Mean-Field and Pairing Calculations in the UCOM Framework

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Overview

- Reminder: UCOM and SRG Basics
- Hartree-Fock and Perturbation Theory with $\boldsymbol{V}_{\mathrm{UCOM}}$
- Pairing in the UCOM Framework
  - Hartree-Fock-Bogoliubov & Projection
  - Quasiparticle RPA
- Conclusions

Current Approaches

Phenomenology
binding energies, radii
nuclear matter

QCD

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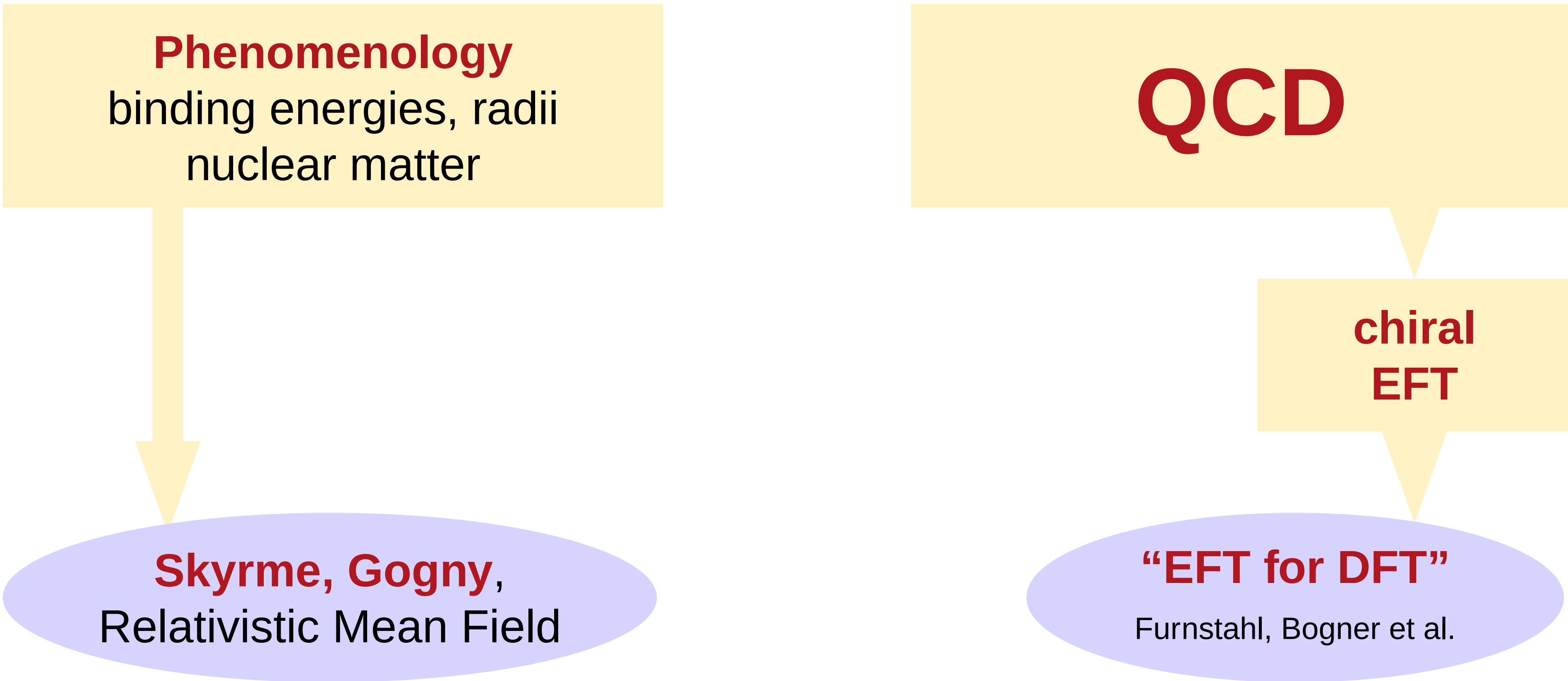
Phenomenology
binding energies, radii
nuclear matter

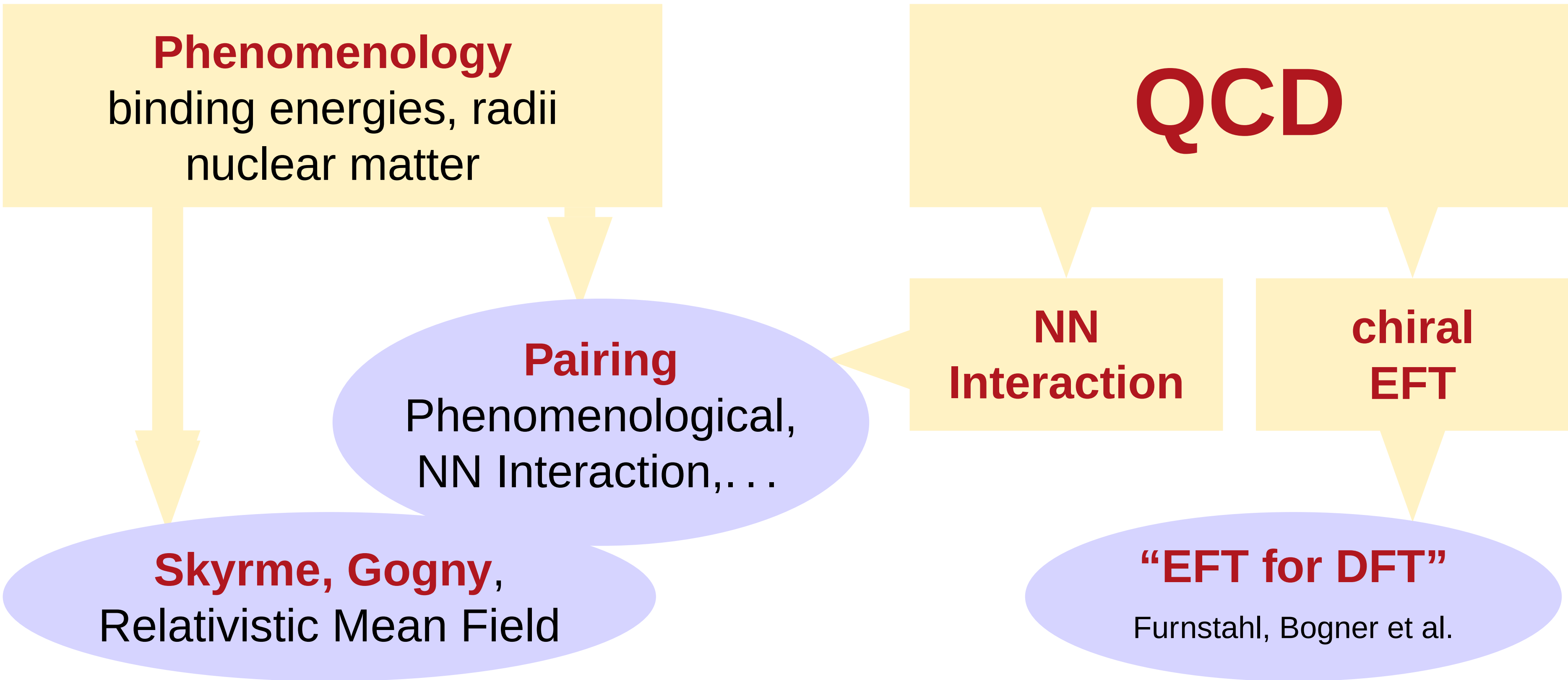
QCD

Skyrme, Gogny,
Relativistic Mean Field

Current Approaches



Current Approaches



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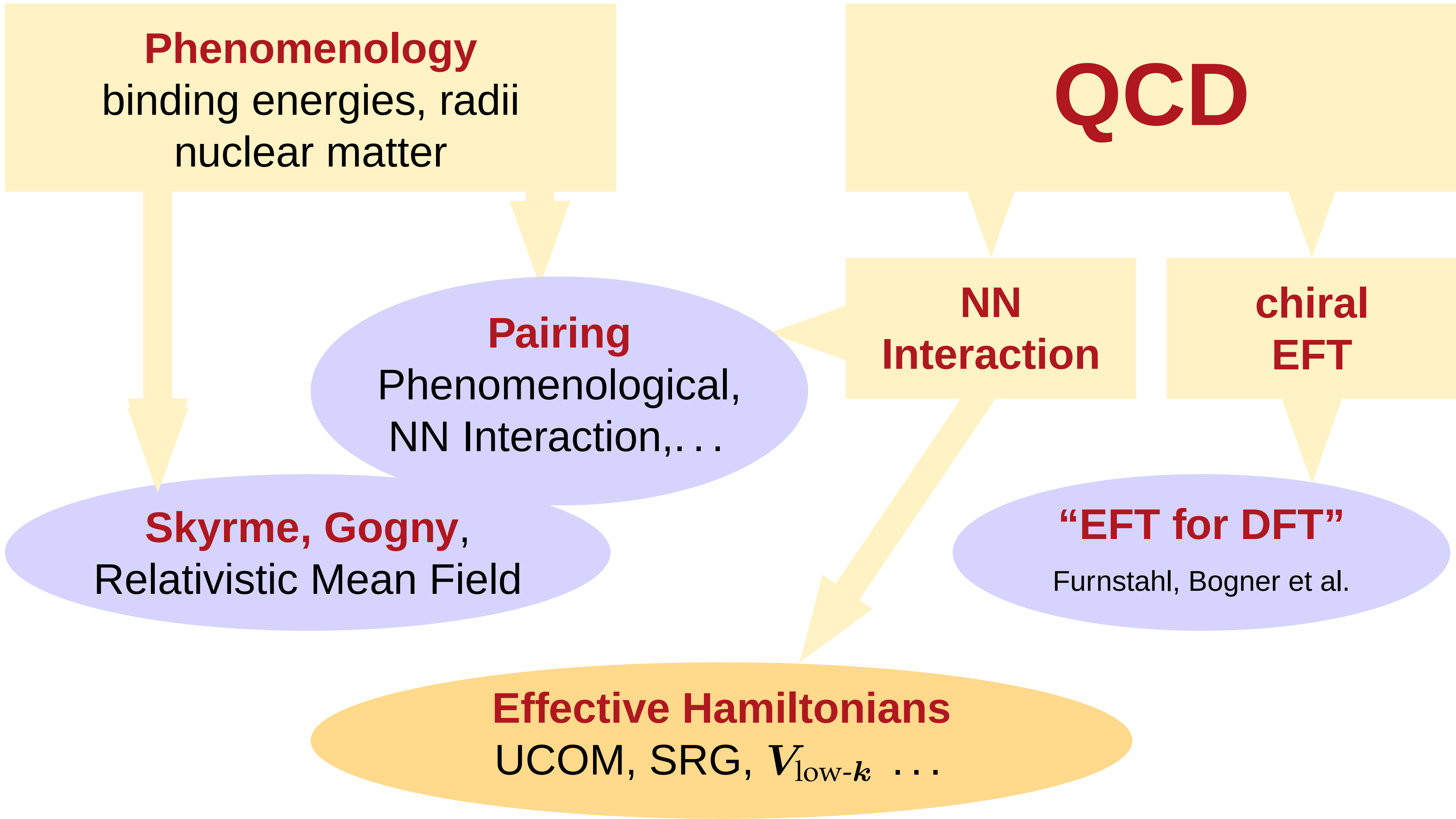

Issues of DFT

- ✘ description of **exotic nuclei** and **spectroscopic observables** is lacking
- ✘ inconsistent treatment of **particle-hole** and **particle-particle** channel treated if separate forces are used
- ✘ local density approximation, gradient expansion essentially **uncontrolled**
- ✘ technical & conceptual difficulties due to **non-analytic terms**

☞ Dobaczewski et al., Phys. Rev. **C76**, 054315 (2007)

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

- ✘ fits of phenomenological functionals obscure underlying physics

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- ✘ fits of phenomenological functionals obscure underlying physics

consistent Hamiltonian approach
avoids most problems

UCOM and SRG Basics

Modern Effective Interactions

phase-shift equivalent interaction from unitary transformation of the Hamiltonian

Unitary Correlation Operator Method

- **transformed Hamiltonian**

$$\widetilde{\mathrm{H}} = \mathrm{C}_r^\dagger \mathrm{C}_\Omega^\dagger \mathrm{H} \mathrm{C}_\Omega \mathrm{C}_r$$

- **central correlations:** radial shift

$$\mathrm{C}_r = \exp(-i \sum_{i<j} \mathrm{g}_{r,ij}[s(r_{ij})])$$

- **tensor correlations:** angular shift

$$\mathrm{C}_\Omega = \exp(-i \sum_{i<j} \mathrm{g}_{\Omega,ij}[\vartheta(r_{ij})])$$

Similarity Renormalization Group

- **transformed Hamiltonian**

$$\widetilde{\mathrm{H}}(\alpha) = \mathrm{C}^\dagger(\alpha) \mathrm{H} \mathrm{C}(\alpha)$$

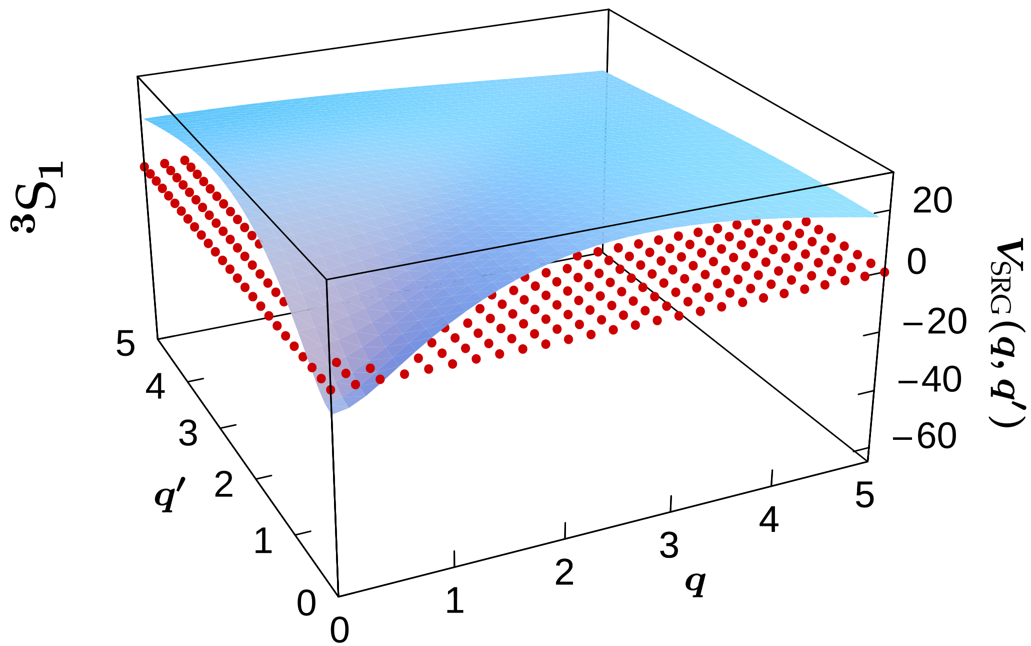
- evolution via RG **flow equation**

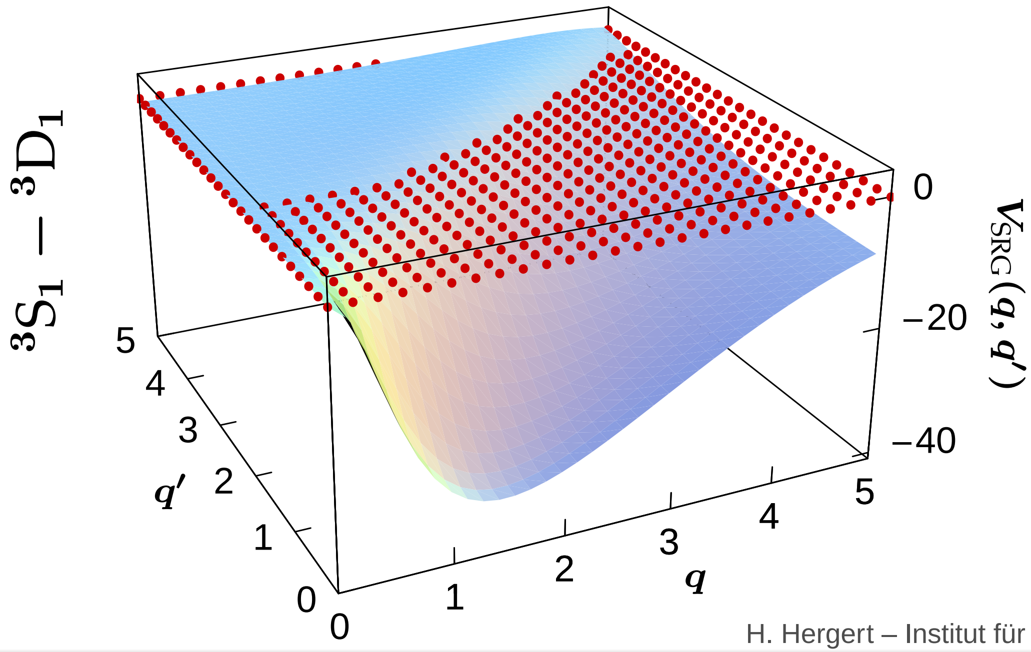
$$\frac{\mathrm{d}}{\mathrm{d}\alpha}\widetilde{\mathrm{H}}(\alpha) = \left[\eta(\alpha), \widetilde{\mathrm{H}}(\alpha)\right]$$

- **dynamical** generator

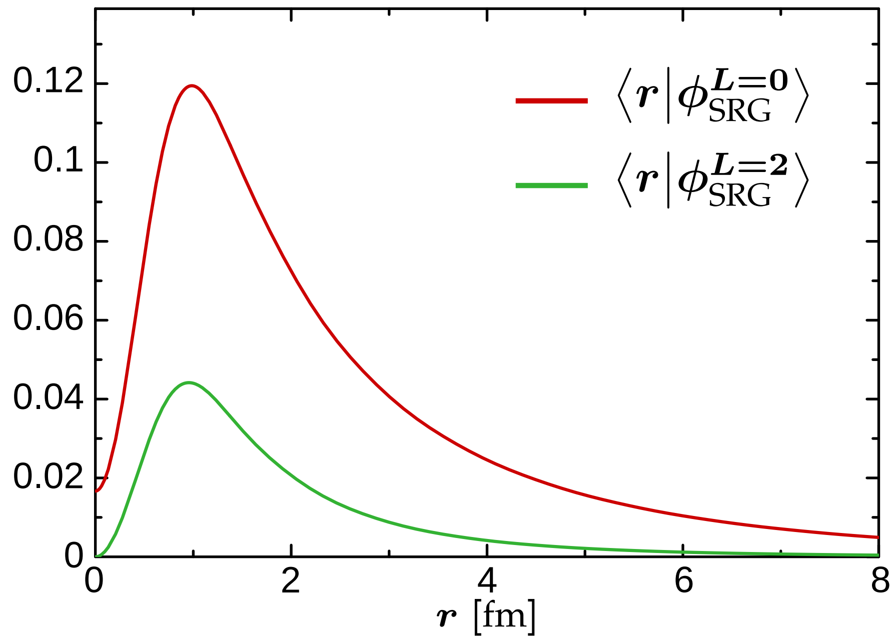
$$\eta(\alpha) = \tfrac{1}{2\mu}\left[\vec{\mathrm{q}}^2, \widetilde{\mathrm{H}}(\alpha)\right]$$

SRG Evolution: The Deuteron





Argonne V18



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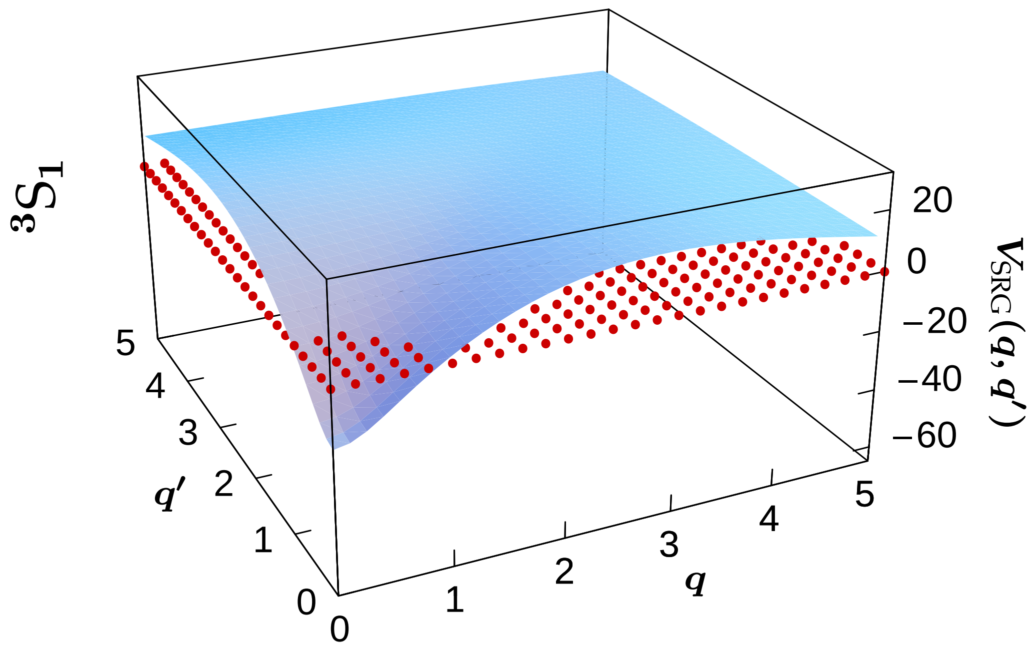
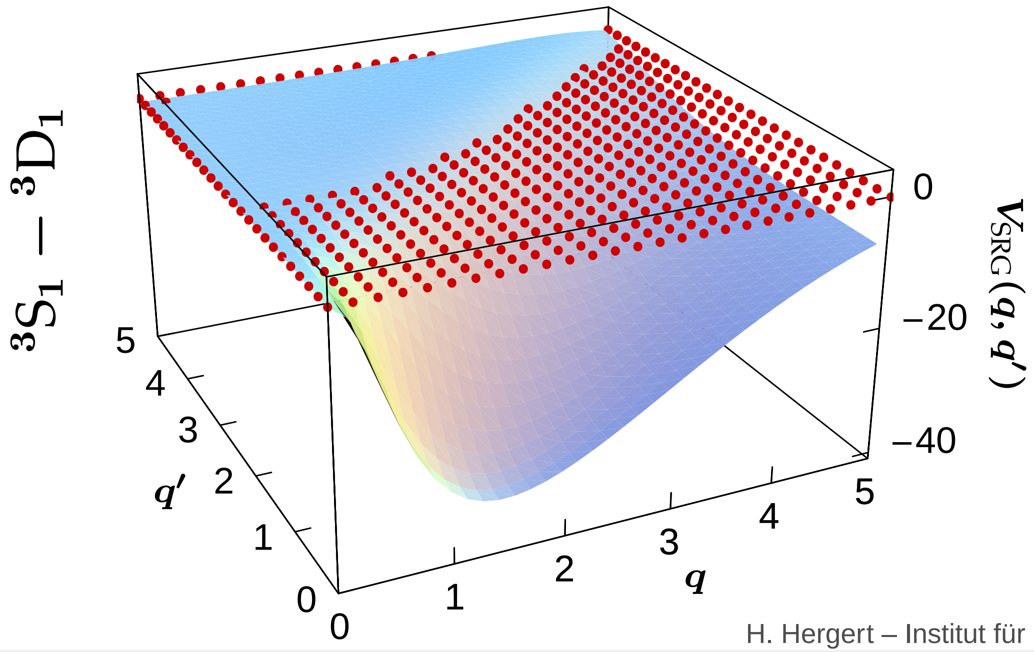
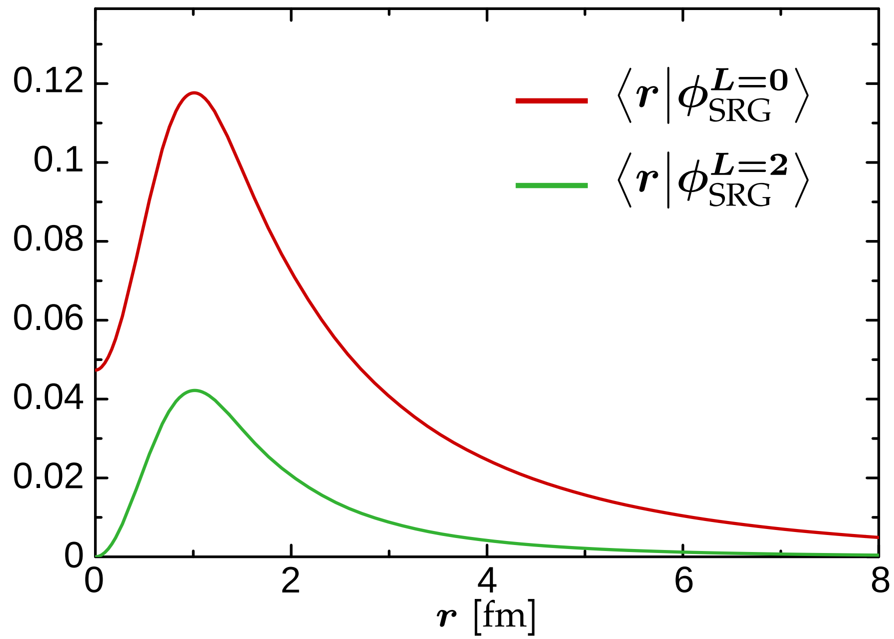




$\alpha = 0.0004\,\mathrm{fm}^4$



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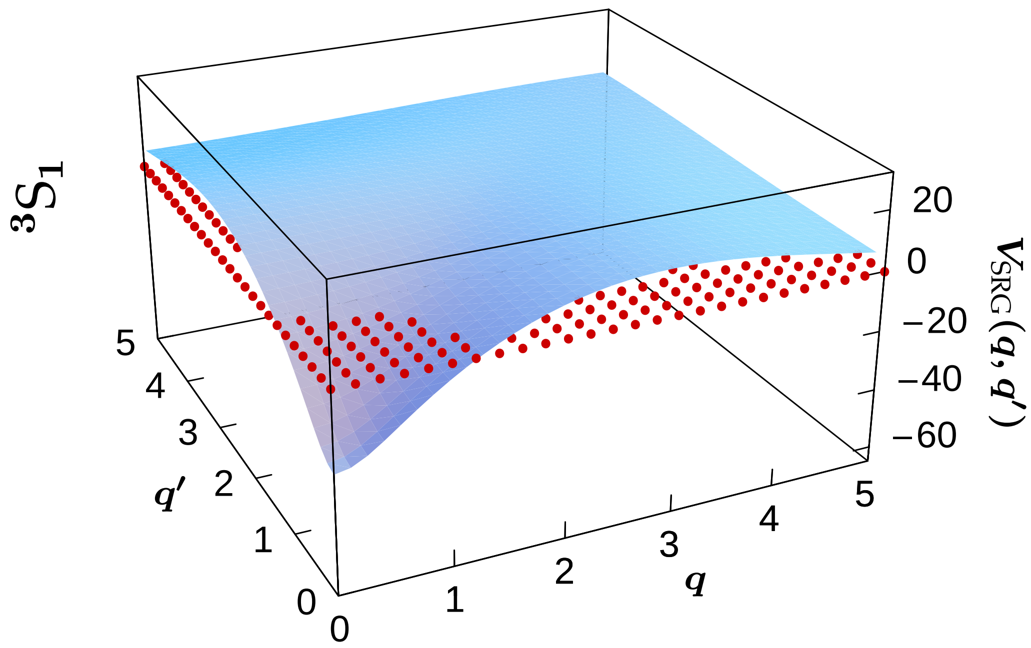

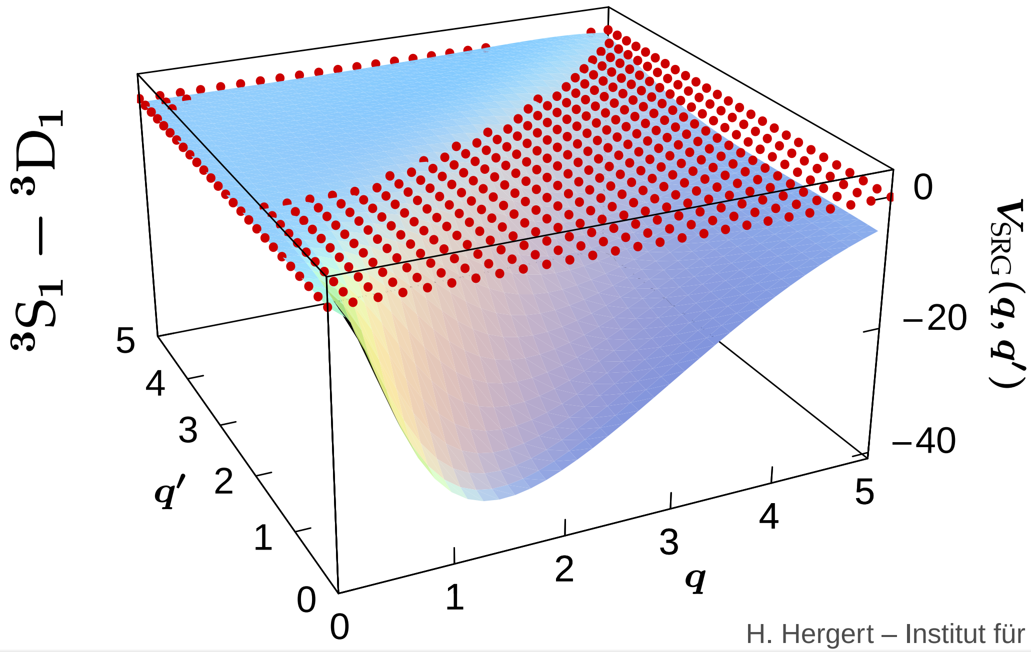

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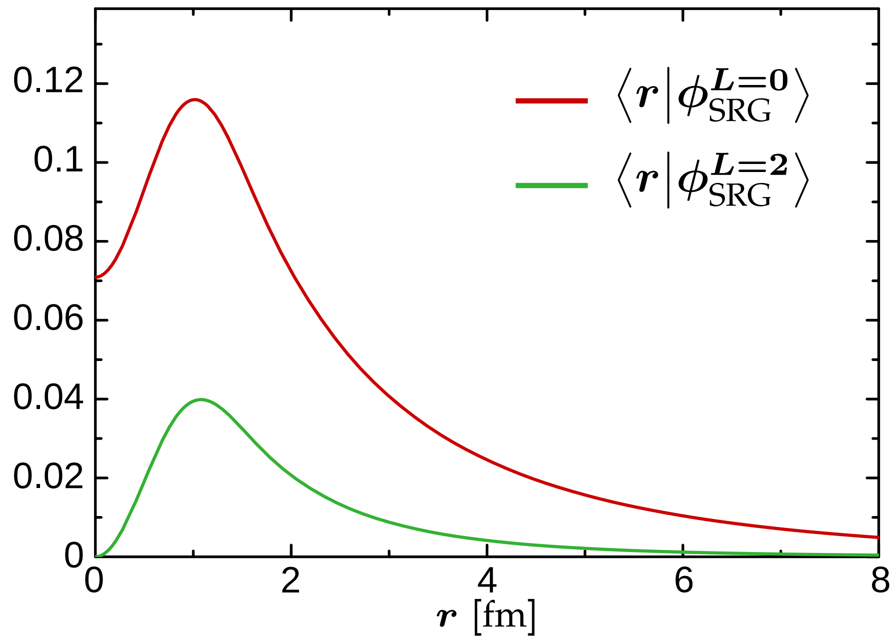
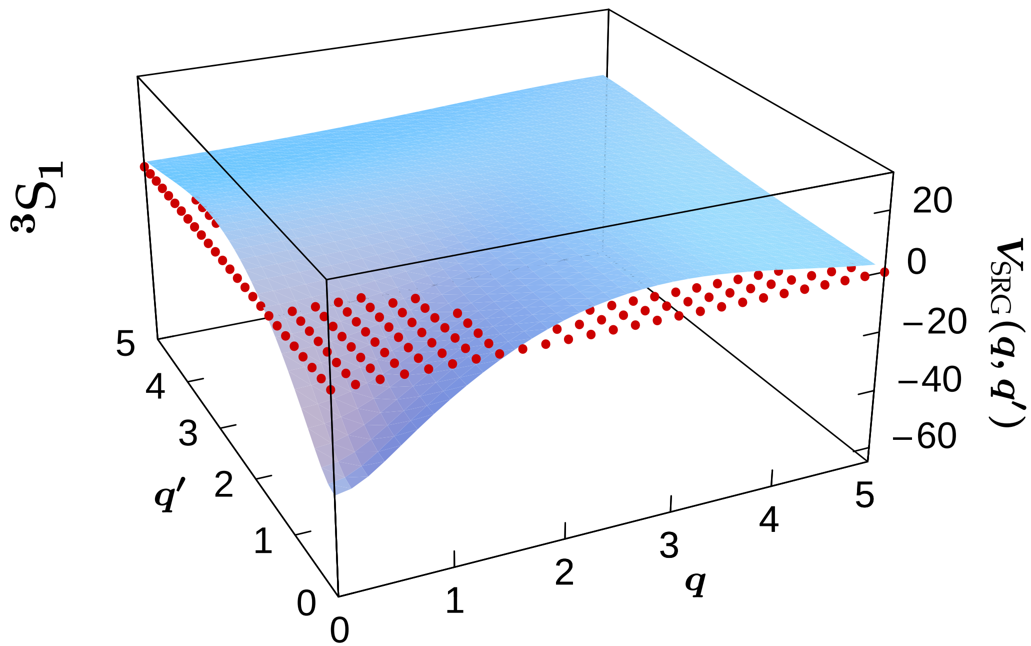
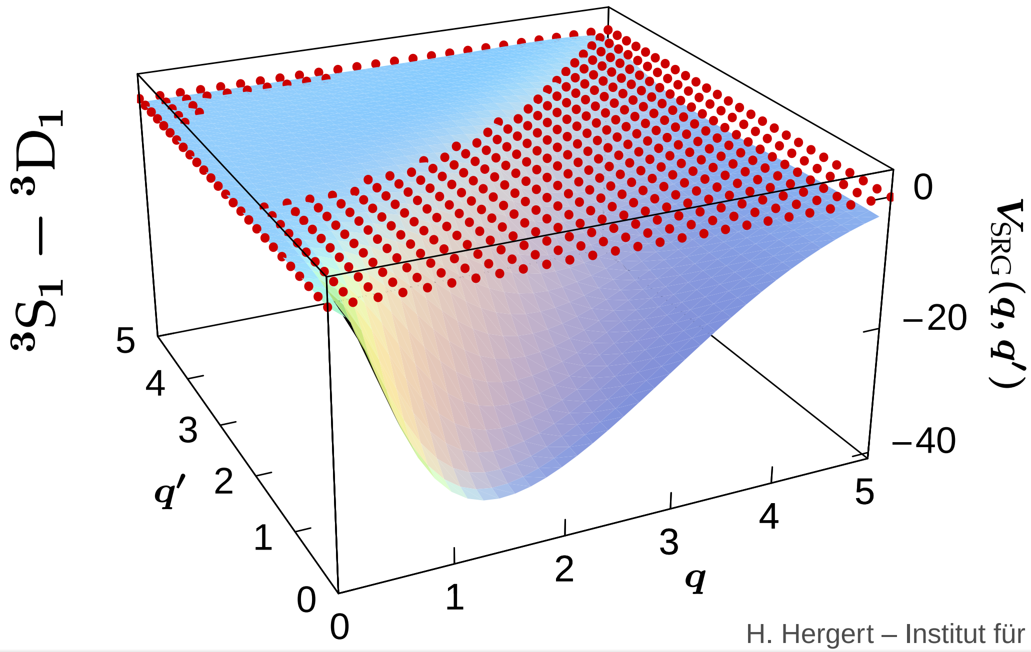


SRG Evolution: The Deuteron





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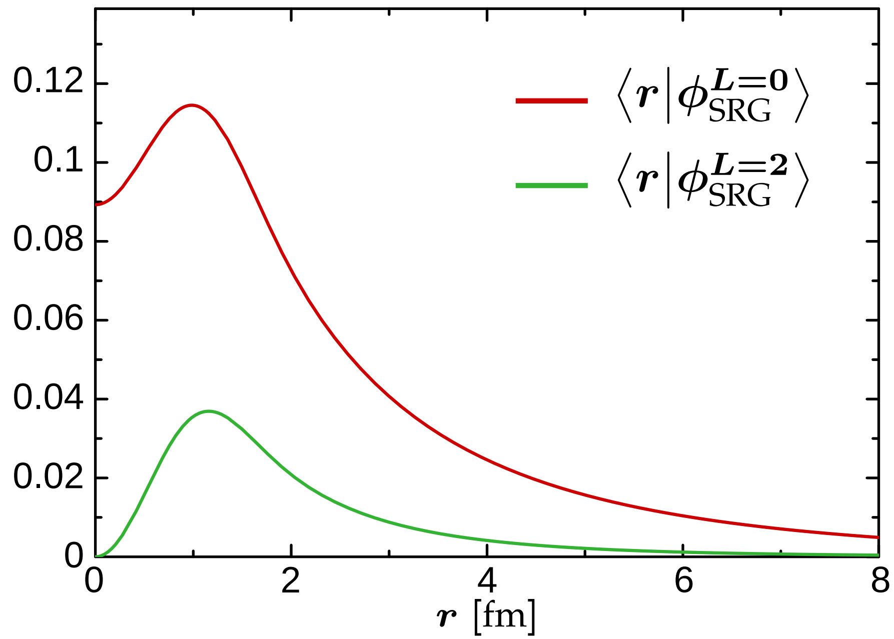

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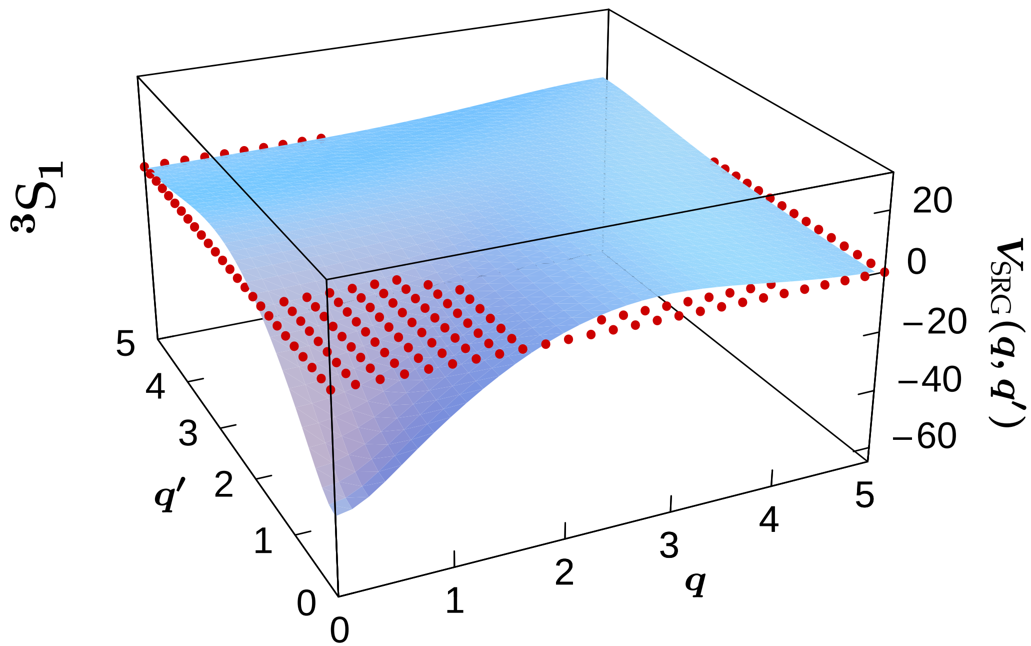

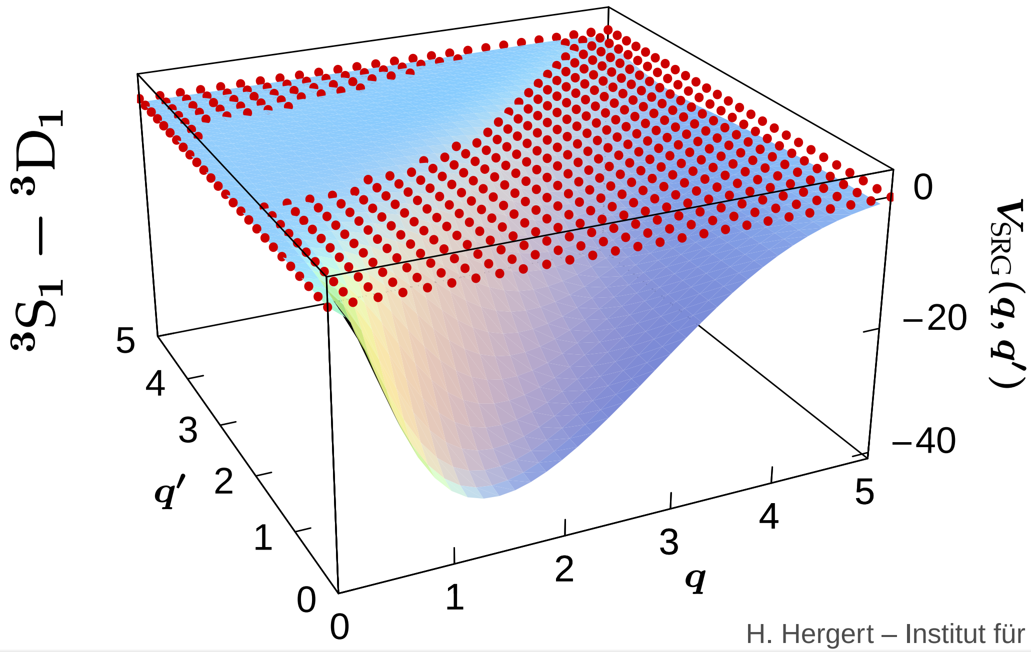

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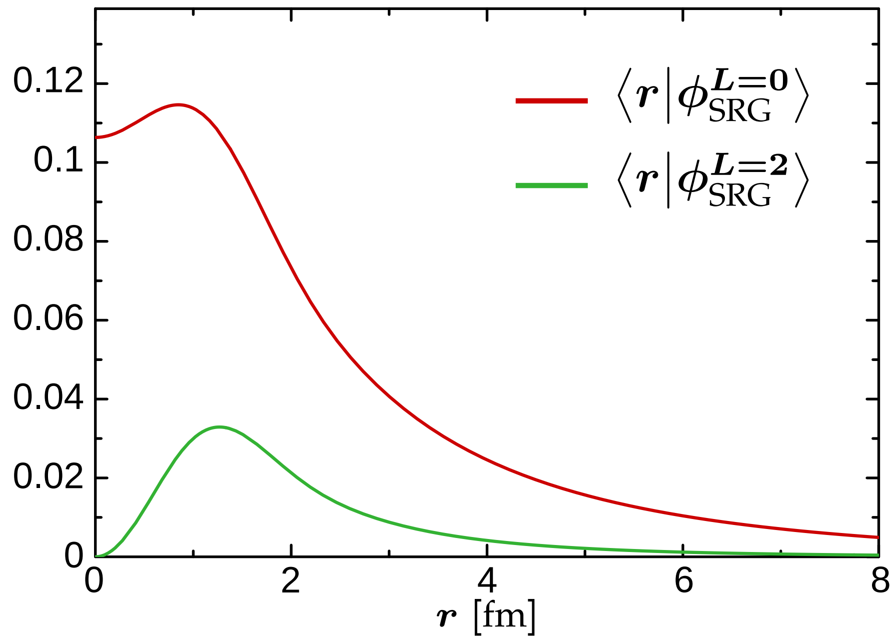

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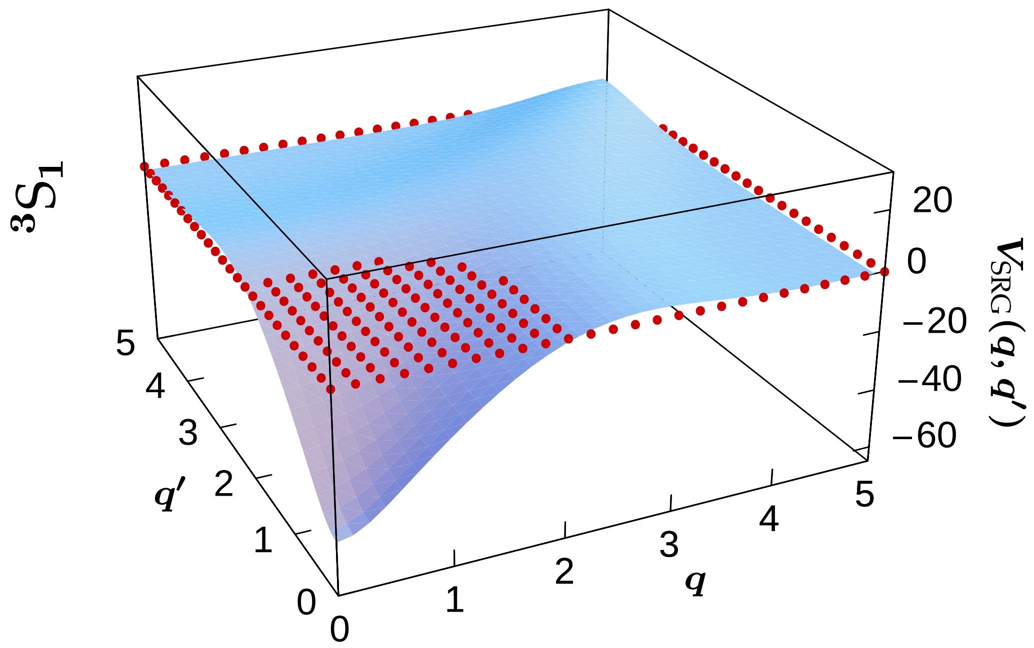

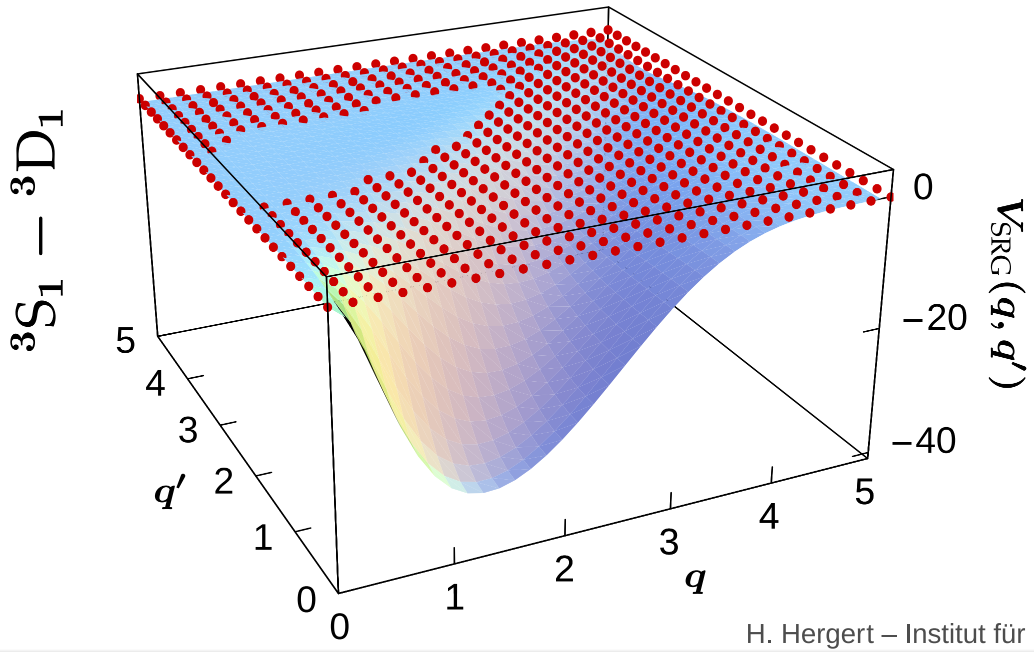

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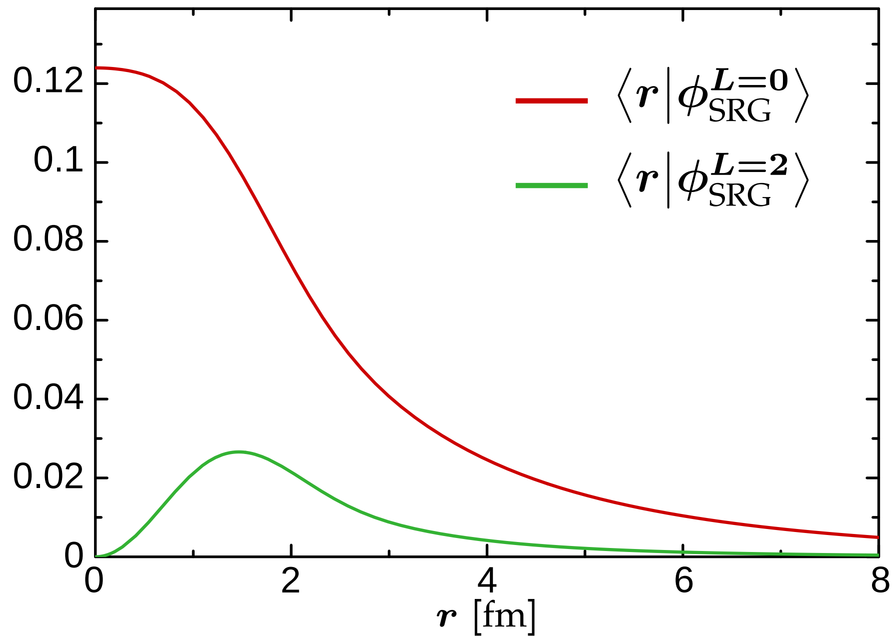

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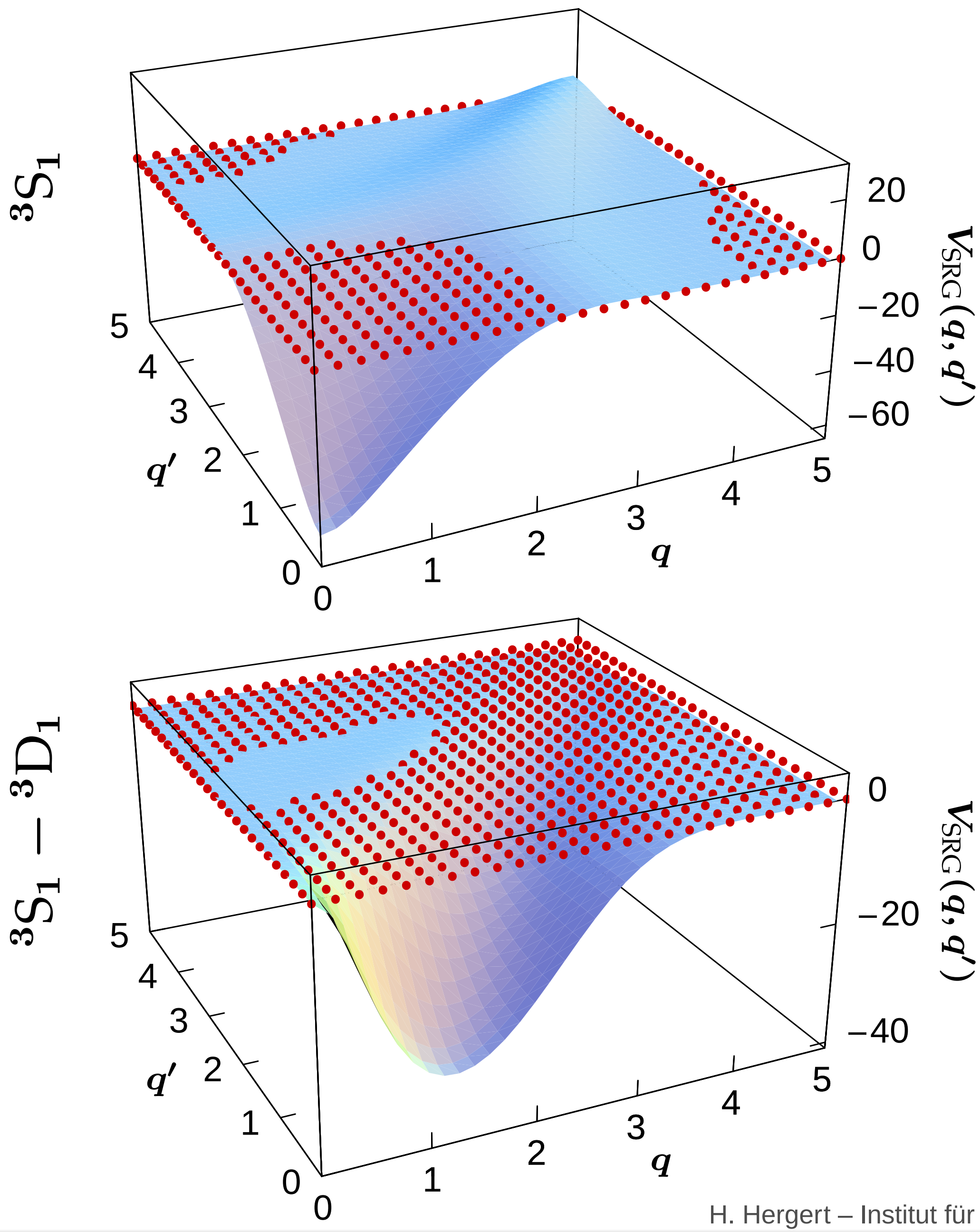

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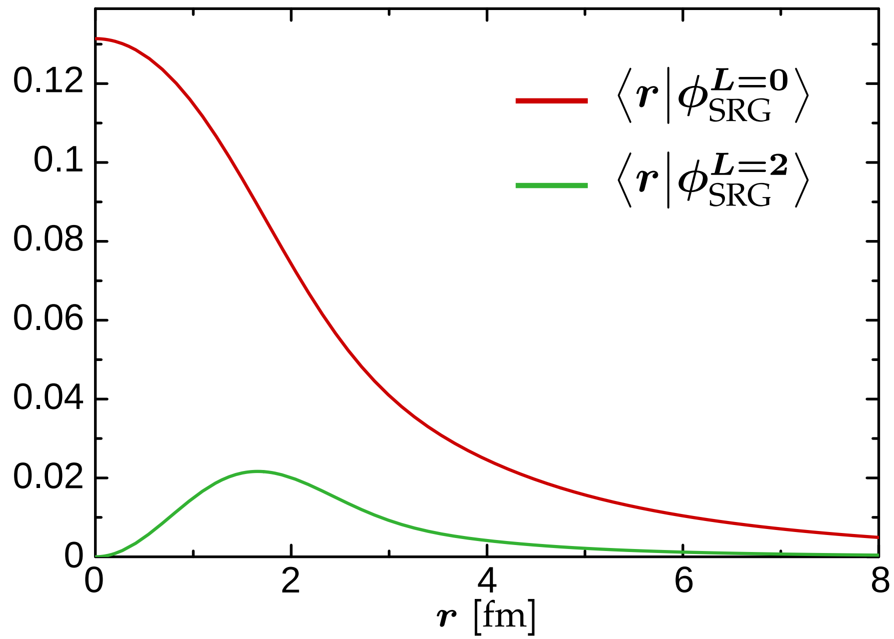

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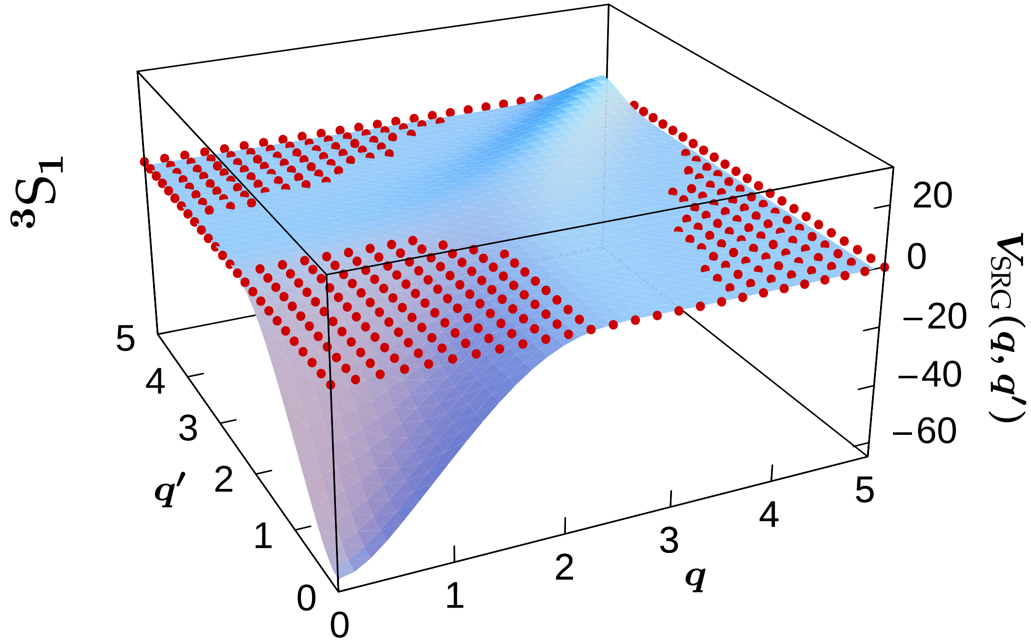

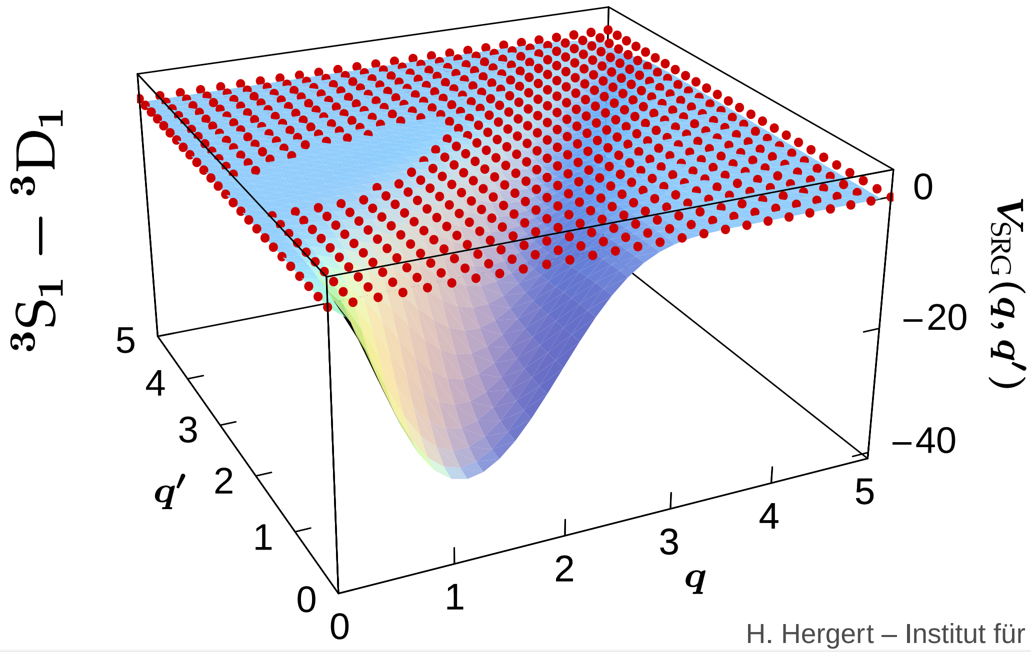

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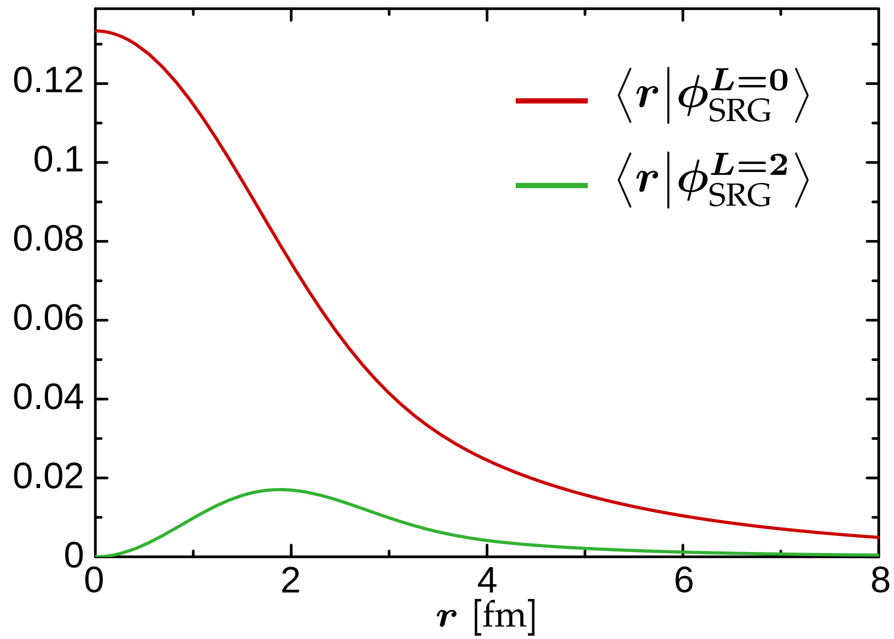
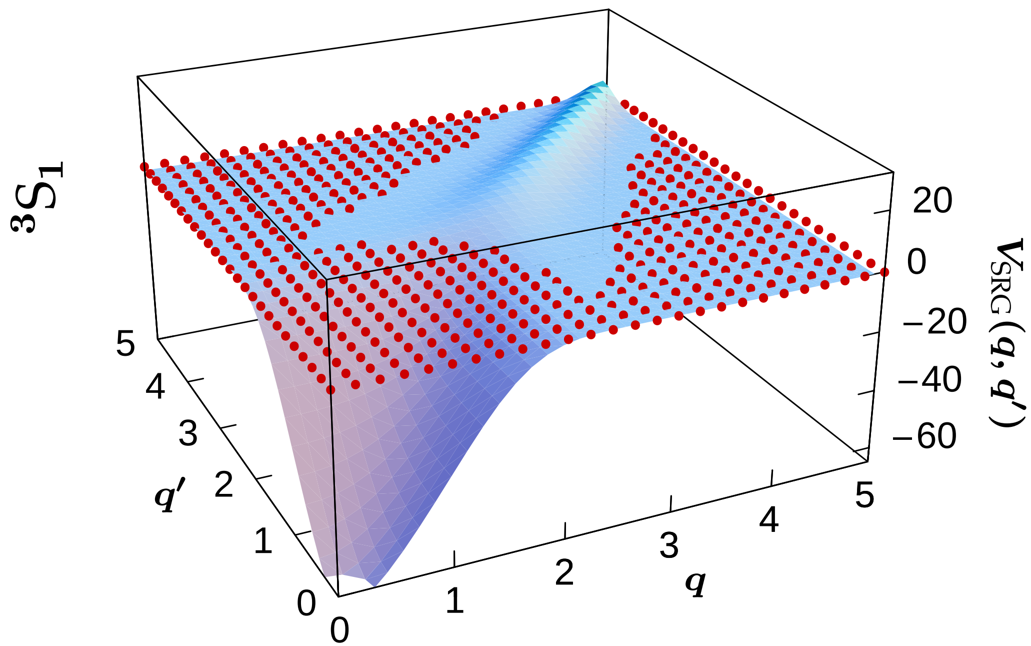
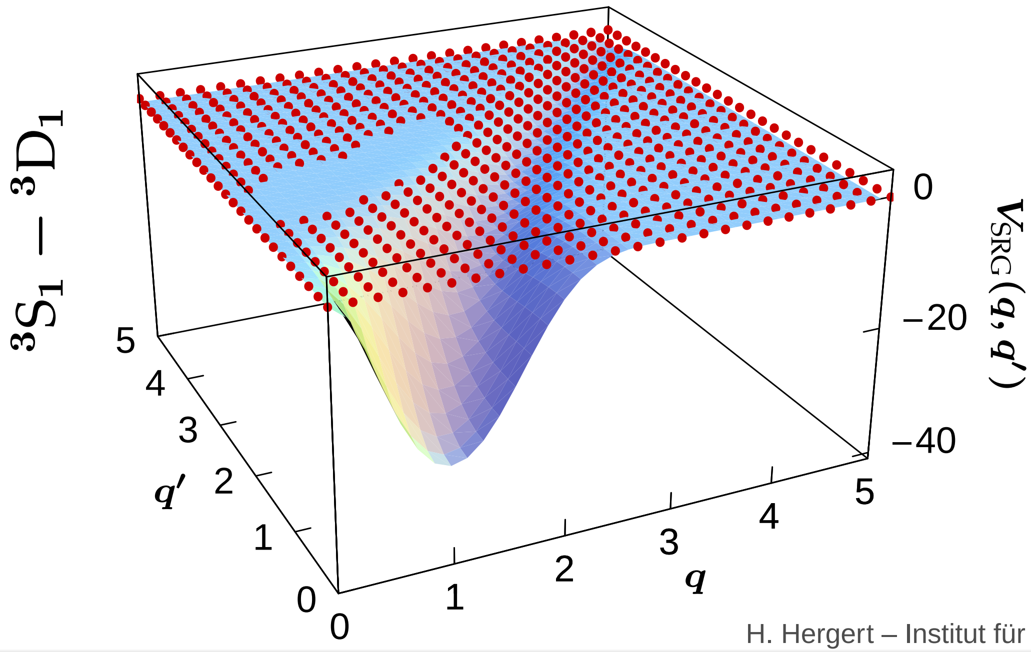
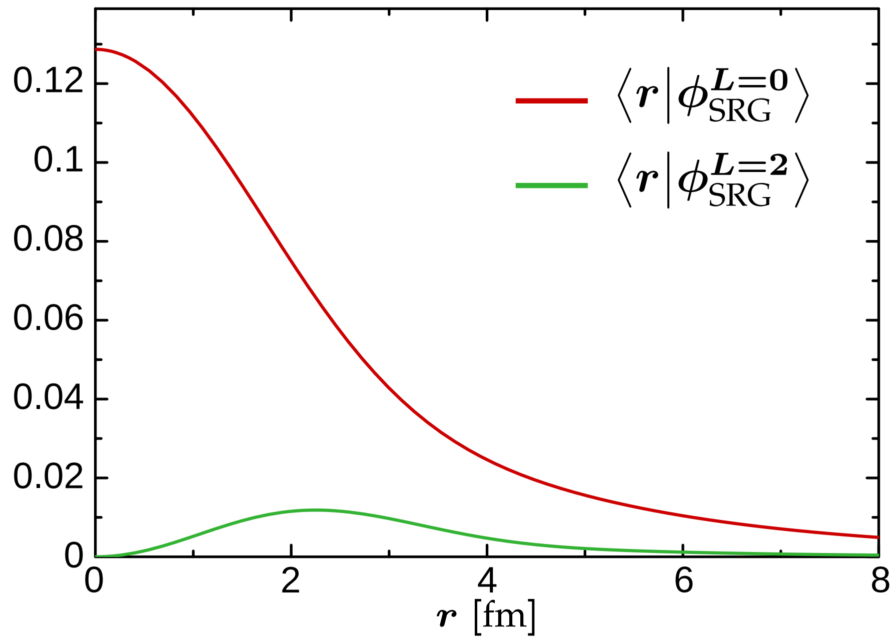


SRG Evolution: The Deuteron

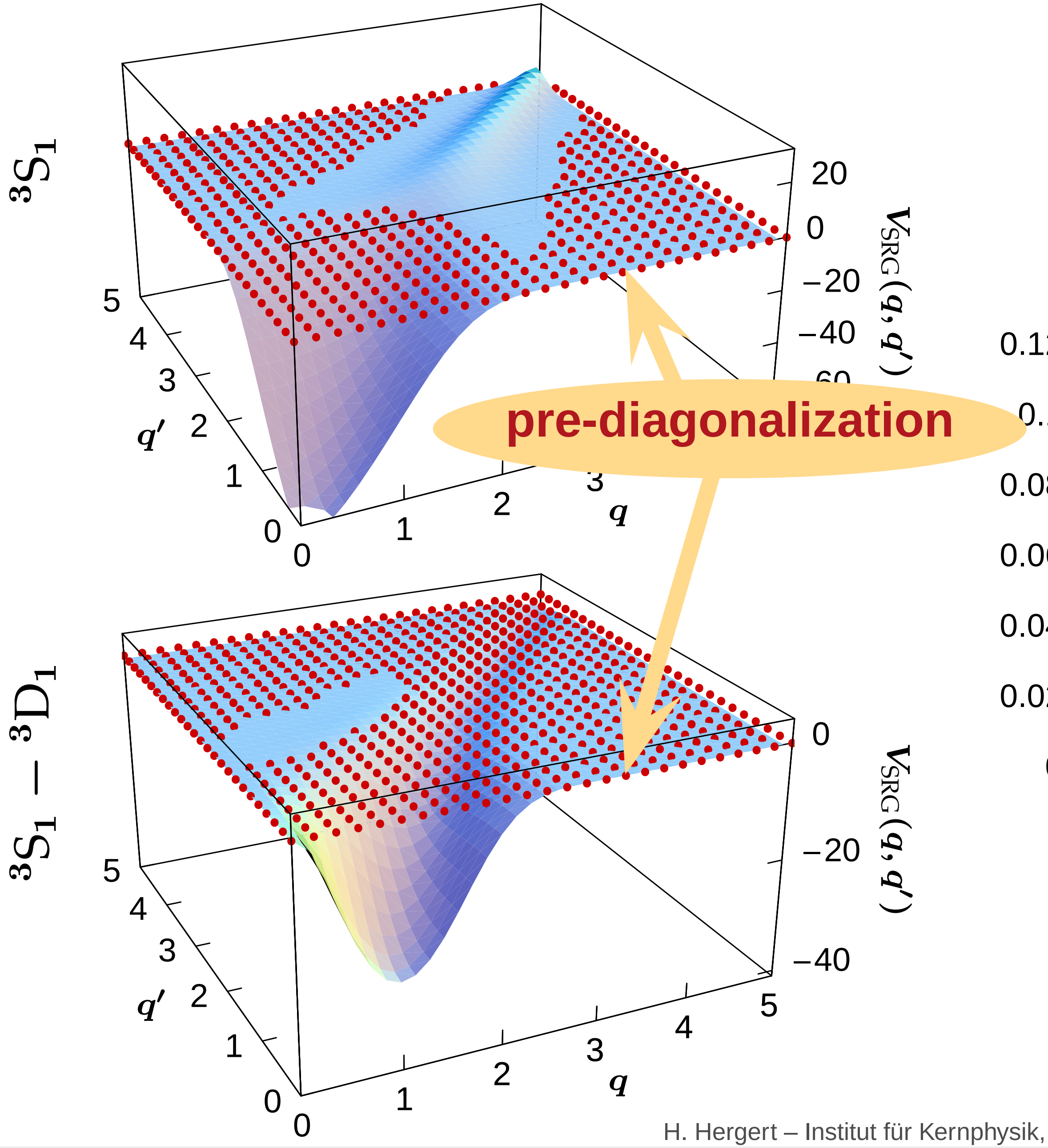




$\alpha = 0.1000\,\text{fm}^4$



SRG Evolution: The Deuteron



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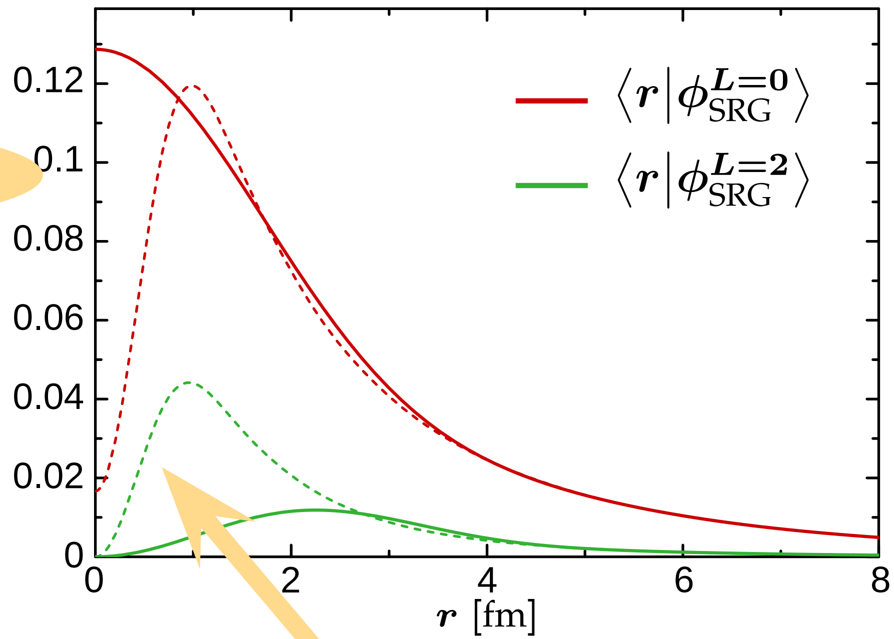
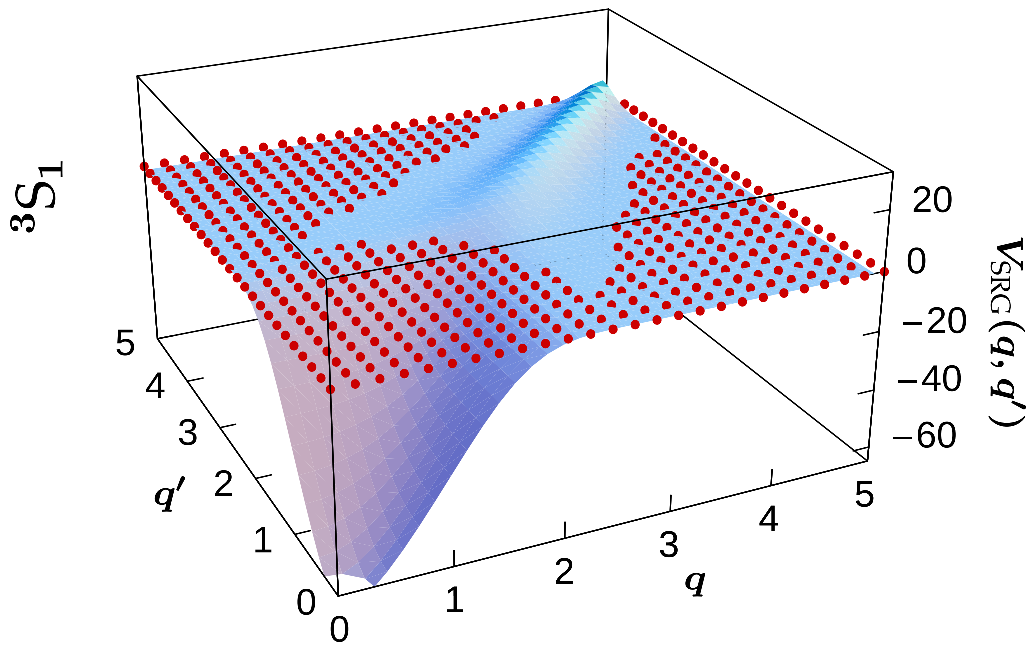
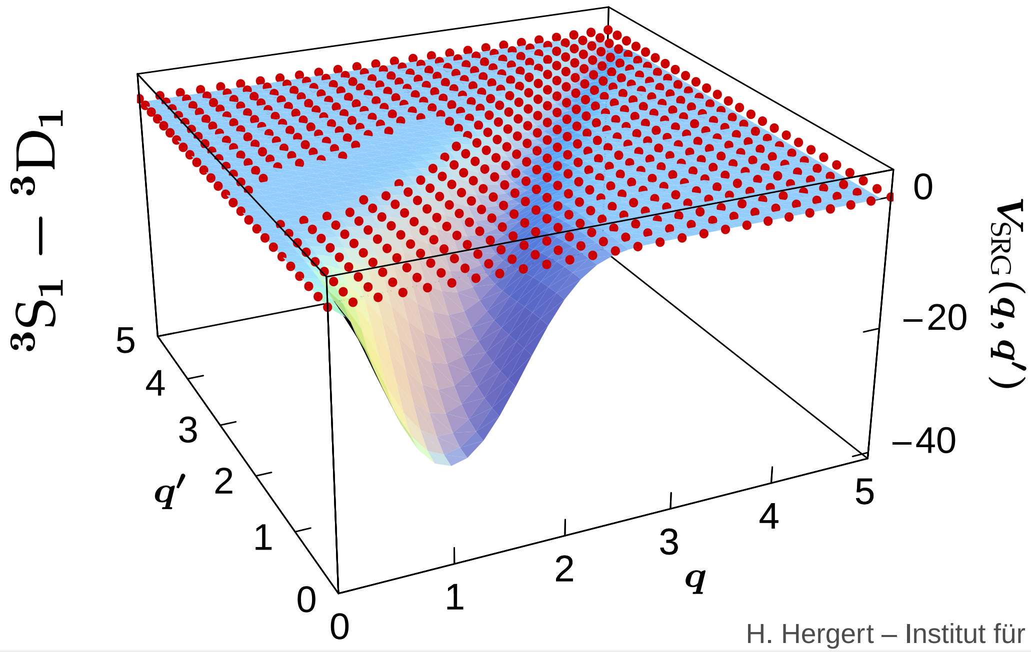


elimination of short-range correlations

SRG-Evolution: The Deuteron





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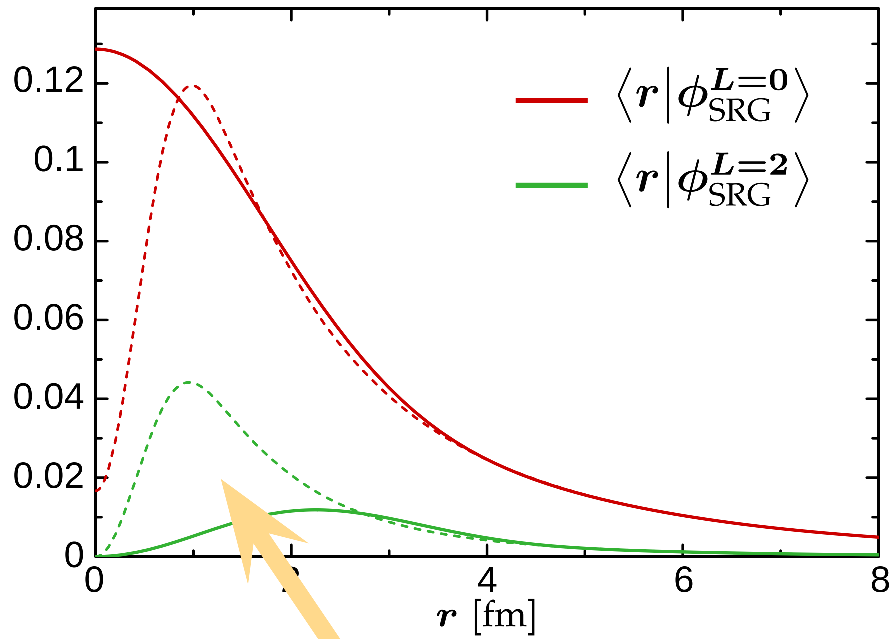
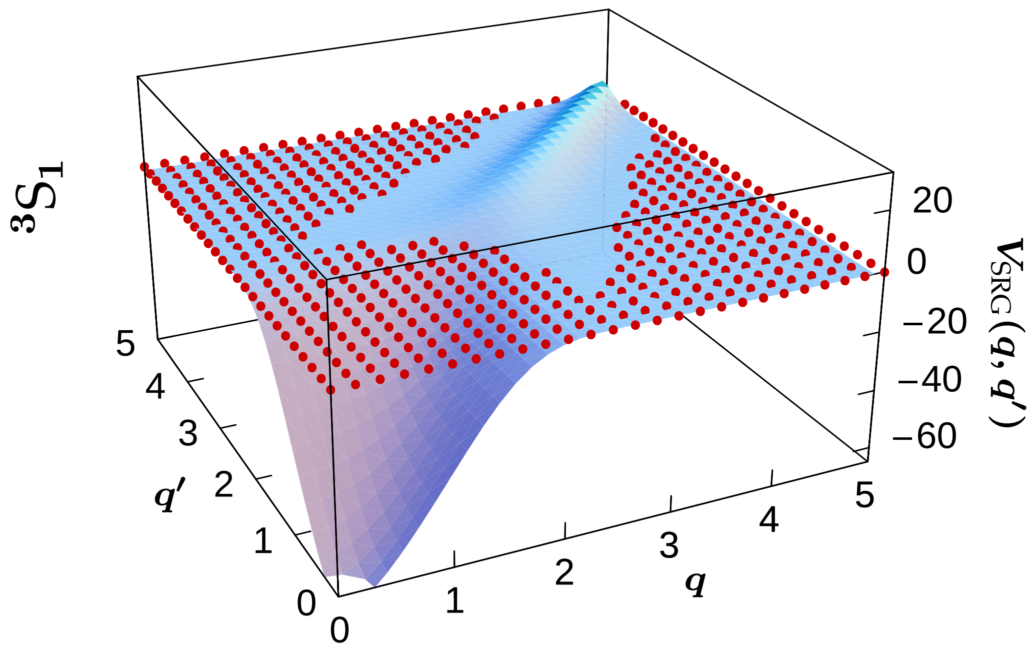
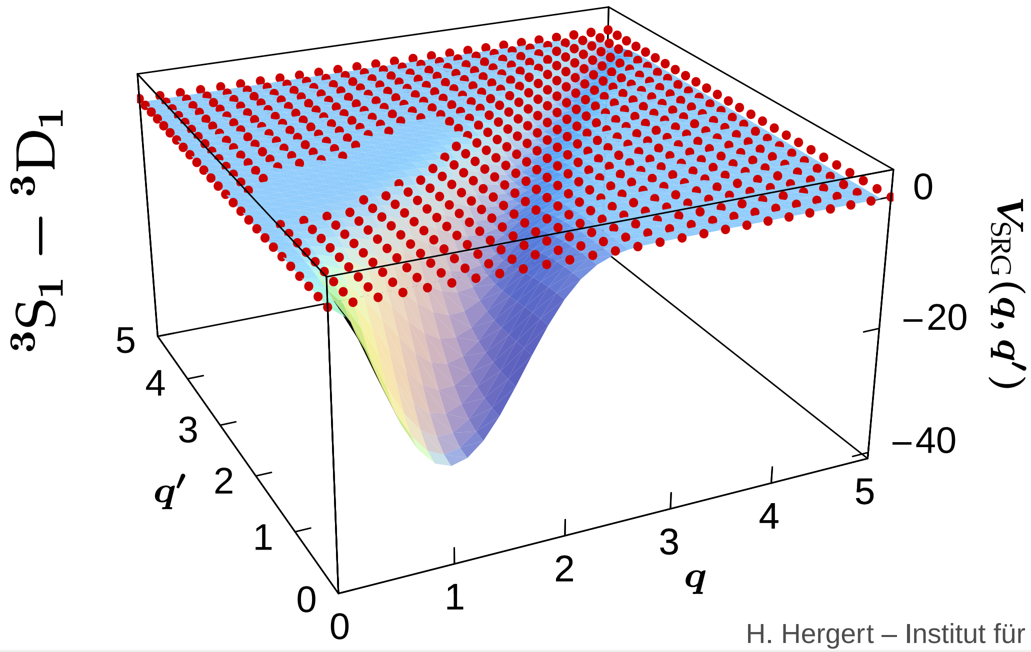


extract UCOM correlation functions

SRG-Evolution: The Deuteron





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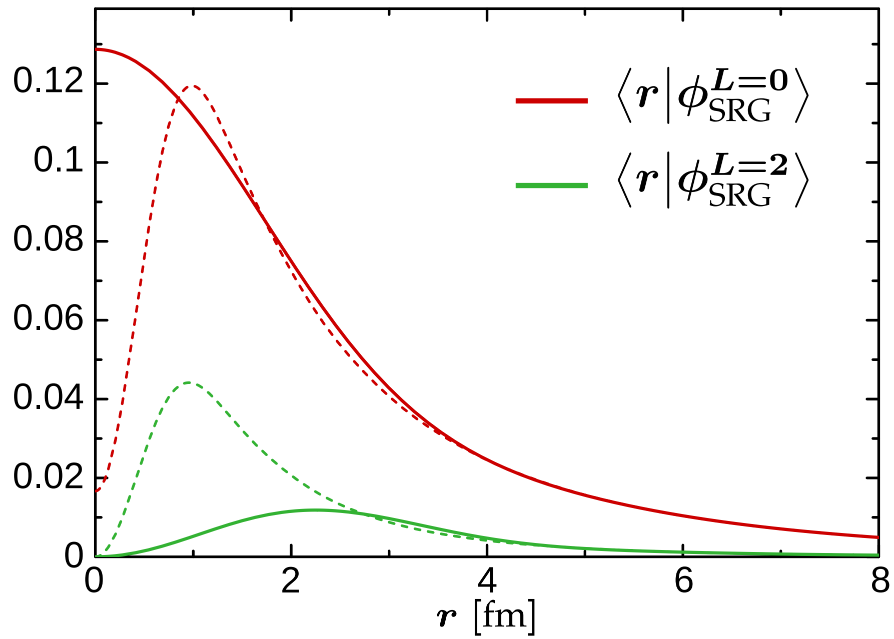
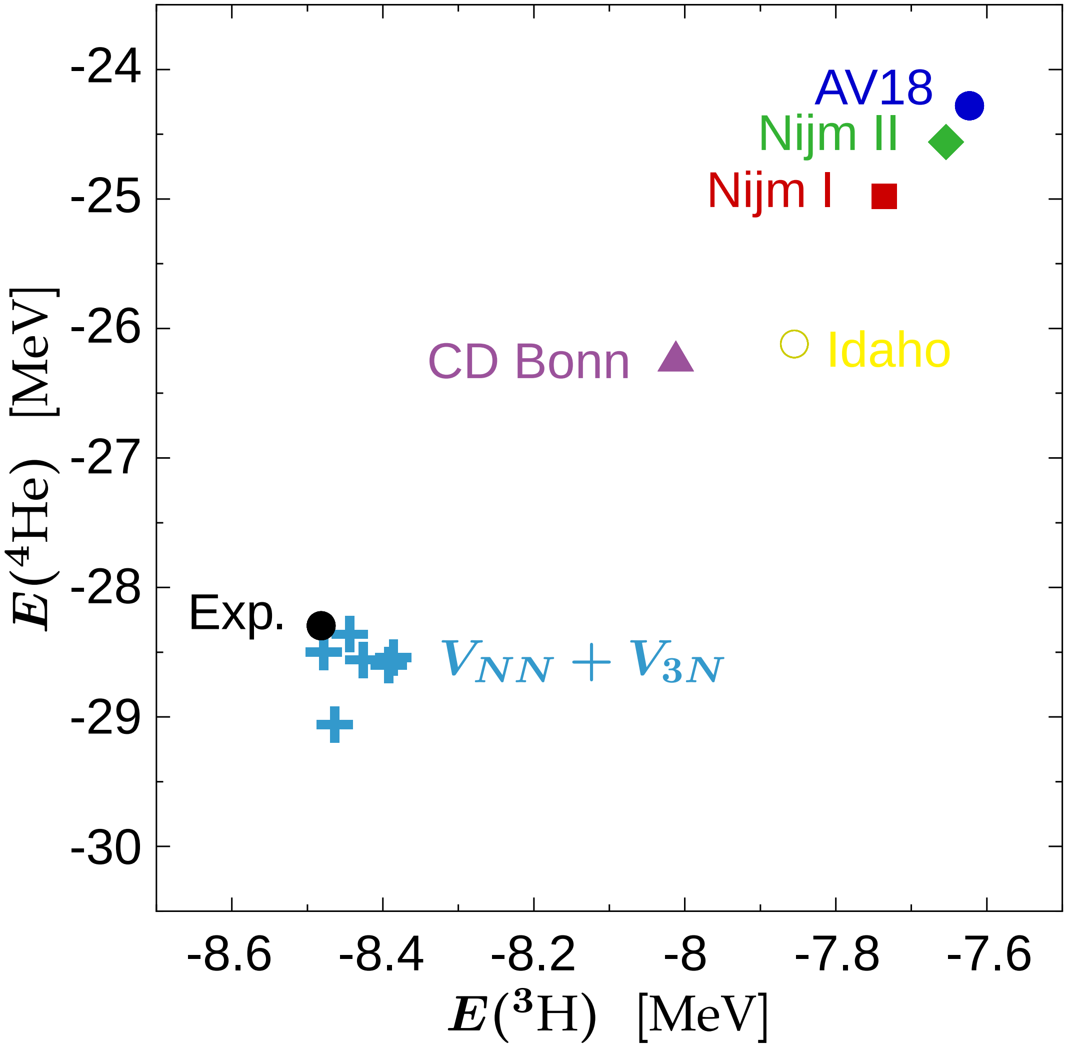


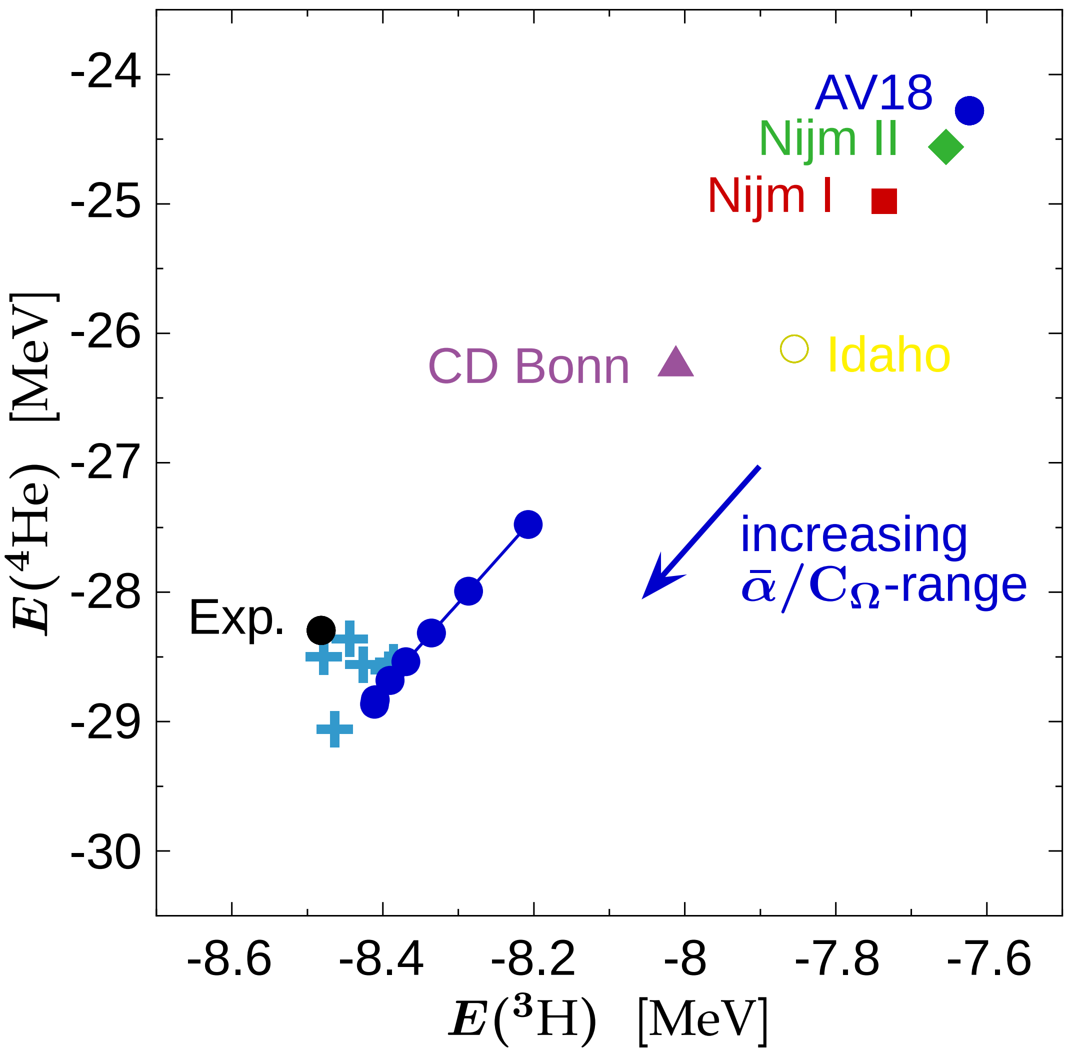
$V_{UCOM} \neq V_{SRG}$!

Tjon Line



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

Tjon Line



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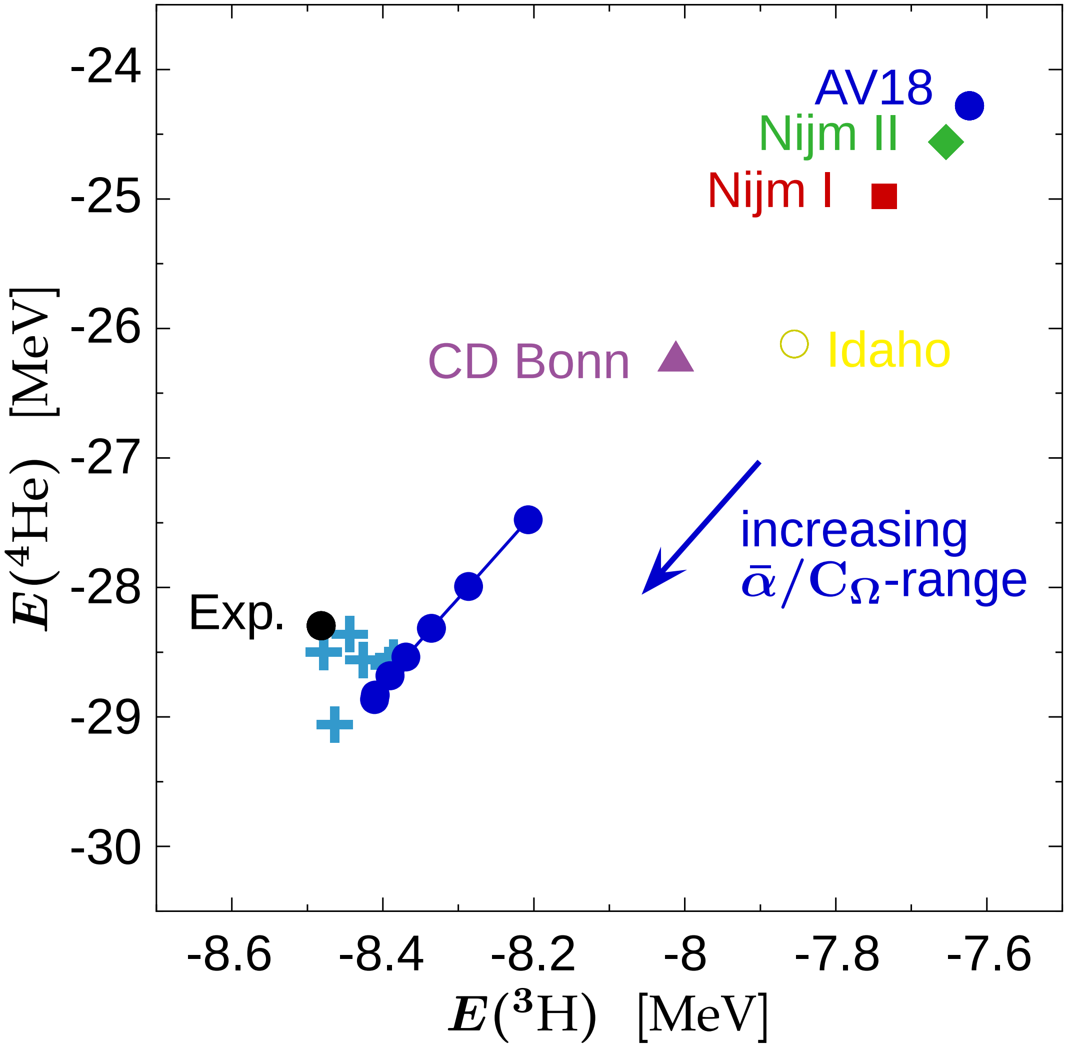

- **Tjon line**: $E(^4\mathrm{He})$ vs. $E(^3\mathrm{H})$ for phase-shift equivalent NN-interactions
- use $\bar{\alpha}$ / range of C_Ω
  - test dependence of $\mathrm{V}_{\mathrm{UCOM}}$
  - tune contributions of **net 3N force**

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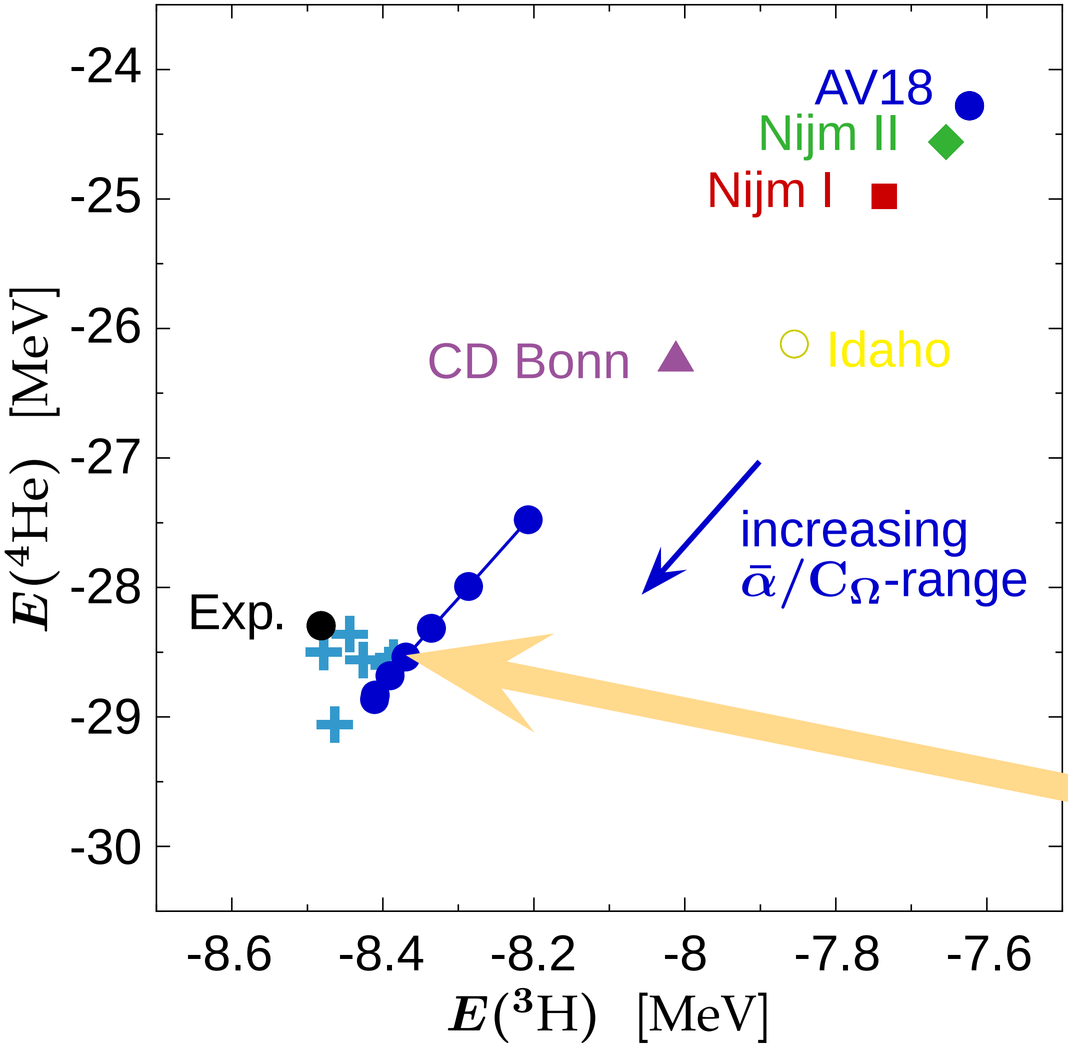
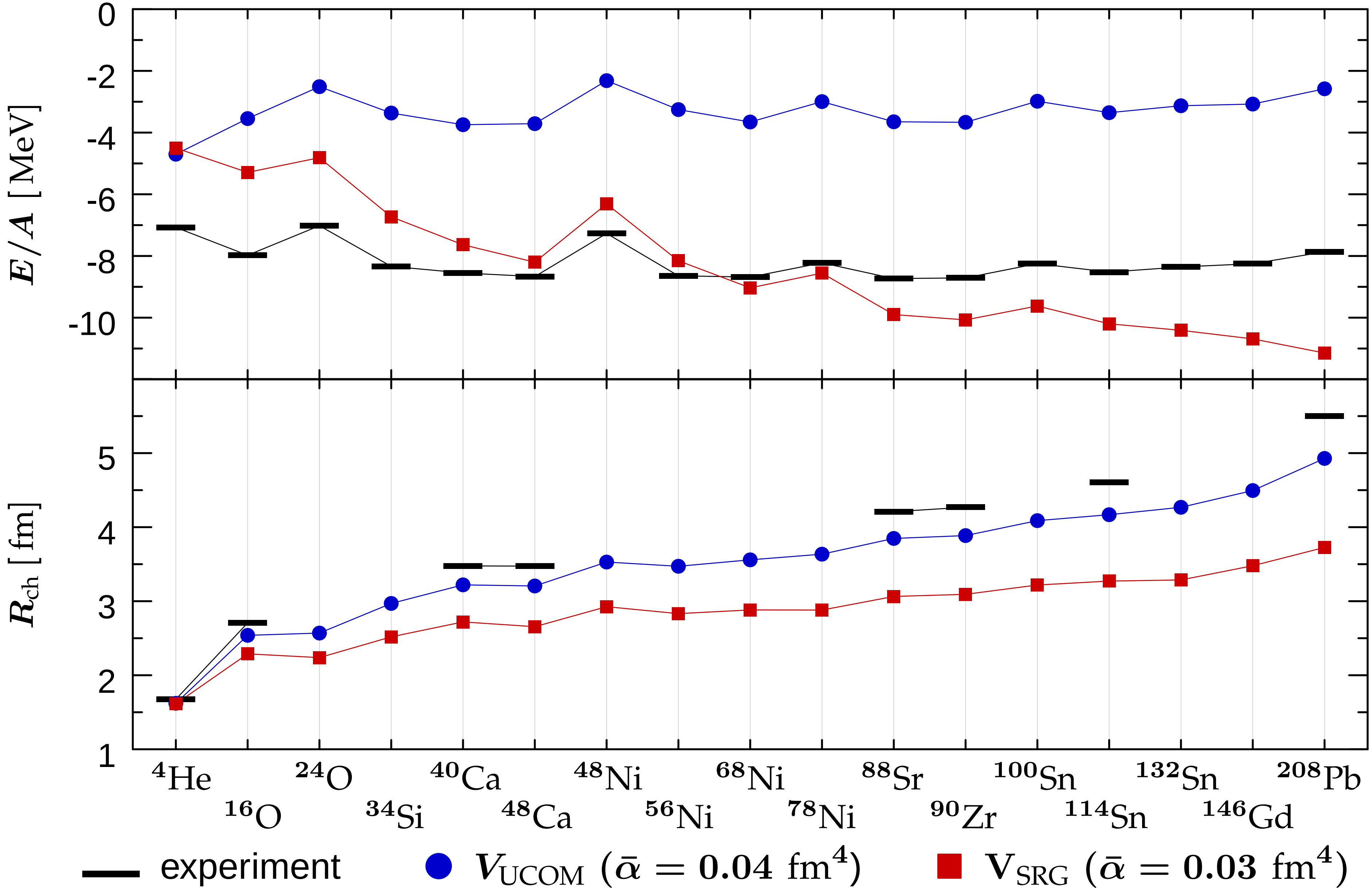


- **Tjon line**: $E(^4\text{He})$ vs. $E(^3\text{H})$ for phase-shift equivalent NN-interactions
- use $\bar{\alpha}$ / range of C_Ω to
  - test dependence of V_{UCOM}
  - tune contributions of **net 3N force**

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

Hartree-Fock and Many-Body Perturbation Theory

Hartree-Fock: UCOM vs. SRG



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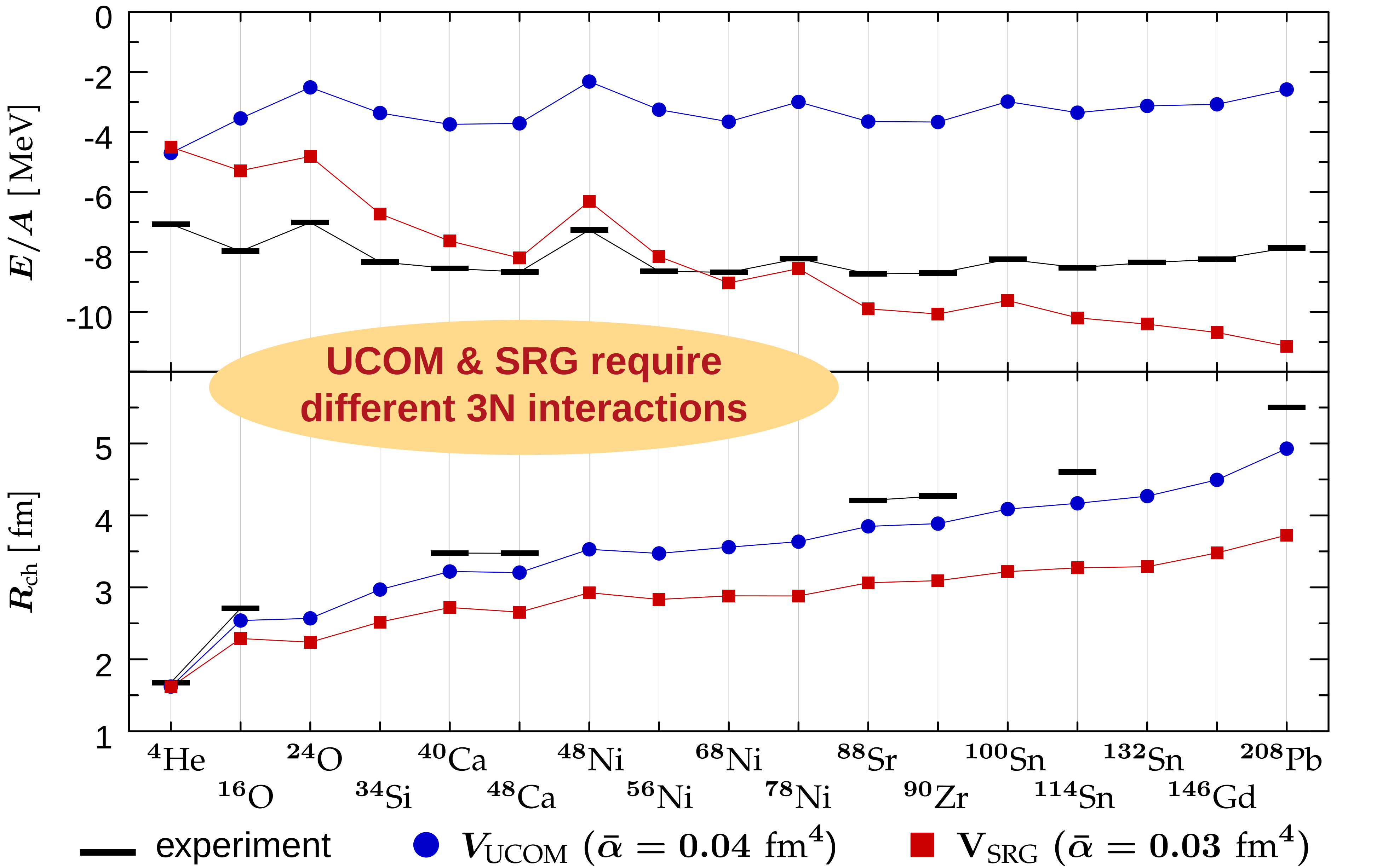
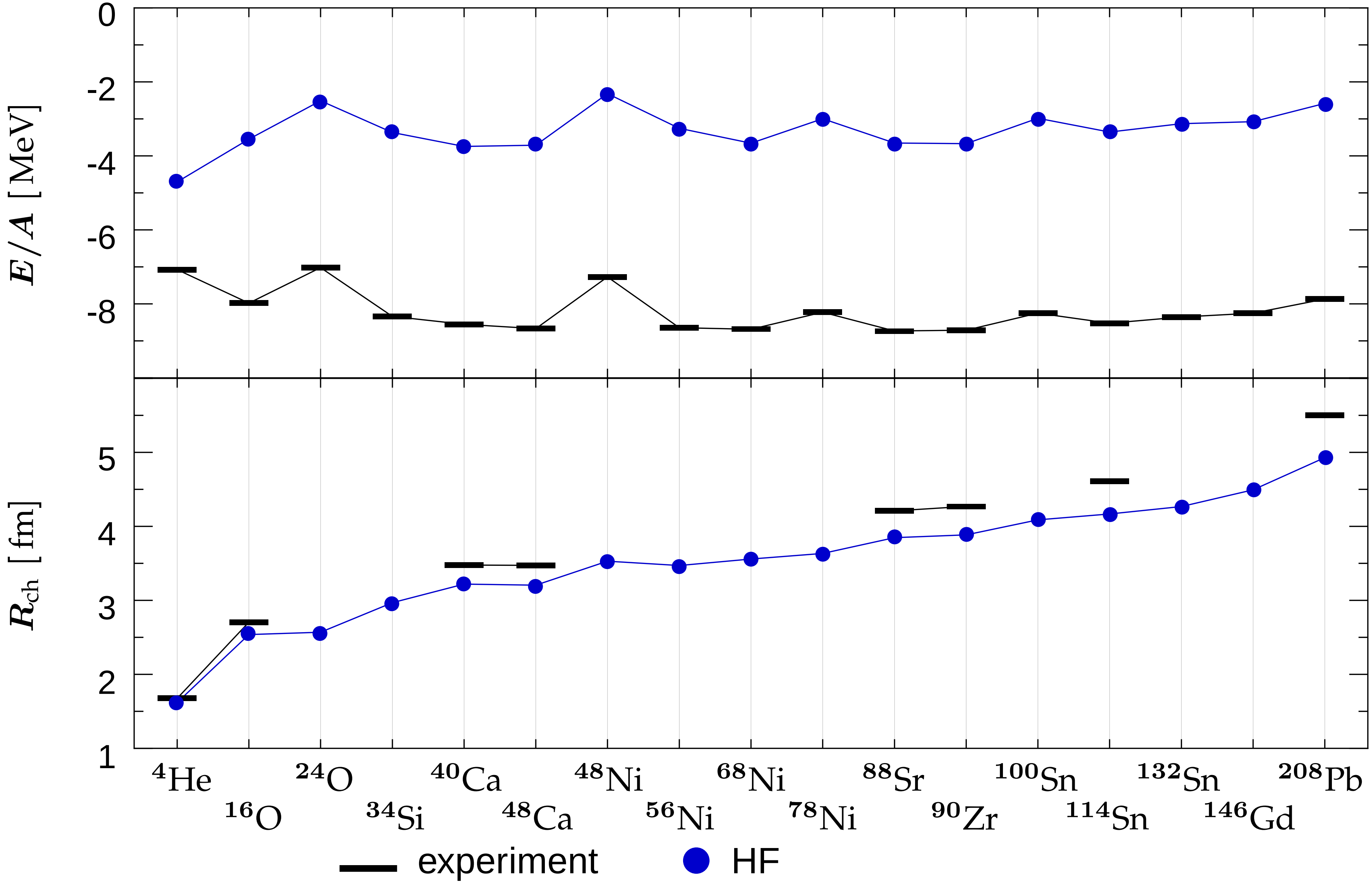


Hartree-Fock & Perturbation Theory



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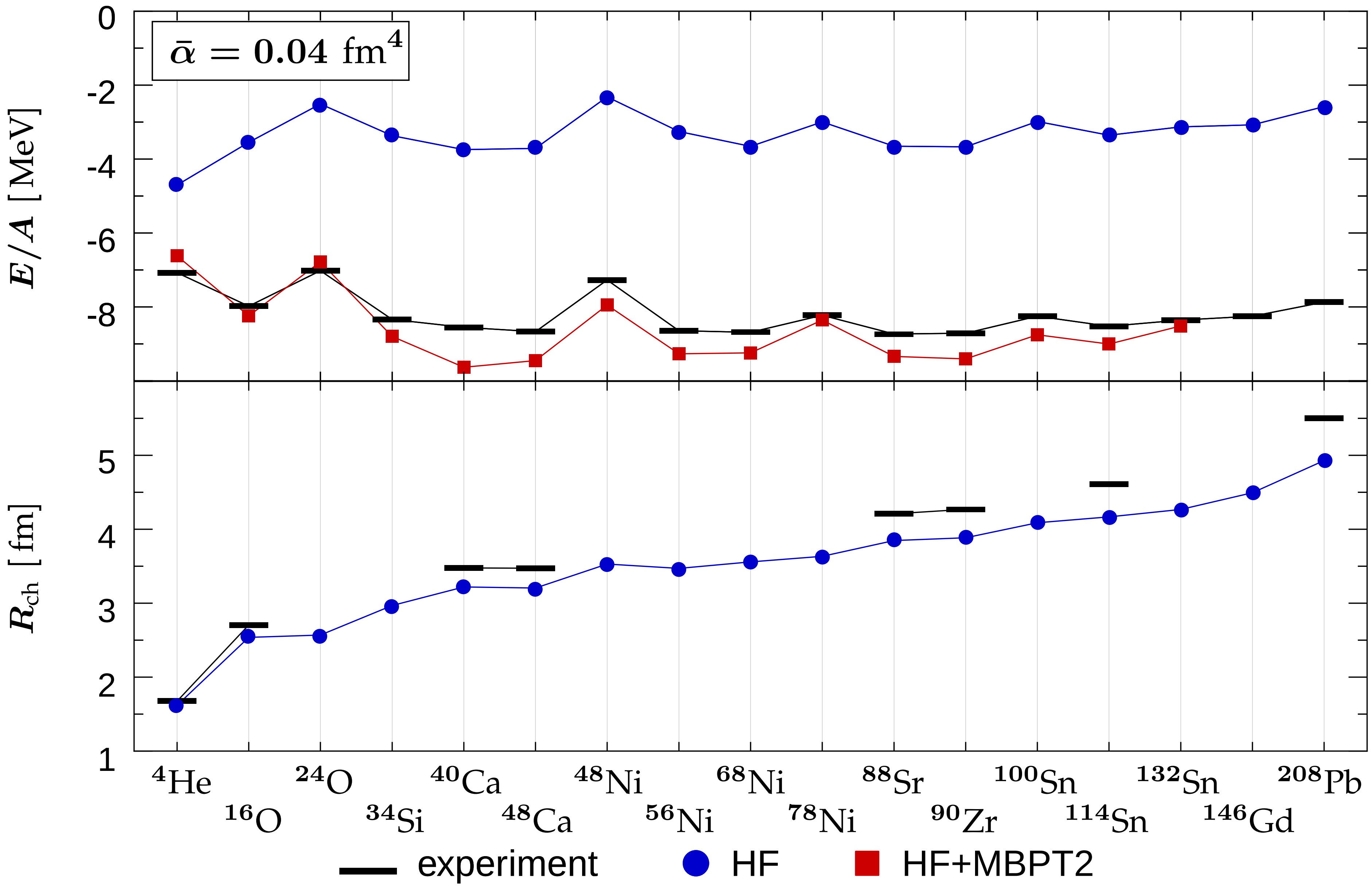

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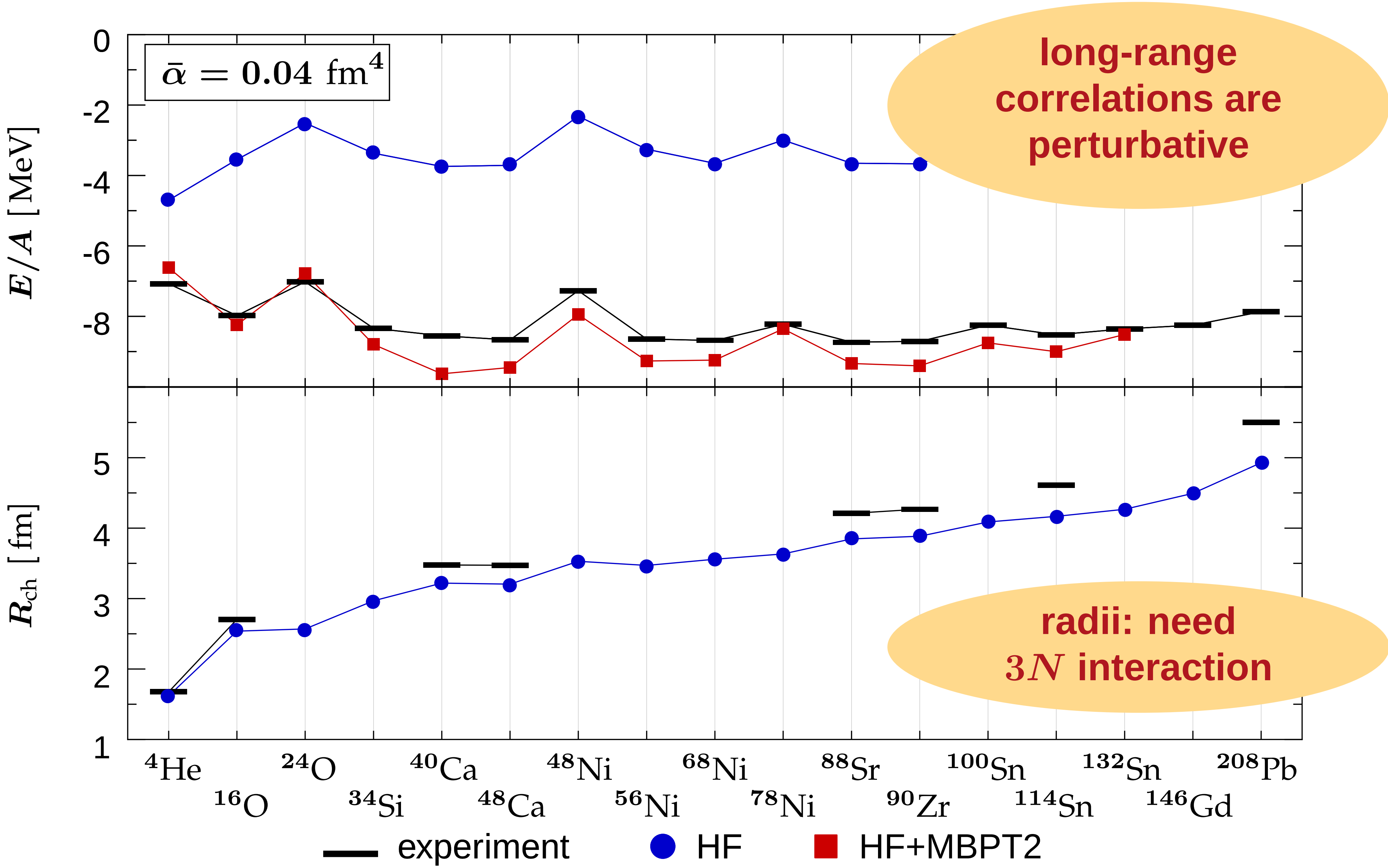

Pairing in the UCOM Framework

Hartree-Fock-Bogoliubov

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

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

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

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

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

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Energy

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

HFB Equations

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

Gap Definitions

Gaps from Experiment

- **binding energy differences**; e.g.

$$\Delta^{(3)}(N) = (-1)^N \frac{1}{2}\left(E(N+1) - 2E(N) + E(N-1)\right)$$

Common Definitions of Theoretical Gap

- lowest canonical state: Δ_μ for state with minimal canonical E_μ
- "correlated" average ($\sim$ averaged **pairing energy**)

$$\langle \Delta \rangle = \frac{\sum_\mu \Delta_\mu u_\mu v_\mu}{\sum_\mu u_\mu v_\mu}$$

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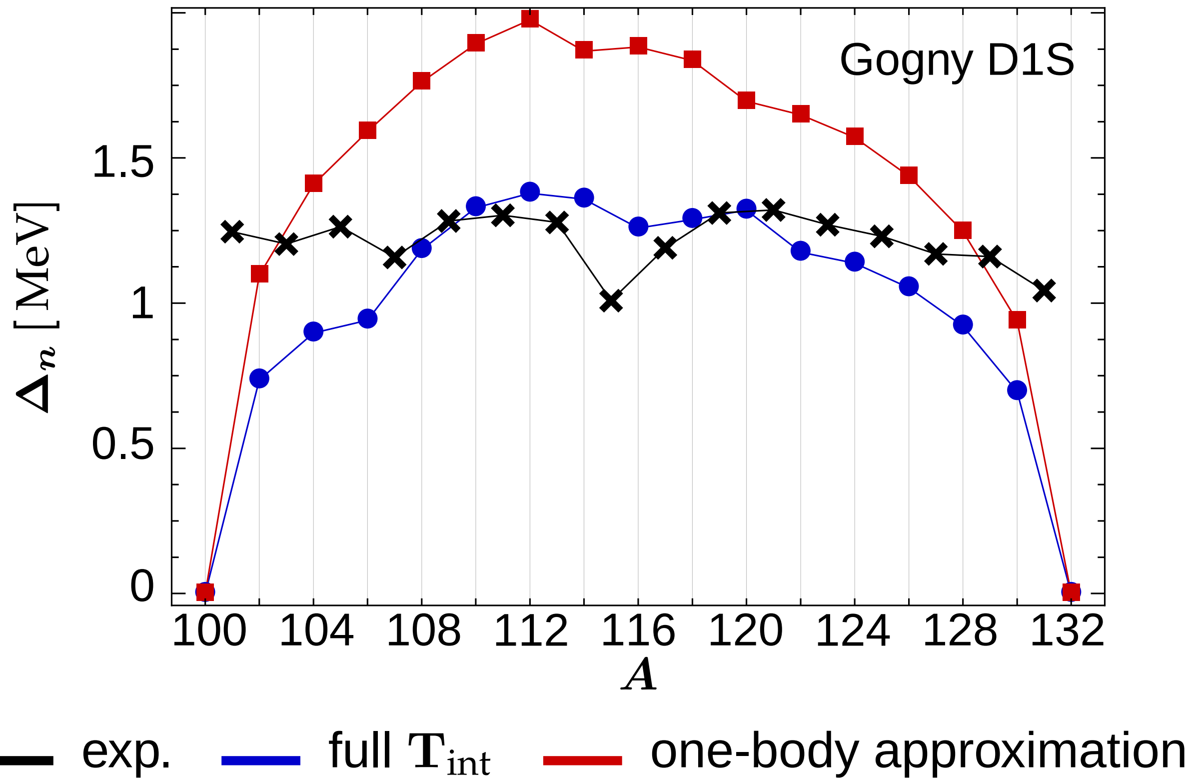
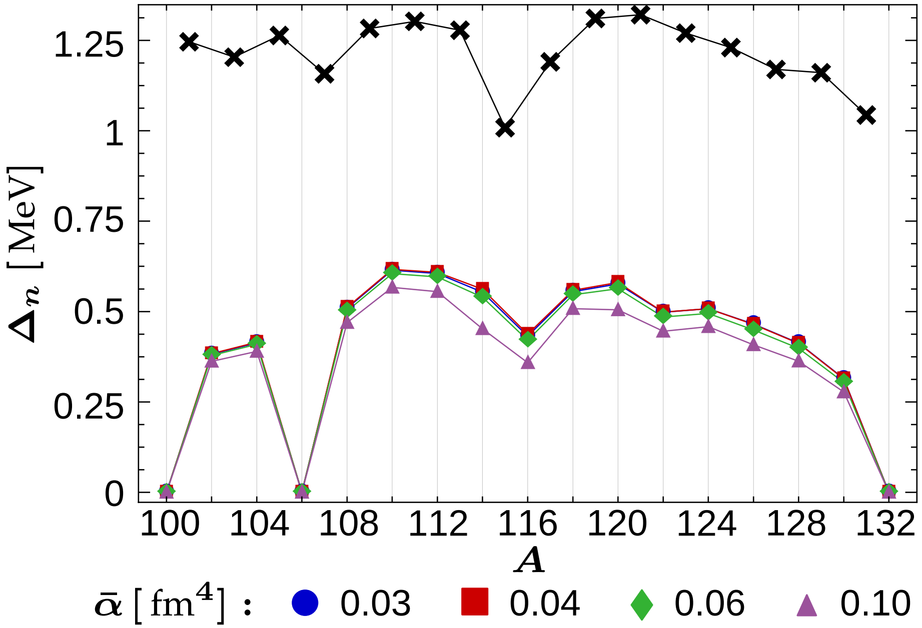
✘ **Such theoretical gaps are not observables!**

Center-of-Mass Correction



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

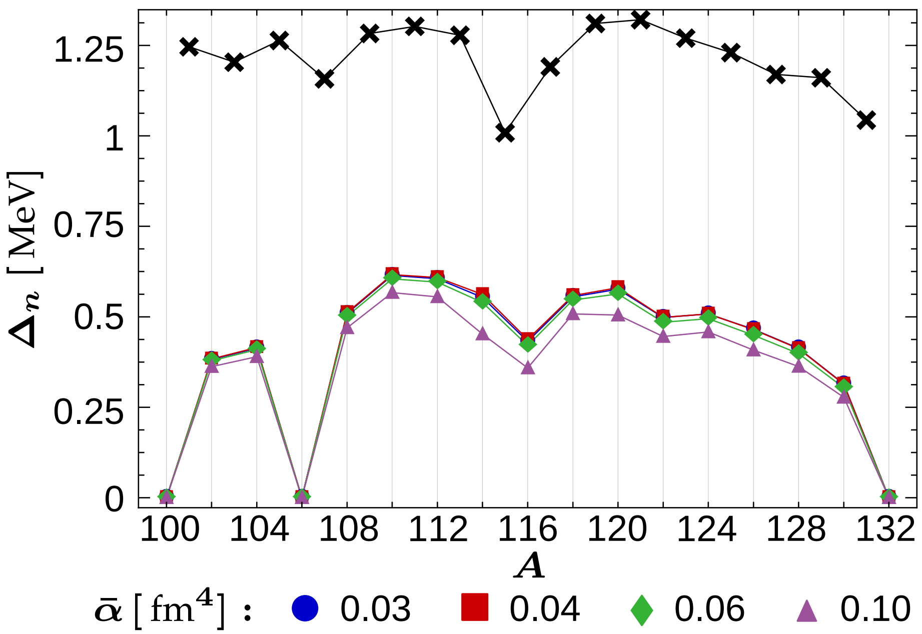
V_{UCOM} as a Pairing Force



variation of $\bar{\alpha}$

- small effect due to **stability** of $^1S_0$ matrix elements
- residual reduction of gaps through **partial wave mixing** by Talmi transformation

V_{UCOM} as a Pairing Force



variation of $\bar{\alpha}$

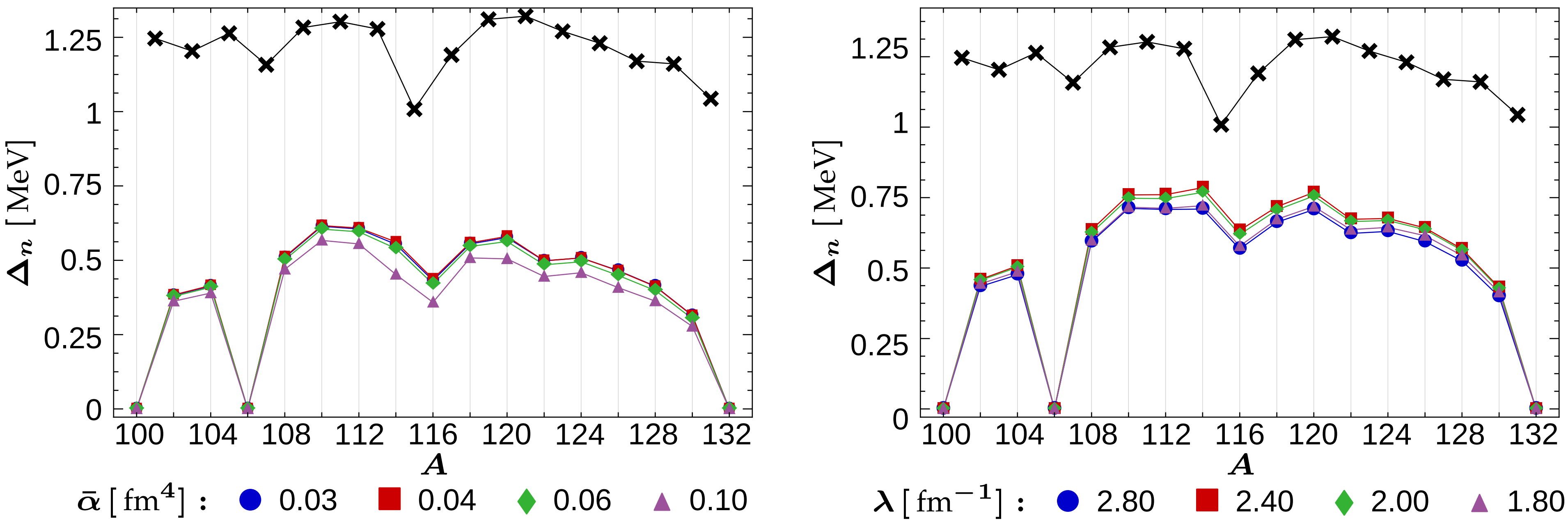
- small effect due to **stability** of $^1S_0$ matrix elements
- residual reduction of gaps through **partial wave mixing** by Talmi transformation

- $^1S_0$ gap in nuclear matter essentially determined by **phase shift**: expect similar gaps for phase-shift equivalent interactions in finite nuclei

✔ Gogny D1S/SLy4 + AV14 pairing
(e.g. F. Barranco et al., EPJ A21 (2004), 57)

✘ $\sim 50\%$ smaller than SLy4 + $V_{\text{low-}k}$ study by Lesinski & Duguet
(arXiv: 0809.2895)

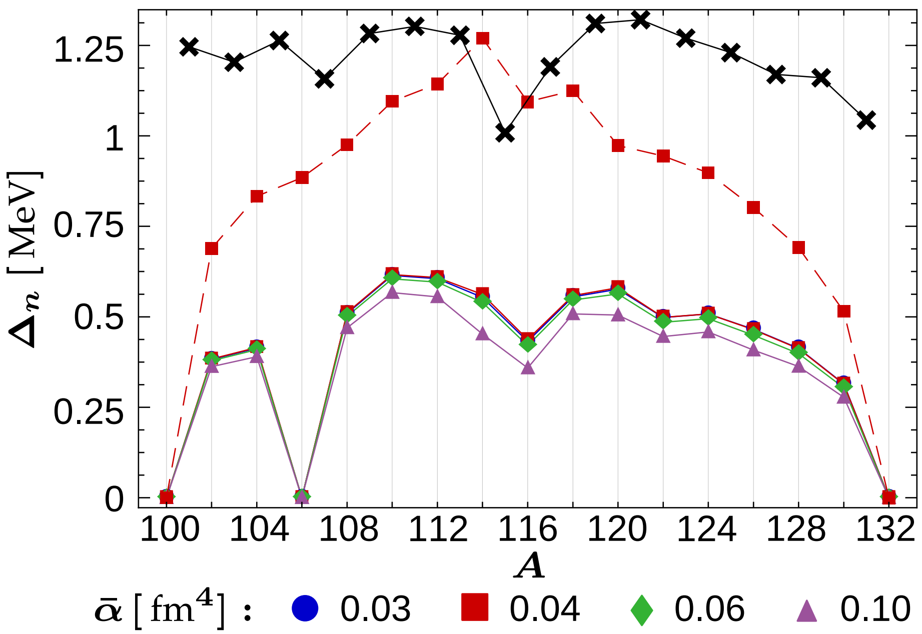
V_{UCOM} vs. V_{SRG}

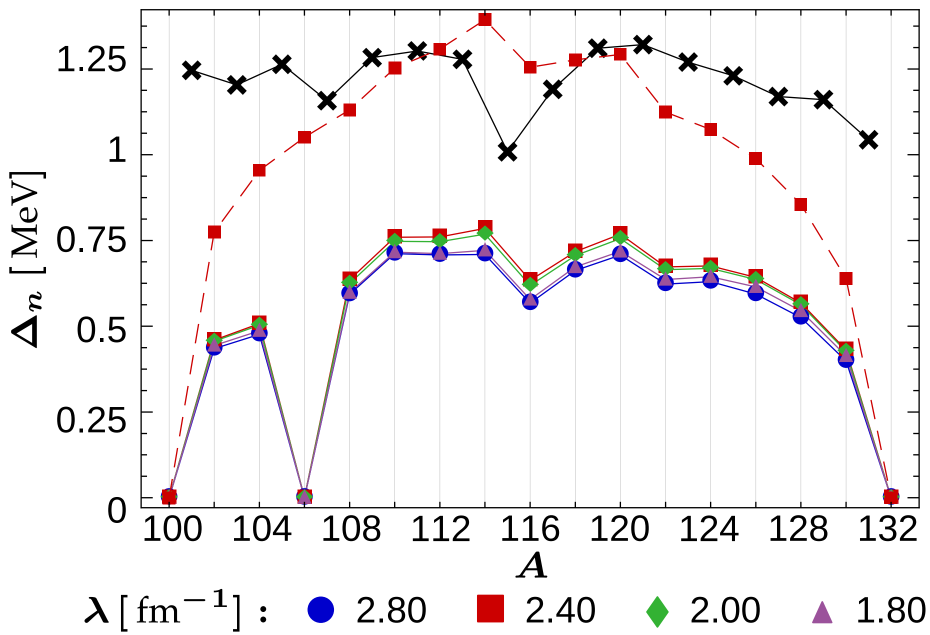


- compare with V_{SRG} (similar properties as $V_{\text{low-}k}$)

☞ **center-of-mass treatment ?**

V_{UCOM} vs. V_{SRG}





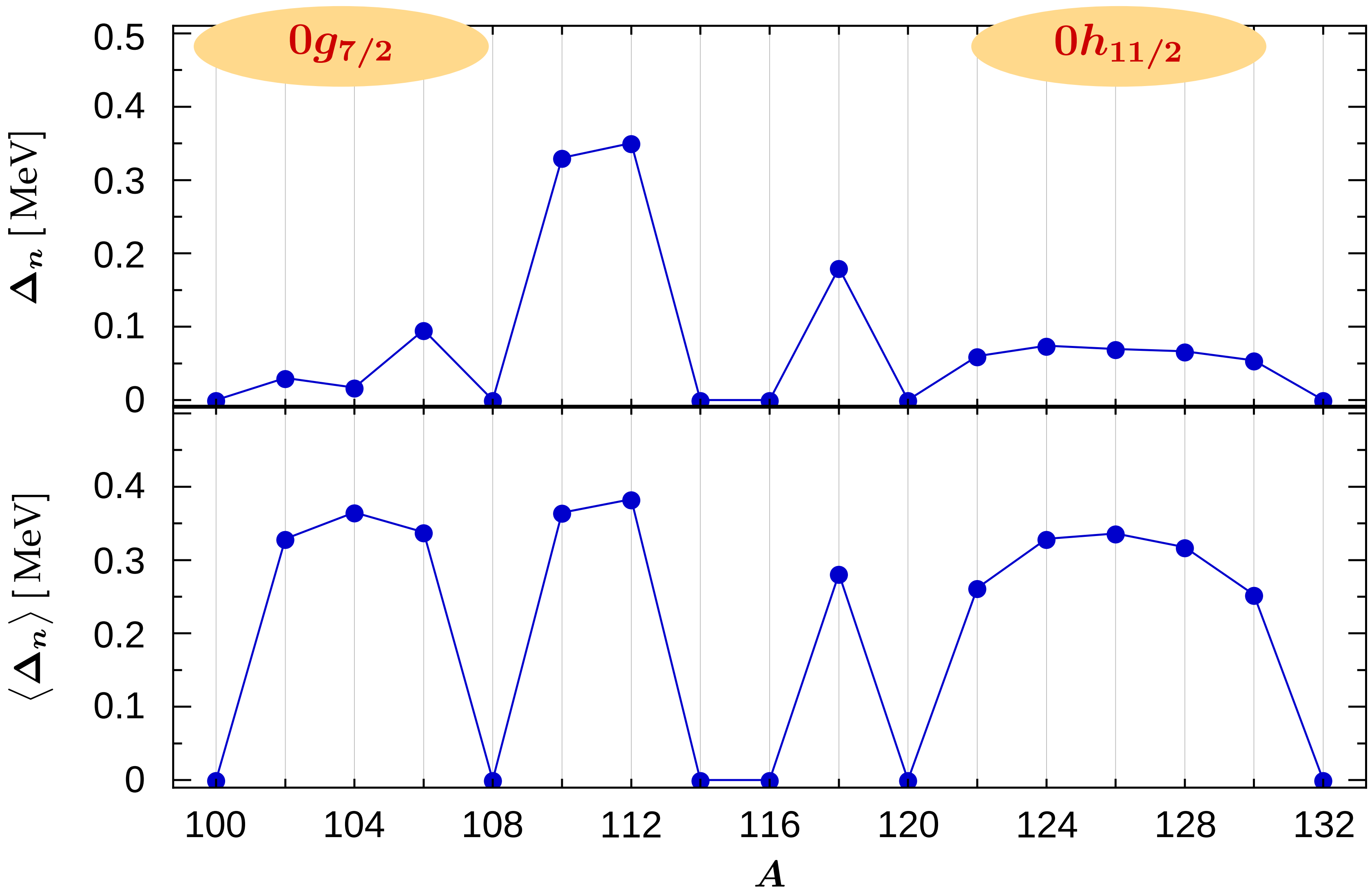
- compare with V_{SRG} (similar properties as $V_{\text{low-}k}$)

✔ different center-of-mass treatment explains discrepancy

Pairing in the UCOM Framework

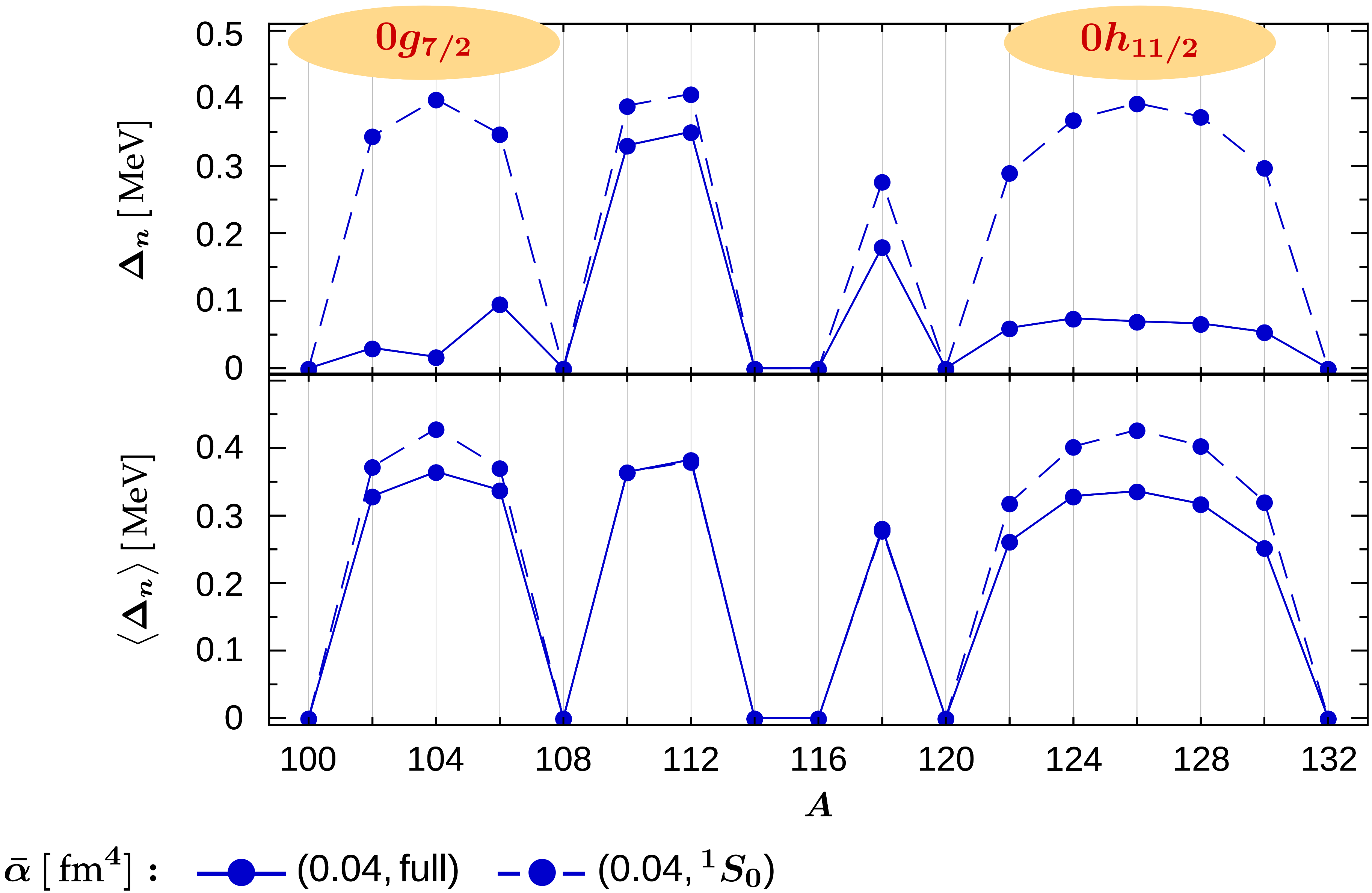
Fully Self-Consistent Hartree-Fock-Bogoliubov

Non-Central Interactions

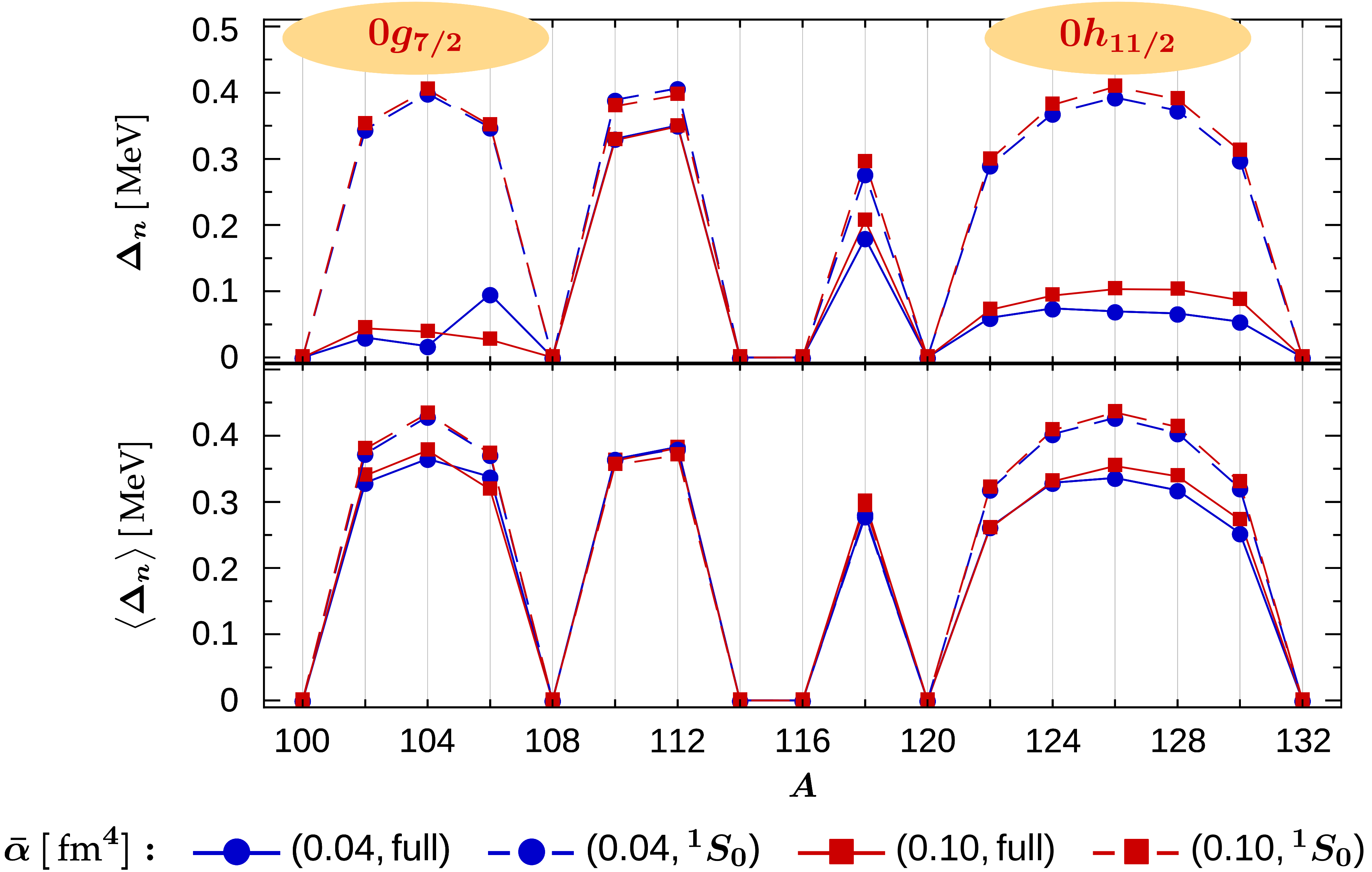


$\bar{\alpha}$ [fm^4] : (0.04, full)

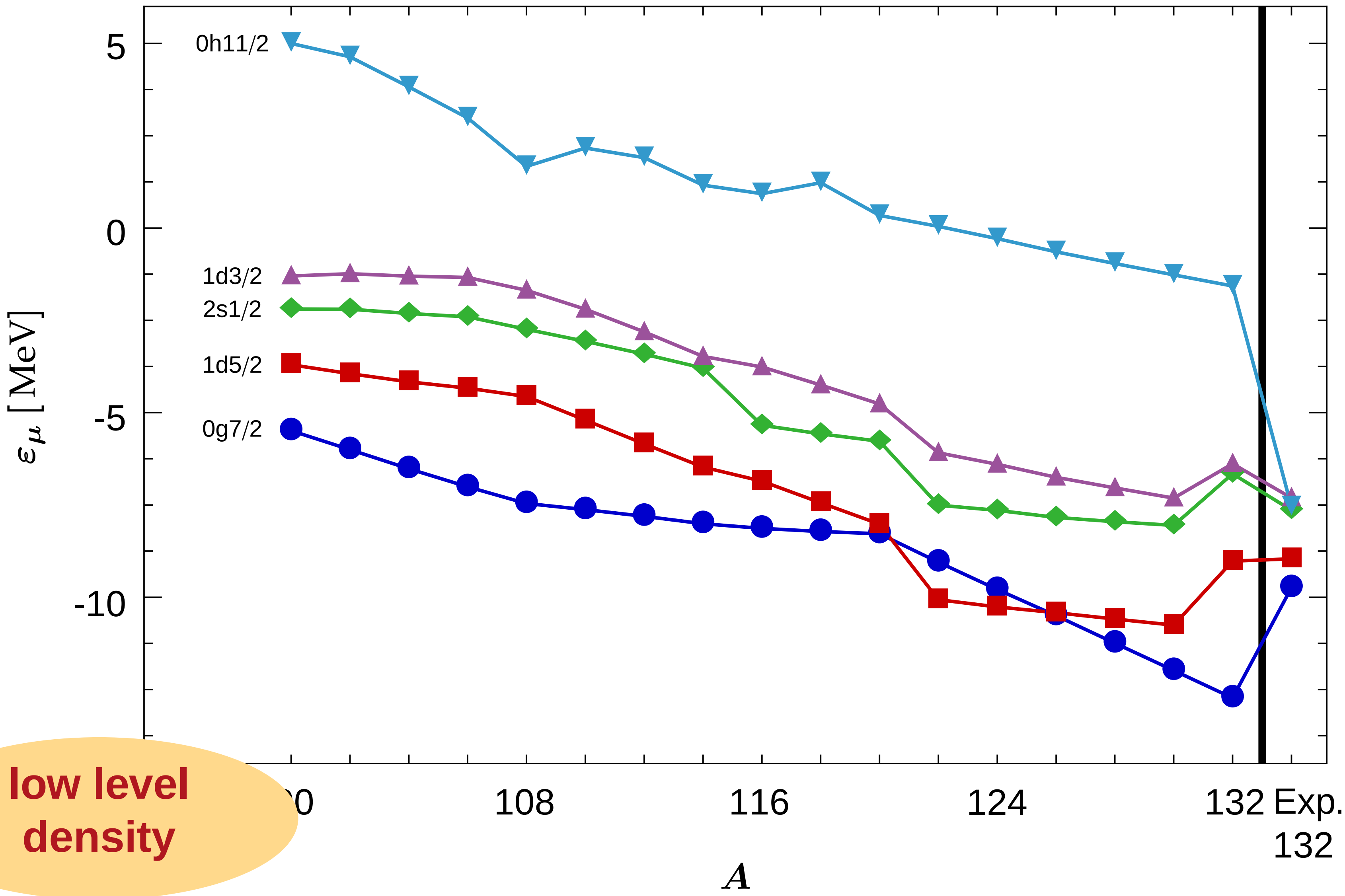
Non-Central Interactions



Non-Central Interactions

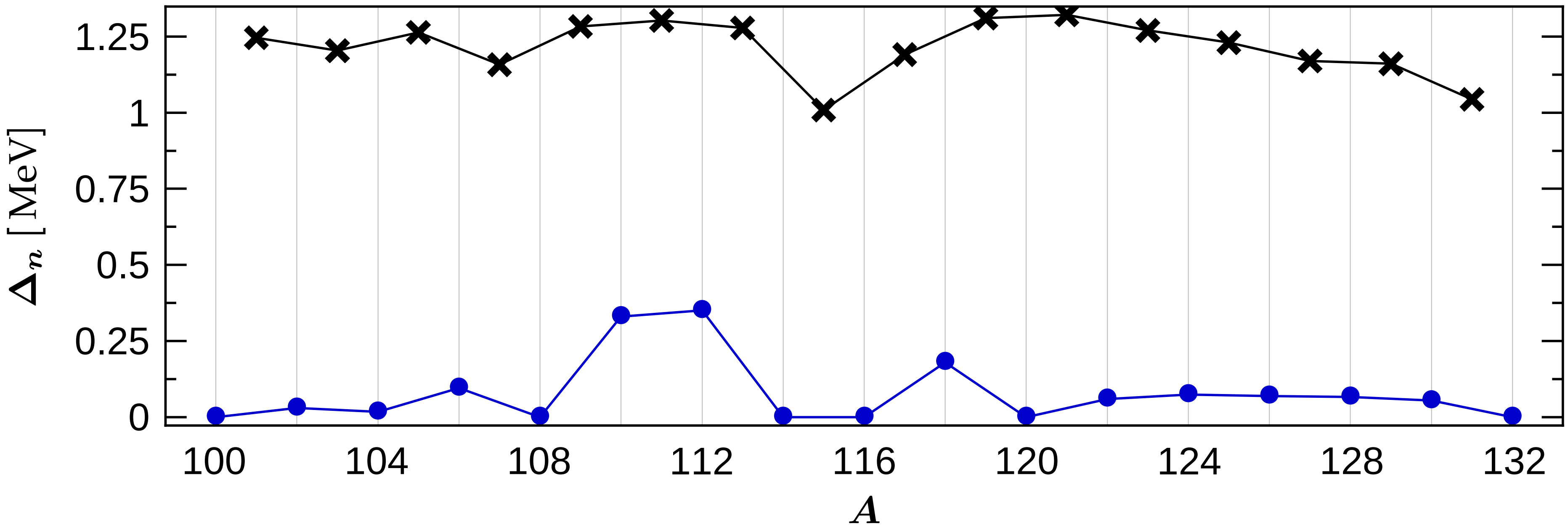


Canonical Single-Particle Spectra



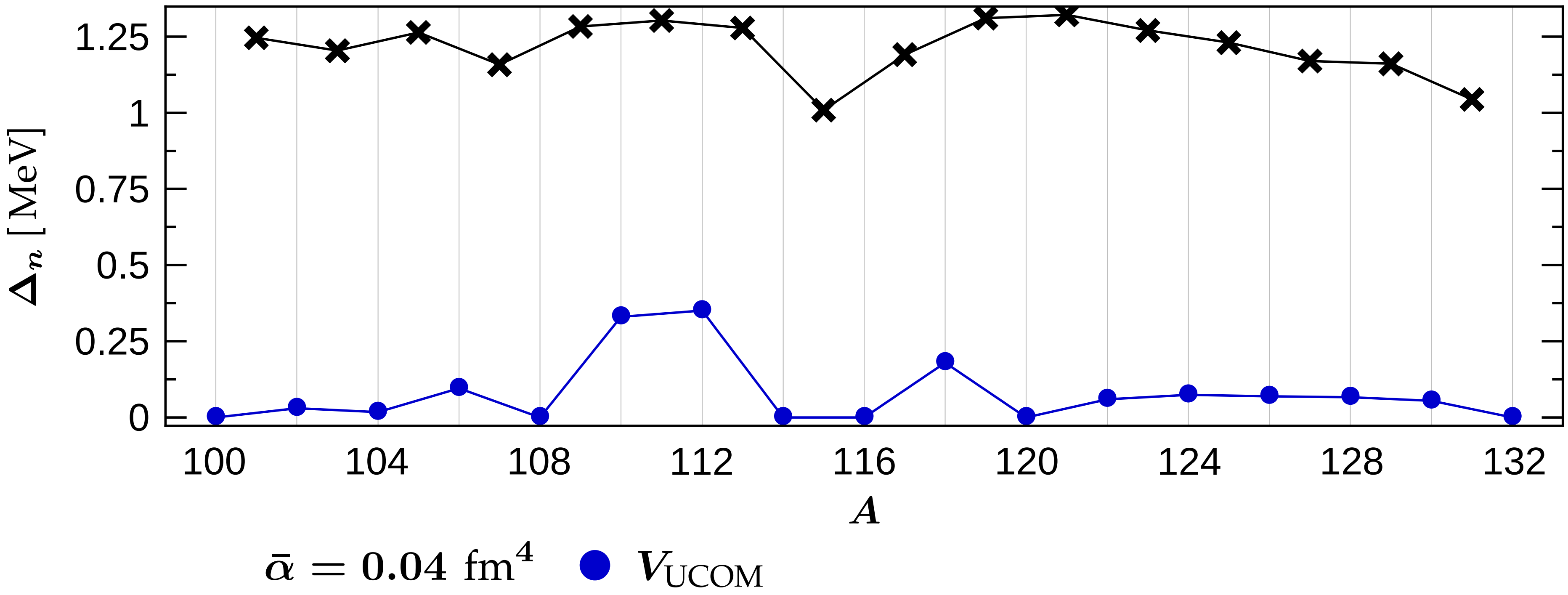
low level density

Gaps



$\bar{\alpha} = 0.04\ \mathrm{fm}^4$ ● V_{UCOM}

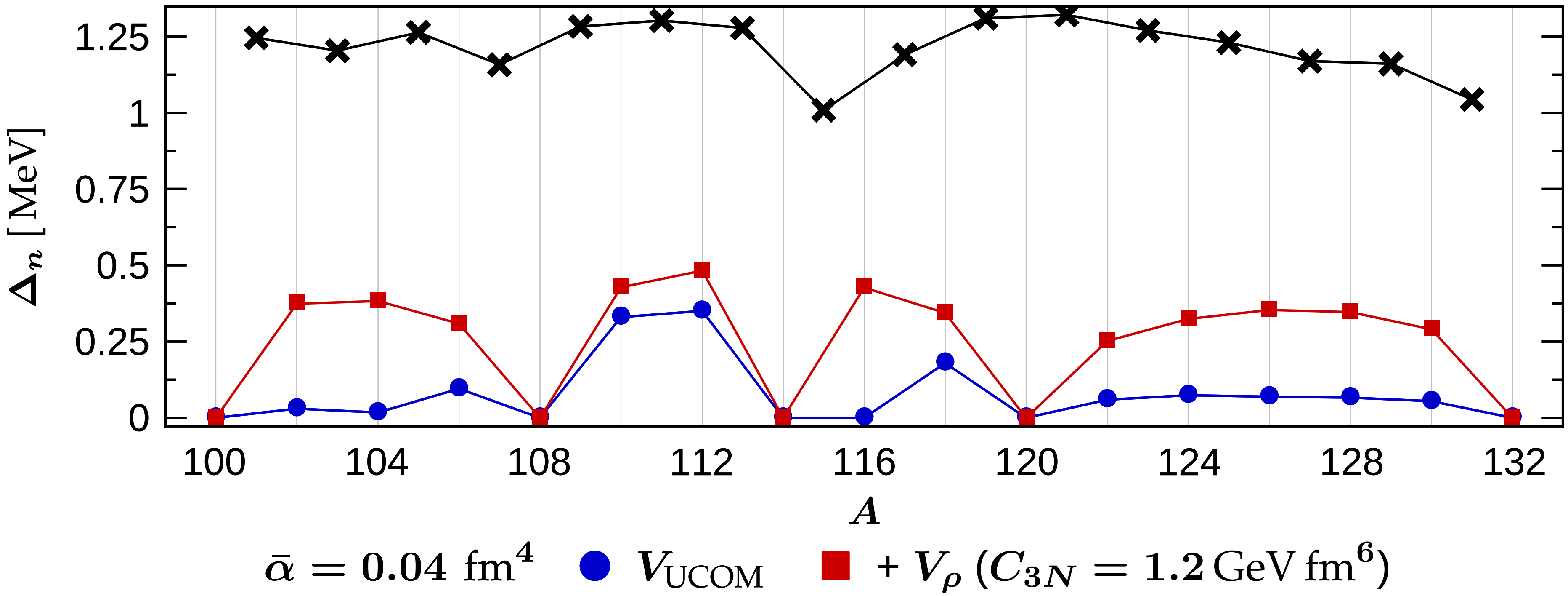
Gaps



- pairing is suppressed due to low level density at Fermi surface
- suppression of theoretical gap in valence shells with high j
- **linear density dependence**:

$$\mathrm{V}_\rho = \frac{C_{3N}}{6} \left(1 + \mathrm{P}_\sigma\right) \rho \left(\tfrac{1}{2}(\vec{\mathbf{r}}_1 + \vec{\mathbf{r}}_2)\right) \delta^3 \left(\vec{\mathbf{r}}_1 - \vec{\mathbf{r}}_2\right)$$

Gaps



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Particle Number Projection

Projected Energy

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

Particle Number Projection

Variation of Projected Energy

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

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

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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**

Particle Number Projection

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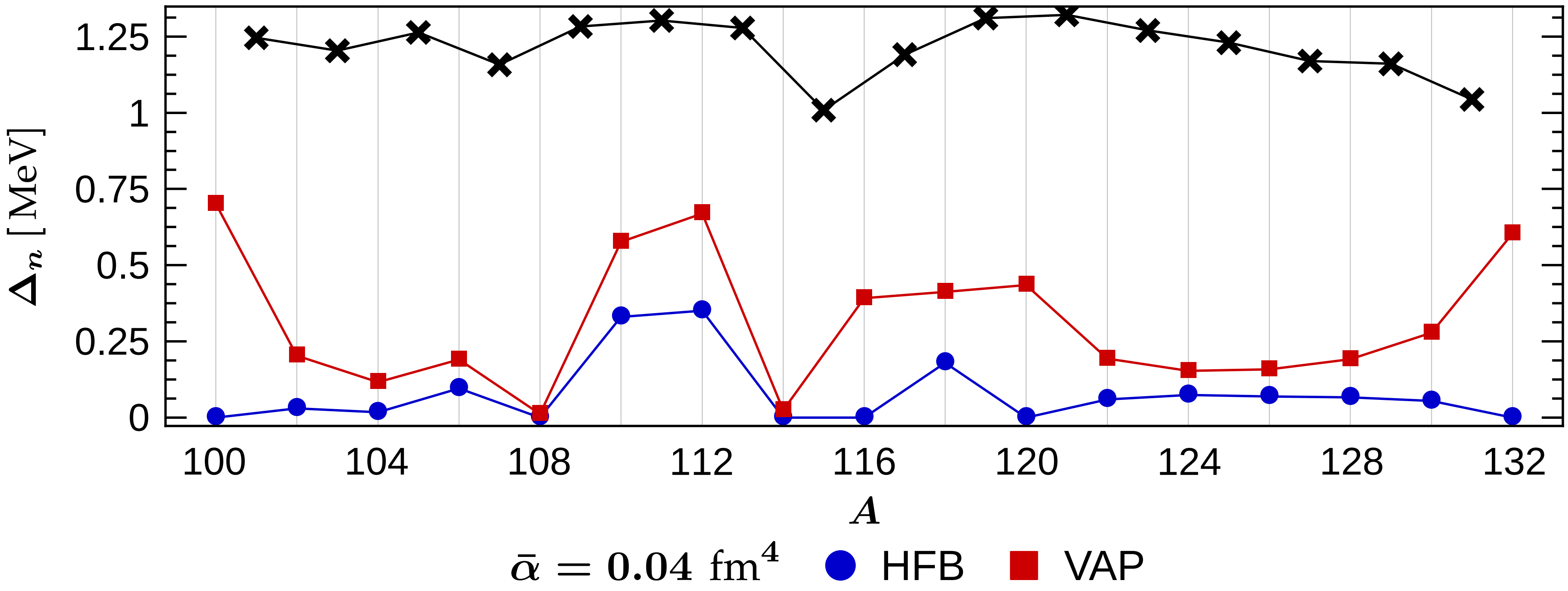
- ✔ managable computational effort for variation after projection (VAP)
- ✔ implement with care: **subtle cancellations between divergences of direct, exchange, and pairing terms**
- ✘ **density-dependent interaction:**
  complex transition density has **poles** (serious problem for projection methods,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

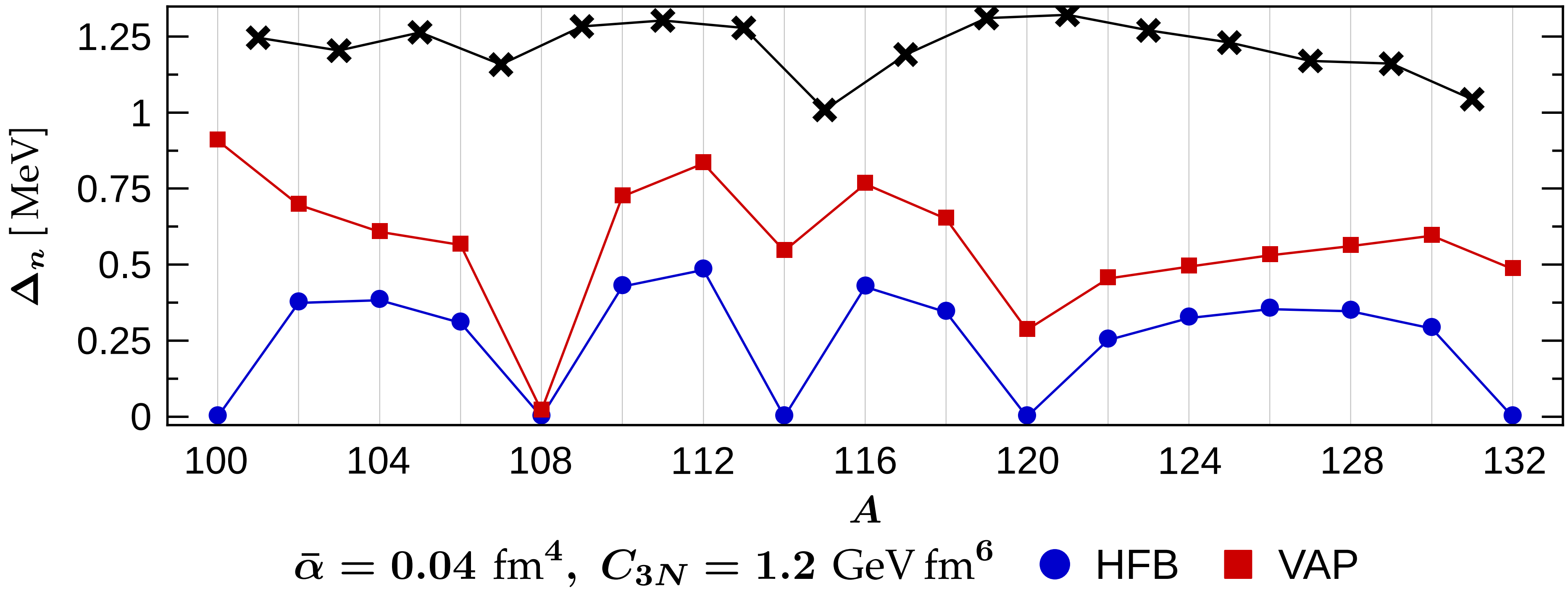
  ☞ Duguet, Lacroix, Bender et al., **arXiv**:0809.2041, 0809.2045, 0809.2049

PNP: Gaps



- consistent inclusion of all two-body terms (**crucial** for particle-number projection)
- projection includes additional **pairing correlations**
- sizable effects at **(major) shell closures**

PNP: Density-Dependent Interaction



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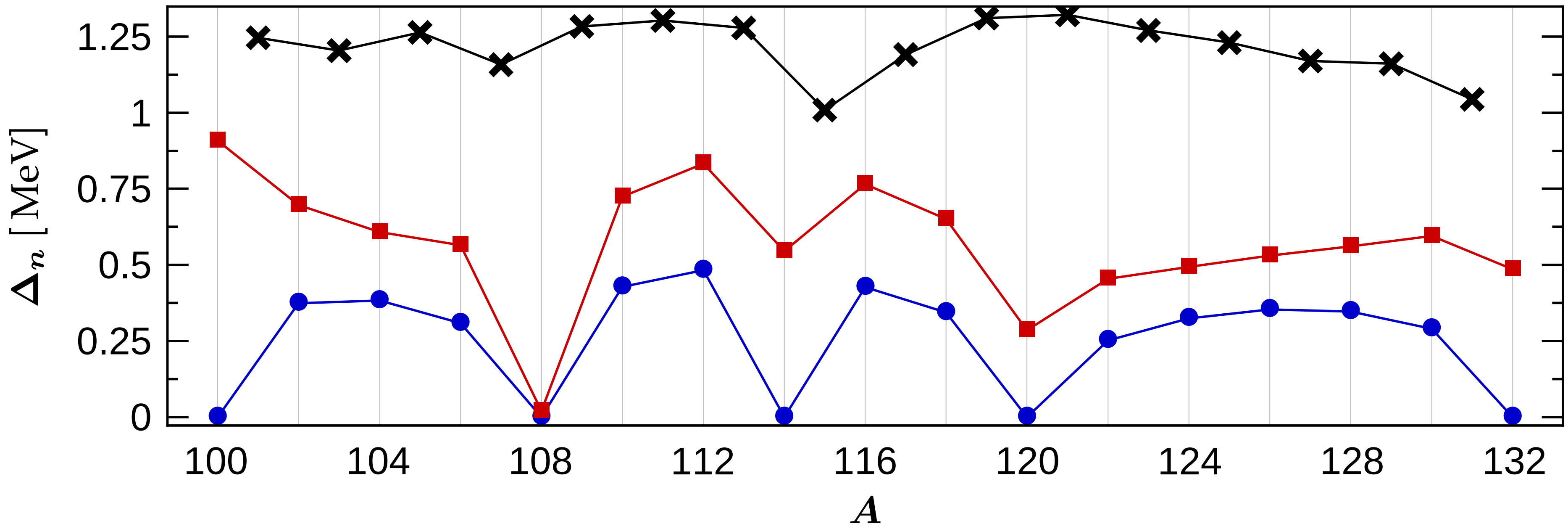

$\bar{\alpha} = 0.04\ \text{fm}^4,\ C_{3N} = 1.2\ \text{GeV fm}^6$ ● HFB ■ VAP

- **linear density-dependence:** isolated poles, check by projecting from neighbouring nuclei

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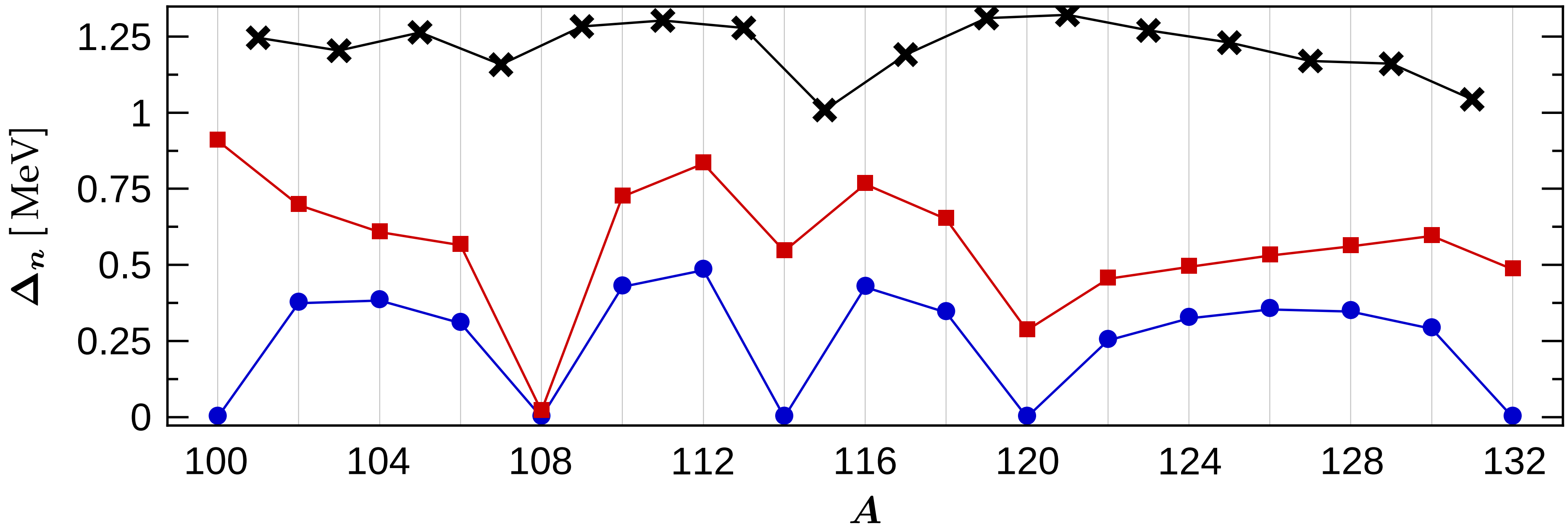

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- **linear density-dependence:** isolated poles, check by projecting from neighbouring nuclei

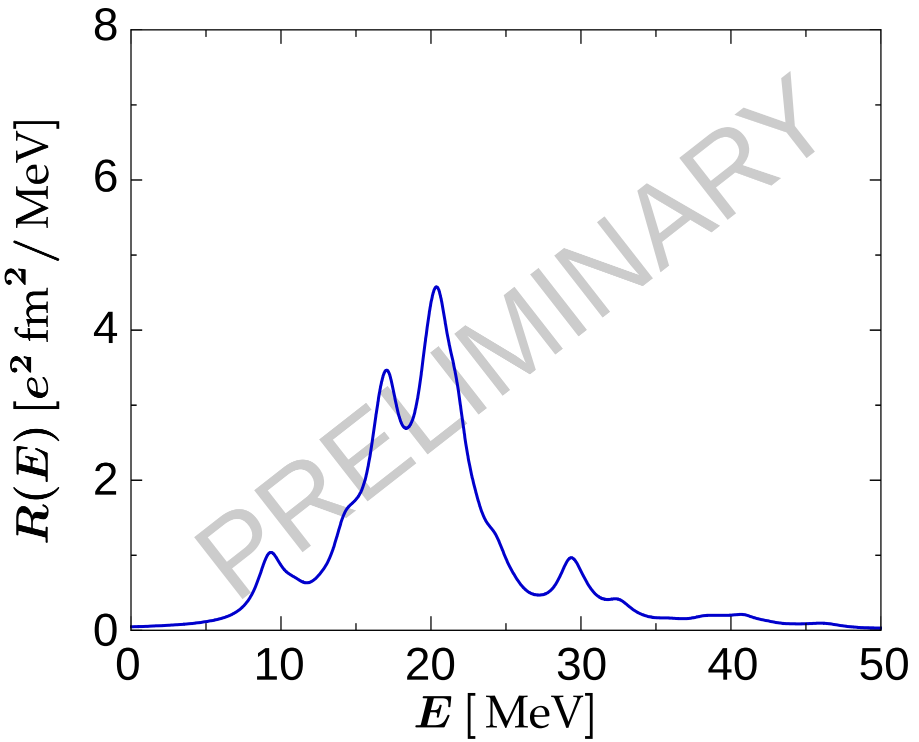
☞ implement explicit correction for isolated spurious poles

Duguet, Lacroix et al.

Pairing in the UCOM Framework

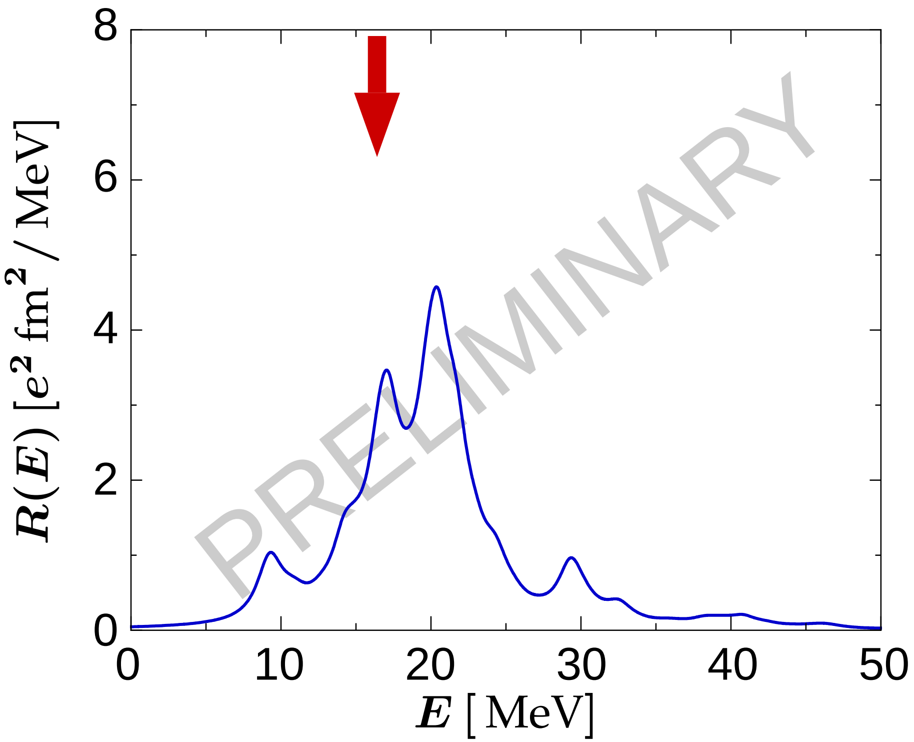
Quasiparticle RPA

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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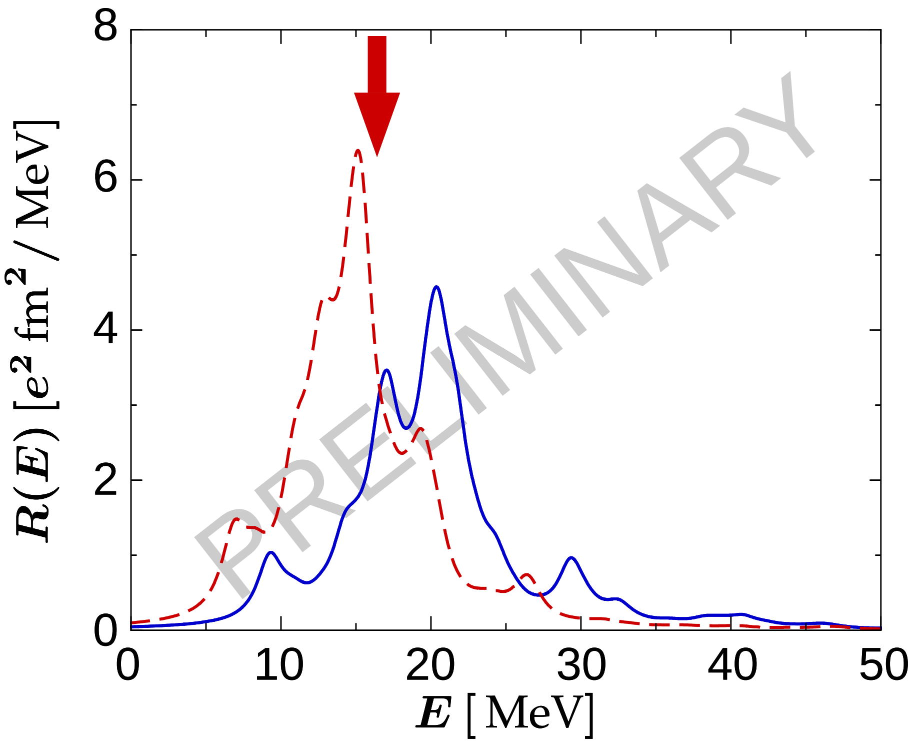

$(\bar{\alpha}[\,\mathrm{fm}^4], C_{3N}[\,\mathrm{GeV\,fm}^6])$ — $(0.04, 0.0)$ - - - $(0.04, 1.2)$

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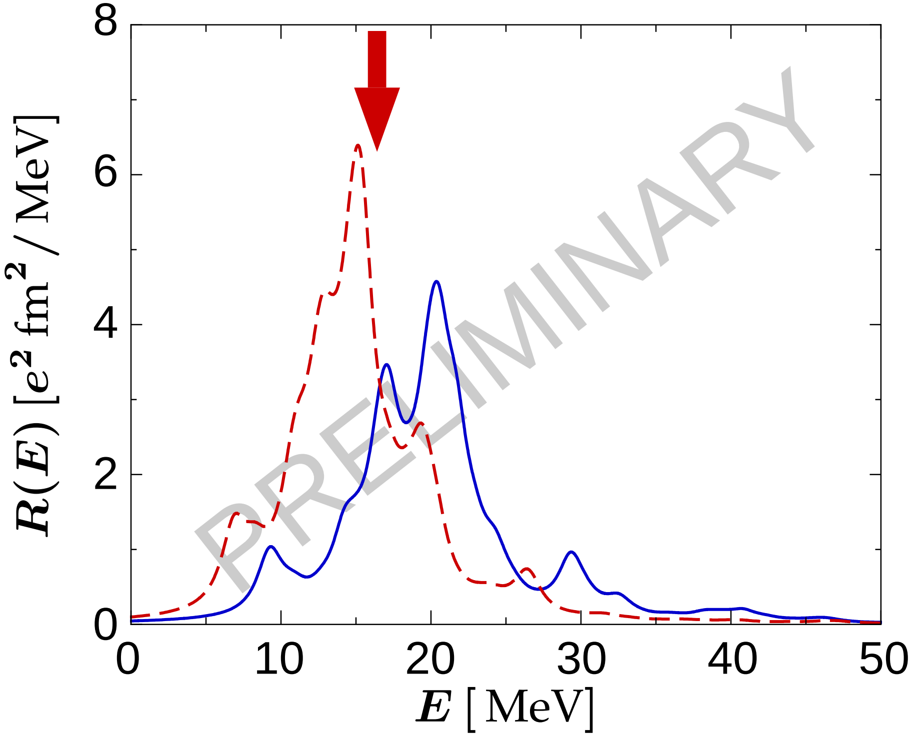

E [MeV]	TRK [%]	N_{neut} [%]
12.86	$\sim$ 9	20.2
15.03	$\sim$ 14	52.2
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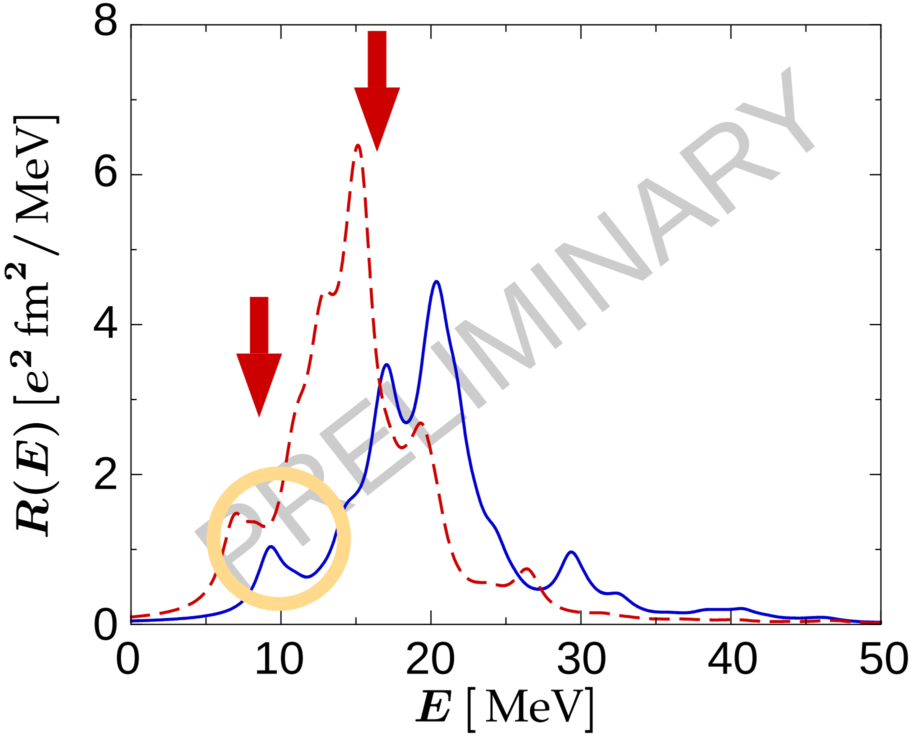
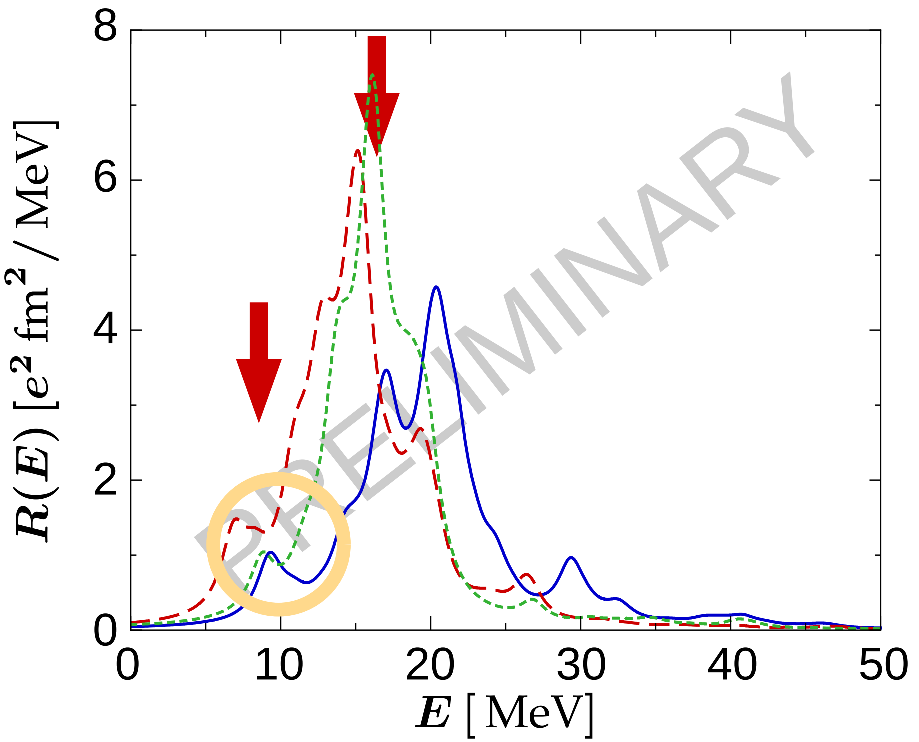


E [MeV]	TRK [%]	N_{neut} [%]
12.86	~ 9	20.2
15.03	~ 14	52.2
15.43	~ 27	24.7
6.86	~ 5	94.7
$\nu 2s_{1/2} \to \nu 2p_{3/2}$		36.0
$\nu 1d_{3/2} \to \nu 2p_{1/2}$		17.6
$\nu 2s_{1/2} \to \nu 2p_{1/2}$		10.6

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

Pygmy Dipole Resonance:
significantly enhanced collectivity in QRPA

QRPA: Dipole Response of ^{130}Sn



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$(\bar{\alpha}[\,\mathrm{fm}^4], C_{3N}[\,\mathrm{GeV\,fm}^6])$ — $(\mathbf{0.04, 0.0})$ - - - $(\mathbf{0.04, 1.2})$ ······ $(\mathbf{0.05, 1.2})$

Pygmy Dipole Resonance:
significantly enhanced collectivity in QRPA

Conclusions

Conclusions

Status

- **fully consistent** framework for HF(B), PNP, like-particle & charge-exchange (Q)RPA
- **inclusion of $3N$ forces**: density-dependent interaction for HFB, QRPA, ...

Outlook & Challenges

- density-dependent interactions in projection methods, GCM, ... (multi-reference scenarios)
- **dressed/renormalized single-particle energies** — e.g. self-consistent coupling to surface modes (HFB+QRPA)
- odd nuclei

Epilogue...

My Collaborators

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- T. Neff, H. Feldmeier

  Gesellschaft für Schwerionenforschung (GSI)

SFB 634

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