Triple-differential cross sections for the ionization of helium by fast electrons

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The triple-differential cross section for the single ionization of helium in the coplanar asymmetric geometry has been calculated by using a second Born approximation which employs an improved choice of the target continuum-state wave function. The contribution of still higher-order terms of the scattering amplitude is also considered via the usual Glauber approximation. The results are compared with the recent data of Jung *et al.* at an incident energy of 600 eV and are found to be in very good agreement with them.

The present paper aims at improving our understanding of atomic ionization by fast electrons. The interest in this area is evinced by the volume of activity, both experimental as well as theoretical, connected with measuring and/or calculating triple-differential cross sections (TDCS) during the last few years. The TDCS for this process are found to be quite sensitive to the model used for its theoretical treatment. This is particularly so in the case of asymmetric (Ehrhardt-type) kinematical arrangement. Most of the ionizing collisions at high incident energies lead to such energy partitioning between the outgoing electrons and a small momentum transfer. In such a situation, for a fast incident electron, the angular distribution of the slow electron at a fixed small scattering angle for the fast (scattered) electron has a two-peaked structure: a peak (binary peak) near the momentum-transfer direction and another subsidiary one (recoil peak) near the opposite direction. Despite significant progress achieved in the understanding of this process during the last few years, the results are generally not satisfying in agreement with experiment even at high incident energies. The development in the theory beyond the first Born (B1) approximation has proceeded along the following lines.

(i) Distorted-wave Born approximation including the Coulomb-projected Born approximation.[1,2]

(ii) Second Born (B2) approximation which has been shown to essentially reproduce all the main characteristic features (angular positions of the binary and recoil peak maxima and the ratio of binary to recoil peak intensities) of the TDCS angular distribution.[3]

(iii) Eikonal-Born series (EBS) approach to consistently include all contributions up to order k^{-2} in the direct scattering amplitude,[4]

$$f_{\mathrm{EBS}}=f_{\mathrm{B1}}+f_{\mathrm{B2}}+f_{\mathrm{G3}} \; . \tag{1}$$

Here f_{B1}, f_{B2}, and f_{G3} are, respectively, the first-order Born, second-order Born, and third-order Glauber (G3) scattering amplitudes.

(iv) Modified Glauber (MG) approximation[5] to include still higher-order ($n>3$) terms of the direct scattering amplitude,

$$f_{\mathrm{MG}}=f_{\mathrm{G}}-f_{\mathrm{G2}}+f_{\mathrm{B2}} \; . \tag{2}$$

Here f_{G2} and f_{G} are, respectively, the second-order Glauber and the full Glauber scattering amplitudes. The MG approximation is found to further improve the B2 results in the cases where the scattering angle θ_a is not too small.[6]

(v) Unitarized Eikonal-Born series (UEBS) approach[7] which contains the MG approximation and consistently includes leading correction to the Glauber phase,

$$f_{\mathrm{UEBS}}=f_{\mathrm{W}}-f_{\mathrm{W2}}+f_{\mathrm{B2}} \; , \tag{3}$$

where f_{W} and f_{W2} are the full Wallace and the second-order Wallace scattering amplitudes, respectively.[8]

(iv) Inclusion of the continuum electron-bound electron correlation, i.e., a proper choice of the low-energy ejected electron wave function in the final state. This has been tried within the framework of the first Born approximation (CB1) and is found to lead to a considerable improvement, in agreement with experiment, in the binary to recoil peak intensity ratio compared to the usual first Born approximation.[9,10] Some of these studies have been summarized in a recent review article by Ehrhardt *et al.*[11] The main findings are that (i) even at fairly high incident energies the second Born approximation term of the direct scattering amplitude must be included, (ii) still higher-order ($n>2$) terms also seem to be important if the scattering angle is not too small, and (iii) any improvement in the description of the low-energy ejected electron improves the binary to recoil peak intensity ratio.

This paper reports our attempt to fuse the above three ingredients for the ionization of helium. A hybrid second-order model in which the first Born approximation amplitude (f_{CB1}) is evaluated by using an improved target continuum wave function and the second Born amplitude (f_{B2}) in the usual way has recently been used by us, with very good results, to analyze the recent absolute TDCS data of Jung *et al.*[12] for the ionization of helium in the coplanar asymmetric geometry at an incident electron energy of $E_0=600$ eV.[10] Notwithstanding the inherent inconsistency of this hybrid model, the good results obtained with it have indicated the direction followed here.

The target ground-state wave function is taken to be an analytical fit to the Hartree-Fock wave function given by Byron and Joachain.[13] The final-state (singlet) wave function $\Phi_{\mathbf{k}_b}(\mathbf{r}_1,\mathbf{r}_2)$ of the helium subsystem is taken to be a symmetrized product of the He^+ ground-state wave function

$$v(\mathbf{r})=(8/\pi)^{1/2}e^{-2r} \tag{4}$$

for the bound electron with the continuum wave function $\Psi_{\mathbf{k}_b}^{(-)}$ (orthogonalized to the ground-state orbital u) for the ejected electron with momentum $\mathbf{k}_b$:

$$\Phi_{\mathbf{k}_b}(\mathbf{r}_1,\mathbf{r}_2)=2^{-1/2}[\Psi_{\mathbf{k}_b}^{(-)}(\mathbf{r}_1)v(\mathbf{r}_2)+v(\mathbf{r}_1)\Psi_{\mathbf{k}_b}^{(-)}(\mathbf{r}_2)]\ , \tag{5}$$

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

The wave function $\psi_{\mathbf{k}_b}^{(-)}$ is written as

$$\psi_{\mathbf{k}_b}^{(-)}(\mathbf{r})=\psi_{C,\mathbf{k}_b}^{(-)}(\mathbf{r})+[\psi_{\mathbf{k}_b}^{(-)}(\mathbf{r})-\psi_{C,\mathbf{k}_b}^{(-)}(\mathbf{r})]\ , \tag{7}$$

where $\psi_{C,\mathbf{k}_b}^{(-)}$ is the Coulomb wave function corresponding to the charge $Z=1$ on the residual ion. The correction $\eta_{\mathbf{k}_b}(\mathbf{r})=[\psi_{\mathbf{k}_b}^{(-)}(\mathbf{r})-\psi_{C,\mathbf{k}_b}^{(-)}(\mathbf{r})]$ is expressed in the partial wave expansion

$$\eta_{\mathbf{k}_b}(\mathbf{r})=\sum_l i^l(2l+1)[e^{-i\delta_l}R_l(r)-e^{-i\delta_l^C}R_l^C(r)]P_l(\hat{\mathbf{k}}_b\cdot\hat{\mathbf{r}})\ . \tag{8}$$

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 potential in the static field of the residual He^+ ion.

The summation over l in Eq. (8) is done up to $l_{max}=2$. For higher partial waves $\psi_{\mathbf{k}_b}^{(-)}(\mathbf{r})$ thus continues to be just the usual Coulomb wave. The improvement introduced here for the lower partial waves is found to be good enough for small ejected electron energies in which we are interested here.

The second Born amplitude f_{CB2} is evaluated with average excitation energy ($\bar{\omega}=0.9$ a.u.) and closure. The details of numerical evaluation of f_{CB1} are given in Ref. 10 while those of f_{CB2} shall be given elsewhere.[14] The choice $\psi_{\mathbf{k}_b}^{(-)}(\mathbf{r})=\psi_{C,\mathbf{k}_b}^{(-)}(\mathbf{r})$, i.e., $\eta_{\mathbf{k}_b}(\mathbf{r})=0$ in Eq. (7) leads to the usual amplitudes f_{B1} and f_{B2} in the first and second order, respectively.

The triple-differential cross section is given by

$$\frac{d^3\sigma_{CB2}}{d\Omega_a\,d\Omega_b\,dE_b}=\frac{k_ak_b}{k_0}\,|f_{CB1}+f_{CB2}|^2\ , \tag{9}$$

where $\mathbf{k}_0$ and $\mathbf{k}_a$ are, respectively, the momenta of the incident and scattered electrons.

Figures 1(a)–1(c) show our coplanar CB2 results at an incident electron energy $E_0=600$ eV for (a) $\theta_a=4°$, $E_b=2.5$ eV; (b) $\theta_a=8°$, $E_b=2.5$ eV; and (c) $\theta_a=4°$, $E_b=10$ eV, along with those obtained by using the usual second Born approximation, the Glauber approximation, and the modified Glauber approximation. These are taken from Ref. 6. 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 momentum transfer in which we are interested here. The theoretical results are compared with the recent absolute measurement of Jung *et al.*[12] The present calculations have been done only at some typical angles θ_b because of computation time limitation.

The present CB2 results (×) are found to be in very good agreement with the experimental data both in the binary and the recoil peak regions. We have also used quantum-defect phase shifts[15] in place of the phase shifts δ_l due to the static potential in calculating $\eta_{\mathbf{k}_b}(\mathbf{r})$. The results change only marginally. The experimental data do not appear to warrant any further improvement in the description of the low-energy ejected electron.

In order to look at the effect of the higher-order terms of the direct scattering amplitude within the present framework we have considered an improved MG approximation in the following way:

$$f_{CMG}=f_{CB1}+f_{CB2}+(f_G-f_{B1}-f_{G2})\ . \tag{10}$$

The higher-order terms are included here just as in the usual MG approximation. The CMG results (⊙) are very close to the CB2 results. However, the trend of the changes with respect to CB2 results in the recoil peak region tend to further improve the agreement (though insignificantly) with data.

The improvement shown by the CB2 and the CMG results is essentially caused by the use of f_{CB1} in place of f_{B1}. Could the second-order term f_{CB2} be completely dispensed with and the higher-order $n\geq 2$ terms included via the Glauber approximation? This aspect has been investigated by considering an improved Glauber approximation:

$$f_{CG}=f_{CB1}+f_G-f_{B1}\ . \tag{11}$$

The CG results (△) are found to be quite good in the binary peak region. The recoil peak is, however, underestimated, and the angular distribution is symmetric about the momentum transfer direction.

In conclusion, the present paper establishes quite conclusively that a second Born calculation with a good choice of the low-energy ejected electron wave function incorporating continuum electron-bound electron correlation is good enough to reproduce the TDCS angular distribution in the asymmetric geometry. Recently Furtado and O'Mahony[16] have also demonstrated the importance of using good helium wave functions in second Born calculations. But a comparison of the present results with those of the present authors' hybrid approach[10] indicates that one needs only to improve the helium wave function in the first Born term, the second Born term being much less sensitive to it. The amplitude f_{CB2} has been evaluated here in the closure approximation with an average excitation energy. In the sum over intermediate states one may exactly incorporate the helium ground state, but the results in the present

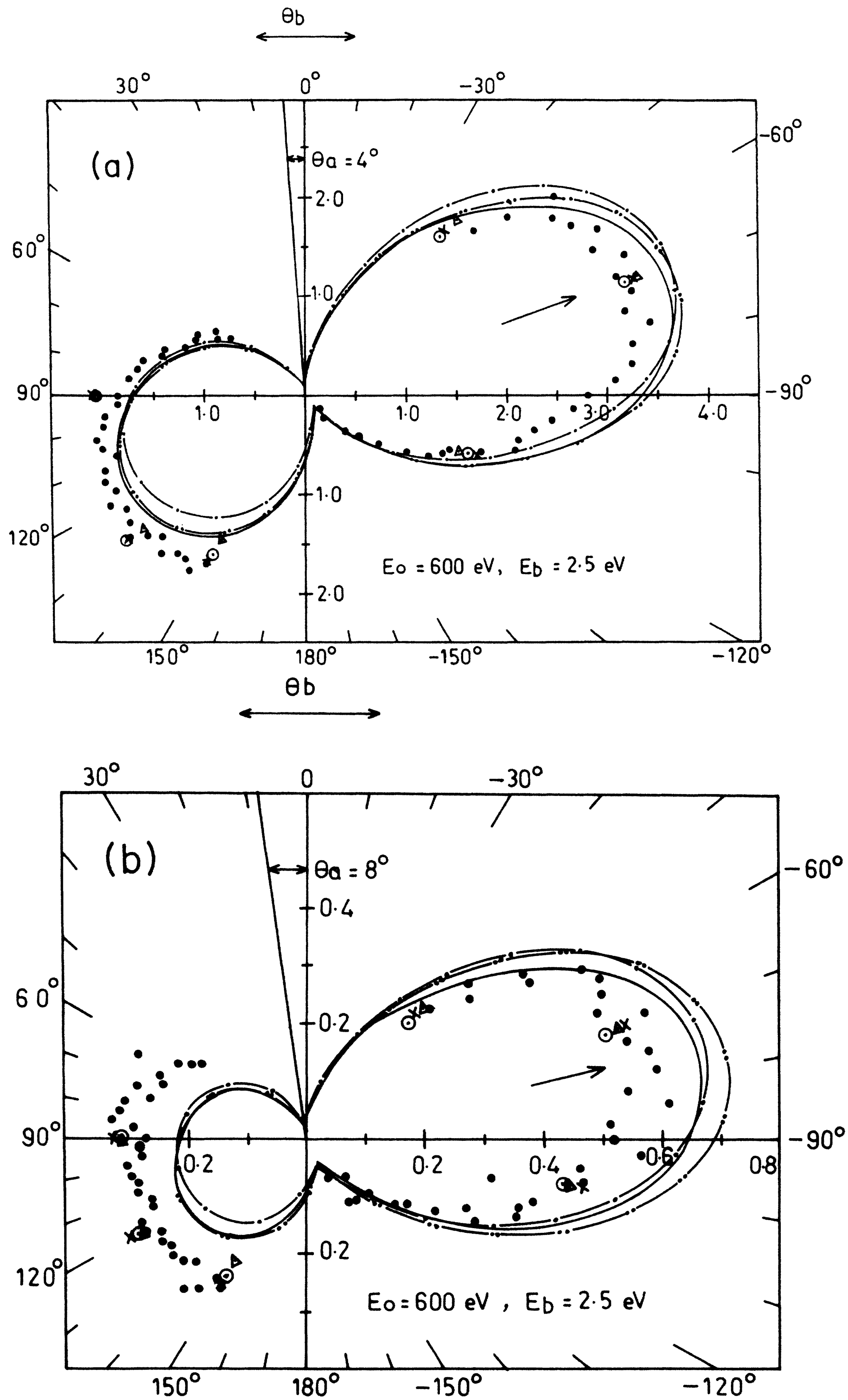

FIG. 1. (a) Triple-differential cross section in units of 10^{-22} $m^2 sr^{-2} eV^{-1}$ for the ionization of helium by electron impact at $E_0 = 600$ eV, $E_b = 2.5$ eV, $\theta_a = 4°$. Theoretical results: Glauber approximation (G), —·—·—·; second Born approximation (B2), —··—··—; modified Glauber approximation (MG), ——; present results (CB2), ×; (CMG), ⊙; (CG), △. The experimental data are the absolute measurements of Jung *et al.* (Ref. 12). The arrow indicates the direction of momentum transfer. (b) Same as (a) but $E_0 = 600$ eV, $E_b = 2.5$ eV, $\theta_a = 8°$. (c) Same as (a) but $E_0 = 600$ eV, $E_b = 10$ eV, $\theta_a = 4°$.

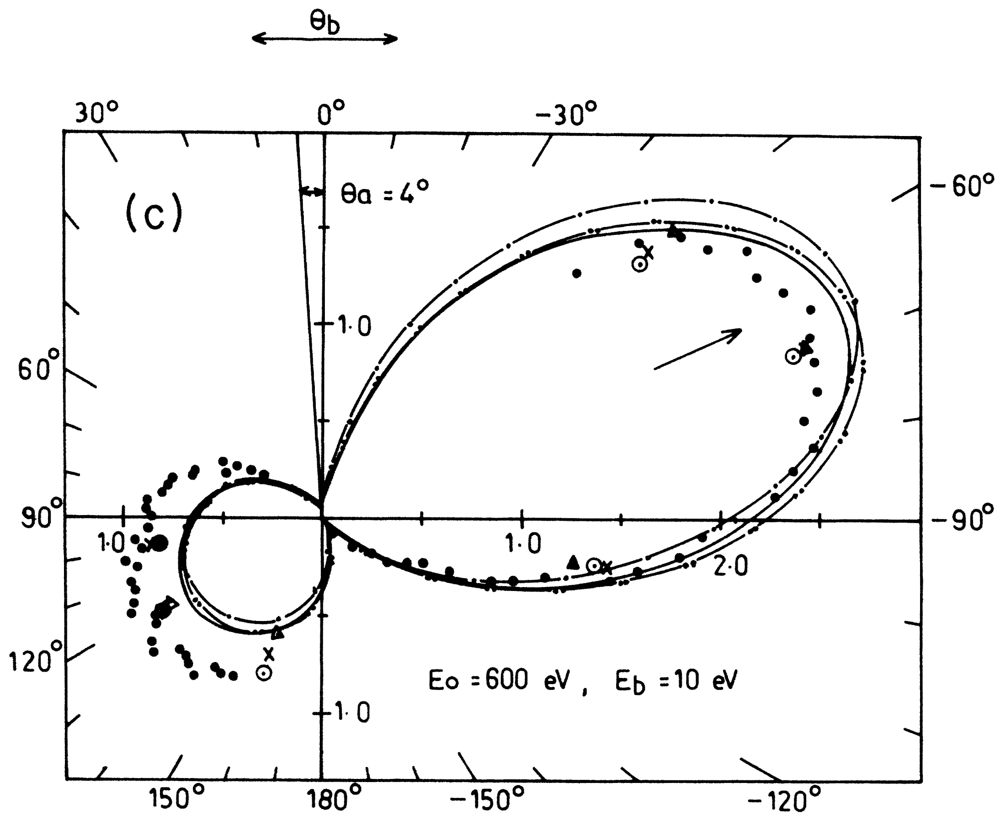

FIG. 1. (*Continued*).

geometry are not expected to change significantly. Still higher-order terms ($n > 2$) of the direct scattering amplitude could be included through the usual Glauber approximation.

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