Approximate analytical solution for two electrons in the continuum

P. A. Macri,[1] J. E. Miraglia,[1] C. R. Garibotti,[2] F. D. Colavecchia,[2] and G. Gasaneo[2]
[1]Instituto de Astronomía y Física del Espacio, Consejo Nacional de Investigaciones Científicas y Técnicas, CC 67, Sucursal 28, 1428 Buenos Aires, Argentina
[2]Centro Atómico Bariloche, Comisión Nacional de Energía Atómica, 8400 San Carlos de Bariloche, Río Negro, Argentina
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In this work we construct a correlated double continuum wave function for the three-body Schrödinger equation valid for large interparticle distances. Genuine three-body effects are considered by taking into account a nondiagonal part of the Hamiltonian written in generalized parabolic coordinates. A solution is found in terms of the confluent hypergeometric function of two variables Φ_2, with similar structure to the first-order Faddeev approximation. The use of such a solution seems to introduce appropriately the interelectronic repulsion. [S1050-2947(97)06804-2]

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I. INTRODUCTION

The three-body Coulomb continuum problem is of fundamental importance in atomic physics. There are several mechanisms leading to three unbounded particles in the final state, such as single ionization by electron impact, double photoionization, or double Compton. In all these cases we have to deal with two electrons in the continuum. Several approximate double continuum wave functions have been used to compute the correspondent cross sections. The most simple approximation consists of neglecting one of the interactions; namely, the electron-electron (e-e) repulsion. This leads to a solution expressed in terms of a product of two Coulomb waves, the so-called C2 approximation. It produces reasonable agreement with measured total cross section for double photoionization [1], but it cannot describe electron angular distributions because it does not consider the electronic correlation. To some extent, this correlation can be taken into account using momentum-dependent effective charges as introduced by Rudge and Seaton [2].

A more comprehensive approximation is found by neglecting all mixed derivatives of the three-body Hamiltonian written in generalized parabolic coordinates [3]. This wave function is expressed in terms of a product of three Coulomb waves, the so-called C3 approximation [3–5]. Unlike the C2, the C3 approximation tends to the exact solution of the problem for large interparticle distances. However, this solution underestimates by orders of magnitude the threshold of total cross sections [6] because of an overestimation of the electronic repulsion.

To avoid this defect it is necessary to find a wave function where the variables of the system are correlated so that, for certain configurations, the repulsion between the electrons becomes shielded by the presence of the nucleus. In recent years, new correlated wave functions have been developed. These solutions have the same structure as the C3 approximation, but with effective momenta [7] or charges [8] depending ''slowly'' on the coordinates. In order to determine to what extent this kind of approach introduces correlation, in Sec. II, we solve numerically a model Hamiltonian considering two electrons in the field of a nucleus for a particular configuration. We find that the use of effective momenta does not provide a fully satisfactory answer to the problem. In Sec. III, we look for a solution beyond the C3 approximation. We find a double continuum wave function in terms of the hypergeometric function of two variables Φ_2, which is an exact solution for large interparticle distances. Finally in Sec. IV, we expose our main conclusions and outlook. Atomic units will be employed throughout this work.

II. THE THREE-BODY COULOMB EQUATION IN GENERALIZED PARABOLIC COORDINATES

Let us consider two electrons in the Coulomb field of a heavy nucleus whose mass is considered infinite. The sets of Jacobi coordinates are shown in Fig. 1. The nonrelativistic Hamiltonian of the three-body system is given by

$$\left(\nabla_1^2+\nabla_2^2+\frac{2Z_1}{r_1}+\frac{2Z_2}{r_2}+\frac{2Z_3}{r_3}-E\right)\overline{\Psi}=0, \tag{1}$$

where $Z_1=Z_2=Z$ is the nuclear charge, $Z_3=-1/2$ represents the strength of the e-e repulsion, and $E=k_1^2/2+k_2^2/2$ is the total energy. It is convenient here to make two transformations. First, we remove the plane-wave asymptotic condition by writing

$$\overline{\Psi}=(2\pi)^{-3}\exp(i\mathbf{k}_1\cdot\mathbf{r}_1+i\mathbf{k}_2\cdot\mathbf{r}_2)\Psi, \tag{2}$$

where $\mathbf{k}_1$ ($\mathbf{k}_2$) is the momentum of the electron ''1'' (''2'') with respect to the heavy nucleus, and $\mathbf{k}_3=(\mathbf{k}_1-\mathbf{k}_2)/2$ is the

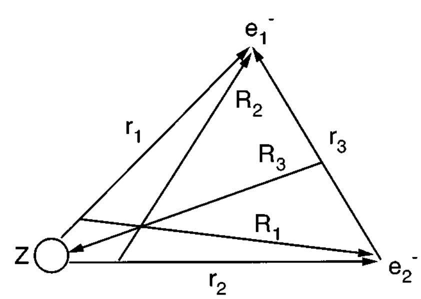

FIG. 1. Set of Jacobi coordinates. When the nucleus mass tends to infinity, then $R_1\to r_2$ and $R_2\to r_1$.

e-e relative momentum. Second, we follow the work of Klar [3] introducing the following generalized parabolic coordinates:

$$\xi_j = r_j + \mathbf{r}_j \cdot \hat{\mathbf{k}}_j, \quad \eta_j = r_j - \mathbf{r}_j \cdot \hat{\mathbf{k}}_j, \quad j=1,2,3. \tag{3}$$

After significant algebra, one can find that Eq. (1) transforms into

$$H\Psi = (H_{\mathrm{C3}} + W_{\mathrm{C3}})\Psi = 0, \tag{4}$$

where H is the total Hamiltonian,

$$H_{\mathrm{C3}} = \sum_{j=1}^{3} 2\frac{1+\delta_{j,3}}{\xi_j + \eta_j}(H_j^- + H_j^+ + Z_j), \tag{5}$$

$$H_j^- = \frac{\partial}{\partial \xi_j}\xi_j \frac{\partial}{\partial \xi_j} + ik_j\xi_j \frac{\partial}{\partial \xi_j}, \tag{6}$$

$$H_j^+ = \frac{\partial}{\partial \eta_j}\eta_j \frac{\partial}{\partial \eta_j} + ik_j\eta_j \frac{\partial}{\partial \eta_j}, \tag{7}$$

$$W_{\mathrm{C3}} = \sum_{l=1}^{2} (-1)^{l+1}\Bigg[\mathbf{t}_l^- \cdot \mathbf{t}_3^- \frac{\partial^2}{\partial \xi_l \partial \xi_3} + \mathbf{t}_l^- \cdot \mathbf{t}_3^+ \frac{\partial^2}{\partial \xi_l \partial \eta_3} + \mathbf{t}_l^+ \cdot \mathbf{t}_3^- \frac{\partial^2}{\partial \eta_l \partial \xi_3} + \mathbf{t}_l^+ \cdot \mathbf{t}_3^+ \frac{\partial^2}{\partial \eta_l \partial \eta_3}\Bigg], \tag{8}$$

and

$$\mathbf{t}_j^{\pm} = \hat{\mathbf{r}}_j \mp \hat{\mathbf{k}}_j, \quad j=1,2,3. \tag{9}$$

If the term W_{C3} is neglected, the solution of H_{C3} with the outgoing condition is the well-known C3 approximation, i.e., $H_{\mathrm{C3}}\Psi_{\mathrm{C3}}^- = 0$, where

$$H_{\mathrm{C3}}^- = \sum_{j=1}^{3} 2\frac{1+\delta_{j,3}}{\xi_j + \eta_j}(H_j^- + Z_j), \tag{10}$$

$$\Psi_{\mathrm{C3}}^- = \prod_{j=1}^{3} N_j^- F_j^-, \tag{11}$$

$$F_j^- = {}_1F_1(i\alpha_j;1;-ik_j\xi_j), \tag{12}$$

$$N_j^- = \exp(-\pi\alpha_j/2)\Gamma(1-i\alpha_j), \tag{13}$$

$\alpha_j = -Z_j/k_j, j=1,2,3$ and ${}_1F_1$ is the degenerate hypergeometric function. In this work we will concentrate on the outgoing solution (similar structure is found for the incoming solution Ψ_{C3}^+). For large interparticle distances, Ψ_{C3}^- tends to the proper asymptotic solution known as Redmond's condition:

$$\lim_{r_j\to\infty} \Psi_{\mathrm{C3}}^- = \prod_{j=1}^{3} E_j^-, \quad E_j^- = \exp[-i\alpha_j \ln(k_j\xi_j)]. \tag{14}$$

The C2 approximation is obtained from Ψ_{C3}^- by neglecting the e-e interaction to give $\Psi_{\mathrm{C2}}^- = \Pi_{j=1}^{2} N_j^- F_j^-$, which does not satisfy the Redmond's conditions. Note that if the e-e interaction is switched off, the C2 function is an exact solution of Eq. (4). Therefore, any approximate double continuum wave function should reduce to C2 when $Z_3 = 0$.

The function Ψ_{C3}^- is a solution of the uncorrelated differential operator H_{C3}. Our goal is to find an approximate solution of Eq. (4) valid for large interparticle distances that account for three-body effects beyond the C3 approximation. In generalized parabolic coordinates, the correlation arises in terms containing mixed derivatives. If we want to account for all the crossing derivatives contained in W_{C3}, the two following problems occur:

(i) Today's computers prohibit solving a six-dimensional differential equation of the type of Eq. (4) in all the variables, i.e., $\xi_1, \xi_2, \xi_3, \eta_1, \eta_2$, and η_3. On physical grounds we will neglect the terms containing $\mathbf{t}^+ \partial/\eta_j$ for the outgoing boundary conditions. Two reasons can be put forward to support this approximation. First, at large distances one can expect that $\mathbf{k}_j$ is nearly parallel to $\mathbf{r}_j$ and so $\mathbf{t}^+$ should vanish. In addition, if we iterate Ψ_{C3}^- thus all the terms containing $\partial \eta_j$ will cancel since it depends only on ξ_j. In conclusion we write the outgoing approximation as

$$W_{\mathrm{C3}} \cong W_{\mathrm{C3}}^- = \sum_{l=1}^{2} (-1)^{l+1} \mathbf{t}_l^- \cdot \mathbf{t}_3^- \frac{\partial^2}{\partial \xi_l \partial \xi_3}. \tag{15}$$

If we are interested in the incoming boundary solution instead, we should approximate $W_{\mathrm{C3}} \cong W_{\mathrm{C3}}^+$, i.e., we should neglect all the terms containing $\mathbf{t}^- \partial/\xi_j$.

(ii) The second problem arises when we try to express the coefficients $\mathbf{t}_l^- \cdot \mathbf{t}_3^-$ as a function of the parabolic coordinates. This task is quite cumbersome since we have to find the roots of a quartic polynomial as shown in Appendix A. Therefore we are forced to approximate $\mathbf{t}_l^- \cdot \mathbf{t}_3^-$, having in mind that the solution should have the following properties: for large interparticle distances it goes to Redmond's solution Eq. (14), it has a regular behavior at total breakup threshold, and the two electrons are treated on equal footing.

A. The use of effective momenta

The wave function Ψ_{C3}^- was designed to hold for large interparticle separations $r_j \to \infty$, but in the semiasymptotic regions, namely,

$$\begin{aligned} \Omega_1&: \quad r_1/r_2 \to 0, \quad r_2, r_3 \to \infty, \\ \Omega_2&: \quad r_2/r_1 \to 0, \quad r_1, r_3 \to \infty, \\ \Omega_3&: \quad r_3/R_3 \to 0, \quad R_3, r_1, r_2 \to \infty \end{aligned} \tag{16}$$

is not appropriated. In this section, we derive the wave function developed by Alt and Mukhamedzhanov [7] Ψ_{AM}^-, which is a correlated solution expected to be valid also in all the semiasymptotic regions. To obtain Ψ_{AM}^- from our general Eq. (4) with the outgoing approximation Eq. (15), we take the following steps. In the region Ω_1 we take into account only the mixed derivative $\partial^2/\partial \xi_1 \partial \xi_3$ and approximate the coefficient $\mathbf{t}_1^- \cdot \mathbf{t}_3^-$ by its projection in the direction $\hat{\mathbf{k}}_1$, i.e.,

$$\mathbf{t}_1^- \cdot \mathbf{t}_3^- \cong (\mathbf{t}_1^- \cdot \hat{\mathbf{k}}_1)(\hat{\mathbf{k}}_1 \cdot \mathbf{t}_3^-) = \frac{\xi_1}{r_1}\hat{\mathbf{k}}_1 \cdot (\hat{\mathbf{k}}_3 + \hat{\mathbf{r}}_3). \tag{17}$$

We look for a solution of the form

$$\Psi^{-}\propto E_2^{-}E_3^{-}F(\mathbf{r}_3;\xi_1), \tag{18}$$

where $\mathbf{r}_3$ is taken parametrically in F. Further, for $r_3\to\infty$, we consider

$$\frac{\partial^2\Psi}{\partial\xi_1\partial\xi_3}\propto E_2^{-}E_3^{-}\frac{i\alpha_3}{r_3(1+\hat{\mathbf{k}}_3\cdot\hat{\mathbf{r}}_3)}\frac{\partial F(\mathbf{r}_3;\xi_1)}{\partial\xi_1}, \tag{19}$$

and then we arrive at a *modified* confluent hypergeometric equation in ξ_1:

$$\left[\frac{\partial}{\partial\xi_1}\xi_1\frac{\partial}{\partial\xi_1}+\imath k_1'(\mathbf{r}_3)\xi_1\frac{\partial}{\partial\xi_1}+Z_1\right]F(\mathbf{r}_3;\xi_1)=0, \tag{20}$$

where $\mathbf{k}_1'$ is an effective momentum defined by

$$\mathbf{k}_1'(\mathbf{r}_3)=\mathbf{k}_1+\frac{\alpha_3}{r_3}\frac{(\hat{\mathbf{k}}_3+\hat{\mathbf{r}}_3)}{(1+\hat{\mathbf{k}}_3\cdot\hat{\mathbf{r}}_3)}. \tag{21}$$

Others asymptotes can be covered in a similar way with momenta

$$\mathbf{k}_2'(\mathbf{r}_3)=\mathbf{k}_2-\frac{\alpha_3}{r_3}\frac{(\hat{\mathbf{k}}_3+\hat{\mathbf{r}}_3)}{(1+\hat{\mathbf{k}}_3\cdot\hat{\mathbf{r}}_3)}, \tag{22}$$

$$\mathbf{k}_3'(\mathbf{r}_3)=\mathbf{k}_3+\frac{\alpha_1}{2r_1}\frac{(\hat{\mathbf{k}}_1+\hat{\mathbf{r}}_1)}{(1+\hat{\mathbf{k}}_1\cdot\hat{\mathbf{r}}_1)}-\frac{\alpha_2}{2r_2}\frac{(\hat{\mathbf{k}}_2+\hat{\mathbf{r}}_2)}{(1+\hat{\mathbf{k}}_2\cdot\hat{\mathbf{r}}_2)}. \tag{23}$$

For large interparticle distances, $\mathbf{k}_j'\to\mathbf{k}_j$, and the Redmond's conditions are then satisfied. In this way, we obtain a product of confluent hypergeometric functions as given by Eq. (11)

$$\Psi_{\mathrm{ASYM}}^{-}=\prod_{j=1}^{3}N_j'^{-}F_j'^{-}, \tag{24}$$

with $\alpha_j'=-Z_j/k_j'$, instead of α_j in Eqs. (12) and (13).

It should be noted that the momenta given by Eqs. (21)–(23) are not identical to those found by Alt and Mukhamedzhanov. These authors considered

$$\mathbf{k}_{1,\mathrm{AM}}'(\mathbf{r}_3)=\mathbf{k}_1+\frac{\alpha_3}{r_2}\frac{(\hat{\mathbf{k}}_3+\hat{\mathbf{r}}_2)}{(1+\hat{\mathbf{k}}_3\cdot\hat{\mathbf{r}}_2)}, \tag{25}$$

instead of Eq. (21), and replaced r_2 by $(r_1+r_2+r_3)/2$ to avoid the singularity as $r_2\to 0$. However, as $r_2\to\infty$ and $r_1/r_2\to 0$ then

$$\mathbf{k}_{1,\mathrm{AM}}'\cdot\mathbf{r}_1\to\mathbf{k}_1'\cdot\mathbf{r}_1+O(r_1^2/r_2^2). \tag{26}$$

Therefore $\Psi_{\mathrm{AM}}\to\Psi_{\mathrm{ASYM}}^{-}$, i.e., both solutions fall down together in Ω_1. In an analogous way, is easy to see that this is also true in each semiasymptotic region. The use of effective momenta was first introduced by Felden [9] in the context of the Vainstein, Presnyakov, and Sobelman approximation, which can be considered as the forerunner of the C3 one [4].

B. A numerical test

In this section we explore how efficiently the effective momenta introduce correlation between coordinates. The benchmark we pose here is an asymptotic Hamiltonian H_∞, in which we have assumed $\eta_1=\eta_2=\eta_3=0$, and so $\mathbf{t}_l^{-}\cdot\mathbf{t}_3^{-}=4\hat{\mathbf{k}}_l\cdot\hat{\mathbf{k}}_3$ to give

$$H_\infty=\sum_{j=1}^{3}2\frac{1+\delta_{j,3}}{\xi_j}(H_j^{-}+Z_j)+4\hat{\mathbf{k}}_1\cdot\hat{\mathbf{k}}_3\frac{\partial^2}{\partial\xi_1\partial\xi_3}-4\hat{\mathbf{k}}_2\cdot\hat{\mathbf{k}}_3\frac{\partial^2}{\partial\xi_2\partial\xi_3}. \tag{27}$$

If we write the series expansion $\Psi_\infty^{-}=\Sigma_{klm}f_{k,l,m}\xi_1^k\xi_2^l\xi_3^m$, one can obtain the following relation [10]

$$\begin{aligned}0=&[(k+1)^2f_{k+1,l-1,m-1}+(Z_1+ik_1k)f_{k,l-1,m-1}]\\&+[(l+1)^2f_{k-1,l+1,m-1}+(Z_2+ik_2l)f_{k-1,l,m-1}]\\&+2[(m+1)^2f_{k-1,l-1,m+1}+(Z_3+ik_3m)f_{k-1,l-1,m}]\\&+\hat{\mathbf{k}}_1\cdot\hat{\mathbf{k}}_3kmf_{k,l-1,m}-\hat{\mathbf{k}}_2\cdot\hat{\mathbf{k}}_3lmf_{k-1,l,m},\end{aligned} \tag{28}$$

which cannot be solved for all values of the subscripts. Three points can be inferred. First, one can easily see that by setting $\hat{\mathbf{k}}_1\cdot\hat{\mathbf{k}}_3=\hat{\mathbf{k}}_2\cdot\hat{\mathbf{k}}_3=0$, we obviously obtain the C3 function, which satisfies

$$f_{k+1,l,m}=-\frac{(Z_1+ik_1k)}{(k+1)^2}f_{k,l,m}, \tag{29}$$

and similar relations for the other variables. Second, Ψ_∞^{-} tends to the Redmond's conditions. And third, the derivative at the origin satisfies Kato's cusp condition [11]

$$\left[\frac{1}{\Psi_\infty^{-}}\frac{\partial}{\partial\xi_j}\Psi_\infty^{-}\right]_{\xi_j=0}=-Z_j, \tag{30}$$

which lets us initialize the numerical calculation. The Redmond's values at large distances and Kato's derivatives at the origin lead us to a Dirichlet-Neumann mixed-boundary condition problem. The determinant of the coefficients multiplying the second derivative terms is positive, and therefore the differential equation is elliptic, as it is the original Eq. (1).

The numerical solution of Eq. (27) is still quite cumbersome. To reduce the problem we have considered $\hat{\mathbf{k}}_2\cdot\hat{\mathbf{k}}_3=0$ and so $\hat{\mathbf{k}}_1\cdot\hat{\mathbf{k}}_3=2k_3/k1$. In this case, we write $\Psi_\infty^{-}=N_2F_2G_{13}'(\xi_1,\xi_3)$, where G_{13}' satisfies

$$\left[\frac{2}{\xi_1}(H_1^{-}+Z_1)+\frac{4}{\xi_3}(H_3^{-}+Z_3)+\frac{8k_3}{k_1}\frac{\partial^2}{\partial\xi_1\partial\xi_3}\right]\times G_{13}'(\xi_1,\xi_3)=0. \tag{31}$$

We have solved Eq. (31) by the finite difference method for $k_1=1$, $k_3=0.4$, and so $k_2=0.6$. Results are shown in Fig. 2 where we represent the square modulus of G_{13}' in parabolic coordinates. G_{13}' is compared with the C3 approximation

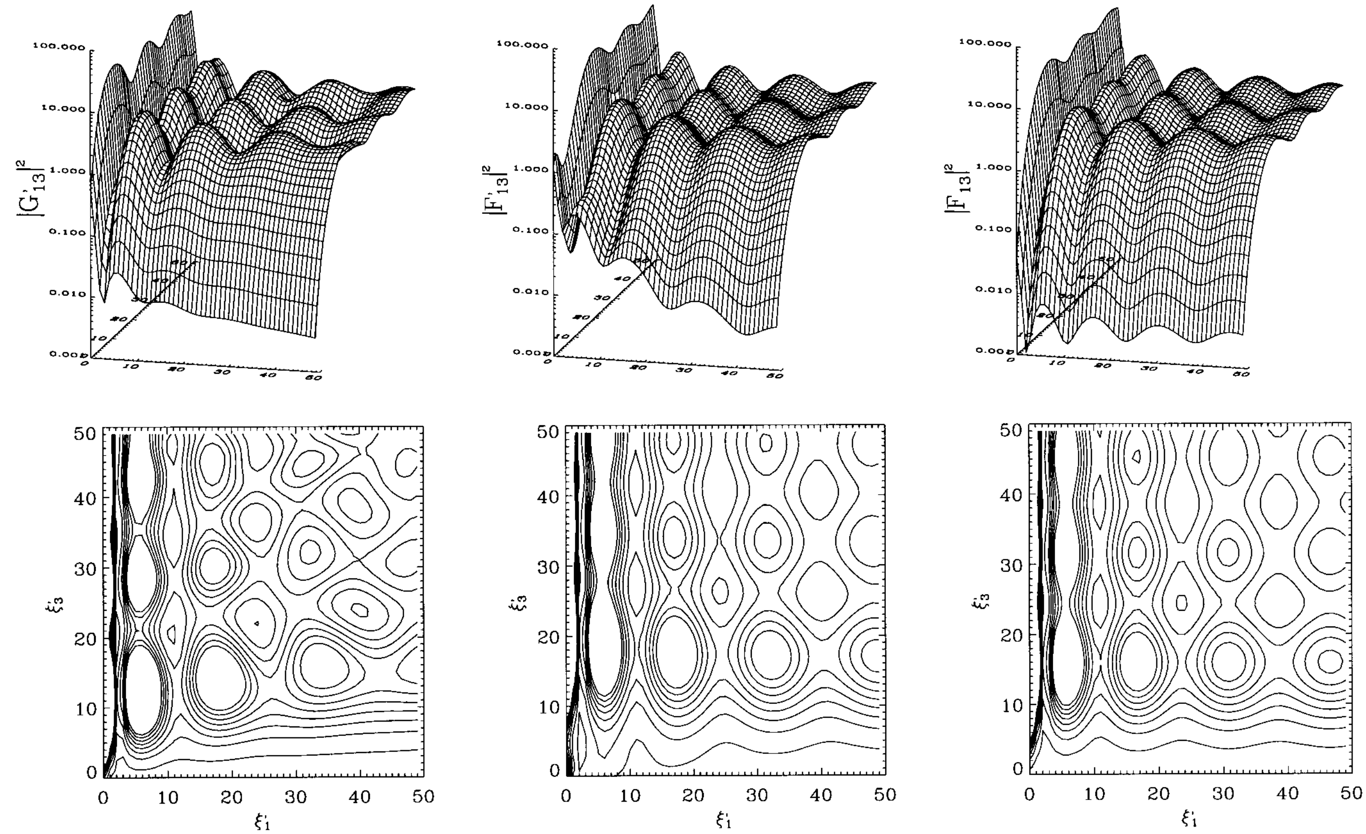

FIG. 2. Upper figures display $|G'_{13}|^2$, $|F_{13}|^2$, and $|F'_{13}|^2$ as a function of $\xi_i'=\xi_i(N-1)/\xi_i^{\mathrm{MAX}} i=1,3$ for $k_1=1.0$ a.u. and $k_3=0.4$ a.u. Lower figures display the corresponding contour plot. The number of nodes N in each direction is $N=50$ and the maximum value of ξ_1 (ξ_3) is $\xi_1^{\mathrm{MAX}}=15$ a.u. ($\xi_3^{\mathrm{MAX}}=65$ a.u.).

$F_{13}=N_1N_3F_1F_3$ and the one having effective momenta $F'_{13}=N'_1N'_3F'_1F'_3$ for $r_2=1$. The effective momenta are now

$$\mathbf{k}'_1=\mathbf{k}_1+\frac{2\alpha_3}{R}(\hat{\mathbf{k}}_3+\hat{\mathbf{k}}_2), \tag{32}$$

$$\mathbf{k}'_3=\mathbf{k}_3+\frac{\alpha_1}{R}\,\frac{(\hat{\mathbf{k}}_1+\hat{\mathbf{R}}_3)}{1+\hat{\mathbf{k}}_1\cdot\hat{\mathbf{R}}_3}-\frac{\alpha_2}{R}\,\frac{(\hat{\mathbf{k}}_2+\hat{\mathbf{R}}_3)}{1+\hat{\mathbf{k}}_2\cdot\hat{\mathbf{R}}_3}, \tag{33}$$

$R=1+r_1+r_3$, and $\mathbf{R}_3=(r_1\hat{\mathbf{k}}_1+\hat{\mathbf{k}}_2)/2$.

Some conclusions can be drawn. First, F'_{13} does not differ appreciably from F_{13}. Similar conclusions can be inferred also from the article of Jones and Madison [12]; the inclusion of effective momenta does not alter appreciably the electronic distributions. By inspecting the contour plot we can note that the enhancements of F_{13}, and even the ones of F'_{13}, are situated in a *rectangular* form, while the ones of G'_{13} are *slanted*. Also the shapes of the enhancement have different forms (similar features have been found also for others values of k_i). The effective momenta method does not seem to be a satisfactory solution of the problem. In the next section we introduce an alternative approximation that, we think, may be a good candidate to tackle the double continuum problem.

III. THE Φ_2 APPROXIMATION

We look for a wave function with the outgoing boundary condition beyond the C3 approximation by taking into account the mixed derivatives. Let us write the exact expression of the coefficient $\mathbf{t}_l^-\cdot\mathbf{t}_3^-$:

$$\mathbf{t}_l^-\cdot\mathbf{t}_3^-=\pm\frac{2\xi_l}{(\xi_3+\eta_3)}\pm\frac{4\xi_3}{(\xi_l+\eta_l)}\mp\frac{2r_l^2+r_3^2\mp\mathbf{r}_l\cdot\mathbf{r}_3}{r_lr_3}$$
$$+\hat{\mathbf{k}}_l\cdot\hat{\mathbf{k}}_3-\frac{\hat{\mathbf{k}}_l}{r_3}\cdot(2\mathbf{r}_l\mp\mathbf{r}_3)+\frac{\hat{\mathbf{k}}_3}{r_l}\cdot(\mathbf{r}_l\mp\mathbf{r}_3), \tag{34}$$

where the upper (lower) sign corresponds to $l=1$ ($l=2$). We here will consider just the first two terms

$$\mathbf{t}_l^-\cdot\mathbf{t}_3^-\cong\pm\left[\frac{2\xi_l}{(\xi_3+\eta_3)}+\frac{4\xi_3}{(\xi_l+\eta_l)}\right] \tag{35}$$

to give

$$W_{\mathrm{C3}}^-\cong W_{\mathrm{corr}}^-=\frac{2\xi_3}{(\xi_1+\eta_1)}\,\frac{\partial^2}{\partial\xi_1\partial\xi_3}+\frac{2\xi_3}{(\xi_2+\eta_2)}\,\frac{\partial^2}{\partial\xi_2\partial\xi_3}$$
$$+\frac{4\xi_1}{(\xi_3+\eta_3)}\,\frac{\partial^2}{\partial\xi_1\partial\xi_3}+\frac{4\xi_2}{(\xi_3+\eta_3)}\,\frac{\partial^2}{\partial\xi_2\partial\xi_3}. \tag{36}$$

As we shall see, the approximation (36) does not alter the Redmond's condition. Considering Eqs. (15) and (36) we can reduce Eq. (4) as $H^-_{\rm corr}\Psi^-_{\rm corr}=(H^-_{\rm C3}+W^-_{\rm corr})\Psi^-_{\rm corr}=0$, where

$$H^-_{\rm corr}=\frac{1}{(\xi_1+\eta_1)}\left[H^-_1+Z_1+\xi_3\frac{\partial^2}{\partial\xi_1\partial\xi_3}\right]+\frac{1}{(\xi_2+\eta_2)}\left[H^-_2+Z_2+\xi_3\frac{\partial^2}{\partial\xi_2\partial\xi_3}\right]+\frac{2}{(\xi_3+\eta_3)}\left[H^-_3+Z_3+\xi_1\frac{\partial^2}{\partial\xi_1\partial\xi_3}+\xi_2\frac{\partial^2}{\partial\xi_2\partial\xi_3}\right]. \tag{37}$$

A closed form of $\Psi^-_{\rm corr}$ is not known to us. The nearest solved case is the fully symmetric system

$$\left[H^-_j+Z_j+\xi_k\frac{\partial^2}{\partial\xi_k\partial\xi_j}+\xi_l\frac{\partial^2}{\partial\xi_l\partial\xi_j}\right]\Phi=0, \tag{38}$$

with $j\neq k\neq l=1,2,3$ whose solution is the degenerate hypergeometric function of *three* variables [13] $\Phi=\Phi_2(i\alpha_1,i\alpha_2,i\alpha_3;1;-ik_1\xi_1,-ik_2\xi_2,-ik_3\xi_3)$, where

$$\Phi_2(\beta,\beta'\beta'';\gamma;x,y,z)=\sum_{klm}\frac{(\beta)_k(\beta')_l(\beta'')_m}{(\gamma)_{k+l+m}}\frac{x^k}{k!}\frac{y^l}{l!}\frac{x^m}{m!}. \tag{39}$$

Note that this solution considers a term $\partial^2/\partial\xi_1\partial\xi_2$, which is missing in our starting Eq. (37). Consequently, by setting $Z_3=0$, it does not reproduce the C2 approximation, and it should be lied aside. However, Eq. (39) should be considered an appropriate wave function for a three equal-mass system of particles. Next we will find an approximation of Eq. (37) valid for large distances.

To start, we correlate only the variables ξ_1 and ξ_3, i.e., we discard $\partial^2/\partial\xi_2\partial\xi_3$. This restriction allows us to separate Eq. (37) as

$$\frac{1}{(\xi_2+\eta_2)}[H^-_2+Z_2]G_2(\xi_2)=0, \tag{40}$$

$$\frac{1}{(\xi_1+\eta_1)}\left[H^-_1+Z_1+\xi_3\frac{\partial^2}{\partial\xi_1\partial\xi_3}\right]G_{13}(\xi_1,\xi_3)=0, \tag{41}$$

$$\frac{2}{(\xi_3+\eta_3)}\left[H^-_3+Z_3+\xi_1\frac{\partial^2}{\partial\xi_1\partial\xi_3}\right]G_{13}(\xi_1,\xi_3)=0. \tag{42}$$

The solution of this system of equation is $G_2(\xi_2)G_{13}(\xi_1,\xi_3)$. Note that it depends only on ξ_1,ξ_2, and ξ_3 even though we have not imposed any condition on the variables η_1,η_2, and η_3.

The solution of Eq. (40) is simply a confluent hypergeometric function; $G_2(\xi_2)=N^-_2F^-_2$. Equations (41) and (42) form a system of partial differential equations studied by Appell and Kampé de Fériet [13]. A solution of this system is a generalization of the confluent hypergeometric function Φ_2 of *two* variables, which is expressed as

$$\Phi_2(\beta,\beta';\gamma;x,y)=\sum_{km}\frac{(\beta)_m(\beta')_k}{(\gamma)_{m+k}}\frac{x^m}{m!}\frac{y^k}{k!}. \tag{43}$$

Afterwards, the correlated solution of Eqs. (40)–(42) is

$$\Psi^-_{13}=N^-_2F^-_2N^-_{1,3}\Phi^-_{1,3}, \tag{44}$$

$$\Phi^-_{l,m}=\Phi_2(i\alpha_l,i\alpha_m;1;-ik_l\xi_l,-ik_m\xi_m), \tag{45}$$

and $N_{l,m}$ is the factor to resume the Redmond's conditions (see Appendix B for details)

$$N^-_{l,m}=\exp[-\pi(\alpha_l+\alpha_m)/2]\Gamma(1-i\alpha_l-i\alpha_m). \tag{46}$$

In similar way, another solution can be obtained accounting $\partial^2/\partial\xi_2\partial\xi_3$ and neglecting $\partial^2/\partial\xi_1\partial\xi_3$:

$$\Psi^-_{23}=N^-_1F^-_1N^-_{2,3}\Phi^-_{2,3}. \tag{47}$$

Considering the asymptotic behavior of $\Phi^-_{l,m}$ and F^-_j showed in Appendix B, is easy to see that for $r_i\to\infty$

$$H_{\rm corr}\Psi_{13}=O(r_i^{-2}),\quad H_{\rm corr}\Psi_{23}=O(r_i^{-2}),\quad H_{\rm corr}\Psi_{\rm C3}=O(r_i^{-2}). \tag{48}$$

At this point is interesting to look for a solution given by

$$\Psi^-=aN^-_1F^-_1N^-_{2,3}\Phi^-_{2,3}+bN^-_2F^-_2N^-_{1,3}\Phi^-_{1,3}+c\Psi^-_{\rm C3}. \tag{49}$$

We found $a=1,b=1$ and $c=-1$ is the unique solution that (i) satisfies Redmond's condition as $r_i\to\infty$, (ii) treats both electrons on equal footing, and (iii) get one order more accuracy as $r_i\to\infty$, since

$$H_{\rm corr}\Psi^-_F=(r_i^{-3}) \tag{50}$$

where

$$\Psi^-_F=N^-_1F^-_1N^-_{2,3}\Phi^-_{2,3}+N^-_2F^-_2N^-_{1,3}\Phi^-_{1,3}-\Psi^-_{\rm C3}. \tag{51}$$

We can easily ''read'' Eq. (51); the first term of the right-hand side contains $\partial^2/\partial\xi_2\partial\xi_3$ to all orders, the second considers $\partial^2/\partial\xi_1\partial\xi_3$, and the third corrects the double counting. Further, if we set $\alpha_3=0$ in Eq. (51), the C2 approximation is recovered, as it is expected. We have used the subscript ''F'' because Eq. (51) has a structure very similar to the first order Faddeev solution found by Macek [14] and Briggs [15]. In fact, we can derive it considering the Green function of $H_{\rm C3}$ instead of the free Green function used in the Faddeev equations [16], and taking $V_{l3}=\pm[2\xi_l/(\xi_3+\eta_3)+4\xi_3/(\xi_l+\eta_l)]\partial^2/\partial\xi_l\partial\xi_3$, $l=1,2$ as the components of the perturbed potential.

Threshold behavior and normalization factors

The cross section of an ionization process is strongly determined by the behavior at small interparticle separations of the final-state wave function. In the C3 approximation the normalization constant is $\Psi^-_{\rm C3}(\xi_i=0)=N^-_{\rm C3}=N^-_1N^-_2N^-_3$, and it is well known that the use of $\Psi^-_{\rm C3}$ leads to cross

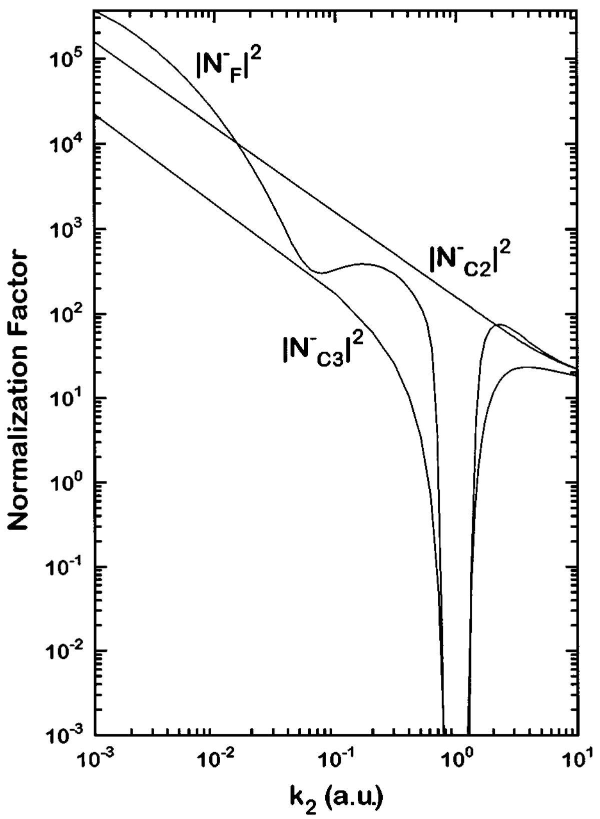

FIG. 3. Square modules $|N^-_{C2}|^2$, $|N^-_{C3}|^2$, and $|N^-_F|^2$, for $k_1=1$ a.u. as a function of $\mathbf{k}_2$ so that $\hat{\mathbf{k}}_2$ is parallel to $\hat{\mathbf{k}}_1$.

sections that underestimate experimental data by orders of magnitude [6] in the threshold of double photoionization, i.e., in the Wannier region [19]. The origin of this failure arises from the overestimation of the *e*-*e* repulsion given by the Coulomb factor N^-_3 . It decreases exponentially for small decreasing excess energy. Figure 3 shows the square modulus of the N^-_{C3} normalization factor for $k_1=1$ as a function of $\mathbf{k}_2$ so that $\hat{\mathbf{k}}_2$ is parallel to $\hat{\mathbf{k}}_1$. It presents a divergence when $k_2=0$ known as the Coulomb cusp and an exclusion hole, the so-called Coulomb depth, which is the footprint of the *e*-*e* repulsion. To some extent the range of this hole is exaggerated and is responsible for the failure to describe the threshold of the double ionization cross section. We include also the normalization factor of the wave function $\Psi^-_{C2}(\xi_i=0)=N^-_{C2}=N^-_1 N^-_2$, which describes reasonably well the total cross section at the threshold [1]. It presents the Coulomb cusp but not the Coulomb depth. In Fig. 3 the normalization factor of Ψ^-_F is also shown:

$$N^-_F=N^-_2 N^-_{1,3}+N^-_1 N^-_{2,3}-N^-_1 N^-_2 N^-_3 , \tag{52}$$

which has the best of both worlds. The Coulomb cusp remains the same, the exclusion hole is also present, and, more important, its range is largely diminished. Moreover, as $k_2\rightarrow 0, N^-_F$ has the same order of magnitude as N^-_{C2}. Therefore, we can expect that Ψ^-_F produces similar double photoionization cross sections to Ψ^-_{C2} in the Wannier threshold region [19]. In this way, the undesirable exponential decreasing of Ψ^-_{C3} in the threshold may be removed. A complete study of such a cross section is planned to publish elsewhere.

IV. SUMMARY

In this work, we present a correlated wave function for the three-body Coulomb problem valid for large interparticle distances. Unlike other works [7,8] where the correlation is introduced parametrically, here we consider the contribution of the mixed derivatives. Let us resume the three steps to obtain Ψ^-_F : (i) from the full Hamiltonian, we take the outgoing approximation, i.e., $W_{C3}\cong W^-_{C3}$ as in Eq. (15); (ii) we further approximate $W^-_{C3}\cong W^-_{\rm corr}$ as in Eq. (36) by considering the first two terms of Eq. (34) as stated in Eq. (35); and (iii) finally, we approximate the solution of Eq. (37) by using the first order of the Faddeev expansion as in Eq. (51).

In this way, we found a genuine many-variable wave function Ψ_F , which treats the electrons on equal footing and it seems to correct the overestimation of the interelectronic repulsion of Ψ^-_{C3}. Other systems can be treated in similar way, e.g., the problem of an electron in the field of two nuclei [17].

It is important to remark that the solution Ψ^-_F is not valid in the semiasymptotic regions. If we want such a solution, we could introduce effective momenta [7] (as shown in Sec. II) or effective charges [8] (using the coordinate system of the reference).

Further work is being carried out to compute transition matrices. A numerical calculation using the hypergeometric function of two variables Φ_2 presents several difficulties due to the complexity of the problem.

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APPENDIX A: CHANGE OF COORDINATES

In Eq. (3) we posed the generalized parabolic transformation $(\mathbf{r}_1,\mathbf{r}_2)\rightarrow(\xi_1,\xi_2,\xi_3,\eta_1,\eta_2,\eta_3)$; in this appendix we look for the inverse transformation. We write $\mathbf{r}_l=(x_l,y_l,z_l), l=1,2, \mathbf{k}_j=(k_{jx},k_{jy},k_{jz}), j=1,2,3$, and for convenience we choose $\vec{x}_1$ parallel to $\mathbf{k}_1$ (i.e., $k_{1y}=k_{1z}=0$). Introducing the variables

$$\sigma_1=(\xi_1-\eta_1)/2, \quad \sigma_2=(\xi_1+\eta_1)^2/4, \tag{A1}$$

$$\sigma_3=(\xi_2-\eta_2)/2, \quad \sigma_4=(\xi_2+\eta_2)^2/4, \tag{A2}$$

$$\sigma_5=(\xi_3-\eta_3)/2, \quad \sigma_6=(\xi_3+\eta_3)^2/4, \tag{A3}$$

$$\sigma_0=\tfrac{1}{2}(\sigma_2+\sigma_4-\sigma_6), \tag{A4}$$

$$\rho_1=\frac{k_2\sigma_3}{k_{2y}}+\frac{k_3\sigma_5}{k_{3y}}-\frac{k_{3x}\sigma_1}{k_{3y}}, \quad \rho_2=\frac{k_2\sigma_3}{k_{2y}}, \tag{A5}$$

$$\tau_1=\frac{k_{3x}}{k_{3y}}-\frac{k_{2x}}{k_{2y}}, \quad \tau_2=-\frac{k_{2x}}{k_{2y}}, \tag{A6}$$

we find the value of x_2 is the solution of the following quartic equation

$$0=[\sigma_2-\sigma_1^2-(\rho_1+\tau_1x_2)^2][\sigma_4-x_2^2-(\rho_2+\tau_2x_2)^2] -[\sigma_0-\sigma_1x_2-(\rho_1+\tau_1x_2)(\rho_2+\tau_2x_2)]. \quad (A7)$$

The inverse transformation is then $x_1=\sigma_1$, and the rest of the variables are related to x_2 through the relations

$$y_1=\rho_1+\tau_1x_2, \quad y_2=\rho_2+\tau_2x_2, \quad (A8)$$

$$z_1=[\sigma_2-\sigma_1^2-(\rho_1+\tau_1x_2)^2]^{1/2}, \quad (A9)$$

$$z_2=[\sigma_4-x_2^2-(\rho_2+\tau_2x_2)^2]^{1/2}. \quad (A10)$$

This procedure to obtain the inverse transformation is quite tedious due to the discrimination of the different roots. Next, we will study some particular cases.

1. The Crothers's condition

This is the case when $\mathbf{k}_l$ is parallel to $\mathbf{r}_l$, for $l=1,2$ [18]. In terms of the generalized parabolic coordinates, it can be expressed as $\eta_1=\eta_2=0$, thus

$$x_2=\frac{\xi_1^2+\xi_2^2-(\xi_3+\eta_3)^2}{4\xi_1}. \quad (A11)$$

The cancellation of $\eta_{1,2}$ constrains the values of ξ_3 and η_3 to

$$\begin{bmatrix}\xi_3\\ \eta_3\end{bmatrix}=\frac{(\xi_1^2+\xi_2^2-2\xi_1\xi_2\hat{\mathbf{k}}_1\cdot\hat{\mathbf{k}}_2)^{1/2}}{2}\begin{bmatrix}+\\ -\end{bmatrix}N, \quad (A12)$$

$$N=\xi_1N_1+\xi_2N_2, \quad N_l=\frac{k_l^2-\hat{\mathbf{k}}_1\cdot\hat{\mathbf{k}}_2}{4k_3k_l}, \quad (A13)$$

and $l=1,2$. It is concluded then that the wave function depends on only *two* variables: ξ_1 and ξ_2.

2. Peterkop's condition

This is the case when the three position vectors $\mathbf{r}_j$ are parallel to $\mathbf{k}_j$, for $j=1,2,3$, and so $\eta_1=\eta_2=\eta_3=0$ [20]. Thus,

$$x_2=\frac{\xi_1^2+\xi_2^2-\xi_3^2}{4\xi_1}. \quad (A14)$$

Therefore only *one* parameter is the independent variable and the following constraint is observed:

$$t=\frac{\xi_1}{[1-(\hat{\mathbf{k}}_2\cdot\hat{\mathbf{k}}_3)^2]^{1/2}}=\frac{\xi_2}{[1-(\hat{\mathbf{k}}_1\cdot\hat{\mathbf{k}}_3)^2]^{1/2}} =\frac{\xi_3}{[1-(\hat{\mathbf{k}}_1\cdot\hat{\mathbf{k}}_2)^2]^{1/2}}, \quad (A15)$$

where t is a parameter that can be seen as the time.

3. Wannier's condition

This is the case when the electrons recede from each other; thus, $\mathbf{r}_1=-\mathbf{r}_2$ and so $x_2=-\sigma_1$ [19]. Under these circumstances only *three* variables are independent, for example ξ_1,ξ_2, and η_1, and the rest of the coordinates are constrained to hold

$$\eta_2=\xi_1+\eta_1-\xi_2,$$

$$\xi_3=\xi_1+\eta_1+\frac{k_1}{2k_3}(\xi_1-\eta_1)+\frac{k_2}{2k_3}(2\xi_2-\xi_1-\eta_1), \quad (A16)$$

$$\eta_3=\xi_1+\eta_1-\frac{k_1}{2k_3}(\xi_1-\eta_1)-\frac{k_2}{2k_3}(2\xi_2-\xi_1-\eta_1)$$

If, in addition, we consider Crother's condition, i.e., $\mathbf{k}_l$ parallel to $\mathbf{r}_l$, for $l=1,2$ (or equivalently $\eta_1=\eta_2=0$), then we find $\eta_3=0,\xi_2=\xi_1$, and $\xi_3=2\xi_1$.

APPENDIX B: ASYMPTOTIC BEHAVIOR

In order to show the asymptotic behavior of the function $\Phi_2(\beta,\beta';\gamma;x,y)$ as $x\to\infty$ and $y\to\infty$, we start by expressing Φ_2 in its integral form

$$\Phi_2(\beta,\beta';\gamma;x,y)=\frac{\Gamma(\gamma)}{\Gamma(\beta)\Gamma(\beta')\Gamma(\gamma-\beta-\beta')} \times\int\int du\,dv\exp(ux+vy)u^{\beta-1}v^{\beta'-1} \times(1-u-v)^{\gamma-\beta-\beta'-1}, \quad (B1)$$

where the integral is taken over the triangular region $u\geqslant0,v\geqslant0$, and $1-u-v\geqslant0$. Using the integral form of the confluent hypergeometric function [21]

$${}_1F_1(\nu,\mu+\nu,\lambda u)=\frac{\Gamma(\mu+\nu)}{\Gamma(\mu)\Gamma(\nu)u^{1-\mu-\nu}} \times\int_0^u ds\,s^{\nu-1}(u-s)^{\mu-1}e^{\lambda s}, \quad (B2)$$

we can reduce Eq. (B1) to a single integral:

$$\Phi_2(\beta,\beta';\gamma;x,y)=\frac{\Gamma(\gamma)}{\Gamma(\beta)\Gamma(\gamma-\beta)}\int_0^1 du\exp(ux)u^{\beta-1} \times(1-u)^{\gamma-\beta-1}{}_1F_1(\beta',\gamma-\beta,(1-u)y). \quad (B3)$$

Since the limit as $|z|\to\infty$ of ${}_1F_1$ for $\mathrm{Re}(b)>0$ is

$${}_1F_1(a,b,z)\to\frac{\Gamma(b)}{\Gamma(b-a)}e^{-i\epsilon\pi a}z^{-a}, \quad (B4)$$

$\epsilon=\mathrm{sgn}[\mathrm{Im}(z)]$, then we find

$$\Phi_2(\beta,\beta';\gamma;x,y)\rightarrow\frac{\Gamma(\gamma)}{\Gamma(\gamma-\beta-\beta')}\exp(-i\epsilon_x\pi\beta)\times\exp(-i\epsilon_y\pi\beta')x^{-\beta}y^{-\beta'},\quad \text{as}\quad x,y\rightarrow\infty \tag{B5}$$

with $\epsilon_x=\mathrm{sgn}[\mathrm{Im}(x)]$, and $\epsilon_y=\mathrm{sgn}[\mathrm{Im}(y)]$. Therefore, the asymptotic behavior of Ψ_{13}^- in Eq. (44) is given by

$$\Phi_2(\imath\alpha_1,\imath\alpha_3,1,-ik_1\xi_1,-ik_3\xi_3)\rightarrow\frac{1}{N_{1,3}}E_1^-E_3^- \tag{B6}$$

with

$$N_{1,3}=\exp(-\pi\alpha_1/2)\exp(-\pi\alpha_3/2)\Gamma(1-i\alpha_1-i\alpha_3) \tag{B7}$$

and similar expressions for any other pair of correlated particles.

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