Semirelativistic model for ionization of atomic hydrogen by electron impact

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We present a semirelativistic model for the description of the ionization process of atomic hydrogen by electron impact in the first Born approximation by using the Darwin wave function to describe the bound state of atomic hydrogen and the Sommerfeld-Maue wave function to describe the ejected electron. This model, accurate to first order in Z/c in the relativistic correction, shows that, even at low kinetic energies of the incident electron, spin effects are small but not negligible. These effects become noticeable with increasing incident electron energies. All analytical calculations are exact and our semirelativistic results are compared with the results obtained in the nonrelativistic Coulomb Born approximation both for the coplanar asymmetric and the binary coplanar geometries.

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I. INTRODUCTION

Relativistic $(e,2e)$ processes have been reviewed both from the experimental and theoretical points of view [1]. As one deals with atomic hydrogen, the value of the parameter $Z\alpha$ is much lower than 1, where Z is the atomic charge number and α is the fine-structure constant. Therefore, it is convenient and sufficient to use approximate wave functions of a mathematically simpler structure than the exact analytical wave functions needed to describe relativistic $(e,2e)$ processes. A numerical approach to an exact description of the relativistic ionization of atomic hydrogen by electron impact could be carried out, but we will focus instead on an alternative approach that will give nearly the same results as the exact description if the condition $Z\alpha \ll 1$ is satisfied. In $(e,2e)$ processes, relativistic effects are important and all electrons (the incident, scattered, and ejected) can have very high velocities. One has to consider many interactions (namingly, retardation interaction, magnetic interaction, and spin-dependent interaction). For atomic hydrogen, many experimental and theoretical contributions have been made [2,3]. Some were successful but the theoretical situation for all setups and kinematics is far from resolved, at least analytically. Many calculations have resorted to various approximations. For example, plane-wave models [4–7] are successful in the coplanar binary geometries [4] and for fast scattered and ejected electrons. The first Born approximation (FBA) has been used to describe asymmetric geometries at nonrelativistic energies [8,9]. In this approximation, the incident and scattered electrons are described by plane waves whereas the ejected electron is treated as a Coulomb wave. Many authors extended this approximation to the relativistic domain. Das *et al.* [10,11] employed a semirelativistic Sommerfeld-Maue wave function to describe the ejected electron. Jakubaßa-Amundsen evaluated the first-order transition matrix element S_{fi} using semirelativistic Coulomb wave functions times a free spinor, i.e., neglecting the relativistic contraction of the bound state and approximating the continuum Coulomb state by a relativistic Coulomb wave times a free spinor. This model did well in predicting integrated cross sections [12] but yielded a value for the absolute triple differential cross section (TDCS) too large. For the Coulomb approximation, Jakubaßa-Amundsen [13] argued that one could not neglect the Coulomb potential in the treatment of inner-shell ionization of high-Z atoms. Agreement with experiment was encouraging for intermediate values of Z. The merits and shortcomings of this theory have been analyzed in [14]. Thereafter, a fully relativistic version was produced [15], which showed that the original physical insight was essentially correct.

In this contribution, we present a theoretical semirelativistic model, the semirelativistic Coulomb Born approximation (SRCBA) in a closed and exact form for the description of the ionization of atomic hydrogen by electron impact in the first Born approximation that is valid for all geometries. In the nonrelativistic Coulomb Born approximation (NRCBA), a well-known integral occurs [16] and is usually denoted by $I(\lambda)$. In this article, we show that the main contribution to the spin-unpolarized triple differential cross section in the SRCBA corresponding to the ionization of atomic hydrogen in its ground state by electron impact comes from this term added to relativistic corrections valid to first order in Z/c. These relativistic corrections contain a new integral, which we have denoted $J(\lambda)$ and in the appendix, we give the formal derivation of this integral. All numerical appropriate tests to check the validity of the analytical result we have found have been carried out with a very good degree of accuracy. It turns out that spin effects can be accounted for

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even at low kinetic energies of the incident electron in the case of the Ehrhardt coplanar asymmetric geometry [17] where, for a given kinetic energy T_i of the fast incident electron, a fast ("scattered") electron of kinetic energy T_f is detected in coincidence with a slow ("ejected") electron of kinetic energy T_B. These spin effects, as well as the relativistic effects, become noticeable with increasing incident electron kinetic energy.

The organization of this paper is as follows: in Sec. II, we present the semirelativistic formalism of $(e,2e)$ reaction and give a detailed account of the various terms that contribute to the spin-unpolarized TDCS. In Sec. III, we discuss the results we have obtained and end by a brief conclusion in Sec. IV. The formal derivation of the integral $J(\lambda)$ is given in the appendix. Throughout this work, atomic units (a.u.) are used ($\hbar=m_e=e=1$), where m_e is the electron rest mass.

II. THE SPIN-UNPOLARIZED TRIPLE DIFFERENTIAL CROSS SECTION

In this section, we calculate the exact analytical expression of the semirelativistic spin-unpolarized TDCS in the SRCBA corresponding to the ionization of atomic hydrogen by electron impact. The spin-unpolarized TDCS is obtained by averaging over the spins of the initial states (projectile electron plus atomic target) and summing over the spins of the final states (scattered electron plus ejected electron). The transition matrix element for the direct channel (exchange effects are not considered) is given by

$$\begin{aligned} S_{fi} &= -i\int dt\langle\psi_{p_f}(x_1)\phi_f(x_2)|V_d|\psi_{p_i}(x_1)\phi_i(x_2)\rangle \\ &= -i\int_{-\infty}^{+\infty} dt\int d\mathbf{r}_1\overline{\psi}_{p_f}(t,\mathbf{r}_1)\gamma^0_{(1)}\psi_{p_i}(t,\mathbf{r}_1) \\ &\quad\times\langle\phi_f(x_2)|V_d|\phi_i(x_2)\rangle. \end{aligned} \tag{1}$$

In Eq. (1), V_d is the direct interaction potential

$$V_d = \frac{1}{r_{12}} - \frac{1}{r_1}, \tag{2}$$

$\mathbf{r}_1$ are the coordinates of the incident and scattered electron, $\mathbf{r}_2$ are the atomic electron coordinates, $r_{12}=|\mathbf{r}_1-\mathbf{r}_2|$ and $r_1=|\mathbf{r}_1|$. The wave function $\psi_{p_i}(x_1)=\psi_p(t,\mathbf{r}_1)=u(p,s)\exp(-ip\cdot x)/\sqrt{2EV}$ is the electron wave function described by a free-Dirac spinor normalized to the volume V and $\phi_{i,f}(x_2)=\phi_{i,f}(t,\mathbf{r}_2)$ are the semirelativistic wave functions of the hydrogen atom where the index i stands for the initial state, namely the ground state, and the index f stands for the final state. The quantity $p\cdot x=p_\mu x^\mu$ is the Lorentz scalar product. The semirelativistic wave function of the hydrogen atom used is the Darwin wave function for bound states [18]

$$\phi_i(t,\mathbf{r}_2) = \exp(-i\varepsilon_b t)\varphi^{(\pm)}(\mathbf{r}_2), \tag{3}$$

where $\varepsilon_b=c^2[\sqrt{1-Z^2\alpha^2}-1]$ is the atomic hydrogen binding energy in the ground state.

$$\varphi^{(\pm)}(\mathbf{r}_2) = \left[1_4 - \frac{i}{2c}\alpha\cdot\nabla_{(2)}\right]u^{(\pm)}\varphi_0(\mathbf{r}_2) \tag{4}$$

is a quasirelativistic bound-state wave function accurate to first order in Z/c in the relativistic corrections (and normalized to the same order) with φ_0 being the nonrelativistic bound-state hydrogenic function. The spinors $u^{(\pm)}$ are such that $u^{(+)}=(1,0,0,0)^T$ and $u^{(-)}=(0,1,0,0)^T$ and represent the basic four-component spinors for a particle at rest with spin up and spin down, respectively. The wave function $\phi_f(t,\mathbf{r}_2)$ in Eq. (1) is the Sommerfeld-Maue wave function for continuum states [18], also accurate to the order Z/c in the relativistic corrections. We have $\phi_f(t,\mathbf{r}_2)=\exp(-iE_Bt)\psi^{(-)}_{p_B}(\mathbf{r}_2)$ and

$$\begin{aligned} \psi^{(-)}_{p_B}(\mathbf{r}_2) &= \exp(\pi\eta_B/2)\Gamma(1+i\eta_B)\exp(i\mathbf{p}_B\cdot\mathbf{r}_2) \\ &\quad\times\left\{1_4 - \frac{ic}{2E_B}\alpha\cdot\nabla_{(2)}\right\} \\ &\quad\times{}_1F_1(-i\eta_B,1,-i(p_Br_2+\mathbf{p}_B\cdot\mathbf{r}_2))\frac{u(p_B,s_B)}{\sqrt{2E_BV}} \end{aligned} \tag{5}$$

normalized to the volume V. The Sommerfeld parameter is given by

$$\eta_B = \frac{E_B}{c^2p_B}, \tag{6}$$

where E_B is the total energy of the ejected electron and $p_B=|\mathbf{p}_B|$ is the norm of the ejected electron momentum. The matrix differential operator $\alpha\cdot\nabla$ is given by

$$\alpha\cdot\nabla = \begin{pmatrix} 0 & 0 & \partial_z & \partial_x-i\partial_y \\ 0 & 0 & \partial_x+i\partial_y & -\partial_z \\ \partial_z & \partial_x-i\partial_y & 0 & 0 \\ \partial_x+i\partial_y & -\partial_z & 0 & 0 \end{pmatrix}. \tag{7}$$

Performing the integration over d^4x, one obtains

$$\int dt\exp[-i(E_i-E_f-E_B-\varepsilon_b)t] = 2\pi\delta(E_i-E_f-E_B-\varepsilon_b), \tag{8}$$

$$\int d\mathbf{r}_2 e^{i(\mathbf{p}_i-\mathbf{p}_f)\cdot\mathbf{r}_1}\left\{\frac{1}{r_{12}}-\frac{1}{r_1}\right\} = \frac{4\pi}{\Delta^2}\{e^{i\mathbf{\Delta}\cdot\mathbf{r}_2}-1\}, \tag{9}$$

where we have used the well-known Bethe integral [17]. The quantity $\mathbf{\Delta}=\mathbf{p}_i-\mathbf{p}_f$ is the momentum transfer. We give the final compact form of the Sommerfeld-Maue wave function

$$\begin{aligned} \psi^{(-)}_{p_B}(\mathbf{r}_2) &= \exp(\pi\eta_B/2)\Gamma(1+i\eta_B)\exp(i\mathbf{p}_B\cdot\mathbf{r}_2)\Bigg\{{}_1F_1(-i\eta_B,1, \\ &\quad -i(p_Br_2+\mathbf{p}_B\cdot\mathbf{r}_2)) + \frac{i}{2cp_B}(\alpha\cdot\mathbf{p}_B+p_B\alpha\cdot\hat{\mathbf{r}}_2) \\ &\quad\times{}_1F_1(-i\eta_B+1,2,-i(p_Br_2+\mathbf{p}_B\cdot\mathbf{r}_2))\Bigg\}\frac{u(p_B,s_B)}{\sqrt{2E_BV}}. \end{aligned} \tag{10}$$

In Eq. (10), the operator $\alpha\cdot\mathbf{p}_B$ acts on the free spinor $u(p_B,s_B)$ and the operator $\alpha\cdot\hat{\mathbf{r}}_2$ acts on the spinor part of the Darwin function. The direct transition matrix element in Eq. (1) becomes

$$S_{fi} = -i\int d\mathbf{r}\frac{\overline{u}(p_f,s_f)}{\sqrt{2E_fV}}\gamma^0_{(1)}\frac{\overline{u}(p_B,s_B)}{\sqrt{2E_BV}}\gamma^0_{(2)}\left\{{}_1F_1(i\eta_B,1,i(p_Br + \mathbf{p}_B\cdot\mathbf{r})1_4) - \frac{i}{2cp_B}(\alpha\cdot\mathbf{p}_B + p_B\alpha\cdot\hat{\mathbf{r}}) \times {}_1F_1(i\eta_B+1,2,i(p_Br+\mathbf{p}_B\cdot\mathbf{r}))\right\}\varphi^{(\pm)}(\mathbf{r})\exp(-i\mathbf{p}_B\cdot\mathbf{r}) \times[\exp(i\boldsymbol{\Delta}\cdot\mathbf{r})-1]\frac{8\pi^2}{\Delta^2}\delta(E_f+E_B-E_i-\varepsilon_b)\frac{u(p_i,s_i)}{\sqrt{2E_iV}} \times\exp(\pi\eta_B/2)\Gamma(1-i\eta_B). \quad (11)$$

This transition matrix element contains three terms, one of which is given by

$$S^{(1)}_{fi} = -i\int d\mathbf{r}\frac{\overline{u}(p_f,s_f)}{\sqrt{2E_fV}}\gamma^0_{(1)}\frac{\overline{u}(p_B,s_B)}{\sqrt{2E_BV}}\gamma^0_{(2)}\{{}_1F_1(i\eta_B,1,i(p_Br + \mathbf{p}_B\cdot\mathbf{r}))\}\varphi^{(\pm)}(\mathbf{r})\exp(-i\mathbf{p}_B\cdot\mathbf{r}) \times[\exp(i\boldsymbol{\Delta}\cdot\mathbf{r})-1]\frac{8\pi^2}{\Delta^2}\delta(E_f+E_B-E_i-\varepsilon_b)\frac{u(p_i,s_i)}{\sqrt{2E_iV}} \times\exp(\pi\eta_B/2)\Gamma(1-i\eta_B). \quad (12)$$

This term can be recast in the form

$$S^{(1)}_{fi} = -i[H_1(\mathbf{q}=\boldsymbol{\Delta}-\mathbf{p}_B)-H_1(\mathbf{q}=-\mathbf{p}_B)]\frac{\overline{u}(p_f,s_f)}{\sqrt{2E_fV}} \times\gamma^0_{(1)}\frac{\overline{u}(p_B,s_B)}{\sqrt{2E_BV}}\gamma^0_{(2)}\frac{u(p_i,s_i)}{\sqrt{2E_iV}}\frac{8\pi^2}{\Delta^2} \times\delta(E_f+E_B-E_i-\varepsilon_b)\exp(\pi\eta_B/2)\Gamma(1-i\eta_B). \quad (13)$$

In the above expression, $H_1(\mathbf{q})$ is given by

$$H_1(\mathbf{q}) = \int d\mathbf{r}\exp(i\mathbf{q}\cdot\mathbf{r})\,{}_1F_1(i\eta_B,1,i(p_Br+\mathbf{p}_B\cdot\mathbf{r}))\varphi^{(\pm)}(\mathbf{r}). \quad (14)$$

For instance, if one considers $\varphi^{(+)}(\mathbf{r})$, the quantity $H_1(\mathbf{q})$ is given by

$$H_1(\mathbf{q}) = (I_1,I_2,I_3,I_4)^T, \quad (15)$$

and one has to evaluate

$$I_1 = \frac{1}{\sqrt{\pi}}\int d\mathbf{r}\exp(i\mathbf{q}\cdot\mathbf{r})e^{-r}\,{}_1F_1(i\eta_B,1,i(p_Br+\mathbf{p}_B\cdot\mathbf{r})). \quad (16)$$

To do that, we introduce the well-known integral [16]

$$I(\lambda) = \int d\mathbf{r}\exp(i\mathbf{q}\cdot\mathbf{r})\frac{e^{-\lambda r}}{r}\,{}_1F_1(i\eta_B,1,i(p_Br+\mathbf{p}_B\cdot\mathbf{r})) = \frac{4\pi}{q^2+\lambda^2}\exp\left[i\eta_B\ln\left(\frac{q^2+\lambda^2}{q^2+\lambda^2+2\mathbf{q}\cdot\mathbf{p}_B-2i\lambda p_B}\right)\right]. \quad (17)$$

The other integrals can be obtained by noting that

$$\cos\theta\exp(i\mathbf{q}\cdot\mathbf{r}) = -\frac{i}{r}\frac{\partial}{\partial q_z}\exp(i\mathbf{q}\cdot\mathbf{r}) \quad (18)$$

and

$$\sin\theta\exp(i\phi)\exp(i\mathbf{q}\cdot\mathbf{r}) = -\frac{i}{r}\left(\frac{\partial}{\partial q_x}+i\frac{\partial}{\partial q_y}\right)\exp(i\mathbf{q}\cdot\mathbf{r}). \quad (19)$$

The second term in the transition amplitude given in Eq. (11) is

$$S^{(2)}_{fi} = S^{(2),1}_{fi} + S^{(2),2}_{fi}, \quad (20)$$

with

$$S^{(2),1}_{fi} = -\int d\mathbf{r}\frac{\overline{u}(p_f,s_f)}{\sqrt{2E_fV}}\gamma^0_{(1)}\frac{u(p_i,s_i)}{\sqrt{2E_iV}}\frac{1}{2cp_B}\frac{\overline{u}(p_B,s_B)}{\sqrt{2E_BV}} \times\gamma^0_{(2)}\left[\gamma^0_{(2)}\frac{E_B}{c}-\not{p}_B\right]\varphi^{(\pm)}(\mathbf{r})\,{}_1F_1(i\eta_B+1,2,i(p_Br + \mathbf{p}_B\cdot\mathbf{r}))\exp(-i\mathbf{p}_B\cdot\mathbf{r})[\exp(i\Delta\cdot\mathbf{r})-1] \times\exp(\pi\eta_B/2)\Gamma(1-i\eta_B)\frac{8\pi^2}{\Delta^2}\delta(E_f+E_B-E_i-\varepsilon_b) \quad (21)$$

and

$$S^{(2),2}_{fi} = -\int d\mathbf{r}\frac{\overline{u}(p_f,s_f)}{\sqrt{2E_fV}}\gamma^0_{(1)}\frac{u(p_i,s_i)}{\sqrt{2E_iV}}\frac{1}{2c}\frac{\overline{u}(p_B,s_B)}{\sqrt{2E_BV}}\gamma^0_{(2)}\varphi'^{(\pm)}(\mathbf{r}) \times{}_1F_1(i\eta_B+1,2,i(p_Br+\mathbf{p}_B\cdot\mathbf{r}))\exp(-i\mathbf{p}_B\cdot\mathbf{r}) \times[\exp(i\Delta\cdot\mathbf{r})-1]\exp(\pi\eta_B/2)\Gamma(1-i\eta_B)\frac{8\pi^2}{\Delta^2}\delta(E_f + E_B-E_i-\varepsilon_b). \quad (22)$$

In Eq. (22), $\varphi'^{(+)}(\mathbf{r})$ for spin up is given by

$$\varphi'^{(+)}(\mathbf{r}) = N_D\begin{pmatrix} i/2c \\ 0 \\ \cos(\theta) \\ \sin(\theta)e^{i\phi}\end{pmatrix}\frac{1}{\sqrt{\pi}}e^{-r}, \quad (23)$$

where $N_D = 2c/\sqrt{4c^2+1}$ is a normalization constant. Using the standard procedures of QED [19], one obtains for the spin-unpolarized TDCS

$$\frac{d\overline{\sigma}}{dE_B d\Omega_B d\Omega_f} = \frac{1}{2}\sum_{s_i,s_f}\sum_{s_B}\frac{1}{2}\sum_{s_t}\frac{d\sigma}{dE_B d\Omega_B d\Omega_f} \tag{24}$$

evaluated for $E_f = E_i + \varepsilon_b - E_B$, where $\Sigma_{s_t}(\cdots)/2$ denotes the averaged sum over the spin states of the target atomic hydrogen with

$$\frac{d\overline{\sigma}}{dE_B d\Omega_B d\Omega_f} = \frac{1}{64c^6\pi^3}\frac{p_f p_B}{p_i}\frac{\exp(\pi\eta_B)}{\Delta^4}|\Gamma(1-i\eta_B)|^2|\tilde{S}_{fi}^{(1)} + \tilde{S}_{fi}^{(2),1} + \tilde{S}_{fi}^{(2),2}|^2. \tag{25}$$

In the expressions of $\tilde{S}_{fi}^{(2),1}$ and $\tilde{S}_{fi}^{(2),2}$, a new integral occurs. We have calculated this integral analytically. Details of its derivation are given in the appendix. This integral is

$$J(\lambda) = \int d\mathbf{r}\exp(i\mathbf{q}\cdot\mathbf{r})\frac{e^{-\lambda r}}{r}{}_1F_1(i\eta_B + 1, 2, i(p_B r + \mathbf{p}_B\cdot\mathbf{r})) = \frac{4\pi}{(q^2+\lambda^2)}{}_2F_1\left(i\eta_B + 1, 1, 2, -2\frac{(\mathbf{q}\cdot\mathbf{p}_B - i\lambda p_B)}{q^2+\lambda^2}\right). \tag{26}$$

All the calculations in Eq. (25) can be done analytically and only five terms out of nine are nonzero, the diagonal terms $|\tilde{S}_{fi}^{(1)}|^2, |\tilde{S}_{fi}^{(2),1}|^2, |\tilde{S}_{fi}^{(2),2}|^2$, and $\tilde{S}_{fi}^{(1)\dagger}\tilde{S}_{fi}^{(2),1}$, as well as $\tilde{S}_{fi}^{(2),1\dagger}\tilde{S}_{fi}^{(1)}$. In Eq. (24), the different sums over spin states give the following results:

$$\frac{1}{2}\sum_{s_i,s_f}|\overline{u}(p_f,s_f)\gamma_{(1)}^0 u(p_i,s_i)|^2 = 2c^2\left(\frac{2E_iE_f}{c^2} - (p_i\cdot p_f) + c^2\right),$$

$$\sum_{s_B}\left|\overline{u}(p_B,s_B)\gamma_{(2)}^0\left[\gamma_{(2)}^0\frac{E_B}{c} - \not{p}_B\right]\right|^2 = 4E_B\left(\frac{E_B^2}{c^2} - c^2\right),$$

$$\sum_{s_B}|(\overline{u}(p_B,s_B)\gamma_{(2)}^0|^2 = 4E_B,$$

$$\frac{1}{2}\sum_{s_t}(\cdots) = 1(\cdots). \tag{27}$$

III. RESULTS AND DISCUSSION

A. Coplanar asymmetric geometries

We begin our discussion by considering well-known results in the nonrelativistic domain, namely the results of Byron and Joachain [17] and those of Berakdar [21].

All these results are obtained in the coplanar asymmetric geometry. Let us consider the process whereby an incident electron with a kinetic energy E_i=250 eV scatters with a hydrogen atom. The ejected electron is observed to have a kinetic energy E_B=5 eV and the scattered electron is observed having an angle θ_f=3°. In this particular case, the CBA is not as accurate as the results obtained by Byron and Joachain within the framework of the Eikonal Born series [17] which contain higher-order corrections. These authors have pushed the numerical calculations up to the third order to obtain a curve that is close to the absolute experimental data of Ehrhardt *et al.* [24]. As we are mainly interested in our comparison by orders of magnitude and as it can be seen in Fig. 1, the agreement between the nonrelativistic and semirelativistic results is good since we obtain two identical curves.

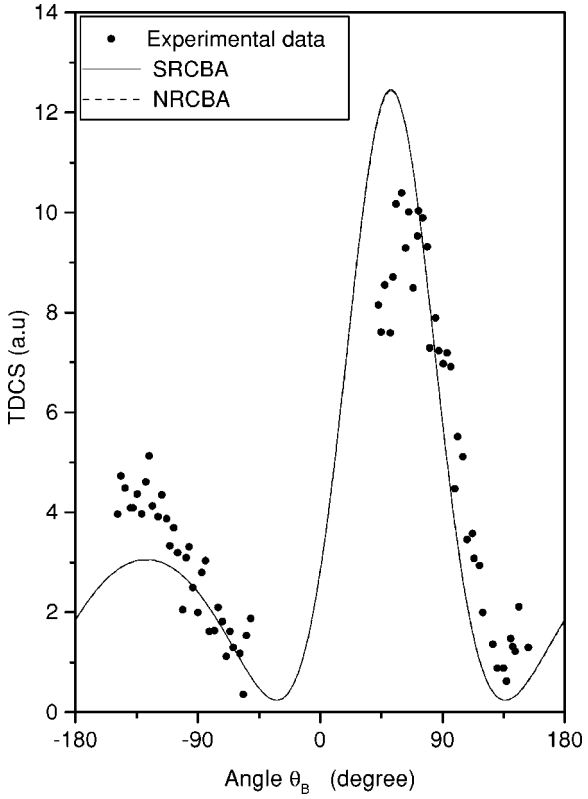

FIG. 1. The two TDCSs. The solid line represents the relativistic TDCS in the semirelativistic Coulomb Born approximation, the long-dashed line represents the corresponding TDCS in the nonrelativistic Coulomb Born approximation. The incident electron kinetic energy is T_i=250 eV and the ejected electron kinetic energy is T_B=5 eV. Experimental data is from [24]. All these TDCSs were obtained in the direct channel.

However, even in this nonrelativistic regime, small effects due to the semirelativistic treatment of the wave functions we have used are present and these can only be tracked back to the spin. Indeed, if we plot the ratio of the semirelativistic TDCS and the nonrelativistic TDCS, it emerges that, however small, these spin effects can reach 0, 45% for some specific angles. We recall that the TDCS has extrema, in particular when the direction of $\mathbf{p_B}$ coincides with that of the vectors Δ and $-\Delta$ and this can be seen in Fig. 2. In the former case, the extremum is always a maximum and in the latter case the extremum is a local maximum. The two TDCSs exhibit in this geometry a forward or binary peak with a maximum in the direction of Δ and a recoil or backward peak in the opposite direction $-\Delta$. The locations of such extrema are $\theta_B \approx -128°$ with a ratio equal to 1.002 34 and $\theta_B \approx 52°$ with a ratio equal to 1.001 85. These mechanisms for the emergence of the binary recoil peak structure are also present even when one uses the simplest description in which plane waves for incoming and outgoing particles are assumed [22]. Now, if we compare our result with the

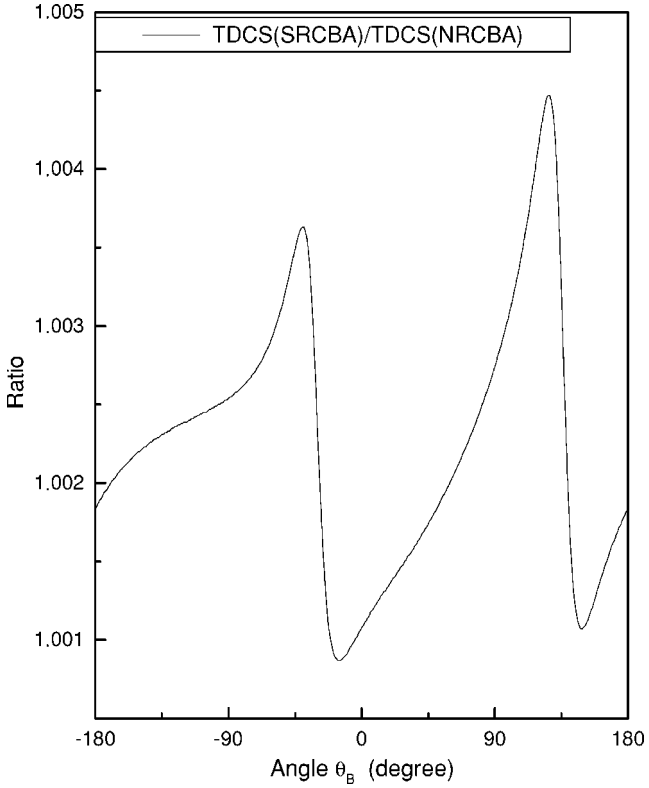

FIG. 2. The ratio TDCS (SRCBA)/TDCS (NRCBA) as a function of the angle θ_B with $\theta_f=3°$. The incident electron kinetic energy is $t_i=250$ eV and the ejected electron kinetic energy is $T_B=5$ eV. Both TDCSs were evaluated in the direct channel.

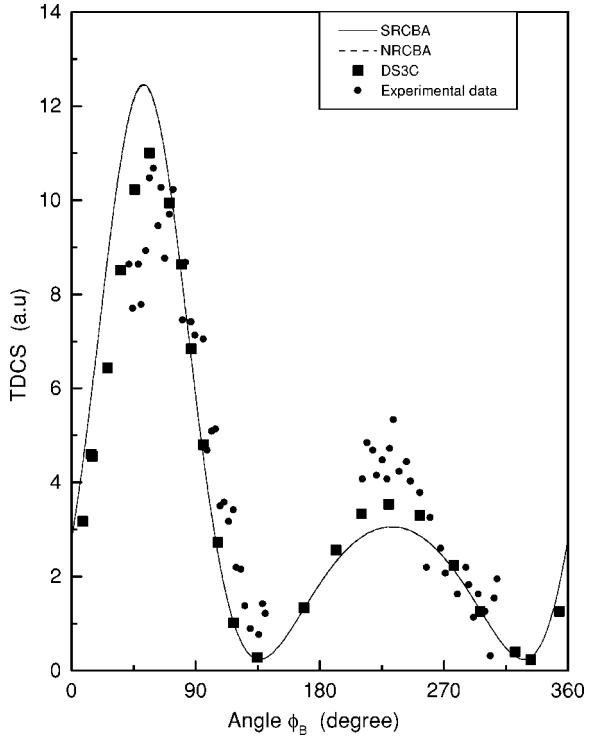

FIG. 3. The two TDCSs. The solid line represents the relativistic TDCS in the semirelativistic Coulomb Born approximation, the long-dashed line represents the corresponding TDCS in the nonrelativistic Coulomb Born approximation, the symbols square and circle, respectively, represent the formalism of DS3C and the experimental data. We keep the same energies as in Fig. 1. Experimental data is from [9]. The results of the DS3C model were obtained by including exchange effects and using correlated wave functions.

result obtained by Berakdar [21], we also obtain a good agreement. But before beginning the discussion proper, let us recall the formalism used by Berakdar. His calculations were performed within a model where the three-body final state is described by a product of three symmetrical, Coulomb-type functions. Each of these functions describes the motion of a particular two-body subsystem in the presence of a third charged particle. The choice he made for the parameters used in his formalism to describe the correlated wave functions stems from the threshold theory of Wannier [25] and is of paramount importance when the energies involved are small or intermediate. Thereafter, he made a comprehensive comparison with available experimental data and with other theoretical models. He ended his study by concluding that generally, good agreement is found with the absolute measurements but that, however, in some cases discrepancies between various theoretical predictions and experimental findings are obvious, which highlights the need for a theoretical and experimental benchmark study of these reactions.

In Fig. 3, we compare our results with those obtained by Berakdar for an incident electron kinetic energy $E_i=250$ eV for the case of a coplanar asymmetric geometric where $\theta_f=\theta_B=90°$. The ejected electron kinetic energy is $E_B=5$ eV and $\phi_f=357°$. What is remarkable is the agreement between our results and his, bearing in mind that he used the DS3C formalism (DS3C stands for dynamical screening theory with three Coulomb-type functions). As it is a three-body final state, the question of the correlations of the various wave functions that intervene in its description is still, nowadays, an unanswered question. The only method that can give a satisfactory answer to this question is the use of the relativistic *R*-matrix method. However, the orders of magnitude of both results are similar and this is a second validity-check of our model bearing in mind the relative simplicity of the wave functions we have used. Another atypical result related to our calculations is the behavior of the ratio of the TDCS (SRCBA)/TDCS (NRCBA), where now the maxima of this ratio correspond nearly to the local minima of the TDCS when plotted as a function of the angle ϕ_B. However, there is no rule that can be inferred from the behavior of this ratio since when performing various simulations even in the coplanar asymmetric geometry but with increasing values of the incident electron kinetic energy, there are many regions not close to the binary or secondary peaks that present maxima or minima.

B. Binary coplanar geometries

The relativistic regime can be defined as follows: when the value of the relativistic parameter $\gamma=[1-(\beta/c)^2]^{-1/2}$ is greater that 1.0053, there begins to be a difference between the nonrelativistic kinetic energy and the relativistic kinetic energy.

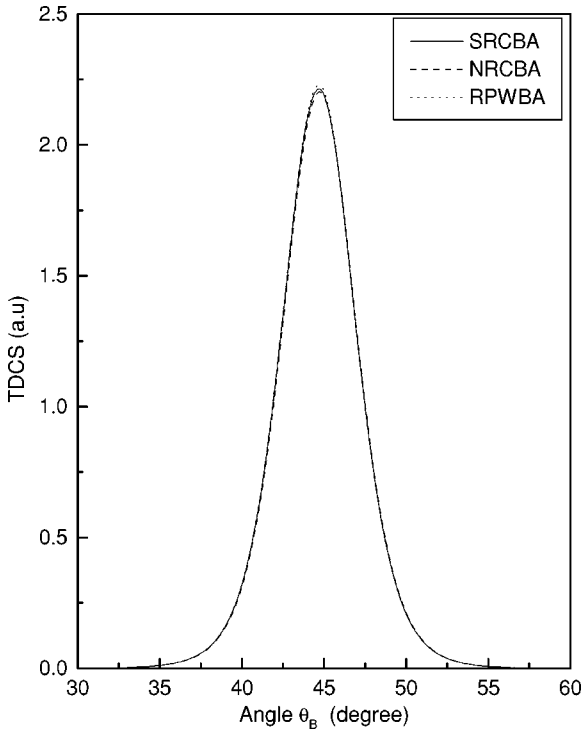

FIG. 4. The three TDCSs scaled in 10^{-3}. The solid line represents the relativistic TDCS in the semirelativistic Coulomb Born approximation, the long-dashed line represents the corresponding TDCS in the nonrelativistic Coulomb Born approximation. The short-dashed line represents the relativistic plane-wave Born approximation. The incident electron kinetic energy is T_i=2700 eV and the ejected electron kinetic energy is T_B=1349.5 eV and θ_f =45°. All these results were obtained in the direct channel.

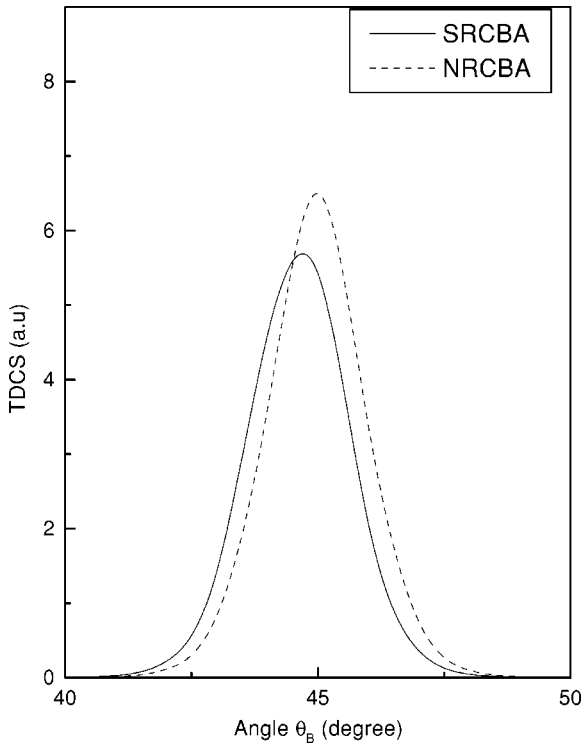

FIG. 5. The two TDCSs scaled in 10^{-5}. The solid line represents the relativistic TDCS in the semirelativistic Coulomb Born approximation, the long-dashed line represents the corresponding TDCS in the nonrelativistic Coulomb Born approximation. The incident electron kinetic energy is T_i=25 000 eV and the ejected electron kinetic energy is T_B=12 499.5 eV and θ_f=45°. All these results were obtained in the direct channel.

This numerical value of the aforementioned relativistic parameter corresponds to an incident electron kinetic energy of E_i=2700 eV. Because there is no experimental data available for this regime, we simply compare our results with those we have previously found when we introduced the relativistic plane-wave Born approximation (RPWBA) [23] to study the ionization of atomic hydrogen by electron impact in the binary geometry. In Fig. 4, it is clearly visible that the three models (NRCBA, SRCBA, and RPWBA) give the same results, which was to be expected since in this geometry, the use of a Coulomb wave function is not necessary.

In Fig. 5, there is a shift of the maximum of the TDCS in the SRCBA towards smaller values than θ_B=45° and this remains the case for increasing values of the kinetic energy of the incident electron. The origin of this shift stems from the fact that the main contribution to the TDCS comes from the term $H_1(q)$ given by Eq. (14). This term contains a dominant integral I_1. When plotting the behavior of I_1 as function of the angle θ_B, and with increasing values of E_i, one observes the shift we have mentioned as well as the fact that in the relativistic regime, the TDCS (SRCBA) is always lower than the TDCS (NRCBA).

IV. CONCLUSION

In this article, we have presented a semirelativistic model that does not rely on heavy numerical computations but yet can be applied to a wide range of kinematic geometries and energies. We have used simple semirelativistic Sommerfeld-Maue wave functions that allow to obtain analytical results in an exact and closed form within the framework of the first Born approximation. This model gives good results if the condition $Z\alpha \ll 1$ is fulfilled. We have compared our results with previous nonrelativistic results and found that the agreement between the different theoretical approaches is good even if our model uses simple uncorrelated wave functions. It contains the coplanar asymmetric geometry, as well as the binary coplanar geometry as particular cases, and shows that the nonrelativistic treatment is no longer reliable for energies higher than 25 keV. We hope that we will be able to compare our theoretical results with forthcoming experimental data.

APPENDIX: ANALYTICAL CALCULATION OF THE INTEGRAL $J(\lambda)$

Before turning to the analytical calculation of the integral $J(\lambda)$ proper, let us recall how the integral $I(\lambda)$ [16] can be obtained. This is explained without any detail in [20]. Using parabolic coordinates, one has to evaluate the following integral:

$$I(\lambda) = \int d\mathbf{r}\, \exp(i\mathbf{Q}\cdot\mathbf{r})\exp(-i\mathbf{p}_B\cdot\mathbf{r})\frac{e^{-\lambda r}}{r} \times {}_1F_1(i\eta_B, 1, i(p_B r + \mathbf{p}_B\cdot\mathbf{r})). \quad \text{(A1)}$$

The choice of the scalar product $\mathbf{Q}\cdot\mathbf{r}$ chosen is [6]

$$\mathbf{Q}\cdot\mathbf{r} = \frac{1}{2}Q(\xi-\eta)\cos\gamma - 4\sqrt{\xi\eta}\cos\varphi\sin\gamma. \quad \text{(A2)}$$

Performing the various integrals, one finds

$$I(\lambda) = \frac{2\pi}{\lambda - i(Q\cos\gamma + p_B)}\int_0^\infty d\xi \exp(-\mu\xi) \times {}_1F_1(i\eta_B, 1, ip_B\xi). \quad \text{(A3)}$$

We use the well-known result [20]

$$\int_0^\infty dt \exp(-\lambda t)\,{}_1F_1(\alpha, 1, kt) = \lambda^{\alpha-1}(\lambda - k)^{-\alpha} \quad \text{(A4)}$$

with

$$\lambda = \mu = \frac{Q^2\sin^2\gamma}{2[\lambda - i(Q\cos\gamma + p_B)]} + \frac{1}{2}[\lambda + i(Q\cos\gamma + p_B)] \quad \text{(A5)}$$

and $\alpha = i\eta_B$ and $k = ip_B$. This gives the result

$$I(\lambda) = \frac{4\pi}{(Q^2 + \lambda^2 + p_B^2 + 2Qp_B\cos\gamma)} \times \exp\left[i\eta_B \ln\left(\frac{Q^2 + \lambda^2 + p_B^2 + 2Qp_B\cos\gamma}{Q^2 + \lambda^2 - p_B^2 - 2i\lambda p_B} \right) \right]. \quad \text{(A6)}$$

To recover the integral $I(\lambda)$ given in Eq. (17) of the text, one has to make the following substitutions:

$$-\mathbf{Q} = \mathbf{q} + \mathbf{p}_B$$

$$Qp_B\cos\gamma = \mathbf{Q}\cdot\mathbf{p}_B = -\mathbf{q}\cdot\mathbf{p}_B - p_B^2. \quad \text{(A7)}$$

It is then straightforward to find that

$$Q^2 + \lambda^2 + p_B^2 + 2Qp_B\cos\gamma = q^2 + \lambda^2$$

$$Q^2 + \lambda^2 - p_B^2 - 2i\lambda p_B = q^2 + \lambda^2 + 2\mathbf{q}\cdot\mathbf{p}_B - 2i\lambda p_B, \quad \text{(A8)}$$

so that

$$I(\lambda) = \frac{4\pi}{(q^2 + \lambda^2)}\exp\left[i\eta_B \ln\left(\frac{q^2 + \lambda^2}{q^2 + \lambda^2 + 2\mathbf{q}\cdot\mathbf{p}_B - 2i\lambda p_B} \right) \right]. \quad \text{(A9)}$$

To calculate

$$J(\lambda) = \int d\mathbf{r}\, \exp(i\mathbf{Q}\cdot\mathbf{r})\exp(-i\mathbf{p}_B\cdot\mathbf{r})\frac{e^{-\lambda r}}{r} \times {}_1F_1(i\eta_B + 1, 2, i(p_B r + \mathbf{p}_B\cdot\mathbf{r})) \quad \text{(A10)}$$

one uses the same procedures to obtain

$$J(\lambda) = \frac{2\pi}{\lambda - i(Q\cos\gamma + p_B)}\int_0^\infty d\xi \exp(-\mu\xi) \times {}_1F_1(i\eta_B + 1, 2, ip_B\xi) = \frac{2\pi}{\lambda - i(Q\cos\gamma + p_B)}\frac{1}{\mu} \times {}_2F_1\left(i\eta_B + 1, 1, 2, \frac{ip_B}{\mu} \right). \quad \text{(A11)}$$

Performing the various substitutions, one gets the following analytical integral:

$$J(\lambda) = \int d\mathbf{r}\, \exp(i\mathbf{q}\cdot\mathbf{r})\frac{e^{-\lambda r}}{r}\,{}_1F_1(i\eta_B + 1, 2, i(p_B r + \mathbf{p}_B\cdot\mathbf{r})) = \frac{4\pi}{(q^2 + \lambda^2)}\,{}_2F_1\left(i\eta_B + 1, 1, 2, -2\frac{[\mathbf{q}\cdot\mathbf{p}_B - i\lambda p_B]}{q^2 + \lambda^2} \right). \quad \text{(A12)}$$

We have tested this analytical result by performing the integral using two Gaussian quadratures because we have assumed without loss of generality both $\mathbf{q}$ and $\mathbf{p}_B$ to be parallel to the *Oz* axis. The first one, a Laguerre Gaussian quadrature (32 points) to integrate over the radial variable *r*, and the second one, using a Legendre Gaussian quadrature (32 points) to integrate over the angular variable θ. The agreement between the analytical result and the numerical result is excellent. To illustrate this point, we give as an example the results obtained by the two methods for the following random values of the relevant parameters: For $\lambda = 1$, $|\mathbf{q}| = 1.015\,055$, $|\mathbf{p}| = 0.105\,509\,8$. The exact result is

$$J_{\text{exact}}(\lambda) = (0.573\,558\,96, 0.124\,585\,10), \quad \text{(A13)}$$

and the numerical result is

$$J_{\text{num}}(\lambda) = (0.573\,558\,99, 0.124\,585\,07). \quad \text{(A14)}$$

[1] W. Nakel and C. T. Whelan, Phys. Rep. **315**, 409 (1999).
[2] C. T. Whelan, R. J. Allan, J. Rasch, H. R. J. Walters, X. Zhang, J. Röder, K. Jung, and H. Ehrhardt, Phys. Rev. A **50**, 4394 (1994).
[3] P. Marchalant, C. T. Whelan, and H. R. J. Walters, J. Phys. B **31**, 1141 (1998).
[4] I. Fuss, J. Mitroy, and B. M. Spicer, J. Phys. B **15**, 3321 (1982).
[5] I. E. McCarthy and E. Weigold, Contemp. Phys. **35**, 377 (1994).
[6] F. Bell, J. Phys. B **22**, 287 (1989).
[7] A. Cavaldi and L. Avaldi, Nuovo Cimento Soc. Ital. Fis., D **16**, 1 (1994).
[8] H. Ehrhardt, Comments At. Mol. Phys., **13**, 115 (1983).

[9] H. Ehrhardt, K. Jung, G. Knöth, and P. Schlemmer, Z. Phys. D: At., Mol. Clusters **1**, 3 (1986).
[10] J. N. Das and A. N. Konar, J. Phys. B, **7**, 2417 (1974).
[11] J. N. Das and S. Chakraborty, Phys. Lett. **92A**, 127 (1982).
[12] B. L. Moïseiwitsch, Prog. At. Mol. Phys. **16**, 281 (1980).
[13] D. H. Jakubaßa-Amundsen, Z. Phys. D: At., Mol. Clusters **11**, 305 (1989).
[14] D. H. Jakubaßa-Amundsen, Phys. Rev. A **53**, 2359 (1996).
[15] L. U. Ancarani, S. Keller, H. Ast, C. T. Whelan, H. R. J. Walters, and R. M. Dreizler, J. Phys. B **31**, 609 (1998).
[16] H. S. W. Massey and C. B. O Mohr, Proc. R. Soc. London **140**, 613 (1933).
[17] F. W. Jr. Byron and C. J. Joachain, Phys. Rep. **179**, 211 (1989).
[18] J. Eichler and W. E. Meyerhof, *Relativistic Atomic Collisions* (Academic, New York, 1995).
[19] W. Greiner and J. Reinhardt, *Quantum Electrodynamics* (Springer-Verlag, Berlin, 1992).
[20] L. Landau and E. Lifchitz, *Mécanique Quantique* (Editions Mir, Moscou, 1967).
[21] J. Berakdar, Phys. Rev. A **56**, 370 (1997).
[22] J. S. Briggs, Comments At. Mol. Phys., **23**, 155 (1989).
[23] Y. Attaourti and S. Taj, Phys. Rev. A **69**, 063411 (2004).
[24] H. Ehrhardt, G. Knoth, P. Schlemmer, and K. Jung, Phys. Lett. **110A**, 92, (1985).
[25] G. Wannier, Phys. Rev. **90**, 817 (1953).