Towards Hartree-Fock calculations based on correlated, realistic interactions

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Novel Approaches to the Nuclear Many-Body Problem: From Nuclei to Stellar Matter
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Overview

- Introductory remarks
- MFT and "realistic" effective interactions
  - The limitations of the Slater-Determinant Wavefunction: Short-range and Tensor Correlations
  - The UCOM "correlated" Hamiltonian
- UCOM and Hartree Fock
  - Standard "HF with finite range forces"
  - Preliminary results
- Perspectives

The Nuclear Many-Body Problem

- Nuclear structure and dynamics starting from the NN interaction
  - Nuclei and Nuclear Matter (NM) described as systems of interacting Fermions - non-relativistic approach
- Fully microscopic calculations: only possible for light nuclei and NM, using advanced Quantum Many-Body Theory
  - GFMC: $A \leq 12$
- For heavier nuclei, we depend upon shell model, mean-field approaches

*** *Effective NN interaction*

NN interaction and MFT

- Phenomenological effective interaction
  - limited predictive power (in our expanding nuclear landscape!)
- Derived from the bare NN interaction *(realistic potentials)*
  - Brückner G-Matrix
  - EFT, RG ... low-momentum expansion: V_{low-k} potential employed with success in shell-model calculations

*** *the UCOM Hamiltonian*

✌ *Possibility to combine realistic interactions with MFT!*

The Unitary Correlation Operator Method (UCOM)

- "A unitary correlation operator method";
  H. Feldmeier, T. Neff, R. Roth and J. Schnack,
  Nucl. Phys. A 632 (1998) 61.

- "Tensor correlations in the unitary correlation operator method";
  T. Neff and H. Feldmeier,
  Nucl. Phys. A 713 (2003) 311.

- "Nuclear Structure based on Correlated Realistic NN-Potentials",
  R. Roth, T. Neff, H. Hergert and H. Feldmeier,
  nucl-th/0406021; tbp in Nucl. Phys. A .

- Diploma, Masters and/or PhD Theses of H. Hergert, T. Neff, R. Roth;
  available on `http://crunch.ikp.physik.tu-darmstadt.de/tnp/`
  or `http://www.gsi.de/forschung/tp/` .

The limitations of the Slater-Determinant Wavefunction: the Independent-Particle Model (IPM) breaks down in small-medium NN distances

- Short-range central correlations: pair distribution vanishes in small relative distance due to strong repulsive core

- Tensor correlations: distribution of particles depends also on relative spin orientation

The limitations of the Slater-Determinant Wavefunction: the Independent-Particle Model (IPM) breaks down in small-medium NN distances

☞ introduce correlations by means of Unitary Correlation Operator (UCO) C acting on relative coordinates of all pairs:

$$C = \exp[-iG] = \exp[-i\sum_{i<j} g_{ij}] \; ; \; g_{ij} = g(\vec{r}_{ij}, \vec{q}_{ij}, \vec{\sigma}_i, \vec{\sigma}_j, \vec{\tau}_i, \vec{\tau}_j)$$

- Short-range central correlations: pair distribution vanishes in small relative distance due to strong repulsive core

☞ radial shift in the relative coordinate of nucleon pair:

$$C_r \; \leftrightarrow \; g_r = \tfrac{1}{2}[s(r)q_r + q_r s(r)] \; ; \; q_r = \tfrac{1}{2}[\tfrac{\vec{r}}{r}\vec{q} + \vec{q}\tfrac{\vec{r}}{r}]$$

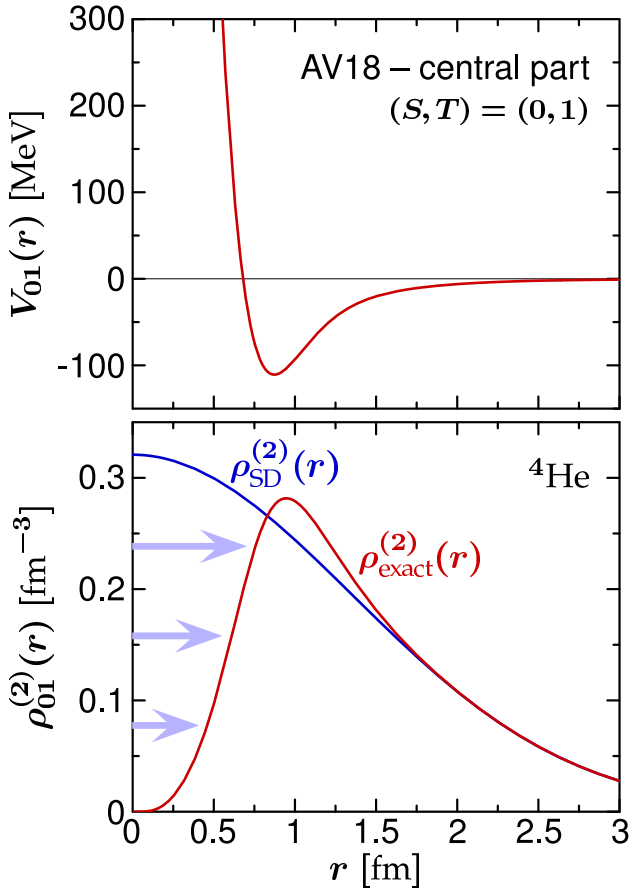
- Tensor correlations: distribution of particles depends also on relative spin orientation

☞ angular shift depending on orientation of spin and relative coordinate:

$$C_\Omega \; \leftrightarrow \; g_\Omega = \tfrac{3}{2}\vartheta(r)[(\vec{\sigma}_i \cdot \vec{q}_\Omega)(\vec{\sigma}_j \cdot \vec{r}) + (\vec{r} \leftrightarrow \vec{q}_\Omega)] \; ; \; \vec{q}_\Omega = \vec{q} - \tfrac{\vec{r}}{r}q_r$$

$$\text{UCO} : C = C_r C_\Omega = \exp[-iG] \; ; \; G^\dagger = G \; ; \; C^\dagger C = 1$$

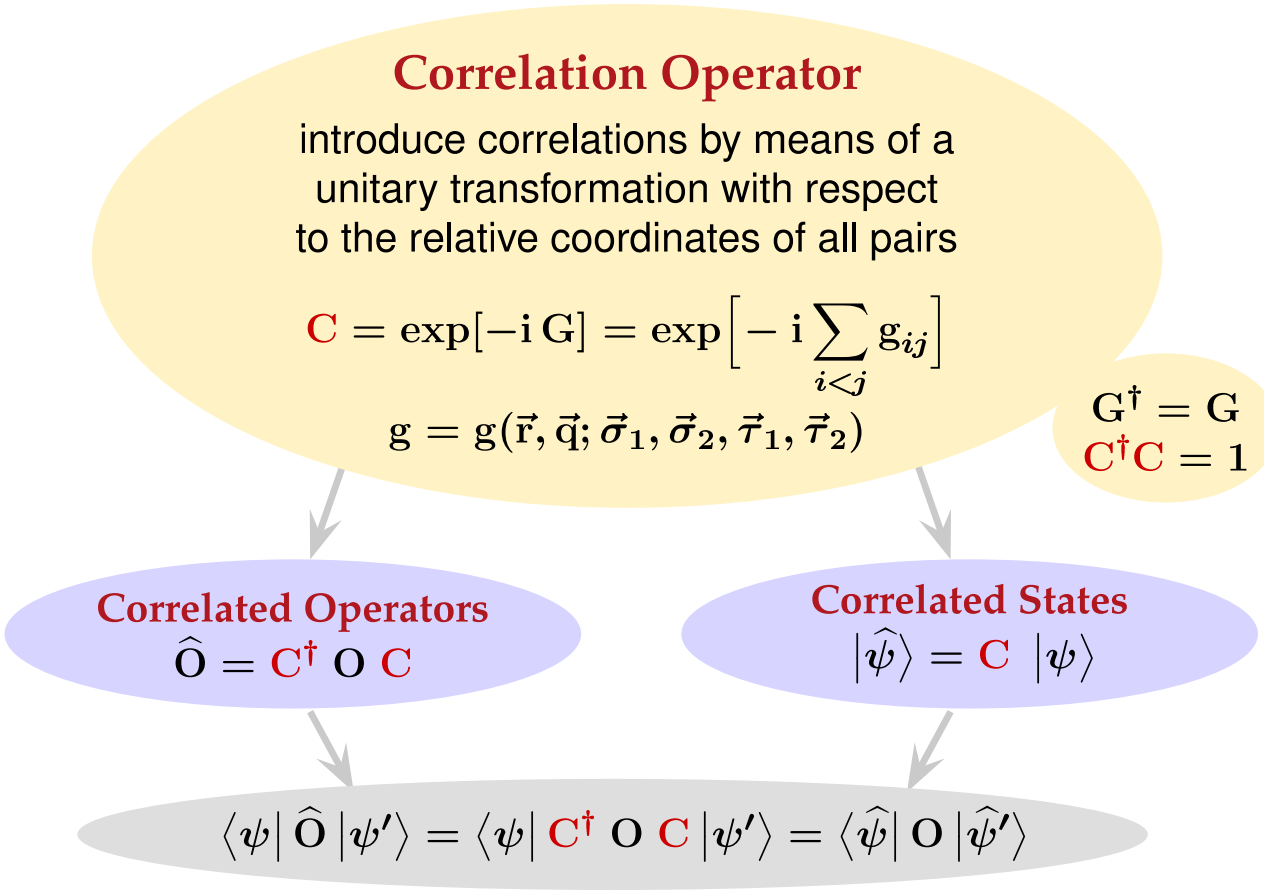
Central Correlations



- two-body density distribution of ^{4}He in the $(S,T) = (0,1)$ channel
- strong repulsive core in the central part of realistic interactions
- suppression of the probability density for finding two nucleons within the core region ➔ **correlation hole**
- short-range central correlations cannot be described by single or superpositions of few Slater determinants

"shift the nucleons out of the core region"

Unitary Correlation Operator Method



Correlated Operators

Cluster Expansion

$$\hat{O} = C^{\dagger}\, O\, C = \hat{O}^{[1]} + \hat{O}^{[2]} + \hat{O}^{[3]} + \cdots$$

Cluster Decomposition Principle

if the correlation range is small compared to the mean particle distance, then higher orders are negligible

restrict range of the correlators in order to minimise higher order contributions

Two-Body Approx.

$$\hat{O}^{C2} = \hat{O}^{[1]} + \hat{O}^{[2]}$$

operators for all observables can be and have to be correlated consistently

Correlated Realistic NN-Potential

$$\widehat{\mathbf{H}}^{C2} = \widehat{\mathbf{T}}^{[1]} + \widehat{\mathbf{T}}^{[2]} + \widehat{\mathbf{V}}^{[2]} = \mathbf{T} + \mathbf{V}_{\mathrm{UCOM}}$$

- **closed operator expression** for the correlated interaction $\mathbf{V}_{\mathrm{UCOM}}$ in two-body approximation
- correlated interaction and original NN-potential are **phase shift equivalent** by construction
- **central correlator**: removes the repulsive core and generates additional momentum dependence
- **tensor correlator**: "rotates" part of tensor force into other operator channels (central, spin-orbit,...)
- momentum-space matrix elements of correlated interaction are **identical to** $V_{\mathrm{low}-k}$

The UCOM interaction

$$
\begin{aligned}
V_{\mathrm{UCOM}} &= \sum_{S,T}[\nu^{c}_{ST}(r) + \{\nu^{qr2}_{ST}(r) q_r^2\}_H + \nu^{L2}_{ST}(r)\vec{L}^2]\Pi_{ST} \\
&+ \sum_{T}[\nu^{LS}_{T}(r)(\vec{L}\cdot\vec{S}) + \nu^{t}_{T}(r) s_{12} + \nu^{tLL}_{T}(r) s_{12}(\vec{L},\vec{L}) \\
&\quad + \nu^{tqq}_{T}(r)\bar{s}_{12}(\vec{q}_\Omega,\vec{q}_\Omega) + \nu^{L2tqq}_{T}(r)\{\vec{L}^2\bar{s}_{12}(\vec{q}_\Omega,\vec{q}_\Omega)\}_H \\
&\quad + \nu^{qr2trq}_{T}(r)\{q_r^2 s_{12}(\vec{r},\vec{q}_\Omega)\}_H + \nu^{L2LS}_{T}(r)\vec{L}^2(\vec{L}\cdot\vec{S})]\Pi_{1T}
\end{aligned}
$$

- the functions $\nu^{\cdots}_{(S)T}$ are parametrized so that they have a simple analytical radial dependence *(sum of gaussians)*
- they are parametrized by energy minimization in the two-body system

*** same parametrization is used for all nuclei

Missing Pieces

"Physical" Points

- genuine three-body forces
- genuine many-body correlations

"Technical" Points

- residual three-body contributions of cluster expansion
- imperfect two-body correlations

Pragmatic Approach

simulate these by a phenomenological correction to the correlated two-body potential

Phenomenological Corrections

Central Correction

- Wigner-type local and momentum-dependent Gaussian potentials

$$\mathrm{V_C} = v_1(\mathrm{r}) + \vec{\mathrm{q}}\, v_{qq}(\mathrm{r})\, \vec{\mathrm{q}}$$

- parameters fixed to reproduce binding energies and cms-radii of $^4\mathrm{He}$, $^{16}\mathrm{O}$, and $^{40}\mathrm{Ca}$

Spin-Orbit Correction

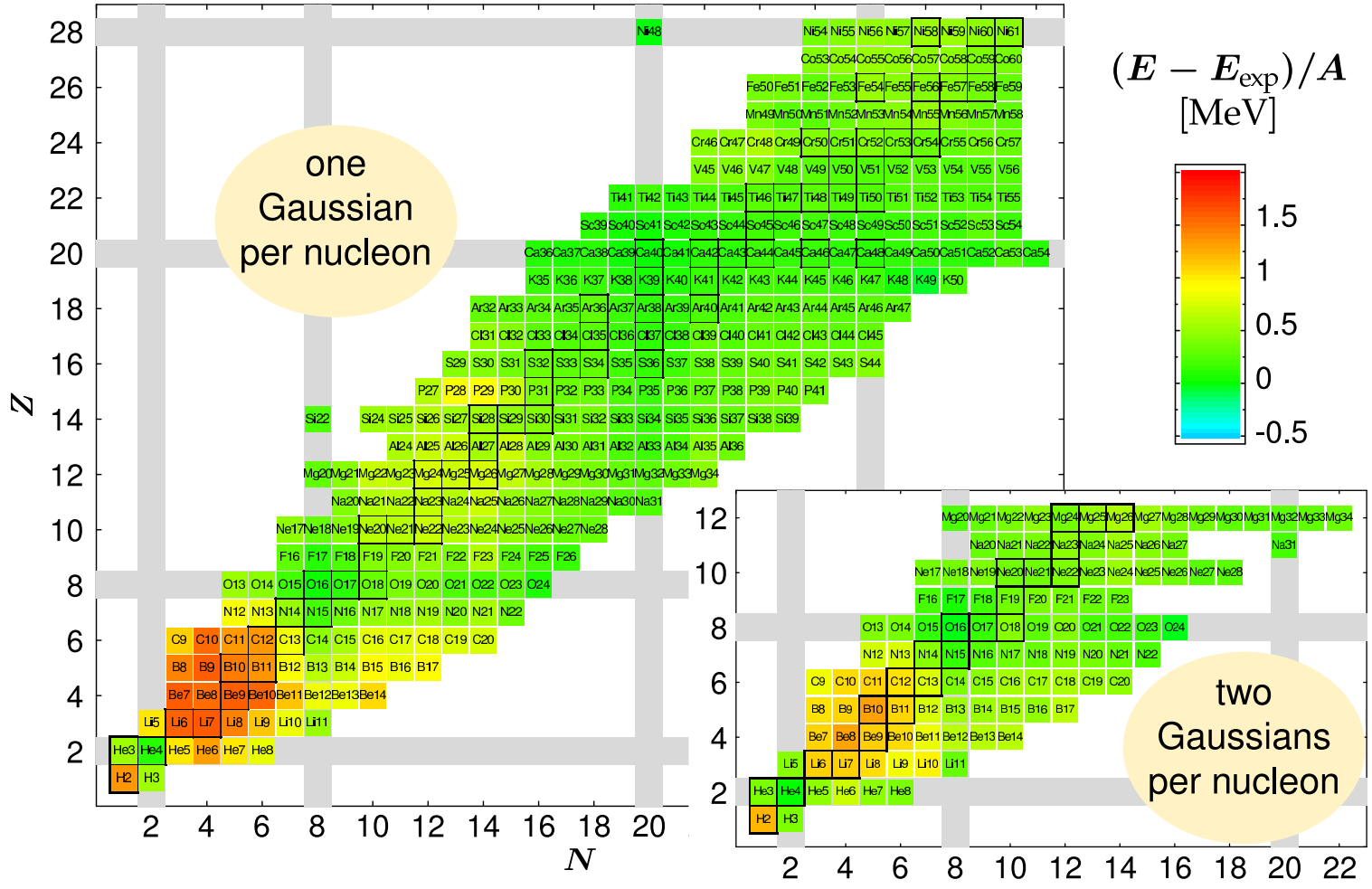
- isospin-independent attractive $\vec{\mathrm{L}}\cdot\vec{\mathrm{S}}$-potential

$$\mathrm{V_{LS}} = v_{LS}(\mathrm{r})\, \vec{\mathrm{L}} \cdot \vec{\mathrm{S}}$$

- parameters adjusted to binding energy of $^{24}\mathrm{O}$ and $^{48}\mathrm{Ca}$

$\sim 15\%$ of potential energy generated by correction

Chart of Nuclei



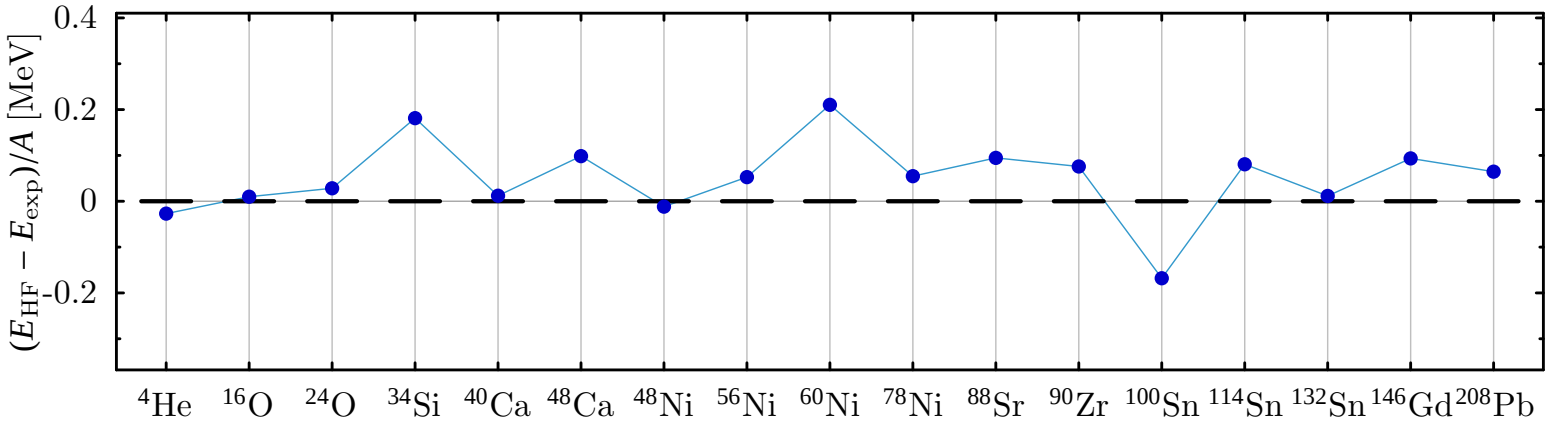
UCOM + HF

- UCOM interaction + K.E. + Coulomb: HF with finite-range forces
- Harmonic Oscillator basis: two-body matrix elements (2bMEs) in analytical form
- 2bMEs of interaction can be calculated separately and stored; same for all nuclei considered

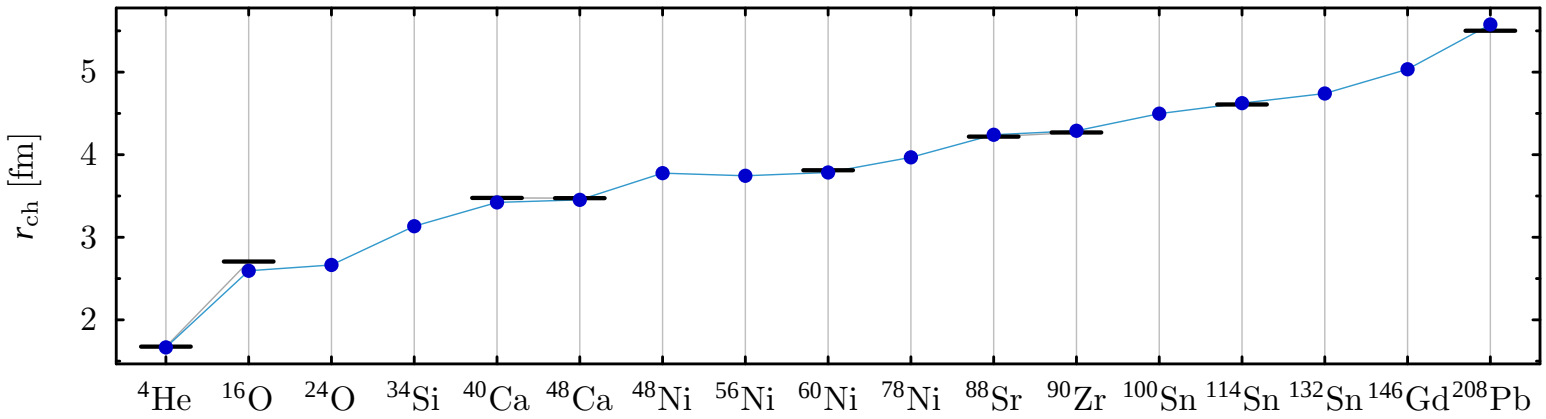
➜ suitable also for shell-model calculations

Preliminary results

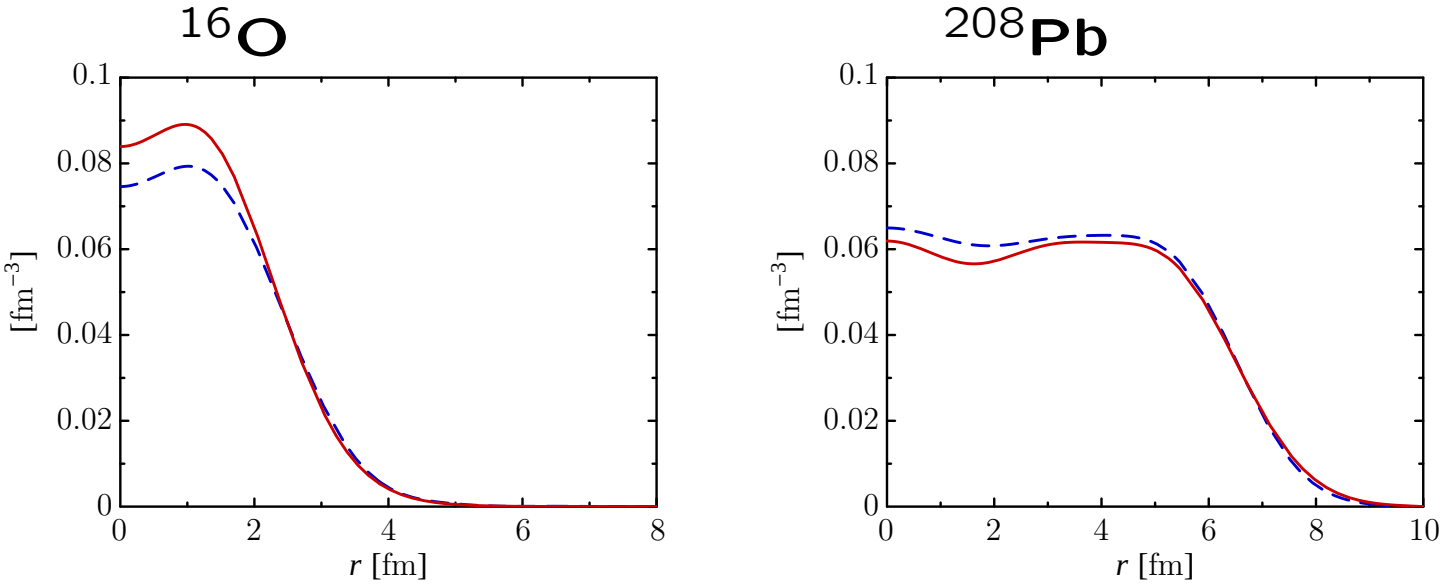
Binding energies



Charge rms radii



Preliminary results: Charge-density distributions



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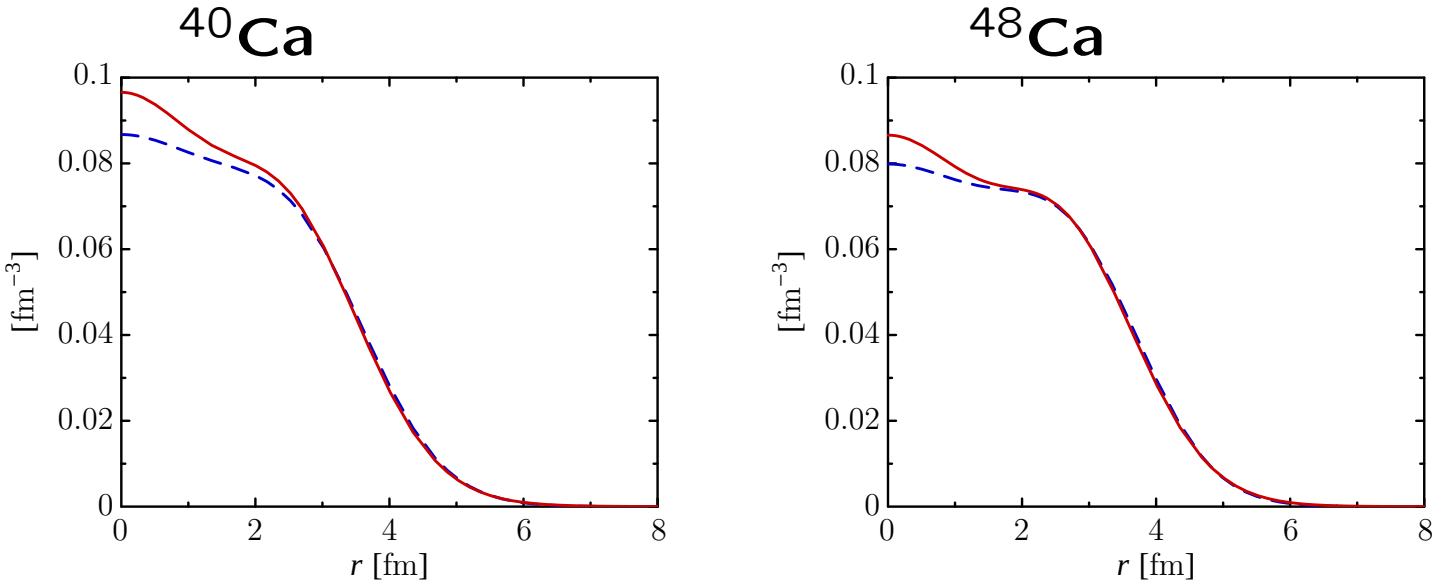

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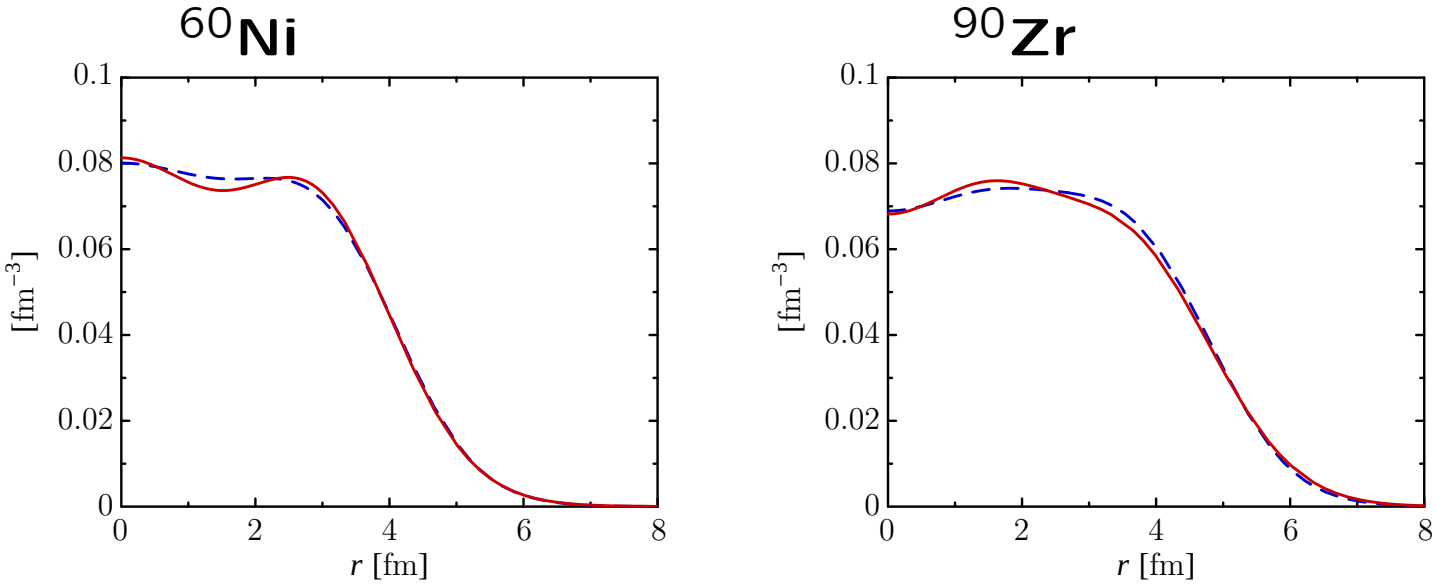

Summary - Perspectives

- The UCOM provides us with effective interactions based on realistic NN potentials
  - in tractable analytical form
  - same for all nuclei
  - suitable for MF-type calculations (simple many-body wave-functions)
  - and for shell-model calculations
- Hartree-Fock calculations now possible
  - Preliminary but promising results

✎ RPA calculations of excited states: coming up!