Projected multicluster model with Jastrow and linear state dependent correlations for $12 \leqslant A \leqslant 16$ nuclei

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(Received 29 July 2004; published 18 November 2004)

Variational wave functions based on a Margenau-Brink cluster model with short-range and state-dependent correlations and angular momentum projection are obtained for some nuclei with $12 \leqslant A \leqslant 16$. The calculations have been carried out starting from the nucleon-nucleon interaction by using the variational Monte Carlo method. The configuration used consists of three alpha clusters located at the apexes of an equilateral triangle and an additional cluster, not necessarily of alpha type, forming a tetrahedron. This cluster is located at the top of its height. Short-range and state dependent correlations are included by means of a central Jastrow factor and a linear operatorial correlation factor, respectively. Angular momentum projection is performed by using the Peierls-Yoccoz operators. Optimal structures are obtained for all the nuclei studied. Some aspects of our methodology have been tested by comparing with previous calculations carried out without short-range correlations. The binding energy, the root mean square radius, and the one- and two-body densities are reported. The effects of correlations on both the energy and nucleon distributions are analyzed systematically.

DOI: 10.1103/PhysRevC.70.054315 PACS number(s): 21.60.Gx, 21.60.Ka, 27.20.+n, 21.10.−k

I. INTRODUCTION

The joint use of short-range dynamic correlations with model wave functions including relevant aspects of nuclear structure constitutes the most commonly used scheme to describe nuclear bound states with realistic or semirealistic interactions. Short-range correlations are essential elements in the wave function because, as is well known, any of the so-called realistic or semirealistic parametrizations of the nuclear potential present a strong short-range repulsive core. On the other hand, the formation of different kinds of clusters in the nuclei can be understood as a collective movement of nucleons governed by the medium- and long-range parts of the nuclear potential. Therefore, for an accurate description of the nuclear states, it is convenient to consider both aspects in any variational approach to the nuclear bound states using this type of interactions. In principle, short-range correlations are mainly governed by the nucleon-nucleon interaction while medium- and long-range effects depend on the particular nuclear state. However—and in a more careful approach—the final form of the short-range correlations will depend on the model wave function giving rise to a nonnegligible dependence of the correlations on the nucleus.

A direct way to include both short-range and medium- and long-range correlations is by using Jastrow-type correlation factors, but the calculation of the expectation values becomes very cumbersome, especially when state dependent correlations are included. There exist several methods to evaluate these expectation values such as those based on cluster expansions [1–3], the Fermi-HiperNetted-Chain method [4,5], or statistical methods such as the variational Monte Carlo method [6,7]. The coupled cluster method allows one to incorporate both types of correlations [8–10]. In this way it is possible to understand how the different correlation mechanisms are incorporated [11,12].

Alpha cluster models—or cluster models in general—have been widely applied in microscopic descriptions of bound and scattering states of nuclear systems [13–15]. Variational wave functions built within this framework constitute an appropriate scheme for nuclei such as ^{8}Be and ^{12}C, which present a clear cluster structure. The use of wave functions including the possibility of the formation of alpha cluster structures or any other kind of grouping of nucleons improves the description of these nuclei and their neighbors with respect to simple mean field approximations [16].

Multicluster models have been used in microscopic calculations—i.e., without effective cluster-cluster interactions—based on the generator coordinate method for some nuclei between $A=12$ and $A=16$ [17,18]. In these works a Volkov nucleon-nucleon potential was used [19]. Other results of microscopic multicluster calculations based on the stochastic variational method have been reported [20,21] for some nuclei using the Minnesota potential. Neither of these potentials presents a strongly repulsive short-range part and, therefore, short-range correlations do not play a significant role. On the other hand, previous studies of alpha clustering based on nuclear potentials with a strongly repulsive core have been mainly restricted to spin-isospin-saturated nuclei—i.e., states of $A=4n$, $Z=N$—nuclei in which each spatial orbital is occupied by two protons and two neutrons [22,23].

The aim of this work is to study the ground state of some p-shell nuclei, $A \neq 4n$, including clustering effects and short-range and state dependent correlations, starting from v_4-type nucleon-nucleon interactions. Here we extend previous works done for $A=4n$ nuclei. The ground state energy and the root mean square radius along with the parameters of the optimal structures have been obtained for several nuclei using two different interactions and several models for the trial

wave function. Local properties such as the one- and two-body spatial densities are reported. The effects of the different correlation mechanisms on these quantities and on the different channels of the interacting potential have been analyzed. In this work we present the extension of the methodology in order to consider $A \neq 4n$ nuclei with angular momentum projection and state dependent correlations within the variational Monte Carlo scheme.

The nucleon clustering is described in terms of model wave functions based on a generalized Margenau-Brink model as in [17]. Short-range correlations are included by means of a Jastrow factor and the dependence on the spin and isospin exchange channels is included by using a linear state dependent correlation factor. Angular momentum projection is carried out in order to obtain variational wave functions that are eigenfunctions of the total angular momentum operator. The calculations are performed by means of the variational Monte Carlo method.

In generalizing to the $A \neq 4n$ case, the angular momentum projection involves a spin mixing not present in spin- and isospin-saturated nuclei. In this paper we present an analytical reduction of the different expectation values for these nuclei, obtaining expressions suitable for the variational Monte Carlo method. By using this scheme, the computing time is hardly increased with respect to the spin-isospin-saturated case. We apply the method to the ground state of ^{13}C, ^{14}C, ^{14}N, and ^{15}N. The results obtained are also valid for the mirror nuclei ^{13}N, ^{14}O, and ^{15}O because the electrostatic energy has been not considered in the minimization process. A systematic analysis of the effects of the different correlations mechanisms included in the wave functions on the total energy and on the contribution of the different channels is carried out. One- and two-body densities are reported and the effect of the correlations are discussed.

The scheme of this work is as follows. In Sec. II the variational wave function and the analytical reduction of the expectation values leading to a form appropriate for the variational Monte Carlo method are detailed. In Sec. III we report and discuss the main results here obtained. The conclusions of the present work can be found in Sec. IV.

II. WAVE FUNCTION

The variational trial wave function used in this work is

$$\Psi^{\pm}_{JKM}(1,2,\ldots,A) = F_{\mathcal{J}}(1,\ldots,A)F_{\mathcal{L}}(1,\ldots,A)$$

$$\Phi^{\pm}_{JKM}(1,\ldots,A). \tag{1}$$

This structure has been used in previous studies of spin- and isospin-saturated nuclei [23,24]. It consists of a central Jastrow correlation factor $F_{\mathcal{J}}$, a linear correlation factor $F_{\mathcal{L}}$ that can include state dependent correlations, and a model wave function $\Phi^{\pm}_{JKM}$ that is antisymmetric and has the proper values of the total angular momentum and parity.

The Jastrow factor depends only on the distance between a pair of nucleons:

$$F_{\mathcal{J}}(1,\ldots,A) = \prod_{i<j}^{A} f(r_{ij}). \tag{2}$$

The linear factor is defined as

$$F_{\mathcal{L}}(1,\ldots,A) = \sum_{i<j}^{A} g(i,j), \tag{3}$$

where the function $g(i,j)$ depends on the radial and intrinsic degrees of freedom of particles, i, j. This is the only part of the trial wave function where state dependent correlations are present explicitly. Here we employ the same parametrization for the correlation functions $g(i,j)$ and $f(r)$, used in previous works [22–24], which has shown to provide good results:

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

where

$$\mathbf{P}^{(1)}(i,j) = 1,$$

$$\mathbf{P}^{(2)}(i,j) = \frac{1}{2}(1 + \vec{\sigma}_i \cdot \vec{\sigma}_j)$$

$$\mathbf{P}^{(3)}(i,j) = \frac{1}{2}(1 + \vec{\tau}_i \cdot \vec{\tau}_j),$$

$$\mathbf{P}^{(4)}(i,j) = \mathbf{P}^{(2)}(i,j)\mathbf{P}^{(3)}(i,j). \tag{5}$$

This dependence on operators of the correlation factor is the same as that of the nucleon-nucleon interactions considered in this work. The functions $g^{(k)}(r)$, $k=1,\ldots,4$, and $f(r)$ are parametrized as a linear combination of Gaussians:

$$g^{(k)}(r) = \sum_{m=0}^{M} a_m^{(k)} e^{-b_m r^2}, \quad f(r) = 1 + \sum_{n=1}^{N} c_n e^{-d_n r^2}. \tag{6}$$

The parameters $a_m^{(k)}$, b_m, c_n, and d_n are taken as variational parameters in such a way that they are fixed by minimizing the expectation value of the ground state energy. The optimum values for $a_m^{(k)}$ have been obtained by solving a generalized eigenvalue problem, with matrix elements calculated by using Monte Carlo quadrature. The other parameters have been obtained by using standard techniques of many dimensional nonlinear optimization. This step is, in general, time consuming. We have verified that the use of the simplification $b_m = d_n$ conveys to accurate results for $M=N=2$ and it has been used throughout this work.

The new aspects of treating $A \neq 4n$ nuclei with respect to spin- and isospin-saturated ones originate in the angular momentum projection. Therefore we shall focus here on the model part of the wave function and on the angular momentum projection. The correlation factors are treated as in the spin- and isospin-saturated cases.

The model wave function used here is based on a generalization of the Margenau-Brink model. Instead of using only alpha-particle-like nucleon clusters, more general groupings are allowed, giving rise to a multicluster description [17,20].

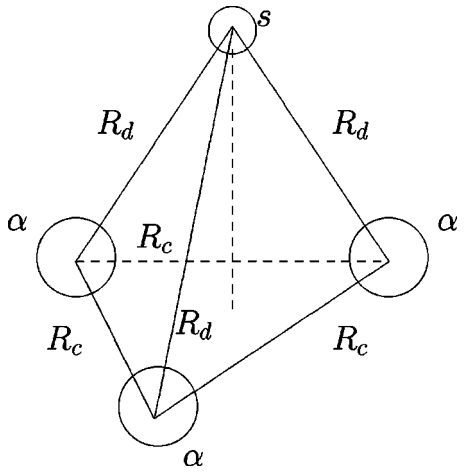

FIG. 1. Cluster description of the nuclei in terms of three alpha particles and a general *s* incomplete cluster with one, two, or three nucleons.

Within the molecular viewpoint of the Margenau-Brink scheme, the model wave function is obtained starting from the functions

$$\Phi_{\vec{\mathbf{C}}}(1,2,\ldots,A) = \mathcal{A}\{\Phi_1(x_1,\ldots,x_{k_1})\cdots\Phi_n(x_{k_{n-1}+1},\ldots,x_A)\}, \tag{7}$$

where $\vec{\mathbf{C}} \equiv \{\vec{c}_k\}_{k=1}^n$ is a set of parameters that represent the centers of the clusters and $\mathcal{A}$ is the corresponding antisymmetrizer. In this work the arrangement of the nucleons, shown in Fig. 1, consists of three α clusters and a fourth incomplete cluster that can be made of one, two, or three nucleons depending on the nucleus under study.

For this configuration, the general form of the function given in Eq. (7) reduces to

$$\Phi_{\vec{\mathbf{C}},S}(1,2,\ldots,A) = \mathcal{A}\left\{\left[\prod_{m=1}^{3}\Phi_{\alpha_m}(x_{4m-3},\ldots,x_{4m})\right]\Phi_{\alpha_s,S}(x_{13},\ldots,x_A)\right\}, \tag{8}$$

where Φ_{α_m} stands for the wave function of an alpha particle centered at $\vec{c}_m$, Φ_s represents the incomplete cluster wave function centered at $\vec{c}_s$, and the label *S* indicates the dependence on the spin of the incomplete cluster.

In this work the Φ_{α_m} functions are taken to be Slater determinants built from harmonic oscillator single-particle orbitals centered at $\vec{c}_m$:

$$\phi_{\beta,\vec{c}}(\vec{r}) = \left(\frac{\beta^2}{\pi}\right)^{3/4} e^{-\beta^2(\vec{r}-\vec{c})^2/2}. \tag{9}$$

The oscillator parameter β is the same for all of the alpha clusters. For the incomplete cluster wave function another Slater determinant centered at $\vec{c}_s$ is employed also built from *s*-wave harmonic-oscillator single-particle orbitals. The oscillator parameter in this case is, in general, different to that for the α cluster wave function. The importance of using a different harmonic oscillator parameter will be discussed. With these choices for the cluster wave functions, the model wave function of the *A* nucleons is a Slater determinant. In general this function is not eigenfunction of parity or total angular momentum operators.

The linear combinations

$$\Phi^{\pm}_{\vec{\mathbf{C}},S}(1,2,\ldots,A) = \Phi_{\vec{\mathbf{C}},S}(1,2,\ldots,A) \pm \Phi_{-\vec{\mathbf{C}},S}(1,2,\ldots,A) \tag{10}$$

have definite parity. Model wave functions with the total angular momentum of the state under study can be obtained from Eq. (10) by using the Peierls-Yoccoz projection operators [25]

$$\Phi^{\pm}_{JKM}(1,\ldots,A) = \frac{2J+1}{8\pi^2}\int d\Theta \mathcal{D}^{J*}_{MK}(\Theta)\mathbf{R}(\Theta)\Phi^{\pm}_{\vec{\mathbf{C}},S}(1,\ldots,A), \tag{11}$$

where $\mathbf{R}(\Theta)$ is the rotation operator, $\mathcal{D}^{J*}_{MK}(\Theta)$ is the rotation matrix, and Θ represents the Euler angles. The quantum number *J* gives the total angular momentum, *K* is its projection along the nuclear *z* axis, and *M* is the projection along the *Z* axis of the laboratory fixed frame. The projection within this scheme is carried out by rotating the intrinsic state and integrating over all angles weighted by the rotation matrix.

The function $\Phi_{\vec{\mathbf{C}},S}(1,\ldots,A)$ in Eq. (8) is the generator function of the model wave functions. Note that we have removed the parametric dependence of the model wave function on the position of the centers, $\vec{\mathbf{C}}$, in order to simplify the notation. The distances between the clusters, R_c and R_d, are determined variationally.

The action of the rotation operator on the generator function is now described in detail. As we have mentioned before, this is the source of the new methodological aspects originated by the fact that the nuclear states are not spin and isospin saturated. We do not need to consider here the correlation factors because they are rotationally invariant. The generator function is a Slater determinant. The action of the rotation operator on it leads to a linear combination of Slater determinants. If the Slater determinant is spin and isospin saturated, this linear combination contains only one Slater determinant that also is spin and isospin saturated, containing the same single-particle orbitals. The only difference is that, after rotation, these orbitals depend on the rotated coordinates. This was exploited previously to study $A=4n$ nuclei [24,26]. When the nuclei are not spin or isospin saturated the rotation gives rise to a mixing of spin states.

When the incomplete shell consists of one nucleon—as, for example, in the ground state of ^{13}C—the action of the rotation operator can be written as follows:

$$\mathbf{R}(\Theta)\Phi_{\vec{\mathbf{C}},\beta s_\beta t_\beta} = \sum_{s_i=\pm 1/2}\mathcal{D}^{1/2}_{s_\beta,s_i}(\Theta)\overline{\Phi}_{\vec{\mathbf{C}},\beta s_i t_\beta}, \tag{12}$$

where β stands for the spatial quantum numbers of the orbital of the incomplete cluster, and s_β and t_β are the third components of spin and isospin, respectively. The overbar indicates that the Slater determinant must be evaluated on the rotated coordinates. Therefore—and concerning the spin de-

pendence of the state—the effect of the rotation is to mix the two possible spin projections of the orbital in the incomplete cluster. The weight of each component is given by the matrix element of the rotation matrix.

When there are two extra nucleons the result of the rotation can be written as follows:

$$\begin{aligned}\mathbf{R}(\Theta)\Phi^{\vec{}}_{\mathbf{C},\beta s_\beta t_\beta,\beta s_\gamma t_\gamma} &= \sum_{s_i,s_j=\pm 1/2} \mathcal{D}^{1/2}_{s_\beta,s_i}(\Theta)\mathcal{D}^{1/2}_{s_\gamma,s_j}(\Theta)\overline{\Phi}^{\vec{}}_{\mathbf{C},\beta s_i t_\beta,\beta s_j t_\gamma} \\ &= \sum_{s_i,s_j=\pm 1/2}\sum_{S=0,1}\left\langle \frac{1}{2}\frac{1}{2}s_\beta s_\gamma | S, s_\beta + s_\gamma \right\rangle \\ &\times \left\langle \frac{1}{2}\frac{1}{2}s_i s_j | S, s_i + s_j \right\rangle \mathcal{D}^{S}_{s_\beta+s_\gamma,s_i+s_j}(\Theta) \\ &\times \overline{\Phi}^{\vec{}}_{\mathbf{C},\beta s_i t_\beta,\beta s_j t_\gamma}, \end{aligned} \tag{13}$$

where $(\beta s_\beta t_\beta)$ and $(\beta s_\gamma t_\gamma)$ stand for the quantum numbers of the orbitals of the incomplete shell. Note that we have considered the same spatial dependence for both single-particle orbitals. Therefore, if one is dealing with two extra protons (^{14}O) or two extra neutrons (^{14}C) with the two possible spin orientations, the term $S=1$ vanishes. Only in the case of one proton and one neutron outside a closed shell (^{14}N) will both total spin components contribute.

Finally, the case of three nucleons outside a closed shell (^{15}N and ^{15}O is a conjugate configuration to that of one nucleon outside a closed shell and it is handled in the same way.

The values allowed for J and K are governed by the symmetry group of the system—i.e., by the spatial positions of the centers of the clusters. For the nuclei here considered the group is C_{3v}. The spin of the extra cluster must be also considered in determining the possible values of K. If M_S is the total spin third component, the allowed K values are given by the selection rule $|K-M_S|=3n$, with n a positive integer [17] and, for any K, $J \geqslant K$, and the parity is $\pi=(-1)^{J\pm S}$. The energy grows with K, providing different rotational bands. In this work we are concerned only with the ground state; therefore, we shall restrict ourselves to $K=1$ for ^{14}N and $K=0$ for all the rest. For one and three extra nucleons $M_S=1/2$ and the ground state is $(1/2)^+$, and for two extra nucleons there are two possibilities: (i) both nucleons are protons or neutrons, $M_S=0$, and the state is 0^+ and (ii) one nucleon is a proton and the other a neutron, $M_S=0$, 1 and the 1^+ ground state must be constructed with $M_S=1$ and $K=1$.

In order to compute the expectation value of the Hamiltonian in the projected wave function it is convenient to use the expression [24,27]

$$\begin{aligned}\langle \Psi^{\pm}_{JKM}|\mathbf{H}|\Psi^{\pm}_{JKM}\rangle &= \frac{2J+1}{8\pi^2}\int d\Theta \mathcal{D}^{J*}_{KK}(\Theta) \\ &\times \langle \Phi^{\pm}_{\vec{\mathbf{C}},S}|F_{\mathcal{L}}F_{\mathcal{J}}\mathbf{H}F_{\mathcal{J}}F_{\mathcal{L}}\mathbf{R}(\Theta)|\Phi^{\pm}_{\vec{\mathbf{C}},S}\rangle. \end{aligned} \tag{14}$$

Let us focus on the spin-isospin configuration of the nuclear state. Note that, because of the rotational invariance property of the Hamiltonian, only the ket is rotated, the bra remaining on its original configuration. This is important because it determines the configurations that give nonzero contributions to the integral when projected onto the bra. The action of the rotation operator is to produce a linear combination of configurations containing the original one. One needs to analyze all of them to determine if, after the action of the spin-isospin operators of $F_{\mathcal{L}}$ and the Hamiltonian, the original configuration is obtained. As a result, only the original configuration appearing after rotation contributes with both central and state dependent correlation factors, except for incomplete clusters made of one proton and one neutron with $S=0$, which we have not studied here, for which two of the configurations appearing after the rotation give a nonzero contribution. Note that the weight factor must be included when doing the integral in all cases. The treatment of state dependent correlations in terms of the intermediate states is not modified with respect to the case of spin- and isospin-saturated nuclei [28,29].

III. RESULTS

First we will test the new methodological aspects implemented in this work by comparing with the results of Dufour and Descouvemont [17] obtained by using a different computational scheme. We will employ for the test both the same nucleon-nucleon interaction (the Volkov V7 potential) and the same wave function as in [17]. It is worth pointing out that the correlation factor is not needed because the interaction does not present a strongly repulsive core. In order to correct for the effects of the center of mass motion, we have worked with an intrinsic Hamiltonian built as the total Hamiltonian minus the kinetic energy of the center of mass. When we use one only parameter for describing all the clusters in the MB wave function this method corrects exactly the spurious effect of the center of mass motion. This is because in that case the center of mass dependence in the total wave function can be exactly factored. If one uses two different parameters to describe the clusters, the wave function cannot be factored. In this case the method here used introduces spurious effects associated with the center of mass and intrinsic wave function coupling. However, the results obtained are still of variational character and the figures are better than those obtained with only one parameter.

In Table I we show for the ground state and some excited states of the nuclei studied in this work the binding energy and the root mean square radius, $\langle r^2\rangle^{1/2}$. As can be seen from the table, both sets of results are in very good agreement. The spin-orbit interaction is not included in our work and therefore one cannot compare directly the results for nuclei with an odd number of nucleons. For these nuclei we have compared with the average value of the states $1/2^-$ and $3/2^-$ of [17]. This average gives a value that it is very close to the Monte Carlo result of this work, especially for ^{13}C where the spin-orbit splitting is smaller than in ^{15}N. From this test it can be concluded that, for $A \neq 4n$, the angular momentum projection scheme of this work provide reliable results.

The ground state of these nuclei has been studied in this work by using a semirealistic potential. We have used the modified Afnan-Tang nuclear potential MS3 [30,31]. This is

TABLE I. Binding energy and root mean square radius $\langle r^2\rangle^{1/2}$ for different nuclear states calculated in this work (mc) as compared with the results of Dufour and Descouvemont (dd) [17]. Both calculations have been performed by using the Volkov V7 interaction [19] and the same variational wave function without correlations. The inverse of the oscillator parameter, β^{-1}, and the distances between the clusters, R_c and R_d, are also included. The energies are in MeV and $\langle r^2\rangle^{1/2}$, β^{-1}, and R_c and R_d in fm. The statistical error in the Monte Carlo calculation is indicated in parentheses. The Coulomb energy has been included in the total energy.

$^AX(K,J^\pi)$	β^{-1}	R_c, R_d	E_{mc}	E_{dd}	$\langle r^2\rangle_{mc}^{1/2}$	$\langle r^2\rangle_{dd}^{1/2}$
$^{12}C(0,0^+)$	1.38	2.65	86.49(4)	86.7	2.31(7)	2.31
$^{12}C(3,3^-)$	1.38	3.14	76.41(4)	76.5	2.49(9)	2.49
$^{13}C(\frac{1}{2},\frac{1}{2}^-)$	1.39	2.29,2.114	88.99(7)	89.6	2.25(9)	2.25
$^{14}C(0,0^+)$	1.39	2.26,2.057	102.26(6)	102.5	2.26(7)	2.26
$^{15}N(\frac{1}{2},\frac{1}{2}^-)$	1.35	1.84,1.887	119.37(7)	121.9	2.15(11)	2.15
$^{16}O(0,0^+)$	1.34	1.49,2.409	147.83(5)	148.0	2.18(3)	2.18
$^{16}O(3,3^-)$	1.37	2.24,1.958	129.46(10)	129.8	2.27(10)	2.26

a v_4-type interaction with a strongly repulsive core. It gives meaningless results when used with noncorrelated trial wave functions. Thus, in order to analyze the effects of nuclear correlations with respect to the noncorrelated case, it is more convenient to use an interaction with a less repulsive short-range part such as the Brink-Boeker BB1 force [32].

The ground state energy and the root mean square radius $\langle r^2\rangle^{1/2}$ for different nuclei calculated from a number of trial wave functions by using the BB1 and the MS3 interactions are reported in Tables II and III, respectively. The optimal parameters of the trial wave functions are also shown. The notation is as follows: MB stands for a noncorrelated trial wave function of Margenau-Brink type, JL is a correlated wave function including both a central Jastrow factor and a linear state independent correlation factor [$g^{(k)}(r)=0$ for $k=2$, 3 4 in Eq. (4)], and JLO is a correlated wave function with both a central Jastrow factor and a linear correlation factor that is state dependent—i.e., depends explicitly on the spin and isospin exchange operators [$g^{(k)}(r)\neq 0$ for $k=1$, 2, 3, 4 in Eq. (4)]. Both types of correlated trial wave functions, JL and JLO, are built from a Margenau-Brink model wave function. In the JLO approach we have used the same non-

TABLE II. Ground state energies calculated by using different trial wave functions without correlations (MB), with state independent correlations (JL), and with linear state dependent correlations (JLO) for the BB1 Brink-Boeker potential. Energies are in MeV, $\langle r^2\rangle^{1/2}$ in fm, β_1, β_2 in fm^{-1}, and R_c, R_d in fm. The statistical error is shown in parentheses. The Coulomb energy is not included in the total energy.

$^AX(K,J^\pi)$	WF	β_1, β_2	R_c, R_d	E	E_c	$\langle r^2\rangle^{1/2}$
	MB	0.70	3.4	−80.01(4)	7.197(1)	2.63(4)
$^{12}C(0,0^+)$	JL	0.72	3.5	−112.36(4)	7.417(1)	2.53(7)
	JLO	0.72	3.5	−117.68(11)	7.397(1)	2.53(7)
	MB	0.68, 0.59	3.5, 3.0	−78.29(6)	7.057(1)	2.71(9)
$^{13}C(\frac{1}{2},\frac{1}{2}^-)$	JL	0.72, 0.54	3.4, 3.0	−112.65(7)	7.558(1)	2.53(8)
	JLO	0.72, 0.54	3.4, 3.0	−119.8(2)	7.613(2)	2.52(15)
	MB	0.69, 0.56	3.2, 2.5	−86.36(5)	7.363(1)	2.64(6)
$^{14}C(0,0^+)$	JL	0.74, 0.58	3.1, 2.8	−122.93(8)	7.836(1)	2.47(5)
	JLO	0.74, 0.58	3.1, 2.8	−131.75(13)	7.854(1)	2.46(8)
	MB	0.68, 0.57	3.2, 2.8	−85.09(6)	9.849(1)	2.65(8)
$^{14}N(1,1^+)$	JL	0.71, 0.57	3.0, 2.5	−121.68(7)	10.438(1)	2.47(7)
	JLO	0.71, 0.57	3.0, 2.5	−131.8(2)	10.381(2)	2.48(10)
	MB	0.66, 0.56	3.0, 2.5	−97.69(10)	9.948(1)	2.65(9)
$^{15}N(\frac{1}{2},\frac{1}{2}^-)$	JL	0.74, 0.63	2.7, 2.4	−139.55(10)	10.821(1)	2.39(9)
	JLO	0.74, 0.63	2.7, 2.4	−152.0(4)	10.837(5)	2.38(18)
	MB	0.66	2.9, 2.4	−118.70(5)	13.470(1)	2.60(3)
$^{16}O(0,0^+)_{C_{3v}}$	JL	0.76	2.8, 2.4	−166.92(6)	14.516(1)	2.36(3)
	JLO	0.76	2.8, 2.4	−179.46(10)	14.515(2)	2.35(5)
	MB	0.67	2.8	−118.52(5)	13.456(1)	2.60(3)
$^{16}O(0,0^+)_t$	JL	0.74	2.6	−166.66(6)	14.446(2)	2.37(4)
	JLO	0.74	2.6	−180.61(8)	14.552(2)	2.35(5)

TABLE III. Ground state energies calculated by using different trial wave functions, with state independent correlations (JL), and with linear state dependent correlations (JLO) for the modified Afnan-Tang MS3 potential. Energies are in MeV, $\langle r^2\rangle^{1/2}$ in fm, β_1, β_2 in fm^{-1}, and R_c, R_d in fm. The statistical error is shown in parentheses. The Coulomb energy is not included in the total energy.

$^AX(K,J^\pi)$	WF	β_1,β_2	R_c,R_d	E	E_c	$\langle r^2\rangle^{1/2}$
$^{12}C(0,0^+)$	JL	0.70	3.5	−74.54(5)	7.571(1)	2.48(4)
	JLO	0.70	3.5	−87.2(4)	7.440(2)	2.49(15)
$^{13}C(\frac{1}{2},\frac{1}{2}^-)$	JL	0.70, 0.46	3.3, 3.1	−73.37(10)	7.833(1)	2.47(8)
	JLO	0.70, 0.46	3.3, 3.1	−88.6(6)	7.864(1)	2.44(13)
$^{14}C(0,0^+)$	JL	0.69, 0.48	3.4, 3.0	−77.52(7)	7.840(1)	2.50(5)
	JLO	0.69, 0.48	3.4, 3.0	−94.6(3)	7.840(1)	2.44(10)
$^{14}N(1,1^+)$	JL	0.69, 0.54	3.2, 2.8	−81.95(9)	10.699(1)	2.42(7)
	JLO	0.69, 0.54	3.3, 3.8	−99.3(4)	10.865(3)	2.37(10)
$^{15}N(\frac{1}{2},\frac{1}{2}^-)$	JL	0.67, 0.54	3.2,2.8	−91.77(12)	10.701(1)	2.45(9)
	JLO	0.67, 0.54	3.2, 2.8	−112.6(6)	10.878(3)	2.39(15)
$^{16}O(0,0^+)$	JL	0.71	2.7	−114.46(7)	14.827(1)	2.32(3)
	JLO	0.71	2.7	−135.6(3)	15.036(2)	2.27(7)

linear parameters as in JL; i.e., the variational freedom is restricted only to the linear parameters of the different operatorial channels. This scheme has shown to work properly for spin- and isospin-saturated nuclei [23,24] in such a way that the loss of energy due to this partial optimization was very small. This is convenient because when state dependent correlations are included, two things happen: first the calculation becomes slower, and second, the statistical error increases. Therefore it is very convenient, from a computational point of view, that the nonlinear parameters can be well determined by means of a state independent optimization. Note that the linear parameters are computed by solving a generalized eigenvalue problem and then only a long run is required to fix them. The expectation value of the Coulomb energy E_c, not included in the total binding energy, is reported separately. For the results shown in this work we have used $2^8\times10^5$ ($2^6\times10^5$) moves per nucleon with state independent (state dependent) correlated wave functions.

The wave functions used in this work include two different oscillator parameters: one for the complete clusters and another for the incomplete one. This gives rise to an improvement in the energy of about 3 or 4 MeV when the incomplete cluster is made of one or two nucleons. The improvement is noticeably reduced if the incomplete cluster contains three nucleons. The smaller value for the oscillator parameter of the incomplete cluster is due to the fact that the nucleons are more localized in the alpha particle cluster than in the incomplete cluster. In general we have obtained oscillator parameters that vary between those of ^{12}C and ^{16}O.

With respect to the optimum parameters of the intercluster distances, we have obtained that the distance between the centers of the complete clusters is bigger than the distance between the incomplete cluster and an alpha particle cluster. The total energy is not very sensitive to variations of the intercluster distances in the neighborhood of the equilibrium values. We have indicated such a situation by giving these distances with only one decimal digit. Finally—and as could be expected—when moving from $A=12$ to $A=15$ the optimal values of the variational parameters tend to those of ^{16}O. This is the case for all of the interactions and wave functions analyzed in this work. It is remarkable that the ground state energy of ^{16}O obtained with the C_{3v} symmetry is practically the same as the one obtained with a tetrahedral symmetry T_d.

In general, the effect of the correlations is to reduce the average size of the nucleus. Therefore, the optimum values in the model wave function will depend on the presence, or not, of the correlation factor. The modification with respect to the noncorrelated wave function is roughly proportional in all of the parameters in such a way that nucleon correlations give rise to an isotropic contraction of the nucleus.

It is interesting to point out the importance of correlations in the binding energy of ^{12}C and ^{14}C as compared with ^{13}C and ^{14}N, respectively. With both interactions, ^{12}C is more bound than ^{13}C with central correlations, but state dependent correlations reverse this situation, obtaining a difference of 1 and 2 MeV with the MS3 and BB1 interactions, respectively. The behavior of the nuclear binding energy of ^{14}C and ^{14}N is different with both potentials. With the BB1 interaction and without correlations, ^{14}C is slightly more bounded than ^{14}N. The difference in their binding energy decreases with the use of central correlations and is zero with state dependent correlations. However, with the MS3 potential, ^{14}N is 4.5 MeV more bounded than ^{14}C with central and state dependent correlations. The reason for this different behavior lies in the contribution of the Bartlett and Heisenberg channels of the MS3 interaction, which are null in the BB1 potential. Finally it is also worth mentioning here that we have obtained a negligible effect of the state dependent correlations on the Coulomb energy, which depends basically on the parameters of the model wave function.

The correlations increase the binding energy by a quantity which grows with the number of nucleons, A. In order to get a deeper insight into the coupling between correlations and the particular nucleus we report in Table IV the increment in energy per number of pairs of nucleons. For example the increase in the binding energy per nucleon pair when state independent correlations are included with respect to the uncorrelated model is given by

TABLE IV. Increase in the binding energy per number of nucleon pairs due to the inclusion of different correlation factors for the nuclei studied in this work. For ^{16}O the symmetry group is C_{3v}. In parentheses is indicated the nuclear interaction. The increment is in MeV per number of nucleon pairs. The error is in the last figure.

$^{A}X(K,J^{\pi})$	$\Delta_{\text{JL-MB}}$ (BB1)	$\Delta_{\text{JLO-JL}}$ (BB1)	$\Delta_{\text{JLO-JL}}$ (MS3)
^{12}C$(0,0^{+})$	−0.49	−0.08	−0.19
^{13}C$(\frac{1}{2},\frac{1}{2}^{-})$	−0.44	−0.09	−0.19
^{14}C$(0,0^{+})$	−0.40	−0.10	−0.19
^{14}N$(1,1^{+})$	−0.40	−0.11	−0.19
^{15}N$(\frac{1}{2},\frac{1}{2}^{-})$	−0.40	−0.12	−0.19
^{16}O$(0,0^{+})$	−0.40	−0.12	−0.18

$$\Delta_{\text{JL-MB}} = \frac{2}{A(A-1)}(E_{\text{JL}} - E_{\text{MB}}),$$

where E_{JL} (E_{MB}) is the energy in the JL (MB) model. The quantity $\Delta_{\text{JLO-JL}}$ is defined in a similar way. As can be seen, the increment per number of pairs is roughly constant for all of the nuclei considered, especially $\Delta_{\text{JLO-JL}}$, which accounts for the effect of state dependent correlations. The increment due to state dependent correlations in the MS3 potential is practically twice the increment in the BB1 case.

A more detailed analysis of the effect of the state dependent correlations on the energy can be done by looking at the contribution of the kinetic energy and of the different channels of the potential energy. In Fig. 2 we plot the differences between these quantities calculated with the JL and JLO wave functions for both the BB1 and MS3 interactions. Both the kinetic energy and energy of the Wigner channel rise with state dependent correlations for both potentials. This increase is more important for the kinetic energy with the MS3 potential than with the BB1 one, whereas the opposite holds for the energy of the Wigner energy. For the BB1 potential, the Majorana channel is the responsible for the decrease in the ground state energy when state dependent correlations are considered. For the MS3 interaction, the effect on the Majorana channel is practically canceled with that on the kinetic and Wigner energies, and the Bartlett and Heisenberg channels make the nuclei more bound. The contribution of these two channels is very close and is nearly independent of the nucleus considered.

The one- and two-body densities give the spatial distribution of the nucleons in the nuclei. The one-body density is the probability density distributions for finding a nucleon around the center of mass of the system and the two-body the probability density distribution for finding a nucleon around another given nucleon. In particular, the spherically averaged one- and two-body densities, normalized to unity, are defined as [33,34]

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

$$\rho_2(r_{12}) = \int \mathrm{d}\tau |\Psi(\tau)|^2 \left\{ \frac{2}{A(A-1)}\sum_{i<j}^{A} \frac{1}{r_{12}^2}\delta(r_{12} - |\vec{r}_i - \vec{r}_j|) \right\}, \quad (16)$$

where τ stands for all of the particles' spatial coordinates and intrinsic degrees of freedom and $\vec{R} = (1/A)\Sigma_{i=1}^{A}\vec{r}_i$. Here we have calculated these densities to analyze the effect of the different correlation mechanisms introduced in the variational wave functions. In Fig. 3 we show the one-body nuclear density calculated with the JL wave function for all of the nuclei here studied and the two interactions considered. As can be seen, the qualitative behavior is similar for both potentials, with a higher value of the maximum as the number of nucleons increases. It is also worth pointing out that as A increases, the density tends to that of ^{16}O. It is for these nuclei and the MS3 interaction where this density is more separated from the others.

The effect of the state-dependent correlations on the one-body density for these nuclei is studied in Fig. 4, where we plot the difference between the single-particle density obtained with the JL and JLO wave functions. The first noticeable fact is that the general behavior is different for the two interactions used here. Thus at short distances state dependent correlations tend to increase the density with the BB1 interaction and the opposite happens with the MS3 potential, except for ^{12}C, for which a negative region at short distances

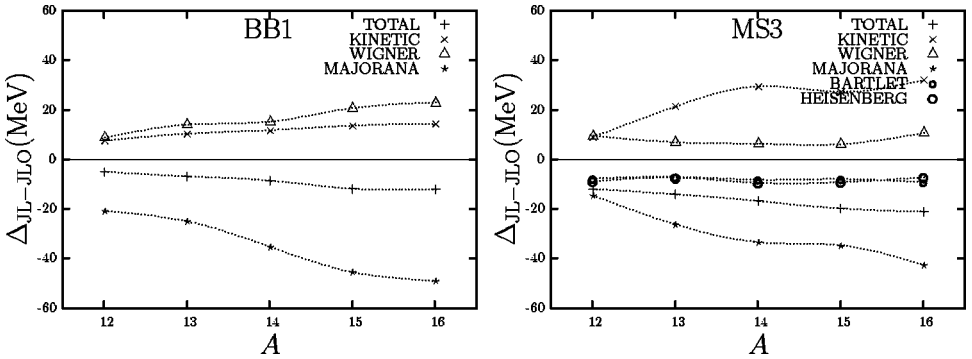

FIG. 2. Increase in the total energy, the expectation values of the kinetic energy, and the different channels of the interacting potential when state-dependent correlations are included with respect to the JL approximation. In the left hand side panel we plot the results for the BB1 potential and in the right hand side panel for the MS3 potential. The lines are for guiding the eyes.

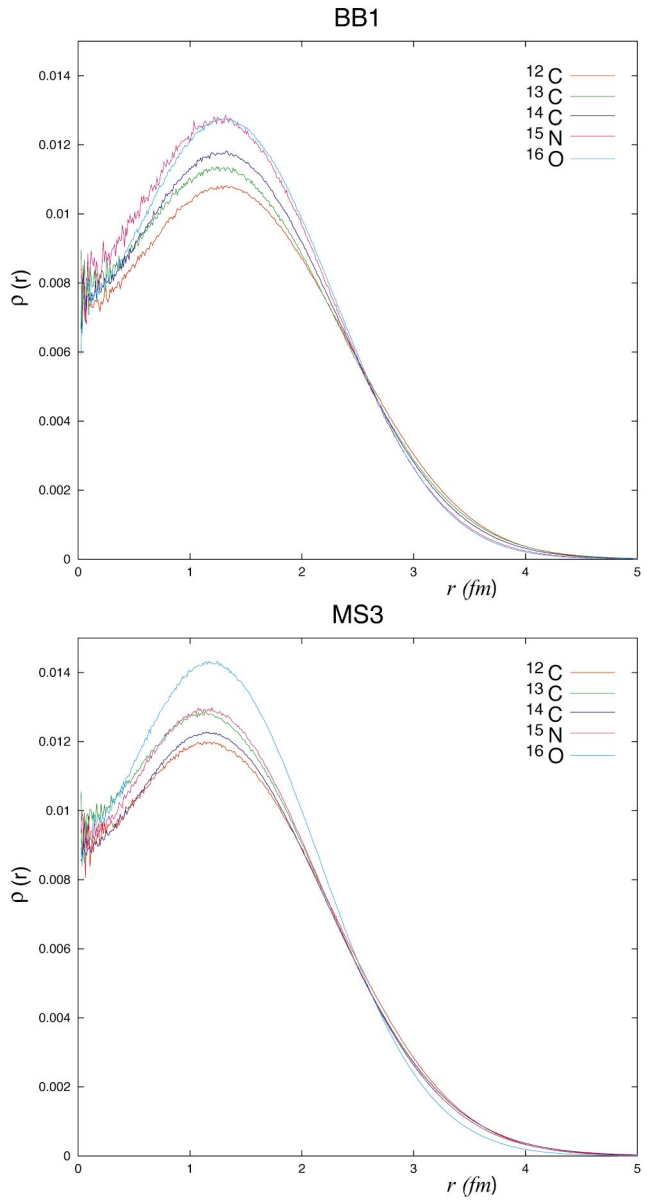

FIG. 3. One-body density for all the nuclei studied in this work calculated with the JL wave function. In the upper panel we plot the results for the BB1 potential and in the lower one for the MS3 potential.

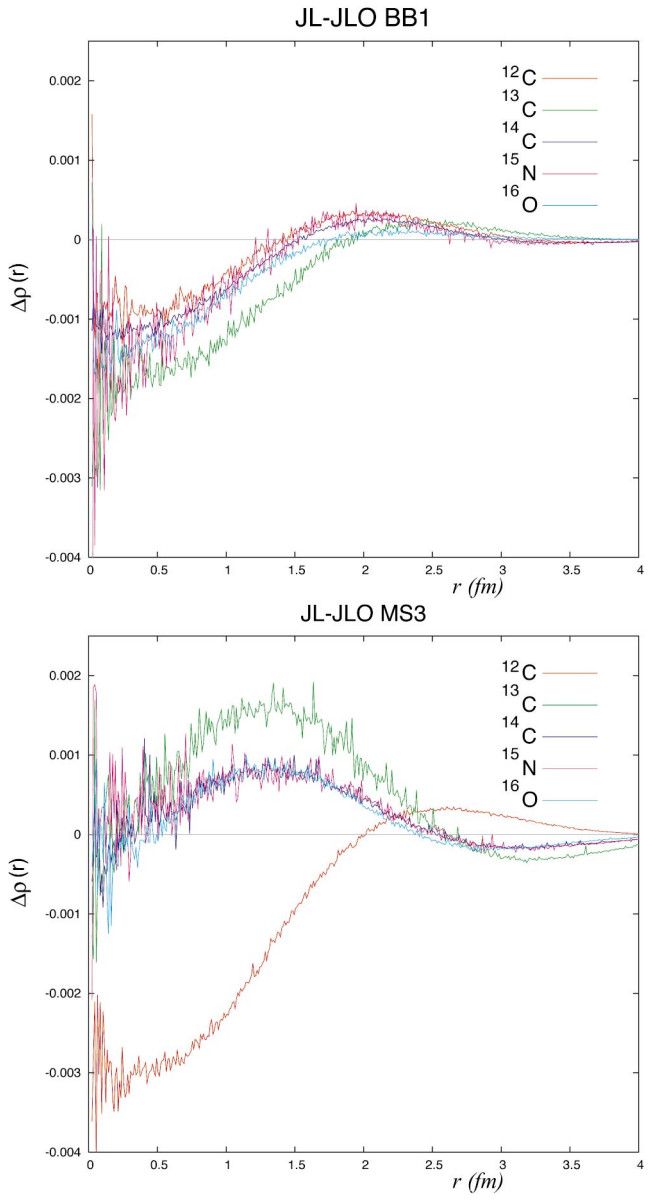

FIG. 4. Effect of the state dependent correlations on the one-body density for the different nuclei considered in this work. In the upper panel we plot the results for the BB1 potential and in the lower one for the MS3 potential.

appears. In addition, for the BB1 potential, the effect of the operatorial correlations is roughly independent of the nucleus while for the MS3 potential effects of the operatorial correlations show a more accused dependence on the nucleus.

The effects of correlations are more important on the two body density than in the one-body density. In Fig. 5 we plot the two-body density obtained from the state independent correlated wave function JL for all of the nuclei studied and the two interactions considered in this work. The behavior of this density is very similar for both potentials, although the effect of the nuclear core is much more important in the MS3 potential. The main difference is that with the MS3 interaction shorter distances are favored with respect to the BB1 potential. At distances between 2 and 3.5 fm the differences among the nuclei considered are more important, with bigger values as the number of nucleons increases from ^{12}C to ^{16}O. This can be understood as a progressive filling of the incomplete cluster that gives rise to a larger number of particles at these intermediate distances.

Finally, the effect of including state dependent correlations on this density is studied in Fig. 6 where we plot the difference between the two-body density calculated from the JL and JLO wave functions. As was the case for the one-body density, the effect of state dependent correlations is roughly independent of the nucleus when the BB1 potential is used and a more accused dependence is observed for the MS3 interaction. For both potentials, state dependent correlations bring together nucleons with respect to the JL case.

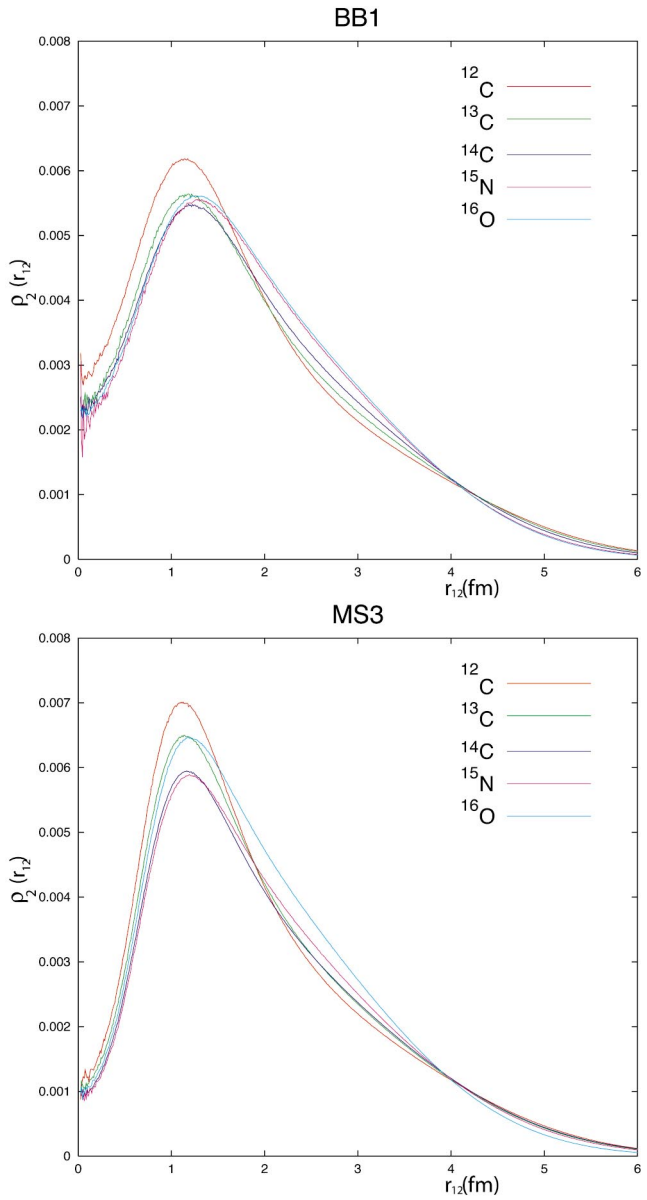

FIG. 5. Two-body density for all the the nuclei studied in this work calculated with the JL wave function. In the upper panel we plot the results for the BB1 potential and in the lower one for the MS3 potential.

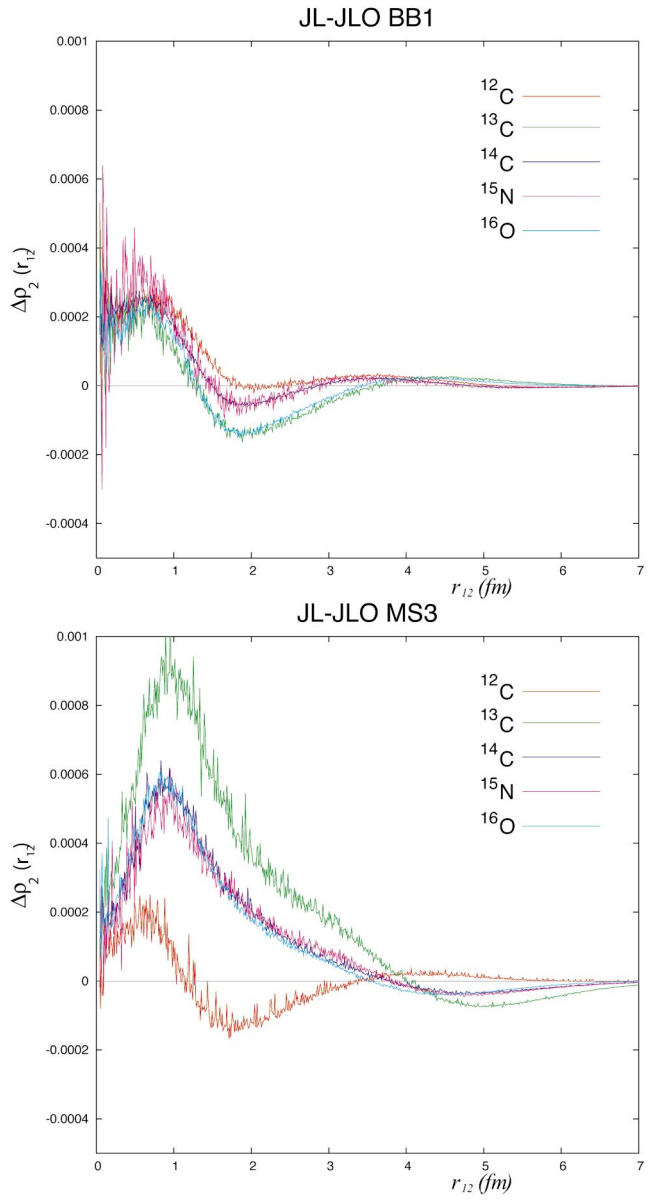

FIG. 6. Effect of the state-dependent correlations on the two-body density for the different nuclei considered in this work. In the upper panel we plot the results for the BB1 potential and in the lower one for the MS3 potential.

IV. CONCLUSIONS

Variational Monte Carlo calculations for *p*-shell, $A \neq 4n$, nuclei starting from the nucleon-nucleon interaction have been presented. The ground state energy and the one- and two-body densities have been calculated. The variational wave function consists of three factors: a central Jastrow term, a spin-isospin dependent linear term, and a model wave function. The model wave function is based on a cluster model allowing for the formation of different kinds of nucleon clusters with centers at fixed positions. The Peierls-Yoccoz projection operators have been used in order to obtain trial wave functions with the proper values of the angular momentum. This work extend previous ones carried out for spin- and isospin-saturated nuclei.

The present scheme has shown to be appropriate for describing two important and complementary aspects of the nuclear dynamics as the short-range correlations and the formation of nucleon clusters. The former is induced by the short-range repulsive part of the nuclear potential while the later is a collective effect due to the medium- and long-range part of the interaction.

In this work, an analytical reduction of the expectation values for $A \neq 4n$ nuclei is presented. The use of the Peierls-Yoccoz projection operators introduces new features when the nuclei are not spin and isospin saturated. Here we obtain a final form of the expectation values which is specially suited for the variational Monte Carlo calculation. This is done for both state-independent and state dependent correlation factors. As a result the different expectation values can

be computed with no significant extra computational cost with respect to the case of spin- and isospin-saturated nuclei.

The scheme is applied to several nuclei with $12 \leqslant A \leqslant 16$. The methodology has been first tested against previous works using a completely different scheme of calculation. Then results obtained by using two different nucleon-nucleon potentials including a repulsive core at short distances and state-dependent interaction channels have been reported. The binding energies and the root mean square radius along with the optimal parameters of the wave functions are shown for the different nuclei and states considered here. The effect of the different correlation mechanisms included in the trial wave function on the energy and on the equilibrium geometries is discussed. The importance of using different oscillator parameters for the different kind of nucleon clusters is shown. The effect of the correlations on the different interaction channels is analyzed in terms of the number of nucleons. Finally one- and two-body densities obtained for the nuclei here studied with several approximations of the wave functions are reported and discussed.

ACKNOWLEDGMENTS

This work has been partially supported by the Ministerio de Ciencia y Tecnología and FEDER under Contract No. BFM2002-00200 and by the Junta de Andalucía.

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