Ground State for Two-Electron and Electron-Muon Three-Body Atomic Systems

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ABSTRACT: In this article, the angular correlated configuration interaction method previously introduced by some of the authors is extended to three-body atomic systems with general masses. A recently proposed angularly correlated basis set is used to construct ground state wave functions which: (i) satisfy exactly Kato cusp conditions at the two-body coalescence points; (ii) have only linear coefficients; and (iii) show a fast convergency rate for the energy. The efficiency of the construction is illustrated by the study of the negatively charged hydrogen-like systems ($^{\infty}H^-$, T^-, D^-, $^1H^-$, and Mu^-), neutral helium-like systems ($e^-e^-\ ^{\infty}He^{+2}$,$e^-e^-\ ^4He^{+2}$, $e^-e^-\ ^3He^{+2}$, $e^-\mu^-\ ^{\infty}He^{+2}$, $e^-\mu^-\ ^4He^{+2}$, and $e^-\mu^-\ ^3He^{+2}$), and positively charged lithium-like systems ($e^-e^-\ ^{\infty}Li^{+3}$, $e^-e^-\ ^7Li^{+3}$, $e^-e^-\ ^6Li^{+3}$, $e^-\mu^-\ ^{\infty}Li^{+3}$, $e^-\mu^-\ ^7Li^{+3}$, and $e^-\mu^-\ ^6Li^{+3}$). The ground state energies and other mean values are compared with those given in the literature, when available. Wave functions with a moderate number of (20 maximum) linear coefficients are given explicitly; they are sufficiently simple and accurate to be used in practical calculations of atomic collision in which multidimensional integrations are involved.
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1. Introduction

The three-body problem plays a fundamental role in atomic physics. From a theoretical point of view, it is very important because it presents most of the properties of the many-body problem. For bound states of three-body atomic systems, and in particular for helium, many trial wave functions have been proposed and optimized to obtain the best ground state energy. They all are not of the same quality and can be grouped in at least three different groups. Highly sophisticated wave functions, built with a large number of basis functions, lead to very accurate energies (see, e.g., [1–9]). A second, analytical, group includes rather simple wave functions possessing some of the correct functional properties (see, e.g., [10–15]). A third category, deals with wave functions (typically Hylleraas-type) and energies of quality, which are intermediate between the two already mentioned (see, e.g., [16–18]). All these trial wave functions have separate, and possibly complementary, purposes: obtain very accurate mean quantities (including the energy), search for a solution as formal as possible, or useful for applications such as collision studies. For the latter, it is useful to remind that the evaluation of fully differential cross sections for processes such as double ionization by electron [19–22] or photon [23, 24] impact involve large dimensional numerical integrations; this is even more true if one considers the second Born approximation [20, 25, 26] or the evaluation of less differential cross sections through further quadratures. The use of bound wave functions with a very large number of terms (first group) can be prohibitive, even with modern computer facilities [23]. It is then not surprising that only simple or intermediate trial wave functions have been employed so far in all such collision calculations. Another reason for this may be related to the practical fact that simpler functions can be easily tabulated and shared by a wider community. This, for example, possibly explains the popularity of Hylleraas-type wave functions, such as that of Kinoshita [16] or simpler versions [17, 27], among the collision community.

Another important issue concerning trial wave functions is their formal structure. In particular, the behavior close to the singular points plays an essential role, for example, in photo-double ionization for which the cusp conditions have fundamental importance at high energy regimes. Indeed, the use of wave functions, which do not satisfy the cusp conditions, leads to errors in the cross sections, see e.g. [28] and references therein. In other processes, like the double ionization of helium by electron impact [29, 30], this issue has been recently under scrutiny. It is now clear now that, in this case, the cusp conditions are not at all determinant as discussed in, e.g.,[30]; however, this conclusion could only be reached through the use of intermediate quality wave functions, with relatively few parameters, and satisfying exactly the cusp conditions. Trial wave functions usually satisfy the so-called Kato cusp conditions [31] in an approximate way; the functions of the first group usually contain so many terms that the conditions are satisfied quite accurately but not exactly. An alternative approach is to build the trial wave functions with intrinsically the correct behavior, for example, by choosing appropriate basis functions. This is one of the issues addressed in this report.

In the last 3 years, we have worked on the construction of trial wave functions of intermediate quality [32–35], in particular, for two-electron atoms. The idea is to provide to the atomic collision community, explicit wave functions (including the parameters and normalization constant), which can be easily used in various cross sections calculations. This article has two main objectives: (i) the extension of the angular correlated configuration interaction (ACCI) method introduced in [32, 33, 35], in combination with the basis functions recently proposed in [35], to more general atomic systems including those with a finite nuclear mass and light particles of different masses (electrons or muons); and (ii) the construction, for this type of atomic three-body systems, of highly correlated wave functions which satisfy exactly the two-body cusp conditions and are as accurate as the traditional Hylleraas wave functions available in the literature for two-electron systems with infinite nuclear mass.

For some collision calculations (for example the calculation within the second Born approximation of double ionization cross sections), a complete set of wave functions is necessary. This article shall deal with the ground state only, but the method can be successfully used to generate excited states. An orthogonal set of S ground and excited states was presented in [36].

The method is based on a decomposition of the three-body wave function in a sum of doubly correlated configurations. Each configuration, noted ϕ, is formed by the product of atomic functions multiplied by a distortion factor, noted χ, which de-

pends explicitly on the inter-electronic coordinate. The functions ϕ solve part of the three-body hamiltonian, diagonalizing the electron-nucleus Coulomb interactions and partially the electron–electron interaction. The second ingredient on the construction of the ACCI method consists in including a factor Ω in the wave function that solves the nondiagonal terms of the kinetic energy not solved by the first factor ϕ. In the original proposal [32, 33], the distortion factor χ did not fully diagonalize the electron–electron interaction. On the other hand, in connection with collisional studies, Gasaneo and Ancarani [35] introduced a *C*3-like basis set for two-electron atomic systems, which fully diagonalizes all the Coulomb interactions. A simplified version of the ACCI method was then used by the authors to define the double bound counterpart of the approximated double continuum wave function known as *C*3 (or BBK in the electron-atom collision community)[37]. Applications of both approaches to the helium isoelectronic sequence in the infinite mass approximation were presented in Refs. [32, 33, 35].

The efficiency of our ACCI method will be illustrated by considering the following two-electron and electron–muon three-body atomic systems: negatively charged hydrogen-like systems ($^{\infty}H^-$, T^-, D^-, $^1H^-$, and Mu^-); neutral helium-like systems ($e^-e^-\,{}^{\infty}He^{+2}$, $e^-e^-\,{}^4He^{+2}$, $e^-e^-\,{}^3He^{+2}$, $e^-\mu^-\,{}^{\infty}He^{+2}$, $e^-\mu^-\,{}^4He^{+2}$, and $e^-\mu^-\,{}^3He^{+2}$), and positively charged lithium-like systems ($e^-e^-\,{}^{\infty}Li^{+3}$, $e^-e^-\,{}^7Li^{+3}$, $e^-e^-\,{}^6Li^{+3}$, $e^-\mu^-\,{}^{\infty}Li^{+3}$, $e^-\mu^-\,{}^7Li^{+3}$, and $e^-\mu^-\,{}^6Li^{+3}$). The calculated energies, with only a moderate number of linear parameters, are of intermediate quality; they lie in between the highly accurate ones presented for example by Frolov (see e.g., [5]) and those obtained with simple wave functions (see e.g., [15]). Our method generates wave functions which (i) are sufficiently simple and accurate to be used in practical atomic collision calculation; and (ii) by construction, satisfy exactly Kato cusp conditions [31]. Wave functions with these characteristics, and in tabulated form, are presently not available in the literature, in particular for the electron–muon systems considered.

Our work is organized as follows: in Section 2, we redefine the ACCI method with the new basis set and extend it to atomic systems with general masses. In Section 3, we present our results for the systems mentioned above: wave functions are given explicitly, and the energies and mean values of others radial physical quantities are compared to "exact" reference values, when available. We also study the stability and the threshold properties of some of the systems. Finally, a summary and some concluding remarks are given in Section 4.

Hartree atomic units ($\hbar = m_e = e = 1$) are used throughout this article.

2. Method

Consider atomic systems composed of three-particles with charges $z_1 < 0$, $z_2 < 0$, $z_3 > 0$, and respective masses m_1, m_2, m_3; we shall note these three-body systems by $m_1^{z_1}m_2^{z_2}m_3^{z_3}$, with the charges z_i as superscripts. Let $\mu_{ij} = m_i m_j/m_i + m_j (i \neq j)$ be the reduced masses. We shall designate as particle 3 the heaviest particle, that is, the nucleus of mass m_3 and charge $z_3 = Z$, and the two lighter particles, labeled 1 and 2, with masses m_1, m_2, and charges $z_1 = z_2 = -1$. The vectors $\mathbf{r}_{13}$ and $\mathbf{r}_{23}$ will denote the two lighter particles positions with respect to the nucleus, and $\mathbf{r}_{12} = \mathbf{r}_2 - \mathbf{r}_1$ their relative position.

For *S*-states, the six-dimensional Schrödinger equation reduces to the three-dimensional Hylleraas equation when Euler angles have been removed. In terms of the interparticles coordinates (r_{13}, r_{23}, r_{12}), and keeping the general charges z_1, z_2, and $z_3 = Z$, it reads

$$H\Psi(r_{13},r_{23},r_{12}) = E\Psi(r_{13},r_{23},r_{12}), \tag{1}$$

where the nonrelativistic Hamiltonian H is given by

$$H = D_0 + D_1. \tag{2}$$

Here, D_0 and D_1 are the operators

$$\begin{aligned} D_0 = &\left[-\frac{1}{2\mu_{13}}\left(\frac{\partial^2}{\partial {r_{13}}^2} + \frac{2}{r_{13}}\frac{\partial}{\partial r_{13}}\right) + \frac{Zz_1}{r_{13}}\right] \\ &+ \left[-\frac{1}{2\mu_{23}}\left(\frac{\partial^2}{\partial {r_{23}}^2} + \frac{2}{r_{23}}\frac{\partial}{\partial r_{23}}\right) + \frac{Zz_2}{r_{23}}\right] \\ &+ \left[-\frac{1}{2\mu_{12}}\left(\frac{\partial^2}{\partial {r_{12}}^2} + \frac{2}{r_{12}}\frac{\partial}{\partial r_{12}}\right) + \frac{z_1z_2}{r_{12}}\right], \end{aligned} \tag{3}$$

$$\begin{aligned} D_1 = -\Bigg(&\frac{1}{m_1}\frac{{r_{13}}^2 - {r_{23}}^2 + {r_{12}}^2}{2r_{13}r_{12}}\frac{\partial^2}{\partial r_{13}\partial r_{12}} \\ &+ \frac{1}{m_2}\frac{{r_{23}}^2 - {r_{13}}^2 + {r_{12}}^2}{2r_{23}r_{12}}\frac{\partial^2}{\partial r_{23}\partial r_{12}} \\ &+ \frac{1}{m_3}\frac{{r_{13}}^2 - {r_{12}}^2 + {r_{23}}^2}{2r_{13}r_{23}}\frac{\partial^2}{\partial r_{23}\partial r_{13}}\Bigg). \end{aligned} \tag{4}$$

When the nucleus is (virtually) considered as infinitely heavy ($m_3 \to \infty$), the last term in D_1 is absent.

It is known that the wave function Ψ of Eq. (1) must satisfy Kato cusp conditions [31]

$$\left[\frac{\partial \bar{\Psi}}{\partial r_{13}}\right]_{r_{13}\to 0} = z_1 Z \mu_{13} \Psi(0, r_{23}, r_{12}), \tag{5a}$$

$$\left[\frac{\partial \bar{\Psi}}{\partial r_{23}}\right]_{r_{23}\to 0} = z_2 Z \mu_{23} \Psi(r_{13}, 0, r_{12}), \tag{5b}$$

$$\left[\frac{\partial \bar{\Psi}}{\partial r_{12}}\right]_{r_{12}\to 0} = z_1 z_2 \mu_{12} \Psi(r, r, 0) \text{ with } r = \frac{1}{2}|\mathbf{r}_{13} + \mathbf{r}_{23}|, \tag{5c}$$

the notation $\bar{\Psi}$ meaning the average of Ψ over a very small sphere of radius r_{13} (respectively, r_{23} or r_{12}) keeping the other values fixed. Relations 5(a–c) provide the linear behavior that Ψ (r_{13}, r_{23}, r_{12}) must have close to the Coulomb singular points. Satisfying these two-body cusp conditions is not only a mathematical requirement but also an important property that any trial wave function should have. This point has been underlined throughout the literature, and again recently in the context of double photoionization (see, e.g., Ref. [28]).

In Ref. [35], we proposed a basis set that solves exactly the D_0 part of the three-body Schrödinger Eq. (1). The basis functions read

$$\phi_{n_1,n_2,n_3}(r_{13}, r_{23}, r_{12}) = \varphi_{n_1}(r_{23}) \varphi_{n_2}(r_{13}) \chi_{C3}(n_3, \mu_{12}, r_{12}) \tag{6}$$

with $\varphi_{n_i}(r_{jk})$, for ($i = 1, 2$, and $i \neq j, k$), are normalized hydrogenic functions with principal quantum numbers n_1 and n_2, and zero angular momenta ($l_1 = l_2 = 0$). The distortion factor χ_{C3} $(n_3, \mu_{12}, r_{12}) = {}_1F_1[-n_3, 2, -2z_1 z_2 \mu_{12}/n_3 r_{12}]$ is the confluent hypergeometric function [38] which reduces to Laguerre polynomials; for a given value of n_3, it is a parameter-free factor which results from the double analytic continuation [34, 35] of an approximated solution for the double continuum wave function known as *C*3 [37] (also called 3C or BBK model). By construction, the basis functions ϕ_{n_1,n_2,n_3} (r_{13}, r_{23}, r_{12}) satisfy the Kato cusp conditions.

Here, we combine this basis set with the ACCI method introduced in [32, 33, 35]. To find approximated solutions to the Eq. (1), we thus use linear combinations of the following functions:

$$\Psi_{n_1,n_2,n_3}(r_{13}, r_{23}, r_{12}) = \phi_{n_1,n_2,n_3}(r_{13}, r_{23}, r_{12}) \Omega_{n_1,n_2,n_3}(r_{13}, r_{23}, r_{12}) \tag{7}$$

According to [32, 33], we use the following definition for Ω_{n_1,n_2,n_3}

$$\Omega^{(N_i,N_j,N_k)}_{n_1,n_2,n_3}(r_{13}, r_{23}, r_{12}) = \sum_{i,j,k\neq 1} c^{n_1 n_2 n_3}_{ijk} r^i_{13} r^j_{23} r^k_{12} \tag{8}$$

where N_i, N_j, and N_k represent the number of coefficients included for each of the coordinates. When dealing with identical light particles, these numbers are restricted by the symmetry properties satisfied by the wave function under the exchange of the coordinate r_{13} and r_{23}. To have the functions of Eq. (7)—noted now $\Psi^{(N_i,N_j,N_k)}_{n_1,n_2,n_3}$ (r_{13}, r_{23}, r_{12})—satisfying Kato cusp conditions, the coefficients $c^{n_1 n_2 n_3}_{ijk}$ corresponding to first powers in the coordinates should not appear. The polynomials $\Omega^{(N_i,N_j,N_k)}_{n_1,n_2,n_3}$ add to the function $\Psi^{(N_i,N_j,N_k)}_{n_1,n_2,n_3}$ extra correlation in addition to the already included in the basis functions ϕ_{n_1,n_2,n_3}.

The ACCI method suggests, as an approximated solution of the Schrödinger Eq. (1), a linear combination of the functions (7),

$$\Psi_{C3-M} = N \sum_{n_1,n_2,n_3} \Psi^{(N_i,N_j,N_k)}_{n_1,n_2,n_3}(r_{13}, r_{23}, r_{12}), \tag{9}$$

where N is the overall normalization factor. The subscript *C*3–*M* recalls the *C*3-like basis functions originating from the *C*3 double continuum, and indicates the total number M of linear coefficients. Two main differences between the ACCI and the traditional configuration interaction (CI) approach (see e.g., [39]) should be underlined. The first one is that the ACCI includes explicitly angular correlation through the introduction of the r_{12} coordinate in each configuration ϕ_{n_1,n_2,n_3}. The second one is associated to the presence of the multiplying functions $\Omega^{(N_i,N_j,N_k)}_{n_1,n_2,n_3}$ which add both radial and angular correlation. The overall amount of correlation included is dictated by the number M of linear coefficients $c^{n_1 n_2 n_3}_{ijk}$. The ACCI method thus ensures a rather fast convergency rate for the energy and other relevant physical quantities, as will be illustrated in the next section.

With the proposal (9) for the wave function, the Schrödinger Eq. (1) can be transformed into a generalized eigenvalue problem [40]:

$$\sum_{n_1,n_2,n_3,i,j,k} [\hat{H} - E\hat{S}] c^{n_1 n_2 n_3}_{ijk} = 0, \tag{10}$$

where the coefficients $c_{ijk}^{n_1n_2n_3}$ are the eigenvectors and E_i the eigenvalues. Our basis functions $\Psi_{n_1,n_2,n_3}^{(N_i,N_j,N_k)}$, as indeed any other containing products of power and exponential functions [41], allow to express in closed form all the elements of the overlap $\hat{S}$ and Hamiltonian $\hat{H}$ matrices. Indeed, they are obtained from one basic integral:

$$I_{i,j,k}(A,B,C) = \int_0^\infty dr_{13} \int_0^\infty dr_{23} \int_{|r_{12}-r_{13}|}^{|r_{12}+r_{13}|} dr_{12} r_{13}{}^i r_{23}{}^j r_{12}{}^k e^{-Ar_{13}-Br_{23}-Cr_{12}}, \quad (11)$$

which can be expressed in closed form [42] as

$$I_{i,j,k}(A,B,C) = \frac{2i!j!k!}{(A+B)^{j+1}(B+C)^{k+1}(A+C)^{i+1}} \Delta\left[-i, -j, -k, j+1, k+1, i+1, -\frac{(A+C)}{(A+B)}, -\frac{(A+B)}{(B+C)}, -\frac{(B+C)}{(A+C)} \right], \quad (12)$$

where $\Delta\,[a_1, a_2, a_3, b_1, b_2, b_3, x, y, z]$ represents a three variable hypergeometric function [43]

$$\Delta[a_1,a_2,a_3,b_1,b_2,b_3,x,y,z] = \sum_{l=0}^{\infty}\sum_{m=0}^{\infty}\sum_{n=0}^{\infty} \frac{(a_1)_l (a_2)_m (a_3)_n (b_1)_{l-m} (b_2)_{m-n} (b_3)_{n-l}}{l!m!n!} x^l y^m z^n. \quad (13)$$

In our particular case, the exponential depending on the r_{12} coordinate does not appear, and the parameter C is zero.

Before presenting our results, we would like to mention that in the papers [32, 33] a different basis set (named GR) was used. It differs from the present one by the use of another distortion factor, χ_{GR} (r_{12}). The latter depends on a nonlinear parameter β, and is not the exact solution of a Coulomb-like problem as it is the case with the χ_{C3} factor in (6). Although the efficiency of the GR basis used in Refs. [32, 33] is good, it introduces the numerical difficulty that the generalized eigenvalue problem (10) has to be solved many times to optimize the value of β. Compared to the GR basis, the $C3$ basis set functions (6) offer an additional advantage. For a fixed number of terms of the function $\Omega_{n_1,n_2,n_3}^{(N_i,N_j,N_k)}$ the correlation factor χ_{C3} (n_3, μ_{12}, r_{12}) allows for the inclusion into the trial wave function Ψ_{C3-M} of different amounts of angular correlation; this is not possible with the χ_{GR} (r_{12}) of the GR basis set. For example, the ground state energies of the $^\infty$He atom obtained with both basis and using the same powers in Ω are: $E_{\Psi GR5} = -2.90286$ and $E_{\Psi C3\text{-}10} = -2.90307$ a.u. (the $C3$–10 result is obtained with $n_1 = n_2 = 1$ and $n_3 = 1, 2$, thus $M = 10$). A similar analysis performed with more accurate functions like Ψ_{GR9} and Ψ_{C3-18} (see section III), for $^\infty$He and $^\infty H^-$, leads to the following mean energies -2.90327 a.u. [33] and -2.90344 a.u., and -0.526529 a.u. [33] and -0.52734 a.u., respectively. The results obtained with the Ψ_{C3-M} wave functions not only show better accuracies but also require only one diagonalization process, while the use of the GR basis requires many to minimize the β parameter. A similar conclusion can be reached by comparing our method with other variational procedures. For example, Harris and Smith [27] presented very accurate ground state wave functions using a reduced number (four) of configurations. Only 12 nonlinear parameters were used but, as stated by the authors, their optimization is a demanding numerical task. Because our method involves only linear parameters, more configurations are needed to reach similar level of accuracy. However, two advantages appear in our method: (i) the optimization of the parameters is direct and straightforward; and (ii) the same optimization also leads to a set of accurate excited states.

3. Results

Let us now illustrate the ACCI method presented above with negatively charged hydrogen-like ions ($Z = 1$), neutral helium-like ($Z = 2$) atoms, and positively charged lithium-like ions ($Z = 3$). As only the ground states are considered here, the principal quantum numbers n_1 and n_2 are both set equal to one when building the wave functions (9). Remains the choice of N_i, N_j, N_k, and n_3. To keep the approximated functions reasonably simple, and at the same time sufficiently accurate, we decided to perform all our calculations with n_3 up to 2.

To show the dependency on the total number M of linear parameters, we have considered several approximated wave functions Ψ_{C3-M}, with $M = 14$, 18, 20, and 30. They are all subcases of the following general formula:

$$\Psi_{C3-M} = Ne^{-Z(\mu_{13}r_{13}+\mu_{23}r_{23})}\{\chi_{C3}(1,\mu_{12},r_{12})[c_{000}^{111} + c_{200}^{111}r_{13}^{\ 2} + c_{020}^{111}r_{23}^{\ 2} + c_{220}^{111}r_{13}^{\ 2}r_{23}^{\ 2} + c_{300}^{111}r_{13}^{\ 3} + c_{030}^{111}r_{23}^{\ 3} + c_{002}^{111}r_{12}^{\ 2} + c_{320}^{111}r_{13}^{\ 3}r_{23}^{\ 2} + c_{230}^{111}r_{13}^{\ 2}r_{23}^{\ 3} + c_{202}^{111}r_{13}^{\ 2}r_{12}^{\ 2} + c_{022}^{111}r_{23}^{\ 2}r_{12}^{\ 2} + c_{302}^{111}r_{13}^{\ 3}r_{12}^{\ 2} + c_{032}^{111}r_{23}^{\ 3}r_{12}^{\ 2} + c_{402}^{111}r_{13}^{\ 4}r_{12}^{\ 2} + c_{042}^{111}r_{23}^{\ 4}r_{12}^{\ 2} + c_{222}^{111}r_{13}^{\ 2}r_{23}^{\ 2}r_{12}^{\ 2}] + \chi_{C3}(2,\mu_{12},r_{12})[c_{000}^{112} + c_{200}^{112}r_{13}^{\ 2} + c_{020}^{112}r_{23}^{\ 2} + c_{220}^{112}r_{113}^{\ 2}r_{23}^{\ 2} + c_{300}^{112}r_{13}^{\ 3} + c_{030}^{112}r_{23}^{\ 3} + c_{002}^{112}r_{12}^{\ 2} + c_{320}^{112}r_{13}^{\ 3}r_{23}^{\ 2} + c_{230}^{112}r_{13}^{\ 2}r_{23}^{\ 3} + c_{202}^{112}r_{13}^{\ 2}r_{12}^{\ 2} + c_{022}^{112}r_{23}^{\ 2}r_{12}^{\ 2} + c_{302}^{112}r_{13}^{\ 3}r_{12}^{\ 2} + c_{032}^{112}r_{23}^{\ 3}r_{12}^{\ 2} + c_{402}^{112}r_{13}^{\ 4}r_{12}^{\ 2} + c_{042}^{112}r_{13}^{\ 4}r_{12}^{\ 2} + c_{222}^{112}r_{13}^{\ 2}r_{23}^{\ 2}r_{12}^{\ 2}]\}, \quad (14)$$

where χ_{C3} (1, μ_{12}, r_{12}) = 1 + $r_{12}/2$ and χ_{C3} (2, μ_{12}, r_{12}) = 1 + $r_{12}/2$ + $r_{12}^{\ 2}$ /24. It should be noted that when the two light particles are identical, the coefficients must satisfy the following symmetry relation $c_{ijk}^{n_1n_2n_3} = c_{jik}^{n_1n_2n_3}$, so that the number of coefficients is reduced.

The mean energy is a very important quality test of any trial wave function. However, the expectation values of other physical quantities allow one to test the wave function with a particular emphasis on a given portion of the configuration space. The mean values of several radial quantities, strongly dependent on the shape of the wave functions, are involved in various calculations of physical quantities such as dipole polarizabilities or magnetic susceptibilities.

For all systems considered, we shall provide, in tabular form, the linear coefficients $c_{ijk}^{n_1n_2n_3}$ and the normalization constant N of a few selected ψ_{C3-M} with a moderate M. We shall then give the calculated mean value of the ground state energy and $< r_{ij}^{\ p} >$ with ($p = -1, 1, 2$) ($i, j = 1, 2, 3$). When the two light particles are identical, we shall give only $< r_{i3}^{\ p} >$ with either $i = 1$ or 2.

To allow for a direct numerical comparison with the reference energy values given by Frolov [5, 6], we have taken the same masses values, which were taken from Ref [44]. For hydrogen-like ions, they read: the proton mass m_p = 1836.152701 m_e, the deuteron mass m_d = 3670.483014 m_e, the tritium nuclear mass m_t = 5496.92158 m_e, and the muonic mass m_μ = 206.768262 m_e. As the He^{2+} nucleus is concerned, we have taken m_3 = 7294.2996 m_e for $^4He^{2+}$ and m_3 = 5495.8852 m_e for $^3He^{2+}$. For the Li^{3+} nucleus, we have taken the same values as Frolov [45], m_3 = 10961.8968 m_e for $^6Li^{+3}$ and m_3 = 12786.3927 m_e for $^7Li^{+3}$.

3.1. THE NEGATIVE IONS $^\infty H^-$, $^1H^-$, D^-, T^-, AND MU^-

Let us start with the negatively charged hydrogen-like three-body systems made of two electrons and a third heavier particle with charge $Z = 1$: the ions $^\infty H^-$, $^1H^-$, D^-, T^-, and the muonium ion $Mu^-(e^-\ e^-\mu^+)$. All these systems are similar to each other in the main property of their spectra, that is, they have only one bound (ground), singlet state with $L = 0$. They differ only by the nuclear mass. For these systems, we shall consider two functions, ψ_{C3-14} and ψ_{C3-18} with, respectively, $M = 14$ and 18 linear coefficients.

For these ions, we present, in Table I, the normalization constant and the linear coefficients corresponding to the functions ψ_{C3-18}. In Table II, the ground state energies and the mean of radial quantities obtained with ψ_{C3-14} and, ψ_{C3-18} are compared with the numerically "exact" values of Ref [5]. The mean energy obtained with ψ_{C3-18} for Mu^- has a relative accuracy of 7.8×10^{-4}; similar accuracies are obtained for all the other systems considered in the table. This is a quite good result in view of the relatively small number of terms used.

Wave functions for these ions have been proposed by Flores-Rivero and Rivas-Silva [46]. They compared their Eckart-Gaussian wave functions with 4- and 10-term Hylleraas functions, denoted ψ_{S4} and ψ_{S10}. The ψ_{S10} trial wave function gives a mean energy of -0.526701 a.u. for D^- and -0.526751 a.u. for T^-. It should be mentioned that, contrary to ours, these trial wave functions do not satisfy Kato cusp conditions. Moreover, the authors do not give the values of the nonlinear parameters of the wave functions. In fact, to the best of our knowledge, there are no reports in the literature presenting the complete wave functions (including the values of the parameters) for all these systems. For the helium atom and its isoelectronic series with infinite mass, on the other hand, details of the wave functions are often provided. For example, in case of the $^\infty H^-$ ion, Harris and Smith [27] have recently proposed a wave function yielding an energy of -0.5277131 a.u. and provide the twelve nonlinear parameters involved.

As we already mentioned, systematic improvement of our approximated wave functions, without breaking the cusp conditions, can be achieved by including (i) more configurations, through an increase of n_3 values, or (ii) more terms in the polynomial Ω. A greater number of linear coefficients is then needed, and tables of reasonable size difficult

TABLE I

The linear coefficients $c_{ijk}^{n_1n_2n_3}$ (rounded off to the seventh digit) and of the normalization constants N of the Ψ_{C3-18} approximated wave functions for the ground state of several negatively charged hydrogen-like three-body systems.

	Mu^-	$^1H^-$	D^-	T^-	$^\infty H^-$
N	0.0320917	0.0321394	0.0321421	0.0321429	0.0321448
c_{000}^{111}	0.8547058	−0.8532817	0.8531894	0.8531581	0.8530970
c_{200}^{111}	0.2217853	−0.2239379	0.2240780	0.2241255	0.2242180
c_{220}^{111}	−0.0174139	0.0178301	−0.0178571	−0.0178661	−0.0178842
c_{300}^{111}	−0.0818877	0.0826078	−0.0826544	−0.0826700	−0.0827008
c_{320}^{111}	0.0007082	−0.0007308	0.0007323	0.0007328	0.0007338
c_{002}^{111}	−0.0009480	0.0009515	−0.0009527	−0.0009531	−0.0009538
c_{202}^{111}	−0.0039553	0.0039946	−0.0039971	−0.0039979	−0.0039996
c_{302}^{111}	−0.0015092	0.0015263	−0.0015274	−0.0015277	−0.0015285
c_{402}^{111}	0.0001816	−0.0001847	0.0001849	0.0001850	0.0001852
c_{000}^{112}	−0.2826039	0.2799913	−0.2798171	−0.2797582	−0.2796431
c_{200}^{112}	−0.1754047	0.1774231	−0.1775543	−0.1775988	−0.1776856
c_{220}^{112}	0.0121321	−0.0124499	0.0124706	0.0124775	0.0124913
c_{300}^{112}	0.0887226	−0.0895564	0.0896104	0.0896285	0.0896642
c_{320}^{112}	−0.0005037	0.0005222	−0.0005234	−0.0005238	−0.0005246
c_{002}^{112}	0.0003381	−0.0004983	0.0005094	0.0005131	0.0005205
c_{202}^{112}	0.0053839	−0.0054488	0.0054529	0.0054543	0.0054571
c_{302}^{112}	−0.0003756	0.0003837	−0.0003842	−0.0003844	−0.0003847
c_{402}^{112}	−0.0000288	0.0000292	−0.0000292	−0.0000292	−0.0000292

to present. For the $^\infty H^-$ ion, for example, the mean energy value obtained with ψ_{C3-14} and n_3 up to 2 is −0.526438 a.u.; if n_3 is taken up to 3 (which implies $M = 27$) the energy improves to −0.526666 a.u. On the other hand, when increasing the number of terms in Ω, for example going from 14 to 18 linear coefficients, an important improvement of the energies is noticed in Table II.

3.2. NEUTRAL HELIUM-LIKE SYSTEMS

Let us now consider the following neutral helium-like systems $e^-e^{-\infty}He^{+2}$, $e^-e^{-4}He^{+2}$, $e^-e^{-3}He^{+2}$, $e^-\mu^{-\infty}He^{+2}$, $e^-\mu^{-4}He^{+2}$, and $e^-\mu^{-3}He^{+2}$.

For the $e^-e^{-\infty}He^{+2}$, $e^-e^{-4}He^{+2}$, $e^-e^{-3}He^{+2}$ three-body systems, the results obtained with the ψ_{C3-14} and ψ_{C3-18} wave functions are practically the same. We therefore give, in Table III, the details only for the simplest function. The mean values of the energy and radial quantities, are listed in Table IV. Except for the energy and for the $e^-e^{-\infty}He^{+2}$ case, we could not find in the literature other mean values to compare with. When compared to "exact" reference value, the mean energy obtained with ψ_{C3-14} for $e^-e^{-\infty}He^{+2}$ has a relative accuracy of 1.2×10^{-4}; similar accuracies are obtained when finite nuclear masses are considered.

For the nonsymmetric helium-like systems $e^-\mu^{-\infty}He^{+2}$, $e^-\mu^{-4}He^{+2}$, and $e^-\mu^{-3}He^{+2}$ we have used a ψ_{C3-20} wave function, the details of which are given in Table V. To check the convergence with M, the corresponding mean values, given in Table VI, are also compared to the results of a ψ_{C3-30} wave function.

When compared to "exact" reference value, the mean energy obtained with ψ_{C3-20} for $e^-\mu^{-\infty}He^{+2}$ has a relative accuracy of 4.3×10^{-8}, and similar accuracies are obtained when finite nuclear masses are taken. Note that, in contrast to the previous three-body systems, the means involving r_{13} and r_{23} are not equal because particles 1 and 2 are now different.

Here, we should underline that the ground state energies, which are essentially proportional to $m_2 = m_\mu$, are of about four hundred atomic units. The apparently excellent agreement between the energy values should thus be taken with care, as one should look at the relative agreement.

3.3. POSITIVELY CHARGED LITHIUM IONS-LIKE SYSTEMS

Let us now consider the following positively charged lithium-like systems $e^-e^{-\infty}Li^{+3}$, $e^-e^{-7}Li^{+3}$, $e^-e^{-6}Li^{+3}$, $e^-\mu^{-\infty}Li^{+3}$, $e^-\mu^{-7}Li^{+3}$, and $e^-\mu^{-6}Li^{+3}$.

TABLE II

The mean energy and the mean of several radial quantities for the ground state of several negatively charged hydrogen-like three-body systems, obtained using the Ψ_{C3-14} and Ψ_{C3-18} approximated wave functions, are compared with the numerically "exact" values of Ref. [5].

		Mu^-	$^1H^-$	D^-	T^-	$^\infty H^-$
$\langle -E \rangle$	Ψ_{C3-14}	0.52373	0.52613	0.52628	0.52633	0.52644
	Ψ_{C3-18}	0.52464	0.52703	0.52719	0.52724	0.52734
	Exact	0.52505	0.52744	0.52760	0.52765	0.52775
$\langle r_{i3} \rangle$	Ψ_{C3-14}	2.56767	2.5552	2.55441	2.55415	2.55362
	Ψ_{C3-18}	2.67316	2.65922	2.65833	2.65804	2.65744
	Exact	2.72718	2.71209	2.71114	2.71082	2.71018
$\langle r_{i3}^2 \rangle$	Ψ_{C3-14}	9.88098	9.7846	9.77849	9.77646	9.77238
	Ψ_{C3-18}	11.1969	11.0769	11.0693	11.0668	11.0617
	Exact	12.0742	11.9317	11.9227	11.9197	11.9137
$\left\langle \frac{1}{r_{i3}} \right\rangle$	Ψ_{C3-14}	0.68758	0.69073	0.69093	0.69099	0.69113
	Ψ_{C3-18}	0.68110	0.68428	0.68448	0.68455	0.68468
	Exact	0.67965	0.68285	0.68306	0.68312	0.68326
$\langle r_{12} \rangle$	Ψ_{C3-14}	4.13923	4.12060	4.11942	4.11903	4.11824
	Ψ_{C3-18}	4.33763	4.31619	4.31483	4.31437	4.31346
	Exact	4.43928	4.41569	4.41419	4.41369	4.41269
$\langle r_{12}^2 \rangle$	Ψ_{C3-14}	21.2139	21.0264	21.0145	21.0105	21.0026
	Ψ_{C3-18}	23.8103	23.5761	23.5613	23.5564	23.5464
	Exact	25.5145	25.2372	25.2196	25.2138	25.2020
$\left\langle \frac{1}{r_{12}} \right\rangle$	Ψ_{C3-14}	0.32140	0.32292	0.32302	0.32305	0.32312
	Ψ_{C3-18}	0.31259	0.31417	0.31427	0.31430	0.31437
	Exact	0.30920	0.31081	0.31092	0.31095	0.31102

TABLE III

The linear coefficients $c_{ijk}^{n_1 n_2 n_3}$ (rounded off to the seventh digit) and of the nor- malization constants N of the Ψ_{C3-14} approximated wave functions for the ground state of several neutral helium-like atoms.

	$e^-e^{-\infty}He^{+2}$	$e^-e^{-4}He^{+2}$	$e^-e^{-3}He^{+2}$
N	0.448367	0.448354	0.448349
c_{000}^{111}	0.7019935	0.7020639	−0.7020870
c_{200}^{111}	0.1521548	0.1520548	−0.1520221
c_{220}^{111}	−0.1718711	−0.1717718	0.1717393
c_{300}^{111}	0.0017437	0.0017295	−0.0017249
c_{002}^{111}	0.0203784	0.0203525	−0.0203440
c_{202}^{111}	0.0006772	0.0006741	−0.0006731
c_{222}^{111}	−0.0043226	−0.0043191	0.0043179
c_{000}^{112}	−0.6054576	−0.6055292	0.6055526
c_{200}^{112}	−0.1361976	−0.1360928	0.1360585
c_{220}^{112}	0.1647337	0.1646368	−0.1646051
c_{300}^{112}	0.0007997	0.0008118	−0.0008157
c_{002}^{112}	−0.0100536	−0.0100339	0.0100275
c_{202}^{112}	0.0002263	0.0002271	−0.0002274
c_{222}^{112}	0.0020219	0.0020201	−0.0020195

TABLE IV

The mean energy and the mean of several radial quantities for the ground state of several helium-like three body systems $e^-e^{-\infty}He^{+2}$, $e^-e^{-4}He^{+2}$, and $e^-e^{-3}He^{+2}$, obtained using the ψ_{C3-14} wave function, are compared with the numerically "exact"values of Ref. [9].

		$e^-e^{-\infty}He^{+2}$	$e^-e^{-4}He^{+2}$	$e^-e^{-3}He^{+2}$
$\langle -E \rangle$	Ψ_{C3-14}	2.90337	2.90295	2.90282
	Exact	2.90372	2.90330	2.90317
$\langle r_{i3} \rangle$	Ψ_{C3-14}	0.92947	0.92961	0.92965
	Exact	0.92947		
$\langle r_{i3}^2 \rangle$	Ψ_{C3-14}	1.19281	1.19316	1.19327
	Exact	1.19348		
$\left\langle \frac{1}{r_{i3}} \right\rangle$	Ψ_{C3-14}	1.68730	1.68706	1.68698
	Exact	1.68832		
$\langle r_{12} \rangle$	Ψ_{C3-14}	1.42163	1.42181	1.42187
	Exact	1.42207		
$\langle r_{12}^2 \rangle$	Ψ_{C3-14}	2.51472	2.51534	2.51555
	Exact	2.51644		
$\left\langle \frac{1}{r_{12}} \right\rangle$	Ψ_{C3-14}	0.94632	0.94620	0.94616
	Exact	0.94582		

TABLE V

The linear coefficients $c_{ijk}^{n_1n_2n_3}$ (rounded off to the seventh digit) and of the nor-malization constants N of the $\Psi_{C3\text{-}20}$ approximated wave functions for the ground state of several neutral helium-like atoms.

	$e^-\mu^{-\infty}He^{+2}$	$e^-\mu^{-4}He^{+2}$	$e^-\mu^{-3}He^{+2}$
N	0.684302	0.60359	0.560566
c_{000}^{111}	−0.2856291	0.2873294	−0.2842373
c_{200}^{111}	0.5880162	−0.5890340	0.5906894
c_{020}^{111}	−0.0049916	0.0032295	−0.0047919
c_{220}^{111}	−0.0064209	0.0039822	−0.0037438
c_{300}^{111}	0.10544208	−0.1255693	0.1371306
c_{030}^{111}	−0.0000493	0.0000381	−0.0000868
c_{002}^{111}	−0.1740855	0.1422221	−0.1226149
c_{202}^{111}	0.0117025	−0.0152402	0.0174262
c_{022}^{111}	−0.0048893	0.0101970	−0.0056564
c_{222}^{111}	0.0025263	−0.0044554	0.0040943
c_{000}^{112}	0.2445510	−0.2407512	0.2340879
c_{200}^{112}	−0.6602520	0.6692177	−0.6754980
c_{020}^{112}	−0.0032731	0.0048711	−0.0049847
c_{220}^{112}	−0.0031702	0.0014265	−0.0037292
c_{300}^{112}	−0.0428220	0.0611165	−0.0716672
c_{030}^{112}	−0.0000397	0.0000337	−0.0000927
c_{002}^{112}	0.1827232	−0.1565263	0.1405741
c_{202}^{112}	−0.0026106	0.0029171	−0.0031578
c_{022}^{112}	−0.0027534	0.0038721	−0.0046499
c_{222}^{112}	−0.0010845	0.0022691	−0.0020406

For the $e^-e^{-\infty}Li^{+3}$, $e^-e^{-7}Li^{+3}$, $e^-e^{-6}Li^{+3}$ three-body systems, the results obtained with the $\psi_{C3\text{–}14}$ and $\psi_{C3\text{–}18}$ wave functions are practically the same. We therefore give, in Table VII, only the values for the simplest function. The mean values of the energy and radial quantities, are given in Table VIII.

When compared to "exact" reference values, the mean energies obtained with $\psi_{C3\text{–}14}$, have approximately a relative accuracy of 5.9×10^{-5} for all the systems considered.

Finally, for the nonsymmetric lithium-like systems $e^-\mu^{-\infty}Li^{+3}$, $e^-\mu^{-7}Li^{+3}$, and $e^-\mu^{-6}Li^{+3}$, we have used a $\psi_{C3\text{–}20}$ wave function, whose details are given in Table IX, and the corresponding mean values in Table X.

When compared to the "exact" reference value, the mean energy obtained with $\psi_{C3\text{–}20}$ for $e^-\mu^{-6}Li^{+3}$ has a relative accuracy of 9.8×10^{-8}, and similar accuracies are obtained for finite nuclear masses are considered. Note that, for these systems, to allow for a direct numerical comparison with the reference energy values given by Frolov [45], we have taken the muon mass as 206.7682838 m_e.

For all systems, more accurate wave functions can be easily constructed by increasing the number of terms in $\Omega_{n_1,n_2,n_3}^{(N_i,N_j,N_k)}(r_{13},r_{23},r_{12})$ and/or including other configurations $(n_1n_2n_3)$ as done in Ref [35]. However, as mentioned in the Introduction, the aim was to provide the details of the wave functions and have therefore kept the number of coefficients reasonably moderate.

Other systems with larger values of Z can be equally considered. The relatively less important role played by the electron–electron correlation gives then even better energy agreement with "exact" values (not shown).

3.4. MINIMUM VALUE OF THE CHARGE REQUIRED TO BIND TWO ELECTRONS

To study the stability of these three-body systems $[m_1m_2m_3]$, one should compare its energy $E[m_1m_2m_3]$ with that of the ground state of the separate two-body sub-systems $E[m_im_j]$ where $i \neq j$. If m_1 denotes the lightest particle, the stability condition reads

$$E[m_1m_2m_3] < -\frac{1}{2}(z_2z_3)^2\mu_{23} = E[m_2m_3]. \quad (15)$$

We have already mentioned that all the considered systems in section 3.1, with $Z = 1$ have only one bound state, the ground state. It is also well known that when the value of Z is decreased, there appears a minimum value, the critical charge ($Z_{th} < 1$), below which the double bound state does not exist, as it becomes a continuum state [47]. In the case of two electrons, the critical charge is the minimum nuclear charge value which allows to bind two electrons. This threshold value is obtained as the zero of the following function [48]:

$$f(Z) \equiv E(Z) + \frac{\mu_{23}}{2}Z^2$$

which results from the stability condition (15).

The calculated values of the threshold charge, Z_{th}, and the corresponding threshold energy E_{th}, obtained with a $\psi_{C3\text{–}18}$ wave function are listed in Table XI for the negatively charged, infinitely heavy, hydrogen ion $e^-e^{-\infty^{Z_3}}$ and its muonic counterpart $e^-e^-\mu^{Z_3}$. The obtained threshold values Z_{th} lie between the lower $Z^{(-)}$ and upper $Z^{(+)}$ bounds found in [49], and are closer to the upper bounds. Note that, for the hydrogenic ion our Z_{th} value is

TABLE VI

The mean energy and the mean of several radial quantities for the ground state of several neutral helium-like systems $e^-\mu^{-\infty}He^{+2}$, $e^-\mu^{-4}He^{+2}$ and $e^-\mu^{-3}He^{+2}$, obtained using the Ψ_{C3-20} and a Ψ_{C3-30} wave function are compared with the numerically "exact" values of Ref. [6].

		$e^-\mu^{-\infty}He^{+2}$	$e^-\mu^{-4}He^{+2}$	$e^-\mu^{-3}He^{+2}$
$\langle -E \rangle$	Ψ_{C3-20}	414.0365192	402.6372416	399.0423138
	Ψ_{C3-30}	414.0365223	402.6372484	399.0423193
	Exact	414.0365369	402.6372630	399.0423368
$\langle r_{13} \rangle$	Ψ_{C3-20}	1.50053	1.49970	1.49945
	Ψ_{C3-30}	1.49996	1.50016	1.50024
	Exact	1.49996	1.50016	1.50022
$\langle r_{13}^2 \rangle$	Ψ_{C3-20}	2.99713	2.99500	2.99443
	Ψ_{C3-30}	2.99955	3.00032	3.00070
	Exact	2.99986	3.00065	3.00090
$\left\langle \frac{1}{r_{13}} \right\rangle$	Ψ_{C3-20}	1.00028	1.00002	0.999919
	Ψ_{C3-30}	1.00003	0.99990	0.999835
	Exact	1.00004	0.99990	0.99986
$\langle r_{23} \rangle$	Ψ_{C3-20}	0.00377	0.00376	0.00376
	Ψ_{C3-30}	0.00363	0.00373	0.00376
	Exact	0.00363	0.00373	0.00376
$\langle r_{23}^2 \rangle$	Ψ_{C3-20}	0.000018898	0.00001890	0.00001889
	Ψ_{C3-30}	0.000017542	0.00001855	0.00001889
	Exact	0.000017543	0.00001855	0.00001889
$\left\langle \frac{1}{r_{23}} \right\rangle$	Ψ_{C3-20}	398.760	398.596	398.542
	Ψ_{C3-30}	413.537	402.137	398.542
	Exact	413.536	402.137	398.532
$\langle r_{12} \rangle$	Ψ_{C3-20}	1.50054	1.49971	1.49945
	Ψ_{C3-30}	1.49996	1.50017	1.50025
	Exact	1.49997	1.50017	1.50023
$\langle r_{12}^2 \rangle$	Ψ_{C3-20}	2.99715	2.99502	2.99444
	Ψ_{C3-30}	2.99955	3.00033	3.00072
	Exact	2.99987	3.00067	3.00009
$\left\langle \frac{1}{r_{12}} \right\rangle$	Ψ_{C3-20}	1.00026	0.99999	0.99989
	Ψ_{C3-30}	1.00003	0.99988	0.99982
	Exact	1.00002	0.99989	0.99985

only 0.5% off the value $Z_{th} = 0.911029$ found in [50] with a 30 basis exponential functions but with 90 nonlinear parameters. In contrast, our result is obtained with a wave function containing only 18 linear coefficients.

It is interesting to investigate also the three-body systems, $e^-\mu^{-\infty^{z_3}}$, and to find the minimal charge z_3 to bind an electron and a muon. In this case, the critical (or threshold) charge Z_{th} corresponding to a stable system is $Z_{th} \simeq 1.11$ (see Table XI). According to our calculations, an infinitely heavy nucleus (and similarly for finite masses such as those of a proton, a deuteron or a tritium) can not bind a muon and an electron; these three-body systems can not be found forming a stable bound state in nature. This is an example of an unstable ion with a unit nuclear charge. This explains why we were able to present results for helium- ($Z = 2$) and lithium-like ($Z = 3$) systems with a muon replacing an electron, but not for hydrogen-like ($Z = 1$).

4. Summary and Concluding Remarks

In this article, we have generalized the *C*3-like basis set [35] to three-body atomic systems with general masses, and have used the basis functions to extend the angular correlated configuration-interaction method presented in [32, 33]. The *C*3-like basis functions are defined as being exact solution

TABLE VII

The linear coefficients $c_{ijk}^{n_1n_2n_3}$ (rounded off to the seventh digit) and of the normalization constants *N* of the Ψ_{C3-14} approximated wave functions for the ground state of several positively charged lithium-like ions.

	$e^-e^{-\infty}Li^{+3}$	$e^-e^{-7}Li^{+3}$	$e^-e^{-6}Li^{+3}$
N	1.4842	1.48403	1.48400
c_{000}^{111}	0.5226780	−0.5228122	−0.5228345
c_{200}^{111}	0.1780267	−0.1779453	−0.1779318
c_{220}^{111}	−0.4327624	0.4326755	0.4326611
c_{300}^{111}	0.0079818	−0.0079668	−0.0079643
c_{002}^{111}	0.0344479	−0.0344364	−0.0344345
c_{202}^{111}	0.0023769	−0.0023721	−0.0023714
c_{222}^{111}	−0.0182345	0.0182282	0.0182272
c_{000}^{112}	−0.4863479	0.4864784	0.4865001
c_{200}^{112}	−0.1690866	0.1690009	0.1689867
c_{220}^{112}	0.4242703	−0.4241833	−0.4241689
c_{300}^{112}	−0.0065276	0.0065139	0.0065117
c_{002}^{112}	−0.0240043	0.0239935	0.0239917
c_{202}^{112}	−0.0000742	0.0000719	0.0000715
c_{222}^{112}	0.0104493	−0.0104453	−0.0104446

of a general three-body Coulomb problem where the nondiagonal terms of the kinetic energy are neglected; hence, the functions naturally satisfy the cusp conditions at the two-body singularities. They are defined as a product of two-body Coulomb wave functions multiplied by a Coulomb distortion factor, being in that way the counterpart of the *C*3 approach used for scattering problems. This distortion factor, which depends on the inter-electronic coordinates, already includes angular correlation in the configuration basis functions [34, 35]. A configuration interaction scheme can then be constructed with these correlated basis elements as done in Ref [35]. However, the convergence rate of the energy and wave functions obtained can be considerably increased by multiplying the basis functions by an additional correlation factor Ω which adds radial and angular correlation to each configuration. Two advantages of the *C*3-like basis set should be mentioned: all the parameters included in the wave functions are linear, thus a single diagonalization gives both energies and eigenvectors. Second, the basis set diagonalizes all the Coulomb interactions and part of the kinetic energy, leading to analytic closed form expressions for the nondiagonalized terms.

TABLE VIII

The mean energy and the mean of several radial quantities for the ground state of several lithium-like three body systems $e^-e^{-\infty}Li^{+3}$, $e^-e^{-7}Li^{+3}$, and $e^-e^{-6}Li^{+3}$, obtained using the Ψ_{C3-14} wave function, are compared with the numerically "exact"values of Ref. [9].

		$e^-e^{-\infty}Li^{+3}$	$e^-e^{-7}Li^{+3}$	$e^-e^{-6}Li^{+3}$
$\langle -E\rangle$	Ψ_{C3-14}	7.27948	7.27889	7.27879
	Exact	7.27991	7.27989	7.27989
$\langle r_{13}\rangle$	Ψ_{C3-14}	0.57285	0.57290	0.57291
	Exact	0.57277		
$\langle r_{13}^2\rangle$	Ψ_{C3-14}	0.44637	0.44644	0.44645
	Exact	0.44628		
$\left\langle \frac{1}{r_{13}} \right\rangle$	Ψ_{C3-14}	2.68651	2.68629	2.68626
	Exact	2.68792		
$\langle r_{12}\rangle$	Ψ_{C3-14}	0.86224	0.86230	0.86231
	Exact	0.86231		
$\langle r_{12}^2\rangle$	Ψ_{C3-14}	0.92709	0.92721	0.92723
	Exact	0.927065		
$\left\langle \frac{1}{r_{12}} \right\rangle$	Ψ_{C3-14}	1.56829	1.56818	1.56816
	Exact	1.56772		

TABLE IX

The linear coefficients $c_{ijk}^{n_1n_2n_3}$ (rounded off to the seventh digit) and of the nor-malization constants *N* of the Ψ_{C3-20} approximated wave functions for the ground state of several positively charged lithium-like ions.

	$e^-\mu^{-\infty}Li^{+3}$	$e^-\mu^{-7}Li^{+3}$	$e^-\mu^{-6}Li^{+3}$
N	0.61255	0.637727	0.641883
c_{000}^{111}	0.3180814	0.3219735	0.3225994
c_{200}^{111}	−0.3445659	−0.3480885	−0.3486838
c_{020}^{111}	0.0003802	0.0006452	0.0006874
c_{220}^{111}	0.0006659	0.0006931	0.0006972
c_{300}^{111}	−0.4256829	−0.4235959	−0.4232422
c_{030}^{111}	0.0000025	0.0000041	0.0000044
c_{002}^{111}	−0.3263497	−0.3199306	−0.3188607
c_{202}^{111}	−0.0602641	−0.0598046	−0.0597278
c_{022}^{111}	0.0023915	0.0024939	0.0025094
c_{222}^{111}	−0.0006798	−0.0007175	−0.0007234
c_{000}^{112}	−0.2473109	−0.2539969	−0.2550630
c_{200}^{112}	0.4651296	0.4678794	0.4683486
c_{020}^{112}	0.0021780	0.0035065	0.0037179
c_{220}^{112}	0.0020573	0.0008832	0.0021482
c_{300}^{112}	0.3629819	0.3608580	0.3604966
c_{030}^{112}	0.0000063	0.0000101	0.0000107
c_{002}^{112}	0.2819142	0.2759202	0.2749235
c_{202}^{112}	0.0009703	0.0008832	0.0008695
c_{022}^{112}	0.0005285	0.0005499	0.0005531
c_{222}^{112}	−0.0003238	−0.0003343	−0.0003358

TABLE X

The mean energy and the mean of several radial quantities for the ground state of several lithium-like three body systems $e^-\mu^{-\infty}Li^{+3}$, $e^-\mu^{-7}Li^{+3}$ and $e^-\mu^{-6}Li^{+3}$, obtained using the Ψ_{C3-20} wave function, are compared with the numerically "exact"values of Ref. [45].

		$e^-\mu^{-\infty}Li^{+3}$	$e^-\mu^{-7}Li^{+3}$	$e^-\mu^{-6}Li^{+3}$
$\langle -E \rangle$	Ψ_{C3-20}	932.45724	917.65013	915.23126
	Exact	—	917.65022	915.23135
$\langle r_{13} \rangle$	Ψ_{C3-20}	0.750004	0.750064	0.750074
	Exact	—	0.750041	0.750050
$\langle r_{13}^2 \rangle$	Ψ_{C3-20}	0.749979	0.750098	0.750118
	Exact	—	0.750085	0.750104
$\left\langle \frac{1}{r_{13}} \right\rangle$	Ψ_{C3-20}	2.00012	1.99996	1.99993
	Exact	—	1.99991	1.99989
$\langle r_{23} \rangle$	Ψ_{C3-20}	0.00241817	0.00245727	0.00246378
	Exact	—	0.00245727	0.00246377
$\langle r_{23}^2 \rangle$	Ψ_{C3-20}	0.0000078	0.0000080	0.0000081
	Exact	—	0.0000080	0.0000081
$\left\langle \frac{1}{r_{23}} \right\rangle$	Ψ_{C3-20}	620.305	610.434	608.821
	Exact	—	610.433	608.8209
$\langle r_{12} \rangle$	Ψ_{C3-20}	0.75001	0.75007	0.75008
	Exact	—	0.75005	0.75006
$\langle r_{12}^2 \rangle$	Ψ_{C3-20}	0.74999	0.75011	0.75012
	Exact	—	0.75009	0.75011
$\left\langle \frac{1}{r_{12}} \right\rangle$	Ψ_{C3-20}	2.00006	1.99989	1.99987
	Exact	—	1.99986	1.99984

The efficiency of the method has been illustrated by considering the ground state of hydrogen-, helium-, and lithium-like three-body systems, in which the nuclear mass can be finite and the two light particles can be equal (two electrons) or different (one electron and one muon). Ground state energies and other mean values for different relevant physical magnitudes were compared to reference values, when available; good agreement is found for all cases. Accurate wave functions, satisfying the two-body Kato cusp conditions, and with a moderate number (maximum 20) of linear coefficients were used, and coefficients and normalization constant tabulated. This has been done with the purpose to provide, for example, to the collisional community, wave functions as accurate as the traditional Hylleraas wave function available in the literature for two-electron systems with infinite nuclear mass. To the best of our knowledge, for all other three-body systems investigated here, no functions (as accurate and simple as those presented here), have been explicitly given in the literature.

TABLE XI

Critical charge Z_{th} to bind two electrons, or an electron and a muon. The energy values E_{th} corresponding to the threshold charge $Z = Z_{th}$, as well as the lower and upper bounds $Z^{(-)}$ and $Z^{(+)}$ found in Ref. [49], are also included.

	$e^-e^-\infty^{z3}$	$e^-e^-\mu^{z3}$	$e^-\mu^-\infty^{z3}$
Z_{th}	0.916	0.916	1.11
E_{th}	−0.41971	−0.41757	−127.38069
$Z_{th}^{(-)}$	0.8909[a]	0.8913[a]	—
$Z_{th}^{(+)}$	0.9171[a]	0.9174[a]	—

[a] Rebane [49].

A study of the stability of some of these three-body systems was also performed, by providing the critical charge to bind two electrons, or an electron and a muon.

The method presented here can be easily extended to excited states. An orthogonal set of S ground and excited states was presented in [36]. The extension to $L > 0$ states is part of these inves-

tigations. It is also possible to extend the methodology to molecular systems; however, in this case, molecular-like basis set have to be used to replace the basis functions $\phi_{n1,n2,n3}(r_{13}, r_{23}, r_{12})$. This is also being studied by some of the authors.

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