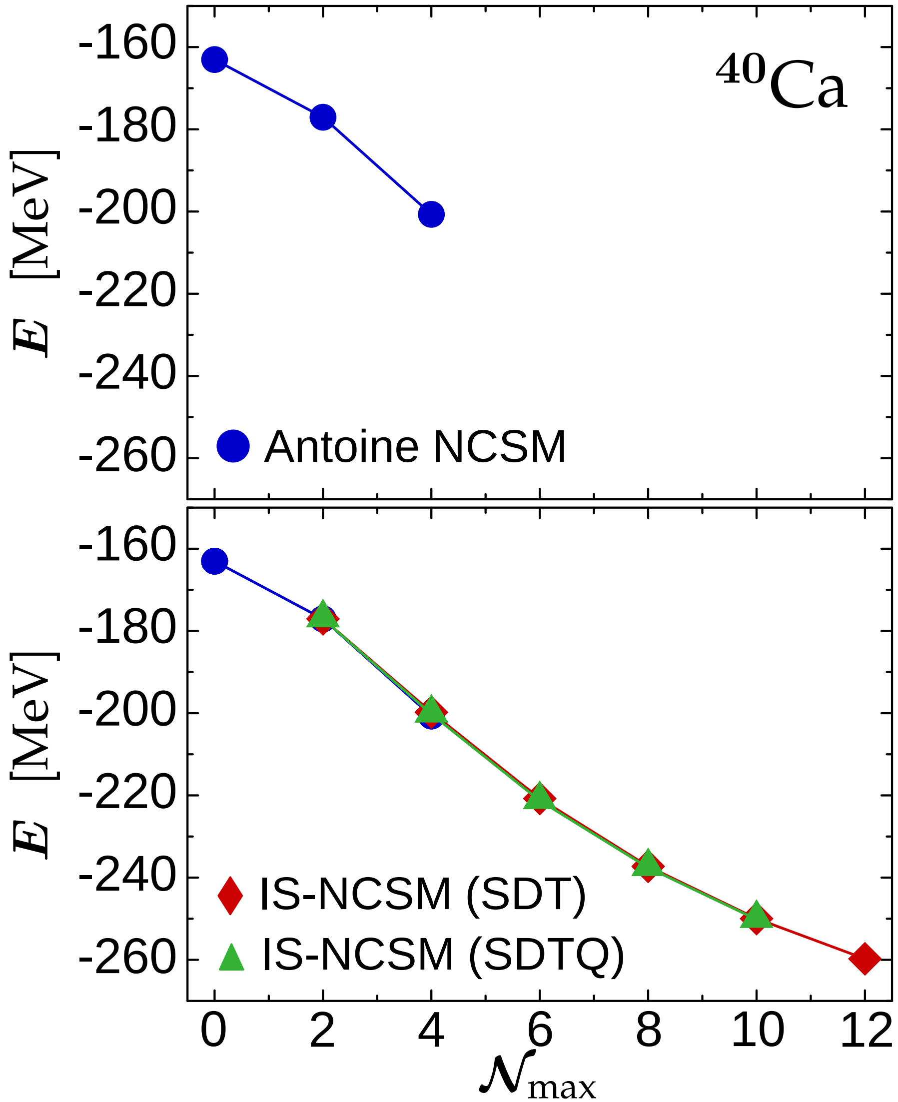
# Outlook: NCSM beyond the p-Shell

## NCSM

- converged calculations essentially restricted to p-shell
- $6\hbar\omega$ calculation for $^{40}\mathrm{Ca}$ presently not feasible ($\sim 10^{10}$ states)

## Importance Sampling NCSM

- diagonalization in space of **impor-tant** many-body configurations
- **a priori importance measure** given by perturbation theory




$\mathbf{V}_{\mathrm{UCOM}},\ \hbar\omega = \mathbf{14}\,\mathrm{MeV}$

# 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, GFRPA,...
  - Fermionic Molecular Dynamics

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

# Epilogue

- **thanks to my group & my collaborators**
  - T. Böhlen, P. Hedfeld, H. Hergert, M. Hild, N. Paar,
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    NSCL, Michigan State University
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