Separable wave equation for three Coulomb interacting particles

F. D. Colavecchia, G. Gasaneo,* and C. R. Garibotti
Centro Atómico Bariloche and Consejo Nacional de Investigaciones Científicas y Técnicas, 8400 San Carlos de Bariloche, Río Negro, Argentina
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We consider a separable approximation to the Schrödinger equation for the three-body Coulomb problem and found its exact solution above the ionization threshold. This wave function accounts for different possible asymptotic behaviors and reduces to the well-known product of three two-body Coulomb waves (C3) for scattering conditions. The momenta and position-dependent modifications recently proposed for the Sommerfeld parameters, as an improvement to the C3 model, are analyzed. We show how these changes can be included in our model as a suitable physically based variations in the separable approximation for the wave equation. [S1050-2947(98)01302-X]

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I. INTRODUCTION

The position of three particles in the center-of-mass frame can be defined in closed form using a set of six variables. However, the choice of this set is by no means trivial, since it is dictated by the physical processes we are interested in describing. Each set of variables leads to a particular expression of the coupled six-dimensional Schrödinger equation. The general solution of this equation is not known and approximate wave functions should be considered instead. The usual method to circumvent this problem is to propose the full separability of the solution into six wave functions, each one related with a specific coordinate. In this way, the original Schrödinger equation splits into six partial uncoupled equations and the complete solution has a set of six quantum numbers that represent integrals of motion of the simplified problem. The underlying assumption is that the simplified model portrays the most important features of the dynamic of the problem.

In the three-body Coulomb problem, in addition to the total energy E, there are two more exact quantum numbers that can be used to label the stationary state of the three particles, these are the total orbital angular momentum L and its projection M along a space-fixed axis. These two quantum numbers represent a certain fundamental symmetry property (isotropy) of our space and does not depend on the nature of interparticle interaction. Hence, the dynamical aspects of the system would be represented by the reduced set of three additional quantum numbers. The main shortcoming is that in the truly three-body Coulomb problem these other three quantum numbers do not exist and then the six-dimensional Schrödinger equation cannot be totally separated.

These considerations have led to different kinds of approximate wave functions for the three-body Coulomb problem along the years [1]. In particular, the high-energy electron or ion collisions with atoms are treated with simple models, which rely on separable wave functions where the different factors correspond to solutions of two-body Coulomb problems. One of the most thoroughly used is known as C3 [2]. In the C3 model, the three-body wave function is represented as a product of three two-body Coulomb wave functions, one for each pair of particles. Each pair is considered to interact separately with a relative energy on the two-body energy shell and with electric charges unscreened by the presence of the third particle. Through the years this model has been modified to obtain a better description of the dynamic of the three-body problem. Some of the modifications of the basic model include the introduction of velocity-dependent charges, and recently, position-dependent charges [3,4]. Using theses charges, which represent the dynamical screening associated with the position or velocities of the particles, the new wave functions give a better description of the problem in contrast with the original model.

In this work we obtain a fully separable approximate solution of the three-body Coulomb problem above the threshold of total breakup, suitable to describe the final state of ionizing collisions. We name this function C6 because it is built upon the superposition of a two-body continuum wave function for each of the six independent subsystems. A particular choice of the separation parameters restricts the C6 model to the usual C3 one. The modified C3 models can be obtained in a similar way, including relevant information of the dynamic of the real problem through the proper election of these parameters as a function of momenta or position of the particles.

The plan of this paper is as follows. After discussing the basic C6 model, Sec. II, we derive the well-known C3 wave function. We discuss the different asymptotic behavior of the C6 model. In Sec. III we introduce the general form of the approximate Hamiltonian, which straightforwardly leads to the variation of the basic model. Finally, conclusions of our work are drawn in Sec. IV.

II. THE C6 MODEL

The Schrödinger equation for three particles with charges Z_i and masses m_i $(i=1,2,3)$ can be expressed in any of the following Jacobi pairs $\{\mathbf{r}_{ij},\mathbf{R}_{ij}\}$ as [5]

*Permanent address: Departamento de Física, Universidad Nacional del Sur, Avenida Alem 1253, 8000 Bahía Blanca, Argentina.

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$$\left[-\frac{1}{2\mu_{ij}}\nabla^2_{\mathbf{r}_{ij}}-\frac{1}{2\nu_{ij}}\nabla^2_{\mathbf{R}_{ij}}+\sum_{m=1}^{3}V_m\right]\overline{\Psi}(\mathbf{r}_{ij},\mathbf{R}_{ij})$$
$$=E\overline{\Psi}(\mathbf{r}_{ij},\mathbf{R}_{ij}) \quad (1)$$

with the reduced masses $\mu_{ij}=m_im_j/(m_i+m_j)$ and $\nu_{ij}=(m_i+m_j)m_k/m_i+m_j+m_k$, while $V_i=Z_jZ_k/r_{jk}$ $(i\neq j\neq k)$ are the three Coulomb potentials. The eigenenergy E will be written considering that all the particles are in the continuum. The ansatz

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

removes the eigenenergy giving a wave equation for the function Ψ. The set $\{\mathbf{k}_{ij},\mathbf{K}_{ij}\}$ are the conjugated momenta. Continuum states, which are the object under study in this work, are infinitely degenerate in L and appropriate linear combinations should be defined regarding asymptotic boundary conditions. So, for high energy one may prefer to abandon L and M for the sake of individual momenta of colliding particles or other quantum numbers characterizing asymptotic behavior of the wave function Ψ. To do that we use the set of generalized parabolic coordinates introduced by Klar [6], which leads the wave equation in a very symmetric form:

$$\xi_1=r_{32}+\hat{\mathbf{k}}_{23}\cdot\mathbf{r}_{32},\quad \eta_1=r_{32}-\hat{\mathbf{k}}_{23}\cdot\mathbf{r}_{32},$$
$$\xi_2=r_{13}+\hat{\mathbf{k}}_{13}\cdot\mathbf{r}_{13},\quad \eta_2=r_{13}-\hat{\mathbf{k}}_{13}\cdot\mathbf{r}_{13},$$
$$\xi_3=r_{12}+\hat{\mathbf{k}}_{12}\cdot\mathbf{r}_{12},\quad \eta_3=r_{12}-\hat{\mathbf{k}}_{12}\cdot\mathbf{r}_{12}, \quad (3)$$

where $\hat{\mathbf{k}}_{13}$ and $\hat{\mathbf{k}}_{23}$ are the unit vectors determined by the directions of the relative momenta. This set of coordinates is adequate for the analysis of the scattering asymptotic behavior. Thus the equation for Ψ results:

$$D\Psi=[D_0+D_1]\Psi=0, \quad (4)$$

where D_0 and D_1 are given by

$$D_0=\sum_{i=1,i\neq j\neq k}^{3}\frac{2}{\mu_{jk}(\xi_i+\eta_i)}[A_i^++A_i^-+\mu_{jk}Z_jZ_k] \quad (5)$$

and

$$D_1=\sum_{i=1}^{2}\sum_{j=i+1}^{3}\frac{(-1)^{i+1}}{m_k}\mathbf{B}_i\cdot\mathbf{B}_j, \quad (6)$$

where we have defined the following operators:

$$A_i^+=\xi_i\frac{\partial^2}{\partial\xi_i^2}+(1+ik_{jk}\xi_i)\frac{\partial}{\partial\xi_i},$$
$$A_i^-=\eta_i\frac{\partial^2}{\partial\eta_i^2}+(1-ik_{jk}\eta_i)\frac{\partial}{\partial\eta_i},$$
$$\mathbf{B}_i=(\nabla_{\mathbf{r}_{jk}}\xi_i)\frac{\partial}{\partial\xi_i}+(\nabla_{\mathbf{r}_{jk}}\eta_i)\frac{\partial}{\partial\eta_i}. \quad (7)$$

As we can see these coordinates appear to be an adequate system to consider all the interactions and particles motions equally. As we pointed out above, Eq. (4) is not totally separable. Nevertheless, it is easy to see from Eq. (5) that if we neglect D_1 from this equation it can be solved in a closed form.

The usual C3 solution has been discussed by Klar [6]. Here we will analyze a general solution for

$$D_0\Psi=0, \quad (8)$$

which is a fully separable function:

$$\Psi=\prod_{i=1}^{3}f_i(\xi_i,\eta_i) \quad (9)$$

and satisfies the equations

$$[A_i^++A_i^-+\mu_{jk}Z_jZ_k]f_i(\xi_i,\eta_i)=\tfrac{1}{2}C_i(\xi_i+\eta_i)f_i(\xi_i,\eta_i). \quad (10)$$

If we choose for f_i the form $f_i(\xi_i,\eta_i)=g_i(\xi_i)h_i(\eta_i)$ we can easily see that the functions $g_i(\xi_i)$ and $h_i(\eta_i)$ satisfy the equations

$$\left[A_i^++\frac{\mu_{jk}}{2}(C_i\xi_i+a_i)\right]g_i(\xi_i)=0, \quad (11)$$

$$\left[A_i^-+\frac{\mu_{jk}}{2}(C_i\eta_i+b_i)\right]h_i(\eta_i)=0, \quad (12)$$

with the constraints

$$\sum_{i=1}^{3}C_i=0\quad\text{and}\quad a_i+b_i=2Z_jZ_k. \quad (13)$$

The solution of these equations can be obtained by transforming the confluent hypergeometric equation. The general solution of Eq. (4) when D_1 is neglected can be written as (see Appendix)

$$\Psi=N\prod_{l=1,l\neq m\neq n}^{3}e^{-i(k_{mn}/2)(1-\gamma_l)(\xi_l-\eta_l)}$$
$$\times{}_1F_1\left(\frac{\gamma_l-1-i\mu_{mn}a_l/k_{mn}}{2\gamma_l},1,-ik_{mn}\gamma_l\xi_l\right)$$
$$\times{}_1F_1\left(\frac{\gamma_l-1+i\mu_{mn}b_l/k_{mn}}{2\gamma_l},1,ik_{mn}\gamma_l\eta_l\right), \quad (14)$$

where $\gamma_l^2=1-2\mu_{mn}C_l/k_{mn}^2$.

By setting specific values for separation parameters we obtain solutions with a particular asymptotic behavior. In this way, any fixed set of separation constants $\{a_l,b_l,C_l\}$ will determine a unique asymptotic condition that the wave function will fulfill.

There are several choices in this case. If C_l are set such that $2\mu_{mn}C_l/k_{mn}^2>1$, the parameters γ_l will be imaginary, transforming the oscillatory exponential factors in Eq. (14) into exponentially increasing or decreasing functions and leading to asymptotically diverging or decaying solutions,

depending on the sign of γ_l. On the other hand, selecting C_l with the condition $2\mu_{mn}C_l/k_{mn}^2<1$ will lead to a real parameter γ_l. The confluent hypergeometric function has the well-known eikonal behavior when the variable goes to infinity, i.e., ${}_1F_1(a,b,z)\rightarrow(-z)^{-a}$ for $z\rightarrow\infty$ and then, since the complex parameter a includes a real part $\mathcal{R}(a)=(\gamma_l-1)/2\gamma_l<0$, the asymptotic behavior of the wave function will contain terms of order $z^{-\mathcal{R}(a)}$ that go to zero. Any complex values for C_l are simple combinations of the previous cases.

From the above discussion it is clear that the election $C_l=0$ is the unique way to obtain the correct outgoing asymptotic behavior for the function $\widetilde{\Psi}_{\mathrm{C3}}$ because the oscillatory factor reduces to the unit and the first parameter of the hypergeometric functions is imaginary. These considerations show that a careful choice of the separation parameters should be done to guarantee the physical properties of any wave function. In order to get the outgoing behavior included in solution Ψ_{C3} we should select $C_l=b_l=0$.

The wave function Ψ is a solution of the separable approximate six-dimensional Schrödinger equation. Therefore it introduces a set of six quantum numbers that represent integrals of motion of an underlying problem of three independent pairs of particles that interact though Coulombic potentials. The set of quantum numbers associated with this problem will be the eigennumber of the three sets:

$$\{H^{ij},A_z^{ij}\}, \tag{15}$$

where H^{ij} and A_z^{ij} represent the Hamiltonian and the components of the Runge-Lenz vector along the direction of $\hat{\mathbf{k}}_{ij}$, respectively. These sets represent a total of six quantum numbers. In this way we have obtained an approximated solution for the three-body Coulomb problem that we call C6. It is a generalization of the model known as C3, which was introduced by Garibotti and Miraglia [2] and it is currently used in collision theory.

In the two-body case, bound states can be derived from continuum wave functions by introducing complex moments. An equivalent procedure can be performed in the three-body case, for each pair of particles [7]. The solution given by Eq. (14) could be analytically continued to negative relative energies to provide bound states with general values for the parabolic quantum numbers. Instead the C3 function is an outgoing wave and can be only extended to a restricted set of bound states.

The function C3 is obtained by choosing the separation constant $C_i=0$ and $b_i=0$:

$$\overline{\Psi}_{\mathrm{C3}}=e^{i\mathbf{K}_i\cdot\mathbf{R}_i+i\mathbf{k}_{ij}\cdot\mathbf{r}_{ij}} \times\prod_{m,n=1;n>m}^{3} N_{mn}\,{}_1F_1(i\alpha_l,1,-i[k_{mn}r_{mn}+\mathbf{k}_{mn}\cdot\mathbf{r}_{mn}]) \tag{16}$$

giving outgoing waves, or incoming waves selecting $C_i=0$ and $a_i=0$. The Sommerfeld parameters α_l are defined by

$$\alpha_l=\frac{\mu_{mn}Z_mZ_n}{k_{mn}}. \tag{17}$$

It is well known that this model is an exact solution of the three-body Coulomb problem only in an asymptotic region of the coordinate space, since

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

when all interparticle distances tend to infinity [8]. Although formally this approximation can reproduce correctly some dominant features of the dynamics of the system only in the mentioned region, it was used as a solution for the three-body Coulomb problem everywhere in the coordinate space. It has been very successful in describing angular distributions of ionized electrons, for both electron impact and photoionization [9,10]; nevertheless it suffers from several deficiencies [9].

The C3 wave function is a usual approximation for the three-body Coulomb problem. Modifications of Eq. (16) have been proposed to obtain improved solutions and will be shown in the following section. An example of these modifications is the position-dependent Sommerfeld parameters introduced by Berakdar [4] or the Sommerfeld parameters, which are functions of all three relative momenta introduced by Berakdar and Briggs [3] and Jetzke and Faisal [11]. The mentioned approximations are based on physical presumptions, however, they can be associated with a particular approach for D_1.

III. ALTERNATIVE C3 WAVE FUNCTIONS

In Sec. II we mention that the C3 wave function is an approximate solution of Eq. (4), which results from neglecting D_1, with a particular choice of the separation constants. Different strategies have been formulated to modify and improve this approximation, still maintaining the form (16) for the wave function. In this section we want to show how particular approaches to the D_1 term lead, in a straightforward way, to usual and well-known variations of the C3 or C6 models [3,4,11].

The Schrödinger equation for the three-body Coulomb problem is essentially nonseparable. The nonseparability of the Schrödinger equation is represented by the term D_1 when written in coordinates defined by (3). It is commonly known as the nonorthogonal kinetic energy and in the parabolic set (6) is a very involved function of the coordinates. When D_1 is considered the Schrödinger equation is a six-dimensional coupled partial differential equation. If we are interested in including in some approximate way the neglected terms of D_1 but keeping the function similar to the C3 model, we can introduce the operator D_1' and separate the Schrödinger equation as

$$(D_0+D_1')\Psi=0, \tag{19}$$

$$(D_1-D_1')\Psi=0, \tag{20}$$

We should note that the solutions of this system represent only a restricted subset of the complete set of solutions of Eq. (4). As above we neglect Eq. (20) and choose the operator D_1' such that the solution Ψ of Eq. (19) keeps the forms of Eqs. (14) or (16).

A. Velocity-dependent charges

Recently different modifications to the C3 model have been introduced and used to evaluate the transition matrix for different collision processes. First we want to show how the introduction of momenta-dependent charges can be included in the C3 model with a particular election of D_1'. As a starting point we consider

$$D_1'=\sum_{i=1}^{3}\frac{\chi_i(\mathbf{k})}{r_{jk}}=\sum_{i=1}^{3}\frac{2\chi_i(\mathbf{k})}{\xi_i+\eta_i}, \tag{21}$$

where $\chi_i(\mathbf{k})$ are momenta-dependent functions that will be selected according to physical criteria. The variable separation proceeds as above, giving a wave function $\tilde{\Psi}_{\mathrm{C6}}$ as Eq. (14) with new separation parameters $\tilde{a}_i$, $\tilde{b}_i$ restricted by

$$\sum_{i=1}^{3} C_i=0,$$

$$\tilde{a}_i+\tilde{b}_i=2[Z_jZ_k+\chi_i(\mathbf{k})]. \tag{22}$$

The separable function $\tilde{\Psi}_{\mathrm{C6}}$ is the solution of the problem of three independent pairs of two-body system with modified Coulomb interactions. The set of dynamic charges $[Z_jZ_k+\chi_i(\mathbf{k})]$ introduces a correlation between the three motions through the parameters $\tilde{a}_i$ and $\tilde{b}_i$. As a three two-body Coulomb problem we can obtain a solution with full outgoing behavior by choosing $C_i=0$ and $\tilde{b}_i=0$,

$$\tilde{\Psi}_{\mathrm{C3}}=e^{i\mathbf{K}_i\cdot\mathbf{R}_i+i\mathbf{k}_{ij}\cdot\mathbf{r}_{ij}}\prod_{m,n=1;n>m\neq l}^{3}N'_{mn}$$
$$\times{}_1F_1(i\tilde{\alpha}_l,1,-i[k_{mn}r_{mn}+\mathbf{k}_{mn}\cdot\mathbf{r}_{mn}]), \tag{23}$$

or with incoming behavior when $C_i=0$ and $\tilde{a}_i=0$. The three Sommerfeld parameters $\tilde{\alpha}_l$ are defined by

$$\tilde{\alpha}_l=\frac{\mu_{mn}[Z_mZ_n+\chi_i(\mathbf{k})]}{k_{mn}}. \tag{24}$$

Now as a three-body Coulomb problem, the wave function (23) should verify $D_1'\tilde{\Psi}=O(1/r_{jk}^2)$. This condition imposes a restriction over the functions χ_i, which can be written as

$$\sum_{i=1}^{3}\frac{\mu_{mn}\chi_i(\mathbf{k})}{k_{mn}}=0. \tag{25}$$

This ensures that the parameters satisfy the Peterkop relation and the wave function $\tilde{\Psi}_{\mathrm{C3}}$ is a good asymptotic solution in the region known as Ω_0. Further modifications must be introduced to have a solution with the correct behavior in the regions Ω_k where particle k is far from the particles i and j, which remain close to each other [12].

A possible choice for χ_i has been proposed by Berakdar and Briggs [3] for a one-proton–two-electron system. For the symmetric case where the modulus of the momenta of the electrons relative to the proton are equal they obtain

$$\chi_{e1}=\chi_{e2}=-\frac{\sin\Theta}{4},$$

$$\chi_{ee}=-\frac{\sin\Theta}{2}, \tag{26}$$

where 2Θ is the angle between those momenta. This choice for the final three-body wave gives a cross section for the e-H ionizing collision in very good agreement with experiments [3].

Another approach that can be included in the previous discussion has been proposed by Jetzke and Faisal [11]. They consider a system of N light charged particles, either electrons or positrons, in the field of a nucleus of charge Z. They replace the action of the e-e field over an electron by its component along the e-nucleus direction, such that the i-electron remains in a central field with effective dynamical charge:

$$\alpha_i/2=Z+\sum_{j\neq i}^{N}\frac{\mathbf{v}_i\cdot\mathbf{v}_{ij}v_i}{v_{ij}^3}, \tag{27}$$

where $\mathbf{v}_i$ is the asymptotic velocity of the i-electron relative to the nucleus and $\mathbf{v}_{ij}=\mathbf{v}_i-\mathbf{v}_j$. For a heavy particle plus two-electron system we have

$$\chi_1=\frac{\mathbf{v}_1\cdot\mathbf{v}_{12}v_1}{v_{12}^3},\quad \chi_2=-\frac{\mathbf{v}_2\cdot\mathbf{v}_{12}v_2}{v_{12}^3},\quad \chi_3=-1. \tag{28}$$

Therefore only two factors contibute to the wave function in Eq. (23). The χ_i given by Eqs. (26) and (28) satisfies the Peterkop condition (25) and then the resulting wave function has the correct asymptotic behavior.

Note that the obtained wave functions are totally separable; this means that there exist a set of six good quantum numbers. Again this corresponds to the set (15). Nevertheless we must note that in this case the eigennumber A_z^{ij} depends of all the relative velocity-though the velocities dependent charges $[Z_jZ_k+\chi_i(\mathbf{k})]$.

B. Position-dependent charges

While the momenta-dependent charges have been widely used, position-dependent effective charges have been recently introduced in the description of the final state of an electron-atom ionization process [4]. The wave function Ψ_B proposed by Berakdar has the form of the C3 with the significant difference that it includes position-dependent parameters. This wave function has the form shown in Eq. (23) with

$$\tilde{\alpha}_l=\alpha_l'=\frac{\mu_{mn}[Z_mZ_n+\chi_i'(\mathbf{r}_{ij},\mathbf{R}_{ij})]}{k_{mn}}. \tag{29}$$

To obtain Ψ_B the wave equation is written in the coordinates set $\Upsilon=\{\xi_1,\xi_2,\xi_3,r_{12},r_{13},r_{23}\}$, which is composed by three parabolic coordinates (3) and the other three are the distances between the particles. The parabolic coordinates define the orientation and r_{12},r_{13},r_{23} the shape of the triangle formed by the three particles. Other sets of variables could be used,

setting the parabolic coordinates according to outgoing or incoming asymptotic conditions for each pair of particles.

It is possible to write the Schrödinger equation in the coordinates Υ and propose a separation similar to the former D_0 and D_1 [4]:

$$\widetilde{D}_0=\sum_{i=1,i\neq j\neq k}^{3}\frac{2}{\mu_{jk}r_{jk}}\left[\xi_i\frac{\partial^2}{\partial\xi_i^2}+(1+ik_{jk}\xi_i)\frac{\partial}{\partial\xi_i}+\mu_{jk}Z_jZ_k\right],$$

$$\widetilde{D}_1=R_{\xi_1,\xi_2,\xi_3}(r_{12},r_{13},r_{23})+S(\xi_1,\xi_2,\xi_3,r_{12},r_{13},r_{23}).$$

As we can see $\widetilde{D}_0$ depends on the variables ξ_i and parametrically on the other three variables. The operator $\widetilde{D}_1$ is formed by two parts R, which depend on r_{12},r_{13},r_{23} and parametrically on ξ_i, and S that mix all the variables. These operators can be associated with $H_{\rm par}$, $H_{\rm in}$, and $H_{\rm mix}$ defined by Berakdar [4]. The wave function Ψ_B is obtained as before, neglecting $\widetilde{D}_1\Psi$. Looking for a separable solution we write

$$\widetilde{D}_0\Psi_B=0. \tag{30}$$

This equation can be solved in a closed form by proposing a separation of variables. Now the separation constants could be chosen as a function of variables $\{r_{12},r_{13},r_{23}\}$ and, in this way, as a function of *all* the Jacobi coordinates. Then if we call this separation function $\widetilde{\chi}_i$, we can proceed as before and obtain the solution of Eq. (30) in terms of the Kummer confluent hypergeometric functions:

$$\Psi_B=Ne^{i\mathbf{K}_i\cdot\mathbf{R}_i+i\mathbf{k}_{ij}\cdot\mathbf{r}_{ij}}\prod_{m,n=1,n>m}^{3}{}_1F_1\left(i\frac{\mu_{mn}[Z_mZ_n+\widetilde{\chi}_i(\mathbf{r}_{ij},\mathbf{R}_{ij})r_{jk}/2]}{k_{mn}},1,-ik_{mn}\xi_m\right), \tag{31}$$

which, apart of a normalization constant N, is the same as that given by Berakdar [4], and where $\chi_i'=(r_{jk}/2)\widetilde{\chi}_i$. However, there exists an important difference between the use of the parabolic coordinates (3) and Υ. If we use the set given by Eq. (3) it is possible to obtain a scattering wave function C6 with coordinate-independent parameters. The asymptotic behavior in the region Ω_0 can be properly selected by choosing the separation constants [6]. Nevertheless using Υ we rewrite the equations in a such way that only one of these asymptotic behaviors could be obtained. This is a direct consequence of the coordinate election. In that case, the wave function Ψ_B has the right behavior also in the regions Ω_k. The application of $\widetilde{D}_1$ over Ψ_B gives a function of order $O(1/d^2)$ where d represents the set of coordinates that tend to infinity in every one of the corresponding regions [12]. However, imposing the asymptotic behaviors to the wave function is not sufficient to fix the functions χ_i, and other conditions are required. Berakdar imposes physical conditions over the coordinate-dependent product of charges in order to verify the right behavior in the Wannier region.

C. Effective momenta

In Sec. III B we have shown that some physically based approximations to the wave functions can be derived within the C6 framework. All these wave functions can be viewed as approximately separable solutions of some effective potentials that give rise to modifications of the charges of the interacting particles. All these functions are asymptotically correct in the region Ω_0 where all particles are far from each other. Besides, modifications in the relative momenta of the particles can be introduced to improve the description of the dynamic of the three-body Coulomb problem in the regions Ω_k where the particle k is far from the particles i and j, which remain close to each other. Then, we can think that the presence of particle k slightly modifies the wave function of the pair (i,j) introducing correlation between the motions of the particles. However, we will consider that the function $f_k(\xi_k,\eta_k)$ of ansatz (9) is weakly dependent on the other variables $w_k=\{\xi_i,\eta_i,\xi_j,\eta_j\}$. In other words, f_k depends parametrically on the other set of variables w_k. Then Eq. (9) in Ω_k reduces to

$$\Psi_k=f_k(\xi_k,\eta_k)\prod_{l=i,j}f_l(\xi_l,\eta_l) \tag{32}$$

and we are interested in solving the Schrödinger equation up to order $\mathcal{O}(1/\xi_l^2,1/\eta_l^2)$, $l=i,j$. We first note that

$$D_1\Psi_k=\frac{(-1)^{i+1}}{m_j}[\mathbf{B}_i\ln\mathcal{E}_i+\mathbf{B}_j\ln\mathcal{E}_j]\cdot(\mathbf{B}_kf_k)+\mathcal{O}\left(\frac{1}{\xi_{i,j}^2},\frac{1}{\eta_{i,j}^2}\right), \tag{33}$$

where $\mathcal{E}_l$ represents the asymptotic expressions of the functions f_l:

$$f_l\to\mathcal{E}_l+\mathcal{O}\left(\frac{1}{\xi_l},\frac{1}{\eta_l}\right)\quad\text{when }\{\xi_l,\eta_l\}\to\infty$$

for all $l\neq k$. Then we can proceed with the separation of the full Schrodinger equation up to order $\mathcal{O}(1/\xi_{i,j}^2,1/\eta_{i,j}^2)$ in the following way:

$$[\widetilde{A}_l^+ +\widetilde{A}_l^- +\mu_{lk}Z_lZ_k]\mathcal{E}_l(\xi_l,\eta_l)=\frac{1}{2}C_l(\xi_l+\eta_l)\mathcal{E}_l(\xi_l,\eta_l),\qquad l\neq k, \tag{34}$$

$$[A_k^+ + A_k^- + \mu_{ij} Z_i Z_j] f_k(\xi_k, \eta_k)$$
$$= \frac{(-1)^{i+1}}{2m_j}(\xi_k + \eta_k)[\mathbf{B}_i \ln \mathcal{E}_i + \mathbf{B}_j \ln \mathcal{E}_j] \cdot (\mathbf{B}_k f_k)$$
$$+ \frac{1}{2} C_k(\xi_k + \eta_k) f_k(\xi_k, \eta_k), \tag{35}$$

where

$$\tilde{A}_l^+ = i k_{lk} \xi_l \frac{\partial}{\partial \xi_l}, \quad \tilde{A}_l^- = -i k_{lk} \eta_l \frac{\partial}{\partial \eta_l} \quad \text{for } l \neq k$$

while $A_k^{\pm}$ remain the same as in definitions (7). It is easy to see that the solutions $\mathcal{E}_l(\xi_l, \eta_l)$ are products of eikonal wave functions,

$$\mathcal{E}_l(\xi_l, \eta_l) = \exp\left[-\left(\frac{1}{2} - \frac{1}{2\gamma_l} - \frac{i\mu_{mn} a_l}{k_{mn}} \right) \ln(k_{mn} \gamma_l \xi_l) \right]$$
$$\times \exp\left[\left(\frac{1}{2} - \frac{1}{2\gamma_l} + \frac{i\mu_{mn} b_l}{k_{mn}} \right) \ln(k_{mn} \gamma_l \eta_l) \right],$$

where a_l, b_l, and γ_l were defined in Sec. II. If we consider outgoing waves, $\mathcal{E}_l(\xi_l, \eta_l)$ reduces to the usual form $\mathcal{E}_l(\xi_l) = \exp[-i\alpha_l \ln(k_{mn}\xi_l)]$ with α_l defined by Eq. (17). Now we can proceed with the solution of Eq. (35). For the sake of simplicity, we will restrict ourselves to the case where the functions $\mathcal{E}_i(\xi_i, \eta_i)$ and $\mathcal{E}_j(\xi_j, \eta_j)$ verify the outgoing asymptotic behavior. Then $C_k = 0$ and using the definitions of the differential operators $\mathbf{B}_l$ [Eq. (7)], we have

$$[A_k^+ + A_k^- + \mu_{ij} Z_i Z_j] f_k(\xi_k, \eta_k)$$
$$= (\Delta \mathbf{k}_i + \Delta \mathbf{k}_j) \cdot \left[(\hat{\mathbf{r}}_{ij} + \hat{\mathbf{k}}_{ij}) \frac{\partial}{\partial \xi_k} + (\hat{\mathbf{r}}_{ij} - \hat{\mathbf{k}}_{ij}) \frac{\partial}{\partial \eta_k} \right] f_k, \tag{36}$$

where we defined ($l \neq k$)

$$\Delta \mathbf{k}_l = \frac{(-1)^{l+1} \mu_{lk}}{m_l} \frac{r_{ij}}{r_{lk}} \left[\frac{(\hat{\mathbf{r}}_{lk} + \hat{\mathbf{k}}_{lk})}{1 + \hat{\mathbf{r}}_{lk} \cdot \hat{\mathbf{k}}_{lk}} \right].$$

As we noted before, since the right-hand side of Eq. (36) contains a term differential in the function f_k, the separable solution will have modified momenta instead of effective charges. These modifications in the momenta $(\Delta \mathbf{k}_i + \Delta \mathbf{k}_j)$ are of order $\mathcal{O}(1/\xi_{i,j}, 1/\eta_{i,j})$, which contributes to orders $\mathcal{O}(1/\xi_{i,j}^2, 1/\eta_{i,j}^2)$ in the Schrödinger equation and can be treated as a small constant. Then the equation reduces to Eq. (10) with momenta $\tilde{\mathbf{k}}_{ij} = \mathbf{k}_{ij} + \Delta \mathbf{k}_i + \Delta \mathbf{k}_j$ and the solution is

$$f_k(\xi_k, \eta_k)$$
$$= {}_1F_1\left(-\frac{i\mu_{ij} a_k}{2\tilde{k}_{ij}}, 1, -i\tilde{k}_{ij}\xi_k \right) {}_1F_1\left(\frac{i\mu_{ij} b_k}{2\tilde{k}_{ij}}, 1, i\tilde{k}_{ij}\eta_k \right). \tag{37}$$

If we select $a_k = 2Z_i Z_j$; $b_k = 0$ we obtain the full solution in Ω_k with outgoing asympotic conditions:

$$\Psi_k = {}_1F_1\left(-\frac{i\mu_{ij} a_k}{2\tilde{k}_{ij}}, 1, -i\tilde{k}_{ij}\xi_k \right)$$
$$\times \prod_{l=i,j} \exp\left[-\frac{i\mu_{lk} Z_l Z_k}{k_{lk}} \ln(k_{lk}\xi_l) \right], \tag{38}$$

which is equivalent to that derived by Alt and Mukhamedzhanov [12]. We would like to stress that this wave function results from the separability of the the wave equation in the set of parabolic coordinates. The solution (38) can be easily extended to give a C6 wave function.

IV. SUMMARY

We have obtained a general solution of an approximate wave equation for three particles interacting with Coulomb potentials, which we denote as C6. It is the product of six hypergeometric functions, each depending of one parabolic coordinate. This solution depends on six separation constants. According to the choice of these constants we can obtain different asymptotic behaviors: outgoing, incoming, exploding, and decaying waves. A particular choice provides the well-known C3 function.

Recent proposals of different authors improve the C3 wave by introducing momentum- and coordinate-dependent charges. These effective charges dynamically correlate the independent motions described by the C6 function. We show that to account for these charges the approximate wave equation must be modified, but it continues to be separable.

The use of the effective momenta enabled us to solve the Schrödinger equation in the region where one particle is far from the other two, which remain close. Furthermore, effective momenta and charges can be combined, resulting in a set of separable wave functions. Anyway, the description of the correct wave function at non-asympotic distances could require the introduction of nonseparable approximations, which leads to multivariable functions, some particular solutions of the hypergeometric kind have been recently discussed [13].

V. APPENDIX

The general form for the equation of the confluent hypergeometric function used in Sec. II is [14]

$$w'' + \left[\frac{2A}{z} + 2f' + \frac{bh'}{h} - h' - \frac{h''}{h'} \right] w' + \left[\left(\frac{bh'}{h} - h' - \frac{h''}{h'} \right) \left(\frac{A}{2} + f' \right) + \frac{A(A-1)}{z^2} + \frac{2Af'}{z} + f'' + f'^2 - \frac{ah'^2}{h} \right] w = 0. \tag{A1}$$

The solution of Eq. (A1) is

$$w = z^{-A} e^{-f(z)}\ {}_1F_1(a,b,h(z)), \tag{A2}$$

where A is a constant and $f(z)$ and $h(z)$ are arbitrary functions. This equation gives us the possibility to obtain more general functions. Equation (11) can be associated with this equation through a change of function and variables. If we set $z_l = -ik_{mn}\xi_l$, Eq. (11) can be written as

$$w_l'' + \left(\frac{1-z_l}{z_l}\right) w_l' - \frac{1}{2z_l}\left(\frac{\mu_{nm}C_l}{k_{mn}^2} z_l + \frac{\mu_{mn}a_l}{ik_{mn}}\right) w_l = 0.$$

The transformations from this equation to Eq. (A1) are not unique. We select $A=0$, $b=1$, and $h(z_l)=\gamma_l z_l$. This choice determines the remaining functions:

$$f(z_l) = \frac{\gamma_l - 1}{2} z_l, \quad \gamma_l = 1 - 2\frac{\mu_{mn}C_l}{k_{mn}^2}, \quad \text{and}$$

$$a = \frac{1}{2\gamma_l}\left[\gamma_l - 1 - \frac{i\mu_{mn}a_l}{k_{mn}}\right],$$

and hence

$$w_l(z_l) = e^{[(\gamma_l - 1)/2]z_l}\ {}_1F_1\left(\frac{1}{2\gamma_l}\left[\gamma_l - 1 - \frac{i\mu_{mn}a_l}{k_{mn}}\right], 1, z_l\right),$$

which represents each factor of the C6 wave function.

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