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Triply differential cross sections for ionization of hydrogen atoms by electron impact using HHOB approximation : the intermediate and high energy region

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Abstract : Triply differential cross sections (TDCS) in coplanar geometry for the ionization of atomic hydrogen by electron impact have been successfully studied within the framework of High energy Higher Order Born approximation (HHOB). The calculations are performed incorporating first three terms of the generalized Born series at intermediate and high incident energies 413.6, 600 and 800 eV. The results at incident energy 413.6 eV are in agreement with the experimental results. Remaining results are compared with other theoretical results as experimental data is not available.

Keywords : Ionization of hydrogen atoms, triply differential cross sections (TDCS), higher order Born approximation (HHOB)

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In the recent years, numerous investigations corresponding to nearly as many theoretical descriptions, have been made of amplitudes of high energy collisions of charged particles with atomic targets. Most of the cited works have had as their objective, the determination of accurate theoretical procedures to avoid the enormous complexity in describing and predicting the results of associated experiments. Two factors provide the motivation for the study. The first is prompted by the work and success of the theory given by Yates [1] and its application to hydrogen and lithium atoms by Rao and Desai [2]. A second consideration is the suggestion of anomalous behaviour of the small angle, high energy differential cross sections in electron atom collisions.

The present investigation reports an application of the High energy Higher Order Born approximation to calculate triple differential cross sections (TDCS) for electron impact ionization of atomic hydrogen avoiding the use of partial wave technique and compares the calculated results with corresponding experimental data of Weigold *et al* [3] and with theoretical results of Mohr [4].

The procedure adopted here, develops partial expansions of the second and third Born terms in reciprocal powers of incident momentum k_i^2, parallels the method of Glauber [5] and is most akin to the high energy, small angle potential scattering analysis of Schiff [6]. It is assumed that potential is slowly varying over the distance of a wavelength of the scattering and that intermediate momenta $\underline{k}_n$ does not differ greatly in either magnitude of direction.

Considering above assumptions, the Born series can be renamed as the Generalized Born series.

The purpose of the present work is to investigate contribution of higher order terms of the generalized Born series [1,2] which were not considered in the limited perturbative expansion.

Accordingly, amplitude of HHOB approximation is given as

$$f_{\mathrm{HHOB}} = f_{i\to f}^{(1)} + \mathrm{Re} f_{\mathrm{HEA}}^{(2)} + i\, \mathrm{Im} f_{\mathrm{HEA}}^{(2)} + f_{\mathrm{HEA}}^{(3)}. \tag{1}$$

The TDCS is given as

$$\frac{d^3\sigma}{d\hat{k}_a\, d\hat{k}_b\, dE_b} = \frac{k_a k_b}{k_i} \left| f_{\mathrm{HHOB}} (\underline{q}, \underline{k}_b) \right|^2 \tag{2}$$

It is important to note that in earlier calculations of Yates [1] for scattering processes, imaginary term of $f_{\mathrm{HEA}}^{(3)}$ was not considered because it was assumed insignificant. In the present case, real as well as imaginary terms of $f_{\mathrm{HEA}}^{(3)}$ are taken into account.

The ground state wave function and free electron Coulomb wave functions employed in persent investigation, are as follows

$$\psi_{1s}(\underline{r}_1) = \frac{\lambda^{-3/2}}{\pi} e^{-\lambda r_1}, \tag{3}$$

$$\psi_{c,k_b}^{(-)}(\underline{r}_1) = (2\pi)^{-3/2} e^{-\pi\alpha/2}\, \Gamma(1-i\alpha)\, e^{i\underline{k}_b\cdot\underline{r}_1}\, {}_1F_1(i\alpha, 1, -i(k_b r_1 + \underline{k}_b\cdot\underline{r}_1)). \tag{4}$$

High energy approximation to the second Born term can be simplified [1] to separate the real and imaginary parts

$$\mathrm{Re}\, f_{\mathrm{HEA}}^{(2)} = -\frac{4\pi^2}{k_i} P \int d\underline{p} \int_{-\infty}^{\infty} \frac{dp_z}{p_z - \beta_i} U_{fi}^{(2)} \left(\underline{q} - \underline{p} - p_z\hat{\xi},\ \underline{p} + p_z\hat{\xi}\right)$$

$$- \frac{2\pi}{k_i^2} \frac{d}{d\beta_i} P \int d\underline{p} \int_{-\infty}^{\infty} dp_z \frac{\left(p^2 + p_z^2\right)}{p_z - \beta_i} U_{fi}^{(2)} \left(\underline{q} - \underline{p} - \beta_i\hat{\xi},\ \underline{p} + \beta_i\hat{\xi}\right), \tag{5}$$

where β_i is an average excitation energy and it is assumed [1] that $\beta_i = \frac{\Delta E}{k_i}$ and

$$U_{fi}^{(2)}\left(\underline{q}-\underline{p}-p_z\hat{\xi},\ \underline{p}+p_z\hat{\xi}\right) = \Big\langle \psi_f \Big| \bar{V}\left(\underline{p}+p_z\hat{\xi},\ \underline{r}_1,\ \underline{r}_2,\ \ldots\ \underline{r}_N\right)$$

$$\bar{V}\left(\underline{p}+p_z\hat{\xi},\ \underline{r}_1,\ \underline{r}_2,\ \ldots\ \underline{r}_N\right)\Big|\psi_i\Big\rangle, \tag{6}$$

$$\mathrm{Im}\ f_{\mathrm{HEA}}^{(2)} = \frac{4\pi^3}{k_i}\int d\underline{p}\ U_{fi}^{(2)}\left(\underline{q}-\underline{p}-\beta_i\hat{\xi},\ \underline{p}+\beta_i\hat{\xi}\right). \tag{7}$$

If β_i is set equal to zero in eq. (5), the first term vanishes and the leading term of the real part of $f_{\mathrm{HEA}}^{(2)}$ is then proportional to $\frac{1}{k_i^2}$. The imaginary term of $f_{\mathrm{HEA}}^{(2)}$, *i.e*. eq. (7) identically becomes Glauber's estimate of the second Born term. Third Born term of the HHOB is given by

$$f_{\mathrm{HEA}}^{(3)} = \frac{1}{2\pi k_i^2}\int d\underline{p}\int_{-\infty}^{\infty} dp_z \int d\underline{p}'\int_{-\infty}^{\infty} d\underline{p}''_z \int d\underline{p}''\int_{-\infty}^{\infty} d\underline{p}''_z\ U_{fi}^{(2)}\left(\underline{p}+p_z\hat{\xi},\right.$$

$$\left.\underline{p}'+p_z'\hat{\xi},\ \underline{p}''+p_z''\hat{\xi}\right)\int d\underline{b}_0\ e^{i(\underline{q}-\underline{p}-\underline{p}'-\underline{p}'')b_0}\int_{-\infty}^{\infty} dz_0$$

$$e^{-i(p_z+p_z'+p_z'')z_0}\int_{\infty}^{\infty} dz_0'\ e^{-i(\beta_i-p_z-p_z'')z_0'}\ H(z_0')\int dz_0''\ e^{-i(\beta_i-p_z'')z_0''}\ H(z_0''), \tag{8}$$

where
$$U_{fi}^{(2)}\left(\underline{p}+p_z\hat{\xi},\ \underline{p}'+p_z'\hat{\xi},\ \underline{p}''+p_z''\hat{\xi}\right) = \Big\langle \psi_f \Big| \bar{V}\left(\underline{p}+p_z\hat{\xi},\ \underline{r}_1,\ \underline{r}_2,\ \ldots,\ \underline{r}_N\right)$$

$$\bar{V}\left(\underline{p}'+p_z'\hat{\xi},\ \underline{r}_1,\ \underline{r}_2,\ \ldots,\ \underline{r}_N\right)\bar{V}\left(\underline{p}''+p_z''\hat{\xi},\ \underline{r}_1,\ \underline{r}_2,\ \ldots,\ \underline{r}_N\right)\Big|\psi_i\Big\rangle \tag{9}$$

The most notable point in eq. (8) is that, apart from Glauber like term, there is a second term of $O(k_i^{-2})$ which contributes to the real part of the third Born term.

The calculations are done for coplanar symmetric geometry. Integrations are performed using different integration techniques. The radial, ϕ and p_z integrations are performed incorporating Gauss-Laguarre quadrature, Gauss-Legendre quadrature and Hermite quadrature techniques respectively. The TDCS are obtained with the Z-axis perpendicular to $\underline{q}$ to avoid approximating the first Born term and to extend the validity of the results of larger values of the momentum transfer.

This work has been conceded with the elucidation of the character of the second and third Born terms for short-wavelength collisions and for small momentum transfers.

$f_{\mathrm{HEA}}^{(2)}$ can be calculated with relative ease for ground state hydrogen; few additional complications arise for atomic wave functions written as antisymmetrised products of one electron orbitals. All of the third Born terms, though straight forward to analyze, are algebraically cumbersome.

Figures 1, 2 and 3 represent results for coplanar TDCS using HHOB alongwith the corresponding results for the ionization of atomic hydrogen by electron impact at incident energies of 413.6, 600 and 800 eV respectively. They show a comparison of the present HHOB calculation with the available coplanar measurements of Weigold *et al* [3] and with the

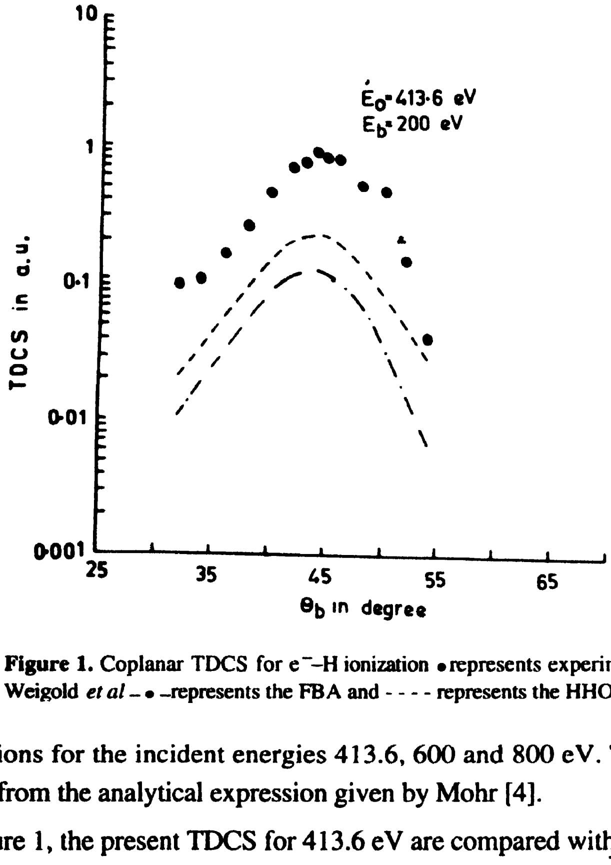

Figure 1. Coplanar TDCS for e^-–H ionization • represents experimental results of Weigold *et al* –•– represents the FBA and - - - - represents the HHOB.

FBA calculations for the incident energies 413.6, 600 and 800 eV. The FBA cross sections are evaluated from the analytical expression given by Mohr [4].

In Figure 1, the present TDCS for 413.6 eV are compared with experimental results of Weigold *et al* [3] and with FBA results. In this case, there is better agreement with the experiments. No lateral shift and a little virtual shift is seen. Figures 2 and 3 show comparison of the present TDCS for 600 and 800 eV with FBA results as corresponding experimental data is not available. Though there is a striking difference in TDCS calculations of FBA and HHOB method, very good agreement in angular distribution between them is seen. The most important conclusion can be drawn through is that the higher order terms are significant in the approximation of a non-zero average excitation energy. It is noticeable that for higher energies, HHOB results approach to FBA. In second and third Born terms, average excitation energy is taken as 0.75 a.u. as it was taken in the case of Byron and Joachain [7]. All the results of HHOB and FBA are divided by $(0.529)^2$ in order to normalize them to achieve experimental peak height. It is worth noting that the variation in average excitation energy is found highly effective to the second and third Born terms.

Since $(e, 2e)$ experiments using atomic hydrogen as a target, unambiguously test the validity of the single ionization reaction, it is obvious that the HHOB method is an appropriate

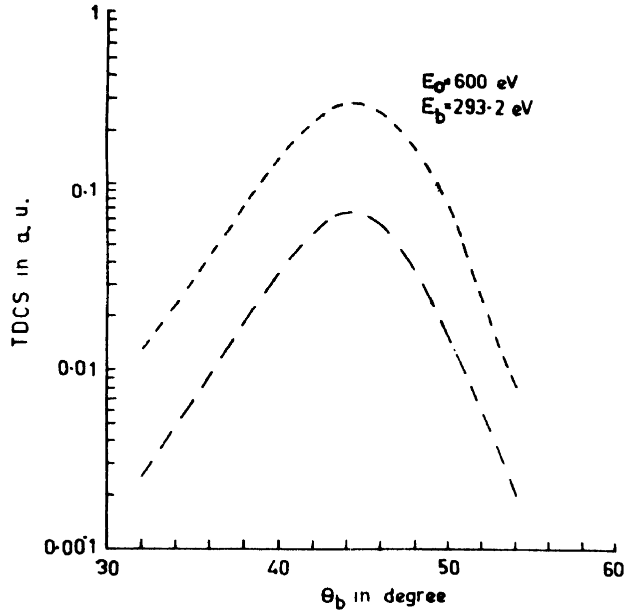

Figure 2. Coplanar TDCS for e^-–H ionization – • –represents the FBA and - - - - represents the HHOB.

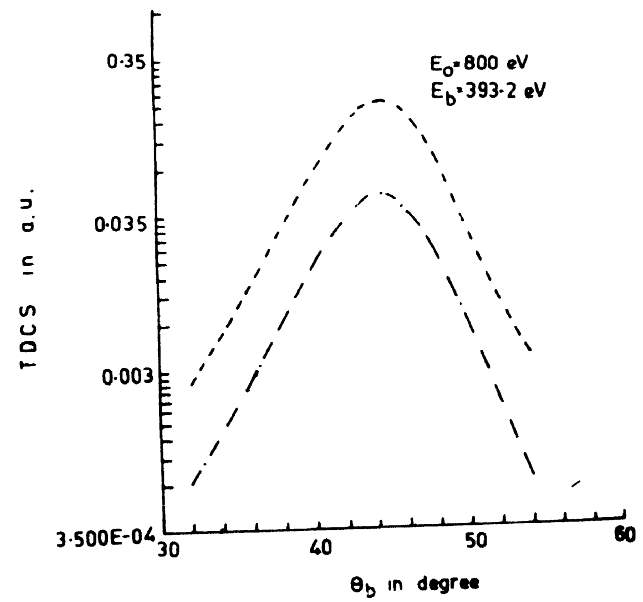

Figure 3. Coplanar TDCS for e^-–H ionization. – • – represents the FBA and - - - - represents the HHOB.

one to understand $(e, 2e)$ processes in more complex targets and for higher energies, where initial and final wave function-effects must be taken into account.

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