Model wave functions and dynamic correlations in light-medium nuclei

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Abstract. The nuclei \(^4\)He, \(^8\)Be, \(^{12}\)C and \(^{16}\)O have been studied starting from nucleon-nucleon interactions of \(v_4\) type. The wave function is built as the product of three terms, a Jastrow correlation factor, a linear correlation factor and a model wave function. The correlation factors account for both the short range repulsive and the spin and isospin dependence of the nuclear potential. The model wave function is antisymmetric and has the values of the angular momentum and parity of the state under description. For the model wave function we have used two different schemes. The first one is based on a Harmonic Oscillator shell model with and without deformation, and the second one is based on the Margenau-Brink model of alpha clustering. Projection operators of parity and total angular momentum are used. The performance of these two models is studied and compared systematically. Wave functions for the ground state and some members of its rotational band and some other bound states of these nuclei have been obtained. Binding energies, root mean square radius and the expectation value of the kinetic energy and the different channels of the nuclear interactions and the one– and two– body densities are reported. The two different model wave functions and the effects of the different nucleon-nucleon correlations have been evaluated on those quantities. All the results here presented have been obtained by using the Variational Monte Carlo method.

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1. Introduction

The use of explicitly correlated trial wave functions to study nuclear bound states constitutes an efficient and compact way to include the complex dynamic mechanisms induced by the nuclear potential in the nuclear structure. Short range correlations along with a model wave function is a scheme widely used as starting point when realistic or semi-realistic interactions are considered. Usually, the model wave function is a Slater determinant built with orbitals obtained from a given mean field. By including in the ansatz correlation factors, one tries to take care of the deficiencies of this model wave function, specially the dependence of the nuclear force on the state of the nucleon pair and the behaviour at short internucleon distances.

Jastrow central correlation factors [1] have shown to be an appropriate way of handling the strongly repulsive short range core of the nuclear force in the operator independent channel. This functional form has been extended to the spin and isospin dependent channels including Jastrow type operatorial correlation factors. In this way the model wave function is corrected, and the two nucleons dynamic is adapted to the behaviour of the different channels of the interaction. A major drawback of this ansatz is the enormous computational difficulties posed by this wave function, mainly due to the presence of operatorial correlations. In fact this correlated wave function has been applied so far only to light nuclei [2], or by using some approximations for heavier nuclear systems [3, 4].

In order to overcome these problems, simpler trial wave functions with a linear state dependent correlation factor [5], and a central Jastrow term times a linear state dependent correlation factor [6] have been proposed. With them medium nuclei have been studied obtaining good results [5, 6, 7, 8, 9, 10]. In this way, the short range effects, at least in the Wigner channel, are adequately described by means of the central Jastrow factor. The linear term can be obtained from the Coupled Cluster method including only two–body translationally and rotationally invariant excitations [5, 11], formally equivalent to a Configuration Interaction expansion. Thus, the use of a linear correlation factor can be viewed either as a linear approximation to the Jastrow operatorial factor or as Configuration Interaction expansion of the trial wave function.

The variational freedom given by the model part of the wave function can be exploited to include medium and long range effects induced by the nuclear interaction. In general, it is difficult to describe these effects by means of a correlation factor. These are typical many body effects that are usually treated in nuclear physics by using, for instance, a deformed mean field. An important example of these kind of effects is the formation of alpha clusters or other type of nucleon groupings. In principle one could describe these effects in terms of correlation factors by, for example, truncating the Coupled Cluster exp(S) wave function at higher orders, considering in this way three--, four--, and larger $n$–body excitations. However, and within the scheme of this work, it is simpler to incorporate long range effects in the model wave function, by making use of the different models developed for effective interactions.
Therefore the different components of the trial wave function are tailored to account for different correlation mechanisms. The aim of this work is to use these wave functions to study the ground and some low lying excited states of the $^4$He, $^8$Be, $^{12}$C and $^{16}$O nuclei and to analyse the interplay between the different dynamical effects included in the wave function. The ansatz consists of three factors: a state independent Jastrow correlation factor, a linear state dependent factor and a model wave function. Two different model wave functions are employed. The first one is based on a shell model built from a deformed Harmonic Oscillator mean field while the second one is based on the $\alpha$-cluster Margenau-Brink model. The determination of the optimal variational wave function and the calculation of the different nuclear properties is carried out by means of the Variational Monte Carlo method.

The structure of this work is as follows. In section 2 we show in detail the variational trial wave function used. Section 3 is devoted to the technical aspects involved in the calculation of the different properties. The results are presented and discussed in section 4. Finally, section 5 summarizes and gives the conclusions of this work.

2. Trial wave function

The variational trial wave functions used are the product of a correlation factor, which includes a central Jastrow correlation factor and a linear state-dendent correlation factor, and a model wave function

$$\Psi_{JKM}^{\pm}(1, \ldots, A) = F_J(1, \ldots, A) F_L(1, \ldots, A) \Phi_{JKM}^{\pm}(1, \ldots, A)$$

The function $F_J$ is the central Jastrow factor that depends only on the distance between pairs of nucleons

$$F_J(1, \ldots, A) = \prod_{i<j}^A f(r_{ij})$$

while $F_L$ is the linear state-dependent correlation factor defined as

$$F_L(1, \ldots, A) = \sum_{i<j}^A g(i, j).$$

where the function $g(i, j)$ depends on the radial and intrinsic degrees of freedom of the particles, $i$ and $j$

$$g(i, j) = g^{(1)}(r_{ij}) + \sum_{k=2}^4 g^{(k)}(r_{ij}) P^{(k)}(i, j),$$

and $P^{(k)}(i, j)$, with $k = 2, 3, 4$, are the exchange spin, isospin and spin–isospin operators, respectively. This is the only part of the trial wave function where state dependent correlations are present explicitly.

The radial correlation functions $g^{(k)}(r)$, $k = 1, \ldots, 4$, and $f(r)$ are parameterized as a linear combination of Gaussian functions

$$g^{(k)}(r) = \sum_{m=0}^M a_m^{(k)} e^{-b_m^2 r^2}, \quad f(r) = 1 + \sum_{n=1}^N c_n e^{-d_n^2 r^2}.$$
The structure of the state dependent correlation factor is the same as that of the nuclear potential. We have used two different $v_4$ type nuclear forces with the same operatorial dependence as the linear correlation factor; the BB1 Brink-Boeker [12] and a modified S3 Afnan-Tang interaction [13]. The first one was fitted by using non correlated wave functions. The second one is a semi-realistic interaction fixed by using explicitly correlated wave functions to reproduce the $s$-wave scattering data up to about 60 MeV for the alpha particle. Some of the parameters of this interaction were modified by Guardiola [14] to include the repulsion in the triplet states, necessary to an adequate description of nuclei heavier than the $\alpha$ particle. Both potentials have been extensively employed in previous works.

For the model wave function, $\Phi_{\bar{C}M}^\pm$, we have considered two possibilities, a shell model wave function built from Cartesian Harmonic oscillator orbitals, and a wave function including the alpha clustering effect by means of the Margenau-Brink model. This model was devised by Margenau [15] as a simpler alternative to the Wheeler model [16], and it was further developed by Brink [17]. Within this scheme, nuclear bound states are described as a composite of $\alpha$ particles centered around some given fixed positions, like the atoms in a molecule. Different arrangements of the $^4$He clusters give rise to different geometries and states. The model function is taken to be antisymmetric with respect to nucleon exchange.

We study $A = 4n$, $n = 1, 2, 3, 4$ nuclei with $N = Z$. The model wave function based on the Margenau-Brink model can be written as

$$
\Phi_{\bar{C}}(1, 2, \ldots, A) = A \left\{ \prod_{k=1}^{n} \xi_{\bar{C}_k}(4k - 3, 4k - 2, 4k - 1, 4k) \right\}
$$

(6)

where $\bar{C} \equiv \{\bar{c}_k\}_{k=1}^n$ is a set of centers of the $\alpha$-cluster, and the operator $A$ is the antisymmetrizer of $A$ particles. The $\xi_{\bar{C}_k}$ functions can be any approximated wave function for the $^4$He nucleus centered at $\bar{c}_k$. In this work we have taken these functions to be of the form

$$
\xi_{\bar{C}_k}(1, 2, 3, 4) = \frac{1}{\sqrt{4!}} \begin{vmatrix}
\phi_{\bar{C}_k}(\beta; r_1) \eta_1(1) & \phi_{\bar{C}_k}(\beta; r_1) \eta_2(1) & \ldots & \phi_{\bar{C}_k}(\beta; r_1) \eta_4(1) \\
\vdots & \vdots & \ddots & \vdots \\
\phi_{\bar{C}_k}(\beta; r_4) \eta_1(4) & \phi_{\bar{C}_k}(\beta; r_4) \eta_2(4) & \ldots & \phi_{\bar{C}_k}(\beta; r_4) \eta_4(4)
\end{vmatrix}
$$

(7)

where $\eta_k(i)$ stands for the four possible spin-isospin states of the nucleon, and the single particle wave function is taken to be a $s$-wave harmonic oscillator orbital centered at $\bar{c}_k$

$$
\phi_{\bar{C}_k}(\beta; r) = \left(\frac{\beta^2}{\pi}\right)^{3/4} e^{-\frac{1}{2} \beta^2 (r - \bar{c}_k)^2}
$$

(8)

It is straightforward to check that the full model wave function becomes a Slater determinant, that allows one to apply the machinery developed to deal with determinants in Variational Monte Carlo calculations.

Regardless the actual values of the centers, this function has total spin equal to zero. By using $\Phi_{\bar{C}}$ and $\Phi_{-\bar{C}}$ (the same function with centers at opposite positions) we
can build eigenfunctions of the parity operator
\[ \Phi^\pm_C(1, \ldots, A) = \Phi_C(1, \ldots, A) \pm \Phi_{-C}(1, \ldots, A). \]  

In general these functions have not a definite value of the total angular momentum. In order to get model wave functions that are eigenfunctions of the angular momentum operator, the Peierls-Yoccoz projection operators [18], \( \mathcal{P}^J_{MK} \), are used. In this way we obtain the model wave function
\[ \Phi^\pm_{J, KM, C}(1, \ldots, A) = \mathcal{P}^J_{MK} \Phi^\pm_C(1, \ldots, A) \]
\[ = \frac{2J + 1}{8\pi^2} \int d\Theta \mathcal{D}^J_{MK}(\Theta) R(\Theta) \Phi^\pm_C(1, \ldots, A) \]  
where \( R(\Theta) \) is the rotation operator, \( \mathcal{D}^J_{MK}(\Theta) \) the rotation matrix and \( \Theta \) represents the Euler angles. The quantum number \( J \) gives the total angular momentum, \( K \) is the projection along the nuclear \( z \) axis and \( M \) is the projection along the \( Z \) axis of the laboratory fixed frame. Therefore the projection is carried out by rotating the intrinsic state and integrating over all angles weighted by the rotation matrix. The projection operation is done only for the model part of the trial wave function because both the Jastrow and the linear correlation factors commute with the projection operator.

Within this scheme a rotational band is associated to each value of \( K \). The states in the band correspond to all the possible values of \( J \) and parity allowed by the symmetry of the spatial arrangements of the \( \alpha \) clusters [17, 19, 20, 21]. For \(^8\text{Be}\) only a linear configuration can be built within this model with the two alpha clusters separated by a distance \( d \). This corresponds to the point symmetry group \( D_{\infty h} \). For \(^{12}\text{C}\) one can build different arrangements of the \( \alpha \) cluster giving rise to different geometries. In a non-correlated calculation the lowest energy is obtained from an equilateral triangle having \( D_{3h} \) as symmetry group. This configuration will be used here to describe, when \( K = 0 \), the \( 0^+ \) ground state of this nucleus and its rotational band, as well the \( J^\pi = 3^- \) excited state, with \( K = 3 \). We shall use a linear configuration of the three alpha particles to study the first excited \( 0^+ \) state whose excitation energy is 7.65 MeV. Finally, the \( 0^+ \) ground state and the first excited state with \( J^\pi = 3^- \) of \(^{16}\text{O}\) will be described with the \( \alpha \) particles lying at the vertices of a regular tetrahedron and therefore with \( T_d \) as symmetry group. For this nucleus we shall also consider the linear configuration of the alpha particles. In table 1 we summarize the different configurations studied here with the corresponding \( K \) and \( J \) values and the parity of the states.

When the distances between the different alpha clusters are taken to be zero some of the Margenau-Brink model functions tend to shell model wave functions. In table 1 we give the limiting Harmonic Oscillator shell model configurations of the corresponding Margenau-Brink wave functions for zero intercluster distance. Any of these wave functions is written as a Slater determinant with not well defined value of the angular momentum, except for the tetrahedron in \(^{16}\text{O}\). For states with axial symmetry we have considered deformed harmonic oscillator wave functions. By including axial symmetry in the model wave functions a noticeable improvement in the binding energy is obtained with respect to the spherical shell model approximation.
### Table 1. Symmetry point group of the different spatial arrangements of the $\alpha$ clusters and the limiting Harmonic Oscillator shell model configurations (HO). The different rotational states that can be obtained are also given.

|       | (K : $J^\pi$) | HO                                      |
|-------|---------------|-----------------------------------------|
| $^{8}$Be | $D_{\infty h}$ | (0 : $0^+$, $2^+$, $4^+$)                |
| $^{12}$C | $D_{3h}$      | [(0, 0, 0)$^4$(0, 0, 1)$^4$]             |
| $^{12}$C | $D_{\infty h}$ | (0 : $0^+$, $2^+$, $4^+$)                |
| $^{16}$O | $T_d$         | [(0, 0, 0)$^4$(0, 0, 1)$^4$]             |
| $^{16}$O | $D_{\infty h}$ | (0 : $0^+$)                              |

#### 3. VMC calculation of the matrix elements

The VMC evaluation of the expectation values involved in the determination of the energy and other properties presents several differences with respect to standard algorithms [22]. The reason for that lies in the presence in the trial wave function of both, the state dependent correlations (by means of $F_L$), and the projection operator $P_{JMK}$. The technical problems induced by each one of these elements can be treated independently. The spin-isospin dependence in the trial wave function is the main source of difficulties and the ultimate reason why the nuclear problem is more complex, from a computational point of view, than other non-relativistic many body systems.

To deal with angular momentum projection we use equation (10) to write the expectation value of the Hamiltonian, $\langle H \rangle$, as

$$\langle H \rangle = \int d\Omega D_{JK}^J(\Omega) \langle \Phi^\pm | F_J F_L H F_J F_L R(\Omega) | \Phi^\pm \rangle$$

In this equation the transformation properties of the rotation matrices and the rotational invariance of the correlation factors have been taken into account [17]. Note that this is an integral over the particle degrees of freedom, intrinsic and spatial considered in the bracket, and the Euler angles of the rotation. The latter can be further simplified for nuclei with axial symmetry. This multi dimensional integration is performed here by using a Monte Carlo quadrature with the Metropolis algorithm. The probability distribution function used will be discussed below. Finally, it is worth to point out that the action of the rotation operator over a spin-isospin saturated Slater determinant is another spin-isospin saturated Slater determinant. This property is important for our treatment of the state-dependent correlations.

To carry out the spin-isospin integral in the expectation value of the Hamiltonian, equation (11), we use the following complete set

$$|\mathcal{R}, \Xi⟩ = |\mathcal{r}_1 \eta_1⟩ |\mathcal{r}_2 \eta_2⟩ \ldots |\mathcal{r}_A \eta_A⟩$$

where $\mathcal{r}_i$ is the spatial coordinate of the $i$-particle and $\eta_i$ represents its spin-isospin variables. $\mathcal{R}$ and $\Xi$ denote the spatial coordinates and spin-isospin components,
respectively, of the whole system.

Thus the expectation value in equation (11), can be written as

$$\langle \Phi^\pm | F_J F_L H F_J F_L R(\Omega) | \Phi^\pm \rangle = \sum \int dR \langle \Phi^\pm | F_J F_L | R, \Xi \rangle \langle R, \Xi | H F_J F_L R(\Omega) | \Phi^\pm \rangle (13)$$

where the sum runs over all the possible spin-isospin components of the $A$ particle system and the integral is extended over all the spatial degrees of freedom of the system. The present scheme is valid for the calculation of the expectation value of any operator that commutes with the rotation operator.

We start from the spin and isospin sum. Let us focus on $\langle \Phi^\pm | F_L | R, \Xi \rangle$ (here we do not include the factor $F_J$ since it is a scalar in the spin–isospin subspace). This factor is not zero only in those cases in which the action of the operators in $F_L$ over $| R, \Xi \rangle$ leads to the same spin–isospin configuration as in $\Phi^\pm$. If we designate by $(0, 0, 0, 0)$ the state saturated in spin–isospin and by $(n_1, n_2, n_3, n_4)$ those states different from $(0, 0, 0, 0)$ in $n_1$ particles with spin and isospin up, $n_2$ particles with spin up and isospin down, $n_3$ particles with spin down and isospin up and $n_4$ particles with spin and isospin down, then the only $| R, \Xi \rangle$ states that contribute in equation (13) are $(1, -1, -1, 1)$ and $(-1, 1, 1, -1)$ as well as $(0, 0, 0, 0)$. Therefore the sum over the spin-isospin coordinates is reduced to only three spin–isospin configurations of the $A$ nucleons.

The spatial integration is carried out by using the VMC in the same way as in the case of state independent correlations. For the Metropolis random walk we have used the following probability distribution function

$$\omega(\mathcal{R}, \Omega) = | F_J(\mathcal{R}) F_L^c(\mathcal{R}) |^2 | \langle \Phi^\pm | \mathcal{R}, \Xi_1 \rangle \langle \mathcal{R}, \Xi_1 | R(\Omega) | \Phi^\pm \rangle | (14)$$

where $F_L^c$ is the central part of the linear state dependent factor $F_L$ and $\Xi_1$ stands for the spin and isospin configuration of the nucleons equal to that of the state under description. This function has been used in previous works providing a good performance.

In order to obtain the optimum set of variational parameters in the wave function we have worked as follows. First we have optimized the state–independent trial wave function. The search of the optimum set of non linear parameters has been performed by means of the simplex algorithm. Once this has been accomplished the state dependent trial wave function is built by using the same Jastrow and model functions. For the non linear parameters in the $g^{(k)}(r)$ functions of equation (5) we use the same ones as in the Jastrow function $f(r)$. The only new variational parameters are the $a_m^{(k)}$ that are fixed by solving the generalized eigenvalue problem. The use of the same set of non linear parameters does not lead to any appreciable loss of accuracy, but it conveys to a substantial reduction of the computing time because the optimization of the non–linear parameters for each trial wave function, as it was done in previous works, is very time consuming. This reduction is specially convenient for heavy nuclei.

4. Results

We have explored three possibilities of the correlation factor and the two models for the intrinsic function. For the correlation factor the three parameterizations considered are:
Figure 1. Jastrow functions for the two potentials and the different trial wave functions studied. The upper plots correspond to the BB1 interaction and the lower plots to the MS3 one. The left hand side figures correspond to HO model wave functions and the right hand side ones to Margenau-Brink model wave functions.

i) a central Jastrow factor only, $J$; ii) a linear state dependent correlation factor, $LO$; and iii) a central Jastrow times a linear state dependent, $JLO$. The $JLO$ is the most general form of the correlation factor used here. For the model part we have used either a shell model built from Harmonic Oscillator orbitals (spherical, HO, or deformed, HOD), or a function based on the Margenau-Brink model, MB. For $^{12}$C and $^{16}$O, and within the MB model, we have also considered a linear geometry for the alpha clusters, describing a different state with symmetry $D_{\infty h}$ and angular momentum and parity given in table 1. These states have been also described by means of the Harmonic Oscillator shell model by using the orbitals obtained in the limit of zero intercluster distance given in table 1. The model wave function for these states is denoted by HO-l and MB-l when using the Harmonic Oscillator and the Margenau-Brink models, respectively.

4.1. Correlation factor

In figure 1 we show the optimal correlation function of the Jastrow factor for both interactions and model wave functions. In general, the qualitative behaviour is the same for all of the cases although quantitatively the function depends on both the model function and the potential. At short distances these functions are mainly governed by the short range part of the potential. The depth of the minimum at the origin is mostly
Figure 2. Correlation functions of the linear correlation factor corresponding to both the LO and JLO trial wave functions for the ground state of the $^{12}$C nucleus. The upper panels correspond to the BB1 interaction and the others to the MS3 force.

determined by the strength of the core of the interaction, that is higher in the MS3 than in BB1. At medium distances, $r \approx 1.2$ fm, the correlation function has a maximum. The value of this maximum depends on the potential used, on the model function and on the state of the nucleus under study. For the ground state, the height of the maximum decreases with the number of nucleons for both models. For the linear configurations of $^{12}$C and $^{16}$O, the maximum is bigger than in the corresponding ground state, and tends to the same values obtained for $^{8}$Be and $^{4}$He, this is because the clustering is more accused in the linear geometry. This is an example of the interplay between the model function and the correlation factor. It is worth mentioning here that the energy is not very sensitive to this part of the correlation function, and it is the short range part the ultimate responsible of the binding.
The correlation functions of the linear correlation factor show, as it could be expected, different forms in different channels. This is due to the different radial dependence of the potential on the different channels. In figure 2 we plot the correlation functions obtained for the ground state of $^{12}$C in the LO and JLO approximations for the two interactions and model functions considered in this work. This nucleus is representative of the different nuclei studied here. Note that the BB1 potential only has Wigner and Majorana channels. Within the LO approximation and for both model wave functions, the correlation functions of the Wigner and Majorana channels present the same qualitative behaviour for both interactions. For the MS3 potential the correlation functions of the Bartlett and Heisenberg channels are practically the same in magnitude but with opposite sign. In principle one could expect that both functions are the same, except for the sign, because of the symmetry of the interaction in these channels. The reason of the difference is not the parameterized solution used in this work because similar differences have been found previously by using a different methodology [5] with the same type of wave function.

The inclusion of the Jastrow factor modifies the correlation functions of the different channels. The effect is more accused in the case of the Wigner channel, where the correlation function practically vanishes. For the other channels, the qualitative structure is similar to that obtained in the LO approach, with the only exception of the Majorana channel with Margenau-Brink model functions for both interactions.

4.2. Energy

In table 2 we report the total energy and the root mean square radius for the lowest energy states of the nuclei studied in this work obtained from different trial wave functions and working with the two potential considered here. The wave functions have been obtained by projecting to $K = 0$ and $J = 0$ the configurations proposed for both the ground state and the states built from the linear geometry for $^{12}$C and $^{16}$O. The values of the variational parameters in the model function are also shown in the table for each nucleus, $\beta$ is the oscillator parameter in both the HO and MB approaches and $d$ is either the deformation in the HOd model or the intercluster distance in the MB model.

The harmonic oscillator parameter $\beta$ is larger with the BB1 interaction than with the MS3 one. Therefore BB1 gives rise to a bigger confinement of the nucleons as compared with MS3. This can be also concluded from the values of the root mean square radius. It is worth to point out here that this quantity and, in general, those related to the one body spatial density are mainly governed by the model part of the wave function. On the other hand, the deformation for HO and intercluster distances for MB, are similar for both interactions. This can be understood by considering that the major differences between the potentials take place at short distances, that are accounted by the Jastrow factor, and to the fact that at medium and large distances both forces are similar and the behaviour is mainly governed by the model part of the
Table 2. Binding energy and root mean square radius for the lowest energy states of a given spatial arrangement calculated with the BB1 and MS3 interactions and the two model functions considered. The variational parameters of the model functions are also reported. Distances are given in fm and energies in MeV and $\beta$ in fm$^{-1}$. In parentheses we show the statistical error.

| Nucleus | wavefunction | Model | $\beta$; $d$ | $E$ | $\langle r^2 \rangle^{1/2}$ | $E$ | $\langle r^2 \rangle^{1/2}$ | $E$ | $\langle r^2 \rangle^{1/2}$ |
|---------|--------------|-------|-------------|-----|----------------|-----|----------------|-----|----------------|
| $^4$He  | HO           | 0.68;1| -37.93(2)   | 1.39(2) | -37.31(2) | 1.41(2) | 38.00(2) | 1.39(2) |
| $^8$Be  | HOd          | 0.76;0.61| -64.41(3) | 2.32(4) | -69.66(3) | 2.36(5) | -71.34(3) | 2.38(5) |
|         | MB           | 0.75;3.95| -73.65(2) | 2.35(3) | -72.59(3) | 2.41(4) | -74.86(3) | 2.30(4) |
| $^{12}$C | HOd          | 0.55;1.40| -101.06(4)| 2.39(4) | -109.72(8)| 2.40(6) | -114.20(7)| 2.39(6) |
|         | MB           | 0.74;3.87| -112.26(4)| 2.50(4) | -109.75(6)| 2.64(7) | -117.64(8)| 2.44(6) |
| $^{16}$O | HO           | 0.64;1.| -151.84(3)| 2.36(2) | -159.2(2) | 2.30(5) | -171.0(1) | 2.34(5) |
|         | MB           | 0.74;2.67| -166.56(5)| 2.37(3) | -170.5(2) | 2.35(5) | -180.7(1) | 2.33(5) |
| $^{12}$C | HO-l         | 0.69;0.56| -90.54(3) | 3.19(4) | -96.80(6)| 3.33(8) | -101.70(6)| 3.27(7) |
|         | MB-l         | 0.64;3.82| -100.48(3)| 3.40(3) | -99.77(4)| 3.55(8) | -107.62(5)| 3.37(5) |
| $^{16}$O | HO-l         | 0.66;0.52| -115.84(3)| 4.12(4) | -121.86(9)| 4.29(8) | -130.6(1) | 4.2(1)   |
|         | MB-l         | 0.70;3.42| -127.19(3)| 4.12(3) | -128.7(1)| 4.17(8) | -135.96(9)| 4.09(8) |

| Nucleus | wavefunction | Model | $\beta$; $d$ | $E$ | $\langle r^2 \rangle^{1/2}$ | $E$ | $\langle r^2 \rangle^{1/2}$ | $E$ | $\langle r^2 \rangle^{1/2}$ |
|---------|--------------|-------|-------------|-----|----------------|-----|----------------|-----|----------------|
| $^4$He  | HO           | 0.61;1.| -27.11(3)   | 1.43(3) | -26.03(3) | 1.52(3) | 30.17(3) | 1.40(2) |
| $^8$Be  | HOd          | 0.67;0.65| -43.09(4) | 2.42(4) | -46.2(1) | 2.51(5) | -54.07(6) | 2.45(5) |
|         | MB           | 0.66;4.43| -50.55(4) | 2.57(4) | -47.9(2) | 2.70(7) | -57.6(2) | 2.51(9) |
| $^{12}$C | HOd          | 0.54;1.42| -66.44(5) | 2.35(4) | -69.7(2) | 2.41(6) | -83.6(1) | 2.36(6) |
|         | MB           | 0.70;3.58| -72.72(5) | 2.55(4) | -69.8(4) | 2.62(9) | -87.3(2) | 2.47(7) |
| $^{16}$O | HO           | 0.62;1.| -104.20(5)| 2.32(2) | -102.1(4)| 2.34(6) | -128.4(2) | 2.30(7) |
|         | MB           | 0.71;2.74| -112.50(6)| 2.40(3) | -101.5(4)| 2.43(6) | -134.3(2) | 2.34(6) |
| $^{12}$C | HO-l         | 0.66;0.58| -57.85(4) | 3.20(4) | -58.9(2) | 3.4(1) | -73.7(2) | 3.26(9) |
|         | MB-l         | 0.64;3.96| -65.77(4) | 3.54(3) | -60.5(1) | 3.66(9) | -77.8(1) | 3.5(1)   |
| $^{16}$O | HO-l         | 0.63;0.54| -72.49(5) | 4.13(5) | -69.1(4) | 4.3(2) | -93.3(2) | 4.2(2)   |
|         | MB-l         | 0.63;3.89| -81.36(4) | 4.60(4) | -70.8(4) | 4.7(1) | -98.0(4) | 4.6(2)   |
wave function. With respect to the binding energies, they are bigger when the BB1 potential is used. This is because this potential was fitted by using non correlated wave function, giving rise to an over binding when a more realistic model is used. In spite of this, the trend is the same for all of the states considered and trial wave functions studied; for example the MB model wave functions always constitute a better variational option than the HO one. In general, within the LO model, the differences between MB and HO are very small for both interactions.

In order to get a deeper insight on the different correlation mechanisms included in the variational wave functions we have analysed the different contributions to the total energy. In figure 3 we plot the contribution to the total energy of the kinetic energy as well as the energy from the Wigner and Majorana channels for the ground state of the nuclei here studied and the linear configurations of the $^{12}$C and $^{16}$O nuclei. This is done for the two potentials and model wave functions considered and including only central Jastrow type correlations, J. For both potentials, the HO functions show larger binding in the Wigner channel than the MB ones while the opposite holds for the Majorana channel. The differences in the Majorana channel are bigger than in the Wigner one giving rise to the lower energy provided by the Margenau-Brink model. The expectation values of the Bartlett and Heisenberg channels calculated from state independent wave functions have the same value with opposite sign, and therefore they cancel out.

The Jastrow factor, J, and the linear operatorial correlations, LO, involve dynamical mechanisms of different nature, and therefore the origin of the binding energy obtained with them can be very different. A hint on the different correlation mechanisms included by the J and LO factors is that, when both are taken into account simultaneously, a significant increase of the binding energy is obtained, specially with the MS3 interaction.
Figure 4. Difference of the kinetic energy and the channels of the nuclear potential between the values obtained from the J and LO wave functions and those calculated from the JLO trial wave function. The upper plots correspond to the BB1 potential and the lower plots to the MS3 interaction. The symbol (-l) stands for harmonic oscillator orbitals of the linear geometry. The lines are for guiding the eyes.
To further elucidate on the effects of the different correlation mechanisms on the binding energy, we plot in figure 4 the differences between several expectation values related to the energy calculated from different wave functions. We show the differences between the expectation values of the kinetic energy and all of the channels of the nuclear potential calculated from the J and the JLO models ((JLO)-(J)) and between the LO and JLO models ((JLO)-(LO)). The former can be interpreted as the effects of the linear state dependent correlations on these quantities while the latter are the effects of the central Jastrow correlations. When these differences take positive values, the action of the corresponding operator is to reduce the binding and the opposite holds for negative values.

The effect of both state-dependent and Jastrow correlations is to increase the expectation value of the kinetic energy, reducing the binding. This effect is more accused when the MS3 interaction is employed. This is also the case of the Wigner channel when operators are included. An exception to this is the $^4$He nuclei with the BB1 interaction that shows the opposite trend. The effect of the Jastrow correlations on the Wigner channel is to increase the binding energy. The effect of the state dependent correlations is more accused for the BB1 potential and the effect of the Jastrow factor is more important for the MS3 interaction. In the latter case, it is an order of magnitude bigger when using MS3 than for BB1 for the ground states and it is reduced for the other states. In the Majorana channel, operators tend to increase the binding energy except for $^4$He with the BB1 interaction. In the case of Jastrow correlations, the effects depend on the potential. Thus when using the MS3 interaction, the tendency is to increase the binding energy. However, for the BB1 potential, it depends on the nucleus and on the model wave function. Finally the effects on the Bartlett and Heisenberg channels, that appear only in the MS3 interaction, are very similar. For these channels, both the Jastrow and the operators tend to increase the binding energy. The effect is more important, by a factor 3-4, for the operators than for the Jastrow.

Therefore the action of the state dependent correlations is to increase the binding by means of the Majorana channel. In the case of the BB1 interaction, the reduction of the energy coming from this channel is bigger than the enhancement coming from the sum of the Wigner channel and the kinetic energy. In the case of the MS3 potential, the increasing in the binding energy given by the Majorana channel is roughly the same as the decreasing provided by the sum of the Wigner channel and the kinetic energy. As a consequence, the gain in the total binding energy due to the operators, is the sum of the Bartlett and Heisenberg channels. The $^4$He nuclei is an exception. In the case of the BB1 interaction, the gain comes from the Wigner channel and it is very small (0.1 MeV). For the MS3 potential, the Majorana is not enough to compensate for the decrease in the binding energy provided by both the Wigner energy and the kinetic energy.

The action of the Jastrow correlation factor is to increase the binding energy by means of the Wigner channel. For the BB1 potential, the effect on Majorana channel depend on the nucleus. This is not the case of the MS3 interaction, for which the effect
Table 3. Excitation energies (in MeV) with respect to the lowest energy state of a given configuration for the nuclei here studied obtained from the different trial wave functions and the two potentials considered. In parentheses we show the statistical error.

|         | J$^*$  | $^{10}$Be  | $^{12}$C  | $^{16}$O  |
|---------|--------|------------|-----------|-----------|
|         | HO/MB  | J(HO/JMB)  | LO(HO/MB) | JLO(HO/MB) |
| $^8$Be  | 2$^+$  | 3.24(3)/3.42(3) | 3.44(3)/3.73(3) | 3.80(4)/3.71(3) | 3.90(4)/3.91(3) | 3.040 |
|        | 4$^+$  | 11.72(4)/11.76(4) | 12.40(5)/12.89(4) | 13.26(6)/12.63(5) | 13.48(5)/13.59(5) | 11.400 |
| $^{12}$C | 2$^+$  | 2.97(4)/3.37(4) | 3.11(4)/3.83(4) | 3.61(8)/3.94(6) | 3.65(6)/4.10(7) | 4.439 |
|        | 4$^+$  | 11.5(1)/12.24(6) | 12.14(9)/13.71(6) | 13.6(2)/13.7(1) | 13.8(2)/14.7(1) | 14.083 |
|        | 0$^+$  | 6.01(8)/10.08(7) | 12.52(7)/11.76(7) | 13.9(1)/10.0(1) | 12.5(1)/10.0(1) | 7.654 |
|        | 3$^-$  | -/- | -/7.8(1) | -/6.6(2) | -/7.7(2) | 9.641 |
| $^{16}$O | 3$^-$  | -/- | -/16.3(1) | -/15.4(5) | -/15.9(4) | 11.600 |

The model used in this work provides the ground state and also some other excited states by means of the projection operation of the total angular momentum and parity. In table 3 we show different excitation energies with respect to their corresponding lowest energy ones reported in table 2. We give those states that can be assigned to some experimental nuclear excited states. The excitation energy is almost independent of the model wave function and the effect of state dependent correlations is to increase slightly the value of the excitation energy. In general it can be concluded that the simple models used here and the physical picture behind them provide a reasonable description of these nuclear states.

4.3. One- and two- body densities

To better understand the differences between the two model wave functions used in this work we study both the single particle and the two–body densities. We shall consider...
Figure 5. One-body radial density for all of the states here studied calculated from a trial wave function with a central Jastrow correlation factor. The upper plots correspond to the BB1 interaction and the lower plots to the MS3 one. The left hand side figures correspond to HO model wave functions and the right hand side ones to MB model wave functions, both of them with a Jastrow factor.

Here the spherical average of these two functions normalized to unity which are defined as

$$\rho^{(1)}(r) = \int d\tau |\Psi(\tau)|^2 \left\{ \frac{1}{A} \sum_{i=1}^{A} \frac{1}{r_i^2} \delta(r - |\vec{r}_i - \vec{R}|) \right\}$$  \hspace{1cm} (15)

$$\rho^{(2)}(r_{12}) = \int d\tau |\Psi(\tau)|^2 \left\{ \frac{2}{A(A-1)} \sum_{i<j}^{A} \frac{1}{r_{12}^2} \delta(r_{12} - |\vec{r}_i - \vec{r}_j|) \right\}$$  \hspace{1cm} (16)

where $\tau$ stands for all of the particles’ spatial coordinates and intrinsic degrees of freedom, and $\vec{R} = \frac{1}{A} \sum_{i=1}^{A} \vec{r}_i$ is the center of mass coordinate. The one– body density is the probability distribution of the nucleons with respect to the center of mass and the two– body density is the probability distribution with respect to a given nucleon.

In figure 5 we plot the one body radial density, $r^2 \rho^{(1)}(r)$, obtained from the Jastrow correlated wave functions for the interactions and model wave functions analysed in this work. For the ground state of the different nuclei, the radial one body density has one maximum whose height and width depend on both the nucleus and the model wave function. For the linear geometry in $^{12}$C and $^{16}$O the situation is different, with two maxima for the two model wave functions considered. Within the Margenau-Brink
model these maxima are interpreted as the position of the alpha clusters. Note that for $^{12}\text{C}$ the center of mass coincides with the center of the central cluster, while for $^{16}\text{O}$ the location of the $\alpha$-clusters is symmetric with respect to the position of the center of mass. When the model part of the wave function is built from a HO shell model, the position of the maxima is related to the extremes of the single particle orbitals, given in table 1. The one body density is mainly governed by the model function of the trial wave function. The effect of the correlations is indirect through the change of the variational parameters of the model function induced by the inclusion of the correlations.

The radial density is very similar for all of the cases considered except for $^4\text{He}$, that is of shorter range. The use of different interactions does not modify the structure of this function for the ground state and only changes slightly the position and height of the maximum, that are reduced when the MS3 potential is used with respect to the BB1 case. The use of a different model wave function, with the same potential, also induces minor changes. With respect to the linear geometry, we have obtained an appreciable dependence on the model wave function, and a nearly negligible dependence on the nuclear interaction. For the linear configuration, the clusterization can be clearly observed on this density when using both model wave functions. Note that the formation of alpha clusters is included explicitly in the MB model but not in the HO one.

In order to analyse the effects of the different correlation mechanisms we have calculated the difference between the densities obtained from a correlated and an uncorrelated trial wave function. For the uncorrelated case we have used the same model wave function as in the correlated trial wave functions

$$\Delta \rho^{(k)}_\mu(r) = r^2 \left[ \rho^{(k)}_\mu(r) - \rho^{(k)}_{\text{uc}}(r) \right], \quad k = 1, 2. \quad (17)$$

where $\rho^{(k)}_{\text{uc}}(r)$ is the $k$-body density calculated from the uncorrelated wave function and $\rho^{(k)}_\mu(r)$, where $\mu$ stands for J, LO, JLO, corresponds to a density calculated from each of these correlation factors. In figure 6 we plot these difference functions for $^{12}\text{C}$, which is representative for all of the nuclei here studied. They have been calculated with the two nuclear potentials and the two model wave functions here considered. The effect of the central Jastrow correlations is to increase the density at distances smaller than roughly 2 fm for the ground state and 4 fm for the linear geometry, and to decrease this density for larger distances. For the wave functions built from HO model functions and using the BB1 potential the effect of the correlations is less important. When only linear state dependent correlations are included, LO, we have not found a systematic trend. In the case of the linear geometry, correlations tend to increase the density in the neighbourhood of the maxima and to reduce the density around the minima as well as at distances greater than 4 fm, close to the nuclear surface. The only exception to this effect is for HO wave functions with the MS3 interaction.

In figure 7 we plot the two body radial density obtained from the Jastrow correlated wave function for the two different interactions and model wave functions considered. As can be seen, when HO wave functions are employed, the results are roughly independent of the nuclear potential and a greater dependence on the potential is found in the case
Figure 6. One-body difference functions for the ground state configuration and the linear configuration of $^{12}$C. The upper plots correspond to the BB1 interaction and the lower plots to the MS3 one. The left hand side figures correspond to the ground state and the right hand side ones to the linear arrangement. For any figure the upper (lower) part corresponds to MB (HO) model. The full, dashed, and dotted lines correspond to J, LO, and JLO wave functions, respectively.

of the MB wave functions. The cluster structure of the nuclei here studied can be seen on this density. The different maxima correspond to interparticle distances of nucleons in the same or in different clusters. This can be clearly noticed in $^8$Be and in the linear configuration of $^{12}$C and $^{16}$O. The ground state two-body density of $^{12}$C and $^{16}$O presents only one maximum, i.e. the two characteristic internucleon distances are very close. This is because, in the ground state, the clusters are not very far from each other. On the other hand one does not have any particular nucleon grouping when the HO wave function is used and therefore there is only one maximum which becomes higher and narrower as the number of nucleons increases.

In figure 8 we plot the functions $\Delta \rho_{\mu}^{(2)}(r)$ with $\mu =$J, LO, JLO for $^{12}$C calculated from the two different models and interactions here considered. As it was the case for the one body density, we have obtained a stronger influence of the model wave function than of the nuclear potential on these difference functions. Two common features to all of the difference functions have been found. The first one is a negative region at short inter-nucleon distances with a minimum located at around 0.5 fm. This structure is generated by the decreasing of the density around a given nucleon in order to avoid the repulsive core of the potential. The second element is a first maximum with a well defined structure in the case of the linear configuration and a little bit more diffuse in the ground state. This maximum is a consequence of the increase of the relative
Figure 7. Two-body radial density for all of the states here studied calculated from a trial wave function with a central Jastrow correlation factor. The upper plots correspond to the BB1 interaction and the lower plots to the MS3 one. The left hand side figures correspond to HO model wave functions and the right hand side ones to Margenau-Brink model wave functions.

density at distances in the neighbourhood of the minimum of the nuclear potential. At larger nucleon-nucleon distances the effects of the correlations, specially in the linear configuration, are smaller. It can be stated that within the Margenau-Brink model correlations are focused on nucleons of the same cluster, while that within the HO shell model, the main effects of correlations take place between nucleons in orbitals with the same spatial part.

5. Conclusions

A variational study of the ground and some bound states of the $^4\text{He}$, $^4\text{Be}$, $^{12}\text{C}$ and $^{16}\text{O}$ nuclei starting from nucleon-nucleon interactions is presented. The binding energy, the root mean square radius and the one– and two– body densities are reported. The calculations have been done by means of the Variational Monte Carlo method.

The variational trial wave function used consists of three factors including several aspects of the nuclear dynamics induced by the nuclear interaction. Short range correlations are accounted by a central Jastrow-type factor, state dependent correlations are incorporated by a linear factor depending on the spin and isospin of the nucleons, and some medium and long range effects by the model part of the wave function, that
Figure 8. Two-body difference functions for the ground state configuration and the linear configuration of $^{12}$C. The upper plots correspond to the BB1 interaction and the lower plots to the MS3 one. The left hand side figures correspond to the ground state and and the right hand side ones to the linear arrangement. For any figure the upper (lower) part corresponds to MB (HO) model. The full, dashed, and dotted lines correspond to J, LO, and JLO wave functions, respectively.

It is also antisymmetric. The medium and long range effects considered here are the deformation of the nuclear potential and the formation of alpha clusters. Projection operators are used to obtain wave functions with the proper values of parity and total angular momentum. This functional form has shown to be able to describe several dynamic effects that give rise to different mechanisms of lowering the energy depending on the nucleus, the state and the potential.

The performance of the two model wave functions employed and the relationship of the different elements of the variational wave function have been studied. The different correlation functions, the size of the nucleus and the deformation parameter or the intercluster distances have been obtained and compared for the two different potentials employed. The effects of the different correlation mechanisms have been analysed by calculating the different contributions to the total energy. It has been found that the inclusion of Jastrow and state dependent correlations increase the expectation value of the kinetic energy. In the former case a substantial reduction in the expectation value of the Wigner channel is obtained, leading to the increase in the total binding energy that is found when these correlations are included. The other channels of the potential, in general, also contribute to a bigger binding when Jastrow correlations are included. In the case of state dependent correlations the effect on the Wigner channel is the opposite, and it is the Majorana channel for the BB1 potential and the
Majorana, Bartlett and Heisenberg channels for the MS3 interaction, the responsible for the bigger binding energy. When using model wave functions including explicitly the alpha clustering effect, lower values of the expectation value of the Majorana channel are obtained, giving rise to the better performance of this ansatz from a variational point of view.

For the one body density, a small dependence on both the potential and the model wave function for the ground state has been found while the dependence on the model wave function is more accused in the linear configuration. The effects of the correlations are to increase the density at short distances for the ground state and to make more accused the alpha clustering for the linear configuration. In the case of the two body radial distribution a stronger dependence on the model wave function has been found. This is due to the two typical internucleon distances that appear in a Margenau-Brink type structure, one between nucleons in the same alpha cluster and the second one between nucleons in different clusters. On this density, the effect of correlations is to decrease the density around a given nucleon and increase it for distances close to the minimum of the potential, avoiding the hard core of the nuclear potential. This is consistent with the short range character assigned to the correlation factor, that is mainly focused on nucleons within the same alpha cluster in the case of Margenau-Brink, and on nucleons with the same spatial part in the case of HO model.

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