UCOM-Hartree-Fock with Realistic NN-Interactions

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The Unitary Correlation Operator Method (UCOM) provides a powerful means of combining numerically affordable many-body Hilbert spaces with the precision of current realistic NN-interactions [1, 2, 3]. Variational calculations in the mass range $A \lesssim 60$ using the Gaussian basis states of Fermionic Molecular Dynamics (FMD) have been reported previously.

Within the UCOM-Hartree-Fock scheme, it is possible to perform calculations using a realistic NN-interaction over the *whole* nuclear chart. Like in FMD, we employ a correlated version of the Argonne V18 interaction. We perform calculations in a configuration space approach, using a basis of spherical harmonic oscillator (HO) eigenstates, which allows us to implement central and tensor correlations in the two-nucleon system exactly. For HO states, one can also separate center-of-mass and relative motion exactly by means of a *Talmi transformation*. The interaction matrix elements are calculated once and stored for subsequent use in Hartree-Fock, No-Core Shell Model, RPA calculations, etc.

Bare realistic interactions usually feature both a strong repulsive core and a strong tensor force, causing a coupling of states of different momentum and energy scales. Converged results can then only be achieved by performing calculations in a Hilbert space of very large dimension, e. g., a spherical HO configuration space with excitations as high as several hundred $\hbar\omega$. The correlation procedure reduces this coupling and effectively pre-diagonalizes the interaction in momentum space. As a direct result, the convergence of self-consistent calculation schemes is improved notably.

In the case of Hartree-Fock calculations, the use of bare interactions does not yield bound systems at all — the treatment of correlations by UCOM techniques is *crucial*. Fig. 1 shows results for the binding energies of closed shell nuclei up to ^{208}Pb. The correlated interaction already reproduces the trends in the experimental binding energies very well.

By construction, the correlation operators are used to describe short-range correlations only. Long-range correlations should be treated by an appropriate choice of the model space. Thus, as a first step, we have used many-body perturbation theory to investigate the effect of the leading non-zero correction to the UCOM-HF results. The relevant term originates at the second order of the Goldstone expansion:

$$\Delta E^{(2)} = -\frac{1}{4}\sum_{i,j}^{\text{occ.}}\sum_{a,b}^{\text{unocc.}} \frac{|\langle ab|\, v_{\text{UCOM}}\, |ij\rangle|^2}{\epsilon_a + \epsilon_b - \epsilon_i - \epsilon_j}\,. \qquad (1)$$

It should be emphasized that the 'standard' Goldstone expansion can be applied because a Brueckner resummation is no longer necessary due to the correlation procedure. The lower line in Fig. 1 displays the improved results obtained with $\Delta E^{(2)}$ included, using HO shells up to $N_{\max} = 10$.

The treatment of long-range correlations can be further improved by performing RPA and coupled cluster calculations. Preliminary results from RPA are in agreement with the trend set by the perturbative treatment. We also plan to include pairing effects by performing Hartree-Fock-Bogoliubov calculations with the correlated interaction.

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References

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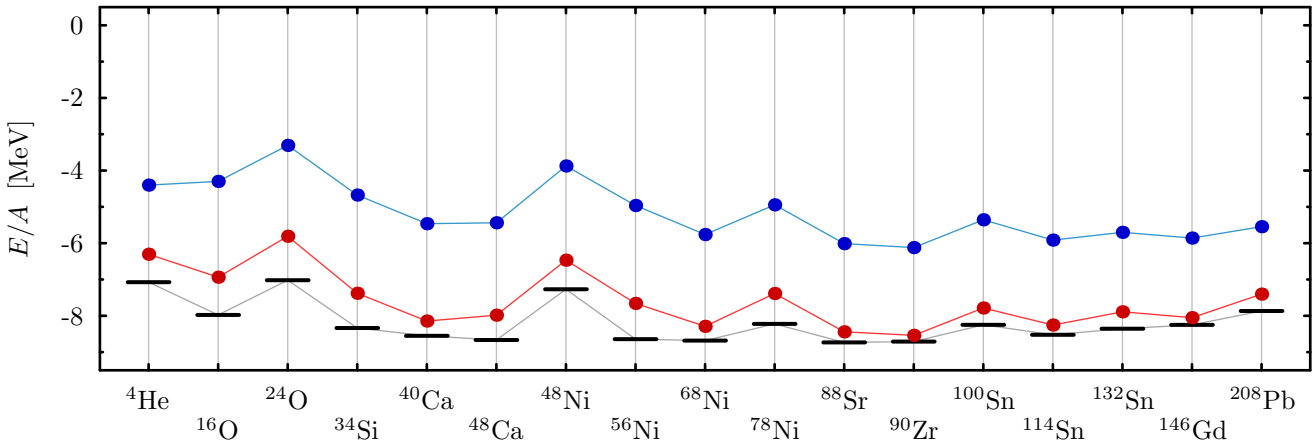

Figure 1: Binding energy per nucleon of closed shell nuclei. The results were obtained using the correlated Argonne V18 interaction alone (upper line), and including the perturbative correction (1) (lower line). Experimental values are indicated by black bars. HO shells up to $N_{\max} = 10$ were included.