Approximate wave functions for two electrons in the continuum of a Coulomb charge

J. E. Miraglia, M. G. Bustamante, and P. A. Macri
Instituto de Astronomía y Física del Espacio, Consejo Nacional de Investigaciones Científicas y Técnicas, Casilla de Correo 67, Sucursal 28, 1428 Buenos Aires, Argentina
(Received 26 January 1999)

The outgoing scattering state describing two electrons in the continuum of a Coulomb charge is investigated. Boundary, simple, and double conditions are used to construct *ab initio* wave functions. Simple conditions describe the limits when the Coulomb charges are switched off, and double conditions take into account the cases when two out of three particles are close and have low relative velocity. A base to expand the double continuum—here called the Λ base—is introduced. All the components of the three-body wave function in this base have the appropriate Coulomb conditions and are versatile enough to build up simple as well as double conditions. [S1050-2947(99)05111-2]

PACS number(s): 34.80.Dp, 32.80.Fb

I. INTRODUCTION

Several approximate double continuum wave functions have been used to compute the corresponding ionization cross sections. The most simple approximation consists of neglecting the electron-electron (e-e) repulsion leading to a state expressed in terms of a product of two Coulomb waves, the so-called $C2$ approximation. It produces a reasonable agreement with measured total cross sections for double photoionization [1], but it fails to 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 it was 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. At threshold, however, it is meaningless since it underestimates by orders of magnitude the experimental total cross sections [6] owing to an overestimation of the electronic repulsion present in the normalization of the wave function. To avoid this defect, it is necessary to find a scattering state 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. Generally, these attempts have the same structure as the $C3$ approximation, but with effective momenta [7] or charges [8] depending on the coordinates. A recent comprehensive work employing these solutions to describe double photoionization of helium [9] shows that the double continuum state is still far from being known.

In this paper, we follow a line initiated a few years ago in our groups, which intends to describe the continuum state of the three Coulomb particle system with the use of the generalized hypergeometric functions of several variables.

To deal with heavy ion-atom ionization (two heavy particles and one electron), a good candidate to examine has been the degenerate hypergeometric function of *two* variables $\Phi_2^{(2)}$ [10–13]. Here the superscript (2) denotes the number of variables corresponding to the relative position of the electron with respect to the heavy target and projectile (as usual in this case, the internuclear interaction is dropped when possible). The first results, using the undistorted wave function in the entrance channel and $\Phi_2^{(2)}$ in the exit one, were very encouraging. At high electron energies, the method provides very good results when compared with the experiments, including a precise description of the asymmetry parameters of the capture to continuum peak [14]. At low electron energies, the approximation overestimates the experiments, especially around the soft electron peak [13]. At present, calculations are carried out to inspect whether improving the initial channel (using distorted wave states) can deal successfully with low-energy electrons [15].

For two electrons in the continuum state of a heavy nucleus, the problem is much more complex; we can no longer disregard an interaction (such as the internuclear potential mentioned before) and the issue remains a truly three-particle problem. Unfortunately, $\Phi_2^{(3)}$ of *three* variables [10,11] is not an entirely suitable choice because it solves a symmetric system of equations while the system to solve is asymmetric due to the mass differences among the particles. In this context, we went forward and assayed a *correlated*-Faddeev approximation Φ_F [11], which essentially separates the three-particle system in clusters of two, and solves each cluster using $\Phi_2^{(2)}$. This approximation corrects the exponential fall of the $C3$ normalization factor at threshold. However, since Φ_F is written in a *linear* form, it may present interference of doubtful physical reality as the ones found by Duncan *et al.* studying the uncorrelated-Faddeev approximation [16,17].

In this paper we continue this line by going further, trying to include new properties. The scheme to follow in this paper is summarized next.

In Sec. II, the total Hamiltonian for two electrons in the continuum state is expressed in terms of generalized curvilinear coordinates and the solution is confined to the outgoing space (*outgoing approximation*).

In Sec. II A, we write the *boundary* and *simple* conditions

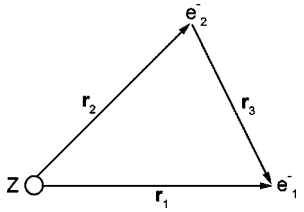

FIG. 1. Set of coordinates.

that the solution should satisfy. We add three *double* conditions which are expected properties representing limit cases when two out of three particles are close with low relative velocity.

In Sec. III, we abridge the preliminary models of interest in this paper, including a *perturbative ansatz* recently posed by Dewangan [18].

In Sec. IV, the here-called base Λ is introduced, which we think is a promising base to expand the solution in the outgoing space. Advantages of using this base are remarked upon.

In Sec. V, two proposals Φ_A and Φ_B are put forward. The first one can be considered as a new degenerate hypergeometric function, which to our knowledge has never been posed before. To fill this vacancy, in Appendix B we calculate all its properties such as integral representation, differential equation, Kummer transformations, etc. For specific parameters, it is found that Φ_A is the *fractional* form of Φ_F as explained in Appendix C. The other function Φ_B is a variation of the $\Phi_2^{(3)}$ functions of three variables. Properties and failures are discussed in each case.

In Sec. VI, future developments are discussed. Atomic units are used.

II. THE THEORETICAL PROBLEM

Let us consider two electrons in the Coulomb field of a heavy nucleus. The coordinates are shown in Fig. 1. The nonrelativistic Hamiltonian equation for the three-particle system is given by

$$\left(\nabla_1^2+\nabla_2^2+\frac{2Z_1}{r_1}+\frac{2Z_2}{r_2}+\frac{2Z_3}{r_3}-k_1^2-k_2^2\right)\Psi=0, \qquad (1)$$

where $Z_1=Z_2=Z$ is the nuclear charge and $Z_3=-1/2$ takes into account the *e-e* repulsion. Although we will concentrate on the continuum of two electrons, the formalism presented here holds if a particle, say ''1,'' is a positron; in this case, $Z_1=-Z$ and $Z_3=+1/2$. Next, two transformations will be made. First, the plane-wave function is removed by writing

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

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 relative *e-e* momentum. Second, the generalized curvilinear coordinates are introduced [3],

$$\xi=r_j+\mathbf{r}_j\cdot\hat{\mathbf{k}}_j, \quad \eta_j=r_j-\mathbf{r}_j\cdot\hat{\mathbf{k}}_j, \qquad (3)$$

and $j=1,2,3$. For short, it will be convenient to use $x_j=-ik_j\xi_j$ and $y_j=-ik_j\eta_j$. In these variables the total Hamiltonian, $H=H_{C3}+W_{C3}$, reads

$$H_{C3}=\sum_{j=1}^{3}2k_j^2\frac{1+\delta_{j,3}}{x_j+y_j}(H_j^-+H_j^+), \quad a_j=Z_j/k_j, \qquad (4)$$

$$H_j^-=x_j\frac{\partial^2}{\partial x_j^2}+(1-x_j)\frac{\partial}{\partial x_j}-(-ia_j), \qquad (5)$$

$$H_j^+=y_j\frac{\partial^2}{\partial y_j^2}+(1-y_j)\frac{\partial}{\partial y_j}, \qquad (6)$$

$$W_{C3}=\sum_{l=1}^{2}(-1)^l k_l k_3\mathbf{t}_3^-\cdot\left(\mathbf{t}_l^-\frac{\partial}{\partial x_l}+\mathbf{t}_l^+\frac{\partial}{\partial y_l}\right)\frac{\partial}{\partial x_3}$$
$$+\sum_{l=1}^{2}(-1)^l k_l k_3\mathbf{t}_3^+\cdot\left(\mathbf{t}_l^-\frac{\partial}{\partial x_l}+\mathbf{t}_l^+\frac{\partial}{\partial y_l}\right)\frac{\partial}{\partial y_3}, \qquad (7)$$

and $\mathbf{t}_j^{\pm}=\hat{\mathbf{r}}_j\mp\hat{\mathbf{k}}_j$. In the generalized curvilinear coordinates, the *correlation* arises in the terms containing mixed derivatives; namely $\partial^2/\partial(x,y)_l\partial(x,y)_3, l=1,2$, in W_{C3}. In this sense H_{C3} is an *uncorrelated* differential operator which is also fully symmetric [3]. Note that H is not symmetric since the crossing derivative $\partial^2/\partial(x,y)_1\partial(x,y)_2$ is missing in W_{C3}.

We will restrict Φ to the outgoing space, *outgoing approximation*, where only the variables x_i are considered. The total Hamiltonian reduces to $H\sim H_{C3}^-+W_{C3}^-$, where H_{C3}^- is given by Eq. (4) with $H_j^+=0$, and W_{C3}^- takes into account only derivatives on x. As we work with generalized curvilinear coordinates, there is a key problem; it is that $\mathbf{t}_j^{\pm}\cdot\mathbf{t}_3^{\pm}$ does not have a suitable expression in terms of these coordinates to attempt to find an approximate solution in closed form. In this paper, we will study some conditions that the exact wave function should satisfy and we will propose some functions to suit such requirements.

Boundary, simple, and double conditions

The function Φ is expected to satisfy a series of conditions—here limited to the outgoing space—that we list next.

(a) When $|x_j|\to\infty, j=1,2,3, \Phi$ must satisfy the Redmond [19] asymptotic condition, namely

$$\Phi\to\Phi_R=\prod_{j=1}^{3}\exp(ia_j\ln|x_j|).$$

This condition led us to determine the normalization factor N.

(b) The Kato cusp condition [20] should be observed, namely, if we write

$$\Phi=N\sum_{klm}P_{klm}\frac{x_1^k}{k!}\frac{x_2^l}{l!}\frac{x_3^m}{m!}, \qquad (8)$$

then

$$P_{1lm}=-ia_1P_{0lm}, \quad P_{k1m}=-ia_2P_{k0m}, \qquad (9)$$

$$P_{kl1} = -ia_3 P_{kl0}. \tag{10}$$

The requirements (a) and (b) can be considered as *boundary conditions* (more precisely Dirichlet-Neuman mixed-boundary conditions) if the differential equation is to be solved numerically in a reduced domain [11].

(c) When $a_3 \to 0$ (or equivalently $Z_3 \to 0$), i.e., when the *e-e* interaction is switched off, the $C2$ approximation must be recovered, which is the exact solution of the two noninteracting electron systems,

$$\Phi \to \Phi_{C2} = \prod_{j=1}^{2} N_j^- F_j^- , \tag{11}$$

$$F_j^- = {}_1F_1(-ia_j;1;x_j), \tag{12}$$

$$N_j^- = \exp(\pi a_j/2)\Gamma(1+ia_j), \quad j=1,2,3. \tag{13}$$

(d) Also, when $a_{1,2} \to 0$ (or equivalently when $Z \to 0$), i.e., when the nucleus charge is switched off, the *e-e* Coulomb continuum wave functions must be recovered, which is the exact solution of two isolated electrons,

$$\Phi \to N_3^- F_3^- . \tag{14}$$

The requirements (c) and (d) are *simple conditions* which are evident properties of the starting Hamiltonian Eq. (1).

(e) If the electron labeled with ''2'' is considered to be nearly motionless at the origin, i.e., $r_2 \sim 0$ and $k_2 \sim 0$, then $\mathbf{r}_3 \sim \mathbf{r}_1, \mathbf{k}_3 \sim \mathbf{k}_1/2$, and $2x_3 = 2x_1/2 = x_1$, and we expect the following limit to hold:

$$\Phi \to N F_2^- {}_1F_1(-ia_1 - ia_3;1;x_1), \tag{15}$$

where $-ia_1 - ia_3 = -i(Z_1 + 2Z_3)/k_1 = -i(Z-1)/k_1$. Thus, the electron ''1'' moves in a Coulomb central charge $Z-1$, which is expected to be the correct condition.

(f) Equivalently, if the electron labeled with ''1'' is considered to be nearly motionless at the origin, i.e., $r_1 \sim 0$ and $k_1 \sim 0$, then $\mathbf{r}_3 \sim -\mathbf{r}_2$, $\mathbf{k}_3 \sim -\mathbf{k}_2/2$, and $2x_3 = 2x_2/2 = x_2$. Thus, the electron ''2'' should move in a central charge $Z-1$,

$$\Phi \to N F_1^- {}_1F_1(-ia_2 - ia_3;1;x_2). \tag{16}$$

(g) If both electrons are very near each other and move along together, i.e., $r_3 \sim 0$ and $k_3 \sim 0$, then $\mathbf{k}_2 \sim \mathbf{k}_1$ and $x_1 \sim x_2$. Thus, the two electrons should behave as a pseudoparticle of charge -2, and so

$$\Phi \to N F_3^- {}_1F_1(-ia_1 - ia_2;1;x_1), \tag{17}$$

involving a Coulomb parameter $-ia_1 - ia_2 \to i(-2)Z/k_1$.

The requirements (e), (f), and (g), which we call *double conditions*, represent limit cases when two out of three particles are *near and with low relative velocities* to each other. We should differentiate these conditions from the ones analyzed by Alt and Mukhamedzhanov [7]. These authors studied the cases when $r_j/r_k \to 0$, independent of the relative moments.

III. SOME PRELIMINARY MODELS

A. The $C3$ approximation

If the term W_{C3}^- is neglected, the solution of H_{C3}^- is the well known $C3$ approximation, i.e., $H_{C3}^- \Phi_{C3} = 0$, where [3–6]

$$\Phi_{C3} = N_{C3}^- \prod_{j=1}^{3} F_j^- , \quad N_{C3}^- = N_1^- N_2^- N_3^- . \tag{18}$$

It is quite simple to show that Φ_{C3} satisfies the first four conditions (a), (b), (c), and (d) but none of the double conditions are observed.

B. Faddeev approximations

It is illustrative here to recall the first-order Faddeev equations to deal with the three body ionization problem introduced by Macek [16]. A simple extension of Macek's formulation to the present case leads us to the first-order *uncorrelated*-Faddeev expression,

$$\Phi_M = N_1^- F_1^- + N_2^- F_2^- + N_3^- F_3^- - 1 - 1. \tag{19}$$

Following this line, in Ref. [11] a first-order *correlated*-Faddeev approximation was found including, to some extent, the crossing derivatives. It reads

$$\Phi_F = N_1^- F_1^- N_{23}^- F_{23}^- + N_2^- F_2^- N_{13}^- F_{13}^- - \Phi_{C3}, \tag{20}$$

with

$$N_{j,k}^- = \exp[(a_j + a_k)\pi/2]\Gamma(1 + ia_j + ia_k), \tag{21}$$

$$F_{j,k}^- = \Phi_2^{(2)}(-ia_j, -ia_k;1;x_j,x_k), \tag{22}$$

$\Phi_2^{(2)}$ is here the degenerate hypergeometric function of *two* variables. This approximation satisfies points (a), (c), and (d). However, Φ_F may produce interference of doubtful physical reality due to its *linear* form [17]. In Sec. V, we will put forward two wave functions to tackle the problem; the first one (Φ_A below) is, as we shall see, the *fractional* form of Φ_F.

C. The perturbative ansatz

In a recent article, Dewangan [18] examined the applicability of the $C3$ approximation for electron-hydrogen excitation. He found that replacing (in our notation)

$$x_3 \to 2x_3, \tag{23}$$

the corresponding amplitude of transition reduces in the high-energy limit to the second Born term calculated with the closure approximation. Good agreement with the experiments was found when compared with the experimental differential cross sections and alignment parameters, particularly at large angles [18]. Very recently, this ansatz has been reexamined by Berakdar [21], who studied the large distance behavior when one of the electrons is bound. Within our scope, we shall prove that the use of the perturbative ansatz gives rise to the observation of the double conditions (e) and (f), sacrificing the simple condition (d).

IV. THE Λ BASE

Our strategy will be to expand the double continuum wave function as

$$\Phi = N\sum_{klm} Q_{klm}\Lambda\left(\begin{array}{ccc|c} -ia_1 & k & c_1 & x_1 \\ -ia_2 & l & c_2 & x_2 \\ -ia_3 & m & c_3 & x_3 \end{array}\right), \tag{24}$$

where

$$\Lambda\left(\begin{array}{ccc|c} -ia_1 & k & c_1 & x_1 \\ -ia_2 & l & c_2 & x_2 \\ -ia_3 & m & c_3 & x_3 \end{array}\right) = (-x_1)^k {}_1F_1(-ia_1+k;c_1;x_1) \times (-x_2)^l {}_1F_1(-ia_2+l;c_2;x_2) \times (-x_3)^m {}_1F_1(-ia_3+m;c_3;x_3), \tag{25}$$

and Q_{klm} are constant, which will be found to be related to a_j as

$$Q_{klm} = \mathcal{Q}_{klm}(-ia_1)_k(-ia_2)_l(-ia_3)_m .$$

In this paper, calligraphic letters denote rational numbers, independent of the electron parameters. It will become evident that it is convenient to work with the *natural* base

$$\Delta_{klm} = (-ia_1)_k(-ia_2)_l(-ia_3)_m \times \Lambda\left(\begin{array}{ccc|c} -ia_1 & k & 1+2k & x_1 \\ -ia_2 & l & 1+2l & x_2 \\ -ia_3 & m & 1+2m & x_3 \end{array}\right). \tag{26}$$

We will prove that Δ is an appropriate base to describe the double continuum state. A series of properties are summarized below.

(i) For the natural base, the first term is precisely the $C3$ approximation.

(ii) If Φ is obtained through a power series in terms of $x_1^k x_2^l x_3^m$, as given by Eq. (8), the corresponding expansion coefficients Q_{klm} can be unequivocally obtained (see Appendix A for details).

(iii) When $|x_j|\to\infty$, Λ tends to the Redmond conditions

$$\Lambda\left(\begin{array}{ccc|c} -ia_1 & k & c_1 & x_1 \\ -ia_2 & l & c_2 & x_2 \\ -ia_3 & m & c_3 & x_3 \end{array}\right) \to R_{klm}\Phi_R , \tag{27}$$

$$R_{klm} = R'\frac{\Gamma(c_1)\Gamma(c_2)\Gamma(c_3)}{(d_1)_k(d_2)_l(d_3)_m}, \tag{28}$$

$$R' = \frac{\exp[-\pi(a_1+a_2+a_3)]}{\Gamma(d_1)\Gamma(d_2)\Gamma(d_3)}, \tag{29}$$

with $d_1 = c_1 - 2k + ia_1$, $d_2 = c_2 - 2l + ia_2$, and $d_3 = c_3 - 2m + ia_3$. Equation (27) holds if, as in our case, $\mathrm{Re}(x_i) = 0$ and $\mathrm{Re}(c) > 0$.The normalization constant can now be simply written as

$$N = \left[\sum_{klm} R_{klm}Q_{klm}\right]^{-1}. \tag{30}$$

It should be noted that if the indexes k, l, and m run up to finite integers in Eq. (24), the *same* upper limits must be considered to determine the normalization constant N. For the natural base, $R' = N_{C3}^{-1}$.

(iv) Any analytical function of variables x_1, x_2, x_3 can be expanded in terms of Δ_{klm}. For example, we found the following expansion of the hypergeometric function $\Phi_2^{(3)}$ in terms of the Δ base as

$$\Phi_2^{(3)}(-ia_1,-ia_2,-ia_3;1;x_1,x_2,x_3) = \sum_{klm} \mathcal{S}_{klm}\Delta_{klm}, \tag{31}$$

and $\mathcal{S}_{klm}$ remains the same under exchange of subindexes. The first coefficients $\mathcal{S}_{klm}$ are listed in Appendix A. To our knowledge, this is the first time that this expansion has been found.

As we shall see, the natural base will allow us to construct the double conditions. If one of the variables tends to zero, $\Phi_2^{(3)}$ reduces to $\Phi_2^{(2)}$, which can also be expressed in terms of a two-dimensional natural base

$$\Phi_2^{(2)}(-ia_2,-ia_3;1;x_2,x_3) = \sum_j \mathcal{S}_j\Delta_j , \tag{32}$$

$$\Delta_j = (-ia_2)_j(-ia_3)_j\Lambda\left(\begin{array}{ccc|c} -ia_2 & j & 1+2j & x_2 \\ -ia_3 & j & 1+2j & x_3 \end{array}\right), \tag{33}$$

$$\mathcal{S}_j = \frac{(-1)^j[2]_j}{(2j)!(2j)!}, \tag{34}$$

where $[2]_j = 1$ if $j = 0$ and 2 otherwise. We can now exploit the fact that $\Phi_2^{(2)}$ satisfies the following property [22]:

$$\Phi_2^{(2)}(-ia_1,-ia_3;1;x,x) = {}_1F_1(-ia_1-ia_3;1;x), \tag{35}$$

in accordance with Eqs. (15)–(17) required by the double conditions. We have found another property which extends Eq. (35),

$$\Phi_2^{(3)}(-ia_1,-ia_3,-ia_3';1;x,x,x) = {}_1F_1(-ia_1-ia_3-ia_3';1;x). \tag{36}$$

This property can be useful to describe a *triple condition* involving three electrons in the continuum. When two out of three electrons are motionless and close to the nucleus, Eq. (36) describes the outer (third) electron moving in a charge $(Z-1-1)$, which is the expected condition.

(v) If the parameters c_j are positive integers, as in the case of the natural base, one can prove that the matrix elements involving the ground state, such as the double photoionization, can be reduced to three-dimensional integrals of closed forms in a similar fashion to the $C3$ approximation (i.e., the integrand does not contain hypergeometric functions of the type ${}_2F_1$). If the parameters c_j are not positive integer, we still have the alternative to expand the hypergeometric functions in power series and reconstruct the function in terms of

the natural base, as developed in Appendix A. Thus, the expansion coefficients will depend on c_j but the matrix elements can be reduced to three-dimensional integrals of closed forms.

(vi) Expressions resulting from some operations on Δ_{klm}, such as $\partial/\partial x_j \Delta_{klm}$ and $x_j^n \Delta_{klm}$, can be cast as a sum of Δ_{klm} (see Appendix D for details). In particular, we found the following useful identities:

$$H_1^- \Delta_{klm} = \frac{k^2}{x_1} \Delta_{klm}, \tag{37}$$

$$x \frac{\partial}{\partial x} \Delta_{klm} = \sum_{K=0}^{\infty} A_K^k \Delta_{k+K\,l\,m}, \tag{38}$$

$$x^n \Delta_{klm} = \sum_{K=0}^{\infty} B_K^{n,k} \Delta_{k+K\,l\,m}. \tag{39}$$

V. TWO PROPOSALS

In this section we put forward two proposals to deal with two electrons in the continuum, which can be written in terms of the Λ base and can be considered as variations of $\Phi_2^{(3)}$. It would be interesting to investigate beforehand the behavior of precisely $\Phi_2^{(3)}(2x_3)$. This generalized confluent hypergeometric function can be easily expanded in the natural base Δ [see Eq. (31)] and can be proven to satisfy (a) and the three double conditions (e), (f), and (g) but it fails to observe (c). We note that $\Phi_2^{(3)}$ may be a good alternative to study electron-positronium ionization, where the three particles have equal masses and so the system becomes fully symmetric. The degenerate hypergeometric function $\Phi_2^{(3)}$ has a lot of physical information of interest. To some extent it includes some previous approximation. For example, as mentioned before, the first term of the natural base is the $C3$ approximation. Further, if we consider the subset for $k=0$ in the $\Phi_2^{(3)}$ expansion, Eq. (31), it results

$$\Phi_2^{(3)}|_{k=0} = \sum_{lm} \mathcal{S}_{0lm} \Delta_{0lm} = F_1^- \sum_{lm} \mathcal{S}_l \delta_{lm} \Delta_{0lm}$$

$$= F_1^- \sum_{l} \mathcal{S}_l \Delta_l = F_1^- \sum_{l} F_{2,3}^-, \tag{40}$$

which is the first term of Φ_F given by Eq. (20). The second term corresponds to the subset with $l=0$.

The approximations introduced below are corrections to $\Phi_2^{(3)}$ so that the condition (c) will be satisfied. It should be a necessary requirement to observe, especially in the case of having a large nuclear charge. The condition (c) turns out results to be the independent electron model.

A. First proposal

Let us introduce the following power series:

$$\Phi_A = N_A \sum_{klm} P_{klm}^A \frac{x_1^k}{k!} \frac{x_2^l}{l!} \frac{x_3^m}{m!},$$

$$P_{klm}^A = \frac{(-ia_1)_k (-ia_2)_l (-ia_3)_m}{(1)_{k+l+m}} \frac{(c_A)_{k+l}}{(c_A)_k (c_A)_l}, \tag{41}$$

and the normalization constant can be found in closed form to give

$$N_A = \begin{cases} N_F = \dfrac{N_{1,3}^- N_{2,3}^-}{N_3^-} & \text{if } c_A = 1 + ia_3, \\ N_{C3} = N_1^- N_2^- N_3^- & \text{if } c_A = 1. \end{cases} \tag{42}$$

The degenerate hypergeometric function $\Phi_2^{(3)}$ can be obtained from Eq. (41) by simply replacing $(c_A)_{k+l}/(c_A)_k (c_A)_l$ by unity. From the mathematical point of view, this term decouples the correlation between the variables x_1 and x_2 as observed in Eq. (B5) removing $\partial^2/\partial x_1 \partial x_2$. Φ_A can be expressed in terms of the natural basis

$$\Phi_A = N_A \sum_{klm} \mathcal{A}_{klm} \Delta_{klm}, \tag{43}$$

where the expansion coefficients $\mathcal{A}_{klm}$ are listed in Appendix A. Due to the symmetry of the series, $\mathcal{A}_{klm} = \mathcal{A}_{lkm}$ and $\mathcal{A}_{k0k} = \mathcal{A}_{0kk} = \mathcal{S}_k$, which guarantees the description of $\Phi_2^{(2)}$ as either x_1 or x_2 vanishes.

Alternatively, we have found a simpler expansion over only the *two*-index sum as follows:

$$\Phi_A = N_A \sum_{kl} A_{kl} \Lambda \left(\begin{matrix} -ia_1 & k & c_A + k \\ -ia_2 & l & c_A + l \\ -ia_3 & k+l & 1+k+l \end{matrix} \middle| \begin{matrix} x_1 \\ x_2 \\ x_3 \end{matrix} \right), \tag{44}$$

$$A_{kl} = \frac{(-ia_1)_k (-ia_2)_l (-ia_3)_{k+l}}{k!\,l!\,(k+l)!} (-x_3)^{-k-l}, \tag{45}$$

but the expansion coefficients A_{kl} are now no longer constant, as one may wish, but they are proportional to $(-x_3)^{-k-l}$.

Φ_A satisfies three conditions introduced in the preceding section, namely (a), (c), and (d). Correlations (crossing derivatives) are included to some extent. In general, if three different c parameters are used, the so-constructed wave function $\Phi_A' = \Phi_A(c_1, c_2, c_3)$ is a solution of $H_A' \Phi_A' = 0$, where $H_A' = H_{C3}^- + U_A'$ so that (see Appendix B for details)

$$U_A' = \frac{4k_3^2}{x_3 + y_3} \left[(1 - c_3) + \sum_{l=1}^{2} x_l \frac{\partial}{\partial x_l} \right] \frac{\partial}{\partial x_3}$$

$$+ \sum_{l=1}^{2} \frac{2k_l^2}{x_l + y_l} \left[(1 - c_l) \frac{\partial}{\partial x_l} + \left(-ia_l + x_l \frac{\partial}{\partial x_l} \right) \frac{\partial}{\partial x_3} \right]. \tag{46}$$

In our case $c_1 = c_2 = c_A$ and $c_3 = 1$. The interaction U_A' tries to approximate W_{C3}^- within its limitations.

The interesting point is that Φ_A verifies a huge amount of properties, which makes it a ''friendly'' function to deal with. Φ_A belongs to the family of the degenerate hypergeometric functions of several variables [10]. Since it has never been proposed before, we abridge their properties in Appen-

dix B. Also Φ_A can be easily extended straightforwardly to describe three or even more electrons.

If we consider $c_A=1$, three advantages are observed; the first term is precisely the $C3$ approximation as noted in paragraph (i) of the preceding section. Second, the matrix elements can be reduced significantly as noted in (v). And third, Kato conditions are not fully lost; the properties

$$P^A_{1,l,0}=(-ia_1)P^A_{0,l,0},\quad P^A_{k,1,0}=(-ia_2)P^A_{k,0,0}, \tag{47}$$

and $P^A_{0,0,1}=(-ia_3)P^A_{0,0,0}$ still stand. Although Eq. (10) is not fully satisfied (and it is a setback as compared with the $C3$ approximation, which fully satisfies the cusp conditions), it is still an improvement as compared with the $C2$ approximation, which also satisfies Eq. (47) but $P^{C2}_{0,0,1}=0$ instead.

If otherwise $c_A=1+ia_3$ in Eq. (44), the three previous advantages are no longer observed, but in turn Φ_A is found to be the fractional form of the first-order correlated-Faddeev approximation Φ_F, as explained in Appendix C.

Application of the perturbative ansatz

If the double argument , i.e., $x_3\to 2x_3$, is considered in the definition of Φ_A, two properties (e) and (f) come out as explained next. Following the item (e) of Sec. II A, if the electron labeled with ''2'' is considered to be close to the nucleus and with low relative velocity, $r_2\sim 0$ and $k_2\sim 0$, then $x_2\sim 0, 2x_3\sim x_1$, and only $l=0$ survives in Eq. (41) (and consequently Φ_A becomes independent on c_A). Thus

$$\Phi_A\sim N_A\sum_{km}\frac{(-ia_1)_k(-ia_3)_m}{(1)_{k+m}}\frac{x_1^k}{k!}\frac{x_1^m}{m!}$$

$$=\Phi_2^{(2)}(-ia_1,-ia_3;1;x_1,x_1)$$

$$={}_1F_1(-ia_1-ia_3;1;x_1), \tag{48}$$

where we have used Eq. (35). In this way the electron ''2'' moves in a Coulomb charge $Z-1$ which should be the correct condition. In a similar fashion, following item (f) of Sec. II A, if the electron labeled with ''1'' is considered to be close to the nucleus and with low relative velocity, $r_1\sim 0$ and $k_1\sim 0$, it can be proven that the electron ''1'' is now the one seeing a charge $Z-1$. The perturbative ansatz then has a solid and independent explanation; the wave function is modified to satisfy two double conditions. Recall that Dewangan just considered the first term of the series (the equivalent of the $C3$ approximation). A price must be paid to satisfy the double conditions, i.e., the property (c) is no longer satisfied. Now, when the nucleus charge is switched off $(a_{1,2}\to 0)$, the proper *e-e* continuum is *not* recovered, but

$$\Phi_A\to 2^{-ia_3}N_3^-{}_1F_1(-ia_3;1;2x_3),$$

instead of $N_3^-F_3^-$. Anyway, the Redmond conditions are *still* satisfied. The region which is altered corresponds to $|x_3|\lesssim 1$, where precisely the *e-e* repulsion reduces the probability. For this reason, that deficiency may not introduce a substantial failure at a level of integrated cross section.

B. Second proposal

Let us introduce the following subset of $\Phi_2^{(3)}$:

$$\Phi_B=N_B\sum_{kl}\mathcal{B}_{k\,l\,k+l}\Delta_{k\,l\,k+l}(2x_3),$$

where the coefficients $\mathcal{B}_{klm}$ satisfy $\mathcal{B}_{0kk}=\mathcal{B}_{k0k}=\mathcal{S}_k$ as given by Eq. (34). There is some freedom to choose these coefficients. A first election may be the expansion coefficients corresponding to the $\Phi_2^{(3)}$ of three variables, i.e., $\mathcal{B}_{k\,l\,k+l}=\mathcal{S}_{k\,l\,k+l}$ (see Appendix A). The normalization constant N_B can be calculated with Eq. (30). This function again follows the perturbative ansatz and it satisfies the two simple conditions (a) and (c) and the two double conditions (e) and (f). The Kato conditions observed are the approximated ones given by Eq. (47).

VI. DISCUSSIONS AND FUTURE DEVELOPMENTS

We have introduced an approach to tackle the problem of two electrons in the continuum, by expanding the wave function in the here-called Λ base. The properties of this base make it very versatile. By construction it tends to the proper Coulomb conditions; simple and/or double conditions can be built up, and the generalization to three or more electrons is rather tedious to deal with but is a possible task.

The future applications of this expansion are quite encouraging. For any numerical purpose, further groundwork is needed, this is the design of an efficient code to solve the matrix elements involving the product of three hypergeometric functions which, as observed in (v), can be reduced to three dimensional integrals.

The Λ base is an ideal outer function to match the inner solution within the scheme of the *R*-matrix theory. The expansion coefficients can be determined to fit the logarithmic derivative at the boundary edge. The mathematical task reduces to simple linear algebra problem.

The Λ base can be also extended to describe also the initial channel in case of studying the ionization of hydrogen by impact of electrons or positrons. In this case, it is convenient to write the base in terms of the incoming variable. Its first term is therefore the usual product of two incoming continuum waves times the bound state. It is possible then to construct a *symmetric* approximation by using Λ bases in both the initial and final channels.

The scattering state expressed in terms of the Λ base has an appropriate structure to be used within the Kohn-type variational principle, since the asymptotic conditions are warranted. Making a variation on the expansion coefficients as trial parameters, the task reduces to a linear algebra problem.

We can even overrun the outgoing approximation which reduces the problem to the variables x_i, neglecting y_i. The generalization is obviously the use of a Δ base of six variables summing on six subindexes, i.e.,

$$\Delta\left(\begin{array}{ccc|c} -ia_1 & n_1 & 1+2n_1 & x_1\\ -ia_2 & n_2 & 1+2n_2 & x_2\\ -ia_3 & n_3 & 1+2n_3 & x_3\\ 0 & n_1' & 1+2n_1' & y_1\\ 0 & n_2' & 1+2n_2' & y_2\\ 0 & n_3' & 1+2n_3' & y_3 \end{array}\right).$$

The function on the incoming variables y_i does not interfere, for $r_i \to \infty$ ($|x_i| \to \infty$ and $|y_i| \to 0$) it survives only $n_1' = n_2' = n_3' = 0$ contributing with unity. The solution is constructed with a superposition of solutions of $H_j^+ - n_j^2/x_j$ (x_i outgoing space) times those of $H_j^+ - n_j'^2/y_j$ (y_i incoming space). The collision state divides in an inner zone, where the variables x_i and y_i compete, and an outer zone where only the x_i variables survive to give the correct Coulomb conditions. This is an alternative approach to the description posed by Berakdar [23] where x_i with r_i are mixed, while here the description remains in parabolic coordinates. Problems arise to manage so large an amount of unknown parameters, especially those connecting variables x_i with y_j. However it may be an advantage; with the help of the variables y_i, the Kato cusp conditions may be reinstalled.

ACKNOWLEDGMENTS

We would like to thank C. R. Garibotti, G. Gasaneo, and F. Colavecchia for useful discussions.

APPENDIX A: THE Λ EXPANSION FROM THE POWER SERIES

The mathematical problem is to find the coefficients Q_{klm} so that

$$\sum_{klm} P_{klm}\ x_1^k x_2^l x_3^m = \sum_{KLM} Q_{KLM} \Lambda \left(\begin{array}{ccc|c} -ia_1 & K & c_1 & x_1 \\ -ia_2 & L & c_2 & x_2 \\ -ia_3 & M & c_3 & x_3 \end{array} \right). \tag{A1}$$

After simple algebra one can find that the following relation holds:

$$P_{klm} = \sum_{KLM=0}^{klm} U_1(K,k-K) U_2(L,l-L) \times U_3(M,m-M) Q_{KLM}, \tag{A2}$$

where

$$U_n(J,j-J) = \frac{(-ia_n+J)_{j-J}}{(c_n)_{j-J}(j-J)!}. \tag{A3}$$

This system of algebraic equations can be solved sequentially exploiting the property that $U_n(J,0)=1$. Using this simple technique we have obtained the expansion of $\Phi_2^{(3)}$ [see Eq. (31)], unknown to us so far, to give

$$\mathcal{S}_{4,4,4} = 1/88720676352000, \quad \mathcal{S}_{1,3,3} = 1/252000, \tag{A4}$$

$$\mathcal{S}_{3,4,4} = -1/352066176000, \quad \mathcal{S}_{2,2,3} = 1/226800,$$

$$\mathcal{S}_{1,4,4} = -1/800150400, \quad \mathcal{S}_{1,2,3} = -1/86400,$$

$$\mathcal{S}_{0,4,4} = 1/812851200, \quad \mathcal{S}_{2,2,2} = 1/3240,$$

$$\mathcal{S}_{3,3,4} = 1/7620480000, \quad \mathcal{S}_{1,2,2} = -1/270,$$

$$\mathcal{S}_{2,3,4} = -1/571536000, \quad \mathcal{S}_{0,2,2} = 1/288,$$

$$\mathcal{S}_{1,3,4} = 1/203212800, \quad \mathcal{S}_{1,1,2} = 1/144,$$

$$\mathcal{S}_{2,2,4} = 1/135475200, \quad \mathcal{S}_{1,1,1} = 2/3,$$

$$\mathcal{S}_{3,3,3} = 17/2449440000, \quad \mathcal{S}_{0,1,1} = -1/2,$$

$$\mathcal{S}_{2,3,3} = -1/3024000, \quad \mathcal{S}_{0,0,0} = 1,$$

$$\mathcal{S}_{0,3,3} = -1/259200.$$

Due to symmetry of the function, $\mathcal{S}_{klm}$ remains the same under exchange of subindexes, and $\mathcal{S}_{kl0} = \mathcal{S}_{k0l} = \mathcal{S}_{0kl} = \mathcal{S}_k \delta_{kl}$. The series seem to be strongly convergent.

In a similar fashion, the expansion coefficients corresponding to Φ_A can be found to give [see Eq. (43)]

$$\mathcal{A}_{3,3,3} = 1/612360000, \quad \mathcal{A}_{2,3,3} = -1/24192000,$$

$$\mathcal{A}_{3,3,2} = 1/36288000, \quad \mathcal{A}_{1,3,3} = 1/504000,$$

$$\mathcal{A}_{3,3,1} = 1/1512000, \quad \mathcal{A}_{0,3,3} = -1/259200,$$

$$\mathcal{A}_{2,2,2} = 1/25920, \quad \mathcal{A}_{2,2,3} = 1/302400,$$

$$\mathcal{A}_{2,3,2} = -1/453600, \quad \mathcal{A}_{1,2,3} = -1/28800,$$

$$\mathcal{A}_{1,3,2} = 1/43200, \quad \mathcal{A}_{2,3,1} = -1/86400,$$

$$\mathcal{A}_{2,2,1} = 1/1080, \quad \mathcal{A}_{1,2,2} = -1/540,$$

$$\mathcal{A}_{0,2,2} = 1/288, \quad \mathcal{A}_{1,1,2} = 1/72,$$

$$\mathcal{A}_{1,2,1} = -1/144, \quad \mathcal{A}_{1,1,1} = 1/3,$$

$$\mathcal{A}_{0,1,1} = -1/2, \quad \mathcal{A}_{1,0,1} = -1/2,$$

$$\mathcal{A}_{0,0,0} = 1,$$

and $\mathcal{A}_{k,j,0} = \mathcal{A}_{0,2,3} = \mathcal{A}_{0,3,2} = \mathcal{A}_{1,1,3} = \mathcal{A}_{1,3,1} = \mathcal{A}_{0,1,3} = \mathcal{A}_{0,3,1} = \mathcal{A}_{0,0,3} = \mathcal{A}_{0,1,2} = \mathcal{A}_{0,2,1} = \mathcal{A}_{0,0,2} = \mathcal{A}_{0,0,1} = 0$ for $c_A = 1$. In the case that $c_A = c \neq 1$, other coefficients are obtained,

$$\mathcal{A}_{2,2,2} = (+1-4c+4c^2)/[12960(c+c^2)],$$

$$\mathcal{A}_{1,2,2} = -(-1+2c)/(540c),$$

$$\mathcal{A}_{2,2,1} = -(2-5c+2c^2)/[540(c+c^2)],$$

$$\mathcal{A}_{2,2,0} = -(-2+3c-c^2)/[288(c+c^2)],$$

$$\mathcal{A}_{1,1,2} = -(-1-c)/(144c),$$

$$\mathcal{A}_{1,2,1} = -(2-c)/(144c),$$

$$\mathcal{A}_{1,1,1} = -(1-2c)/(3c),$$

$$\mathcal{A}_{1,1,0} = -(-1+c)/(2c),$$

$$\mathcal{A}_{0,2,2} = 1/288, \mathcal{A}_{0,0,0} = 1, \mathcal{A}_{0,1,1} = 1/2,$$

and $\mathcal{A}_{0,1,2} = \mathcal{A}_{0,2,1} = \mathcal{A}_{1,2,0} = \mathcal{A}_{0,0,2} = \mathcal{A}_{0,2,0} = \mathcal{A}_{0,0,1} = \mathcal{A}_{0,1,0} = 0$.

APPENDIX B: MATHEMATICAL PROPERTIES OF THE Φ_A HYPERGEOMETRIC FUNCTION

The mathematical properties of the hypergeometric function Φ_A are summarized here. We had to develop all the formulas here presented since Φ_A never had been studied before nor, to our knowledge, even proposed. Such proofs required some degree of tedious algebra here avoided. We have tried to be as general as possible, following the items of a mathematical table [24,25]. $\Phi_0(\alpha_1,\alpha_2,\alpha_3;\gamma_1,\gamma_2,\gamma_3;z_1,z_2,z_3)$ (shortly denoted by Φ_0) is a generalization of Φ_A. In particular, $\Phi_A=\Phi_0(\gamma_1=\gamma_2=\gamma_3-\alpha_3)$. In this appendix the following notation is used: $\delta_j=\gamma_j-\alpha_j, j=1,2,3$.

(i) *Differential equations*. Introducing the degenerate hypergeometric operator

$$H(\alpha,\gamma,z)=z\frac{\partial^2}{\partial z^2}+(\gamma-z)\frac{\partial}{\partial z}-\alpha, \tag{B1}$$

so that $H(\alpha,\gamma,z)_1F_1(\alpha;\gamma;z)=0$, we proved that Φ_0 satisfies the following system of differential equations:

$$\left[H(\alpha_1,\gamma_1,z_1)+\left(\alpha_1+z_1\frac{\partial}{\partial z_1}\right)\frac{\partial}{\partial z_3}\right]\Phi_0=0,$$

$$\left[H(\alpha_2,\gamma_2,z_2)+\left(\alpha_2+z_2\frac{\partial}{\partial z_2}\right)\frac{\partial}{\partial z_3}\right]\Phi_0=0, \tag{B2}$$

$$\left[H(\alpha_3,\gamma_3,z_3)+z_1\frac{\partial^2}{\partial z_1\partial z_3}+z_2\frac{\partial^2}{\partial z_2\partial z_3}\right]\Phi_0=0.$$

(ii) *Series expansions*. From Eq. (B2), one can obtain the power series expansion

$$\Phi_0=\sum_{klm}P_{klm}\frac{z_1^k}{k!}\frac{z_2^l}{l!}\frac{z_3^m}{m!}, \tag{B3}$$

where

$$P_{klm}=\frac{(\alpha_1)_k(\alpha_2)_l(\alpha_3)_m(\gamma_3-\alpha_3)_{k+l}}{(\gamma_1)_k(\gamma_2)_l(\gamma_3)_{k+l+m}}. \tag{B4}$$

(iii) *Integral representations*. The hypergeometric function Φ_0 has the following integral representations:

$$\Phi_0=\Gamma_3\int_0^1 du_3\exp(u_3z_3)u_3^{\alpha_3-1}K_3(u_3)\times\prod_{l=1}^{2}{}_1F_1(\alpha_l;\gamma_l;(1-u_3)z_l) \tag{B5}$$

$$=\int\int\int_{\mathcal{R}}du_1du_2du_3\prod_{j=1}^{3}\Gamma_j\exp(u_jz_j)u_j^{\alpha_j-1}\times\mathcal{K}_0(u_1,u_2,u_3) \tag{B6}$$

$$=\int_0^1\int_0^1\int_0^1du_1du_2du_3\prod_{j=1}^{3}\Gamma_j\exp(u_jz_j)u_j^{\alpha_j-1}\times K_j(u_j)\exp(-u_3u_1z_1-u_3u_2z_2), \tag{B7}$$

$$\mathcal{K}_0(u_1,u_2,u_3)=\frac{\mathcal{K}_{13}(u_3,u_1)\mathcal{K}_{23}(u_3,u_2)}{K_3(u_3)}, \tag{B8}$$

$$\mathcal{K}_{l3}(u_l,u_3)=[1-u_l-u_3]^{\gamma_l-1+\alpha_l}, \tag{B9}$$

$$K_j(u_j)=[1-u_j]^{\gamma_j-\alpha_j-1}, \tag{B10}$$

$$\Gamma_j=\frac{1}{\Gamma(\alpha_j)}\Gamma_j',\quad \Gamma_j'=\frac{\Gamma(\gamma_j)}{\Gamma(\gamma_j-\alpha_j)} \tag{B11}$$

with $l=1,2$ and $=1,2,3$. The lower limits of integration of $\mathcal{R}$ are $u_1\geqslant0$, $u_2\geqslant0$, and $u_3\geqslant0$, and the upper one are $1-u_1-u_3\geqslant0$, $1-u_2-u_3\geqslant0$, and $1-u_3\geqslant1$. As a rule, the base of the kernels [the terms in squared brackets in Eqs. (B9) and (B10)] must always be positive. Note that $\mathcal{K}_{1,3}(u_1,u_3)[\mathcal{K}_{2,3}(u_2,u_3)]$ is a $\Phi_2^{(2)}$ kernel which ''constructs'' the Coulomb interactions represented by the Coulomb parameters α_1 and α_3 (α_2 and α_3). On the other hand, $K_3(u_3)$ is a $_1F_1$ kernel which ''deconstructs'' α_3 interaction since it is accounted twice.

(iv) *Asymptotic limits*. Using the limit, when $|z_j|\to\infty$,

$${}_1F_1(\alpha_j;\gamma_j;z_j)\to\Gamma_j'z_j^{-\alpha}e^{i\epsilon_j\pi\alpha}, \tag{B12}$$

where $\mathrm{Re}(\gamma_j)>0,\epsilon_j=\mathrm{sgn}[\mathrm{Im}(z_j)]$, it can be found that the following limit holds:

$$\Phi_0\to\Gamma_1'\Gamma_2'\Gamma_3'z_1^{-\alpha_1}z_2^{-\alpha_2}z_3^{-\alpha_3}\exp\left(i\sum_{j=1}^{3}\epsilon_jz_j\pi\alpha_j\right), \tag{B13}$$

as $|z_j|\to\infty, j=1,2,3$ providing the Redmond asymptotic conditions.

(v) *Differential relations.* The derivatives of Φ_0 satisfy

$$z_1\frac{\partial}{\partial z_1}\Phi_0=-\alpha_1\Phi_0+\alpha_1\Phi_0(\alpha_1+1), \tag{B14}$$

$$z_2\frac{\partial}{\partial z_2}\Phi_0=-\alpha_2\Phi_0+\alpha_2\Phi_0(\alpha_2+1), \tag{B15}$$

$$(\gamma_3)_n\frac{\partial^n}{\partial z_3^n}\Phi_0=(\alpha_3)_n\Phi_0(\alpha_3+n;\gamma_3+n),$$

$$\frac{\partial}{\partial z_1}\Phi_0=\frac{\alpha_1}{\gamma_1}\frac{\alpha_2}{\delta_2}\epsilon_{2,3}\Phi_0(\alpha_2+1;\gamma_1+1,\gamma_2+1,\gamma_3+1)+\frac{\alpha_1}{\gamma_1}\epsilon_{2,3}\Phi_0(\gamma_1+1,\gamma_2+1,\gamma_3+1), \tag{B16}$$

with

$$\epsilon_{2,3}=\frac{\delta_2}{\gamma_2}\frac{\delta_3}{\gamma_3}. \tag{B17}$$

(vi) *Kummer relations.* One can prove the following identities:

$$\Phi_0=e^{z_1}\Phi_0(\delta_1,\alpha_{2-3};\gamma_{1-3};-z_1,z_2,z_3-z_1), \tag{B18}$$

$$\Phi_0 = e^{z_2}\Phi_0(\alpha_1, \delta_2, \alpha_3; \gamma_{1-3}; z_1, -z_2, z_3 - z_2). \tag{B19}$$

For the third variable z_3, the Kummer rule is not so evident, but for Φ_A the relation is simple and it reads

$$\Phi_A = e^{z_3}\Phi_A(\alpha_{1-2}, \delta_3 - \alpha_1; \gamma_3; z_1 - z_3, z_2, -z_3), \tag{B20}$$

$$\Phi_A = e^{z_3}\Phi_A(\alpha_{1-2}, \delta_3 - \alpha_2; \gamma_3; z_1, z_2 - z_3, -z_3). \tag{B21}$$

(vii) *Hypergeometric expansions*. Expanding the ${}_1F_1$ functions in Eq. (B5), we can prove the following relations:

$$\Phi_0 = \sum_{kl} \frac{(\alpha_1)_k}{(\gamma_1)_k}\frac{(\alpha_2)_l}{(\gamma_2)_l}\frac{(\alpha_3)_{k+l}}{(\gamma_3)_{k+l}} \times \frac{(-z_1)^k}{k!}\frac{(-z_2)^l}{l!}\,{}_1F_1(\alpha_3 + k + l; \gamma_3 + k + l; z_3) \times {}_1F_1(\alpha_1 + k; \gamma_1 + k; z_1)\,{}_1F_1(\alpha_2 + l; \gamma_2 + l; z_2). \tag{B22}$$

Other transformations can be obtained using Eq. (49) of Ref. [22],

$$\Phi_A = \sum_r \frac{(\alpha_1)_r(\alpha_2)_r}{(\gamma - \alpha_3)_r(\gamma - \alpha_3)_{2r}}\frac{(z_1 z_2)^r}{r!} \times \Phi_2(\alpha_1 + r, \alpha_2 + r, \alpha_3; \gamma - \alpha_3 + 2r; z_1, z_2, z_3). \tag{B23}$$

(viii) *Contiguous relations*. The following contiguous relations hold:

$$0 = \Phi_0 - \Phi_0(\alpha_1 - 1) - \frac{1}{\gamma_1}\epsilon_{2,3} z_1 \Phi_0(\gamma_1 + 1, \gamma_2 + 1, \gamma_3 + 1) - \frac{1}{\gamma_1}\frac{\alpha_2}{\delta_2}\epsilon_{2,3} z_1 \Phi_0(\alpha_2 + 1; \gamma_1 + 1, \gamma_2 + 1, \gamma_3 + 1), \tag{B24}$$

$$0 = \Phi_0 - \Phi_0(\alpha_1 + 1) + \frac{1}{\gamma_1}\epsilon_{2,3} z_1 \Phi_0(\alpha_1 + 1; \gamma_1 + 1, \gamma_2 + 1, \gamma_3 + 1) + \frac{1}{\gamma_1}\frac{\alpha_2}{\delta_2}\epsilon_{2,3} z_1 \Phi_0(\alpha_1 + 1, \alpha_2 + 1; \gamma_1 + 1, \gamma_2 + 1, \gamma_3 + 1), \tag{B25}$$

and similar relations.

(ix) *Special cases*. When one of the coefficients is zero, then

$$\Phi_A(\alpha_1 = 0) = \Phi_A(z_1 = 0) = \Phi_2^{(2)}(\alpha_2, \alpha_3; \gamma; z_2, z_3), \tag{B26}$$

$$\Phi_A(\alpha_2 = 0) = \Phi_A(z_2 = 0) = \Phi_2^{(2)}(\alpha, \alpha_3; \gamma; z_1, z_3), \tag{B27}$$

$$\Phi_A(\alpha_1 = 0, \alpha_2 = 0) = \Phi_A(z_1 = 0, z_2 = 0) = {}_1F_1(\alpha_3; \gamma; z_3), \tag{B28}$$

$$\Phi_A(z_3 = 0) = \sum_{r=0}^{\infty} (-1)^r \frac{(\alpha_1)_r(\alpha_2)_r(\alpha_3)_r(\gamma)_{2r}}{(\gamma)_r^4(\gamma + r - 1)_r(\gamma - \alpha_3)_r(1_r)} \times z_1^r z_2^r\,{}_1F_1(\alpha + r; \gamma + 2r; z_1) \times {}_1F_1(\alpha_2 + r; \gamma + 2r; z_2). \tag{B29}$$

APPENDIX C: CONNECTION WITH THE FIRST PERTURBATIVE ORDER OF THE CORRELATED-FADDEEV APPROXIMATION

We prove here that Φ_A with $c_A = 1 + ia_3$ can be considered as the fractional form of the correlated-Faddeev approximation Φ_F, as explained next. The integral representation of Φ_A contains a normalized kernel $\mathcal{K}_A$ in the tridimensional space u_1, u_2, u_3 [see Eq. (B6) of Appendix B] which can be rewritten as

$$\mathcal{K}_A(u_1, u_2, u_3) = \mathcal{K}_A = \frac{[\mathcal{K}_{1,3}\mathcal{K}_2][\mathcal{K}_{2,3}\mathcal{K}_1]}{\mathcal{K}_1\mathcal{K}_2\mathcal{K}_3}. \tag{C1}$$

$\mathcal{K}_{l,3} = N_{l,3}^{-}\mathcal{K}_{l,3}(u_l, u_3)(l = 1,2)$ and $\mathcal{K}_j = N_j^{-}\mathcal{K}_j(u_j)(j = 1,2,3)$ are the kernels of the $\Phi_{l,3}^{-}$ and F_j^{-} hypergeometric functions, respectively, multiplied by the normalization constant. The kernel corresponding to Φ_F is simply

$$\mathcal{K}_F = \mathcal{K}_{1,3}\mathcal{K}_2 + \mathcal{K}_{2,3}\mathcal{K}_1 - \mathcal{K}_1\mathcal{K}_2\mathcal{K}_3. \tag{C2}$$

Now it is evident that this expression contains the same terms as the fractional form given by Eq. (C1), but in a linear form. Conceptually, fractional forms become linear forms transforming multiplication by sum and division by subtraction operations. In this way the kernels seem to behave in a similar pattern to the Green operators; a many-body operator can be cast in linear [26] as well as fractional forms [27].

Further, when the pair interaction is discoupled, by setting $\mathcal{K}_{l,3} \to \mathcal{K}_l\mathcal{K}_3$, in either Eq. (C1) or in Eq. (C2), we arrive at the same result,

$$\mathcal{K}_A, \mathcal{K}_F \to \mathcal{K}_1\mathcal{K}_2\mathcal{K}_3 = \mathcal{K}_{C3},$$

which is the kernel of the $C3$ approximation.

APPENDIX D: EXPANSIONS IN TERMS OF THE NATURAL BASIS

The first coefficients $\tilde{A}_K^k = A_K^k/(a + k)_K$, corresponding to Eq. (38) are

$$A_0^k = k a_k, \tag{D1}$$

$$A_1^k = -\frac{-ia + k}{1 + 2k} a_k,$$

$$A_2^k = \frac{(-ia + k)(-ia + k + 1)}{2(1 + k)(1 + 2k)(3 + 2k)} a_k,$$

and for $K \geqslant 2$ the coefficients may be defined recursively by the formula

$$A_K^k = \frac{(ia - k - K + 1)}{2^{K-1}(k + K - 1)(2k + K + 1)} A_{K-1}^k. \tag{D2}$$

The first coefficients $\tilde{B}_K^{n,k}=B_K^{n,k}/(a+k)_K$, corresponding to Eq. (39) with $n=1$ are

$$B_0^{1,k}=0,$$

$$B_1^{1,k}=-a_k,$$

$$B_2^{1,k}=\frac{-2ia-1}{(1+2k)(3+2k)}a_k, \tag{D3}$$

$$B_3^{1,k}=\frac{3a^2-3ia-(1+k)(2+k)}{4(1+k)(2+k)(1+2k)(5+2k)}a_k,$$

$$B_4^{1,k}=\frac{2ia^3+3a^2-i(7+8k+2k^2)a-(1+k)(3+k)}{2(1+k)(3+k)(1+2k)(3+2k)(5+2k)(7+2k)}a_k.$$

The first coefficients corresponding to Eq. (39) with $n=2$ are

$$B_0^{2,k}=B_1^{2,k}=0,$$

$$B_2^{2,k}=1a_k,$$

$$B_3^{2,k}=\frac{4ia+2}{(1+2k)(5+2k)}a_k,$$

$$B_4^{2,k}=\frac{-5a^2+5ia+(1+k)(3+k)}{2(1+k)(3+k)(1+2k)(7+2k)}a_k.$$

The first coefficients corresponding to Eq. (39) with $n=3$ are

$$B_0^{3,k}=B_1^{3,k}=B_2^{3,k}=0,$$

$$B_3^{3,k}=-1a_k,$$

$$B_4^{3,k}=\frac{-6ia-3}{(1+2k)(7+2k)}a_k, \tag{D4}$$

$$B_5^{3,k}=\frac{21a^2-21ia-3(1+k)(4+k)}{4(1+k)(4+k)(1+2k)(9+2k)}a_k.$$

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