Nuclear Structure with Correlated Realistic Interactions

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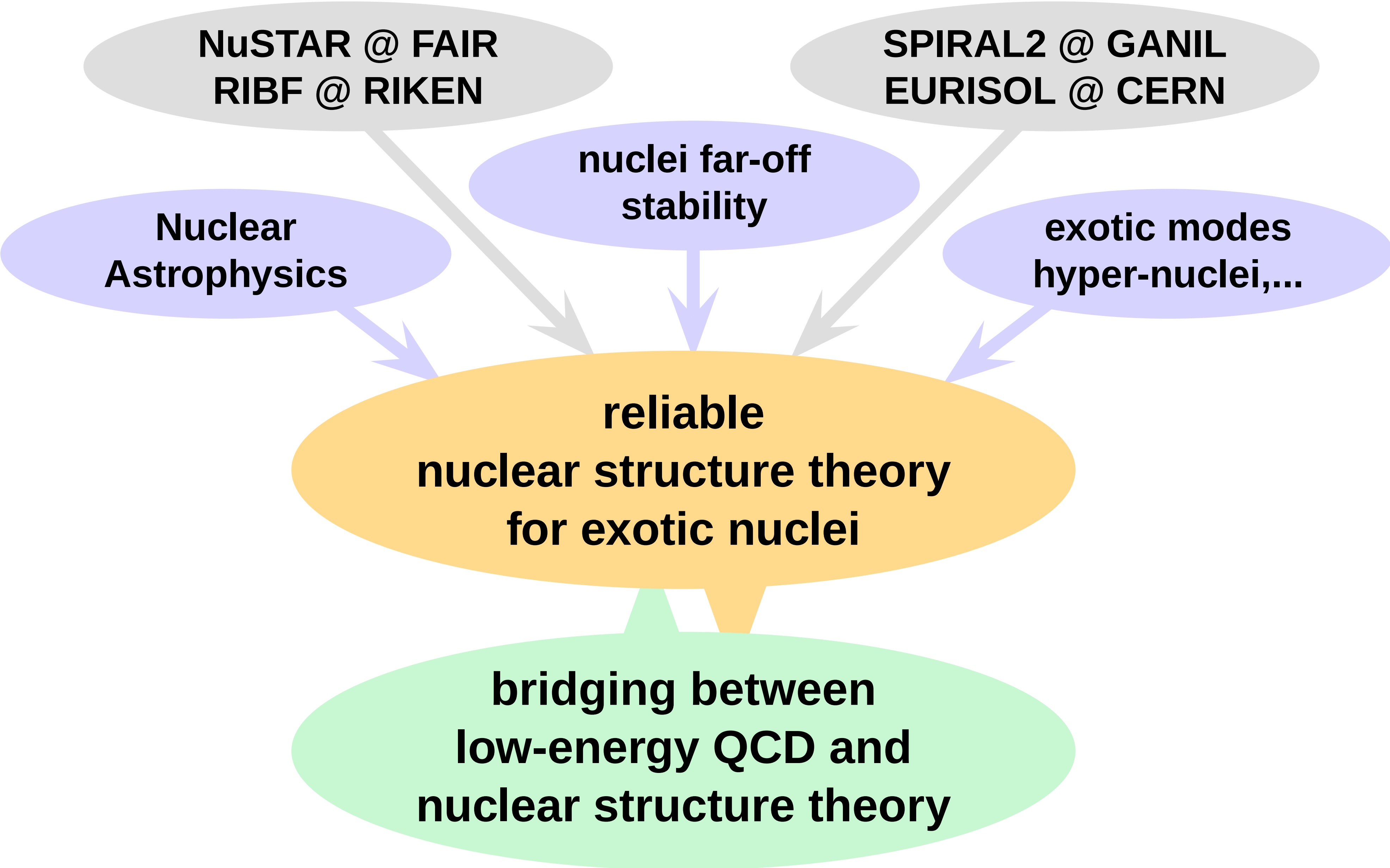
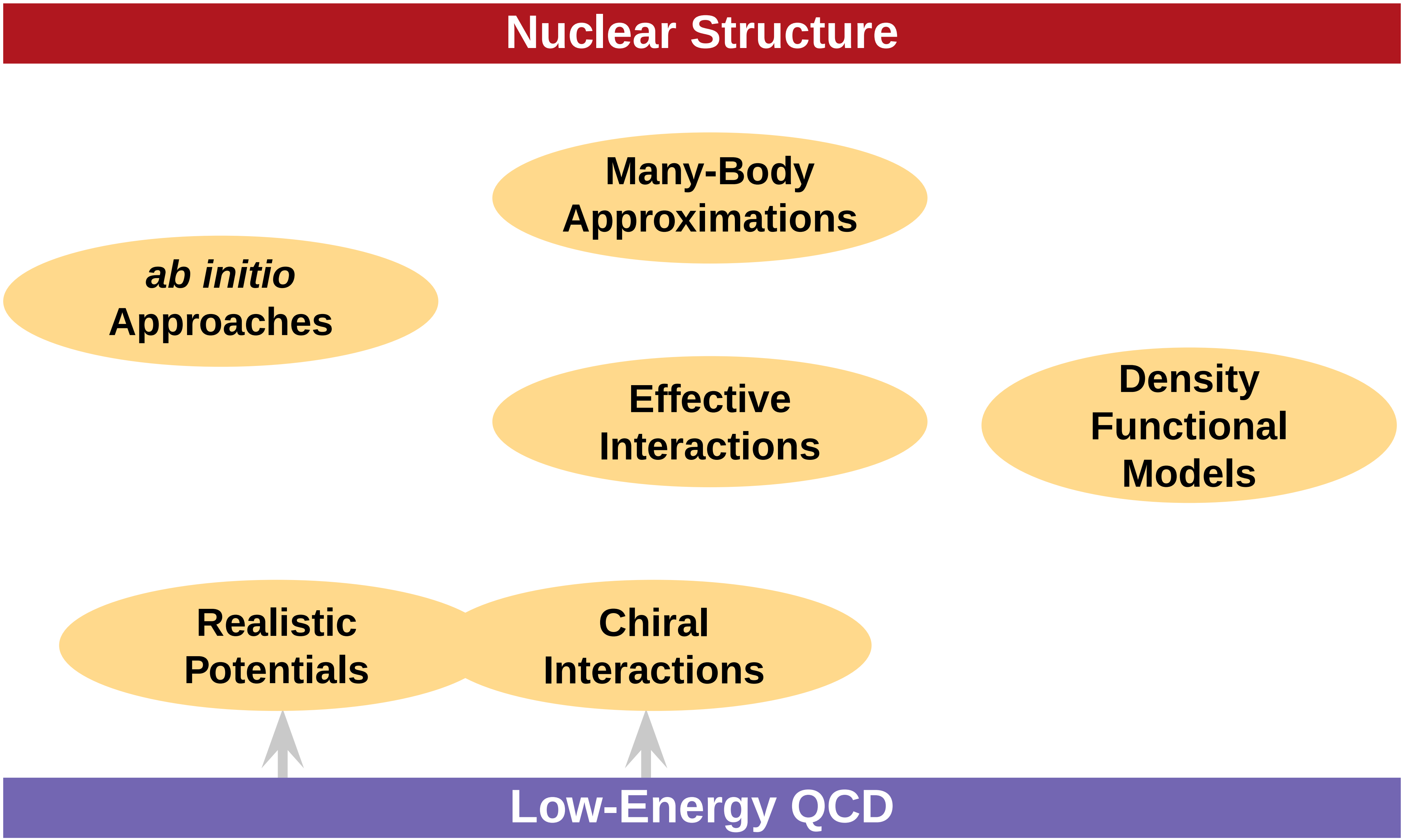
Overview

- Motivation
- Modern Effective Interactions
  - Unitary Correlation Operator Method
  - Similarity Renormalization Group
- Many-Body Methods
  - No Core Shell Model & Beyond
  - Hartree-Fock & Beyond
  - Random Phase Approximation & Beyond

Nuclear Structure in the 21st Century



Modern Nuclear Structure Theory



Realistic Interactions

- **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

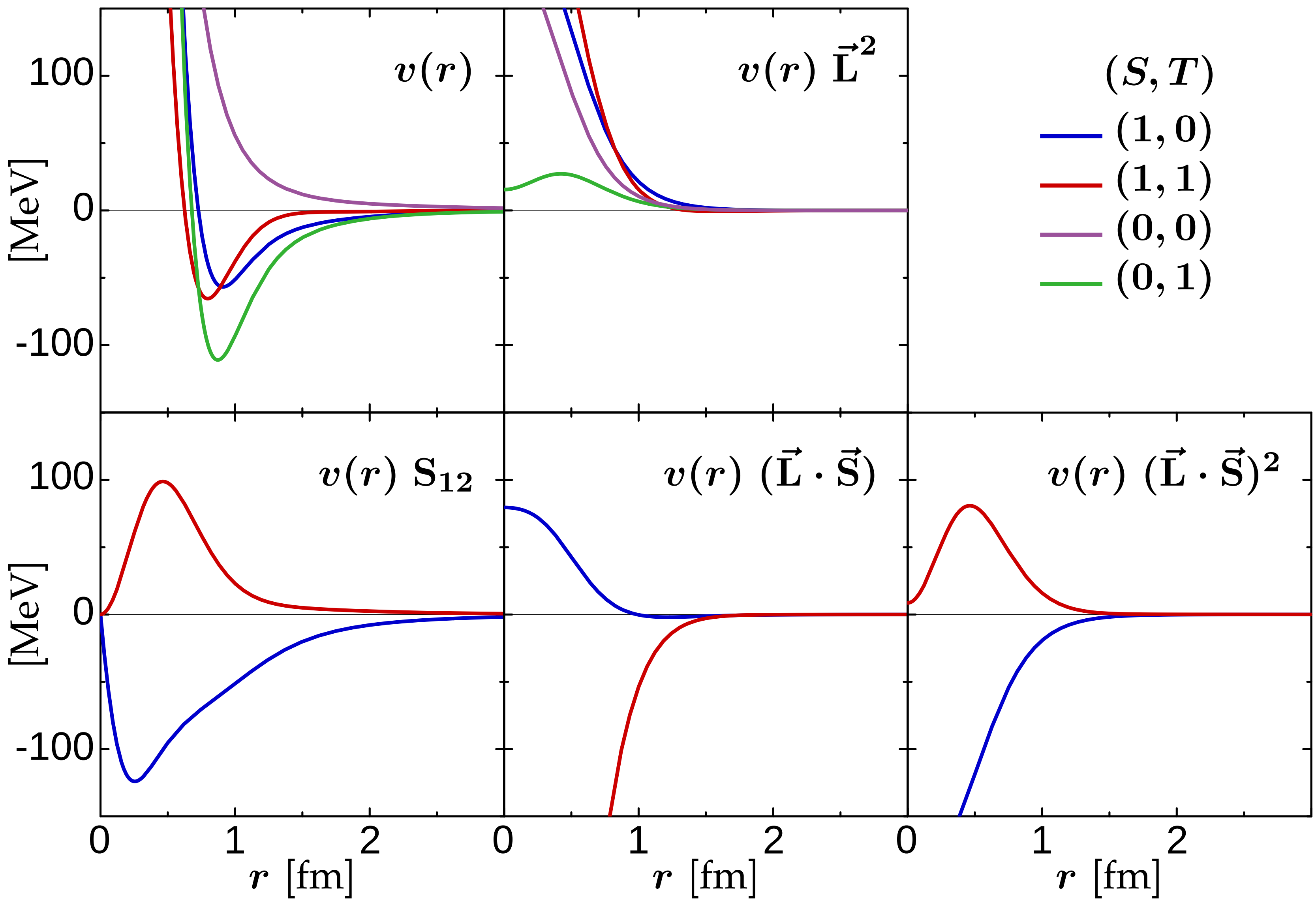
Nijmegen I/II

Chiral N3LO

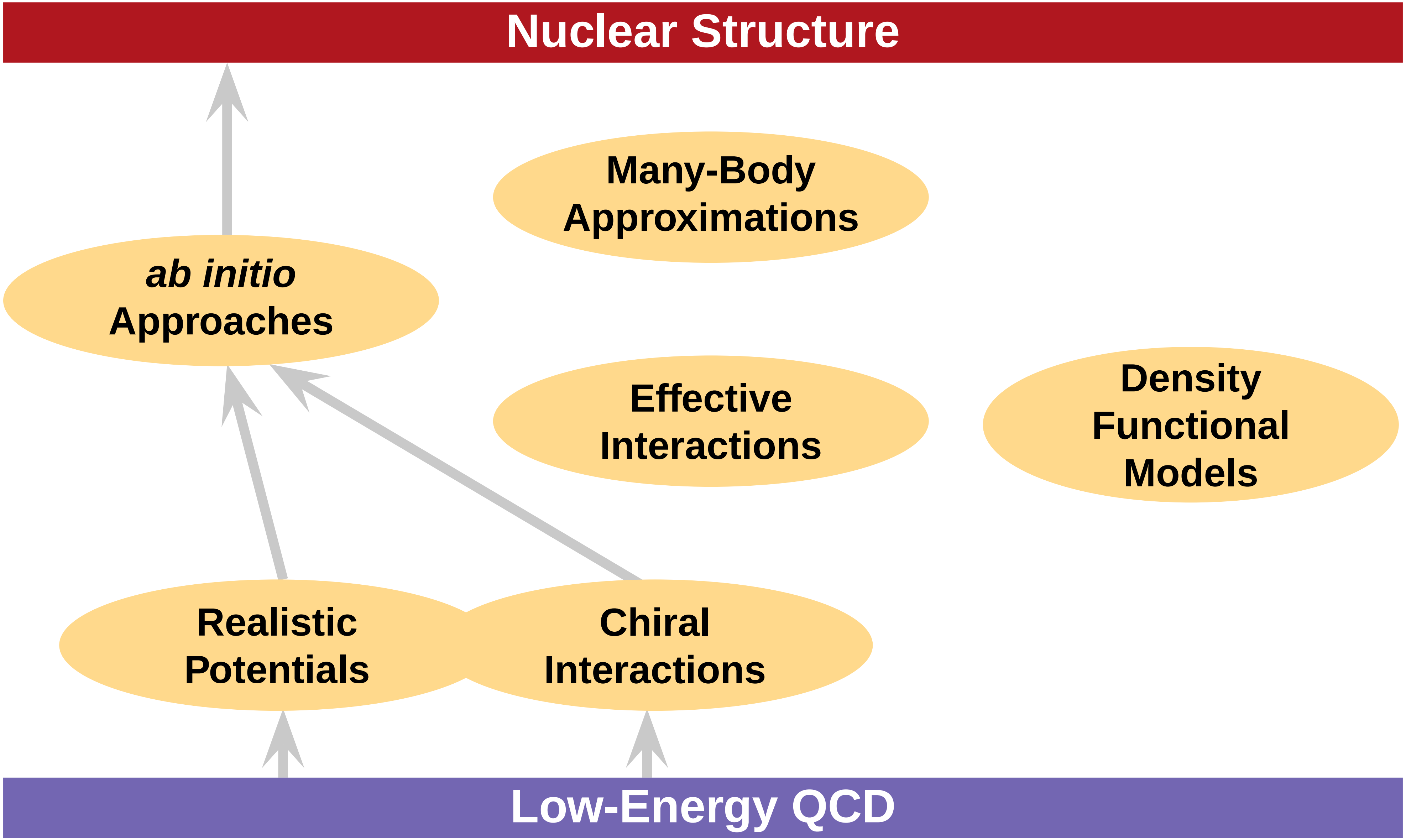
Argonne V18 + **Illinois 2**

Chiral N3LO + **N2LO**

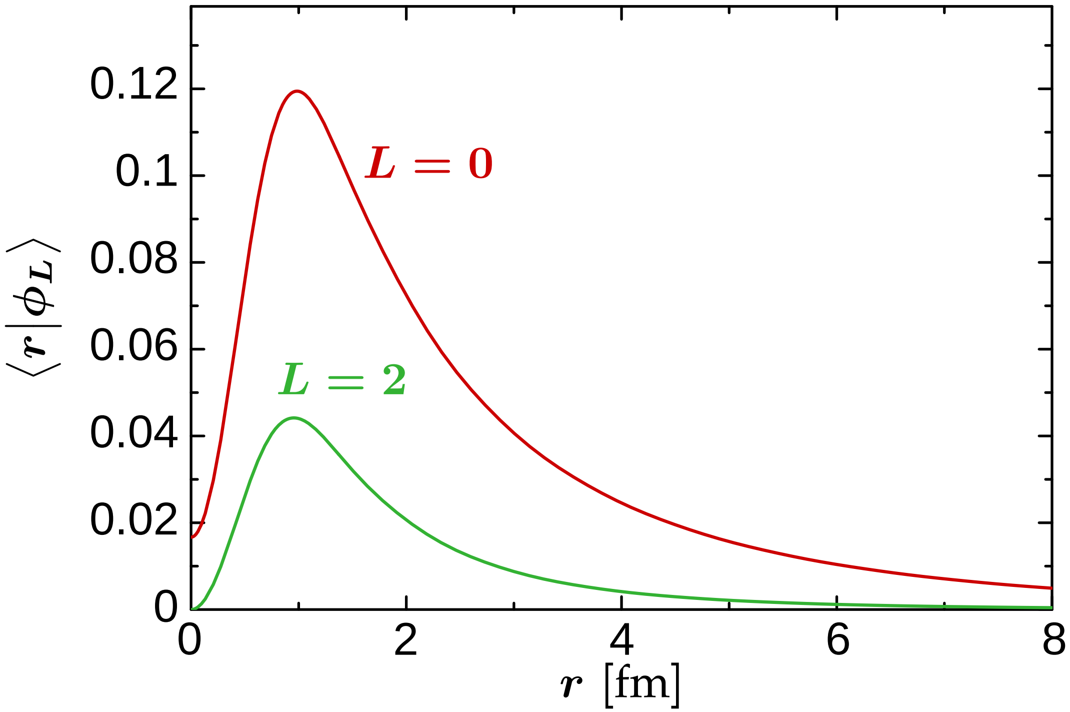
Argonne V18 Potential



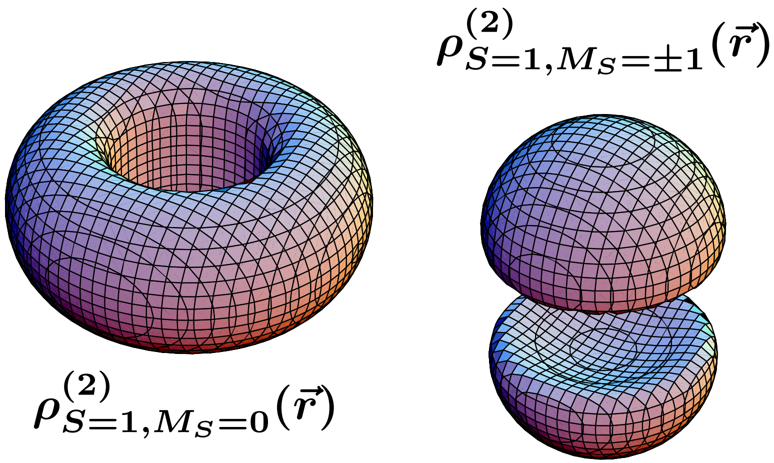
Modern Nuclear Structure Theory



Deuteron: Manifestation of Correlations



- **exact deuteron solution** for Argonne V18 potential



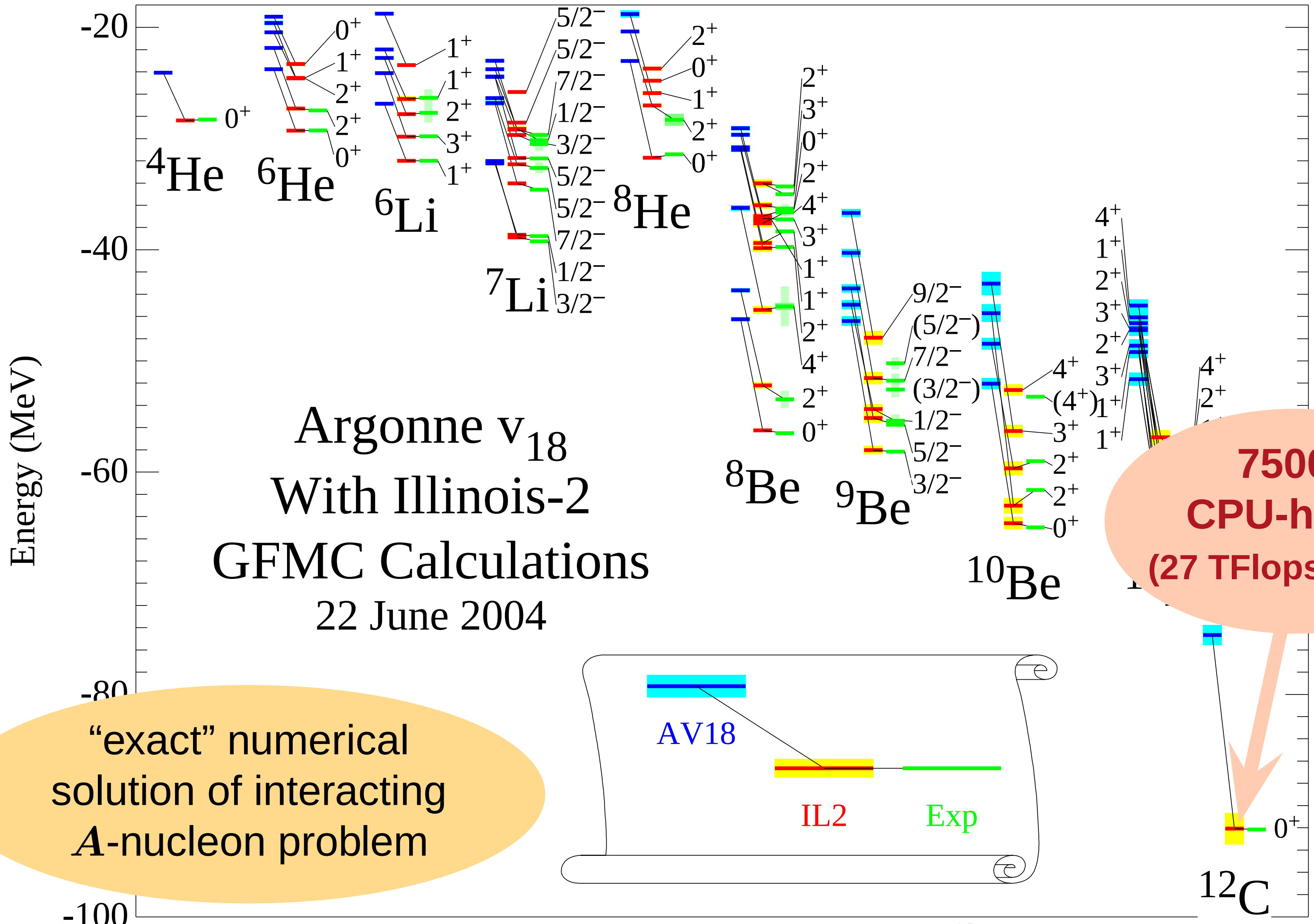
short-range repulsion supresses wavefunction at small distances r

central correlations

tensor interaction generates D-wave admixture in the ground state

tensor correlations

Ab initio Approaches: GFMC



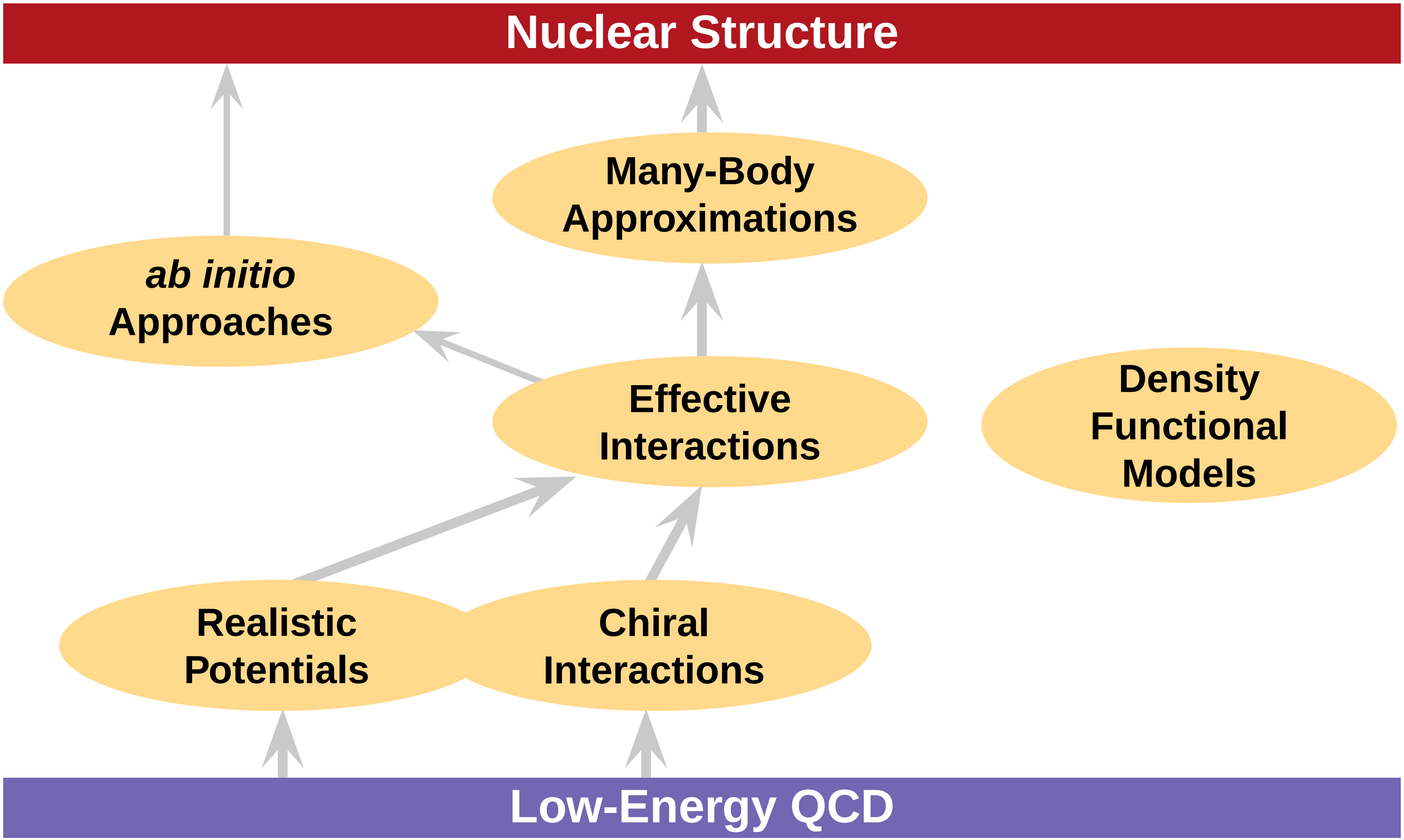
75000 CPU-hours (27 TFlops-hours)

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

[S. Pieper, private comm.]

^{12}C results are preliminary.

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 Approximations

- rely on truncated many-nucleon Hilbert spaces (model space)
- 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 space
- conserve experimentally constrained properties (phase shifts)

can be viewed as realistic interactions

Modern Effective Interactions I

Unitary Correlation Operator Method (UCOM)

Unitary Correlation Operator Method

Correlation Operator

define an unitary operator C to describe the effect of short-range correlations

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

Correlated States

imprint short-range correlations onto uncorrelated many-body states

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

Correlated Operators

adapt Hamiltonian and all other observables to uncorrelated many-body space

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

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

Unitary Correlation Operator Method

explicit ansatz for the correlation operator motivated by the **physics of short-range central and tensor correlations**

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

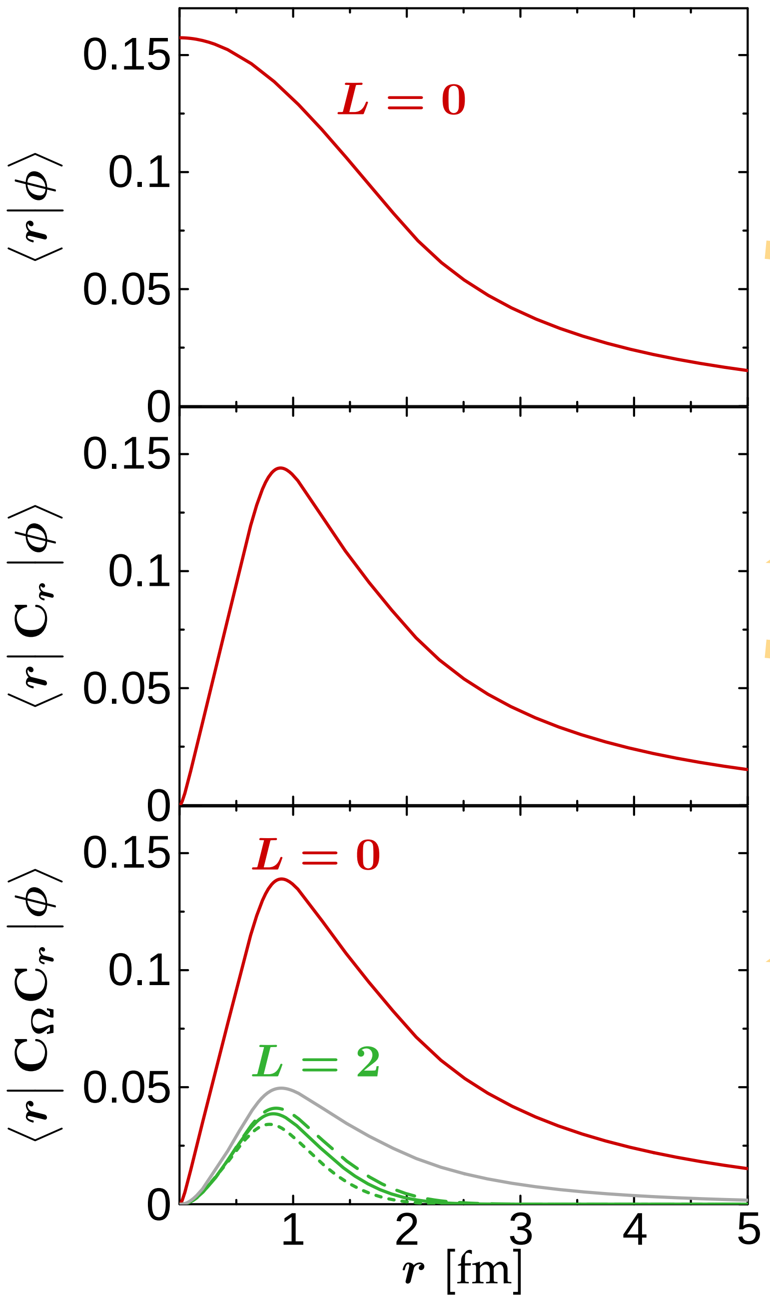
- angular shift depending on the orientation of spin and relative coordinate of a nucleon pair

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

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

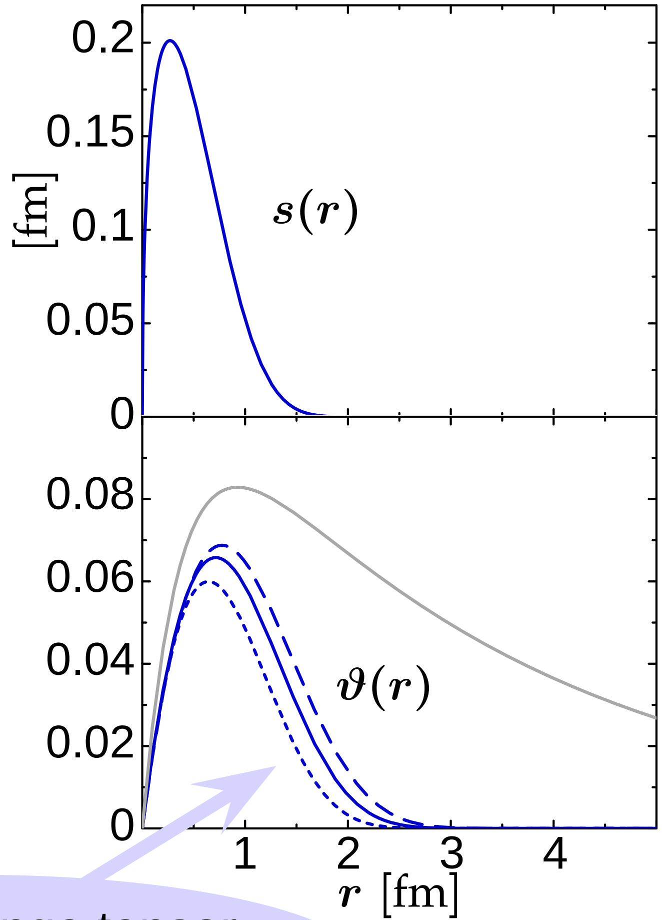
- $s(r)$ and $\vartheta(r)$ for given potential determined by energy minimization in the two-body system (for each S, T)

Correlated States: The Deuteron



central correlations

tensor correlations



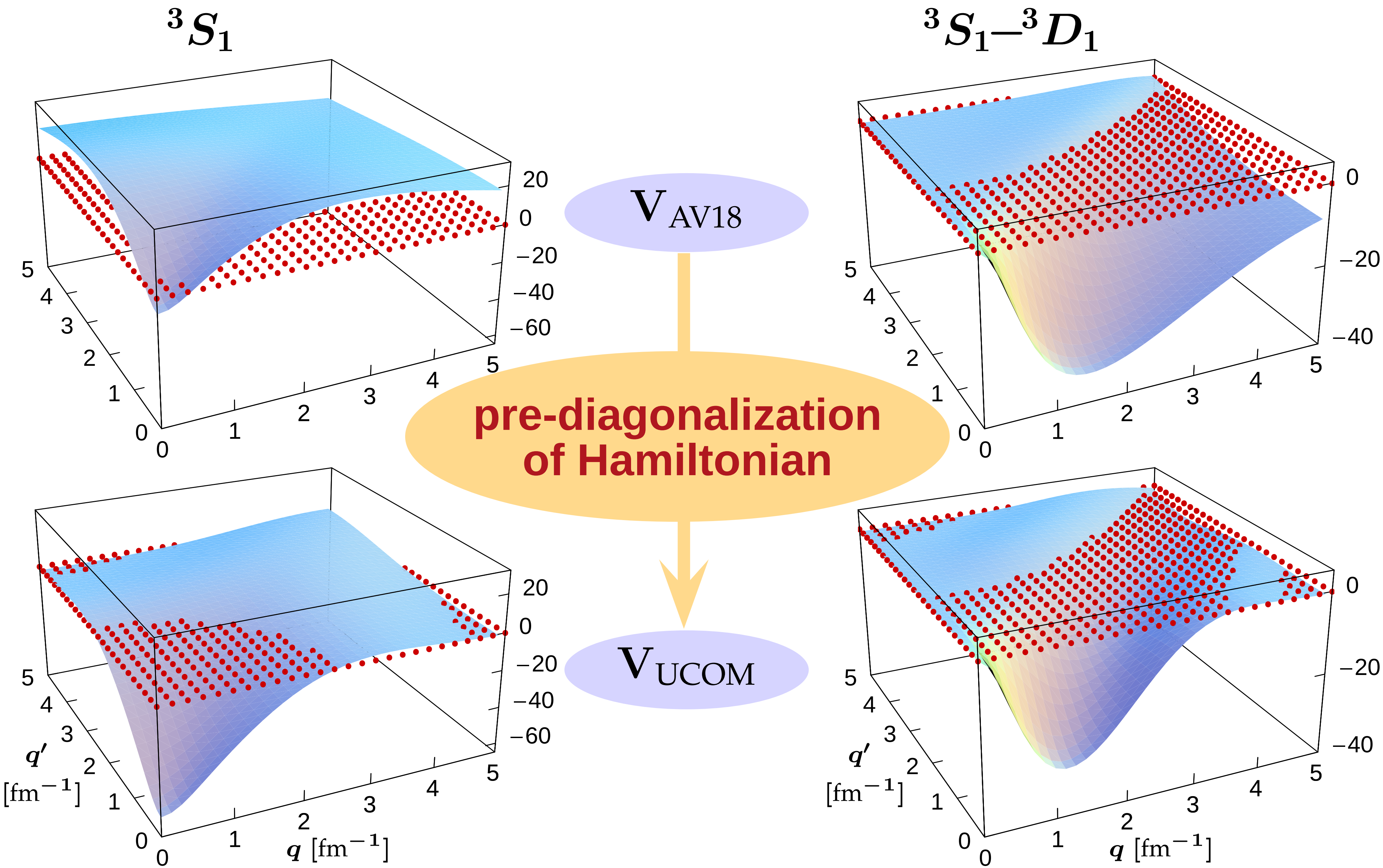
only short-range tensor correlations treated by C_Ω

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**

Momentum-Space Matrix Elements



Modern Effective Interactions II

Similarity Renormalization Group (SRG)

Similarity Renormalization Group

unitary transformation of the **Hamiltonian to a band-diagonal form** with respect to a given uncorrelated many-body basis

Flow Equation for Hamiltonian

- evolution equation for Hamiltonian

$$\widetilde{\mathrm{H}}(\alpha) = \mathrm{C}^{\dagger}(\alpha)\,\mathrm{H}\,\mathrm{C}(\alpha) \qquad \longrightarrow \qquad \frac{\mathrm{d}}{\mathrm{d}\alpha}\widetilde{\mathrm{H}}(\alpha) = \left[\eta(\alpha), \widetilde{\mathrm{H}}(\alpha)\right]$$

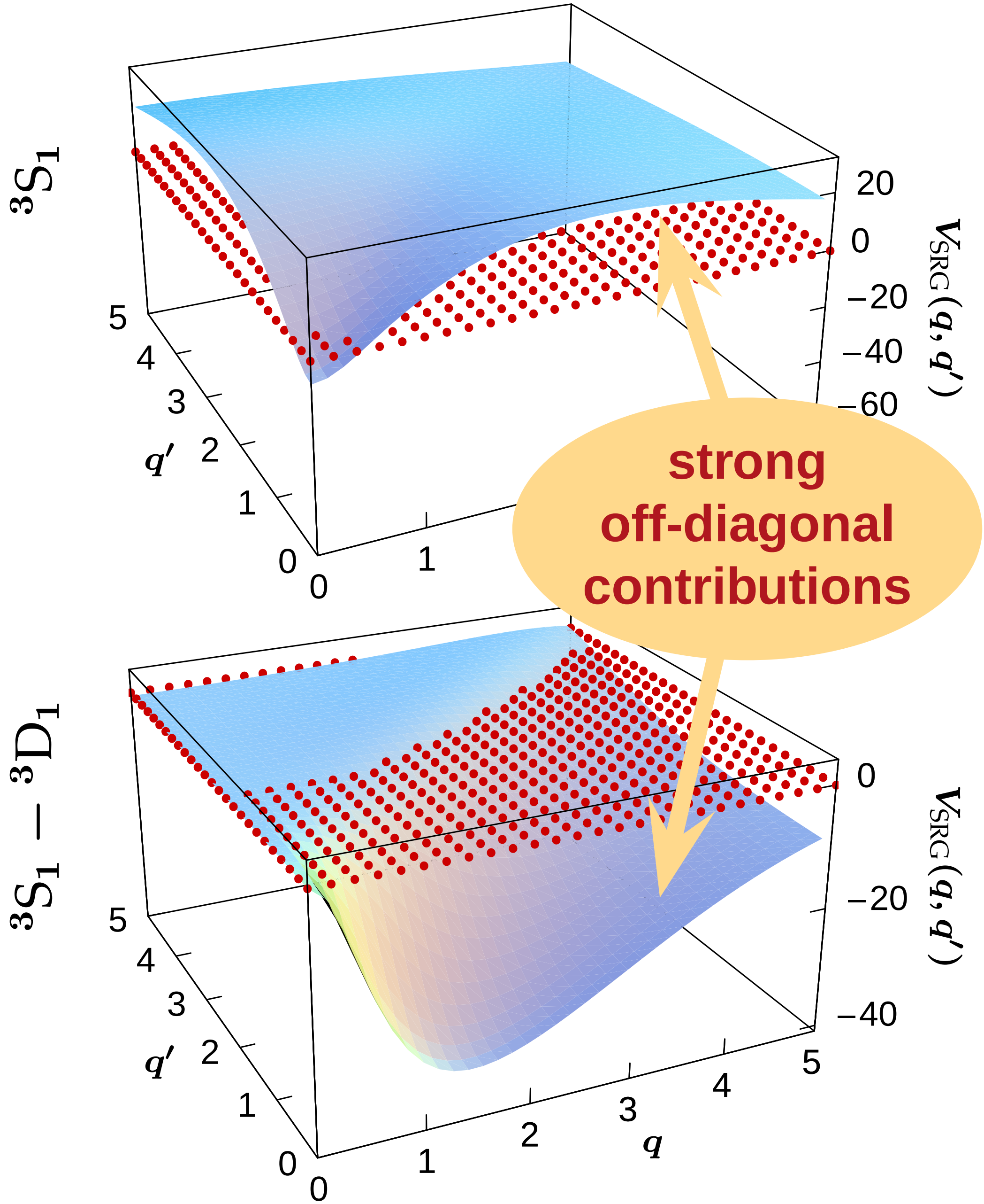
- dynamical generator defined as commutator with the operator in whose eigenbasis H shall be diagonalized

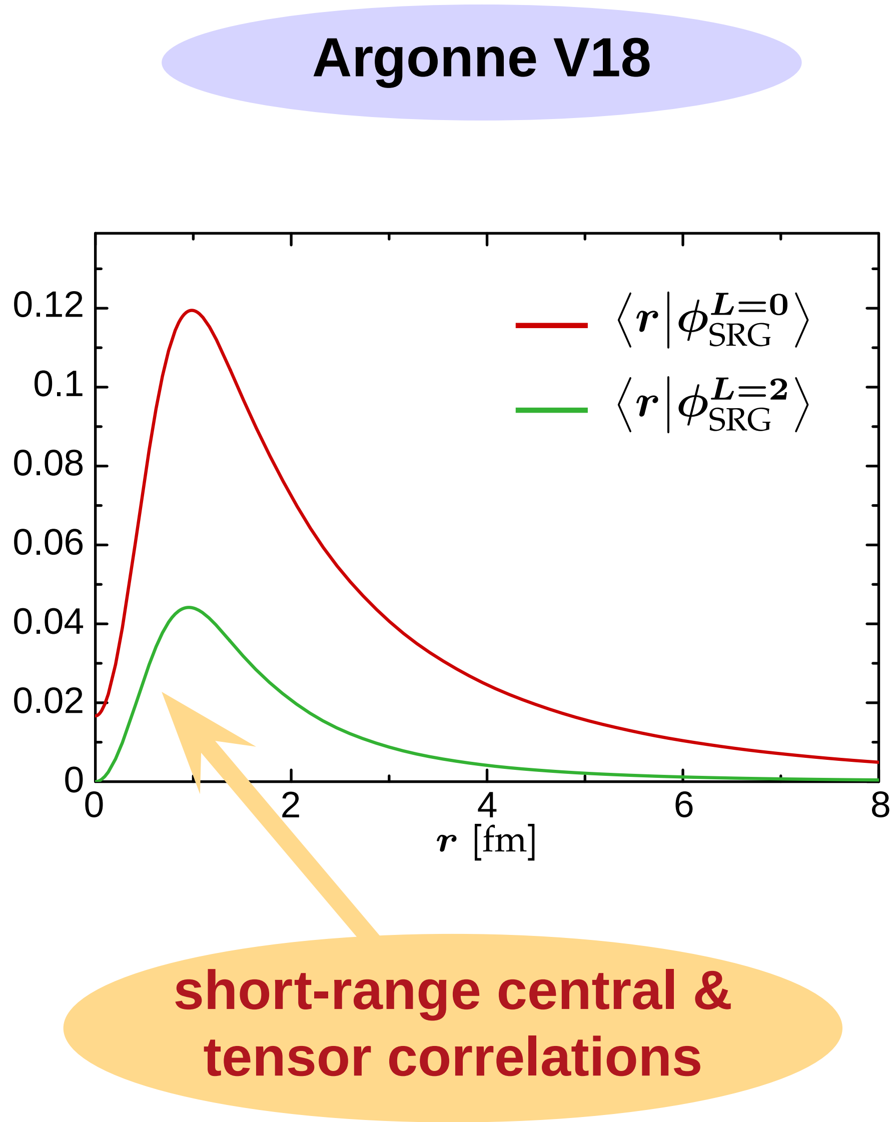
$$\eta(\alpha) = \left[\mathrm{T}_{\mathrm{int}}, \widetilde{\mathrm{H}}(\alpha)\right] \overset{2\mathrm{B}}{=} \tfrac{1}{2\mu}\left[\vec{\mathrm{q}}^{\,2}, \widetilde{\mathrm{H}}(\alpha)\right]$$

- $\eta(0)$ has the same structure as the UCOM generators g_r and g_Ω

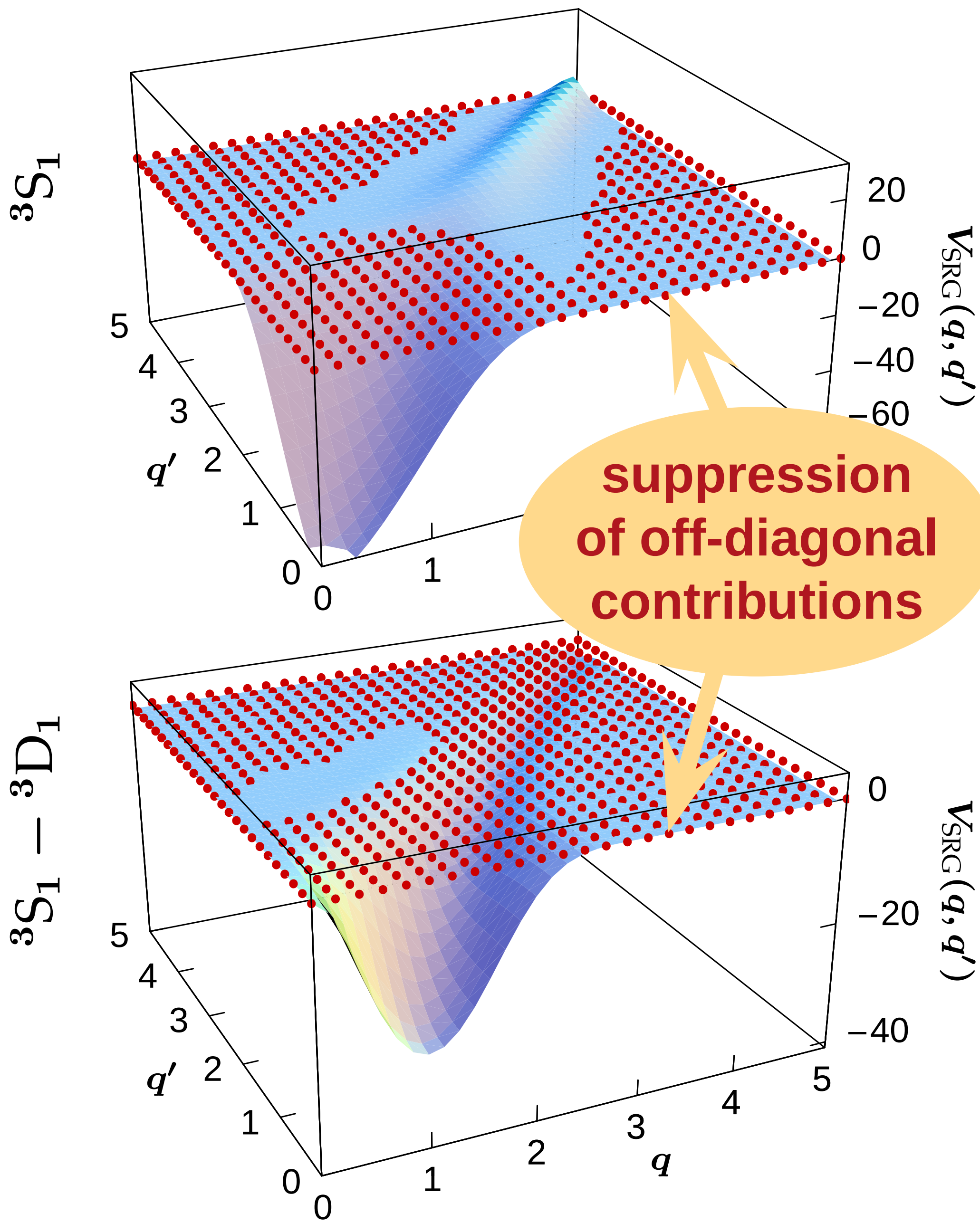
[Bogner et al., nucl-th/0611045; Hergert et al., PRC (2007), nucl-th/0703006]

SRG Evolution: The Deuteron



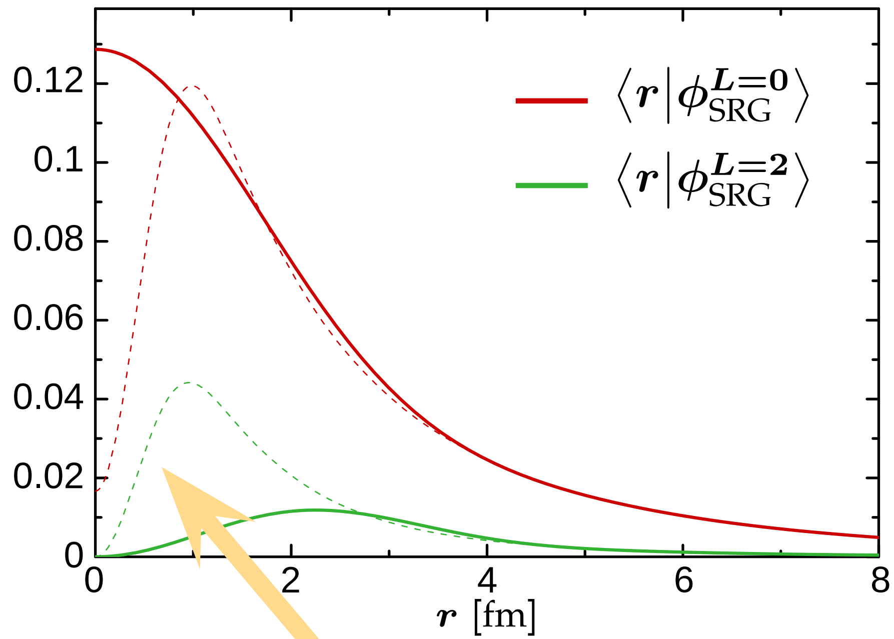


SRG Evolution: The Deuteron



suppression of off-diagonal contributions

$$\alpha = 0.1000\,\text{fm}^4$$



elimination of short-range correlations

Many-Body Methods 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

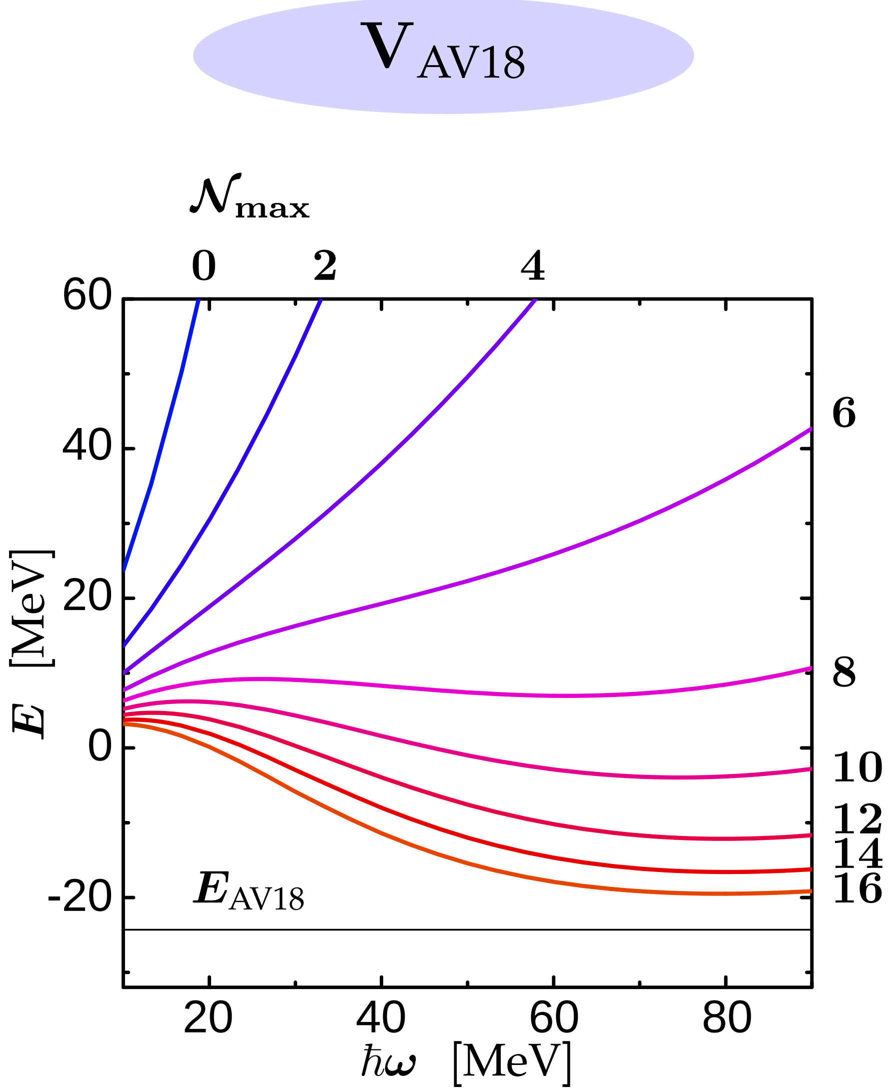
$$|\Psi\rangle = \sum_i C_i \, |\mathrm{SD}_i\rangle$$

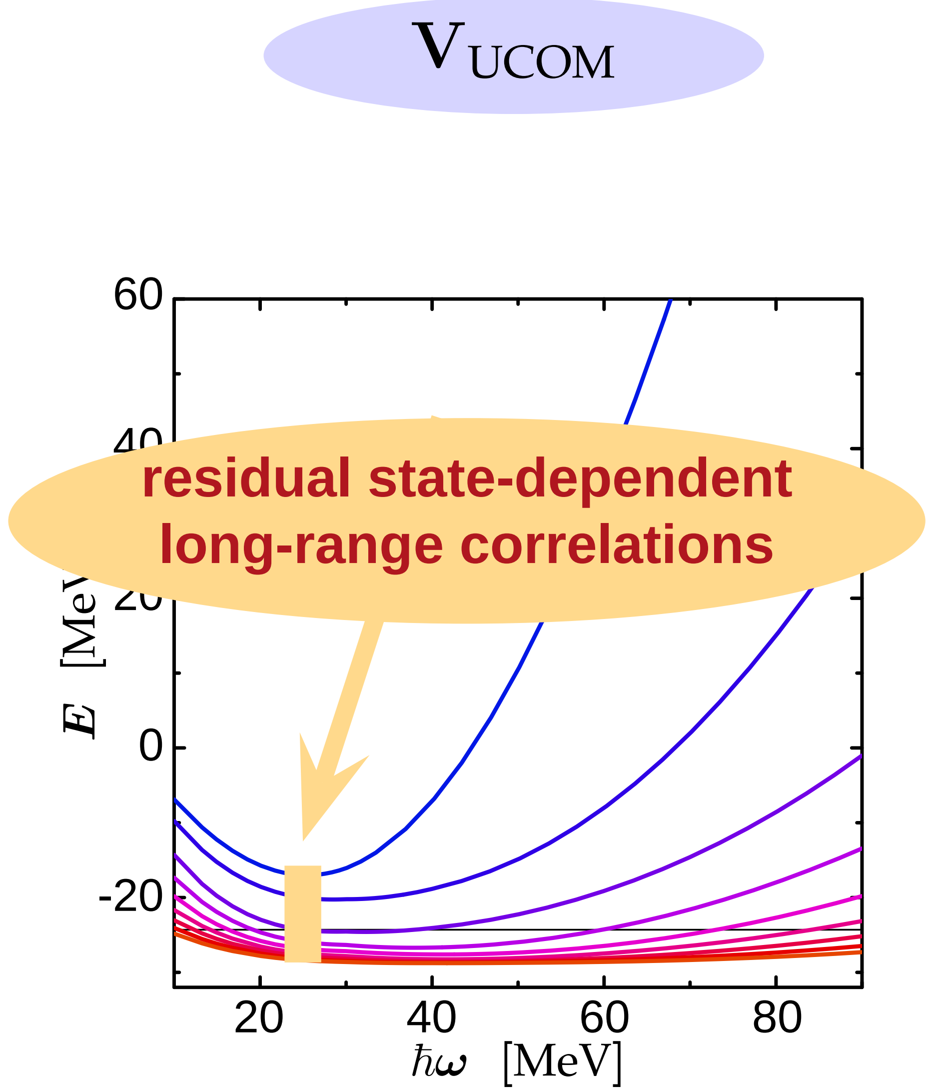
- $\mathcal{N}_{\max}\hbar\omega$ **model space**: truncate basis of Slater determinants with respect to number of oscillator quanta (unperturbed excitation energy)

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

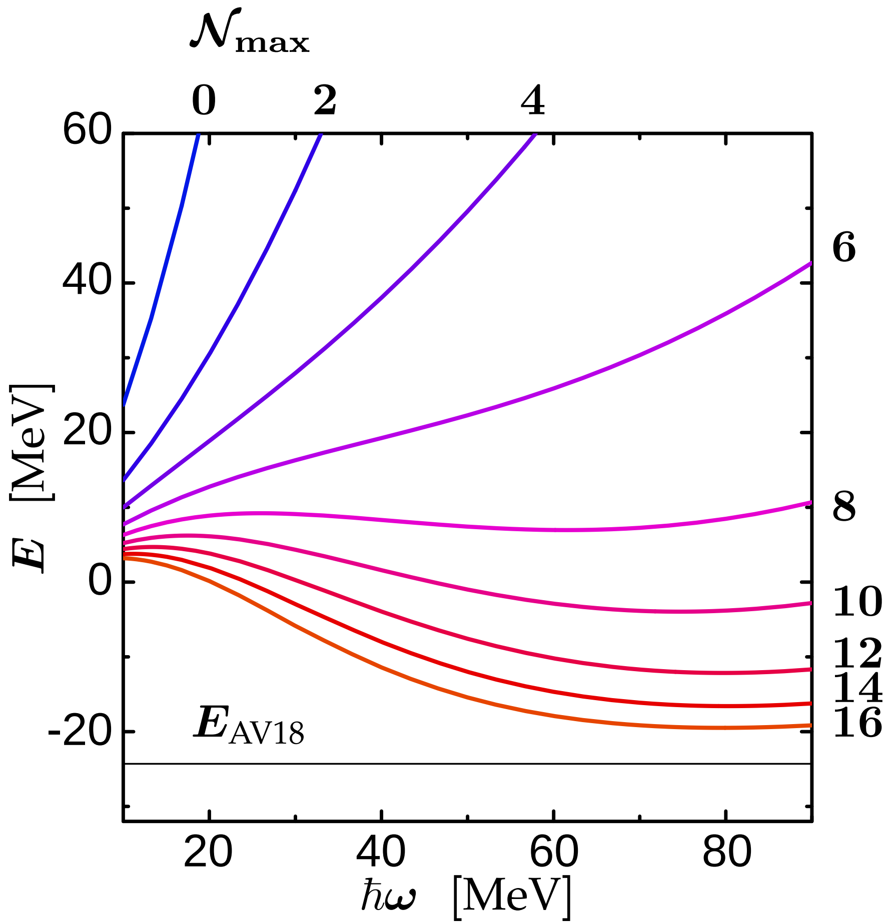
^{4}He: Convergence



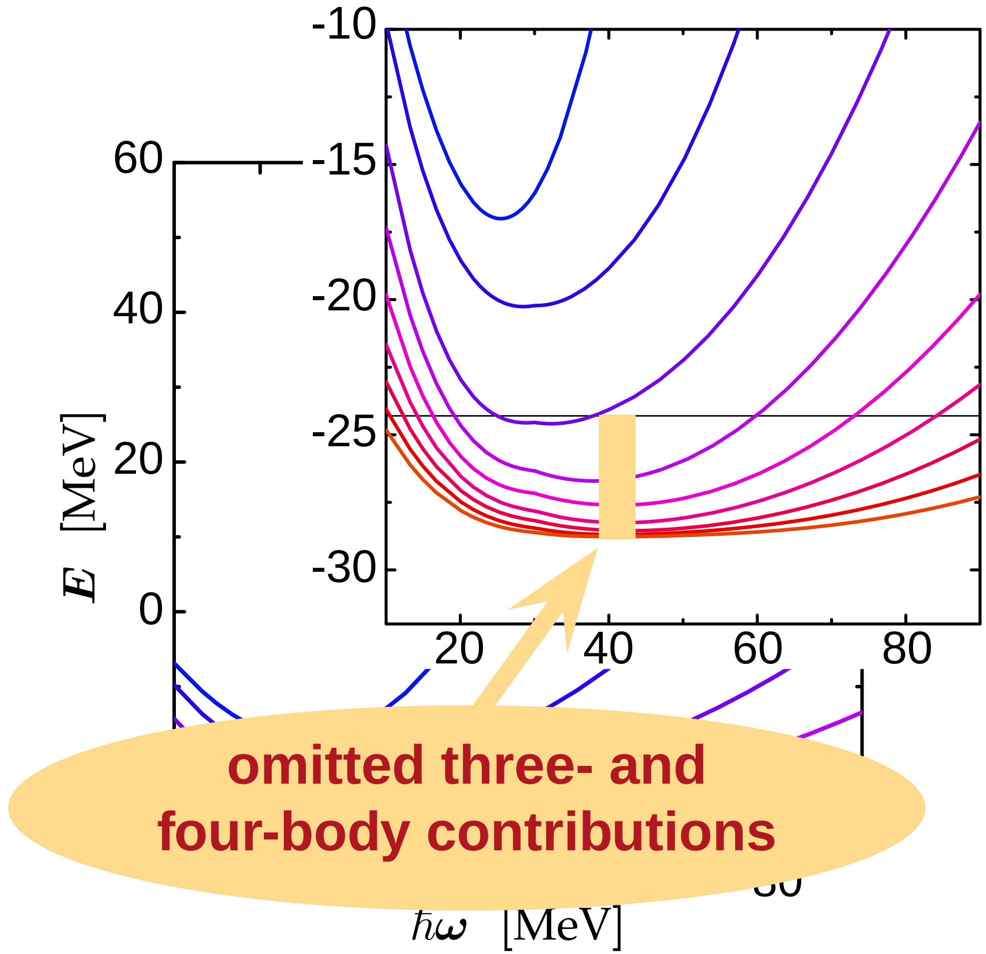


^{4}He: Convergence

V AV18



V UCOM



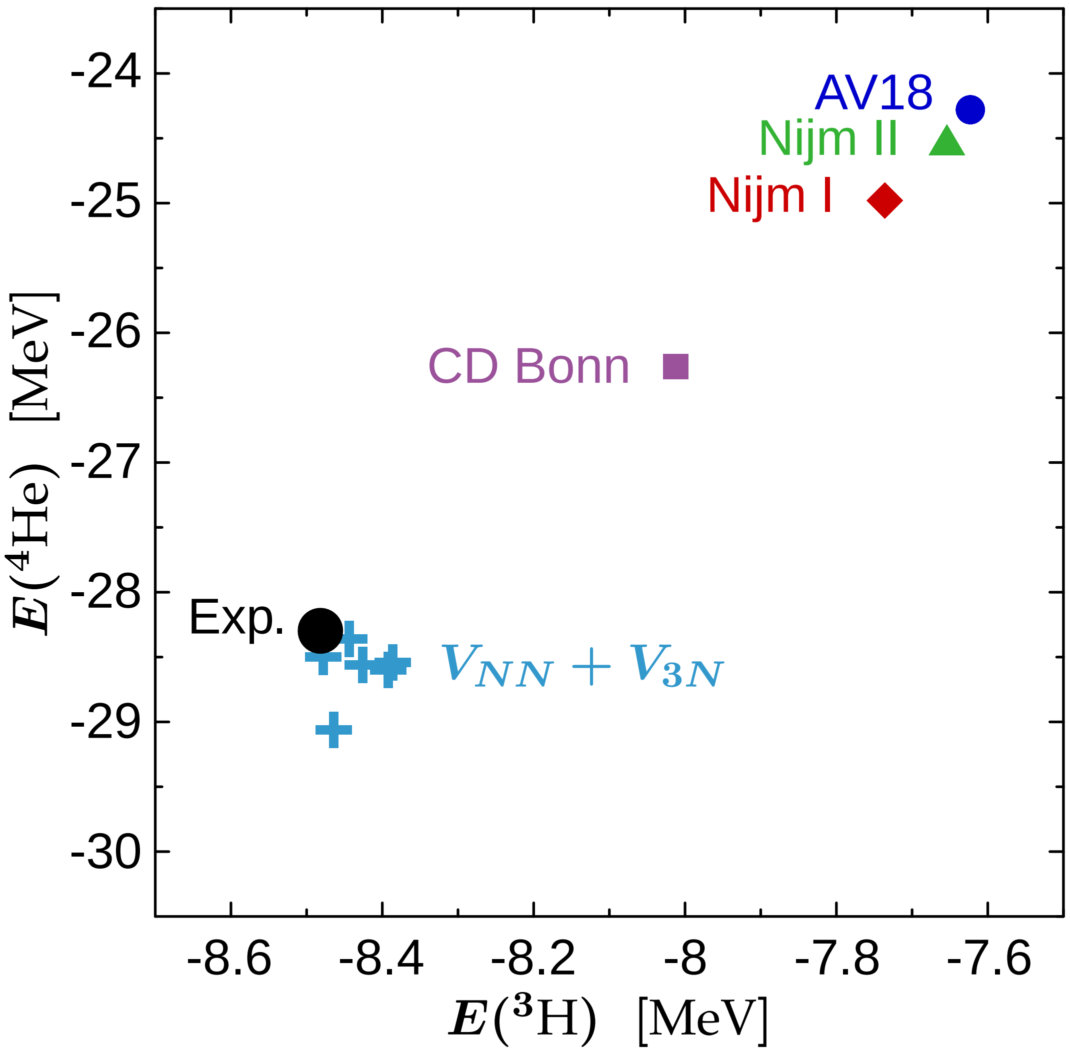
Three-Body Interactions — Strategies

Correlated Hamiltonian in Many-Body Space

$$\begin{aligned}\widetilde{\mathrm{H}} &= \mathrm{C}^{\dagger}\,(\mathrm{T} + \mathrm{V}_{NN} + \mathrm{V}_{3N})\,\mathrm{C} \\ &= \widetilde{\mathrm{T}}^{[1]} \;+\; (\widetilde{\mathrm{T}}^{[2]} + \widetilde{\mathrm{V}}_{NN}^{[2]}) \;+\; (\widetilde{\mathrm{T}}^{[3]} + \widetilde{\mathrm{V}}_{NN}^{[3]} + \widetilde{\mathrm{V}}_{3N}^{[3]}) \;+\; \cdots \\ &= \mathrm{T} \;+\; \mathrm{V}_{\mathrm{UCOM}} \;+\; \mathrm{V}_{\mathrm{UCOM}}^{[3]} \;+\; \cdots\end{aligned}$$

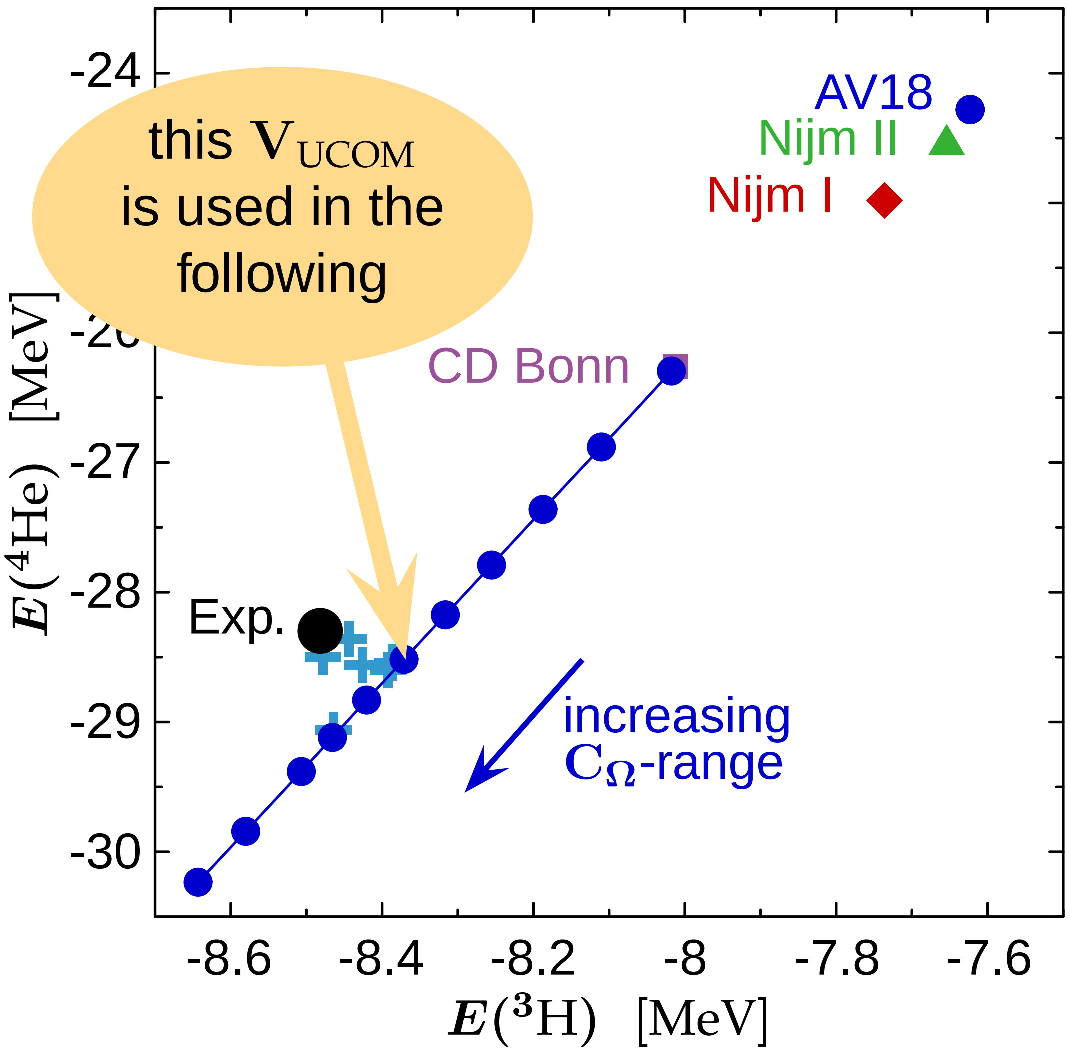
- **include full** $\mathrm{V}_{\mathrm{UCOM}}^{[3]}$ consisting of genuine and induced 3N terms
  (not really feasible beyond lightest isotopes)
- **replace** $\mathrm{V}_{\mathrm{UCOM}}^{[3]}$ by phenomenological three-body force
  (tractable also for heavier nuclei)
- **minimize** $\mathrm{V}_{\mathrm{UCOM}}^{[3]}$ by proper choice of unitary transformation
  (calculation with a pure two-body interaction)

Three-Body Interactions — Tjon Line



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

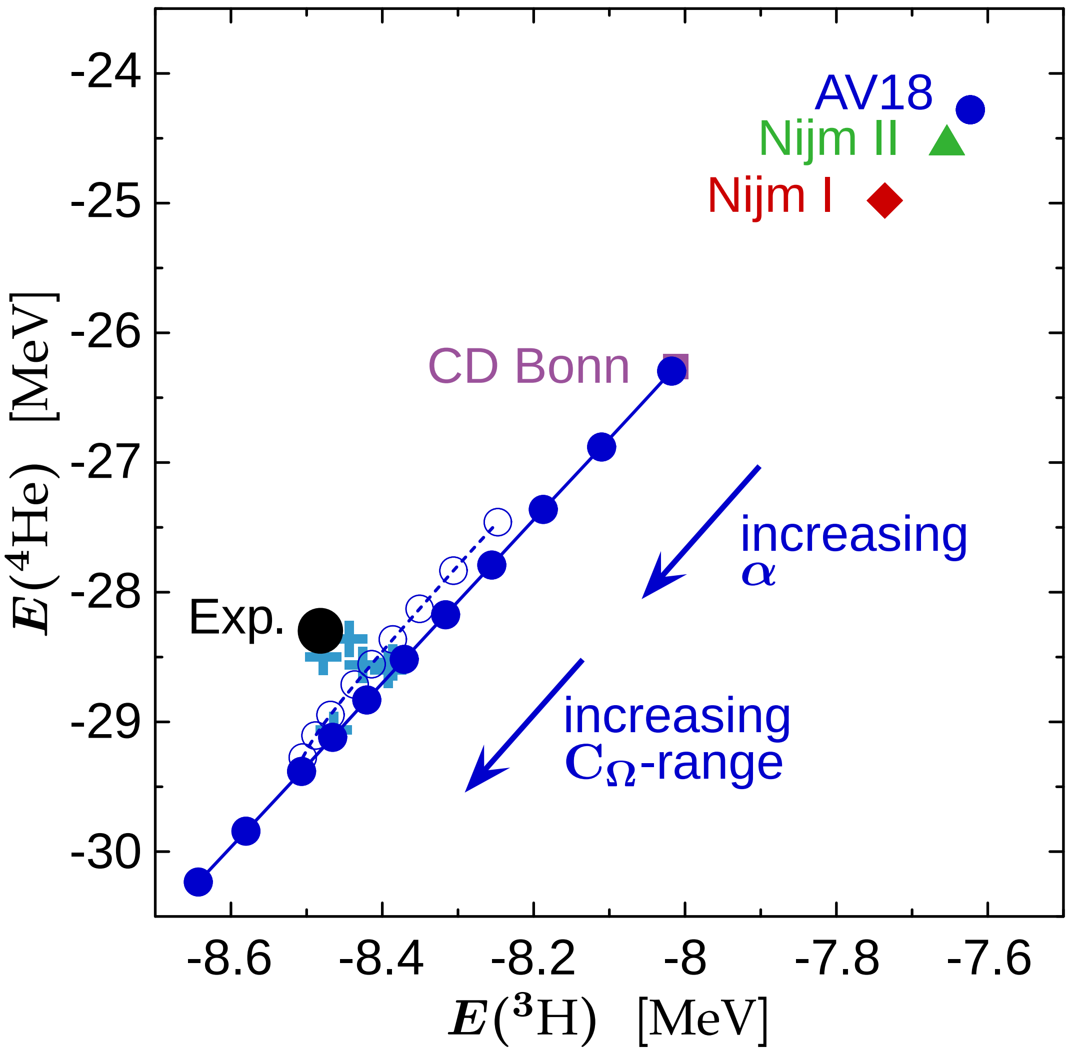
Three-Body Interactions — Tjon Line



- **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

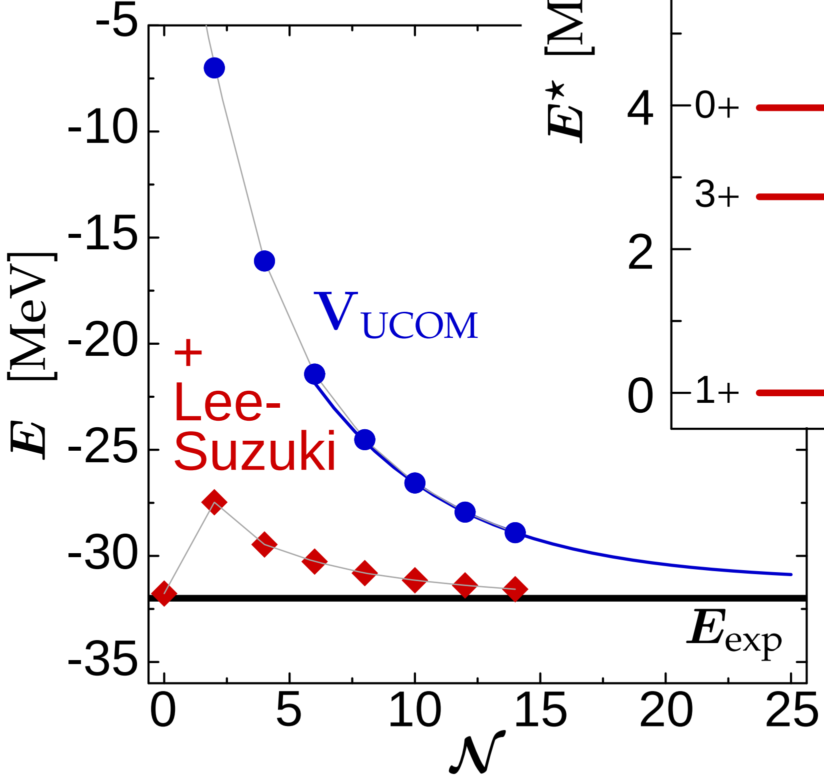
Three-Body Interactions — Tjon Line

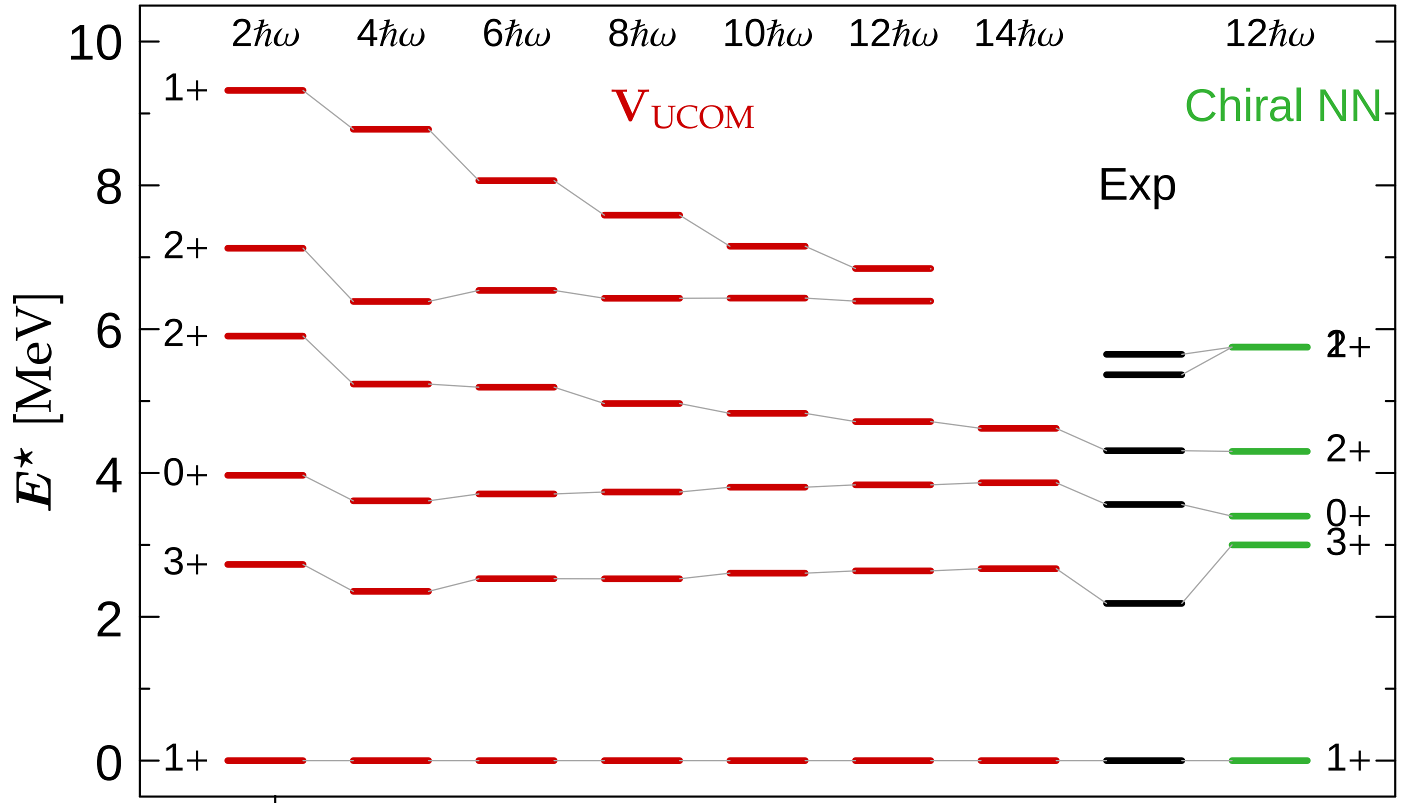


- **Tjon-line**: $E(^4\mathrm{He})$ vs. $E(^3\mathrm{H})$ for phase-shift equivalent NN-interactions
- same behavior for the SRG interaction as function of α

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

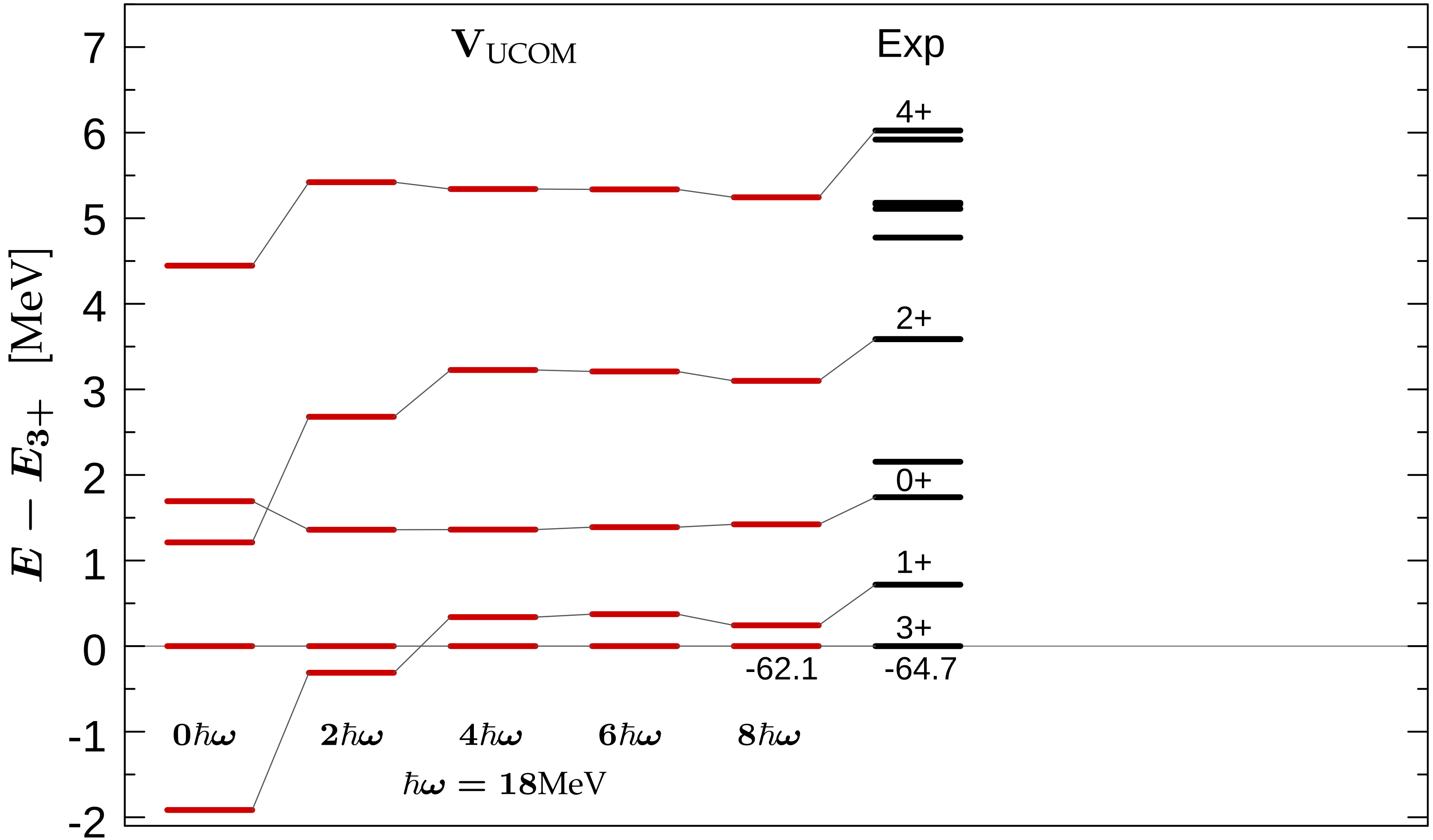
^{6}Li: NCSM throughout the p-Shell



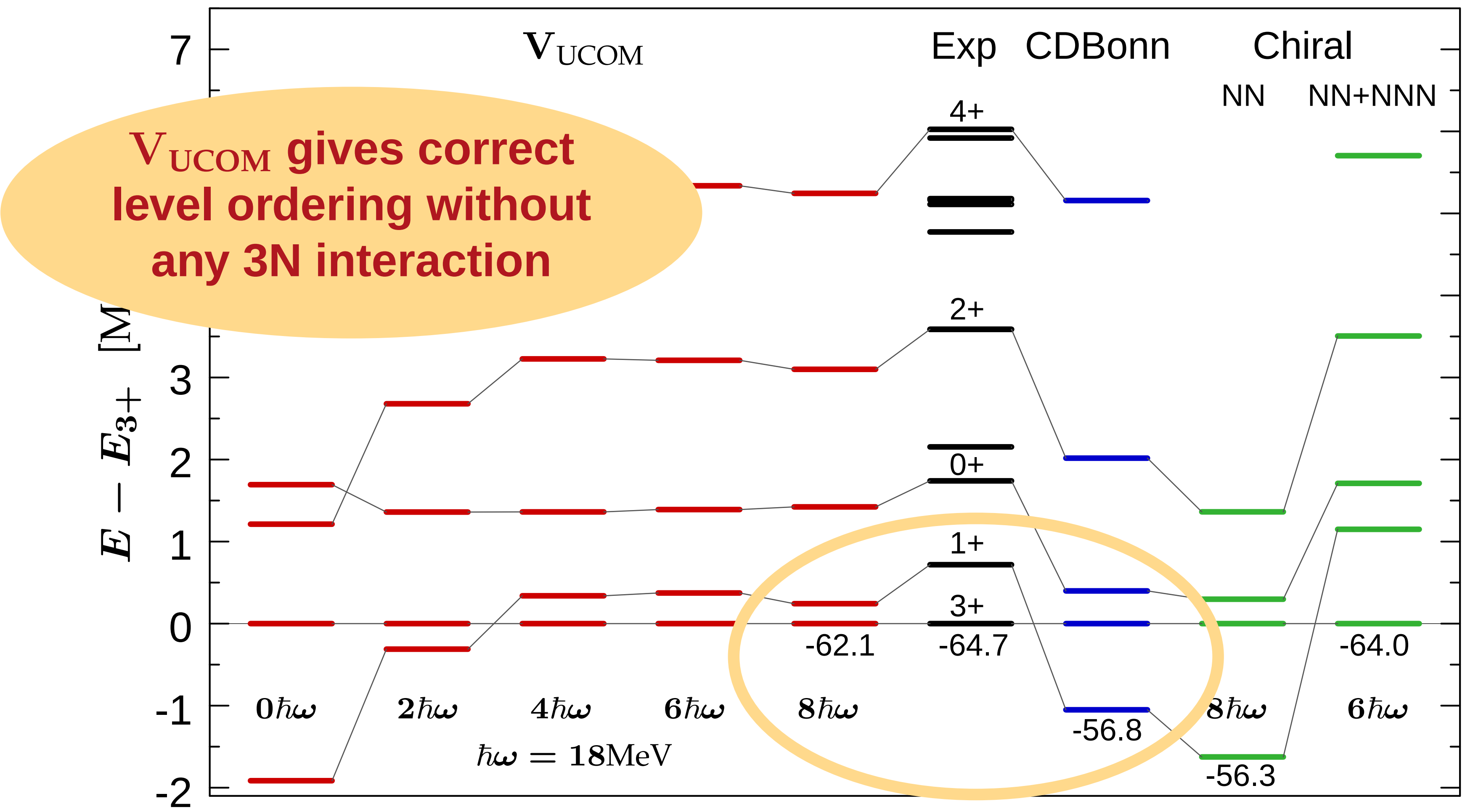


systematic NCSM studies
throughout p-shell with V_{UCOM}
(+ Lee-Suzuki transformation)

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



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



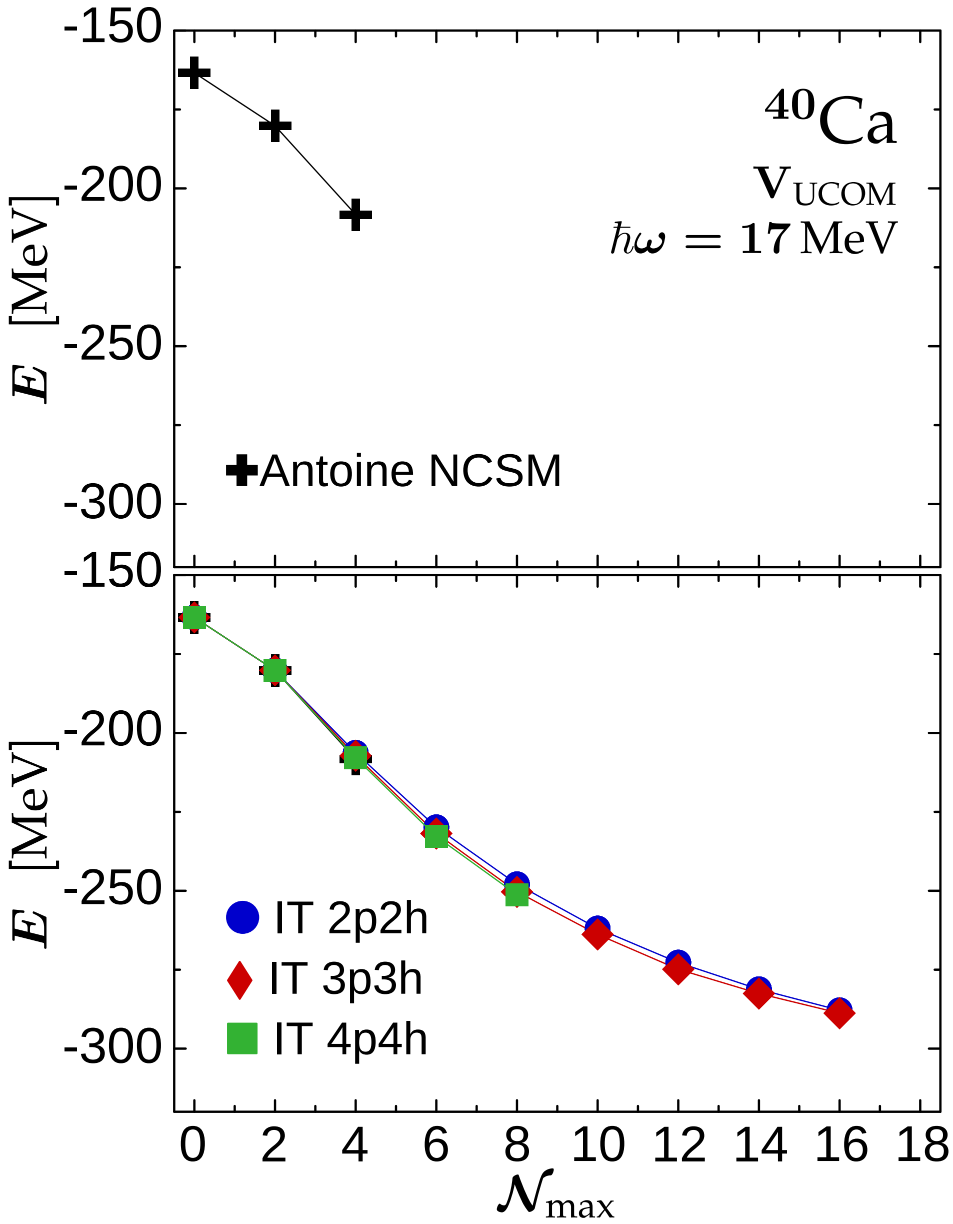
Importance Truncated NCSM

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



Many-Body Methods II:

Hartree-Fock & Beyond

Reminder: Hartree-Fock Approximation

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

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

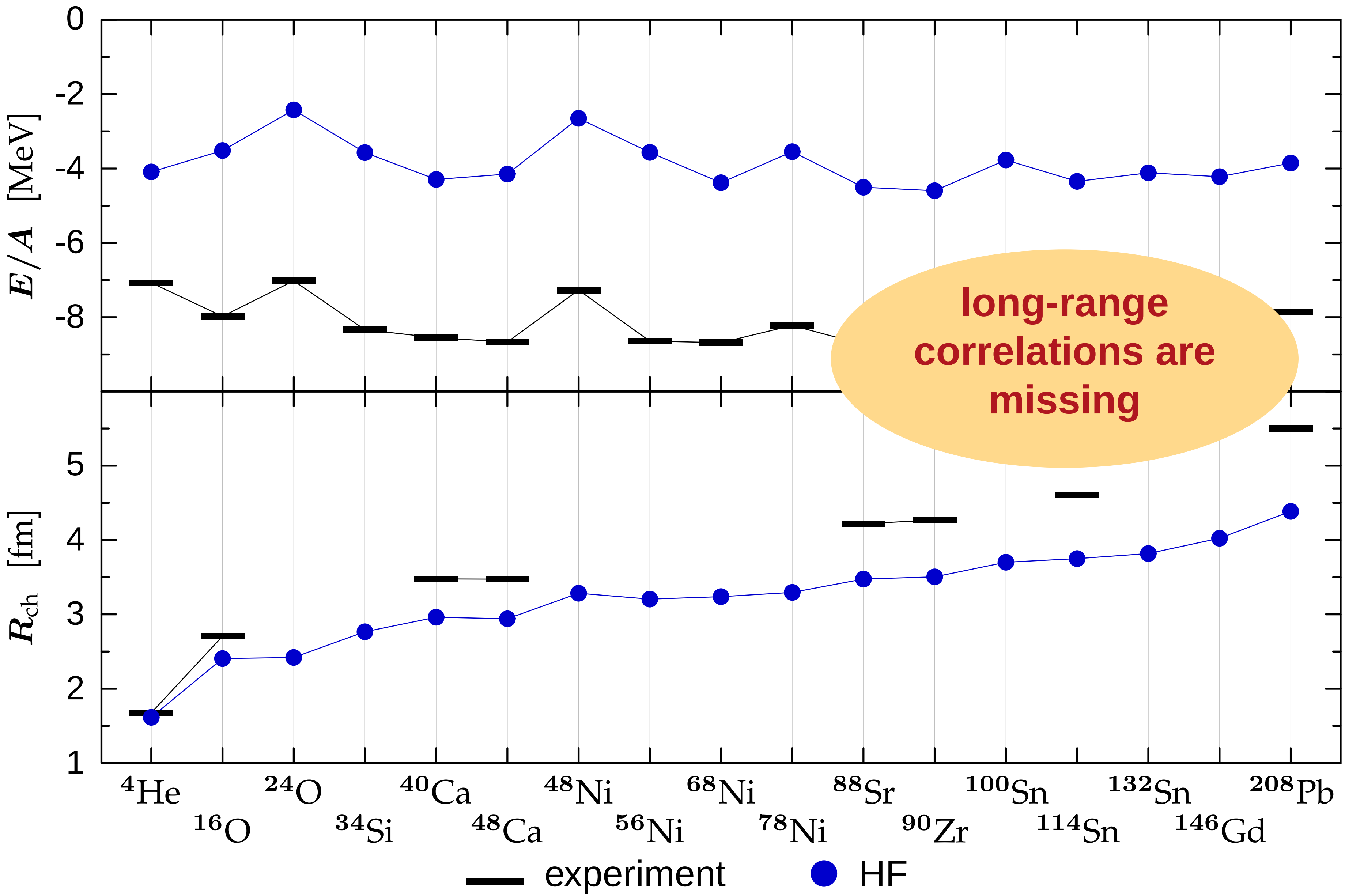
- **variational calculation**: single-particle states $\left|\phi_i\right\rangle$ determined by minimizing the energy expectation value

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

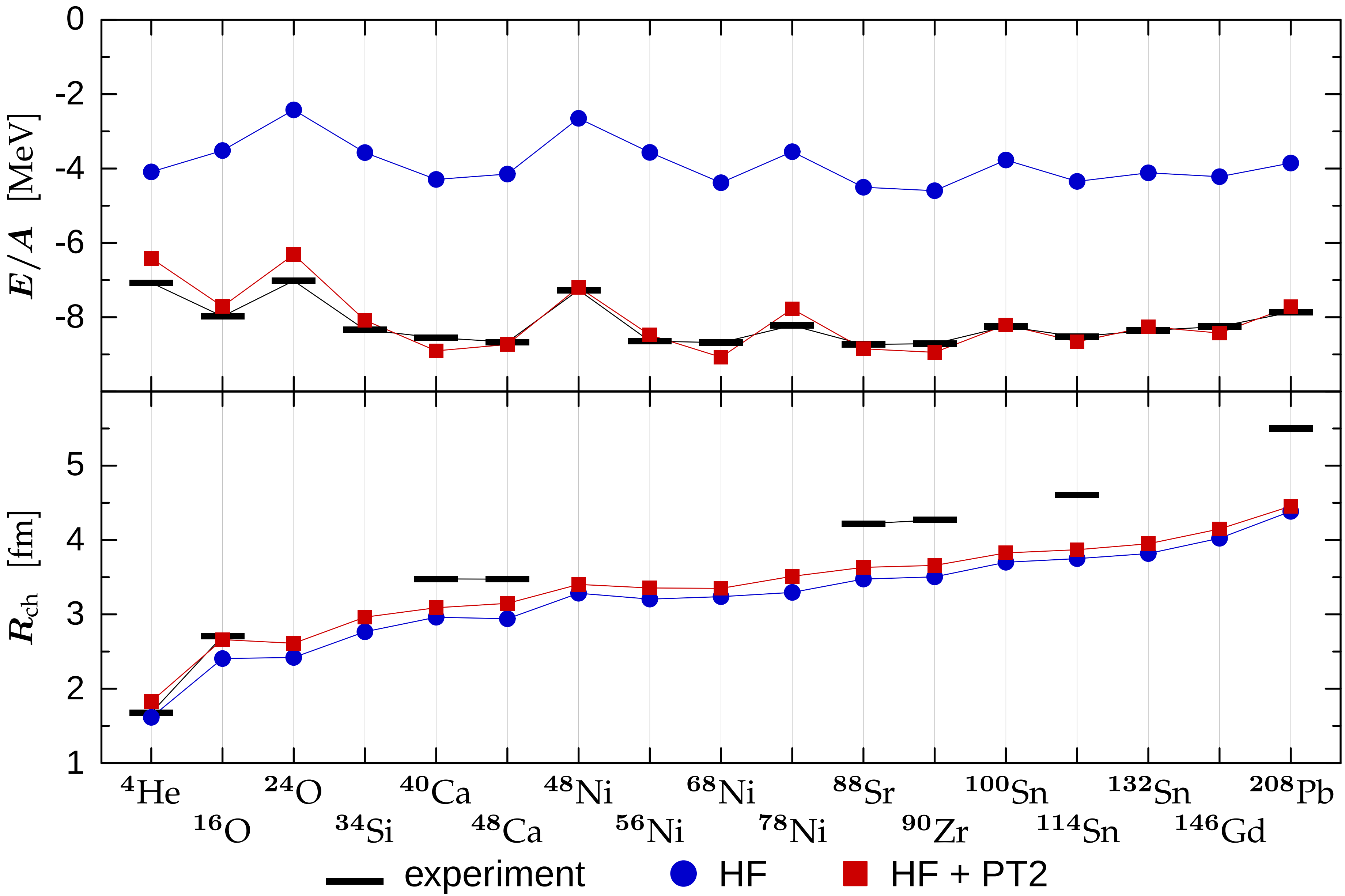
single Slater determinant by definition **cannot describe any correlations** (independent particle state)

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

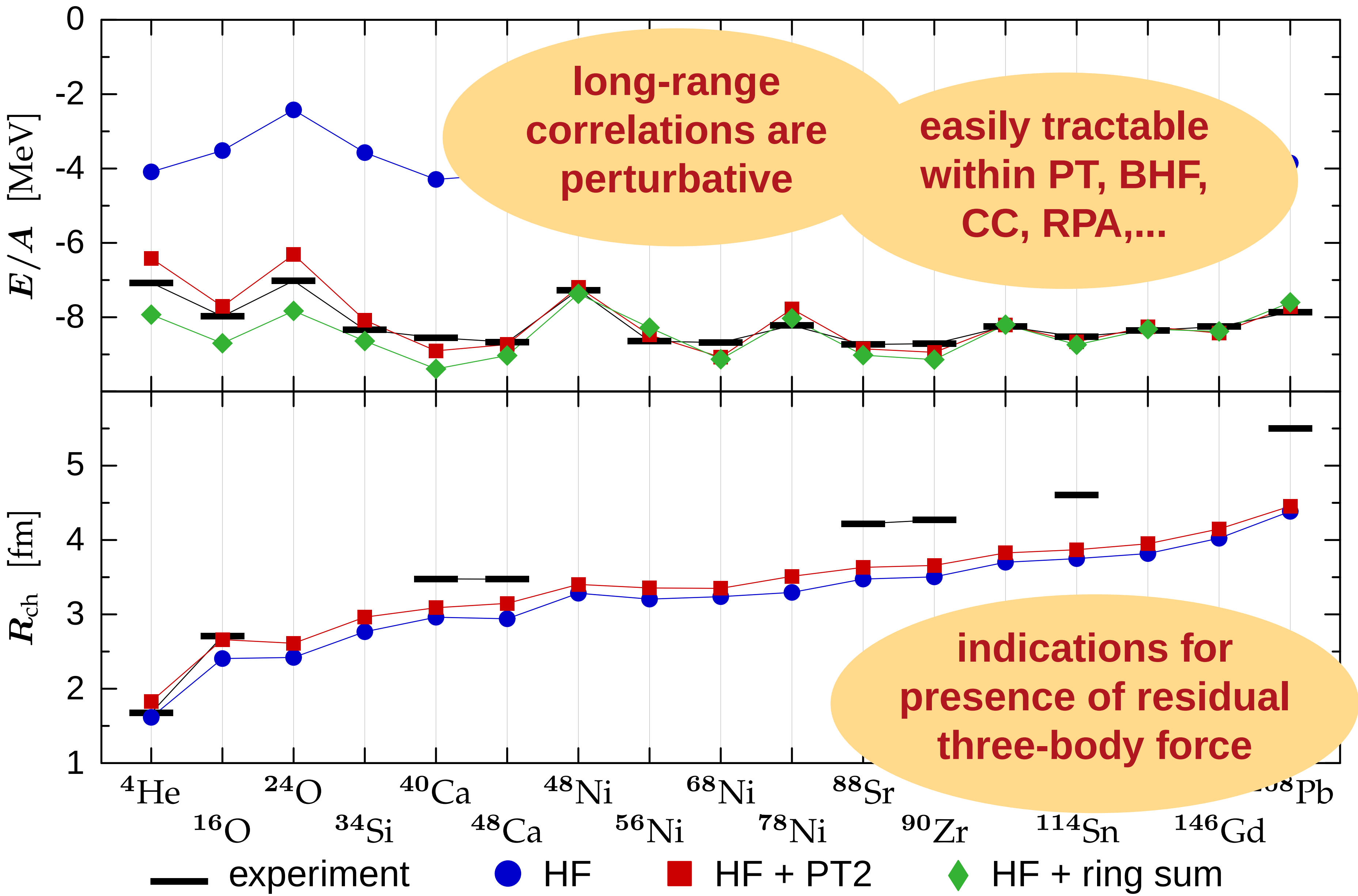
Hartree-Fock with V_{UCOM}



Perturbation Theory with V_{UCOM}



RPA Ring Summation with V_{UCOM}



Many-Body Methods III

RPA & Beyond

Reminder: Random Phase Approximation

- describe **excited states** via vibration creation operator $Q_\nu^\dagger$

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

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

$$Q_\nu^\dagger = \sum_{ph} X_{ph}^\nu a_p^\dagger a_h - \sum_{ph} Y_{ph}^\nu a_h^\dagger a_p$$

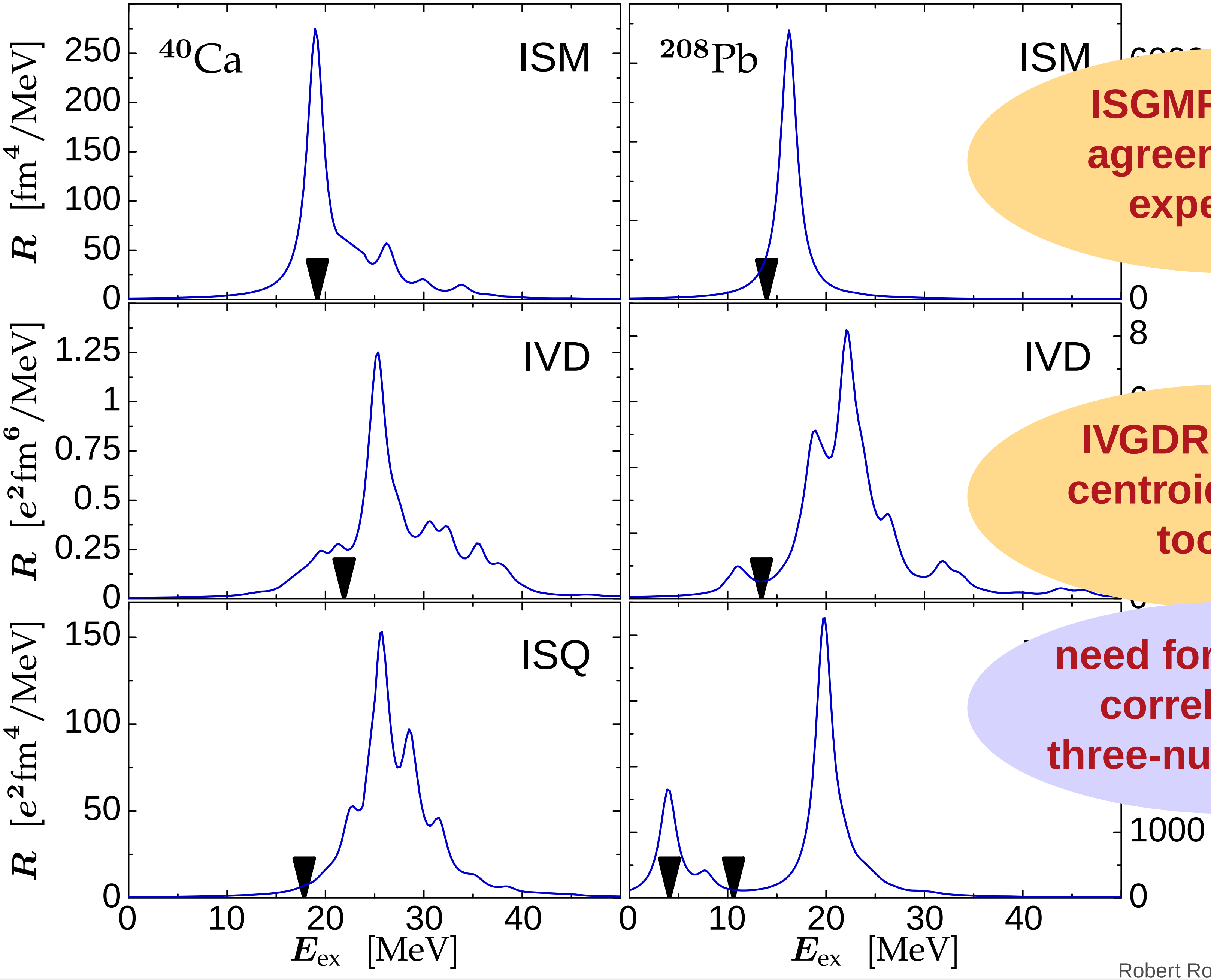
- formal solution of eigenvalue problem via equations of motion method approximating vacuum state by $|\mathrm{HF}\rangle$ yields **RPA equations**

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

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

- **self-consistent** solution using the same Hamiltonian $\mathrm{H}_{\mathrm{int}}$ as in HF

RPA with V_{UCOM}

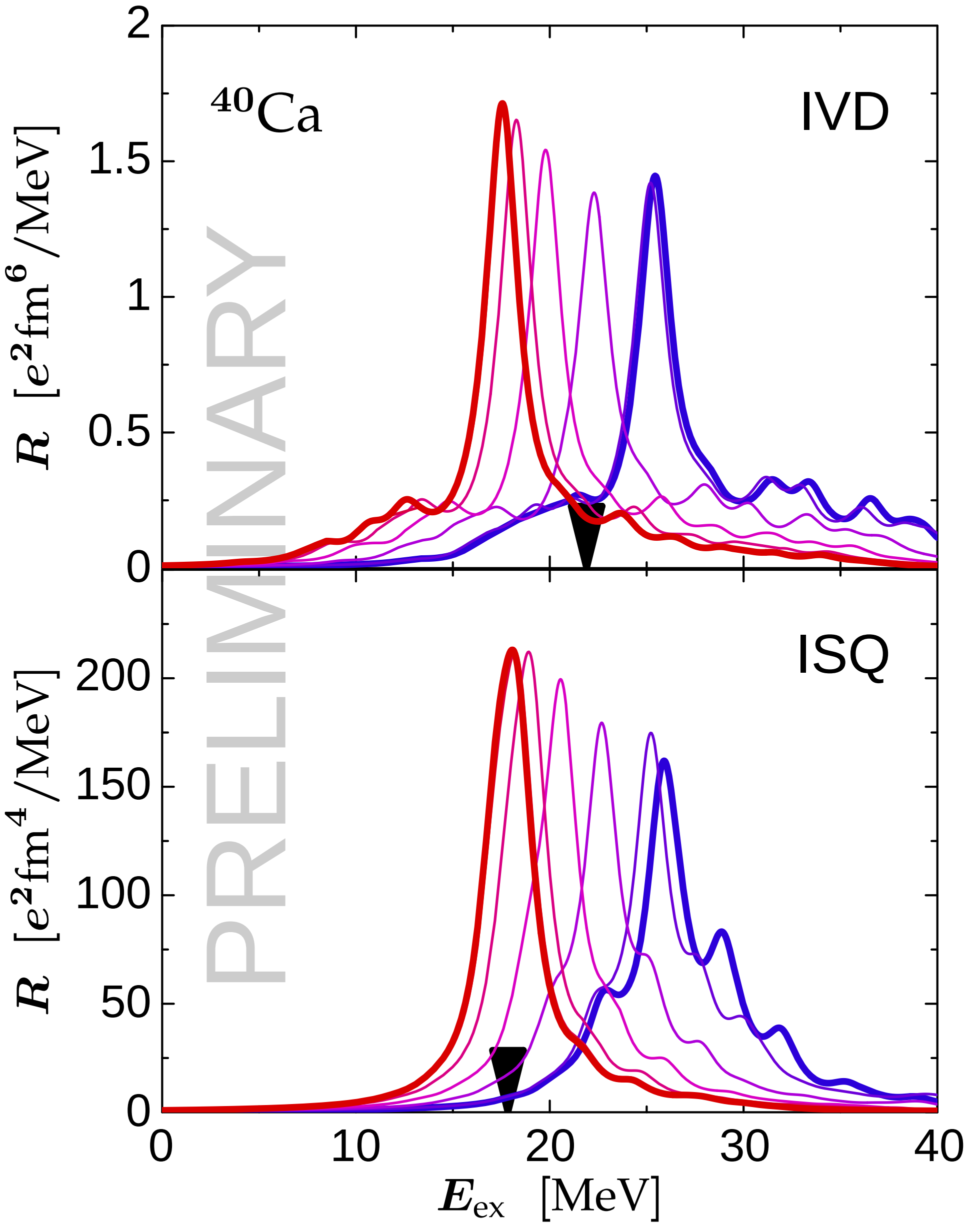


ISGMR in good agreement with experiment

IVGDR & ISGQR centroid energies too high

need for additional correlations & three-nucleon force

SRPA: Complex Configurations



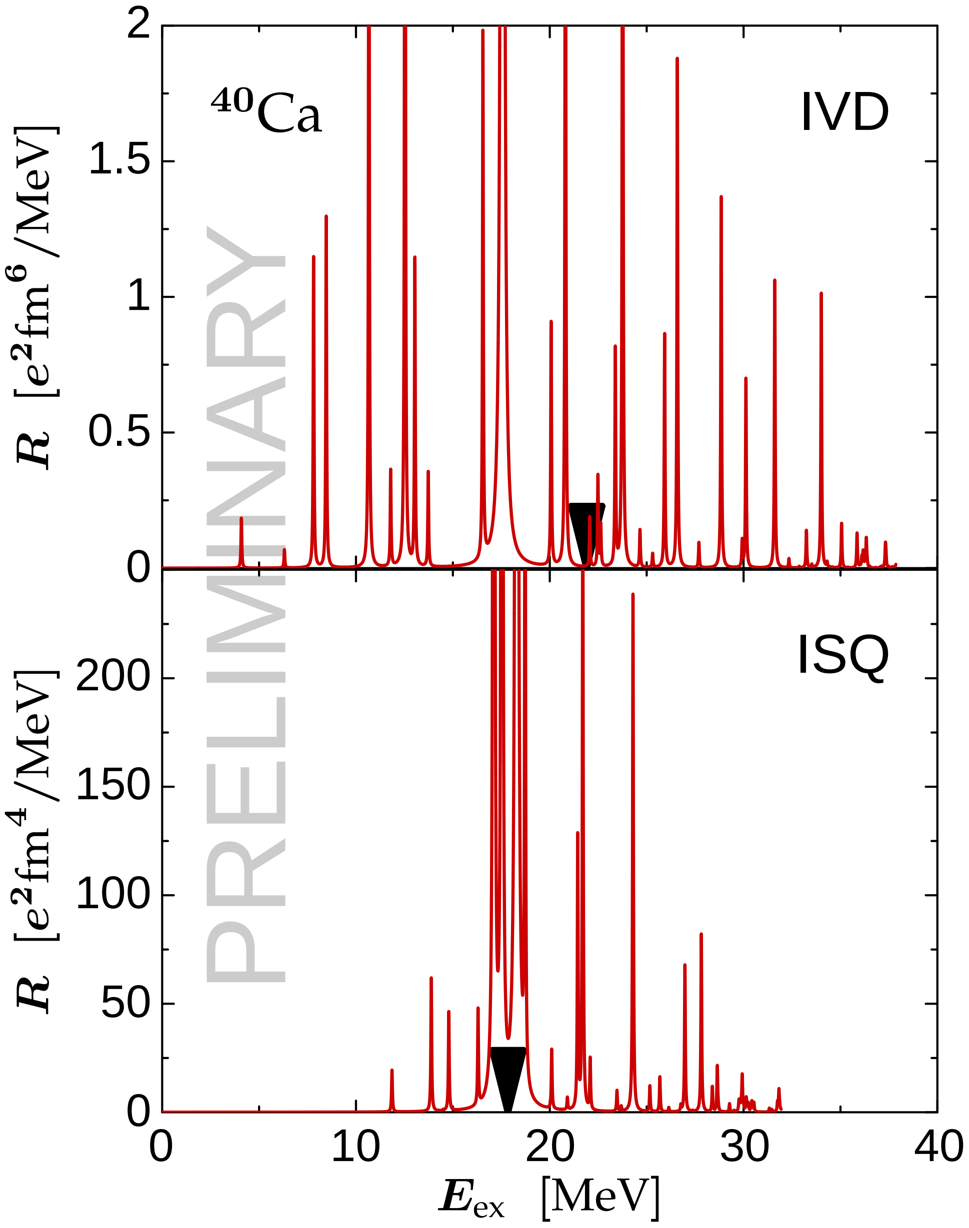
RPA (full 1p1h space)

SRPA (full 1p1h+2p2h space)

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

complex configurations have significant impact on response

SRPA: Complex Configurations



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

- **Modern Effective Interactions**
  - treatment of short-range central and tensor correlations by unitary transformations: UCOM, SRG, Lee-Suzuki,...
  - universal phase-shift equivalent correlated interaction $\mathbf{V}_{\mathrm{UCOM}}$

- **Innovative Many-Body Methods**
  - No-Core Shell Model, Importance Truncation
  - Hartree-Fock, MBPT, 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**
  - S. Binder, P. Hedfeld, H. Hergert, M. Hild, P. Papakonstantinou, S. Reinhardt, F. Schmitt, I. Türschmann, A. Zapp

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