Correlated continuum wave functions for three particles with Coulomb interactions

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We present an approximate solution of the Schrödinger equation for the three-body Coulomb problem. We write the Hamiltonian in parabolic curvilinear coordinates and study the possible separation of the wave equation as a system of coupled partial differential equations. When two of the particles are heavier than the others, we write an approximate wave equation that incorporates some terms of the Hamiltonian that before had been considered as a perturbation. Its solution can be expressed in terms of a confluent hypergeometric function of two variables. We show that the proposed wave function includes a correlation between the motion of the light particle relative to the heavy particles and verifies the correct asymptotic behavior when all particles are far from each other. Finally, we discuss the possible uses of this function in the calculation of transition matrices and differential cross sections in ionizing collisions. [S1050-2947(97)00504-0]

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INTRODUCTION

The full three-body Coulomb problem has particular importance in many areas of physics, especially in atomic collisions. The initial and the final channel of ion-atom or electron-atom collisions can be considered as three-body Coulomb states in a first approximation when we assume that only one electron of the target atom is active. The characteristics of these processes are described by the transition matrix in the post or prior form $T_{if} = \langle \psi_f | V_f | \Psi_i^+ \rangle = \langle \Psi_f^- | V_i | \psi_i \rangle$, respectively. The exact channel functions Ψ_i^+ (Ψ_f^-) are not known in the three-body case and then they should be replaced by proper approximations. These approximate wave functions also determine the channel potential V_f (V_i) [1]. From an experimental point of view, the spectra of electrons emitted in the collisions reveal the main features of these processes. Nowadays many double differential cross sections (DDCSs), in terms of the energy and direction of the emitted electrons are available for a variety of processes (ion-atom or electron-atom ionization, charge transfer, excitation, etc.). Recently, measurements of differential cross sections that take into account the momenta of the recoil atom have been reported [2]. Triply differential cross sections (TDCSs), in which the momentum of the projectile is considered, are known in some particular geometries of electron-atom ionization [3]. However, they remain an open question for ion-atom collisions.

The choice of approximate wave functions has been found to be critical when comparing theory with experimental results. Initial attempts to describe total cross sections (TCSs) were carried out decades ago. The wave functions included in that theory were simply plane waves for the three outgoing particles and their results described the TCS very roughly in fast ion-atom collisions. The main drawback of this approach is that it does not take into account the long-range behavior of the Coulomb potential among the particles. Further approximate wave functions were based on the exact solution of the two-body Coulomb problem that can be written in terms of the confluent hypergeometric function ${}_1F_1$. The first Born approximation (FBA) relies on the assumption that the ejected electron completely screens the target potential, including a final state described by the free wave function of the projectile leaving the collision region, while the electron interacts with the target through the Coulomb potential [4]. In this way, the final wave function is a product of a plane wave and the solution of the two-body Coulomb problem electron target. This approximation has been useful in describing the single differential cross sections in the high-impact-energy regime, but fails to reproduce the well-known electron capture to the continuum peak that appears in the double differential cross sections. This effect can only be understood with the introduction of the projectile-electron interaction, which is treated perturbatively in the FBA [5,6].

If we focus our attention on ion-atom ionization processes, there are many theories that incorporate the projectile-electron interaction at the final channel, but with different approximate initial states. The continuum distorted wave (CDW) eikonal initial state (EIS) approximation [7] and the impulse approximation (IA) [8] include the electron-target and the electron-projectile interactions in the final channel and the projectile-target interaction is introduced in an eikonal way. The Coulomb projectile-target interaction is included on an equal basis in the multiple scattering (MS) approximation [9]. All these theories show qualitative agreement with DDCS in fast bare ion-atom ionizations. In spite of the relative success of these theories in the description of the overall features of the DDCS, many discrepancies remain unexplained.

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The final state in the CDW-EIS approximation, the IA, and the MS approximation is constructed through a *superposition* of two-body wave functions, relying on the assumption that the target does not play any role in the projectile-electron interaction and, similarly, the projectile does not exert any influence on the electron-target interaction. These final wave functions are built as products of confluent hypergeometric functions related to each two-body interaction. In this way coupling between the pairs of motions is not considered in any of these theories.

On the other hand, there have been many improvements to the simple product of two-body wave functions in electron-atom collision processes since the pioneering works of Peterkop [10] and Rudge and Seaton [11], where the correlation between the two-body motions is incorporated through velocity-dependent charges. Berakdar and Briggs [12] extended these results to the MS wave function. Effective charges dependent on spatial positions of the particles were recently proposed by Berakdar [13]. In this way he was able to write MS-like wave functions that are asymptotically correct not only when all particles are far from each other, but also when two particles are close and the third one is far from them. In another approach devised by Alt and Mukhamedzhanov, correlation is accounted for by introducing space-dependent relative momenta and requiring the correct behavior in all the asymptotic regions [14]. This wave function has been used by Jones and Madison to calculate cross sections of ionization processes in electron-atom collisions [15]. It is clear that a better description of the final states of ionization processes is needed and some investigation should be carried out in order to solve the wave equations in a more accurate way.

Following this point of view, we present in this work a wave function that can be obtained as an approximate solution of the Schrödinger equation for three charged particles when two of them have large masses than the third one. We show that under some approximations, the wave equation could be separated as a system of coupled differential equations. The solution can be written as a product of a two-body wave function for the heavy particles and a hypergeometric function of two variables, which includes the correct Coulomb asymptotic conditions. In Sec. I we introduce the notation and a set of curvilinear parabolic coordinates useful for our purposes. In Sec. II we show the procedure in order to obtain the wave function, while in Sec. III we analyze the general properties and the asymptotic behavior of the wave function obtained. We briefly discuss the results we should expect when using this function in the calculation of transition matrices and differential cross sections. Finally, the conclusions of our work are drawn. The Appendix summarizes some important properties of hypergeometric functions of two variables. Atomic units are used thorough this paper unless otherwise noted.

I. STATEMENT OF THE PROBLEM

We will focus our attention on the problem of three charged particles labeled 1, 2, and 3 with the masses m_i and charges Z_i $\{i=1,2,3\}$, respectively. We choose the set of relative coordinates $\mathbf{r}_{ij}$ defined as

$$\mathbf{r}_{12}=\mathbf{r}_1-\mathbf{r}_2, \quad \mathbf{r}_{13}=\mathbf{r}_3-\mathbf{r}_1, \quad \mathbf{r}_{23}=\mathbf{r}_3-\mathbf{r}_2$$

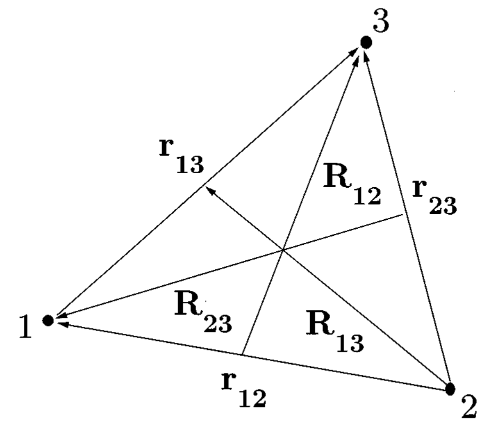

FIG. 1. Scheme of the coordinates system used in this work.

and, of course, $\mathbf{r}_{ij}=-\mathbf{r}_{ji}$. Associated with these coordinates, we define the position vectors $\mathbf{R}_{12}$, $\mathbf{R}_{13}$, and $\mathbf{R}_{23}$. The vectors $\mathbf{R}_{ij}$ describe the position of the particle k relative to the center of mass (c.m.) of the particles i and j $(i\neq j\neq k)$ as indicated in Fig. 1. The Jacobi pairs $\{\mathbf{r}_{ij},\mathbf{R}_{ij}\}$ diagonalize the kinetic energy in the c.m. of the three-particle system. There are simple relations between the Jacobi pairs that are described elsewhere [16]. In this work it will be enough to write down the relations between coordinates $\mathbf{r}_{ij}$ and $\mathbf{R}_{12}$:

$$\mathbf{R}_{12}=a_{12}\mathbf{r}_{23}+b_{12}\mathbf{r}_{13}, \quad \mathbf{r}_{23}=\mathbf{R}_{12}+b_{12}\mathbf{r}_{12},$$
$$\mathbf{r}_{12}=\mathbf{r}_{23}-\mathbf{r}_{13}, \quad \mathbf{r}_{13}=\mathbf{R}_{12}-a_{12}\mathbf{r}_{12}, \tag{1}$$

where

$$a_{12}=\frac{m_2}{m_1+m_2}=\frac{\mu_{12}}{m_1}, \quad b_{12}=\frac{m_1}{m_1+m_2}=\frac{\mu_{12}}{m_2} \tag{2}$$

and we define the reduced masses $\mu_{ij}=m_im_j/(m_i+m_j)$ and $\nu_{ij}=(m_i+m_j)m_k/(m_i+m_j+m_k)$, $i\neq j\neq k$. Since the particles interact in pairs through Coulombic potentials $V_{ij}=Z_iZ_j/r_{ij}$, the Schrödinger equation for any given Jacobi pair $\{\mathbf{r}_{ij},\mathbf{R}_{ij}\}$ is

$$\left[-\frac{1}{2\mu_{ij}}\nabla^2_{\mathbf{r}_{ij}}-\frac{1}{2\nu_{ij}}\nabla^2_{\mathbf{R}_{ij}}+V_{12}+V_{23}+V_{13}\right]\overline{\Psi}(\mathbf{r}_{ij},\mathbf{R}_{ij})$$
$$=E\overline{\Psi}(\mathbf{r}_{ij},\mathbf{R}_{ij}), \tag{3}$$

where the eigenenergy will be written considering that all the particles are in the continuum and the pair $\{\mathbf{k}_{ij},\mathbf{K}_{ij}\}$ represents the conjugated momenta to $\{\mathbf{r}_{ij},\mathbf{R}_{ij}\}$. We choose the Jacobi pair $\{\mathbf{r}_{12},\mathbf{R}_{12}\}$, but the selection of this pair is arbitrary. The use of other Jacobi coordinates leads to equivalent equations, which do not affect the following results.

The set of the six Cartesians coordinates $\{\mathbf{r}_{12}=(x,y,z),\mathbf{R}_{12}=(X,Y,Z)\}$ completely defines the problem. These coordinates can be replaced by any convenient set of curvilinear ones. The particular case of the parabolic set resembles the treatment of the two-body Coulomb problem and it has been successfully used by some authors when studying the approximate solution to Eq. (3). These coordinates have been proposed by Klar and allow one to separate the Schrödinger equation when all the particles are far from each other [17]. Using relations (1), this parabolic set of coordinates $\{\xi_i,\eta_i\}$ can be defined in terms of $\mathbf{r}_{ij}$ as

$$\xi_1=r_{32}+\hat{\mathbf{k}}_{23}\cdot\hat{\mathbf{r}}_{32},\quad \eta_1=r_{32}-\hat{\mathbf{k}}_{23}\cdot\hat{\mathbf{r}}_{32},$$

$$\xi_2=r_{13}+\hat{\mathbf{k}}_{13}\cdot\hat{\mathbf{r}}_{13},\quad \eta_2=r_{13}-\hat{\mathbf{k}}_{13}\cdot\hat{\mathbf{r}}_{13},\quad \xi_3=r_{12}+\hat{\mathbf{k}}_{12}\cdot\hat{\mathbf{r}}_{12},$$

$$\eta_3=r_{12}-\hat{\mathbf{k}}_{12}\cdot\hat{\mathbf{r}}_{12}, \tag{4}$$

where $\hat{\mathbf{k}}_{13}$ and $\hat{\mathbf{k}}_{23}$ are the unit vectors determined by the directions of the relative momenta

$$\mathbf{k}_{13}=\frac{\mu_{13}}{\nu_{12}}\mathbf{k}_{12}-\frac{a_{12}\mu_{13}}{\mu_{12}}\mathbf{K}_{12},\quad \mathbf{k}_{23}=\frac{\mu_{23}}{\nu_{12}}\mathbf{k}_{12}+\frac{b_{12}\mu_{23}}{\mu_{12}}\mathbf{K}_{12}. \tag{5}$$

Coordinates given by Eqs. (4) allow a natural expression of Coulombic asymptotic conditions for the three-body wave function.

II. APPROXIMATE SOLUTIONS TO THE WAVE EQUATION

Consider a final state of a collision process between a charged projectile 1 and a target arrangement. The final state is the one in which the target is formed by a particle labeled 3, which may be an electron, and a charged particle 2, both interacting through Coulomb potentials giving rise to a three-body final continuum state. The dynamic of the particles is governed by the three-body Schrödinger equation. Because we are looking for continuum states, we remove the kinetic energy by

$$\overline{\Psi}(\mathbf{r}_{12},\mathbf{R}_{12})=(2\pi)^{-3/2}e^{i\mathbf{K}_{12}\cdot\mathbf{R}_{12}+i\mathbf{k}_{12}\cdot\mathbf{r}_{12}}\Psi(\mathbf{r}_{12},\mathbf{R}_{12}) \tag{6}$$

in Eq. (3), which leads to

$$\left[\frac{1}{2\mu_{12}}\nabla^2_{\mathbf{r}_{12}}+\frac{1}{2\nu_{12}}\nabla^2_{\mathbf{R}_{12}}+\frac{i}{\mu_{12}}\mathbf{K}_{12}\cdot\nabla_{\mathbf{r}_{12}}+\frac{i}{\nu_{12}}\mathbf{k}_{12}\cdot\nabla_{\mathbf{R}_{12}}-\frac{Z_1Z_2}{r_{12}}-\frac{Z_2Z_3}{r_{23}}-\frac{Z_1Z_3}{r_{13}}\right]\Psi(\mathbf{r}_{12},\mathbf{R}_{12})=0 \tag{7}$$

since the eigenenergy in the state $\Psi(\mathbf{r}_{12},\mathbf{R}_{12})$ is $E=k_{12}^2/2\mu_{12}+K_{12}^2/2\nu_{12}$.

As was shown by Klar [17], the Schrödinger equation acquires a symmetric aspect written in term of the set (4),

$$D\Psi=[D_0+D_1]\Psi=0, \tag{8}$$

where D_0 and D_1 are given by

$$D_0=\sum_{i=1,i\neq j\neq k}^{3}[A_i^{+}+A_i^{-}+V_{jk}], \tag{9}$$

$$D_1=\sum_{i=1}^{2}\sum_{j=i+1}^{3}\frac{(-1)^{i+1}}{m_k}\mathbf{B}_i\cdot\mathbf{B}_j \tag{10}$$

and we have defined the operators

$$A_i^{+}=\frac{2}{\mu_{jk}(\xi_i+\eta_i)}\left[\xi_i\frac{\partial^2}{\partial\xi_i^2}+(1+ik_{jk}\xi_i)\frac{\partial}{\partial\xi_i}\right],$$

$$A_i^{-}=\frac{2}{\mu_{jk}(\xi_i+\eta_i)}\left[\eta_i\frac{\partial^2}{\partial\eta_i^2}+(1-ik_{jk}\eta_i)\frac{\partial}{\partial\eta_i}\right],$$

$$\mathbf{B}_i=(\nabla_{\mathbf{r}_{jk}}\xi_i)\frac{\partial}{\partial\xi_i}+(\nabla_{\mathbf{r}_{jk}}\eta_i)\frac{\partial}{\partial\eta_i}. \tag{11}$$

The vector scalar products in D_1 can be expressed in the terms of parabolic coordinates. We observe that D_0 contains one-variable derivatives and the mixed derivatives are all included in D_1. The D_1 term contains the well-known non-orthogonal kinetic energy of CDW theories [7].

Equation (8) is a six-variable elliptical partial differential equation with a non-denumerable infinite number of solutions. We will look for some of those solutions with physical meaning, assuming that Eq. (8) is separable in a system of coupled differential equations. A possible separation is given by [17]

$$D_0\Psi=0, \tag{12}$$

$$D_1\Psi=0. \tag{13}$$

The main feature of this system is that the first equation itself is totally separable. All three terms in D_0 are equivalent to the two-body Coulomb problem, where azimuthal symmetry was imposed around the relative momenta $\mathbf{k}_{ij}$. Equation (12) describes the dynamic of a problem where each pair of particles interacts through a Coulombic potential while the other particle is considered free. The D_1 term couples the three ''independent'' pairs and correlates their kinetic energy.

Neglecting D_1, a general solution to Eq. (12) can be obtained by proposing a separable function

$$\Psi=\prod_{l=1}^{3}f_l(\xi_l,\eta_l) \tag{14}$$

such that (12) splits in three equations. As was analyzed by Klar, the different solutions depend on the asymptotic behavior imposed on the wave function [17]. For outgoing asymptotic conditions the ansatz (14) reduces to

$$\Psi_{C3}=\prod_{l=1}^{3}f_l(\xi_l) \tag{15}$$

and the corresponding solutions $f_l(\xi_l)$ are $(l\neq m\neq n)$ [18]

$$f_l(\xi_l)=N_l\,{}_1F_1(i\alpha_{mn},1,-ik_{mn}\xi_l), \tag{16}$$

where N_l are the constants that normalize the wave function to outgoing unit flux

$$N_l=e^{-\pi\alpha_{mn}/2}\Gamma(1-i\alpha_{mn}) \tag{17}$$

and $\alpha_{mn}=Z_mZ_n/k_{mn}$.

The wave function (15) is commonly known as the $C3$ function and was proposed by Garibotti and Miraglia [9] to study the ion-atom ionization process. As was shown by Berakdar, Ψ_{C3} is an exact asymptotic solution of Eq. (7) only in a limited region of the coordinate space since

$$D_1\Psi_{C3}\sim O\left(\frac{1}{r_{ij}^2}\right) \tag{18}$$

when all the interparticle distances tend to infinity [13]. Consequently, Ψ_{C3} is not a suitable solution for the three-body problem in the condensation region where the distances between the particles are small.

Similar solutions can be written for other asymptotic conditions, which are dictated by the physical properties of the system. For example, the final state of an ion-atom ionization process should correspond to a boundary condition with three outgoing waves, while two incoming and one outgoing wave would be a proper boundary condition for the final state of a capture to the continuum process. The $C3$ function has been widely used to calculate transition matrices and differential cross sections of atomic ionization by electron and ion impact.

The function Ψ_{C3} is physically aceptable in the asymptotic region [19]. However, for finite distances, coupling between two-body motion and the third particle must be relevant. This means that we should look for other decompositions of the operator D, alternative to that given by Eqs. (12) and (13). This can be done in infinite ways. Therefore, rather than propose a decomposition of the operator and then look for solutions, we will assume a definite shape for the wave function and then derive the proper decomposition for D. First, we should point out that there are different masses included in D_0 and D_1 that introduce a particular asymmetry that results in an important problem at the moment of proposing solutions in a general case. Assuming $m_1, m_2 \gg m_3$, we deal with continuum states from an ionization process of atomic systems by heavy particles, where the particle labeled m_3 represents the electron. This allows us to neglect the two terms of Eq. (10) that contain the heavy masses m_1 and m_2. Thus the expression for D_1 reduces to

$$D_1=\frac{1}{m_3}\left[a^{-+}\frac{\partial^2}{\partial\xi_1\partial\xi_2}+a^{--}\frac{\partial^2}{\partial\xi_1\partial\eta_2}+a^{++}\frac{\partial^2}{\partial\eta_1\partial\xi_2}+a^{+-}\frac{\partial^2}{\partial\eta_1\partial\eta_2}\right],$$

where we have defined

$$a^{\pm\pm}\equiv a^{\pm\pm}(\xi_1,\eta_1,\xi_2,\eta_2,\xi_3,\eta_3)=(\hat{\mathbf{r}}_{23}\pm\hat{\mathbf{k}}_{23})\cdot(\hat{\mathbf{r}}_{13}\pm\hat{\mathbf{k}}_{13}).$$

On this basis, the simplest generalization to Eq. (14) is

$$\Psi=\varphi(\xi_1,\eta_1,\xi_2,\eta_2)\chi(\xi_3,\eta_3). \tag{19}$$

This ansatz introduces a coupling between the motion of the light particle relative to the two heavy ions.

The application of operator D to the wave function (19) gives

$$\frac{1}{\chi}[A_3^{+}+A_3^{-}+V_{12}]\chi+\frac{1}{\varphi}\left[\sum_{j=1}^{2}(A_j^{+}+A_j^{-}+V_{j3})+D_1\right]\varphi=0,$$

where the $A_j^{\pm}$ operators are defined by Eqs. (11). We separate this equation as

$$[A_3^{+}+A_3^{-}+V_{12}]\chi=0, \tag{20}$$

$$\left[\sum_{j=1}^{2}(A_j^{+}+A_j^{-}+V_{j3})+D_1\right]\varphi=0. \tag{21}$$

This separation of the wave equation is an alternative to that given by Eqs. (12) and (13). It is also arbitrary because the coefficients $a^{\pm\pm}$ in D_1 depend on the six parabolic variables, but guided by the physical assumptions, i.e., in the description of the dynamics of the heavy particles we neglect the influence of the light one. Equation (20) has as a solution a two-body Coulomb wave function that can be outgoing or incoming according to the required asymptotic conditions.

Now we consider Eq. (21), which is a four-variable partial differential equation. The operator D_1 depends on ξ_3 and η_3 and therefore φ would be parametrically dependent on these two variables. To obtain a solution that couples the relative motion between the pairs of particles (1,3) and (2,3) we should take into account in Eq. (21) the mixed derivatives included in D_1 at least in a suitable approximated way.

We will look for solutions of this system that verify outgoing asymptotic conditions. As in Eq. (15), one way to satisfy these requirements is to assume

$$\varphi=\varphi(\xi_1,\xi_2). \tag{22}$$

Then Eq. (21) reduces to a two-variable equation

$$\left[\sum_{j=1}^{2}(A_j^{+}+V_{j3})+D_1\right]\varphi=0. \tag{23}$$

Equation (23) still includes the dependence on the other parabolic coordinates in a parametric way. The evaluation of the function a^{-+} requires the expressions of Cartesian coordinates in terms of the parabolic ones. This must be interpreted as a transformation in the six-dimensional phase space from $(\mathbf{r}_{ij},\mathbf{R}_{ij},\mathbf{k}_{ij},\mathbf{K}_{ij})$ to $(\boldsymbol{\xi}_i,\eta_i,\mathbf{k}_{13},\mathbf{k}_{23})$ and shows that a^{-+} is a very involved algebraic function of the parabolic variables.

The solution of Eq. (23) is unknown. When D_1 is neglected, Eq. (23) separates in two independent equations and its solution is a product of two single-variable confluent hypergeometric functions. Even when D_1 is not neglected, Eq. (23) can be separated in a system of two *coupled* second-order differential equations. The best-known systems of this kind are associated with two-variable hypergeometric functions [20]. However, the reduction of Eq. (23) to one of those systems requires a particular choice of a^{-+} that should lead to a solution with correct physical properties. We observe that a^{-+} contains the additive terms

$$a_1^{-+}=\frac{1}{m_3}\left[\frac{\xi_1}{\xi_2+\eta_2}+\frac{\xi_2}{\xi_1+\eta_1}\right] \tag{24}$$

such that $a^{-+}=a_1^{-+}+a_2^{-+}$. Then we are able to separate Eq. (23) as

$$\left[\sum_{j=1}^{2}(A_j^{+}+V_{j3})+a_1^{-+}\frac{\partial^2}{\partial\xi_1\partial\xi_2}\right]\varphi=0, \quad (25)$$

$$a_2^{-+}\frac{\partial^2\varphi}{\partial\xi_1\partial\xi_2}=0. \quad (26)$$

Equation (25) can be separated again into

$$\left[\xi_1\frac{\partial^2}{\partial\xi_1^2}+\frac{\mu_{23}}{m_3}\xi_2\frac{\partial^2}{\partial\xi_1\partial\xi_2}+(1+ik_{23}\xi_1)\frac{\partial}{\partial\xi_1}+\mu_{23}Z_2Z_3\right]\varphi=0,$$

$$\left[\xi_2\frac{\partial^2}{\partial\xi_2^2}+\frac{\mu_{13}}{m_3}\xi_1\frac{\partial^2}{\partial\xi_2\partial\xi_1}+(1+ik_{13}\xi_2)\frac{\partial}{\partial\xi_2}+\mu_{13}Z_1Z_3\right]\varphi=0. \quad (27)$$

Thus an outgoing analytical solution of Eq. (8) for one electron and two heavy ions when $a_2^{-+}(\partial^2\varphi/\partial\xi_1\partial\xi_2)$ is neglected can be given in terms of confluent hypergeometric functions as

$$\Psi_1=N\varphi(\xi_1,\xi_2)\chi(\xi_3), \quad (28)$$

where

$$\varphi(\xi_1,\xi_2)=\Phi_2(i\alpha_{23},i\alpha_{13},1,-ik_{23}\xi_1,-ik_{13}\xi_2), \quad (29)$$

$$\chi(\xi_3)={}_1F_1(i\alpha_{12},1,-ik_{12}\xi_3). \quad (30)$$

That is to say, Eq. (29) is an exact solution of Eq. (27) and N is a normalization constant. The function $\Phi_2(a,a',b,x,y)$ is a generalized confluent hypergeometric defined by (see the Appendix)

$$\Phi_2(a,a',b,x,y)=\sum_{m,n}\frac{(a)_m(a')_n}{(b)_{m+n}}\frac{x^m}{m!}\frac{y^n}{n!}. \quad (31)$$

In Sec. III we will prove that Ψ_1 has correct physical properties.

Even though Eq. (28) is an approximate solution of Eq. (8), we see that it is possible to find solutions that couple the variables. This can be considered as a first step to solve the Schrödinger equation in a closed form through the use of generalized multiple-variable functions. Of course a complete coupling of the six variables $\{\xi_i,\eta_i\}$ should be expected in a general solution. There exists the possibility that the full equation (8) could be separated into a set of six coupled differential equations. This system could have solutions expressed as many-variable hypergeometric functions. However, the study of this topic is precluded by the poor knowledge of the mathematical properties of Lauricella functions and their corresponding systems of differential equations.

In addition to the wave function (29), there exist other approximate solutions, with the form of Eq. (19), that can be written in terms of generalized confluent hypergeometric functions (see the Appendix)

$$\Psi=\begin{cases} N\ {}_1F_1(i\alpha_{12},1,-ik_{12}\xi_3)G_1, & \left|\frac{k_{23}\xi_1}{k_{13}\xi_2}\right|<1\\ N\ {}_1F_1(i\alpha_{12},1,-ik_{12}\xi_3)G_2, & \left|\frac{k_{23}\xi_1}{k_{13}\xi_2}\right|>1,\end{cases} \quad (32)$$

where

$$G_1=\left(\frac{k_{23}\xi_1}{k_{13}\xi_2}\right)^{i\alpha_{13}}\Phi_1\left(i\alpha_{23}+i\alpha_{13},i\alpha_{13},1+i\alpha_{13},\frac{k_{23}\xi_1}{k_{13}\xi_2},-ik_{23}\xi_1\right), \quad (33)$$

$$G_2=\left(\frac{k_{23}\xi_1}{k_{13}\xi_2}\right)^{-i\alpha_{23}}\Phi_1\left(i\alpha_{23}+i\alpha_{13},i\alpha_{23},1+i\alpha_{23},\frac{k_{13}\xi_2}{k_{23}\xi_1},-ik_{13}\xi_2\right), \quad (34)$$

and N is a normalization constant. All the features of these wave functions will be analyzed elsewhere [21].

There are eight different solutions to equations similar to Eq. (28). These are all the different ways to group the variables that lead to alternative asymptotic behavior. If we take the normalization constant N in such a way that we have a unit of outgoing flux, then the wave function (29) is written as

$$\Psi_1=N\ \ \Phi_2(i\alpha_{23},i\alpha_{13},1,-ik_{23}\xi_1,-ik_{13}\xi_2)\times{}_1F_1(i\alpha_{12},1,-ik_{12}\xi_3), \quad (35)$$

with

$$N=e^{(\pi/2)(\alpha_{12}+\alpha_{13}+\alpha_{23})}\Gamma(1-i\alpha_{12})\Gamma(1-i\alpha_{13}-i\alpha_{23}). \quad (36)$$

We have obtained a set of approximate solutions to the Schrödinger equation for three charged particles under the condition that two of them are heavier than the other one. This solution should fulfill some physical properties in order to be eligible for the calculation of transition matrices. These properties are analyzed in detail in the following section.

III. PROPERTIES OF THE WAVE FUNCTION

In this section we will perform a detailed analysis of the properties of this two-center continuum wave function. First, we analyze the general properties and then we discuss the asymptotic behavior of the wave function.

A. General properties

According to the previous sections, the function Ψ_1 constructed with the coupled variables (19) describes the motion of Coulomb particles in generalized parabolic coordinates $\{\xi_i\}$ as is the case of Ψ_{C3}, assuming, of course, the same asymptotic behavior, i.e., outgoing waves. In contrast to Ψ_{C3}, the wave function Ψ_1 does not separate into a product of three two-body Coulomb continuum states, but decouples the problem into a two-body Coulomb continuum state for the dynamic of the heavy particles and a function that correlates the motion of the electron to them. An interesting result can be obtained using the series expansion in terms of the coordinates [Eq. (A6)]

$$\Psi_1 = N\ {}_1F_1(i\alpha_{12},1,-ik_{12}\xi_3)\sum_m (-1)^m \frac{(i\alpha_{13})_m(i\alpha_{23})_m}{m!(m)_m(1)_{2m}} \times [k_{23}\xi_1]^m[k_{13}\xi_2]^m {}_1F_1(i\alpha_{23}+m,1+2m,-ik_{23}\xi_1) \times {}_1F_1(i\alpha_{13}+m,1+2m,-ik_{13}\xi_2). \tag{37}$$

It can be seen from Eq. (37) that the Ψ_{C3} is included as a first order of this series expansion. Certainly, it is a consequence of the two-center behavior of Ψ_1. Thus, if the interaction between the two pairs of particles (1,3) and (2,3) does not exist, the best representation is the product of the two independent one-center wave functions, as in the $C3$ case. Now, to make a comparative analysis of this wave function we take the square module of Eq. (35), which can be considered as a quantum-mechanical particle distribution. We define

$$\tilde{n}(\alpha,\xi) = |\Psi_1|^2 = \tilde{n}(\alpha,0)|\Phi_2(i\alpha_{23},i\alpha_{13},1,-ik_{23}\xi_1,-ik_{13}\xi_2) \times {}_1F_1(i\alpha_{12},1,-ik_{12}\xi_3)|^2, \tag{38}$$

where we have included the constant of normalization given by Eq. (36) to the unit of outgoing flux as $\tilde{n}(\alpha,0)=|N|^2$, which gives the density along the directions $\hat{\mathbf{k}}_{ij}$. In these directions $a_2^{-+}(\partial^2\varphi/\partial\xi_1\partial\xi_2)=0$ and the above density agrees with the exact one. As we can see, the dependence of the particle distribution on the position vector $\mathbf{r}_{ij}$ is through the variables $\xi=\{\xi_i,\ i=1,2,3\}$, but it also depends on the Sommerfeld parameters $\alpha=\{\alpha_{12},\alpha_{23},\alpha_{13}\}$ corresponding to each interaction.

Thus the function $\tilde{n}(\alpha,\xi)$ describes the particle distribution of the three-body problem through the approximated solution Ψ_1. Now, as stated before, the differences between $C3$ and the solution (35) come from the function Φ_2. Then, to see these differences we define a reduced particle distribution $n(\alpha_{13},\alpha_{23},\xi_1,\xi_2)$,

$$n(\alpha_{13},\alpha_{23},\xi_1,\xi_2) = n(\alpha_{13},\alpha_{23},0)|\Phi_2(i\alpha_{23},i\alpha_{13},1,-ik_{23}\xi_1,-ik_{13}\xi_2)|^2, \tag{39}$$

where

$$n(\alpha_{13},\alpha_{23},0) = |e^{\pi[(\alpha_{13}+\alpha_{23})/2]}\Gamma(1-\alpha_{13}-\alpha_{23})|^2 = \frac{2\pi(\alpha_{13}+\alpha_{23})}{1-e^{-2\pi(\alpha_{13}+\alpha_{23})}}. \tag{40}$$

We may write a particle distribution associated with the dynamics of the electron in the potential of particles 1 and 2 as described by our approximate solution of Eq. (8). The function $n(\alpha_{13},\alpha_{23},0)$ in Eq. (40) gives us the density along the directions $\hat{\mathbf{k}}_{23}\cdot\hat{\mathbf{r}}_{23}=0$ and $\hat{\mathbf{k}}_{13}\cdot\hat{\mathbf{r}}_{13}=0$.

The first distinctive characteristic between Ψ_{C3} and Ψ_1 is related to the normalization factor, that is through the particle distribution $n(\alpha_{13},\alpha_{23},0)$ and $n_{C3}(\alpha_{13},\alpha_{23},0)$. As we can see from Eqs. (17) and (40)

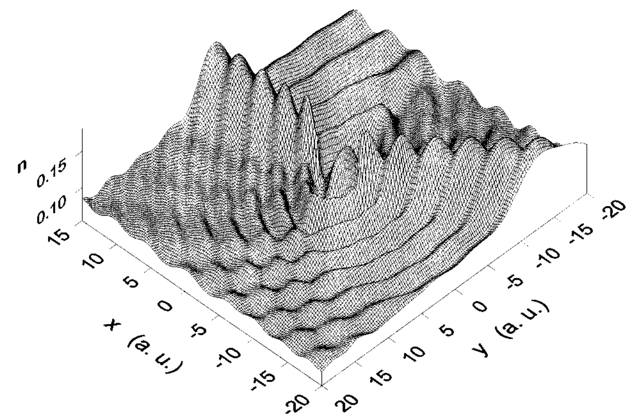

FIG. 2. Reduced particle distribution $n(\alpha_{13},\alpha_{23},\mathbf{r}_{12},\mathbf{R}_{12})/n(\alpha,0)$ as a function of the $\mathbf{r}_{23}$ coordinate for $\mathbf{k}_{23}=(1\ \text{a.u.})\hat{\mathbf{x}}$, $\mathbf{k}_{13}=(1\ \text{a.u.})(\hat{\mathbf{x}}+\hat{\mathbf{y}})$, and $\mathbf{r}_{12}=-(6\ \text{a.u.})\hat{\mathbf{x}}$.

$$n_{C3}(\alpha_{13},\alpha_{23},0) = N_2N_3 = \frac{4\pi^2\alpha_{13}\alpha_{23}}{(e^{2\pi\alpha_{13}}-1)(e^{2\pi\alpha_{23}}-1)}. \tag{41}$$

the functional form of this equation is very different. In fact, $n(\alpha_{13},\alpha_{23},0)$ presents the characteristics of the two-center function, that is, the density is not separable as the product of two coefficients as in the case of Eq. (41).

Since in the spectra of the electrons emitted in bare ion-atom collisions the normalization factor $\tilde{n}(\alpha,0)$ gives rise to the forward cusps known as soft electron (SE) and electron capture to the continuum (ECC) peaks in the double differential cross sections, as a function of the electron velocity, the differences between $n(\alpha_{13},\alpha_{23},0)$ and $n_{C3}(\alpha_{13},\alpha_{23},0)$ become important [22–24]. The principal shortcoming presented by $\tilde{n}_{C3}(\alpha,0)$ is that it describes the ECC and the soft electron as two independent structures [25]; however, only for large relatives velocities between the projectile and target can this assumption be considered correct. On the other hand, $\tilde{n}(\alpha,0)$, given by Eq. (38), may give a better description of these structures due to the two-center form introduced by Eq. (40). The ECC peak is located at a velocity of the electron relative to the projectile that is equal to zero and the SE peak appears at a velocity equal to zero relative to the target. These peaks are due to the diverging number of states available at the threshold of the projectile and the target continuum and their asymmetry results from the residual two-center effect. Even though the principal features of asymmetry of the soft electron and ECC peaks are due to the behavior of the wave function for small relative velocities, the two-center particle density $\tilde{n}(\alpha,0)$ can take an important role in its description because it could be interpreted as a Jost function for a two-center wave function [26]. Furthermore, it is possible that $\tilde{n}(\alpha,0)$ also improves the description of the collision process in the zone between the target and projectile, in the velocity space, because Eq. (40) is larger than $\tilde{n}_{C3}(\alpha,0)$ in this region.

In Fig. 2 we show an example of the particle distribution given by Eq. (39) in the configuration space where we have

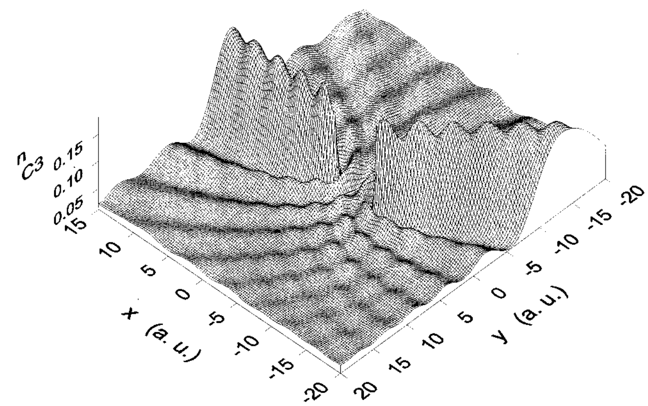

FIG. 3. Similar to Fig. 2, but for $n_{C3}(\alpha_{13},\alpha_{23},\mathbf{r}_{12},\mathbf{R}_{12})/n_{C3}(\alpha,0)$.

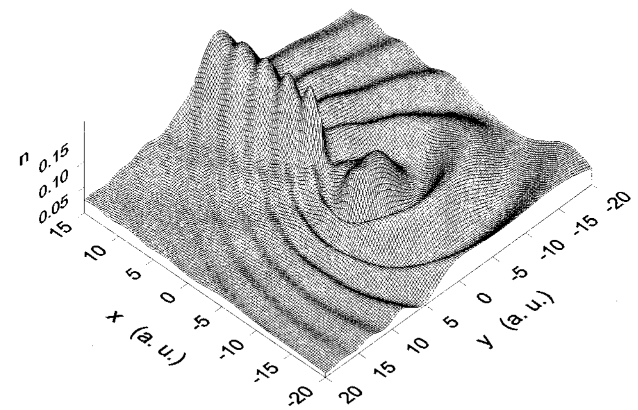

FIG. 4. Reduced particle distribution $n(\alpha_{13},\alpha_{23},\mathbf{r}_{12},\mathbf{R}_{12})/n(\alpha,0)$ with $\mathbf{k}_{23}=10^{-2}$ (a.u.)$\hat{\mathbf{x}}$. The other magnitudes are the same as in Fig. 2.

set the origin at $\mathbf{r}_{23}=0$. The figure shows $n(\alpha_{13},\alpha_{23},\mathbf{r}_{12},\mathbf{R}_{12})/n(\alpha,0)$ for a fixed distance between the heavy particles. Here $r_{12}=6$ a.u. along the x coordinate and $k_{23}=k_{13}=1$ a.u., where $\hat{\mathbf{k}}_{23}$ is antiparallel to the relative position vector $\mathbf{r}_{12}$. The unit vector $\hat{\mathbf{k}}_{13}$ forms an angle of $\pi/4$ with the $\hat{\mathbf{k}}_{23}$ direction, which defines the value of $k_{12}=1.41$ a.u. The charge of the particles are $Z_1=Z_2=1$ and $Z_3=-1$.

In Fig. 3 we show a representation of $n_{C3}(\alpha_{13},\alpha_{23},\mathbf{r}_{12},\mathbf{R}_{12})/n_{C3}(\alpha,0)$ for the same conditions. Evident in both distributions are the confluent hypergeometric fins along the directions defined by the conditions $\hat{\mathbf{k}}_{23}\cdot\hat{\mathbf{r}}_{23}=-1$ and $\hat{\mathbf{k}}_{13}\cdot\hat{\mathbf{r}}_{13}=1$. In other directions, n_{C3} shows the simple superposition of the hyperbolically shaped waves associated with both one-variable hypergeometric functions without any correlation between them. Meanwhile, in $n(\alpha_{13},\alpha_{23},\mathbf{r}_{12},\mathbf{R}_{12})$ the fins are connected through the coordinate space, showing that the relative motions are correlated. We observe that a two-center symmetry dominates over the hyperbolic one in the region where the interactions are competitive. Furthermore, the n distribution is enhanced relatively to n_{C3} in the region between the heavy particles, i.e., the saddle between the Coulomb potentials. This shows that the wave function accounts for two-center effects. In addition, the n distribution exhibits a shape similar to n_{C3} for large values of r_{23}. This indicates that the corresponding wave functions have the same correct asymptotic behavior. These general features of the particle distributions remain similar for others set of values $\{R_{12},k_{23},k_{13},Z_1,Z_2\}$. We should note that $n(\alpha_{13},\alpha_{23},\mathbf{r}_{12},\mathbf{R}_{12})$ is exact along the directions of k_{13} and k_{23} since the function Ψ_1 is a solution of the wave equation in this case.

When the particle densities for the two-body Coulomb problems are described, the mentioned fins become a unique maximum along one particular direction, the direction of the relative momentum between the particles. For this case the maximum could be associated with a well-known optical effect: the glory or the rainbow caustics depending of the sign of the intervening charges. When these charges are taken as, for example, our 2 and 3 particles, then we are dealing with the glory effect [26]. Thus, even when this phenomenon is unknown for the three-body Coulomb problem we may think that the maxima result for an effect similar to that occurring in the two-body problem.

Now we will discuss several limiting cases of physical interest. The wave function gives a description equivalent to the $C3$ approach for the relative motion of the heavy particles. However, it is well known that the normalization factor corresponding to the projectile-target wave function leads to an exponential decrease in the cross sections for large values of the corresponding Bohr parameter attained either for small relative momenta k_{12} or large Z_1. This can be avoided through a suitable modification of the Born parameter that appears in the normalization factor N_3 and has been discussed elsewhere [13].

The limit for soft electron emission results when the module of the asymptotic momentum k_{23} becomes small. In this case the wave function is expressed by

$$\Psi_1=N\ {}_1F_1(i\alpha_{12},1,-ik_{12}\xi_3)\sum_m \frac{1}{(Z_2Z_3)^m}\frac{(i\alpha_{13})_m}{m!(m)_m}\times[k_{23}\xi_1]^m J_{2m}(-2i\sqrt{Z_2Z_3\xi_1})\times{}_1F_1(i\alpha_{13}+m,1+2m,-ik_{13}\xi_2), \tag{42}$$

which has a significative different functional form when compared with the behavior of $C3$ [27]. As we can see the series (42) depends on the position and momentum of the electron relative to the target and therefore includes a two-center effect in the description of the electron wave function near the ionization threshold.

In Fig. 4 the particle density $n(\alpha_{13},\alpha_{23},\mathbf{r}_{12},\mathbf{R}_{12})/n(\alpha,0)$ is shown for $k_{23}=10^{-2}$ a.u. and $k_{13}=1$ a.u. The coordinates, angles, etc. are the same as those in Figs. 2 and 3. The three-body problem considered again is one formed by two charged heavy particles and one electron. It is clear from the figure that the density of electrons is dominated by the target-electron interaction still in $n_{C3}(\alpha_{13},\alpha_{23},\mathbf{r}_{12},\mathbf{R}_{12})$; see Fig. 5. The electrons are distributed around the target in a way similar to the two-body Coulomb problem and an evident correlation still exists between the different maxima of the distribution. The mentioned maxima have superposed oscillations, reminiscence of the

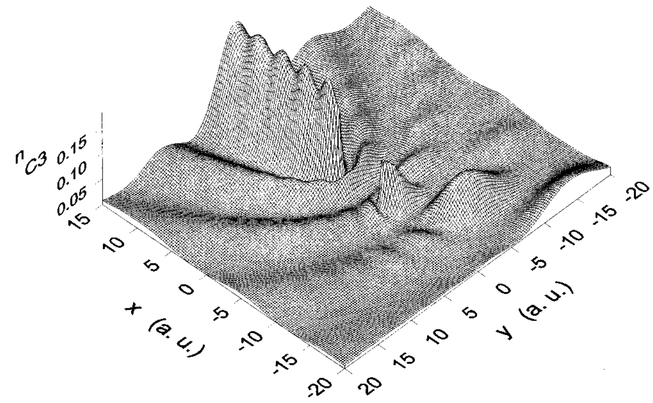

FIG. 5. Similar to Fig. 4, but for $n_{C3}(\alpha_{13},\alpha_{23},\mathbf{r}_{12},\mathbf{R}_{12})/n_{C3}(\alpha,0)$.

two-body Coulomb problem, just as in the case of $n_{C3}(\alpha_{13},\alpha_{23},\mathbf{r}_{12},\mathbf{R}_{12})$; see Fig. 5.

As we see, the dynamic of the electron is correlated even for small relatives velocities, which is not the case of the density given by $n_{C3}(\alpha_{13},\alpha_{23},\mathbf{r}_{12},\mathbf{R}_{12})$. Having in mind the behavior of the electron in this field, we can suggest that the correlation shown by $n(\alpha_{13},\alpha_{23},\mathbf{r}_{12},\mathbf{R}_{12})$ gives rise to the enhancement presented by the DDCS all along the velocities comprised between the ECC and the soft electron peaks.

An equation similar to Eq. (42) could be written when $k_{13}\to 0$. The ECC peak asymmetry is associated with the wave function at this limit. The expression for Ψ_{C3} function in this region is easy to obtain and gives the continuation through the threshold predicted by the two-body Coulomb problem. Nevertheless, our wave function gives a very different description since it leaves the electron correlated to the target still in the case $k_{13}=0$.

For small values of the total energy E the form of the wave function is

$$\Psi_1 = C\sum_m \frac{1}{(Z_1 Z_3)^m}\frac{(-1)^m}{(Z_2 Z_3)^m}\frac{(i\alpha_{23})_m}{m!(m)_m} \times J_{2m}(-2i\sqrt{Z_2 Z_3 \xi_1})J_{2m}(-2i\sqrt{Z_1 Z_3 \xi_2}) \times J_0(-2i\sqrt{Z_1 Z_2 \xi_3}). \tag{43}$$

The behavior of the wave function when all the momenta are small, that is, the Wannier zone, could give us some information about the behavior of the transition matrix for a collision process in this energy range.

There are two important differences between Ψ_1 and Ψ_{C3}. The function Ψ_1 modifies the form of the Coulomb factor and the asymmetry of the SE and ECC peaks. A quantitative analysis through the evaluation of a TDCS or a DDCS with our wave function could show some details of these differences.

B. Asymptotic behavior

A critical point of every approximate solution for a three-body Coulomb problem is its asymptotic behavior. There are two kind of asymptotic regions that should be analyzed: Ω_0, all the interparticle distances tend to infinity in an arbitrary manner, i.e., $r_{ij}\to\infty$, and Ω_j, where the distance between particle j and the center of mass of the pair (k,l) tends to infinity, i.e., $R_{kl}\to\infty$, while the distance between particles k and l satisfies the constraint $r_{kl}/R_{kl}\to 0$.

As was shown by Alt and Mukhamedzhanov [14], the Schrödinger equation can be solved in a closed form up to order $1/d_j^2$, where d_j stands for the interparticle distances that go to infinity in each asymptotic region Ω_j. Furthermore, a test for every new approximate wave function is that, asymptotically, it should be a solution of the wave equation in this sense.

Just for simplicity we confine the treatment to outgoing waves and restrict the analysis only for Eq. (35) since similar conclusions can be obtained with the other asymptotic conditions. As a first step we study the case Ω_0. The behavior of the confluent hypergeometric ${}_1F_1(a,b,z)$ for large values of the argument is well known and the generalized confluent hypergeometric function $\Phi_2(a,a',b,x,y)$ is representable by a convergent series of two variables, as we have shown in Eqs. (31)–(37). In the same way as for ${}_1F_1(a,b,z)$, Φ_2 has an asymptotic representation in terms of generalized Whittaker's functions of two variables, see the Appendix. There are different representation of Φ_2 in term of Whittaker's functions depending on which variable, x or y, tends to infinity. If we use the expansion for the case $x\to\infty$, $y\to\infty$, and $y-x\to\infty$ [Eq. (A7)] and write it in terms of the coordinates $\mathbf{r}_{ij}$, the asymptotic expansion for Φ_2 outside of the nonsingular region, i.e., $\hat{\mathbf{k}}_{ij}\cdot\hat{\mathbf{r}}_{ij}\neq 1$, reads

$$\begin{aligned}\Phi_2 \sim & \frac{e^{\pi(\alpha_{13}+\alpha_{23})}}{\Gamma(1-i\alpha_{13}-i\alpha_{23})} e^{-i\alpha_{23}\ln k_{23}\xi_1} e^{-i\alpha_{13}\ln k_{13}\xi_2} \\ & \times\left\{1+O\left(\frac{1}{k_{23}\xi_1},\frac{1}{k_{13}\xi_2}\right)\right\} \\ & -\frac{e^{\pi(\alpha_{13}-2\alpha_{13}-1)}}{\Gamma(i\alpha_{23})} e^{i(\alpha_{13}+\alpha_{23})\ln k_{23}\xi_1 - i\alpha_{13}\ln(k_{23}\xi_1-k_{13}\xi_2)} \\ & \times\frac{e^{ik_{23}\xi_1}}{k_{23}\xi_1}\left\{1+O\left(\frac{1}{k_{23}\xi_1},\frac{1}{k_{13}\xi_2}\right)\right\} \\ & -\frac{e^{\pi(\alpha_{13}-1)}}{\Gamma(i\alpha_{13})} e^{i(\alpha_{13}+\alpha_{23})\ln k_{13}\xi_2 - i\alpha_{23}\ln(k_{23}\xi_1-k_{13}\xi_2)} \\ & \times\frac{e^{ik_{13}\xi_2}}{k_{13}\xi_2}\left\{1+O\left(\frac{1}{k_{23}\xi_1},\frac{1}{k_{13}\xi_2}\right)\right\}.\end{aligned} \tag{44}$$

An inspection clearly shows that the leading term is

$$\Phi_2 \sim \frac{e^{(\pi/2)(\alpha_{13}+\alpha_{23})}}{\Gamma(1-i\alpha_{13}-i\alpha_{23})} e^{-i\alpha_{23}\ln k_{23}\xi_1} e^{-i\alpha_{13}\ln k_{13}\xi_2} + O\left(\frac{1}{\xi_1},\frac{1}{\xi_2}\right). \tag{45}$$

Hence, taking in account the asymptotic behavior of ${}_1F_1(a,b,z)$, Eq. (31) reduces to

$$\Psi_1 \sim \frac{e^{(\pi/2)(\alpha_{13}+\alpha_{12}+\alpha_{23})}}{\Gamma(1-i\alpha_{12})\Gamma(1-i\alpha_{13}-i\alpha_{23})} \times N e^{-i\alpha_{23}\ln k_{23}\xi_1 - i\alpha_{13}\ln k_{13}\xi_2 - i\alpha_{12}\ln k_{12}\xi_3}, \tag{46}$$

which has, in fact, exactly the same functional asymptotic behavior as the $C3$ wave function apart from a normalization constant. From Eq. (46) it is clear that we must take the constant N as given by Eq. (36) in order to normalize the wave function to an outgoing unit of flux.

We should note, as we said before, that the asymptotic functional form of our wave function Ψ_1 in this region is equal to Ψ_{C3}. However, they have different normalization factors: the first is a two-center factor, while the second is the superposition of two single-center factors. As we see, we may have different functions with the same asymptotic behavior and this can lead to different outgoing or incoming units of flux. This can be considered as the starting point in the search for normalization and the wave function, which take in account the three-center behavior. The main feature of our wave function is the two-center representation for the dynamics of the electron as depending on the coordinates associated with particles 1 and 2. This kind of representation leads to a normalization factor with the corresponding two-center behavior.

The wave function (35) gives the *Redmond asymptotic behavior* when all the interparticle distances tend to infinity. In the same way as for $C3$, our wave function is an exact solution up to $O(1/r_{ij}^2)$ of the total Schrödinger equation (8).

We can now consider the behavior of the wave function Ψ_1 in the regions Ω_j. First, we should point out that neither Ψ_{C3} nor Ψ_1 is an exact solution in Ω_j in the sense mentioned before because the neglected terms of the Hamiltonian in each approximation are of order $1/d_j$. However these terms can be considered as small corrections in each of the regions Ω_j and can be incorporated in the wave functions through a modification of relative momenta of each pair of particles. Alt and Mukhamezdanov have studied the case of the Ψ_{C3} function [14] and Colavecchia *et al.* devised a general method to obtain modifications required for a correct asymptotic behavior of the wave function in Ω_j [28].

We will briefly discuss the application of this method in the region Ω_1, where the target and the electron (particles 2 and 3, respectively) are close to each other, while the projectile is far from them. The asymptotic behavior of Eq. (35) when, for example, $\mathbf{r}_{23}$ is finite but $\mathbf{r}_{12}$ and $\mathbf{r}_{13}$ go to infinity, corresponding to the region of Ω_1, can be carried out using the asymptotic expansion of the hypergeometric function Φ_2 given by Eq. (A9), specialized to the present case. A fast inspection clearly shows that the leading term in that expansion is

$$\Phi_2 \sim \frac{e^{\pi\alpha_{13}}}{\Gamma(1-i\alpha_{13})} e^{-i\alpha_{13}\ln k_{13}\xi_2} \times \Phi_5\left(i\alpha_{23}, i\alpha_{13}, 1-i\alpha_{23}, -ik_{23}\xi_1, -\frac{1}{ik_{13}\xi_2}\right). \tag{47}$$

Hence, taking again into account the asymptotic behavior of the ${}_1F_1(a,b,z)$, Eq. (35) reduces to

$$\Psi_1 \sim N \frac{e^{\pi(\alpha_{12}+\alpha_{13})}}{\Gamma(1-i\alpha_{12})\Gamma(1-i\alpha_{13})} e^{-i\alpha_{12}\ln k_{12}\xi_3 - i\alpha_{13}\ln k_{13}\xi_2} \times \Phi_5\left(i\alpha_{23}, i\alpha_{13}, 1-i\alpha_{13}, -ik_{23}\xi_1, -\frac{1}{ik_{13}\xi_2}\right), \tag{48}$$

where $\Phi_5(a,a',c,x,1/y)$ is the generalized confluent hypergeometric of Whittaker given in the Appendix. Since this function is defined by a series convergent for small values of $|x|$ and large values of $|y|$, the partial derivative $\partial\Phi_5/\partial y$ is proportional to $1/y^2$. This will allow us to properly include the terms neglected in the Hamiltonian. Let us consider the leading orders of Ψ_1 as a function of parabolic coordinates

$$\Psi_1 \propto \mathcal{E}(\xi_3)\mathcal{E}(\xi_2) f(\xi_1, 1/\xi_2), \tag{49}$$

where $\mathcal{E}(\xi_j) = \exp(-i\alpha_{mn}\ln k_{mn}\xi_j)$ is an eikonal function and f represents the leading orders of the function Φ_5,

$$f(\xi_1, 1/\xi_2) \propto F(\xi_1) + G(\xi_1)/\xi_2, \tag{50}$$

where F and G are confluent hypergeometric functions of one variable and $\partial f/\partial\xi_2 \propto 1/\xi_2^2$. In this way we are considering that the asymptotic representation in the variables ξ_2 and ξ_3 is mainly given by the eikonal functions, while f introduces only a small coupling between ξ_1 and ξ_2. If we replace this ansatz in the Schrödinger equation and take into account the leading orders of each function, we obtain:

$$\frac{1}{\mu_{23}r_{23}}\left[\xi_1 \frac{\partial^2 f}{\partial \xi_1} + (1-ik_{23}\xi_1)\frac{\partial f}{\partial \xi_1} + \mu_{23}Z_2Z_3 f\right] + \frac{1}{m_3}\left[\frac{a^{-+}}{\mathcal{E}(\xi_2)} \frac{\partial \mathcal{E}(\xi_2)}{\partial \xi_2}\right]\frac{\partial f}{\partial \xi_1} + \frac{a^{-+}}{m_3}\frac{\partial^2 f}{\partial\xi_1\partial\xi_2} = 0. \tag{51}$$

The term that includes the partial derivative of the eikonal $\mathcal{E}(\xi_2)$ is of order $1/\xi_2$ and will be included as a small correction of the relative momenta k_{23}. In this way we can define

$$\mathbf{k}'_{23} = \mathbf{k}_{23} - \frac{\alpha_{13}}{r_{13}} \frac{\hat{\mathbf{r}}_{13} - \hat{\mathbf{k}}_{13}}{1 - \hat{\mathbf{k}}_{13}\cdot\hat{\mathbf{r}}_{13}}.$$

Now, the term that contains the mixed partial derivatives of the function f can be written as

$$a^{-+}\frac{\partial^2 f}{\partial\xi_1\partial\xi_2} = a_1^{-+}\frac{\partial^2 f}{\partial\xi_1\partial\xi_2} + a_2^{-+}\frac{\partial^2 f}{\partial\xi_1\partial\xi_2}. \tag{52}$$

If we take into account that f represents the asymptotic behavior of the wave function Ψ_1, the first term of the right-hand side of Eq. (52) is exactly considered, even in the region Ω_1. However, in this region $\partial^2 f/\partial\xi_1\partial\xi_2 \propto \xi_2^{-2}$ and therefore $a_2^{-+}(\partial^2 f/\partial\xi_1\partial\xi_2)$ will be included as a small correction of order $1/\xi_2$. Then we obtain the equation for f (up to order $1/\xi_2$)

$$\xi_1 \frac{\partial^2 f}{\partial \xi_1} + \xi_2 \frac{\partial^2 f}{\partial\xi_1\partial\xi_2} + (1+\gamma - ik'_{23}\xi_1)\frac{\partial f}{\partial \xi_1} + \mu_{23}Z_2Z_3 f = 0, \tag{53}$$

where

$$\gamma=\lim_{\Omega_1}\frac{\mathbf{r}_{12}}{r_{13}^2}\cdot\left(\frac{\mathbf{r}_{12}}{r_{13}r_{23}}+\frac{\hat{\mathbf{k}}_{13}}{r_{23}}+\frac{\hat{\mathbf{k}}_{23}}{r_{13}}\right).$$

It is clear that the solution of Eq. (53) is the leading order of the function Φ_5. We should remember that the two-variable function Φ_5 verifies a coupled system of two equations. However, it is easy to see that the second equation is of order greater than $1/\xi_2^2$ and can be neglected in this treatment. Therefore, we can obtain an exact solution in Ω_1, introducing small corrections in the function Ψ_1. This solution will match also the solution in Ω_0. In a similar way, we obtain the asymptotic functions in regions Ω_2 and Ω_3. In short, we have avoided the details of these calculations by writing down the final solution, exact up to order $1/d_j^2$ in all asymptotic regions:

$$\Psi_1'(\mathbf{r},\mathbf{R})=N'\,{}_1F_1(i\alpha_{tp}',1,-ik_{12}'\xi_3)\times\Phi_2(i\alpha_{23}',i\alpha_{13}',1+\gamma,-ik_{23}'\xi_1,-ik_{13}'\xi_2),\tag{54}$$

where the primed momenta are defined as

$$\mathbf{k}_{12}'=\mathbf{k}_{12}-\frac{\alpha_{23}b_{12}}{r_{23}}\frac{\hat{\mathbf{r}}_{23}+\hat{\mathbf{k}}_{23}}{1+\hat{\mathbf{k}}_{23}\cdot\hat{\mathbf{r}}_{23}}+\frac{\alpha_{13}a_{12}}{r_{13}}\frac{\hat{\mathbf{r}}_{13}-\hat{\mathbf{k}}_{13}}{1-\hat{\mathbf{k}}_{13}\cdot\hat{\mathbf{r}}_{13}},$$

$$\mathbf{k}_{13}'=\mathbf{k}_{13}-\frac{\alpha_{23}}{r_{23}}\frac{\hat{\mathbf{r}}_{23}+\hat{\mathbf{k}}_{23}}{1+\hat{\mathbf{k}}_{23}\cdot\hat{\mathbf{r}}_{23}},$$

and $\alpha_{mn}'=Z_mZ_n/k_{mn}'$, etc., while $\mathbf{k}_{23}'$ and γ have been defined above.

The wave function (35) is a generalization of Ψ_1 obtained in Sec. II. The coordinate-dependent momenta modify asymptotically the wave function in such way that the obtained function fulfills the correct asymptotic conditions in both Ω_0 and Ω_j.

CONCLUSION

In this work we have obtained a class of approximate wave functions for the three-body Coulomb problem in the case of a system composed of one light and two heavy particles, which can be interpreted as a state resulting from an ion-atom ionization collision. These functions can be written in terms of hypergeometric functions of two variables. We have shown that they couple the electron-target and electron-projectile interactions, but treating them on an equal footing. We would like to point out that the main features of these wave functions correctly include the Coulomb asymptotic conditions.

The functions obtained here can be considered a good alternative to the functions previously used in the calculation of transition matrices and DDCSs. For example, these functions can replace the Ψ_{C3} function in a CDW or a multiple-scattering approach [9]. Numerical examples show that Ψ_1 has a two-center symmetry in the inner region, i.e., when the distances between the three particles are comparable. This seems to be a remarkable improvement over Ψ_{C3}, which shows the asymptotic hyperbolic symmetry even in the condensation region. However, as it has been pointed out before, a suitable change in the normalization factor N_{12} should be seriously considered to avoid the exponential decrease in the cross section when the projectile charge is large or the impact energy is small [29]. Such modifications have been successfully used in a multiple-scattering approximation in $(e,2e)$ processes [12], but, to the best of our knowledge, the application of this method in ion-atom collisions has not been investigated yet. Another alternative would be an impact parameter approximation where the hypergeometric function of the heavy pair is replaced by an eikonal phase in Ψ_1 [1].

The computation of these transition matrices with the general function Ψ_1' can be an involved task since each calculation of the function Φ_2 would imply the evaluation of a series of products of one-variables hypergeometric functions with coordinate-dependent parameters. Preliminary results recently obtained show that the introduction of coordinate-dependent momenta in the wave function is very expensive in terms of computational time [15]. As a first step we consider that the function Ψ_1, instead of the function Ψ_1' would be a suitable election for the development of new scattering theories in ion-atom processes.

Finally, we would like to remark that the properties of systems of coupled partial differential equations involving three or more variables are poorly known. This seriously restricts the study of possible separations of the wave equations and a complete investigation of those systems is needed in order to improve the results presented in this work. Further research is being carried out in order to obtain an analytical expression of the transition matrix in some adequate approximation.

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APPENDIX

In this appendix we summarize the basic definitions of the hypergeometric function introduced in Sec. III. The principal formulas can be found in the works of Appell and Kampé de Feriet [20] and Erdelyi [30,31].

The generalized confluent hypergeometric function $\Phi_2(a,a',b,x,y)$ is defined by the double series

$$\Phi_2(a,a',b,x,y)=\sum_{m,n}\frac{(a)_m(a')_n}{m!n!(b)_{m+n}}x^my^n,\tag{A1}$$

which converges for every finite value of x and y; the parameters a and a' are arbitrary and $b\neq 0,-1,-2,\ldots$. If a or a' is a negative integer number, the function $\Phi_2(a,a',b,x,y)$ reduces to a polynomial in the variable x (y) of degree $|a|$ (degree $|a'|$). If both a and a' are negative integer numbers then the function represents a polynomial in

x and y of degree $|a|$ and $|a'|$. For general values of the variables and parameters, the function can be defined in terms of contour integrals [30].

The function (A1) satisfies the pair of differential equations

$$\left[x\frac{\partial^2}{\partial x^2}+y\frac{\partial^2}{\partial x\partial y}+(b-x)\frac{\partial}{\partial x}-a\right]\Phi_2=0,$$
$$\left[y\frac{\partial^2}{\partial y^2}+x\frac{\partial^2}{\partial x\partial y}+(b-y)\frac{\partial}{\partial y}-a'\right]\Phi_2=0. \quad \text{(A2)}$$

This set has, in general, three linearly independent solutions that can be represented in terms of the generalized hypergeometric functions

$$z_0=\Phi_2(a,a',b,x,y), \quad \text{(A3)}$$

$$z_1=x^{a'-b+1}y^{-a'}\Phi_1\left(a+a'-b+1,a',a'-b+2,\frac{x}{y},x\right),$$
$$|x|<|y| \quad \text{(A4)}$$

$$z_2=x^{-a}y^{a-b+1}\Phi_1\left(a+a'-b+1,a,a-b+2,\frac{y}{x},y\right),$$
$$|y|<|x|, \quad \text{(A5)}$$

where $\Phi_1(a,b,c,x,y)$ is a generalized confluent hypergeometric function of two variables defined by [32]

$$\Phi_1(a,b,c,x,y)=\sum_{m,n}\frac{(a)_{m+n}(b)_m}{m!n!(c)_{m+n}}x^my^n, \quad |x|<1.$$

Thus a general solution of the system can be write as

$$z=Az_0+Bz_1+Cz_2,$$

where A, B, and C are arbitrary constants.

In addition to the functions defined in Eqs. (A3)–(A5) there is another solution of Eq. (A2) that is expressible by convergent hypergeometric series of two variables [30], but this can be written in terms of the functions already defined.

The relations

$$\frac{\partial}{\partial x}\Phi_2(a,a',b,x,y)=\frac{a}{b}\Phi_2(a+1,a',b+1,x,y),$$

$$\frac{\partial}{\partial y}\Phi_2(a,a',b,x,y)=\frac{a'}{b}\Phi_2(a,a'+1,b+1,x,y)$$

show that the derivatives of the Φ_2 function are expressible in terms of the function itself in a way similar to the confluent hypergeometric ${}_1F_1(a,b,z)$. One of the multiple series expansions for Φ_2 is

$$\Phi_2(a,a',b,x,y)=\sum_r(-1)^r\frac{(a)_r(a')_r}{r!(b+r-1)_r(b)_{2r}}x^ry^r\times{}_1F_1(a+r,b+2r,x)\ {}_1F_1(a'+r,b+2r,y). \quad \text{(A6)}$$

The asymptotic behavior of $\Phi_2(a,a',b,x,y)$ when $|x|\to\infty$, $|y|\to\infty$, and $|y-x|\to\infty$ can be written as

$$z_0=\frac{e^{i\pi(a+a')}\Gamma(b)}{\Gamma(1-a-a')}z_4+\frac{e^{i\pi(a+2a'-b)}\Gamma(b)}{\Gamma(a)}z_5+\frac{e^{i\pi(a'-b)}\Gamma(b)}{\Gamma(a')}z_6, \quad \text{(A7)}$$

with

$$z_4=x^{-a}y^{-a'}\Phi_4\left(a+a'-b+1,a,a',-\frac{1}{x},-\frac{1}{y}\right),$$

$$z_5=(-x)^{a+a'-b}(y-x)^{-a'}e^x\times\Phi_4\left(1-a,b-a-a',a',\frac{1}{x},\frac{1}{x-y}\right),$$

$$z_6=(x-y)^{-a}(-y)^{a+a'-b}e^y\times\Phi_4\left(1-a',a,b-a-a',\frac{1}{y-x},\frac{1}{y}\right),$$

where Φ_4 is one of the generalized Whittaker functions and is defined by the series

$$\Phi_4\left(c,a,a',-\frac{1}{x},-\frac{1}{y}\right)=\sum_{m,n}\frac{(c)_{m+n}(a)_m(a')_n}{m!n!(-x)^m(-y)^n}. \quad \text{(A8)}$$

The expansion of Eq. (A7) when x, y, and $x-y$ go to infinity leads to the asymptotic expression (44) of Sec. IV B since the function Φ_4 can be considered a constant in this limiting case. On the other hand, in the case in which one of the variables is small (for example, x) and the other tends to infinity (the y variable, for example) the asymptotic expansion of z_0 is

$$\Phi_2=\frac{e^{i\pi(a'-1)}}{\Gamma(a')}(x-y)^{-a}(-y)^{a+a'-1}\times e^y\Phi_4\left(1-a',a,1-a-a',\frac{1}{y-x},\frac{1}{y}\right)+\frac{e^{i\pi a'}}{\Gamma(1-a')}y^{-a'}\Phi_5\left(a,a',1-a',x,\frac{1}{y}\right), \quad \text{(A9)}$$

with Φ_5 given by the series

$$\Phi_5\left(a,a',c,x,\frac{1}{y}\right)=\sum_{m,n}\frac{(a)_m(a')_n}{(c)_{m-n}}\frac{x^m}{m!}\frac{y^{-n}}{n!}, \quad \text{(A10)}$$

which is another Whittaker function. Expanding the function Φ_5 up to first order in $1/y$, we obtain Eq. (50).

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