Towards Ab Initio Nuclear Structure Calculations Based on Realistic NN-Potentials

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Abstract

The Unitary Correlation Operator Method (UCOM) provides a novel route towards *ab initio* nuclear structure calculations starting from realistic NN-potentials. The basic idea is to describe the dominant correlations—namely short-range central correlations generated by the repulsive core of the NN-potential and tensor correlations induced by the strong attractive tensor force—explicitly by means of a unitary transformation. The application of UCOM to the Argonne V18 potential is discussed and variational calculations within Fermionic Molecular Dynamics up to mass numbers $A \sim 60$ are presented.

1 Introduction

In recent years several realistic nucleon-nucleon interactions, like the Argonne V18 and the Bonn CD potentials, have been constructed on the basis of high-precision nucleon-nucleon scattering data. These potentials serve as a basis for *ab initio* nuclear structure calculations, e.g., in the framework of the Green's function Monte Carlo method which are presently feasible for nuclei up to mass numbers $A \lesssim 12$ [1]. The use of these realistic potentials for nuclear structure studies in heavier nuclei poses an enormous challenge. Traditional many-body methods, like Hartree-Fock or the multi-configuration shell-model, cannot be used in connection with the bare NN-interaction. The reason is the inability of the restricted model spaces to describe the dominant correlations, which are present in the exact many-body eigenstates.

The two most important types of correlations manifest themselves in the deuteron. Figure 1 depicts the diagonal elements of the spin-projected two-body density matrix $\rho^{(2)}_{1,M_S}(\vec{r})$ for the deuteron calculated with the AV18 potential. Two prominent features of the two-body density distribution are evident: (i) a complete suppression at small relative distances $\vec{r}$ and (ii) a pronounced angular structure relative to and depending on the spin orientation.

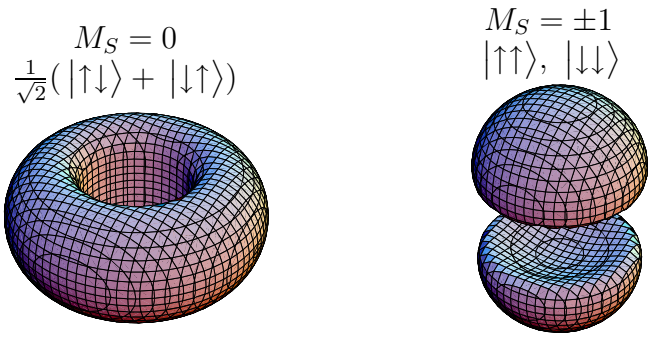

Figure 1: Spin-projected two-body density $\rho^{(2)}_{1,M_S}(\vec{r})$ of the deuteron calculated with the AV18 potential. Shown is an iso-density surface for 0.005 fm^{-3}.

The suppression of the two-body density at small interparticle distances is a direct signature of the *central correlations* induced by the repulsive core in the central part of the realistic potential. For energetic reasons the nucleons avoid the repulsive core which results in a suppression of the probability density for finding two nucleons at small distances. The pronounced angular structure is a manifestation of *tensor correlations*. Depending on the relative alignment of the spins of proton and neutron (parallel for $M_S = \pm 1$ or antiparallel for $M_S = 0$) the spatial two-body density distribution changes dramatically. For $M_S = 0$ the probability density is concentrated in the plane perpendicular to the spin direction (doughnut), whereas the probability density for $M_S = \pm 1$ is largest along the spin axis (dumb-bell). The situation is analogous to the classical dipole-dipole interaction: for parallel dipoles the interaction energy is minimal if the distance vector is parallel to the dipole orientation. For anti-parallel dipoles the distance vectors perpendicular to the dipole moments are energetically favoured. Neither of these correlations can be modelled by a single or a superposition of few Slater determinants. Therefore, a naive inclusion of the bare realistic NN-potential into a Hartree-Fock or multi-configuration shell-model calculation has to fail.

2 Unitary Correlation Operator Method

The basic idea of the Unitary Correlation Operator Method (UCOM) is to include the dominant correlations into the many-body state by means of a unitary transformation [2, 3]. Starting from an uncorrelated many-body state $|\Psi\rangle$, in the simplest case just a Slater determinant, a correlated state $|\widehat{\Psi}\rangle$ is

defined through the application of the unitary correlation operator $\mathbf{C}$:

$$\big|\widehat{\Psi}\big\rangle = \mathbf{C}\,\big|\Psi\big\rangle\ . \tag{1}$$

Alternatively one can perform a similarity transformation of the operators of all relevant observables (e.g. the Hamiltonian, coordinate and momentum space densities, transition operators, etc.):

$$\widehat{\mathbf{O}} = \mathbf{C}^{\dagger}\mathbf{O}\mathbf{C}\ . \tag{2}$$

Due to unitarity both approaches are equivalent. For the following many-body calculations the formulation through correlated operators is, however, more convenient.

We decompose the correlation operator $\mathbf{C}$ into a central correlator $\mathbf{C}_r$ and a tensor correlator $\mathbf{C}_\Omega$, reflecting the two dominant types of correlations in the many-body problem

$$\mathbf{C} = \mathbf{C}_\Omega\mathbf{C}_r = \exp\Big[-\mathrm{i}\sum_{i<j}\mathbf{g}_\Omega(ij)\Big]\exp\Big[-\mathrm{i}\sum_{i<j}\mathbf{g}_r(ij)\Big]\ . \tag{3}$$

Both operators are defined as exponentials of Hermitian two-body generators $\mathbf{g}_\Omega$ and $\mathbf{g}_r$, respectively. They are given in a closed analytic form and determine quite intuitively the way the correlation operators act.

Central Correlations. The task of the central correlator $\mathbf{C}_r$ is to generate the hole in the two-body density distribution at small particle distances caused by the strong repulsive core in the central part of the interaction. Pictorially speaking, $\mathbf{C}_r$ has to shift those pairs of particles, which are closer than the core radius, apart from one another. The two-body generator for this distance-dependent shift can be written as $\mathbf{g}_r = \frac{1}{2}[s(\mathbf{r})\mathbf{q}_r + \mathbf{q}_r s(\mathbf{r})]$, where $\mathbf{q}_r = \frac{1}{2}[\vec{\mathbf{q}}\cdot(\vec{\mathbf{r}}/\mathbf{r}) + (\vec{\mathbf{r}}/\mathbf{r})\cdot\vec{\mathbf{q}}]$ is the radial component of the relative momentum $\vec{\mathbf{q}}$ of a particle pair. The function $s(r)$ determines the distance dependence of the shift. It is large for small r and vanishes for large distances.

Tensor Correlations. The tensor correlation operator $\mathbf{C}_\Omega$ has to generate the complex angular structure of the two-body density distribution with respect to the spin orientation. Two nucleons with parallel spin are preferentially oriented with their relative position vector aligned with the spin. Nucleons with antiparallel spins prefer relative position vectors perpendicular to the spin direction. The tensor correlator has to generate this angular shift towards or away from the spin direction. An essential ingredient is the component of the relative momentum $\vec{\mathbf{q}}$ perpendicular to $\vec{\mathbf{r}}$, the so-called orbital momentum $\vec{\mathbf{q}}_\Omega = \vec{\mathbf{q}} - \frac{\vec{\mathbf{r}}}{\mathbf{r}}\ \mathbf{q}_r$. The generator has the form

$\mathbf{g}_\Omega = \frac{3}{2}\vartheta(\mathbf{r})\big[(\vec{\boldsymbol{\sigma}}_1\cdot\vec{\mathbf{q}}_\Omega)(\vec{\boldsymbol{\sigma}}_2\cdot\vec{\mathbf{r}}) + (\vec{\mathbf{r}}\leftrightarrow\vec{\mathbf{q}}_\Omega)\big]$ which is similar to the tensor operator. The function $\theta(r)$ describes the magnitude of the shift as a function of distance.

Correlated Operators and Cluster Expansion. For the following many-body calculations the notion of correlated operators is advantageous. The operators of all observables under consideration have to be transformed consistently. Since the correlation operators are defined as exponentials of two-body operators, the correlated operators contain irreducible contributions for all particle numbers. We organise the different irreducible terms according to their rank in a cluster expansion

$$\widehat{\mathbf{H}} = \mathbf{C}^\dagger\mathbf{H}\mathbf{C} = \widehat{\mathbf{H}}^{[1]} + \widehat{\mathbf{H}}^{[2]} + \widehat{\mathbf{H}}^{[3]} + \cdots \ . \tag{4}$$

Here we used the Hamiltonian $\mathbf{H} = \mathbf{T} + \mathbf{V}$ as an example, the same holds true for any other operator. If the range of the correlators is sufficiently small compared to the average particle distance in the many-body system, three-body and higher order terms in the cluster expansion are negligible and we can restrict ourselves to the computationally simple two-body approximation

$$\widehat{\mathbf{H}}^{C2} = \widehat{\mathbf{T}}^{[1]} + \widehat{\mathbf{T}}^{[2]} + \widehat{\mathbf{V}}^{[2]} = \mathbf{T} + \mathbf{V}_{\mathrm{UCOM}} \ , \tag{5}$$

where $\widehat{\mathbf{T}}^{[1]} = \mathbf{T}$ and $\widehat{\mathbf{T}}^{[2]}$ are the one- and two-body contributions of the correlated kinetic energy, resp., and $\widehat{\mathbf{V}}^{[2]}$ is the two-body part of the correlated NN-potential. All two-body contributions are subsumed in the correlated interaction $\mathbf{V}_{\mathrm{UCOM}}$. It is by construction *phase-shift equivalent* to the original, uncorrelated NN-potential as long as the correlators have finite range.

In order to ensure the validity of the two-body approximation, we restrict the range of the correlation functions—most notably for the tensor correlator. The correlation functions for a given potential are determined for each spin-isospin channel by a constrained energy minimisation in the two-body system.

3 Correlated Realistic NN-Potentials

We employ the Unitary Correlation Operator Method to construct a correlated interaction based on the Argonne V18 potential [4]. The charge independent components of the AV18 potential can be written in the following operator representation

$$\begin{aligned}\mathbf{V} = &\sum_{S,T}\left[v_{ST}^{c}(\mathbf{r}) + v_{ST}^{l2}(\mathbf{r})\ \vec{\mathbf{L}}^2\right]\boldsymbol{\Pi}_{ST} \\ &+ \sum_{T}\left[v_{T}^{t}(\mathbf{r})\ \mathbf{S}_{\mathbf{12}} + v_{T}^{ls}(\mathbf{r})\ (\vec{\mathbf{L}}\cdot\vec{\mathbf{S}}) + v_{T}^{ls2}(\mathbf{r})\ (\vec{\mathbf{L}}\cdot\vec{\mathbf{S}})^2\right]\boldsymbol{\Pi}_{1T}\ ,\end{aligned} \tag{6}$$

where $\mathbf{\Pi}_{ST}$ is the projection operator onto the different spin S and isospin T channels. Applying the central and tensor correlators leads to a correlated interaction $\mathbf{V}_{\mathrm{UCOM}}$ with transformed radial dependencies $\widehat{v}^{\circ}_{ST}(r)$. These functions depend on the original radial dependencies $v^{\circ}_{ST}(r)$ as well as on the tensor and central correlation functions. Moreover, new operator terms emerge. Correlating the kinetic energy, for example, leads to an additional momentum dependent two-body term of the form $\vec{\mathbf{q}}\ \hat{v}^{qq}_{ST}(\mathbf{r})\ \mathbf{\Pi}_{ST}\ \vec{\mathbf{q}}$. The tensor correlator generates various additional terms, e.g., operators containing the angular momentum $\vec{\mathbf{L}}$ or the orbital momentum $\vec{\mathbf{q}}_{\Omega}$.

The nature of the correlated interaction $\mathbf{V}_{\mathrm{UCOM}}$ can be understood in different ways. By means of the unitary transformation the bare potential is *tamed*, meaning that the exact eigenstates of the correlated Hamiltonian do not exhibit the dominant central and tensor correlations anymore (compare Fig. 1). The correlated Hamiltonian is thus well suited for an approximate treatment of the many-body problem in a simplified Hilbert space. Alternatively one may say that the unitary transformation pre-diagonalises the Hamiltonian with respect to a simple many-body basis of Slater determinants. From another point of view the correlator separates low- and high-momentum degrees of freedoms in that it treats the high-momentum, short-range features of the many-body state, i.e. the short-range correlations, explicitly and leaves a correlated Hamiltonian for describing the low-momentum properties. At this point the connection to the $V_{\mathrm{low}-k}$ [5] approach is evident.

Phenomenological Corrections. So far, we have restricted ourselves to a two-body interaction. It is well known, that these two-body interactions alone cannot adequately describe the properties of finite nuclei. Quasi-exact Green's function Monte Carlo calculations for light nuclei have demonstrated that binding energies and the charge radii obtained with realistic two-body potentials are significantly smaller than the experimental values [1]. This discrepancy is remedied by introducing a local three-body force which is adjusted to ground and low-lying excited states of light nuclei. Recent developments in chiral perturbation theory might supersede these phenomenological three-body forces and lead towards realistic, first-principles three-body interactions.

In principle the inclusion of three-body forces is also possible in our framework. However, the computational effort to evaluate three-body matrix elements within a many-body system would be enormous. Within a pragmatic approach we, therefore, utilise a momentum dependent two-body correction to simulate the effect of genuine three-body forces. The correction also accounts for residual higher-order contributions of the cluster expansion and missing long-range tensor correlations.

We use a spin-isospin independent (Wigner type) correction consisting of a local, a momentum dependent and a spin-orbit term

$$\mathbf{V}_{\rm corr} = v^c(\mathbf{r}) + \vec{\mathbf{q}}\, v^{qq}(\mathbf{r})\, \vec{\mathbf{q}} + v^{ls}(\mathbf{r})\, (\vec{\mathbf{L}} \cdot \vec{\mathbf{S}}) \; . \tag{7}$$

Each of the three radial dependencies is described by a single Gauss function. The parameters of the central and momentum dependent part (2 range and 2 strength parameters) are adjusted such that the binding energy and the rms-radii of ^{4}He, ^{16}O, and ^{40}Ca agree with experiment. The strength of the spin-orbit correction is chosen such that the binding energy of ^{24}O and ^{48}Ca are consistent with experiment. For finite nuclei the correction will contribute roughly 15% to the total potential energy.

4 Variational Ground State Calculations

In a first step we tackle the many-body problem in the framework of a variational model. The many-body trial state is given by a simple Slater determinant

$$\big|Q\big\rangle = \mathcal{A}(\, \big|q_1\big\rangle \otimes \, \big|q_2\big\rangle \otimes \cdots \otimes \, \big|q_A\big\rangle) \tag{8}$$

composed of single-particle states

$$\big|q\big\rangle = \sum_{\nu=1}^{n} c_\nu \;\, \big|a_\nu, \vec{b}_\nu\big\rangle \otimes \, \big|\chi_\nu\big\rangle \otimes \, \big|m_t\big\rangle \; . \tag{9}$$

Their coordinate space part is given by a Gaussian wave packet $\big\langle \vec{x}\big|a_\nu, \vec{b}_\nu\big\rangle = \exp[-(\vec{x} - \vec{b}_\nu)^2/(2\, a_\nu)]$ with a complex vector $\vec{b}_\nu$ encoding mean position and mean momentum of the wave packet and a complex width parameter a_ν. Several wave packets with different spin orientations can be superposed to enhance the flexibility of the single-particle trial states. These trial states—the basis of the Fermionic Molecular Dynamics (FMD) approach [6]—prove to be extremely versatile. Spherical shell-model type states as well as intrinsically deformed and α-cluster configurations can be described.

Figures 2 and 4 summarise the results of large-scale variational calculations for nuclei up to $A \sim 60$. For each nucleus the intrinsic energy, i.e. the expectation value of $\widehat{\mathbf{H}}^{C2} + \mathbf{V}_{\rm corr} - \mathbf{T}_{\rm cm}$, is minimised. Over all, the binding energies and the charge radii of the ground state show a nice agreement with experimental data. Sizable deviations from the experimental binding energies appear for p-shell and to a lesser extend for sd-shell nuclei. This deviation has two origins: (i) A single Gaussian wave packet for the wave function of each nucleon is not optimally suited for light isotopes. A generalisation of the single particle trial-states by considering a superposition of two Gaussians leads to

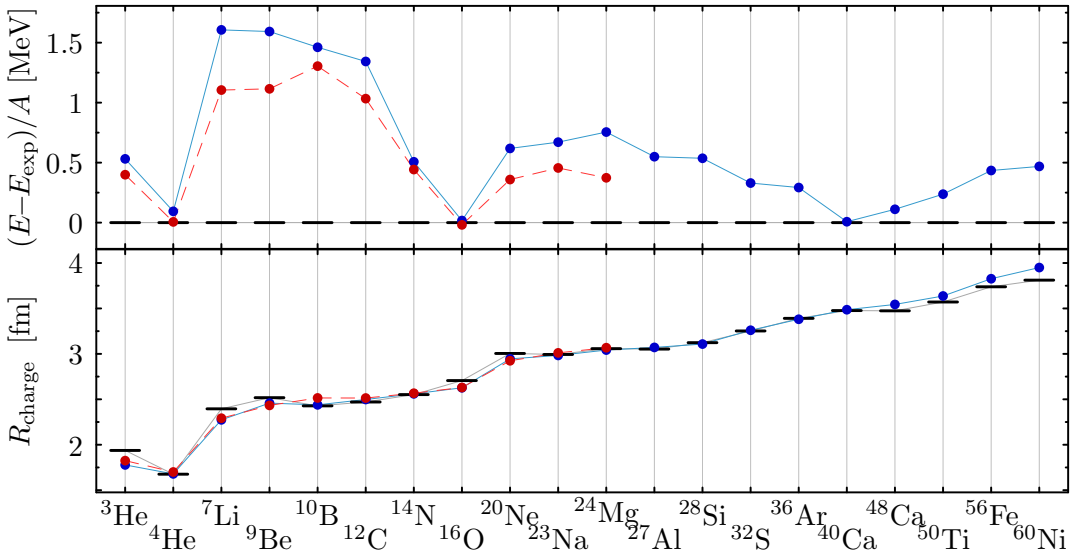

Figure 2: Deviation from the experimental binding energy per nucleon (upper panel) and charge radius (lower panel) for various stable isotopes. Shown are the results with one Gaussian wave packet per nucleon (——) and with two Gaussians per nucleon (– – –).

a significant improvement as Figs. 2 and 3 show. (*ii*) Away from the magic numbers the variational ground states exhibit strong intrinsic deformations. A projection of these intrinsic states onto angular momentum eigenstates becomes necessary and leads to a further reduction of the ground state energy. At the same time one obtains information on the whole rotational band. A detailed discussion of angular momentum projection and multi-configuration calculations within the UCOM/FMD framework is presented in a separate contribution in this volume.

In summary, the Unitary Correlations Operator Method is a promising tool to facilitate nuclear structure calculations on the basis of realistic NN-potentials. The correlated interaction can be used in connection with a variety of traditional nuclear structure methods. Beyond the variational calculations presented here, Hartree-Fock calculations for larger nuclei are a natural next step.

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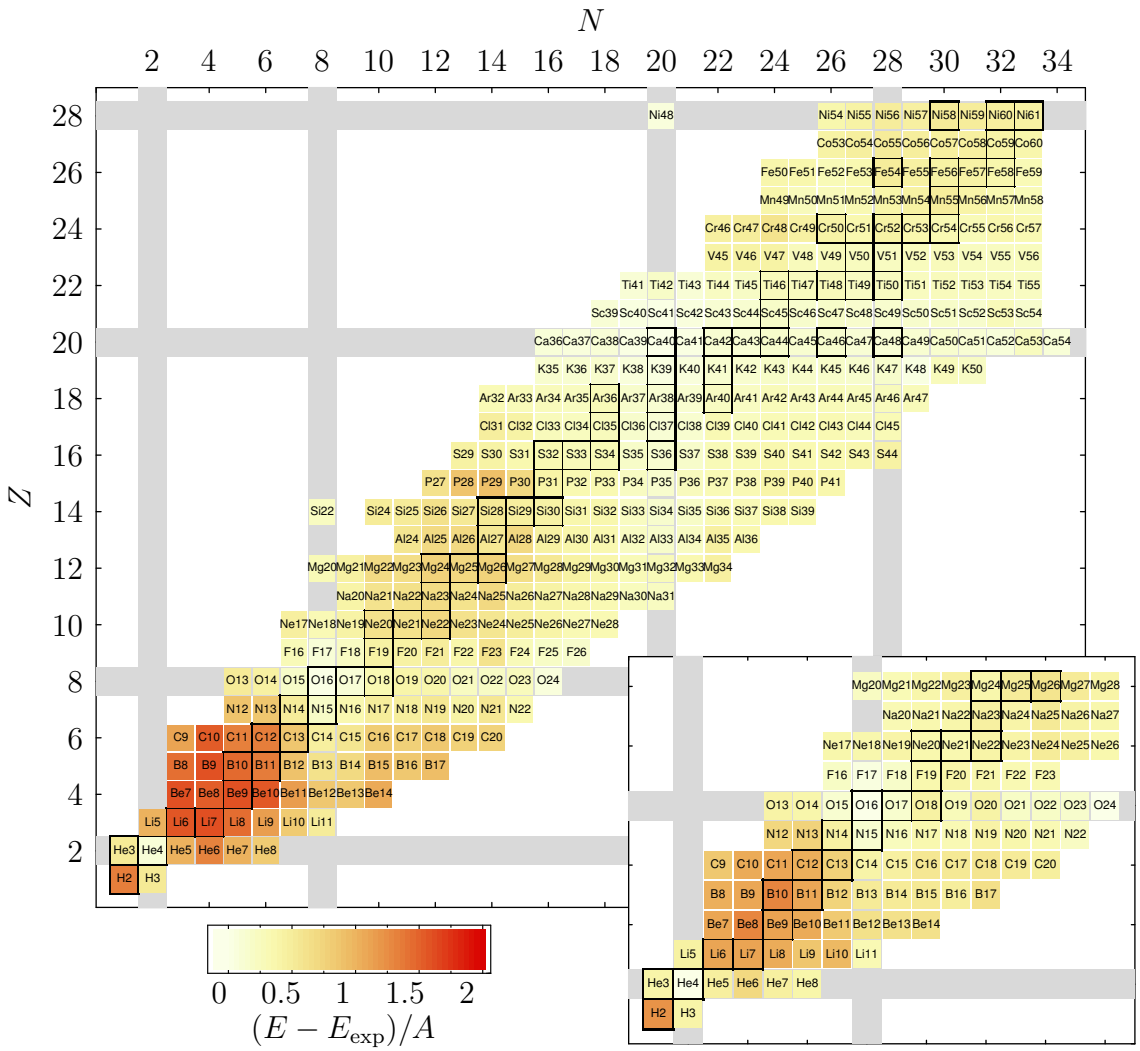

Figure 3: Chart of isotopes. The colour coding represents the difference between the variational and the experimental binding energy per nucleon $(E - E_{\rm exp})/A$. The main chart was obtained with a single Gaussian wave packet per nucleon. The inset shows results with two Gaussians per nucleon.

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