From Realistic Interactions to Shell Model, Hartree-Fock and RPA:

Correlations in the Nuclear Many-Body Problem

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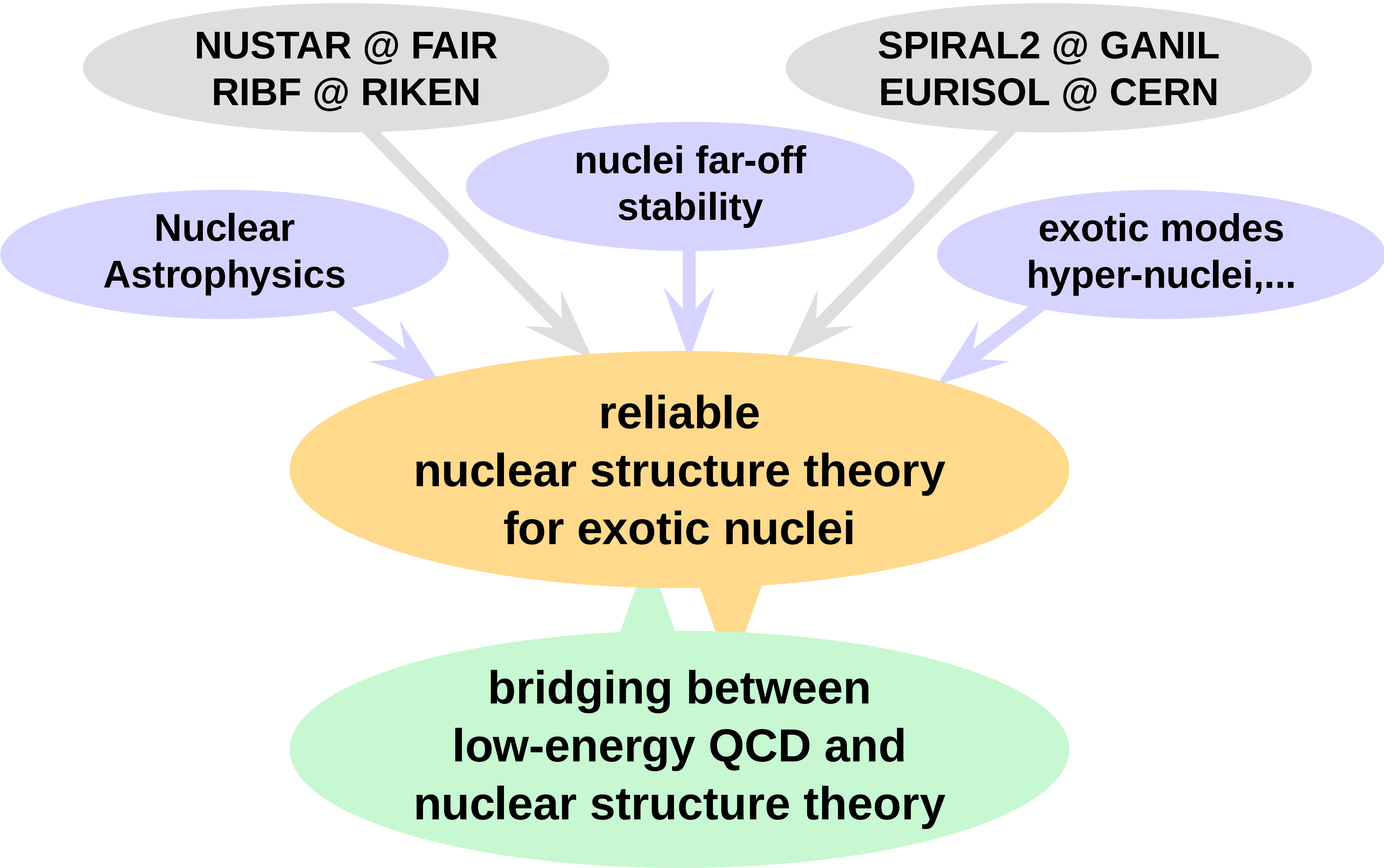
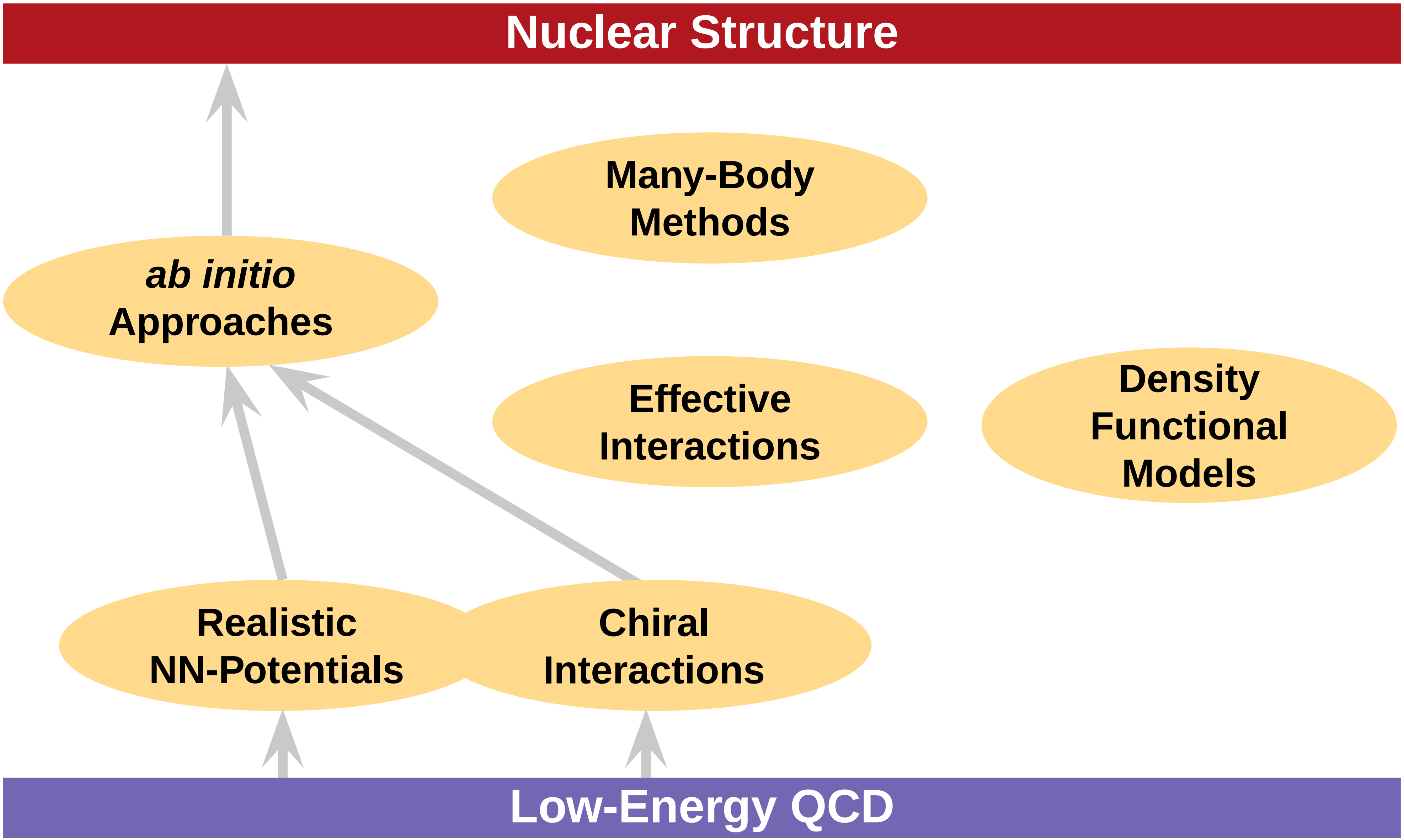
Overview

- Motivation
- Modern Effective Interactions
  - Correlations & Unitary Correlation Operator Method
- Applications
  - No Core Shell Model
  - Hartree-Fock & Beyond
  - Random Phase Approximation & Beyond

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 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

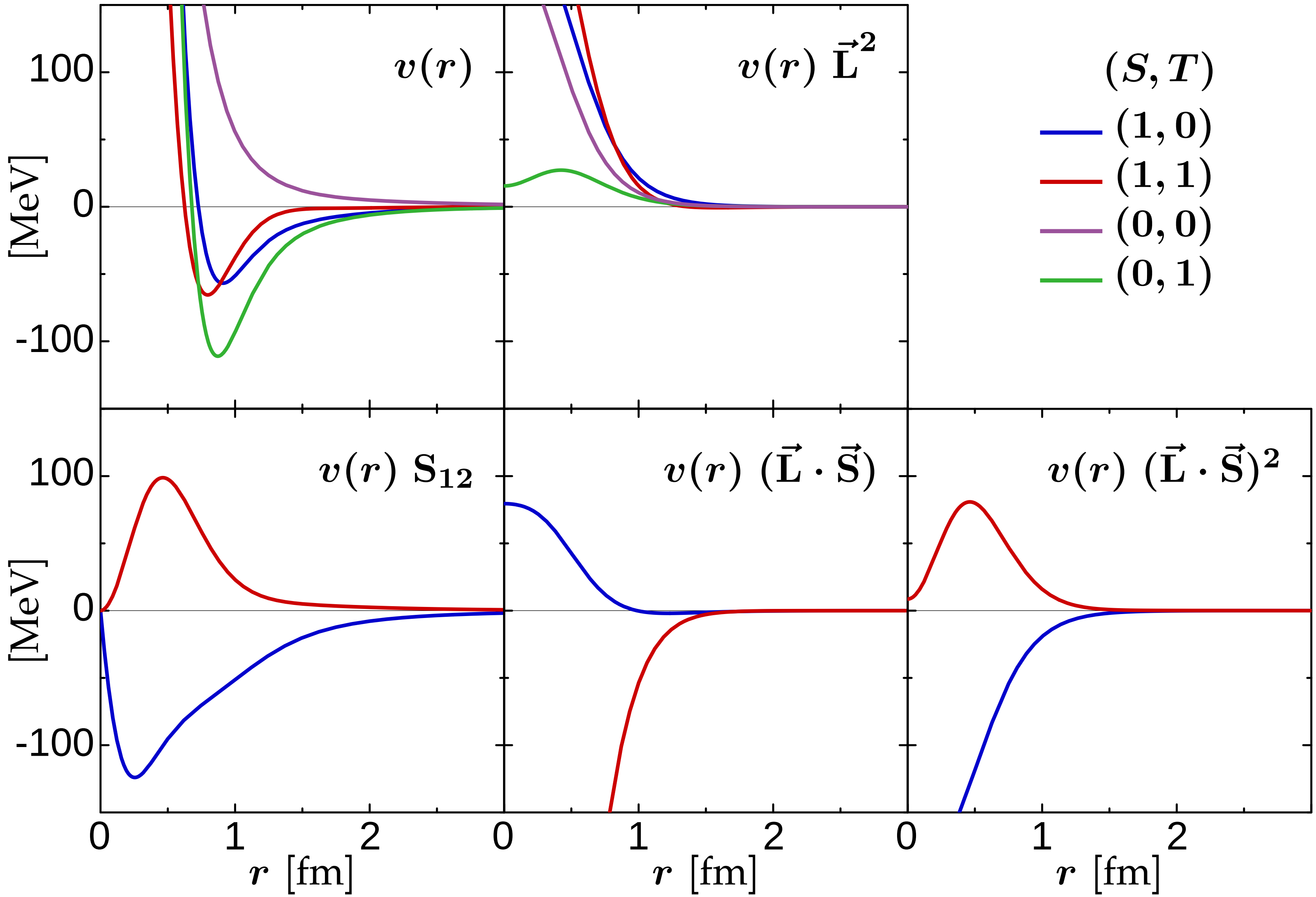
Nijmegen I/II

Chiral N3LO

Argonne V18 +
Illinois 2

Chiral N3LO +
N2LO

Argonne V18 Potential



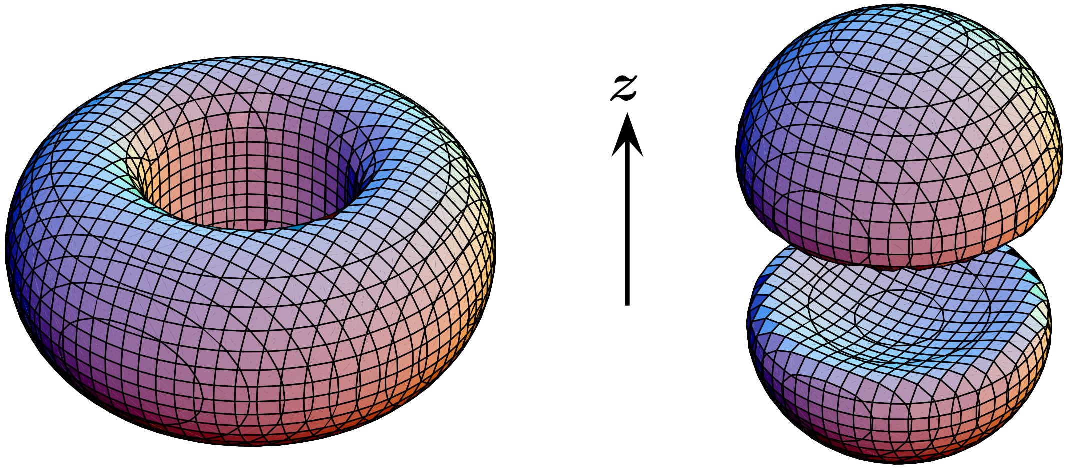
Deuteron: Manifestation of Correlations

$M_S = 0$

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

$M_S = \pm 1$

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



- spin-projected two-body density $\rho^{(2)}_{1,M_S}(\vec{r})$
- **exact deuteron solution** for Argonne V18 potential

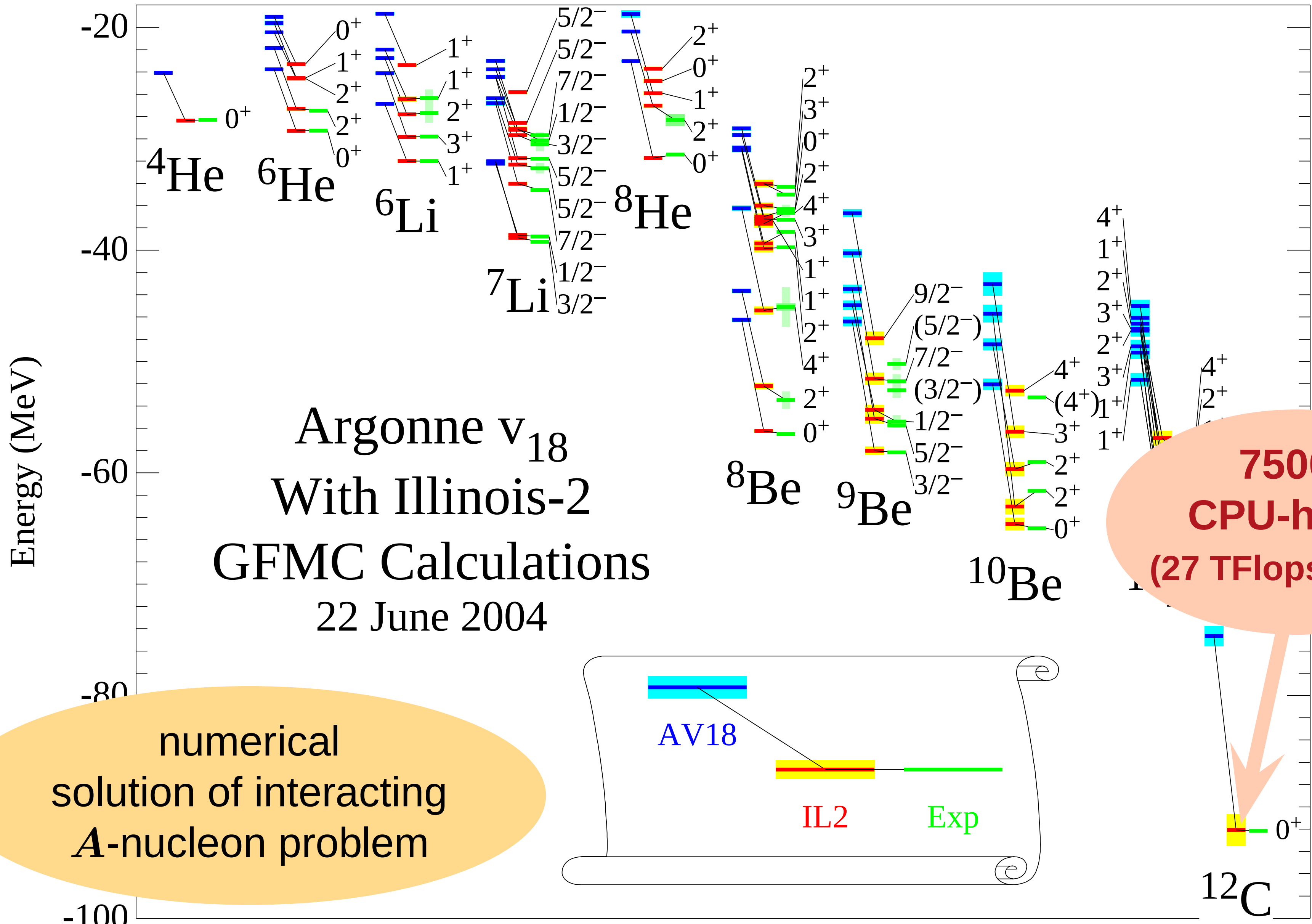
two-body density fully suppressed at small particle distances $|\vec{r}|$

central correlations

angular distribution depends strongly on relative spin orientation

tensor correlations

Ab initio Methods: GFMC



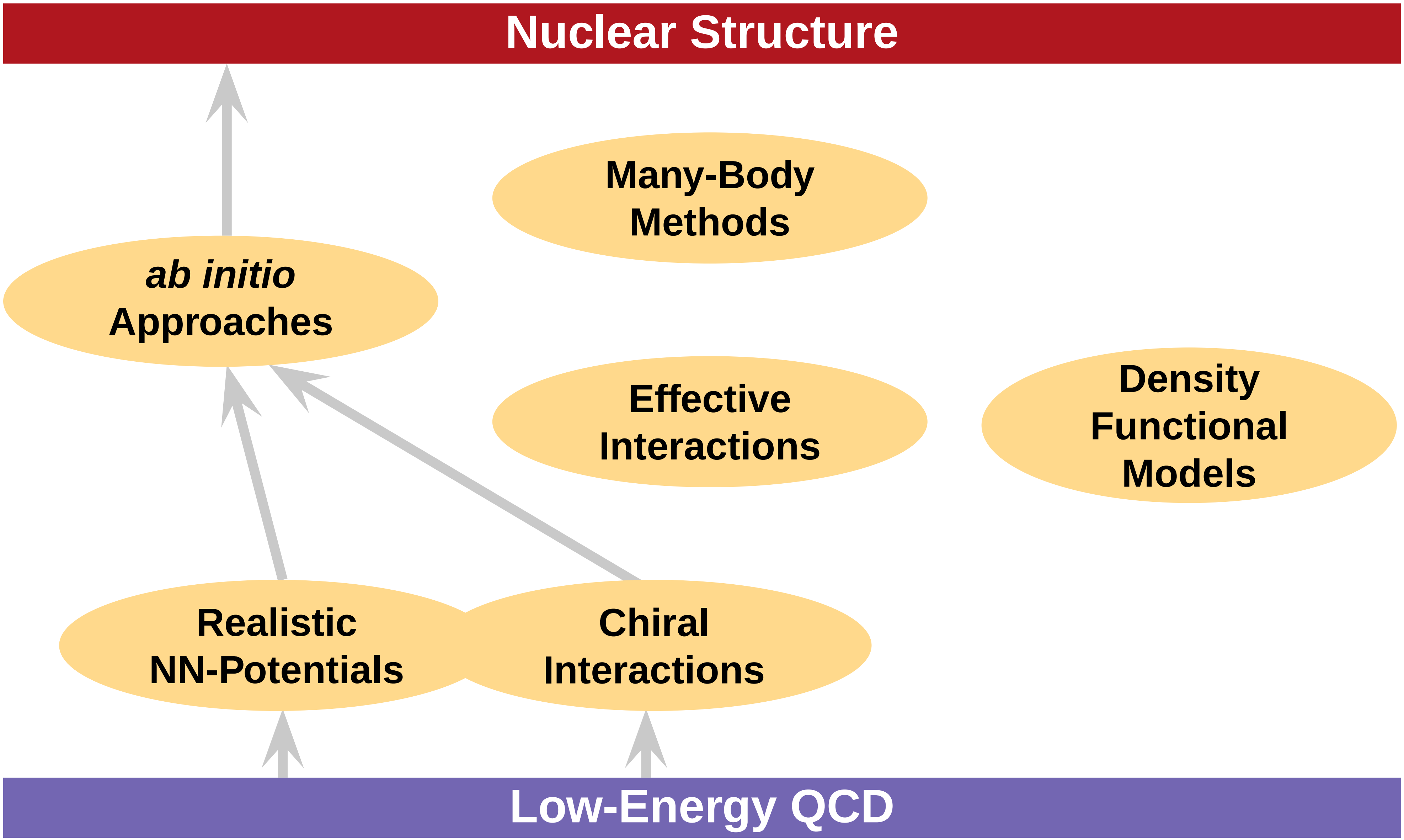
numerical solution of interacting *A*-nucleon problem

75000 CPU-hours (27 TFlops-hours)

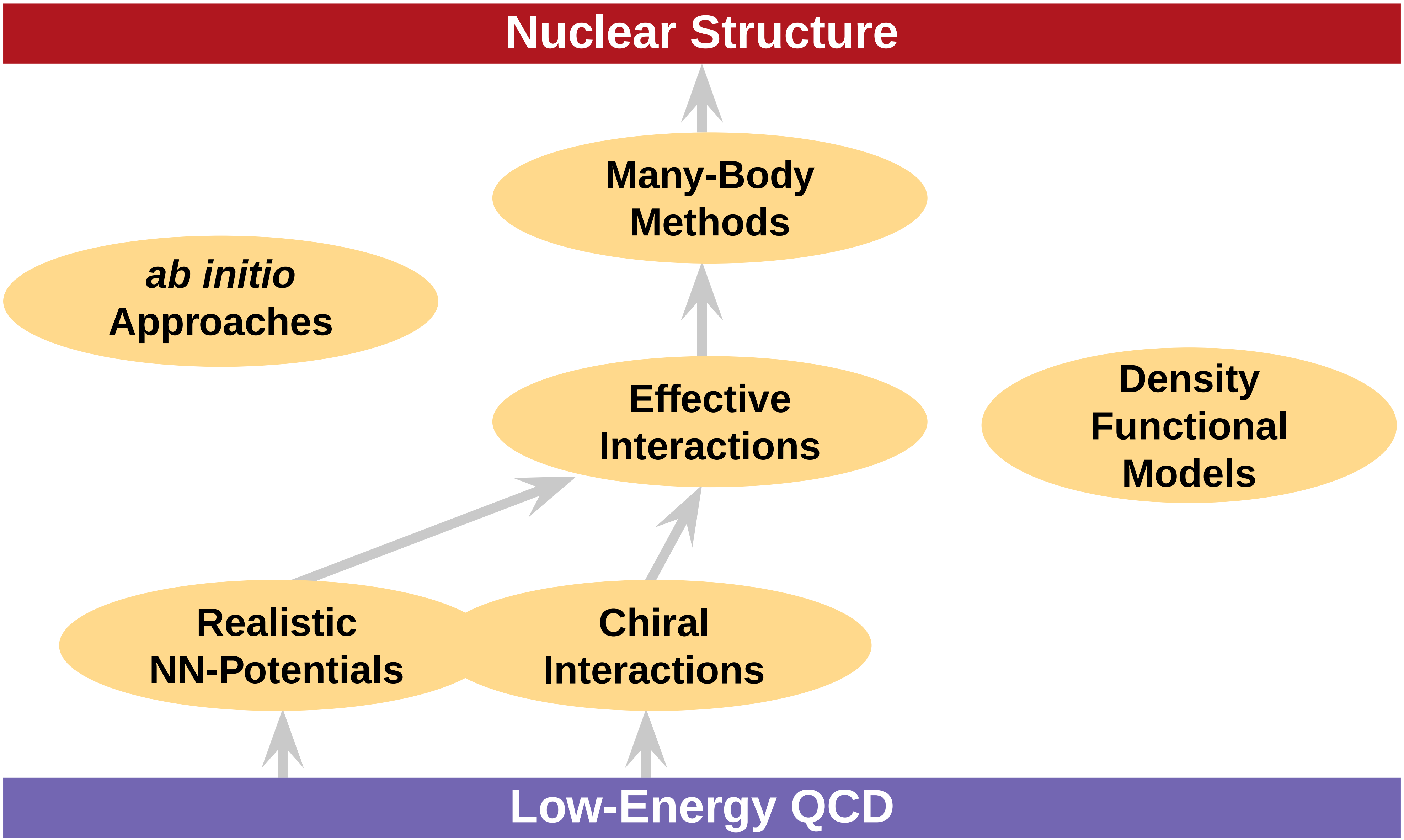
[S. Pieper, private comm.]

^{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
- 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

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

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

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

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

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

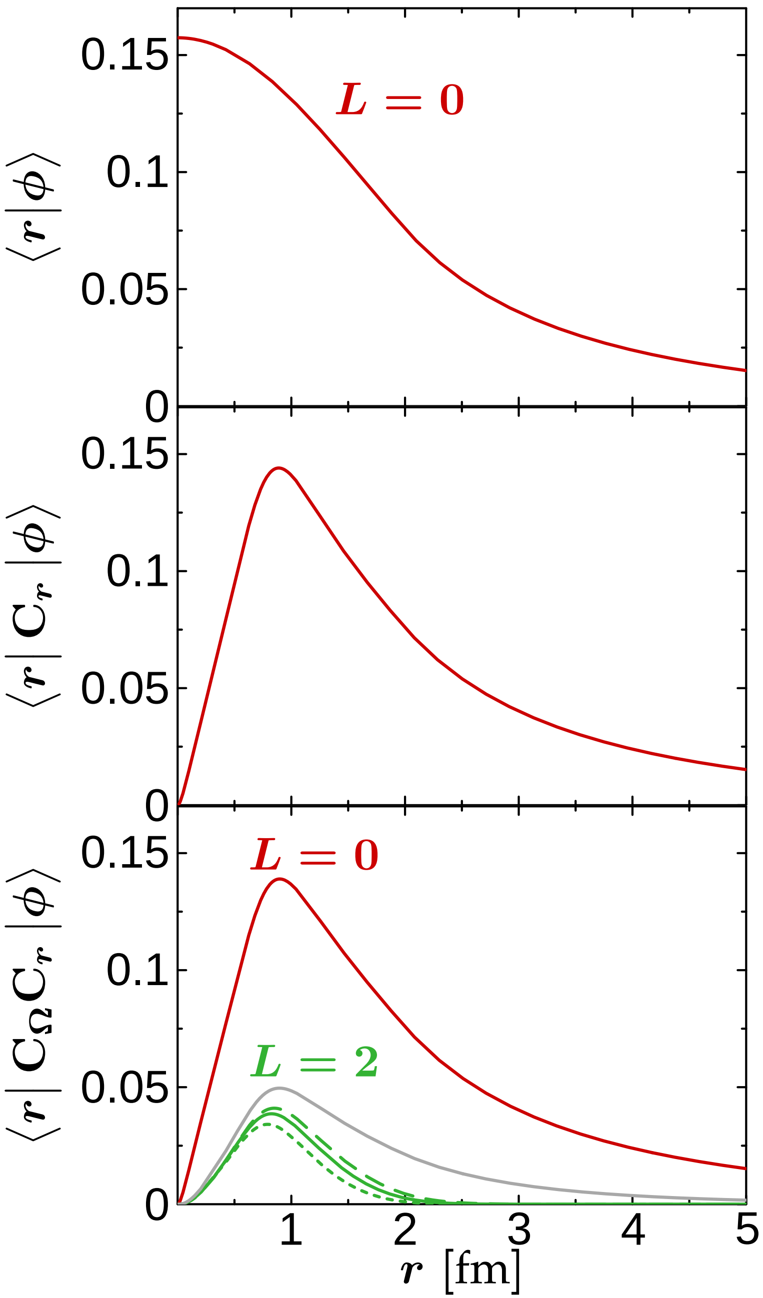
- angular shift depending on the orientation of spin and relative coordinate of a nucleon pair

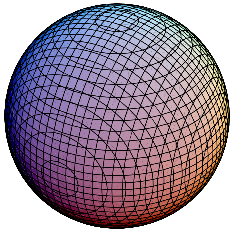
$$\mathrm{g}_\Omega = \frac{3}{2}\vartheta(\mathrm{r})\big[(\vec{\sigma}_1 \cdot \vec{\mathrm{q}}_\Omega)(\vec{\sigma}_2 \cdot \vec{\mathrm{r}}) + (\vec{\mathrm{r}} \leftrightarrow \vec{\mathrm{q}}_\Omega)\big]$$

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

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

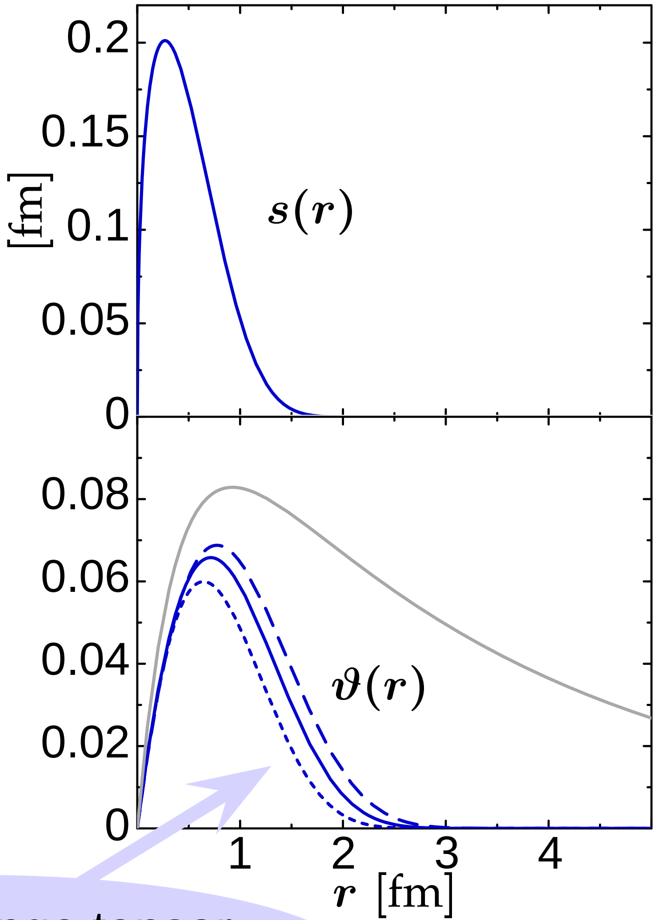
Correlated States: The Deuteron

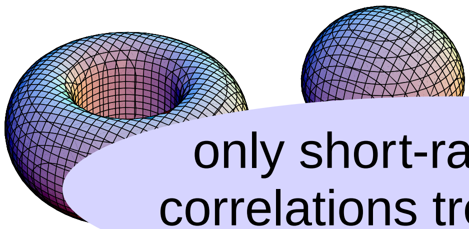




central correlations

tensor correlations





only short-range tensor correlations treated by C_Ω

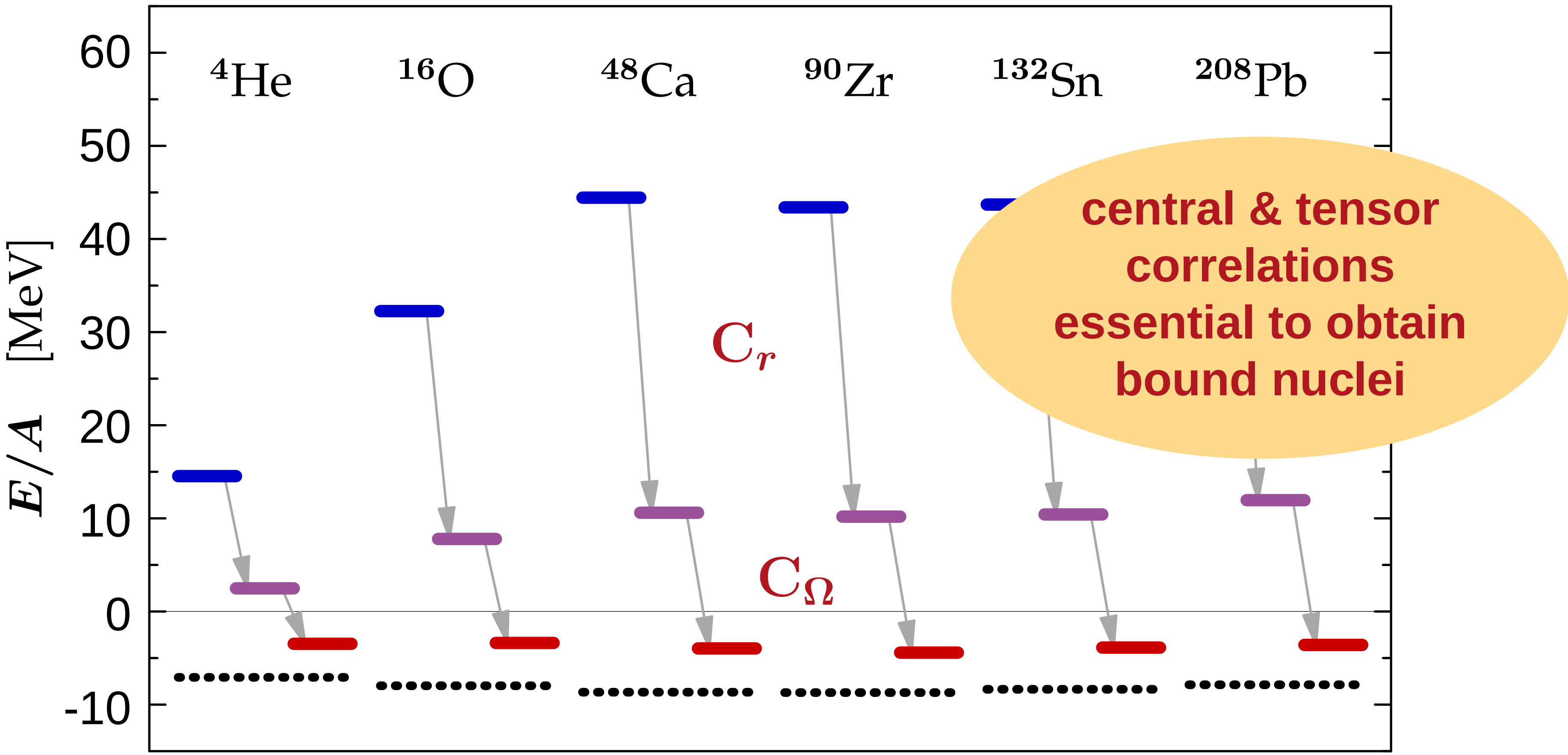
Correlated Interaction: V_{UCOM}

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

- **closed operator expression** for the correlated interaction $\mathrm{V}_{\mathrm{UCOM}}$ in two-body approximation
- correlated interaction and original NN-potential are **phase shift equivalent** by construction
- unitary transformation results in a **pre-diagonalization** of Hamiltonian (similar to renormalization group methods)
- operators of **all observables** (densities, transitions) have to be and can be **transformed consistently**

Simplistic "Shell-Model" Calculation

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



Application I

No-Core Shell Model

in collaboration with

Petr Navrátil (LLNL)

Reminder: No-Core Shell Model

- many-body state is **expanded in Slater determinants** $|\mathrm{SD}_i\rangle$ composed of harmonic oscillator single-particle states

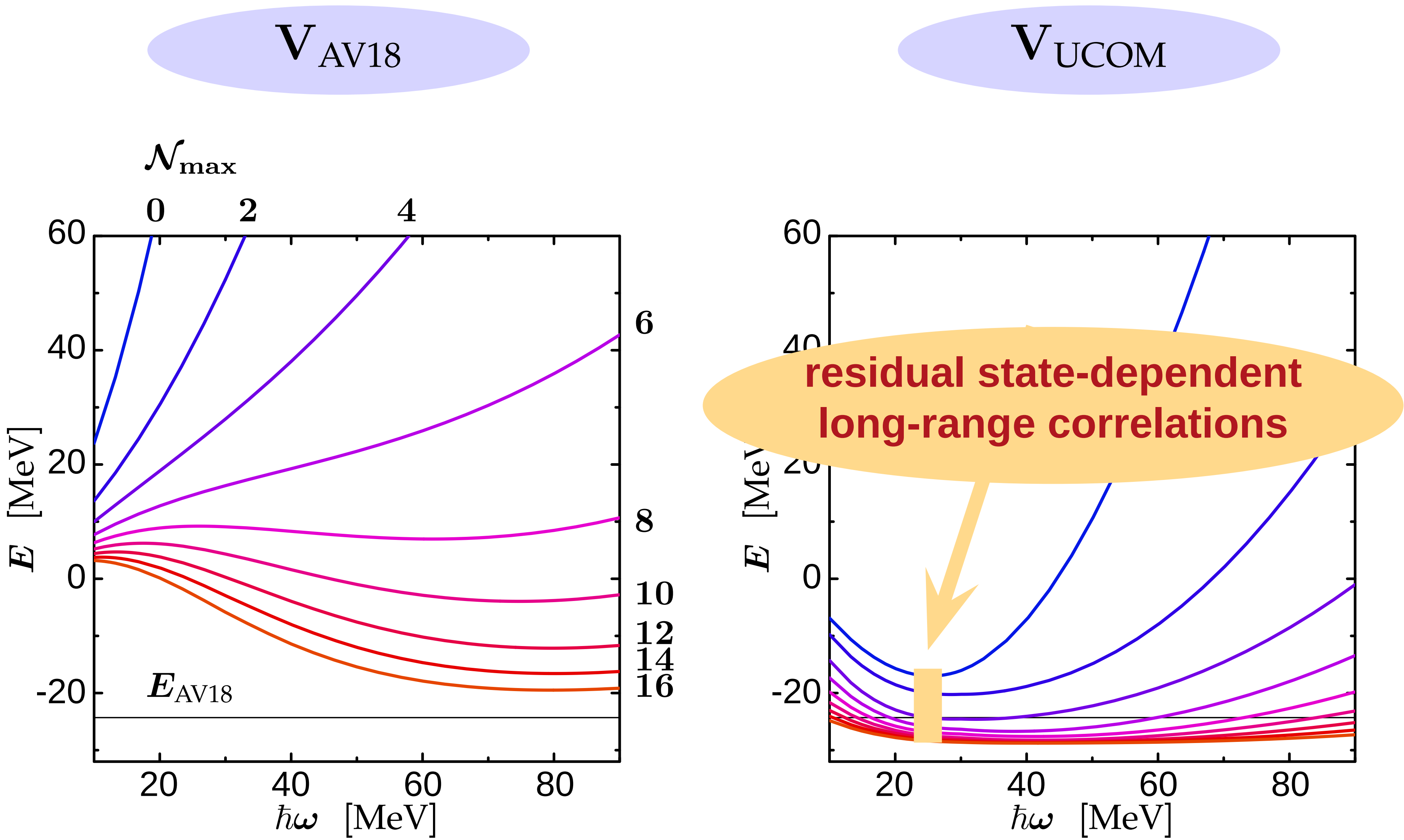
$$|\Psi\rangle = \sum_i C_i \, |\mathrm{SD}_i\rangle$$

- $\mathcal{N}_{\max}\hbar\omega$ **model space**: truncate basis of Slater determinants with respect to number of oscillator quanta (unperturbed excitation energy)

with increasing model space size more and more **correlations can be described** by the shell model states

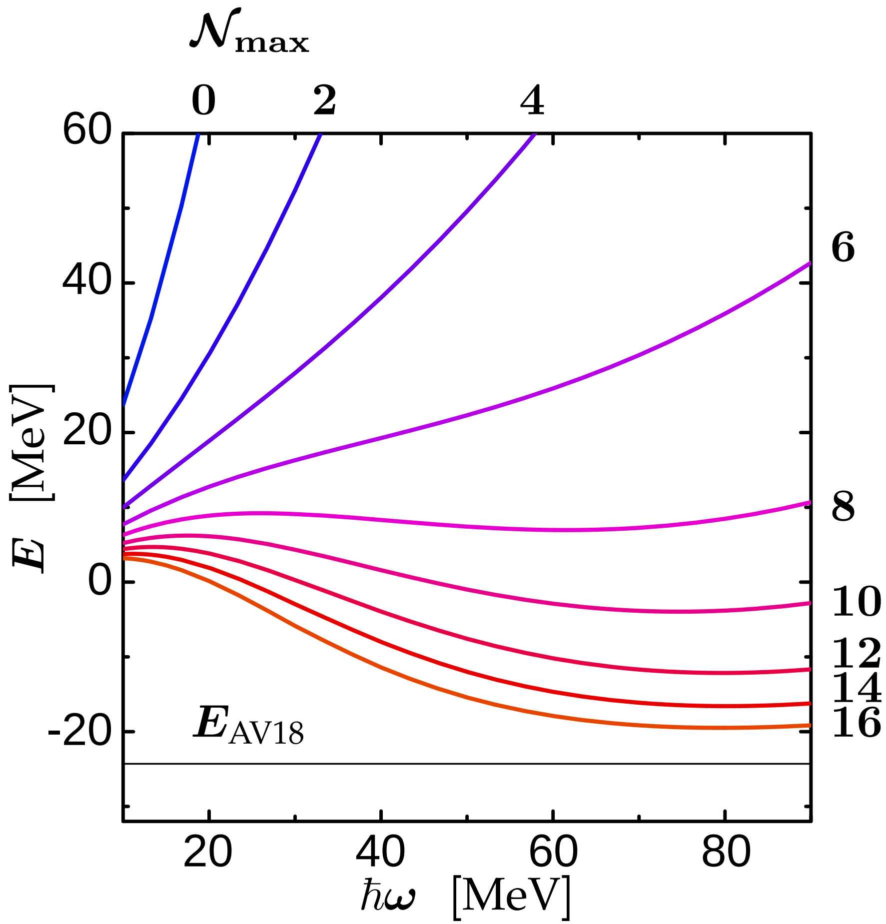
facilitates systematic study of short- and long-range correlations

^{4}He: Convergence

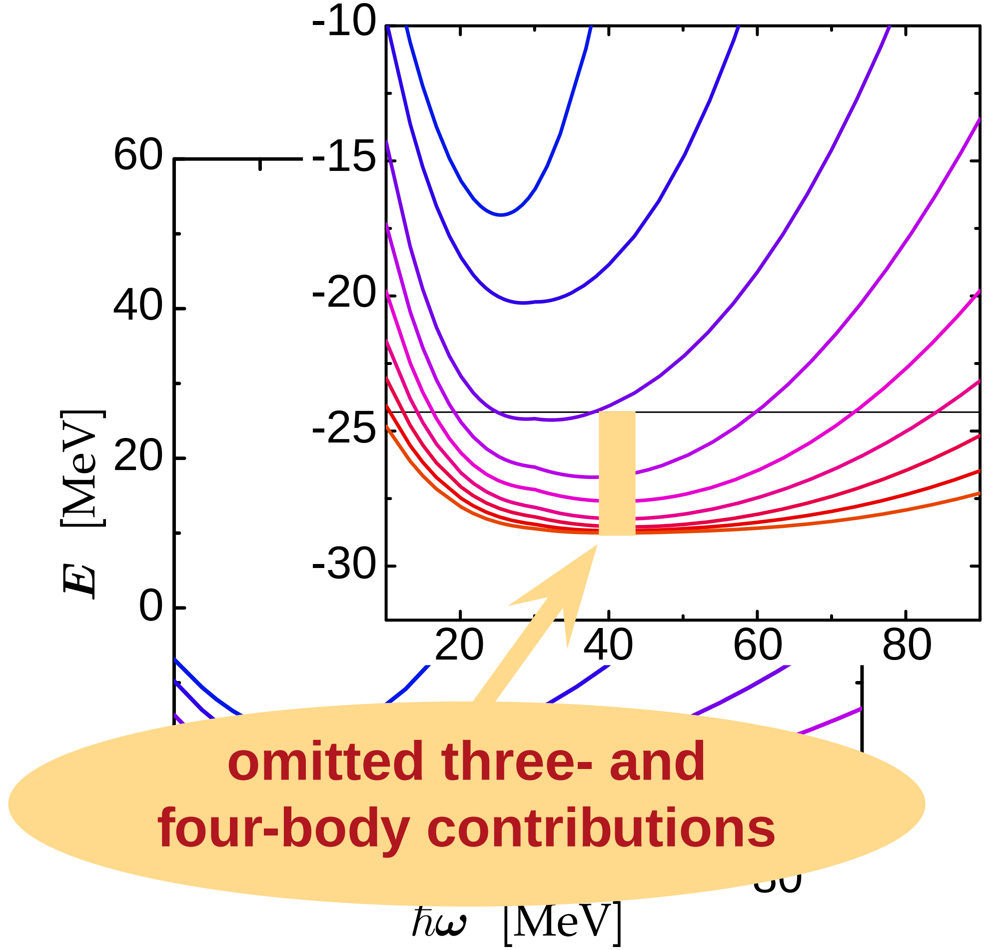


^{4}He: Convergence

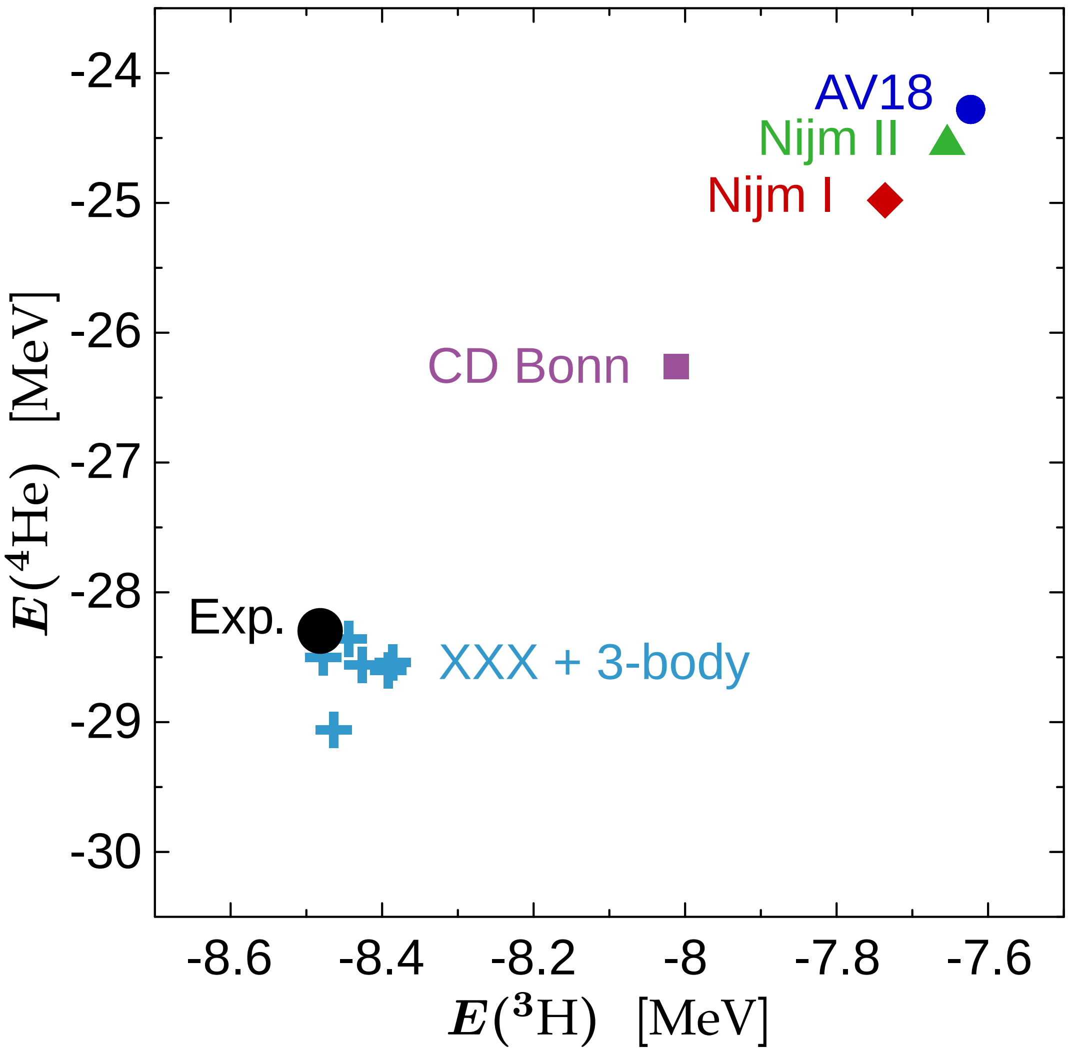
V_{AV18}



V_{UCOM}

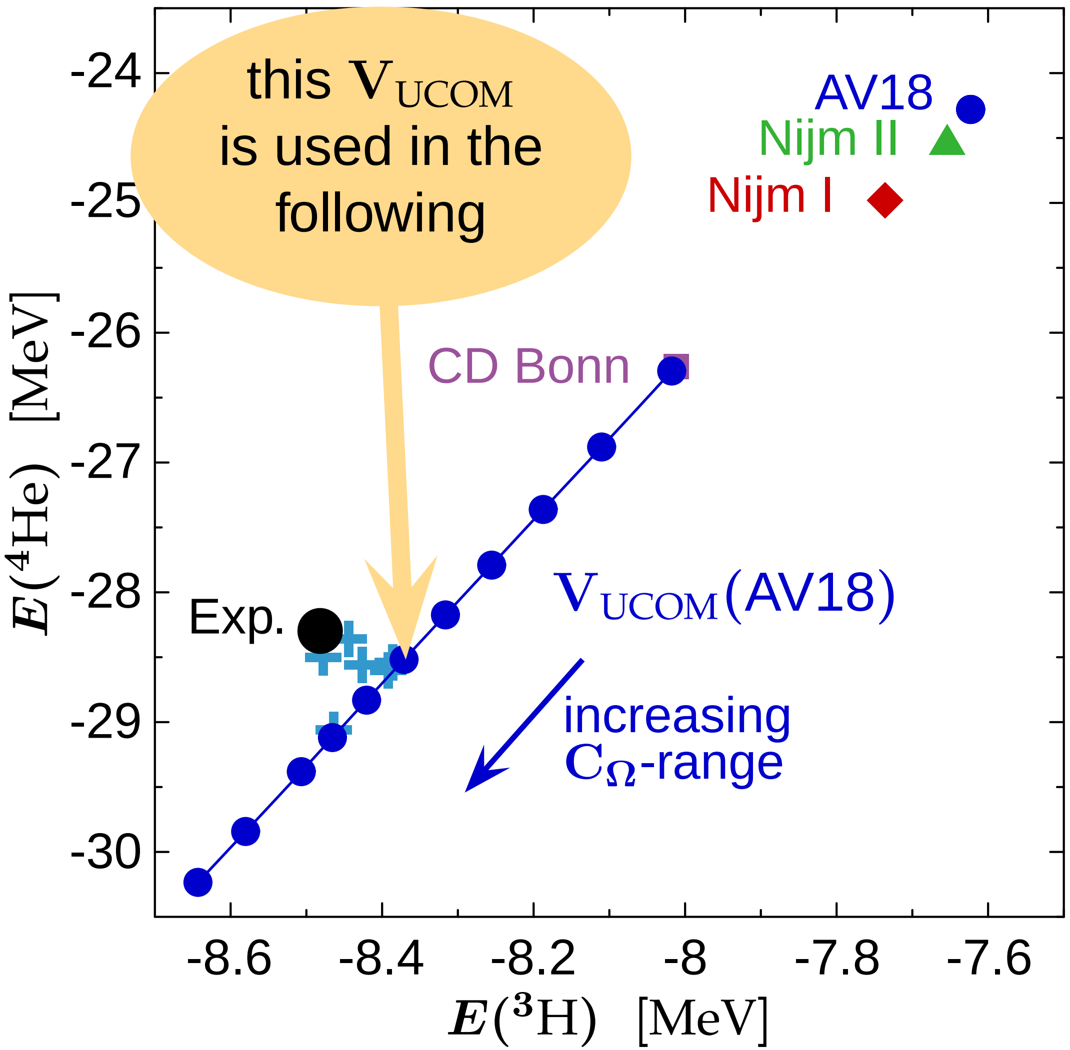


Tjon-Line and Correlator Range



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

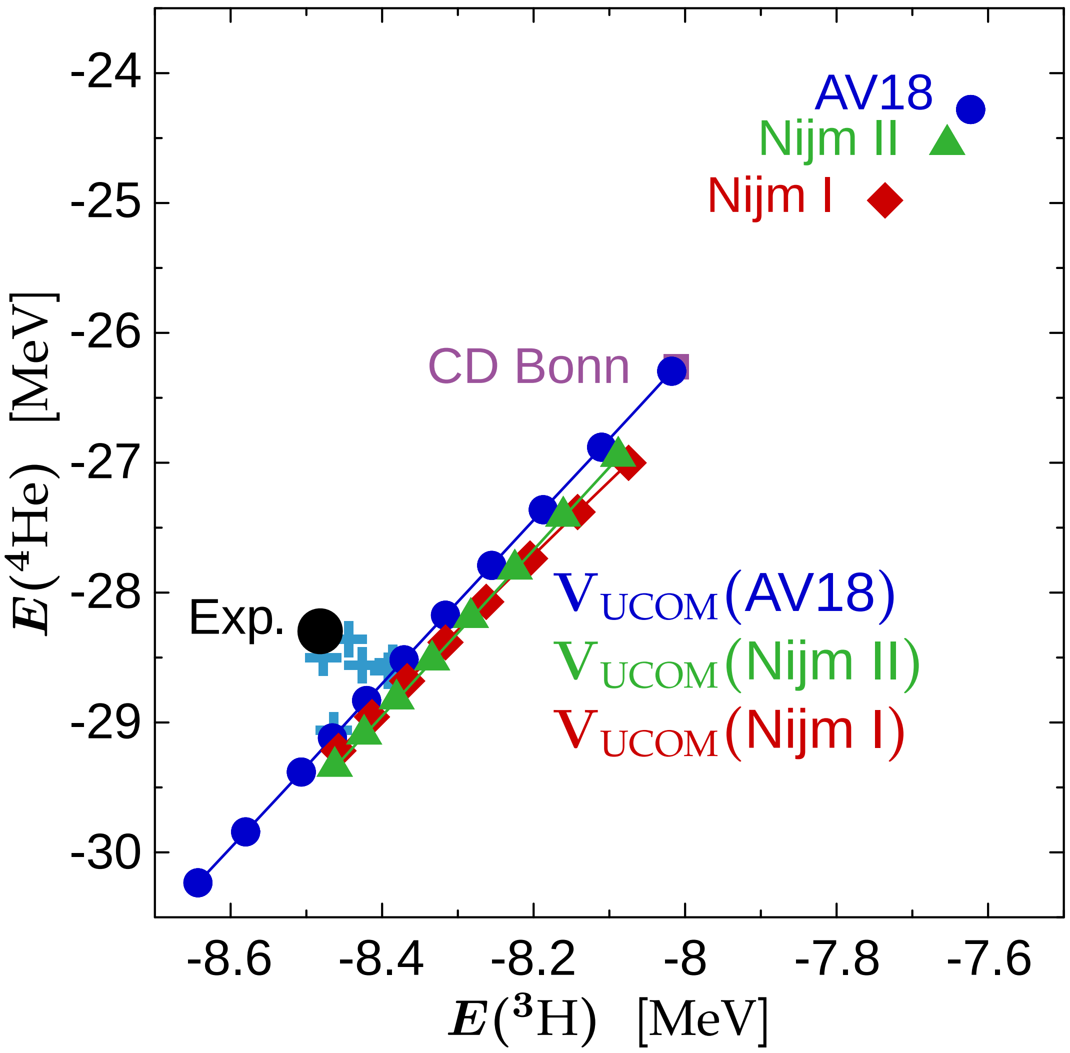
Tjon-Line and Correlator Range



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

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

Tjon-Line and Correlator Range



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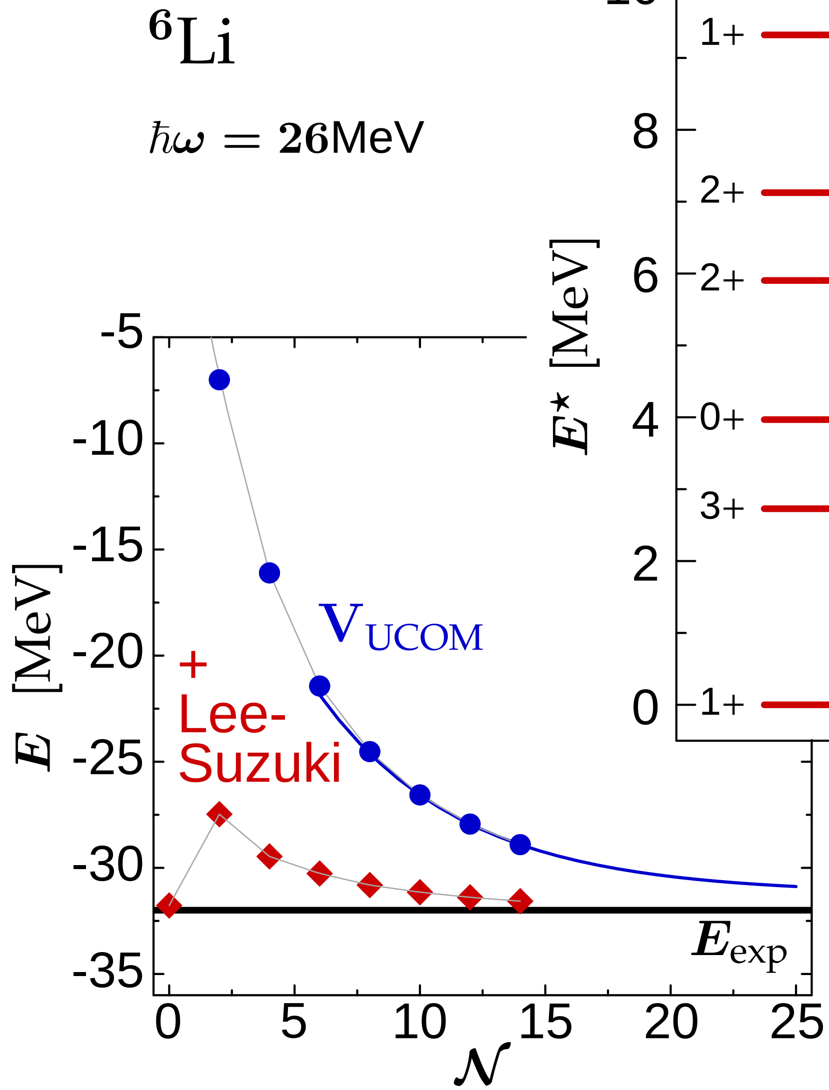
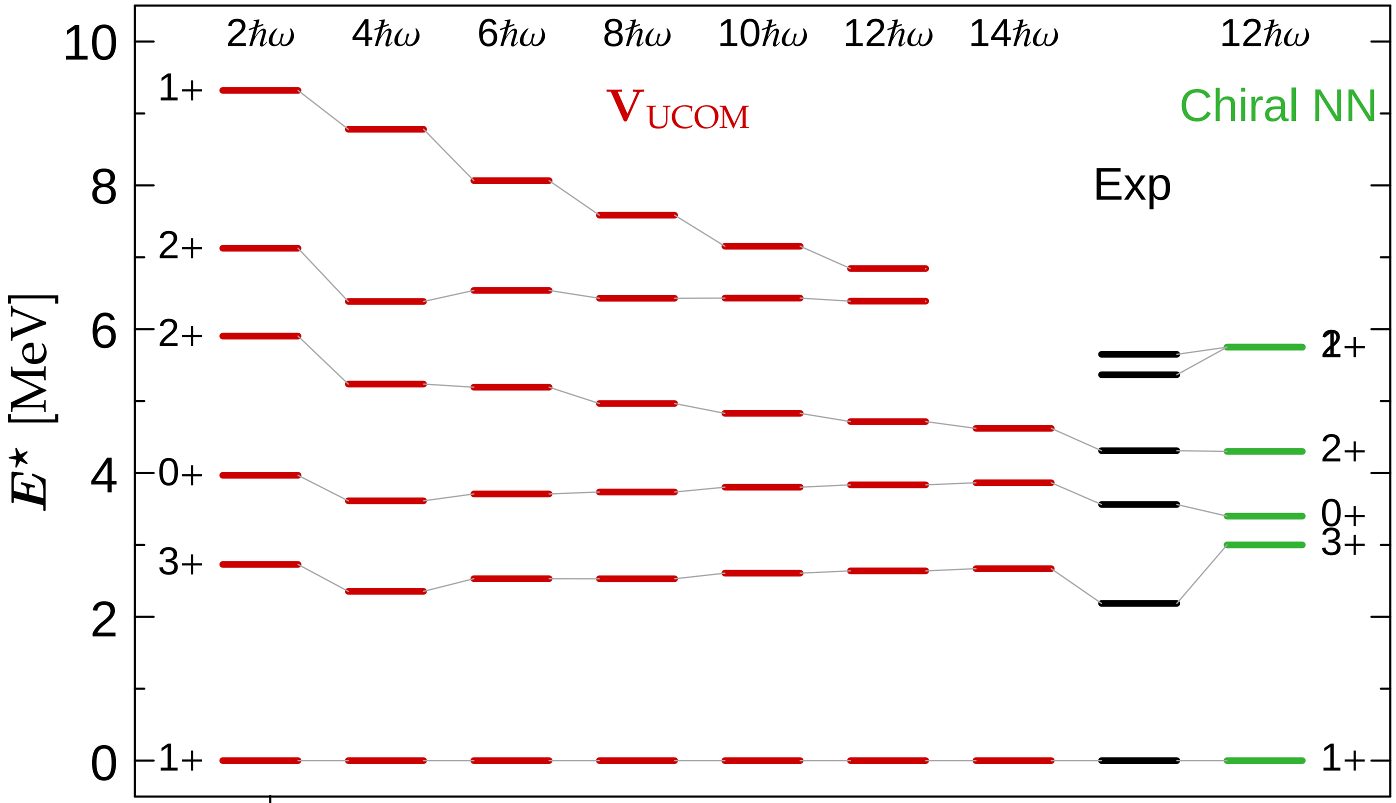
minimize net three-body force by choosing correlator with energies close to experimental value

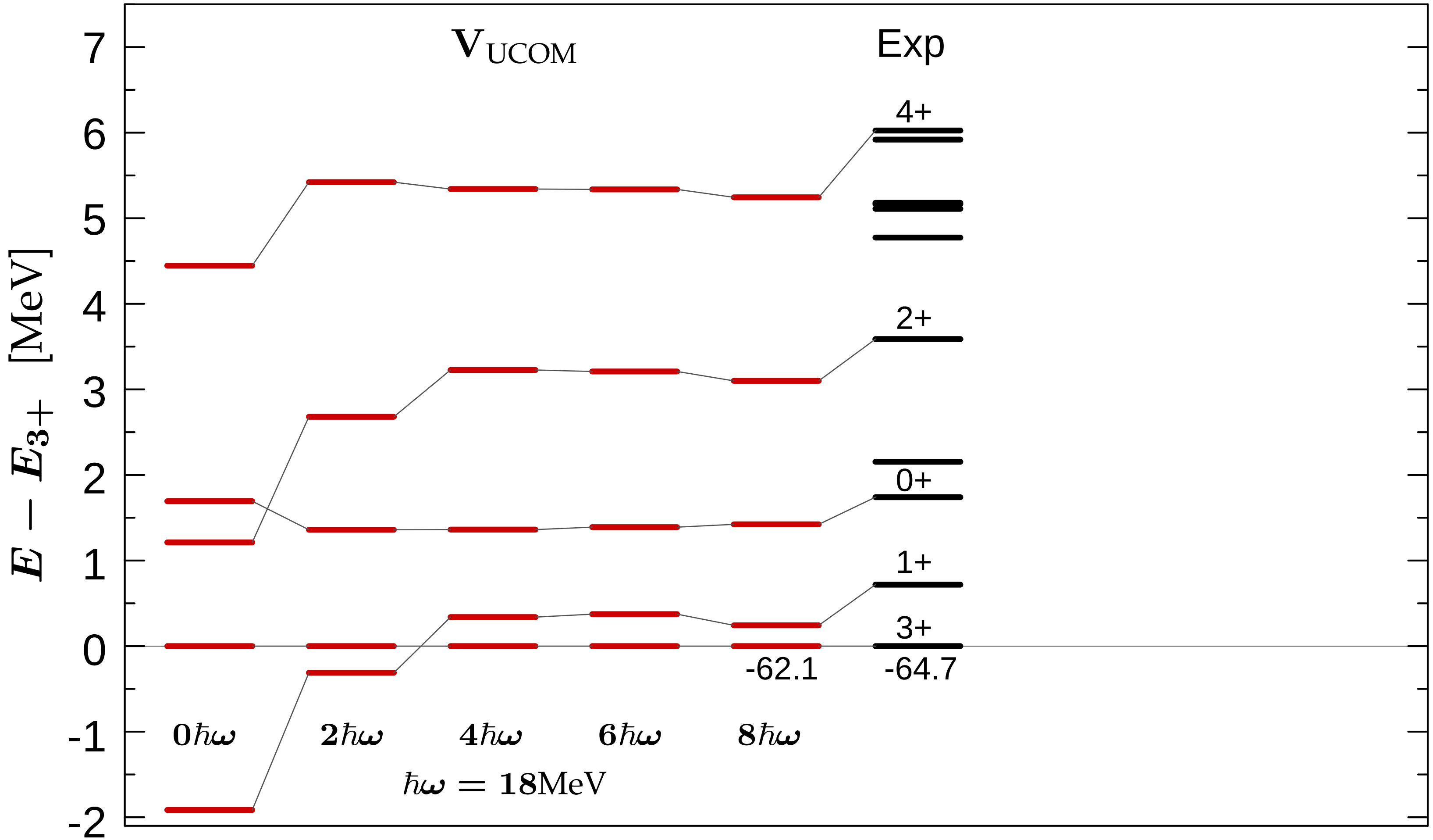
^{6}Li: NCSM throughout the p-Shell



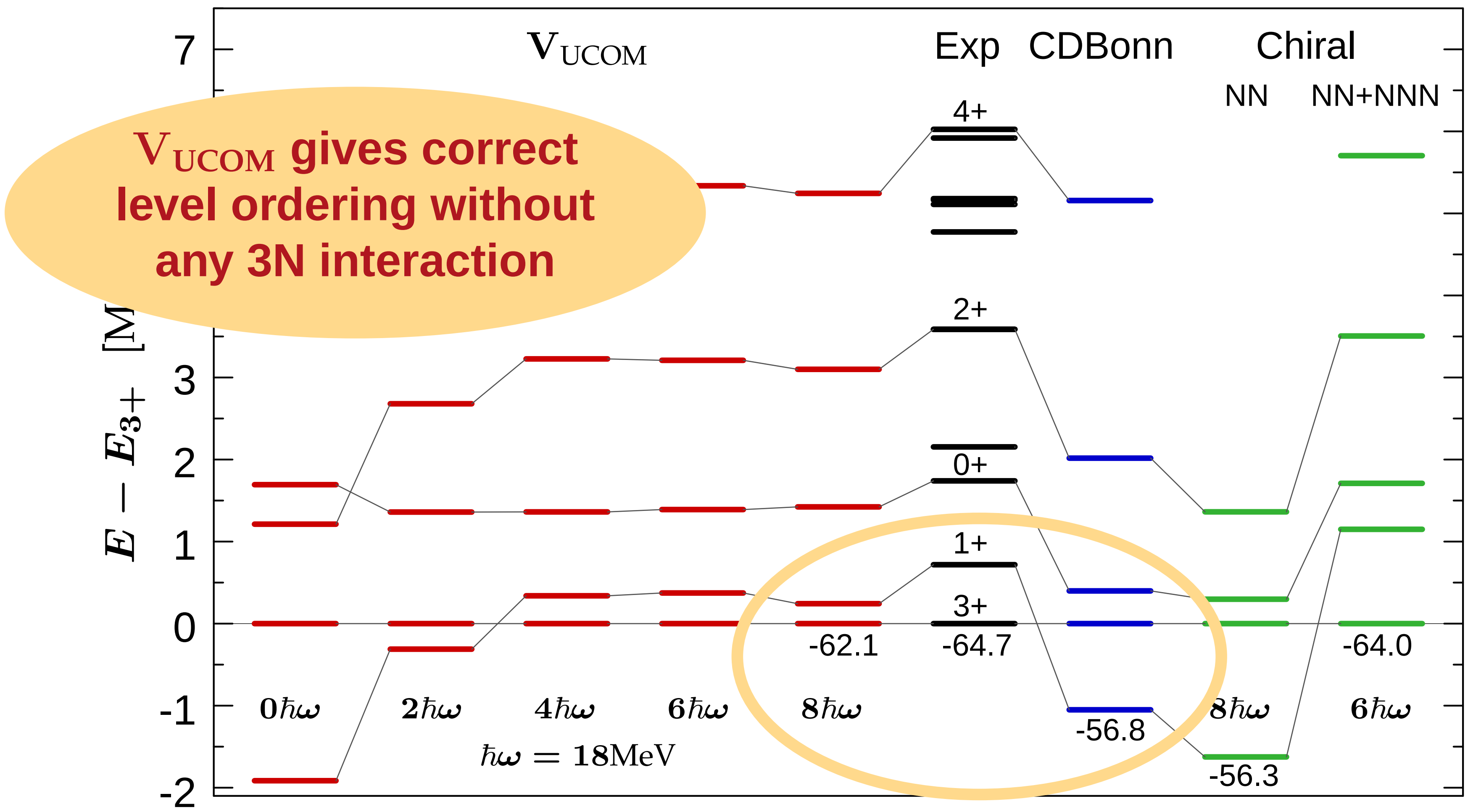


systematic NCSM studies throughout p-shell with $\mathbf{V}_{\text{UCOM}}$ (+ Lee-Suzuki transformation)

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



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



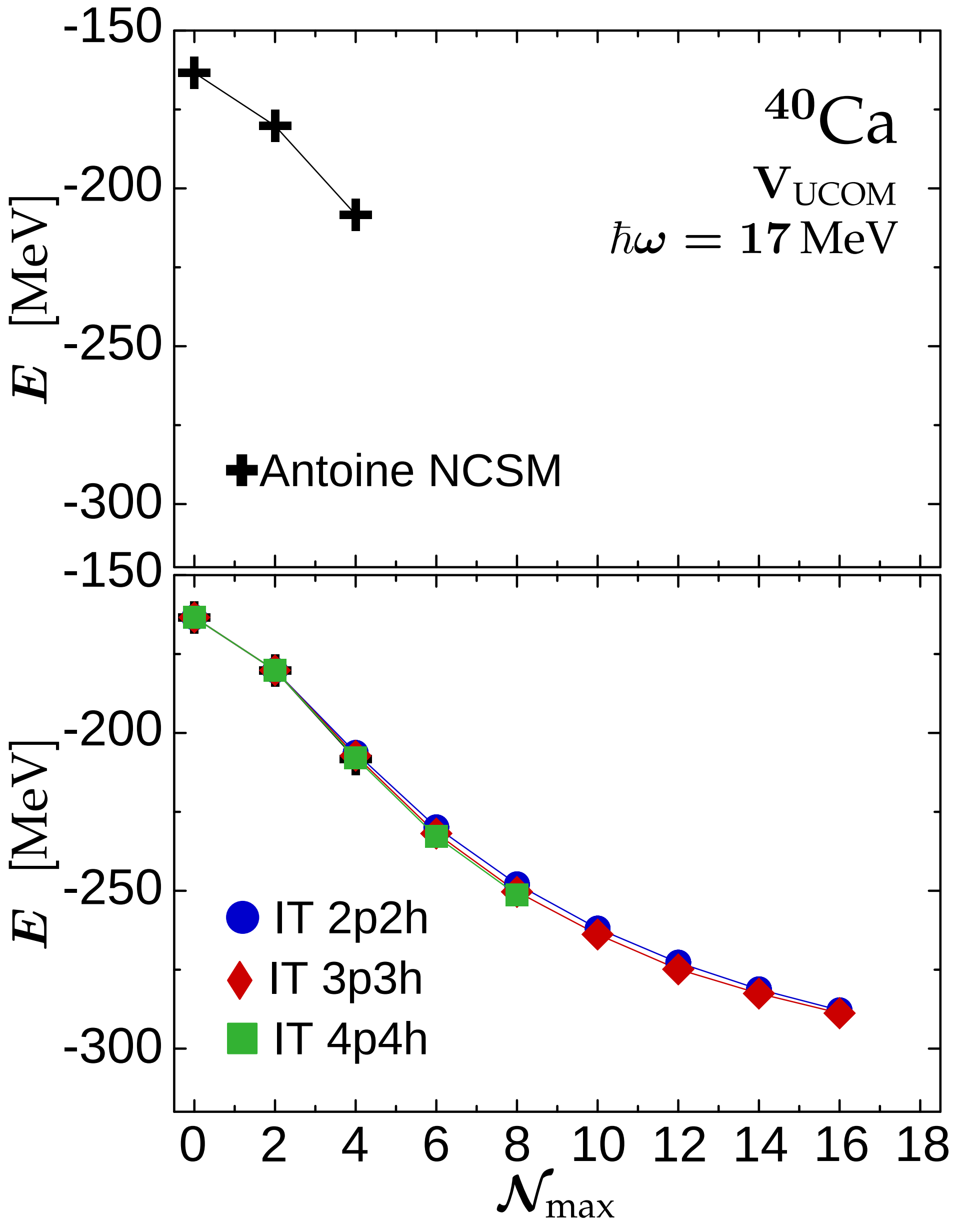
Outlook: NCSM beyond the p-Shell

NCSM

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

Importance Truncation

- diagonalization in space of **important** configurations
- **a priori importance measure** given by perturbation theory



Application II:

Hartree-Fock & Beyond

Reminder: Hartree-Fock Approximation

- ground state approximated by a **single Slater determinant**

$$\left|\Psi\right\rangle \approx \left|\mathrm{HF}\right\rangle = \left|\phi_1, \phi_2, \ldots, \phi_A\right\rangle_a$$

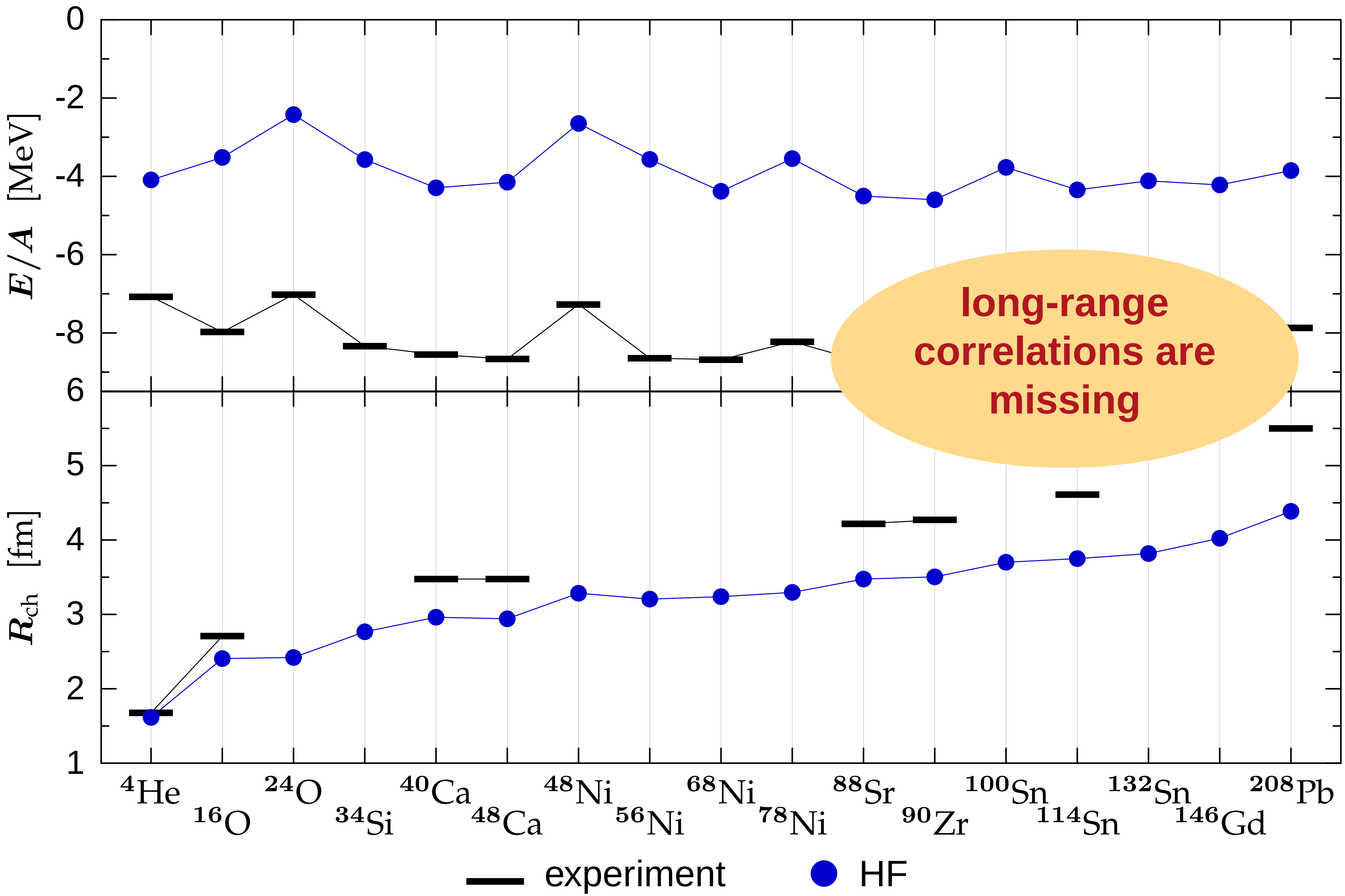
- **variational calculation**: single-particle states $\left|\phi_i\right\rangle$ determined by minimizing the energy expectation value

$$E_{\mathrm{HF}} = \left\langle \mathrm{HF}\right| \mathrm{H}_{\mathrm{int}} \left|\mathrm{HF}\right\rangle = \frac{1}{2} \sum_{i,j=1}^{A} {}_a\!\left\langle \phi_i \phi_j \right| (\mathrm{T}_{\mathrm{int}} + \mathrm{V}) \left|\phi_i \phi_j\right\rangle_a$$

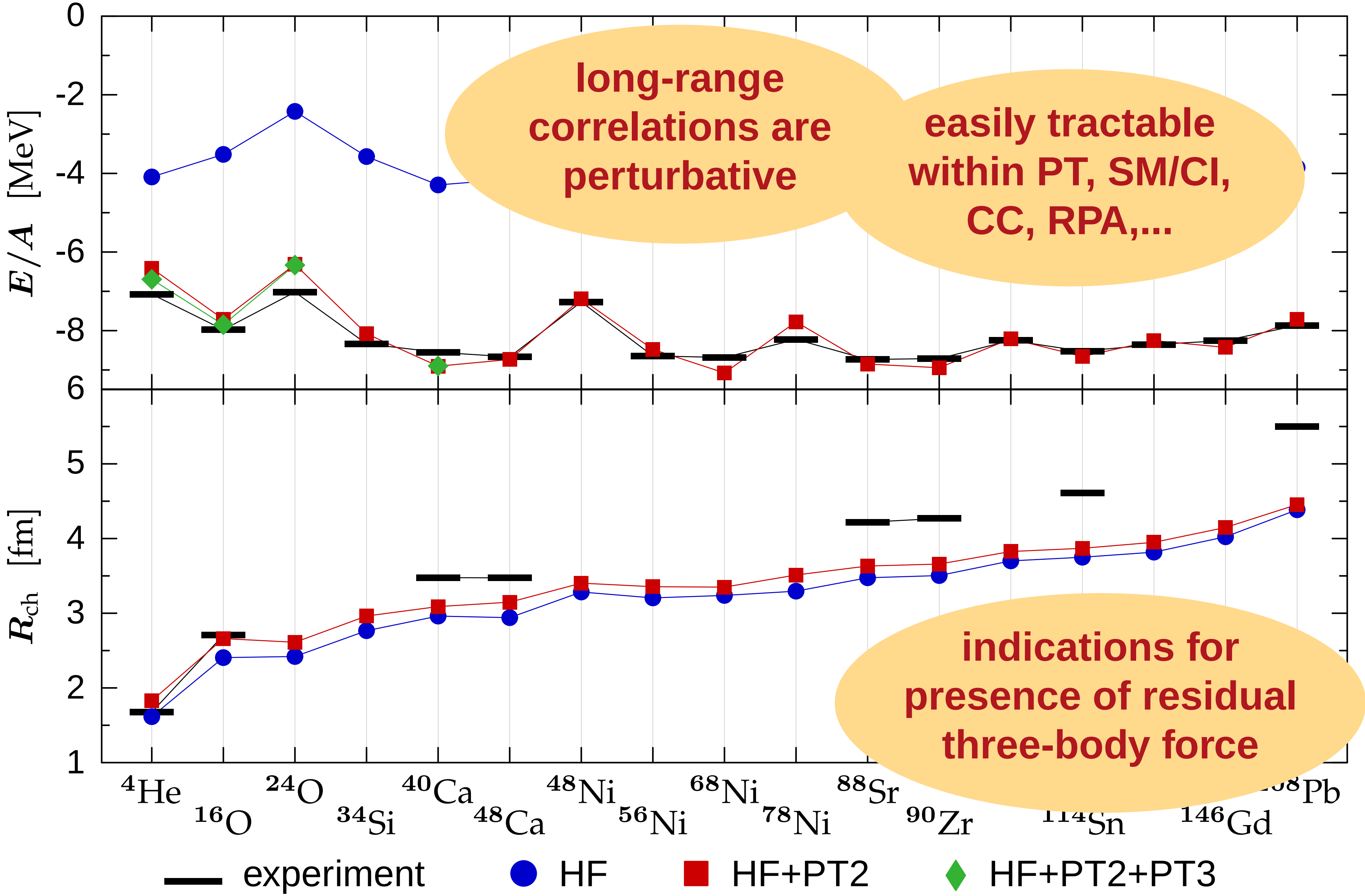
single Slater determinant by definition **cannot describe any correlations** (independent particle state)

Hartree-Fock solution is **starting point for improved calculations**

Hartree-Fock with V_{UCOM}



Perturbation Theory with V_{UCOM}



Application III

RPA & Beyond

Reminder: Random Phase Approximation

- describe **excited states** via vibration creation operator $Q^\dagger_\nu$

$$Q_\nu|\mathrm{RPA}\rangle = 0 \qquad\qquad Q^\dagger_\nu|\mathrm{RPA}\rangle = |\nu\rangle$$

- ansatz for **vibration creation operator $Q^\dagger_\nu$** including 1p1h excitations with respect to HF single-particle basis

$$Q^\dagger_\nu = \sum_{ph} X^\nu_{ph} a^\dagger_p a_h - \sum_{ph} Y^\nu_{ph} a^\dagger_h a_p$$

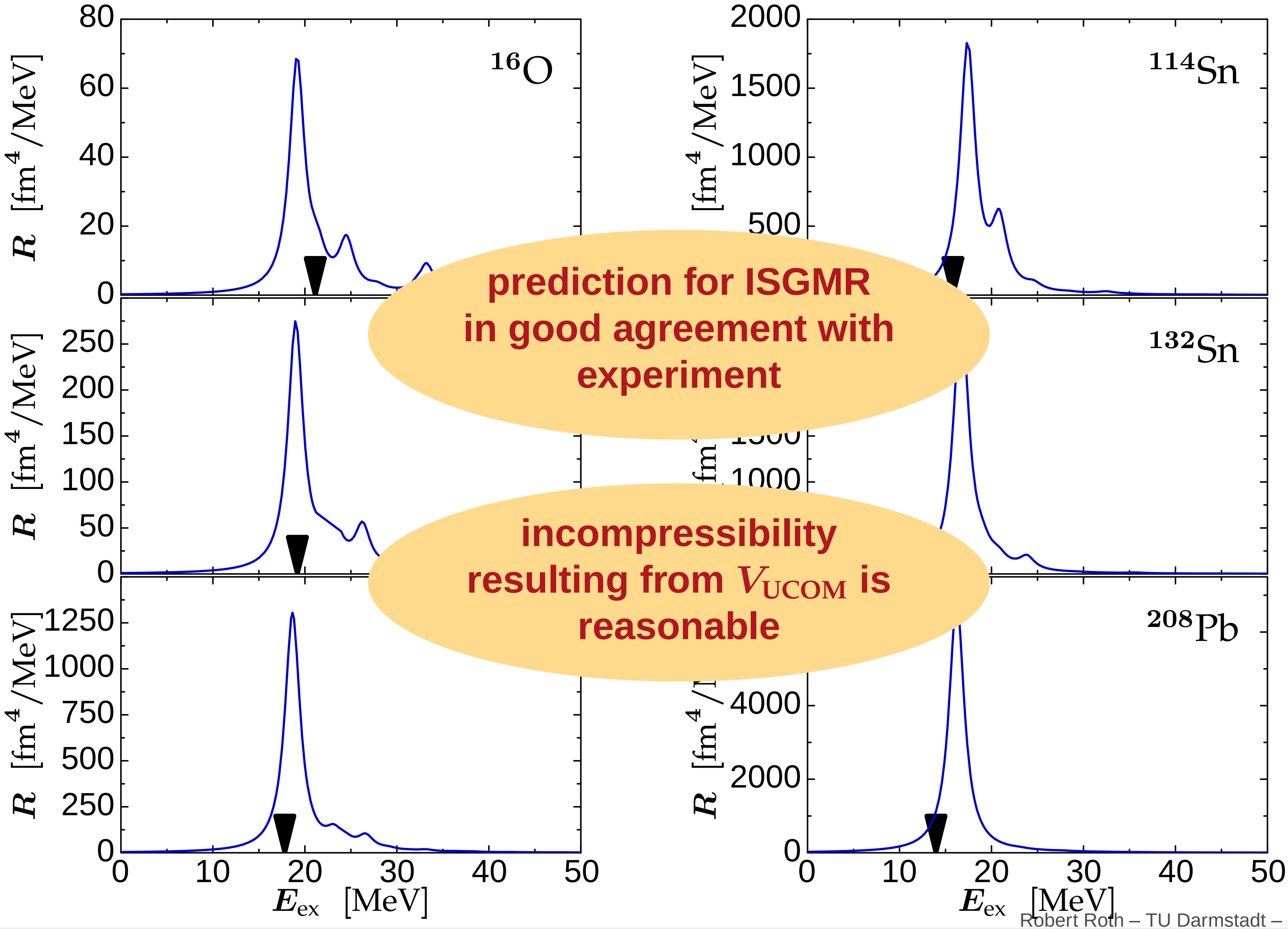
- formal solution of eigenvalue problem via equations of motion method approximating vacuum state by $|\mathrm{HF}\rangle$ yields **RPA equations**

$$\begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix} \begin{pmatrix} X^\nu \\ Y^\nu \end{pmatrix} = E_\nu \begin{pmatrix} X^\nu \\ Y^\nu \end{pmatrix}$$

$$A_{ph,p'h'} = \delta_{pp'}\delta_{hh'}(\epsilon_p - \epsilon_h) + \langle hp'|\,\mathrm{H}_{\text{int}}\,|ph'\rangle \qquad\qquad B_{ph,p'h'} = \langle hh'|\,\mathrm{H}_{\text{int}}\,|pp'\rangle$$

- **self-consistent** solution using the same Hamiltonian H_{int} as in HF

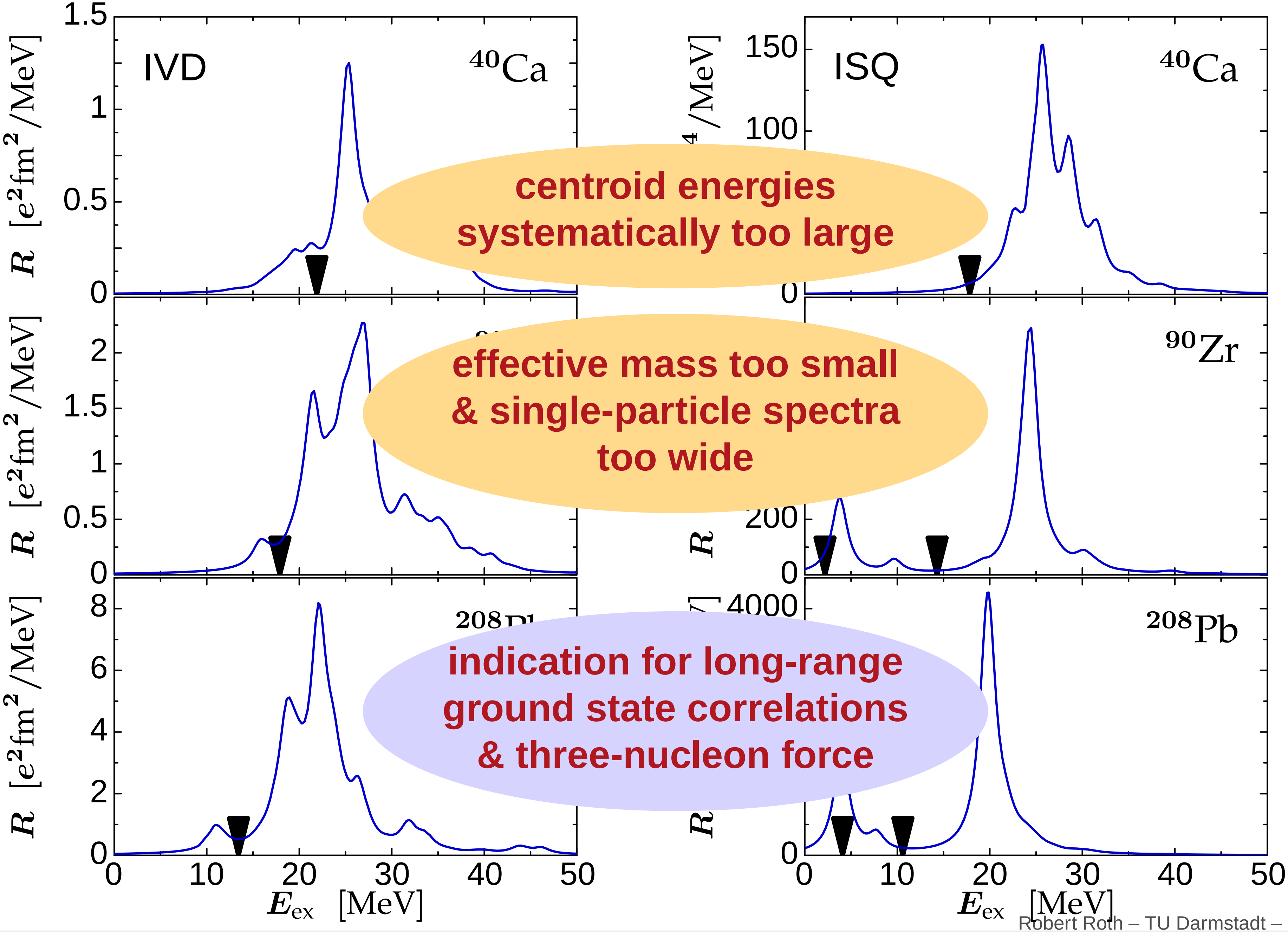
Isoscalar Giant Monopole



prediction for ISGMR in good agreement with experiment

incompressibility resulting from V_{UCOM} is reasonable

Isovector Dipole & Isoscalar Quadrupole

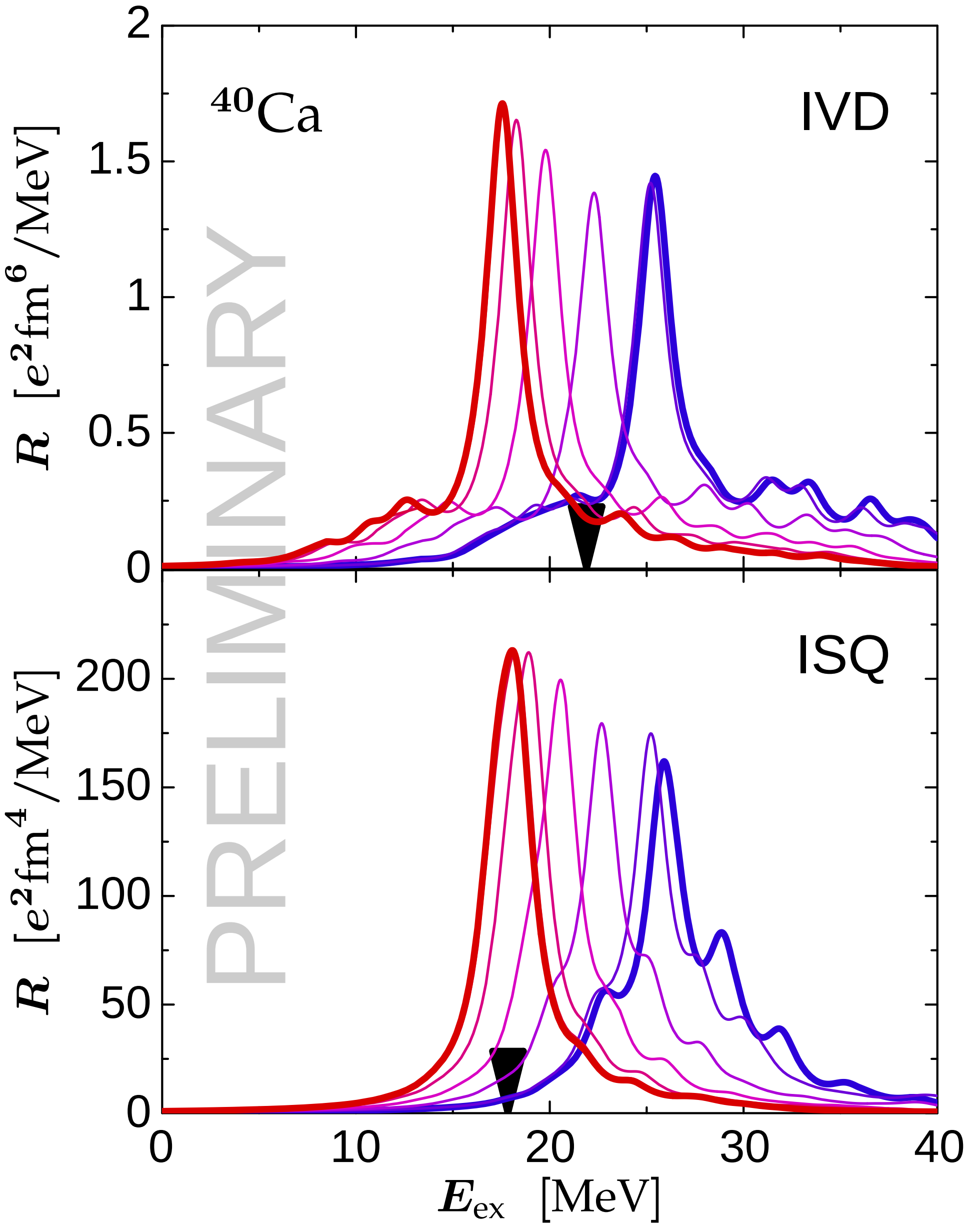


centroid energies
systematically too large

effective mass too small
& single-particle spectra
too wide

indication for long-range
ground state correlations
& three-nucleon force

Outlook: Second-RPA

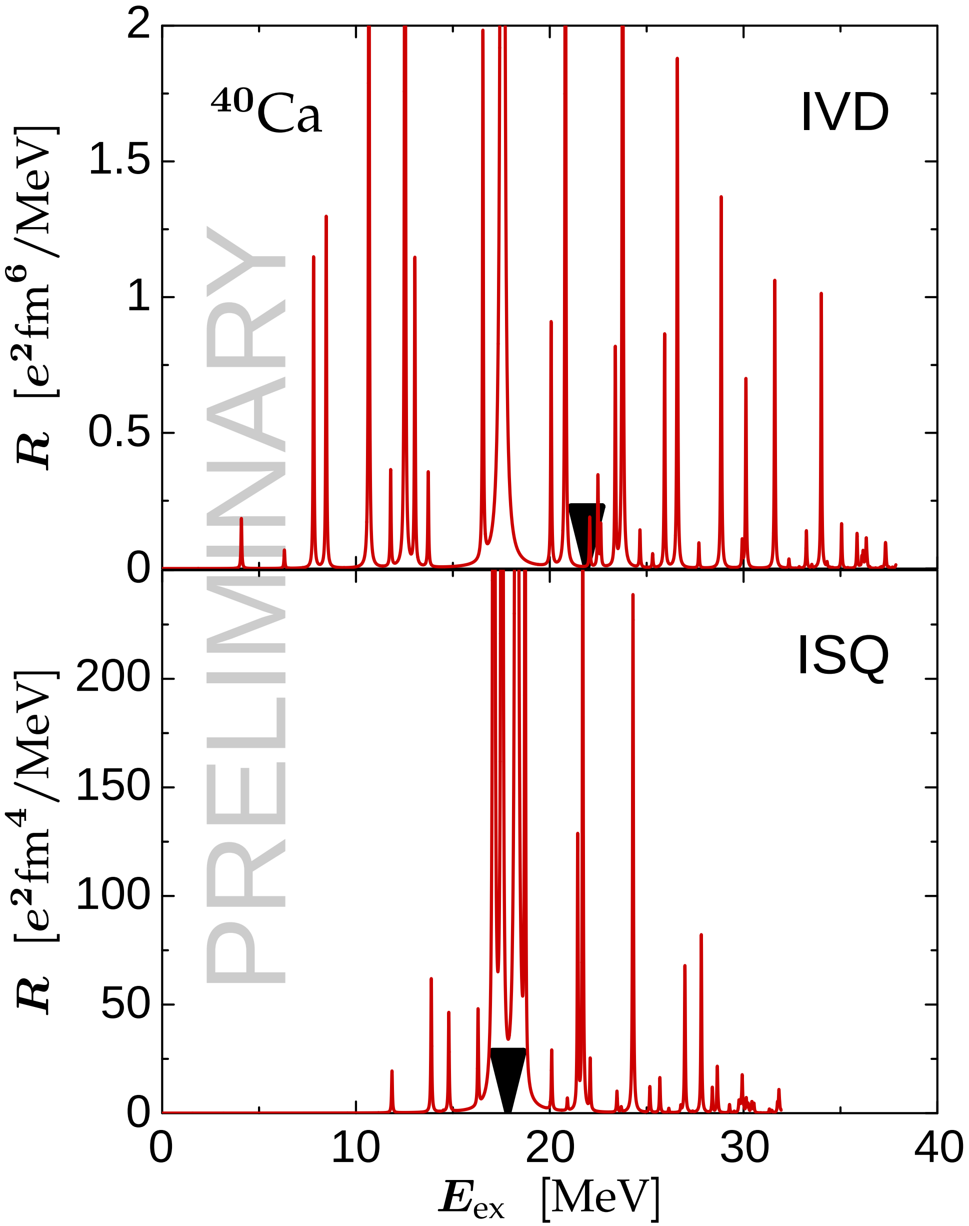


- RPA (full 1p1h space)
- SRPA (full 1p1h+2p2h space)

(11 major shells, $\Gamma = 2\,\mathrm{MeV}$)

complex configurations have significant impact on response

Outlook: Second-RPA



RPA (full 1p1h space)

SRPA (full 1p1h+2p2h space)

(11 major shells, $\Gamma = 50\,\mathrm{keV}$)

complex configurations have significant impact on response

possibility to investigate fine structure

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**
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