Hartree-Fock-Bogoliubov with Correlated Realistic Interactions

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Overview

- The Unitary Correlation Operator Method (UCOM)
- Hartree-Fock & Hartree-Fock-Bogoliubov
  - Particle-Number Projection
  - Inclusion of $3N$-Forces
- Summary & Outlook

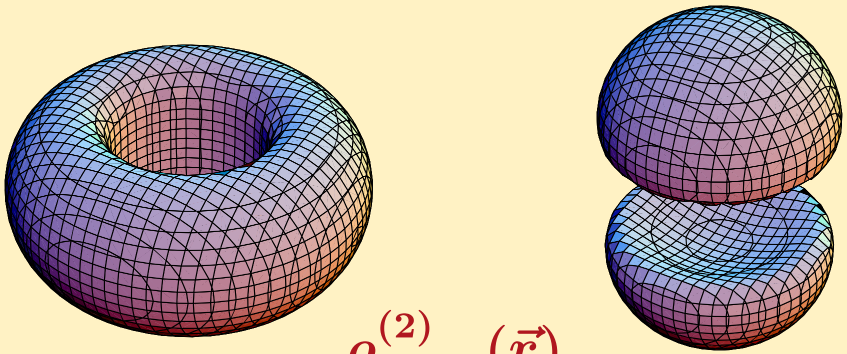
Unitary Correlation Operator Method (UCOM)

Motivation

Argonne V18 Deuteron Solution

$M_S = 0$ $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$

$M_S = \pm 1$ $|\uparrow\uparrow\rangle, |\downarrow\downarrow\rangle$



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

- **central correlations:** two-body density is suppressed at low distances
- **tensor correlations:** angular distribution depends on the relative spin alignments

Central Correlator C_r

radial distance-dependent shift in the relative coordinate of a nucleon pair

$$C_r = \exp(-i \sum_{i,j}^{A} g_{r,ij}[s(r_{ij})])$$

Tensor Correlator C_Ω

angular shift, depending on orientation of spin and relative coordinate

$$C_\Omega = \exp(-i \sum_{i,j}^{A} g_{\Omega,ij}[\vartheta(r_{ij})])$$

$s(r)$ and $\vartheta(r)$ encapsulate the physics of short-range correlations

Correlated Interaction

Correlated Hamiltonian

$$\widetilde{\mathrm{H}} = \mathrm{T}^{[1]} + \mathrm{V}_{\mathrm{UCOM}} + \mathrm{V}_{\mathrm{UCOM}}^{[3]} + \ldots$$

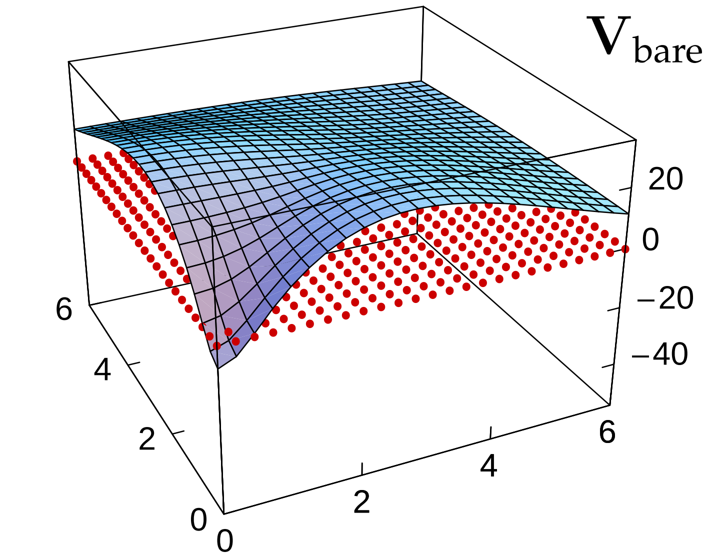
- **closed operator representation** of $\mathrm{V}_{\mathrm{UCOM}}$ in two-body approximation

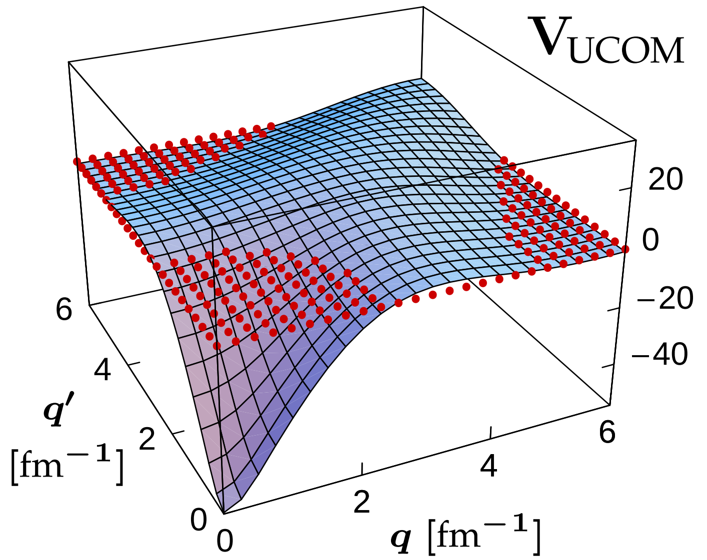
  $\Rightarrow$ usable with **arbitrary many-body basis**

- $\mathrm{V}_{\mathrm{UCOM}}$ is **phase-shift equivalent** to the underlying bare nucleon-nucleon interaction

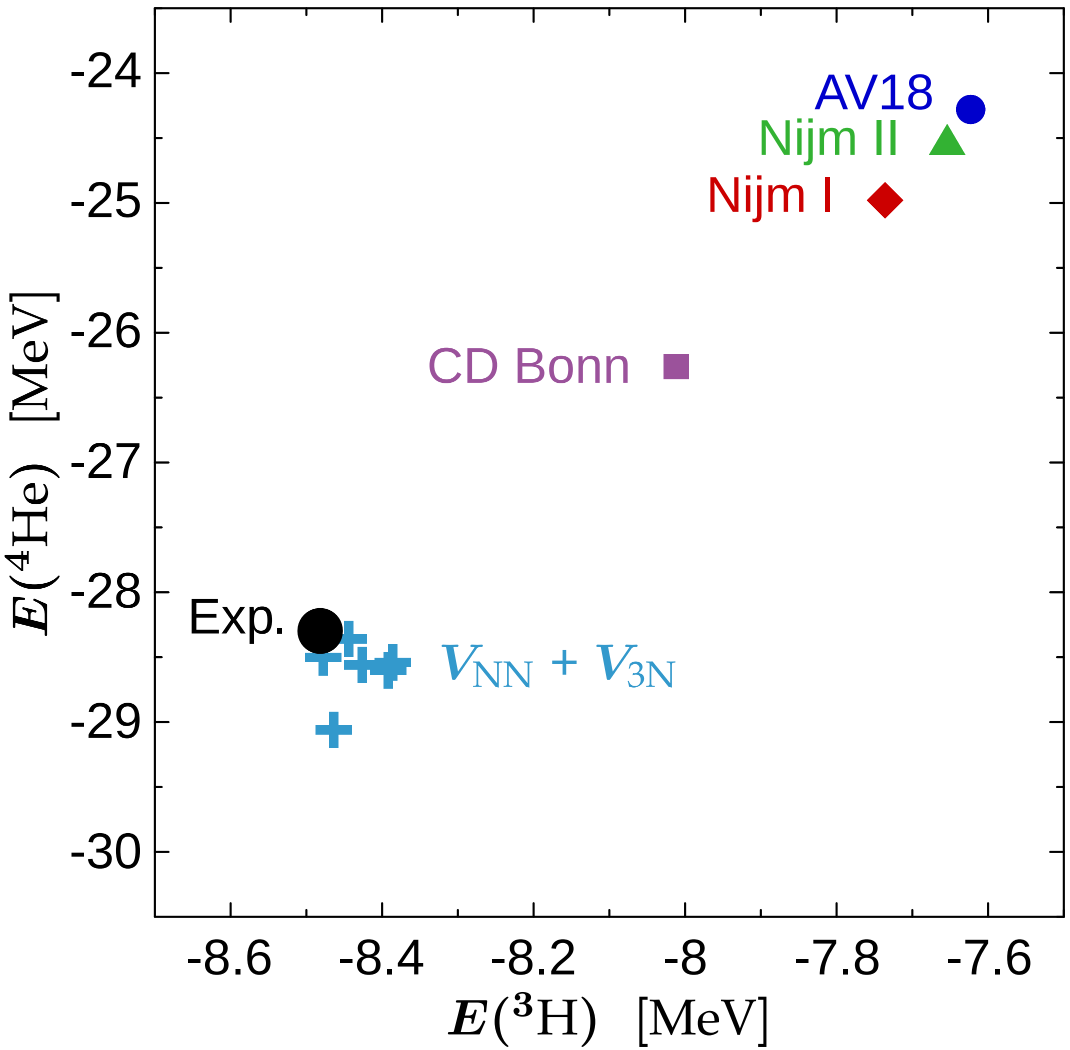
- $\mathrm{V}_{\mathrm{UCOM}}$ is pre-diagonalized in momentum space, i. e. **high-momentum components are decoupled** (similar to $\mathrm{V}_{\text{low-k}}$)

AV18 $^3S_1$





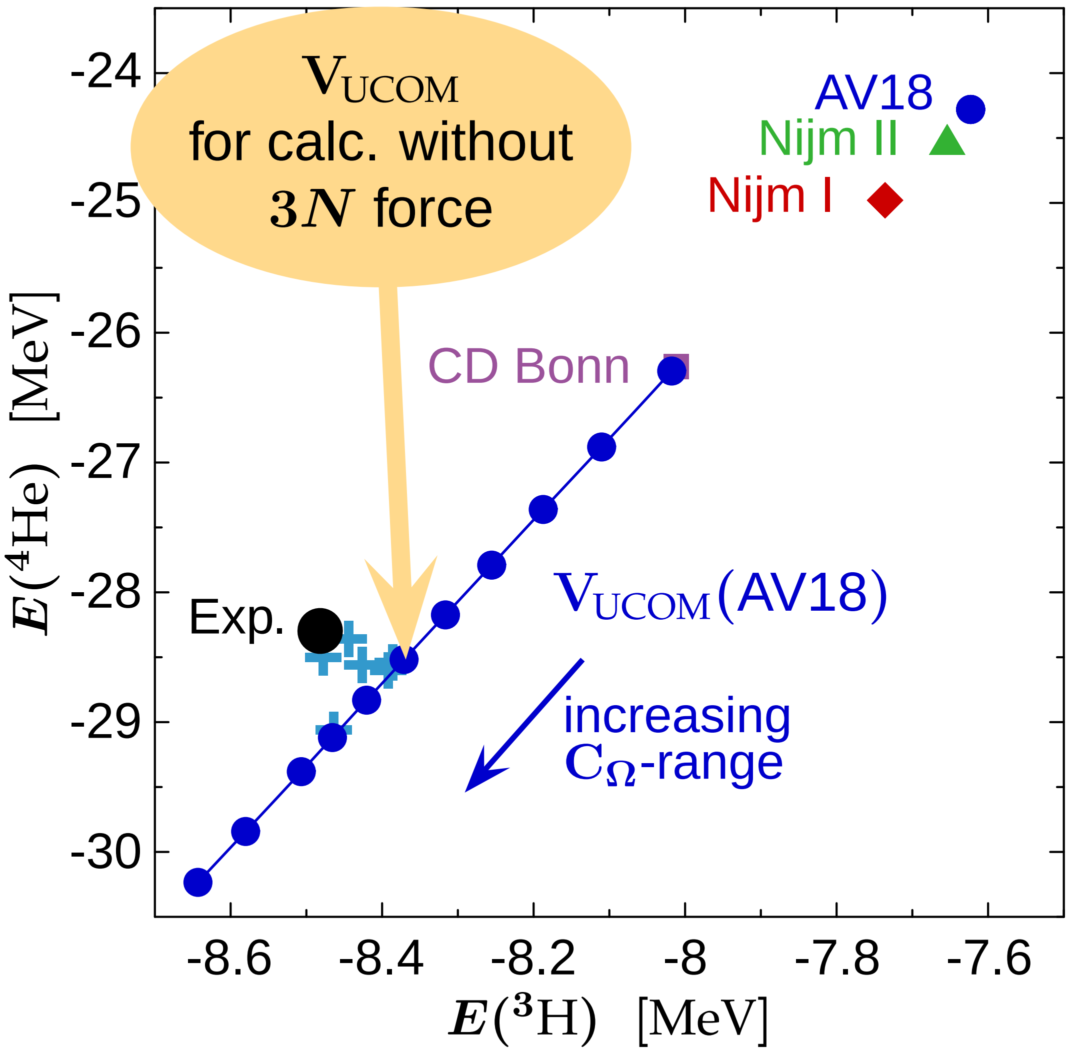
Tjon-Line and Correlator Range



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

Data points: A. Nogga et al., Phys. Rev. Lett. **85**, 944 (2000)

Tjon-Line and Correlator Range



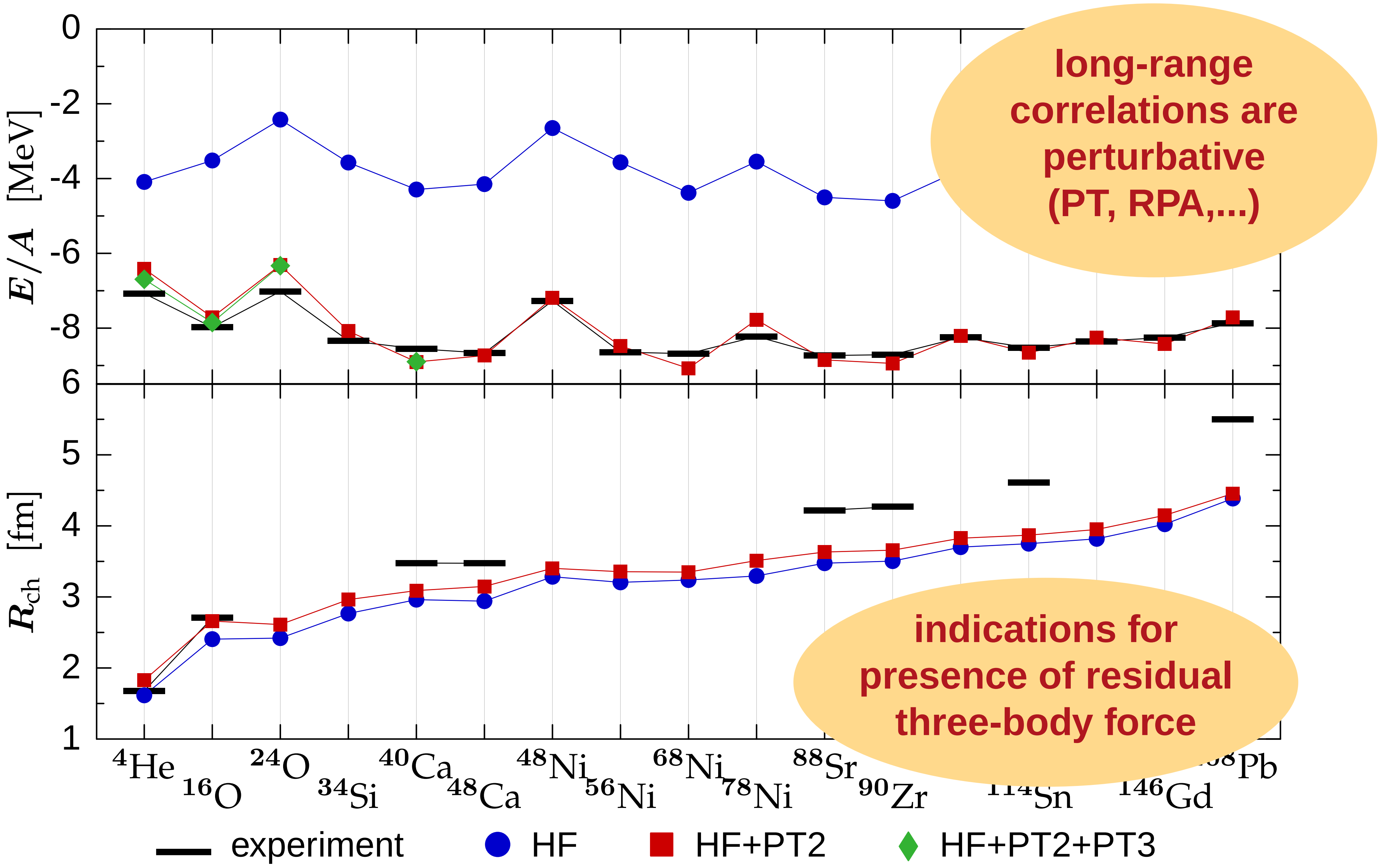
- **Tjon-line**: $E(^4He)$ vs. $E(^3H)$ for phase-shift equivalent NN-interactions
- change of C_Ω-correlator range results in shift along Tjon-line

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

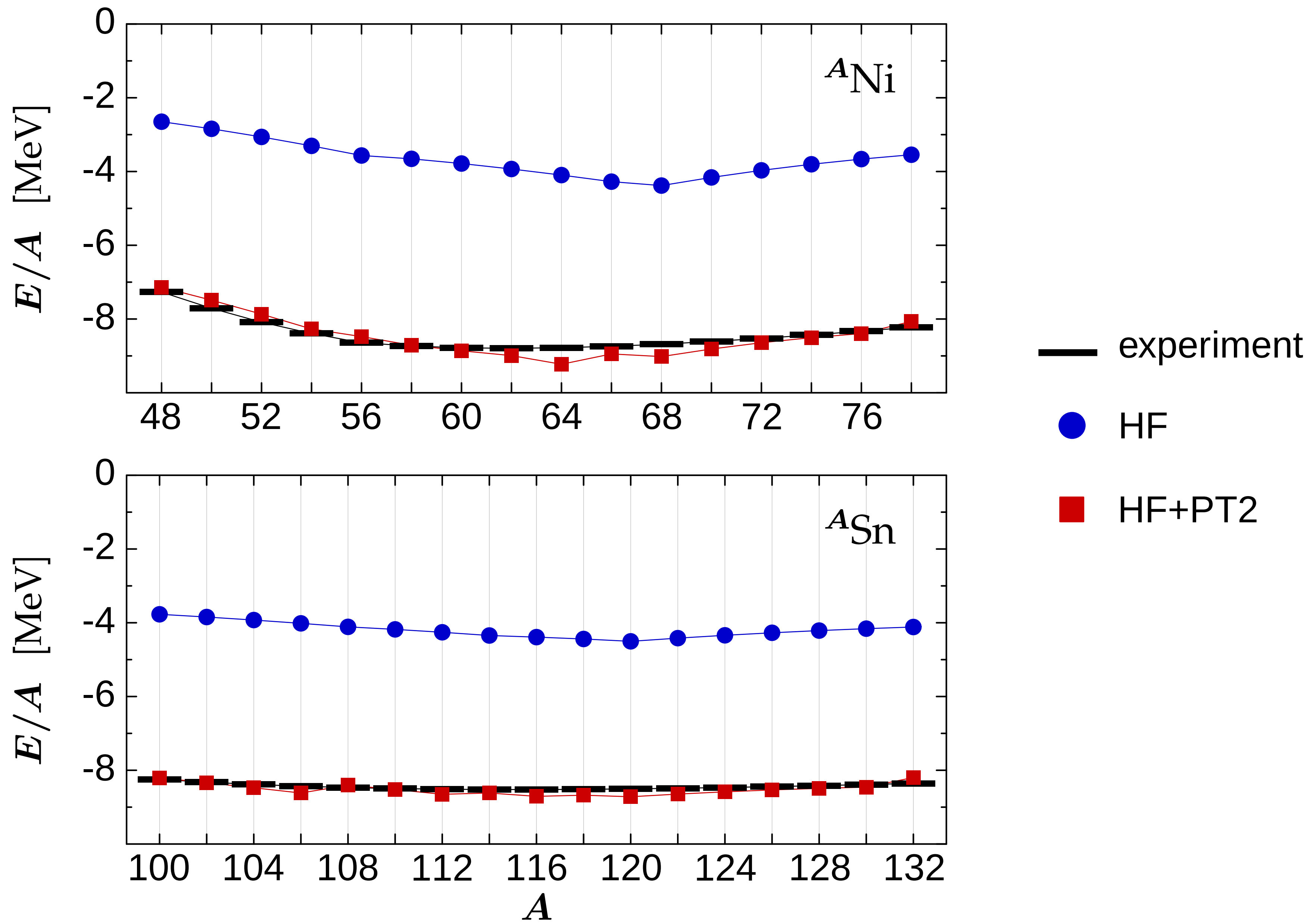
Data points: A. Nogga et al., Phys. Rev. Lett. **85**, 944 (2000)

Hartree-Fock &
Hartree-Fock-Bogoliubov

Binding Energies & Radii



Isotope Chains



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

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

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

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

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

Energy

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

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

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

Lipkin-Nogami Method

- power series expansion
- expansion coefficients **not varied**
- indeterminate / numerically unstable at shell closures

M-Periodic Approximation

- expansion in periodic functions
- fully variational
- higher numerical effort, but **well-defined weak-pairing limit**

☞ Structure of **HFB equations is preserved** by approximations!

☞ exact particle number projection after variation

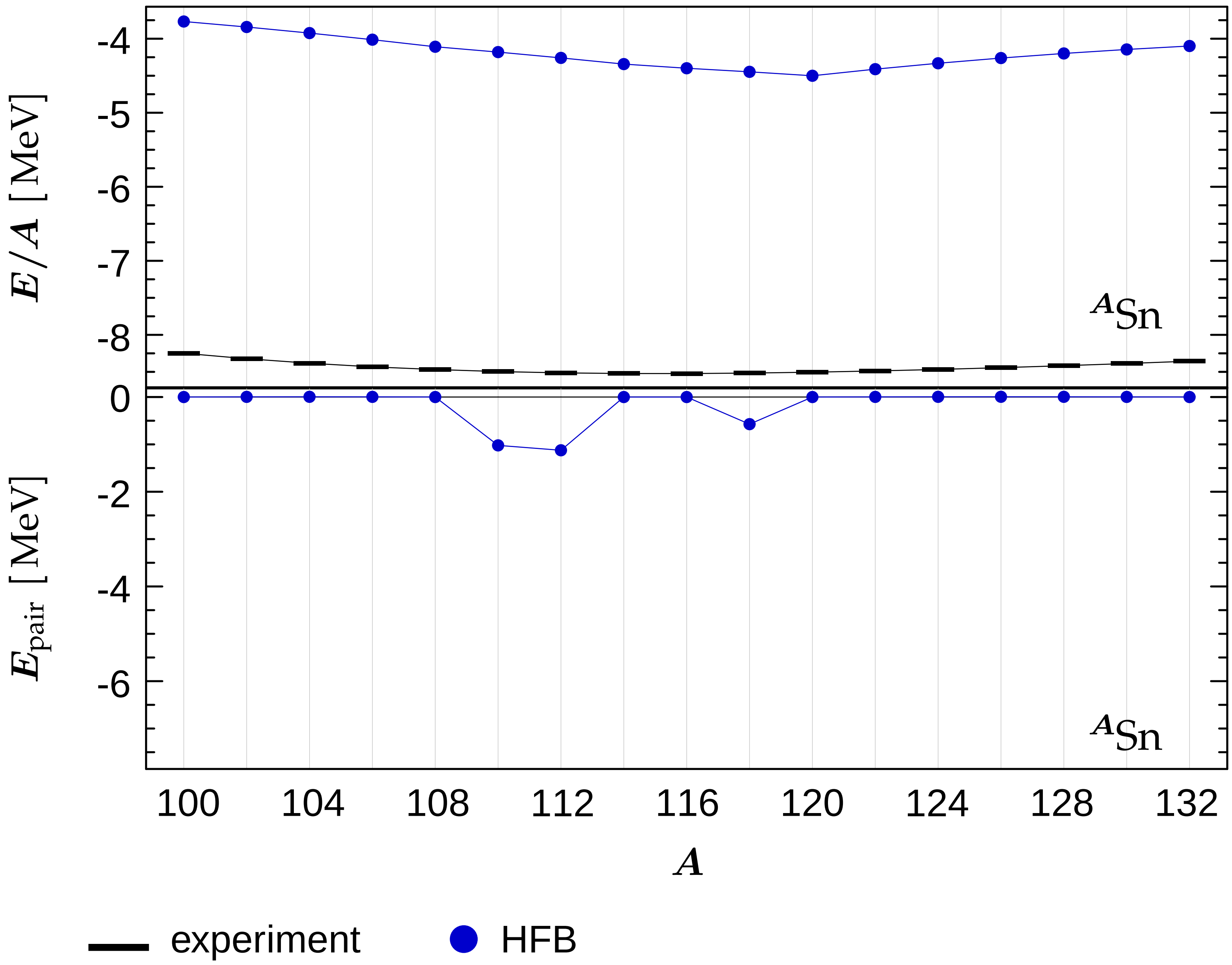
Flocard & Onishi, Ann. Phys. 254, **275** (1997, approx. PNP); Sheikh et al., Phys. Rev. **C66**, 044318 (2002, exact PNP)

Implementation

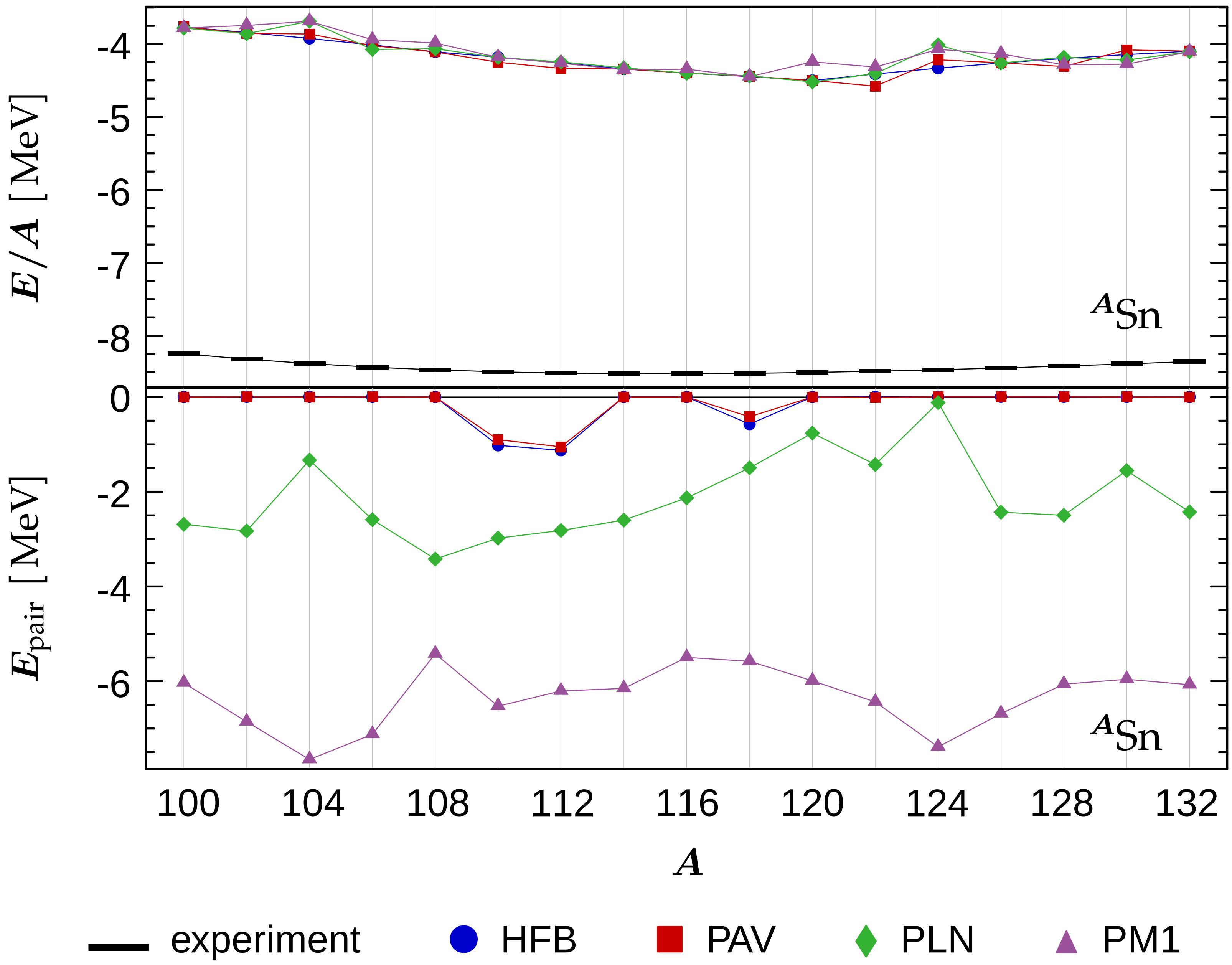
fully consistent treatment of direct, exchange & pairing terms

- $\mathbf{V}_{\mathrm{UCOM}}$ in **ph- and pp-channel** !
- vary **intrinsic energy** $\mathbf{H}_{\mathrm{int}} = \mathbf{H} - \mathbf{T}_{\mathrm{cm}}$
- include (anti-)pairing effects from intrinsic kinetic energy and Coulomb interaction
- quasi-particle Slater determinants expanded in **spherical HO basis** (typically 12–14 major shells sufficient for converged results)
- project on proton and neutron numbers simultaneously:
  $\mathbf{P}_{N_0 Z_0} = \mathbf{P}_{N_0} \mathbf{P}_{Z_0}$

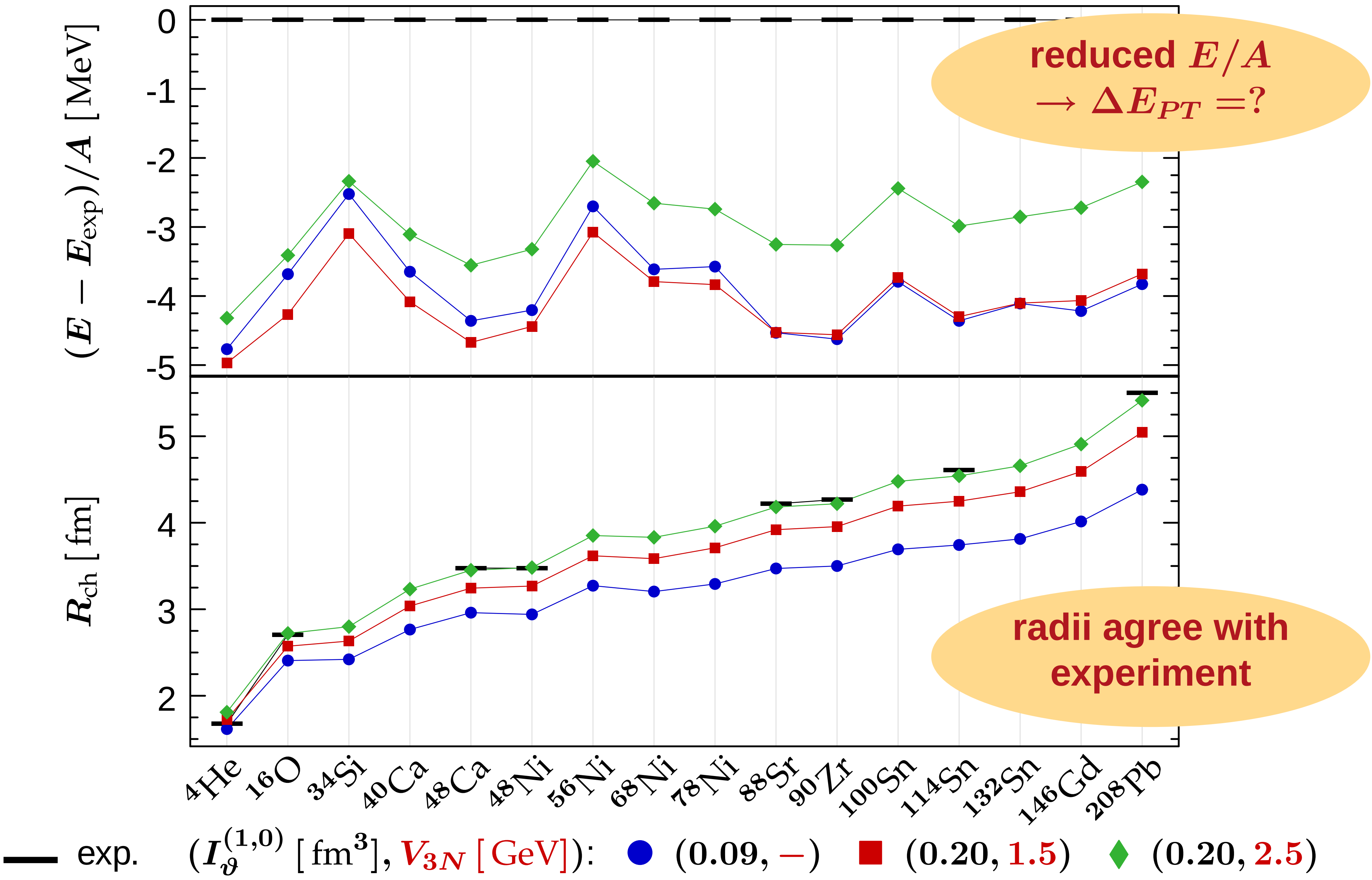
Sn Isotopes: Binding & Pairing Energies



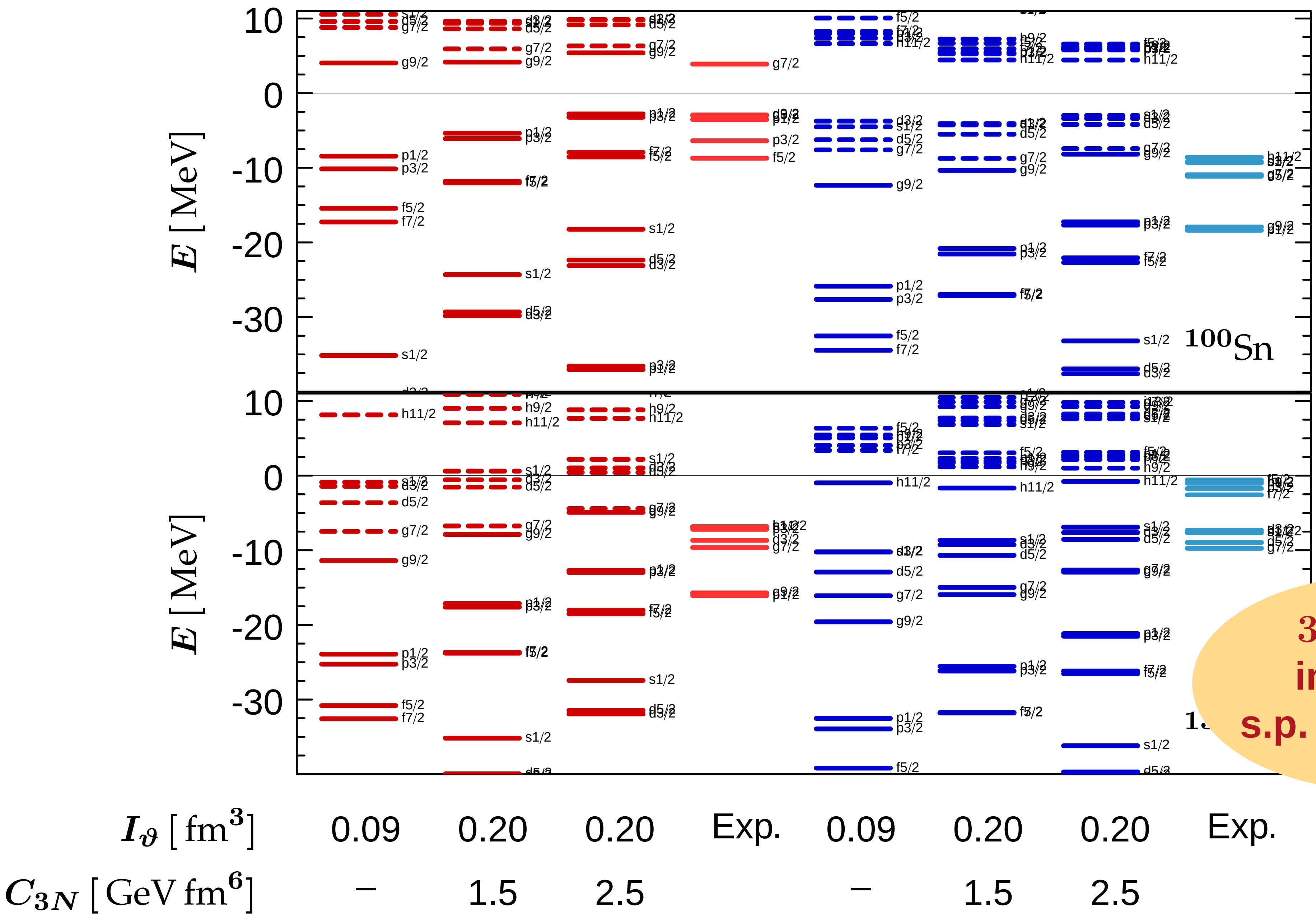
Sn Isotopes: Binding & Pairing Energies



$3N$ Forces: Energies & Radii



$3N$ Forces: HF Single-Particle Energies

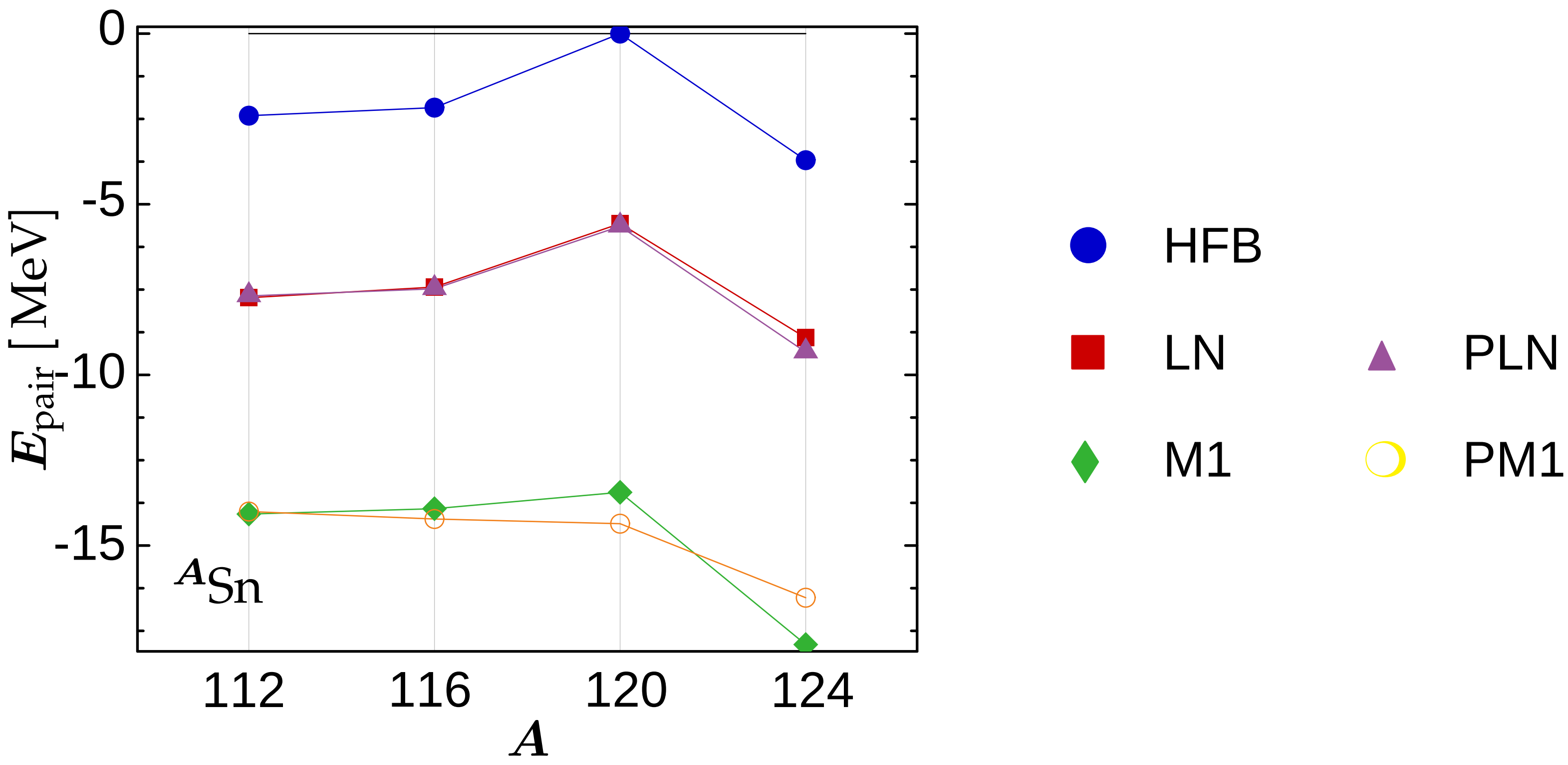


protons

neutrons

$3N$ force improves s.p. spectrum !

$3N$ Forces: Pairing



$$\bar{v}^{[2]}_{kk',qq'} \;\longrightarrow\; \bar{v}^{[2]}_{kk',qq'} + f \cdot \sum_{rr'} \bar{v}^{[3]}_{kk'r,qq'r'} \rho^{HF}_{r'r}\,, \quad f = \begin{cases} \frac{1}{3} & \text{expect. values} \\ \frac{1}{2} & \text{fields} \end{cases}$$

Gogny D1 VAP calc.: $E_{\text{pair}} \simeq -20\ \text{MeV}$ (Anguiano et al., Phys. Lett. **B545** (2002), 62)

Summary & Outlook

Summary

- $\mathbf{V}_{\mathrm{UCOM}}$ is suited for a wide range of many-body methods: HF(B), MBPT, RPA, NCSM, FMD, ...

  $\Rightarrow$ **"Universal" phase-shift equivalent** NN-interaction!

- **fully consistent** HFB calculations with particle number projection, **based on a Hamiltonian**

- **inclusion of** $3N$**-forces** fixes the two-body $\mathbf{V}_{\mathrm{UCOM}}$'s problems with radii and single-particle spectra

- HF and HFB results look promising

$\Rightarrow$ another step towards a **consistent description of different aspects** of nuclear structure based on $\mathbf{V}_{\mathrm{UCOM}}$

Outlook ("Roadmap")

- UCOM-HFB calculations with fewer symmetry constraints
  ⇒ parity and angular momentum projection
- variation after PNP
- finite-range $3N$-force (usable in perturbative methods)
- investigation of pn pairing
  ⇒ isospin projection
- long-range correlations - quasi-particle RPA ...

(In)Famous Last Words...

My Collaborators

- R. Roth, N. Paar, P. Papakonstantinou, A. Zapp

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- T. Neff

  NSCL, Michigan State University

- H. Feldmeier

  Gesellschaft für Schwerionenforschung (GSI)

Recent References

- R. Roth, H. Hergert, P. Papakonstantinou, T. Neff, and H. Feldmeier, Phys. Rev. C**72**, 034002 (2005)
- R. Roth, P. Papakonstantinou, N.Paar, H. Hergert, T. Neff, and H. Feldmeier, Phys. Rev. C**73**, 044312 (2006)
- N. Paar, P. Papakonstantinou, H. Hergert, and R. Roth, Phys. Rev. C**74**, 014318 (2006)
- http://crunch.ikp.physik.tu-darmstadt.de/tnp/

Appendices

Central and Tensor Correlators

Central Correlator C_r

- radial distance-dependent shift in the relative coordinate of a nucleon pair

$$C_r = \exp(-i \sum_{i,j}^{A} g_{r,ij})$$

$$g_r = \frac{1}{2}\left[s(r)\, q_r + q_r\, s(r)\right]$$

$$q_r = \tfrac{1}{2}\left[\tfrac{\vec{r}}{r} \cdot \vec{q} + \vec{q} \cdot \tfrac{\vec{r}}{r}\right]$$

Tensor Correlator C_Ω

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

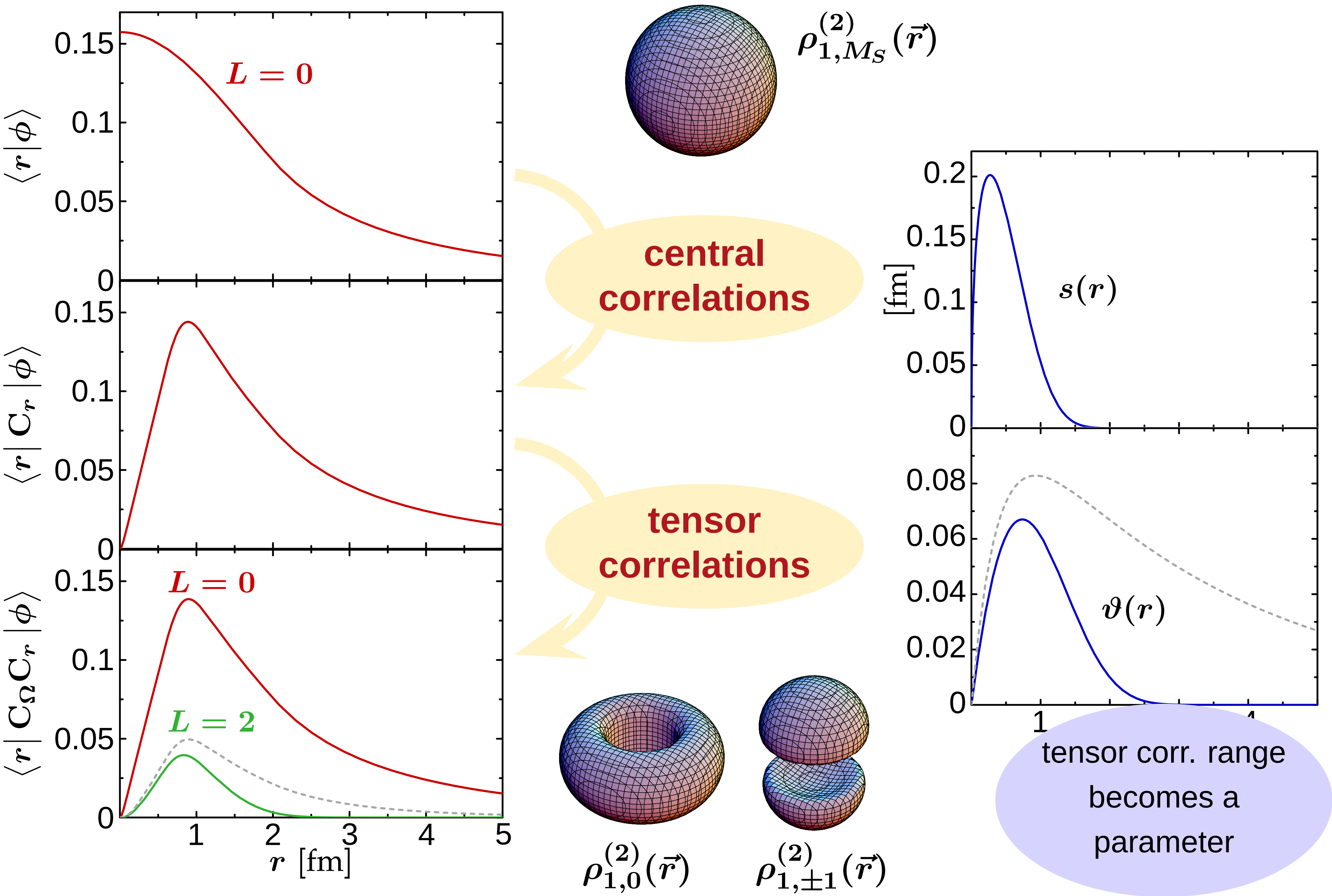
$$C_\Omega = \exp(-i \sum_{i,j}^{A} g_{\Omega,ij})$$

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

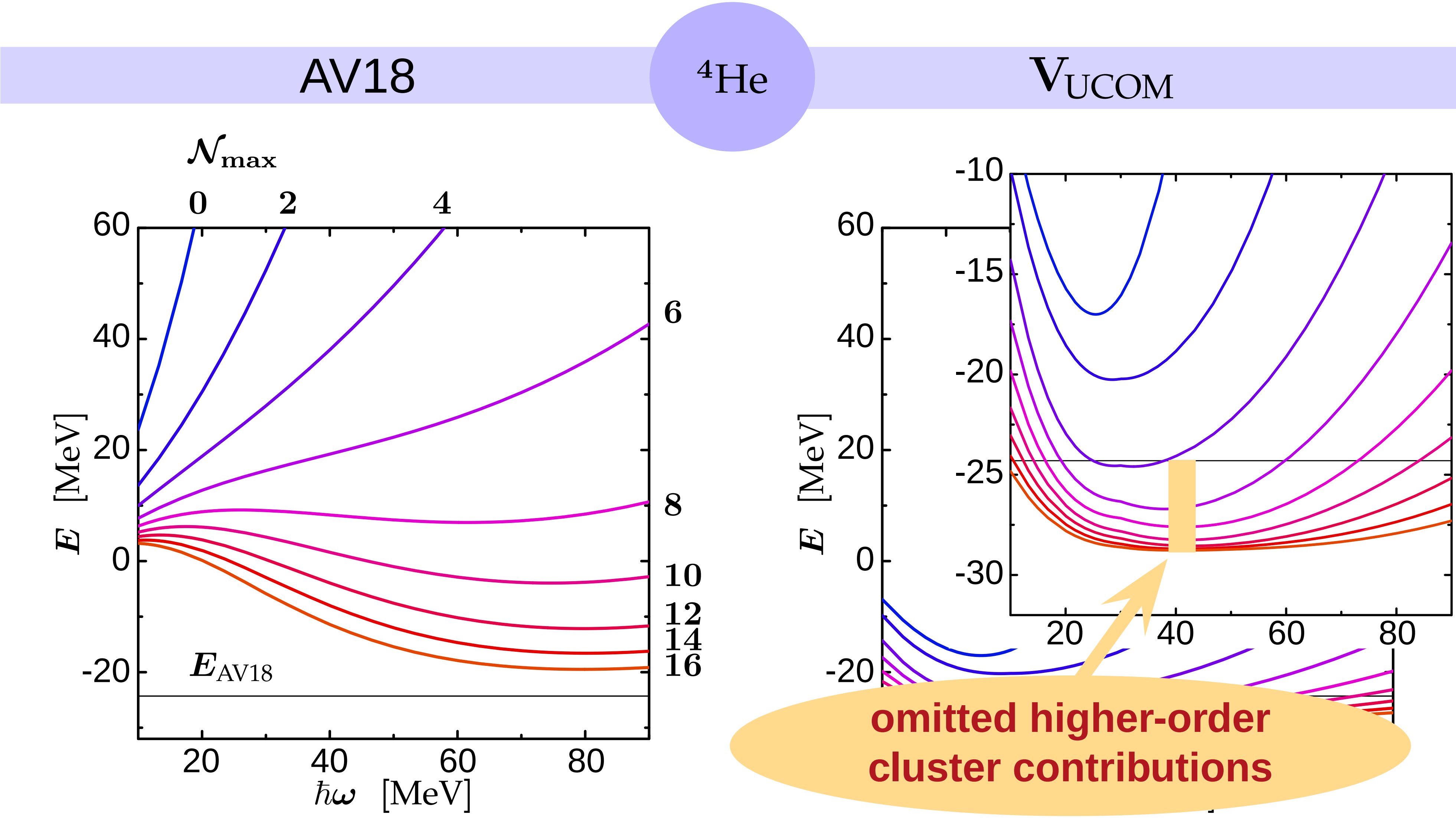
$$\vec{q}_\Omega = \vec{q} - \tfrac{\vec{r}}{r}\, q_r$$

$s(r)$ and $\vartheta(r)$
encapsulate the physics of
short-range correlations.

Correlated States



^{4}He: Convergence



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