A unitary correlation operator method

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Abstract

The short range repulsion between nucleons is treated by a unitary correlation operator which shifts the nucleons away from each other whenever their uncorrelated positions are within the replusive core. By formulating the correlation as a transformation of the relative distance between particle pairs, general analytic expressions for the correlated wave functions and correlated operators are given. The decomposition of correlated operators into irreducible n–body operators is discussed. The one– and two–body–irreducible parts are worked out explicitly and the contribution of three–body correlations is estimated to check convergence. Ground state energies of nuclei up to mass number $A = 48$ are calculated with a spin–isospin–dependent potential and single Slater determinants as uncorrelated states. They show that the deduced energy– and mass–number–independent correlated two–body Hamiltonian reproduces all "exact" many–body calculations surprisingly well.

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1 Introduction

In many–body physics the most convenient trial states are products of single–particle states which for identical bosons or fermions are symmetrized or anti-symmetrized with respect to particle exchange. An adequately selected set of those product states spans a subspace of the Fock space called model space. In the following we shall use the term product state for bosons and fermions as well and proper statistics is implied without mentioning.

For particles with a rigid internal structure like atoms or nucleons the two–body interaction between the particles contains a short–ranged repulsive core. For this situation product states are not appropriate because a numerically tractable number of them can usually not represent the strong depletion of probability in the two–body density distribution at short distances between the particles. Or in other words, the true eigenstates of the exact Hamiltonian contain components which lie outside the model space in the so–called Q–space.

There are in general two types of methods to remedy the incompatibility of the Hamiltonian with the trial states which span the model space [1]. The first is to adapt the Hamiltonian by replacing the interaction with an effective one which takes the scattering between model space and Q–space into account. The Brueckner G–Matrix formalism is of this type [2]. The method of effective operators allows to calculate the whole spectrum of low lying states including transitions between them.

The second way is to introduce the short–range repulsive correlations into the many–body state by applying correlation operators [3] onto the trial product state. In the simplest case it is a multiplication with Jastrow correlation functions [4]. This approach is mainly used to find ground–state energies by minimizing with respect to the parameters contained in the correlated trial state. Spectra and transitions cannot be calculated easily in this scheme.

In this article we propose the Unitary Correlation Operator Method (UCOM), which to a certain extend combines the advantages of the above mentioned schemes. It correlates the product state, $|\,\Phi\,\rangle$, by means of a unitary correlator, C. The identity

$$\langle\,\Psi\,|\,H\,|\,\Psi'\,\rangle = \langle\,\Phi\,|\,C^\dagger\,H\,C\,|\,\Phi'\,\rangle = \langle\,\Phi\,|\,C^{-1}\,H\,C\,|\,\Phi'\,\rangle = \langle\,\Phi\,|\,\widehat{H}\,|\,\Phi'\,\rangle \quad (1)$$

shows that one may either speak of the original "untamed" Hamiltonian H sandwiched between correlated states $|\,\Psi\,\rangle = C\,|\,\Phi\,\rangle$ or of a correlated Hamiltonian $C^{-1}\,H\,C$ represented in the model space of the uncorrelated product states $|\,\Phi\,\rangle$. The task of the correlator C is to "tame" the short–ranged repulsive part of H by means of a unitary transformation. This general idea exists

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for a long time [5–7] but has not been pursued very much.

When the correlator C is applied to the Hamiltonian the method can be regarded as a pre-diagonalization such that large matrix elements connecting model space and Q–space are removed. $\widehat{H} = C^{-1} H C$ can then for example be diagonalized in a shell model configuration space in order to describe long–range many–body correlations in low lying eigenstates. In this sense it is similar to the method of effective operators, although there a projection onto the model space is used rather than a unitary transformation.

When C acts on the uncorrelated state $\mid \Phi \rangle$ one has more the picture of a trial ansatz for the many–body state as for example used in Jastrow–type methods. However, the advantage of a unitary C is that the norms $\langle \Psi \mid \Psi \rangle = \langle \Phi \mid C^\dagger C \mid \Phi \rangle = \langle \Phi \mid \Phi \rangle$ of correlated and uncorrelated states are identical so that there is no need to develop expansion methods when calculating the denominator in expectation values like $\langle \Phi \mid C^\dagger H C \mid \Phi \rangle / \langle \Phi \mid C^\dagger C \mid \Phi \rangle$ [8].

We propose to write C as a generalized shift operator, which moves two particles away from each other whenever they are within the classically forbidden region of the repulsive core. In section 2 we discuss the many–body nature of the correlator C and of the correlated operators and give analytic expressions for C and the correlated Hamiltonian in terms of a coordinate transformation of the relative distance. In the two–body space the resulting correlated Hamiltonian has no repulsive core anymore, instead a non-locality occurs at short distances which is written in terms of a quadratic momentum dependence with a reduced mass which is a function of the distance. The eigenstates, bound as well as scattering states, of the correlated Hamiltonian coincide with the exact eigenstates of the original Hamiltonian outside the range of the correlator, therefore the two interactions are completely phase–shift equivalent [9,10].

For the many–body system our aim is to devise a correlator which does not depend on energy and particle number so that the same correlated Hamiltonian $\widehat{H}$ can be used for many nuclei. In section 4 results will be given for mass numbers ranging from $A = 2$ to $A = 48$. The main problem consists in separating the variational degrees of freedom residing in the correlator C from those in the product state $\mid \Phi \rangle$ such that the irreducible three– and higher–body parts of $\widehat{H}$ remain small. These aspects are discussed in section 2.4 and in section 3, where the concept is applied to spin–isospin–independent forces and small nuclei first. The convergence of the expansion of the correlated Hamiltonian into one–, two– and three–body parts is discussed in terms of a smallness parameter which is the product of the density times a correlation volume.

Then in section 4 the correlator is extended to spin–isospin–dependent forces which are more realistic for heavier nuclei. We calculate ground state energies up to ^{48}Ca and compare them to existing "exact" results. The agreement is

astonishing considering that the uncorrelated many–body states are single Slater determinants.

2   The concept of a unitary correlator

In this section the advantage of representing improved trial states by a unitary transformation of product states will be elucidated in a quite general way. The following subsections will explain in detail the explicit form of the correlator C and the expansion of a correlated operator into n–body operators, in particular the expansion of the correlated Hamiltonian.

Throughout this section we use the convention that $|\Psi\rangle$ or $|\psi\rangle$ stand for correlated states and $|\Phi\rangle$ or $|\phi\rangle$ for uncorrelated states. The states $|\Phi_n\rangle$ denote a basis set of many–body product states (symmetrized or antisymmetrized if necessary).

The eigenstates $|n\rangle$ of the many–body eigenvalue problem

$$H\,|\,n\,\rangle = E_n\,|\,n\,\rangle \tag{2}$$

can be written as

$$|\,n\,\rangle = C[H,\Phi]\ |\,\Phi_n\,\rangle \tag{3}$$

where $C\,[H,\Phi]$ is the unitary operator

$$C[H,\Phi] = \sum_k\ |\,k\,\rangle\langle\,\Phi_k\,| \tag{4}$$

which diagonalizes the Hamiltonian H.

The idea is to devise a unitary correlation operator C which approximates $C[H,\Phi]$ for low energies, i.e. for states $|\,k\,\rangle$ with E_k in the vicinity of the ground state. From (4) it is clear that C depends on the choice of the product states $|\,\Phi_k\,\rangle$ and on the Hamiltonian H via its eigenstates $|\,k\,\rangle$.

Since there is a certain amount of freedom in choosing the single–particle states which build the product states $|\,\Phi_n\,\rangle$ there is no need to be so ambitious to really approximate $C[H,\Phi]$ in the sense of an operator equality $C = C[H,\Phi]$. One rather divides the burden among C and $|\,\Phi_n\,\rangle$ in such a way that $|\,\Phi_n\,\rangle$ or linear combinations of a small number of $|\,\Phi_n\,\rangle$ describe the long–range correlations (mean field, deformations) while C takes care of the short–range repulsive correlations.

In other words the physical task of C is to provide a mapping between the Hilbert space spanned by low lying correlated states $|\,k\,\rangle$ and the Hilbert space of uncorrelated product states $|\,\Phi_k\,\rangle$ which do not contain (repulsive) short–range correlations.

One main advantage of a unitary correlator C is that the correlated state

$$|\,\Psi\,\rangle = C\,|\,\Phi\,\rangle \tag{5}$$

has the same norm as the uncorrelated state $|\,\Phi\,\rangle$ so that the norm in the denominator of an expectation value

$$\langle\,\Psi\,|\,B\,|\,\Psi\,\rangle = \frac{\langle\,\Phi\,|\,C^\dagger\,B\,C\,|\,\Phi\,\rangle}{\langle\,\Phi\,|\,C^\dagger C\,|\,\Phi\,\rangle} \tag{6}$$

does not require special treatment as for example in the Jastrow method [4,8].

If the correlator C is chosen to be state independent one may equivalently use correlated states $|\,\Psi\,\rangle$ and uncorrelated operators B or uncorrelated states $|\,\Phi\,\rangle$ and correlated operators $\widehat{B}$

$$\langle\,\Psi\,|\,B\,|\,\Psi'\,\rangle = \langle\,\Phi\,|\,\widehat{B}\,|\,\Phi'\,\rangle\,, \tag{7}$$

where the correlated operator

$$\widehat{B} = C^\dagger\,B\,C = C^{-1}\,B\,C \tag{8}$$

does not dependent on the particular states $|\,\Phi\,\rangle$ and $|\,\Phi'\,\rangle$.

If C is not unitary as for example in the Jastrow method [4] one may from eq. (6) also define a correlated operator $\widehat{B}_{\text{Jastrow}}$ as

$$\widehat{B}_{\text{Jastrow}} = \frac{C^\dagger_{\text{Jastrow}}\,B\,C_{\text{Jastrow}}}{\langle\,\Phi\,|\,C^\dagger_{\text{Jastrow}}C_{\text{Jastrow}}\,|\,\Phi\,\rangle}\,, \tag{9}$$

but this depends on the state $|\,\Phi\,\rangle$.

For a unitary correlator C there is the duality that one may regard C as a part of the trial state $C\,|\,\Phi\,\rangle$ which provides further variational degrees of freedom beyond those already contained in $|\,\Phi\,\rangle$. Or one may view C as a unitary transformation of the Hamiltonian which amounts to a pre-diagonalization

$$\langle\,\Psi_k\,|\,H\,|\,\Psi_l\,\rangle = \langle\,\Phi_k\,|\,C^{-1}\,H\,C\,|\,\Phi_l\,\rangle = \langle\,\Phi_k\,|\,\widehat{H}\,|\,\Phi_l\,\rangle\,. \tag{10}$$

This means that the transformed Hamiltonian $\widehat{H} = C^{-1} H C$ is much better represented in the product basis $|\Phi_n\rangle$ than the original Hamiltonian.

Both ways of viewing the correlator C are mathematically equivalent. The first, where C is part of the trial state, is more suited for the Ritz variational principle where one wants to find only the ground state and its energy. The second is better adopted to the language of multi–configuration mixing and effective operators. In any case the physics contained in C is the same, namely to describe the short range correlations.

2.1 Decomposition of correlated operators into n–body operators

In order to ensure unitarity the correlator C is written as

$$C = \exp\{-iG\} , \qquad G = G^\dagger , \tag{11}$$

where G is the hermitean generator of the correlations. Because we treat fermion systems in this work, particle number conserving generators are considered only. Furthermore the generator G is invariant under permutations of the particles. G has to be a two–body operator or higher because a one–body operator would only cause a unitary transformation of the single–particle states and this variational degree of freedom is already present in the product–state $|\Phi\rangle$.

$$G = \sum_{i<j}^{A} g(i,j) + \text{three–body} + \text{higher} \tag{12}$$

Any correlated operator

$$\widehat{B} = C^{-1} B C = \exp\{+iG\} B \exp\{-iG\} \tag{13}$$

will therefore be in general a superposition of zero–, one–, two–, three– and higher–particle operators.

In order to avoid confusion we will use the following notation. An irreducible n–body operator B in an A–particle space is denoted as

$$B_A^{[n]} = \sum_{i_1 < \cdots < i_n}^{A} b^{[n]}(i_1, \cdots, i_n) , \tag{14}$$

where $b^{[n]}(i_1, \cdots, i_n)$ is the actual operator with the n particle indices $i_1, \cdots, i_n$. If $n > A$ then $B_A^{[n]} = 0$. For example, the Hamiltonian which consists of a one–body kinetic energy T and a two–body potential V is written in this elaborate way as

$$H = T + V \equiv H_A = T_A^{[1]} + V_A^{[2]} = \sum_i^A t^{[1]}(i) + \sum_{i<j}^A v^{[2]}(i,j) \ . \tag{15}$$

A missing superscript $[n]$ means that the operator is a combination of different many–body operators. Of course later on when there is no danger of confusion, superscripts and subscripts are omitted again.

The decomposition of the correlated operator $\widehat{B} \equiv \widehat{B}_A$ into a sum of irreducible n–body operators is written as

$$\widehat{B}_A \equiv C_A^{-1} \, B_A \, C_A = \sum_{n=0}^A \widehat{B}_A^{[n]} \ , \tag{16}$$

where in the A–body space the n–body operator

$$\widehat{B}_A^{[n]} = \sum_{i_1 < \cdots < i_n}^A \widehat{b}^{[n]}(i_1, \cdots, i_n) \qquad \text{for} \quad n \geq 1 \tag{17}$$

is given by

$$\widehat{b}^{[n]} := \widehat{B}_n - \sum_{k=1}^{n-1} \widehat{B}_n^{[k]} \tag{18}$$

$$= C_n^{-1} \, B_n \, C_n - \sum_{k=1}^{n-1} \sum_{i_1 < \cdots < i_k}^n \widehat{b}^{[k]}(i_1, \cdots, i_k) \ .$$

The first non-vanishing $\widehat{b}^{[n]}$ depends on how many particles the operator B connects. The trivial case is when B is proportional to the unit operator then $\widehat{B}_A = C_A^{-1} B_A C_A = \widehat{B}_A^{[0]} = B_A$. If $B = \sum_{i_1 < \cdots < i_m}^A b^{[m]}(i_1, \cdots, i_m)$ is an m–body operator then the first non-vanishing contribution comes from $\widehat{b}^{[m]}$ and is given by

$$\widehat{b}^{[m]} = C_m^{-1} \, b^{[m]} \, C_m \ . \tag{19}$$

The decomposition (16) is often called "cluster expansion". This is at this stage somewhat misleading as the particles $i_1, i_2, \cdots, i_n$ whose coordinates show up in $\widehat{b}^{[n]}(i_1, \cdots, i_n)$ need not be close to each other.

From now on we assume the generator to be a two–body operator $G = \sum_{i<j}^{A} g(i,j)$. Of particular interest is the effect of the correlation on one– and two–body operators. For example the kinetic energy, a one–body operator, transforms to

$$\widehat{T}_A \equiv C_A^\dagger \, T_A \, C_A = \widehat{T}_A^{[1]} + \widehat{T}_A^{[2]} + \widehat{T}_A^{[3]} + \cdots \;, \tag{20}$$

where the one–body part is just the regular uncorrelated kinetic energy

$$\widehat{T}_A^{[1]} = \sum_i^A \widehat{t}^{[1]}(i) = \sum_i^A t^{[1]}(i) = T_A^{[1]} \tag{21}$$

because the generator is a two–body operator. The two–body part $\widehat{T}_A^{[2]}$ is obtained from the general eqs. (17) and (18) as

$$\widehat{T}_A^{[2]} = \sum_{i<j}^A \widehat{t}^{[2]}(i,j) \qquad \text{with} \tag{22}$$

$$\widehat{t}^{[2]}(i,j) = c(i,j)^{-1}\Big(t^{[1]}(i) + t^{[1]}(j)\Big)\, c(i,j) - \Big(t^{[1]}(i) + t^{[1]}(j)\Big)$$

and $c(i,j) = \exp\{-ig^{[2]}(i,j)\}$ denotes the correlator between particle i and j. The obvious meaning is that for each pair (i,j) the two–body part is the difference between correlated and uncorrelated kinetic energy for the pair. The three–body part of the correlated kinetic energy operator is according to eqs. (17) and (18) given by

$$\widehat{T}_A^{[3]} = \sum_{i<j<k}^A \widehat{t}^{[3]}(i,j,k) \qquad \text{and} \tag{23}$$

$$\widehat{t}^{[3]}(i,j,k) = c(i,j,k)^{-1}\Big(t^{[1]}(i) + t^{[1]}(j) + t^{[1]}(k)\Big)\, c(i,j,k)$$
$$\qquad - \Big(\widehat{t}^{[2]}(i,j) + \widehat{t}^{[2]}(i,k) + \widehat{t}^{[2]}(j,k)\Big)$$
$$\qquad - \Big(t^{[1]}(i) + t^{[1]}(j) + t^{[1]}(k)\Big)$$

with $c(i,j,k) = \exp\{-i(g^{[2]}(i,j) + g^{[2]}(i,k) + g^{[2]}(j,k))\}$. The three–body part correlates all triples (i,j,k) of the system. But it is important to note that only the genuine irreducible three–body correlations appear in (23) because all two–body correlations and the uncorrelated kinetic energy are subtracted out.

When transforming a two–body operator $V_A^{[2]} = \sum_{i<j} v^{[2]}(i,j)$ like the potential, the correlated operator

$$\widehat{V}_A \equiv C_A^{-1} \, V_A \, C_A = \widehat{V}_A^{[2]} + \widehat{V}_A^{[3]} + \cdots \tag{24}$$

starts with a two–body part which is already correlated

$$\widehat{V}_A^{[2]} = \sum_{i<j}^A \widehat{v}^{[2]}(i,j) \qquad \text{with} \tag{25}$$

$$\widehat{v}^{[2]}(i,j) = c(i,j)^{-1} \, v^{[2]}(i,j) \, c(i,j) \ .$$

This means that the bare interaction $v^{[2]}$ is in lowest order replaced by the correlated interaction $\widehat{v}^{[2]}$ which will be much less repulsive at short distances.

The specific form of eq. (18) for the three–body part is

$$\widehat{V}_A^{[3]} = \sum_{i<j<k}^A \widehat{v}^{[3]}(i,j,k) \qquad \text{with} \tag{26}$$

$$\widehat{v}^{[3]}(i,j,k) = c(i,j,k)^{-1} \left(v^{[2]}(i,j) + v^{[2]}(i,k) + v^{[2]}(j,k) \right) c(i,j,k)$$
$$- \left(\widehat{v}^{[2]}(i,j) + \widehat{v}^{[2]}(i,k) + \widehat{v}^{[2]}(j,k) \right) \ .$$

From the explicit way of writing eqs. (23) and (26) it is obvious that the three–body part will only contribute appreciably if the probability of finding three particles simultaneously in the correlation volume is high. The importance of the three–body correlations will be discussed in more detail in section 3.3.

Another very important issue is the "cluster decomposition property". If a system decomposes into locally separated subsystems with particle numbers $A, B, \ldots, Z$, which means that the uncorrelated state can be written as

$$| \, \Phi \, \rangle = | \, \Phi_A \, \rangle \otimes | \, \Phi_B \, \rangle \otimes \cdots \otimes | \, \Phi_Z \, \rangle \tag{27}$$

where $| \, \Phi_A \, \rangle$, $| \, \Phi_B \, \rangle$ and so on are locally disconnected, then

$$C \, | \, \Phi \, \rangle = C_A \, | \, \Phi_A \, \rangle \otimes C_B \, | \, \Phi_B \, \rangle \otimes \cdots \otimes C_Z \, | \, \Phi_Z \, \rangle \ . \tag{28}$$

From the construction of C, which is

$$C = \exp\left\{ - i \sum_{i<j}^{A+B+\cdots+Z} g^{[2]}(i,j) \right\} , \tag{29}$$

the validity of the decomposition property is obvious because first, $g^{[2]}(i,j) = 0$ if i and j do not belong to the same subsystem and second, $[g^{[2]}(i,j), g^{[2]}(k,l)] = 0$ if $(i,j) \in A$ and $(k,l) \notin A$. Therefore, C can be decomposed as

$$C \,|\, \Phi \,\rangle = \exp\Big\{ -i \sum_{i<j}^{A} g^{[2]}(i,j) \Big\} \,|\, \Phi_A \,\rangle \otimes \cdots \tag{30}$$

$$\cdots \otimes \exp\Big\{ -i \sum_{i<j}^{Z} g^{[2]}(i,j) \Big\} \,|\, \Phi_Z \,\rangle$$

and hence the "cluster decomposition property" is fulfilled.

It is easy to see that the cluster decomposition property of the correlator C is carried over to each irreducible n–body term in $\widehat{B}$ (see eq. (16)).

2.2 Representation as coordinate transformation

The repulsion at short distances will keep the particles from getting too close to each other. This feature is not included in a (symmetrized/antisymmetrized) product state where the probability to find two particles (with different spin) at the same place is just the product of the one–body densities ($\pm$ exchange term). Therefore, the task of the correlator is to shift two particles away from each other whenever they are close.

In this section we define a generator $g(1,2)$ which is producing an outward radial shift depending on the uncorrelated distance of the particles. We express the action of the correlator in the two–body space $c(1,2) = \exp\{-ig(1,2)\}$ in terms of a coordinate transformation $R_\pm(r)$ of the radial distance r.

The relative distance and the relative momentum for equal mass particles are denoted by

$$\vec{r} = \vec{x}(1) - \vec{x}(2) \;, \qquad \vec{q} = \frac{1}{2}\left(\vec{p}(1) - \vec{p}(2)\right) \;, \tag{31}$$

respectively. A generator $g(1,2) = g(\vec{r},\vec{q})$ which creates a position–dependent shift may be written in the hermitean form

$$g(\vec{r},\vec{q}) = \frac{1}{2}\left\{ \left(\vec{q}\cdot\frac{\vec{r}}{r}\right) s(r) + s(r) \left(\frac{\vec{r}}{r}\cdot\vec{q}\right) \right\} \;, \qquad r \equiv |\vec{r}| \;. \tag{32}$$

One expects the unitary operator $c(1,2) = \exp\{-ig(\vec{r},\vec{p})\}$ to shift a relative position $\vec{r}$ to about $\vec{r} + s(r)\frac{\vec{r}}{r}$. The exact transformation will be derived below. The idea is to find a suited function $s(r)$ such that $g(\vec{r},\vec{p})$ moves the probability amplitude out of the classically forbidden region of the repulsion.

In coordinate representation the action of the generator $g(\vec{r},\vec{q})$ on a relative wave function $\langle\,\vec{r}\,|\,\phi\,\rangle$ is given by

$$\langle \vec{r} \,|\, g \,|\, \phi \rangle = -i \left(\frac{1}{2} \frac{\partial s}{\partial r} + \frac{s}{r} + s(r) \frac{\partial}{\partial r} \right) \langle \vec{r} \,|\, \phi \rangle \tag{33}$$

$$= -i \frac{1}{r\sqrt{s(r)}} \; s(r) \frac{\partial}{\partial r} \; r\sqrt{s(r)} \, \langle \vec{r} \,|\, \phi \rangle \; . \tag{34}$$

From that we obtain the coordinate representation of the correlator

$$\langle \vec{r} \,|\, c \,|\, \phi \rangle = \exp \left\{ -\frac{1}{r\sqrt{s(r)}} \; s(r) \frac{\partial}{\partial r} \; r\sqrt{s(r)} \right\} \, \langle \vec{r} \,|\, \phi \rangle \tag{35}$$

$$= \frac{1}{r\sqrt{s(r)}} \; \exp \left\{ -s(r) \frac{\partial}{\partial r} \right\} \, r\sqrt{s(r)} \, \langle \vec{r} \,|\, \phi \rangle \; . \tag{36}$$

The last line can be verified using the power expansion of the exponential. Writing c in this way suggests a coordinate transformation

$$s(r) \frac{\partial}{\partial r} \longrightarrow \frac{\partial}{\partial y} \; , \tag{37}$$

such that c amounts to a shift of -1 in the coordinate y. The transformations between y and r are denoted by $Y(r)$ and $R(y)$

$$r \xrightarrow{\;Y\;} y = Y(r) \tag{38}$$
$$y \xrightarrow{\;R\;} r = R(y) \; . \tag{39}$$

They are by construction the inverse of each other

$$R(Y(r)) = r \qquad \text{and} \qquad Y(R(y)) = y \; . \tag{40}$$

From (37) follow the differential equations

$$\frac{\partial}{\partial r} Y(r) = \frac{1}{s(r)} \qquad \text{and} \qquad \frac{\partial}{\partial y} R(y) = s(R(y)) \tag{41}$$

and the integral equation

$$y = \int^{R(y)} \frac{\mathrm{d}\xi}{s(\xi)} \; , \tag{42}$$

which defines the transformation $R(y)$. Rewriting eq. (36) in terms of y and $r = R(y)$ one obtains

$$\langle R(y)\frac{\vec{r}}{r} \,|\, c \,|\, \phi \rangle = \frac{1}{R(y)\sqrt{s(R(y))}} \, \exp\left\{-\frac{\partial}{\partial y}\right\} R(y)\sqrt{s(R(y))} \, \langle R(y)\frac{\vec{r}}{r} \,|\, \phi \rangle \tag{43}$$

$$= \frac{R(y-1)}{R(y)}\sqrt{\frac{s(R(y-1))}{s(R(y))}} \, \langle R(y-1)\frac{\vec{r}}{r} \,|\, \phi \rangle \; .$$

The action of $\exp\{-\frac{\partial}{\partial y}\}$ is to shift y by -1 and to leave the direction $\frac{\vec{r}}{r}$ unchanged. Rewriting (43) in terms of r yields

$$\langle \vec{r} \,|\, c \,|\, \phi \rangle = \frac{R(Y(r)-1)}{r}\sqrt{\frac{s(R(Y(r)-1))}{s(r)}} \, \langle R(Y(r)-1)\frac{\vec{r}}{r} \,|\, \phi \rangle \tag{44}$$

or for the inverse transformation

$$\langle \vec{r} \,|\, c^{-1} \,|\, \phi \rangle = \frac{R(Y(r)+1)}{r}\sqrt{\frac{s(R(Y(r)+1))}{s(r)}} \, \langle R(Y(r)+1)\frac{\vec{r}}{r} \,|\, \phi \rangle \; . \tag{45}$$

These two equations show that the transformations R and Y appear only in the form $R(Y(r)\pm 1)$. Therefore it is convenient to introduce the functions

$$R_{\pm}(r) \equiv R(Y(r)\pm 1) \tag{46}$$

with which we also express the terms under the square root as

$$R'_{\pm}(r) \equiv \frac{\partial}{\partial r} \, R_{\pm}(r) = \frac{s(R_{\pm}(r))}{s(r)} \; . \tag{47}$$

From the integral equation (42) follows

$$\int_{R(y)}^{R(y\pm 1)} \frac{\mathrm{d}\xi}{s(\xi)} = y \pm 1 - y \qquad \text{or} \qquad \int_{r}^{R_{\pm}} \frac{\mathrm{d}\xi}{s(\xi)} = \pm 1 \tag{48}$$

which is the formal definition of $R_{\pm}(r)$. From the fact that $Y(r)$ and $R(y)$ are inverse of each other follows

$$R_{\pm}(R_{\mp}(r)) = r \; , \tag{49}$$

which means that R_+ is the inverse of R_- and hence

$$R'_{\pm}(r) = \left[R'_{\mp}(R_{\pm}(r))\right]^{-1} \; . \tag{50}$$

With help of the coordinate transformations $R_+(r)$ and $R_-(r)$ the correlated wave function for the relative motion of two particles given in (44) can be written as

$$\langle \vec{r} \mid c \mid \phi \rangle = \frac{R_-(r)}{r}\sqrt{R'_-(r)} \ \langle R_-(r)\frac{\vec{r}}{r} \mid \phi \rangle \tag{51}$$

and the inverse transformation as

$$\langle \vec{r} \mid c^{-1} \mid \phi \rangle = \frac{R_+(r)}{r}\sqrt{R'_+(r)} \ \langle R_+(r)\frac{\vec{r}}{r} \mid \phi \rangle \ . \tag{52}$$

Hence, the unitary correlator $c = \exp\{-ig\}$ is uniquely given by the coordinate transformation $R_+(r)$.

With the correlated state given in (51) one can define the correlation volume V_c by the square of the defect wave–function which is the difference between a uniform uncorrelated state $\langle \vec{r} \mid \phi \rangle$ and $\langle \vec{r} \mid \psi \rangle = \langle \vec{r} \mid c \mid \phi \rangle$

$$V_c := 4\pi \int_0^\infty \mathrm{d}r \ \left[r - R_-(r)\sqrt{R'_-(r)} \right]^2 \tag{53}$$
$$= 4\pi \int_0^\infty \mathrm{d}r \ \left[r - R_+(r)\sqrt{R'_+(r)} \right]^2 \ .$$

A typical case is illustrated in fig. 2.

By looking at a matrix element $\langle \psi_1 \mid b(\vec{r}) \mid \psi_2 \rangle$ of a local operator $b(\vec{r})$, which acts on the relative distance, the meaning of the different parts in (51) and (52) becomes clear

$$\langle \psi_1 \mid b(\vec{r}) \mid \psi_2 \rangle = \int r^2 \mathrm{d}r \, \mathrm{d}\Omega \ \langle \psi_1 \mid \vec{r} \rangle \, b(\vec{r}) \, \langle \vec{r} \mid \psi_2 \rangle \tag{54}$$
$$= \int r^2 \mathrm{d}r \, \mathrm{d}\Omega \ \langle \phi_1 \mid c^\dagger \mid \vec{r} \rangle \, b(\vec{r}) \, \langle \vec{r} \mid c \mid \phi_2 \rangle$$
$$= \int r^2 \mathrm{d}r \, \mathrm{d}\Omega \ \left(\frac{R_-(r)}{r} \right)^2 R'_-(r) \ \langle \psi_1 \mid R_-(r)\frac{\vec{r}}{r} \rangle \, b(\vec{r}) \, \langle R_-(r)\frac{\vec{r}}{r} \mid \psi_2 \rangle$$
$$= \int r_-^2 \mathrm{d}r_- \mathrm{d}\Omega_- \ \langle \psi_1 \mid \vec{r}_- \rangle \, b\left(R_+(r_-)\frac{\vec{r}_-}{r_-} \right) \ \langle \vec{r}_- \mid \psi_2 \rangle \ .$$

The factor $\frac{R_-(r)}{r}\sqrt{R'_-(r)}$ in (51) is just the square root of the Jacobian of the transformation

$$\vec{r} \longrightarrow \vec{r}_- \equiv R_-(r)\frac{\vec{r}}{r} \tag{55}$$

$$\mathrm{d}^3 r_- = r_-^2 \mathrm{d}r_- \mathrm{d}\Omega_- = \left(\frac{R_-(r)}{r}\right)^2 R_-'(r) \, r^2 \mathrm{d}r \, \mathrm{d}\Omega \;, \tag{56}$$

where $\mathrm{d}\Omega = \mathrm{d}\Omega_- = \sin\theta \mathrm{d}\theta \mathrm{d}\phi$ remains unchanged.

Thus, the correlated wave function (51) at a relative distance $\vec{r}$ is given by the uncorrelated one taken at a closer distance $R_-(r)\frac{\vec{r}}{r}$ times the square root of the Jacobian which takes care of unitarity.

Equivalently one can use the correlated relative distance

$$\widehat{\vec{r}} = c^{-1} \vec{r} \, c = R_+(r)\frac{\vec{r}}{r} \;. \tag{57}$$

Due to the unitarity property $c^\dagger c = 1$ any local operator $b(\vec{r})$ can be readily transformed to the correlated one

$$\widehat{b(\vec{r})} = c^\dagger \, b(\vec{r}) \, c = c^{-1} \, b(\vec{r}) \, c = b\left(R_+(r)\frac{\vec{r}}{r}\right) \;. \tag{58}$$

The correlated operator $\widehat{b(\vec{r})}$ is just the uncorrelated one taken at the transformed relative distance $R_+(r)\frac{\vec{r}}{r}$. This is also the physical meaning of the last line in eq. (54).

The correlated radial momentum $\widehat{q}_r$ can be calculated in analogy to (54) by using the coordinate transformation (55) $\vec{r} \to \vec{r}_-$ and the relation (50) between R_-' and R_+'. The result is

$$\widehat{q}_r = c^{-1} q_r \, c = \frac{1}{\sqrt{R_+'(r)}} \frac{1}{r} q_r \, r \frac{1}{\sqrt{R_+'(r)}} \tag{59}$$

where

$$\langle \vec{r} \, | \, q_r \, | \, \phi \rangle = \langle \vec{r} \, | \, \frac{\vec{r}}{r} \cdot \vec{q} \, | \, \phi \rangle = -i \frac{\partial}{\partial r} \, \langle \vec{r} \, | \, \phi \rangle \;. \tag{60}$$

The correlated relative angular momentum is the same as the uncorrelated one

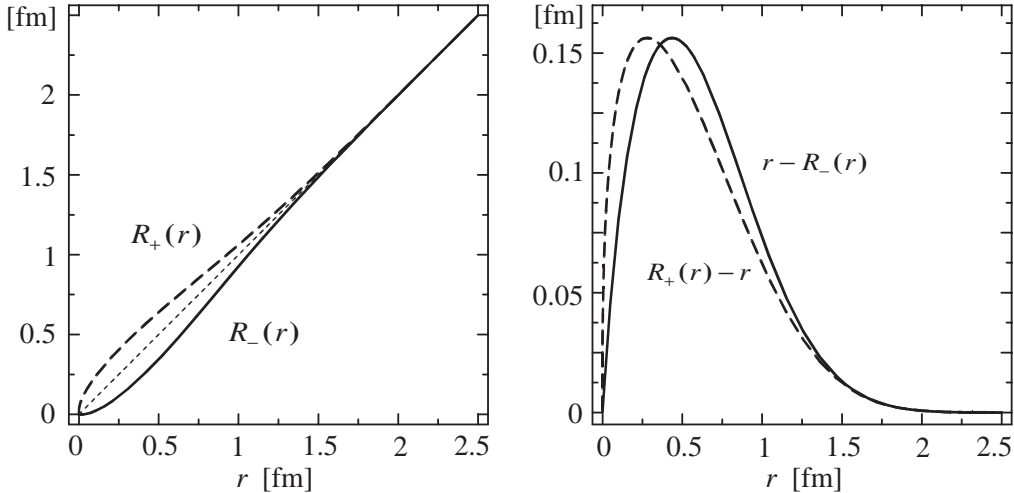$$\widehat{\vec{l}} = c^{-1} \vec{l} \, c = c^{-1} \vec{r} \times \vec{q} \, c = \vec{l} \;. \tag{61}$$

Fig. 1. L.h.s.: typical coordinate transformation $R_+(r)$ and its inverse $R_-(r)$; r.h.s: shifts $r - R_-(r)$ (full line) and $R_+(r) - r$ (dashed line).

The present correlator conserves angular momentum and spin for fermions. The realistic nucleon–nucleon interaction, however, induces strong tensor correlations. For such a situation, which will be subject of a forthcoming paper, the coordinate transformation $\vec{R}_-(\vec{r}, \vec{\sigma}_1, \vec{\sigma}_2)$ will not only depend on the relative distance $|\vec{r}|$ but also on the angles between $\vec{r}$ and the spins $\vec{\sigma}_1$ and $\vec{\sigma}_2$ of the two particles.

An intuitive relation between the coordinate transformation $R_\pm(r)$ and the original $s(r)$ in eq. (32) can be obtained from the first term of the Taylor expansion around y using (41)

$$R_\pm(r) = R(Y(r) \pm 1) = R(Y(r)) \pm R'(Y(r)) + \cdots \tag{62}$$
$$= r \pm s(r) + \cdots .$$

For $s(r)$ small compared to r, $s(r)$ is the amount by which the two particles are shifted away from their original distance r, as anticipated earlier.

Instead of discussing the shift function $s(r)$ as the variational degree of freedom we will consider the equivalent coordinate transformation $R_\pm(r)$ directly.

In order to avoid unphysical transformations, $R_\pm(r)$ has to increase monotonically with r and has to be differentiable everywhere. For correlations of finite range $R_\pm(r) \to r$ for large r. A typical example which will be used later is shown in fig. 1 in terms of $R_\pm(r)$ on the l.h.s.. The r.h.s. displays the shifts $r - R_-(r)$ and $R_+(r) - r$ which is the essential information. The shifts rise rapidly at $r = 0$ to a maximum of 0.15 fm around $r = 0.4$ fm. This results in a strong depletion of the relative wave function as can be seen in fig. 2 where a uniform uncorrelated state is compared with the correlated one as given in
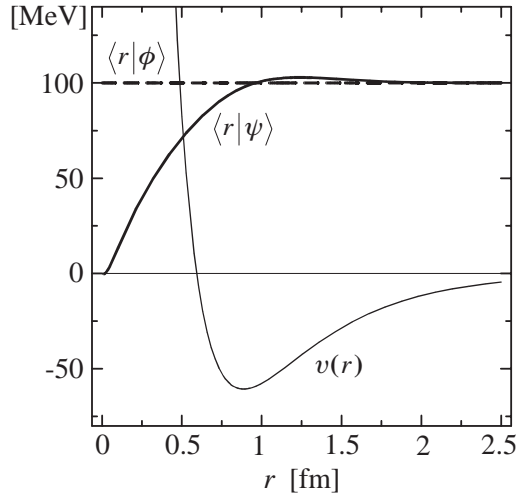
Fig. 2. Uncorrelated state $\langle r \, | \, \phi \rangle$ (dashed line), correlated state $\langle r \, | \, \psi \rangle$ (full line) and potential $v(r)$ (thin line) as a function of the relative distance r.

eq. (51). The corresponding potential is also included in the figure.

2.3 One– and two–body part of the correlated Hamiltonian

Of particular interest is the n–body expansion of the correlated Hamiltonian. Starting from eq. (58) the two–body part of the correlated potential is given by

$$\widehat{v}^{[2]}(i,j) = c(i,j)^{-1} \, v^{[2]}(i,j) \, c(i,j) = v\left(R_+(r_{ij})\right) \tag{63}$$

where $\vec{r}_{ij} = \vec{x}(i) - \vec{x}(j)$ and $r_{ij} = |\vec{r}_{ij}|$.

The three-body part $\widehat{v}^{[3]}(i,j,k)$ assumes the more complicated form given in (26). It will be discussed in section 3.3.

The correlated kinetic energy contains the uncorrelated kinetic energy as the first term

$$\widehat{t}^{[1]}(i) = t(i) \tag{64}$$

because $g^{[2]}(i,j)$ is a two–body operator and hence $C_1 = 1$ in the one–body space. The two–body part can be calculated by first separating the kinetic energy of two particles into relative and centre of mass energy

$$t(i) + t(j) = \frac{1}{m}\, \vec{q}_{ij}^2 + \frac{1}{4m}\, (\vec{p}(i) + \vec{p}(j))^2 \tag{65}$$

where $\vec{q}_{ij} = (\vec{p}(i) - \vec{p}(j))/2$ is the relative momentum. Since $g^{[2]}(i,j)$ commutes with the centre of mass coordinate, only the relative momentum is correlated

$$c(i,j)^{-1}\, (t(i) + t(j))\, c(i,j) \tag{66}$$
$$= \frac{1}{m}\, c(i,j)^{-1}\, \vec{q}_{ij}^2\, c(i,j) + \frac{1}{4m}\, (\vec{p}(i) + \vec{p}(j))^2 \ .$$

Decomposing $\vec{q}_{ij}^2$ into a radial and angular momentum part

$$\vec{q}_{ij}^2 = q_{r\,ij}^\dagger\, q_{r\,ij} \ + \ \frac{1}{r_{ij}^2}\vec{l}_{ij}^2 \ , \tag{67}$$

where $q_r = \frac{\vec{r}}{r} \cdot \vec{q}$ and $\vec{l} = \vec{r} \times \vec{q}$, one can utilize eqs. (59) and (61) to obtain

$$c(i,j)^{-1}\, \vec{q}_{ij}^2\, c(i,j) \tag{68}$$
$$= \frac{r_{ij}}{\sqrt{R_+'(r_{ij})}}\, q_{r\,ij}^\dagger\, \frac{1}{r_{ij}^2 R_+'(r_{ij})}\, q_{r\,ij}\, \frac{r_{ij}}{\sqrt{R_+'(r_{ij})}} \ + \ \frac{1}{(R_+(r_{ij}))^2}\vec{l}_{ij}^2 \ .$$

Commuting the two radial momenta $q_{r\,ij}$ in the first term on the r.h.s. to the left and to the right of $r_{ij}/\sqrt{R_+'(r_{ij})}$, respectively, yields

$$c(i,j)^{-1}\, \vec{q}_{ij}^2\, c(i,j) \tag{69}$$
$$= q_{r\,ij}^\dagger\, \frac{1}{(R_+'(r_{ij}))^2}\, q_{r\,ij} \ + \ \frac{1}{(R_+(r_{ij}))^2}\vec{l}_{ij}^2 + m\, \widehat{u}^{[2]}(i,j) \ ,$$

where

$$\widehat{u}^{[2]}(i,j) = \frac{1/m}{(R_+'(r_{ij}))^2} \left\{ 2\frac{R_+''(r_{ij})}{r_{ij} R_+'(r_{ij})} - \frac{5}{4}\left(\frac{R_+''(r_{ij})}{R_+'(r_{ij})}\right)^2 + \frac{1}{2}\frac{R_+'''(r_{ij})}{R_+'(r_{ij})}\right\} \ . \tag{70}$$

$R_+''(r)$ and $R_+'''(r)$ are the second and the third derivative of $R_+(r)$ with respect to r. Thus, the two–body part of the correlated kinetic energy may be split into three parts

$$\widehat{t}^{[2]}(i,j) \tag{71}$$
$$= q_{r\,ij}^\dagger\, \frac{1}{m}\left[\frac{1}{(R_+'(r_{ij}))^2} - 1\right] q_{r\,ij} + \frac{1}{m}\left[\frac{1}{(R_+(r_{ij}))^2} - \frac{1}{r_{ij}^2}\right]\vec{l}_{ij}^2 + \widehat{u}^{[2]}(i,j) \ .$$

The first is a two–body radial kinetic energy with a reduced radial mass

$$\mu_r(r) = \frac{m}{2} \left[\frac{1}{(R'_+(r))^2} - 1 \right]^{-1} \tag{72}$$

which depends on the distance r between the particles in the pair. The second part is a relative rotational energy with a reduced angular mass

$$\mu(r) = \frac{m}{2} \left[\frac{r^2}{(R_+(r))^2} - 1 \right]^{-1} . \tag{73}$$

The third part $\widehat{u}^{[2]}(i,j)$ is a local two–body potential which depends on derivatives of $R_+(r)$ as given by eq. (70). All three parts vanish outside the correlation range when $R_+(r) \to r$.

The one– and two–body parts of the correlated Hamiltonian add up to

$$\widehat{H}^{[1]} + \widehat{H}^{[2]} = \sum_i^A t(i) \tag{74}$$
$$+ \sum_{i<j}^A \left[q^\dagger_{r\,ij} \frac{1}{2\mu_r(r_{ij})} q_{r\,ij} + \frac{1}{2\mu(r_{ij})r_{ij}^2} \vec{l}_{ij}^{\,2} \right]$$
$$+ \sum_{i<j}^A \left[\widehat{u}^{[2]}(i,j) + \widehat{v}^{[2]}(i,j) \right] .$$

The first part is the uncorrelated one–body kinetic energy. The second is a momentum dependent two–body interaction which is restricted to the correlation area. The third is the tamed two–body potential which has no repulsive core anymore. Its shape will be determined in the following section where the choice of $R_+(r)$ is discussed. The taming of $v(r)$ has to be paid by the momentum dependent two–body interaction. In Cartesian coordinates this part may also be written as

$$q^\dagger_r \frac{1}{2\mu_r(r)} q_r + \frac{1}{2\mu(r)r^2} \vec{l}^{\,2} = \vec{q}\frac{1}{2\mu(r)} \vec{q} + q^\dagger_r \frac{1}{2\mu^*_r(r)} q_r , \tag{75}$$

where

$$\mu^*_r(r) = \frac{m}{2} \left[\frac{1}{(R'_+(r))^2} - \frac{r^2}{(R_+(r))^2} \right]^{-1} . \tag{76}$$

2.4 Choice of the correlation function $R_\pm(r)$

The correlator is a functional of $s(r)$ or equivalently of the coordinate transformation $R_-(r)$

$$| \Psi \rangle = C[R_-] \ | \Phi \rangle \ . \tag{77}$$

Therefore, $R_-(r)$ represents additional variational freedom and according to the Ritz variational principle $R_-(r)$ could be determined by minimizing the ground state energy

$$\langle \Psi | H | \Psi \rangle = \langle \Phi | C^\dagger[R_-] H C[R_-] \ | \Phi \rangle \tag{78}$$

not only with respect to $| \Phi \rangle$ but also with respect to $R_-(r)$.

However, since only the first terms in the n–body expansion of the correlated Hamiltonian $\widehat{H} = \widehat{H}^{[1]} + \widehat{H}^{[2]} + \cdots$ (see eq. (16)) will be used, the exact ground state energy is in general no lower bound on $\langle \Phi | \widehat{H}^{[1]} | \Phi \rangle + \langle \Phi | \widehat{H}^{[2]} | \Phi \rangle$ anymore because contributions $\langle \Phi | \widehat{H}^{[n]} | \Phi \rangle$ for $n \geq 3$ can be positive and negative so that only the complete sum up to the total particle number A has the lower bound.

In order to make the three– and higher–body correlation part as small as possible one should use the freedom in the separation of short and long range correlations, i.e. what should be taken care of by $C[R_-]$ and $| \Phi \rangle$ respectively, to find an optimal correlated two–body Hamiltonian. One expects the three–body part of the correlated Hamiltonian which is induced by $C[R_-]$ to be small if the correlation range in which $R_-(r) \neq r$ (or $s(r) \neq 0$) is short compared to the mean distance between the particles. A measure of the smallness is the uncorrelated density ρ_0 times the correlation volume V_c, defined in (53). In section 3.3 where we calculate three–body terms a relation between $\rho_0 V_c$ and the three–body correlations is given. From that one can judge how small $\rho_0 V_c$ actually should be.

In the following we investigate for a two–body system the general idea that the correlator C can be imagined as a unitary mapping of uncorrelated states onto correlated states which approximately diagonalize the Hamiltonian H.

$$H | \psi_E \rangle = E | \psi_E \rangle \tag{79}$$

$| \psi_E \rangle$ are the exact bound and scattering eigenstates of the Hamiltonian $H = \frac{1}{2\mu} \vec{q}^{\,2} + v(r)$ for the relative motion. The repulsive core of $v(r)$ will suppress the wave function $\langle \vec{r} | \psi_E \rangle$ for small r. The goal is to find for a range of energies

an optimal correlator $c[R_-]$ which removes these repulsive correlations from $|\psi_E\rangle$.

If one demands that in a range $r \leq \lambda$ the correlated trial state and the exact state coincide

$$\langle \vec{r} \,|\, c[R_-] \,|\, \phi \rangle \overset{!}{=} \langle \vec{r} \,|\, \psi_E \rangle \quad \text{for} \quad 0 \leq |\vec{r}| \leq \lambda \tag{80}$$

one obtains for angular momentum equal zero from eq. (51)

$$\sqrt{R'_-(r)} \, u(R_-(r)) = u_E(r) \tag{81}$$

or the integral equation

$$R_-(r) = \int_0^r d\xi \left(\frac{u_E(\xi)}{u(R_-(\xi))} \right)^2 , \tag{82}$$

where $R_-(r=0)=0$ is assumed and the radial wave functions are denoted as

$$u_E(r) = r\langle \vec{r} \,|\, \psi_E \rangle \quad \text{and} \quad u(r) = r\langle \vec{r} \,|\, \phi \rangle . \tag{83}$$

As already discussed in a more general frame in section 2 the correlator C or the coordinate transformation $R_-(r)$ as defined in eq. (82) depend on the trial function $u(r)$ and on the Hamiltonian via its eigenfunctions $u_E(r)$.

For systems at small energies a first attempt is to assume the trial state $\langle \vec{r} \,|\, \phi \rangle = 1/\sqrt{N_0}$ to be uniform across the repulsive core [11]. For this special case the coordinate transformation $R_-(r)$ is given by the differential equation

$$R'_-(r) = N_0 \left(\frac{u_E(r)}{R_-(r)} \right)^2 , \tag{84}$$

where the norm N_0 is still to be chosen.

The dependence of $R_-(r)$ on N_0, which is displayed in fig. 3 l.h.s. in terms of the deviation $r - R_-(r)$, will now be used to limit the range of the correlation. For this the MTV potential ([13] and eq. (A.1)), already shown in fig. 1, is chosen as an example and the energy E is set to zero. Among the set of curves there is one which touches the x–axis at a distance λ which means

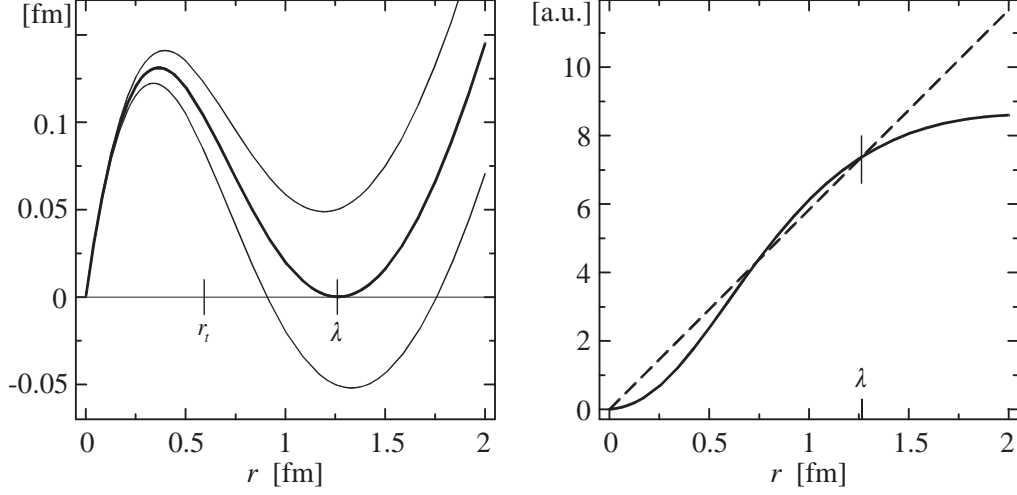$$R_-(\lambda) = \lambda \quad \text{and} \quad R'_-(\lambda) = 1 . \tag{85}$$

Fig. 3. L.h.s.: Coordinate transformation $R_-(r)$ plotted as $r - R_-(r)$ for $E = 0$ and different N_0. R.h.s: Exact radial wave function $u_{E=0}(r)$ (solid line) and trial function $u(r)$ for which $R_-(\lambda) = \lambda$ and $R'_-(\lambda) = 1$.

From the Schrödinger equation for angular momentum zero

$$u''_E(r) = m \, (v(r) - E) \, u_E(r) \tag{86}$$

one sees that at the classical turning point $v(r_t) = E$ the curvature of $u_E(r)$ switches sign so that a linear radial function $u(r) = r/\sqrt{N_0}$ can be found which intersects the exact solution twice, see fig. 3 r.h.s., such that at $r = \lambda$ trial and exact state coincide

$$u(\lambda) = u_E(\lambda) \tag{87}$$

and their norms up to λ are also equal

$$\int_0^\lambda \mathrm{d}r \, (u(r))^2 = \int_0^\lambda \mathrm{d}r \, (u_E(r))^2 \; . \tag{88}$$

The transformation $R_-(r)$ which fulfills the conditions (85) or equivalently (87) and (88) provides a natural division into a short and a long range part. This division is an inherent property of all methods which derive effective interactions [12]. At $r = \lambda$ one may split $c[R_-]$ into

$$c[R_-] = c[R^I_-] \, c[R^{II}_-] \tag{89}$$

where

$$R_-^I = \begin{cases} R_-(r) \text{ for } 0 \le r \le \lambda \\ r \quad \text{ for } \quad \lambda \le r \end{cases} \quad \text{and} \quad R_-^{II} = \begin{cases} r \quad \text{ for } 0 \le r \le \lambda \\ R_-(r) \text{ for } \quad \lambda \le r \end{cases} \tag{90}$$

because $c[R_-^I]$ commutes with $c[R_-^{II}]$ if (85) is fulfilled. For $r > \lambda$ the uncorrelated state $\langle \vec{r} \,|\, \phi \rangle$ is supposed to describe the long range part so that we set $R_-^{II} = r$ or $c[R_-^{II}] = 1$.

The schematic case of a uniform uncorrelated state illustrates nicely how the method works. As the correlation function $R_-(r)$ is chosen such that the correlated state equals the exact solution for a given energy E (see eq. (80)) it also solves the Schrödinger equation (86)

$$\langle \vec{r} \,|\, \left(\frac{1}{m} q_r^\dagger q_r + v(r) \right) c[R_-] \,|\, \phi \rangle = E \,\langle \vec{r} |\, c[R_-] \,|\, \phi \rangle \tag{91}$$

or

$$\langle \vec{r} \,|\, \left(\frac{1}{m} c[R_-]^{-1} q_r^\dagger q_r \, c[R_-] + c[R_-]^{-1} v(r) \, c[R_-] \right) \,|\, \phi \rangle = E \,\langle \vec{r} | \phi \rangle . \tag{92}$$

Since $\langle \vec{r} \,|\, \phi \rangle = 1/\sqrt{N_0}$ is uniform, the relative kinetic energy reduces to (c.f. eqs. (69) and (70))

$$\langle \vec{r} \,|\, \frac{1}{m} c[R_-]^{-1} q_r^\dagger q_r \, c[R_-] \,|\, \phi \rangle = \widehat{u}^{[2]}(r) \frac{1}{\sqrt{N_0}} \tag{93}$$

and hence

$$\widehat{u}^{[2]}(r) + \widehat{v}^{[2]}(r) = E \quad \text{for} \quad r \le \lambda . \tag{94}$$

This means that a correlator obtained from eq. (84) for $E = 0$ transforms the original Hamiltonian for small distances $r < \lambda$, where the potential is strongly repulsive, into a correlated Hamiltonian with a vanishing local potential $\widehat{u}^{[2]}(r) + \widehat{v}^{[2]}(r) = 0$. Thus the repulsive core is completely absent in the correlated Hamiltonian.

If the potential is purely repulsive ($v(r) \ge 0$ for all r) there is no natural scale for the division into long and short ranged components. In this case the quest for a correlation volume small enough for the two–body approximation will determine the range of the correlation. Further discussions on repulsive potentials can be found in section 4.1 where we treat spin–isospin–dependent correlators.

The next point is the dependence on the energy. Fig. 4 displays $r - R_-(r)$ for a separable correlation at different energies between 0 and 80MeV which
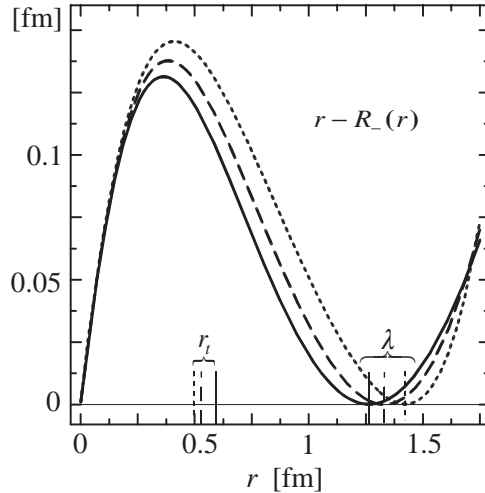
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Fig. 4. Energy dependence of the coordinate transformation $R_-(r)$, $E = 0$ (full line), $E = 40\,\mathrm{MeV}$ (dashed line), $E = 80\,\mathrm{MeV}$ (dotted line). r_t classical turning points, λ range of correlators.

is the kinetic energy of two nucleons colliding with opposite Fermi momenta. As the uncorrelated state we choose the spherical Bessel function so that the radial function $u(r) = r j_0(\sqrt{mE}r)/\sqrt{N_0} = \sin(\sqrt{mE}r)/\sqrt{N_0}$ is the $l = 0$ solution of the free Schrödinger equation. It turns out that for distances $r < r_t$ the correlation function $R_-(r)$ is rather energy independent. For $r > r_t$ one expects an influence from the uncorrelated state so that the shape of $R_-(r)$ may differ for $r_t < r < \lambda$ from the one shown in fig. 4 depending on the choice of the uncorrelated state.

The kink in the wave function at $r = \lambda$ (see fig. 3 r.h.s.) caused by cutting off $R_-(r)$ at $r = \lambda$ in a non-analytic way should be removed. Therefore, the short range part $R_-^I(r)$ will be parameterized by an analytic function which approximates $R_-(r)$ for $0 < r < r_t$ rather well and leaves some freedom for $r > r_t$ for adjusting to the actual trial states used.

Since later on in the many–body case the product state will consist of Gaussian shaped single–particle states, the uncorrelated state of the two–particle system, from which the coordinate transformation $R_-(r)$ is deduced, is also assumed to be a Gaussian at small r (and not a constant or a Bessel function) which joins smoothly to an exponential radial function at $r = \rho$

$$\langle \vec{r} \,|\, \phi \rangle = \frac{1}{\sqrt{N(\rho)}} \begin{cases} \exp\left\{ -\frac{\rho+\kappa}{2\rho^2\kappa} r^2 \right\} & \text{for} \quad r \le \rho \\ \frac{\rho}{r} \exp\left\{ \frac{\rho-\kappa}{2\kappa} - \frac{r}{\kappa} \right\} & \text{for} \quad r \ge \rho \end{cases} . \tag{95}$$

The length $\kappa = (-mE_0)^{-1/2}$ is chosen such that the long range part, where the correlator should not modify the trial state, has the correct fall off.
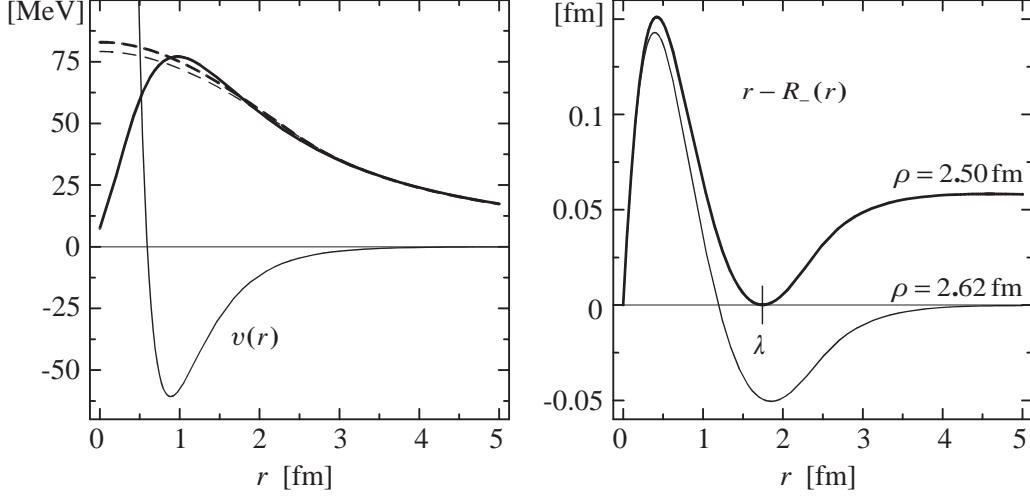
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Fig. 5. L.h.s.: MTV potential $v(r)$ in MeV, uncorrelated wave functions for $\rho = 2.62\,\mathrm{fm}$ (thin dashed line) and $\rho = 2.5\,\mathrm{fm}$ (thick dashed line) and corresponding correlated ones which both equal the exact one (thick solid line). R.h.s: correlation functions in terms of $r - R_-(r)$ for uncorrelated states which map on the exact ground state.

Fig. 5 displays on the left hand side the uncorrelated trial state $\langle \vec{r} \,|\, \phi \rangle$ for $\rho = 2.62\,\mathrm{fm}$ and the exact ground state $\langle \vec{r} \,|\, \psi_E \rangle$ together with the MTV potential. The exact solution is pushed out of the repulsive region compared to the uncorrelated state. The coordinate transformation $R_-(r)$ obtained from (82), which transforms $\langle \vec{r} \,|\, \phi \rangle$ into $\langle \vec{r} \,|\, \psi_E \rangle$, is shown on the r.h.s. in terms of the shift distance $r - R_-(r)$ (thin line). Due to the attraction this shift turns out to be negative beyond $r = 1.2\,\mathrm{fm}$ so that more probability is accumulated around $r \approx 1\,\mathrm{fm}$ where the potential is most attractive. This long range effect should not be corrected by the correlator but an improved trial state should be employed, otherwise the three– and higher–body terms in the correlated Hamiltonian will be too large.

Similar to the uniform trial state discussed above we vary the norm $N(\rho)$ by moving the matching point ρ until we achieve a separable correlator which is the case for $\rho = 2.5\,\mathrm{fm}$ (thick line in fig. 5 r.h.s.). This correlation function differs only little from the one where trial and exact state coincide for very large r ($\rho = 2.62\,\mathrm{fm}$). The resulting shifts $r - R_-(r)$ are displayed on the r.h.s. of fig. 5. For $r < r_t = 0.6\,\mathrm{fm}$ they are identical and similar to the case of a uniform uncorrelated state. The separation point λ turns out to be inside $r = \rho$, so that the correlation acts only on the Gaussian part.

3 Few–body systems with spin–isospin–independent forces

In this section we apply the concept of the unitary correlation operator to the two–, three– and four–body systems ^{2}H and ^{3,4}He. The correlation function $R_+(r)$ is first parameterized and then the binding energies of the three nuclei are minimized with respect to the parameters of $R_+(r)$. It turns out that the resulting correlation functions are almost identical. This shows that the general concept of a state–independent correlator discussed in the previous section is applicable. The last subsection investigates an approximate treatment of the three–body term in the correlated Hamiltonian.

Throughout this section the Malfliet–Tjon V potential (MTV) [13] is used, which is a central interaction without spin and isospin dependence (see appendix eq. (A.1)). This potential is widely used in the literature, for instance to compare different theoretical many–body approaches [14,15] because it has a repulsive core and an attractive long range part chosen by considering the phase shifts of the scattering problem. However, already for ^{4}He it overbinds. For larger nuclei it gives completely unrealistic results. Therefore another potential will be used in section 4 where nuclei up to $A = 48$ are investigated.

3.1 Parameterization of $R_\pm(r)$

For the two–body system everything can be calculated with a correlation function $R_+(r)$ that is derived as described before and at least numerically known at all r. But for many–body systems it is advisable to have an analytic form with a limited number of parameters. Therefore we parameterize the numerically determined $R_+(r)$ by

$$R_+(r) = r + \alpha \left(\frac{r}{\beta}\right)^\eta \exp\left\{-\exp\left(\frac{r}{\beta}\right)\right\} \ . \tag{96}$$

The parameter α controls the overall amount of the shift and β the length scale. η determines the steepness around $r = 0$. The double–exponential fall off is required to reproduce the exact correlation function in the vicinity of the separation distance $r = \lambda$, which has been derived in the previous section. Figure 6 compares the exact correlation function for the bound state with the parameterization (96), where $\alpha = 0.935\,\mathrm{fm}$, $\beta = 0.95\,\mathrm{fm}$ and $\eta = 0.39$. A similar fit can be achieved with a Gaussian replacing the double–exponential fall off.
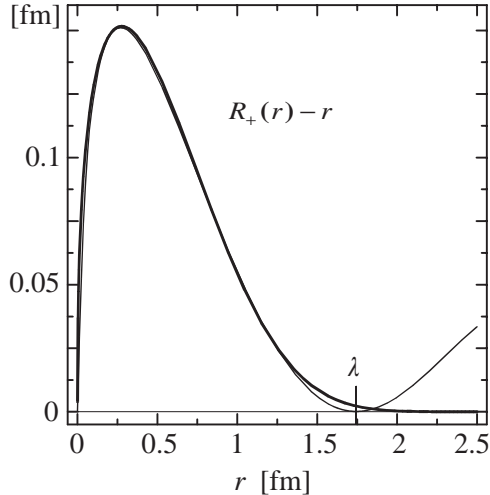
Fig. 6. Exact correlation function $R_+(r)$ for the ground state (thin line) and the parameterization (96) plotted as $R_+(r) - r$.

3.2 ^2H and $^{3,4}He$ with the Malfliet–Tjon V potential

In this section the particle number dependence of the correlation function is investigated. For that the three parameters α, β, η of the ansatz for $R_+(r)$ given in eq. (96) are varied in order to minimize the binding energy of the two–, three– and four–nucleon system. The uncorrelated trial states are kept as simple as possible because the short range correlations are supposed to be described by the unitary correlator alone. Therefore, the uncorrelated ^3He and ^4He states are taken to be a product of three and four identical Gaussians in coordinate space, respectively. The antisymmetry is taken care of by an appropriate spin–isospin part of the many–body state. This excludes for ^3He the admixture of relative p–states which are important for a correct ground state energy.

Thus all three uncorrelated many–body wave functions are characterized by only one variational parameter, which for ^2H is ρ as defined in (95) and for $^{3,4}He$ is the width a of the Gaussian shaped single–particle state.

The correlated Hamiltonian is calculated up to its two–body part as defined in section 2.1

$$\widehat{H}^{C2} = T_{int} + \widehat{T}^{[2]} + \widehat{V}^{[2]} \tag{97}$$

where the intrinsic kinetic energy

$$T_{int} = T - T_{cm} \ , \quad T_{cm} = \frac{1}{2mA} \Big(\sum_{i=1}^{A} \vec{p}(i) \Big)^2 \tag{98}$$

is the kinetic energy minus the centre of mass kinetic energy T_{cm}.

Table 1 summarizes the result of minimizing the expectation value of the correlated intrinsic Hamiltonian $\widehat{H}^{C2}$. The first and very important result is that the correlation functions $R_+(r)$ (represented by their parameters α, β, η), which result from minimizing the energy, are very similar for the two–, three– and four–body system. This can also be seen in fig. 7 where they are plotted together with the $R_+(r)$ which results from mapping the uncorrelated deuteron ground state (95) to the exact relative wave function up to $r = \lambda$ as defined in (82) and discussed in section 2.4.

Since all correlation functions turn out to be almost identical, the initial concept of a unitary state–independent correlator, which does not depend on the actual system it is applied to, is strongly supported.

The second result is that despite of the simplistic nature of the uncorrelated states the binding energies of the $A = 2$ and $A = 4$ systems are very close to the exact values. The $A = 3$ system is still $1.8\,\mathrm{MeV}$ above the value of a Green's function Monte Carlo calculation [16]. Responsible for that are the missing exponential tails in the Gaussian radial functions and a missing component in the uncorrelated state in which the spins of the two protons are coupled to one and the relative motion is in a p–state.

One should keep in mind that the total energy results from the subtraction of two large numbers, the kinetic and the potential energy, both depending sensitively on $R_+(r)$. As will be demonstrated with an example below, the potential energy almost doubles when including the correlator.

A	α	β	η	a	ρ	$\langle \widehat{T}_{int}^{C2} \rangle$	$\langle \widehat{V}^{C2} \rangle$	$\langle \widehat{H}^{C2} \rangle$	exact
	[fm]	[fm]		[fm^2]	[fm]	[MeV]	[MeV]	[MeV]	[MeV]
2	0.939	0.996	0.394	–	2.42	4.78	-5.17	-0.40	-0.41
3	0.944	1.018	0.389	2.06	–	34.97	-41.49	-6.52	-8.26±0.01
4	0.954	1.121	0.369	1.51	–	76.37	-107.2	-30.78	-31.3±0.2

Table 1
Parameters α, β, η of the correlator and a, ρ of the uncorrelated many–body state which minimize the energy $\langle \widehat{H}^{C2} \rangle$. $\langle T_{int}^{C2} \rangle = \langle T_{int} + \widehat{T}^{[2]} \rangle$ is the intrinsic correlated kinetic energy and $\langle \widehat{V}^{C2} \rangle = \langle \widehat{V}^{[2]} \rangle$ the correlated potential energy. The exact binding energies are taken from [16].
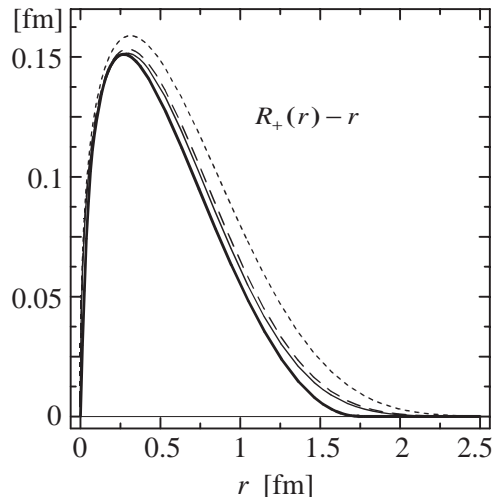
Fig. 7. Comparison between exact correlation function for the ground state of ^{2}H (thick line) and parameterized functions obtained by minimizing the ground state energies of ^{2}H (thin line), ^{3}He (long dashed line) and ^{4}He (short dashed line) in terms of $R_+(r) - r$.

Since the difference between the correlation functions is so small a standard correlator with the parameters

$$\alpha = 0.94 \, \text{fm} \quad \beta = 1 \, \text{fm} \, , \quad \eta = 0.37 \tag{99}$$

is used for all three systems and the minimization is done only with respect to a single parameter, ρ or a, which determines the radial wave functions. As expected their values differ very little from those given in table 1. The resulting energies are decomposed into their components in fig. 8.

For each system the uncorrelated expectation values of kinetic, potential and total energy are compared with their respective correlated counter parts. The uncorrelated energies are calculated with the uncorrelated states which minimize the correlated energy. In all three cases the kinetic correlation energy $\langle \widehat{T}^{[2]} \rangle$ (indicated by a vertical line) is much less than the potential correlation energy $\langle \widehat{V}^{[2]} \rangle - \langle V \rangle$ so that the sum of both reduces the uncorrelated total energy from positive values (unbound) down to almost the exact ground state energies.

Figure 9 illustrates the action of the unitary correlator. On the left hand side one sees that the repulsive maximum of $r^2 v(r)$ is reduced by almost a factor of three, while the attractive region is enlarged. This corresponds to the shift of the wave function away from the repulsive core towards the attractive region, c.f. (54). The correlated kinetic energy contributes a potential like part $\widehat{u}^{[2]}(r)$ which is given in eq. (70) and depicted in the middle of fig. 9. For short distances $r \lesssim 1$ fm it has a pattern opposite to the correlated potential,
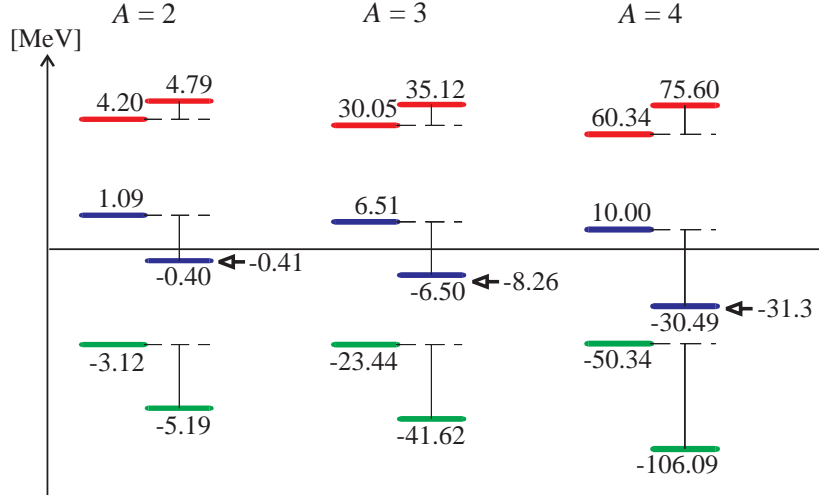
Fig. 8. Energies for $A = 2, 3, 4$ and MTV potential. Left columns: expectation values of kinetic energy $\langle T_{int} \rangle$, potential $\langle V \rangle$ and sum of both $\langle H \rangle$. Right columns: expectation values of correlated kinetic energy $\langle T_{int} + \widehat{T}^{[2]} \rangle$, correlated potential $\langle \widehat{V}^{[2]} \rangle$ and sum of both $\langle \widehat{H}^{C2} \rangle$. Arrows indicate exact values from [16].
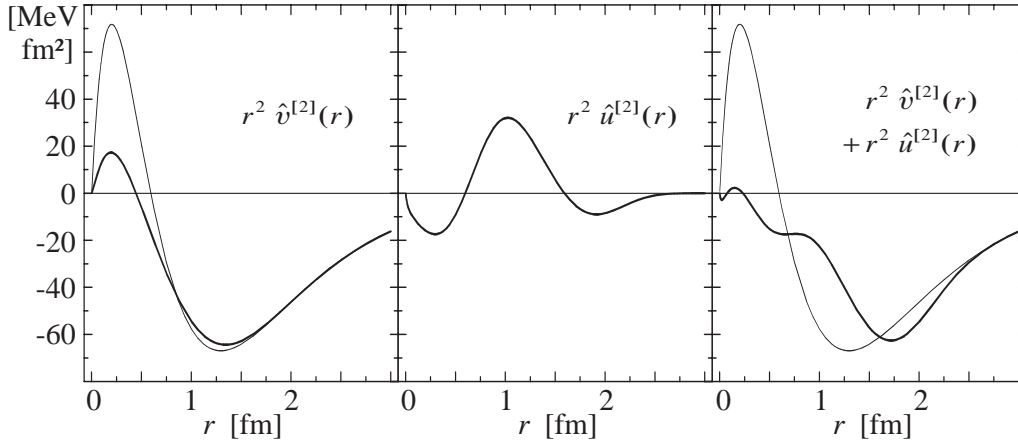

Fig. 9. L.h.s.: correlated $(\widehat{v}^{[2]}(r) = v(R_+(r))$, full line) and uncorrelated $(v(r)$, thin line) MTV potential. Centre: potential like part of the correlated kinetic energy $\widehat{u}^{[2]}(r)$. R.h.s.: MTV potential (thin line) and "tamed" potential $\widehat{u}^{[2]}(r) + \widehat{v}^{[2]}(r)$. All potentials are multiplied with r^2.

attractive at short and repulsive at larger values of r, so that the sum of both $\widehat{u}^{[2]}(r) + \widehat{v}^{[2]}(r)$ (r.h.s. of fig. 9) almost vanishes in the region of the repulsive core of the MTV potential. As discussed in section 2.4 a uniform uncorrelated state which is mapped by the unitary correlator c onto the exact eigenstate of the Hamiltonian at energy E leads to $\widehat{u}^{[2]}(r) + \widehat{v}^{[2]}(r) = E$ for small r. This explains the small values of $\widehat{u}^{[2]}(r) + \widehat{v}^{[2]}(r)$ at small distances. The deviations from a constant E are due to the fact that $R_+(r)$ is parameterized (96) and the trial state is not uniform.
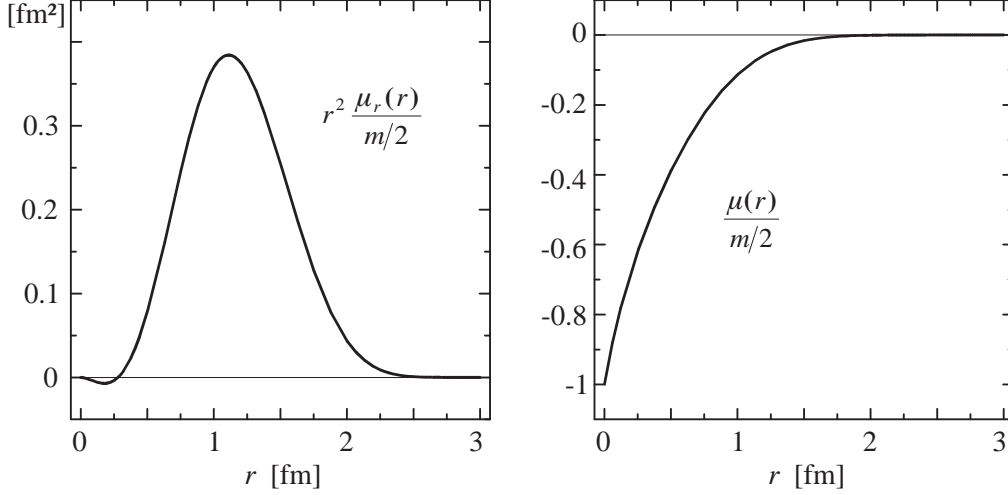
Fig. 10. L.h.s.: Inverse reduced mass in radial direction. R.h.s.: Inverse relative moment of inertia. The values are multiplied with r^2 and in units of $m/2$.

The r.h.s. of fig. 9 shows that the repulsive core of the original potential is completely transformed away by the unitary correlator. The uncorrelated states feel only a tamed potential which is purely attractive.

Since the correlator creates "holes" in the many–body state it induces the additional kinetic energy $\widehat{t}^{[2]}$. One part of that is $\widehat{u}^{[2]}(r)$, the other part can be understood as a momentum dependent two–body potential which is written in eq. (69) in terms of a reduced mass and a reduced moment of inertia. Their dependence on the relative distance r is displayed in fig. 10. The l.h.s. shows the inverse of the reduced mass for the radial direction as calculated from eq. (72) in units of $m/2$ and multiplied by r^2. It results in an increase of the correlated kinetic energy. The r.h.s. of fig. 10 depicts the inverse of the reduced moment of inertia times r^2 which is given by eq. (73). For relative angular momenta $l = 0$ this part does not contribute. But for components with $l \neq 0$ it is always negative. This is due to the fact that the correlator shifts the particles away from each other so that their moment of inertia increases or the inverse of that decreases. Therefore, the correlation energy which is the difference between correlated and uncorrelated energy has to be negative. Altogether the expectation value of the momentum–dependent part of $\widehat{T}^{[2]} = \sum_{i<j} \widehat{t}^{[2]}(i,j)$ is for $A = 4$ only 3.3 MeV compared to 12 MeV for $\langle \widehat{u}^{[2]} \rangle$.

3.3   Three–body part of the correlated Hamiltonian

The ansatz for the correlator discussed in section 2 includes only a two–body generator $g^{[2]}(i,j)$. Nevertheless the correlated operators contain three– and

higher–body operators because $g^{[2]}(i,j)$ appears in the exponent (see eq. (26)). In principle it is possible that the nuclear many–body system requires also genuine three–body correlations so that the corresponding unitary correlator would be written as

$$C = \exp\left(-i \sum_{i<j}^{A} g^{[2]}(i,j) - i \sum_{i<j<k}^{A} g^{[3]}(i,j,k) \right) . \qquad (100)$$

In the n–body expansion of a correlated operator $\widehat{B} = C^{-1}BC$ the three–body correlations induced by $g^{[3]}$ would appear first in the three–body part together with the three–body part originating from $g^{[2]}$. It will be very hard or even impossible to distinguish between the two contributions just from the three– or four–particle ground state energies. This uncertainty together with the complicated calculation of the three–body contribution of $g^{[2]}$ as given in (26) suggests to estimate the three–body contribution first before doing elaborate calculations. A small three–body contribution to $C^{-1}BC$ from $C = \exp\{-i \sum_{i<j}^{A} g^{[2]}(i,j)\}$ is of course desirable for justifying the two–body approximation. On the other hand if it turns out to be small even a small genuine three–body generator $g^{[3]}$ might be of equal or more significance and one would have to discuss its shape and importance. Thus the idea is that either it is sufficient to consider the correlated operators only up to the two–body part or the method becomes too complicated for practical purposes.

The two–body approximation will be tested by calculating the correlated Hamiltonian up to three–body operators with the following approximation which is a partial sum of a power expansion of $C^{-1}HC$ [17].

$$c(i,j,k)^{-1} \, h(i,j,k) \, c(i,j,k) \qquad (101)$$
$$\approx \frac{1}{3!} \sum_{P\{\alpha,\beta,\gamma\}} c(\alpha)^{-1} c(\beta)^{-1} c(\gamma)^{-1} \, h(i,j,k) \, c(\gamma) \, c(\beta) \, c(\alpha)$$

where $h(i,j,k) = t^{[1]}(i) + t^{[1]}(j) + t^{[1]}(k) + v^{[2]}(i,j) + v^{[2]}(i,k) + v^{[2]}(j,k)$. The greek indices α, β, γ denote the three possibilities to pick a pair of particle indices out of $\{i,j,k\}$. The summation runs over all 3! possibilities to order the triple $\{\alpha, \beta, \gamma\}$. $c(\alpha)$ is the two–body correlation operator acting on the pair labeled by α. This approximation correlates all pairs — so to speak — one after the other in all different orderings instead of simultaneously as $\exp\{-i \sum_{i<j}^{A} g^{[2]}(i,j)\}$ would do.

It is not exactly unitary anymore but it conserves the norm in the sense that the correlated unit operator remains unchanged

$$\widehat{1}^{C3} = 1 . \qquad (102)$$

The actual calculations for the three–body and four–body system are done by Monte Carlo integration. The derivatives of the kinetic energy are calculated numerically.

For example in the three–body system the potential energy is given by

$$\langle\,\widehat{V}^{C3}\,\rangle = \frac{1}{3!}\sum_{P\{\alpha,\beta,\gamma\}}\int \mathrm{d}^3x_1\mathrm{d}^3x_2\mathrm{d}^3x_3 \tag{103}$$

$$\times\sum_{i<j}^{3} v(\vec{x}_i - \vec{x}_j)\,|\langle\,\vec{x}_1,\vec{x}_2,\vec{x}_3\,|\,c(\alpha)\,c(\beta)\,c(\gamma)\,|\,\Phi\,\rangle|^2$$

and the kinetic energy is calculated as

$$\langle\,\widehat{T}^{C3}\,\rangle = \frac{1}{3!}\sum_{P\{\alpha,\beta,\gamma\}}\int \mathrm{d}^3x_1\mathrm{d}^3x_2\mathrm{d}^3x_3 \tag{104}$$

$$\times\frac{1}{2m}\sum_{i}^{3}|\frac{\partial}{\partial\vec{x}_i}\,\langle\,\vec{x}_1,\vec{x}_2,\vec{x}_3\,|\,c(\alpha)\,c(\beta)\,c(\gamma)\,|\,\Phi\,\rangle|^2\ .$$

The uncorrelated states $|\,\Phi\,\rangle$ are those which minimize the two–body correlated Hamiltonian together with the standard correlation function $R_+(r)$ defined in section 3.2.

The results are summarized and compared with the two–body approximation (for which analytical expressions exist) in table 2.

The correlated three–body kinetic energy $\langle\,\widehat{T}_{int}^{C3}\,\rangle$ is for both nuclei within the error bars of the Monte Carlo integration the same as the correlated two–body kinetic energy $\langle\,\widehat{T}_{int}^{C2}\,\rangle$. This means that the three–body contribution $\langle\,\widehat{T}^{[3]}\,\rangle = \langle\,\widehat{T}_{int}^{C3}\,\rangle - \langle\,\widehat{T}_{int}^{C2}\,\rangle$ is within $\pm 0.06\,\mathrm{MeV}$ for $A = 4$.

The three–body contribution to the correlated potential $\langle\,\widehat{V}^{[3]}\,\rangle = \langle\,\widehat{V}^{C3}\,\rangle - \langle\,\widehat{V}^{C2}\,\rangle$ is of the order of $0.14\,\mathrm{MeV}$ for $A = 3$ and $1.09\,\mathrm{MeV}$ for $A = 4$. Both corrections are small compared to the difference $\langle\,\widehat{V}^{C2}\,\rangle - \langle\,V\,\rangle$ between the two–body correlated and the uncorrelated potential which is $-18.08\,\mathrm{MeV}$ for $A = 3$ and $-55.89\,\mathrm{MeV}$ for $A = 4$.

It is interesting to note that the three–body contribution shifts up the energy again slightly by 2% of the gain in binding achieved by the two–body part of the correlation. However, the uncorrelated state is not varied for the three–body approximation separately but taken from the energy minimization within the two–body approximation. A variation could lower the energy again.

The three–body part of the correlated potential is positive in all cases we considered. The reason is that a simultaneous action of $c(i,j,k)$ on three particles

which are close shifts them further away from each other than the sum of pair wise shifts $c(i,j)$, $c(i,k)$ and $c(j,k)$. As $c(i,j)$ is optimized to move probability from the repulsive into the attractive region (see fig. 5) a further shift results in a loss of binding.

In order to see the dependence on density of the three–body contribution to the total kinetic energy and potential energy we calculate $\langle \widehat{T}^{[3]} \rangle$ and $\langle \widehat{V}^{[3]} \rangle$ as a function of the width parameter a for ^{3}He. In fig. 11 the ratios $\langle \widehat{T}^{[3]} \rangle / \langle \widehat{T}^{C3} \rangle$ and $\langle \widehat{V}^{[3]} \rangle / \langle \widehat{V}^{C3} \rangle$ between the three–body part and the total correlated energies are plotted versus $\kappa = \rho_{max} V_c$, where ρ_{max} is the maximum of the one–body density and $V_c = 0.16$fm^3 is the correlation volume defined in eq. (53) for the correlation function (parameters in eq. (99)) used in this section. While the three–body part of the correlated kinetic energy stays rather small the three–body part of the correlated potential energy grows linearly with κ. The ratios stay below 1% for $0 \leq \kappa \leq 0.1$. The ground state values for ^{3}He

	$A = 3$	Error	$A = 4$	Error
a [fm^2]	2.07		1.55	
$\langle T_{int} \rangle$	30.05		60.39	
$\langle \widehat{T}^{C2}_{int} \rangle$	35.12		75.58	
$\langle \widehat{T}^{C3}_{int} \rangle$	35.13	± 0.02	75.56	± 0.06
$\langle \widehat{T}^{[2]} \rangle$	5.07		15.19	
$\langle \widehat{T}^{[3]} \rangle$	0.01	± 0.02	-0.02	± 0.06
$\langle V \rangle$	-23.54		-50.23	
$\langle \widehat{V}^{C2} \rangle$	-41.62		-106.12	
$\langle \widehat{V}^{C3} \rangle$	-41.48	± 0.001	-105.03	± 0.002
$\langle \widehat{V}^{[2]} \rangle$	-18.08		-55.89	
$\langle \widehat{V}^{[3]} \rangle$	0.14	± 0.001	1.09	± 0.002
$\langle H \rangle$	6.51		10.16	
$\langle \widehat{H}^{C2} \rangle$	-6.50		-30.54	
$\langle \widehat{H}^{C3} \rangle$	-6.35	± 0.02	-29.47	± 0.06
$\langle \widehat{H}^{[2]} \rangle$	-13.01		-40.70	
$\langle \widehat{H}^{[3]} \rangle$	0.15	± 0.02	1.07	± 0.06

Table 2
Uncorrelated energies, two– and three–body approximation of corre-
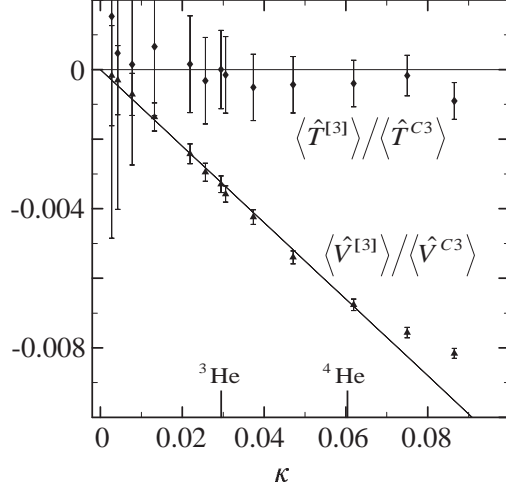lated energies, all in MeV.

Fig. 11. Ratios of correlated three–body part to total kinetic $\langle \widehat{T}^{[3]} \rangle / \langle \widehat{T}^{C3} \rangle$ and potential energy $\langle \widehat{V}^{[3]} \rangle / \langle \widehat{V}^{C3} \rangle$ as function of $\kappa = \rho_{max} V_c$ ($V_c = 0.16\text{fm}^3$) for ^{3}He. Values of κ for the ground states of ^{3}He and ^{4}He are indicated. Lines are only guiding the eye.

and ^{4}He are in this range. One should however keep in mind that the error induced in the total energy $\langle \widehat{T}^{C2} \rangle + \langle \widehat{V}^{C2} \rangle$ by neglecting the three–body contributions is larger because kinetic and potential energy have opposite sign and are of similar size. A rule of thumb is to stay with κ below 0.1 if an accuracy of less then 1% is desired for the effective potential in two–body approximation.

Since the estimated three–body contribution turns out to be so small compared to the leading two–body contribution it is not worthwhile to pursue it further. The other uncertainties, like a genuine three–body contribution, the parameterization of the correlation function $R_+(r)$ or the simplicity of the uncorrelated many–body state are too large.

4 Many–body systems with spin–isospin–dependent forces

In this section the unitary correlation operator method is applied to nuclei up to mass $A = 48$. Since the Malfliet–Tjon V potential overbinds nuclei beyond $A = 4$ strongly the so called modified Afnan–Tang S3 potential [18,19] for which several calculations exist in the literature [19–22] is used. It is specified in the appendix in eq. (A.2). The radial dependence of the potential in the two even–parity states with $S = 0$ and $S = 1$ and in the odd state is depicted in fig. 12.

The uncorrelated many–body states are Slater determinants composed of

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single–particle states

$$\langle \vec{x} \, | \, q_k \rangle = \exp\left\{ -\frac{(\vec{x} - \vec{b}_k)^2}{2a_k} \right\} \otimes \, | \, m_{s,k} \rangle \otimes \, | \, m_{t,k} \rangle \tag{105}$$

with a Gaussian–shaped coordinate space part, a two–component spinor $| \, m_{s,k} = \pm\frac{1}{2} \rangle$ and an isospin part $| \, m_{t,k} = \{\text{proton, neutron}\} \rangle$. The complex parameters $\vec{b}_k$ and a_k are the variational degrees of freedom of the uncorrelated many–body state $| \, \Phi \rangle$. They contain the mean positions, the mean momenta and the complex width of the packets. For details see ref. [23].

All proton and neutron spins are paired to zero except if the number is odd.

4.1   Spin–isospin–dependent correlator

Analogue to the central potential the generator of the unitary correlator is decomposed into the four spin–isospin channels

$$g^{[2]}(\vec{r}, \vec{q}, \vec{\sigma}_1, \vec{\sigma}_2, \vec{\tau}_1, \vec{\tau}_2) = \sum_{S,T}^{\{0,1\}} g_{ST}^{[2]}(\vec{r}, \vec{q}) \, \Pi_S \otimes \Pi_T \tag{106}$$

with the projection operators $\Pi_{S=0} = \frac{1}{4}(1 - \vec{\sigma}_1\vec{\sigma}_2)$, $\Pi_{S=1} = \frac{1}{4}(3 + \vec{\sigma}_1\vec{\sigma}_2)$ and $\Pi_{T=0}, \Pi_{T=1}$ accordingly.

The unitary correlator in A–body space is herewith

$$C_A = \exp\left\{ -i \sum_{k<l}^{A} g^{[2]}(\vec{r}_{kl}, \vec{q}_{kl}, \vec{\sigma}_k, \vec{\sigma}_l, \vec{\tau}_k, \vec{\tau}_l) \right\} . \tag{107}$$

For the two–body approximation of the correlated operator only $c \equiv C_2$ in the two–body space is needed

$$\begin{aligned} c &= \exp\left\{ -i \sum_{S,T}^{\{0,1\}} g_{ST}^{[2]}(\vec{r}, \vec{q}) \, \Pi_S \otimes \Pi_T \right\} \\ &= \sum_{S,T}^{\{0,1\}} \exp\left\{ -i g_{ST}^{[2]}(\vec{r}, \vec{q}) \right\} \Pi_S \otimes \Pi_T . \end{aligned} \tag{108}$$

Since Π_S and Π_T are projection operators the correlator becomes a direct sum of four commuting unitary correlators, one for each channel. Compared to the
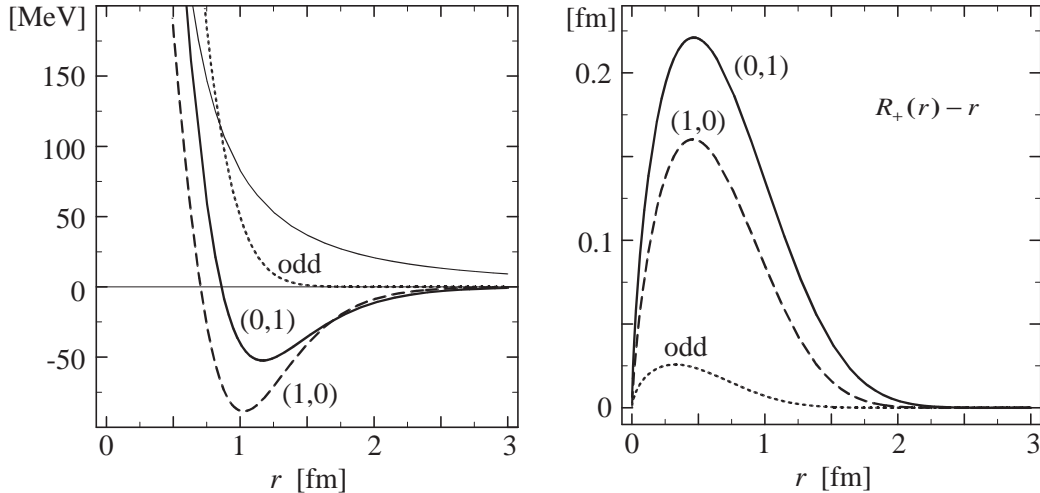
Fig. 12. L.h.s.: Radial dependence of the potentials for even parity channels $(S, T) = (1, 0)$ and $(0, 1)$, the odd channels $(S, T) = (0, 0)$ and $(1, 1)$ and centrifugal potential for $l = 1$ (thin line). R.h.s.: Corresponding correlation functions $R_+^{01}(r)$, $R_+^{10}(r)$, $R_+^{\mathrm{odd}}(r)$ in terms of $R_+(r) - r$.

spin–isospin–independent case there are now four correlation functions $R_+^{ST}(r)$ which have to be determined. For the ATS3M potential [18,19] there are only three because the odd channels $(S, T) = (0, 0)$ and $(1, 1)$ have the same purely repulsive radial dependence. The $(S, T) = (0, 1)$ and $(1, 0)$ potentials have a repulsive core and an attractive tail so that the procedure discussed in 2.4 is used to construct a correlation function of finite range from eq. (82) which is then parameterized in the form (96). The resulting parameters are given in table 3 together with the correlation volumes. The correlation functions are shown on the r.h.s. of fig. 12.

For the repulsive channels $(S, T) = (0, 0)$ and $(1, 1)$ with an odd parity in the relative wave function the exact correlation function obtained by eq. (82) does not provide a unique scale parameter β. As can be seen from fig. 12 the centrifugal barrier for $l = 1$ states dominates the repulsive potential for

channel	α [fm]	β [fm]	η	V_c [fm^3]
even, $S = 0, T = 1$	1.81	1.07	0.67	0.43
even, $S = 1, T = 0$	1.43	0.95	0.78	0.21
odd, $S = 0$, $T = 0$ odd, $S = 1$, $T = 1$	2.30	1.00	0.90	0.004

Table 3
Parameters of the different correlation functions $R_+^{ST}(r)$ and corresponding correlation volumes V_c.
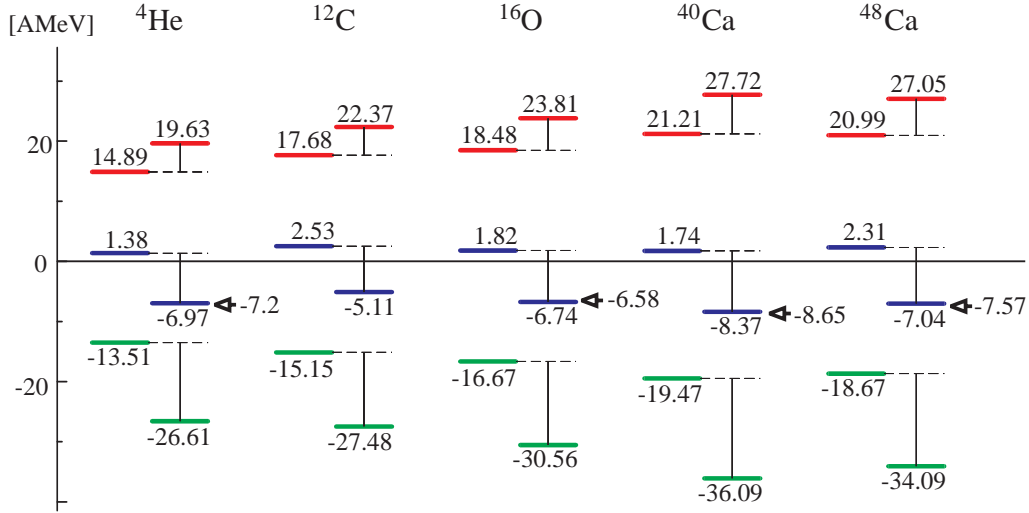
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Fig. 13. Uncorrelated and correlated kinetic, potential and total energies for the modified Afnan-Tang S3 potential, otherwise same as fig. 8. Arrows indicate the results of a Yakubovski calculation for ^{4}He [20], of a FHNC calculation for ^{16}O [21] and of CBF calculations for ^{40,48}Ca [22].

distance $r > 0.7$fm and hence even the uncorrelated $l = 1$ state $u(r) = rj_1(\sqrt{mE}\,r)/\sqrt{N_0} \overset{E \to 0}{\longrightarrow} r^2/\sqrt{N_0}$ has already a small amplitude in the repulsive region. Therefore, a rather small correlation function is needed to correct the small distance behaviour of the repulsive wave function. η which controls the correlation function at small r is chosen to minimize the repulsion in the two–body system, while the ^{16}O ground state was employed to choose α and β. The resulting parameters are given in table 3 and the corresponding $R_+^{\text{odd}}(r) \equiv R_+^{00}(r) = R_+^{11}(r)$ is depicted on the r.h.s. of fig. 12.

4.2 $A = 2 \cdots 48$ nuclei with the modified Afnan–Tang force

The correlation functions given by the parameters of table 3 are now used to calculate the energies of several nuclei. The results for ^{4}He, ^{12}C, ^{16}O, ^{40}Ca and ^{48}Ca are summarized in fig. 13 in terms of the uncorrelated and correlated kinetic and potential energies as already explained in connection with fig. 8. The total energy $\langle \widehat{H}^{C2} \rangle$ is compared to results of different methods such as Yakubovsky calculations [20], FHNC [21] and CBF [22].

Considering the simplicity of the uncorrelated state and the fact that the correlated two–body Hamiltonian is the same for mass number $A = 2$ up to $A = 48$ the agreement with much more elaborate methods is striking. For deformed nuclei like ^{12}C, ^{20}Ne or ^{28}Si the variational many–body calculations are very difficult in terms of computing. With the new Unitary Correlation Op-

	$\langle\,\widehat{T}_{int}^{C2}\,\rangle$	$\langle\,\widehat{V}^{C2}\,\rangle$	$\langle\,\widehat{H}^{C2}\,\rangle$	"exact" energy	$\langle\,\widehat{R}_s^{C2}\,\rangle^{1/2}$
^{2}H	12.33	-14.50	-2.17	-2.22	1.93
^{4}He	78.5	-106.4	-27.9	-28.8 [20]; -24.2 [19]	1.35
^{6}Li	99.3	-113.7	-14.4		1.97
^{12}C	268.5	-329.8	-61.3		2.36
^{16}O	381.0	-488.9	-107.9	-105.3 [21]; -107.7 [19]	2.28
^{19}F	448.2	-558.8	-110.6		2.52
^{20}Ne	501.1	-628.4	-127.4		2.56
^{24}Mg	606.7	-757.6	-150.9		2.74
^{27}Al	678.2	-851.1	-172.9		2.82
^{28}Si	705.4	-896.1	-190.7		2.88
^{40}Ca	1108.7	-1443.6	-334.9	-346.0 [22]; -335.6 [19]	2.93
^{48}Ca	1298.4	-1636.1	-337.7	-363.36 [22]	3.20

Table 4
Results of a variational calculation with a single Slater determinant
(except for ^{2}H) and a fixed correlator for several nuclei with the ATS3M
potential. Energies are given in MeV, radii in fm.

erator Method combined with the uncorrelated states of Fermionic Molecular
Dynamics [23] deformed nuclei do not pose special problems. For example for
^{20}Ne the minimization takes about 3 minutes CPU time on an IBM RS6000,
for ^{40}Ca about one hour.

In table 4 ground state energies of a variety of nuclei, including those of fig. 13,
are listed and compared to literature values if available.

Considering the fact that for all nuclei the energy results from the subtraction
of a large positive kinetic energy and a similarly large potential energy, which
are about 4 respectively 5 times larger than the total energy, it is surprising
that the outcome of the present method lies within the uncertainties of "ex-
act" many–body calculations. One reason is probably that the probability in
the two–body density which is moved out of the repulsive core region is put
where the potential is most attractive, so that a large part of the attractive
correlations are also taken care of. Otherwise it is hard to imagine that a single
Slater determinant which represents only the mean–field behavior is sufficient
as an uncorrelated state.

The root–mean–square radii of the matter distribution which are given in the last column of table 4 are calculated with the correlated operator in two–body approximation.

$$\widehat{R}_s = C^{-1}\frac{1}{A}\sum_i^A \left(\vec{x}(i) - \vec{X}_{cm}\right)^2 C = \frac{1}{A}\Big[C^{-1}\sum_i^A \vec{x}(i)^2 C - \vec{X}_{cm}^2\Big] \tag{109}$$

$$\approx \widehat{R}_s^{C2} = R_s + \widehat{R}_s^{[2]} = \frac{1}{A}\Big[\sum_i^A \vec{x}(i)^2 - \vec{X}_{cm}^2\Big] + \frac{1}{2A}\sum_{i<j}^A \left(R_+(r_{ij})^2 - r_{ij}^2\right)$$

where the centre of mass position operator

$$\vec{X}_{cm} = \frac{1}{A}\sum_i^A \vec{x}(i) \tag{110}$$

commutes with the correlator C. The expression (109) is a straightforward result of the unitary correlator method explained in section 2.

The contribution $\langle\, \widehat{R}_s^{[2]}\, \rangle$ of the second order to $\langle\, \widehat{R}_s^{C2}\, \rangle^{1/2}$ is in all cases only in the last digit which is displayed. This shows that the matter distribution in coordinate space is changed very little by the repulsive two–body correlations.

5 Summary

A new concept, the Unitary Correlation Operator Method (UCOM), has been developed to describe short range correlations brought about by the repulsive part of the interaction.

The unitary correlator reduces the probability to find two particles in the classically forbidden region of the repulsive core by shifting them away from each other. The relation between uncorrelated and new correlated distances are expressed in terms of the coordinate transformation $r \rightarrow R_+(r)$. With this key quantity, which may depend on spin and isospin, analytic expressions for the correlated states and the correlated kinetic and potential energies are derived. Due to unitarity correlated operators can be evaluated easily, for example a local potential $v(r)$ between two particles transforms as $c^\dagger\, v(r)\, c = c^{-1}\, v(r)\, c = v(c^{-1}\, r\, c) = v(R_+(r))$.

For a many–body system the physical challenge is to find an optimal $R_+(r)$ which describes well the depletion in the two–body density at short distances, which cannot be represented by the uncorrelated states. Due to unitarity this

reduction in probability results in an increase at larger distances. If the two–body potential has an attractive area outside the repulsion it is natural to enhance the probability there. These type of repulsive–attractive potentials provide an inherent length scale for the range of the correlator.

For numerical ease one wants to use the two–body approximation for correlated operators and states and hence the correlation range should be smaller than the mean particle distance so that the probability to find two particles within the correlation volume V_c is small and the chance that three particles are simultaneously inside V_c is negligible. If this condition is not fulfilled because the density is too high, the correlation range in which $R_+(r)$ differs from r has to be reduced and at the same time the flexibility of the uncorrelated states has to be increased to include medium range correlations. This is an important aspect of the method: the unitary correlator and the uncorrelated states have to harmonize.

For nuclei (at least without tensor forces which we have not investigated yet) this seems to be the case because the calculations presented show that a single Slater determinant plus a suitably chosen unitary correlator reproduce the "exact" ground–state energies of nuclei between $A = 2$ and 48 within a few percent.

Acknowledgments

A   Appendix

A.1   Malfliet–Tjon V potential

The MTV potential [13] is given by

$$v(r) = \sum_{i=1}^{2} \gamma_i \frac{\exp\{-\beta_i\, r\}}{r} \quad \text{with}$$

i	γ_i [MeV fm]	β_i [fm^{-1}]
1	-584	1.55
2	1458	3.11

. (A.1)

A.2   Modified Afnan–Tang S3 potential

The modified Afnan–Tang S3 potential [19] is given by

$$v = v_0(r)\, \Pi_{01} + v_1(r)\, \Pi_{10} + v_{\text{odd}}(r)\, (\Pi_{00} + \Pi_{11}) \quad \text{with} \tag{A.2}$$

$$v_S(r) = \sum_{i=1}^{3} \gamma_{S,i} \exp\left\{-\beta_{S,i}\, r^2\right\}$$

and the parameters

	$S = 0$		$S = 1$		odd	
i	$\gamma_{S,i}$ [MeV]	$\beta_{S,i}$ [fm^{-2}]	$\gamma_{S,i}$ [MeV]	$\beta_{S,i}$ [fm^{-2}]	$\gamma_{S,i}$ [MeV]	$\beta_{S,i}$ [fm^{-2}]
1	1000	3.0	1000	3.0	1000	3.0
2	-166	0.8	-326.7	1.05		
3	-23	0.4	1000	0.6		

Table A.1
Parameters of the modified Afnan–Tang S3 potential.

The operators $\Pi_{ST} = \Pi_S \otimes \Pi_T$ project on two–body states with total spin S and total isospin T, respectively.

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