Triply differential cross sections for electron-impact ionization of helium

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We report numerical results for the triply differential cross sections (TDCS) for electron-impact ionization of helium in the Glauber approximation in the incident energy range 224.58–2824.58 eV. The present calculation is based upon the technique of Roy *et al.*, which has an advantage over the conventional partial-wave method in calculating TDCS in that the latter requires substantial computer time where many partial waves are involved. A comparison is made of the present TDCS with the results of available theoretical calculations and absolute measurements.

I. INTRODUCTION

Triply differential cross sections (TDCS) provide the most detailed information of an ionization process. So the validity and usefulness of a theory can be tested well from a comparison of theoretical TDCS with the corresponding measurements. To date, a large number of TDCS measurements have been made on various atomic systems, but most of them are relative in nature.[1–5] Although, theoretically, atomic hydrogen is advantageous as a target since it is the simplest of all atoms and its wave functions are exactly known, no absolute measurement of TDCS is available in the case of hydrogen. However, absolute values of TDCS are available for helium. The first absolute data on helium were reported by Beaty *et al.*[2] at the incident energy of 100 eV. Next Stefani *et al.*[3] reported absolute measurements of TDCS for the He(e,2e)He^+ process in the energy range 200–4000 eV. Unfortunately, both experiments yield data that are uncertain by a factor of 2. Recently, van Wingerden *et al.*[4,5] have made absolute measurements for TDCS for electron-impact ionization of He in the energy range 224.58–2824.58 eV in a coplanar symmetric geometry. The experimental error involved has been reported to be smaller than 20%.

Since the first measurement of TDCS for the He(e,2e)He^+ process in 1969, a number of theoretical calculations[6] have been performed. In a previous paper Roy *et al.*[7] have applied the Glauber approximation[8] (GA) to calculate TDCS for electron-impact ionization of H at incident energies of 100, 113.6, and 250 eV. Their procedure has an advantage over the conventional partial-wave technique in calculating TDCS in that the latter requires substantial computer time where many partial waves are involved. Owing to the nonavailability of absolute measurements they could not, however, make a detailed examination with regard to the effectiveness of the GA.

This paper reports the first application of GA to calculate the TDCS for electron-impact ionization of He and compares the calculated cross sections with the corresponding absolute experimental data of van Wingerden *et al.*[5] The calculation is based upon the method of Roy *et al.*, which avoids the use of partial-wave technique. This method reduces the eight-dimensional Glauber amplitude for the He(e,2e)He^+ process to a two-dimensional integral. The integrand of this integral, however, contains a sum of two one-dimensional integral functions that are computed numerically. The final expression for the amplitude obtained in the case of He differs from that in the case of H in that the integral functions involved in the latter case can be evaluated analytically.

The plan of this paper is as follows. Section II gives the method of reduction of the He(e,2e)He^+ amplitude to a form that can be computed numerically with convenience. In Sec. III we present the results of our numerical calculation of the TDCS and compare them with the existing theoretical and experimental findings. Section IV contains the conclusions. Atomic units are used throughout, unless otherwise indicated.

II. THEORY

The Glauber amplitude for the ionization of He by electron impact is given by

$$F(\vec{q},\vec{k}_2)=\frac{ik}{2\pi}\int d\vec{b}\,d\vec{r}_1 d\vec{r}_2 \phi_f^*(\vec{r}_1,\vec{r}_2)\Gamma(\vec{b};\vec{r}_1,\vec{r}_2)\times\phi_i(\vec{r}_1,\vec{r}_2)e^{i\vec{q}\cdot\vec{b}}\ , \tag{1}$$

where

$$\Gamma(\vec{b};\vec{r}_1,\vec{r}_2)=1-\left[\frac{|\vec{b}-\vec{s}_1|}{b}\right]^{2i\eta}\left[\frac{|\vec{b}-\vec{s}_2|}{b}\right]^{2i\eta},$$

$$\vec{q}=\vec{k}-\vec{k}_1\ ,$$

and $\eta=1/k$. Here $\vec{k}$, $\vec{k}_1$, and $\vec{k}_2$ are the momenta of the incoming, scattered, and ejected electrons, respectively, and $\vec{q}$ represents the momentum transfer. $\vec{b}$, $\vec{s}_1$, and $\vec{s}_2$ are the respective projections of the position vectors of the incident particle and the two bound electrons onto the plane perpendicular to the direction of the Glauber path integration. In Eq. (1), $\vec{q}$, $\vec{b}$, $\vec{s}_1$, and $\vec{s}_2$ are all coplanar; $\phi_i(\vec{r}_1,\vec{r}_2)$ and $\phi_f(\vec{r}_1,\vec{r}_2)$ represent, respectively, the wave functions of the initial and the final states of the target. For the initial state of He we have chosen the following form:

$$\phi_i(\vec{r}_1,\vec{r}_2)=u(\vec{r}_1)u(\vec{r}_2)\ , \tag{2}$$

where

$$u(\vec{r})=\lambda^{3/2}\pi^{-1/2}e^{-\lambda r}\ , \tag{3}$$

whereas for the final state of He, we have adopted the following:

$$\phi_f(\vec{r}_1,\vec{r}_2)=2^{-1/2}[\nu(\vec{r}_1)\chi^{-}_{\vec{k}_2}(\vec{r}_2)+\nu(\vec{r}_2)\chi^{-}_{\vec{k}_2}(\vec{r}_1)]\ , \tag{4}$$

where

$$\chi^{-}_{\vec{k}_2}(\vec{r})=(2\pi)^{-3/2}e^{\gamma\pi/2}\Gamma(1+i\gamma)e^{i\vec{k}_2\cdot\vec{r}}\times{}_1F_1(-i\gamma,1,-i(k_2r+\vec{k}_2\cdot\vec{r})) \tag{5}$$

with

$$\nu(\vec{r})=\lambda'^{3/2}\pi^{-1/2}e^{-\lambda' r}\ , \tag{6}$$

and

$$\gamma=Z/k_2\ . \tag{7}$$

In the present formalism, we have chosen $Z=\lambda$ so that $\phi_i(\vec{r}_1,\vec{r}_2)$ and $\phi_f(\vec{r}_1,\vec{r}_2)$ are orthogonal to each other.

Using Eqs. (2) and (4) in Eq. (1) we can express the scattering amplitude as

$$F(\vec{q},\vec{k}_2)=-C\frac{\partial}{\partial\lambda_1}\frac{\partial}{\partial\lambda}I(\vec{q},\vec{k}_2)\ , \tag{8}$$

where the generating function I is defined by

$$I(\vec{q},\vec{k}_2)=\int d\vec{b}\,d\vec{r}_1 d\vec{r}_2\frac{e^{-\lambda_1 r_1}}{r_1}\frac{e^{-\lambda r_2}}{r_2}\exp(-i\vec{k}_2\cdot\vec{r}_2+i\vec{q}\cdot\vec{b})\times{}_1F_1(i\gamma,1,i(k_2r_2+\vec{k}_2\cdot\vec{r}_2))\left[\frac{|\vec{b}-\vec{s}_1|}{b}\right]^{2i\eta}\left[\frac{|\vec{b}-\vec{s}_2|}{b}\right]^{2i\eta},$$

$$C=\frac{ik}{4}\pi^{-4}\lambda^3\lambda'^{3/2}e^{\gamma\pi/2}\Gamma(1-i\gamma)\ ,$$

and (9)

$$\lambda_1=\lambda+\lambda'\ .$$

With the use of the technique of Ref. 7 the eight-dimensional integral in Eq. (9) can be reduced to the following form:

$$F(\vec{q},\vec{k}_2)=-16\pi^2CD_1D_2^2\left[2\pi q^{-2}[f(p_\rho=0)H(\eta)+f(\vec{p}_\rho=\vec{q})H(-\eta)]+\int_0^\infty dp\frac{1}{p^{1-2i\eta}}\int_0^{2\pi}d\phi\frac{f(\vec{p}_\rho)-q^{-1}[(p^2+q^2-2pq\cos\phi)^{1/2}f(p_\rho=0)+p_\rho f(\vec{p}_\rho=\vec{q})]}{(p^2+q^2-2pq\cos\phi)^{1+i\eta}}\right], \tag{10}$$

where

$$f(\vec{p}_p)= -2\lambda_1[2\lambda(i\gamma-1)A^{i\gamma-2}(A-B)^{-i\gamma}-2i\gamma(\lambda-ik_2)A^{i\gamma-1}(A-B)^{-i\gamma-1}]$$
$$\times\left[\int_0^1 dz\frac{z^{-1-2i\eta}}{(p_p^2z^2+\lambda_1^2)^2}\,{}_2F_1(1-2i\eta,1-2i\eta;1;z^2)\right.$$
$$\left.+\int_0^1 dz\frac{z^{5-2i\eta}}{(p_p^2+\lambda_1^2z^2)^2}\,{}_2F_1(1-2i\eta,1-2i\eta;1;z^2)\right] \quad (11)$$

with

$$H(\eta)=\sum_{r=0}^{\infty}\frac{(\frac{1}{2}+i\eta)_r(\frac{1}{2}+i\eta)_r}{(1)_r r!}\times\left[\frac{1}{2(r+i\eta)}+\frac{1}{2r+1}\right], \quad (12)$$

$$A=k_2^2+\lambda^2+(\vec{p}_p-\vec{q})^2+2(\vec{p}_p-\vec{q})\cdot\vec{k}_{2p}, \quad (13)$$

$$B=2[k_2^2+i\lambda k_2+(\vec{p}_p-\vec{q})\cdot\vec{k}_{2p}], \quad (14)$$

and

$$D_1=\frac{\Gamma(2-4i\eta)\Gamma(\frac{1}{2})}{\Gamma(2i\eta)\Gamma(\frac{3}{2}+i\eta)}, \quad (15)$$

$$D_2=\frac{\Gamma(2+2i\eta)\Gamma(\frac{1}{2})}{\Gamma(-i\eta)\Gamma(\frac{3}{2}+i\eta)}. \quad (16)$$

The notations adopted here are those of Ref. 7.

The triply differential cross section for electron-impact ionization of He is given by[9]

$$\frac{d^3\sigma}{d\hat{k}_1 d\hat{k}_2 dE_2}=\frac{k_1k_2}{k}\,|F(\vec{q},\vec{k}_2)|^2, \quad (17)$$

where $d\hat{k}_1$ and $d\hat{k}_2$ denote, respectively, the elements of solid angle for the scattered and ejected electrons, and dE_2 represents the energy interval of the ejected electron.

III. NUMERICAL RESULTS AND DISCUSSION

We have adopted the numerical procedure of Ref. 7 to calculate the coplanar TDCS for the $He(e,2e)He^+$ process. The calculation is based upon the choice of z axis along the Glauber path integration, which is taken to be perpendicular to $\vec{q}$. We note that the numerical procedure described in Ref. 7 applies only to the coplanar geometry, i.e., $\Phi_2=0$ or π. This means that the Eqs. (33) and (34) of Ref. 7 cannot be used in general, although they hold good in the present coplanar case where $\Phi_2=\pi$.

The present calculation has been performed with two different choices of wave functions for the ground state of helium. Choice 1 involves the adoption of Hylleraas wave function[10] with $\lambda=1.6875$ whereas choice 2 concerns the use of the single-parameter Hartree-Fock wave function[11] with $\lambda=1.618$. The orthogonality condition of the initial and final states of the target is satisfied by the choice $Z=\lambda$ in Eq. (5). Table I presents our GA results for the coplanar TDCS along with the corresponding experimental data for the ionization of He by electron impact in the incident energy range 224.58–2824.58 eV for $E_1=E_2$, $\theta_1=\theta_2=45°$, $\Phi_1=0°$, and $\Phi_2=\pi$. We see that the GA cross sections obtained with the Hylleraas wave function (choice 1) are always smaller than those obtained with the single-parameter Hartree-Fock wave function (choice 2). At the incident energy of 2824.58 eV the cross section predicted by the Hartree-Fock choice differs from those by the Hylleraas choice by

TABLE I. Coplanar ($\Phi_1=0°$, $\Phi_2=\pi$) triply differential cross sections $d^3\sigma/d\hat{k}_1d\hat{k}_2dE_2$ in units of $10^{-5}a_0^2$ $eV^{-1}sr^{-2}$ for electron-impact ionization of He for various incident energies E with $E_1=E_2$ and $\theta_1=\theta_2=45°$.

$E-\epsilon$(eV)[a]	GA-HF[b]	GA-H[c]	Experiment[d]
200	75.6	66.4	58.6
300	53.9	47.5	47.6
400	40.6	35.9	42.0
500	31.9	28.3	29.8
600	25.9	23.0	27.4
800	18.3	16.3	17.4
1000	13.8	12.3	14.7
1500	8.08	7.21	9.19
2000	5.45	4.86	5.86
2800	3.39	3.03	3.44

[a]ϵ denotes the binding energy and is defined by $E-E_1-E_2$.
[b]Present Glauber approximation calculated with the single-parameter Hartree-Fock wave function for He.
[c]Present Glauber approximation calculated with the Hylleraas wave function for He.
[d]Reference 5.

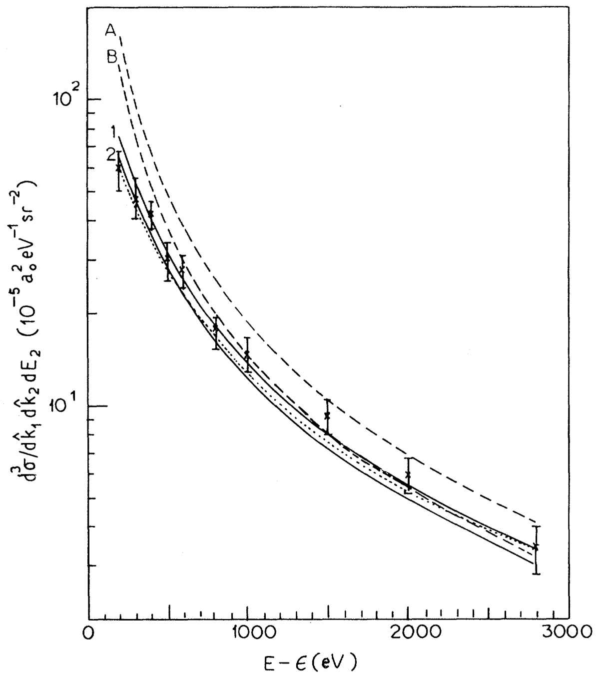

FIG. 1. Triply differential cross sections $d^3\sigma/d\hat{k}_1 d\hat{k}_2 dE_2$ vs energy $E-\epsilon$, where E is the incident energy and ϵ is the binding energy, for electron-impact ionization of helium. The solid curves 1 and 2 represent the present Glauber calculations with the single-parameter Hartree-Fock and Hylleraas wave functions for He, respectively. The dashed curves A and B are the first Born results with the Hartree-Fock and Hylleraas wave functions for He, respectively (Ref. 5). The dotted curve represents the eikonal-impulse approximation results of McCarthy with $\bar{V}=20$ (Ref. 5). The crosses are the experimental results of Ref. 5. All the cross sections are for $E_1=E_2$, $\theta_1=\theta_2=45°$, $\Phi_1=0$, and $\Phi_2=\pi$.

12% while at the incident energy of 224.58 eV they differ by about 14%. This means that with the decrease in incident energy the difference of cross sections predicted by the two choices does not alter substantially. In addition, we notice that the GA cross sections are in reasonably good agreement with experiment. As expected, the agreement decreases at lower energies.

Figure 1 shows a comparison of the present GA calculations with the first Born approximation[12] (FBA) and the eikonal-impulse approximation[13] (EIA) calculations and with the measurements of van Wingerden *et al.* We see that the EIA cross sections agree closely with the GA results. At lower energies the GA cross sections show improvement over the FBA cross sections. At high energies, however, the cross sections predicted by all the three methods nearly coincide with experiment.

IV. CONCLUSIONS

We have presented a method of obtaining triply differential cross sections for electron-impact ionization of helium in the Glauber approximation. This method reduces the eight-dimensional Glauber amplitude for the $He(e,2e)He^+$ process to a two-dimensional integral. The integrand of this integral, however, contains a sum of two one-dimensional integral functions that are computed numerically.

We have calculated coplanar TDCS for electron-impact ionization of He in the incident energy range 224.58−2824.58 eV with $E_1=E_2$, $\theta_1=\theta_2=45°$, $\Phi_1=0°$, and $\Phi_2=\pi$. The GA shows a definite improvement over the FBA, especially at low energies and yields cross sections in close agreement with the eikonal-impulse approximation of McCarthy. In addition, it shows reasonably good agreement with experiment. However, in order to study the usefulness of various theories, detailed absolute measurements involving asymmetric as well as noncoplanar cases would be extremely valuable.

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[12]See Ref. 5.

[13]See Ref. 5. The values plotted are those with $\bar{V}=20$.