Ab-Initio Calculations across the Nuclear Chart:

Interactions and Methods

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Overview

- Unitarily Transformed Interactions
- Hartree-Fock and Perturbation Theory
- Pairing in the UCOM Framework
  - Hartree-Fock-Bogoliubov & Projection
  - Quasiparticle RPA
- 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

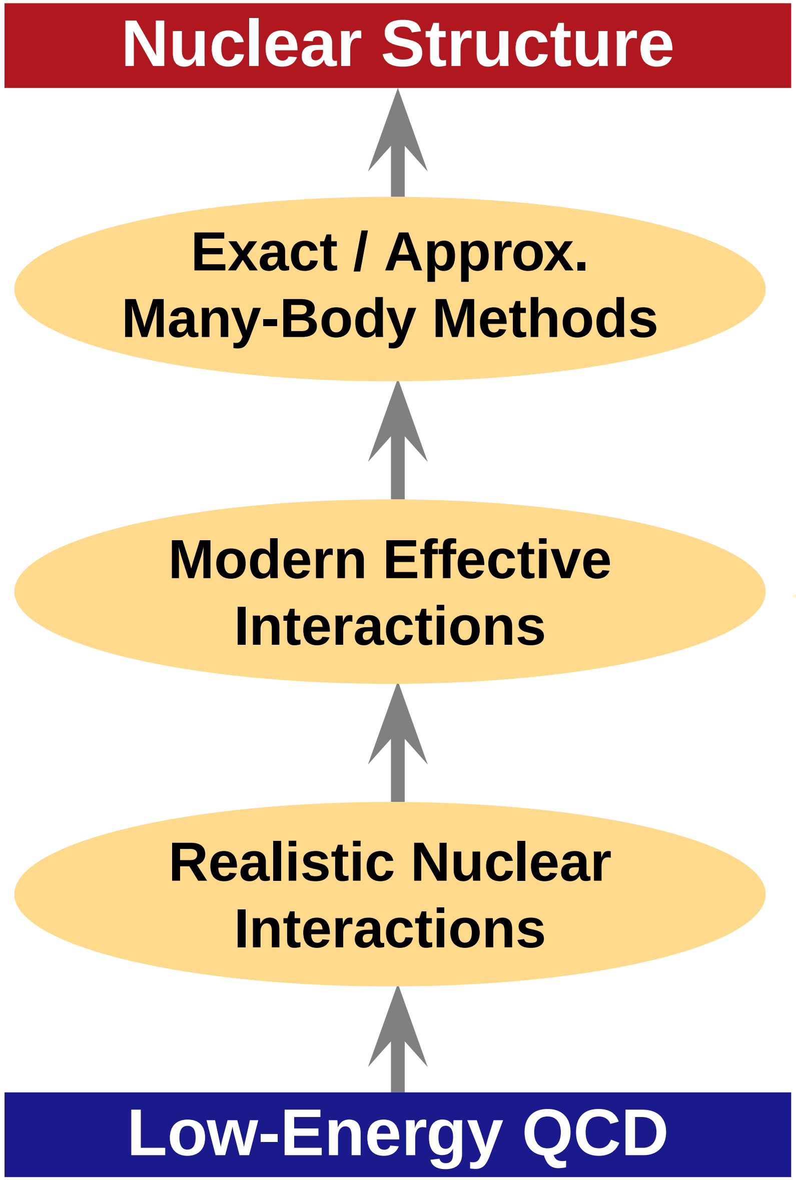
- 'exact' solution of the many-body problem for light and intermediate masses (GFMC, NCSM, CC,...)
- controlled approximations for heavier nuclei (HF & MBPT,...)
- rely on restricted model spaces of tractable size
- not suitable for the description of short-range correlations

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

Unitarily Transformed Interactions

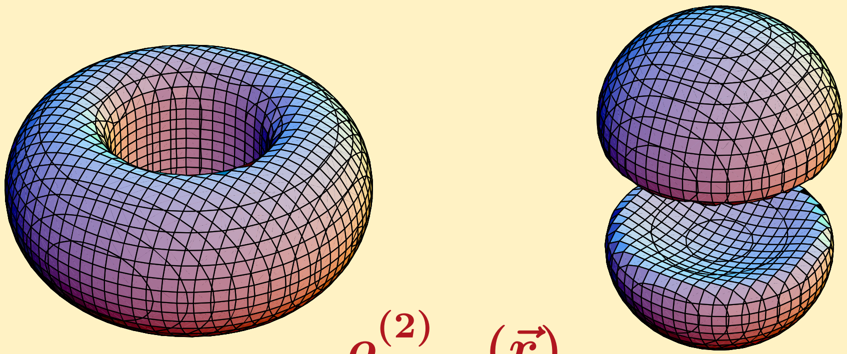
Unitary Correlation Operator Method (UCOM)

Deuteron: Manifestation of Correlations

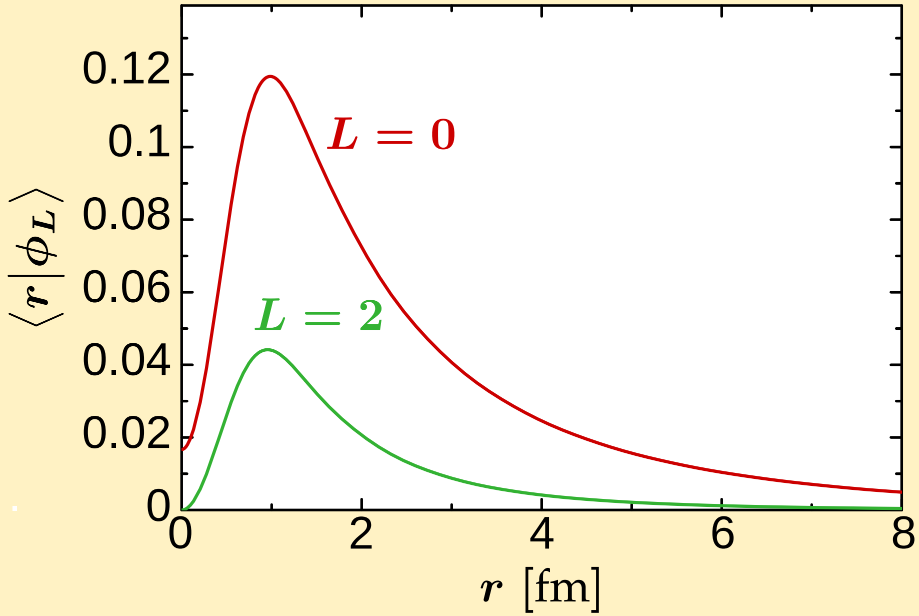
Realistic Deuteron Solution

$M_S = 0$ $\qquad\qquad$ $M_S = \pm 1$

$\frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle \right)$ $\qquad\qquad$ $|\uparrow\uparrow\rangle, \; |\downarrow\downarrow\rangle$



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



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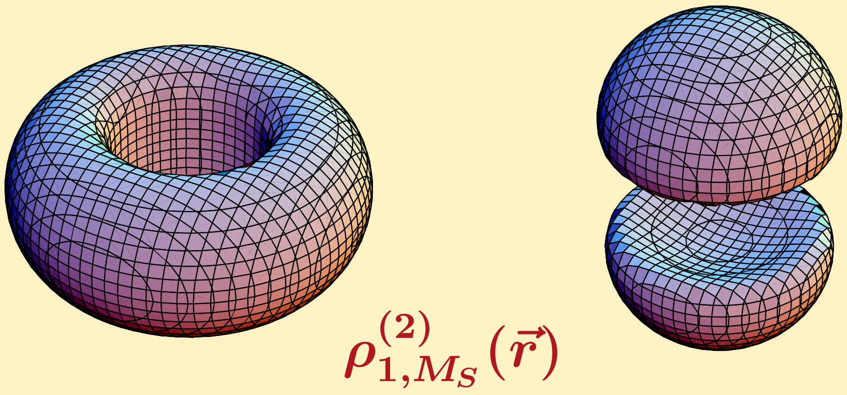

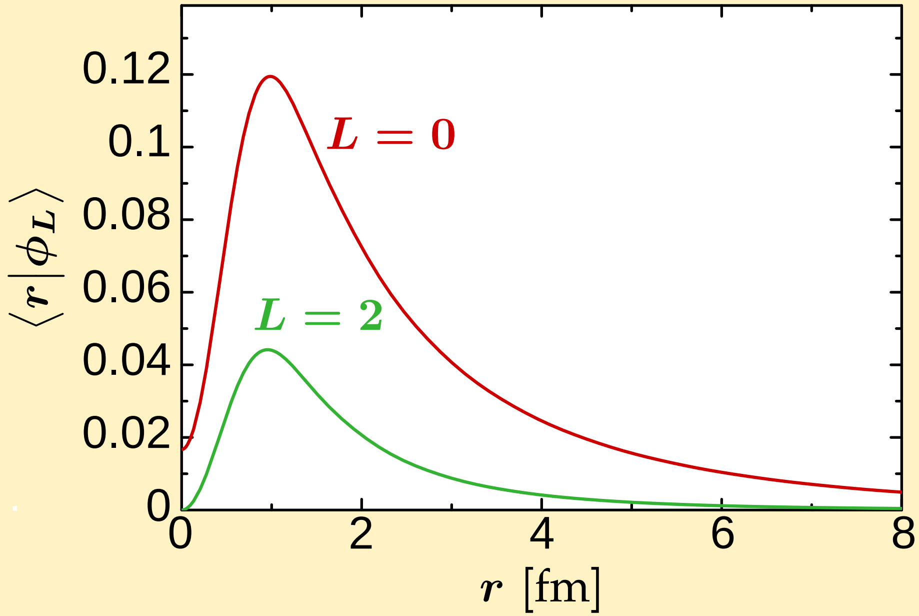

short-range repulsion supresses wavefunction at small distances r

central correlations

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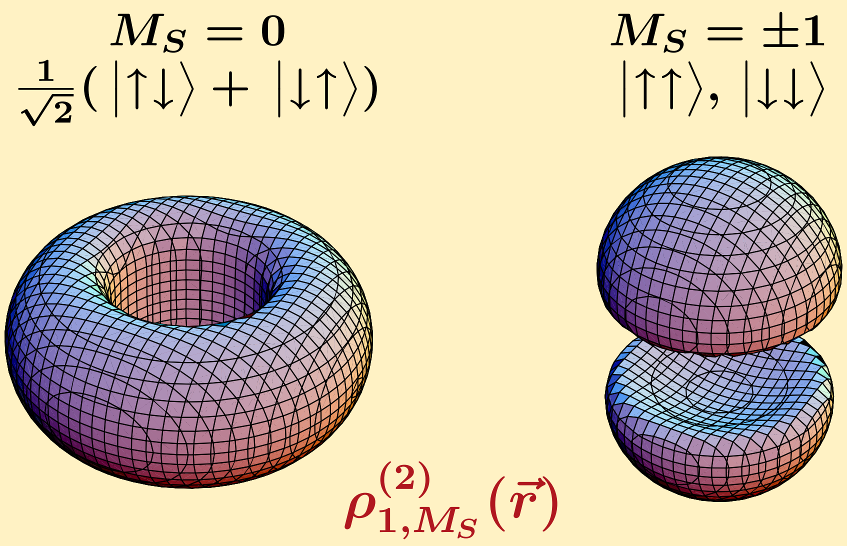
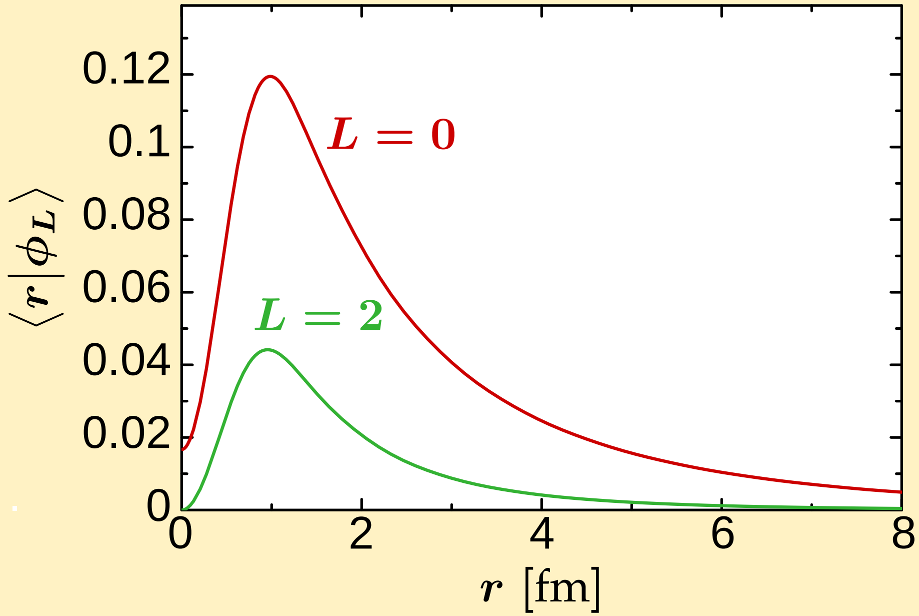




short-range repulsion supresses wavefunction at small distances r

central correlations

tensor interaction generates D-wave admixture in the ground state

tensor correlations

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

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

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

Tensor Correlator C_Ω

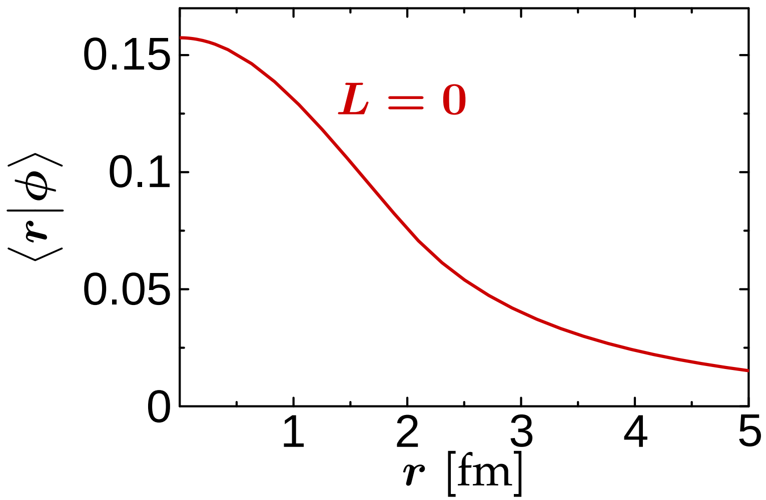
- angular shift depending on the orientation of spin and relative coordinate of a nucleon pair

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

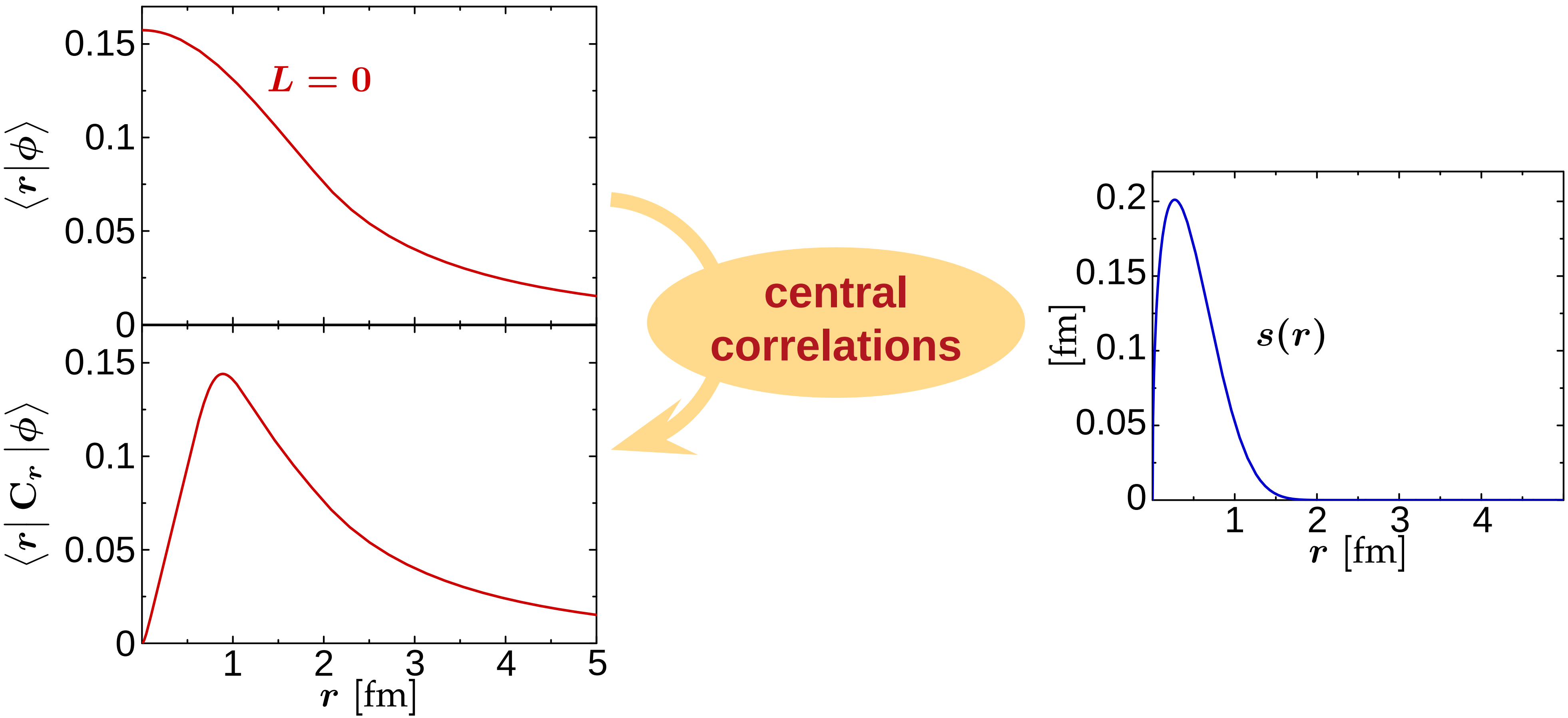
$$\vec{\mathbf{q}}_\Omega = \vec{\mathbf{q}} - \tfrac{\vec{\mathbf{r}}}{\mathbf{r}}\ \mathbf{q}_r$$

- $s(r)$ and $\vartheta(r)$ optimized for given initial potential

Correlated States: The Deuteron



Correlated States: The Deuteron



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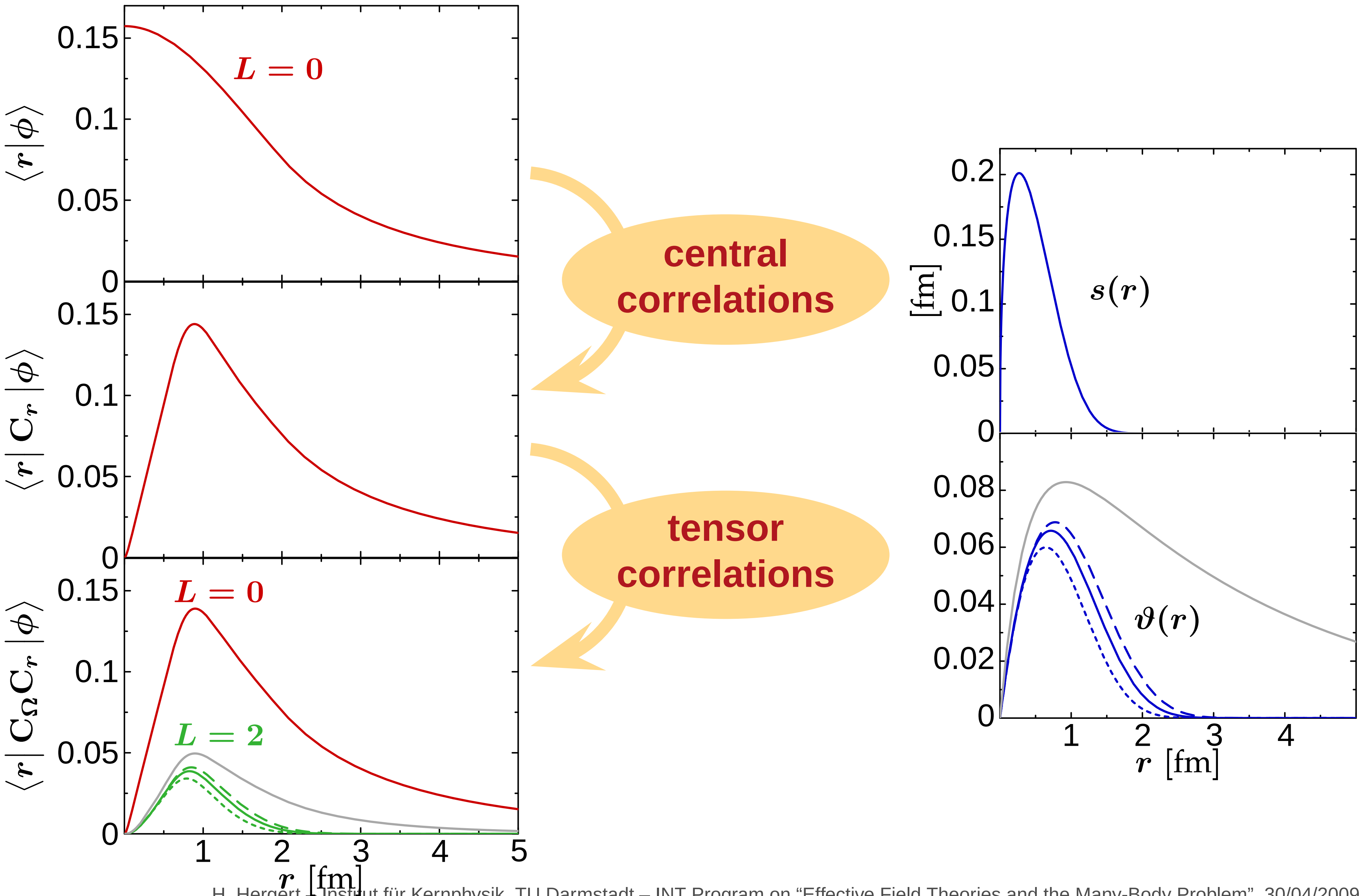

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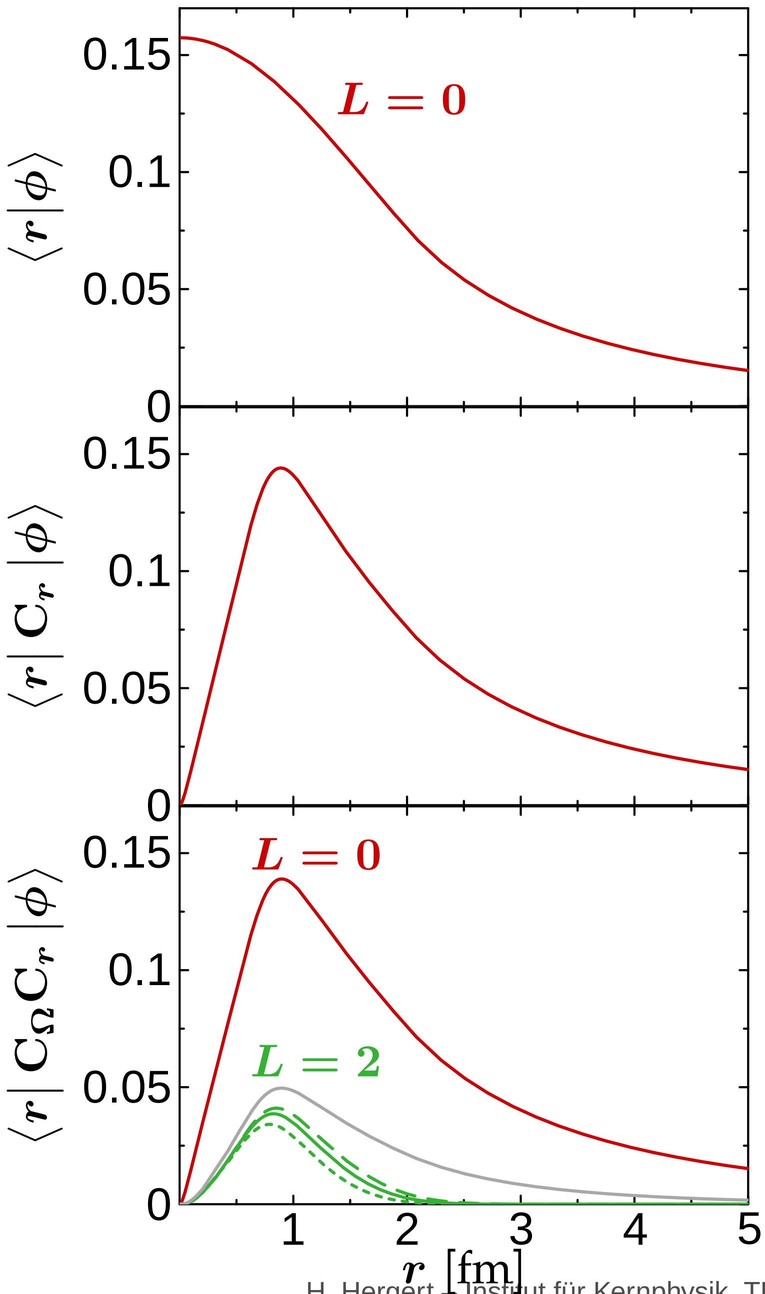
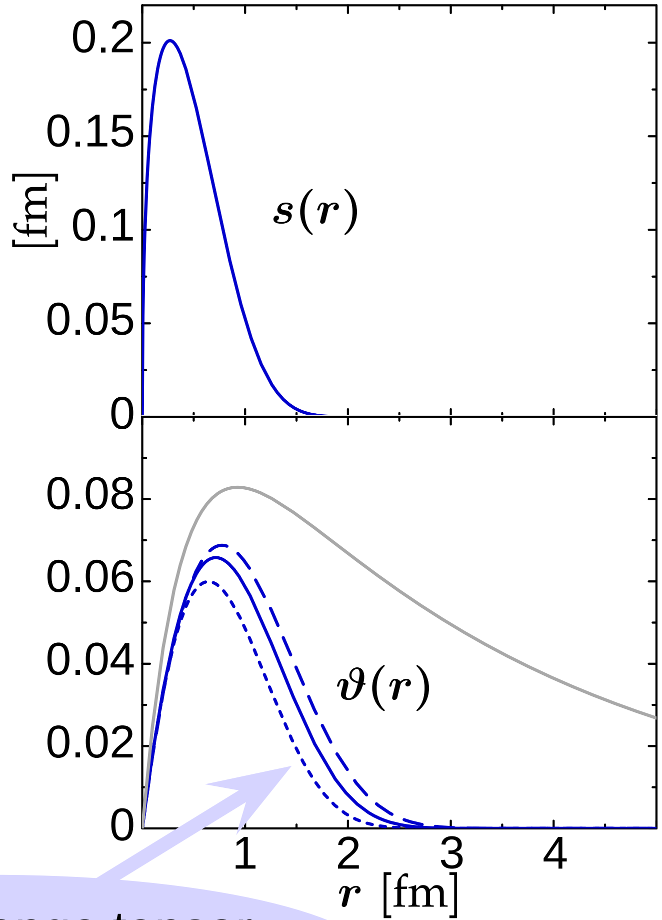


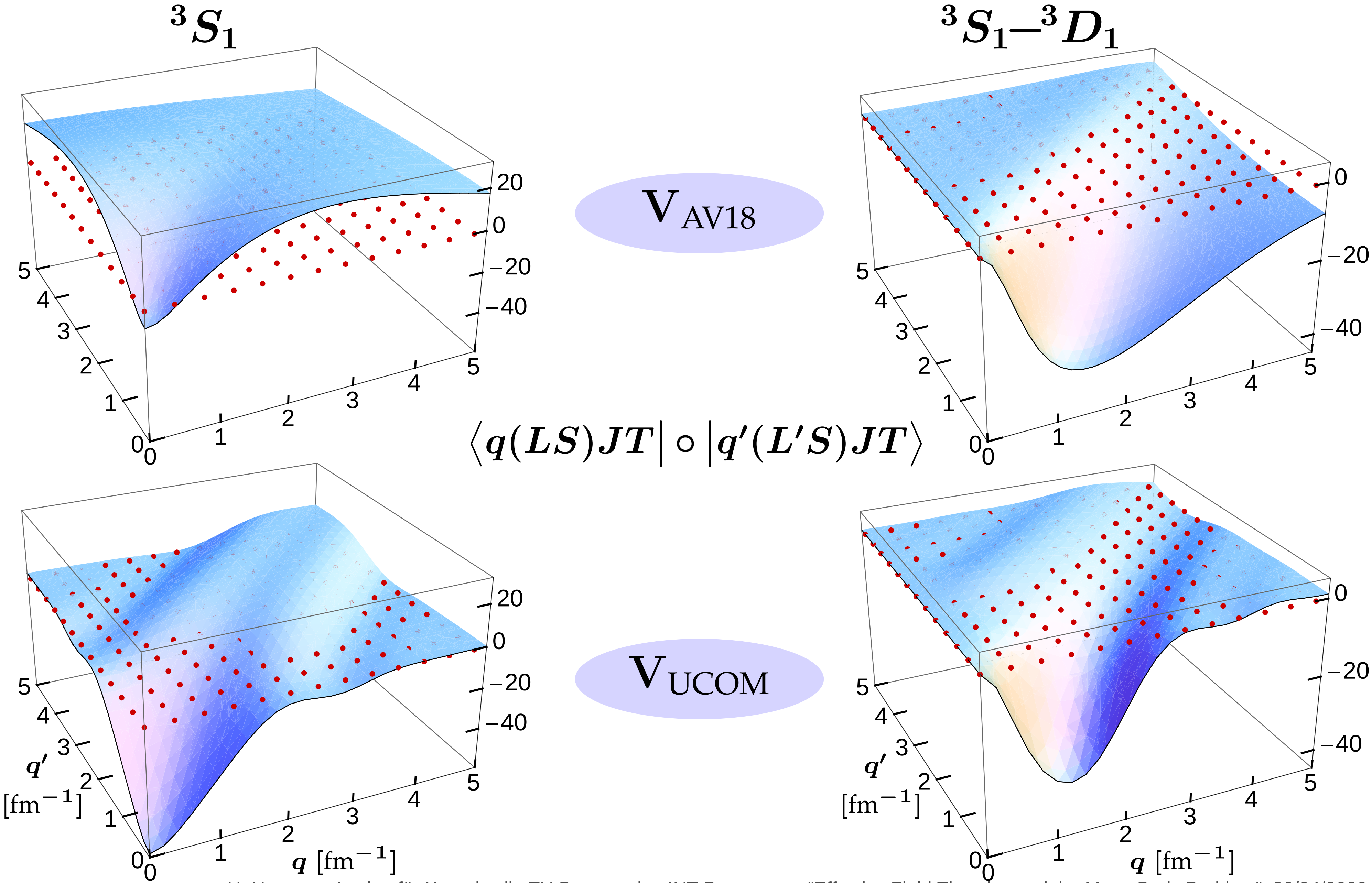
central correlations

tensor correlations



only short-range tensor correlations treated by C_Ω

Correlated Interaction: V_{UCOM}



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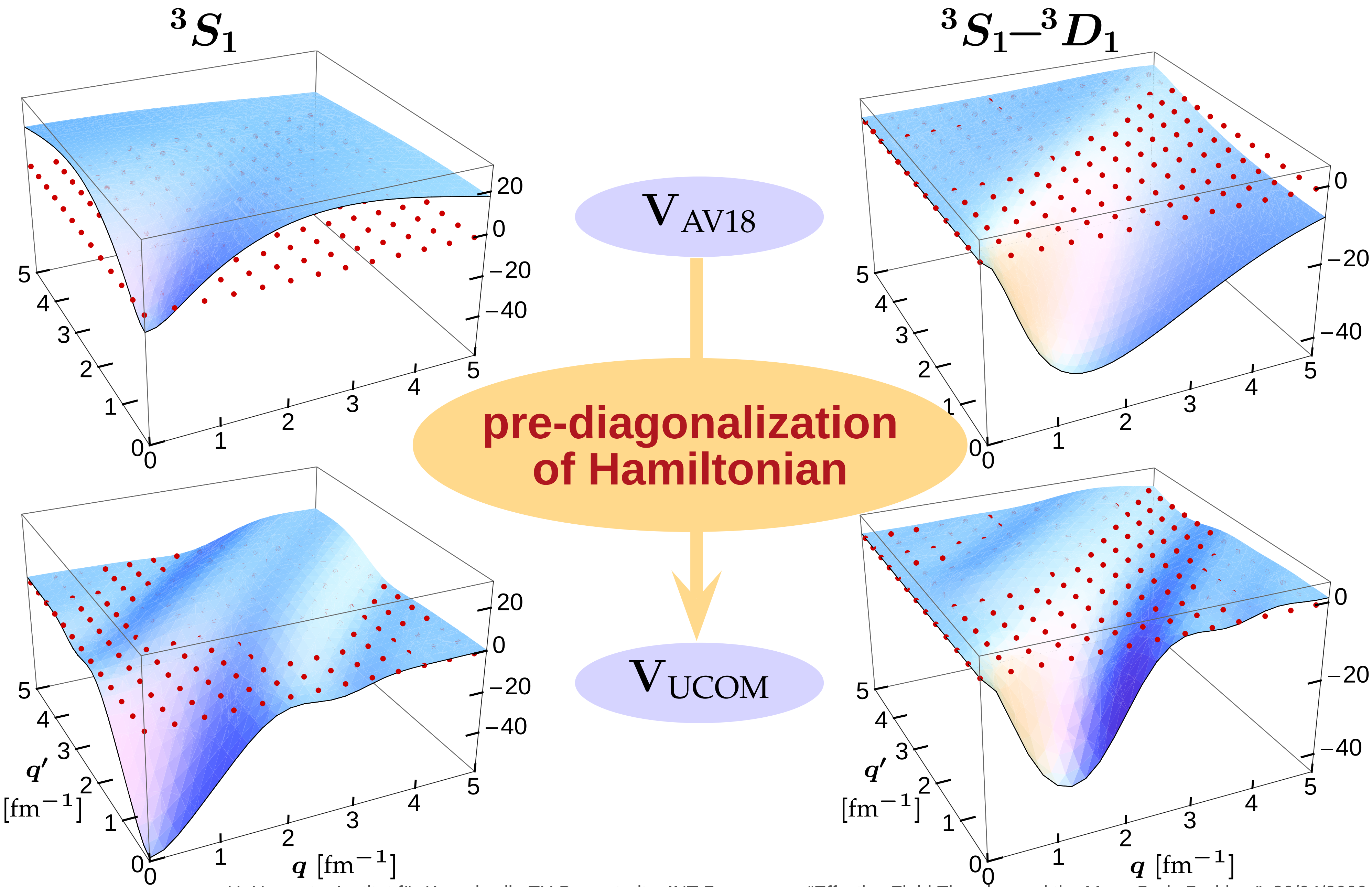

Unitarily Transformed Interactions

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

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

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

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

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

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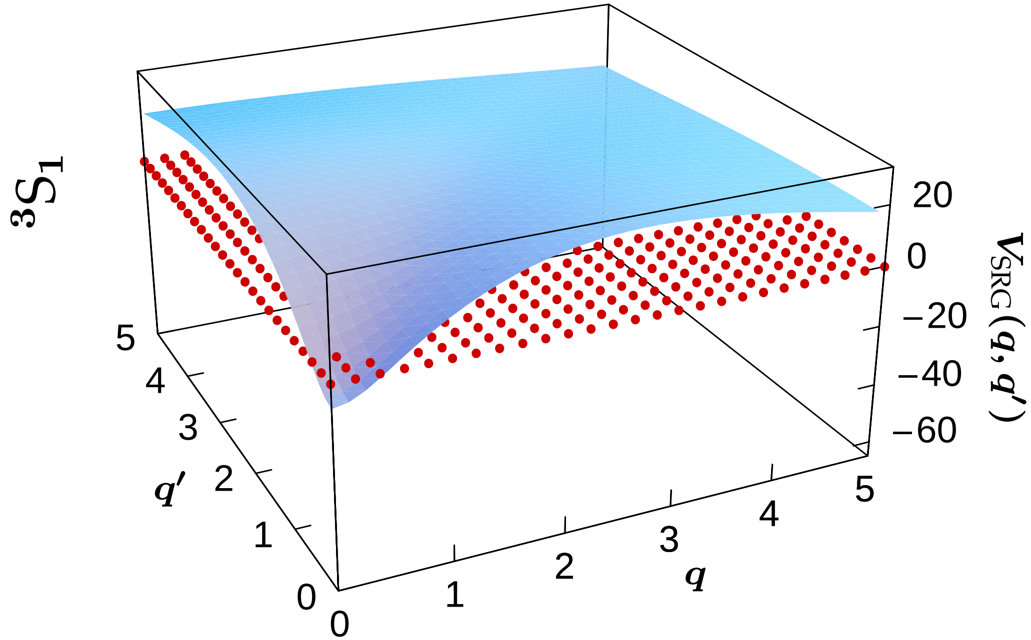
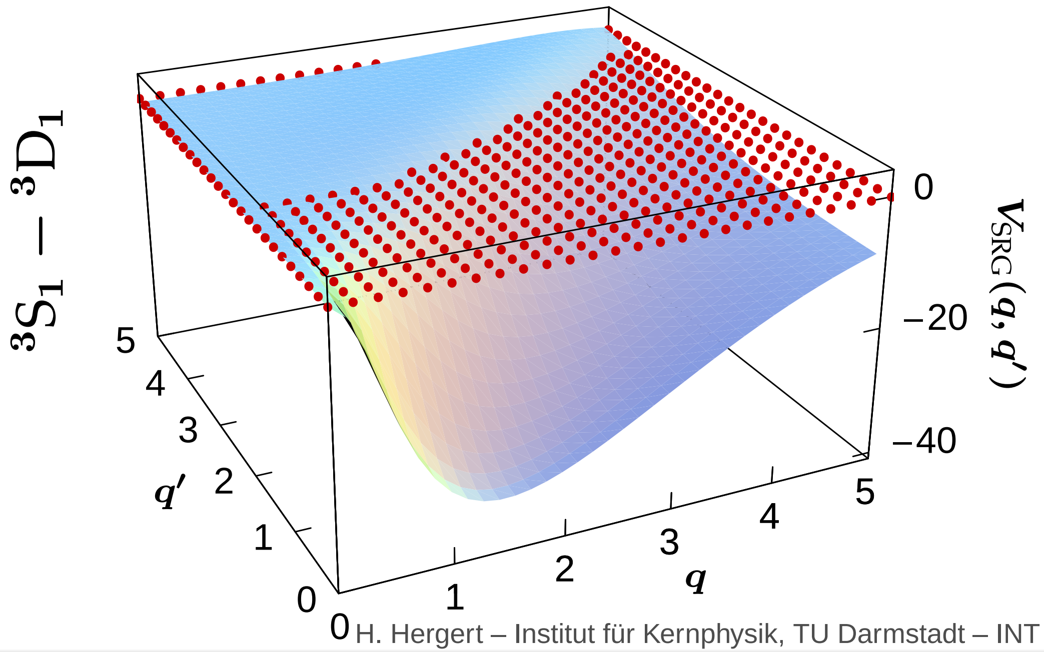
$\eta(0)$ has the **same structure** as the UCOM generators g_r and g_Ω

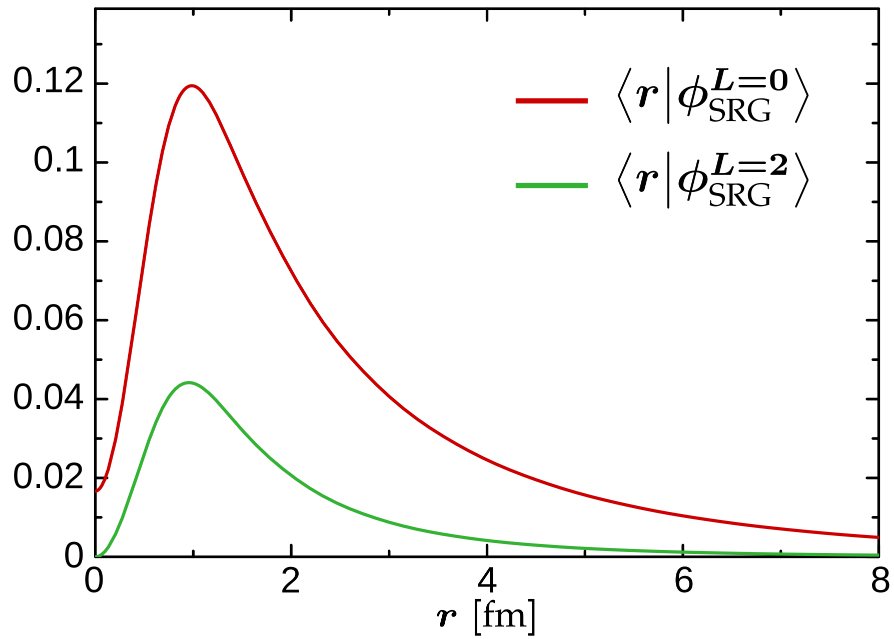
[Bogner et al., PRC**75** 061001(R) (2007); Hergert & Rot...

SRG: The Deuteron





Argonne V18



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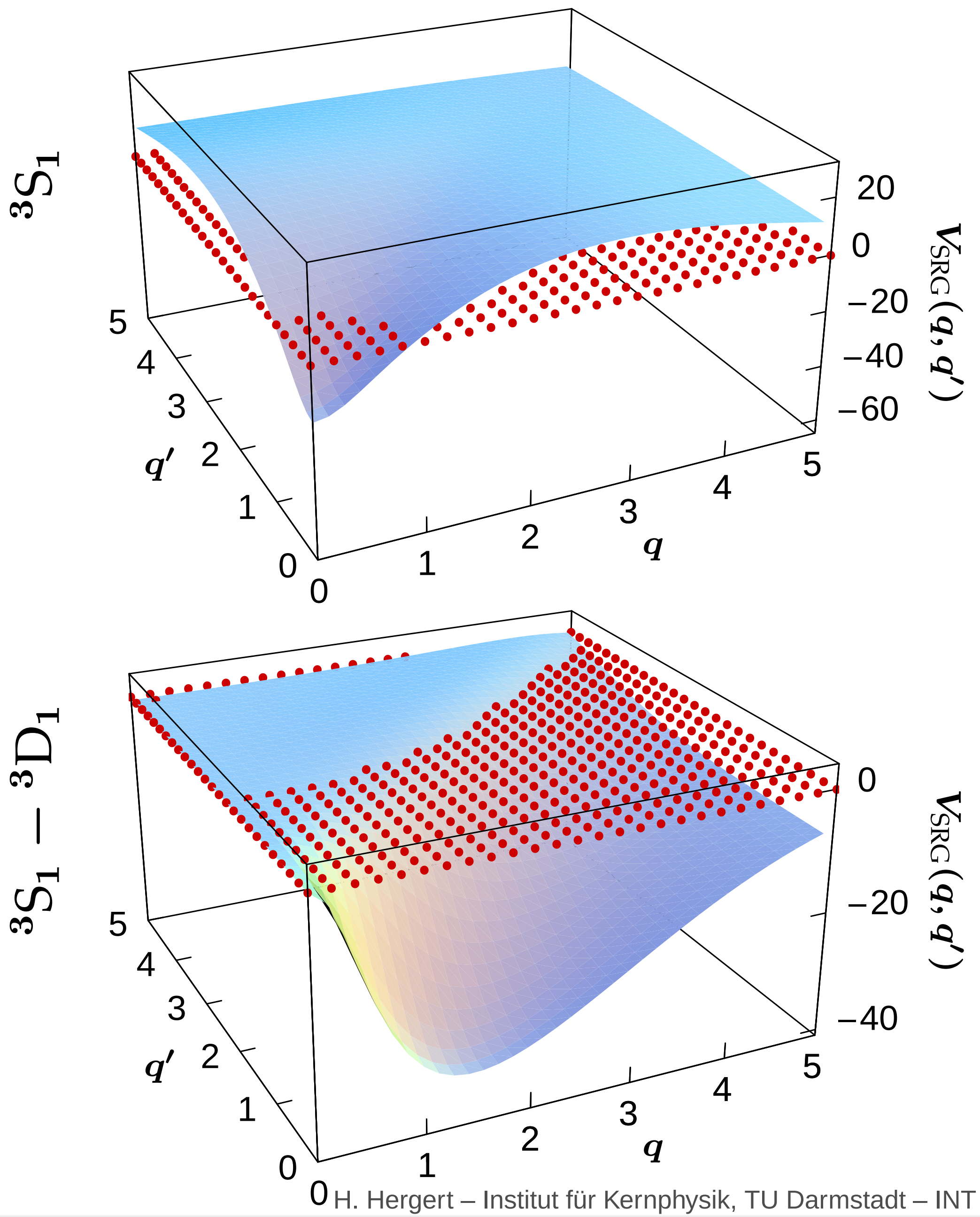
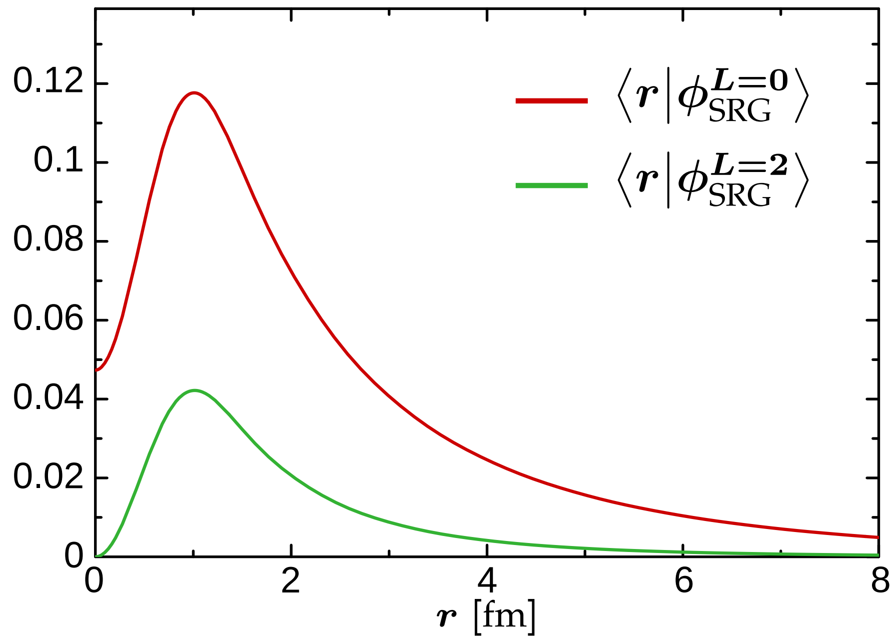


$$\bar{\alpha} = 0.0004\,\text{fm}^4$$



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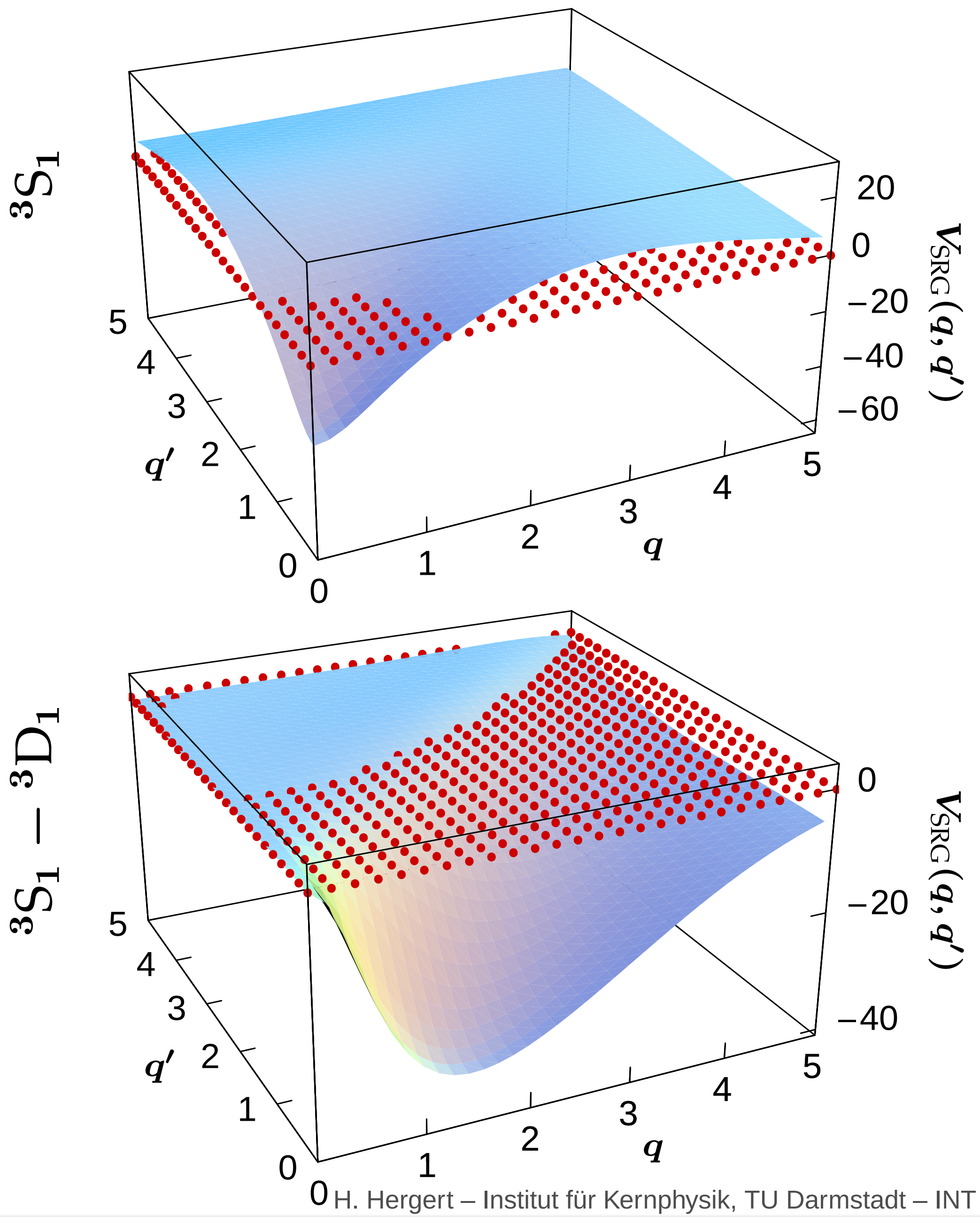
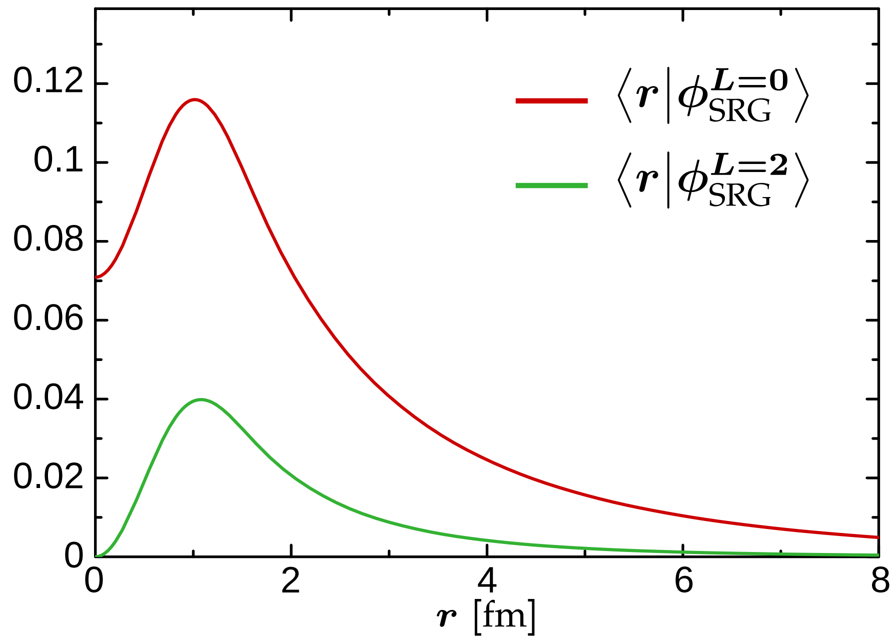


$$\bar{\alpha} = 0.0010\,\mathrm{fm}^4$$



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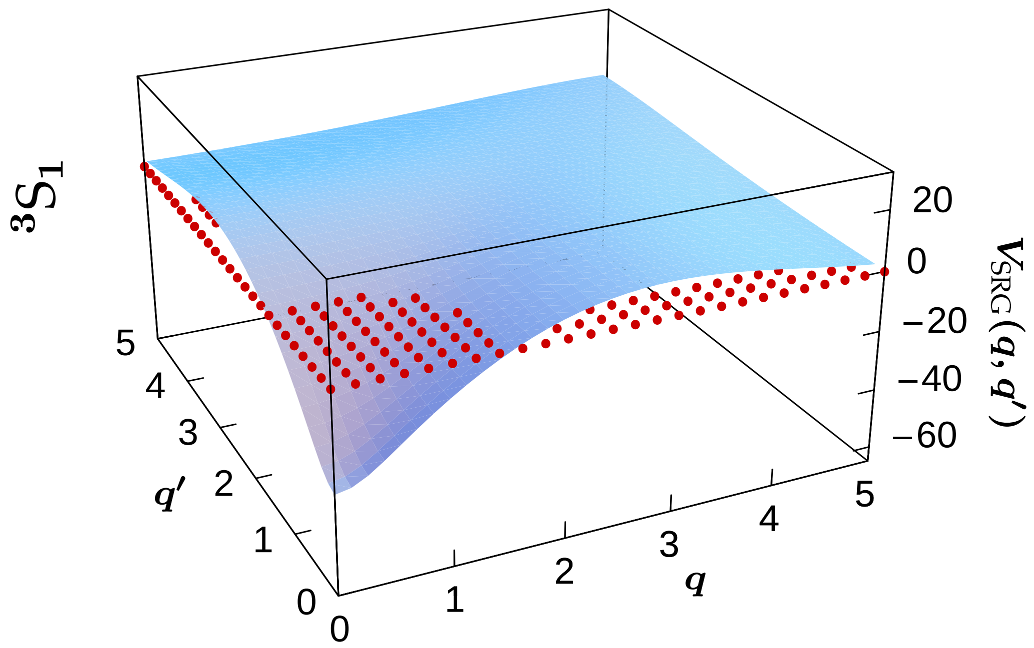
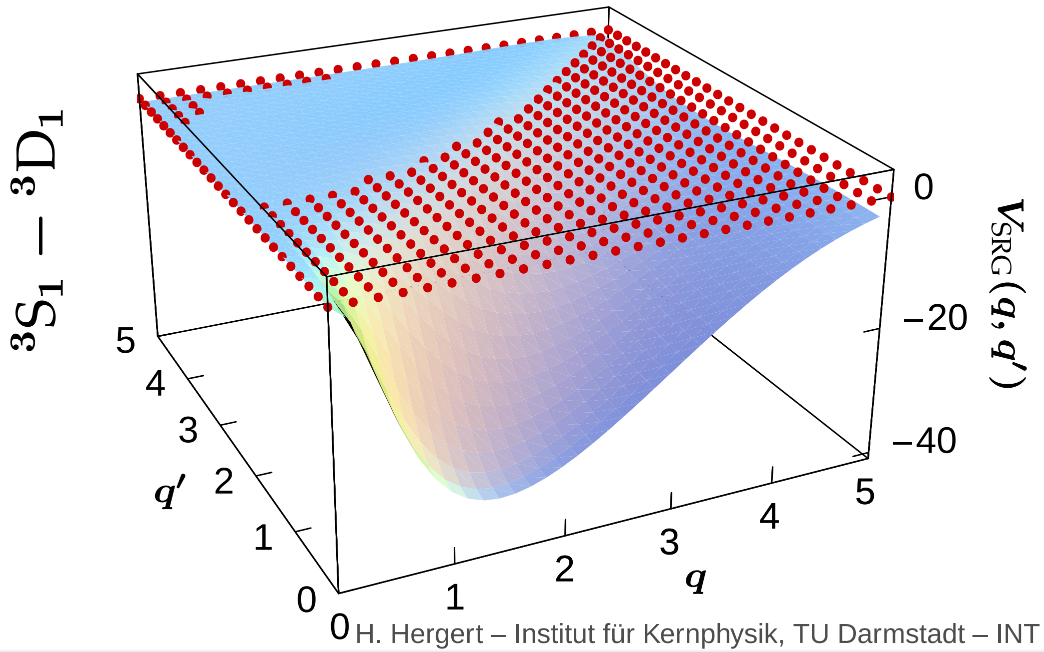
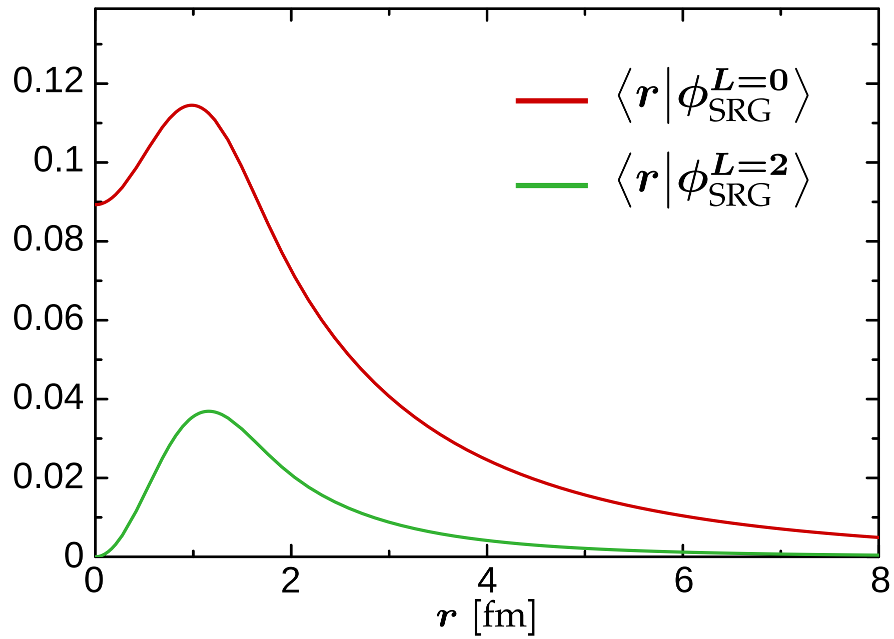




$$\bar{\alpha} = 0.0020\,\text{fm}^4$$



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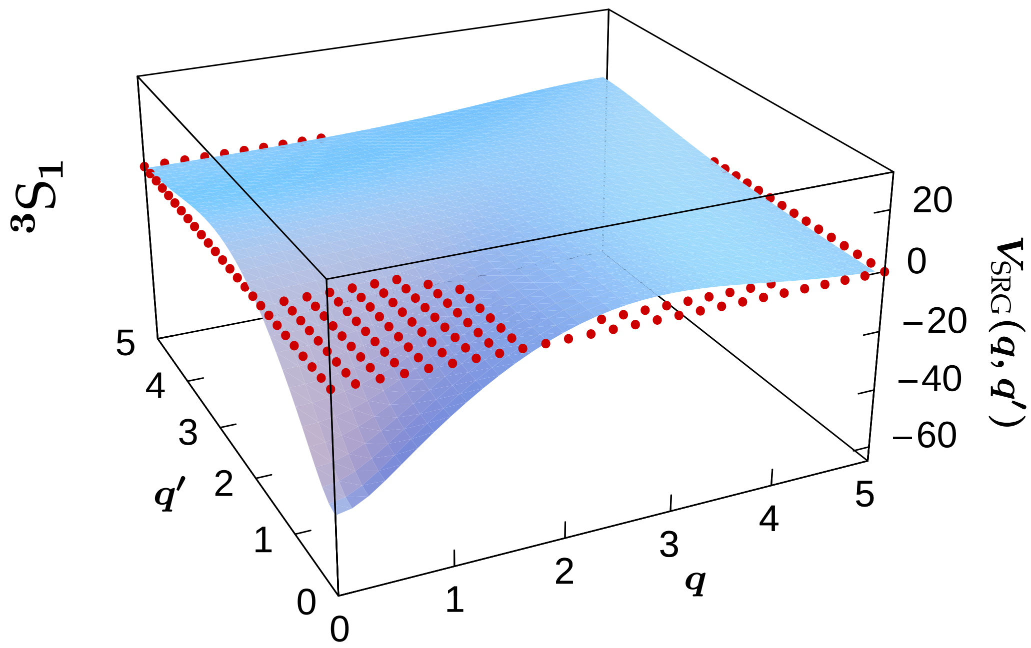
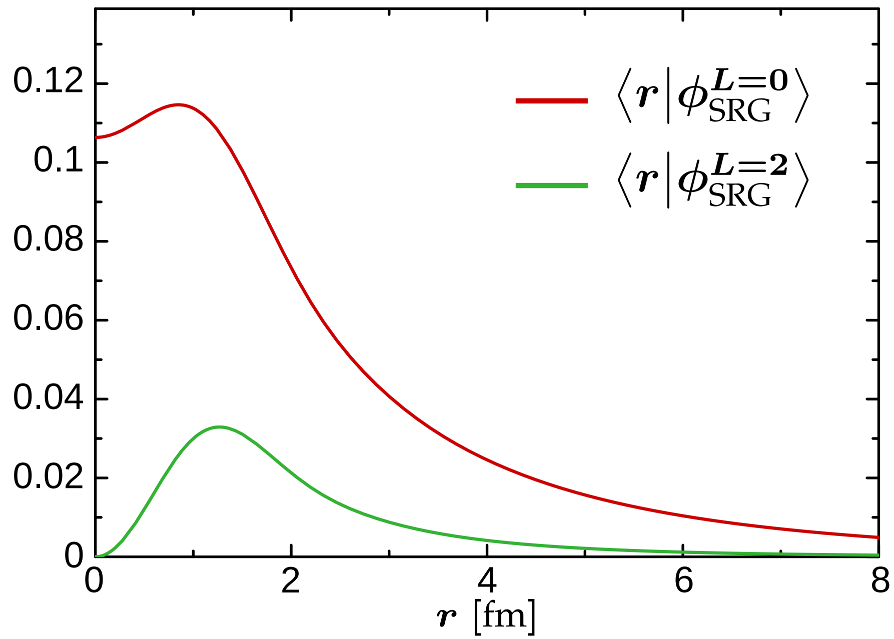
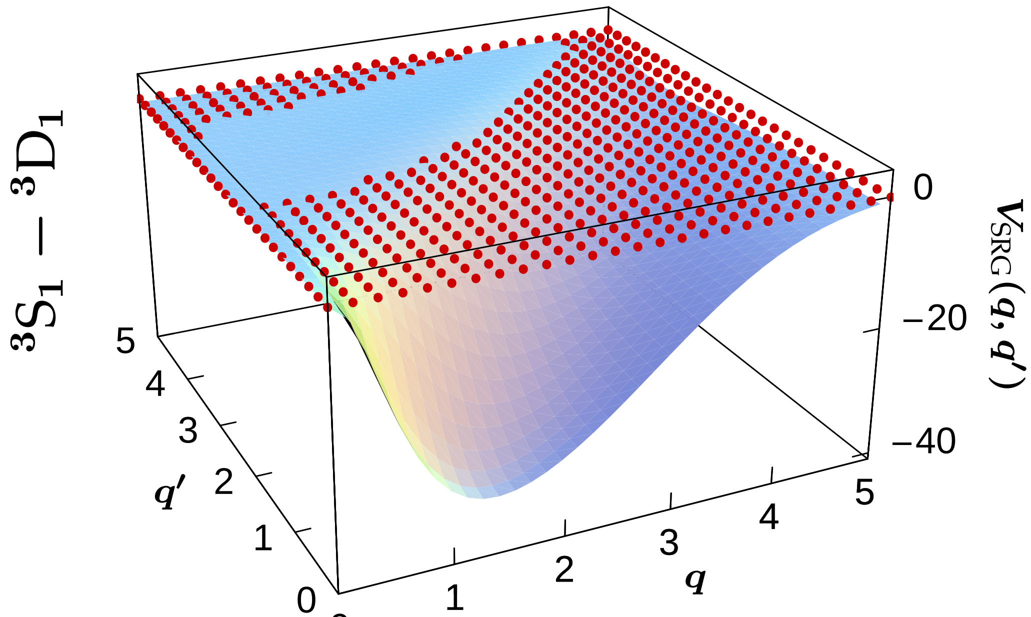


$\bar{\alpha} = 0.0040\,\mathrm{fm}^4$





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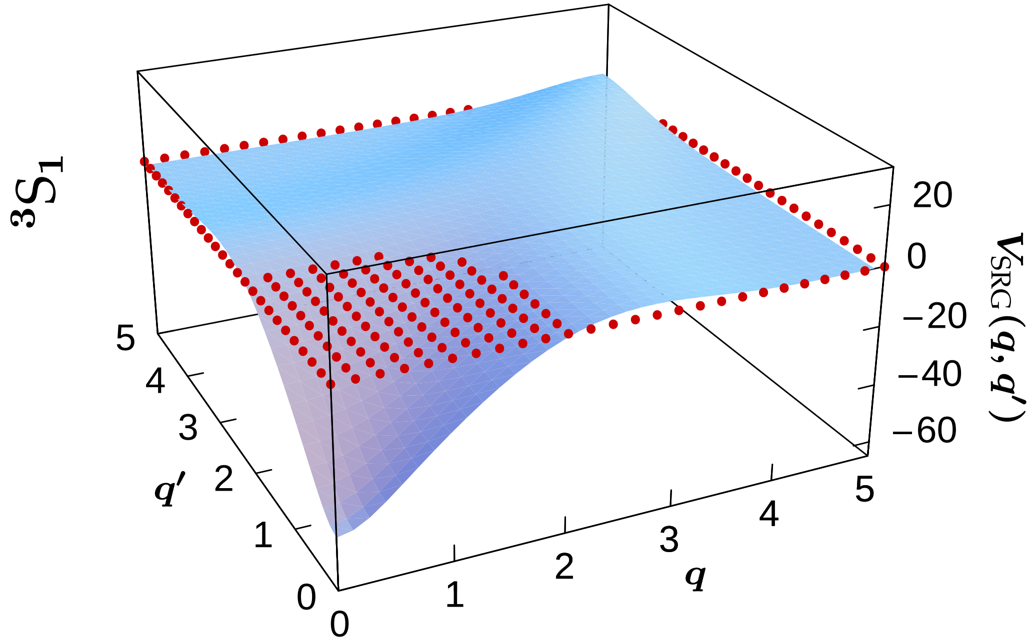
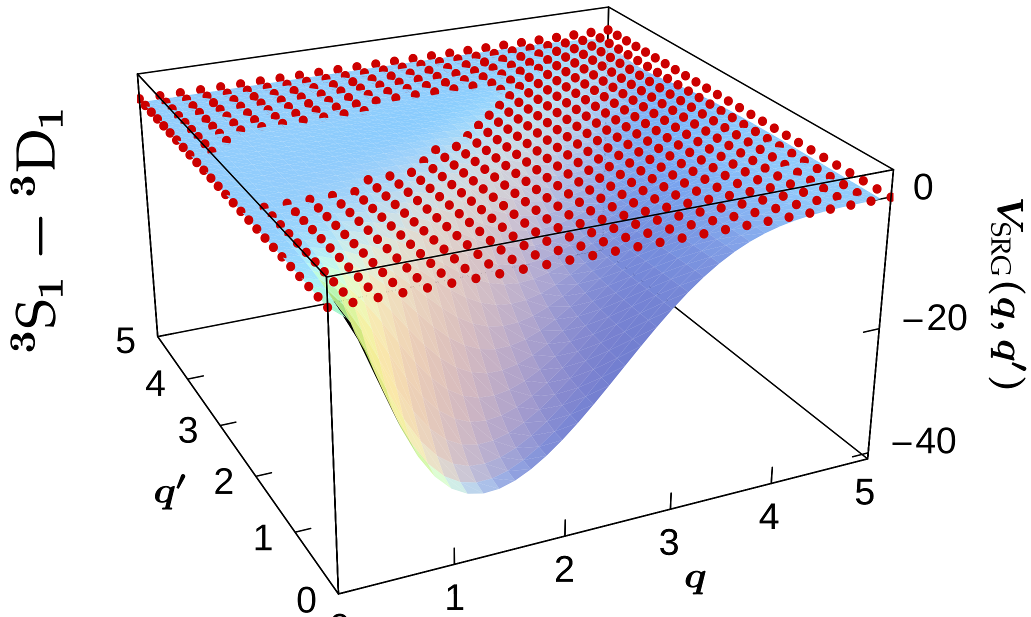
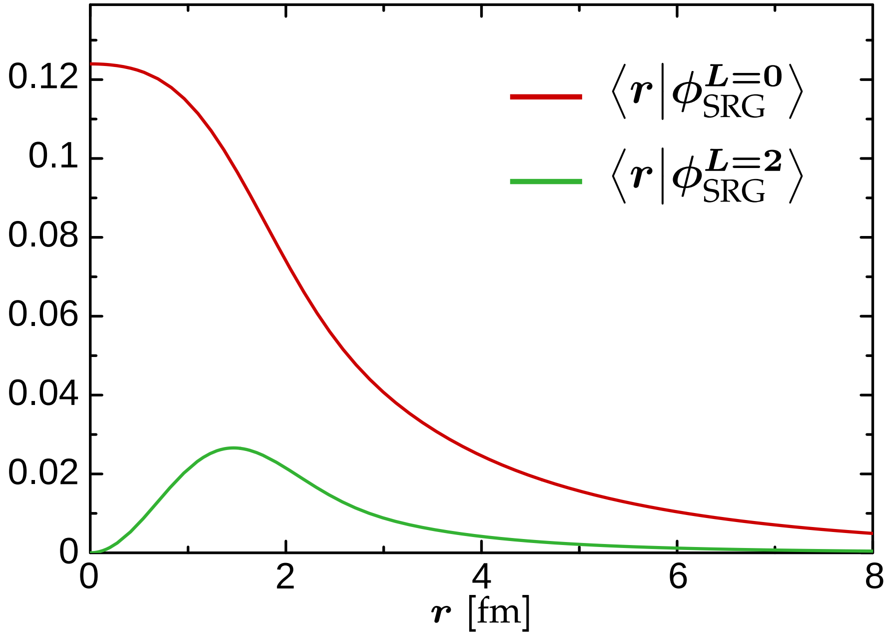




$\bar{\alpha} = 0.0100\,\mathrm{fm}^4$



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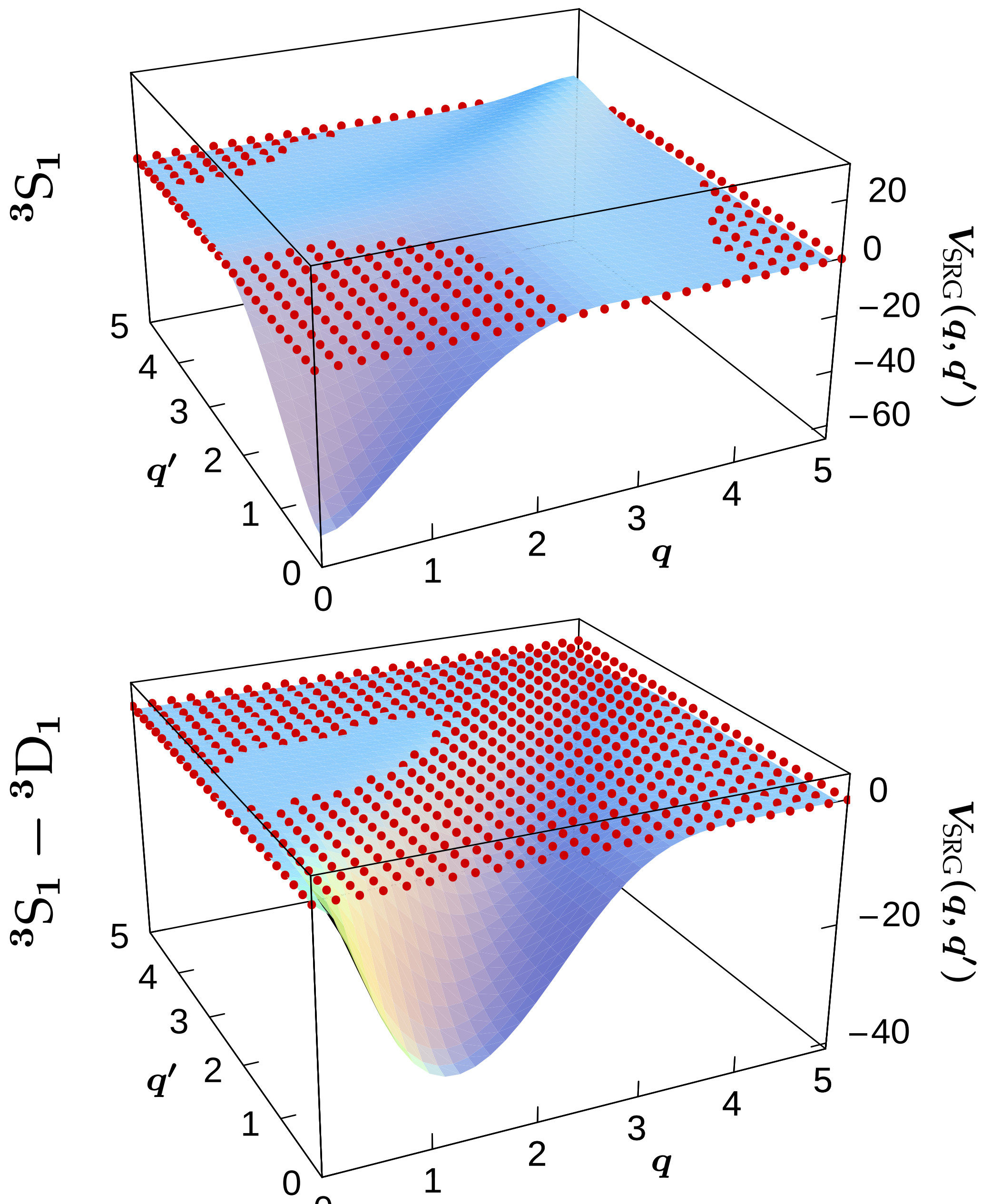
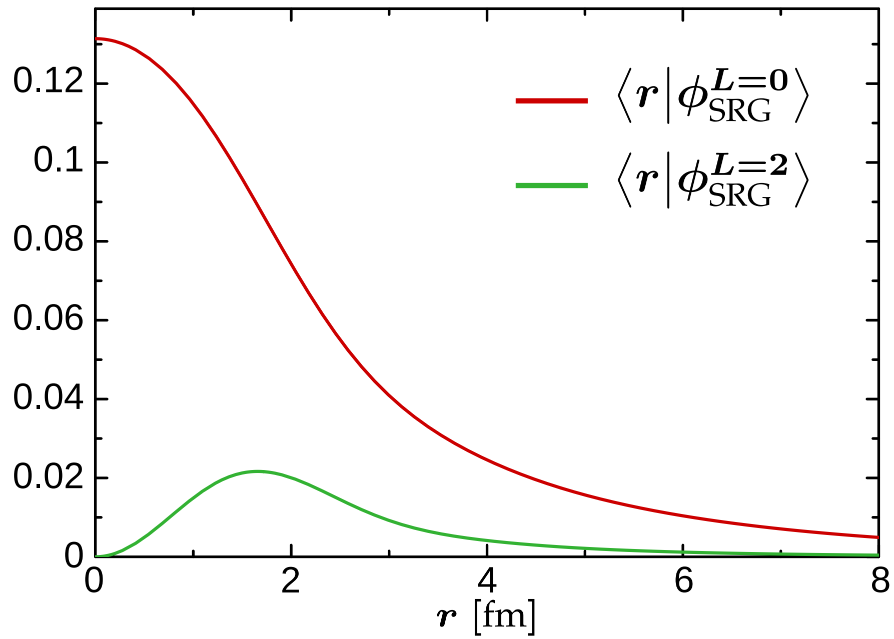


$$\bar{\alpha} = 0.0200\,\mathrm{fm}^4$$



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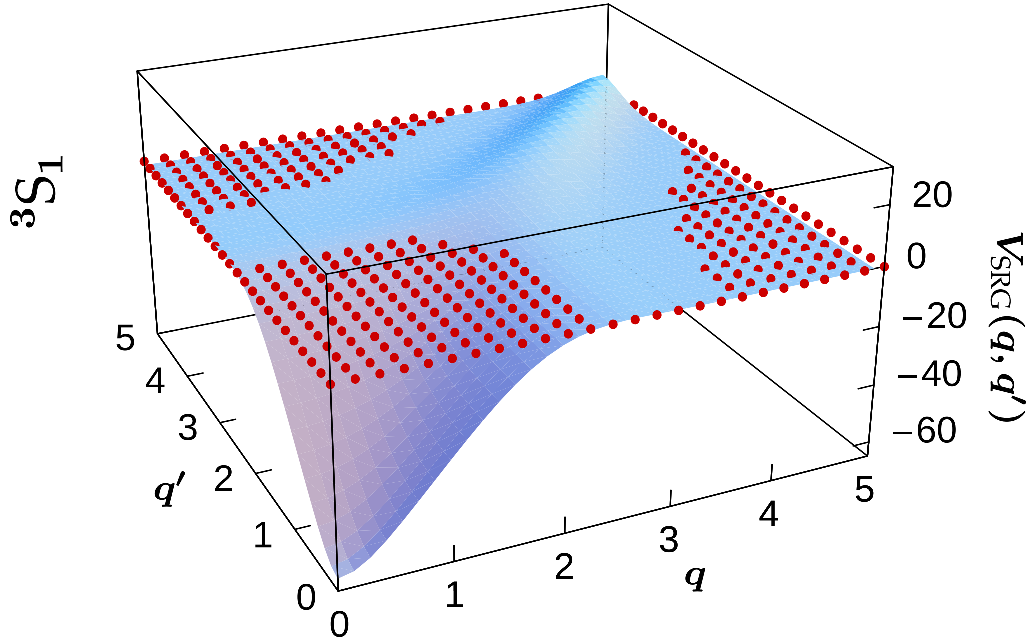
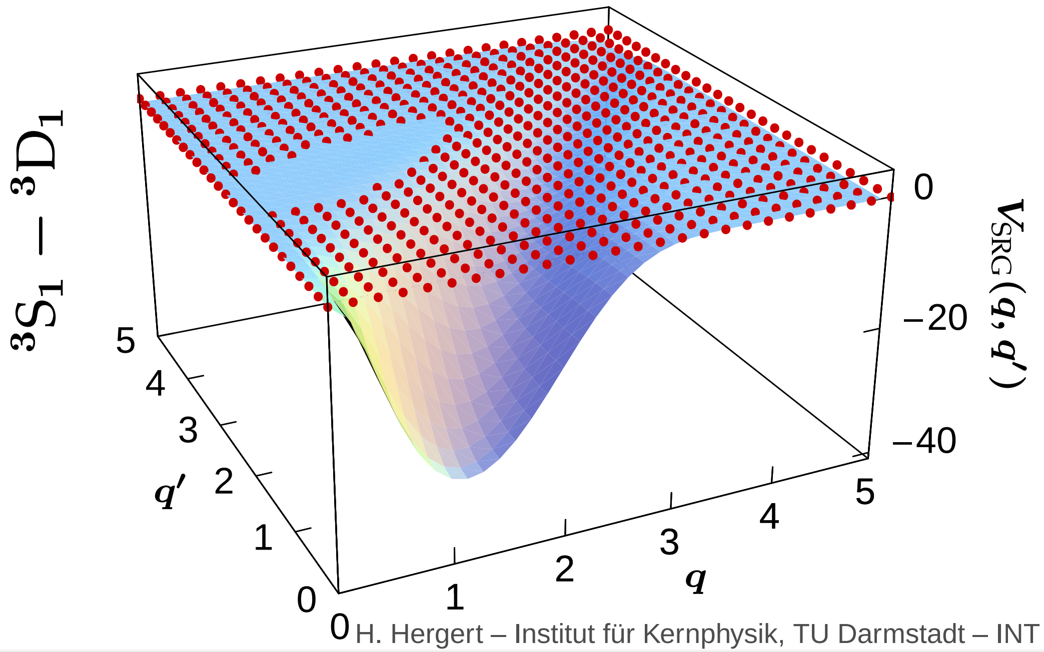
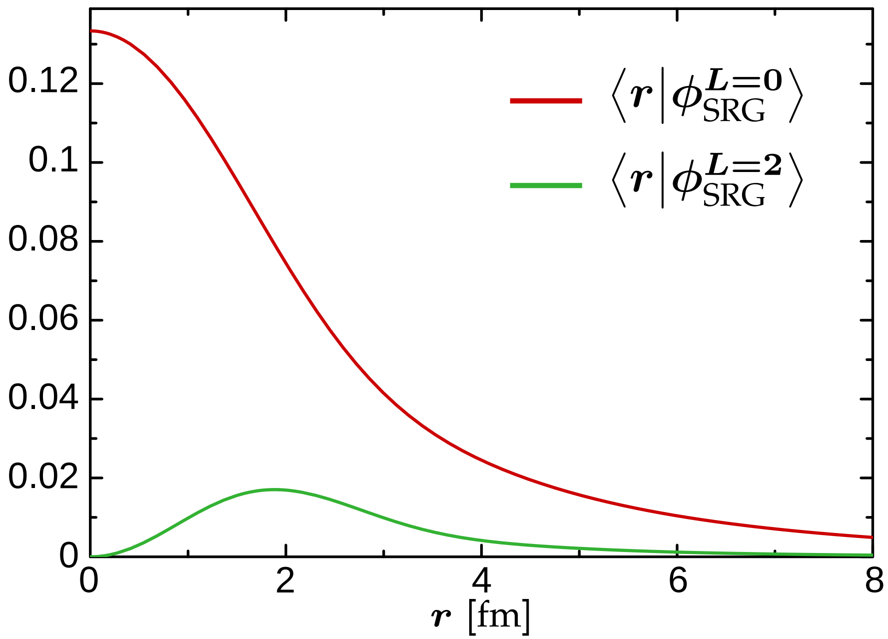




$\bar{\alpha} = 0.0400\,\mathrm{fm}^4$



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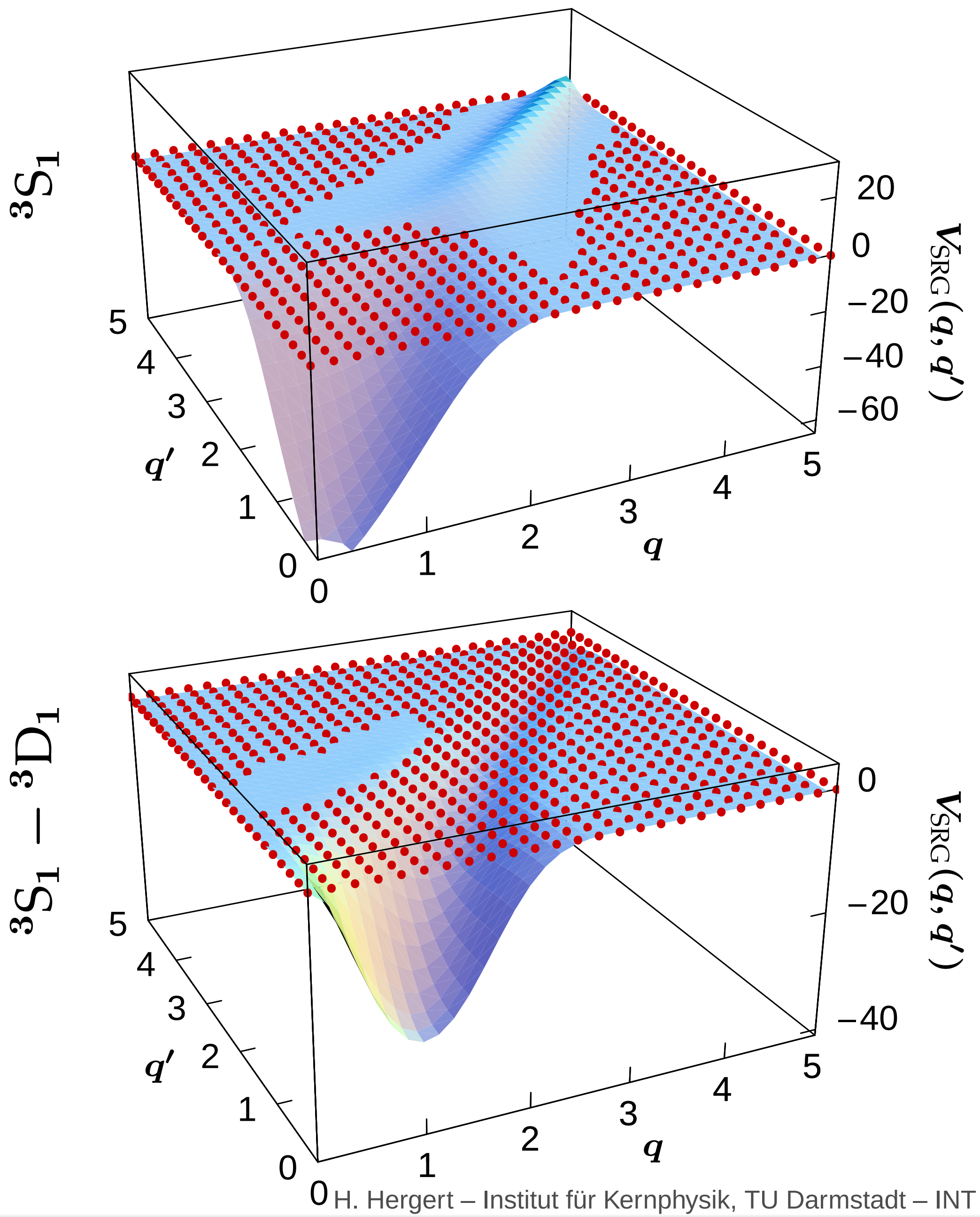
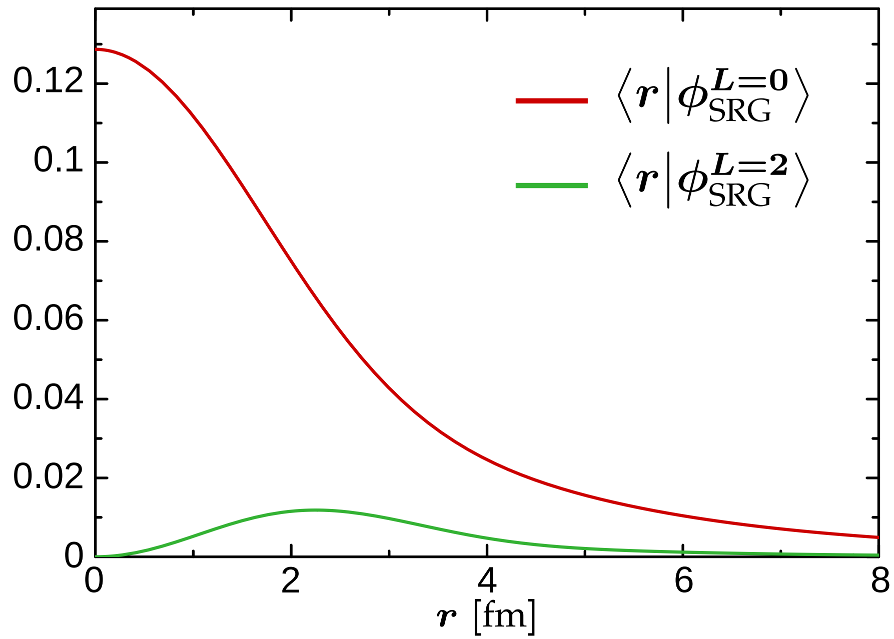


$\bar{\alpha} = 0.1000\,\mathrm{fm}^4$



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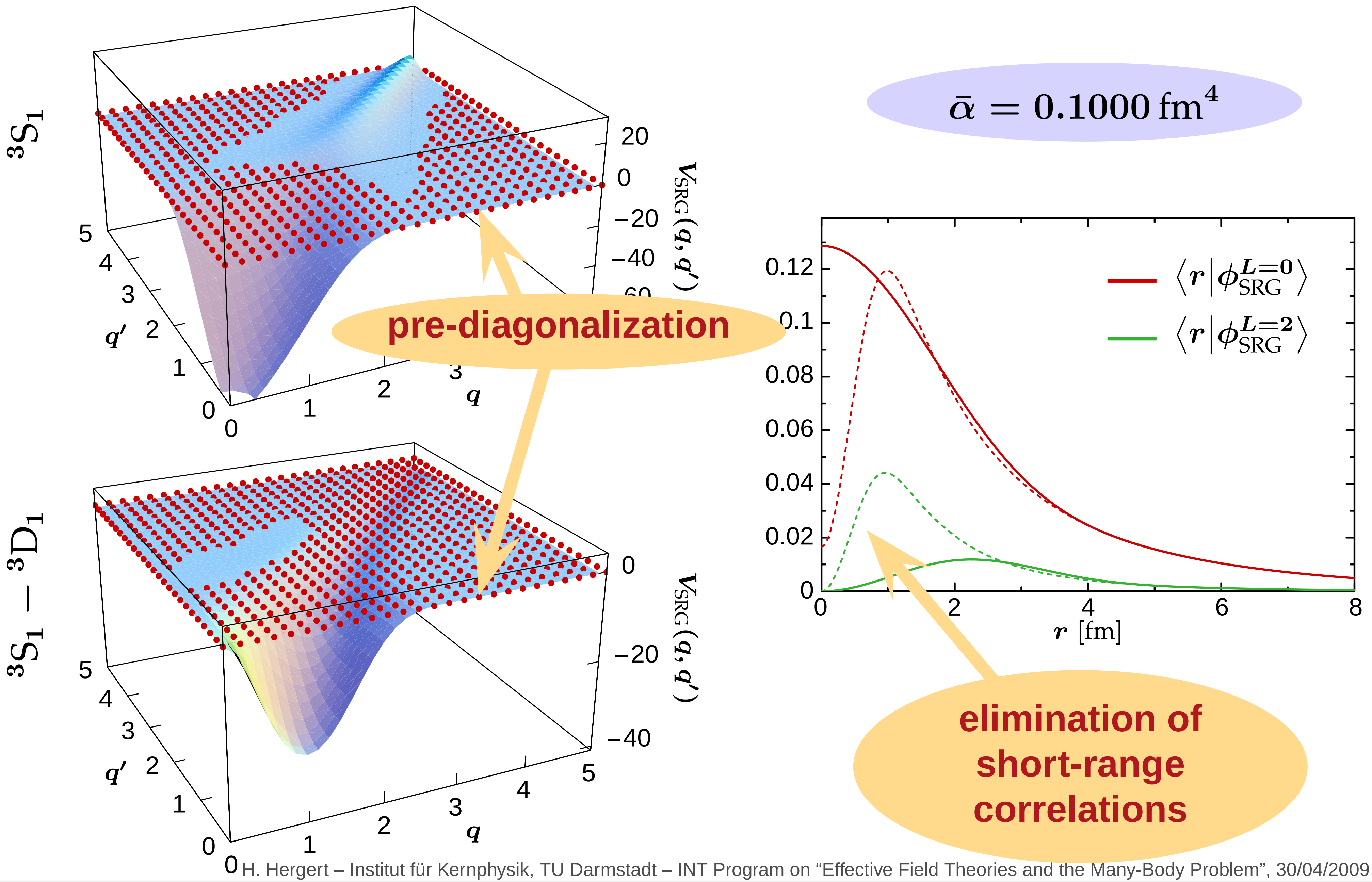

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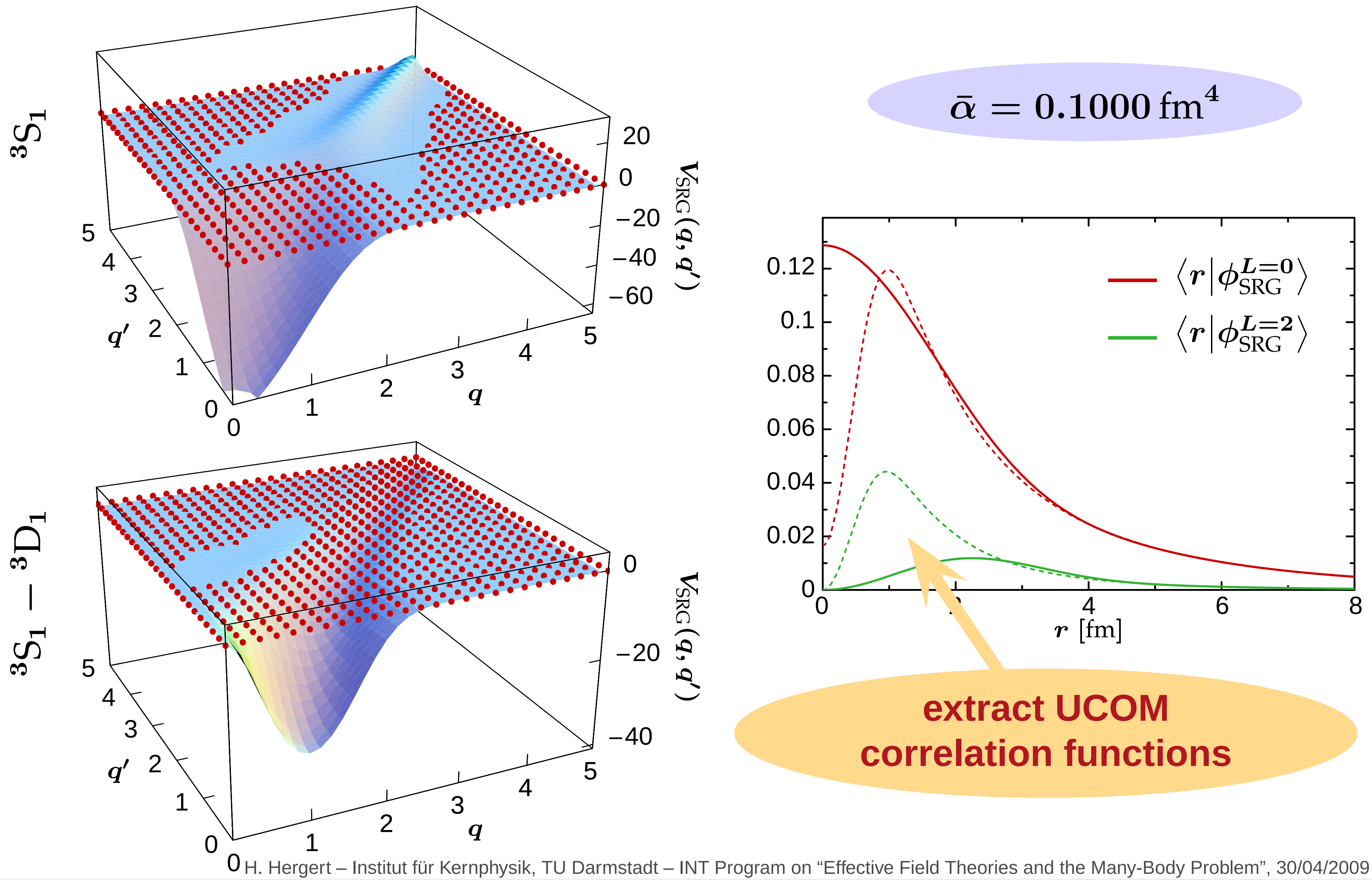

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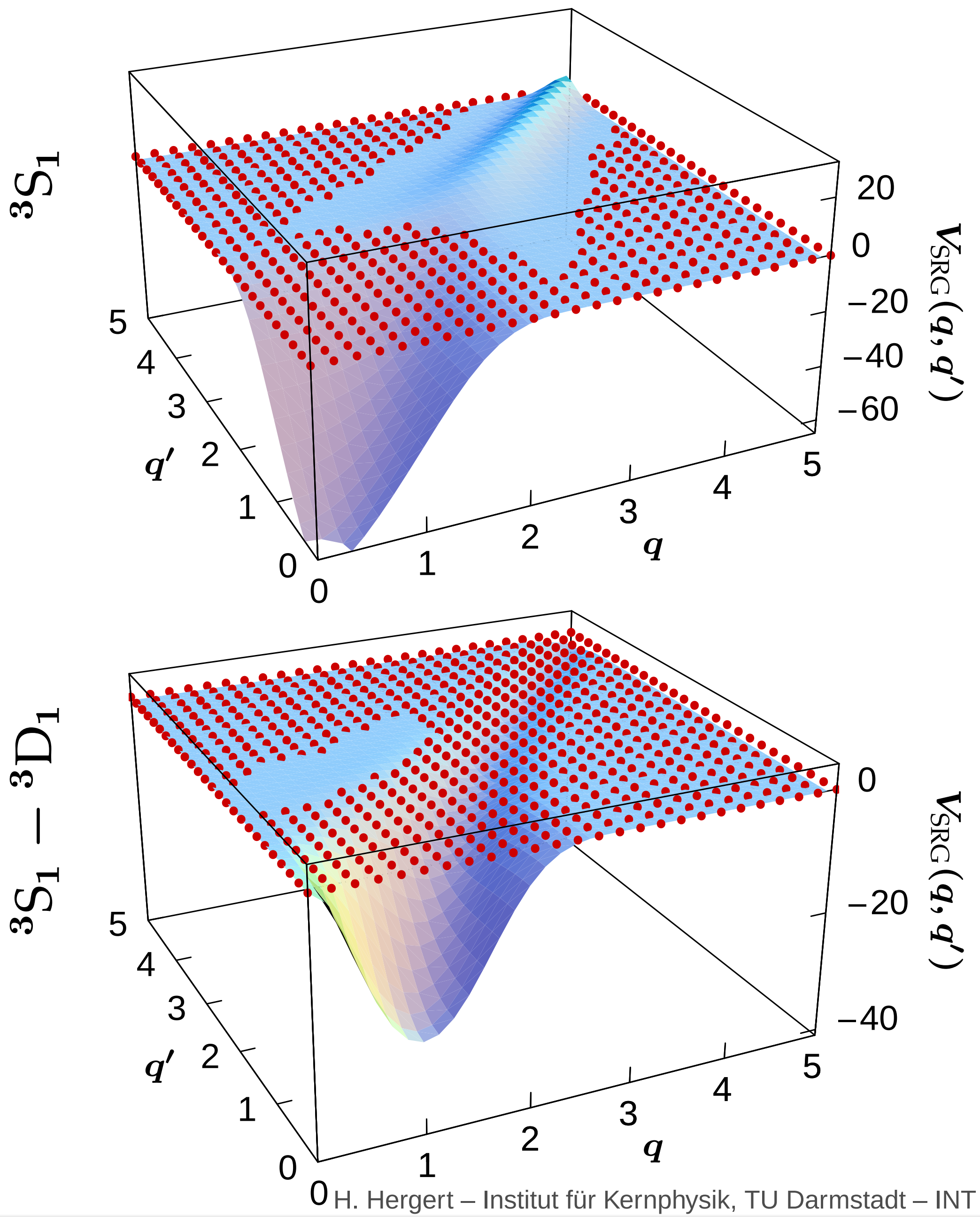

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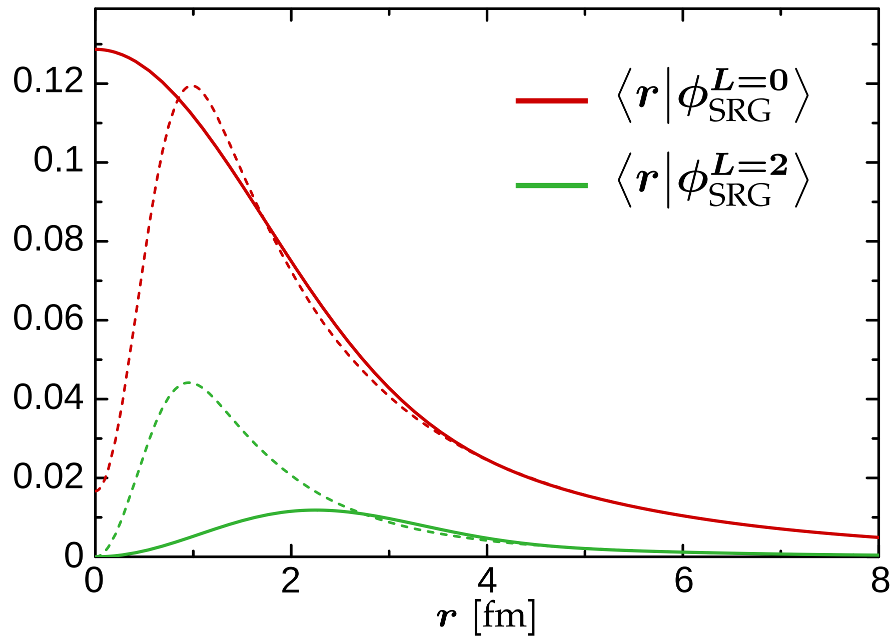
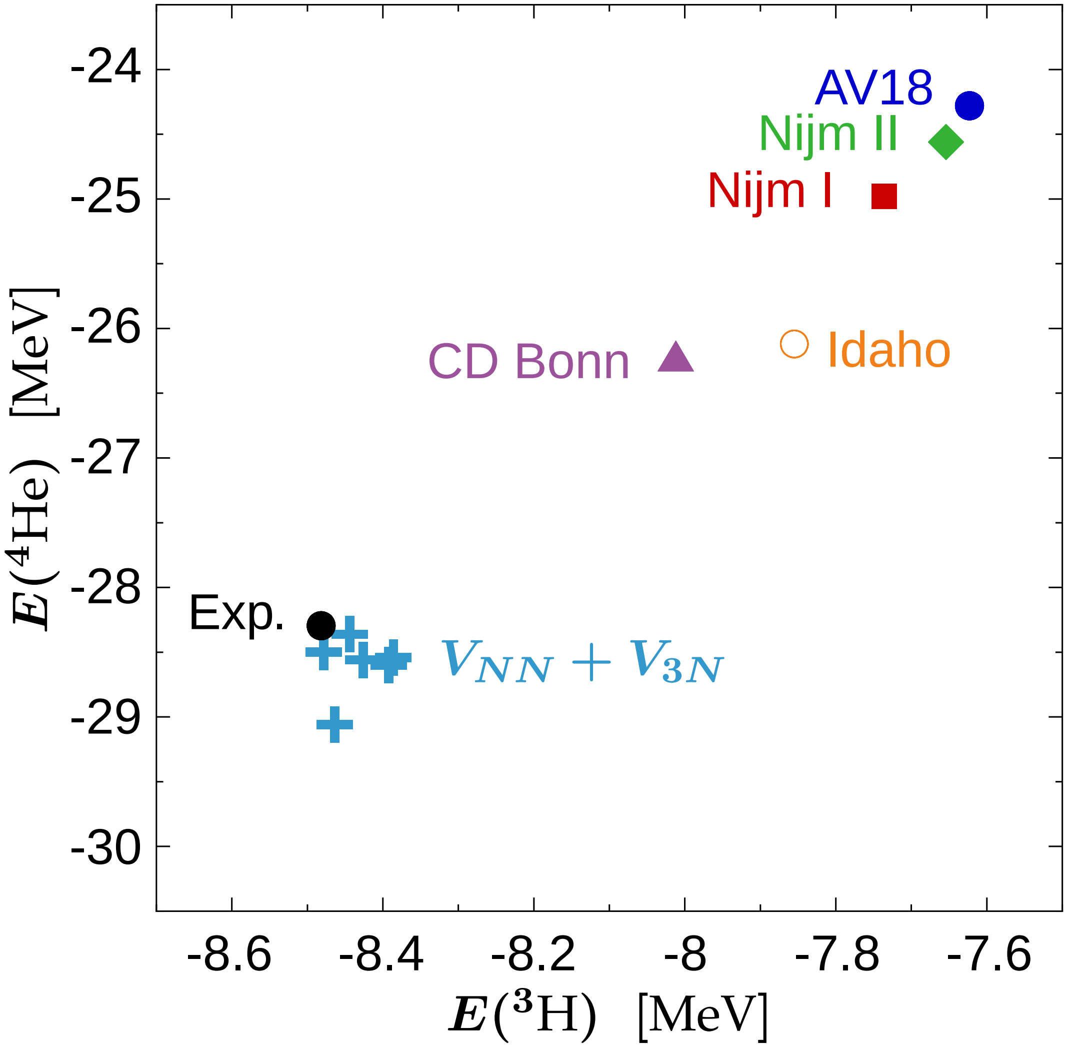


$V_{UCOM} \neq V_{SRG}$!

Tjon Line



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

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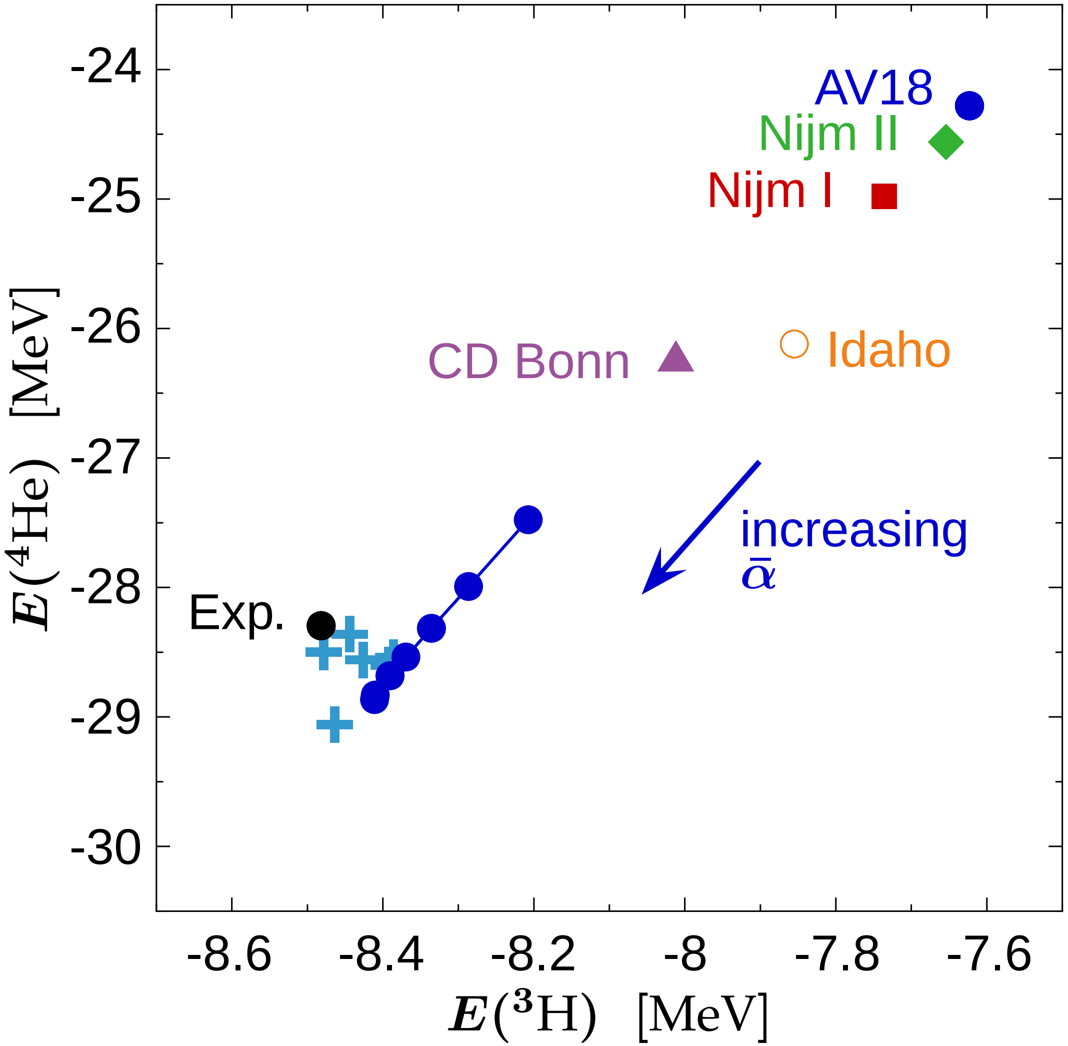

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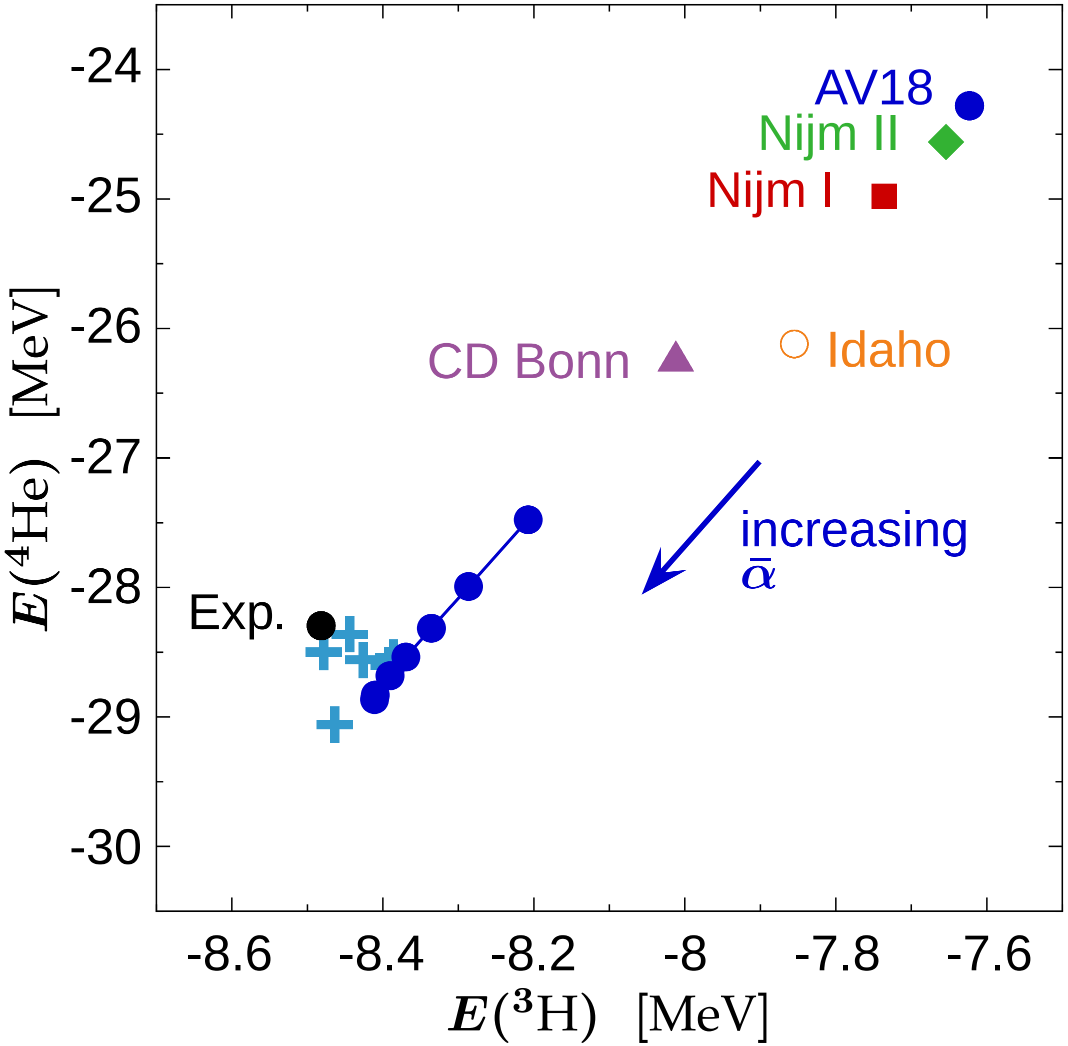

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- use $\bar{\alpha}$ to
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  - provide theoretical “error” estimates

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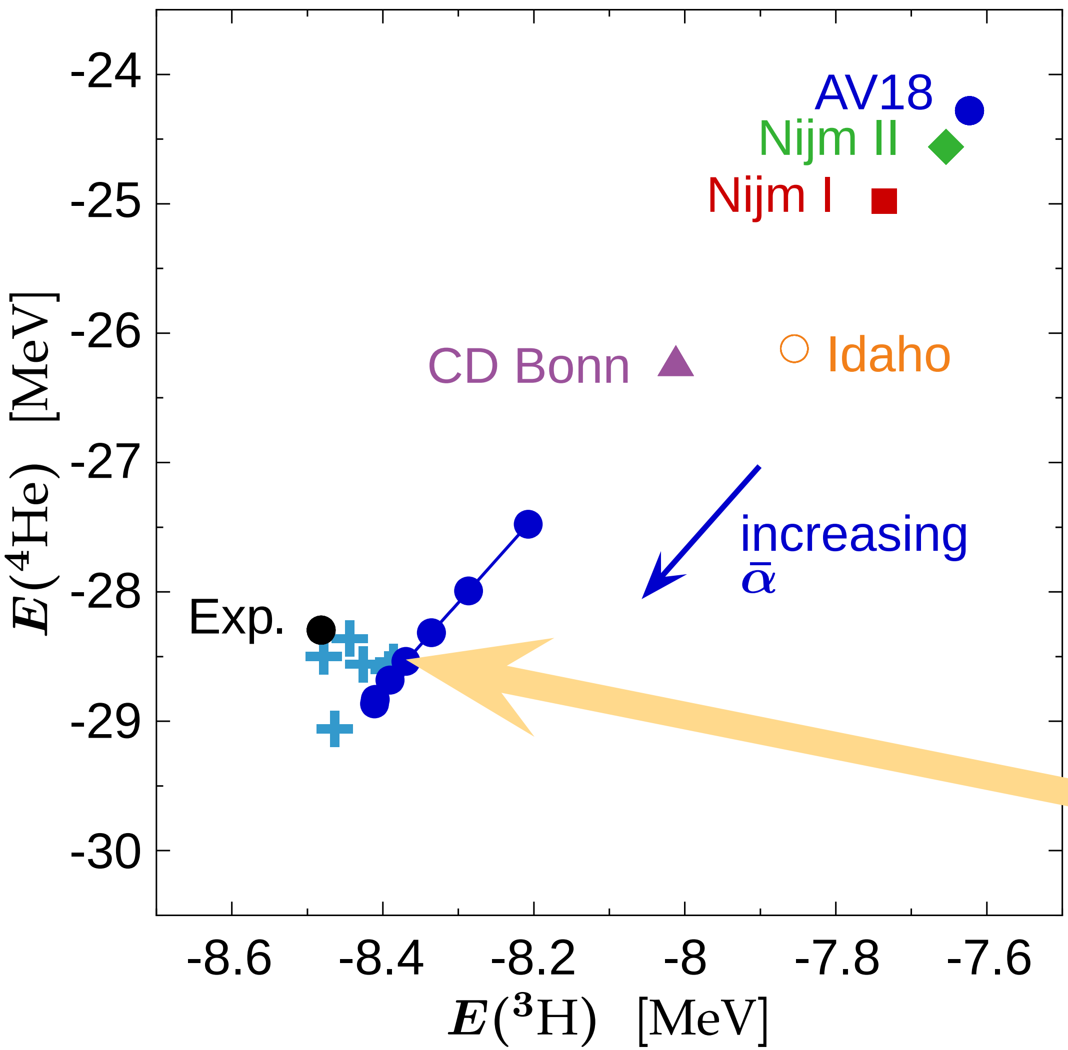

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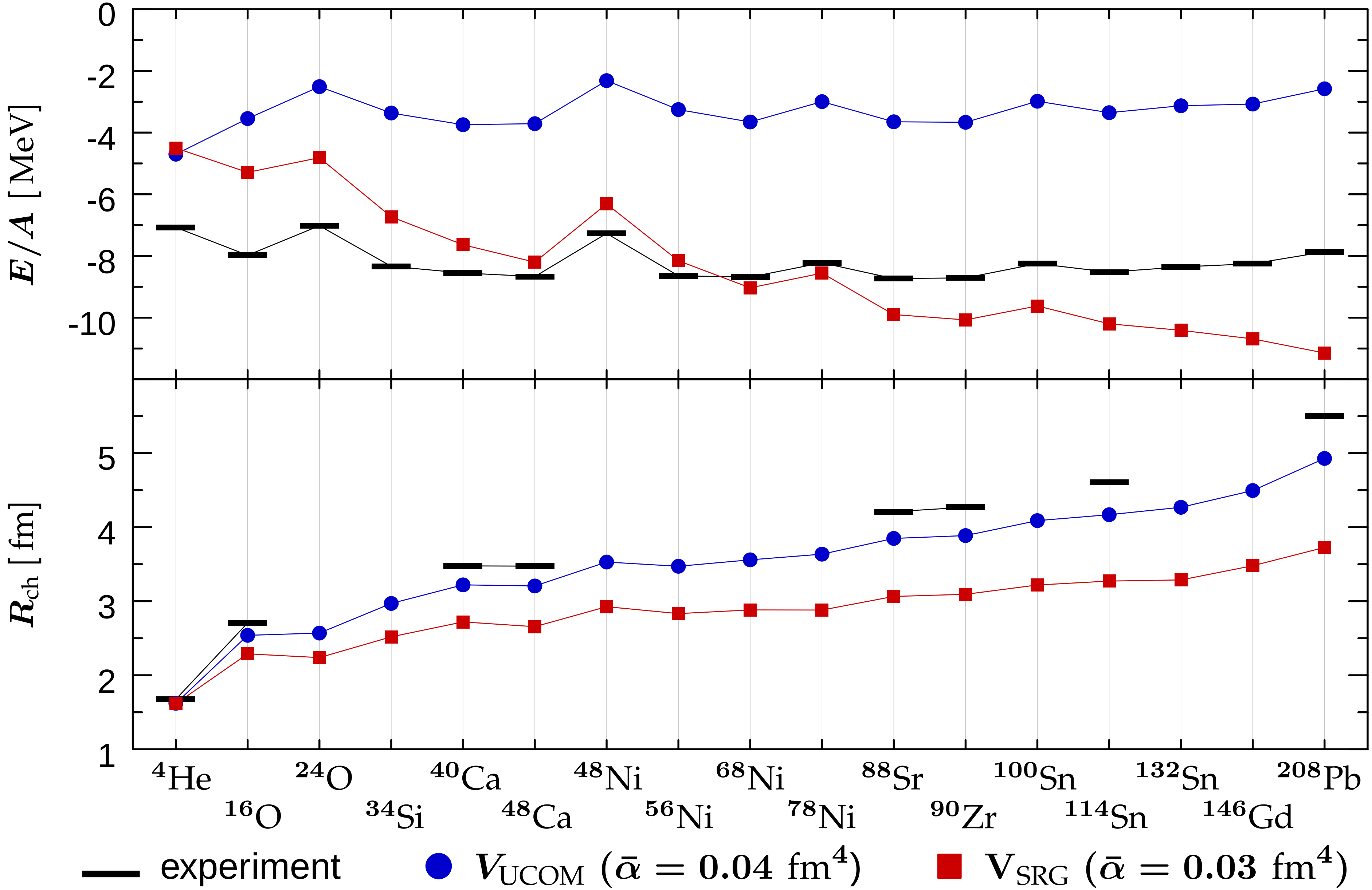
minimal net 3N interaction
use V_{UCOM} with $\bar{\alpha} = 0.04\ \mathrm{fm}^4$

Applications

Hartree-Fock: UCOM vs. SRG



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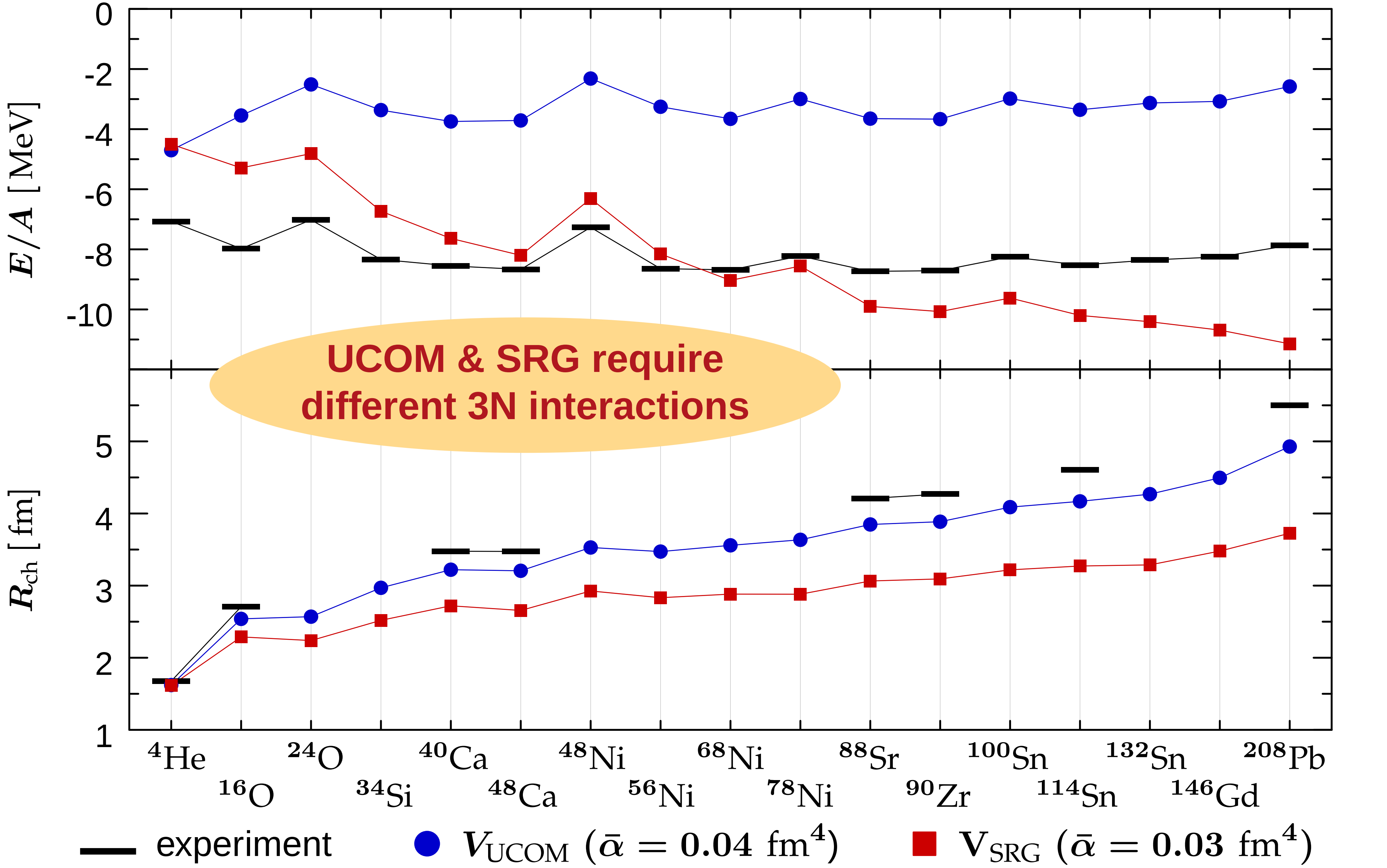
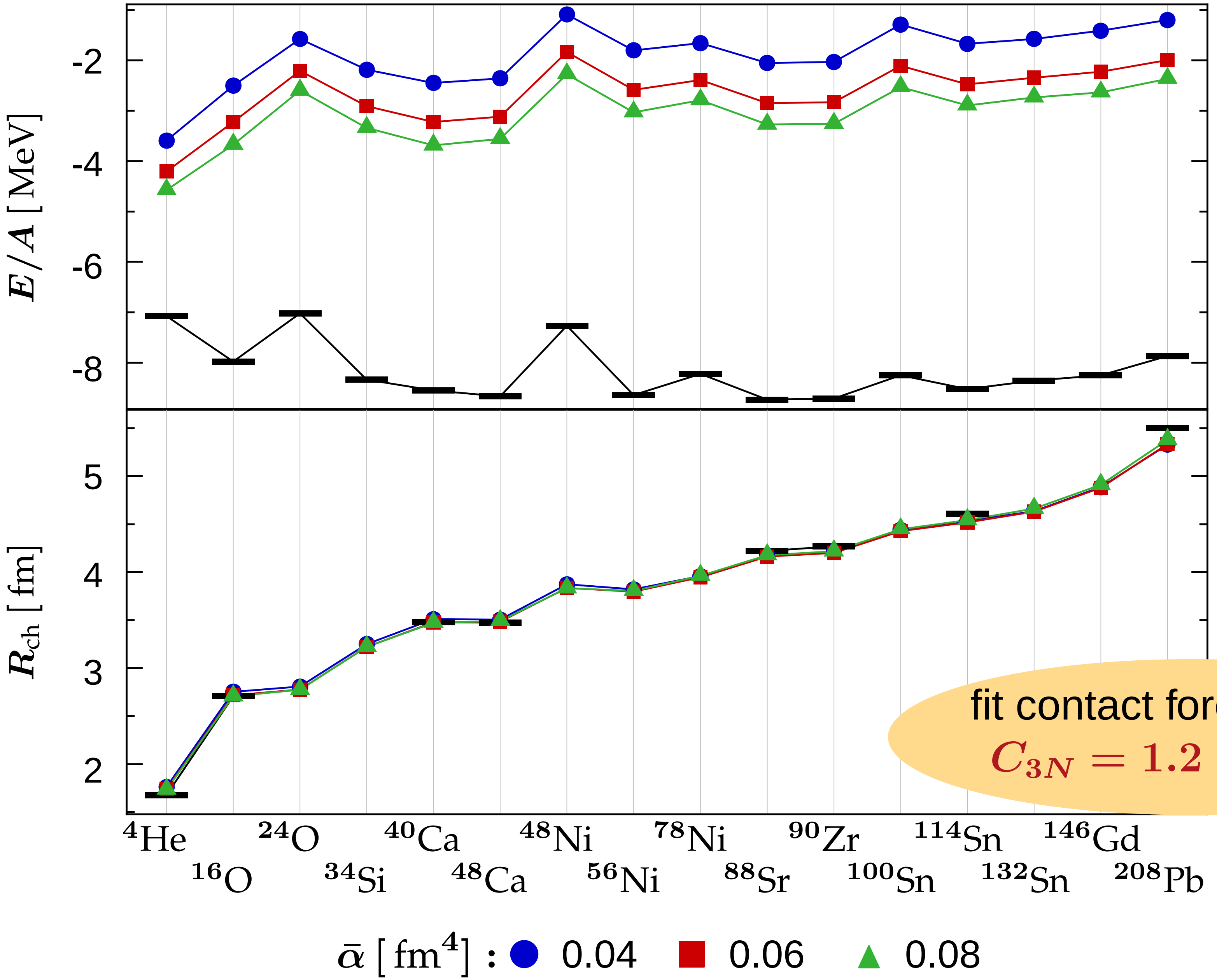
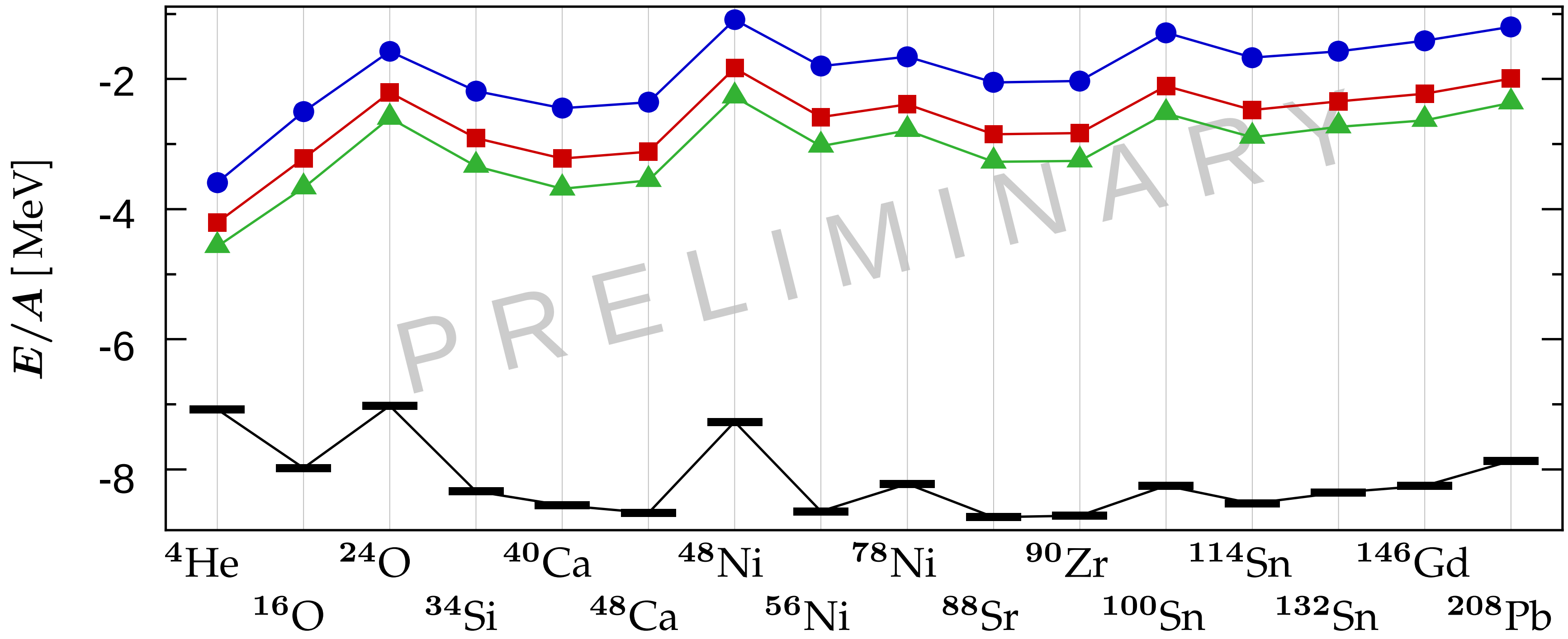


HF: V_{UCOM}+3N Contact Interaction



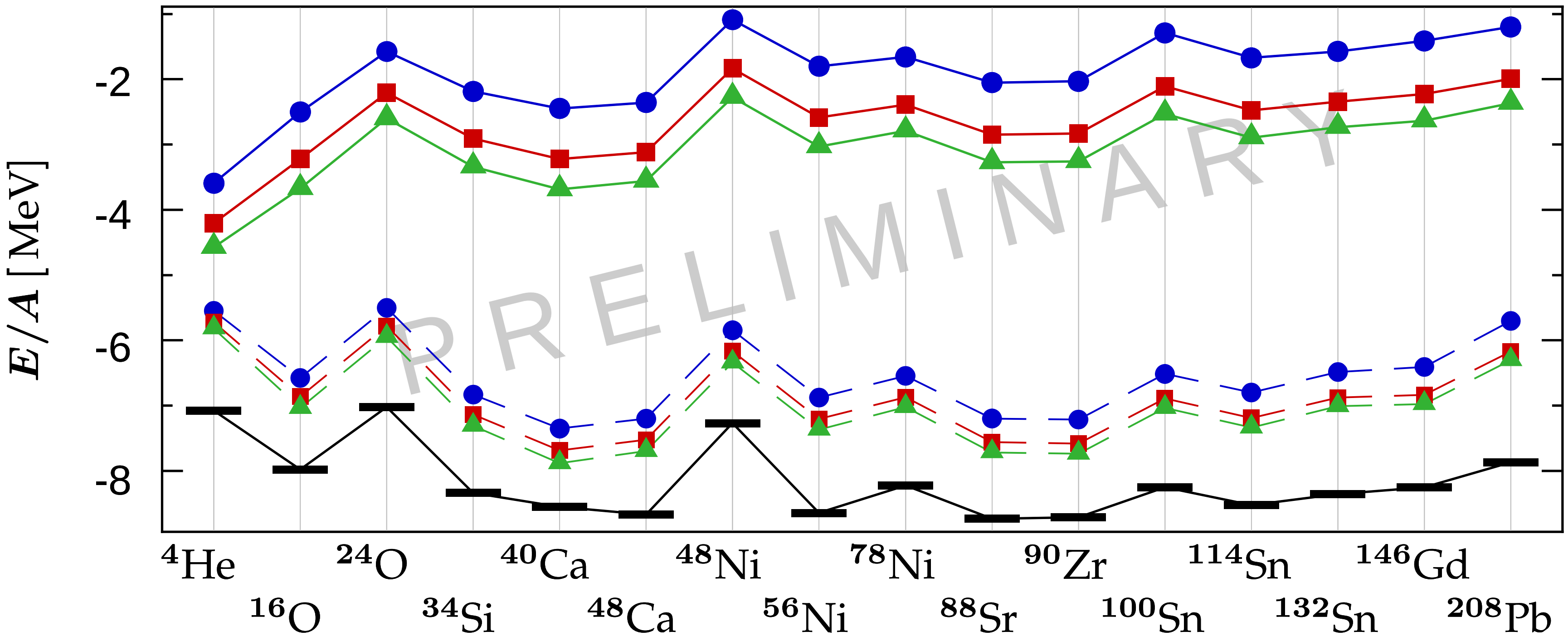
fit contact force to radii:
$C_{3N} = 1.2\ \text{GeV fm}^6$

Many-Body Perturbation Theory



$e_{\mathrm{Max}} = 12, C_{3N} = 1.2$ GeV fm^6, $\bar{\alpha}$ [fm^4] : ● 0.04 ■ 0.06 ▲ 0.08

Many-Body Perturbation Theory



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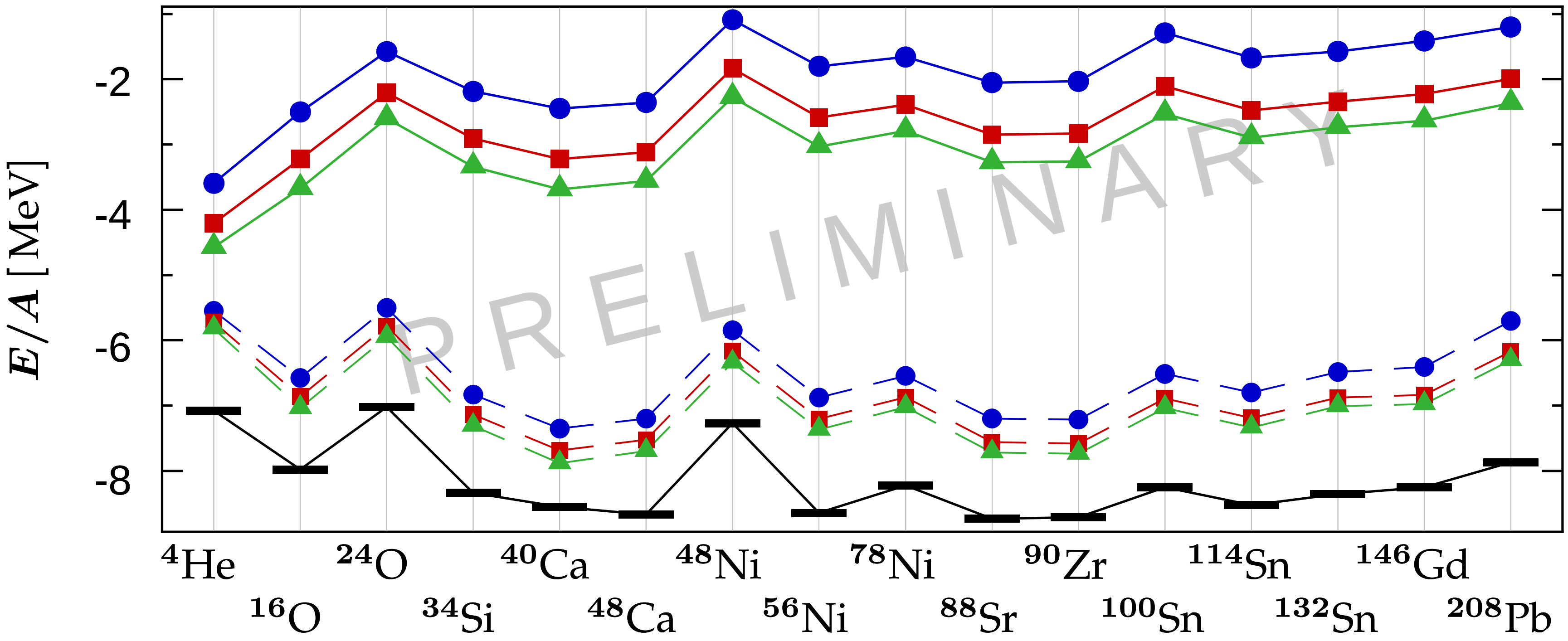

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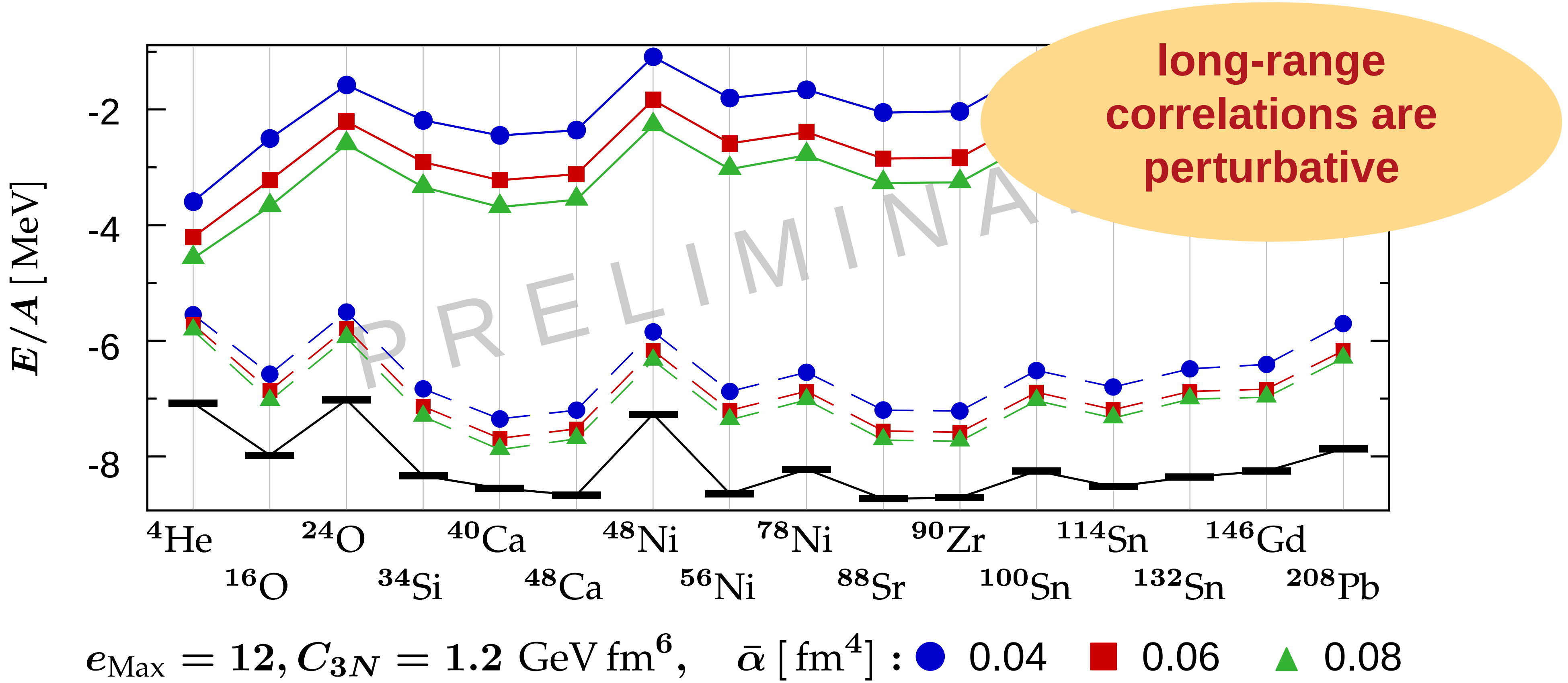
- second order MBPT **correction to radii is small**
- **$\bar{\alpha}$-dependence** of HF+MBPT energy is **reduced notably**

Many-Body Perturbation Theory



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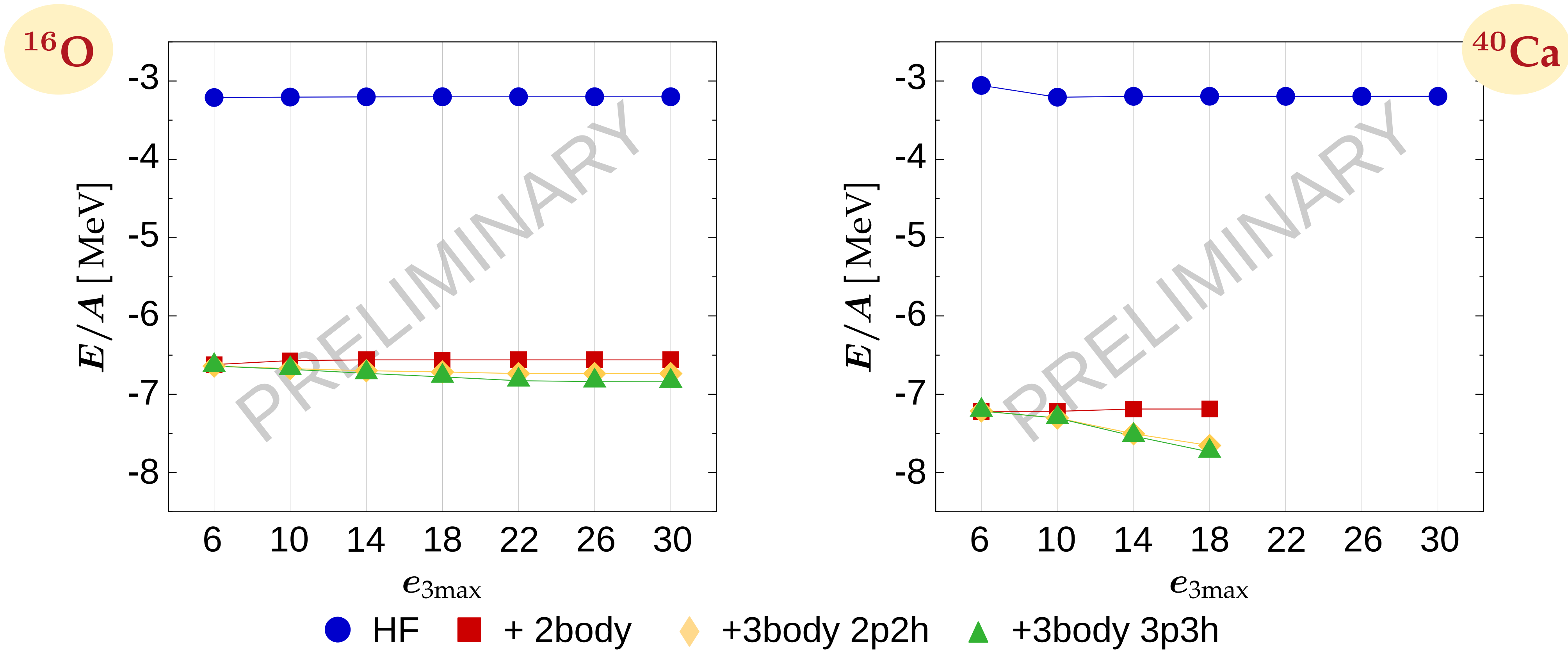
Many-Body Perturbation Theory



$$E_0^{(2)} = \frac{1}{4} \sum_{\alpha\alpha'}^{<\varepsilon_F} \sum_{\beta\beta'}^{>\varepsilon_F} \frac{\left| \langle \alpha\alpha' | T_{\text{int}} + V_{\text{UCOM}} | \beta\beta' \rangle + \sum_{\nu}^{<\varepsilon_F} \langle \alpha\alpha'\nu | V_{3\text{N}} | \beta\beta'\nu \rangle \right|^2}{\varepsilon_\alpha + \varepsilon_{\alpha'} - \varepsilon_\beta - \varepsilon_{\beta'}}$$

$$+ \frac{1}{36} \sum_{\alpha\alpha'\alpha''}^{<\varepsilon_F} \sum_{\beta\beta'\beta''}^{>\varepsilon_F} \frac{\left| \langle \alpha\alpha'\alpha'' | V_{3\text{N}} | \beta\beta'\beta'' \rangle \right|^2}{\varepsilon_\alpha + \varepsilon_{\alpha'} + \varepsilon_{\alpha''} - \varepsilon_\beta - \varepsilon_{\beta'} - \varepsilon_{\beta''}}$$

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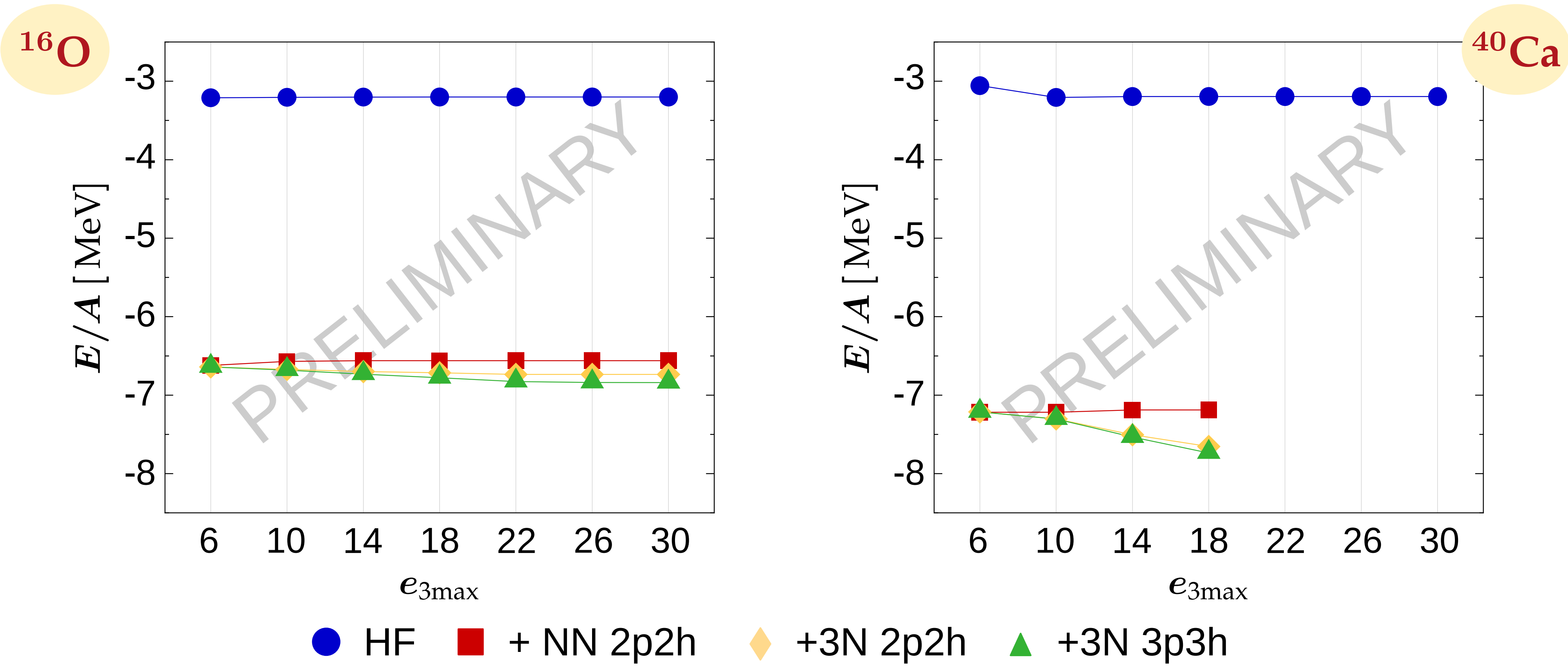
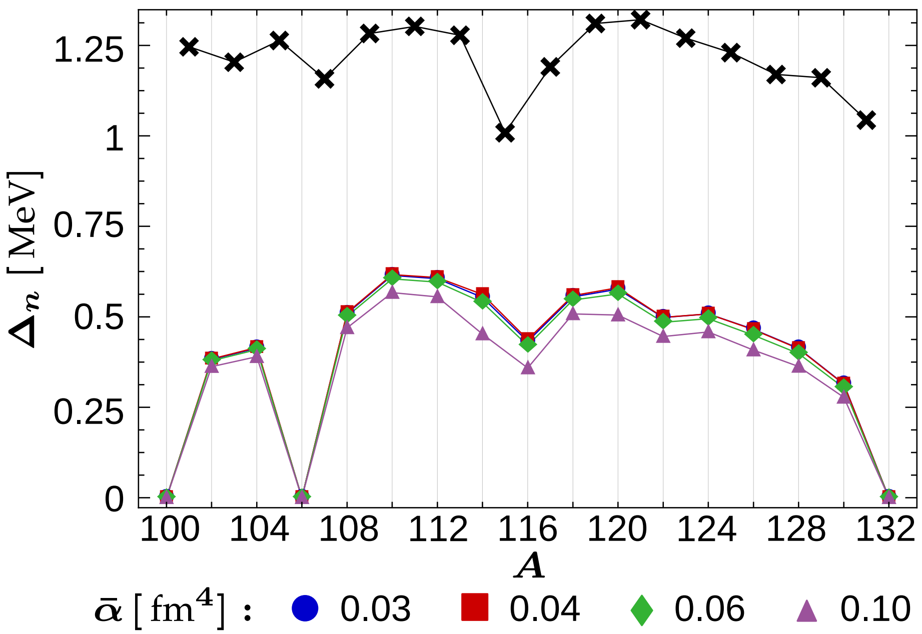


- main 3N energy contributions from contractions w. r. t. ground state
- **residual 3N interaction** gives small contributions in MBPT

☞ justification for **density-dependent two-body interaction**

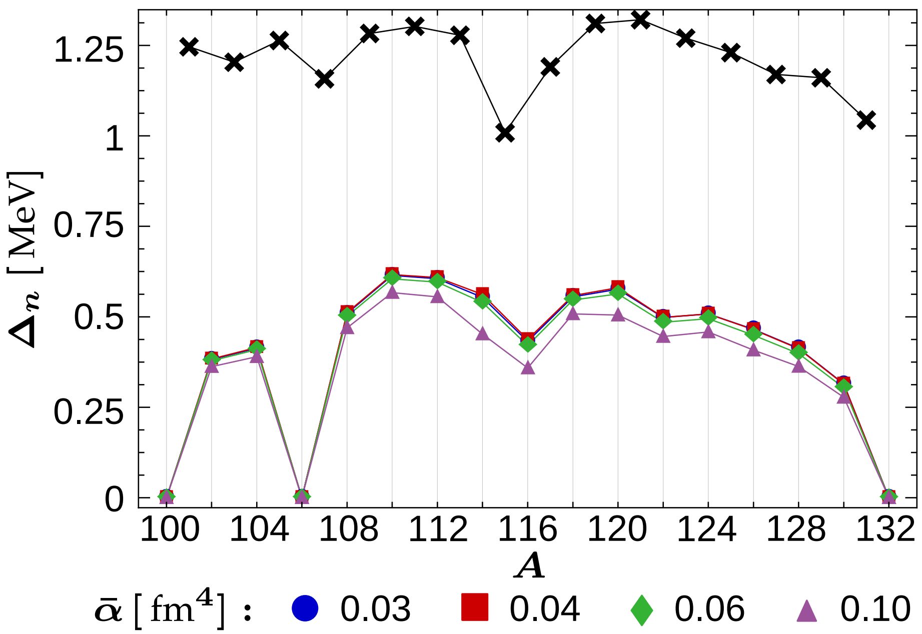
V_{UCOM} as a Pairing Force: Sn Isotopes



hybrid HFB calculation:
Gogny D1S + V_{UCOM}

- **stability** of gaps for wide range of $\bar{\alpha}$: stable ${}^1S_0$ matrix elements
- residual reduction of gaps through contributions from **higher partial waves**

V_{UCOM} as a Pairing Force: Sn Isotopes

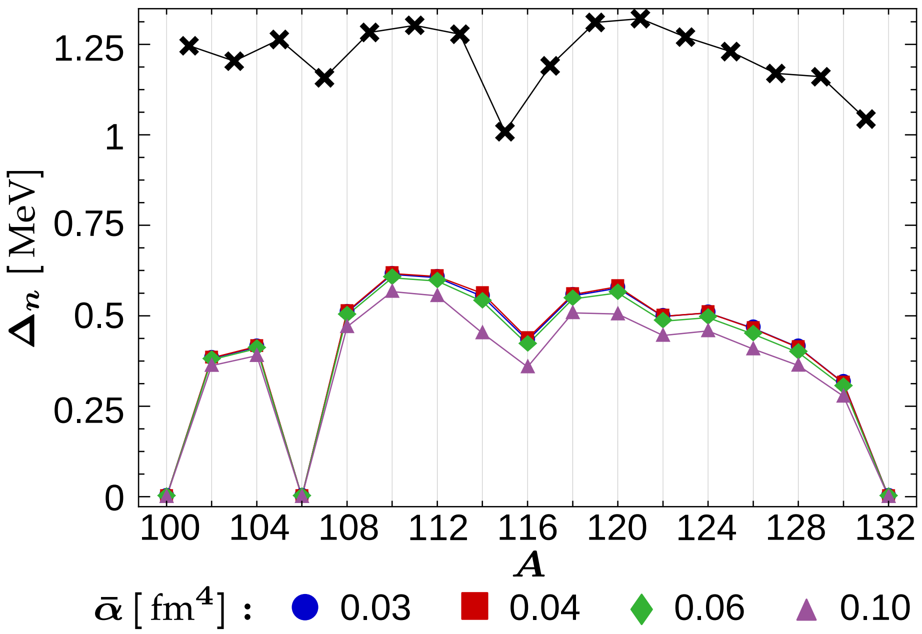


hybrid HFB calculation:
Gogny D1S + V_{UCOM}

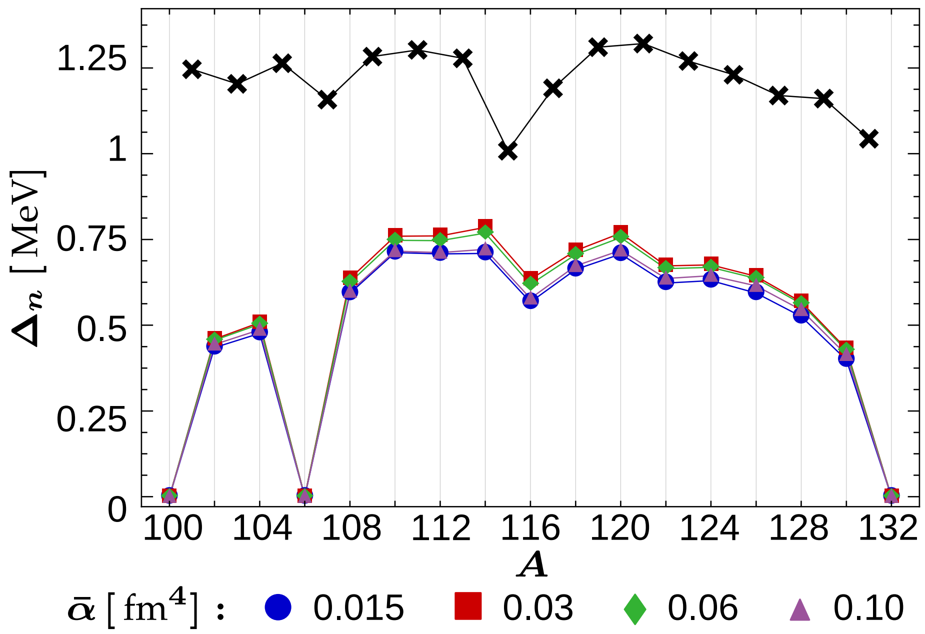
- **stability** of gaps for wide range of $\bar{\alpha}$: stable ${}^1S_0$ matrix elements
- residual reduction of gaps through contributions from **higher partial waves**
- ✘ $\sim 50\%$ smaller than SLy4 + $V_{\text{low-}k}$ study by Lesinski & Duguet
  (arXiv: 0809.2895)

V_{UCOM} vs. V_{SRG}

D1S + V_{UCOM}

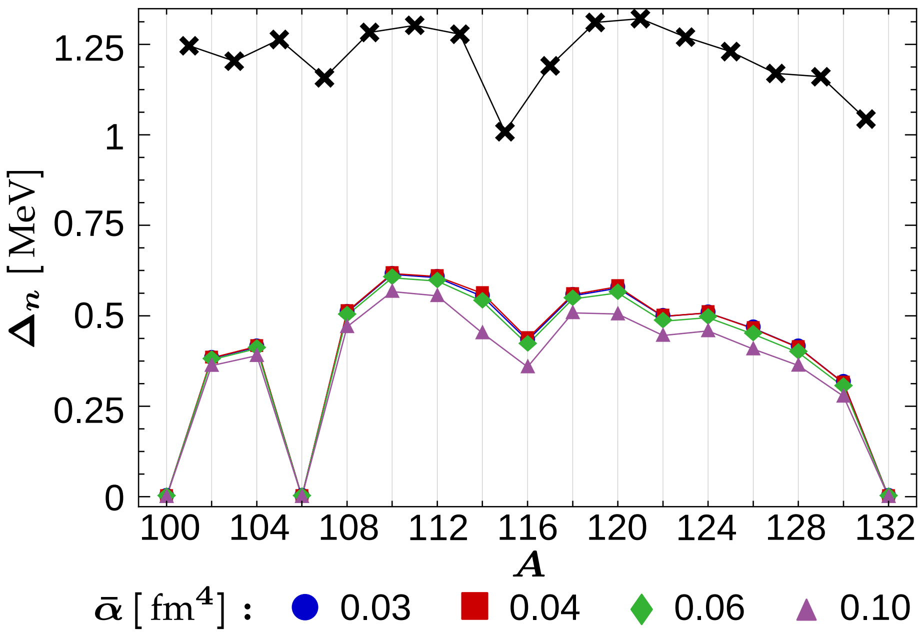


D1S + V_{SRG}

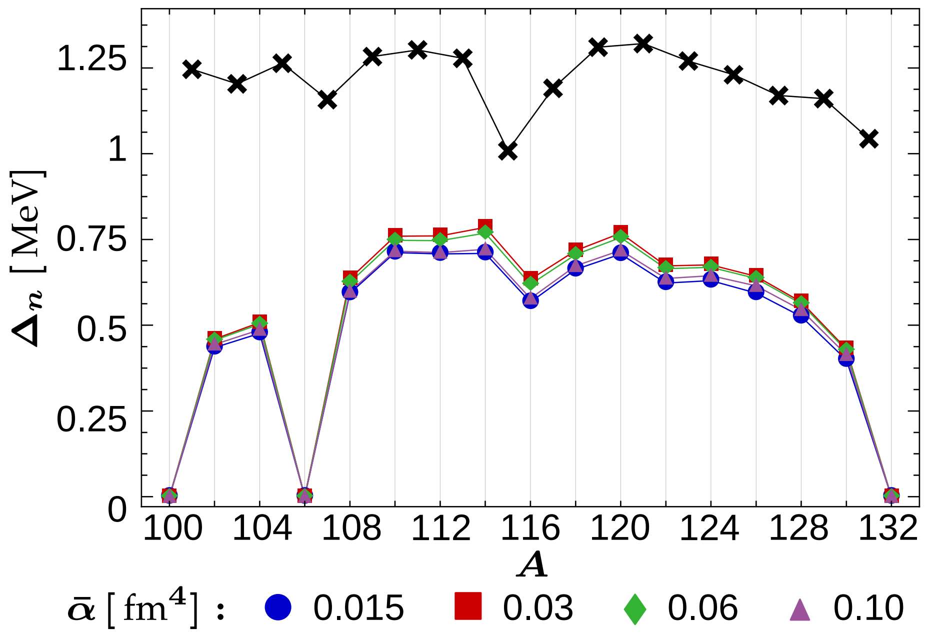


V_{UCOM} vs. V_{SRG}

D1S + V_{UCOM}



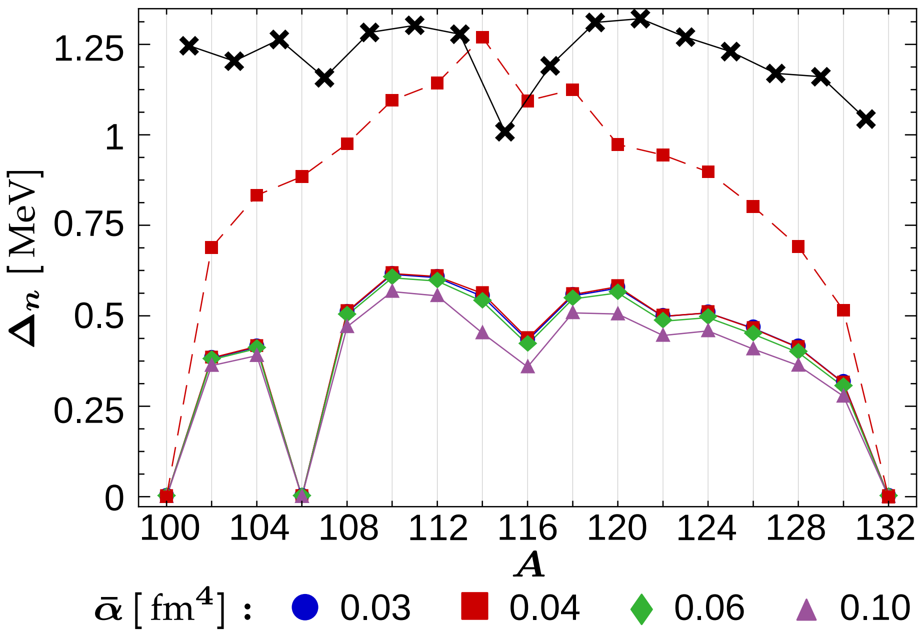
D1S + V_{SRG}



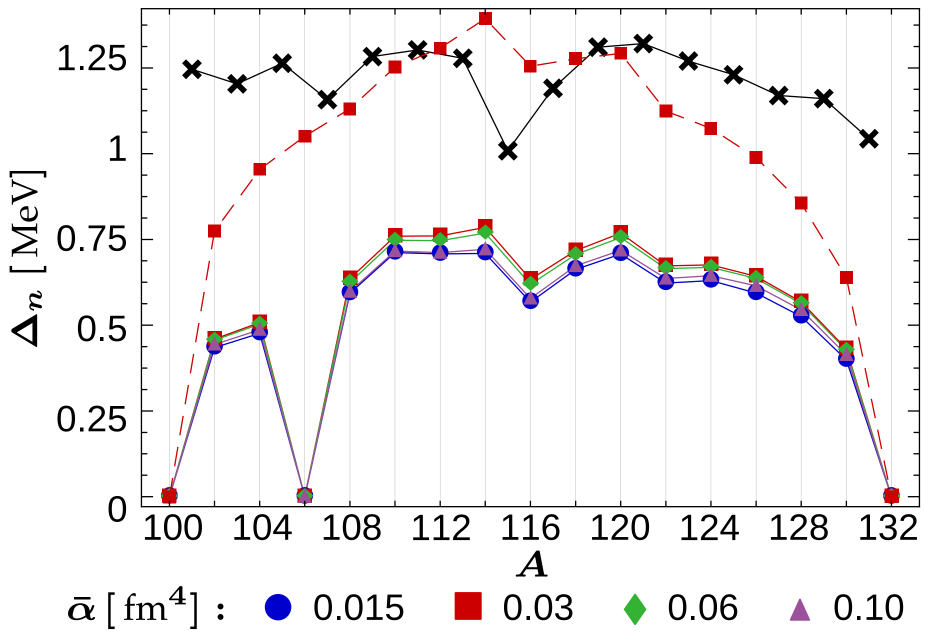
$$T_{\text{int}} = \frac{2}{A}\sum_{i<j}\frac{\vec{q}_{ij}^{\,2}}{2\mu} = \underbrace{\left(1-\frac{1}{A}\right)\sum_i \frac{\vec{p}_i^{\,2}}{2m}}_{\text{one-body}} - \underbrace{\frac{1}{Am}\sum_{i<j}\vec{p}_i\cdot\vec{p}_j}_{\text{two-body}}$$

V_{UCOM} vs. V_{SRG}

D1S + V_{UCOM}



D1S + V_{SRG}



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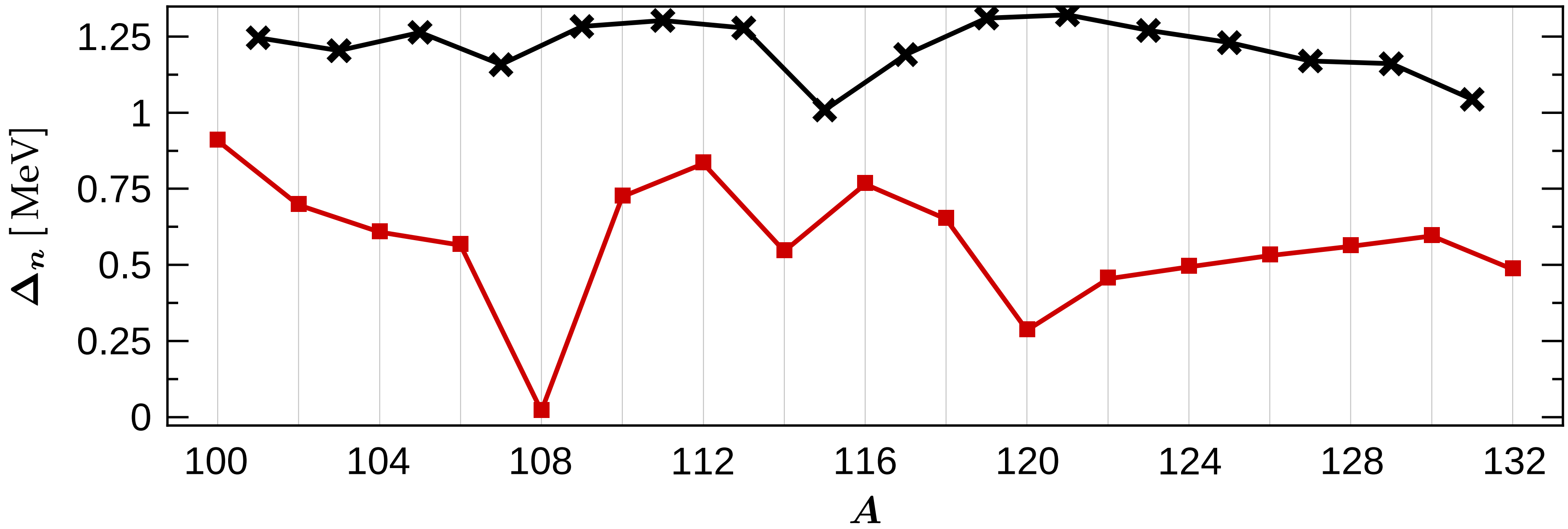
Fully Self-Consistent HFB+PNP

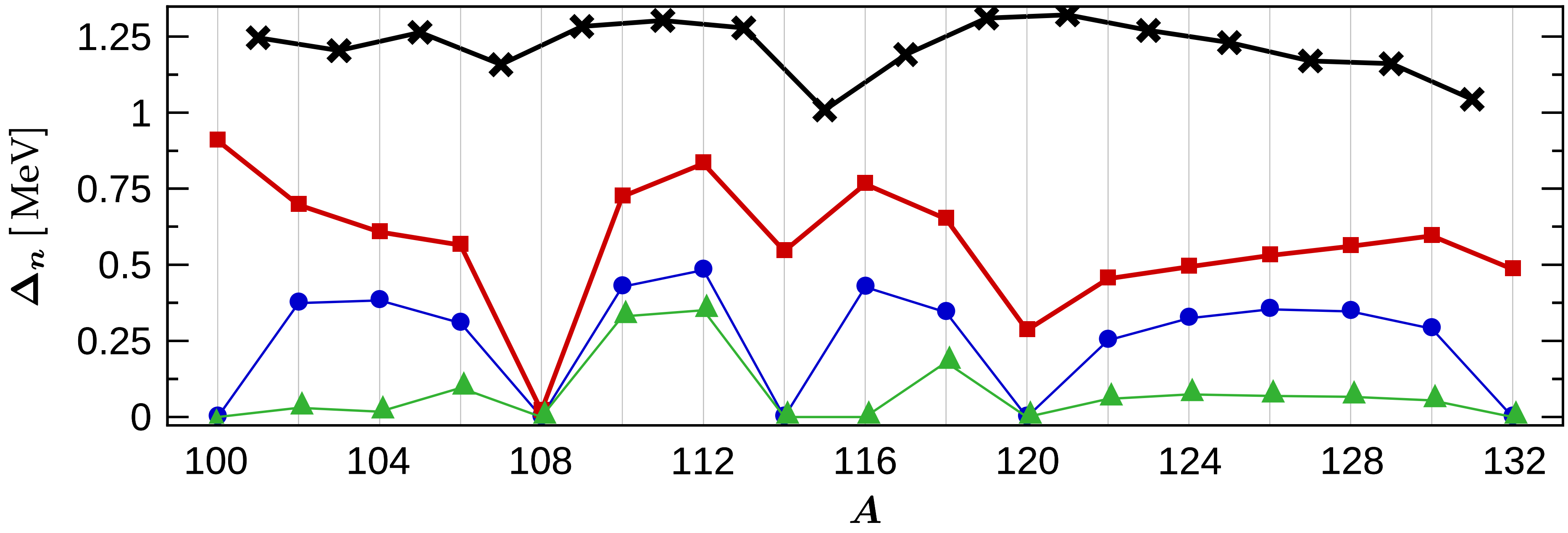
- use V_{UCOM} in both interaction channels
  - include **all partial waves** in the pairing channel
- consistent treatment of all two-body terms: **NN and Coulomb** interaction, **intrinsic kinetic energy**
  - ☞ **crucial** for beyond mean-field methods like particle-number projection
- reduce **3N contact force** to **density-dependent two-body interaction**
- variation after particle-number projection (PNP)

HFB+PNP: Sn Isotopes



$\bar{\alpha} = 0.04\ \text{fm}^4,\ C_{3N} = 1.2\ \text{GeV fm}^6$ ■ VAP NN+3N

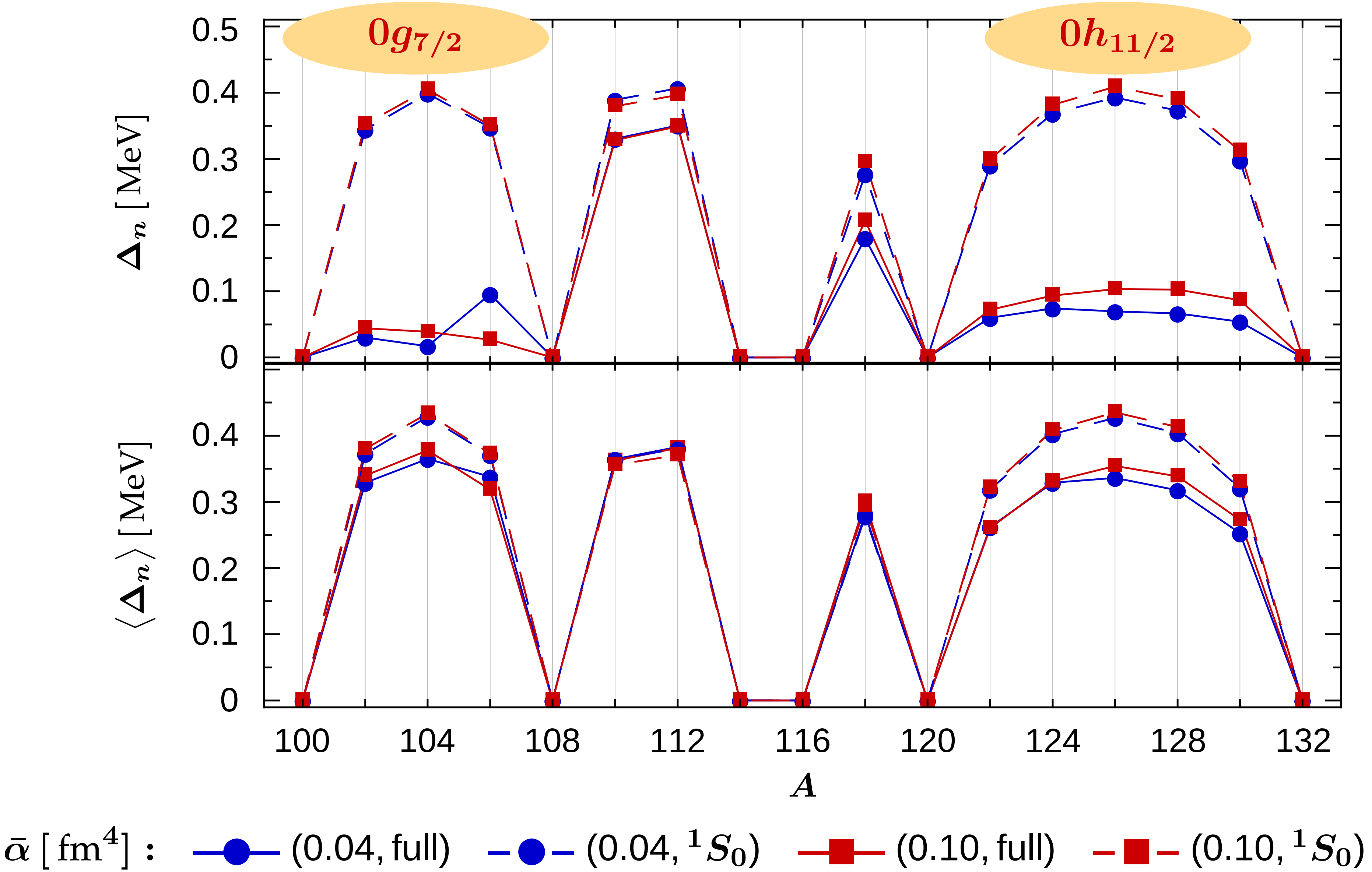
HFB+PNP: Sn Isotopes



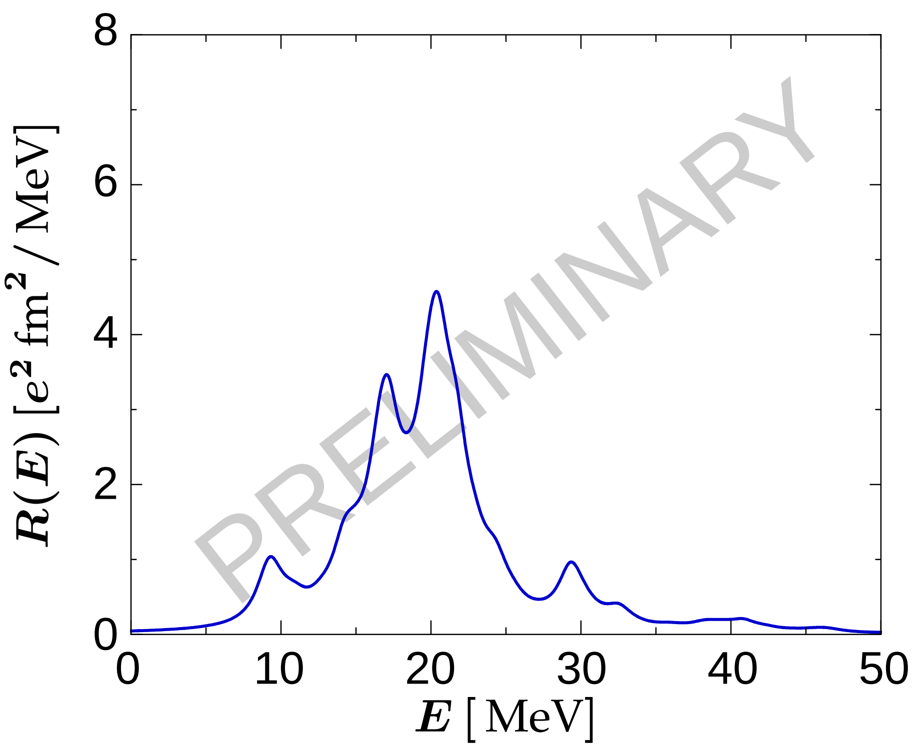
$\bar{\alpha} = 0.04\ \mathrm{fm}^4,\ C_{3N} = 1.2\ \mathrm{GeV\,fm}^6$ ■ VAP NN+3N ● HFB NN+3N ▲ HFB NN

- **low level density** (general feature of soft NN interactions)
  - ☞ 3N interaction **compresses single-particle spectra**
  - ☞ VAP includes **dynamical pairing** correlations

Non-Central Interactions

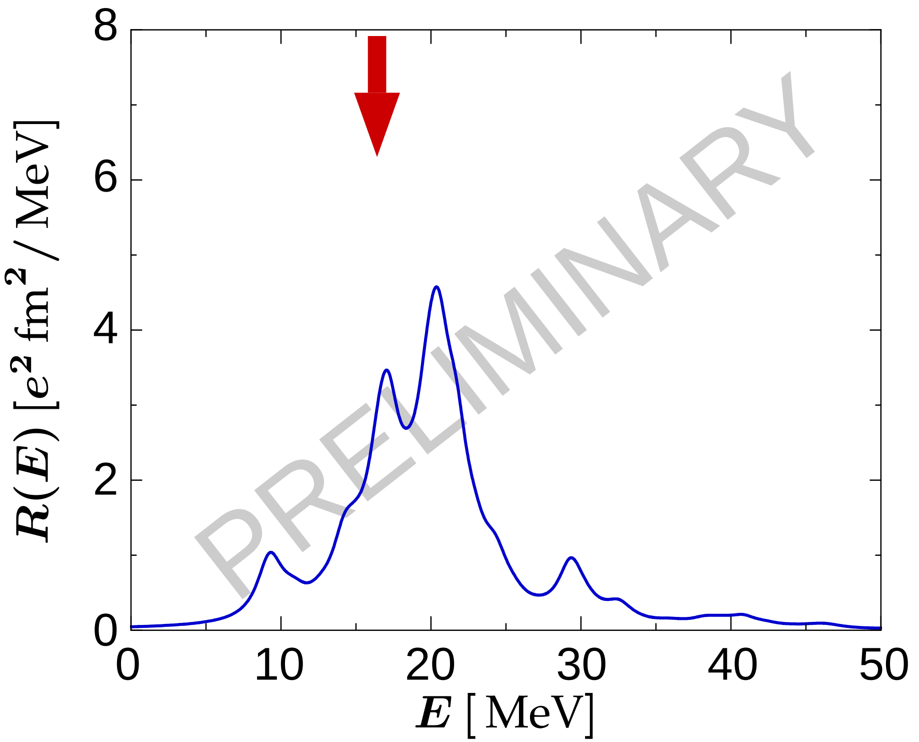


QRPA: Dipole Response of ^{130}Sn



$(\bar{\alpha}[\,\mathrm{fm}^4], C_{3N}[\,\mathrm{GeV\,fm}^6])$ — $(0.04, 0.0)$

QRPA: Dipole Response of ^{130}Sn



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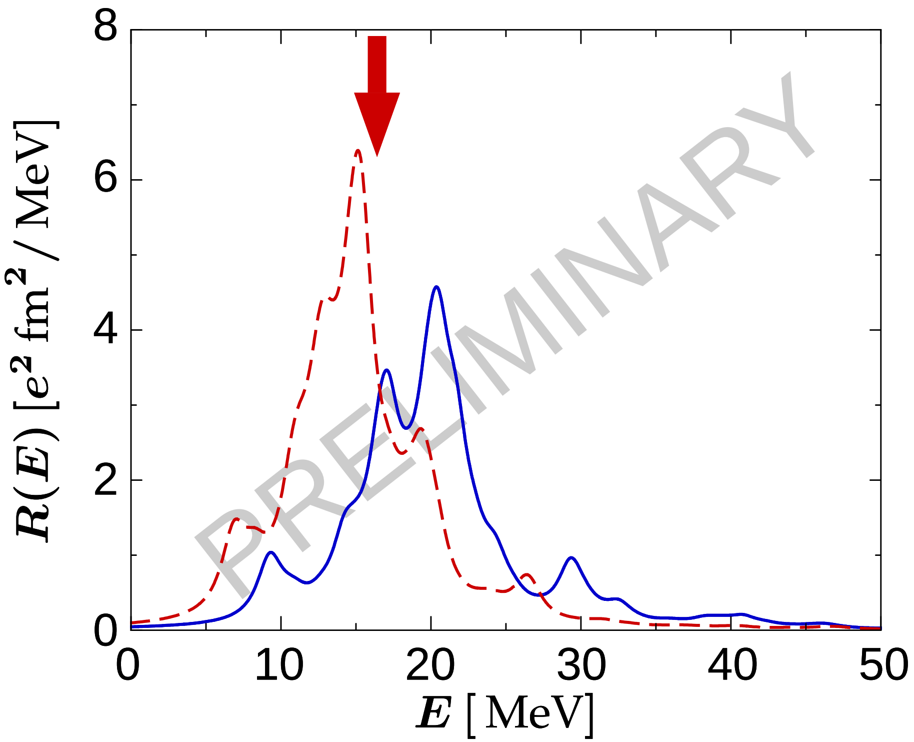

$(\bar{\alpha}[\,\mathrm{fm}^4], C_{3N}[\,\mathrm{GeV\,fm}^6])$ —— $(0.04, 0.0)$ - - - $(0.04, 1.2)$

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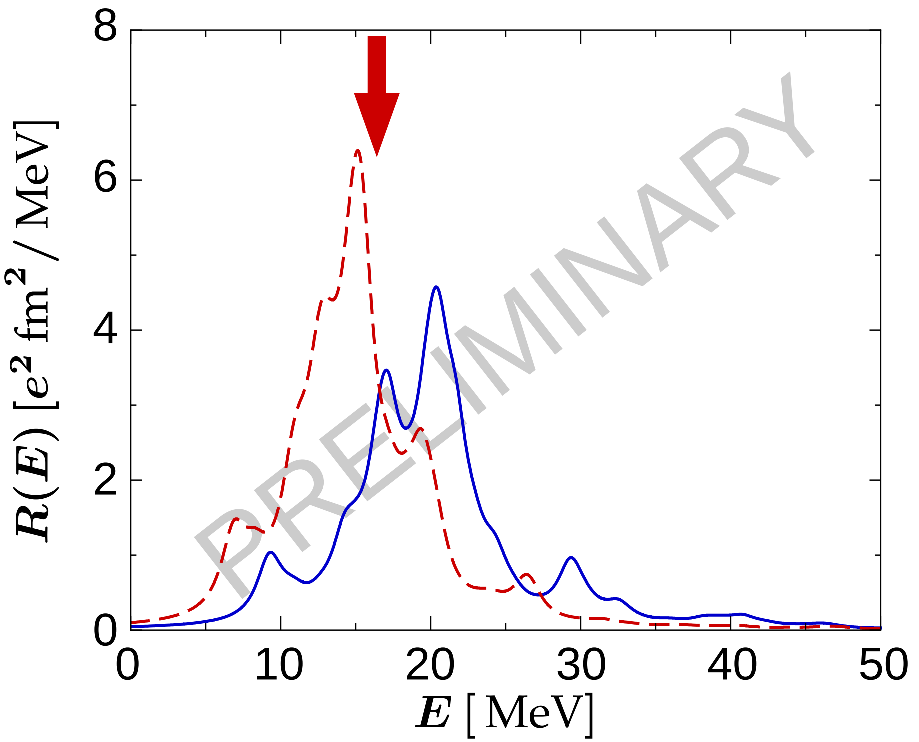

E [MeV]	TRK [%]	N_{neut} [%]
12.86	~ 9	20.2
15.03	~ 14	52.2
15.43	~ 27	24.7

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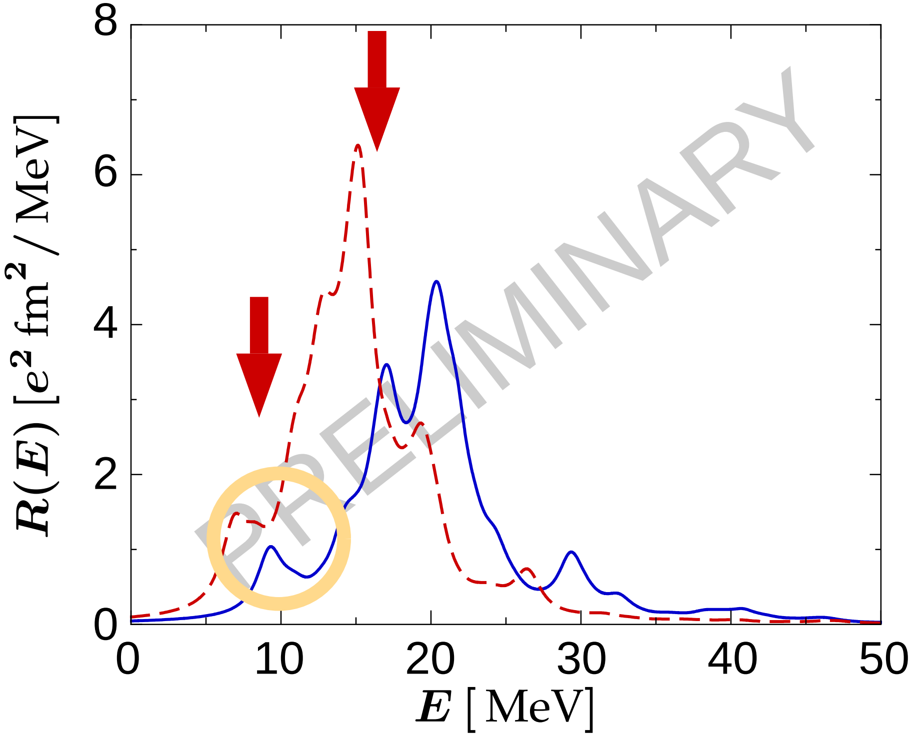

E [MeV]	TRK [%]	N_{neut} [%]
12.86	~ 9	20.2
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15.43	~ 27	24.7
6.86	~ 5	94.7
$\nu 2s_{1/2} \rightarrow \nu 2p_{3/2}$		36.0
$\nu 1d_{3/2} \rightarrow \nu 2p_{1/2}$		17.6
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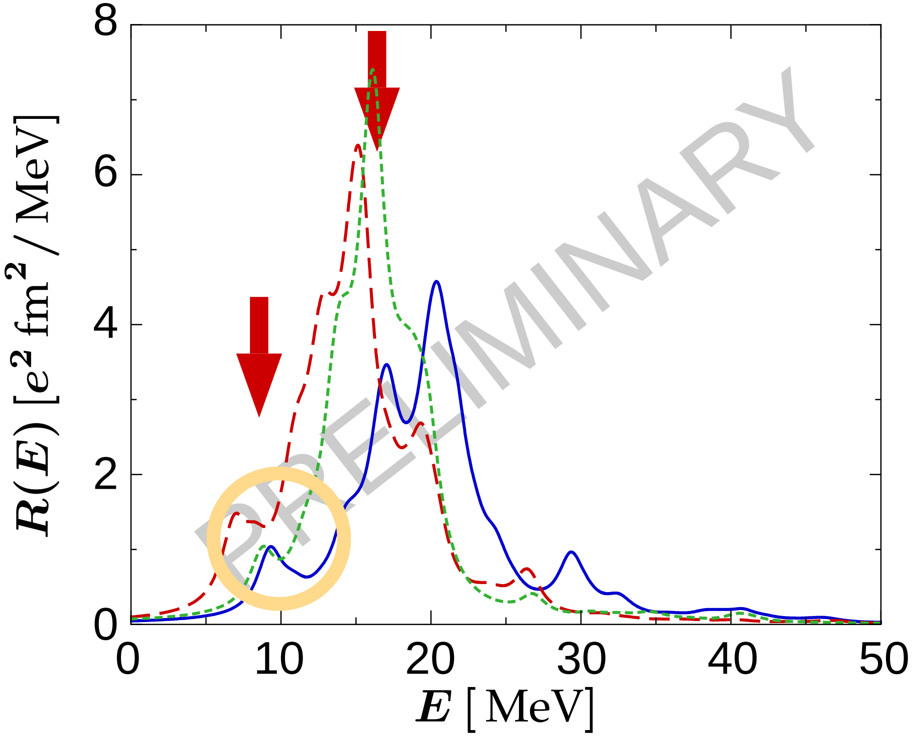
$(\bar{\alpha}[\text{fm}^4], C_{3N}[\text{GeV fm}^6])$ —— $(0.04, 0.0)$ - - - $(0.04, 1.2)$

Pygmy Dipole Resonance:
significantly enhanced collectivity in QRPA

QRPA: Dipole Response of ^{130}Sn



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Pygmy Dipole Resonance:
significantly enhanced collectivity in QRPA

Conclusions

Status

- **fully consistent** framework for HF(B), PNP, like-particle & charge-exchange (Q)RPA, SRPA
- inclusion of (regularized) **3N contact interaction** / **density-dependent interaction**

Outlook & Challenges

- **chiral NN and 3N interactions**
- UCOM/SRG for 3N interaction
- beyond mean-field methods: projection, GCM, higher (Q)RPAs

☞ density-dependent interactions?

Epilogue...

Thanks to my collaborators:

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- T. Neff, H. Feldmeier

  Gesellschaft für Schwerionenforschung (GSI)

Deutsche Forschungsgemeinschaft DFG

SFB 634

HIC for FAIR

LOEWE – Landes-Offensive zur Entwicklung Wissenschaftlich-ökonomischer Exzellenz

Supplements

HFB Theory Overview

Bogoliubov Transformation

$$\beta^\dagger_k = \sum_q U_{qk} c^\dagger_q + V_{qk} c_q$$

$$\beta_k = \sum_q U^*_{qk} c_q + V^*_{qk} c^\dagger_q$$

where

$$\{\beta_k, \beta_{k'}\} \stackrel{!}{=} \{\beta^\dagger_k, \beta^\dagger_{k'}\} \stackrel{!}{=} 0$$

$$\{\beta_k, \beta^\dagger_{k'}\} \stackrel{!}{=} \delta_{kk'}$$

HFB Densities & Fields

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

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

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

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

HFB Theory Overview

Bogoliubov Transformation

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

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

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

Energy

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

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

Projected Energy

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

Particle Number Projection

Variation of Projected Energy

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

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

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- ✔ Structure of **HFB equations is preserved**!
- ✔ managable computational effort for variation after projection (VAP)
- ✔ implement with care: **subtle cancellations between divergences of direct, exchange, and pairing terms**

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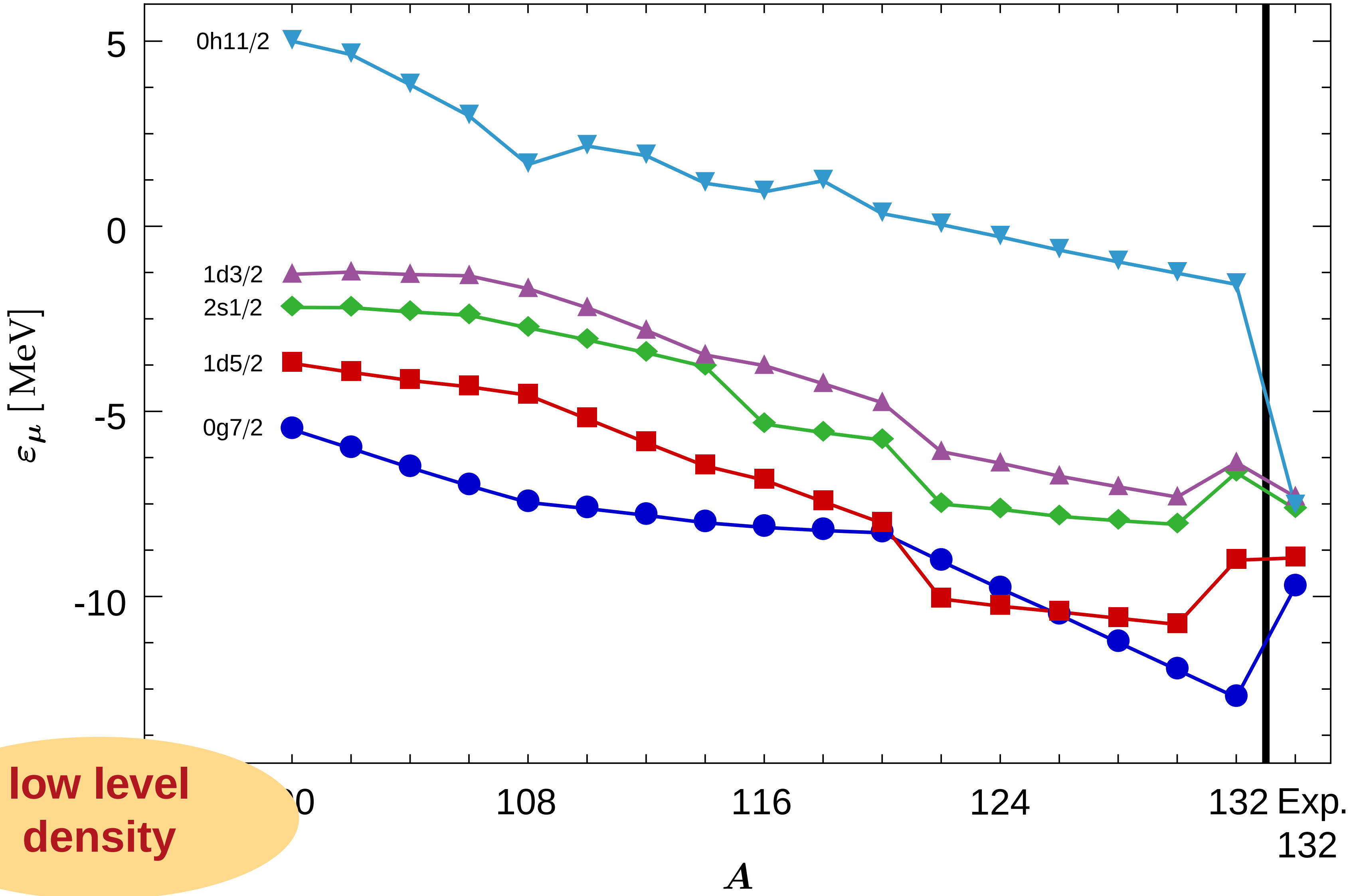
- ✔ Structure of **HFB equations is preserved**!
- ✔ managable computational effort for variation after projection (VAP)
- ✔ implement with care: **subtle cancellations between divergences of direct, exchange, and pairing terms**
- ✘ **density-dependent interaction:**
  complex transition density has **poles** (serious problem for projection methods, GCM, ...)

☞ Duguet, Lacroix, Bender et al., **arXiv**:0809.2041, 0809.2045, 0809.2049

Canonical Single-Particle Spectra



low level density

Quasiparticle RPA

- **equations-of-motion method**: assume $\mathrm{Q}_{\boldsymbol{k}}^{\dagger}$ generates exact excited state from exact ground state of H:

$$\left|\boldsymbol{k}\right\rangle = \mathrm{Q}_{\boldsymbol{k}}^{\dagger}\left|0\right\rangle \quad \Longleftarrow \quad \mathrm{Q}_{\boldsymbol{k}}^{\dagger} = \left|\boldsymbol{k}\right\rangle\!\left\langle 0\right| + \sum_{\boldsymbol{i},\boldsymbol{j}\perp\boldsymbol{k},0} C_{\boldsymbol{ij}}\left|\boldsymbol{i}\right\rangle\!\left\langle \boldsymbol{j}\right|$$

- reformulate Schrödinger equation, project on $\delta\mathrm{Q}_{\boldsymbol{k}}^{\dagger}\left|0\right\rangle$:

$$\left\langle 0\right|\left[\delta\mathrm{Q}_{\boldsymbol{k}},\left[\mathrm{H},\mathrm{Q}_{\boldsymbol{k}}^{\dagger}\right]\right]\left|0\right\rangle = \hbar\omega_{\boldsymbol{k}}\left\langle 0\right|\left[\delta\mathrm{Q}_{\boldsymbol{k}},\mathrm{Q}_{\boldsymbol{k}}^{\dagger}\right]\left|0\right\rangle$$

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- reformulate Schrödinger equation, project on $\delta\mathrm{Q}_k^\dagger \left|0\right\rangle$:

$$\left\langle 0\right| \left[\delta\mathrm{Q}_k, \left[\mathrm{H}, \mathrm{Q}_k^\dagger\right]\right] \left|0\right\rangle = \hbar\omega_k \left\langle 0\right| \left[\delta\mathrm{Q}_k, \mathrm{Q}_k^\dagger\right] \left|0\right\rangle$$

- approximate $\mathrm{Q}_k^\dagger$ (phonon operator) in canonical basis:

$$\mathrm{Q}_k^\dagger = \sum_{\mu<\mu'} \left(X^k_{\mu\mu'} \alpha^\dagger_\mu \alpha^\dagger_{\mu'} - Y^k_{\mu\mu'} \alpha_\mu \alpha_{\mu'} \right)$$

- let $\left|0\right\rangle = \left|\mathrm{HFB}\right\rangle$ (**quasi-boson aproximation**) and obtain:

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} X^k \\ Y^k \end{pmatrix} = \hbar\omega_k \begin{pmatrix} 1 & \\ & -1 \end{pmatrix} \begin{pmatrix} X^k \\ Y^k \end{pmatrix}$$