Triple-differential cross sections for the electron- and positron-impact ionization of helium in an improved second Born approximation

Sadhana Sharma and M. K. Srivastava
Department of Physics, University of Roorkee, Roorkee 247 667, India
(Received 14 September 1987)

The triple-differential cross sections for the electron-impact ionization of helium in coplanar asymmetric geometry have been calculated by use of a second Born approximation which employs an improved choice for the target continuum-state wave function. The results are compared with the absolute experimental data of K. Jung *et al.* [J. Phys. B **18**, 2955 (1985)] at an incident energy of 600 eV and are found to be in very good agreement with them. The corresponding results for the positron-impact case are also presented.

I. INTRODUCTION

In the last few years there has been much activity, both experimental and theoretical, related to measuring or calculating triple-differential cross sections (TDCS) for the electron-impact ionization of atoms. The TDCS for this process are found to be quite sensitive to the model used for their theoretical description. This is particularly true in the case of an asymmetric (Ehrhardt-type) kinematical arrangement. Most of the ionizing collisions at high incident-electron energies lead to (i) an asymmetric partitioning of energy between the two outgoing electrons in the final state and (ii) a small momentum transfer. For a fast incident electron (energy E_0, momentum $\mathbf{k}_0$) and a fixed asymmetric energy partitioning, the angular distribution of the slow "ejected" electron (energy E_b, momentum $\mathbf{k}_b$), at a fixed small scattering angle θ_a for the fast "scattered" electron (energy E_a, momentum $\mathbf{k}_a$) shows a two-peaked structure; a peak (called the binary peak) near the momentum transfer ($\mathbf{q}=\mathbf{k}_0-\mathbf{k}_a$) direction and a subsidiary one (called the recoil peak) near the opposite direction. The calculations aim at predicting this angular distribution and, in particular, the magnitudes and angular positions of the binary- and recoil-peak intensities.

The calculations have been carried out using the second Born (B2) approximation,[1,2] the eikonal-Born series[3] and the unitarized eikonal-Born series approaches,[4] the modified Glauber (MG) approximation,[5,6] and the close-coupling method with pseudostates.[7] It is found that even at fairly high incident energies the second Born term of the direct scattering amplitude must be included to obtain symmetry-breaking of the angular distribution about the momentum-transfer direction and a reasonable ratio of the binary-to-recoil peak intensity maxima. The higher-order terms included in the MG approximation are important only if the scattering angle is not too small. In general, one is able to get better results in the case of hydrogen than in the case of helium. The reason is that the standard Coulomb-wave-function description (in the field of a point charge $Z=1$) for the slow ejected electron in the final state is alright in the case of hydrogen but a similar description for the ejected electron in the field of the residual He^+ ion is not good enough. All the calculations referred to above describe the ejected electron by the standard Coulomb wave function. A better choice of the low-energy ejected-electron wave function taking some account of continuum-electron–bound-electron correlations has been tried by Franz and Klar[8] within the framework of the first Born (CB1) approximation and is found to lead to a considerable improvement in the binary-to-recoil peak intensity ratio compared to the usual first Born (B1) approximation. A hybrid second-order model, in which the first-Born amplitude is calculated by using an improved target continuum wave function and the second Born amplitude in the usual way, though inherently inconsistent, has recently been used by us[9] successfully, with very good results to analyze the absolute TDCS data of Jung *et al.*[10] for the ionization of helium in coplanar asymmetric geometry at an incident electron energy $E_0=600$ eV.

We report in this paper a calculation of TDCS for the ionization of helium using an improved second Born (CB2) approximation. It consistently employs an improved wave function for the low-energy electron instead of its being described by just a Coulomb wave, both in the first Born and the second-Born amplitudes. Preliminary results obtained by using this approach have already been reported.[11] They show a very good agreement with the data of Jung *et al.*[10] A similar calculation using correlated initial- and final-state wave functions for helium has recently been reported by Furtado and O'Mahony.[12]

In Sec. II we present details of the calculation. The results are described and discussed in Sec. III. Atomic units have been used throughout.

II. CALCULATION

The direct scattering amplitude in the present second Born approximation is given by

$$F_{\mathrm{CB2}}=f_{\mathrm{CB1}}+f_{\mathrm{CB2}}\ , \tag{1}$$

where f_{CB1} and f_{CB2} are, respectively, the improved first-and second-order Born amplitudes. The amplitude $f_{\rm CB1}$ is given by

$$f_{\rm CB1}=-\frac{1}{2\pi}\left\langle e^{i\mathbf{k}_a\cdot\mathbf{r}_0}\Phi_{\mathbf{k}_b}(\mathbf{r}_1,\mathbf{r}_2)\left|\frac{1}{r_{01}}+\frac{1}{r_{02}}\right|\times\Phi_0(\mathbf{r}_1,\mathbf{r}_2)e^{i\mathbf{k}_0\cdot\mathbf{r}_0}\right\rangle . \quad (2)$$

Here $\mathbf{r}_0$, $\mathbf{r}_1$, and $\mathbf{r}_2$ are, respectively, the position vectors of the incident particle and two bound electrons. For the initial state of helium we have chosen the analytical fit to the Hartree-Fock wave function given by Byron and Joachain:[13]

$$\Phi_0(\mathbf{r}_1,\mathbf{r}_2)=u(\mathbf{r}_1)u(\mathbf{r}_2) ,$$
$$u(\mathbf{r})=\sum_{i=1}^{2}\gamma_i e^{-\alpha_i r} , \quad (3)$$

with $\alpha_1=1.41$, $\alpha_2=2.61$, $\gamma_1=0.734\,85$, $\gamma_2=0.587\,15$.

The final-state wave function $\Phi_{\mathbf{k}_b}$ is taken to be the symmetrized product of the He^+ ground-state wave function $v(\mathbf{r})$ for the bound electron with the continuum wave function $\Psi_{\mathbf{k}_b}^{(-)}(\mathbf{r})$ [orthogonalized to the ground-state orbital $u(\mathbf{r})$] for the ejected electron:

$$\Phi_{\mathbf{k}_b}(\mathbf{r}_1,\mathbf{r}_2)=\frac{1}{\sqrt{2}}[\Psi_{\mathbf{k}_b}^{(-)}(\mathbf{r}_1)v(\mathbf{r}_2)+\Psi_{\mathbf{k}_b}^{(-)}(\mathbf{r}_2)v(\mathbf{r}_1)] , \quad (4)$$

$$v(\mathbf{r})=\left[\frac{\lambda^3}{\pi}\right]^{1/2}e^{-\lambda r} , \quad \lambda=2 \quad (5)$$

$$\Psi_{\mathbf{k}_b}^{(-)}(\mathbf{r})=\psi_{\mathbf{k}_b}^{(-)}(\mathbf{r})-\langle u\mid\psi_{\mathbf{k}_b}^{(-)}\rangle u(\mathbf{r}) . \quad (6)$$

Using Eqs. (3)–(6) in Eq. (2) and integrating with respect to $\mathbf{r}_0$, we get

$$f_{\rm CB1}=\frac{-2\sqrt{2}}{q^2}\langle v\mid u\rangle[\langle\psi_{\mathbf{k}_b}^{(-)}(\mathbf{r})\mid e^{i\mathbf{q}\cdot\mathbf{r}}\mid u(\mathbf{r})\rangle-\langle u(\mathbf{r})\mid\exp(i\mathbf{q}\cdot\mathbf{r})\mid u(\mathbf{r})\rangle\times\langle\psi_{\mathbf{k}_b}^{(-)}\mid u\rangle] , \quad (7)$$

where $\mathbf{q}=\mathbf{k}_0-\mathbf{k}_a$. The wave function $\psi_{\mathbf{k}_b}^{(-)}$ is written as

$$\psi_{\mathbf{k}_b}^{(-)}(\mathbf{r})=\psi_{C,\mathbf{k}_b}^{(-)}(\mathbf{r})+[\psi_{\mathbf{k}_b}^{(-)}(\mathbf{r})-\psi_{C,\mathbf{k}_b}^{(-)}(\mathbf{r})]$$
$$=\psi_{C,\mathbf{k}_b}^{(-)}(\mathbf{r})+\chi_{\mathbf{k}_b}^{(-)}(\mathbf{r}) , \quad (8)$$

where $\psi_{C,\mathbf{k}_b}^{(-)}$ is the Coulomb wave (corresponding to $Z=1$) with appropriate boundary conditions

$$\psi_{C,\mathbf{k}_b}^{(-)}=e^{-\pi\eta/2}\overline{\Gamma(1-i\eta)}e^{i\mathbf{k}_b\cdot\mathbf{r}}\,{}_1F_1(i\eta;1,-ik_br-i\mathbf{k}_b\cdot\mathbf{r}) ,$$
$$\eta=-1/k_b . \quad (9)$$

The correction $\chi_{\mathbf{k}_b}^{(-)}(\mathbf{r})=[\psi_{\mathbf{k}_b}^{(-)}(\mathbf{r})-\psi_{C,\mathbf{k}_b}^{(-)}(\mathbf{r})]$ is expressed in the partial-wave form

$$\chi_{\mathbf{k}_b}^{(-)}(\mathbf{r})=\sum_l i^l(2l+1)[e^{-i\delta_l}R_l(r)-e^{-i\delta_l^C}R_l^C(r)]\times P_l(\hat{\mathbf{k}}_b\cdot\hat{\mathbf{r}}) . \quad (10)$$

Here $R_l^C(r)$ is the lth partial Coulomb wave and δ_l^C is the corresponding Coulomb phase shift. The radial solution $R_l(r)$ and the phase shift δ_l are obtained by solving the radial Schrödinger equation in the static field of the He^+ ion. Using Eqs. (8) and (10) in Eq. (7), one obtains finally

$$f_{\rm CB1}=f_{\rm B1}-\frac{2^{7/2}\pi}{q^2}C_1(0)[\sum_l(2l+1)P_l(\hat{\mathbf{q}}\cdot\hat{\mathbf{k}}_b)D_l(q)-C_2(q)D_0(0)] , \quad (11)$$

where

$$C_1(q)=\int v(\mathbf{r})u(\mathbf{r})e^{i\mathbf{q}\cdot\mathbf{r}}d\mathbf{r}$$
$$=(512\pi)^{1/2}\sum_i\gamma_i\frac{\alpha_i+2}{[(\alpha_i+2)^2+q^2]^2} , \quad (12)$$

$$C_2(q)=\int u^2(\mathbf{r})e^{i\mathbf{q}\cdot\mathbf{r}}d\mathbf{r}$$
$$=8\pi\sum_i\sum_j\gamma_i\gamma_j\frac{\alpha_i+\alpha_j}{[(\alpha_i+\alpha_j)^2+q^2]^2} , \quad (13)$$

and

$$D_l(q)=\int u(r)j_l(qr)[e^{i\delta_l}R_l(r)-e^{i\delta_l^C}R_l^C(r)]r^2dr . \quad (14)$$

The amplitude $f_{\rm B1}$ is the usual first Born amplitude which is evaluated in the standard way.[2,6] The second term in Eq. (11) represents the correction due to the improved choice, Eq. (8), in place of $\psi_{C,\mathbf{k}_b}^{(-)}(\mathbf{r})$ for the ejected-electron wave function. The radial integral in Eq. (14) is evaluated numerically.

The second Born term $f_{\rm CB2}$ may be written as

$$f_{\rm CB2}=\frac{1}{8\pi^4}\int d\mathbf{q}'\frac{1}{q'^2-p^2-i\epsilon}M , \quad (15)$$

where

$$M=\frac{16\pi^2}{q_i^2q_f^2}\langle\Phi_{\mathbf{k}_b}(\mathbf{r}_1,\mathbf{r}_2)\mid(e^{-i\mathbf{q}_f\cdot\mathbf{r}_1}+e^{-i\mathbf{q}_f\cdot\mathbf{r}_2}-2)\times(e^{i\mathbf{q}_i\cdot\mathbf{r}_1}+e^{i\mathbf{q}_i\cdot\mathbf{r}_2}-2)\mid\Phi_0(\mathbf{r}_1,\mathbf{r}_2)\rangle ,$$
$$p^2=k_0^2-2\bar{\omega} , \quad (16)$$
$$\mathbf{q}_i=\mathbf{k}_0-\mathbf{q}' , \quad \mathbf{q}_f=\mathbf{k}_a-\mathbf{q}' .$$

The excitation energies of the intermediate states have been approximated by an average excitation energy $\bar{\omega}$ (=0.9 a.u.) and the sum over them carried out by using the closure property. Using Eqs. (3), (4), and (12)–(14) in Eq. (16), one obtains

$$M=\frac{16\sqrt{2}\pi^2}{q_i^2q_f^2}[C_1(q_f)\langle\Psi_{\mathbf{k}_b}^{(-)}(r_1)\,|\,e^{i\mathbf{q}_i\cdot\mathbf{r}_1}\,|\,u(r_1)\rangle+C_1(q_i)\langle\Psi_{\mathbf{k}_b}^{(-)}(r_2)\,|\,e^{-i\mathbf{q}_f\cdot\mathbf{r}_2}\,|\,u(r_2)\rangle$$
$$+C_1(0)\langle\Psi_{\mathbf{k}_b}^{(-)}(r_1)\,|\,e^{i\mathbf{q}\cdot\mathbf{r}_1}-2e^{i\mathbf{q}_i\cdot\mathbf{r}_1}-2e^{-i\mathbf{q}_f\cdot\mathbf{r}_1}\,|\,u(r_1)\rangle]\ , \tag{17}$$

which, by using Eqs. (6), (8), and (10) and partial-wave decomposition, finally leads to

$$M=M_C+\frac{16\sqrt{2}\pi^2}{q_i^2q_f^2}\Bigg[4\pi\sum_l(2l+1)\{C_1(0)D_l(q)P_l(\hat{\mathbf{q}}\cdot\hat{\mathbf{k}}_b)+[C_1(q_f)-2C_1(0)]D_l(q_i)P_l(\hat{\mathbf{q}}_i\cdot\hat{\mathbf{k}}_b)$$
$$+[C_1(q_i)-2C_1(0)]D_l(q_f)P_l(\hat{\mathbf{q}}_f\cdot\hat{\mathbf{k}}_b)\}$$
$$-\{C_2(q)-2[C_2(q_i)+C_2(q_f)]+4\pi[C_1(q_f)C_2(q_i)+C_1(q_i)C_2(q_f)]\}D_0(0)\Bigg] \tag{18}$$

where M_C corresponds to the contribution in the usual second-Born amplitude f_{B2}. It is evaluated by following the method of Ehrhardt *et al.*[2] and Baliyan and Srivastava.[6] The second term on the right-hand side of Eq. (18) represents the correction due to the choice $\psi_{\mathbf{k}_b}^{(-)}(\mathbf{r})$ rather than the standard Coulomb wave $\psi_{C,\mathbf{k}_b}^{(-)}(\mathbf{r})$ for the ejected electron.

The summation over l in Eqs. (11) and (18) is carried out only up to $l=2$. This is found to be good enough for low-energy ejected electrons in which we are interested here. The integration over $\mathbf{q}'$ in Eq. (15) is performed numerically and the TDCS are finally calculated by using expression

$$\frac{d^3\sigma_{\text{CB2}}}{d\Omega_a d\Omega_b dE_b}=\frac{k_ak_b}{k_0}\,|\,F_{\text{CB2}}\,|^2\ . \tag{19}$$

The exchange contribution has been ignored as it is expected to be unimportant for highly asymmetric energy sharing between the two outgoing electrons and for small q in which we are interested here.

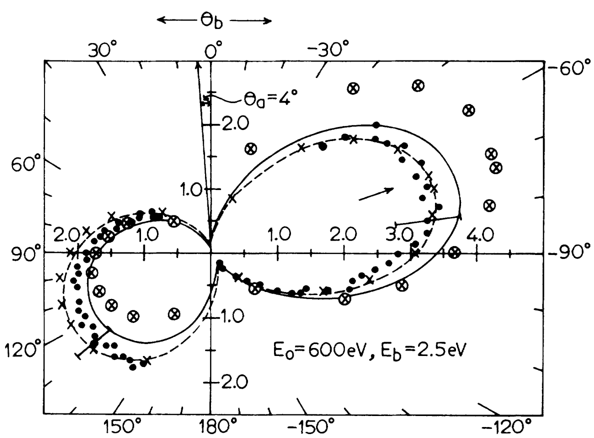

FIG. 1. Triple-differential cross sections in units of 10^{-22} $\text{m}^2\,\text{sr}^{-2}\,\text{eV}^{-1}$ for the ionization of helium at $E_0=600$ eV, $E_b=2.5$ eV, $\theta_a=4°$. Theoretical results: usual second Born approximation (B2) (Ref. 6) ——, and hybrid approach (Ref. 9) —·— — for electrons; present results for e^-, ×; for e^+, ⊗. Experimental data ● are the absolute measurements of Jung *et al.* (Ref. 10). The arrow indicates the direction of momentum transfer.

III. RESULTS AND DISCUSSION

Figures 1–4 show our coplanar CB2 results at an incident electron energy $E_0=600$ eV for Fig. 1: $\theta_a=4°$, $E_b=2.5$ eV, Fig. 2: $\theta_a=8°$, $E_b=2.5$ eV, Fig. 3: $\theta_a=4°$, $E_b=10$ eV, Fig. 4: $\theta_a=8°$, $E_b=10$ eV along with those obtained by using the usual second Born approximation B2 (Ref. 6) and hybrid approach (Ref. 9). The arrow indicates the direction of the momentum transfer $\mathbf{q}$. The theoretical results are compared with the recent absolute measurement of Jung *et al.*[10] The present calculations have been done only at some typical angles θ_b because of computation time limitations.

The present results are in very good agreement with the experimental data for all the cases considered here. There is a remarkable reduction in size of binary peak and a significant enhancement in the size of recoil peak compared to usual second Born results. Quantitatively, the CB2 results reduce the binary-peak maximum by about 10–15 % compared to B2 in the cases considered here. The corresponding changes on the recoil side range from about 20% to 50%. The improvement in the description of the low-energy ejected electron in the final state thus leads to relatively more dominant changes on the recoil side. There is no perceptible change in the angular positions of the binary and recoil peaks. The closeness of the present CB2 results to those obtained by using

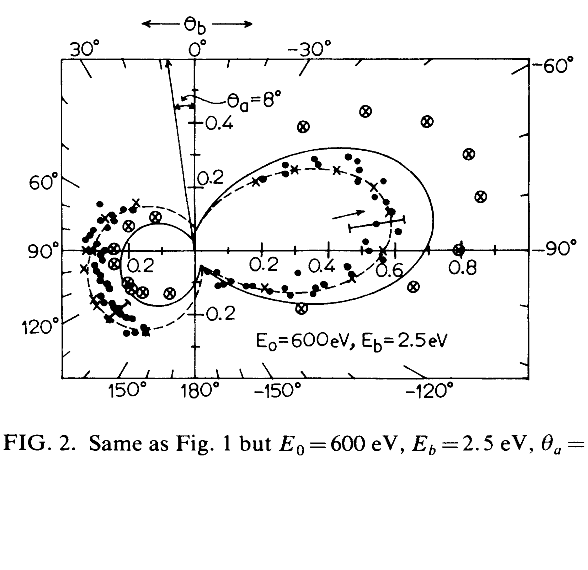

FIG. 2. Same as Fig. 1 but $E_0=600$ eV, $E_b=2.5$ eV, $\theta_a=8°$.

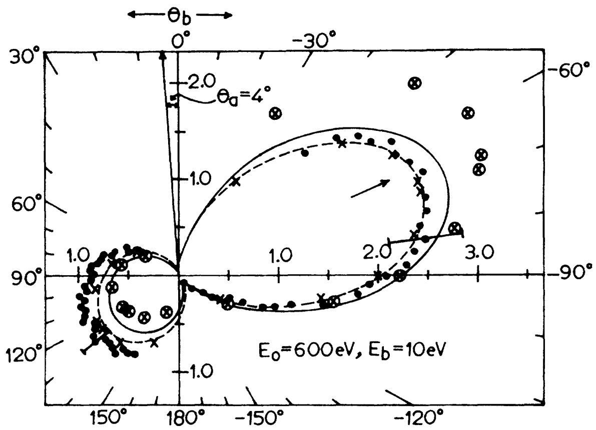

FIG. 3. Same as Fig. 1 but $E_0 = 600$ eV, $E_b = 10.0$ eV, $\theta_a = 4°$.

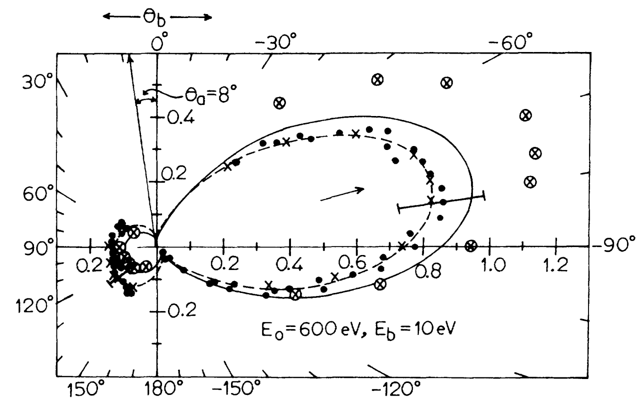

FIG. 4. Same as Fig. 1 but $E_0 = 600$ eV, $E_b = 10.0$ eV, $\theta_a = 8°$.

the hybrid approach[9] shows that one needs only to improve the helium continuum wave function in the first-Born term. The second-Born term is found to be much less sensitive to this change at this energy. The same is expected to be true for still higher-order terms which are needed when the momentum transfer is not small.

Taking advantage of the good agreement of the present CB2 results with the experimental data, we have also indicated in Figs. 1–4 the corresponding results for the positron-impact ionization of helium. The effect of the positronium formation channel has been ignored in the present kinematical situations where one of the outgoing particles is very energetic compared to the other. The binary peak is found to shift towards smaller angle θ_b relative to the momentum-transfer direction. A similar shift is observed in the recoil-peak region. The binary-(recoil-) peak intensity here is of larger (smaller) magnitude compared to the electron-impact case. There are, however, no experimental data with which to compare.

To conclude, the present results underscore the importance of a proper description of the low-energy ejected electron along with at least a second-order treatment of the ionization process. The available experimental data, however, do not warrant the use of any sophisticated wave function in the second Born term of the scattering amplitude.

ACKNOWLEDGMENTS

This work was supported by the Indian Space Research Organization. One of us (S.S.) would like to thank the University Grants Commission for support.

[1]F. W. Byron, Jr., C. J. Joachain, and B. Piraux, J. Phys. B **13**, L673 (1980); **15**, L293 (1982).

[2]H. Ehrhardt, M. Fischer, K. Jung, F. W. Byron, Jr., C. J. Joachain, and B. Piraux, Phys. Rev. Lett. **48**, 1807 (1982).

[3]F. W. Byron, Jr., C. J. Joachain, and B. Piraux, Phys. Lett. **99A**, 427 (1983); **106A**, 299 (1984); J. Phys. B **18**, 3203 (1985).

[4]F. W. Byron, Jr., C. J. Joachain, and R. M. Potvliege, J. Phys. B **14**, L609 (1981); **15**, 3915 (1982); **18**, 1637 (1985).

[5]K. S. Baliyan and M. K. Srivastava, Phys. Rev. A **32**, 3098 (1985); **33**, 2155 (1986).

[6]K. S. Baliyan and M. K. Srivastava, J. Phys. B **19**, 3603 (1986).

[7]E. P. Curran and H. R. J. Walters, J. Phys. B **20**, 337 (1987).

[8]A. Franz and H. Klar, Z. Phys. D **1**, 33 (1986).

[9]Sadhana Sharma and M. K. Srivastava, Phys. Rev. A **35**, 1939 (1987).

[10]K. Jung, R. Muller-Fiedler, P. Schlemmer, H. Ehrhardt, and H. Klar, J. Phys. B **18**, 2955 (1985).

[11]M. K. Srivastava and Sadhana Sharma, Phys. Rev. A (to be published).

[12]F. Mota Furtado and P. F. O'Mahony, J. Phys. B **20**, L405 (1987).

[13]F. W. Byron, Jr. and C. J. Joachain, Phys. Rev. **146**, 1 (1966).