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Triple differential cross section in ionization of hydrogen by electron impact

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A novel model is proposed to study the ionization of atomic hydrogen by fast election impact in coplanar asymmetric geometry making use of the post form of the transition matrix element for the energy shell and the two-potential formula. Based on the approximation of projectile plane waves and three-body problems, the transition matrix element is decomposed into two parts: the structure and scattering factor and the correlation factor. The contributions of these factors to triple differential cross sections are investigated using the method of asymptotic and convergent series.

Keywords: (e ,2e), triple differential cross sections, binary peak, recoil peak
PACC: 3480D, 3450H

1. Introduction

The ionization of atomic hydrogen by electron impact is important as one of the basic atomic processes in plasma physics and astrophysics.[1−4] In spite of decades of extensive research, even single ionization processes occurring in collisions of charged particle and hydrogen atom are not yet completely understood. From a theoretical point of view, the basic problem is that the Schrödinger equation is not solvable in closed form for more than two mutually interacting particles. A comprehensive description of the entire collision, involving the interactions between the projectile, the election and the residual proton, therefore requires approximation. In recent years, a number of powerful theoretical methods have been used to compute scattering amplitudes and cross sections. Among these approximations particularly noteworthy are the calculations of Brauner, Briggs and Klar[5−7] using a final state wavefunction that satisfied the asymptotic three body Schrödinger equation exactly, the second-order Coulomb–Born calculation of Srivastara and Sharma,[8] and the pseudostatic close-coupling calculation by Curran and Walters.[9] All of these calculations provided at least qualitative agreement with experimental data for electron impact in high and intermediate incident energy ranges.

For electron impact, kinematical complete experiments on single ionization of hydrogen have been performed for more than 30 years. There is now a large body of measurements available for different geometries and for incident energies from near threshold to several keV. Most of these measurements focused on the ionization processes where the electron is ejected into the scattering plane defined by the momentum vector of the incident electron $\boldsymbol{k}_{\rm i}$ and that of the faster final state electron $\boldsymbol{k}_{\rm a}$. When the incident electron energy is large, the angular distribution of the ejected electrons exhibits a characteristic shape with one maximum occurring near the direction of the momentum transfer vector $\Delta = \boldsymbol{k}_{\rm i} - \boldsymbol{k}_{\rm a}$, called the binary peak, and a second maximum at an angle close to 180° relative to Δ, which is called the recoil peak.[10,11]

In this paper we describe a novel method based on the use of the convergent and asymptotic series to understand the analytic properties of the persistence of binary peak and recoil peak.[12,13] Based on the approximation of the projectile plane wave, the transition matrix element is decomposed into two parts: the structure and scattering factor and the correlation factor. Triple differential cross sections (TDCS) have been calculated for the single ionization of hydrogen atoms from the ground state in coplanar asymmetric geometry, in the framework of a two-potential formula and post form of transition matrix elements.

Atomic units are used throughout except where otherwise specified.

2. Theory

In this section we sketch the theoretical model briefly. Here we consider a hydrogen target being singly ionized by the impact of an electron with an incident energy of several hundred eV. At the energies considered in this work, exchange and relativistic effects are negligible. The TDCS in the coplanar geometry is given by

$$\frac{\mathrm{d}^3\sigma}{\mathrm{d}\Omega_\mathrm{a}\mathrm{d}\Omega_\mathrm{b}\mathrm{d}E_\mathrm{b}} = (2\pi)^4\frac{k_\mathrm{a}k_\mathrm{b}}{k_\mathrm{i}}|T_\mathrm{if}|^2, \tag{1}$$

where $\boldsymbol{k}_\mathrm{i}$, $\boldsymbol{k}_\mathrm{a}$ and $\boldsymbol{k}_\mathrm{b}$ are the momenta of the incident, the scattered and ejected electrons, respectively. Ω_a and Ω_b are the solid angles subtended by the two outgoing electrons, and E_b is the energy of the ejected electron.

The post form of the transition matrix element (on the energy shell) reads as

$$T_\mathrm{if} = \langle\Phi_\mathrm{b}|V_\mathrm{f}|\psi_\mathrm{a}^{(+)}\rangle. \tag{2}$$

Thus, for the two-potential problem considered here,[14] we find that

$$T_\mathrm{if} = \langle\chi_\mathrm{B}^{(-)}|W_\mathrm{f}|\psi_\mathrm{a}^{(+)}\rangle, \tag{3}$$

where $\chi_\mathrm{B}^{(-)}$ and $\psi_\mathrm{a}^{(+)}$ are the final distorted wavefunction and the exact initial wavefunction under the correct outgoing condition, respectively, and W_f is the interaction between the two electrons in the final channel. The final distorted wavefunction is chosen as a product of two Coulomb wavefunctions that describe the two final continuum electrons distorted by the nucleus field,

$$\chi_\mathrm{B}^{(-)}(\boldsymbol{r}_\mathrm{a},\boldsymbol{r}_\mathrm{b}) = F_\mathrm{c}(\boldsymbol{k}_\mathrm{b},\boldsymbol{r}_\mathrm{b})F_\mathrm{c}(\boldsymbol{k}_\mathrm{a},\boldsymbol{r}_\mathrm{a}). \tag{4}$$

We consider the screen effect of slow election and asymmetric geometry $\boldsymbol{k}_\mathrm{a} \gg \boldsymbol{k}_\mathrm{b}$; consequently, the corresponding hypergeometric function of the fast electron tends to unity from the final channel:

$$\begin{aligned}\chi_\mathrm{B}^{(-)}(\boldsymbol{r}_\mathrm{a},\boldsymbol{r}_\mathrm{b}) =& F_\mathrm{c}(\boldsymbol{k}_\mathrm{b},\boldsymbol{r}_\mathrm{b})F_\mathrm{c}(\boldsymbol{k}_\mathrm{a},\boldsymbol{r}_\mathrm{a})\\ \approx& (2\pi)^{-3/2}\exp(\mathrm{i}\boldsymbol{k}_\mathrm{a}\cdot\boldsymbol{r}_\mathrm{a})F_\mathrm{c}(\boldsymbol{k}_\mathrm{b},\boldsymbol{r}_\mathrm{b}),\end{aligned} \tag{5}$$

where

$$F_\mathrm{c}(\boldsymbol{k}_\mathrm{b},\boldsymbol{r}_\mathrm{b}) =_1 F_1(\mathrm{i}\eta_\mathrm{b},1,-\mathrm{i}k_\mathrm{b}r_\mathrm{b}-\mathrm{i}\boldsymbol{k}_\mathrm{b}\cdot\boldsymbol{r}_\mathrm{b}). \tag{6}$$

${}_1F_1$ is the confluent hypergeometric function and η_b is the Sommerfeld parameter ($\eta_\mathrm{b} = 1/k_\mathrm{b}$).

The perturbation interaction in the final channel W_f is given by

$$W_\mathrm{f} = \frac{1}{r_\mathrm{ab}} = \frac{1}{|\boldsymbol{r}_\mathrm{a}-\boldsymbol{r}_\mathrm{b}|}. \tag{7}$$

The exact initial wavefunction $\psi_\mathrm{A}^{(+)}(\boldsymbol{r}_\mathrm{a},\boldsymbol{r}_\mathrm{b})$ is a solution of the three-body problem. The key point of this work is to neglect the exponential term of the wavefunctions of the relative motion and the centre of mass and to replace the Coulomb distorted wave by the plane wave in this wavefunction. The wavefunction is then approximately written as

$$\psi_\mathrm{A}^{(+)} \approx A\mathrm{e}^{\mathrm{i}k_\mathrm{i}\cdot k_\mathrm{a}}\mathrm{e}^{-\beta r_\mathrm{b}}{}_1F_1(\mathrm{i}\alpha_{12},1,k_\mathrm{ab}r_\mathrm{ab}-\boldsymbol{k}_\mathrm{ab}\cdot\boldsymbol{r}_\mathrm{ab}), \tag{8}$$

where ${}_1F_1$ is also the confluent hypergeometric function and $\alpha_{12} = 1/\eta_\mathrm{ab}$ (η_ab is the Sommerfeld parameter). Substituting Eqs.(5), (7) and (8) into Eq.(3) and then performing the space integration over $\boldsymbol{r}_\mathrm{a}$ and $\boldsymbol{r}_\mathrm{b}$, we arrive at the following expression:

$$T_\mathrm{if} = CT_\mathrm{ab}T_\mathrm{b}, \tag{9}$$

where C is a normalization constant;

$$T_\mathrm{b} = \frac{1}{2\pi\mathrm{i}}\oint_\Gamma \mathrm{d}t_2 p(\eta_\mathrm{b},t_2)\frac{M}{[M^2+(\Delta+\boldsymbol{k}_\mathrm{b}(t_2-1))^2]^2} \tag{10}$$

is called the structure and scattering factor, with $\Delta = \boldsymbol{k}_\mathrm{i}-\boldsymbol{k}_\mathrm{a}$, $M = \beta - k_\mathrm{b}t_2$ and $\beta = \left(\frac{1}{1-\gamma}\right)^{1/2}$. β is the structure parameter and $0<\gamma<1$.

$$\begin{aligned}T_\mathrm{ab} =& \frac{1}{2\pi\mathrm{i}}\oint_\Gamma \mathrm{d}t_{12}p(\eta_\mathrm{ab},t_{12})\\ &\times\frac{1}{(\Delta-\boldsymbol{k}_\mathrm{ab}t_{12})^2-\boldsymbol{k}_\mathrm{ab}t_{12}^2}\end{aligned} \tag{11}$$

is called the correlation factor, with $\boldsymbol{k}_\mathrm{ab} = \boldsymbol{k}_\mathrm{a}-\boldsymbol{k}_\mathrm{b}$.

In the integral expressions of Eqs.(10) and (11) the index Γ indicates a closed contour encircling each of the two points 0 and once counterclockwise, and

$$P(\eta,t) = t^{\mathrm{i}\eta-1}(1-t)^{-\mathrm{i}\eta}, \tag{12}$$

with $\eta_\mathrm{b} = 1/k_\mathrm{b}$ and $\eta_\mathrm{ab} = \frac{1}{2(1-\gamma)}\frac{1}{k_\mathrm{ab}}$.
Carrying out the integrations over t_2 and t_{12}, we can obtain

$$\begin{aligned}T_\mathrm{b} =& \frac{1}{[\beta^2+(\boldsymbol{k}_\mathrm{b}-\Delta)^2]^2}\sum_{n=0}^{\infty}2^n(n+1)\\ &\times\left[\frac{(\mathrm{i}\eta_2)_n\beta}{n!}-\mathrm{i}k_2\frac{(\mathrm{i}\eta_2)_{n+1}}{(n+1)!}\right]\\ &\times\left\{\frac{[\beta k_\mathrm{b}\mathrm{i}+\boldsymbol{k}_\mathrm{b}\cdot(\boldsymbol{k}_\mathrm{b}-\Delta)]}{\beta^2+(\boldsymbol{k}_\mathrm{b}-\Delta)^2}\right\}^n\end{aligned} \tag{13}$$

and

$$T_{\rm ab} = \frac{1}{\Delta^2} \sum_{m=0}^{\infty} \frac{2^m(-{\rm i}\eta_{\rm ab})_m}{m!} \left(\frac{\Delta \cdot \boldsymbol{k}_{\rm ab}}{\Delta^2} \right)^m . \qquad (14)$$

3. Results and discussion

We have computed the TDCS for single ionization of the ground state of hydrogen atoms by fast electron impact for coplanar asymmetric geometries. Moreover, in order to express a general form of the correlation factor, the analytic properties of the asymptotic series (14) are also discussed. At the impact energy considered and with the coplanar asymmetric collision in our theory, the angular distribution of TDCS consists basically of two peaks, which can be assigned to the binary and recoil processes. The calculations show that the correlation factor strongly affects the recoil peak, but it influences the binary peak rather weakly. On the other hand, $T_{\rm b}$, the structure and scattering factor, mainly affects the binary peak.

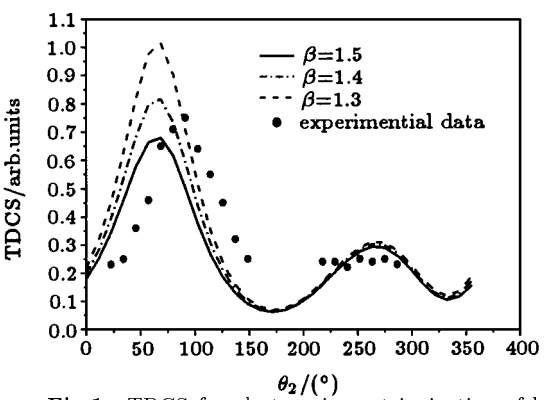


Fig.1. TDCS for electron impact ionization of hydrogen at an incident energy $E_{\rm i}$=150 eV, ejected energy $E_{\rm b}$=5 eV in a coplanar asymmetric geometry, and scattering angle θ_1=16°. The structure parameter β takes values 1.3, 1.4 and 1.5 for the structure and scattering factor. Dots denote the absolute experimental data taken from Ref.[3].

Figure 1 displays the present TDCS results, for the following asymmetric kinematics, the incident energy $E_{\rm i}$=150 eV, ejected energy $E_{\rm b}$=5 eV, and scattering angle θ_1=16°. It also shows the corresponding experimental data of the absolute measurement, and indicates that the present model can well account for the two-peak structure, which is the most important feature of the single ionization process. As may be noted from Fig.1, the present results are in quantitative agreement with the experimental data. As the structure parameter β increases from 1.3 to 1.5 in $T_{\rm b}$, the binary peak decreases sharply but the recoil peak is almost independent of the structure parameter. Regarding the location of the peaks, the present position of the recoil peak is in good agreement with experiment, while the binary peak is shifted slightly toward a smaller ejection angle as compared with the experimental data. The theoretical curve and experimental data are very close to each other in the recoil region.

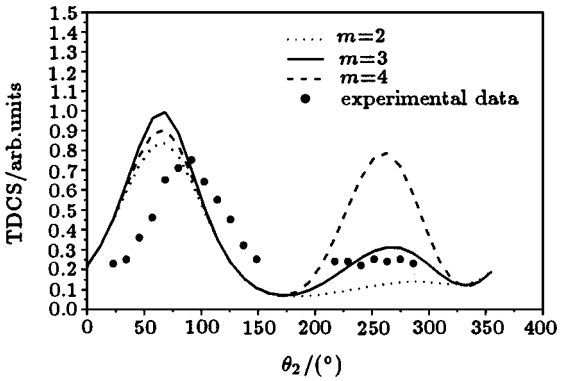


Fig.2. The asymmetric kinematics $E_{\rm b}$=5 eV, $E_{\rm i}$=150 eV, keeping θ_1 fixed at 16°; the truncation integer takes the value of 2, 3 and 4 respectively in the asymmetric series $T_{\rm ab}$.

Figure 2 displays another asymmetric kinematics $E_{\rm b}$=5 eV, $E_{\rm i}$=150 eV while keeping θ_1 fixed at 16° again. The presence of the two-peak structure of the TDCS is noted. In order to illustrate how the correlation factor strongly affects the recoil peak, TDCS against the θ_2 curve is shown in Fig.2, and the optimal truncation integer takes $m-1$, m and $m+1$ respectively in the asymmetric series $T_{\rm ab}$. As may be noted from Fig.2, the magnitude and location of the binary peak is almost independent of the truncating integer m, while the height of the recoil peak depends strongly on the truncating integer m.

In fact, the calculation of (e,2e) in the convergence problem is a difficulty to overcome. To circumvent this, many methods have been proposed.[12,13] In our calculation the truncation of asymptotic series (14) has been adopted. In this measurement condition, for the asymptotic series the first few terms of series (14) fall off. After the truncation m, the terms increase in size and produce divergence. If the summation up to the smallest term is taken, T_{12} may be considered as the sum of the series (14).

Figure 3 shows the relation between the term number m of the summation and the absolute value of the asymptotic series $T_{\rm ab}$. At $E_{\rm i}$=150 eV, $E_{\rm b}$=5 eV and θ_1=16°, β=1.3, the minimal absolute value of this asymptotic series corresponds to the optimal truncation integer m=3, for either $\eta_{\rm ab} = \dfrac{1}{2(1-\gamma)}(k_{\rm a}-k_{\rm b})^{-1}$ or $\eta_{\rm ab} = \dfrac{1}{2(1-\gamma)}(k_{\rm a}+k_{\rm b})^{-1}$.

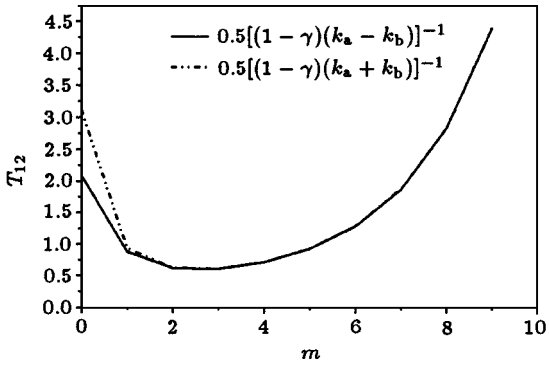


Fig.3. The relation between the term number m of the summation and the absolute value of asymptotic series T_{ab}, at incident energy E_i=150 eV, E_b=5 eV and θ_1=16°.

To sum up, using the post form of the two-potential formula and the plane wave approximation of fast electrons, the transition amplitude of TDCS is decomposed into two parts: the structure and scattering factor and the correlation factor. In the present theoretical computation, the angular distribution still consists of a two-peak structure. The structure and scattering factor strongly affect the binary peak, while the height and position of the recoil peak depend sensitively on optimal truncation integers m of the correlation factor. Clearly, although the present theory is a simple approximate method, we expect our formalism to open up vistas for TDCS analytic calculation.

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