Hartree-Fock and Hartree-Fock-Bogoliubov with Modern Effective Interactions

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Overview

- Motivation
- Modern Effective Interactions
  - Unitary Correlation Operator Method
  - Similarity Renormalization Group
- Few-Body Systems
- Many-Body Systems
  - Hartree-Fock, Many-Body Perturbation Theory & Beyond
  - Hartree-Fock-Bogoliubov
- Conclusions

From QCD to Nuclear Structure

Nuclear Structure

Low-Energy QCD

From QCD to Nuclear Structure

Nuclear Structure

Realistic Nuclear Interactions

Low-Energy QCD

- chiral interactions: consistent NN & 3N interaction derived within χEFT
- traditional NN-interactions: Argonne V18, CD Bonn,...
- reproduce experimental NN phase-shifts with high precision
- induce strong short-range central & tensor correlations

From QCD to Nuclear Structure

Nuclear Structure

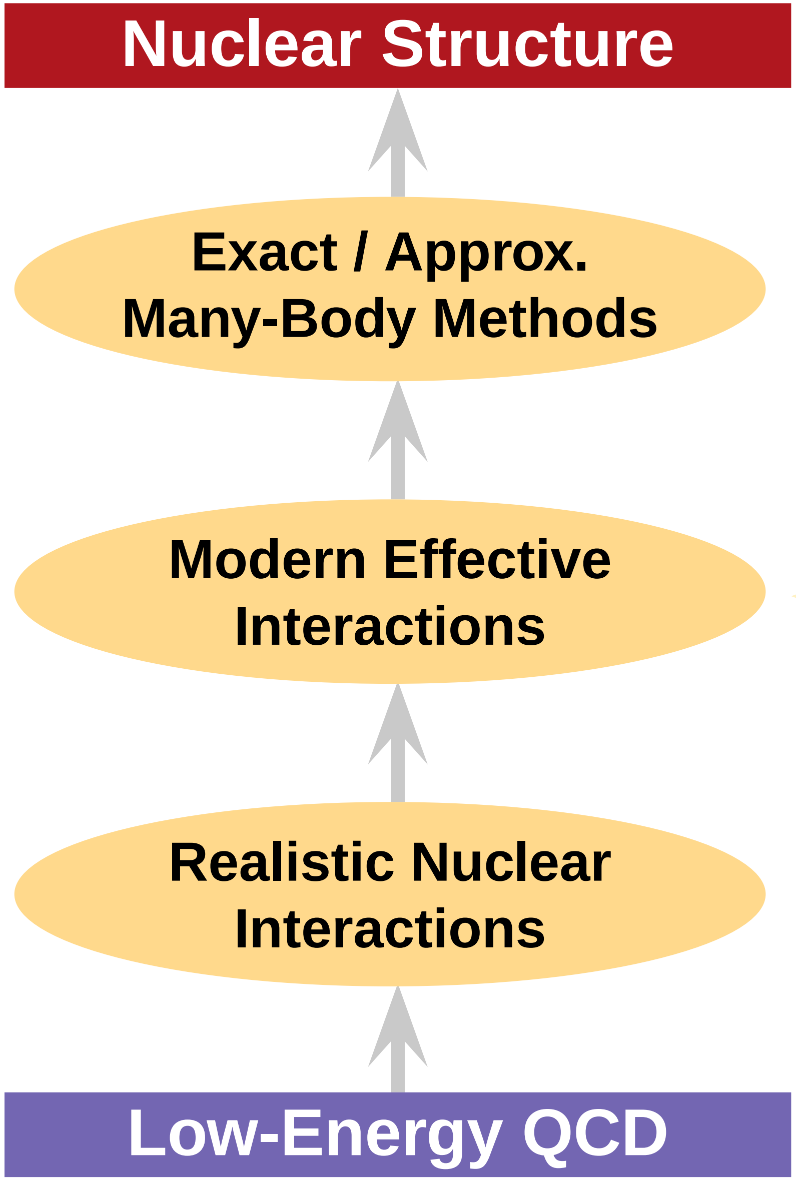
Exact / Approx. Many-Body Methods

- ‘exact’ solution of the many-body problem for light and intermediate masses (GFMC, NCSM, CC,...)
- controlled approximations for heavier nuclei (HF & MBPT,...)
- rely on restricted model spaces of tractable size
- not suitable for the description of short-range correlations

Realistic Nuclear Interactions

Low-Energy QCD

From QCD to Nuclear Structure



- adapt realistic potential to the available model space
  - tame short-range correlations
  - improve convergence behavior
- conserve experimentally constrained properties (phase shifts)
  - generate new realistic interaction
- provide consistent effective interaction & effective operators
- unitary transformations most convenient

Deuteron: Manifestation of Correlations

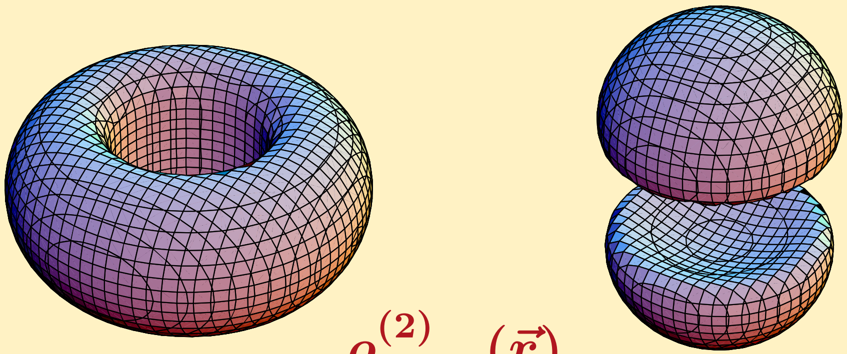
Argonne V18 Deuteron Solution

$M_S = 0$

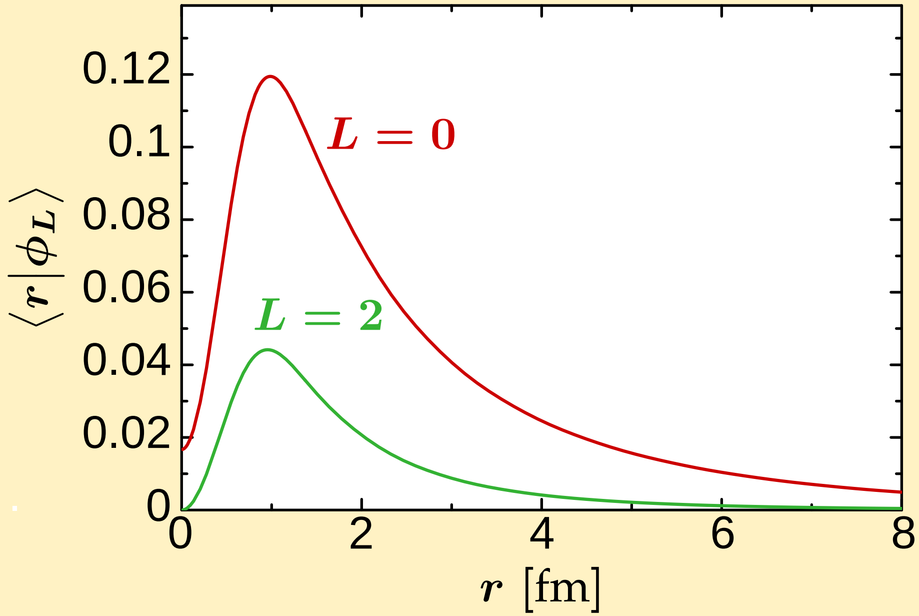
$\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$

$M_S = \pm 1$

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



$\rho^{(2)}_{1,M_S}(\vec{r})$



short-range repulsion supresses wavefunction at small distances r

central correlations

tensor interaction generates D-wave admixture in the ground state

tensor correlations

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

$$\mathbf{g}_r = \frac{1}{2}\big[s(\mathrm{r})\, \mathrm{q}_r + \mathrm{q}_r\, s(\mathrm{r})\big]$$

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

Tensor Correlator C_Ω

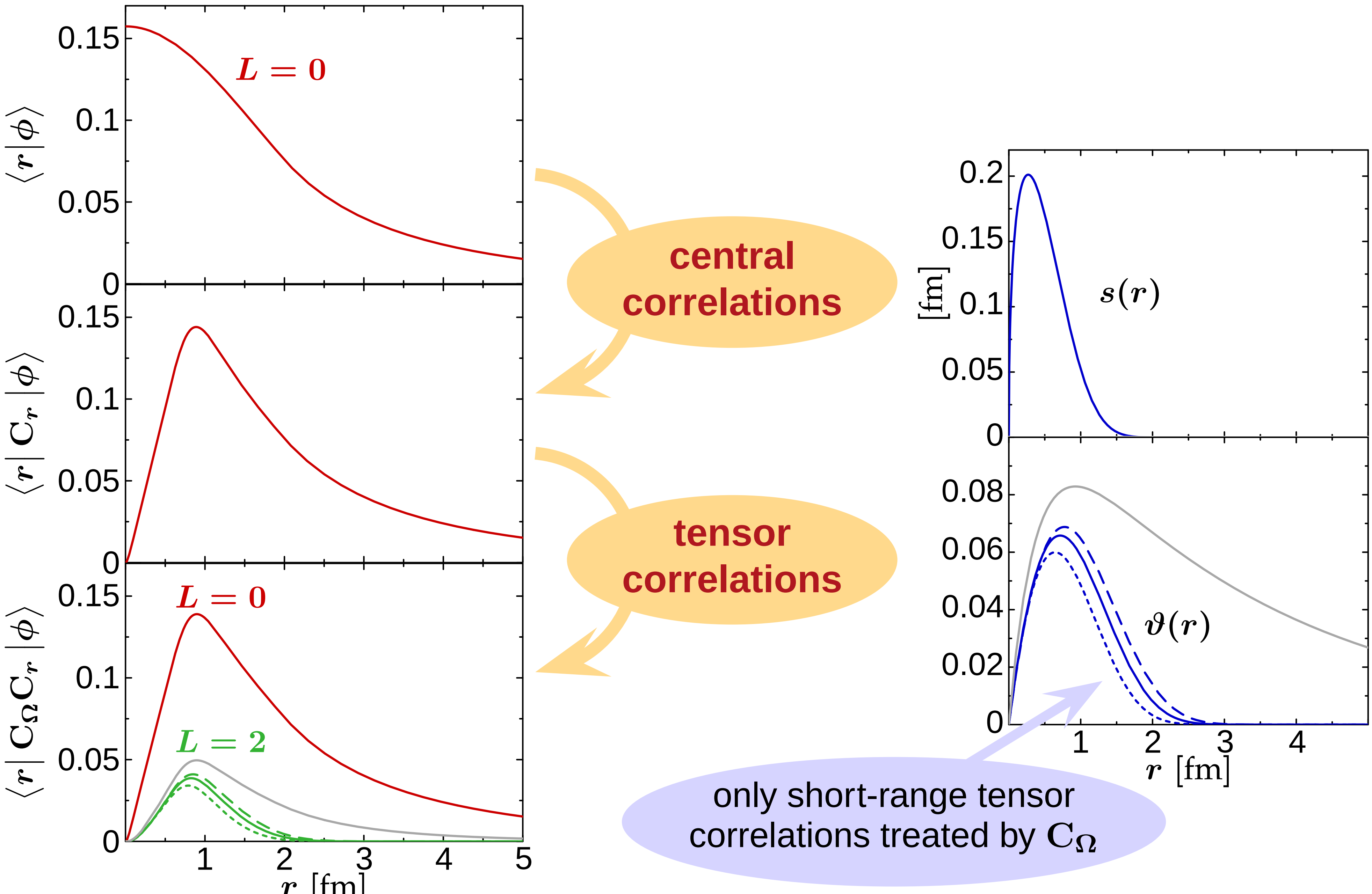
- angular shift depending on the orientation of spin and relative coordinate of a nucleon pair

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

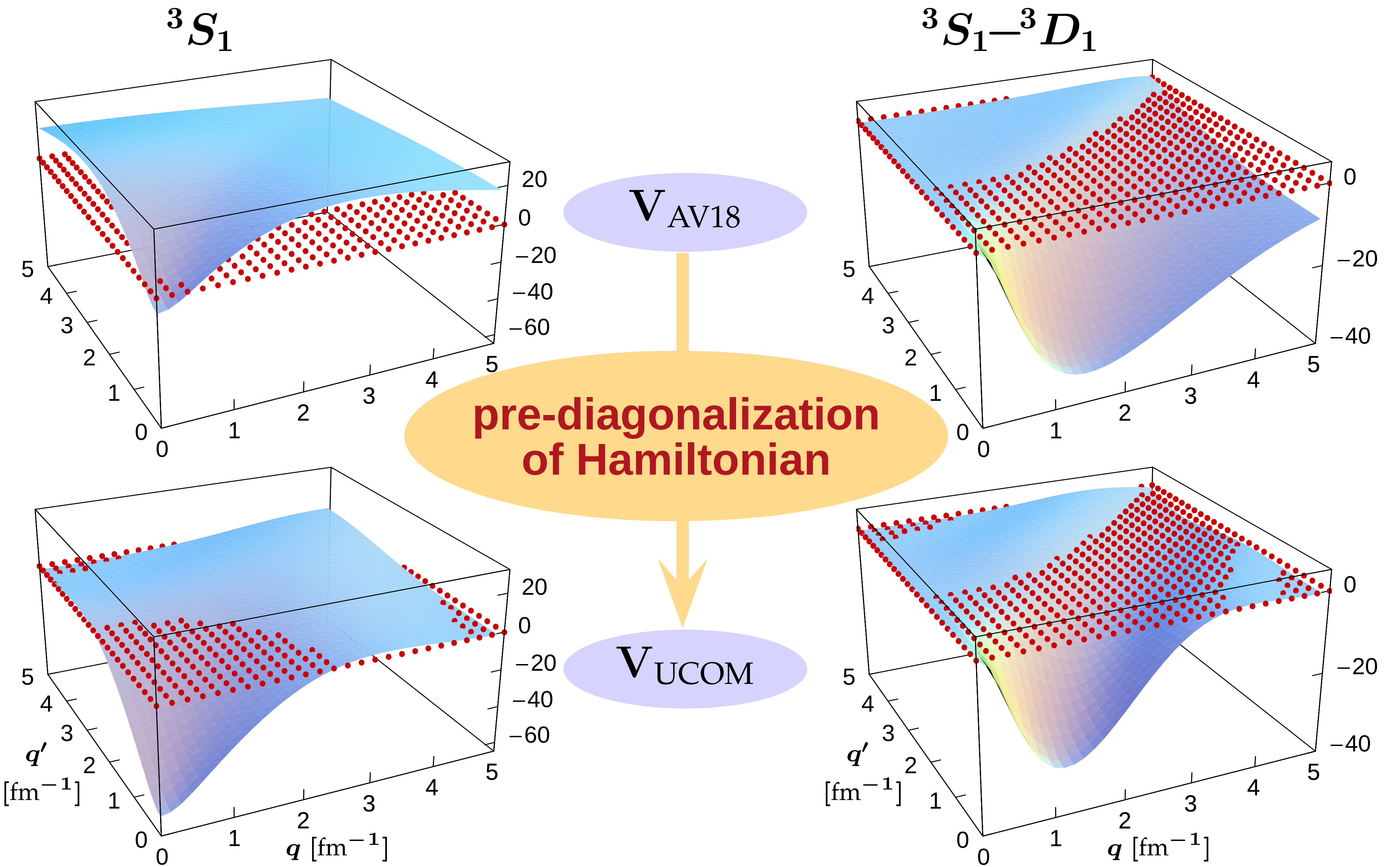
$$\vec{\mathrm{q}}_\Omega = \vec{\mathrm{q}} - \tfrac{\vec{\mathrm{r}}}{\mathrm{r}}\, \mathrm{q}_r$$

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

Correlated States: The Deuteron



Correlated Interaction: V_{UCOM}



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

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

[Bogner et al., PRC**75** 061001(R) (2007); Hergert & Roth, PRC**75** 051001(R) (2007)]

The SRG Generator: A Closer Look

- typical NN interaction operators:

$$\mathbf{O}_p \in \{\mathbb{1}, \vec{\boldsymbol{\sigma}}_1 \cdot \vec{\boldsymbol{\sigma}}_2, \vec{\mathbf{l}}^2, \vec{\mathbf{l}} \cdot \vec{\mathbf{s}}, \mathbf{s}_{12}(\vec{\mathbf{r}}, \vec{\mathbf{r}}), \ldots\} \otimes \{\mathbb{1}, \vec{\boldsymbol{\tau}}_1 \cdot \vec{\boldsymbol{\tau}}_2, \ldots\}$$

Radial Kinetic Energy

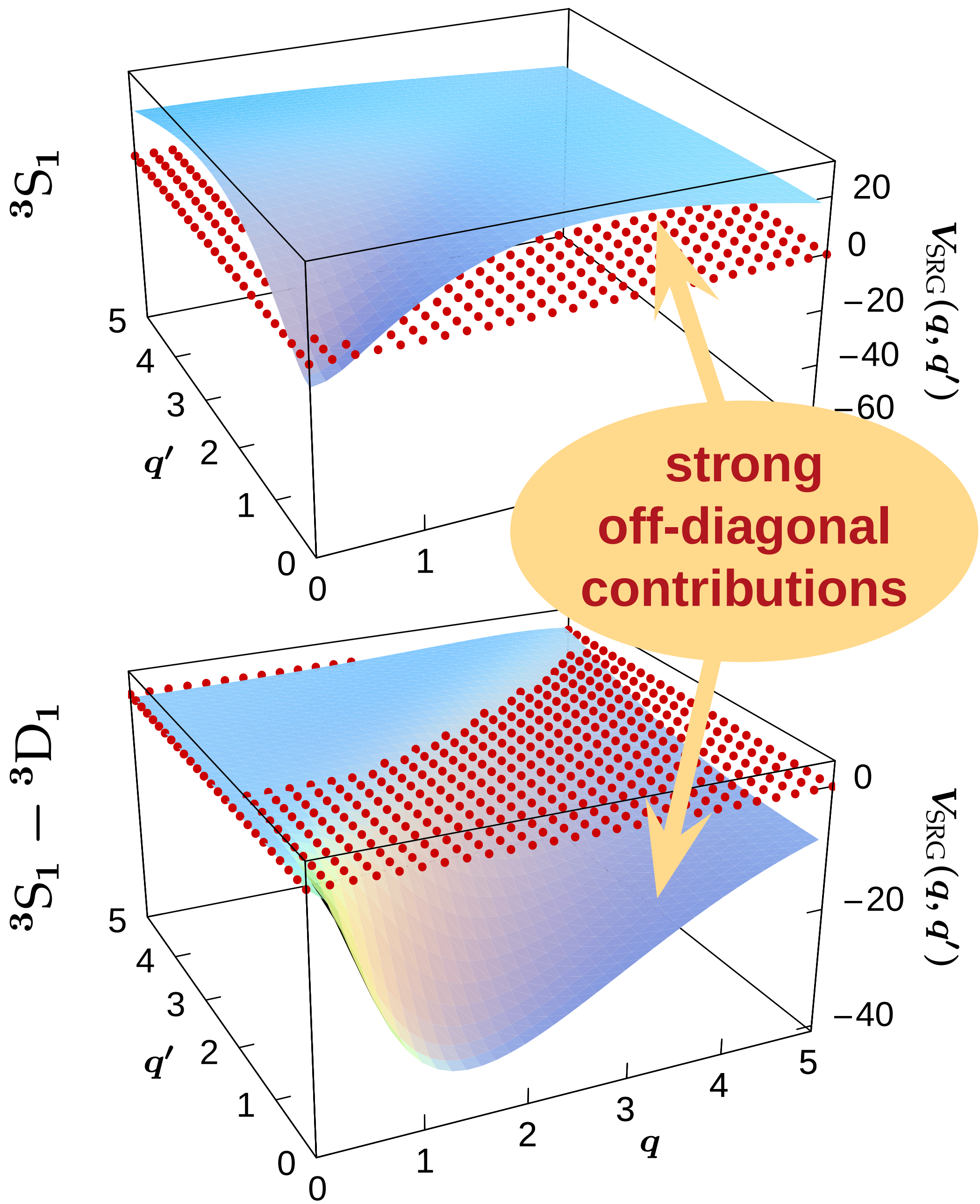
$$\boldsymbol{\eta}_r(0) \sim \left[\mathbf{q}_r^2, \mathbf{V}\right] = \sum_p \left[\mathbf{q}_r^2, v_p(\mathbf{r})\mathbf{O}_p\right] = \sum_p \left(\mathbf{q}_r v_p'(\mathbf{r})\mathbf{O}_p + \mathbf{O}_p v_p'(\mathbf{r})\mathbf{q}_r\right)$$

Angular Kinetic Energy

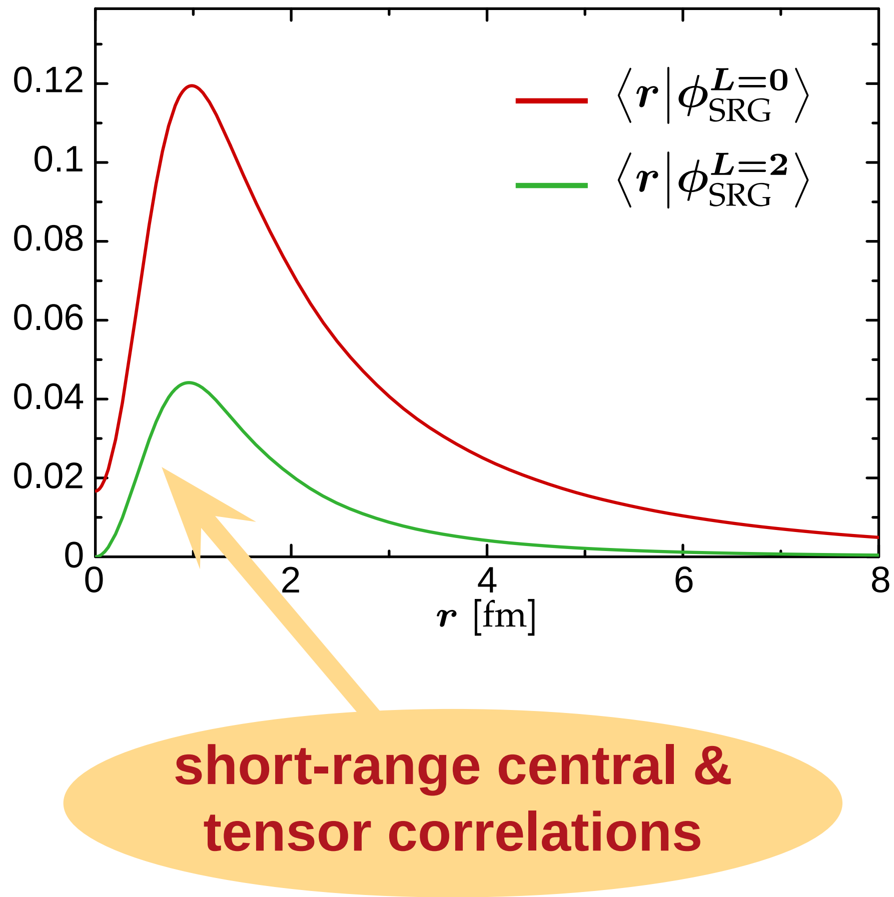
$$\boldsymbol{\eta}_\Omega(0) \sim \left[\vec{\mathbf{l}}^2, \mathbf{V}\right] = \left[\vec{\mathbf{l}}^2, v_t(\mathbf{r})\mathbf{s}_{12}(\vec{\mathbf{r}}, \vec{\mathbf{r}})\right] = -4i v_t(\mathbf{r})\mathbf{s}_{12}(\vec{\mathbf{r}}, \vec{\mathbf{q}}_\Omega)$$

☞ $\boldsymbol{\eta}(0)$ has the same structure as the UCOM generators $\mathbf{g}_r$ and $\mathbf{g}_\Omega$

SRG Evolution: The Deuteron



Argonne V18



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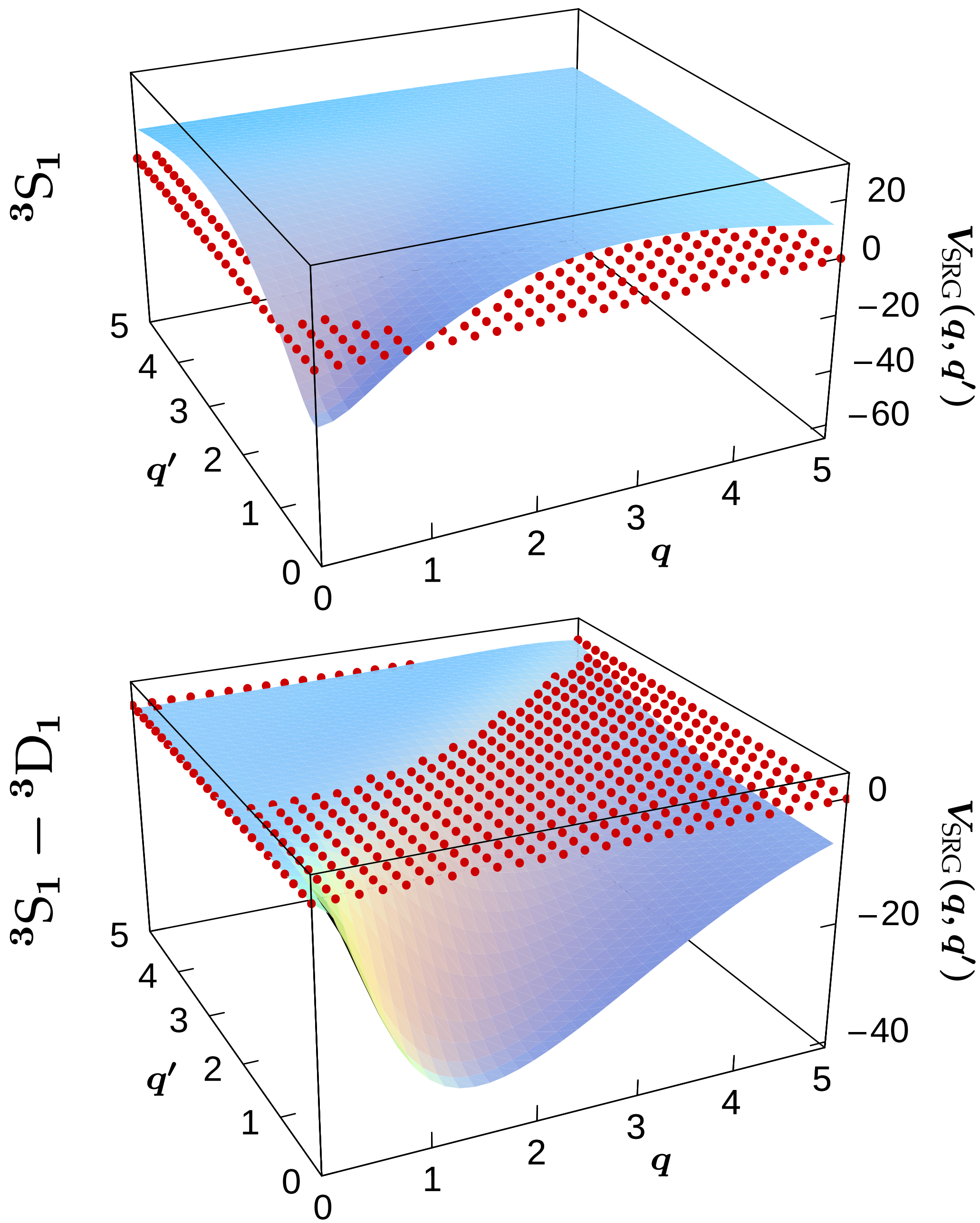
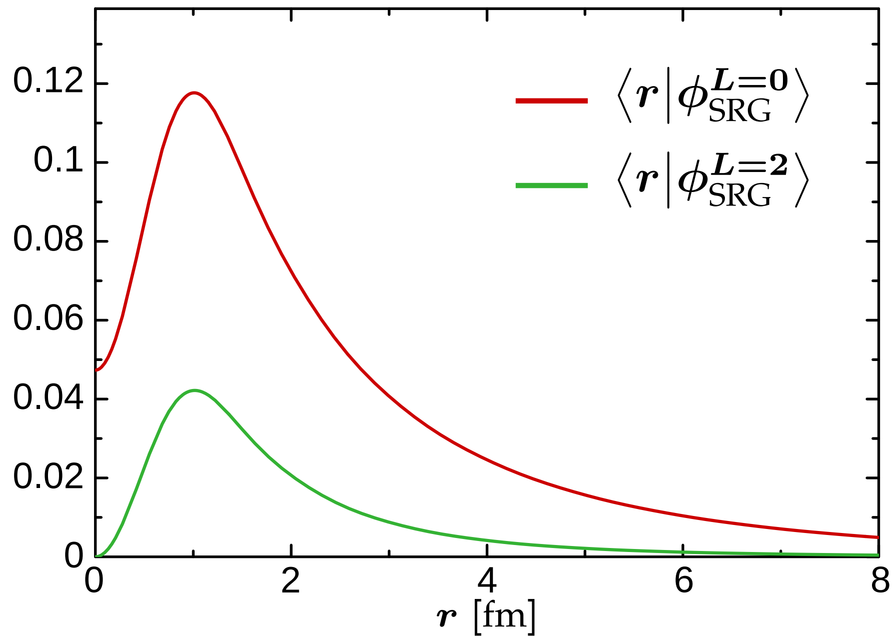


$\alpha = 0.0004\,\mathrm{fm}^4$



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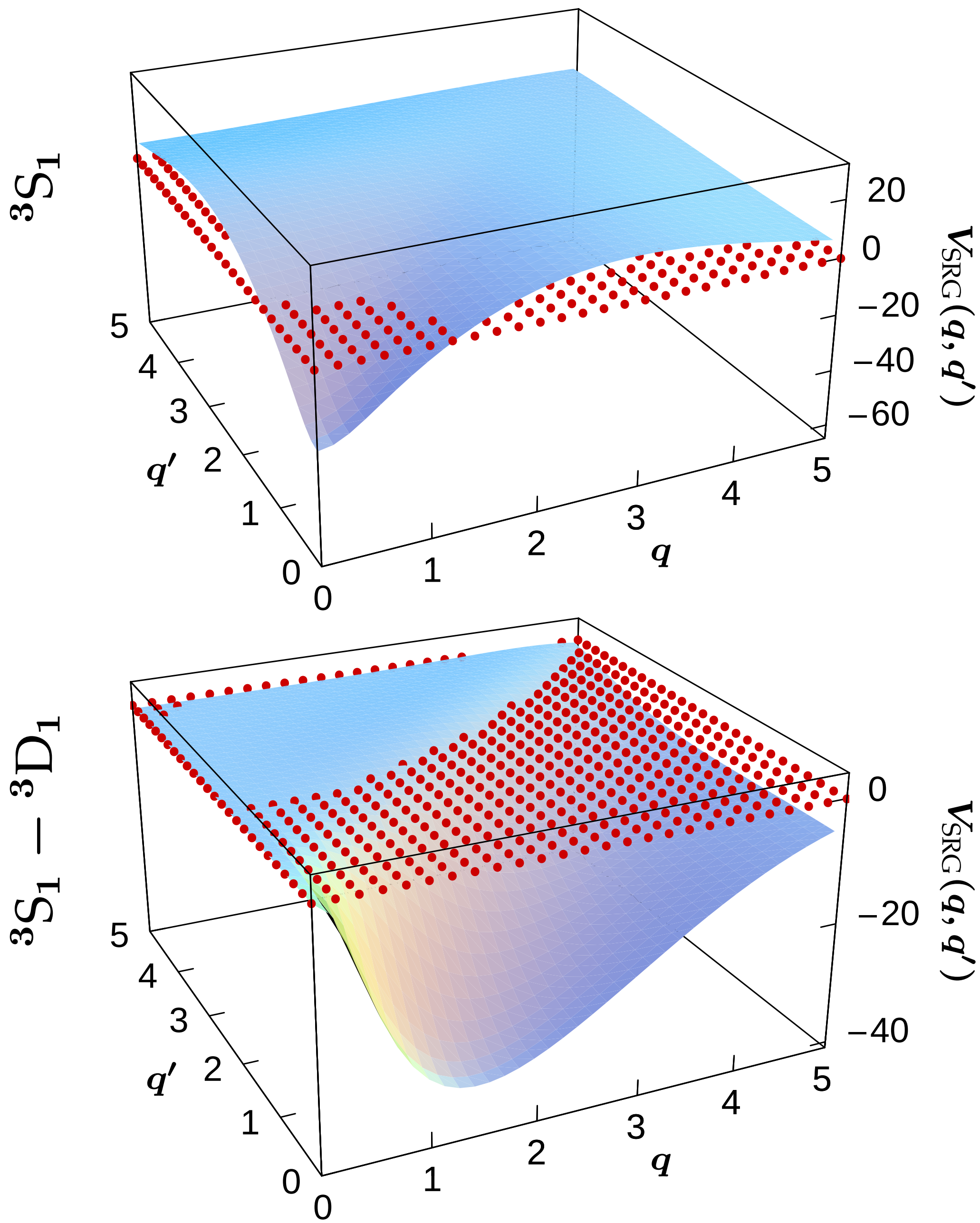
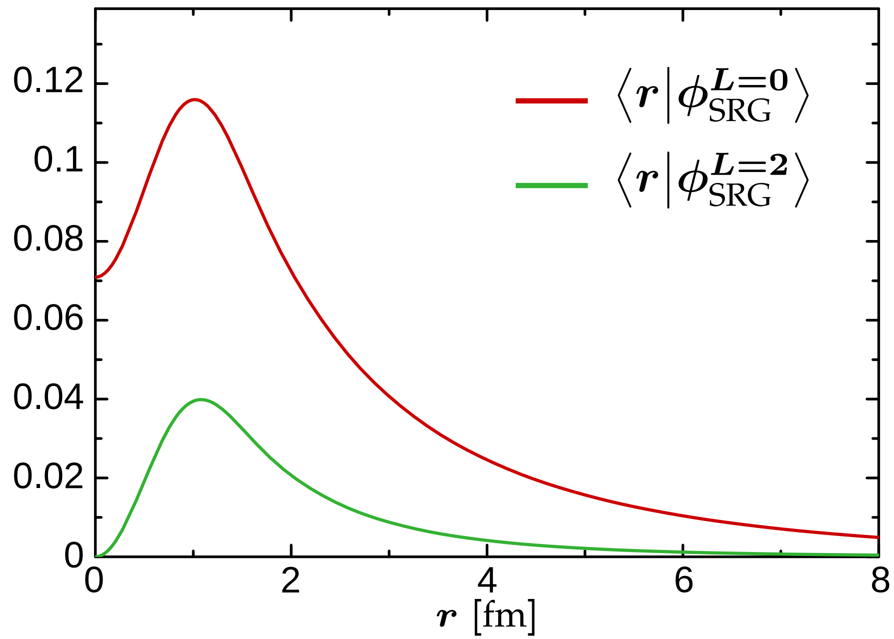
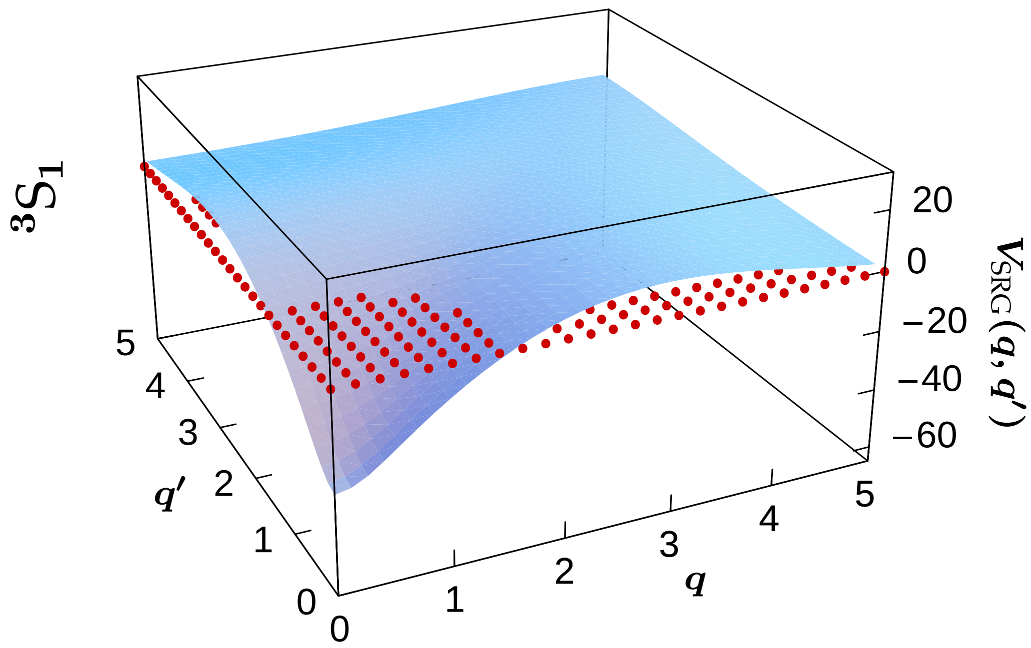
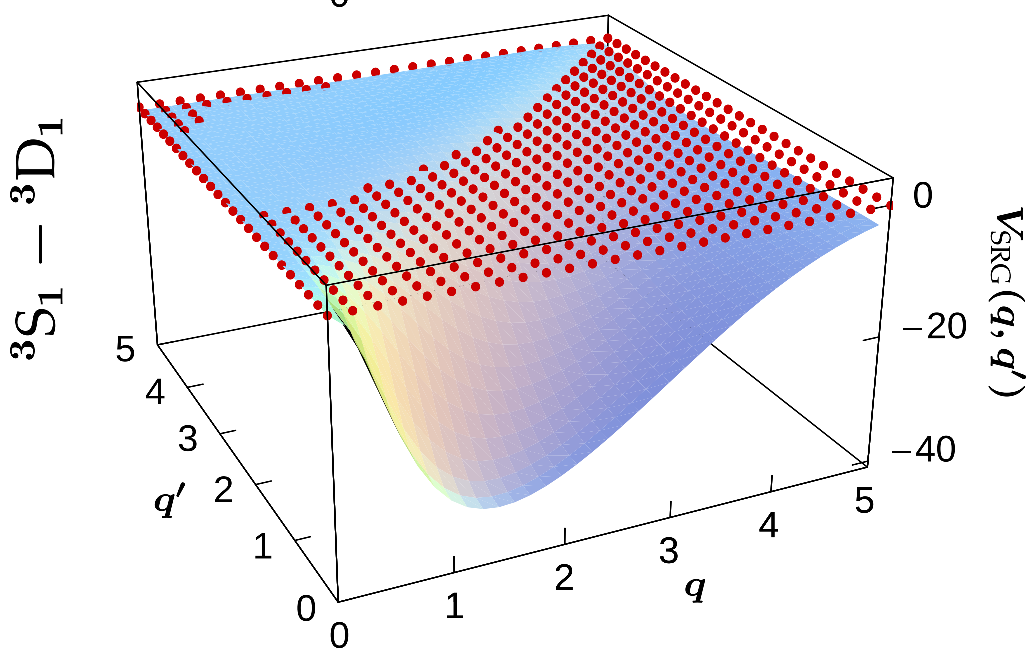


$\alpha = 0.0010\,\text{fm}^4$

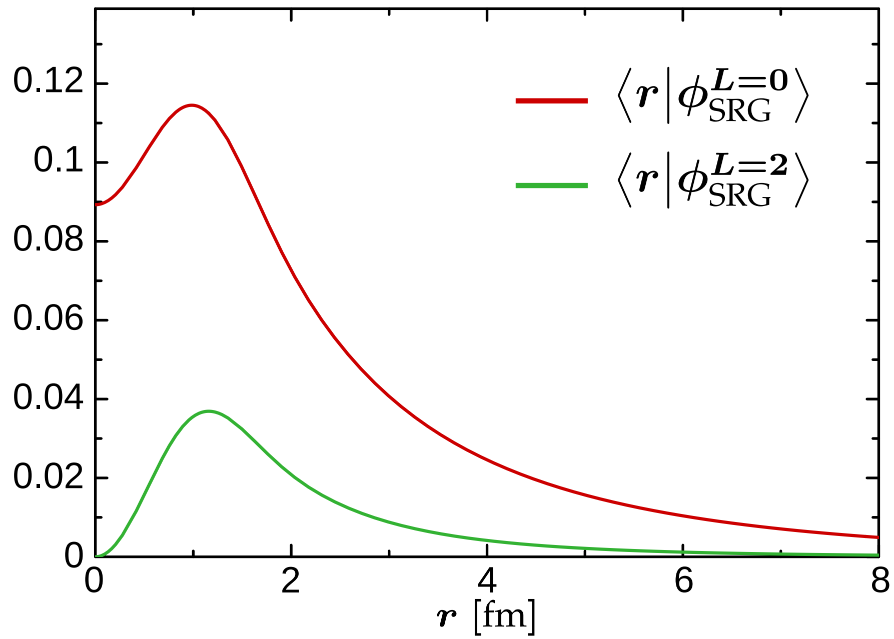


SRG Evolution: The Deuteron

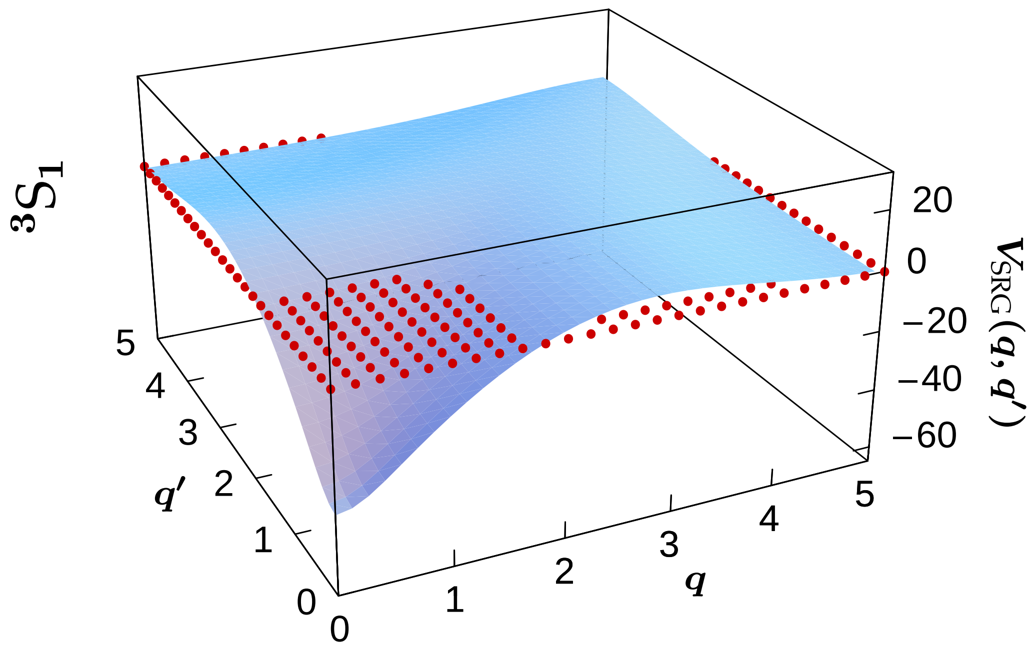


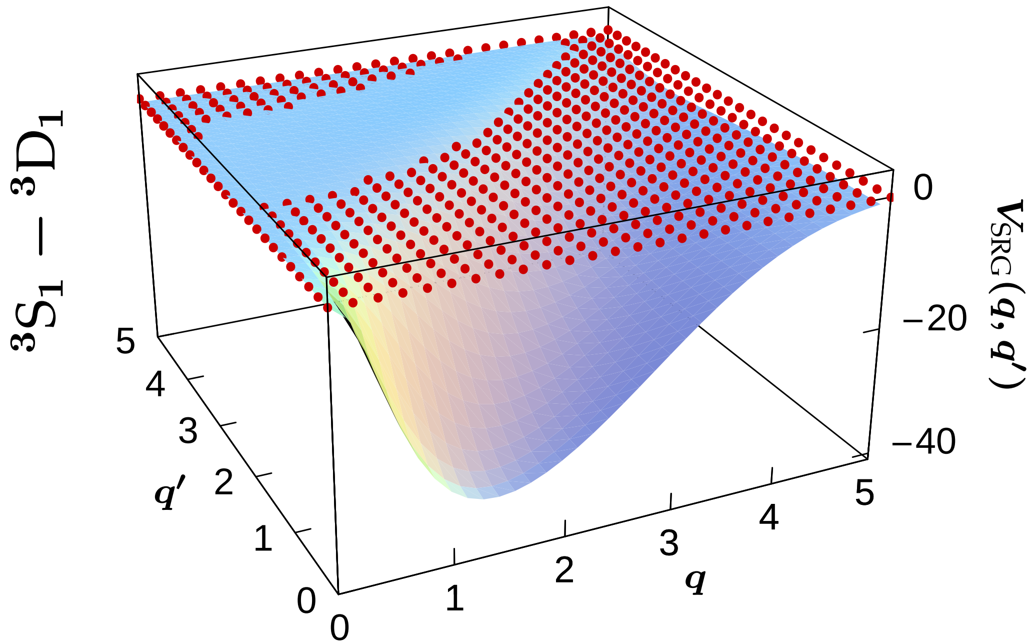


$\alpha = 0.0020\,\mathrm{fm}^4$

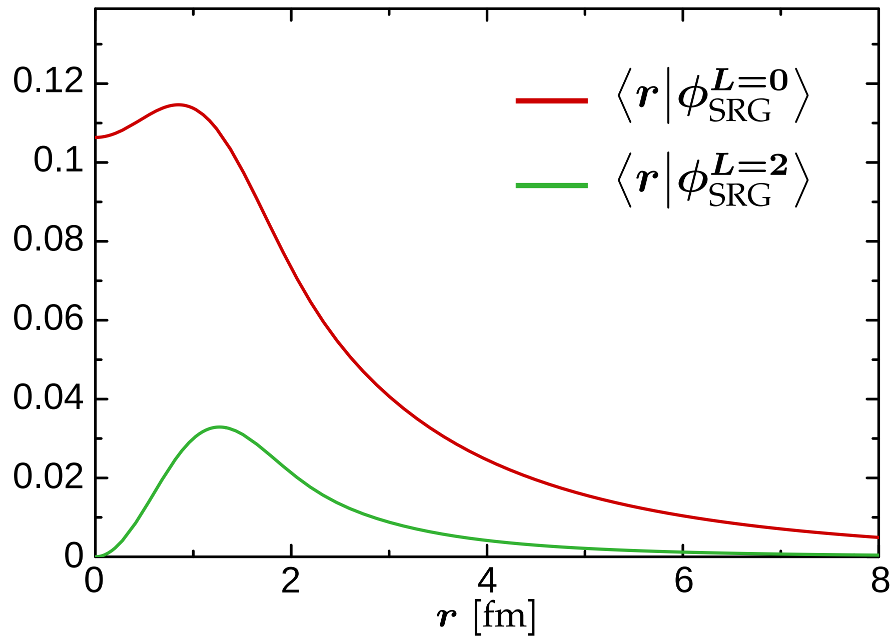


SRG Evolution: The Deuteron

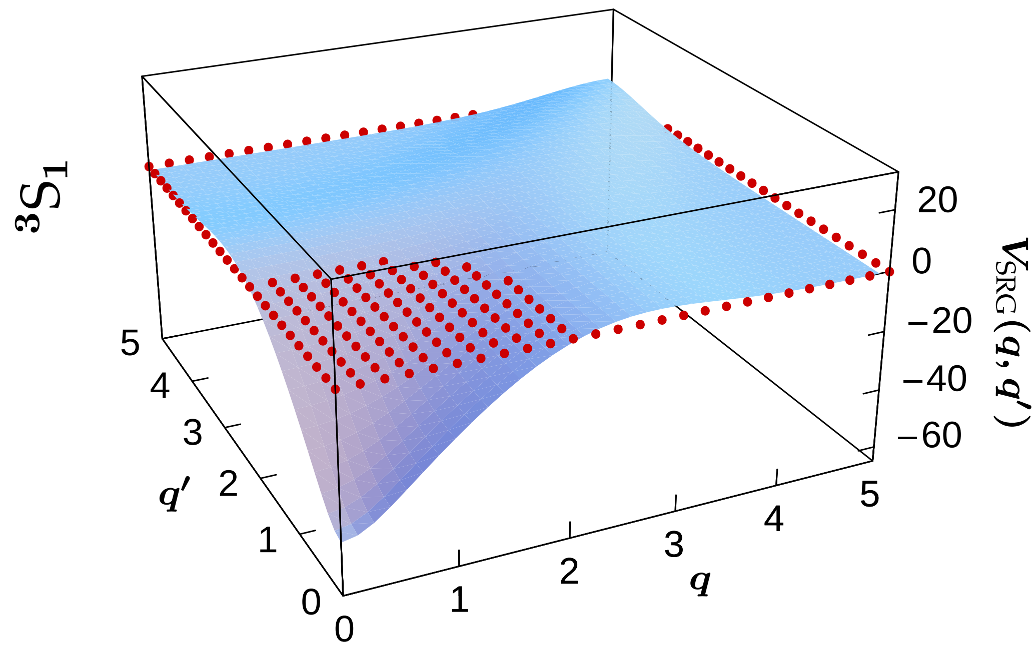


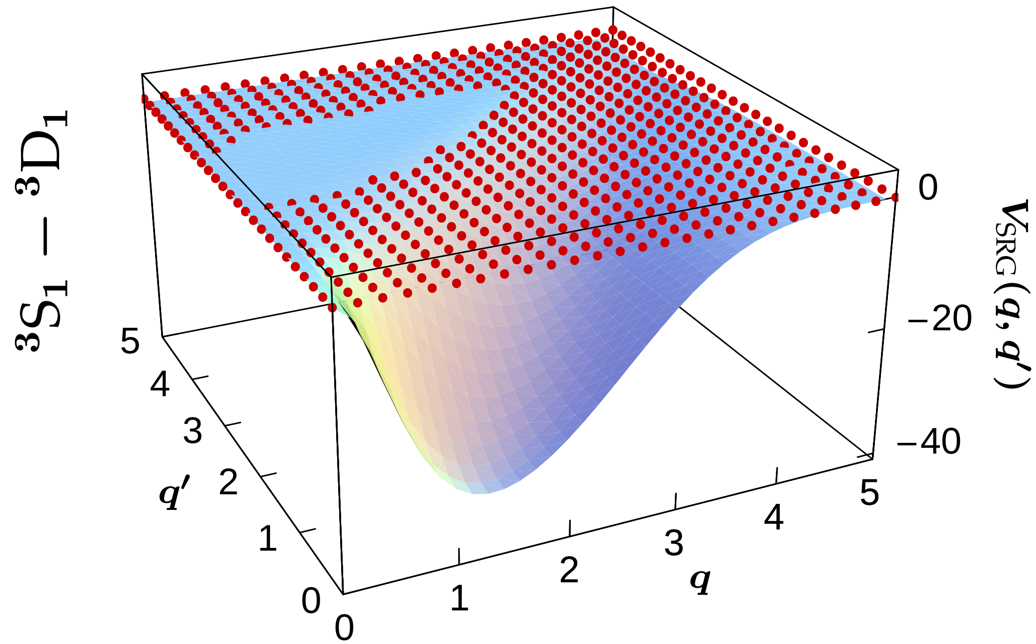


$\alpha = 0.0040\,\mathrm{fm}^4$

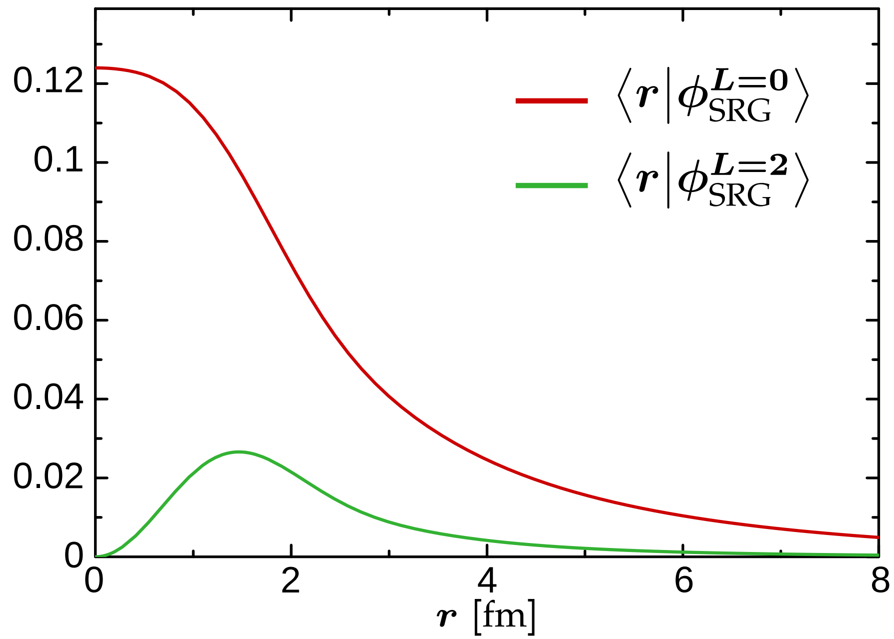


SRG Evolution: The Deuteron

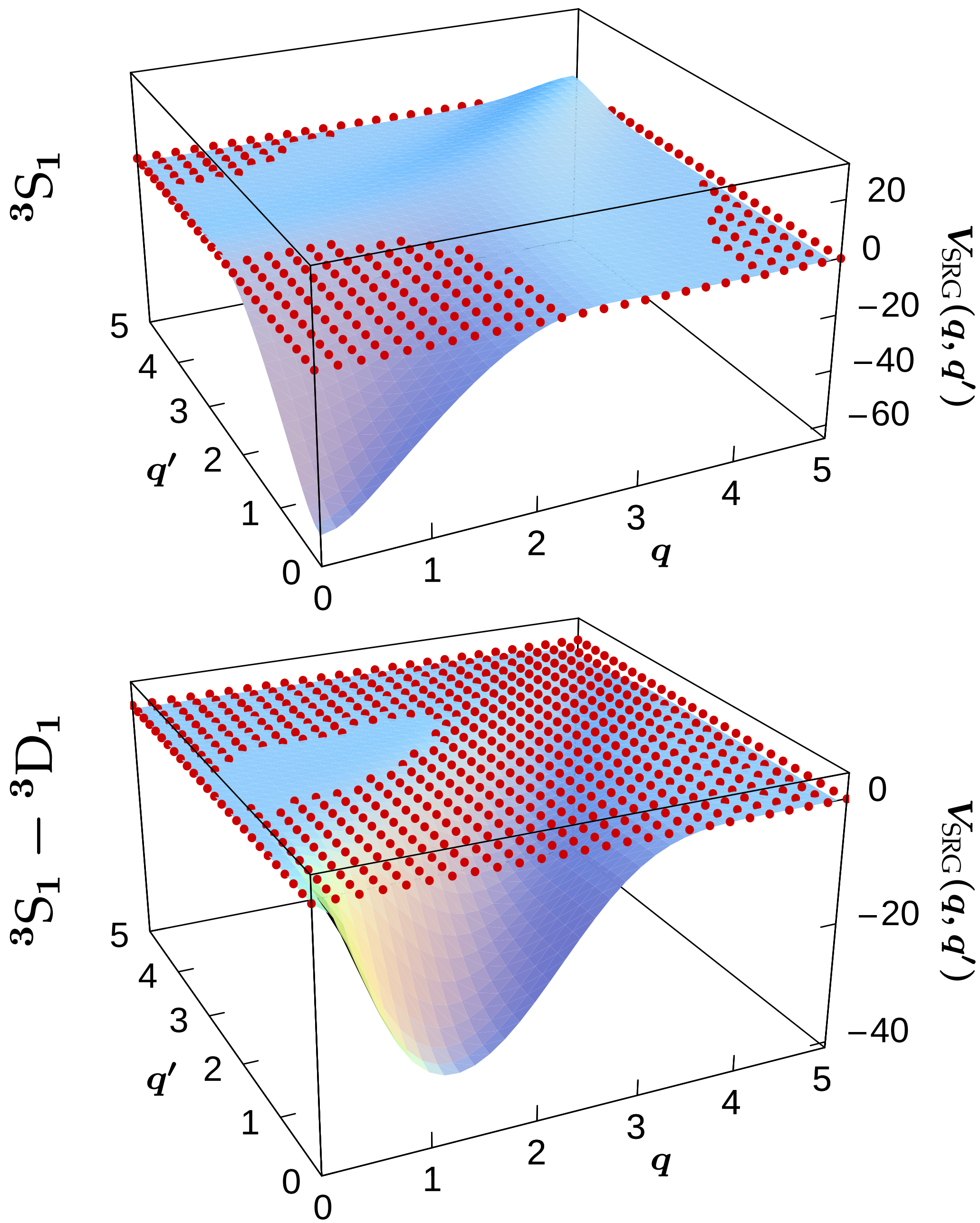




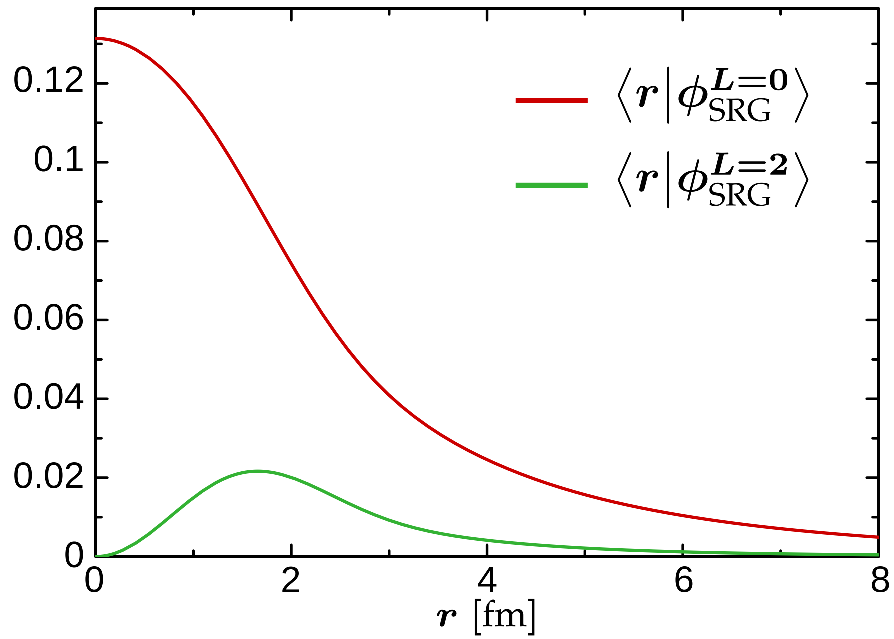
$\alpha = 0.0100\,\mathrm{fm}^4$



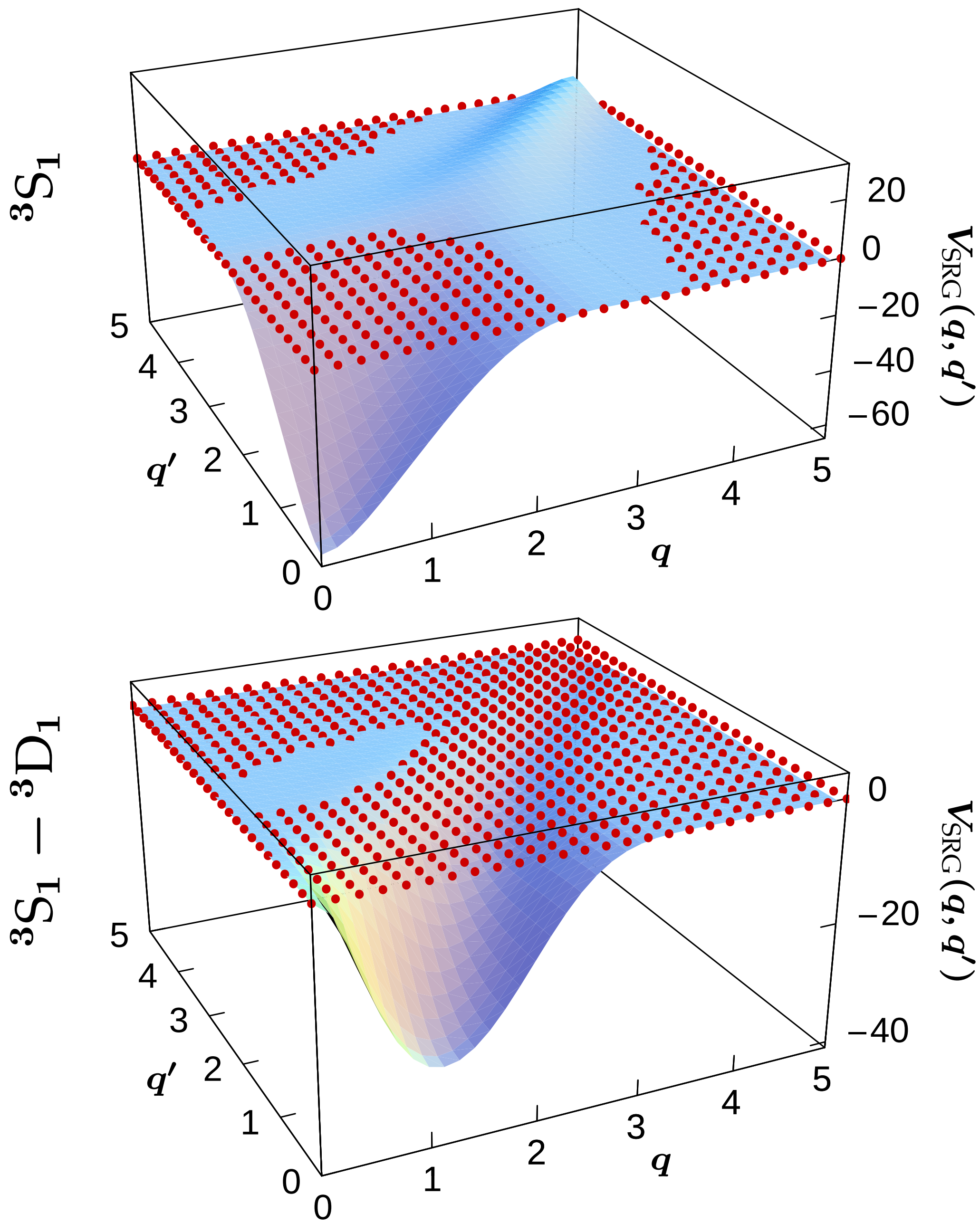
SRG Evolution: The Deuteron



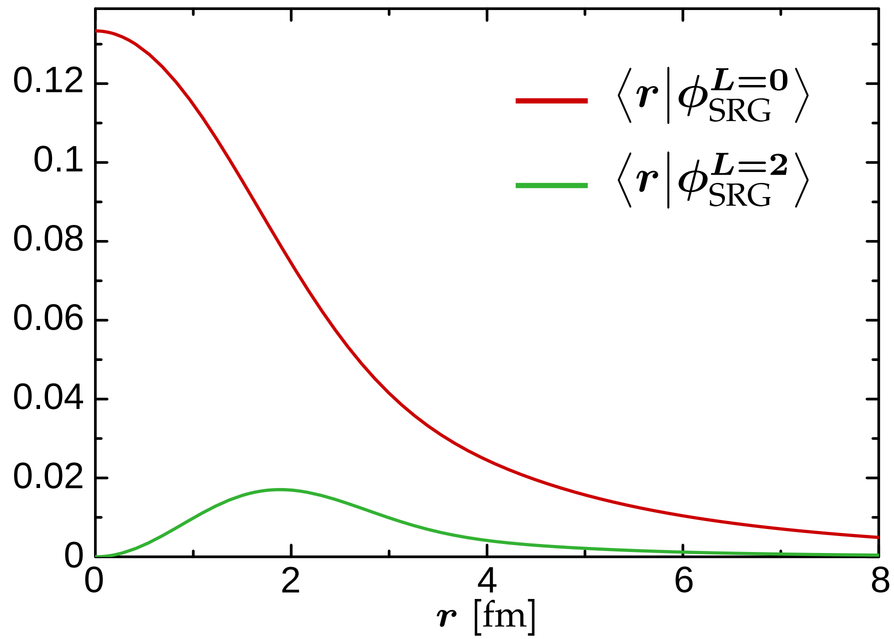
$\alpha = 0.0200\,\mathrm{fm}^4$



SRG Evolution: The Deuteron



$\alpha = 0.0400\,\mathrm{fm}^4$



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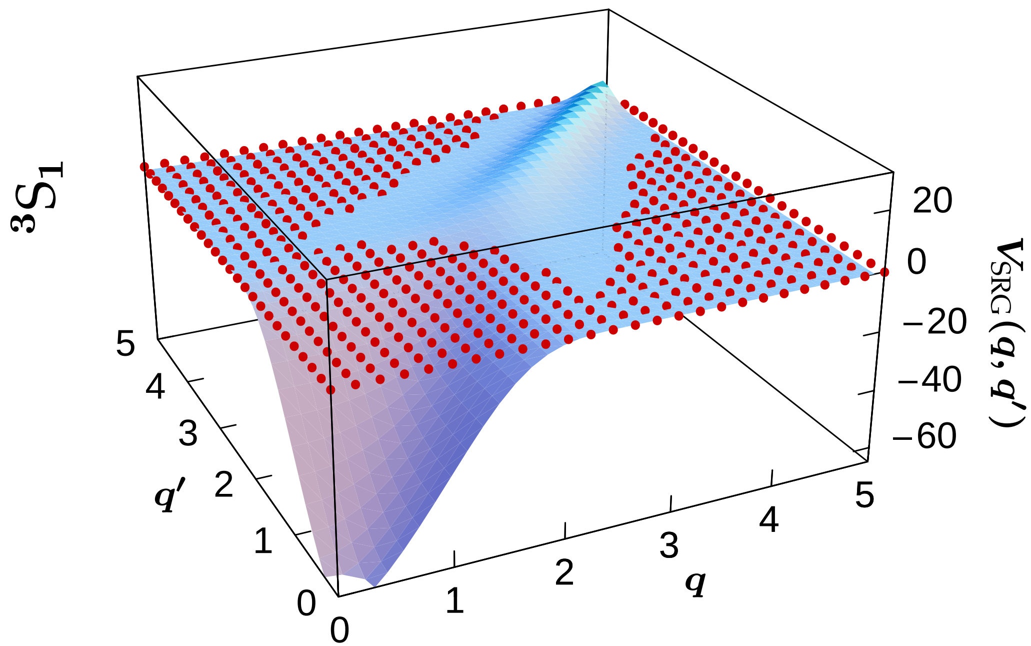
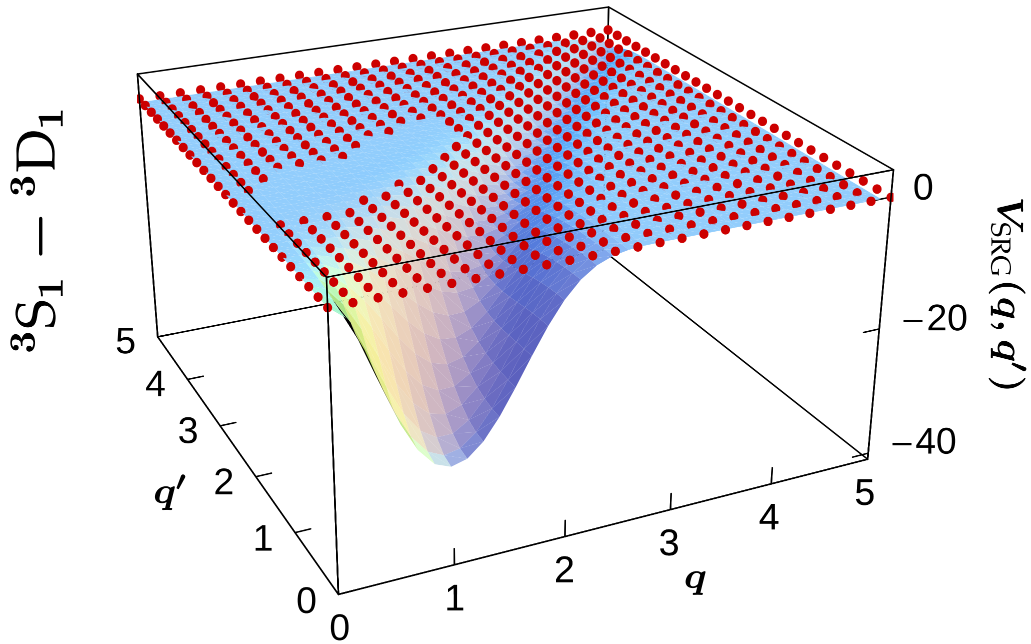
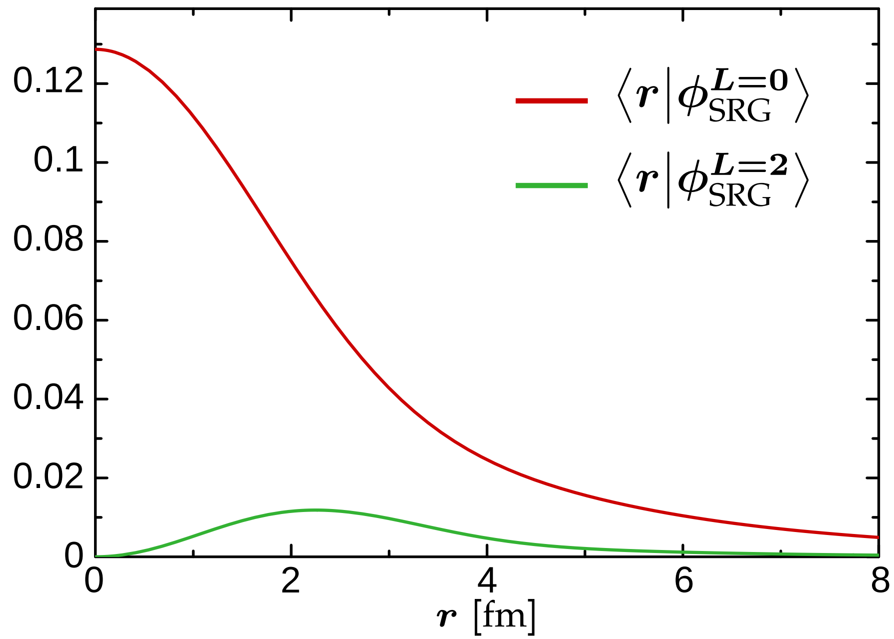
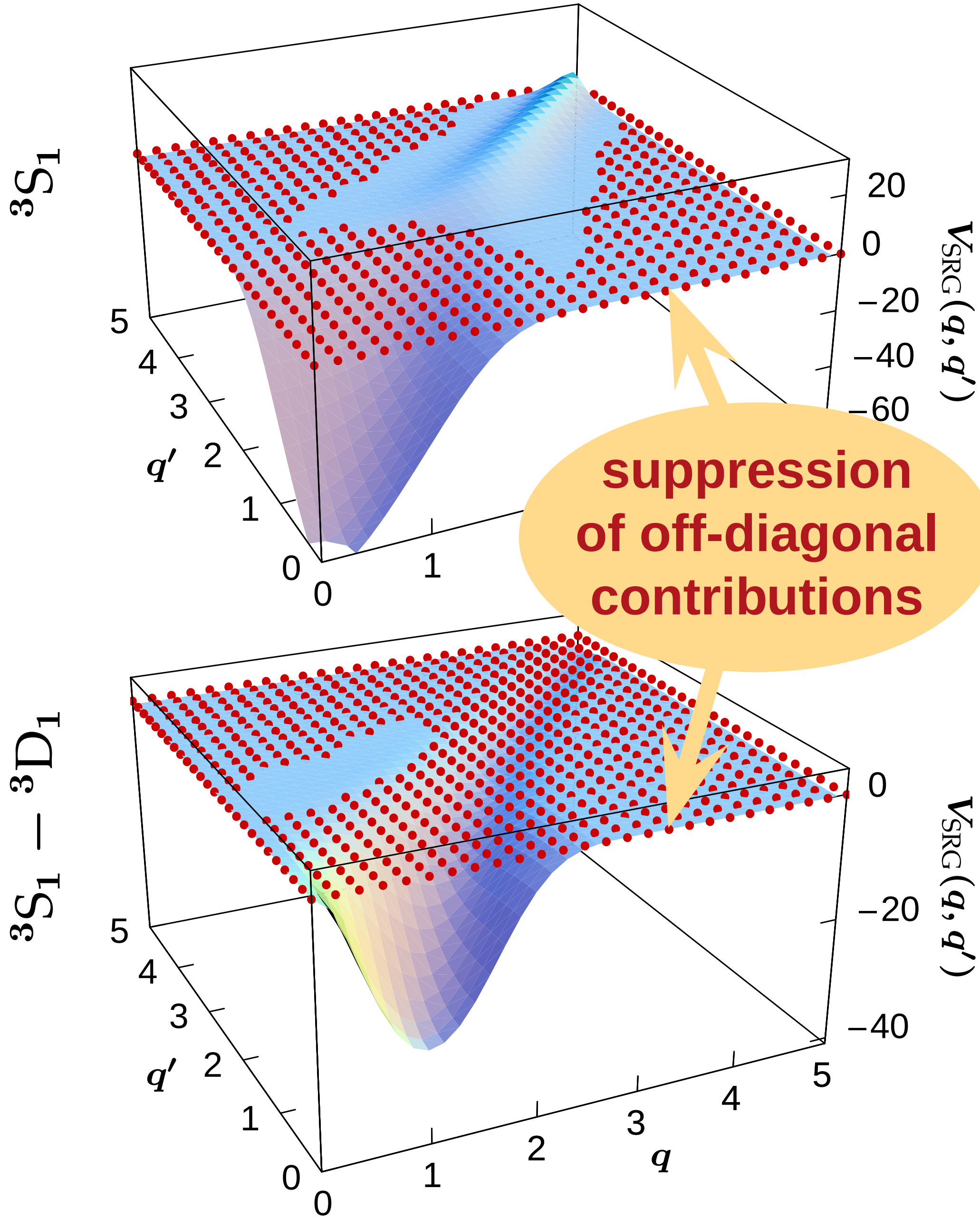




$$\alpha = 0.1000\,\mathrm{fm}^4$$

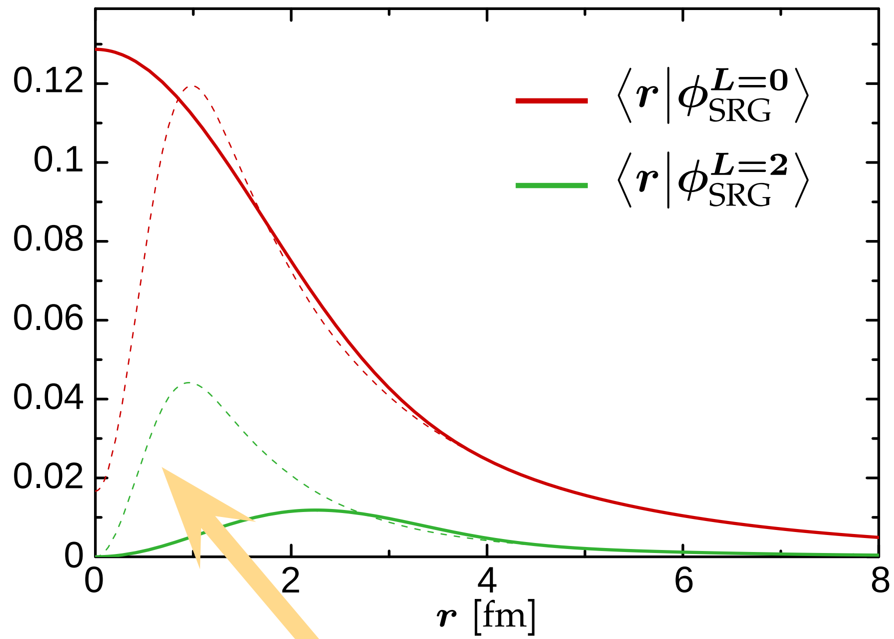


SRG Evolution: The Deuteron



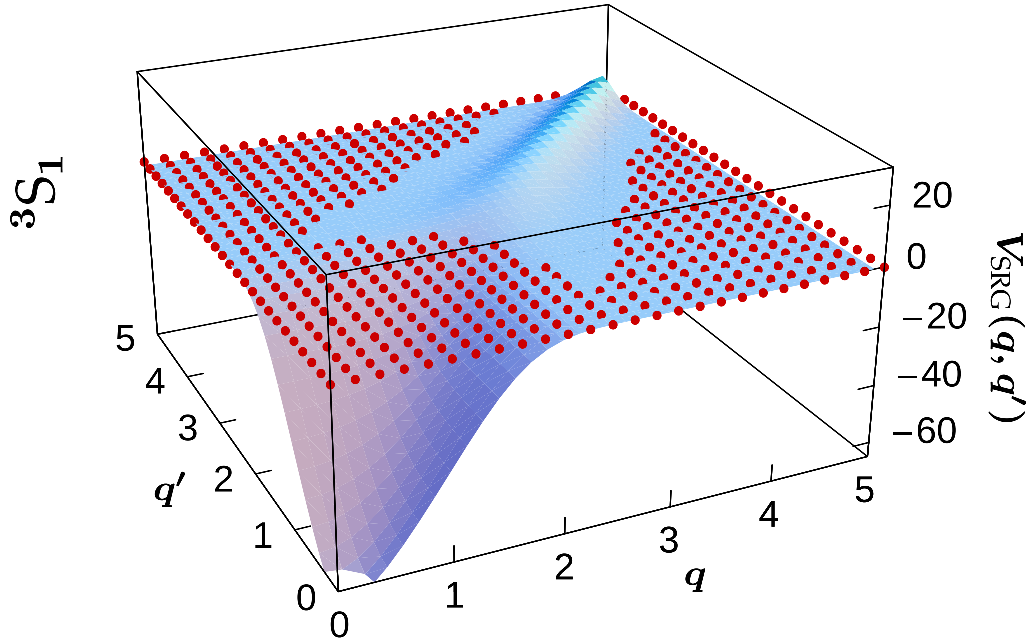
suppression of off-diagonal contributions

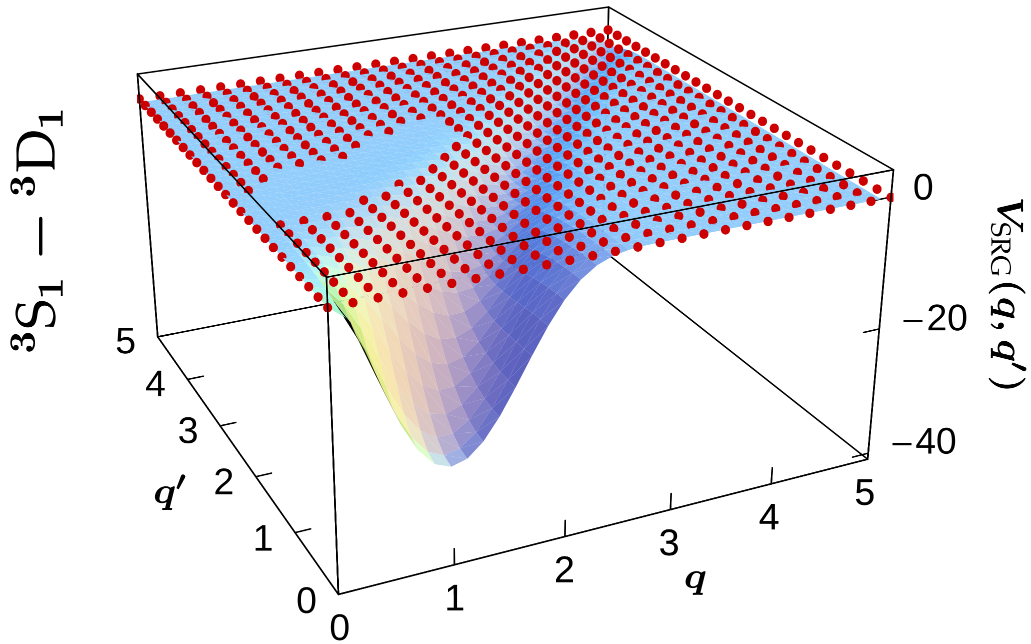
$\alpha = 0.1000\,\mathrm{fm}^4$



elimination of short-range correlations

SRG Evolution: The Deuteron





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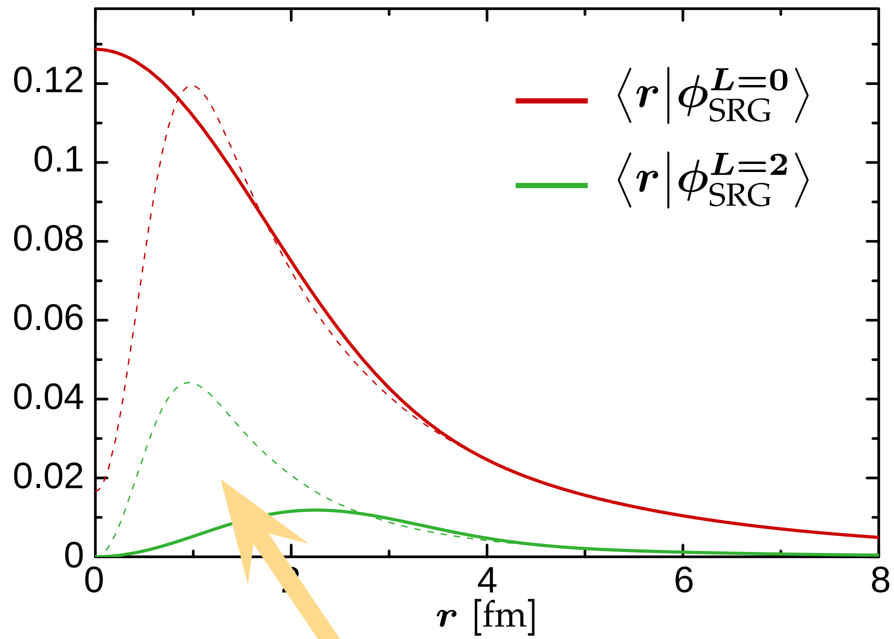
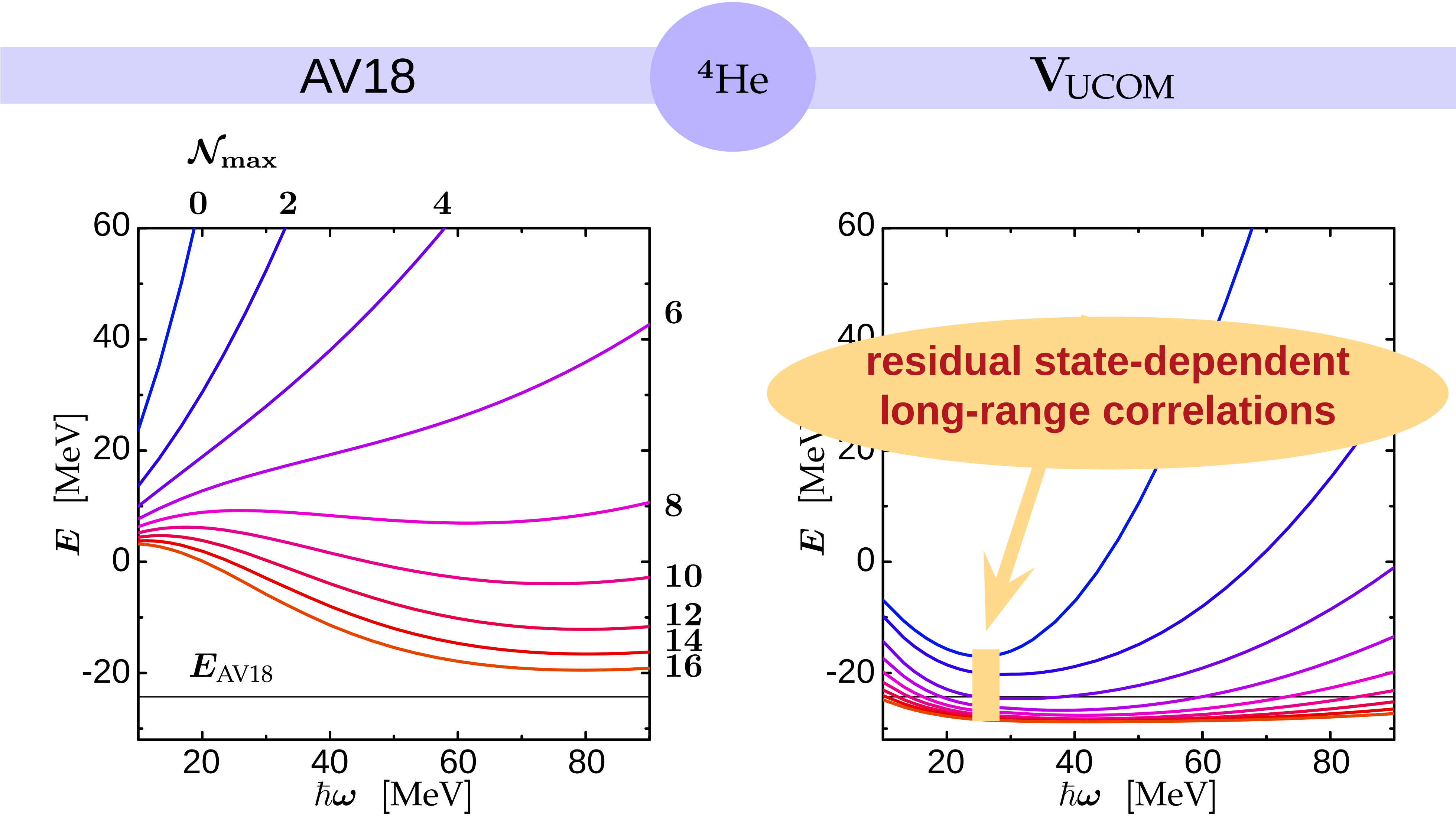


extract UCOM correlation functions $s(r)$ and $\vartheta(r)$

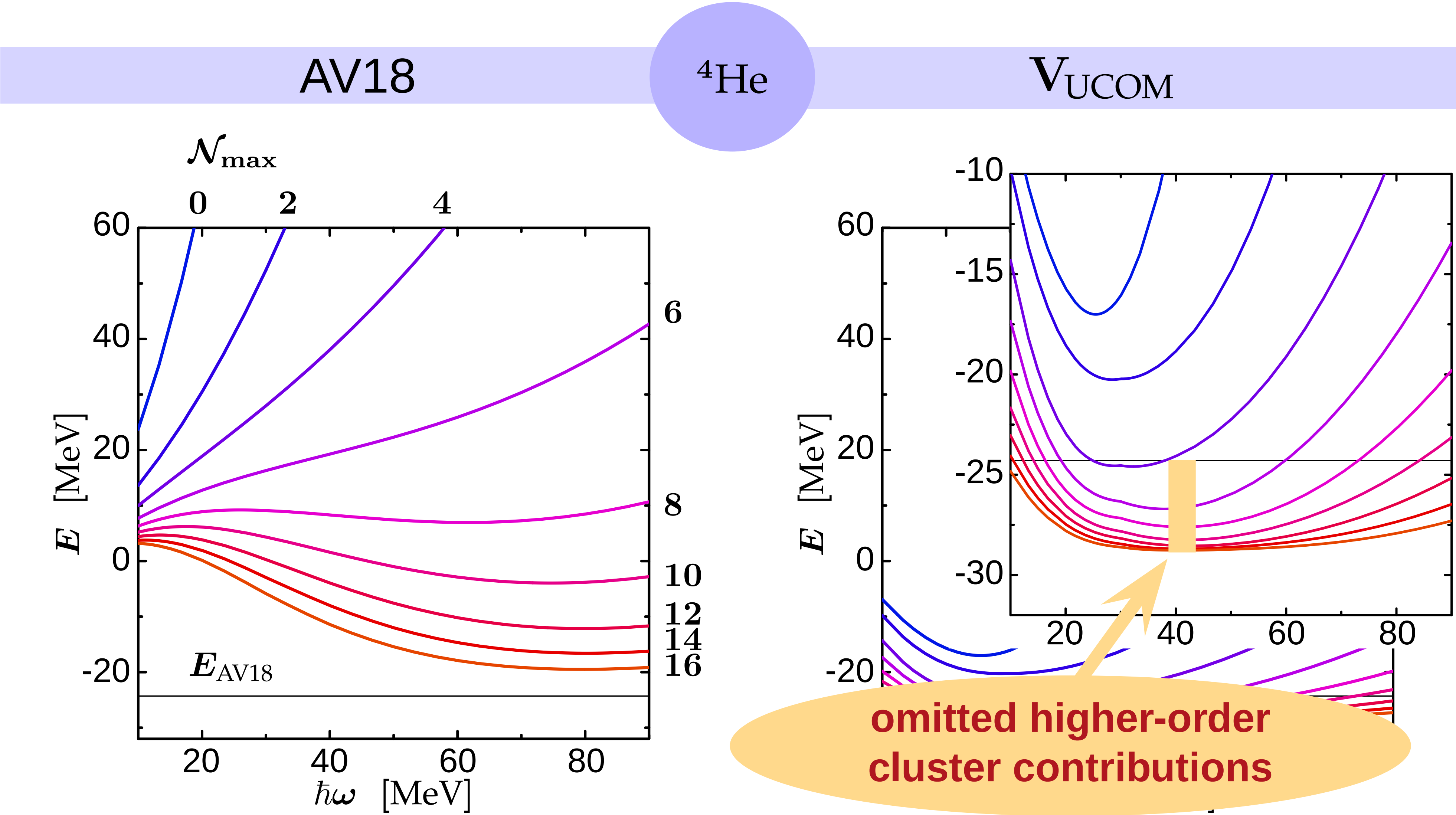
Few-Body Systems

^{4}He: Convergence



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

^{4}He: Convergence



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

Three-Body Interactions — Strategies

Correlated Hamiltonian in Many-Body Space

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

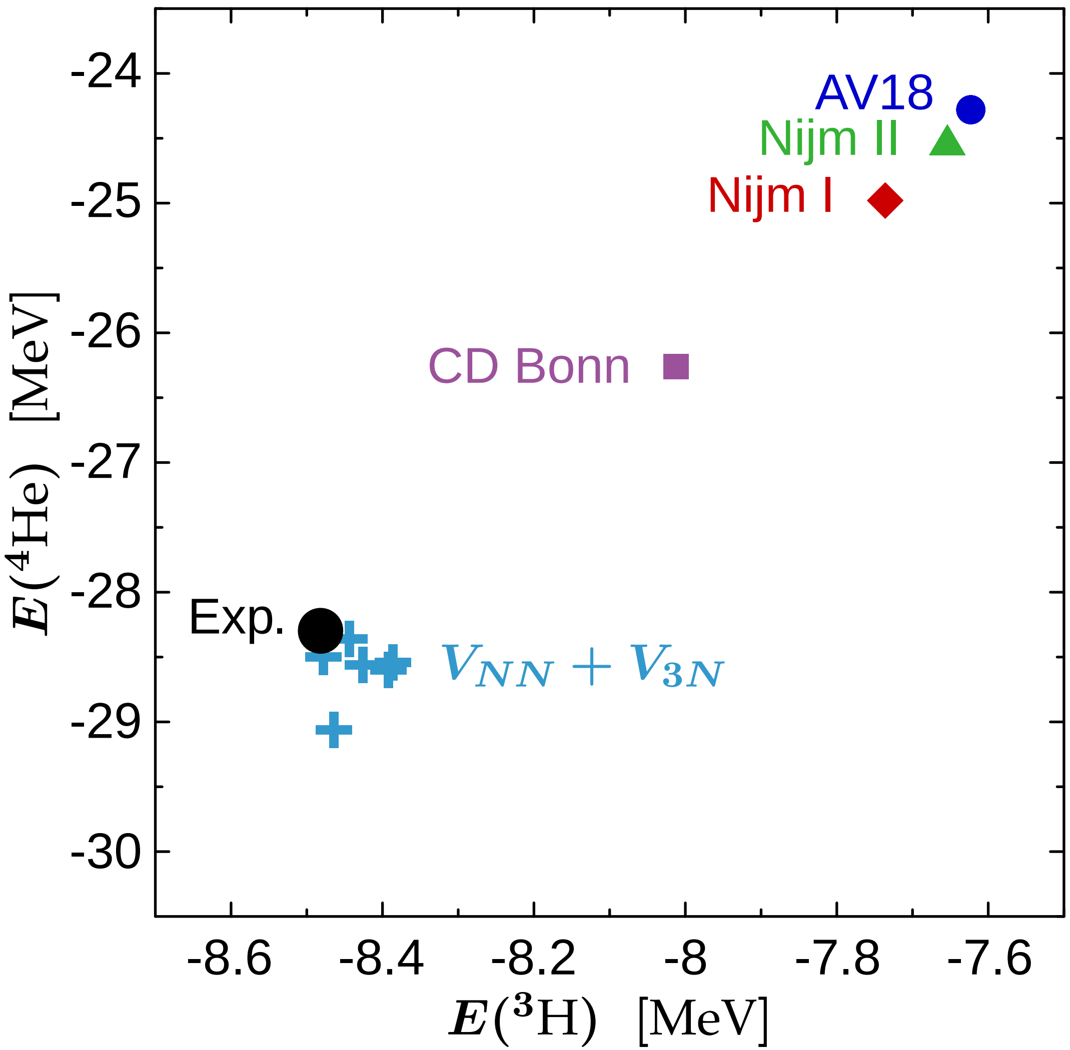
- strategies for treating the three-body contributions:

❶ **include full $\mathrm{V}^{[3]}_{\mathrm{UCOM}}$** consisting of genuine and induced 3N terms

❷ **replace $\mathrm{V}^{[3]}_{\mathrm{UCOM}}$** by “phenomenological” three-body force

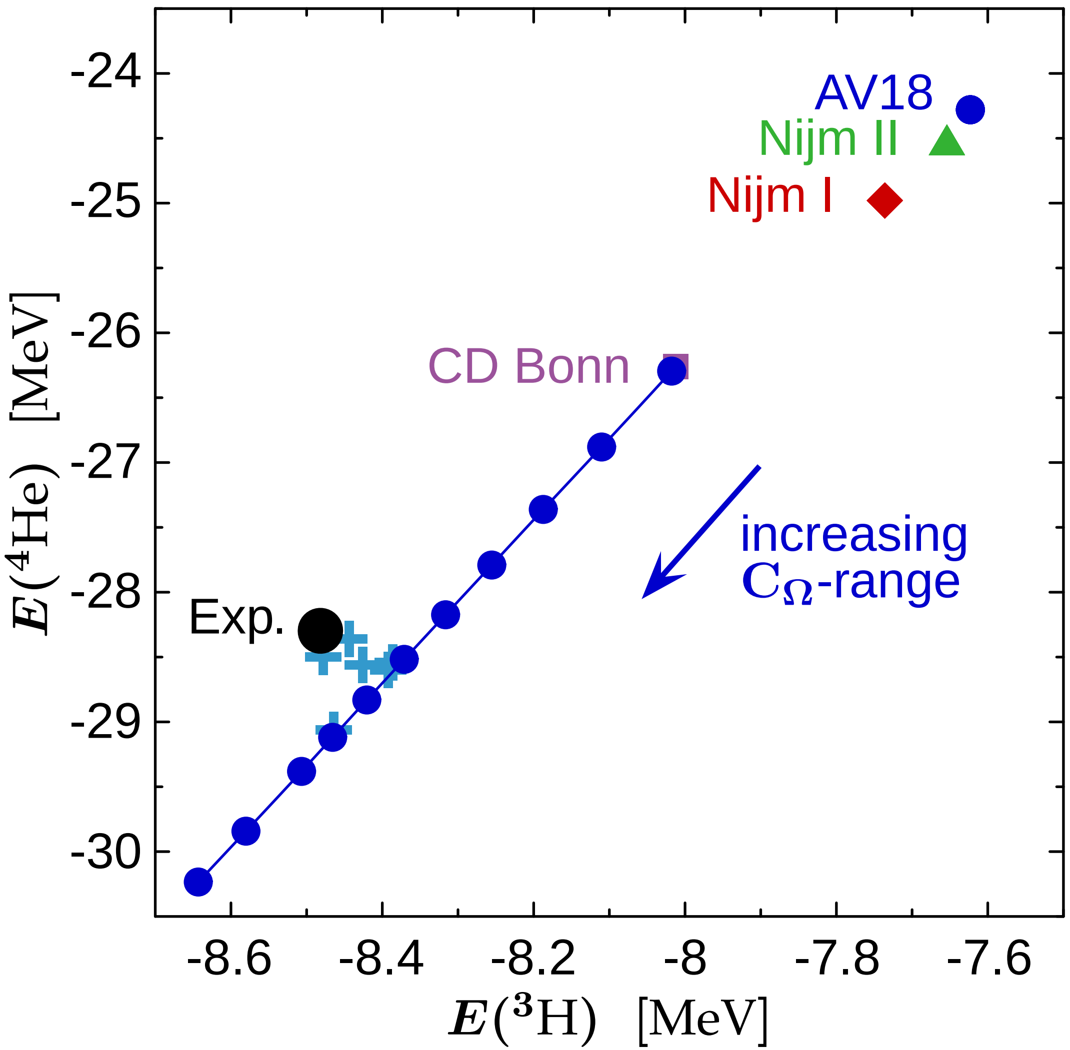
❸ **minimize $\mathrm{V}^{[3]}_{\mathrm{UCOM}}$** by proper choice of unitary transformation

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



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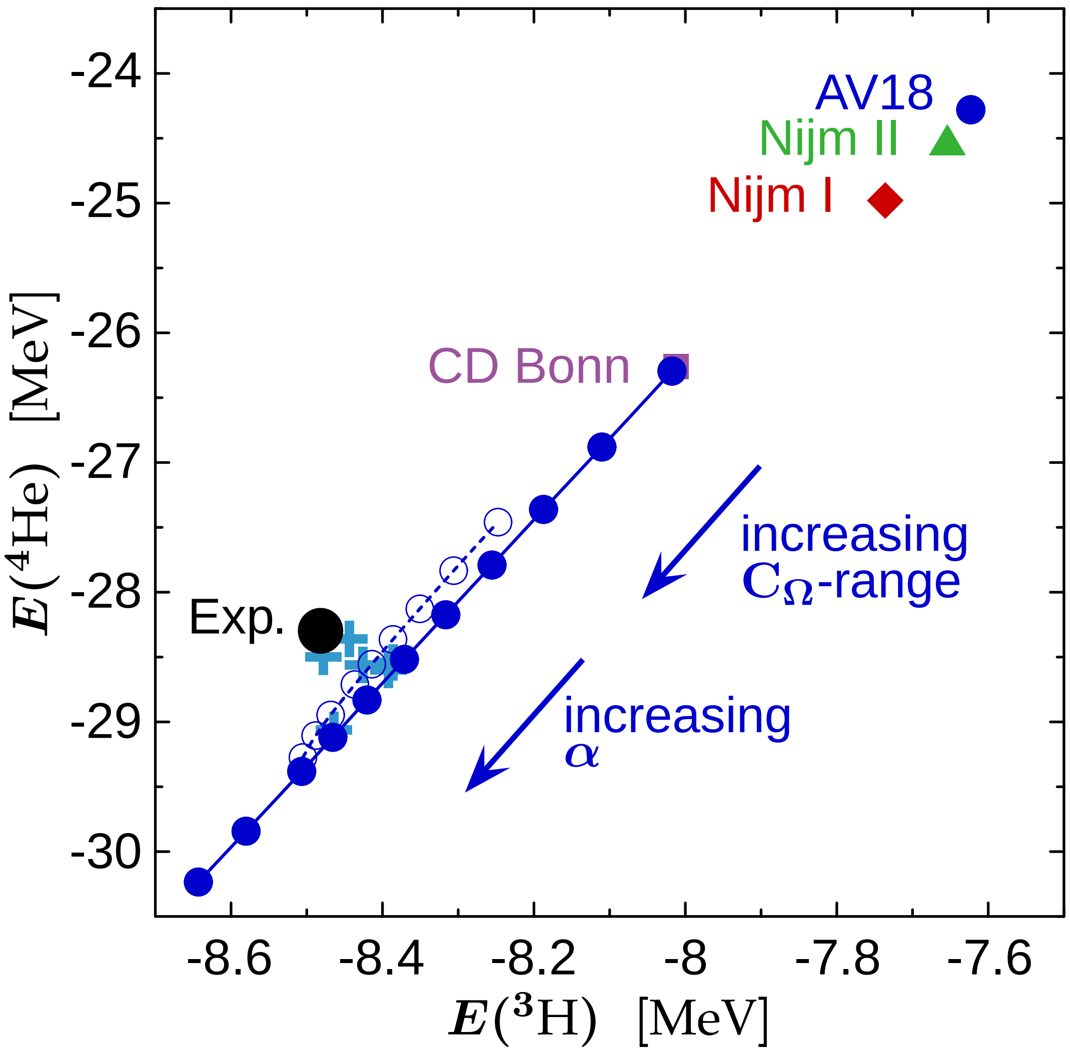
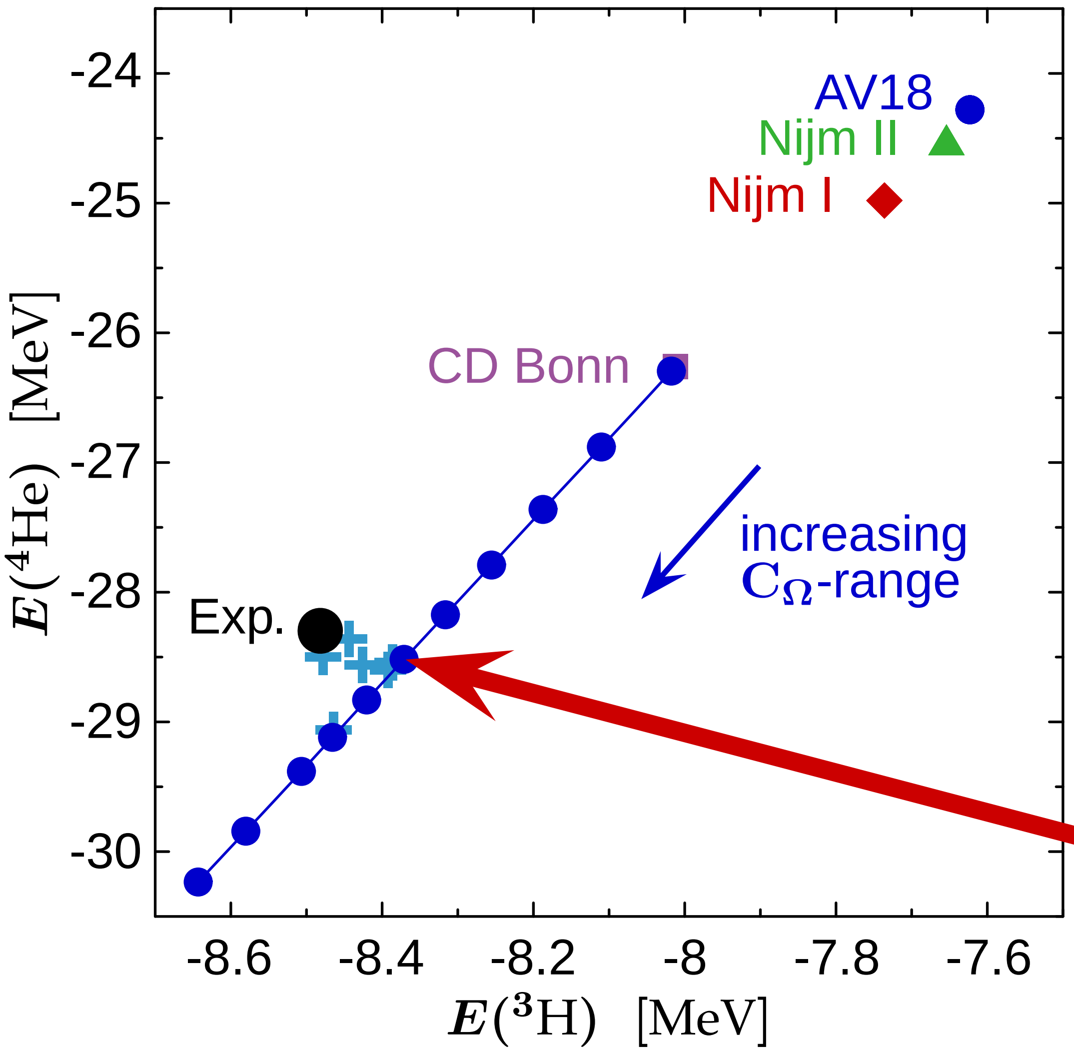
Three-Body Interactions — Tjon Line



- **Tjon-line**: $E(^4\mathrm{He})$ vs. $E(^3\mathrm{H})$ for phase-shift equivalent NN-interactions
- use α / range of C_Ω to
  - test dependence of V_α or V_{UCOM}
  - tune contributions of **net 3N force**

Three-Body Interactions — Tjon Line



- **Tjon-line**: $E(^4\mathrm{He})$ vs. $E(^3\mathrm{H})$ for phase-shift equivalent NN-interactions
- use α / range of C_Ω to
  - test dependence of V_α or $\mathrm{V}_{\mathrm{UCOM}}$
  - tune contributions of **net 3N force**

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

- **min. net $3N$ force**:

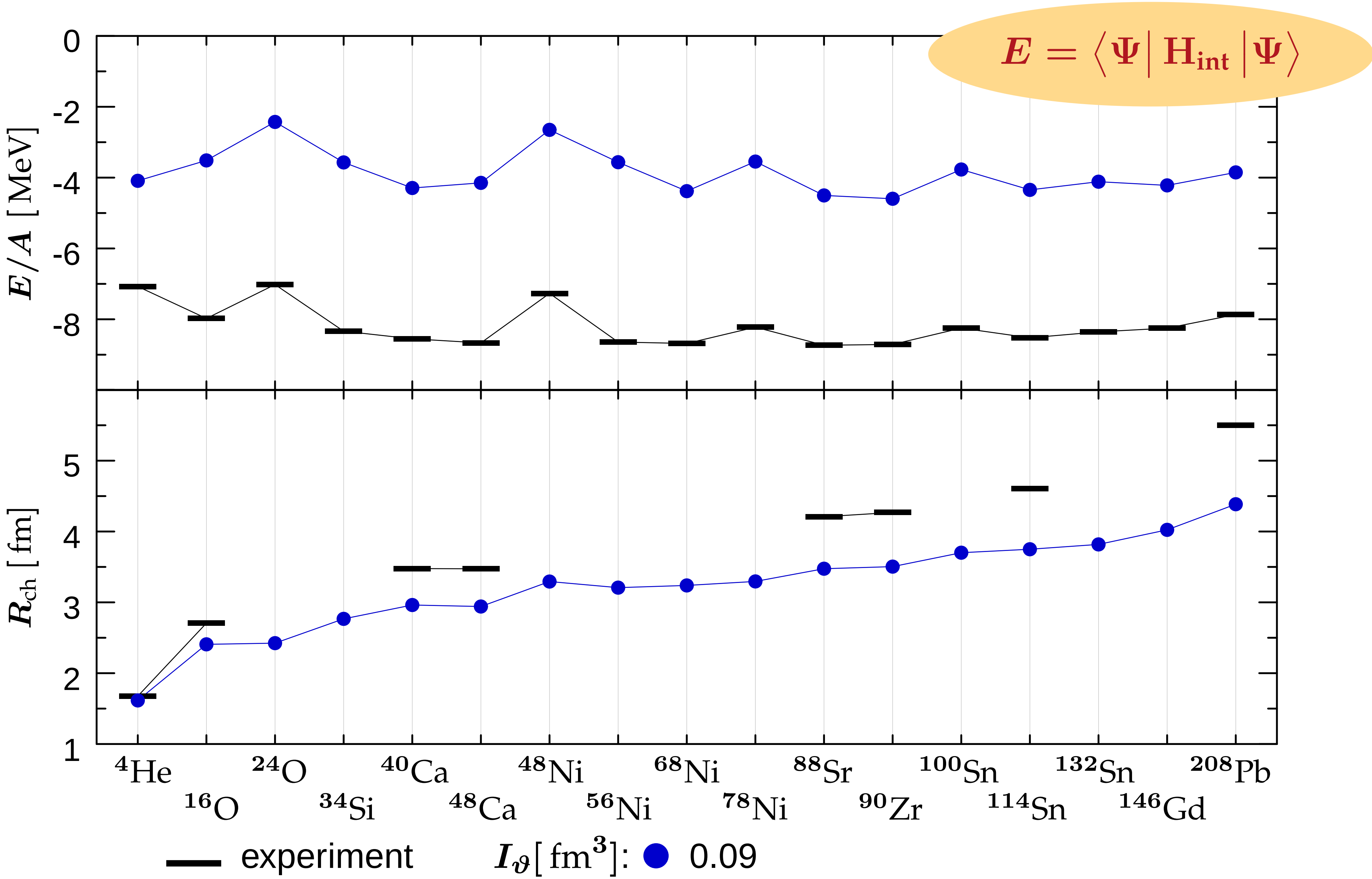
$$I_\vartheta = 0.09\,\mathrm{fm}^3$$

- with **phen. $3N$ force**:

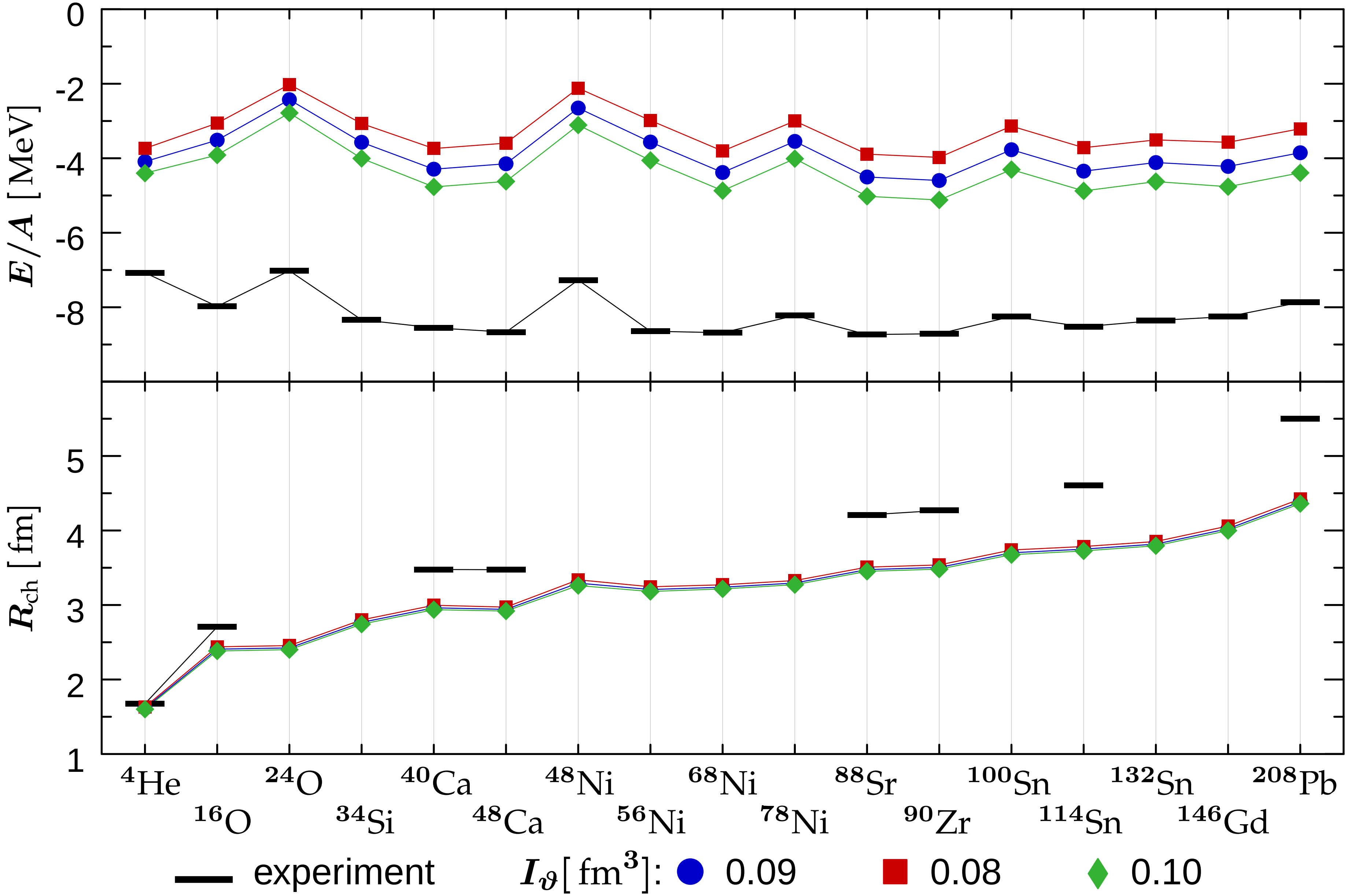
$$I_\vartheta = 0.20\,\mathrm{fm}^3$$

Many-Body Systems

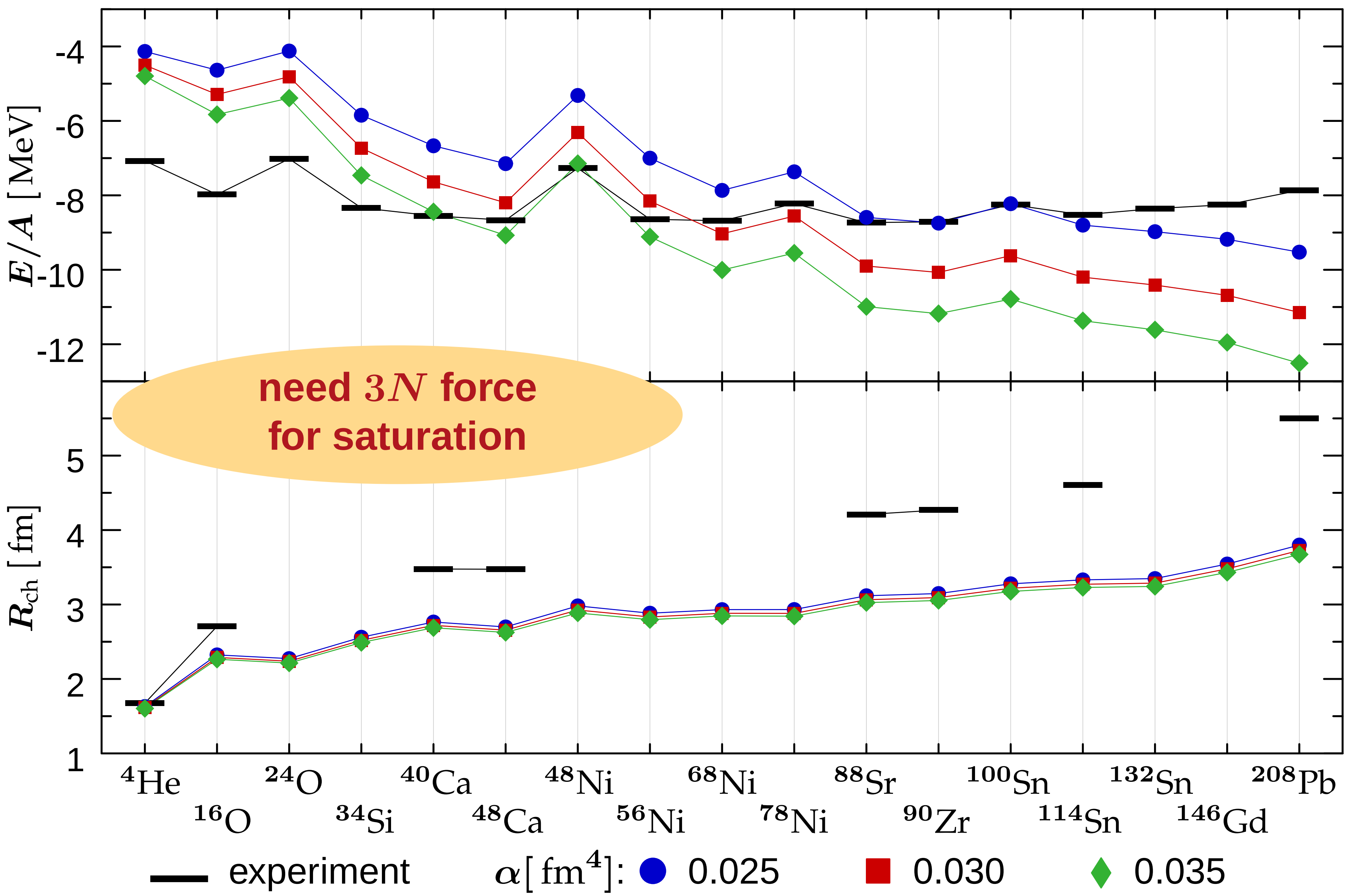
Hartree-Fock with V_{UCOM}



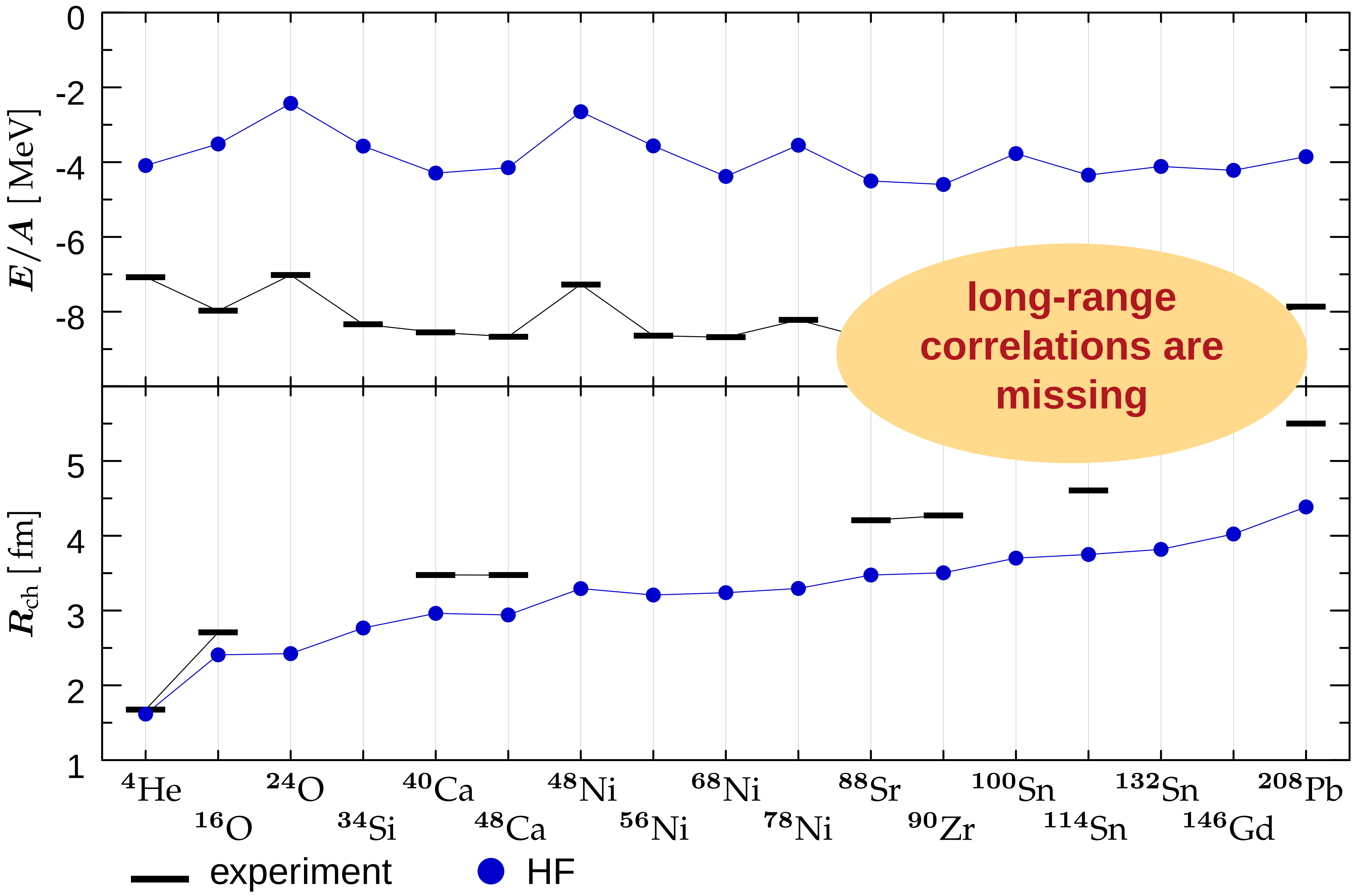
Hartree-Fock with V_{UCOM}



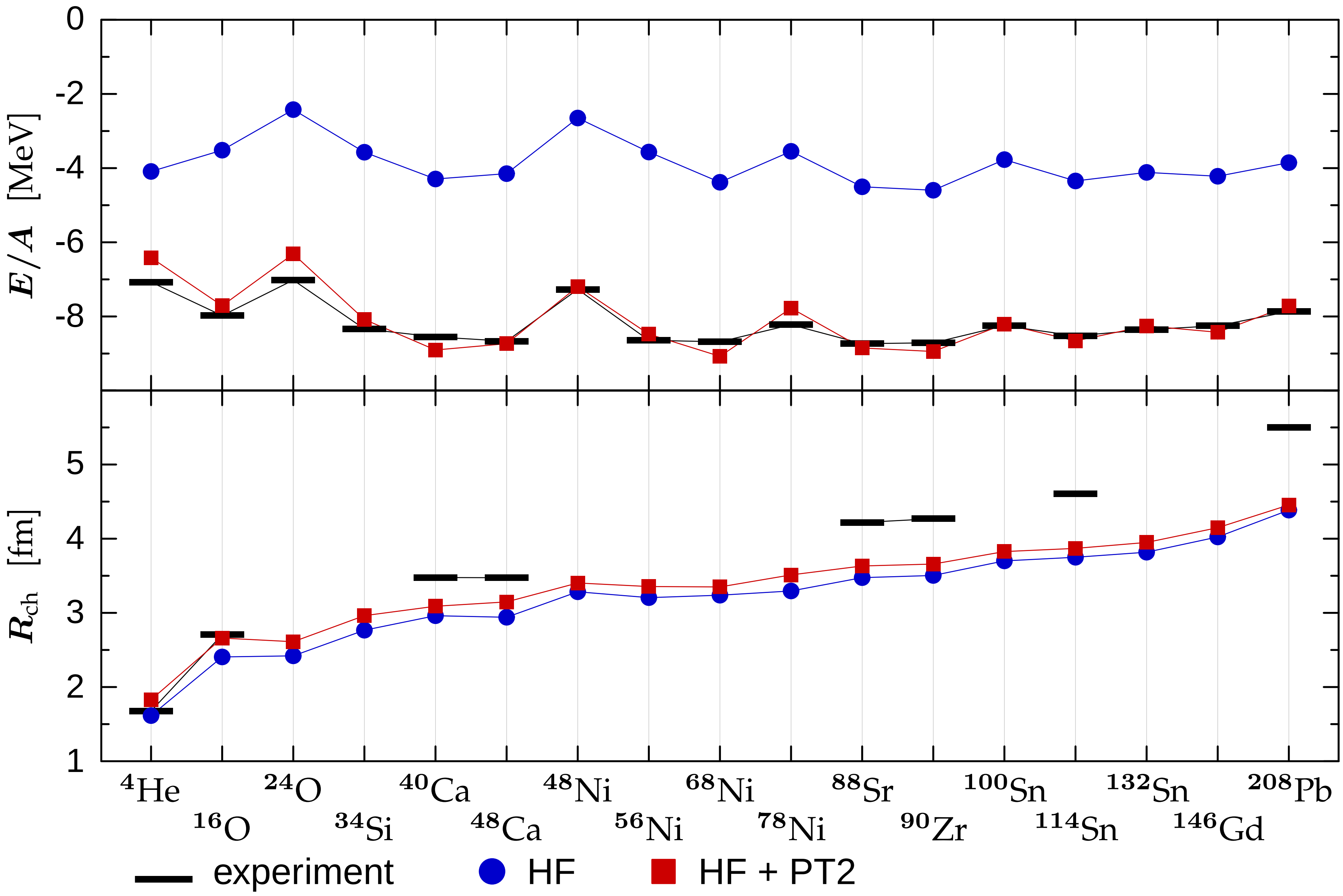
Hartree-Fock with SRG Potentials



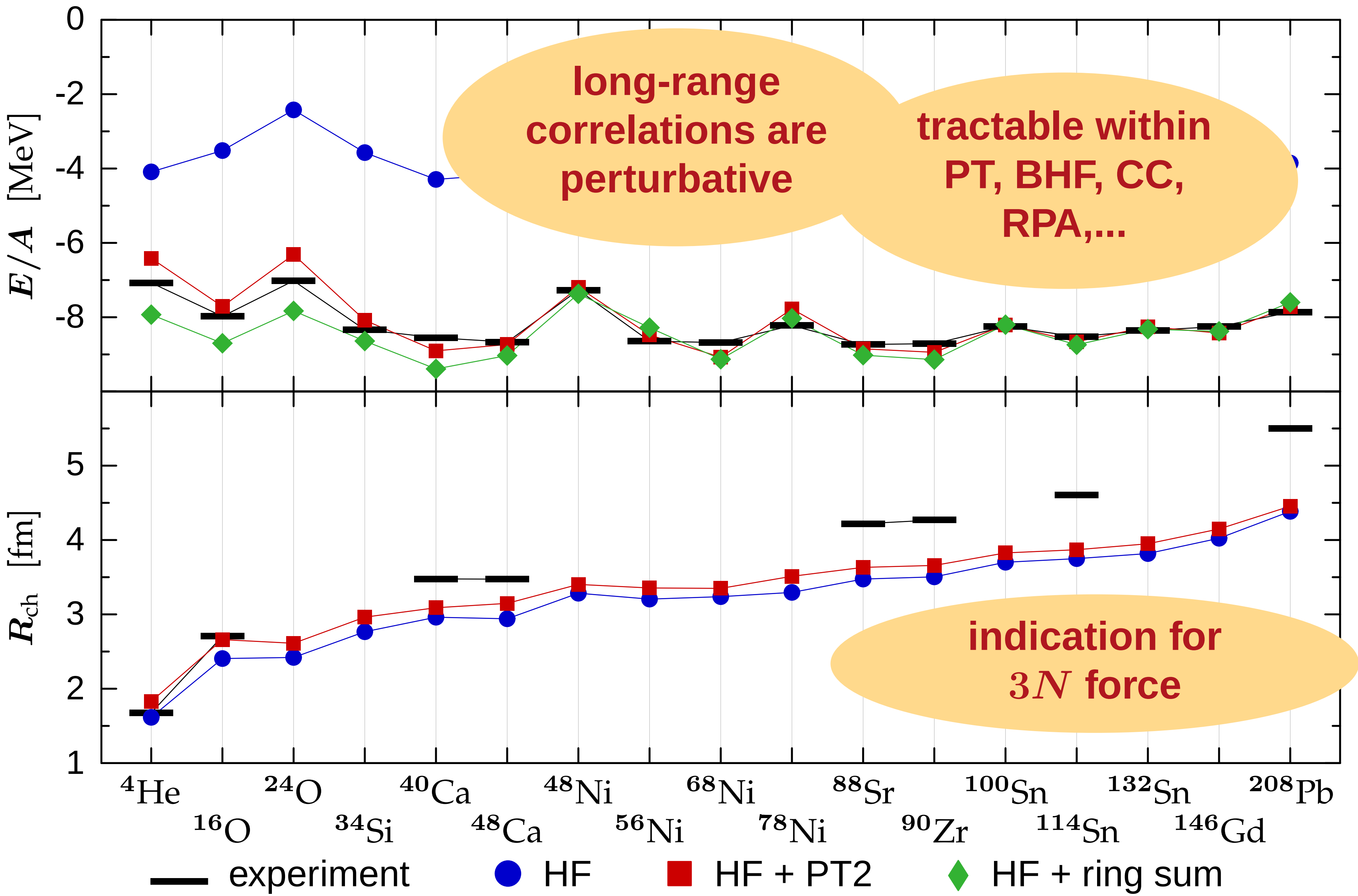
Hartree-Fock with V_{UCOM}



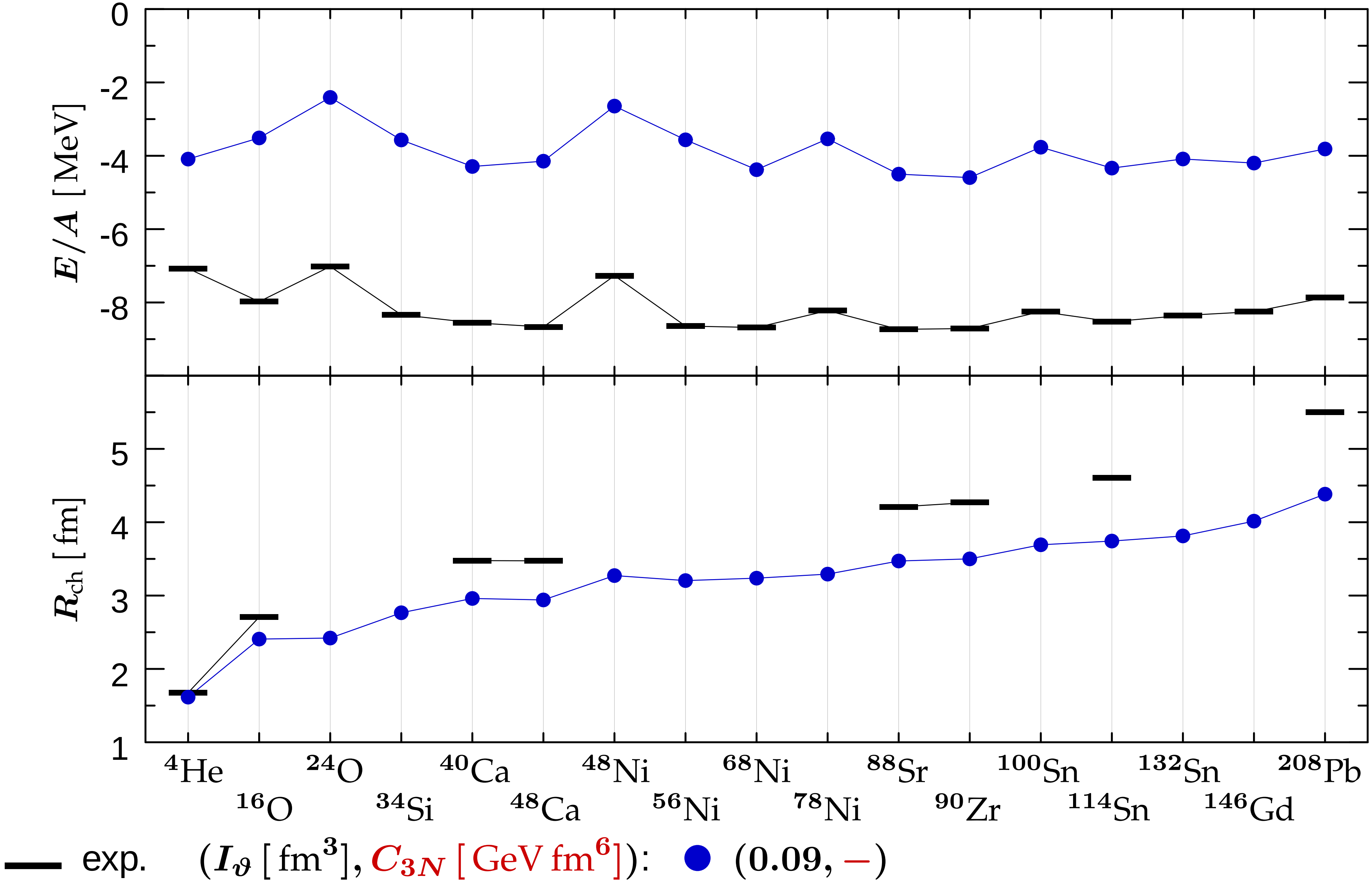
Perturbation Theory with V_{UCOM}



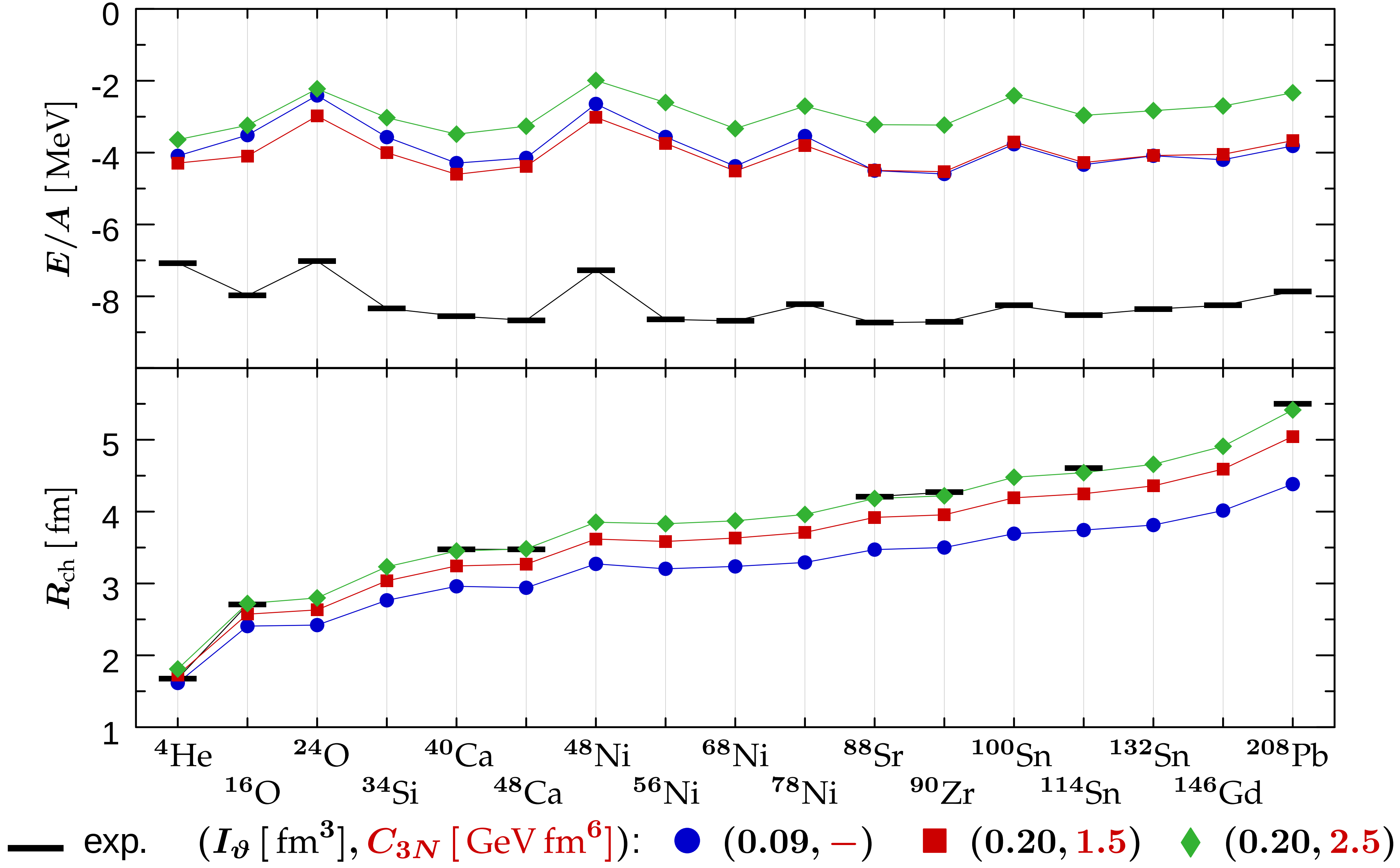
RPA Ring Summation with V_{UCOM}



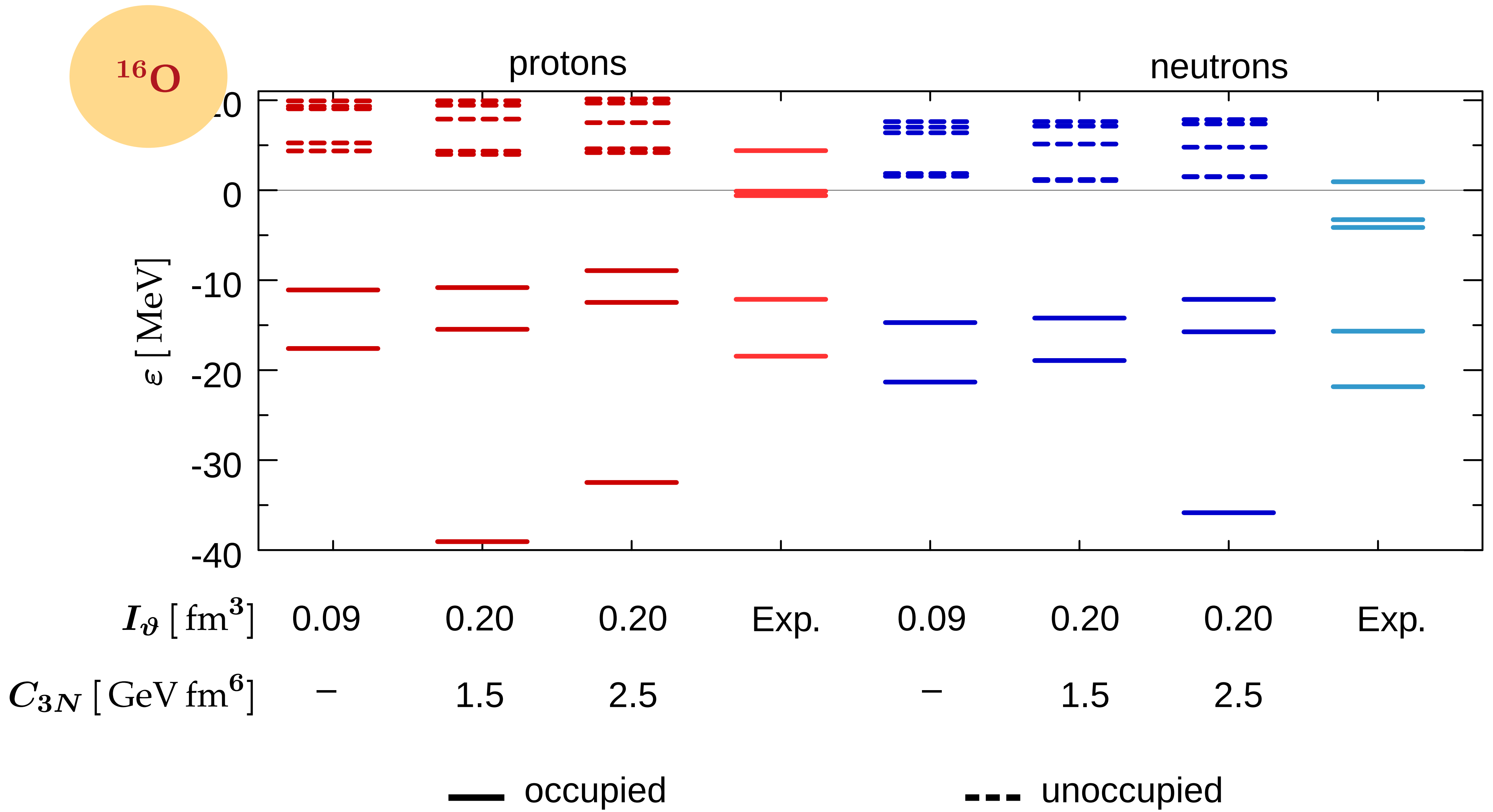
$3N$ Forces: Energies & Radii



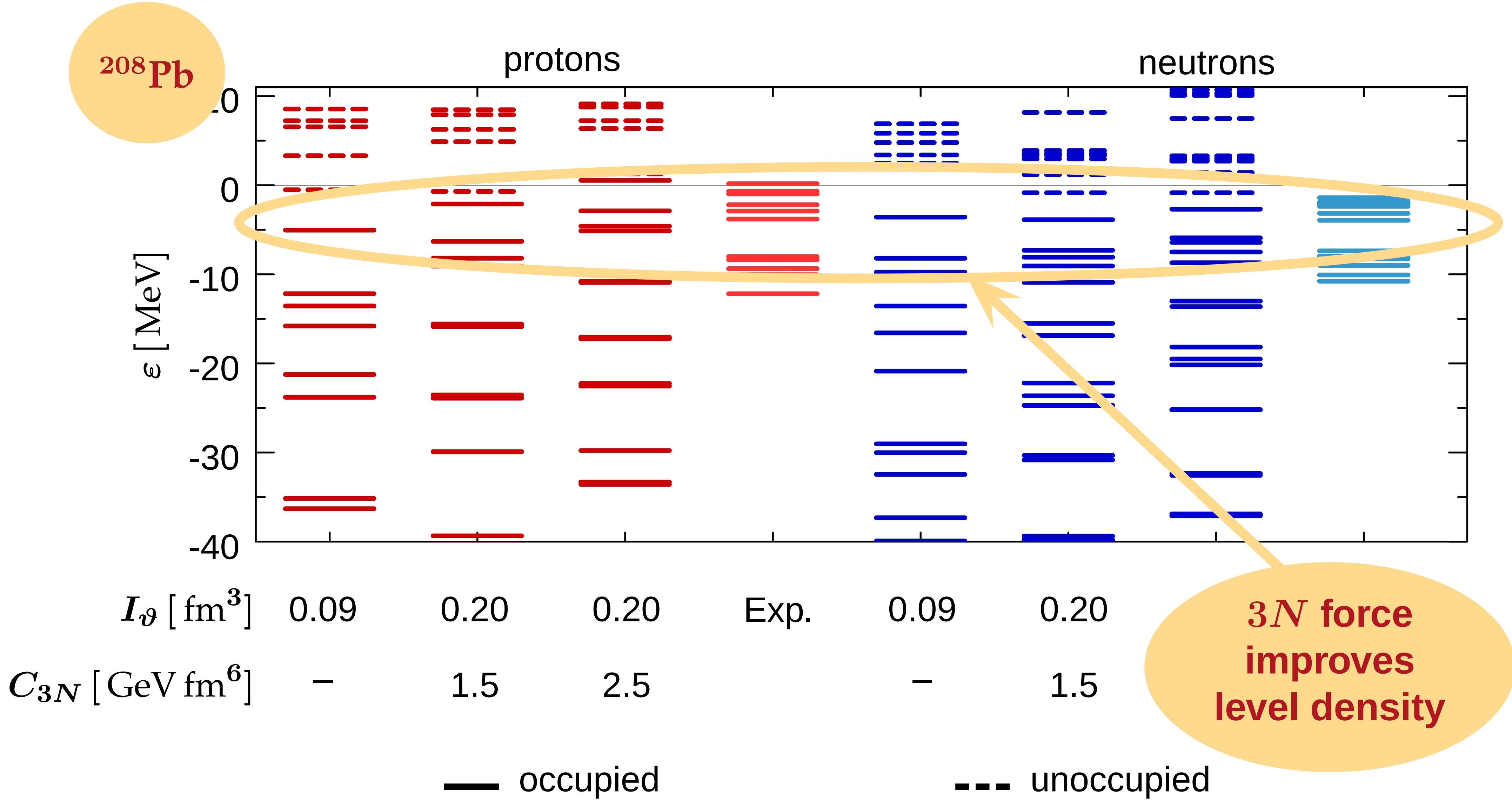
$3N$ Forces: Energies & Radii



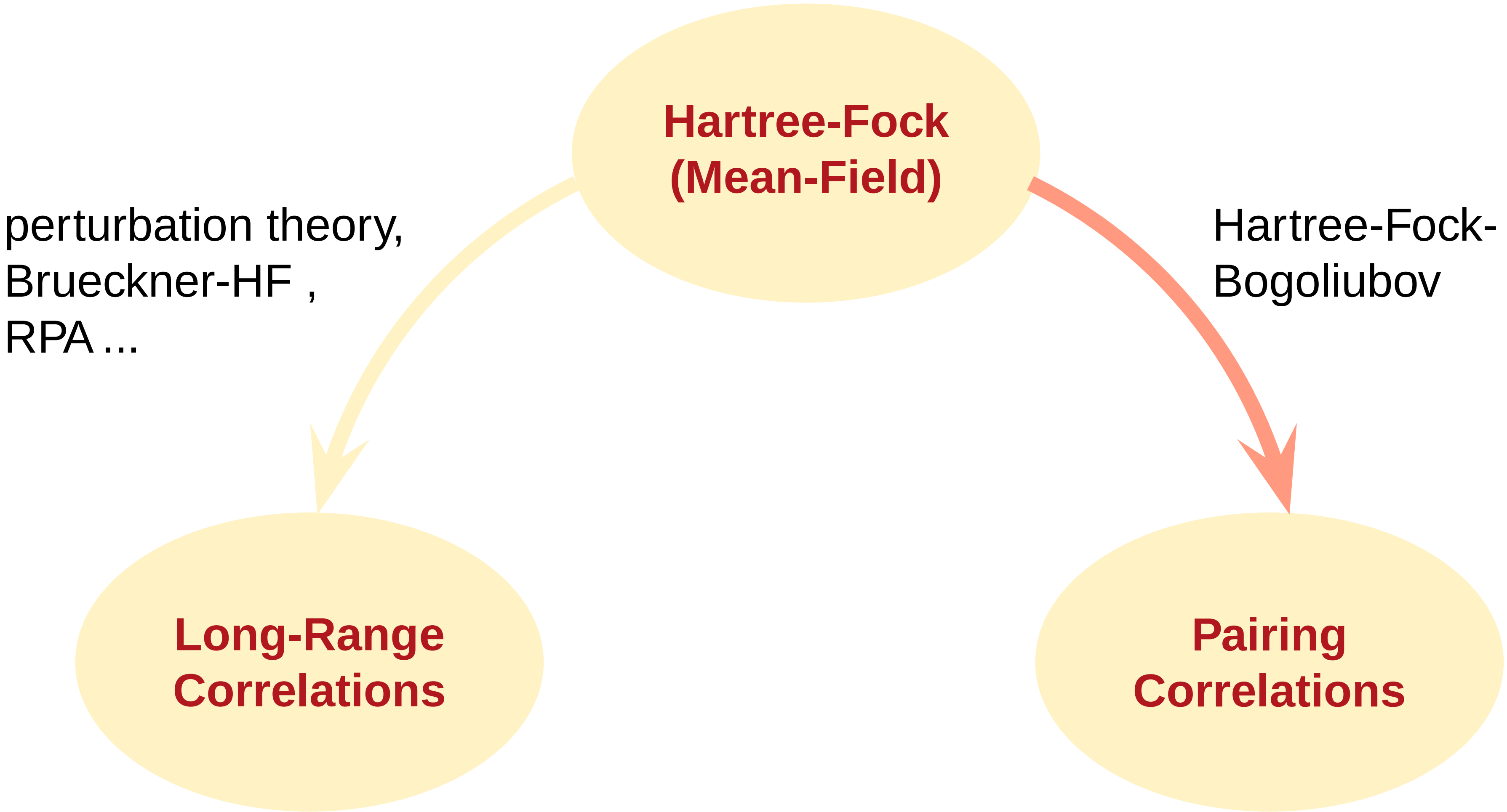
$3N$ Forces: HF Single-Particle Energies



$3N$ Forces: HF Single-Particle Energies



Beyond Hartree-Fock



HFB Theory Overview

Bogoliubov Transformation

$$\beta_k^\dagger = \sum_q U_{qk} c_q^\dagger + V_{qk} c_q$$

$$\beta_k = \sum_q U_{qk}^* c_q + V_{qk}^* c_q^\dagger$$

where

$$\{\beta_k, \beta_{k'}\} \stackrel{!}{=} \{\beta_k^\dagger, \beta_{k'}^\dagger\} \stackrel{!}{=} 0$$

$$\{\beta_k, \beta_{k'}^\dagger\} \stackrel{!}{=} \delta_{kk'}$$

HFB Densities & Fields

$$\rho_{kk'} \equiv \left\langle \Psi \right| c_{k'}^\dagger c_k \left| \Psi \right\rangle = (V^* V^T)_{kk'}$$

$$\kappa_{kk'} \equiv \left\langle \Psi \right| c_{k'} c_k \left| \Psi \right\rangle = (V^* U^T)_{kk'}$$

$$\Gamma_{kk'} = \sum_{qq'} \left(\frac{2}{A} \bar{\mathrm{t}}_{\mathrm{rel}} + \bar{\mathrm{v}} \right)_{kq',k'q} \rho_{qq'}$$

$$\Delta_{kk'} = \sum_{qq'} \left(\frac{2}{A} \bar{\mathrm{t}}_{\mathrm{rel}} + \bar{\mathrm{v}} \right)_{kk',qq'} \kappa_{qq'}$$

Energy

$$E[\rho, \kappa, \kappa^*] = \frac{\left\langle \Psi \right| \mathrm{H} \left| \Psi \right\rangle}{\left\langle \Psi | \Psi \right\rangle} \equiv \frac{1}{2} \left(\mathrm{tr}\ \Gamma\rho - \mathrm{tr}\ \Delta\kappa^* \right)$$

HFB Equations

$$(\mathcal{H} - \lambda\mathcal{N}) \begin{pmatrix} U \\ V \end{pmatrix} \equiv \begin{pmatrix} \Gamma - \lambda & \Delta \\ -\Delta^* & -\Gamma^* + \lambda \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix} = E \begin{pmatrix} U \\ V \end{pmatrix}$$

Particle Number Projection

Variation of Projected Energy

$$\delta E(N_0) = \frac{1}{2\pi\langle \mathrm{P}_{N_0}\rangle} \int_0^{2\pi} d\phi \, \left\langle e^{i\phi(\mathrm{N}-N_0)}\right\rangle \left\{ \delta \langle \mathrm{H} \rangle_\phi - \left(E(N_0) - \langle \mathrm{H} \rangle_\phi \right) \delta \log \left\langle e^{i\phi \mathrm{N}} \right\rangle \right\}$$

$$\langle \mathrm{H} \rangle_\phi \equiv \langle \mathrm{H} e^{i\phi\mathrm{N}} \rangle / \langle e^{i\phi\mathrm{N}} \rangle$$

Lipkin-Nogami + PAV

- power series expansion
- expansion coefficients **not varied**
- indeterminate / numerically unstable at shell closures
- exact PNP after variation

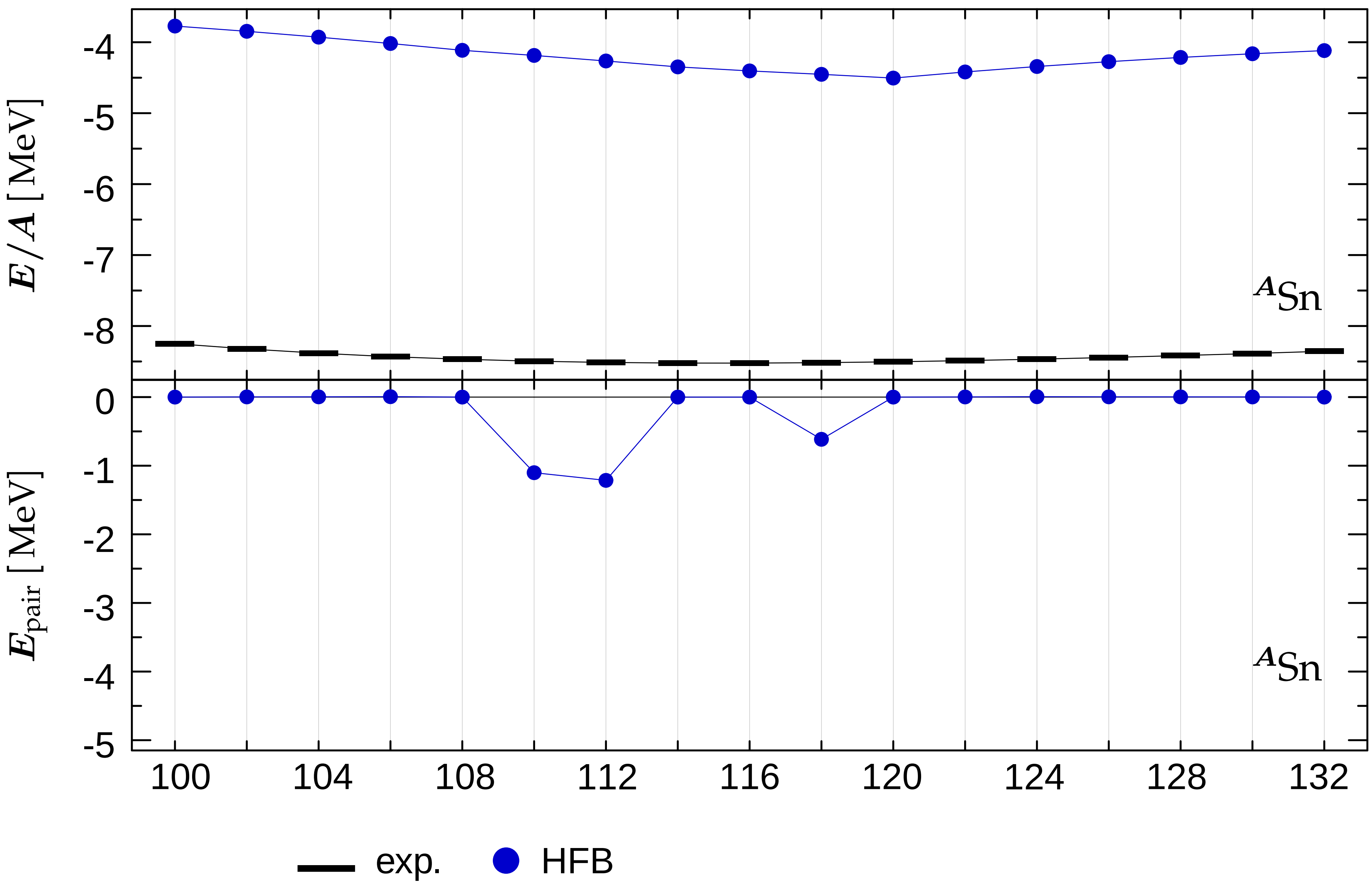
VAP

- higher (but managable) computational effort
- implement with care: **subtle cancellations between divergences of direct, exchange, and pairing terms**

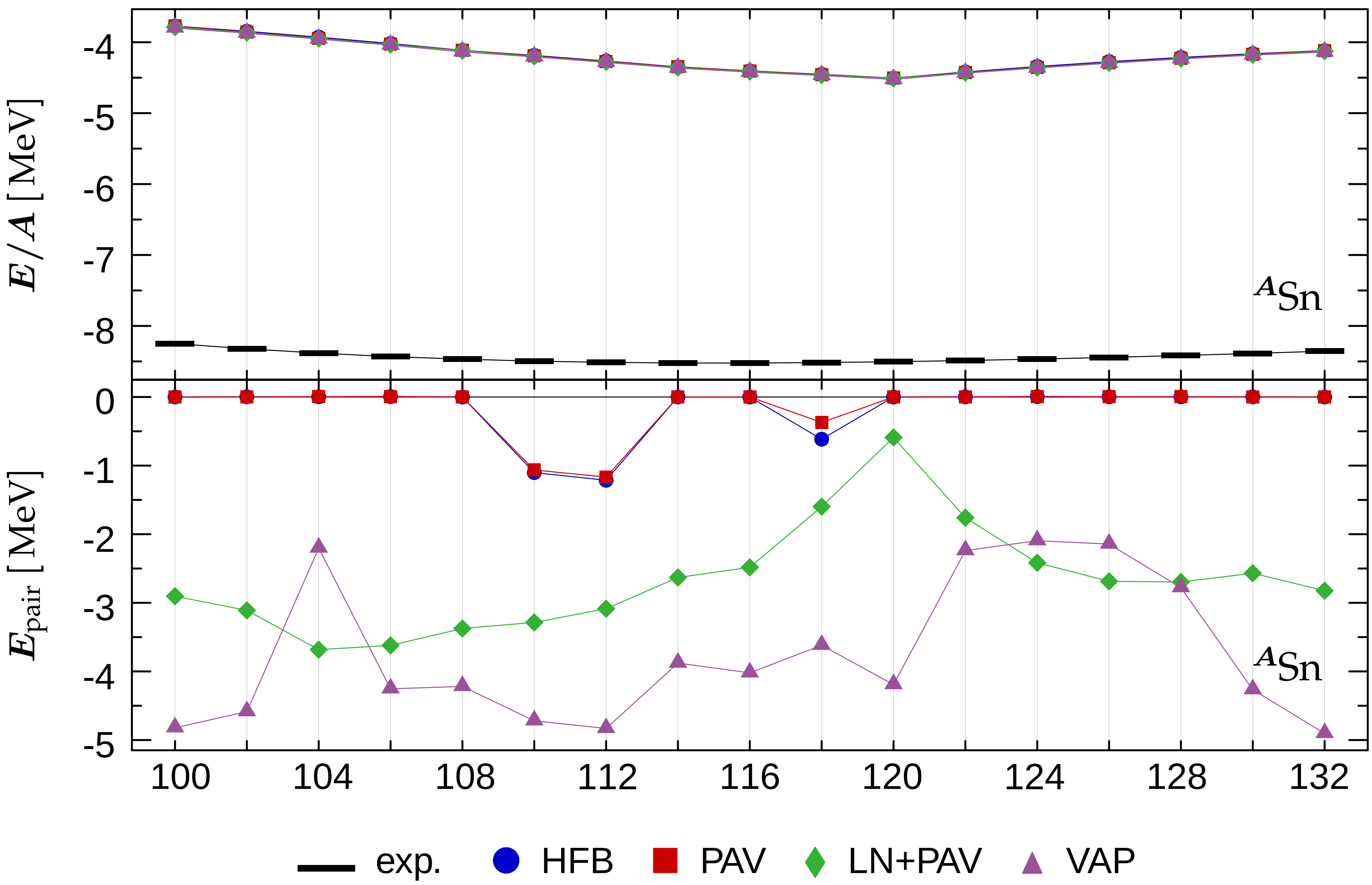
☞ Structure of **HFB equations is preserved** by both methods!

Flocard & Onishi, Ann. Phys. 254, **275** (1997, approx. PNP); Sheikh et al., Phys. Rev. **C66**, 044318 (2002, exact PNP)

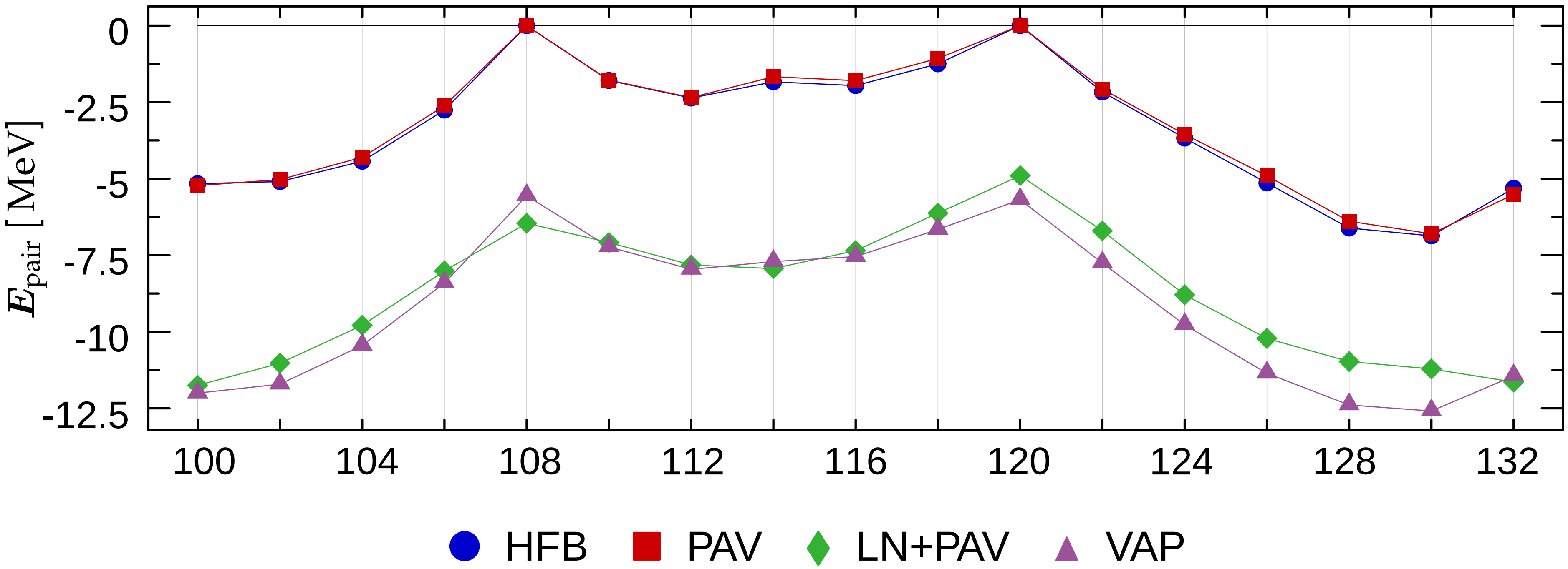
Sn Isotopes: Binding & Pairing Energies



Sn Isotopes: Binding & Pairing Energies



Density-Dependent Force: Pairing



- **linear density dependence**, $t_0 = \frac{1}{6} C_{3N}$:

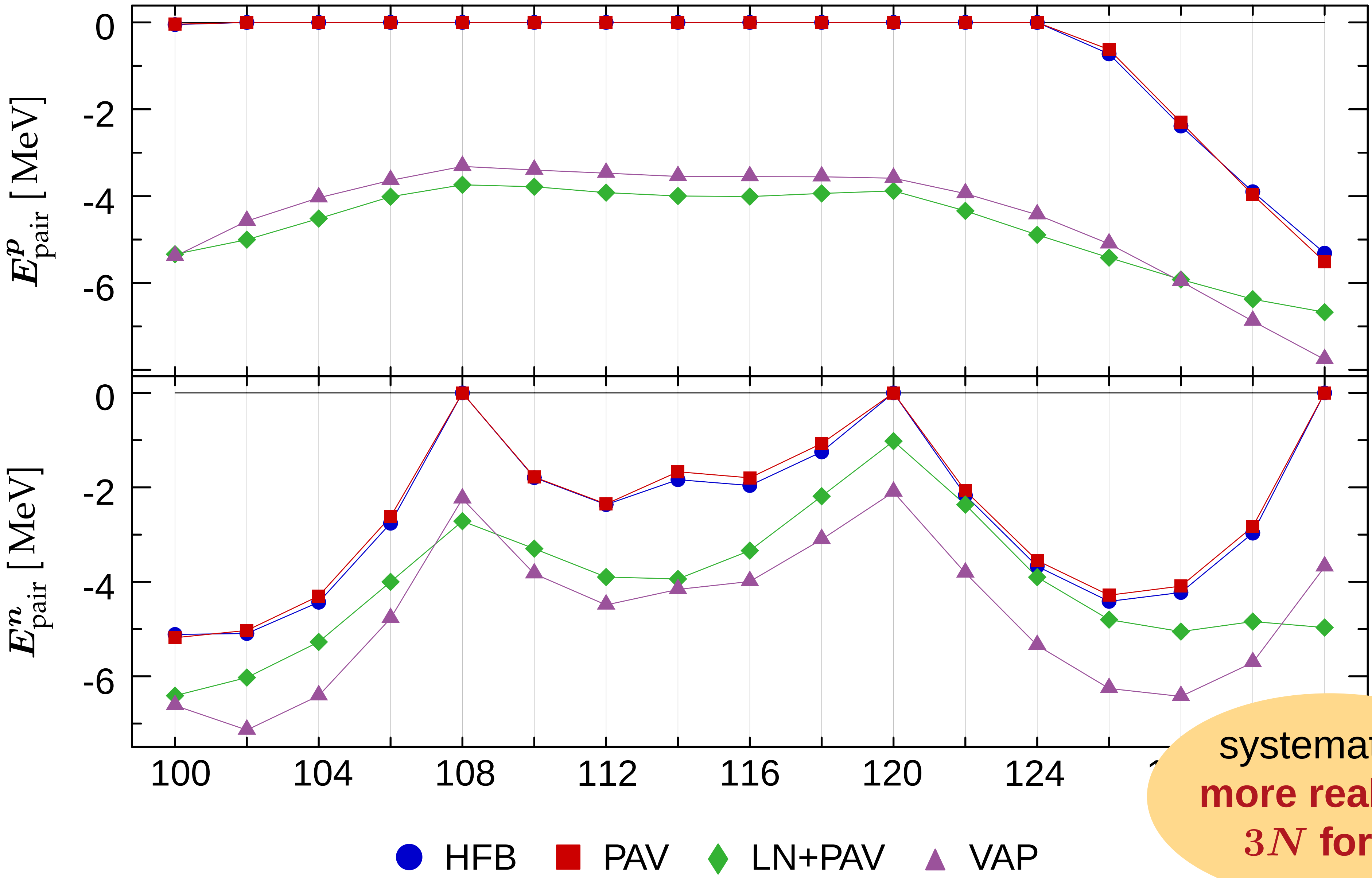
$$\mathrm{V}_\rho = t_0 \, (1 + \mathrm{P}_\sigma) \, \rho \left(\tfrac{1}{2}(\vec{\mathrm{r}}_1 + \vec{\mathrm{r}}_2) \right) \delta^3 \, (\vec{\mathrm{r}}_1 - \vec{\mathrm{r}}_2)$$

- **mixed density** for PAV/VAP: $\rho(\vec{\mathrm{R}}) \longrightarrow \rho_{\phi_p,\phi_n}(\vec{\mathrm{R}})$
- phenomenological VAP calculations: $E_{\text{pair}} \simeq 10 - 20 \text{ MeV}$

(Stoitsov et al., nucl-th/0610061; Anguiano et al., Phys. Lett. **B545** (2002), 62)

"correct" order of magnitude **with realistic NN int.**

Density-Dependent Force: Pairing



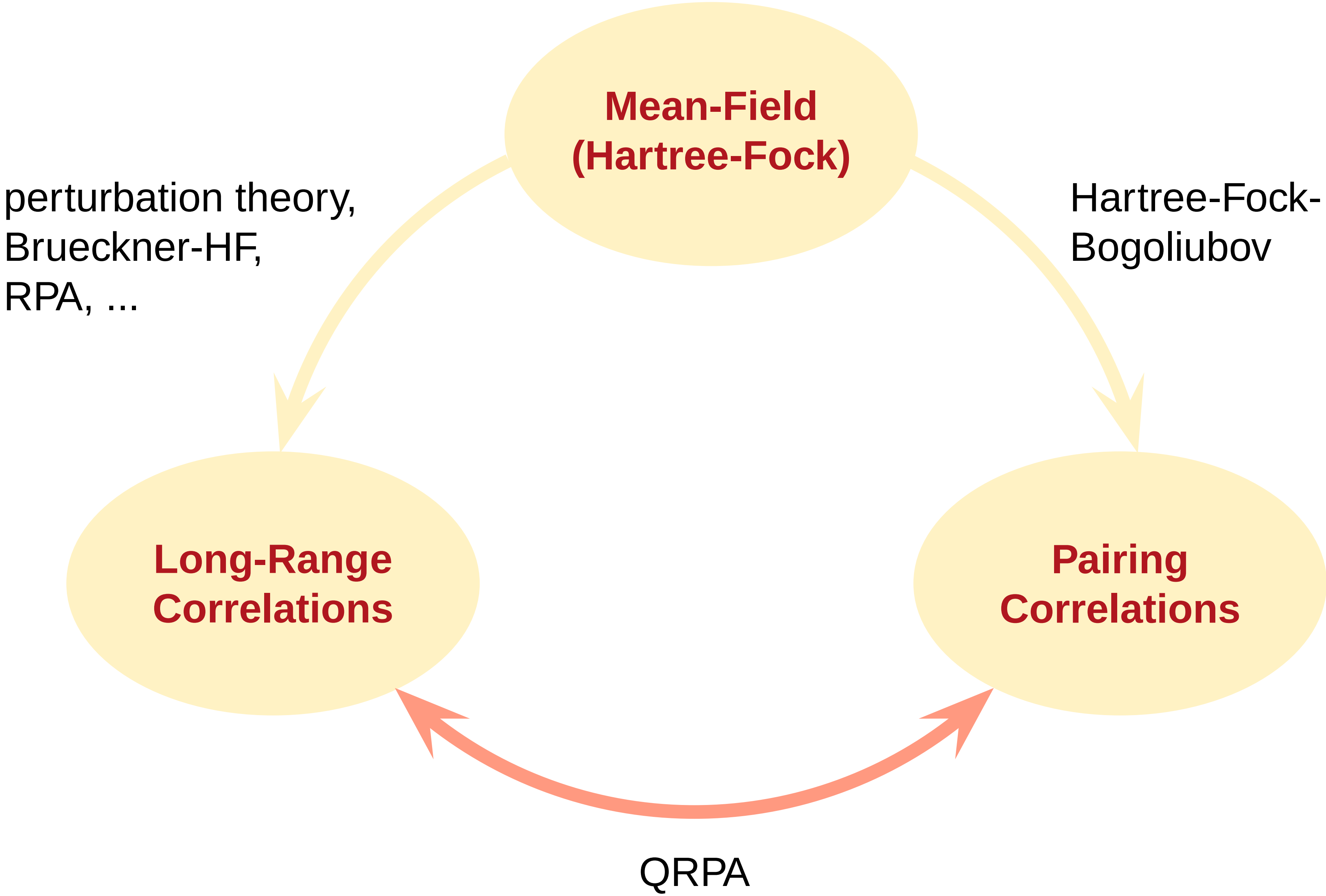
systematics:
more realistic $3N$ force

Conclusions

Modern Effective Interactions

- **Status**
  - treatment of **short-range central** and **tensor correlations** by unitary transformations:
    - Unitary Correlation Operator Method
    - Similarity Renormalization Group
  - **universal phase-shift equivalent** correlated interaction $\mathbf{V}_{\mathrm{UCOM}}$
- **Outlook**
  - **connections** between UCOM and SRG
  - inclusion & treatment of $3N$ **Forces**, in particular...
  - **chiral interactions**

HF, HFB, and Beyond



HF, HFB, and Beyond

- **Status**
  - **fully consistent** HFB calculations with particle number projection
  - **inclusion of $3N$-forces**: **contact & finite range** matrix elements for HF, density-dependent force for HFB, RPA, ...
  - **Like-particle-** & pn**-QRPA** (benchmarked)
- **Outlook**
  - pn **pairing**, Isobaric Analog & Gamow-Teller Resonances
  - **deformation** and **symmetry restoration** by projection (isospin, parity, angular momentum)
  - **caveat:** analytic structure of density-dependent forces is very important in symmetry-projected HFB (J. Dobaczewski, arXiv: 0708.0441)

Perspectives

- **Modern Effective Interactions**
  - treatment of short-range central and tensor correlations by unitary transformations: UCOM, SRG, Lee-Suzuki,...
  - phase-shift equivalent correlated interaction $\mathbf{V}_{\mathrm{UCOM}}$
  - universal input for...
- **Innovative Many-Body Methods**
  - No-Core Shell Model,...
  - Importance Truncated NCSM, Coupled Cluster Method,...
  - Hartree-Fock plus MBPT, Padé Resummed MBPT, BHF, HFB, RPA,...
  - Fermionic Molecular Dynamics,...

Last Words...

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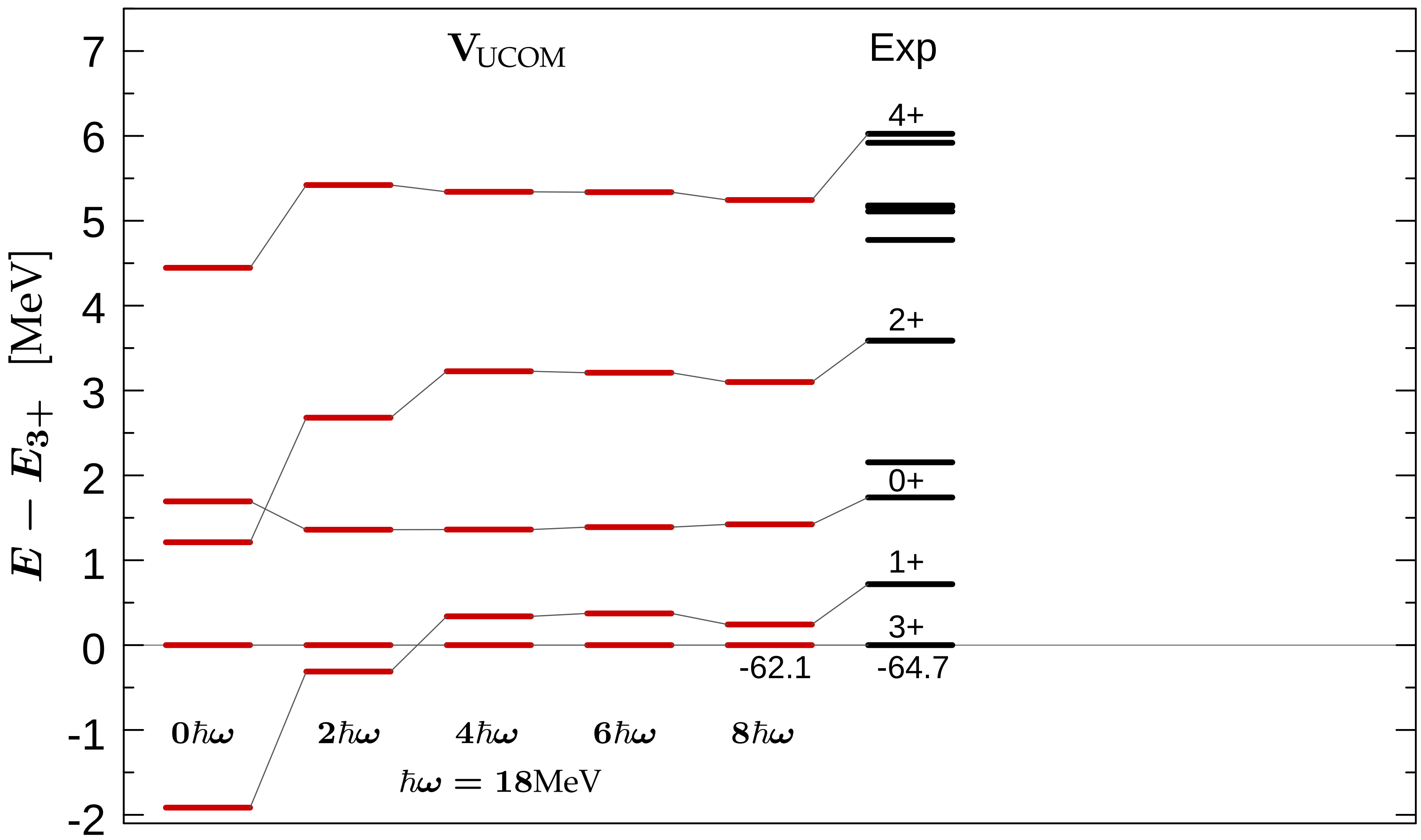
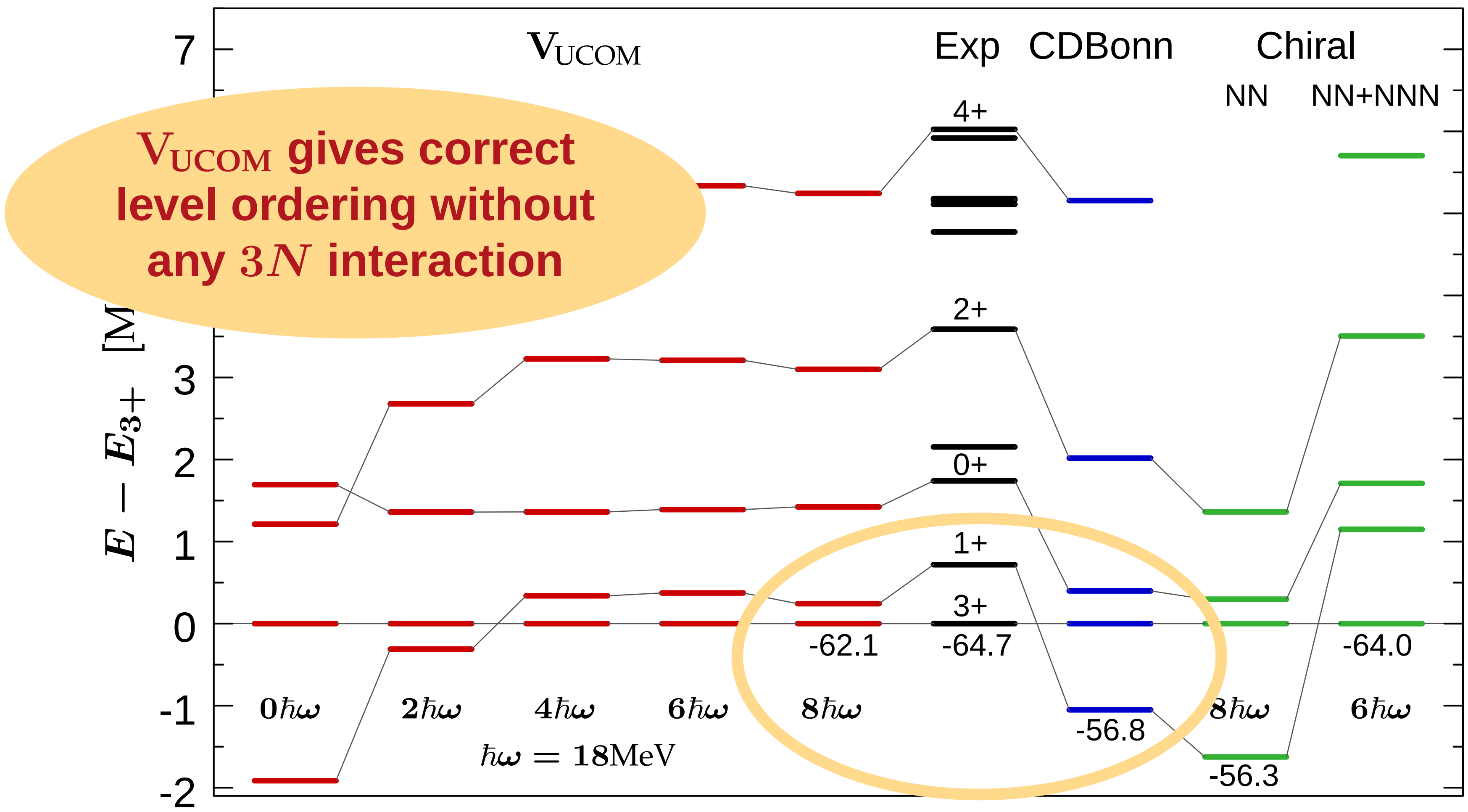
- N. Paar, P. Papakonstantinou, H. Hergert, and R. Roth, Phys. Rev. C**74**, 014318 (2006)
- R. Roth, P. Papakonstantinou, N.Paar, H. Hergert, T. Neff, and H. Feldmeier, Phys. Rev. C**73**, 044312 (2006)
- http://crunch.ikp.physik.tu-darmstadt.de/tnp/

Appendix

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



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

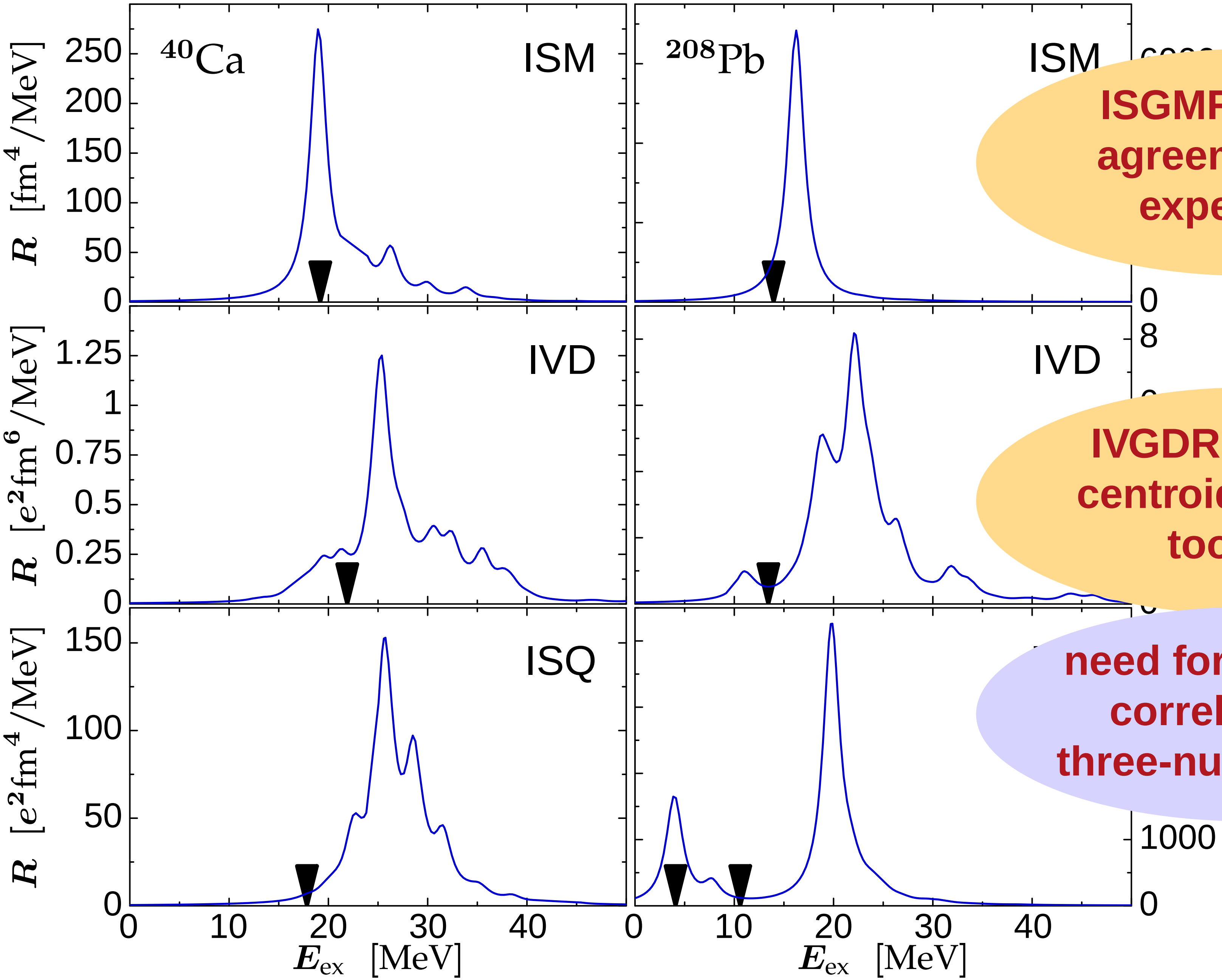


RPA + Realistic Interactions

RPA, ERPA & SRPA
+
Matrix Elements of Correlated Realistic Interaction $\mathrm{V}_{\mathrm{UCOM}}$

- **fully self-consistent RPA** based on the Hartree-Fock orbits using the same V_{UCOM}
- recovering sum rules with high precision, spurious center-of-mass mode fully decoupled at ~ 10 keV
- **Extended-RPA and Second-RPA** to include effects of ground state correlations and complex configurations

RPA with V_{UCOM}

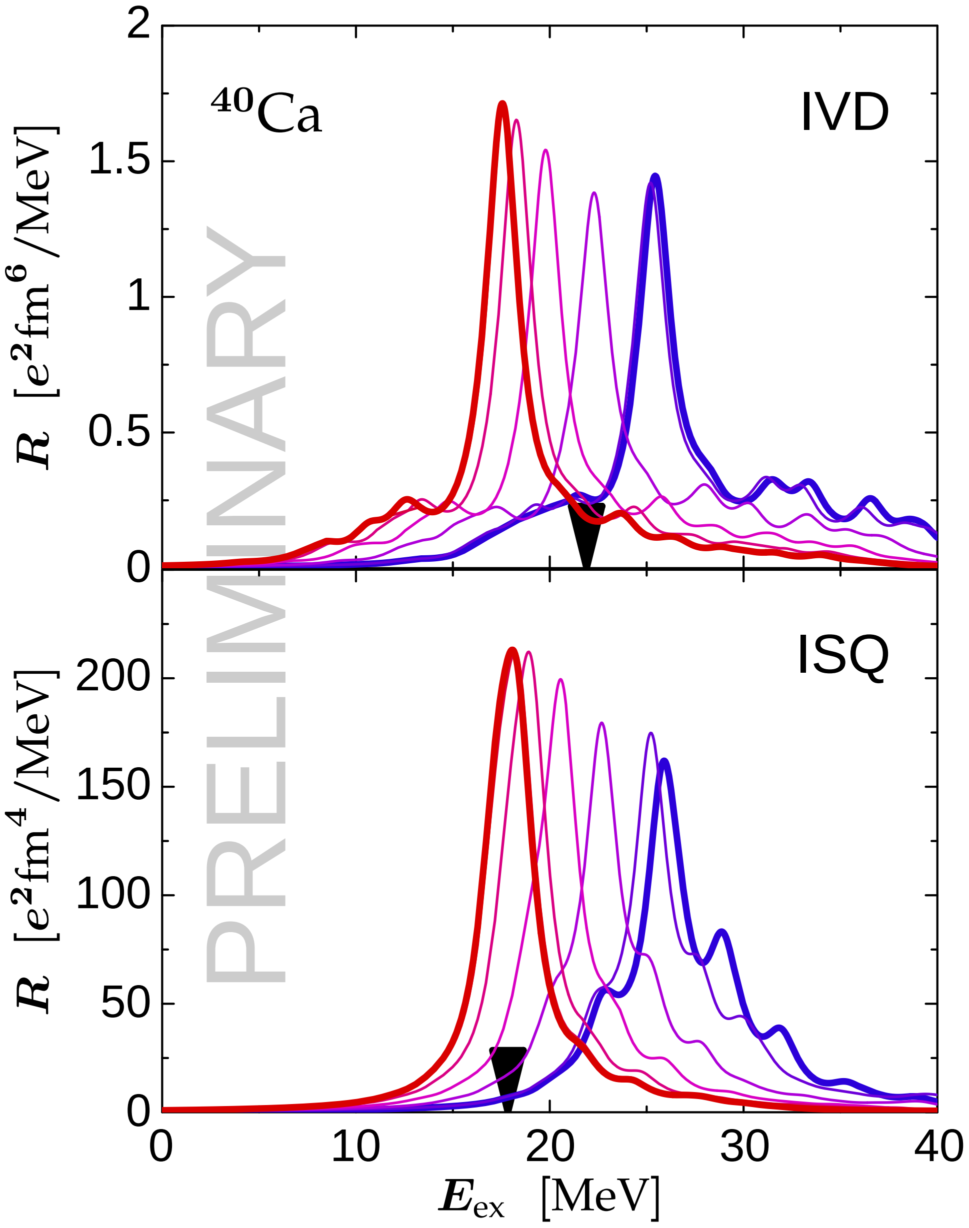


ISGMR in good agreement with experiment

IVGDR & ISGQR centroid energies too high

need for additional correlations & three-nucleon force

SRPA: Complex Configurations



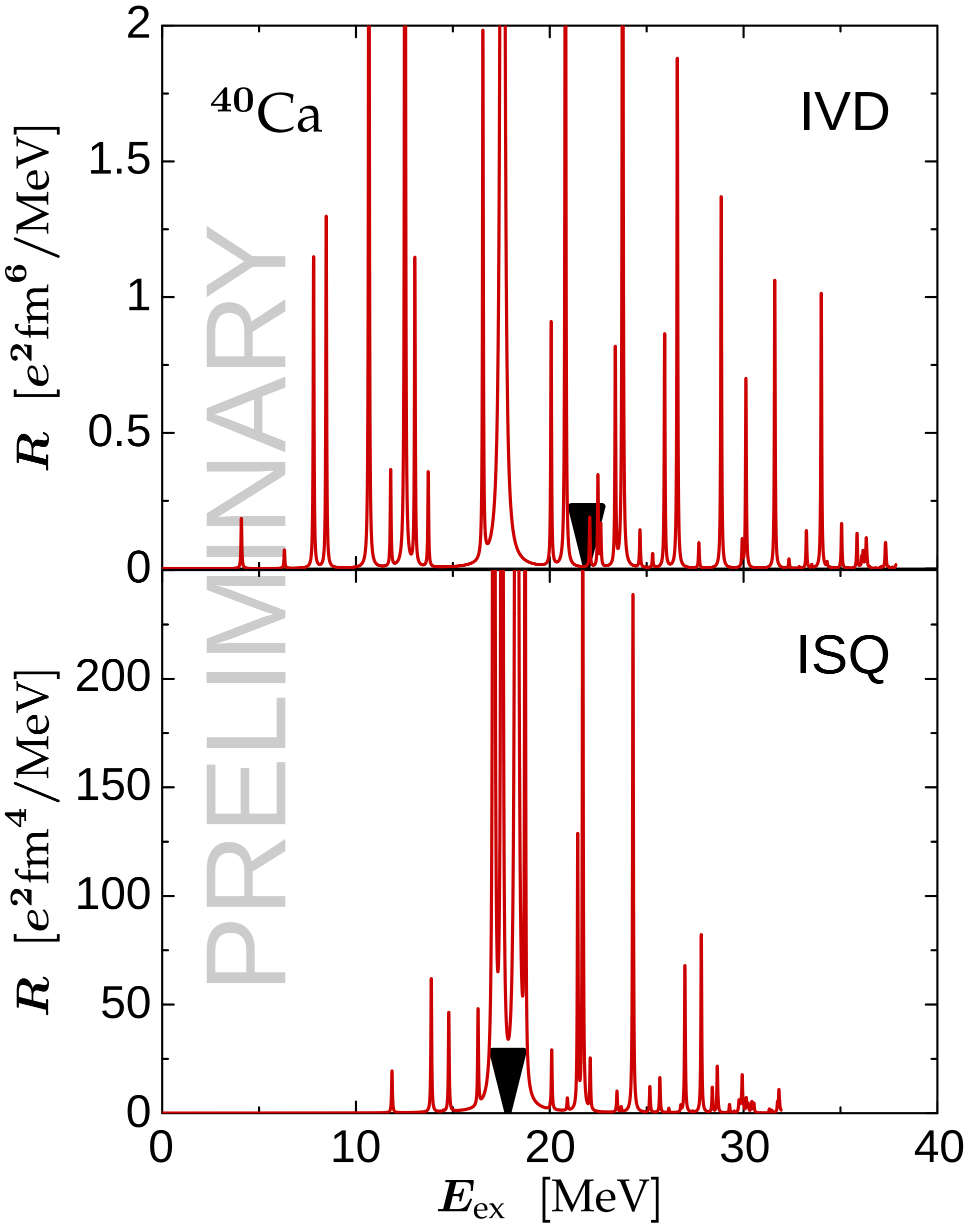
RPA (full 1p1h space)

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)

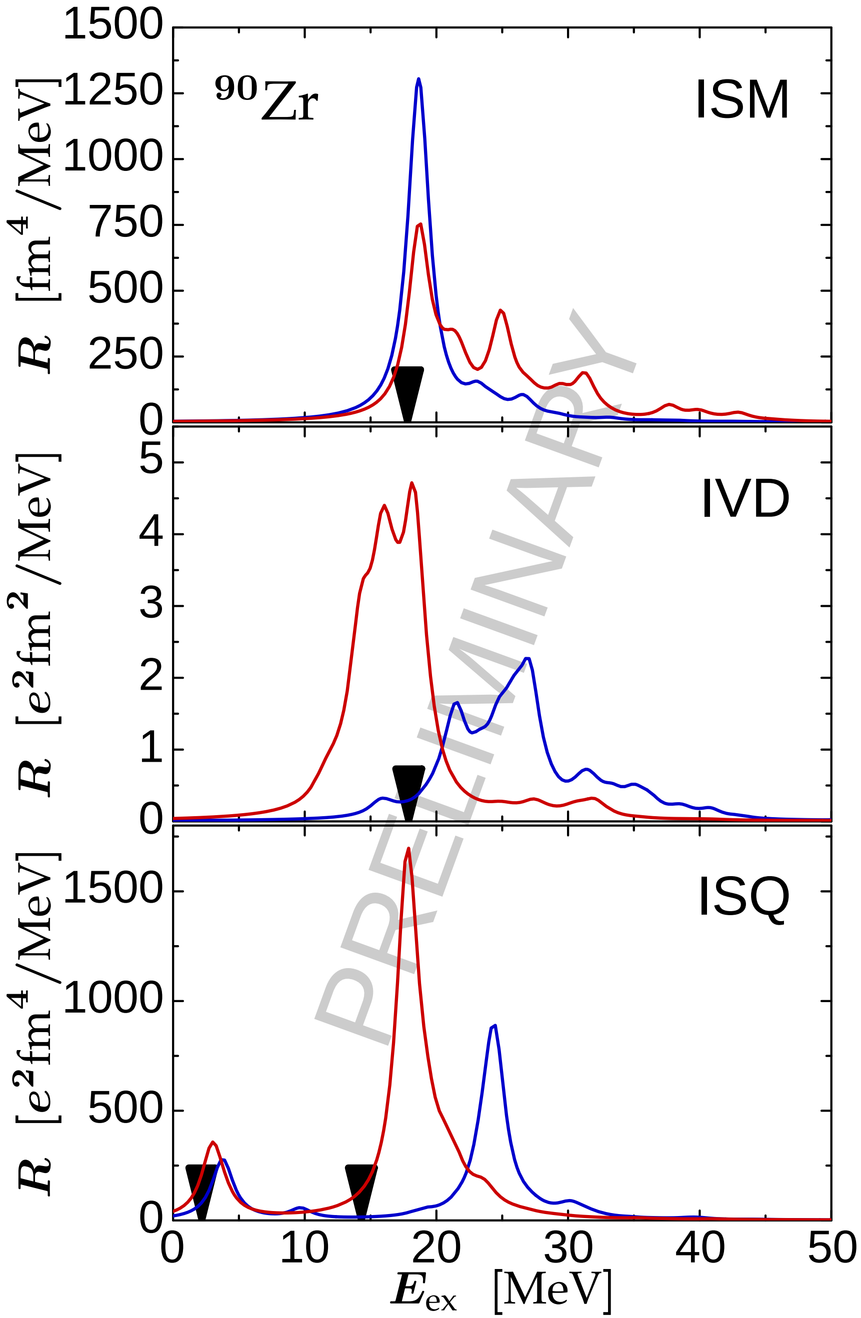
SRPA (full 1p1h+2p2h space)

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

complex configurations have significant impact on response

possibility to investigate fine structure

Outlook: RPA with Three-Body Forces



- long-range tensor correlator & **repulsive three-body contact interaction**

- systematic improvement of
  - → rms-radii
  - → single-particle spectra
  - → strength distributions

standard V_{UCOM}

V_{UCOM} with long-range tensor & three-body contact interaction