Three-body-continuum Coulomb problem using a compact-kernel-integral-equation approach

M. Silenou Mengoue*

Centre for Atomic, Molecular Physics and Quantum Optics, Faculty of Science, University of Douala, P.O. Box 8580, Douala, Cameroon

(Received 4 December 2012; published 5 February 2013)

We present an approach associated with the Jacobi matrix method to calculate a three-body wave function that describes the double continuum of an atomic two-electron system. In this approach, a symmetrized product of two Coulomb waves is used to describe the asymptotic wave function, while a smooth cutoff function is introduced to the dielectronic potential that enters its integral part in order to have a compact kernel of the corresponding Lippmann-Schwinger-type equation to be solved. As an application, the integral equation for the (e^-, e^-, He^{2+}) system is solved numerically; the fully fivefold differential cross sections (FDCSs) for (e,3e) processes in helium are presented within the first-order Born approximation. The calculation is performed for a coplanar geometry in which the incident electron is fast (∼6 keV) and for a symmetric energy sharing between both slow ejected electrons at excess energy of 20 eV. The experimental and theoretical FDCSs agree satisfactorily both in shape and in magnitude. Full convergence in terms of the basis size is reached and presented.

DOI: 10.1103/PhysRevA.87.022701 PACS number(s): 34.80.Dp, 03.65.Nk, 34.10.+x

I. INTRODUCTION

The three-body-continuum Coulomb problem is one of the fundamental unresolved problems of theoretical physics. In atomic physics, a prototype example is a two-electron continuum which arises as a final state in electron-impact ionization and double photoionization of atomic systems such as helium. Several discrete-basis-set methods for the calculation of such processes have recently been developed including the Coulomb-Sturmian separable expansion method [1,2], the convergent close coupling (CCC) [3,4], the J-matrix method combined to Faddeev-Merkuriev equations [5–7]. In all these approaches the continuous Hamiltonian spectrum is represented in the context of complete square integrable bases. Despite the enormous progress made so far in discretization and subsequent numerical solutions of three-body differential and integral equations of the Coulomb scattering theory, a number of related mathematical problems remain open. Actually, the use of a product of two fixed charge Coulomb waves for the two outgoing electrons as an approximation to the three-body-continuum state is typical of these approaches. As a consequence, a long-range potential appears in the kernel of the corresponding Lippmann-Schwinger (LS) equation. Long-range potentials have been suspected to give rise to such severe singularities in the kernels, that their compactness properties are lost. The corresponding solutions therefore are divergent as the size of the basis used is increased.

To try to solve such a problem, many approaches have been developed. One can underline here the work of Mukhamedzhanov *et al.* [8,9] who within an effective two-body formulation of the three-particle theory, have proved that, for all energies, the nondiagonal kernels occurring in the integral equations which determine the transition amplitudes for all binary collision processes, possess on and off the energy shell only integrable singularities. They also proved that diagonal kernels possess only one nonintegrable singularity and then the latter can, however, be isolated explicitly and dealt with in a well-defined manner. Hence, after a few iterations these kernels become compact. But it is very important to stress that this is true provided all three particles have charges of the same sign, i.e., all Coulomb interactions are purely repulsive. Therefore the applicability of this technic to atomic target will not work since there, the nucleus and the electron have charges of the opposite sign. Another approach based on the modified Faddeev-Merkuriev integral equations has been proposed by Yakolev *et al.* [10]. Recently, Zaytsev *et al.* have proposed an approach where the generalized parabolic coordinates are used to treat the three-body-continuum Coulomb problem. The development of the method is chiefly based upon the fact that the asymptotic wave operator is separable in terms of generalized parabolic coordinates [11]. A resulting compact integral equation for the expansion coefficients as the solution for a back-to-back electron emission from helium atom has been obtained. With the use of the Lanczos smoothing factor defined in [12], they showed the convergence behavior of these coefficients as the number N of the basis used is increased. But they were not able to go further than $N = 15$ basis functions.

In this paper, we calculate a three-body wave function that describes the double continuum of an atomic two-electron system. An approximate solution is expressed in the form of a Lippmann-Schwinger-type equation. Since in this work, we address the question of compactness of the kernel of this integral equation, a symmetrized product of two Coulomb waves is used to describe the asymptotic part of the wave function, while a smooth cutoff function is introduced to the dielectronic potential that enters the integral part in order to have a compact kernel. The integral equation for the (e^-, e^-, H_e^{++}) system is then solved numerically. We apply our method to the calculation within first Born approximation, of the FDCS for (e,3e) processes in helium in the small momentum transfer regime. The calculation is performed for a coplanar geometry in which the incident electron is fast (∼6 keV) and for a symmetric energy sharing between both slow ejected electrons at excess energy of 20 eV. As our aim is to study the rate of convergence as the basis used is enlarged, we arbitrary choose and present FDCS for four or five different fixed values of one of the ejected electron θ_1(while the other one θ_2 varies) and show the convergence of FDCS when the size of the basis is increased.

*smengoue@yahoo.fr

The paper is organized as follows. After this introduction, in Sec. II, we briefly present the theoretical approach used to generate the double continuum wave function of an atomic two-electron system. Section III is devoted to the results and discussion. We first give some small details about how we calculate the FDCS for the $(e,3e)$ process we study in helium, then the experimental and theoretical FDCSs are compared. Finally, we study, the convergence of our results as a function of the basis parameters. The paper ends in Sec. IV with a brief summary. Atomic units are used throughout.

II. THEORY

The two-electron continuum wave function with an asymptotic ingoing wave behavior is a solution of the following Schrödinger equation:

$$\left[E+\frac{1}{2}\triangle_1+\frac{1}{2}\triangle_2+\frac{Z}{r_1}+\frac{Z}{r_2}-\frac{1}{r_{12}}\right]\Psi^{(-)}(\mathbf{k}_1,\mathbf{k}_2;\mathbf{r}_1,\mathbf{r}_2)=0, \tag{1}$$

where $\mathbf{r}_1$ and $\mathbf{r}_2$ are the position vectors of electron 1 and 2 and $\mathbf{k}_1$ and $\mathbf{k}_2$ their corresponding momentum. $r_{12}=|\mathbf{r}_2-\mathbf{r}_1|$ is the interelectronic distance. $Z=2$ denotes the charge of the infinitely massive nucleus the position of which coincides with the origin of the laboratory system. E is the total energy of the two electrons.

Both electrons are identical particles, so we can introduce the new functions $\Psi_i^{(-)}(\mathbf{k}_1,\mathbf{k}_2;\,\mathbf{r}_1,\mathbf{r}_2)$ $(i=1,2)$, such that $\Psi^{(-)}=(1/\sqrt{2})[\Psi_1^{(-)}+\Psi_2^{(-)}]$. Taking into account the exchange symmetry of the solution of Eq. (1), $\Psi^{(-)}(\mathbf{k}_1,\mathbf{k}_2;\,\mathbf{r}_1,\mathbf{r}_2)=g\Psi^{(-)}(\mathbf{k}_1,\mathbf{k}_2;\,\mathbf{r}_2,\mathbf{r}_1)$, where $g=+1$ (-1) for a singlet (triplet) state, we have

$$\Psi_2^{(-)}(\mathbf{k}_1,\mathbf{k}_2;\,\mathbf{r}_1,\mathbf{r}_2)=g\,\widehat{P}_{12}\Psi_1^{(-)}(\mathbf{k}_1,\mathbf{k}_2;\,\mathbf{r}_1,\mathbf{r}_2). \tag{2}$$

Let us now rewrite Eq. (1) in the following way:

$$\left[E+\frac{1}{2}\triangle_1+\frac{1}{2}\triangle_2+\frac{Z}{r_1}+\frac{Z}{r_2}\right]\Psi_1^{(-)}=V(\mathbf{r}_1,\mathbf{r}_2)\Psi_1^{(-)}, \tag{3}$$

where

$$V(\mathbf{r}_1,\mathbf{r}_2)=\frac{1}{r_{12}}. \tag{4}$$

Equation (3) is the basic equation for the numerical calculation of the double continuum wave function. The operator in the left-hand side of Eq. (3) act in the two independent subspaces $\mathbf{r}_1$ and $\mathbf{r}_2$. Its free solution is a symmetrized product of two Coulomb wave functions $\varphi^{(-)}(\mathbf{k}_i,\mathbf{r}_2;\,Z)\,\varphi^{(-)}(\mathbf{k}_j,\mathbf{r}_1;\,Z)$. Instead of solving this equation directly, however, it is more convenient to write it in the integral form [7],

$$\begin{aligned}\Psi_1^{(-)}&(\mathbf{k}_1,\mathbf{k}_2;\mathbf{r}_1,\mathbf{r}_2)\\ &=[\varphi^{(-)}(\mathbf{k}_2,\mathbf{r}_2;\,Z)\,\varphi^{(-)}(\mathbf{k}_1,\mathbf{r}_1;\,Z)\theta(k_1-k_2)\\ &\quad+g\varphi^{(-)}(\mathbf{k}_1,\mathbf{r}_2;\,Z)\,\varphi^{(-)}(\mathbf{k}_2,\mathbf{r}_1;\,Z)\theta(k_2-k_1)]\\ &\quad+\iint d\mathbf{r}_1'\,d\mathbf{r}_2'G^{(-)}(\mathbf{r}_1,\mathbf{r}_2;\,\mathbf{r}_1',\mathbf{r}_2';\,E)\\ &\quad\times V(\mathbf{r}_1',\mathbf{r}_2')\,\Psi_1^{(-)}(\mathbf{k}_1,\mathbf{k}_2;\mathbf{r}_1',\mathbf{r}_2').\end{aligned} \tag{5}$$

This new equation incorporates the boundary conditions through the Green's function $G^{(-)}$ associated with the operator of the left-hand size of Eq. (3). θ is the modified step function with $\theta(0)=1/2$.

The Green's function $G^{(-)}$ can be evaluated as a convolution integral along a contour $\mathcal{C}$ in the complex energy $\mathcal{E}$ plane [5]:

$$\begin{aligned}G^{(-)}&(\mathbf{r}_1,\mathbf{r}_2;\,\mathbf{r}_1',\mathbf{r}_2';\,E)\\ &=\frac{1}{2\pi i}\int_{\mathcal{C}}d\mathcal{E}\,g^{(-)}(\mathbf{r}_1,\mathbf{r}_1';\,\mathcal{E}-\mathrm{i}0;\,Z)\\ &\quad\times g^{(-)}(\mathbf{r}_2,\mathbf{r}_2';E-\mathcal{E}-\mathrm{i}0;\,Z).\end{aligned} \tag{6}$$

The contour $\mathcal{C}$ runs from $-\infty$ to $+\infty$ along the real axis of the complex $\mathcal{E}$ plane. We now perform a partial wave decomposition of the wave function $\Psi_1^{(-)}$ and write

$$\begin{aligned}\Psi_1^{(-)}(\mathbf{k}_1,\mathbf{k}_2;\,\mathbf{r}_1,\mathbf{r}_2)=\frac{2}{\pi}\frac{1}{k_1\,k_2}\sum_{L,M,\lambda_0,l_0}&\left\{\psi_{l_0\lambda_0}^{LM}(\mathbf{r}_1,\mathbf{r}_2;k_1,k_2)\right.\\ &\times\mathcal{Y}_{l_0\lambda_0}^{LM^*}(\widehat{\mathbf{k}}_1,\widehat{\mathbf{k}}_2)\theta(k_1-k_2)\\ &+g\;\psi_{l_0\lambda_0}^{LM}(\mathbf{r}_1,\mathbf{r}_2;k_2,k_1)\\ &\left.\times\;\mathcal{Y}_{l_0\lambda_0}^{LM^*}(\widehat{\mathbf{k}}_2,\widehat{\mathbf{k}}_1)\;\theta(k_2-k_1)\right\}.\end{aligned} \tag{7}$$

L is the total angular momentum and M its projection on the quantization axis. l_0 and λ_0 are the individual angular momenta of the two electrons. $\mathcal{Y}_{l_0\lambda_0}^{LM}(\widehat{\mathbf{p}},\widehat{\mathbf{q}})$ is the bipolar harmonics. The partial wave function $\psi_{l_0\lambda_0}^{LM}$ in Eq. (7) can be further expanded in a basis of Coulomb Sturmian functions [13] and bipolar harmonics:

$$\psi_{l_0\lambda_0}^{LM}(\mathbf{r}_1,\mathbf{r}_2)=\sum_{l,\,\lambda,\,n,\,\nu}C_{n\nu}^{L(l\lambda)}(E)\;\langle\mathbf{r}_1,\mathbf{r}_2|n\,l\,\nu\,\lambda;\;LM\rangle\,, \tag{8}$$

with

$$\langle\mathbf{r}_1,\mathbf{r}_2|n\,l\,\nu\,\lambda;\;LM\rangle=\frac{\phi_{nl}^{\kappa}(r_1)}{r_1}\,\frac{\phi_{\nu\lambda}^{\kappa}(r_2)}{r_2}\,\mathcal{Y}_{l\,\lambda}^{LM}(\widehat{\mathbf{r}}_1,\widehat{\mathbf{r}}_2). \tag{9}$$

The Coulomb Sturmian functions $\phi_{\nu\lambda}^{\kappa}(r)$ form a complete and discrete set of $\mathcal{L}^2$-integrable functions defined as follows:

$$\begin{aligned}\phi_{\nu\lambda}^{\kappa}(r)&=\left[\frac{\kappa(\nu-\lambda-1)!}{\nu(\nu+\lambda)!}\right]^{1/2}(2\kappa r)^{\lambda+1}e^{-\kappa r}L_{\nu-\lambda-1}^{2\lambda+1}(2\kappa r),\\ &\nu\geqslant 1+\lambda,\end{aligned} \tag{10}$$

where κ is a nonlinear basis parameter. $L_n^{\alpha}(x)$ is a Laguerre polynomial. These functions are known to be orthogonal with the weight $1/r$,

$$\int_0^{\infty}\frac{dr}{r}\phi_{\nu\lambda}^{\kappa}(r)\phi_{\nu'\lambda}^{\kappa}(r)=\frac{\kappa}{\nu}\delta_{\nu\nu'},$$

and lead to a representation of the Coulomb potential in the form of an infinite tridiagonal (Jacobi) matrix [14–16]. Note that any radial Coulomb eigenstate $\varphi_{\alpha l}(r;Z)$ can be expanded into a series of Sturmian functions:

$$\varphi_{\alpha l}(r;Z)=\sum_{\nu}\mathcal{S}_{\nu l}(\alpha,Z)\phi_{\nu l}^{\kappa}(r). \tag{11}$$

For the continuum states with which we are concerned, the expansion coefficient takes the form,

$$\mathcal{S}_{\nu l}(k;Z) = \left[\frac{\nu(\nu+l)!}{\kappa(\nu-l-1)!}\right]^{1/2} 2^l (\sin\zeta)^{l+1}\, e^{-\pi t/2}\, \xi^{-it} \times \frac{|\Gamma(l+1-\mathrm{i}t)|}{(2l+1)!}(\xi)^{-(\nu-l-1)} \times {}_2F_1(-\nu+l+1, l+1-it;\ 2l+2;\ 1-\xi^2), \tag{12}$$

where $t = -Z/k$ and $\xi = \exp(\mathrm{i}\zeta) = (ik-\kappa)/(ik+\kappa)$.

Collecting all above expansions together, we finally obtain from Eq. (8) the following system of equations for the coefficients $C_{n\nu}^{L(l\lambda)}(k_1,k_2)$:

$$C_{n\nu}^{L(l\lambda)}(k_1,k_2) = i^{l_0+\lambda_0}\delta_{(l\lambda)(l_0\lambda_0)} e^{-i(\sigma_{l_0}(k_1,Z)+\sigma_{\lambda_0}(k_2,Z))}\, \mathcal{S}_{nl_0}(k_1,Z)\mathcal{S}_{\nu\lambda_0}(k_2,Z) + \sum_{n'\nu',\, n''\nu''=0}^{N-1}\left[\frac{1}{2\pi\mathrm{i}}\int_{\mathcal{C}} d\mathcal{E}\; g_{nn'}^{(-)l}(\mathcal{E},Z)\; g_{\nu\nu'}^{(-)\lambda}(E-\mathcal{E},Z)\right] \times \sum_{l''\lambda''} V_{n'\nu',n''\nu''}^{L(l\lambda)(l''\lambda'')}\, C_{n''\nu''}^{L(l''\lambda'')}(E), \tag{13}$$

where

$$V_{n\nu,n'\nu'}^{L(l\lambda)(l'\lambda')} = \langle n\, l\, \nu\, \lambda;\ LM|\frac{1}{r_{12}}\eta(r_1,r_2)|n'\, l'\, \nu'\, \lambda';\ LM\rangle \tag{14}$$

denotes the modified matrix element of the potential defined by Eq. (4) in the basis (9). The upper limit in the sum in Eq. (13) means that the matrix elements of the mutual potential are assumed to be zero for any value of the index n exceeding $(N-1)$. It is known that the potential in $1/r_{12}$ contains long-range terms. And therefore the kernel of the corresponding LS equation is no more compact. In order to solve this problem and to have a compact kernel in the Lippmann-Schwinger Eq. (13), we introduced (14) in the matrix element of the potential defined by Eq. (4), the cutoff function $\eta(r_1,r_2)$ defined as

$$\eta(r_1,r_2) = e^{-\alpha r_1}e^{-\alpha r_2}\sum_{m_1=0}^{M}\frac{(\alpha r_1)^{m_1}}{m_1!}\sum_{m_2=0}^{M}\frac{(\alpha r_2)^{m_2}}{m_2!}, \tag{15}$$

where m_1, m_2, and M are constant, and $M = 10$ is sufficient to achieve convergence. The optimal value for the parameter $\alpha \approx 5$ has proved to be appropriate in practical calculations (as it is shown in Fig. 2, its variation does not lead to a significant change on the cross sections). The convergence behavior of the cross sections as the number N of the basis function (10) is increased is presented in Fig. 3.

Taking into account that partial Coulomb Green's function $g^{(\pm)l}(r,r';E;Z)$ can be standardly represented by a sum over the Coulomb eigenstates $\varphi_{\alpha l}(r;Z)$,

$$g^{(\pm)l}(r,r';E;Z) = \sum_{\alpha}\frac{\varphi_{\alpha l}^*(r;Z)\varphi_{\alpha l}(r';Z)}{E-\varepsilon_\alpha \pm \mathrm{i}0}, \tag{16}$$

and keeping in mind the decomposition (11) of the Coulomb eigenfunctions, the contour integral in Eq. (13) becomes

$$\frac{1}{2\pi\mathrm{i}}\int_{\mathcal{C}} d\mathcal{E}\; g_{nn'}^{(-)l}(\mathcal{E},Z)\; g_{\nu\nu'}^{(-)\lambda}(E-\mathcal{E},Z) = \sum_{\alpha}\mathcal{S}_{nl}^*(\alpha,Z)\,\mathcal{S}_{n'l}(\alpha,Z)\; g_{\nu\nu'}^{(-)\lambda}(E-\varepsilon_\alpha,Z). \tag{17}$$

At this step we could apply Eq. (16) again and obtain a double summation integration in (17), but it is not convenient for the numerical calculations. It is useful now to remember the following representation for the matrix element $g_{\nu\nu'}^{(\pm)\lambda}(E)$ [17]:

$$g_{\nu\nu'}^{(\pm)\lambda}(E;Z) = -\frac{2}{p}\,\mathcal{S}_{\nu_<\lambda}(p,Z)\,\mathcal{C}_{\nu_>\lambda}^{(\pm)}(p,Z), \qquad \nu_< = \min\{\nu,\nu'\},\ \nu_> = \max\{\nu,\nu'\}, \tag{18}$$

with $p = \sqrt{2E}$. $\mathcal{C}_{nl}^{(\pm)}(p,Z)$ is a Pollaczek function that can be written as follows [14,18]:

$$\mathcal{C}_{nl}^{(\pm)}(p,Z) = \frac{1}{2}\left[\frac{n(n-l-1)!}{\kappa(n+l)!}\right]^{1/2} \times \frac{e^{\pi t/2}\xi^{\mathrm{i}t}}{(2\sin\zeta)^{l+1}|\Gamma(l+1\mp\mathrm{i}t)|}q_n^{\pm l}, \tag{19}$$

where

$$q_n^{\pm l} = -2\frac{(n+l)!\Gamma(l+1\mp\mathrm{i}t)}{\Gamma(n+1\mp\mathrm{i}t)}(\xi)^{\mp(n-l)} \times {}_2F_1(-l\mp\mathrm{i}t, n-l;\ n+1\mp\mathrm{i}t;\ \xi^{\mp 2}).$$

The function $\mathcal{C}_{nl}^{(+)}(p,Z)$ $[\mathcal{C}_{nl}^{(-)}(p,Z)]$ is determined for $\mathrm{Im}(p) > 0$ $[\mathrm{Im}(p) < 0$] in the complex p plane and the analytical continuation writes [18]

$$\mathcal{C}_{nl}^{(+)}(p,Z) = \mathcal{C}_{nl}^{(-)}(p,Z) + 2\mathrm{i}\mathcal{S}_{nl}(p,Z). \tag{20}$$

Equation (17) can be effectively used if $E < 0$, i.e., for low energy $(e,2e)$ reactions. Details are presented in [5]. For $E > 0$, the direct evaluation of the contour integral in Eq. (13) can be performed rotating the contour of integration. This method was proposed by Shakeshaft [19]. We only give the final result here. For this purpose, we first move from the energy to the momentum space. For the sake of clarity, we change the notations; we replace $g_{\nu\nu'}^{(\pm)\lambda}(E;Z)$ by $\mathcal{G}_{\nu\nu'}^{\lambda(-)}(p;Z)$ and rewrite the matrix element of the three-body Green's function (6) in the basis (10) as follows:

$$G_{nn',\nu\nu'}^{l\lambda(-)}(E) = \frac{1}{4\pi\mathrm{i}}\int_{\mathcal{C}} d\mathcal{E}\;\mathcal{G}_{nn'}^{l(-)}(\sqrt{\mathcal{E}_0+\mathcal{E}};Z-1) \times \mathcal{G}_{\nu\nu'}^{\lambda(-)}(\sqrt{\mathcal{E}_0-\mathcal{E}};Z), \tag{21}$$

where $\mathcal{E}_0 = E$. Now we rotate the contour $\mathcal{C}$ by a positive angle φ. This may be done by the following change of variable $\mathcal{E} \to \mathcal{E}_0 e^{\mathrm{i}\varphi}t$ with t real and varying from $-\infty$ to $+\infty$. This contour crosses cuts of both Green's functions in the complex $\mathcal{E}$ plane. By using the analytical continuation (20) while integrating along unphysical sheets, we arrive at the following

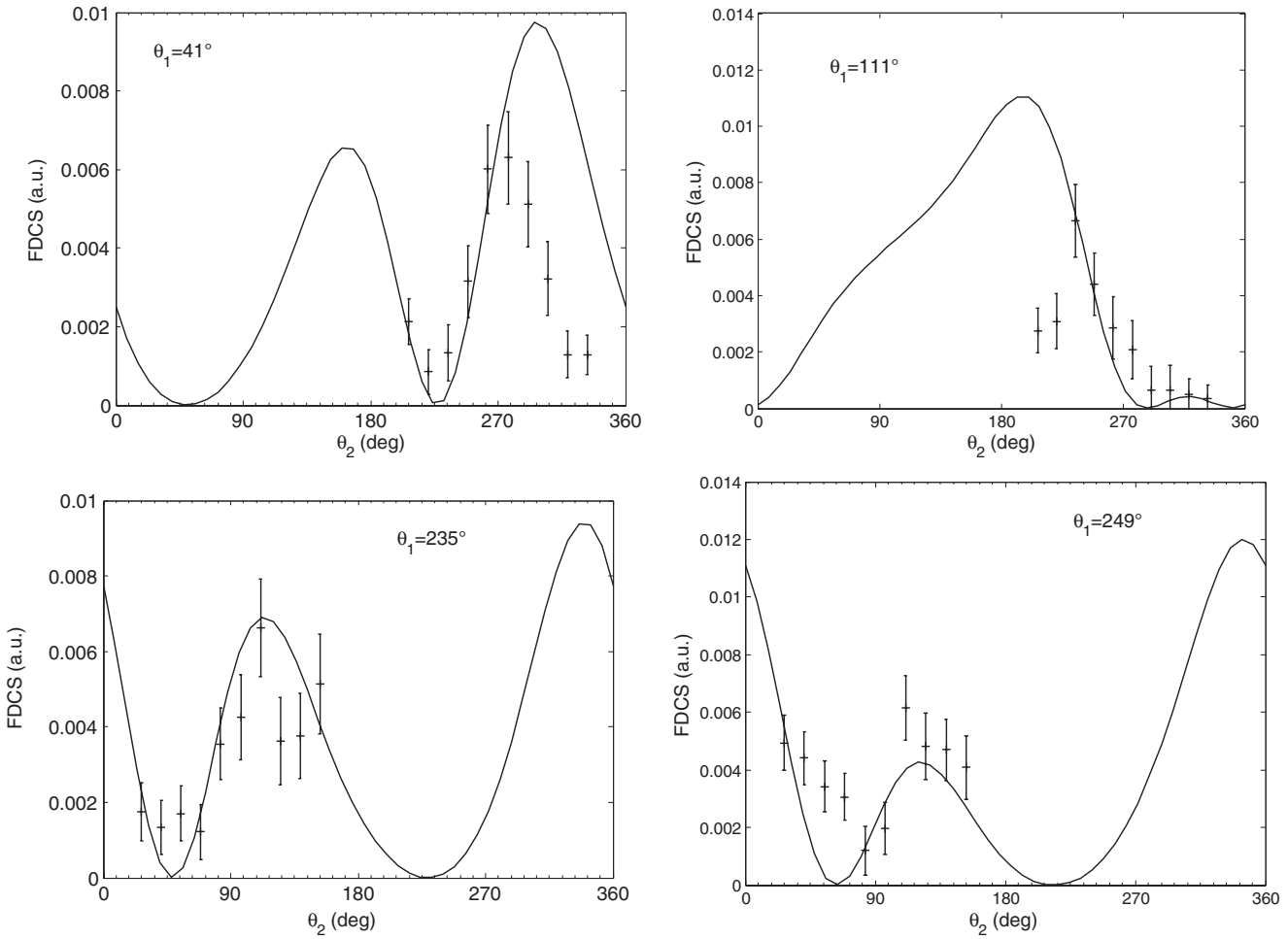

FIG. 1. Fully fivefold differential cross section (FDCS) for electron impact double ionization reaction of helium. The incident energy is $E_0 = 5599$ eV and the energies of the slow ejected electrons are $E_1 = E_2 = 10$ eV. The scattering angle θ_s of the fast incident electron is fixed and equal to 0.45° while the angles of the ejected electrons are θ_1 and θ_2. One of these angles, θ_1, is fixed and the other varies. The solid dots with error bars are the absolute experimental data of Lahmam-Bennani [3].

expression:

$$G^{\lambda l(-)}_{\nu\nu',nn'}(E) = \frac{\mathcal{E}_0 e^{i\varphi}}{4\pi i}\Bigg\{\int_0^\infty dt\Bigg[\Bigg(\mathcal{G}^{\lambda(+)}_{\nu\nu'}(k;Z) + \frac{4i}{k}\mathcal{S}_{\nu\lambda}(k;Z)\mathcal{S}_{\nu'\lambda}(k;Z)\Bigg)\mathcal{G}^{l(-)}_{nn'}(p;Z) + \Bigg(\mathcal{G}^{l(+)}_{nn'}(k;Z) + \frac{4i}{k}\mathcal{S}_{nl}(k;Z)\mathcal{S}_{n'l}(k;Z)\Bigg) \times \mathcal{G}^{\lambda(-)}_{\nu\nu'}(p;Z)\Bigg]\Bigg\}, \tag{22}$$

where $k = \sqrt{\mathcal{E}_0(1+te^{i\varphi})}$, and $p = \sqrt{\mathcal{E}_0(1-te^{i\varphi})}$. The integration (22) is reduced from 0 to ∞ since $k(-t) = p(t)$. This last integral is calculated fully numerically and we checked that the results do not depend on the angle φ.

III. RESULTS AND DISCUSSION

To illustrate the efficiency of the numerical scheme described above, calculations of the fully fivefold differential cross section FDCS for the He$(e,3e)$He^{2+} reaction on the helium atom were performed. Here, we consider the case of very high incident energies and small momentum transfer. In this dipole limit, it is expected that a first Born treatment is sufficient. The FDCS is given by

$$\sigma^{(5)} \equiv \frac{d^5\sigma}{d\Omega_s dE_1 d\Omega_1 dE_2 d\Omega_2} = \frac{4p_s p_1 p_2}{p_i}\frac{1}{Q^4} \mid \langle \Psi^{(-)}(\mathbf{p}_1,\mathbf{p}_2)| \exp(i\mathbf{Q}\cdot\mathbf{r}_1) + \exp(i\mathbf{Q}\cdot\mathbf{r}_2) - 2|\Psi_0\rangle \mid^2, \tag{23}$$

where $(E_i,\mathbf{p_i})$, $(E_s,\mathbf{p_s})$, $(E_1,\mathbf{p_1})$, and $(E_2,\mathbf{p_2})$ are the energy and momentum of the incident, scattered, and the two ejected electrons, respectively; $\mathbf{Q} = \mathbf{p_i} - \mathbf{p_s}$ is the momentum transfer. Ψ_0 and $\Psi^{(-)}$ are the initial and the final double continuum wave function of helium. The helium ground-state wave function Ψ_0 is obtained as a result of diagonalization of the matrix of the Hamiltonian of the three-body system. This ground-state wave function can be expanded in a basis of the Coulomb Sturmian functions (10) for the radial coordinates and bipolar harmonics for the angular coordinates [13]. In the present calculation, we

put $n_{\max} = \nu_{\max} = 15$ and $l_{\max} = 3$. By choosing the nonlinear parameter $\kappa_0 = 2$, we obtain $E_0 = -2.90327$ a.u. for the ground-state energy [20].

The wave function $\Psi^{(-)}$ for the final state of the (e^-, e^-, H_e^{++}) system is obtained by the method outlined above. In these calculations, it is sufficient to take into account three values (0, 1, and 2) of the total angular momentum L and a maximum value $l_{\max}$ of 3 for the individual angular momenta. The number N of Coulomb Sturmian functions is 50 with the dilation parameter $\kappa = 0.4$. The α parameter of the splitting function (15) is equal to 5.

In Fig. 1, we present the results of the FDCS (23). We consider the same kinematic as in the experiments of Lahmam-Bennani *et al.* [3,21] where the geometry of the $(e,3e)$ process is coplanar asymmetric and both ejected electrons share the excess energy of 20 eV, with a momentum transfer of 0.24 a.u.. The FDCS is measured as a function of one of the ejection angles, say θ_2 for fixed values of θ_1, the other angle.

In Fig. 1, the results of the FDCS are presented for four values of θ_1, the two first are for an ejection in the half front plane ($\theta_1 = 41^\circ, 111^\circ$) and the two last for an ejection in the half rear plane ($\theta_1 = 235^\circ, 249^\circ$). The presented results are just to demonstrate that the shape and the magnitude of cross sections agree satisfactorily with the experiment of Lahmam-Bennani *et al.* [3,21] and do not necessitate any renormalization of the data as it is usually needed with other approaches. This constitutes an evident proof that the cutoff function (15) introduced in (14), in order to have a compact kernel, does not lead to a considerable loss of information. We keep in mind that our aim is to study the rate of convergence of our results with the increases of the basis size "N". It can also be easily seen from the pictures in Fig. 1, that in the optical limit [21,22], the positions of the minima at $\hat{p}_1 = \pm\hat{p}_2(\theta_1 = \pm\theta_2)$ are well reproduced.

In the following, we study the convergence of our results as a function of the Coulomb Sturmian basis parameters. Before starting our discussion, it is worth mentioning that we have tested the behavior of the cross sections by changing the smoothing parameter α of (15). As we can see in Fig. 2, no significant change has been observed on the FDCS, by changing this parameter. We have also tested the calculations of the matrix elements in (14) by using different techniques of quadrature (that are known to be very fast and stable) and checked that the results are stable even for very large values of the Sturmian function indices. The same conclusions apply to the calculation of the Green function (22). The matrix elements associated with the dielectronic interaction potential have been evaluated by means of the technic outlined in [13].

The convergence of our results has been studied as a function of the number of pairs (l,λ) of electron angular momenta, as a function of the number of pairs (n,ν) of Sturmian indices for a fixed value of N (the maximum value of n or ν) and as a function of N. Choosing $l_{\max} \leqslant 5$, we checked that the results for the FDCS are stable with respect to the number of pairs (l,λ) of electron angular momenta. For a fixed value of N, we also checked that the results converge with respect to the number of pairs (ν,n). The partial sums of each pair contribution converge to five-digit accuracy. We also used the ϵ algorithm [23] based on Padé approximants to accelerate the convergence of the partial sums. In that case, we reach at least eight-digit accuracy.

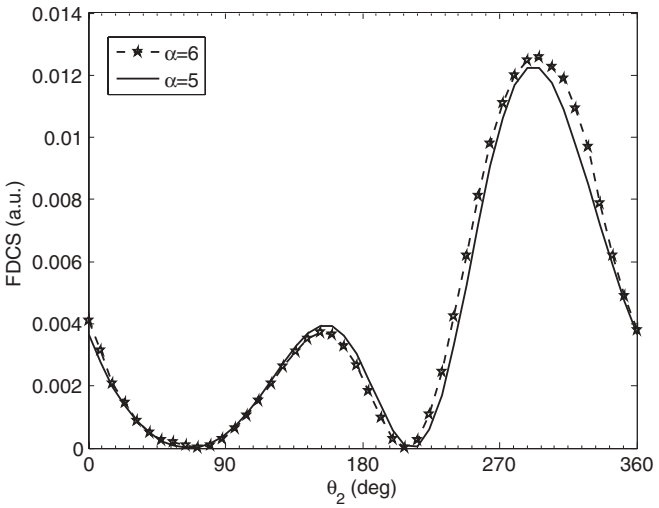

FIG. 2. Dependance of the fully fivefold differential cross section (FDCS) for electron impact double ionization reaction He$(e,3e)$He^{2+} on the α parameter of the cutoff function (15). The incident energy is $E_0 = 5599$ eV and the energies of the slow ejected electrons are $E_1 = E_2 = 10$ eV. The scattering angle θ_s of the fast incident electron is fixed and equal to 0.45° while the angles of the ejected electrons are θ_1 and θ_2. $\theta_1 = 27^\circ$ and θ_2 varies. The calculations are performed for two different values of α.

In Fig. 3 we show the evolution of FDCS for $l_{\max} = 3$ and three different values of N. It is clearly seen that convergence is reached.

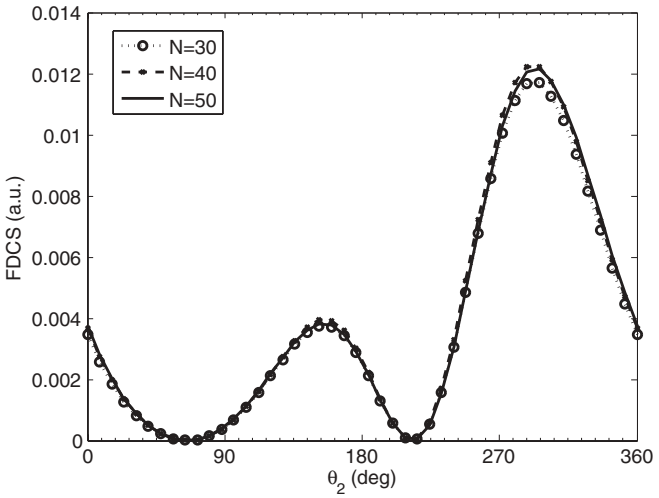

FIG. 3. Convergence of the fully fivefold differential cross section (FDCS) for electron impact double ionization reaction He$(e,3e)$He^{2+} on the number N of the radial basis functions. The incident energy is $E_0 = 5599$ eV and the energies of the slow ejected electrons are $E_1 = E_2 = 10$ eV. The scattering angle θ_s of the fast incident electron is fixed and equal to 0.45° while the angles of the ejected electrons are θ_1 and θ_2. $\theta_1 = 27^\circ$ and θ_2 varies. The calculations are performed for $l_{\max} = 3$ and three different values of N.

IV. CONCLUSIONS

In this paper, we have presented an approach to calculate a three-body wave function that describes the double continuum of an atomic two-electron system. The wave function is calculated in such a way as the corresponding Lippmann-Schwinger-type equation for the (e^-, e^-, H_e^{++}) system possess a compact kernel. In order to achieve our aim that was to study the rate of convergence as the basis used is enlarged, we performed a first Born calculation of the fully differential cross section for electron impact double ionization of helium. In particular, we considered the most studied case of a coplanar kinematic that has been treated experimentally by the Lahmam-Bennani group. This kinematic involves a very high incident energy ($\sim$6 keV), a very small momentum transfer ($Q = 0.24$ a.u.) and slow ejected electrons sharing the excess energy of 20 eV.

The results of the theoretical FDCSs obtained agree satisfactorily with the experimental data both in shape and in magnitude. These results need no scaled parameter to be compared to experimental data. This is an evident proof that the cutoff function introduced inside the dielectronic potential, in order to have a compact kernel of the corresponding Lippmann-Schwinger-type equation, does not lead to a considerable loss of information compared to the absolute data. We have examined the convergence of our results with respect to the basis parameters. The convergence is reached in terms of the number of electron angular momenta, in terms of the partial sums of each pair (ν,n) for a fixed N and in terms of the total number of Sturmian basis functions used. We think that the proposed scheme can also be effective for various application in atomic physics. Its application for the study of double ionization of helium by photon impact will be presented.

ACKNOWLEDGMENTS

I thank Professor Yuri V. Popov for helpful suggestions and comments on the manuscript. I would also like to thank the Centre de Physique Atomique Moléculaire et Optique Quantique (CEPAMOQ) and the Université Catholique de Louvain for providing me with access to the supercomputer of the Calcul Intensif et de Stockage de Masse (CISM) which is supported by the Fonds National de la Recherche Scientifique (FNRS).

[1] Z. Papp and W. Plessas, Phys. Rev. C **54**, 50 (1996).
[2] Z. Papp, J. Darai, C.-Y. Hu, Z. T. Hlousek, B. Kónya, and S. L. Yakovlev, Phys. Rev. A **65**, 032725 (2002).
[3] A. Kheifets, I. Bray, A. Lahmam-Bennani, A. Duguet, and I. Taouil, J. Phys. B **32**, 5047 (1999).
[4] A. S. Kheifets and I. Bray, Phys. Rev. A **69**, 050701(R) (2004).
[5] S. A. Zaytsev, V. A. Knyr, Yu. V. Popov, and A. Lahmam-Bennani, Phys. Rev. A **75**, 022718 (2007).
[6] V. A. Knyr, S. A. Zaytsev, Yu. V. Popov, and A. Lahmam-Bennani, in *The J-matrix Method: Recent Developments and Selected Applications*, edited by A. Alhaidari, E. J. Heller, H. A. Yamani, and M. S. Abdelmonem (Springer, Dordrecht, 2008).
[7] M. S. Mengoue, M. G. Kwato Njock, B. Piraux, Yu. V. Popov, and S. A. Zaytsev, Phys. Rev. A **83**, 052708 (2011).
[8] A. M. Mukhamedzhanov, E. O. Alt, and G. V. Avakov, Phys. Rev. C **61**, 064006 (2000).
[9] A. M. Mukhamedzhanov, E. O. Alt, and G. V. Avakov, Phys. Rev. C **63**, 044005 (2001).
[10] S. L. Yakovlev and Z. Papp, Theor. Math. Phys. **163**, 666 (2010).
[11] S. A. Zaytsev, J. Phys. A: Math. Theor. **41**, 265204 (2008); **42**, 015202 (2009).
[12] Z. Papp, Phys. Rev. C **38**, 2457 (1988).
[13] E. Foumouo, G. L. Kamta, G. Edah, and B. Piraux, Phys. Rev. A **74**, 063409 (2006).
[14] E. J. Heller and H. A. Yamani, Phys. Rev. A **9**, 1201 (1974).
[15] H. A. Yamani and L. Fishman, J. Math. Phys. **16**, 410 (1975).
[16] J. T. Broad and W. P. Reinhardt, Phys. Rev. A **14**, 2159 (1976).
[17] E. J. Heller, Phys. Rev. A **12**, 1222 (1975).
[18] J. T. Broad, Phys. Rev. A **31**, 1494 (1985).
[19] R. Shakeshaft, Phys. Rev. A **70**, 042704 (2004).
[20] G. W. F. Drake, *Handbook of Atomic, Molecular and Optical Physics* (Springer, New York, 2006).
[21] A. Lahman-Bennani, I. Taouil, A. Duguet, M. Lecas, L. Avaldi, and J. Berakdar, Phys. Rev. A **59**, 3548 (1999).
[22] J. Berakdar and H. Klar, J. Phys. B **26**, 4219 (1993).
[23] E. J. Weiniger, Comput. Phys. Rep. **10**, 191 (1989).