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Correlated wave functions to approach the bound excited states of Li$^-$ and Be$^-$

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Abstract. Explicitly correlated wave functions including a Jastrow factor to take into account the dynamical correlation effects, and a multi determinant model wave function to account for the non–dynamical correlations are used to study some metastable excited states of the negative ions Li$^-$ and Be$^-$. A detailed analysis of one– and two–body properties has been carried out for these states. In particular the single–particle density as well as both the two–body inter electronic and center of mass densities have been obtained. All the calculations have been performed by using the variational Monte Carlo method.

PACS. 31.10.+z Theory of electronic structure, electronic transitions, and chemical binding – 31.25.-v Electron correlation calculations for atoms and molecules – 31.25.Jf Electron correlation calculations for atoms and ions: excited states – 02.70.Ss Quantum Monte Carlo methods

1 Introduction

The problem of the atomic structure including correlations has been usually tackled starting from large expansions of the atomic wave function on Slater determinants. The use of explicitly correlated wave functions, including explicitly the inter-electronic coordinate, constitutes an alternative to deal with this problem. For few electron systems, highly accurate results have been obtained by expanding the variational wave function on large basis sets that depend on the inter electronic distance [1,2]. However the generalization of this kind of ansatz to more complex systems is very complicated due to the difficulties involved in the calculation of the expectation values. These problems can be efficiently dealt with the Variational Monte Carlo (VMC) method, see e.g. [3]. With this method, the expectation value of the atomic Hamiltonian between wave functions of practically any form can be accurately computed. Starting from relatively large expansions on the inter-electronic coordinate, highly accurate energies have been recently reported for four and five electron atoms and ions [4,5]. A different option, within the VMC scheme, is the development of compact explicitly correlated wave functions that depend on few variational parameters and contain the most important features of the electronic correlations in the system under study, with a common structure of the wave function for different atoms [6]. The accuracy reached by using these simpler wave functions is not as high as in large expansions. However they lead to a very accurate description of the system and allow for a reliable calculation of other interesting properties. Besides they can be used for the description of atoms with a greater number of electrons. Therefore by using this ansatz a consistent and systematic analysis of the electronic correlations can be completed.

Within the problem of the electronic structure of atomic systems, the calculation of anions is of particular interest. For example, it is well-known that some negative ions can exist in several bound excited states. In particular the bound states of Li$^-$ and Be$^-$ have been the focus of much research interest. Thus, it has been found [7,8] that the only long-lived states of the negative lithium ion are the ground state and the core excited $1s2s2p^2$–^{5}P and $1s2p^3$–^{5}S ones which lie below their corresponding parent terms $1s2s2p$–^{4}P and $1s2p^2$–^{4}P of the neutral Li atom. Both excited states correspond to the highest total spin value. For Be$^-$ it is known that its ground configuration, $1s^22s^22p$–^{2}P is not stable, but it has been demonstrated theoretically [9,10] that Be$^-$ has three metastable bound terms $1s^22s2p^2$–^{4}P, $1s^22p^3$–^{4}S and $1s2s2p^3$–^{6}S which lie below their parent terms $1s^22s2p$–^{3}P, $1s^22p^2$–^{3}P and $1s2s2p^2$–^{5}P of the neutral atom, respectively.

These and other results are based on extensive Configuration Interaction or Multi Configuration Hartree Fock calculations [11,12] that provide very accurate values of the energy and allow for a precise determination of relativistic corrections and some other interesting properties

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such as oscillator strengths. However the knowledge of the one and, especially, the two body densities and related properties such as their radial moments is much more scarce. This is due to the difficulties involved in their calculation by using these wave functions. These distribution functions give insight into the spatial arrangement of the electrons and play a key role in the understanding of the dynamics and structure of the atomic systems [13–16]. In addition, these distribution functions can be used to study some other properties such as electronic correlations, exchange effects, information entropy of atoms, see e.g. references [15,17–24].

In this work we study the bound states of Li^- and Be^- ions by using compact and accurate explicitly correlated wave functions. Both the wave function and the densities and related properties have been obtained by using the Variational Monte Carlo method. The variational ansatz employed here has been previously applied to study the ground and the first excited states of the neutral and positive ions of four [25,26] and five [27,28] electronic systems leading to a reliable description of the radial density and some other related properties.

The wave function used in this work is written as the product of a symmetric correlation factor, F, accounting for the dynamic correlation effects, times a model wave function Φ that gives some of the properties of the state such as the spin and the angular momentum of the atom, and it is antisymmetric in the electronic coordinates

$$\Psi = F\Phi. \tag{1}$$

For the correlation factor we use the form of Boys and Handy [29] with the prescription proposed by Schmidt and Moskowitz [6]. We have worked with 17 variational nonlinear parameters in the correlation factor. For the model wave function we use a multi configuration expansion

$$\Phi = \sum_k C_k \phi_k, \tag{2}$$

where ϕ_k is each one of the states with the proper values of the total spin and orbital angular momentum arising from the configurations selected to describe the state under consideration. The orbitals in ϕ_k and the initial values of the linear coefficients C_k have been fixed by using the parameterized optimized effective potential (POEP) method [30]. When using this model wave function with the correlation factor proposed here, it is not necessary to use a great number of configurations to obtain the energy of the states studied with a relatively good precision. In particular between one and three configurations have been used, depending on the state considered.

Once the model wave function is built, the total trial wave function is obtained by multiplying it by the correlation factor, F. The nonlinear parameters of the correlation factor, and the linear coefficients C_k of the expansion of the model wave function, equation (2), are taken as variational parameters. This constitutes a correlated basis set expansion of the trial wave function where the Hamiltonian is diagonalized. This step involves the solution of a generalized eigenvalue problem, with matrix elements computed by Monte Carlo, obtaining a new set of the linear coefficients C_k. The optimization of the wave function has been carried out by minimizing the total energy.

Starting from the best wave function, several one– and two–body properties have been obtained. One–body properties in position space can be studied in terms of the single particle density, $\rho(\boldsymbol{r})$,

$$\rho(\boldsymbol{r}) = \left\langle \Psi | \sum_i \delta[\boldsymbol{r} - \boldsymbol{r}_i] | \Psi \right\rangle \tag{3}$$

which gives the charge distribution around the nucleus.

Two–electron properties can be studied in terms of both the inter electronic, or intracule, $I(\boldsymbol{r}_{12})$, and the center of mass, or extracule, $E(\boldsymbol{R})$, densities [14,15] defined as

$$I(\boldsymbol{r}_{12}) = \left\langle \Psi | \sum_{i>j} \delta[\boldsymbol{r}_{12} - (\boldsymbol{r}_i - \boldsymbol{r}_j)] | \Psi \right\rangle \tag{4}$$

$$E(\boldsymbol{R}) = \left\langle \Psi | \sum_{i>j} \delta[\boldsymbol{R} - (\boldsymbol{r}_i + \boldsymbol{r}_j)/2] | \Psi \right\rangle \tag{5}$$

respectively. These two distribution functions provide insight into the spatial arrangement of the electronic charge. They represent the probability density function for a pair of electrons having a relative vector $\boldsymbol{r}_{12}$ or a center of mass vector $\boldsymbol{R}$, respectively. Their spherical averages will be denoted by $h(r_{12})$ and $d(R)$, respectively. Besides, the radial moment of order -1 of the single particle and the intracule densities give the electron-nucleus attraction and the electron-electron repulsion energy, respectively. Note that the one body density is normalized to the number of electrons and both the intracule and extracule densities to the number of electron pairs in the atom. Atomic units are used throughout.

2 Results

We have studied the ground $1s^2 2s^2$–^{1}S as well as the highly excited states $1s2p^3$–^{5}S and $1s2s2p^2$–^{5}P of Li^- and the $1s^2 2s2p^2$–^{4}P, $1s^2 2p^3$–^{4}S and $1s2s2p^3$–^{6}S metastable states of Be^-.

For the ground state of Li^- we have used, in addition to the low–lying $1s^2 2s^2$ configuration, the $1s^2 2p^2$ one, to include the $2s$–$2p$ near degeneracy effect, and the $1s^2 2s3s$ configuration. The weight of these last two configurations is of about 30% for this state. For the $1s2p^3$–^{5}S states we have used only one configuration whereas for the $1s2s2p^2$–^{5}P term we have included in the expansion the configurations $1s2s2p^2$, $1s3s2p^2$ and $1s2s2p3p$. If the correlation factor F is taken equal to 1, the use of three configurations improves largely the energy obtained with only one configuration. However, when the correlation factor F is included the difference in the total energy obtained with one and with three configurations is of about 1 mhartree. For the ^{4}P state of Be^- we have used the following three configurations, $1s^2 2s2p^2$, $1s^2 3s2p^2$ and $1s^2 2s2p3p$. The weight of the later two is about 22%. For the ^{4}S state we

Table 1. Energy of the different states of the two ions studied here obtained in this work (VMC) as compared with the non-correlated (NC) and others that we shall consider as exact. In parentheses we give the error in the last figure.

	Li$^-$			Be$^-$		
	^{1}S	^{5}P	^{5}S	^{4}P	^{4}S	^{6}S
NC	-7.428232^a	-5.364274	-5.222489	-14.509028^c	-14.32752^c	-10.428833^c
VMC	$-7.49909(2)$	$-5.38329(1)$	$-5.25355(1)$	$-14.57160(2)$	$-14.40106(2)$	$-10.46624(2)$
Exact	-7.500758^a	-5.3865728^b	-5.2560969^b	$-14.577877(36)^d$	$-14.406282(26)^d$	

^{a}Reference [31], ^{b}reference [11], ^{c}reference [10], ^{d}reference [12].

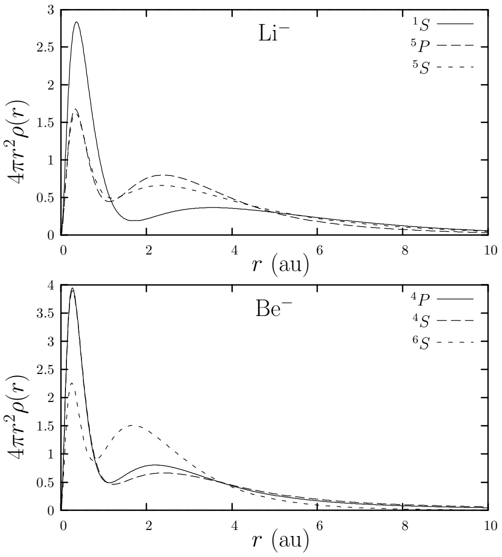

Fig. 1. One body radial density for the different states of the ions of Li$^-$ and Be$^-$ studied here.

have mixed the $1s^22p^3$ and the $1s^22p^23p$ configurations. The weight of the second one is approximately 13%. Finally, for the ^{6}S state we have considered only the $1s2s2p^3$ configuration. All the relative weights discussed here correspond to the correlated basis set.

In Table 1 we show the energy of all these states as compared with the non–correlated ones obtained either within the Hartree–Fock framework for Be$^-$ as well as for the ground state of Li$^-$, or within the POEP method for the two excited states of Li$^-$. We also report the energy obtained from extensive configuration interaction calculations [11,12,31], that we shall consider as exact. The wave functions obtained here recover partially the total correlation energy, providing similar results to those of [10]. For the states of Li$^-$ the greatest difference between the results obtained here and the exact ones is of 3.5 mhartree for ^{5}P, while the smallest one is found for the ground state. Thus the percentage of correlation energy recovered with our wave functions goes from about 86% for the ^{5}P state (the term with the smallest correlation energy), to more than 98% for the ground state. For the states of Be$^-$ the difference between the VMC energy of this work and the exact one is lower than 7 mhartree and the percentage of correlation energy recovered is above than 90%. These results show the good performance of these relatively simple trial wave functions.

The spatial arrangement of the electrons is studied in terms of the one and two electron densities. The one body density provides a direct information about the distribution of the electrons with respect to the nucleus. In Figure 1 we plot the radial single–particle density $(4\pi r^2\rho(r))$ for the states considered here of Li$^-$ and Be$^-$.

The electronic distribution near the nucleus is very similar for the ^{5}P and ^{5}S excited states of Li$^-$ and different to that of the ground state, that shows a higher charge density in this region. At intermediate and large distances the effects of the different coupling of the outermost electrons become more apparent. Between the first minimum, corresponding to the inter-shell separation, up to around $r = 4$ au, the charge density of the excited states is larger than in the ground state. The largest values in this region correspond to the ^{5}P term. Finally, at large distances all the states considered here present a similar behavior, with bigger values of the density in the ground state. In the case of Be$^-$, the ^{4}P and ^{4}S terms present similar values of the density close to the nucleus, different to those of the ^{6}S term. This is due to the fact that the former two terms have two $1s$ core electrons, whereas the latter has only one. The differences between the ^{4}P and ^{4}S excited states become relevant at intermediate distances, i.e. there where the L shell is more important. In this region, the ^{6}S term presents the highest values of the charge density and it is the one that decays faster at large distances.

In Figure 2 we plot both the intracule density and the radial intracule density for the different states of the two ions studied here. The intracule density starts from zero at the coalescence point, $r_{12} = 0$, for the ^{5}P and ^{5}S terms of Li$^-$ and for the ^{6}S term of Be$^-$ due to the Pauli principle. The radial intracule density shows one or two maxima, in such a way that the terms with two $1s$ core electrons present two maxima. In these cases, the first maximum corresponds to the separation of the two $1s$ electrons, and the second one to the other relative interparticle distances, i.e. $1s$–$2s$, $2s$–$2p$ and $2p$–$2p$. The first maximum is dropped out of this radial density in the ^{5}P and ^{5}S terms of Li$^-$ and in the ^{6}S term of Be$^-$. This is also supported by the following. If we define

$$N_{\rm p}(r_{12}) = 4\pi \int_0^{r_{12}} ds s^2 h(s),$$

this function can be interpreted as the number of electron pairs separated by distances lower or equal than r_{12}. We have found that $N_p = 1$, i.e. only one electron pair, at the following values: $r_{12} \approx 1.57, 2.43$ and 2.51 for the ^{1}S, ^{5}P

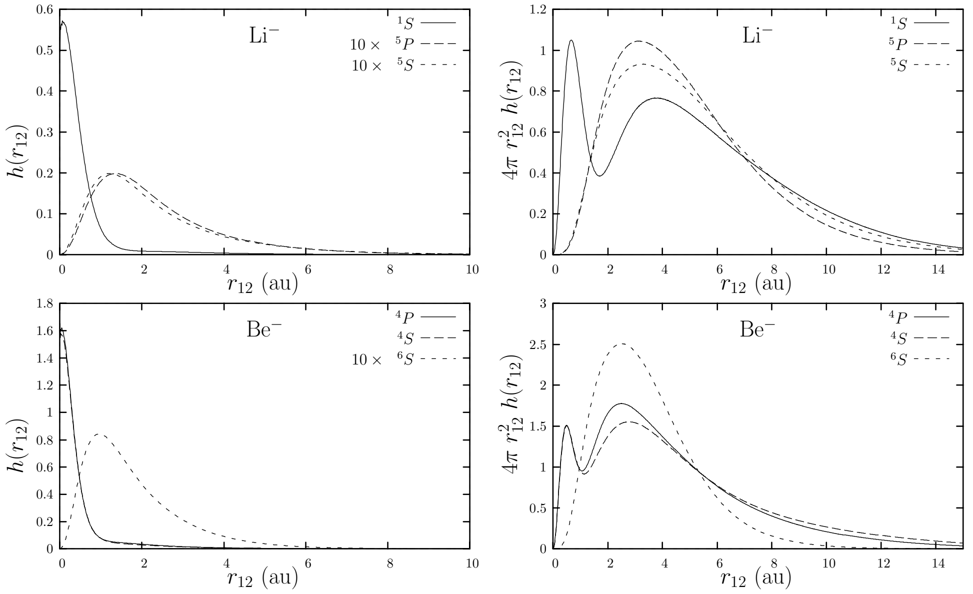

Fig. 2. Intracule density and radial intracule density for the different states of the two ions studied here. The intracule density $h(s)$ for the ^{5}P and ^{5}S states of Li$^-$ and for the ^{6}S state of Be$^-$ are multiplied by ten.

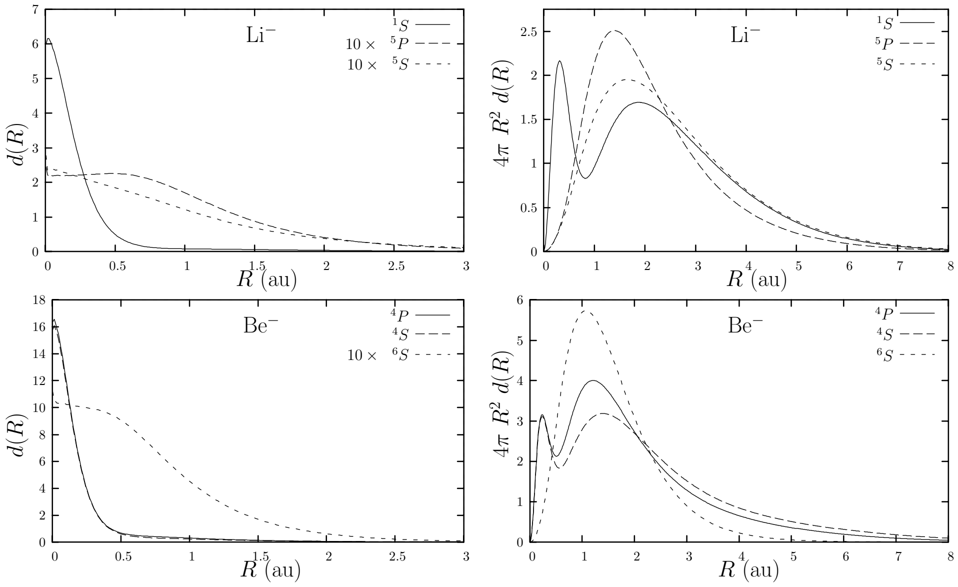

Fig. 3. Extracule density and radial extracule density for the different states of the two ions studied here. The extracule $d(R)$ for the ^{5}P and ^{5}S states of Li$^-$ and for the ^{6}S state of Be$^-$ are multiplied by ten.

and ^{5}S terms of Li$^-$, respectively, and $r_{12} \approx 0.986, 0.988$ and 1.46 for the ^{4}P, ^{4}S and ^{6}S states of Be$^-$, respectively. These values show the role played by the 1s electrons in the intracule density. Finally it is worth to point out that the r_{12} value where $N_p = 2, 3, ...$ depends on the ion considered but they are nearly independent of the LS term.

In Figure 3 we plot both the extracule density and the radial extracule density for the different states of the two ions considered here. It is remarkable the nearly flat region that the extracule density presents for low values of the center of mass coordinate for the states in which all the electron spin are parallel. The radial extracule density shows a shell structure similar to the intracule density, with two maxima for the case of two 1s electrons in the more internal configuration and only one maximum for the states with only one core electron.

Finally, to study how the addition of an extra electron to a bound system to form a new state modifies both the one and the two body densities, we plot in Figure 4 the radial single–particle and both the radial intracule and extracule densities for the $1s^22p^3$–^{4}S state of the ion Be$^-$ and its parent term $1s^22p^2$–^{3}P of the Be atom. The differences between the radial densities of the anion and the neutral atom are also plotted. These figures show that the addition of one electron to the ^{3}P state of the Be atom giving rise to the ^{4}S term of the Be$^-$ ion, does not significantly alter

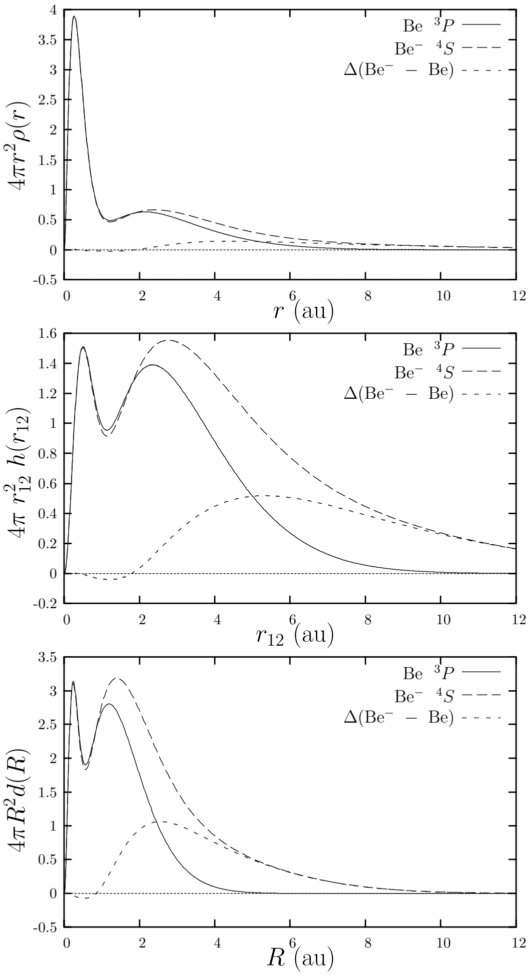

Fig. 4. Radial single particle, intracule, and extracule densities for the ^{4}S term of the ion Be^- and its parent term, the ^{3}P state of the Be atom. The difference between the radial densities of the anion and the neutral atom is also plotted.

the internal structure of the atom up to the beginning of the L shell.

In Table 2 we report the value at the origin and some radial moments of the the single–particle, intracule and extracule densities of the different states of Li^- and Be^- studied here. The values of these quantities are governed by the behavior of the corresponding densities previously studied. For Li^-, the single particle density at the origin and the negative radial values are reduced in both excited states with respect to the ground state. In particular, the $\langle r^{-1}\rangle$ expectation value, proportional to the electron-nucleus attraction energy is reduced by a factor $\sim 2/3$. This is due to the different electronic configuration in the ground state, with two electrons $1s$, as compared with the other states with only one $1s$ electron. The value at the origin and the negative moments of the single particle density of both excited states are very similar, due to the close resemblance of their radial densities near the nucleus. The positive moments are related to the electronic density at medium and large distances from the nucleus. The average size of the system can be analyzed, for example, in terms of the root mean square radius $\sqrt{\langle r^2\rangle}$. The results show that the less extended term is ^{5}P, whereas the ^{5}S state has practically the same size as the ground state.

For Be^- the density at the origin is reduced in the ^{6}S term with respect to the others two states. This is due again to the different electronic configuration for the core. As it was the case for Li^-, the two terms with the same core present similar values for the negative radial moments of the single particle density as well as for the value of the density at the nucleus. The state ^{4}P, the one with the lowest energy, presents the highest value of the moment of order −1. i.e. the strongest electron-nucleus attraction. With respect to the average size, we find that the less extended term is ^{6}S.

At the middle part of Table 2 we show the value at the origin and some radial moments of the intracule density for the states studied here of Li^- and Be^-. It is worth noting here that $h(0)$ is zero, within the statistical error, for both quintuplets in Li^- and for the ^{6}S term of Be^-. This is expected because of the Pauli principle such as it has been pointed out previously. As it was the case of the single particle energy, the negative radial moments of the intracule density are similar for the ^{5}P and ^{5}S terms of Li^- and for the ^{4}P and ^{4}S terms of Be^-. The average size of the inter electronic distribution follows a similar trend as that for the single–particle density. As it is apparent from the data, the main effect of the Pauli principle takes place at short distances.

In the bottom part of Table 2 we report the value at the origin, $d(0)$ and some radial moments of the extracule density. It is remarkable the big differences between the moments of negative order of the states with parallel spin and those corresponding to the other terms. This is a consequence of the nearly–flat shape of the extracule density at low values of the variable R for the states with parallel spin (see Fig. 3).

A systematic analysis of the angular correlations between the electrons can be done by using the angular correlation factor $\tau_{\boldsymbol{r}}$, introduced by Kutzelnigg, Del Re, and Berthier [32]

$$\tau_{\boldsymbol{r}} = \frac{2\sum\limits_{i>j}\langle \boldsymbol{r}_i\cdot\boldsymbol{r}_j\rangle}{(N-1)\sum\limits_{i}\langle r_i^2\rangle}. \qquad (6)$$

This quantity is bounded by [33] $-(N-1)^{-1} \le \tau_{\boldsymbol{r}} \le 1$. $\tau_{\boldsymbol{r}} = 1$ means perfect positive correlation and $\tau_{\boldsymbol{r}} = 0$ stands for either non-correlated variables in the statistical sense or for independent variables. For atomic systems, statistically non-correlated variables means that the position vectors of any pair of particles are, on average, orthogonal, while independent variables means that the diagonal term of the two body density matrix is the product of the one-body distribution functions. These angular correlation factor in both position and momentum spaces are reported in Table 3. We also report in Table 3 some correlated momentum expectation values which are directly obtained in the Monte Carlo calculation. In particular we show the expectation values $\langle p^2\rangle$ (twice the kinetic energy), $\langle p_{12}^2\rangle$, $\langle P^2\rangle$ and $\langle \boldsymbol{p}_1\cdot\boldsymbol{p}_2\rangle$. These two body expectation values

Table 2. Value at the origin and some radial moments of the single–particle (top), the intracule (middle) and the extracule (bottom) densities for the different states of the four and five electron atomic ions studied here. In parentheses we give the statistical error in the last figure.

	$\rho(0)$	$\langle r^{-2}\rangle$	$\langle r^{-1}\rangle$	$\langle r\ \rangle$	$\langle r^{2}\rangle$	$\langle r^{3}\rangle$
Li$^-$ ^{1}S	13.81(4)	30.19(8)	5.8977(6)	11.718(2)	71.30(2)	573.1(4)
Li$^-$ ^{5}P	8.86(3)	19.04(6)	4.1548(6)	11.7410(5)	57.726(8)	388.9(1)
Li$^-$ ^{5}S	8.39(2)	18.23(5)	4.0475(5)	12.9592(6)	72.73(1)	554.5(2)
Be$^-$ ^{4}P	34.7(1)	56.7(2)	8.5525(7)	12.478(1)	66.86(2)	532.9(4)
Be$^-$ ^{4}S	34.06(7)	55.7(1)	8.4140(8)	14.135(2)	89.97(3)	848.7(6)
Be$^-$ ^{6}S	21.1(2)	34.6(3)	6.2137(7)	10.5831(4)	34.785(4)	151.78(4)
	$h(0)$	$\langle r_{12}^{-2}\rangle$	$\langle r_{12}^{-1}\rangle$	$\langle r_{12}\rangle$	$\langle r_{12}^{2}\rangle$	$\langle r_{12}^{3}\rangle$
Li$^-$ ^{1}S	0.5466(4)	4.486(6)	2.6855(2)	31.029(4)	232.75(8)	2168(1)
Li$^-$ ^{5}P	0.00001(5)	0.68646(4)	1.67489(4)	29.647(3)	190.45(2)	1513.8(4)
Li$^-$ ^{5}S	0.00002(5)	0.66895(5)	1.61157(5)	31.942(2)	225.17(3)	1974.8(5)
Be$^-$ ^{4}P	1.576(1)	9.56(1)	5.0279(2)	43.060(5)	281.77(9)	2456(2)
Be$^-$ ^{4}S	1.532(2)	9.32(2)	4.8185(2)	48.271(6)	365.7(1)	3726(3)
Be$^-$ ^{6}S	0.0001(2)	2.1857(1)	3.8844(1)	34.605(1)	151.91(2)	812.0(2)
	$d(0)$	$\langle R^{-2}\rangle$	$\langle R^{-1}\rangle$	$\langle R\ \rangle$	$\langle R^{2}\rangle$	$\langle R^{3}\rangle$
Li$^-$ ^{1}S	6.228(1)	20.83(4)	5.7265(4)	14.279(2)	48.76(2)	207.1(1)
Li$^-$ ^{5}P	0.2203(4)	4.219(4)	3.8941(1)	13.1870(7)	38.975(6)	147.89(4)
Li$^-$ ^{5}S	0.2370(1)	3.616(6)	3.4272(1)	15.4272(8)	52.801(7)	225.97(6)
Be$^-$ ^{4}P	16.631(3)	43.54(5)	10.7696(5)	20.110(3)	63.28(2)	273.6(2)
Be$^-$ ^{4}S	16.226(3)	41.78(5)	9.9966(5)	23.679(3)	88.52(3)	447.9(3)
Be$^-$ ^{6}S	1.039(1)	13.44(2)	8.9518(3)	15.5755(7)	31.593(4)	80.14(2)

Table 3. Several two body position and momentum properties for the different states studied here. In parentheses we give the statistical error in the last figure.

	$\langle \boldsymbol{r}_1 \cdot \boldsymbol{r}_2\rangle$	$\tau_{\boldsymbol{r}}$	$\langle p^2\rangle$	$\langle p_{12}^2\rangle$	$\langle P^2\rangle$	$\langle \boldsymbol{p}_1 \cdot \boldsymbol{p}_2\rangle$	$\tau_{\boldsymbol{p}}$
Li$^-$ ^{1}S	−9.425(4)	−0.08813(4)	15.017(4)	44.44(1)	11.416(3)	0.3069(4)	0.01362(2)
Li$^-$ ^{5}P	−8.638(1)	−0.09976(2)	10.813(3)	32.87(1)	8.001(3)	−0.2160(3)	−0.01332(2)
Li$^-$ ^{5}S	−3.492(2)	−0.03201(2)	10.555(3)	32.21(1)	7.779(3)	−0.274(3)	−0.0173(2)
Be$^-$ ^{4}P	−7.166(2)	−0.05359(3)	29.221(6)	116.42(2)	29.337(6)	0.2328(6)	0.00398(1)
Be$^-$ ^{4}S	−2.900(3)	−0.01612(2)	28.873(6)	115.07(2)	28.978(6)	0.212(1)	0.00367(2)
Be$^-$ ^{6}S	−6.3854(7)	−0.09178(1)	21.008(6)	85.61(3)	20.615(6)	−0.787(4)	−0.0187(1)

and $\langle p^2\rangle$ are not linearly independent but they satisfy the relations [25,27]

$$\langle \boldsymbol{p}_1 \cdot \boldsymbol{p}_2\rangle = \langle P^2\rangle - \frac{1}{4}\langle p_{12}^2\rangle \tag{7}$$

$$\langle p^2\rangle = \frac{2}{N-1}\left(\langle P^2\rangle + \frac{1}{4}\langle p_{12}^2\rangle\right) \tag{8}$$

where N is the electron number. In position space all the states present negative spatial angular correlation. In momentum space the situation is different. We have found a negative angular correlation for the terms with the highest possible total spin value and positive in the other states studied. Positive angular correlation in momentum space indicate that the main contribution to the kinetic energy comes from the center of mass movement of the electron pairs whereas it is more important the inter electronic movement if $\tau_{\boldsymbol{p}}$ is negative (see Eqs. (7) and (8)). Finally it is worth to point out that $\tau_{\boldsymbol{p}}$ presents similar values for those states with the same total spin value in both ions.

3 Conclusions

Explicitly correlated compact wave functions have been obtained for some bound states of the negative ions Li$^-$ and Be$^-$ within a VMC framework. Single or multi determinant wave functions multiplied by a correlation factor have been used. The Boys and Handy form of the correlation factor with the parameterization of Schmidt and Moskowitz has been employed. The free parameters have been optimized by using an algorithm that minimized the expectation value of the energy. The correlation energy recovered is greater than 90% for most of the cases studied. Starting from these wave function the total, one and two body properties as the single particle density, the intracule and extracule densities and some of their radial moments are reported here. A systematic analysis of these properties focusing on the analogies and differences between the different states has been carried out. All the results reported here have been obtained by means of the Variational Monte Carlo method.

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