TRIPLE DIFFERENTIAL CROSS-SECTION FOR THE ELECTRON IMPACT IONIZATION OF ATOMIC HYDROGEN IN THE COPLANAR ASYMMETRIC GEOMETRY

MUKHERJEE, K. K.,[1] MAZUMDAR, P. S.,[2] Imphal

The triple differential cross-section for the electron impact ionization of atomic hydrogen in coplanar asymmetric geometry has been calculated using the distorted wave polarized orbital method. The present results are in fair agreement with the recent experimental findings.

1. INTRODUCTION

The most detailed information available about the single ionization process can be obtained by analysing the triple diferential cross-section (TDCS) measured in $(e, 2e)$ coincidence experiments. The TDCS is a measure of the probability that in an $(e, 2e)$ reaction an incident electron of energy E_0 and momentum $\boldsymbol{k}_0$ will produce on collision with the target two electrons one faster and the other slower with energies E_1 and E_2 and momenta $\boldsymbol{k}_1$ and $\boldsymbol{k}_2$, respectively and are emitted into the solid angles $\mathrm{d}\hat{k}_1$ and $\mathrm{d}\hat{k}_2$ centred about the directions (Θ_1, Φ_1) and (Θ_2, Φ_2). Of the possible kinematic choices, coplanar asymmetric geometry pioneered by Ehrhardt [1] has been found to provide a particularly sensitive probe of the reaction dynamics. Here, the scattering angle Θ_1 of the faster electron is kept fixed and small and the coincidence rate is measured as a function of the angle Θ_2 of the slower electron. The scattered and ejected electrons show a very strong angular correlation. The angular distribution shows two peaks [2], a peak (binary peak) near the momentum transfer $(\boldsymbol{k} = \boldsymbol{k}_0 - \boldsymbol{k}_1)$ direction and another subsidiary one (recoil peak) near the opposite direction.

A good theoretical description of this process is complicated by a long range three-body break up nature of the problem. Another complication is introduced

[1] Manipur Public School, Koirengei, IMPHAL — 795002, India
[2] Department of Physics, Manipur University, Canchipur, IMPHAL — 795003, India

by the uncertainty in the description of both the ground state and the final continuum state of the target. The ionization of the atomic hydrogen is free from this undesirable as the initial and final states are known exactly. Recently absolute measurements of TDCS in the coplanar asymmetric geometry have been performed. Actually there are two sets of experimental data one by Ehrhardt et al. (quoted in Byron et al. [3]) and the other by Schlemmer et al. (quoted in Joachain et al. [4]).

Byron et al. [3] and Joachain et al. [4] have shown that the Eikonal-Born Series (EBS) and the Unitarized Eikonal-Born Series (UEBS) theories can satisfactorily explain all features exhibited by TDCS measured in complanar asymmetrics ionization of the atomic hydrogen from the ground state. They have also shown that the First Born Approximation (FBA) fails to explain the experimental results. Now, the EBS and UEBS theories are very elaborate and require extensive computation. It is worth-while to seek methods to implement the necessary nonlinear elements of the theory with less mathematical effort. Distorted wave calculations are some sort of intermediate between FBA and more elaborate theoretical calculations. Distorted wave calculations for the TDCS for electron impact ionization from the ground state of atomic hydrogen were performed by Smith et al. [5]. The results of Smith et al. [5] were in fair agreement with the experimental data of Wiegold et al. [6]. The literature contains evidence [7, 8] of successful applications of the distorted wave method in electron atom scattering for inelastic processes. In the present investigation we have employed the Distorted Wave Polarized Orbital (DWPO) method of Scott and McDowell [9] to calculate the TDCS for the (e-H) ionization for coplanar asymmetric geometry.

In the First Born Approximation (FBA) the slower electron is represented by a Coulomb wave but the faster electron by a plane wave. But Geltman [10] initiated a different approach. He represented the wave functions of both the slower and the faster electrons by attractive Coulomb waves of unit charge. This choice is physically reasonable because after ionization both electrons move in the field of the residual proton of the unit positive charge. Moreover, since the wave function of the first outgoing electron is calculated in the attractive Coulomb field of the residual nucleus, which is a part of the complete interaction potential, this theory might be regarded as a higher order theory. It was noted by Smith et al. [5] and Pathak and Srivastava [11] that this type of choice of the final state wave function leads to the theoretical predictions of TDCS which are in better agreement with the experimental findings of Wiegold et al. [6] than FBA. In our present calculation we have represented both the slower and the faster electrons by attractive Coulomb functions of the unit charge. We also note that it was shown by Peterkop [12, 13] and by Rudge and Seaton [14] that in the case of electron impact ionization

the effective charges z_1 and z_2 as seen by the faster and slower electrons should satisfy the relation

$$\frac{z_1}{k_1}+\frac{z_2}{k_2}=\frac{1}{k_1}+\frac{1}{k_2}+\frac{1}{|\boldsymbol{k}_1-\boldsymbol{k}_2|}$$

where $\boldsymbol{k}_1$ and $\boldsymbol{k}_2$ are the momenta of the faster and slower electrons, respectively. Our choice $z_1 = z_2 = 1$ satisfied the above condition in the case of the Ehrhardt coplanar asymmetric geometry in which $|\boldsymbol{k}_1 - \boldsymbol{k}_2| \gg 1$.

2. THEORY AND NUMERICAL METHODS

The TDCS for electron impact ionization may be expressed in atomic units (a.u) as [15]

$$\frac{\mathrm{d}^5\sigma}{\mathrm{d}\boldsymbol{k}_1\,\mathrm{d}\boldsymbol{k}_2\,\mathrm{d}E_2}=\frac{k_1k_2}{k_0}\left[0.25\,|f^+(\boldsymbol{k}_1,\boldsymbol{k}_2)|^2+0.75\,|f^-(\boldsymbol{k}_1,\boldsymbol{k}_2)^2\right] \tag{1}$$

where $f^{\pm}(\boldsymbol{k}_1, \boldsymbol{k}_2)$ is the ionization amplitude and the superscripts ($\pm$) stand for the singlet and triplet spin states, respectively, $\boldsymbol{k}_0$, $\boldsymbol{k}_1$ and $\boldsymbol{k}_2$ are the momenta of the incident, faster and slower electrons, respectively. E_2 is the energy of the slower electron. Now,

$$f^{\pm}(\boldsymbol{k}_1,\boldsymbol{k}_2)=(2\pi)^{-5/2}\langle X_{\boldsymbol{k}_1}(z_1,\boldsymbol{r}_1)\,X_{\boldsymbol{k}_2}(z_2,\boldsymbol{r}_2)\,|V_i|\,\Psi^{\pm}(\boldsymbol{r}_1,\boldsymbol{r}_2)\rangle \tag{2}$$

where $\Psi^{\pm}(\boldsymbol{r}_1, \boldsymbol{r}_2)$ is the total wave function of the (e-H) system and is written as

$$\Psi^{\pm}(\boldsymbol{r}_1,\boldsymbol{r}_2)=(1\pm P_{12})[\Phi_{1S}(\boldsymbol{r}_2)+\Phi_{pol}(\boldsymbol{r}_1,\boldsymbol{r}_2)]\,F^{\pm}(\boldsymbol{r}_1) \tag{3}$$

P_{12} is the permutation operator which interchanges the labels 1 and 2, $\Phi_{1S}(\boldsymbol{r})$ is the ground state wave function of atomic hydrogen and $\Phi_{pol}(\boldsymbol{r}_1, \boldsymbol{r}_2)$ is the polarized (distorted) atomic wave function [16], z_1 and z_2 are the effective charges seen by the faster and slower electrons, respectively. In our present calculation we have taken $z_1 = z_2 = 1$. The interaction potential is taken in the direct channel and is written as

$$V_i=-\frac{1}{r_1}+\frac{1}{r_{12}} \tag{4}$$

$X_{\boldsymbol{k}}(z, \boldsymbol{r})$ stands for the Coulomb wave function [9] in the field of the reduced charge z. The radial part of the scattering function $F^{\pm}(\boldsymbol{r})$ satisfied the integro differential equation given by Temkin and Lamkin [16] and corrected for the p-waves by Sloan [17]. $f^{\pm}(\boldsymbol{k}_1, \boldsymbol{k}_2)$ can be written as [9]

$$f^{\pm}(\boldsymbol{k}_1,\boldsymbol{k}_2)=[f_D^{\pm}(\boldsymbol{k}_1,\boldsymbol{k}_2)+f_{PD}^{\pm}(\boldsymbol{k}_1,\boldsymbol{k}_2)]\pm[f_E^{\pm}(\boldsymbol{k}_1,\boldsymbol{k}_2)+f_{PE}^{\pm}(\boldsymbol{k}_1,\boldsymbol{k}_2)] \tag{5}$$

where $f_D^{\pm}(\boldsymbol{k}_1, \boldsymbol{k}_2)$, $f_{PD}^{\pm}(\boldsymbol{k}_1, \boldsymbol{k}_2)$, $f_E^{\pm}(\boldsymbol{k}_1, \boldsymbol{k}_2)$ and $f_{PE}^{\pm}(\boldsymbol{k}_1, \boldsymbol{k}_2)$ are direct, polarized direct, exchange and polarized exchange amplitudes, respectively. Now,

$$f_D^{\pm}(\boldsymbol{k}_1, \boldsymbol{k}_2) = (2\pi)^{-5/2} \langle X_{\boldsymbol{k}_1}(z_1, \boldsymbol{r}_1)\, X_{\boldsymbol{k}_2}(z_2, \boldsymbol{r}_2) | V_i | F^{\pm}(\boldsymbol{r}_1)\, \Phi_{1S}(\boldsymbol{r}_2) \rangle \tag{6}$$

and

$$f_{PD}^{\pm}(\boldsymbol{k}_1, \boldsymbol{k}_2) = (2\pi)^{-5/2} \langle X_{\boldsymbol{k}_1}(z_1, \boldsymbol{r}_1)\, X_{\boldsymbol{k}_2}(z_2, \boldsymbol{r}_2) | V_i | F^{\pm}(\boldsymbol{r}_1)\, \Phi_{pol}(\boldsymbol{r}_1, \boldsymbol{r}_2) \rangle . \tag{7}$$

The other two scattering amplitudes can be obtained as

$$f_E^{\pm}(\boldsymbol{k}_1, \boldsymbol{k}_2) = f_D^{\pm}(\boldsymbol{k}_2, \boldsymbol{k}_1) \tag{8}$$

$$f_{PE}^{\pm}(\boldsymbol{k}_1, \boldsymbol{k}_2) = f_{PD}^{\pm}(\boldsymbol{k}_1, \boldsymbol{k}_2) . \tag{9}$$

We have carried out the partial wave analysis of equation (6) and (7) following Scott and McDowell [9].

The integro differential equation for the incident distorted wave has been solved by using the Numerov method [17] up to a radial distance of 40 a.u. The Coulomb wave functions have been obtained by solving the corresponding differential equation with a step size of 0.002 a.u. Radial integrations occurring in the ionization amplitude have been performed up to a radial distance of 80 a.u. The contributions of $f_{PD}^{\pm}$ and $f_{PE}^{\pm}$ are found to be negligible for $l_0 > 8$, where l_0 is the orbital angular momentum quantum number of the incident electron. Higher partial wave amplitudes (for $l_0 > 8$) have been replaced by the Coulomb Born amplitudes of Roy et al. [18]. Now once $f_D^{\pm}(\boldsymbol{k}_1, \boldsymbol{k}_2)$, $f_E^{\pm}(\boldsymbol{k}_1, \boldsymbol{k}_2)$ and $f_{PE}^{\pm}(\boldsymbol{k}_1, \boldsymbol{k}_2)$ are evaluated from equations (6) to (9) we can determine $f^{\pm}(\boldsymbol{k}_1, \boldsymbol{k}_2)$ from equation (5) and finally knowing $f^{\pm}(\boldsymbol{k}_1, \boldsymbol{k}_2)$ we can compute TDCS from equation (1) and compare it with experimental findings.

3. RESULTS AND DISCUSSIONS

In figure 1 we have compared our present results with the experimental findings of Ehrhardt et al. (as quoted in [3]) corresponding to the case in which the energy of the incident electron is $E_0 = 250$ eV, the energy of the slower electron is $E_2 = 5$ eV and the angle of scattering of the faster electron is $\Theta_1 = 3°$. We find that in the binary peak region our results are in good agreement with the experimental results and the Eikonal Born Series (EBS) results of Byron et al. [3]. As in the EBS, the binary peak is shifted to larger ejection angles and is also reduced in magnitude when comparisons are made with the FBA. In the recoil peak region, our results although not in good agreement with those of EBS and the experiment, are still better than those of the FBA. In

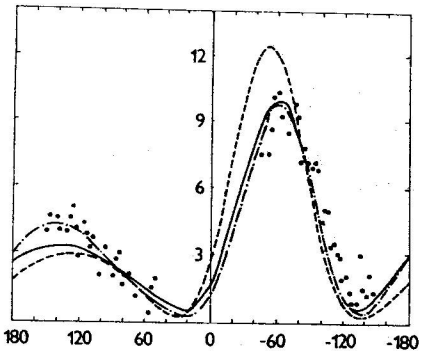

Fig. 1: The TDCS (in atomic units) for the ionization of the atomic hydrogen from the ground state by electron impact for the case $E_0 = 250$ eV, $E_2 = 5$ eV and $\Theta_1 = 3°$, as a function of the angle of ejection (Θ_2) of the slower electron: ——— present DWPO results; - - - - FBA results; -·-·-· EBS results of Byron et al. [3]; . absolute experimental data of Ehrhardt et al. (as quoted in [3]).

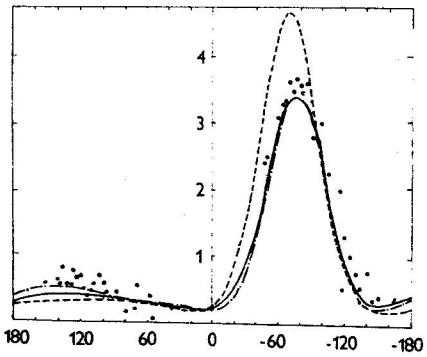

Fig. 2: Same as for fig. 1 but for the case $E_0 = 250$ eV, $E_2 = 5$ eV and $\Theta_1 = 8°$.

figure 2 we have compared our theoretical predictions with the experimental findings for $E_0 = 250$ eV, $E_2 = 5$ eV and $\Theta_1 = 8°$. Here also the situation is the same as that in the case of figure 1. In figure 3 we have compared our theoretical predictions with the experimental results of Schlemmer et al. (as quoted in

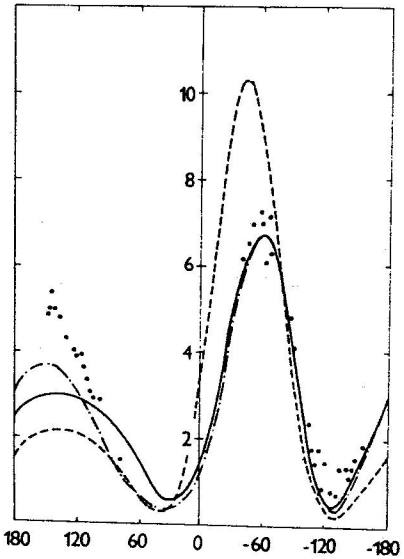

Fig. 3: TDCS (in atomic units) for the ionization of the atomic hydrogen from the ground state by electron impact for the case $E_0 = 150$ eV, $E_2 = 5$ eV and $\Theta_1 = 4°$: ——— present DWPO results; - - - - FBA results; -·-·- UEBS results of Joachain et al. [4] . absolute experimental results of Schlemmer et al. (as quoted in [4]).

[4]) for the case $E_0 = 150\,\text{eV}$, $E_2 = 5\,\text{eV}$ and $\Theta_1 = 4°$. We find that in the binary peak region our results are in fair agreement with those of the experiment and the Unitarized Eikonal Born Series (UEBS) results of Joachain et al. [4]. In contrast with the earlier case in the recoil peak region the predictions of Joachain et al. [4] are not in good agreement with the experimental findings, although they are still better than our results. Our predictions near the recoil peak region are better than those in the cases of figures 1 and 2. In figure 4 we have reported our results for the case $E_0 = 150\,\text{eV}$, $E_2 = 5\,\text{eV}$ and $\Theta_1 = 10°$. The situation is similar to that of figure 3.

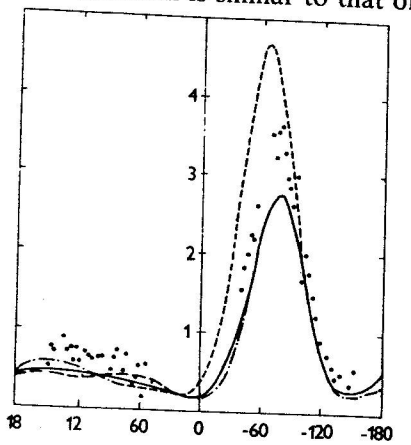

Fig. 4: Same as in fig. 3 but for $\Theta_1 = 10°$.

So we find that the predictions of the present method are better than those of the FBA and in the binary peak region are in good agreement with the absolute experimental results and also with the predictions of elaborate theoretical methods such as the EBS and the UEBS. In the recoil peak region the predictions of the present method improve with the decrease of the energy of the incident electron. This is in agreement with the findings of Scott and McDowell [9] in the case of the electron impact excitation of atomic hydrogen. They noted that the importance of the exchange polarization in deciding the scattering parameters for large angle scattering decreases with the increase in the energy of the incident electron.

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ТРОЙНОЕ ДИФФЕРЕНЦИАЛЬНОЕ СЕЧЕНИЕ ДЛЯ ЭЛЕКТРОННОЙ УДАРНОЙ ИОНИЗАЦИИ АТОМА ВОДОРОДА В КОМПЛАНАРНОЙ АССИМЕТРИЧЕСКОЙ ГЕОМЕТРИИ

На основе метода искаженных волн поляризованных орбит вычислено тройное дифференциальное сечение для электронной ударной ионизации атома водорода в компланарной ассиметрической геометрии. Приведенные результаты хорошо согласуются с недавными экспериментальными данными.