Analytic properties of three-body continuum Coulomb wave functions

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We study the analytic properties of the functions known as C3 and Φ_2, used in atomic collision theory for the description of the three-body continuum state. We analyze the bound states for both models obtained by analytic continuation in the case of ion-atom collision. The C3 wave function is an uncorrelated model represented by the product of two-body Coulomb functions and the bound states are found for negative relative energies of electron-target or electron-projectile pairs. On the other hand, the Φ_2 model is based on a two-variable hypergeometric function that correlates the electron motion relative to both the target and projectile. We found that only decaying bound states are allowed and the atomic spectra becomes continuous. The bound states of the Φ_2 model have a complex energy due to the action of the projectile. Expressions for the wave functions in the different thresholds are given and studied.

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I. INTRODUCTION

The study of the structures of the velocity spectrum of electrons emitted in atomic collision processes has been a matter of active research during the last three decades. The calculations of transition matrices is the main tool used to investigate the evolution of the particles systems. Calculation of these matrices requires an accurate representation of the final state of the system, which is given by a continuum three- or many-body wave function. Some structures of the spectra are linked to specific characteristics of the final channel wave function. In ion-atom single ionization it is a well-known fact that the peaks observed on the emitted electron cross sections, known as soft electrons (SE) and electron capture to the continuum (ECC), originate from divergences in the normalization of the final channel continuum three-body wave functions. [1]. Besides, the shape of those structures are intimately related with characteristics of the wave function. On the other hand, the theoretical interpretations of the occurrence of these cusps are visualized as a smooth continuation across the ionization limit of excitation or capture into highly excited bound states [2].

A standard requirement on the wave function are the ''correct'' asymptotic conditions, when the three particles are far away from each other (Ω_0 region). Some studies also considered the limit of the continuum state when the relative coordinate between two particles is small [3]. This spatial region has been denoted as Ω_α. However, we can say that two particles are ''close'' only when they are in a bound state. In this sense it seems more physical to require that the three-body continuum state goes to bound states when the two-body energy crosses the ionization threshold. This information is displayed when the wave function is analytically continued in the complex energy variable.

Here we discuss the analytic continuation of two particular wave functions used in the calculation of transition matrices for ion-atom collision processes. In Sec. II we review the analytic continuation of the two Coulomb problem and show how the bound state can be obtained from the continuum states. Next, in Sec. III we obtain and study the analytic extension of the three-body wave functions known as C3 and Φ_2 [4–6]. In Sec. IV we study the state density and the functions in the thresholds. Finally the results are summarized in Sec. V. Atomic units are used unless otherwise noted.

II. THE TWO-BODY COULOMB PROBLEM

The study of the analytical properties of the wave function in the two-body quantum collision theory is based on a theorem due to Poincaré [7,8]. From the characteristics of the Schrödinger radial wave equation, the asymptotic properties of the solution and the Poincaré theorem it is possible to ensure the analyticity of the total wave function in a region of the complex plane k, where k represent the modulus of the momentum of the particle. Since the wave function is an analytic function in the complex k plane, a complete study of its behavior in the continuum and discrete spectra can be achieved [8].

In the two-body Coulomb problem a complete analysis can be performed without reference to the Poincaré's theorem. In parabolic coordinates the general solution can be written in terms of confluent hypergeometric functions [9,10]

$$\begin{aligned}\psi_k(\mathbf{r})=&C_{k,m}e^{ikr}e^{im\phi}[-ik(r+\hat{\mathbf{k}}\cdot r)]^{|m|2}\\&\times[-ik(r-\hat{\mathbf{k}}\cdot r)]^{|m|/2}\\&\times{}_1F_1\left(-i\frac{\alpha}{k}+\frac{|m|+1}{2},1+|m|,-ik(r+\hat{\mathbf{k}}\cdot r)\right)\\&\times{}_1F_1\left(-i\frac{\beta}{k}+\frac{|m|+1}{2},1+|m|,-ik(r-\hat{\mathbf{k}}\cdot r)\right),\end{aligned}\quad(1)$$

where $\alpha+\beta=-\mu Z_1Z_2$, μ is the reduced mass of the two particles, Z_i $(i=1,2)$ are their respective charges, m is the magnetic number related to the azimuthal angle ϕ, and $\mathbf{k}$ is the relative momentum of the particles.

To obtain $\psi_k(\mathbf{r})$ given by Eq. (1), we only request regularity in $r=0$ and we have not imposed any asymptotic be-

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havior. Now, it is well known that ${}_1F_1[b,c,x]$ is an analytic function of the complex parameters b, c and the argument x, except when $c=-1,-2,\ldots$. Using this general property of the Kummer functions a complete analysis of $\psi_k(\mathbf{r})$ in the complex k plane is possible.

For positive real energy, k is real and Eq. (1) gives outgoing waves (plus sign) with the choice $\{\alpha=-ik/2,\ m=0\}$ and incoming waves (minus sign) when $\{\beta=ik/2,\ m=0\}$. When an asymptotic unit flux is imposed the normalization factor is

$$C_k^{\pm}=e^{-(\pi/2)(\mu Z_1 Z_2/k)}\Gamma\left(1\mp i\frac{\mu Z_1 Z_2}{k}\right). \tag{2}$$

The resulting states are

$$\psi_k^{\pm}(\mathbf{r})=e^{-(\pi/2)(\mu Z_1 Z_2/k)}\Gamma\left(1\pm i\frac{\mu Z_1 Z_2}{k}\right)e^{i\mathbf{k}\cdot\mathbf{r}}\times{}_1F_1\left(\mp i\frac{\mu Z_1 Z_2}{k},1,\pm ik(r\mp\hat{\mathbf{k}}\cdot r)\right). \tag{3}$$

For negative energies, k is imaginary, and for an atomic hydrogen bound state with energy $E=-(\mu[Z_1Z_2]^2/2n^2)$, we choose

$$k=\mp i\frac{\mu Z_1 Z_2}{n} \tag{4}$$

for outgoing and incoming waves, respectively, and Eq. (3) becomes

$$\psi_{lig}^{\pm}(\mathbf{r})=C_k^{\pm}e^{(\mu Z_1 Z_2/n)r}{}_1F_1\left(1-n,1,-\frac{\mu Z_1 Z_2}{n}(r\pm\hat{\mathbf{k}}\cdot\mathbf{r})\right). \tag{5}$$

For particles with opposite sign charges Z_1 and Z_2 and integer $n=1,2,3\ldots$, these are the wave functions for a two-body Coulomb bound state, with $n_1\geqslant 0$, $n_2=0$, and $m=0$, for the minus sign, and $n_2\geqslant 0$, $n_1=0$, and $m=0$, for the plus sign [9,10].

The analytically continued normalization factors

$$C_k^{\pm}=e^{\mp i(n\pi/2)}\Gamma(1-n) \tag{6}$$

present a pole for every natural number n. At the points of the k-complex plane corresponding to bound states the normalization constants $C_k^{\pm}$ has poles. When we consider the choice

$$\alpha=-ik\left[\frac{1}{2}(|m|+1)+n_1\right]$$

and

$$\beta=-ik\left[\frac{1}{2}(|m|+1)+n_2\right], \tag{7}$$

Eq. (1) gives the bound Coulomb wave function with parabolic quantum numbers (n_1,n_2,m) such that $n_1+n_2+|m|+1=n$ [9].

An infinite number of bound states exist for the Coulomb potential. Due to the long range of this potential there exists an accumulation of states below the threshold, as $n\to\infty$. This accumulation produces a zero-energy resonance in the scattering amplitude. The square modulus of $|C_k^{\pm}|^2$ is given by

$$|C_k^{\pm}|^2=\frac{\mu Z_1 Z_2}{k}\frac{2\pi}{1-e^{-2\pi(\mu Z_1 Z_2/k)}}.$$

For $k\to 0$ the Kummer function tends to a smooth Bessel function of order zero, independent of k. On the other hand, $|C_k^{\pm}|^2$ shows a $1/k$ divergence which is the responsibility of the enhancement of the amplitude $|\psi_k^{\pm}(\mathbf{r})|^2$.

Therefore from the analytic properties of the ${}_1F_1(b,c,x)$ functions, we can analyze those of the continuum wave functions. On the other hand, we see that the normalization factor, closely related to the Jost function for this problem, has all the information about the position of the bound states in the complex plane k and how they accumulate in the threshold region [11].

III. THE THREE-BODY COULOMB PROBLEM

In this section we want to discuss some of the analytical approximated solutions for the three-body Coulomb problem used in atomic collision theory, in particular the C3 model, that has been successfully used since 1980 [4], and the Φ_2 model, that was recently introduced by the authors and coworkers [5].

The SE and the ECC cusps observed in the electron double differential cross section (DDCS) in ion-atom collisions are the consequence of zero-energy resonances produced by the long-range attractive Coulomb interaction between pairs of particles. These resonances result from the accumulation of the bound states below the threshold for every one of the possible subclusters of the particles system [2]. Nowadays it is a well-known fact that the normalization factors in the final wave functions for the attractive Coulomb interactions are responsible for these cusps. Meanwhile, the asymmetry and other characteristics of the peaks depend on the functional form of the wave function. In this way, we can see that information about the bound states, which are below threshold for every one of the possible subclusters of the particles system, are contained in the three-body continuum wave functions. Here we will show how the bound states arise from the continuum states wave functions known as C3 and Φ_2.

A. The C6 model

First we will discuss the C6 model, which is a generalization of the C3 model [12]. There, the wave function has all the information about the dynamic of the three body Coulomb system and is given by a separable function in parabolic coordinates:

$$\Psi_{C6}=N_{C6}e^{i\mathbf{k}_{23}\cdot\mathbf{r}_{23}+i\mathbf{K}_{23}\cdot\mathbf{R}_{23}}\times\prod_{l=1}^{3}{}_1F_1\left[\frac{i\mu_{ij}\alpha_l}{k_{ij}},1,-ik_{ij}\xi_l\right]{}_1F_1\left[\frac{i\mu_{ij}\beta_l}{k_{ij}},1,-ik_{ij}\eta_l\right] \tag{8}$$

where

$$\xi_i = r_{jk} + \hat{\mathbf{k}}_{jk}\cdot\mathbf{r}_{jk} \quad \text{and} \quad \eta_i = r_{jk} - \hat{\mathbf{k}}_{jk}\cdot\mathbf{r}_{jk}$$

with $i\neq j\neq k$; $i,j,k=1,2,3$ and $\alpha_l+\beta_l=2Z_jZ_k$, μ_{ij} is the reduced mass of each pair of particles, $\mathbf{k}_{ij}$ and $\mathbf{r}_{ij}$ are the relative momentum and relative position vector of every pair of particles, $\mathbf{R}_{ij}$ is the position vector from the center of mass of the pair (i,j) to particle l, $\mathbf{K}_{ij}$ is the conjugate momentum of $\mathbf{R}_{ij}$, and N_{C6} is a normalization constant [12]. The vectors can be expressed in terms of the Jacobi pair (for example, $\mathbf{k}_{23}$ and $\mathbf{K}_{23}$).

We should remember that the relative momenta are restricted by the center-of-mass relations

$$\frac{1}{\mu_{23}}\mathbf{k}_{23} = \frac{1}{\mu_{13}}\mathbf{k}_{13} + \frac{1}{\mu_{12}}\mathbf{k}_{12}, \tag{9}$$

$$\mathbf{k}_{13} = \frac{\mu_{13}}{m_3}\mathbf{k}_{23} - \frac{\mu_{13}}{\nu_{23}}\mathbf{K}_{23}, \tag{10}$$

$$\mathbf{k}_{12} = \frac{\mu_{12}}{m_2}\mathbf{k}_{23} + \frac{\mu_{12}}{\nu_{23}}\mathbf{K}_{23},$$

with $\nu_{23}=[(m_2+m_3)m_1]/(m_1+m_2+m_3)$.

The Ψ_{C6} represent a system of three pairs of two-body Coulomb functions, $l=1,2,3$, correlated by kinematic relations between the momentum and coordinate vectors and it is valid for particles with any masses. We must choose the values of $\{\alpha_l,\beta_l\}$ to fix the asymptotic behavior, which determines the normalization constant. The Ψ_{C6}, or the simplified version known as the C3 model, are valid as solutions of the three-body Coulomb problem only in a region where the distances between the particles tends to infinity, i.e., the Ω_0 region [13]. However, they are used as wave functions valid for all the region of the coordinate space, and give relatively good results in different areas of the atomic collision physics, like ion-atom collisions, electron-atom collisions, and double-photoionization processes [14–17].

As in the two-body Coulomb problem, it is possible to study the analytic properties of Ψ_{C6}. We will assume that the particles 1 and 2 are heavy and have positive charges and the third is light and negative (e.g., two protons and one electron). The Ψ_{C3} wave results from Eq. (8) choosing $\beta_i=0$:

$$\Psi_{C3} = N_{C3} e^{i\mathbf{k}_{23}\cdot\mathbf{r}_{23}+i\mathbf{K}_{23}\cdot\mathbf{R}_{23}}\, {}_1F_1[i\alpha_{23},1,-ik_{23}\xi_1] \times {}_1F_1[i\alpha_{13},1,-ik_{13}\xi_2]\, {}_1F_1[i\alpha_{12},1,-ik_{12}\xi_3] \tag{11}$$

with $\alpha_{ij}=\mu_{ij}(Z_iZ_j/k_{ij})$. That choice of the constants β_i fixes the asymptotic behavior as incoming waves in the Ω_0 region [3,18] and gives, for unit outgoing flux, the normalization constant

$$N_{C3} = [e^{-(\pi/2)\alpha_{23}}\Gamma(1-i\alpha_{23})][e^{-(\pi/2)\alpha_{13}}\Gamma(1-i\alpha_{13})] \times [e^{-(\pi/2)\alpha_{12}}\Gamma(1-i\alpha_{12})]. \tag{12}$$

The energy of the system can be written as

$$E = \frac{K_{23}^2}{2\nu_{23}} + \frac{k_{23}^2}{2\mu_{23}}. \tag{13}$$

In the two-body problem there exist only one center to build bound states. In the three-body problem (TBP), and for the particular case under consideration, we can have the particle 3 bound to the 1, or 2, or bound in both centers. To construct a (2,3) bound state we must consider that the energy of a pair $\varepsilon_i=k_{23}^2/2\mu_{23}$ is negative, in particular for an hydrogen atom:

$$k_{23} = i\,\frac{\mu_{23}Z_2Z_3}{n_{23}}. \tag{14}$$

The correct expression for the total-energy requires a real $\mathbf{K}_{23}$, and we will keep k_{13} as a real number. Replacing Eq. (14) in Eq. (11) results in

$$\Psi^{C3}_{n_1,k_{13},k_{12}} \propto e^{i\mathbf{K}_{23}\cdot\mathbf{R}_{23}} \varphi^{C3}_{n_1}\, {}_1F_1[i\alpha_{13},1,-ik_{13}\xi_2] \times {}_1F_1[i\alpha_{12},1,-ik_{12}\xi_3] \tag{15}$$

with

$$\varphi^{C3}_{n_1} = e^{(\mu_{23}Z_2Z_3/n_{23})r_{23}}\, {}_1F_1\left[-n_1,1,-\frac{\mu_{23}Z_2Z_3}{n_{23}}\xi_1\right] \tag{16}$$

where $n_1=n_{23}-1$ and $n_{23}=1,2,3\ldots$. In Eq. (15) the particle's pairs (1,2) and (1,3) are represented by two continuum Coulomb wave functions. For Z_2 and Z_3 with opposite signs, the pair (2,3) bounded, with the parabolic and magnetic numbers given by $n_1\geqslant 0$ and $n_2=m=0$ [12]. As we pointed out before, the bound states of the two-body Coulomb problems correspond to points into the complex k plane that produce a divergence in the normalization constant. A simple analysis of the poles of N_{C3} [Eq. (12)] shows that the value given by Eq. (14) produces in the TBP a divergence similar to that present in C_k^-, Eq. (2).

A more general result can be obtained using the C6 wave function: with $\beta_2=\beta_3=0$ only four variables are involved [12]. With the same analytic extension as before we obtain

$$\Psi^{C6}_{n_1,n_2,K_{23}} \propto e^{i\mathbf{K}_{23}\cdot\mathbf{R}_{23}} \varphi_{n_1,n_2}\, {}_1F_1[i\alpha_{12},1,-ik_{12}\xi_3] \times {}_1F_1[i\alpha_{13},1,-ik_{13}\xi_2], \tag{17}$$

where φ_{n_1,n_2} is given by

$$\varphi_{n_1,n_2} = e^{(\mu_{23}Z_2Z_3/n_{23})r_{23}}\, {}_1F_1[-n_1,1,-(\mu_{23}Z_2Z_3/n_{23})\xi_1] \times {}_1F_1\left[-n_2,1,-\frac{\mu_{23}Z_2Z_3}{n_{23}}\eta_1\right] \tag{18}$$

and $n_1+n_2+1=n_{23}$. The function φ_{n_1,n_2} is the hydrogen-atom wave function with parabolic quantum numbers n_1,n_2 and the magnetic number equal to zero. The continuum C6 wave function is correct in the asymptotic Ω_0 region:

$r_{23}, R_{23} \to \infty$ $(r_{23}/R_{23} \to 1)$. In the Ω_{23} region, where particle 1 is far from the center of mass of the pair (2,3) $(r_{23}/R_{23} \to 0)$ [3], Eq. (17) becomes

$$\Psi^{C6}_{n_1,n_2,K_{23}} \to \frac{e^{-\pi/2(\alpha_{12}+\alpha_{13})}}{\Gamma(1-i\alpha_{12})\Gamma(1-i\alpha_{13})} \times e^{i\mathbf{K}_{23}\cdot\mathbf{R}_{23}} \varphi_{n_1,n_2} e^{-i\alpha_{13}\ln k_{13}\xi_2 - i\alpha_{12}\ln k_{12}\xi_3}. \quad (19)$$

Apart from the normalization constant and restricted to $m=0$, Eq. (19) shows the right asymptotic behavior known as distorted eikonal initial bound-state used in ion-atom collision theory [17]. It is also possible to bound the pair (1,3) obtaining similar expressions as that written for the (2,3) pair. We conclude that $\Psi^{C3}_{n_1,K_{23}}$ and $\Psi^{C6}_{n_1,n_2,K_{23}}$ have the right behavior in these asymptotic conditions.

B. The Φ_2 model

As we said in the preceding section, the C3 wave function represents the TBP by a product of three pairs of two-body Coulomb wave functions only correlated by kinematical relations between coordinates and momenta vectors. The Φ_2 model was recently obtained for two particular cases: one light and two heavy particles [5] and two light and one heavy particles [19].

In the first case, the state for the TBP, denoted as Ψ^{Φ_2}, is a product of confluent hypergeometric functions of two kinds: a degenerate Appell's hypergeometric function times a Kummer function [20]. This two-variable Appell's function was labeled by Horn [21] as $\Phi_2(b,b',c,x,y)$ and studied by Erdélyi [22,23]. The Φ_2 model is a confluent hypergeometric function which is an analytical function for all the complex values of the parameters b, b', c and arguments x, y; except when $c=0,-1,-2,\ldots$. Then, using the analytical properties of the hypergeometric functions we can study the analyticity of the approximated wave Ψ^{Φ_2}. As above we assume two positive (Z_1,Z_2) heavy particles and a negative light particle $(-|Z_3|)$.

The wave function is

$$\Psi^{\Phi_2} = N_{\Phi_2} e^{i\mathbf{k}_{23}\cdot\mathbf{r}_{23} + i\mathbf{K}_{23}\cdot\mathbf{R}_{23}} {}_1F_1(i\alpha_{12},1,-ik_{12}\xi_3) \times \Phi_2(i\alpha_{23}, i\alpha_{13}, 1, -ik_{23}\xi_1, -ik_{13}\xi_2), \quad (20)$$

and with the normalization constant

$$N_{\Phi_2} = [e^{-(\pi/2)(\alpha_{23}+\alpha_{13})}\Gamma(1-i\alpha_{23}-i\alpha_{13})] \times [e^{-(\pi/2)\alpha_{12}}\Gamma(1-i\alpha_{12})] = \overline{N}_{\Phi_2}[e^{-(\pi/2)\alpha_{12}}\Gamma(1-i\alpha_{12})], \quad (21)$$

the incoming flux is one. The Φ_2 model sets a correlation between the motion of the light particle relative to the heavy ones. This correlation is also incorporated in Eq. (21).

For $\mathbf{R}_{23} \to \infty$ is $\xi_2 \to \infty$ (avoiding the singular directions) we have [5]

$$\Phi_2(\alpha,\beta,1,x,y) \to \frac{e^{i\pi(\beta-1)}}{\Gamma(\beta)} (x-y)^{-\alpha}(-y)^{\alpha+\beta-1} e^{y} \times \Phi_4\left(1-\beta, \alpha, 1-\alpha-\beta, \frac{1}{y-x}, \frac{1}{y}\right) + \frac{e^{i\pi\beta}}{\Gamma(1-\beta)} y^{-\beta} \Phi_5\left(\alpha,\beta,1-\beta,x,\frac{1}{y}\right) \quad (22)$$

and

$$\Phi_5\left(\alpha,\beta,1-\beta,x,\frac{1}{y}\right) \to {}_1F_1(\alpha,1-\beta,x),$$

$$\Phi_4\left(1-\beta,\alpha,1-\alpha-\beta,\frac{1}{y-x},\frac{1}{y}\right) \to 1 + \vartheta\left(\frac{1}{y}\right). \quad (23)$$

Further $\xi_3 \to \infty$ gives

$$\Psi^{\Phi_2} \to C e^{i\mathbf{K}_{23}\cdot\mathbf{R}_{23}} \chi_{23} e^{-i\alpha_{13}\ln k_{13}\xi_2 - i\alpha_{12}\ln k_{12}\xi_3} \quad (24)$$

where φ_{23} is given by

$$\chi_{23} = e^{ik_{23}(\hat{\mathbf{k}}_{23}\cdot\mathbf{r}_{23})} {}_1F_1(i\alpha_{23}, 1-i\alpha_{13}, -ik_{23}\xi_1) = e^{-ik_{23}r_{23}} {}_1F_1(1-i\alpha_{13}-i\alpha_{23}, 1-i\alpha_{13}, ik_{23}\xi_1) \quad (25)$$

and C represents a constant which includes the normalization N_{Φ_2}.

The continuum-bound states given by $\Psi^{C3}_{n_1,K_{23}}$ or $\Psi^{C6}_{n_1,n_2,K_{23}}$ [Eqs. (15) and (17)] result when Ψ^{C3} or Ψ^{C6} are analytically continued to the complex k_{23} plane, and evaluated, for negative energies, at the position of the bound states.

Replacement of Eq. (14) on Eq. (25) gives

$$\chi^{I}_{n_{23}} = e^{(\mu_{23}Z_2Z_3/n_{23})r_{23}} \times {}_1F_1\left(1-i\alpha_{13}-n_{23}, 1-i\alpha_{13}, -\frac{\mu_{23}Z_2Z_3}{n_{23}}\xi_1\right). \quad (26)$$

According to the Φ_2 theory, this is the state of the (2,3) subsystem, with negative energy and, when the particle 1 is at infinity. For $\xi_1 \to \infty$ the exponential divergence of the hypergeometric function overcomes the first factor. Therefore it does belong to L^2 and cannot be considered a bound state.

From Eqs. (22) and (23) we observe that exponential decaying states are obtained for values of k_{23} which lead to poles in the normalization factor of the Φ_2 function. Equation (21) has a pole when

$$i\alpha_{13} + i\alpha_{23} = n_{23}$$

for each natural number n_{23}. This gives a relation between k_{23}, k_{13}, and n_{23},

$$k_{23}=-\frac{1}{\frac{\mu_{13}Z_1}{k_{13}\mu_{23}Z_2}+i\frac{n_{23}}{\mu_{23}Z_2Z_3}} \qquad (27)$$

from the kinematic equations, Eq. (10), and defining $v=K_{23}/\nu_{23}$ as a real number results in

$$a_4k_{13}^4+a_3k_{13}^3+a_2k_{13}^2+a_1k_{13}+a_0=0, \qquad (28)$$

where a_i are complex coefficents depending on K_{23}, n_{23}, charges, and masses. For proton-hydrogen forward scattering

$$a_4=n_{23}^2,$$

$$a_3=2in_{23},$$

$$a_2=-2in_{23}v-(n_{23}v)^2,$$

$$a_1=2v(1-in_{23}v),$$

$$a_0=v^2.$$

In this case, Eq. (28) has simple analytical solutions,

$$k_{13}=\frac{1}{2n_{23}}[n_{23}v\mp\sqrt{n_{23}v}\sqrt{4i+n_{23}v}],$$

$$k_{13}=\frac{1}{2n_{23}}[-2i-n_{23}v\pm\sqrt{(n_{23}v)^2-4}].$$

From Eq. (27) we obtain the corresponding k_{23}. Only the last root leads to a bounded χ_{23}. This is a complex root as shown in Fig. 1 as a parametric function of v, for $n_{23}=1$, 2, and 3. For $v\to0$ the root goes to $-2i/n_{23}$. As the velocity v increases, it moves in the k_{23} complex plane, going to $-i/n_{23}$ for $v\to\infty$.

Replacing Eq. (27) in Eq. (20) and using the relation

$$\Phi_2(\alpha,\beta,\gamma,x,y)=e^x\Phi_2(\gamma-\alpha-\beta,\beta,\gamma,-x,y-x),$$

we obtain

$$\Psi^{\Phi_2}=N_{\Phi_2}e^{-ik_{23}r_{23}+i\mathbf{K}_{23}\cdot\mathbf{R}_{23}}{}_1F_1(i\alpha_{12},1,-ik_{12}\xi_3)$$
$$\times\Phi_2(1-n_{23},i\alpha_{13},1,ik_{23}\xi_1,ik_{23}\xi_1-ik_{13}\xi_2). \qquad (29)$$

For $\mathbf{R}_{23}\to\infty$ is $\xi_2\to\infty$ and Ψ^{Φ_2} takes the form as Eq. (24). But, now χ_{23} is replaced by $\chi_{n_{23}}^C$, which is given by

$$\chi_{n_{23}}^C=e^{-ik_{23}r_{23}}{}_1F_1(1-n_{23},1-i\alpha_{13},ik_{23}\xi_1). \qquad (30)$$

For $r_{23}\to\infty$, we have $\xi_1\to\infty$ and $\chi_{n_{23}}^C$ tends exponentially to zero, which means that Eq. (30) is a bounded function. Therefore Ψ^{Φ_2} is asymptotically a L^2 function distorted by two eikonal phases, for any real value of K_{23}.

In the limit $v\to\infty$, $k_{23}\to-i/n_{23}$, we obtain a similar result to the C3 model and the wave function $\chi_{n_{23}}^C$ matches with that given by Eq. (16), which is the bound state for a hydrogen atom. Otherwise, when $v\to0,k_{23}\to-2i/n_{23}$, and the $\chi_{n_{23}}^C$ now presents the exponential decay as a bound state with nuclear charge equal to 2.

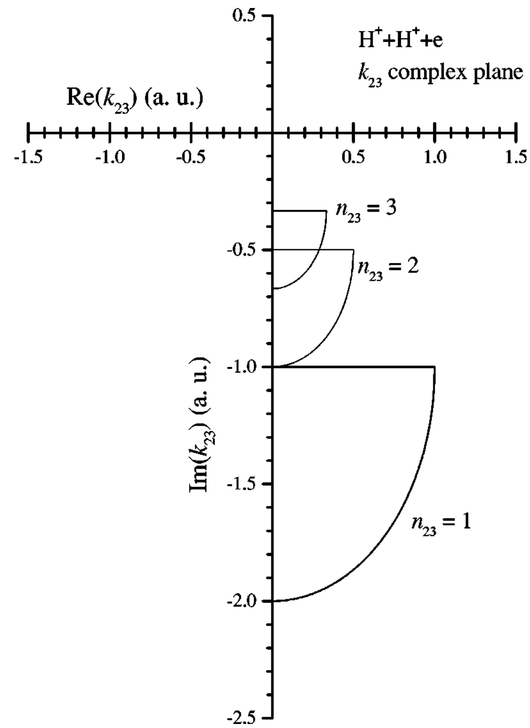

FIG. 1. Trajectory of the poles of N_{Φ_2} as a function of v in the k_{23} complex plane for different values of the quantum number n_{23}.

From Eq. (13) we note that the energy E associated with this wave function has a complex value

$$E=\frac{K_{23}^2}{2\nu_{23}}+\varepsilon_R(K_{23},n_{23})+i\varepsilon_I(K_{23},n_{23}). \qquad (31)$$

Therefore the function given by Eq. (30) is an L^2 exponentially decaying wave function even when it does not correspond to an eigenvalue of the bound electron-target system. However, for $K_{23}\to\infty$, the imaginary part of this energy ε_I goes to 0 and $\varepsilon_R\simeq-1/2n_{23}^2$; meanwhile for $K_{23}\to0$, also $\varepsilon_I\simeq0$ and $\varepsilon_R\simeq-2/n_{23}^2$. In these cases the energy becomes real and negative.

Then, the analytical extension of the Φ_2 function to imaginary k_{23} is not a bounded state. Meanwhile for the complex E values given by Eq. (31) it has an exponential decay. The poles on the normalization factor are responsible for cusps in the density of continuous states in the nearby negative E axis.

The eigenvalue spectrum of the Hamiltonian for an isolated atom is discrete for negative energies and continuous for the positive ones. When the projectile-electron Coulomb potential is introduced the spectra on the negative-energy axis becomes continuous, with a high density of states near the position of the unperturbated bound states. When the collision velocity is very large, the time of the interaction between both systems is small and we can say that the perturbation is small. When the incident velocity tends to zero, for an asymptotic electron, the hydrogen nucleus and the incident particle behave as a molecular system, which resembles an united atom.

The situation is similar to the Stark effect. When a hydrogen atom is placed in a electric field of constant field strength, all the bound eigenvalues that are originally discrete and located on the negative real axis of the energy degenerate into a continuous spectra [24]. The levels with negative real energy become instantaneously dense packets of continuous energy levels, as soon as the field is turned on. As the field intensity increases the packets spread out. Each packet is associated with the presence of a complex pseudoeigenvalue, which is a pole of the perturbed Green function, in the negative and imaginary energy half-plane [25]. Application of the perturbation theory gives the splitting and displacement of the packet centers with the field intensity [26].

The Φ_2 model for the three-body problem gives a similar prediction. The Φ_2 wave function is the solution of a stationary wave equation which includes the electron-target and electron-projectile potentials. Therefore the electron motion is correlated with both centers, even at asymptotic distances.

From another point of view, the projectile-electron interaction could be considered as time dependent. In this case the atomic state becomes time dependent and the imaginary part of the energy in Eq. (31) represents the inverse of the mean decaying time. The electron-projectile interaction allows for the opening of other channels as electron emission or capture by the projectile.

In Fig. 2 we compare the unperturbate hydrogenic bound states $|\varphi_{n_{23}}(\xi_1)|^2$ with $|\chi^C_{n_{23}}(\xi_1)|^2$ for different values of n_{23} and v. The distortion generated by the projectile produces a substantial change in the function that represents the bound state and gives eigenstates ($\chi^C_{n_{23}}$). We note that the nodes of $|\chi^C_{n_{23}}(\xi_1)|^2$ becomes minima. For v larger than 10 a.u. the functions are very similar, but differ considerably for small v.

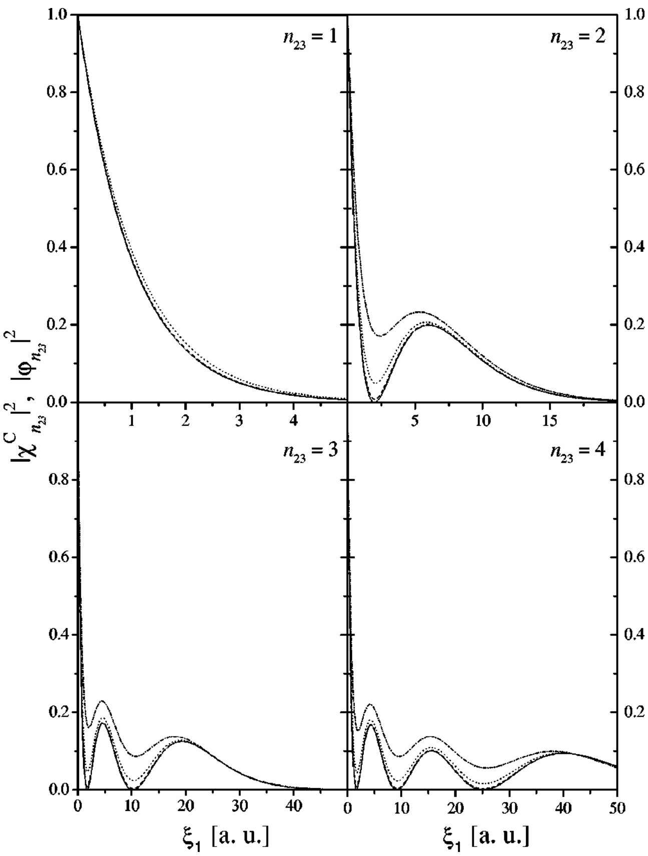

FIG. 2. Square module of the asymptotic wave functions in the Ω_1 region in the C3 and Φ_2 models as a function of ξ_1. We have chosen $n_{23}=1,2,3,4$ and $n_2=m=0$. The solid line represents $|\varphi_{n_{23}}(\xi_1)|^2$, while $|\chi^C_{n_{23}}(\xi_1)|^2$ is given by broken lines: the long-dashed line was obtained with a ratio $v=2$ a.u., the short-dashed line with $v=4$ a.u., and the dash-dotted line with $v=10$ a.u.

IV. THE UNITED ATOM LIMIT AND THE THRESHOLDS

When the distance between the ions and their relative velocity goes to zero the wave function must approach that of an atom with added charge. In this case we have $k_{23}=k_{13}=k$, $\alpha_{23}/Z_2=\alpha_{13}/Z_1=m_3Z_3/k$, and $\xi_1=\xi_2$ for two heavy ions and one electron. From the power series we obtain

$$\Phi_2(i\alpha_{23},i\alpha_{13},1,-ik_{23}\xi_1,-ik_{13}\xi_2)$$
$$={}_1F_1(im_3(Z_1+Z_2)Z_3/k,1,-ik\xi_1).$$

The continuous state Φ_2 reduces correctly to that of the united atom. Continuation to bound states follows as in the two-body case, and they are found in the imaginary k axis. A simple inspection shows that the C3 model does not satisfy this limit.

In the previous sections we study the bound-continuum states obtained by the analytic extension of the continuum three-body eigenfunctions. We mention that the cusps (ECC and SE) observed in the electronic spectra are consequences of the accumulation of bound states for $n_{ij}\to\infty$ in every one of the centres. Then, there must be continuity of the wave functions across the thresholds [27]. The wave function which results for $k_{ij}\to 0$ should be the same that the obtained for $n_{ij}\to\infty$. In the two-body Coulomb problem when k tends to zero the scattering wave function $\psi^{\pm}_k(\mathbf{r})$, Eq. (3), becomes

$$\psi^-_{k\to 0}(\mathbf{r})=C^-_{sca}J_0(\sqrt{4Z_1Z_2(r+\hat{\mathbf{k}}\cdot\mathbf{r})}). \qquad (32)$$

$J_0(x)$ denotes the Bessel function of zeroth order. The continuity across the threshold means that in the limit $n\to\infty$, the $\psi^-_{lig}(\mathbf{r})$, Eq. (5), has the same expression as $\psi^-_k(\mathbf{r})$ [Eq. (32)]. The eigenvalue of the energy becomes zero and, for the scattering wave function given by Eq. (32), the Runge-Lenz eigenvalue is the product of the charges of the interacting particles [2,27].

It is possible to obtain an expression for the normalization (the density of states) of the continuum in terms of the density of bound states. The continuation across the threshold of the scattering eigenfunction leads to a density of states ρ which is proportional to n^4,

$$\rho=\frac{n^4}{Z_1Z_2\mu} \tag{33}$$

rather than $n^5/(Z_1Z_2\mu)$ corresponding to general bound states. This is a consequence of the elimination of states which are accessible when the magnetic number m is different than zero.

A similar analysis could be done for the three-body problem using the C3 and Φ_2 models. The C3 model is represented by three, kinematically uncorrelated, two-body Coulomb problems. The procedure which gives origin to the approximation supposes the existence of six separation constants associated with the Runge-Lenz vector of every pair [6,12]. Therefore, using a similar procedure as for the two-body Coulomb problem we can obtain information about the analytic properties of Ψ^{C3} in the threshold associated with each couple of particles.

The description that results using the Φ_2 model is substantially different from that obtained using the C3 (or C6) model. The limit, $k_{23}\to 0$ leads Ψ^{Φ_2} to

$$\Psi^{\Phi_2}_{k_{23}\to 0}=N_{\Phi_2}e^{i\mathbf{K}_{23}\cdot\mathbf{R}_{23}}{}_1F_1(-i\alpha_{12},1,-ik_{12}\xi_3)\times\Phi_3[-i\alpha_{13},1,-Z_2Z_3\xi_1,-ik_{13}\xi_2], \tag{34}$$

where the Φ_3 represents a confluent hypergeometric function in two variables [21]:

$$\Phi_3[\beta,\gamma,x,y]=\sum\frac{(\beta)_r}{(\gamma)_{r+p}r!p!}x^ry^p, \tag{35}$$

where $(\beta)_r=\Gamma(\beta+r)/\Gamma(\beta)$. It is straighforward that Eq. (34) is also the limit of Eq. (29) for $n_{23}\to\infty$. Writing Eq. (34) in terms of the Bessel and Kummer functions [22,23],

$$\Psi^{\Phi_2}_{k_{23}\to 0}=N_{\Phi_2}e^{i\mathbf{K}_{23}\cdot\mathbf{R}_{23}}\,{}_1F_1(-i\alpha_{12},1,-ik_{12}\xi_3)\times\sum_{m=0}^{\infty}\frac{(-i\alpha_{13})_m}{m!(m)_m}[-ik_{13}\xi_2]^mJ_{2m}(2\sqrt{Z_2Z_3\xi_1})\times{}_1F_1(-i\alpha_{13}+m,1+2m,-ik_{13}\xi_2). \tag{36}$$

The term $m=0$ in this equation equals that given by Ψ^{C3} (except for the normalization constant), but it is modified by the following terms $(m\neq 0)$, which introduce the correlation.

The asymmetry and other characteristics of SE and ECC peaks depend on the spatial electron distribution given by both continuum and bound wave functions. The correlation introduced by the terms included in Eq. (36) modifies in a correct way the shape of these peaks. This has beeen shown in recent work, where the Φ_2 model is applied to the ionization of hydrogen [19] and helium [16] by proton impact.

V. CONCLUSIONS

The Redmond condition is the usual requirement imposed to declare acceptable an approximate wave function, for a three-body system with Coulomb interactions. This is a condition on the behavior in what was called the Ω_0 region where the three particles are asymptotically far one from other. The regions where two particles are near and the other is far away was denoted Ω_α. The wave functions in these regions have been studied in Refs. [3,28]. However, the meaning of ''near'' is unclear for two particles in a continuum state. It seems more appropiate to apply that name to a bound state, and Ω_α should be the region where pairs of the opposite charge particles are in a bound state and the third is in the continuum. In two-particle systems bound states are derived by an analytical extension of continuum states to negative energies, or imaginary momentum.

The definition of an appropiate wave function requires a good behavior in Ω_0 and in each allowed Ω_α. The C3 is the more usual wave functions used for evaluation of the ionization cross sections at high energies. Recently the three-body function Φ_2 has been introduced [5], which improves the C3 approximation by correlating the electron-target and electron-projectile relative motions. Both of these functions satisfies the Redmond condition in Ω_0 and here we have considered the Ω_α regions.

We have studied the analytical extension of the scattering wave functions C3 and Φ_2 to complex values of the relative momentun k_{ij}, between a given attractive pair of particles. This can be done from the analytic properties of the corresponding hypergeometric functions. The C3 wave function is the product of three hypergeometric functions, each describing the relative motion of a pair of particles, and bound states are found when the relative energy of the attractive pair is negative, as in the two-body problem. In the Φ_2 model the electron-ion motion is coupled to the motion of the other ion. Bound states are found when the Φ_2 is continued to complex eigenenergies. This means that the continued Φ_2 is a metastable state. This shows that, under the action of the projectile, the unperturbed atomic discrete spectra becomes continuous, as in the Stark effect. We also prove that the Φ_2 function reduces to the correct wave function in the united atom limit. An expression for the thresholds waves is obtained and analyzed. We note that, in these regions of the energy, the wave functions do not depend on the momenta, which tends to zero, or the principal quantum number that goes to infinity, but on the product of the charges that produce the bound state. In the C6 model this fact is related with the conservation of the Runge-Lenz vector; the charges product is the eigenvalue of a component of the vector.

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