### Double- and triple-differential cross sections for electron-impact ionization of helium

R. Biswas and C. Sinha

# Department of Theoretical Physics, Indian Association for the Cultivation of Science, Jadavpur, Calcutta 700 032, India (Received 15 August 1994; revised manuscript received 9 December 1994)

Triple- (TDCS) and double- (DDCS) differential cross sections have been calculated for single ionization in electron-helium collisions for asymmetric geometry at intermediate and medium high energies. The TDCS and DDCS results have been presented for different kinematical situations and have been compared with the corresponding experiments. In the present prescription, the final-state wave function involves the correlation between the two continuum electrons and satisfies the three-body asymptotic boundary condition (for asymmetric geometry), which is an important criterion for reliable ionization cross sections. The sensitivity of the ionization cross sections (particularly of the TDCS) with respect to the choice of the bound-state wave function of the He atom has also been studied, using two different forms of wave function of the He atom. The binary-to-recoil peak intensity ratio against momentum transfer in TDCS is found to be in closer agreement with the experiment for the simple Hylleraas wave function than for the Hartree-Fock wave function. The DDCS results are found to be in good agreement with the experimental data of Müller-Fiedler *et al.* [J. Phys. B 19, 1211 (1986)] for lower ejected energy  $(E_2)$ , while for higher  $E_2$  the results are closer to the measurements of Shyn *et al.* [Phys. Rev. A 19, 557 (1979)] and Avaldi *et al.* [Nuovo Cimento D 9, 97 (1987)].

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# **INTRODUCTION**

Recently much attention is being paid to the measurements of differential ionization cross sections (e.g. triple, double, and single) for electron- or positron-impact ionization of atoms. From the theoretical point of view, the triple-differential cross sections (TDCS's) are most important since they carry the most detailed information of the ionization process. The double-differential cross sections (DDCS's), on the other hand, though less sensitive to the details of the process, are much more relevant for practical applications in various branches of physics. Thus it is also equally worthwhile to calculate the DDCS and to compare it with experiments.

In the present work we have calculated the triple- and double-differential cross sections of the helium atom by electron impact. The theoretical model is mainly based on our earlier theory [1] developed for the hydrogen atom, where excellent agreement was noted with experiments in the TDCS calculation for electron-impact ionization in the intermediate- and high-energy region and for asymmetric and coplanar geometry. For ionization of helium atoms, however, further complications arise in the dynamics because of the presence of the two bound electrons, and effectively the problem turns into a four-body one in the final channel. Theoretically it thus becomes a rather difficult task to frame the model of the problem and one has to resort to some approximations. Apart from the dynamics, an additional difficulty arises due to inaccuracies of the approximate bound-state wave function of the helium atom in the initial channel. As for the dynamical description of the present model, the faster electron is treated in the framework of the eikonal approximation while for the ejected slower electron a screened Coulomb wave is considered. The final-state wave function involves a projectile-ejected-electron correlation term and satisfies the three-body asymptotic boundary condition for the ionization process in the asymmetric geometry (i.e.,  $k_1 \gg k_2$ ). It is now well established [2,3] that the validity of the three-body asymptotic boundary condition is one of the most important factors for prediction of reliable ionization cross sections. It should be mentioned in this context that the above asymptotic condition is also satisfied in the Brauner-Briggs-Klar (BBK) [2] model even for symmetric geometry, while the present prescription is particularly suitable for asymmetric geometry. The exchange effect between the two continuum electrons has also been taken into account for low incident energy (e.g., 150 eV).

In order to study the sensitivity of the ionization cross sections, particularly of the TDCS's, with respect to the choice of the initial bound-state wave functions, we have performed the calculations for two different wave functions of the He atom.

### THEORY

The prior form of the matrix elements for the direct and exchange process of  $e^-$  + He ionization is given by

$$f = \langle \Psi_f^-(\vec{r}_1, \vec{r}_2, \vec{r}_3) | V_i | \psi_i(\vec{r}_1, \vec{r}_2, \vec{r}_3) \rangle$$
(1a)

and

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$$g = \langle \Psi_f^-(\vec{r}_2, \vec{r}_1, \vec{r}_3) | V_i | \psi_i(\vec{r}_1, \vec{r}_2, \vec{r}_3) \rangle .$$
 (1b)

The total Hamiltonian H of the system is written as

$$H = \left[H_0 - \frac{Z_t}{r_1} - \frac{Z_t}{r_2} - \frac{Z_t}{r_3} + \frac{1}{r_{12}} + \frac{1}{r_{13}} + \frac{1}{r_{23}}\right], \quad (2)$$

where  $Z_t = 2$  is the charge of the target ion. The full

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kinetic-energy operator is given by

$$H_0 = -\frac{1}{2}\vec{\nabla}_1^2 - \frac{1}{2}\vec{\nabla}_2^2 - \frac{1}{2}\vec{\nabla}_3^2 , \qquad (3)$$

where  $\vec{r}_1, \vec{r}_2$ , and  $\vec{r}_3$  are the position vectors of the incoming electron 1 and the two bound electrons 2 and 3, respectively, with respect to the target nucleus;

$$\vec{r}_{12} = \vec{r}_1 - \vec{r}_2, \ \vec{r}_{23} = \vec{r}_2 - \vec{r}_3, \ \vec{r}_{13} = \vec{r}_1 - \vec{r}_3$$

The initial-channel wave function is chosen as

$$\psi_i(\vec{r}_1, \vec{r}_2, \vec{r}_3) = \exp(ik_i \cdot \vec{r}_1)\phi_i(\vec{r}_2, \vec{r}_3) , \qquad (4)$$

 $\vec{k}_i$  being the initial momentum of the incident particle.  $\phi_i$  is the bound-state wave function of the ground state of the helium atom. In the present work the following two forms of  $\phi_i$  are chosen: the simple Hylleraas wave function

$$\phi_i(\vec{r}_2, \vec{r}_3) = u(\vec{r}_2)u(\vec{r}_3) , \qquad (5)$$

where

$$u(r) = \frac{Z_t'^{3/2}}{\sqrt{\pi}} \exp(-Z_t'r)$$
,

 $Z'_{t}$  being the screened charge  $Z'_{t}=Z_{t}-\frac{5}{16}$ , and the Hartree-Fock wave function given by Byron and Joachain [4]. For single ionization the bound-state correlation effect can safely be neglected. From Eqs. (1)-(4) the perturbation interaction  $V_{i}$  [in Eq. (1)] in the initial channel is obtained as

$$V_i = -\frac{Z_i}{r_1} + \frac{1}{r_{12}} + \frac{1}{r_{13}}$$
 (6)

Equation (6) shows that the perturbation  $V_i$  vanishes asymptotically (for  $r_1 \rightarrow \infty$  and  $r_2, r_3$  finite).

In order to construct the final-channel wave function  $(\Psi_f^-)$ , which involves four particles, we assume that the bound passive electron plays no other role than to screen the nucleus from the two outgoing particles, thereby reducing the problem to a three-body one. The final-channel wave function  $\Psi_f^-$  in Eq. (1a) effectively satisfies the equation

$$\left[H_0 - \frac{Z_{\rm SC}}{r_1} - \frac{Z_{\rm SC}}{r_2} - \frac{Z_t}{r_3} + \frac{1}{r_{12}} - E\right] \Psi_f^- = 0 \tag{7}$$

with the screened charge  $Z_{\rm SC} = 1$ . *E* is the total energy of the system given by  $E = \frac{1}{2}k_1^2 + \frac{1}{2}k_2^2 + \varepsilon$ ;  $\varepsilon$  being the binding energy of the He<sup>+</sup> ground state. We thus write  $\Psi_f^-$  as

$$\Psi_{f}^{-}(\vec{r}_{1},\vec{r}_{2},\vec{r}_{3}) = \chi(\vec{r}_{1})\Phi(\vec{r}_{2},\vec{r}_{3}) .$$
(8)

The wave function  $\Phi(\vec{r}_2, \vec{r}_3)$  of the helium subsystem in the final channel is represented [5] by a symmetrized product of the He<sup>+</sup> ground-state wave function for the bound electron and the continuum wave function  $\bar{\phi}_{\vec{k}_2}$  for the ejected electron with momentum  $\vec{k}_2$  (orthogonalized to the ground-state orbital *u*). For the slower ejected electron ( $\vec{r}_2$ , say) we assume the following screened Coulomb wave function:

$$\phi_{\vec{k}_{2}}(\vec{r}_{2}) = (2\pi)^{-3/2} \exp(i\vec{k}_{2}\cdot\vec{r}_{2}) \exp(\frac{1}{2}\pi\alpha_{2})\Gamma(1+i\alpha_{2})$$
$$\times {}_{1}F_{1}(-i\alpha_{2};1;-i(k_{2}r_{2}+\vec{k}_{2}\cdot\vec{r}_{2}))$$
(9)

with  $\alpha_2 = 1/k_2$ ,  $\vec{k}_2$  being the momentum of the ejected electron. The wave function of the faster electron treated in the eikonal framework assumes the following form:

$$\chi(\vec{r}_1) = \exp(i\vec{k}_1 \cdot \vec{r}_1) \exp\left[i\eta_f \int_{z_1}^{\infty} \left(\frac{1}{r_{12}} - \frac{1}{r_1}\right) dz_1'\right]$$
(10)

with  $\eta_f = Z_{SC}/k_1$  and  $Z_{SC} = 1$ ;  $\vec{k}_1$  being the final momentum of the outgoing electron. Evaluating the phase integral in Eq. (10) we obtain

$$\exp\left[\int_{z_{1}}^{\infty} i\eta_{f}\left[\frac{1}{r_{12}}-\frac{1}{r_{1}}\right] dz_{1}'\right]$$
$$=\left[\frac{r_{1}+z_{1}}{r_{12}+z_{12}}\right]^{i\eta_{f}}$$
$$\equiv\exp[i\eta_{f}\ln(r_{1}+z_{1})-i\eta_{f}\ln(r_{12}+z_{12})], \quad (11)$$

 $z_1$  and  $z_{12}$  being the z components of the respective vectors. When evaluating the phase integral Eq. (11), the z axis is chosen along the direction of  $\vec{k}_1$ . It is evident from Eqs. (8) and (9)-(11) that the present final-state wave function that takes account of the electron-electron correlation effect satisfies the asymptotic three-body boundary condition for asymmetric geometry (i.e., for  $k_1 \gg k_2$ ).



FIG. 1. TDCS for the ionization of helium from the ground state by electron impact as a function of ejection angle  $\theta_2$ , for the case of incident energy  $E_i = 600 \text{ eV}$ , ejected energy  $E_2 = 10$ eV, and scattering angle  $\theta_1 = 4^{\circ}$ . —, present results using the Hylleraas wave function [Eq. (5)] for the ground state of the helium atom (without exchange); —, present results using the Hartree-Fock wave function [4] for the ground state of the helium atom (without exchange); --- results of Brauner, Briggs, and Broad [3]; •, experimental data (normalized) of Jung et al. [7].



FIG. 2. Same as Fig. 1 but with  $E_2 = 2.5$  eV.

Finally, the TDCS and DDCS are, respectively, given by (including exchange)

$$\frac{d^{3}\sigma}{d\Omega_{1}d\Omega_{2}dE_{2}} = \frac{k_{1}k_{2}}{k_{i}} \left[\frac{1}{4}|f+g|^{2} + \frac{3}{4}|f-g|^{2}\right], \quad (12)$$

$$\frac{d^2\sigma}{d\Omega_2 dE_2} = \int \left| \frac{d^3\sigma}{d\Omega_1 d\Omega_2 dE_2} \right| d\Omega_1 . \tag{13}$$

The ionization amplitude as described in Eq. (1) finally involves a two-dimensional integration, which has been evaluated numerically following the procedure adopted in our previous work for ionization of the hydrogenic atom [1,6] with necessary modifications for the helium atom.

### **RESULTS AND DISCUSSION**

We have computed the TDCS and DDCS for electronimpact ionization of the ground-state helium atom for cordance with the corresponding experiments. The present TDCS results for two different bound-state wave functions, mentioned earlier in the Theory section, are shown in Figs. 1-6 along with their corresponding experimental data [7,8] as well as some other theoretical results [3,5,9]. Figures 1 and 2 demonstrate a comparison between the present TDCS, the theoretical results of Brauner, Briggs, and Broad [3] and the experimental data of Jung et al. [7] for two different kinematical situations with the same incident energy  $(E_i)$  600 eV. The experimental data (normalized) of Jung et al. [7] have been taken from the work of Brauner, Briggs, and Broad [3]. As is observed from Figs. 1 and 2, the present results with the Hylleraas wave function are in quite good agreement with those of Brauner, Briggs, and Broad [3] (who also used the same wave function) as well as with the normalized experimental data [7], whereas with the Hartree-Fock (HF) wave function the present binary peak overestimates the experiment in both cases. As for the comparison of the present TDCS with the most exhaustive experiment of Schlemmer et al. [8] (see Figs. 3-6) it may be mentioned that the experimental data are absolute only at the impact energies 400 and 250 eV and the results for other energies are normalized to some theoretical results. It may be inferred from Figs. 1-6 that, in general, for lower scattering angles the results with the simple form [Eq. (5)] of wave function are in better agreement with experiment [8] than those with the HF wave function [4], while for higher scattering angles the reverse is true. The binary peak intensities are always higher with the HF wave function than with the Hylleraas type, while the recoil peak in some cases is lower (e.g., for higher  $E_2$ ) and in some cases higher (for lower  $E_2$ ) with the HF wave function. The percentage of change in the peak intensities varies from 2% to 30% for the different kinematical situations considered here for the two different wave functions.

some selected sets of dynamical parameters chosen in ac-

Figures 3 and 5 indicate that the theoretical models [5,9] that take account of the short-range correlation effect between the continuum and bound electrons give



FIG. 3. TDCS for the ionization of helium from the ground state by electron impact as a function of ejection angle  $\theta_2$ , for the case of  $E_i = 400 \text{ eV}$  and  $\theta_1 = 4^\circ$ . Set I for  $E_2 = 5 \text{ eV}$ and set II for  $E_2 = 10 \text{ eV}$ . —, present results using the Hylleraas wave function [Eq. (5)] for the ground state of the helium atom (without exchange); —, present results using the Hartree-Fock wave function [4] for the ground state of the helium atom (without exchange); —, results of Franz and Altick [9]; experimental points are those of Schlemmer *et al.* [8] ( $\bigcirc$  for set I and  $\bullet$  for set II).



FIG. 4. Same as Fig. 3 but set I for  $E_i = 250$ eV,  $E_2 = 10$  eV,  $\theta_1 = 10^\circ$  and set II for  $E_i = 400$ eV,  $E_2 = 10$  eV,  $\theta_1 = 10^\circ$ .





FIG. 6. Same as Fig. 1 but set I for  $E_i = 150$ eV,  $E_2 = 10$  eV,  $\theta_1 = 4^\circ$  and set II for  $E_i = 150$ eV,  $E_2 = 10$  eV,  $\theta_1 = 8^\circ$ . —, present result using the Hylleraas wave function [Eq. (5)] for the ground state of He (with exchange); —••--••-, present result using the Hylleraas wave function [Eq. (5)] for the ground state of He (without exchange); —, present result using the Hartree-Fock wave function [4] for the ground state of He (with exchange); —•--, present result using the Hartree-Fock wave function [4] for the ground state of He (without exchange). Experimental results are those of Schlemmer *et al.* [8] ( $\bigcirc$  for set I and  $\bullet$  for set II).

better TDCS results for low ejected energy. It should be pointed out that in the calculations of the other two theories [5,9] the HF wave function [4] was used.

The ratio of binary to recoil peak intensities  $I_{\rm bin}/I_{\rm rec}$ being independent of any normalization error is known to be a very sensitive parameter for testing both the dynamical description of the process and the quality of the wave functions. We have thus calculated this ratio for both the initial-state wave functions of the He atom and compared them with the corresponding experimental [8] and other theoretical [5,10] values for three different incident energies (400, 250, and 150 eV). Figures 7 and 8 demonstrate a comparative study of this ratio against the momentum transfer  $(\vec{Q})$ , for two fixed ejected energies ( $E_2 = 5$  and 10 eV). It may be noted from Fig. 7 that at 250 eV the present  $I_{bin}/I_{rec}$  ratio with the Hylleraas wave function is in good agreement with experiment [8] while at the other two energies (400 and 150 eV) the corresponding present curve lies a little above the experiment. However, at 400 eV, the agreement is better than at 150 eV. In these two cases the CB2 (second Born approximation with improved final state) curves [5] that take account of the short-range correlation effect are in better agreement with the experiment [8]. In contrast, for the HF wave



FIG. 7. Binary-to-recoil peak intensity ratio  $(I_{\rm bin}/I_{\rm rec})$  has been plotted against the momentum transfer  $\vec{Q}$  for three different incident energies (400, 250, and 150 eV) and for fixed ejected energy  $E_2 = 5$  eV. \_\_\_\_, present ratio for the Hylleraas wave function [Eq. (5)]; \_\_\_\_\_, present ratio for the Hartree-Fock wave function [4]; \_\_\_\_\_, second Born approximation with Coulomb wave function [10]; \_\_\_\_, second Born approximation with improved final state [5]; \_\_\_\_\_\_, modified Glauber approximation [5]; •, experimental results of Schlemmer *et al.* [8].



FIG. 8. Same as Fig. 7 but for  $E_2 = 10$  eV.

function, the present  $I_{\rm bin}/I_{\rm rec}$  ratio is always much higher than the experimental values [8]. It thus appears that with the improved wave function the  $I_{\rm bin}/I_{\rm rec}$  ratio always increases. The reason is that, with improvement in the bound-state wave function, the binary peak always increases, sometimes quite appreciably for certain kinematical situations, whereas the change in the recoil peak is not very significant. This feature, which is also in conformity with the findings of Franz and Klar [11], seems to be quite reasonable since the binary-peak distribution is mostly governed by the initial momentum distribution. For higher value of the ejection energy,  $E_2=10$ eV (vide Fig. 8), the  $I_{\rm bin}/I_{\rm rec}$  ratios are always much closer to experiment than for  $E_2=5$  eV, as expected. In this case also the ratio increases for the HF wave function.

The closer agreement of the present TDCS results with experiment obtained with the simpler bound-state wave function [Eq. (5)] than with the improved one [4] may possibly be attributed to the fact that the former is more or less consistent with the present final-state prescription of the target continuum while for the latter the description may not be proper. To obtain similar or even better (for some kinematical situations) agreement with the improved wave function, simultaneous improvement should be made particularly in the description of the target-state continuum. In other words, the continuum-boundelectron correlation effect should also be taken into account instead of considering the target-ejected-electron interaction to be purely Coulombic (as is done in the present model). This will also improve the corresponding



FIG. 9. DDCS for the ionization of helium from the ground state by electron impact as a function of ejection angle  $\theta_2$ , for the case of  $E_i = 300 \text{ eV}$  and  $E_2 = 10 \text{ eV}$ . —, present results using the Hylleraas wave function [Eq. (5)] for the ground state of the helium atom; —, present results using the Hartree-Fock wave function [4] for the ground state of the helium atom;  $\bigcirc$ , experimental data of Shyn and Sharp [13];  $\blacklozenge$ , experimental data of Müller- Fiedler, Jung, and Ehrhardt [12].

 $I_{\rm bin}/I_{\rm rec}$  ratio towards the experimental data, since as mentioned before the improvement in the initial bound-state wave function influences mostly the binary peak, whereas a better description of the low-energy ejected electron leads to relatively more dominant changes in the recoil intensity.

Regarding the comparison of the present DDCS's with experiment, it should first be pointed out that large discrepancies exist in the absolute values as well as in the shapes of the angular distributions obtained from the experimental data due to different groups [12-14]. Since the DDCS calculation with the HF wave function [4] in-



FIG. 10. Same as Fig. 9 but  $E_i = 300 \text{ eV}$  and  $E_2 = 20 \text{ eV}$ .



FIG. 11. Same as Fig. 9 but  $E_i = 200 \text{ eV}$  and  $E_2 = 20 \text{ eV}$ .

volves a lot of computer time, we have run our DDCS program with the Hylleraas wave function only, except for two cases to be described below, in order to save our computer time. Further, the  $I_{\rm bin}/I_{\rm rec}$  ratio in the TDCS for the Hylleraas wave function has been found to be in much better agreement with experiment than the same obtained from the HF wave function. This adds further justification for the calculation of DDCS's with the Hylleraas wave function.

For lower ejected energy (e.g.,  $E_2 = 10$  eV, Fig. 9), the present DDCS (with the Hylleraas wave function) is in better accord with the measurements of Müller-Fiedler, Jung, and Ehrhardt [12] while for higher  $E_2$  (e.g., 20 and 40 eV), the results compare better with the findings of Shyn and Sharp [13]. (see Figs. 10 and 11) and Avaldi *et al.* [14] (see Fig. 12). However, it may be noted that there is a marked difference between the present DDCS's



FIG. 12. Same as Fig. 9 but  $E_i = 500$  eV and  $E_2 = 40$  eV.  $\Delta$ , experimental data of Avaldi *et al.* [14].

and the results of Shyn and Sharp [13] at low ejection angles  $(0^{\circ}-30^{\circ})$  where the experiment shows a sharp rise at around 6° for all sets of parameters quoted here (see Figs. 9–11). In fact, this particular feature is not present in any other DDCS experiments [12,14] nor in other existing theories [15,16].

In order to have a feeling of how the effect of the change in the wave function of the He atom is reflected in the DDCS results, we have also calculated the DDCS with the HF wave function for the parameters  $E_i = 300$ eV and  $E_2 = 10$  and 20 eV (see Figs. 9 and 10). For lower  $E_2$  (Fig. 9), the results with the HF wave function are found to be higher than those obtained with the Hylleraas wave function throughout the range of the ejection angle  $(\theta_2)$ , while for higher  $E_2$  (see Fig. 10) the curves intersect each other at two points in the angular range 45°-100°. Figures 9 and 10 also demonstrate that with increasing  $E_2$  the separation between the two curves corresponding to the two different wave functions decreases in the peak region. It may also be seen from Figs. 9 and 10 that for a particular incident energy the DDCS peak that occurs in the range of 45°-90° for the ejection angle becomes sharper but less in magnitude with increasing ejected energy. This feature, which is physically understood [17], is also manifested in the experimental results [12-14,17].

#### CONCLUSIONS

The present TDCS and DDCS results are in good agreement particularly for higher ejected energy  $(E_2)$ .

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This is quite justified since for low ejected energy (e.g., 5 eV) a better description for the ejected electron (e.g., taking account of short-range effects) is needed [5,9], while for higher  $E_2$  a screened Coulomb wave, as is usually considered, is expected to be adequate. This is also reflected in the binary-to-recoil ratio curves (see Figs. 7 and 8). In fact, any improvement in the description of the low-energy electron improves the binary-to-recoil ratio. Improvement in the helium wave function does not necessarily mean a better  $I_{\rm bin}/I_{\rm rec}$  ratio. In fact, the ratio obtained from the improved wave function [4] increases appreciably as compared to experiment. To obtain a better TDCS result (as well as the ratio) with the improved bound-state wave function, the inclusion of short-range correlation between the continuum and bound electrons is probably needed.

It thus appears that improvement in the final-state wave function plays a much more important role than the quality of the initial bound-state wave function in obtaining a better agreement of ionization cross sections (particularly the triple one) with experiment. Finally, in view of the agreement of the present DDCS's with experiment, it may be inferred that even with the simple Hylleraas wave function a first-order theory in which the final-state wave function satisfies the proper asymptotic boundary condition can yield reasonably reliable DDCS results. The remaining discrepancies between the present DDCS results and experiment may be attributed to the neglect of exchange and the short-range correlation effect in the final channel.

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