
Correlated $n^{1,3}S$ States for Coulomb Three-Body Systems

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ABSTRACT: $n^{1,3}S$ ($n = 1 - 4$) states for atomic three-body systems are studied with the Angular Correlated Configuration Interaction method. A recently proposed angularly correlated basis set is used to construct, simultaneously and with a single diagonalization, ground and excited states wave functions which: (i) satisfy exactly Kato cusp conditions at the two-body coalescence points; (ii) involve only linear parameters; (iii) show a fast convergency rate for the energy; and (iv) form an orthogonal set. The efficiency of the method is illustrated by the study a variety of three-body atomic systems [$m_1^- m_2^- m_3^{z3+}$] with two negatively charged light particles, with diverse masses m_1^- and m_2^- , and a heavy positively charged nucleus m_3^{z3+} . The calculated ground 1^1S and excited $n^{1,3}S$ ($n = 2 - 4$) state energies are compared with those given in the literature, when available.

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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 two-electron systems, the ground state—and to a lesser extent excited states—have been extensively

studied. For exotic three-body systems, involving for example muons and antihydrogen nuclei, the literature is on the other hand less abundant. Excited states, in particular, have not or very little investigated. The main aim of this article is to study some of these atomic systems, providing relatively simple but accurate wave functions for ground and excited $n^{1,3}S$ ($n = 2 - 4$) states.

Exotic three-body systems, involving electrons, muons, and antihydrogen nuclei, are of interest in many branches of physics, including atomic spectroscopy and quantum electrodynamics (see, e.g., the discussion and the references given in the Introduction of Refs. [1, 2]). Negatively charged hydrogen

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ions, and their isotopes, have also astrophysical applications: their photoionization is the primary source of the continuum opacity in stellar photospheres and their relative abundance is of great interest for predicting the thermonuclear efficiency of our Sun [2]. Moreover exotic systems serve to test the general theory of three-body systems and to study interparticle correlations, going further than two-electron atoms with infinite nuclear mass. Some of the muonic and antihydrogen nuclei three-body systems (atoms or ions) considered in this article have been studied in details only recently (see references below), the focus being set mainly on the ground state.

For two-electron atoms, and in particular for helium, many trial wave functions have been proposed and optimized to obtain the best ground state energy. They are not all 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 and involving both linear and nonlinear parameters, lead to extremely accurate energies (see, e.g., Refs. [1–16] and references therein). A second, analytical, group includes rather simple wave functions possessing some of the correct functional (local) properties (see, e.g., Refs. [17–23]). 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., [24–31]). 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 differential cross sections for processes such as double ionization by electron or photon impact involve multi-dimensional numerical integrations; moreover, for calculations within the second Born approximation, a complete orthogonal set of wave functions is necessary. The use of bound wave functions with a very large number of terms (first group) can be prohibitive, even with modern computer facilities [32]. 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 [24] or simpler versions [25], amongst the collision community.

The formal structure of trial wave functions for three-body systems is also an important issue. There is abundant literature, in particular for two-electron atoms, on the relation between the convergence rate and the choice of basis functions (see, e.g., Ref. [16]). The latter may or may not present the correct behavior in asymptotic regions [19, 33], close to the points where the interaction potential present singularities (two-body coalescence [34, 35]), or close to the three-body coalescence (Fock's expansion, see e.g., Ref. [36]). As the two-body coalescence regions are concerned, the quality of any function is tested through the evaluation of the expectation values of the so-called two-particle operators. An adequate description is crucial for example for annihilation calculations (see, e.g., Ref. [37]), for the evaluation of hyperfine splitting (see, e.g., Refs. [8, 9, 14]), and may even play an essential role in collisional problems such as photoionization (see, e.g., Ref. [38]). Advanced trial wave functions (first group) usually satisfy quite accurately but not exactly the so-called Kato cusp conditions [34, 35] [see Eq. (12) below]. An alternative approach is to build the trial wave functions with intrinsically the correct behavior (second, and some of the third, group), for example by choosing appropriate basis functions. This is one of the issues addressed in this report.

Motivated by collisional studies involving two-electron atoms, Gasaneo and Ancarani [30, 31] introduced a C3-like basis set which fully diagonalizes the whole diagonal part of the kinetic energy and all the Coulomb interactions (see Section 2 below). The use of such a correlated basis in a Configuration Interaction approach is based on a decomposition of the three-body wave function in a sum of doubly correlated configurations [31]; each configuration depends explicitly on the three interelectronic coordinates. The efficiency of the method, called Angular Correlated Configuration Interaction (ACCI), has been illustrated with applications to the helium isoelectronic sequence in the infinite mass approximation [31]. The method presents important advantages: (i) only linear parameters are involved; (ii) a single diagonalization provides the energies and the wave functions of the ground and a number of excited states, which form an orthogonal set; (iii) the results can be systematically improved by adding more configurations; and (iv) by construction, all constructed wave functions satisfy exactly Kato cusp conditions [34, 35]. However, the resulting trial wave functions do not possess all the necessary correct ingredients, like the correct behavior in asymptotic regions or close to the three-body

coalescence. Moreover, the fact that no nonlinear parameters are involved, reduces the variational flexibility, which allows to obtain extremely accurate energies.

The present contribution has two main objectives: (i) the extension of the ACCI method with the C3-like basis functions, to general three-body atomic systems with two negatively singly-charged light particles and a heavy positively charged nucleus, with diverse finite masses; and (ii) the construction of highly correlated wave functions, for both ground and excited $n^{1,3}S$ states, for a number of Coulomb three-body systems including muonic atoms and antihydrogenic nuclei "quasi-atoms." The method generates wave functions, which (i) are sufficiently simple and sufficiently accurate (as the traditional Hylleraas wave functions available in the literature for two-electron systems with infinite nuclear mass) to be used in practical atomic collision calculation; and (ii) by construction, satisfy exactly Kato cusp conditions [34, 35]. Ground state wave functions with these characteristics are not available in the literature, in particular for finite nuclear mass systems and exotic systems. It is important to underline that almost no results for excited states of exotic systems have been given in the literature.

The article is organized as follows: in Section 2 we define the ACCI method with the C3 basis set in order to apply it to atomic systems with general masses. In Section 3, we present our results for both ground and excited states for several Coulomb three-body systems. The energies are compared to "exact" reference values, when available. The doubly excited state $2s^2$ is briefly discussed in Section 4. Finally a summary and some perspectives are given in Section 5.

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

2. Method and Basis Functions

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 $[m_1^{z_1} m_2^{z_2} m_3^{z_3}]$, with the charges z_i as superscripts. Let $\mu_{ij} = \frac{m_i m_j}{m_i + m_j}$ ($i \neq j$) be the reduced masses. We shall designate as particle 3 the heaviest particle, *i.e.* the nucleus of mass m_3 and charge z_3 , 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.

As we consider here only S states (the extension to generate other $L > 0$ excited states will be briefly sketched in Section 5), we may use the interparticle (Hylleraas) coordinates (r_{13}, r_{23}, r_{12}) . For the general charges z_1 , z_2 and z_3 , the six-dimensional Schrödinger equation reduces to the following Hylleraas equation

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

where the nonrelativistic Hamiltonian H is given by

$$H = D_0 + D_1. \quad (2)$$

Here, D_0 and D_1 are the kinetic energy operators (see, e.g., Ref. [5])

$$D_0 = \left[-\frac{1}{2\mu_{13}} \left(\frac{\partial^2}{\partial r_{13}^2} + \frac{2}{r_{13}} \frac{\partial}{\partial r_{13}} \right) + \frac{z_1 z_3}{r_{13}} \right] + \left[-\frac{1}{2\mu_{23}} \left(\frac{\partial^2}{\partial r_{23}^2} + \frac{2}{r_{23}} \frac{\partial}{\partial r_{23}} \right) + \frac{z_2 z_3}{r_{23}} \right] + \left[-\frac{1}{2\mu_{12}} \left(\frac{\partial^2}{\partial r_{12}^2} + \frac{2}{r_{12}} \frac{\partial}{\partial r_{12}} \right) + \frac{z_1 z_2}{r_{12}} \right], \quad (3)$$

$$D_1 = - \left(\frac{1}{m_1} \frac{r_{13}^2 - r_{23}^2 + r_{12}^2}{2r_{13}r_{12}} \frac{\partial^2}{\partial r_{13}\partial r_{12}} + \frac{1}{m_2} \frac{r_{23}^2 - r_{13}^2 + r_{12}^2}{2r_{23}r_{12}} \frac{\partial^2}{\partial r_{23}\partial r_{12}} + \frac{1}{m_3} \frac{r_{13}^2 - r_{12}^2 + r_{23}^2}{2r_{13}r_{23}} \frac{\partial^2}{\partial r_{23}\partial r_{13}} \right). \quad (4)$$

Here, no assumptions are made that some parts of the Hamiltonian are negligible in comparison to others. The operator D_1 contains no singularities, and is nondiagonal as it mixes the three relative coordinates. When the nucleus is (virtually) considered as infinitely heavy ($m_3 \rightarrow \infty$), the last term in D_1 is absent. Such limit is often taken as reference system.

In Ref. [31], two of us proposed a basis set that solves exactly the diagonal D_0 part of the three-body Schrödinger Eq. (1). The basis functions read

$$\phi_\nu(r_{13}, r_{23}, r_{12}) = \varphi_{n_1, l_1}(r_{23}) \varphi_{n_2, l_2}(r_{13}) \chi_{C3}(n_3, l_3, r_{12}) \quad (5)$$

where ν stands for the quantum numbers $\{n_1, l_1, n_2, l_2, n_3, l_3\}$, and where for $i = 1, 2$

$$\varphi_{n_i, l_i}(r_{i3}) = N_{n_i, l_i} e^{z_i z_3 \mu_{i3} r_{i3} / n_i} \left(\frac{-2z_i z_3 \mu_{i3}}{n_i} r_{i3} \right)^{l_i} \times {}_1F_1 \left(1 + l_i - n_i, 2l_i + 2, -2 \frac{z_i z_3 \mu_{i3}}{n_i} r_{i3} \right) \quad (6)$$

are normalized hydrogenic functions with principal quantum numbers n_i and angular momenta l_i [39]; the normalization is given by

$$N_{n_i, l_i} = \frac{1}{(2l_i + 1)!} \sqrt{\left(\frac{-2z_i z_j \mu_{ij}}{n_i}\right)^3 \frac{(n_i + l_i)!}{2n_i(n_i - 1 - l_i)!}}$$

and ${}_1F_1$ is the confluent hypergeometric function [40]. The distortion factor is defined by

$$\begin{aligned} \chi_{C3}(n_3, l_3, r_{12}) &= \left(-2 \frac{z_1 z_2 \mu_{12}}{n_3} r_{12}\right)^{l_3} \\ &\times {}_1F_1\left(l_3 - n_3, 2l_3 + 2, -2 \frac{z_1 z_2 \mu_{12}}{n_3} r_{12}\right), \end{aligned} \quad (7)$$

where $n_3 > l_3$ is a positive integer, and reduces to a polynomial. In particular, for $l_3 = 0$, $\chi_{C3}(n_3, 0, r_{12})$ reduces to a Laguerre polynomial $L_{n_3}^{(1)}(-2z_1 z_2 \mu_{12} r_{12}/n_3)$. If only S states are considered, the angular momenta are taken to be equal to zero $l_1 = l_2 = l_3 = 0$ in the above formulas. For a given set of quantum numbers $\{n_1, n_2, n_3\}$ —one for each coordinate—the basis functions are thus parameter-free. They have been proposed [30, 31] following ideas based on an approximated solution for the double continuum wave function known as C3 [41] (also called 3C or BBK model). We have called the basis C3-like, and will use the label C3 for the three-body bound wave functions constructed from it.

In the case of S states, the ACCI method constructs an approximated solution of the Hylleraas equation (1), as a linear combination of the basis functions (5),

$$\Psi_{C3-M} = N \sum_{n_1, n_2, n_3} c_{n_1 n_2 n_3} \phi_{n_1, n_2, n_3}(r_{13}, r_{23}, r_{12}), \quad (8)$$

where N is the overall normalization factor, and all traces of angular momenta (which are set to zero) have been removed. The functions Ψ_{C3-M} include explicitly angular correlation through the introduction of the r_{12} coordinate in each function ϕ_{n_1, n_2, n_3} . This ensures a rather fast convergency rate for the energy (and other relevant physical quantities), as will be illustrated in the next section. The overall amount of correlation included is dictated by the number M of linear coefficients $c_{n_1 n_2 n_3}$. It should be noted that when the two light particles are identical, the coefficients must satisfy the following symmetry relation $c_{n_1 n_2 n_3} = c_{n_2 n_1 n_3}$, so that the number of coefficients is reduced.

The action of the Hamiltonian H over the basis functions $\phi_{n_1 n_2 n_3}(r_{13}, r_{23}, r_{12})$, defined by Eq. (5) for $l_1 = l_2 = l_3 = 0$, is given by

$$\begin{aligned} H\phi_{n_1 n_2 n_3}(r_{13}, r_{23}, r_{12}) &= E_{n_1, n_2}^{(0)} \phi_{n_1 n_2 n_3}(r_{13}, r_{23}, r_{12}) \\ &+ \left(D_1 + \frac{z_1 z_2}{n_3} \frac{\partial}{\partial r_{12}}\right) \phi_{n_1 n_2 n_3}(r_{13}, r_{23}, r_{12}) \end{aligned} \quad (9)$$

where

$$E_{n_1, n_2}^{(0)} = -\frac{\mu_{13}}{2} \frac{(z_1 z_3)^2}{n_1^2} - \frac{\mu_{23}}{2} \frac{(z_2 z_3)^2}{n_2^2} \quad (10)$$

is the energy corresponding to the solved operator D_0 . The Hylleraas equation can then be transformed into a generalized eigenvalue problem [39]:

$$\sum_{n_1, n_2, n_3} [\hat{H} - E\hat{S}]c_{n_1 n_2 n_3} = 0, \quad (11)$$

where the M coefficients $c_{n_1 n_2 n_3}$ are the eigenvectors and E the eigenvalues for the three-body system. The basis functions $\phi_{n_1 n_2 n_3}$ solve $(D_0 - E_{n_1, n_2}^{(0)})\phi_{n_1 n_2 n_3} = 0$, thus only the nondiagonal part of the kinetic energy has to be diagonalized. Besides, the functions $\phi_{n_1 n_2 n_3}$, as indeed any other containing products of power and exponential functions, allow to express in closed form all the elements of the overlap \hat{S} and Hamiltonian \hat{H} matrices. The results obtained with the Ψ_{C3-M} wave functions, require only one diagonalization process and no further optimization process is needed. According to the number M of basis functions included, a certain amount of excited states $n^{1,3}S$ states is also obtained.

Mathematically, the solution $\Psi(r_{13}, r_{23}, r_{12})$ of Eq. (1) satisfies the two-body Kato cusp conditions [34, 35]

$$\left[\frac{\partial \bar{\Psi}}{\partial r_{ij}}\right]_{r_{ij} \rightarrow 0} = z_i z_j \mu_{ij} \Psi(0, r_{kj}, r_{ik}), \quad (12)$$

for ($i \neq j, i \neq k, j \neq k$), the notation $\bar{\Psi}$ meaning the average of Ψ over a very small sphere of radius r_{ij} keeping the other values fixed. Relations (12) provide the linear behavior that $\Psi(r_{13}, r_{23}, r_{12})$ must have close to the Coulomb singular points $r_{ij} = 0$; they are not only a mathematical requirement but also an important property that any trial wave function should have, as underlined throughout the literature. By construction, our basis functions $\phi_{n_1, n_2, n_3}(r_{13}, r_{23}, r_{12})$ satisfy them exactly, and

therefore so does the trial wave functions Ψ_{C3-M} given by Eq. (8).

Before presenting our results, we would like to mention that the convergence rate of the energy and wave functions obtained can be considerably increased [28, 29] by multiplying the basis functions $\phi_{n_1, n_2, n_3}(r_{13}, r_{23}, r_{12})$ by an additional correlation factor $\Omega(r_{13}, r_{23}, r_{12})$, which adds radial and angular correlation to each configuration. In this advanced ACCI approach, the factor Ω can be represented by a polynomial of the relative coordinates (not affecting the cusps conditions) that solves the nondiagonal terms of the kinetic energy not solved by the functions ϕ_{n_1, n_2, n_3} . The efficiency of this advanced ACCI method has been illustrated by the study of ground states of two-electrons and electron-muon three-body atomic systems [42]. 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. Refs. [8, 11, 14]) and those obtained with simple wave functions (see e.g. Refs. [22, 23]). Similarly to the method presented above, the advanced ACCI also generates an orthogonal set of excited states.

3. Ground 1^1S and Excited $n^{1,3}S$ States

As we want to obtain approximate wave functions - at the same time - for the ground 1^1S and the excited states n^1S and n^3S ($n = 2$ to 4), we have performed calculations with n_1 and n_2 up to 4 , and included the following configurations:

$$1s1s + (1s2s + 2s1s) + (1s3s + 3s1s) + (1s4s + 4s1s). \quad (13)$$

Satisfactory convergence was obtained with $n_3 = 1$ to 5 ; this choice keeps the approximated functions reasonably simple, and at the same time sufficiently accurate. For symmetric three-body systems, i.e. with $m_1 = m_2, z_1 = z_2$, this means $M = 20$ terms while for asymmetric systems, $m_1 \neq m_2, M = 35$. All our calculated energies are presented below with 9 significant digits.

Our ACCI method is applied here to a number of normal and exotic atomic three-body systems: negatively charged hydrogen-like ions ($z_3 = 1$), neutral helium-like ($z_3 = 2$) atoms, and positively charged lithium-like ions ($z_3 = 3$). In this contribution, we shall focus only on the mean energies

of ground and excited states; we should remind though that expectation values $\langle A \rangle$ of other physical operators A are also very useful to test the trial wave functions putting a particular emphasis on a given portion of the configuration space. When possible, we shall compare our energy results with reference values, hereafter named numerically "exact," which are generally obtained with highly accurate variational procedures involving very large numbers of linear and nonlinear parameters. The relative accuracy is then given by $\frac{\langle -E \rangle - \langle -E \rangle_{\text{exact}}}{\langle -E \rangle_{\text{exact}}}$. To allow for a direct comparison with these numerically "exact" energies, it is necessary to take the same mass values for the involved particles. Since for most systems highly accurate results have been provided by Frolov [7-9], we have taken the same masses values as in these references (which are taken from Ref. [43]). 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 $m_\mu = 206.768262 m_e$. [More recently, Frolov [11, 14] used a slightly different muon mass recommended by NIST, $m_\mu = 206.7682838 m_e$ [44]. While the use of this modified mass value produces slight energy shifts, this will affect digits of our calculated energy, which are not given in the tables below.] For the exotic three-body systems (quasi-atoms) where anti-hydrogen nuclei are considered as particle 2, the masses of the antiparticles m_2^- are taken as being the same as those of the particles m_2^+ (i.e. the same choice as in Ref. [1]), i.e.: p^- ($m_2 = m_{p^-} = m_p$), d^- ($m_2 = m_{d^-} = m_d$) or t^- ($m_2 = m_{t^-} = m_t$). As the He^{2+} nucleus is concerned, we have taken $m_3 = 7294.2996 m_e$ for ${}^4\text{He}^{2+}$ and $m_3 = 5495.8852 m_e$ for ${}^3\text{He}^{2+}$. For the Li^{3+} nucleus, we have taken the same values as used by Frolov [14]: $m_3 = 10961.8968 m_e$ for ${}^6\text{Li}^{3+}$ and $m_3 = 12786.3927 m_e$ for ${}^7\text{Li}^{3+}$.

Let us start with the ground singlet state 1^1S . Our calculated mean energies $\langle -E \rangle$ are reported in Table I, and compared with numerically "exact" results collected from the literature.

For negatively charged hydrogen-like three-body systems made of two electrons and a third heavier particle with charge $z_3 = 1$ we considered the ions ${}^\infty\text{H}^-$, ${}^1\text{H}^-$, D^- , T^- , and the muonium ion $\text{Mu}^- [e^- e^- \mu^+]$. All these systems are similar to each other in the main property of their spectra, i.e. they have only one bound (ground), singlet state with $L = 0$. They differ only by the nuclear mass. The mean energies have a relative accuracy of 1.7×10^{-3} for Mu^- ; similar accuracies are obtained for the other systems. These are quite good result in view of the

TABLE I

The ground state 1^1S mean energies for several negatively three-body systems, obtained using the Ψ_{C3-20} (for symmetric systems) or Ψ_{C3-35} (for asymmetric systems) approximated wave functions, are compared with accurate reference values.

$Z_3 = 1$ [$m_1^- m_2^- m_3^+$]	$\langle -E \rangle$	$Z_3 = 2$ [$m_1^- m_2^- m_3^{2+}$]	$\langle -E \rangle$	$Z_3 = 3$ [$m_1^- m_2^- m_3^{3+}$]	$\langle -E \rangle$
$\infty H^- [e^- e^- \infty^+]$	0.526860162 0.527751017^a	$\infty He [e^- e^- \infty He^{2+}]$	2.90107544 2.90372438^c	$\infty Li [e^- e^- \infty Li^{3+}]$	7.27657671 7.27991341^c
$^1 H^- [e^- e^- p^+]$	0.526554804 0.527445881^a	$^4 He [e^- e^- ^4 He^{2+}]$	2.90065336 2.90330456^c	$^7 Li [e^- e^- ^7 Li^{3+}]$	7.27603060 7.27932152^c
$D^- [e^- e^- d^+]$	0.526707359 0.527598325^a	$^3 He [e^- e^- ^3 He^{2+}]$	2.90051530 2.90316721^c	$^6 Li [e^- e^- ^6 Li^{3+}]$	7.27588119 7.27922302^c
$T^- [e^- e^- t^+]$	0.526860161 0.527649048^a	$[e^- \mu^- \infty He^{2+}]$	414.036395 414.036537^d	$[e^- \mu^- \infty Li^{3+}]$	932.456800
$Mu^- [e^- e^- \mu^+]$	0.524161999 0.525054806^a	$[e^- \mu^- ^4 He^{2+}]$	402.637158 402.637263^d	$[e^- \mu^- ^7 Li^{3+}]$	917.649469 917.650220^f
$[\mu^- \mu^- \infty^+]$	108.937959	$[e^- \mu^- ^3 He^{2+}]$	399.042262 399.042337^d	$[e^- \mu^- ^6 Li^{3+}]$	915.230650 915.231355^f
$[\mu^- \mu^- p^+]$	97.3747607 97.5669834^b	$[\mu^- \mu^- \infty He^{2+}]$	599.850338	$[\mu^- \mu^- \infty Li^{3+}]$	1504.56570
$[\mu^- \mu^- d^+]$	102.803286 102.991911^b	$[\mu^- \mu^- ^4 He^{2+}]$	582.399626	$[\mu^- \mu^- ^7 Li^{3+}]$	1479.62095
$[\mu^- \mu^- t^+]$	104.756883 104.944115^b	$[\mu^- \mu^- ^3 He^{2+}]$	576.934471	$[\mu^- \mu^- ^6 Li^{3+}]$	1475.56380
		$[e^- p^- \infty He^{2+}]$	3672.80537	$[e^- p^- \infty Li^{3+}]$	8445.76213
		$[e^- p^- ^4 He^{2+}]$	2934.29713 2934.29719^e	$[e^- p^- ^7 Li^{3+}]$	7227.14146
		$[e^- p^- ^3 He^{2+}]$	2753.15461 2753.15468^e	$[e^- p^- ^6 Li^{3+}]$	7079.22839
		$[e^- d^- \infty He^{2+}]$	7341.46599	$[e^- d^- \infty Li^{3+}]$	16519.1735
		$[e^- d^- ^4 He^{2+}]$	4884.06275 4884.06285^e	$[e^- d^- ^7 Li^{3+}]$	12836.7229
		$[e^- d^- ^3 He^{2+}]$	4401.92755	$[e^- d^- ^6 Li^{3+}]$	12375.8962
		$[e^- t^- \infty He^{2+}]$	11052.6571	$[e^- t^- \infty Li^{3+}]$	24740.6194
		$[e^- t^- ^4 He^{2+}]$	6269.82985 6269.82989^e	$[e^- t^- ^7 Li^{3+}]$	17301.1660
		$[e^- t^- ^3 He^{2+}]$	5538.06345	$[e^- t^- ^6 Li^{3+}]$	16555.5250

^aFrolov [7, 11].

^bFrolov *et al.* [46].

^cDrake [13].

^dFrolov [8].

^eSmith and Frolov [1].

^fFrolov [14].

relatively small number $M = 20$ of basis functions used.

For these ions, intermediate quality wave functions have been proposed, for example, by Flores-Rivero and Rivas-Silva [45]. 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; this was one of the motivations behind the work presented in [42]. For the helium atom and its isoelectronic series with infinite mass, however, 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 12 nonlinear parameters involved. As stated by the authors, their optimization is a demanding numerical task. Since 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 (see below).

Three-body systems where the two electrons are replaced by muons have also been considered; our results are compared with those given (in muonic units) in Ref. [46], and have a relative accuracy of at most 2×10^{-4} . We should also point out that the system $[e^{-}\mu^{-}\infty^{+}]$ is not stable [42], and thus is absent from the table. Finally, negatively charged exotic systems $[e^{-}e^{-}(nm_e)^{+}]$, with a variable quasi-nuclear mass (n integer), have also been studied [3, 47, 48]; these systems go from the negative positronium Ps^{-} ($n = 1$) to the negative hydrogen ion H^{-} ($n \rightarrow \infty$) and allow for a discussion of energy interpolation with the mass.

Let us now turn to three-body systems with $z_3 \geq 2$. In this case, also excited states exist and results will be presented below.

For $z_3 = 2$, we have studied a variety of neutral helium-like systems with a heavy positively charged nucleus m_3^{2+} ; the cases of infinite nuclear mass, and the two isotopes 3He and 4He are considered. The two negatively charged light particles can be equal or different. When both are electrons, we have the standard helium atom; for the ground state of ${}^{\infty}He$, we found a relative accuracy of 9×10^{-4} , and similar values when finite nuclear masses are considered.

When one electron is replaced by a muon, we have the so-called muonic helium $[e^{-}\mu^{-}He^{2+}]$; its ground state has been studied in details by Frolov [8] (and references therein). Our ground state energies are in very good agreement with reference values, relative accuracies not exceeding 3.5×10^{-7} . Such muonic-atoms have a particularly simple structure (see below); their energies are essentially proportional to $m_2 = m_{\mu}$. Similar comments apply to the exotic systems ("quasi-atoms") in which one electron is replaced by antihydrogen nuclei p^{-} , d^{-} , or t^{-} , the found relative accuracy being even better.

Next, we consider the following positively charged lithium-like systems with a heavy positively charged nucleus m_3^{3+} ; the cases of infinite nuclear mass, and the two isotopes 7Li and 6Li are

considered. For the standard ${}^{\infty}Li^{+}$ ion, the mean energies have – approximately – a relative accuracy of 4.6×10^{-4} , and similar values are found for the two finite nuclear mass cases.

The ground state of muonic lithium ions $[e^{-}\mu^{-}Li^{3+}]$ have been studied in detail by Frolov [14]. Our values are very accurate when compared to "exact" reference values (relative accuracy of, at most, 8.2×10^{-7}). For systems involving antihydrogen nuclei we have not found in the literature any calculated energies to compare with.

From the detailed study of mean radial quantities (see, e.g., Refs. [9, 14] and references therein), it appears that the muonic helium atoms (and muonic lithium ions) have a two-shell cluster structure. This means that the actual structure is represented as a one-electron motion in the field of a quasi-nucleus, which is a hydrogen-like ion of charge $z_3 - 1$: singly charged $[He^{2+}\mu^{-}]$ or doubly charged $[Li^{3+}\mu^{-}]$. The bound spectrum of these muonic three-body systems should thus be similar to that of the one-electron ions. Due to the ratio m_{μ}/m_e , the muon shell radius is much times smaller than the outside electron shell radius. For muonic helium atoms (respectively, muonic lithium ions) this ratio is about 413 [8] (respectively, 465 [14]). This implies that, compared with the two-electron He atom (respectively Li^{+} ion), the overall correlation is much smaller for the electron-muon case. Similarly, for systems involving antinuclei (p^{-} , d^{-} , or t^{-}), the electron moves in the field of a positive charged quasi-nucleus. In all these systems, the complex structure of the pseudonucleus is practically insignificant. This essentially one-electron structure explains the very good accuracies presented in Table I.

When solving the generalized eigenvalue problem (11), the single diagonalization provides also bound energies and wave functions for a number of $n^{1,3}S$ excited states. All constructed wave functions form an orthogonal set. Their number and their quality depend on the configurations included in the trial wave function (8).

The results of our calculations are displayed in Table II, for the same systems as in Table I for $z_3 = 2$ and $z_3 = 3$. This is one of the main objectives of this work since only very few results are available in the literature for exotic systems. For the two-electron systems, the accuracy varies from about 1.3×10^{-4} (2^3S) to 3.4×10^{-3} (4^1S), the results for the lithium ion being slightly better. For the muonic helium, the energy of the first excited state (the so-called electron excited state $[1s_{\mu}2s_e]$) has been calculated quite accurately by Frolov [9]. Our accuracy is of the order

TABLE II

Mean energies of the excited states n^1S and n^3S for several negatively three-body systems, obtained using the Ψ_{C3-20} (for symmetric systems) or Ψ_{C3-35} (for asymmetric systems) approximated wave functions, are compared with accurate reference values.

	$\langle -E \rangle_{2^3S}$	$\langle -E \rangle_{2^1S}$	$\langle -E \rangle_{3^3S}$	$\langle -E \rangle_{3^1S}$	$\langle -E \rangle_{4^3S}$	$\langle -E \rangle_{4^1S}$
$e^-e^- \infty\text{He}^{2+}$	2.17493965 2.17522938^a	2.14541020 2.14597405^a	2.06858102 2.06868907^a	2.06107284 2.06127199^a	2.03193872 2.03651208^a	2.02660791 2.03358672^a
$e^-e^- {}^4\text{He}^{2+}$	2.17464057 2.17493019^a	2.14511445 2.14567859^a	2.06829724 2.06840524^a	2.06078978 2.06098908^a	2.03165943 2.03623283^a	2.02633010 2.03330782^a
$e^-e^- {}^3\text{He}^{2+}$	2.17454273 2.17483231^a	2.14501773 2.14558192^a	2.06820440 2.06831238^a	2.06069722 2.06089652^a	2.03156807 2.03614146^a	2.02623837 2.03321657^a
$e^-\mu^- \infty\text{He}^{2+}$	413.661509 413.661526^b	413.592074	413.567502	413.550045	413.519711	413.466971
$e^-\mu^- {}^4\text{He}^{2+}$	402.262291 402.262302^b	402.192862	402.168313	402.151997	402.124186	402.076234
$e^-\mu^- {}^3\text{He}^{2+}$	398.667389 398.667391^b	398.597957	398.573482	398.558098	398.531748	398.488673
$\mu^-\mu^- \infty\text{He}^{2+}$	449.708491	443.602738	427.716903	426.164448	420.140441	419.038311
$\mu^-\mu^- {}^4\text{He}^{2+}$	437.282598	431.329114	415.923494	414.406552	408.536567	407.457197
$\mu^-\mu^- {}^3\text{He}^{2+}$	433.367758	427.467280	412.206764	410.702258	404.879938	403.808994
$e^-p^- \infty\text{He}^{2+}$	3672.43040	3672.36096	3672.33635	3672.31794	3672.28551	3672.22673
$e^-p^- {}^4\text{He}^{2+}$	2933.92222	2933.85279	2933.82845	2933.81429	2933.78990	2933.74337
$e^-p^- {}^3\text{He}^{2+}$	2752.77972	2752.71029	2752.68579	2752.66729	2752.63585	2752.58384
$e^-d^- \infty\text{He}^{2+}$	7341.09102	7341.02158	7340.99683	7340.97617	7340.93684	7340.86131
$e^-d^- {}^4\text{He}^{2+}$	4883.68787	4883.61844	4883.59504	4883.58792	4883.56467	4883.51851
$e^-d^- {}^3\text{He}^{2+}$	4401.55263	4401.48320	4401.45880	4401.44316	4401.41603	4401.36417
$e^-t^- \infty\text{He}^{2+}$	10994.3431	10993.9682	10993.8987	10993.8742	10993.8577	10993.8290
$e^-t^- {}^4\text{He}^{2+}$	6269.45491	6269.38548	6269.36106	6269.34497	6269.31719	6269.26585
$e^-t^- {}^3\text{He}^{2+}$	5496.90325	5496.52832	5496.45889	5496.43417	5496.41420	5496.37711
$e^-e^- \infty\text{Li}^{3+}$	5.11015939 5.11072731^c	5.03941025 5.04087674^c	4.75173831 4.75207644^c	4.73309441 4.73375186^c	4.63433035 4.63713654^c	4.62515508 4.62977459^c
$e^-e^- {}^7\text{Li}^{3+}$	5.10975862	5.03913196	4.75136656	4.73315062	4.63396662	4.62641756
$e^-e^- {}^6\text{Li}^{3+}$	5.10969189	5.03894691	4.75130451	4.73266048	4.63390581	4.62472771
$e^-\mu^- \infty\text{Li}^{3+}$	930.957127	930.679386	930.582187	930.545785	930.512877	930.429896
$e^-\mu^- {}^7\text{Li}^{3+}$	916.150116	915.872416	915.775327	915.728570	915.693136	915.595106
$e^-\mu^- {}^6\text{Li}^{3+}$	913.731280	913.453578	913.356344	913.308876	913.256344	913.155126
$\mu^-\mu^- \infty\text{Li}^{3+}$	1056.61881	1041.99032	982.508707	978.653675	958.232493	956.335166
$\mu^-\mu^- {}^7\text{Li}^{3+}$	1039.75829	1025.32989	966.866304	963.060874	942.961199	941.079444
$\mu^-\mu^- {}^6\text{Li}^{3+}$	1037.00586	1022.61597	964.312364	960.519661	940.467046	938.591610
$e^-p^- \infty\text{Li}^{3+}$	8293.02191	8264.68708	8263.18714	8262.90937	8262.81215	8262.76518
$e^-p^- {}^7\text{Li}^{3+}$	7225.64170	7225.36393	7225.26669	7225.21819	7225.16651	7225.04622
$e^-p^- {}^6\text{Li}^{3+}$	7077.73086	7077.67822	7077.45109	7077.35367	7077.30009	7077.22961
$e^-d^- \infty\text{Li}^{3+}$	16517.6736	16517.3958	16517.2985	16517.2489	16517.1824	16517.0418
$e^-d^- {}^7\text{Li}^{3+}$	12835.2417	12833.7419	12833.4641	12833.3669	12833.3186	12833.2597
$e^-d^- {}^6\text{Li}^{3+}$	12374.3964	12374.1186	12374.0214	12373.9725	12373.9107	12373.7814
$e^-t^- \infty\text{Li}^{3+}$	24738.1471	24736.6471	24736.3693	24736.2721	24736.2242	24736.1721
$e^-t^- {}^7\text{Li}^{3+}$	17299.6661	17299.3883	17299.2911	17299.2440	17299.1817	17299.0050
$e^-t^- {}^6\text{Li}^{3+}$	16476.7604	16475.2605	16474.9828	16474.8855	16474.8387	16474.7871

^a Drake [13].

^b Frolov [9].

^c Accad et al. [49].

of 10^{-8} whether for finite or infinite nuclear masses. To the best of our knowledge, for the other systems, no data have been published to compare with.

Other three-body systems with larger values of z_3 can be equally considered. The relatively less important role played by the electron-electron or electron-muon correlation gives then even better relative energy agreement with "exact" values (not shown).

Finally, for all the systems considered, more accurate wave functions can be easily constructed by including more configurations (n_1n_2) and increasing the number of correlation terms (n_3) (as discussed in Ref. [31]). However, as mentioned in the Introduction, the aim is to provide relatively simple, yet accurate, wave functions and have therefore kept the number of coefficients reasonably moderate. The linear coefficients and normalization constants for the wave functions presented here are available in tabular form upon request [50].

4. Doubly Excited States $2s^2$

Before concluding, let us make some comments on the first doubly excited state. We have performed calculations by including also the $2s2s$ configuration in the trial wave function (13). By doing so, for example for ${}^\infty\text{He}$, the first excited states energies are only slightly improved (by 10^{-5} a.u. at best), while the ground state energy is -2.90147948 a.u., thus 4×10^{-4} better than the value given in Table I (this, incidentally, illustrates that improved values can be obtained by systematically adding more configurations in the trial wave function). More interestingly, the doubly excited state $2s^2\ ^1S$ appears through the diagonalization of the eigenvalue problem (11); its energy -0.7698 a.u. is in good agreement with the value -0.7685 a.u. reported by the Lipsky et al. [51] and the -0.7776 a.u. reported by Dulieu and Le Sech [52].

Next, we have considered the three-body system $[\mu^-\mu^-p^+]$ because recently an excited state energy of -84.891397 a.u. for 2^1S was published [53] (note that, in Table II of [53], the energy is given in muonic mass units). We were surprised by this result since this three-body system does not possess proper simply excited states. This level energy is above the two-body $[\mu^-p^+]$ threshold, so that it must correspond to a doubly - and not a simply - excited state. To check this, we performed a calculation including the $2s2s$ configuration in the trial wave function. We found a ground state energy of -97.418009 a.u.,

thus improving the value -97.374760 a.u. given in Table I. A doubly excited state $2s^2\ ^1S$ appears, with a value of -92.621499 a.u., which is much lower than that given in Ref. [53]. Similar conclusions apply: for $[\mu^-\mu^-d^+]$ for which we found -97.506661 a.u. instead of -89.499228 a.u. [53]; for $[\mu^-\mu^-t^+]$ -99.268382 a.u. instead of -91.168261 a.u. [53]; and for $\text{Mu}^- [e^-e^-\mu^+]$ -0.495784 a.u. instead of -0.455748 a.u. [53].

5. Summary and Perspectives

We have generalized the C3-like basis set [31] to three-body atomic systems with general masses, and have used the basis functions to extend the Angular Correlated Configuration-Interaction method presented in [28, 29]. The C3-like basis functions are defined as being exact solution 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 function multiplied by a Coulomb distortion factor, being in that way the counterpart of the C3 approach used for scattering problems. This distortion factor, which depends on the distance between the two light particles, already includes angular correlation in the configuration basis functions [30, 31]. A configuration interaction scheme can then be constructed with these correlated basis elements as done in Ref. [31]. Two technical advantages of the C3-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 interaction and part of the kinetic energy, leading to analytic closed form expressions for the non-diagonalized terms.

The efficiency of the method has been illustrated by considering S states of several standard and exotic hydrogen-, helium-, and lithium-like three-body systems in which the nuclear mass can be finite and the two light particles can be equal or different. Ground and excited states $n^{1,3}S$ energies have been compared, when possible, to highly accurate values, obtained with large variational calculations; good agreement is found for all cases. For most exotic systems, the energy of excited states has not been given before in the literature. Accurate wave functions, satisfying exactly two-body Kato cusp conditions, and with a moderate number of linear coefficients were

used (the results can be systematically improved by including more terms in the expansion). This has been done with the purpose to provide, e.g., 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 given in the literature.

The extension of the present method to $L > 0$ states is part of our current investigations. There exist a significative number of publications on this topic starting from the first article of Breit [54] to, e.g., Ref. [55]. Without going here into details, we briefly sketch the line of work we are following and refer only to one closely associated article. For general $L > 0$, linear combinations of radial basis functions $\phi_{n_1 n_2 n_3}(r_{13}, r_{23}, r_{12})$ and rotation matrices $D_L^{M,K}(\alpha, \beta, \gamma)$ can be used to expand the different states [56]. The rotation matrices are simultaneously eigenfunctions of \hat{L}^2 and the projections, \hat{L}_z and \hat{L}'_z along space-fixed and body-fixed axes, with eigenvalues $L(L+1)$, M , and K , respectively. Following [56], the rotation matrices can be expressed in terms of the polar and azimuthal angles (θ_{ik}, ϕ_{ik}) of \mathbf{r}_{ik} and the angular momentum lowering operator \hat{L}_- . The general L states Ψ_{C3-M}^L can be written in terms of the radial basis functions together with the angular functions as follows:

$$\Psi_{C3-M}^L = N \sum_{l_1+l_2=L} [(\hat{L}_-)^L (r_{13}\xi_{13})^{l_2} (r_{23}\xi_{23})^{l_1}] \times \sum_{n_1, n_2, n_3} c_{n_1 n_2 n_3, l_1 l_2}^L \phi_{n_1 n_2 n_3}(r_{13}, r_{23}, r_{12})$$

where N is the overall normalization factor and $\xi_j = \sin(\theta_j)e^{i\phi_j}$ where the subscript j stands for 13 or 23. The advantage of expanding with the radial basis functions $\phi_{n_1 n_2 n_3}$ is that they fully diagonalize the Coulomb interactions and remove the diagonal part of the kinetic energy. More details and numerical applications will be presented elsewhere.

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