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Electron and positron impact ionization of atomic hydrogen and helium using CPB approximation with post-collision interaction

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Abstract. Triple differential cross-sections for the electron and positron impact ionization of atomic hydrogen and helium are calculated in a first order model using a product of two Coulomb wavefunctions for the final state continuum electrons supplemented by post-collision interaction effects.

Keywords. Ionization; electron impact; positron impact; Coulomb-projected Born approximation; post-collision interaction.

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1. Introduction

The triple differential cross-sections (TDCS) for electron and positron impact ionization of atoms provide not only a detailed information of the ionization process but also a sensitive meeting ground between theories and experiments. Helium and atomic hydrogen as targets are obviously preferable for such studies. The asymmetric geometry, in which the energies of the two continuum electrons (or the continuum positron and electron) in the final state are very different, is known to provide particularly sensitive probe to the reaction dynamics. In this geometry for a given fast incident electron (or positron) of energy E_0 (momentum $\mathbf{k}_0$) and a fixed small scattering angle θ_a of the fast electron (or positron) of energy E_a (momentum $\mathbf{k}_a$), the coplanar angular distribution of the slow 'ejected' electron of energy E_b (momentum $\mathbf{k}_b$) shows a two-peaked structure: a peak (binary peak) near the momentum transfer ($\mathbf{K} = \mathbf{k}_0 - \mathbf{k}_a$) direction and another subsidiary one (recoil peak) near the opposite direction. In this paper we are interested in this geometry.

A large number of experimental and theoretical investigations have been made on the ionization of helium and atomic hydrogen by electrons. There are no TDCS measurements for ionization by positron impact. The second Born (B2) approximation (Byron *et al* 1980, 1982; Ehrhardt *et al* 1982) has been shown to essentially reproduce the main features (angular positions of the binary and recoil peak maxima and the ratio of binary to recoil peak intensity) of the TDCS angular distribution for the electron impact ionization. The eikonal Born series (EBS) (Byron *et al* 1983, 1984, 1985; Joachain *et al* 1985) and the modified Glauber (MG) approximations (Baliyan and Srivastava 1985, 1986a, b) have also been used. The MG approximation is found to further improve the B2 results in the cases where the scattering angle θ_a is not too small. All these calculations involve considerable computational labour. The Coulomb-projected Born (CPB) approximation (Geltman 1971, 1974; Geltman and Hidalgo 1971, 1974; Hidalgo and Geltman 1972; Schulz 1973; Schubert *et al* 1979; Lal *et al* 1979; Pathak and Srivastava 1980, 1981; Ghosh *et al* 1984 a, b) has also been tried as a simple alternative. It is found to lead to quite good results for the binary to recoil peak intensity ratio and the angular position of the binary peak maximum. However, the CPB approximation, at variance with experiment and B2, EBS and MG approximations, leads to a deviation of the recoil peak maximum to smaller angles of ejection compared to the first Born results. This is unphysical since the two outgoing electrons repel each other.

Some calculations on positron impact ionization using the above approximation have also been reported recently (Joachain 1984; Basu *et al* 1985; Ghosh *et al* 1985a, b; Mandal *et al* 1986; Saxena and Srivastava 1987). A comparison of positron-induced and electron-induced ionization results under identical conditions is expected to provide some additional insight into this process. The two cases differ in the interference between the projectile-target nucleus and the projectile-target electron interactions. The positron results are found to differ from the corresponding electron results in the sense that they lead to a larger binary peak, a smaller recoil peak and peak maxima at smaller angles θ_b.

Klar and Franz (1986) have recently shown that the inclusion of the post-collision interaction (PCI) effects, which correspond to energy exchange and trajectory modifications of the two outgoing electrons in the final state, leads to an improvement in (i) the binary to recoil peak intensity ratio and (ii) the angular positions of the binary and recoil peak maxima.

In the present paper we supplement the CPB approximation with PCI effects to obtain TDCS for electron and positron impact ionization of hydrogen and helium. The incorporation of PCI takes care of the unphysical recoil peak maximum position given by the CPB approximation in the sense that the binary and recoil peak intensity maxima get shifted to larger (smaller) angle θ_b in the case of electron (positron) impact. The PCI effects have been estimated classically by following the procedure of Klar and Franz (1986), Popov and Benayoun (1981), Popov and Erokhin (1983) and Klar *et al* (1986). The electron results are compared with the recent absolute data of Ehrhardt *et al* (1985) for atomic hydrogen and of Jung *et al* (1985) for helium in the coplanar asymmetric geometry.

The method of calculation is outlined in the next section. Section 3 contains our results and their discussion.

2. Calculation

The TDCS is calculated by using the expression

$$\frac{d^3\sigma}{d\Omega_a\, d\Omega_b\, dE_b} = \frac{k_a k_b}{k_0} |f_{\mathrm{CPB}}|^2, \tag{1}$$

where f_{CPB} is the Coulomb-projected Born scattering amplitude.

In the case of hydrogen, the electron/positron-target interaction is given by

$$V = \mp \frac{1}{r_0} \pm \frac{1}{|\mathbf{r}_0 - \mathbf{r}_1|}, \tag{2}$$

where the upper sign refers to the electron and the lower sign to the positron. $\mathbf{r}_0$ and $\mathbf{r}_1$ are respectively the position vectors of the incident electron/positron and the target electron. The nucleus is taken to be infinitely heavy and fixed at the origin. The amplitude f_{CPB} is evaluated by following the method of Pathak and Srivastava (1980). In the case of helium the projectile-target interaction is given by

$$V(\mathbf{r}_0,\mathbf{r}_1,\mathbf{r}_2) = \mp\frac{2}{r_0} \pm \frac{1}{|\mathbf{r}_0-\mathbf{r}_1|} \pm \frac{1}{|\mathbf{r}_0-\mathbf{r}_2|}, \tag{3}$$

where $\mathbf{r}_1$, $\mathbf{r}_2$ are the position vectors of the two target electrons. The amplitude f_{CPB} is evaluated by following the method of Pathak and Srivastava (1981). For the helium ground state we have taken the analytical fit to the Hartree-Fock wave function given by Byron and Joachain (1966). The final state wavefunction of the $\mathrm{He}^+ + e^-$ subsystem is taken to be the symmetrized product of the He^+ ground state wavefunction for the bound electron with the continuum wavefunction for the ejected electron. The latter is taken to be a Coulomb wave (with $Z = 1$) orthogonalized to the ground state orbital.

There is an exchange contribution to the scattering in the electron impact case. However, it is expected to be small under the highly asymmetric conditions considered here and hence has been ignored. Likewise in the positron case, the positronium formation channel is not expected to contribute significantly as in the cases considered here the scattered positron and the ejected electron have very widely different energies. It has, therefore, not been considered.

The PCI effects are incorporated by calculating the scattering amplitude at the initial values (at the boundary of the reaction zone) $E_a(0)$, $E_b(0)$, $\theta_a(0)$ and $\theta_b(0)$ for obtaining the cross-section at E_a, E_b, θ_a and θ_b which are the energies and the angles at the position of the detectors. The former can be obtained by using the following relations:

$$\theta_i(0) = \theta_i - \sin(\theta_a+\theta_b)\int_0^\infty r_a r_b r_{ab}^{-3}\,\mathrm{d}t\int_t^\infty [r_i(t')]^{-2}\,\mathrm{d}t', \quad i = a, b, \tag{4}$$

$$E_a(0) \simeq E_a + \frac{1}{r_a}\bigg|_{t=0} - \int_0^\infty \dot{r}_a r_{ab}^{-3}[r_a - r_b\cos(\theta_a+\theta_b)]\,\mathrm{d}t, \tag{5}$$

$$E_b(0) \simeq E_b - \int_0^\infty \dot{r}_b r_{ab}^{-3}[r_b - r_a\cos(\theta_a+\theta_b)]\,\mathrm{d}t. \tag{6}$$

At intermediate incident energies, the PCI effects are not dominant and equation (4) to (6) may be solved by assuming straight-line trajectories

$$E_a = \tfrac{1}{2}\dot{r}_a^2 \tag{7}$$

$$E_b = \tfrac{1}{2}\dot{r}_b^2 - (1/r_b) \tag{8}$$

with initial values $r_a(0) \equiv r_{0a}$ and $r_b(0) \equiv r_{0b}$. Details are given in Klar and Franz (1986) and Klar *et al* (1986). We have chosen the boundary values r_{0a} and r_{0b} to be 2·5 Å and 0·529 Å for hydrogen and 3·5 Å and 0·2254 Å for helium respectively. The choice for r_{0b} corresponds to the position where the target electron is most likely to be found.

3. Results and discussion

3.1 *Hydrogen*

We have calculated TDCS at an incident energy $E_0 = 250\,\text{eV}$ for $\theta_a = 8°$, $E_b = 5{\cdot}0\,\text{eV}$ corresponding to the electron impact absolute data of Ehrhardt *et al* (1985). Figure 1 shows the angular distribution of the results obtained by using the CPB approximation with and without PCI for electron and positron impact ionization. The results for the electron case are compared with those obtained by using the first Born approximation with PCI (BI-PCI).

In the e^- case the CPB approximation leads to a deviation of the recoil peak maximum to smaller angles of ejection (relative to the momentum transfer direction), while in the e^+ case it moves towards larger angles of ejection compared to the first Born approximation results. This is unphysical since the outgoing scattered electron (positron) and ejected electron repel (attract) each other. With the incorporation of PCI effects the situation moves towards the agreement with the experimental data i.e. in the electron impact case the recoil peak shifts towards the larger angle of ejection while in the positron impact case it shifts towards the smaller angle of ejection. Likewise the binary peak, with PCI, shifts to the larger angle (smaller angle) of ejection for electron (positron) impact ionization. The size of the recoil peak increases (decreases) for electron (positron) impact case. These changes improve the binary to recoil peak maxima ratio (I_b/I_r). This ratio is larger in the positron impact case compared to the corresponding electron impact case.

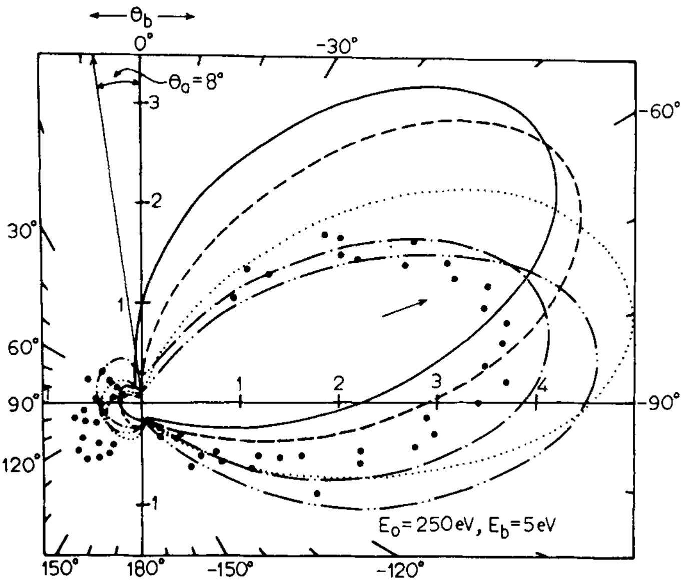

Figure 1. Triple differential cross-section for electron and positron impact on atomic hydrogen in units of $10^{-22}\,\text{m}^2\,\text{Sr}^{-2}\,\text{eV}^{-1}$, for $E_0 = 250\,\text{eV}$, $E_b = 5\,\text{eV}$ and $\theta_a = 8°$. The curves are: CPB with PCI (for positron)—, CPB (for positron)– – – –, CPB with PCI (for electron)– · · –, CPB (for electron)— · —, and BI with PCI (for electron)... The experimental data are the absolute measurements of Ehrhardt *et al* (1985). The arrow indicates the direction of momentum transfer **K**.

3.2 *Helium*

The calculations have been carried out at an incident energy $E_0 = 600\,\mathrm{eV}$ for $\theta_a = 4^\circ$ and 10° with $E_b = 2{\cdot}5\,\mathrm{eV}$ and $10{\cdot}0\,\mathrm{eV}$ corresponding to electron impact absolute data of Jung *et al* (1985). Figures 2(a–d) demonstrate our TDCS results for electron and positron impact ionization in CPB approximation with and without PCI at (a) $\theta_a = 4^\circ$, $E_b = 2{\cdot}5\,\mathrm{eV}$, (b) $\theta_a = 10^\circ$, $E_b = 2{\cdot}5\,\mathrm{eV}$, (c) $\theta_a = 4^\circ$, $E_b = 10{\cdot}0\,\mathrm{eV}$ and (d) $\theta_a = 10^\circ$, $E_b = 10{\cdot}0\,\mathrm{eV}$. The BI-PCI results for the electron case are also shown.

The CPB-PCI electron results in the recoil peak region at $E_b = 2{\cdot}5\,\mathrm{eV}$ are found to be in good agreement with the experimental data. However, at $E_b = 10\,\mathrm{eV}$, it is still underestimated. The binary peak is overestimated in all the cases considered here although it is better than the one obtained by using BI-PCI approximation. The introduction of PCI effects lead to similar changes as in the case of hydrogen. The corresponding positron results show a binary peak of almost the same magnitude as in the electron case with maximum at smaller θ_b as expected. The PCI effects reduce this angle further. The recoil peak here is of smaller magnitude and becomes still smaller when PCI effects are included.

4. Conclusions

The inclusion of PCI effects shifts the angular positions of the binary and recoil peak maxima in such a way that the unphysical feature of the CPB approximation gets

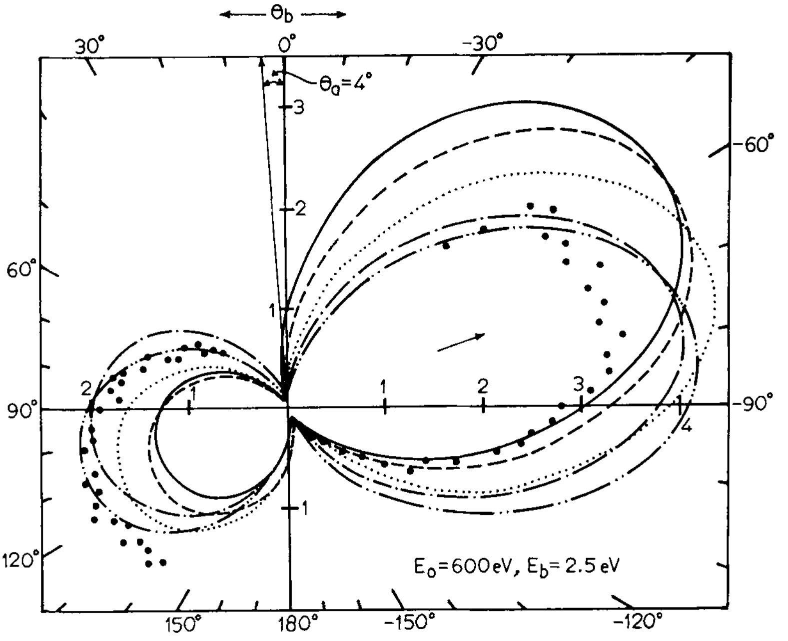

Figure 2(a). Triple differential cross-section for electron and positron impact on helium in units of $10^{-22}\,\mathrm{m}^2\,\mathrm{Sr}^{-2}\,\mathrm{eV}^{-1}$, for $E_0 = 600\,\mathrm{eV}$, $E_b = 2{\cdot}5\,\mathrm{eV}$ and $\theta_a = 4^\circ$. The curves are: CPB with PCI (for positron)—, CPB (for positron) ——, CPB with PCI (for electron)—··—, CPB (for electron)—·—·, and BI with PCI (for electron)··· The experimental data are the absolute measurements of Jung *et al* (1985). The arrow indicates the direction of momentum transfer **K**.

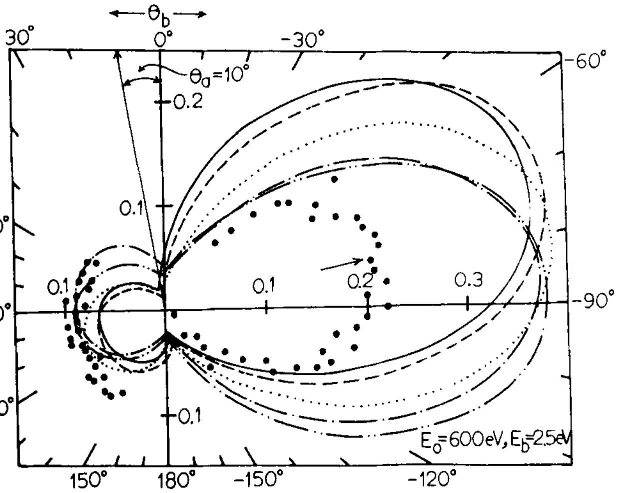

Figure 2(b). Same as in figure 2(a), but for $E_0 = 600\,\text{eV}$, $E_b = 2{\cdot}5\,\text{eV}$, $\theta_a = 10°$.

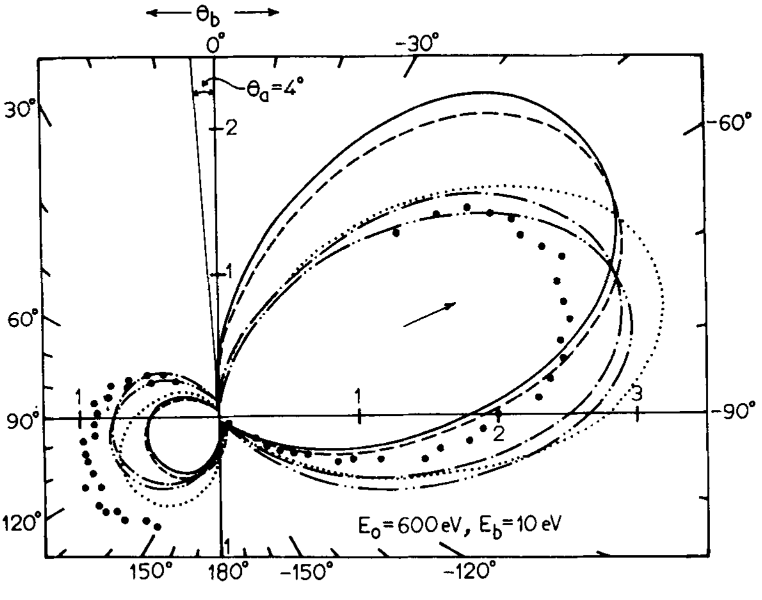

Figure 2(c). Same as in figure 2(a), but for $E_0 = 600\,\text{eV}$, $E_b = 10\,\text{eV}$, $\theta_a = 4°$.

eliminated. Furthermore the size of the recoil peak increases (decreases) for the electron (positron) impact case. The ratio of binary to recoil peak maxima (I_b/I_r) is larger in the positron impact case. Thus the CPB approximation, which has already been shown to yield quite good value for the ratio I_b/I_r also leads to correct angular positions of the peak maxima when PCI effects are included. This approach, which is no more difficult than the BI-PCI approximation can, therefore, be followed as a simple alternative to the more sophisticated models. The description of the initial and final states of the target may, of course, be improved as has been done recently in connection with the second Born approximation (Furtado and O'Mahony 1987; Srivastava and Sharma 1988).

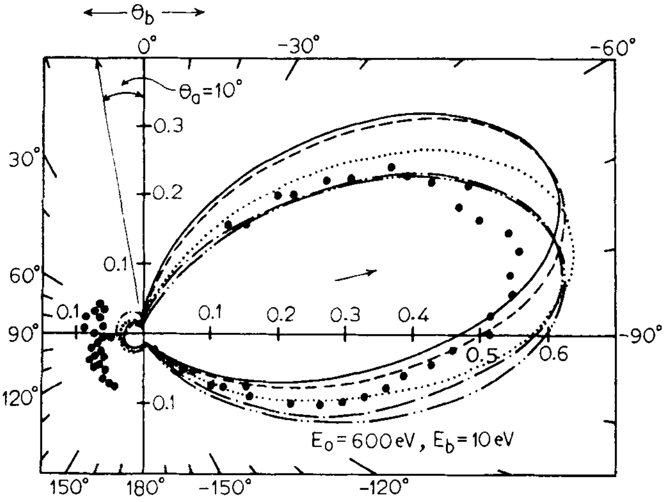

Figure 2(d). Same as in figure 2(a), but for $E_0 = 600\,\text{eV}$, $E_b = 10\,\text{eV}$, $\theta_a = 10°$.

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