

Comparative Analysis on Theoretical TDCS Hydrogenic 3S-State and DDCS for the Ionization of Hydrogenic 2S-State

Tania Noor

Assistant Professor, Department of Mathematics, Premier University, Chittagong, Bangladesh

Abstract:

This paper investigates the differences between double differential cross-sections (DDCS) for the ionization of the hydrogenic 2S metastable state and the calculation of triple differential cross-sections (TDCS) for the ionization of the 3S state hydrogen atoms. We explore the theoretical frameworks used for each and analyze the additional information gained by TDCS measurements. Finally, In order to compare the theoretical hydrogenic 3S and a theoretical setup was created and implemented by electrons in coplanar geometry to compare with 2S state atoms.

Keywords: Hydrogenic, Cross sections, Coplanar geometry

1. Introduction:

Hydrogenic atoms refer to systems with one electron orbiting a nucleus with a single positive charge. The 2S and 3S states represent specific electron configurations within the hydrogen atom.Electron impact ionization is a fundamental process in atomic physics, with applications in plasma physics, astrophysics, and fusion research. Understanding the dynamics of this process requires knowledge of differential cross-sections, which quantify the probability of ionization as a function of various parameters. One of the major issues in the study of the atomic ionization process is the ionization of atoms by charged particles like electrons and positrons. Applied mathematics is faced with fascinating and challenging difficulties while calculating different cross-section findings, such as single, double, and triple differential under diverse kinematic conditions. A new avenue for research in this area has been made possible by the availability of theoretical and experimental results during the last five decades.

The investigation of atomic ionization by electrons and positrons is a significant and crucial challenge for astrophysics, plasma physics, and radiation physics. Bethe [1] initially investigated the ionization of atoms by high-energy particles using quantum mechanics. In recent decades, triple differential cross-sections (TDCS) and double differential cross-sections (DDCS) in collisions between electrons and hydrogen atoms are of increasing interest. In the 20th century, significant advancements were made in both theoretical and experimental studies of triple differential cross sections (TDCS) for both relativistic [2-12] and non-relativistic [13-24] energies, in relation to the multiple scattering theory.Double Differential Cross-Section (DDCS) measures the probability of ionization as a function of the ejected electron's energy and angle with respect to the incident electron's direction.Triple Differential Cross-Section (TDCS) provides a more comprehensive picture by additionally including the momentum of the ejected electron.



Recent studies have focused on calculating DDCS for the ionization of the hydrogenic 2S metastable state using theoretical methods like multiple scattering theory. These calculations provide valuable insights into the dynamics of this process, particularly the ejected electron's energy and angular distribution. However, due to the lack of experimental data for 2S state DDCS, validation remains a challenge.

While DDCS offers valuable information, TDCS provides a more complete picture. Calculating TDCS for the ionization of the 3S state hydrogen atom involves more complex theoretical frameworks. However, advancements in computational techniques and experimental setups with multi-parameter detection are enabling researchers to perform these calculations and measurements.

2. Theory:

A detailed description of how electrons ionize hydrogen atoms can be found in [10]. For the ionization of hydrogen atoms by electrons [10], the T-matrix element is provided by

$$T_{fi} = \langle \Psi_{\mathcal{F}}^{(-)}(\bar{r}_1, \bar{r}_2) | V_i(\bar{r}_1, \bar{r}_2) | \Phi_i(\bar{r}_1, \bar{r}_2) \rangle \quad , \tag{1}$$

Here the perturbation potential $V_i(\bar{r}_1, \bar{r}_2)$ is given by

$$V_i(\bar{r}_1, \bar{r}_2) = \frac{1}{r_{12}} - \frac{Z}{r_2}$$
(2)

For hydrogen atom nuclear charge $(\mathcal{Z}) = 1$, \mathcal{T}_1 and \mathcal{T}_2 are the distance of the atomic electrons and of projectile electron from the nucleus and \mathcal{T}_{12} is the distance between the two electrons. The initial channel unperturbed hydrogenic 3s wave function is,

$$\Phi_{i}(\bar{r}_{1},\bar{r}_{2}) = \frac{e^{\iota \bar{p}_{i}\cdot\bar{r}_{2}}}{(3\pi)^{3/2}} \varphi_{3S}(\bar{r}_{1}) \\
= \frac{e^{\iota \bar{p}_{i}\cdot\bar{r}_{2}}}{(3\pi)^{3/2}} \cdot \frac{1}{81\sqrt{3\pi}} \left(27 - 18\bar{r}_{1} + 2\bar{r}_{1}^{2}\right) e^{-\lambda_{1}r_{1}} \tag{3}$$

Where

$$\varphi_{3S}(\bar{r}_1) = \frac{1}{81\sqrt{3\pi}} (27 - 18\bar{r}_1 + 2\bar{r}_1^2) e^{-\lambda_1 r_1}$$
(4)
and
 $\lambda_1 = 1/3$

Whereas the initial channel unperturbed hydrogenic 2S wavefunction is,

$$\Phi_{i}(\bar{r}_{1},\bar{r}_{2}) = \frac{e^{i\bar{p}_{i}\cdot\bar{r}_{2}}}{(2\pi)^{3/2}} \varphi_{2S}(\overline{r_{1}})$$
(5)

Where

$$\varphi_{2S}(\bar{r_1}) = \frac{1}{4\sqrt{2\pi}} (2 - \bar{r_1}) e^{-\lambda_1 r_1}$$

and
 $\lambda_1 = 1/2$

The ultimate three-particle scattering state wave function is represented by $\Psi_{\mathcal{F}}^{(-)}(\bar{\mathcal{F}}_1, \bar{\mathcal{F}}_2)$ where the electrons are in the continuum with momenta \bar{p}_1 , \bar{p}_2 . The two electrons' coordinates are determined to be $\bar{\mathcal{F}}_1$ and $\bar{\mathcal{F}}_2$.

Here $\Psi_{\mathcal{F}}^{(-)}(\bar{r}_1, \bar{r}_2)$ is approximate wave function for hydrogenic 3S and 2S is given by [14]



$$\begin{split} \Psi_{\mathcal{F}}^{(-)}(\bar{r_{1}},\bar{r_{2}}) &= N(\overline{p_{1}},\overline{p_{2}}) \Big[\phi_{\overline{p_{1}}}^{(-)}(\bar{r_{1}}) e^{i\overline{p_{2}}\cdot\overline{r_{2}}} + \phi_{\overline{p_{2}}}^{(-)}(\overline{r_{2}}) e^{i\overline{p_{1}}\cdot\overline{r_{1}}} + \phi_{\overline{p}}^{(-)}(\overline{r}) e^{i\overline{p_{.}R}} - 2e^{i\overline{p_{1}}\cdot\overline{r_{1}} + i\overline{p_{2}}\cdot\overline{r_{2}}} \Big] / \\ (3\pi)^{3} \\ \psi_{\mathcal{F}}^{(-)}(\bar{r_{1}},\bar{r_{2}}) &= N(\overline{p_{1}},\overline{p_{2}}) \Big[\phi_{\overline{p_{1}}}^{(-)}(\bar{r_{1}}) e^{i\overline{p_{2}}\cdot\overline{r_{2}}} + \phi_{\overline{p_{2}}}^{(-)}(\overline{r_{2}}) e^{i\overline{p_{1}}\cdot\overline{r_{1}}} + \phi_{\overline{p}}^{(-)}(\overline{r}) e^{i\overline{p_{.}R}} - 2e^{i\overline{p_{1}}\cdot\overline{r_{1}} + i\overline{p_{2}}\cdot\overline{r_{2}}} \Big] / \\ (2\pi)^{3} \end{split}$$

(7)

Where

$$\bar{r} = \frac{\overline{r_1} - \bar{r_2}}{2} , \quad \bar{R} = \frac{\overline{r_1} + \bar{r_2}}{2} , \quad \bar{p} = (\overline{p_2} - \overline{p_1}) , \quad \bar{P} = \overline{p_2} + \overline{p_1}$$

The normalization constant $\mathcal{N}(\bar{p}_1, \bar{p}_2)$ is given by

 $\left| \mathcal{N}(\bar{p}_{1,}\bar{p}_{2}) \right|^{-2} = \left| 7 - 2[\gamma_{1} + \gamma_{2} + \gamma_{3}] - \left[\frac{2}{\gamma_{1}} + \frac{2}{\gamma_{2}} + \frac{2}{\gamma_{3}} \right] + \left[\frac{\gamma_{1}}{\gamma_{2}} + \frac{\gamma_{1}}{\gamma_{3}} + \frac{\gamma_{2}}{\gamma_{1}} + \frac{\gamma_{3}}{\gamma_{3}} + \frac{\gamma_{3}}{\gamma_{1}} + \frac{\gamma_{3}}{\gamma_{2}} \right] \right|$ (8)

here

$$\begin{split} \gamma_1 &= e^{\frac{\pi\alpha_1}{2}} \Gamma(1 - i\alpha_1), & \alpha_1 &= \frac{1}{P_1} \\ \gamma_2 &= e^{\frac{\pi\alpha_2}{2}} \Gamma(1 - i\alpha_2), & \alpha_2 &= \frac{1}{P_2} \\ \gamma_3 &= e^{\frac{\pi\alpha}{2}} \Gamma(1 - i\alpha), & \alpha &= -\frac{1}{P} \end{split}$$

And $\phi_{\overline{q}}^{(-)}(\bar{r})$ is the Coulomb wave function and is given by $\phi_{\overline{q}}^{(-)}(\bar{r}) = e^{\frac{\pi\alpha}{2}}\Gamma(1+i\alpha)e^{i\overline{q}\cdot\bar{r}} \mathcal{F}_1(-i\alpha, 1, -i[qr + \overline{q}\cdot\bar{r}]).$

The general one-dimensional integral representation of confluent hypergeometric function is given by $\prod_{1}^{II} \mathcal{F}_{1}(a, c, z) = \frac{\Gamma(c)}{(a)\Gamma(c-a)} \int_{0}^{1} dx \, x^{a-1} (1-x)^{c-a-1} exp(xz)$

For the electron impact ionization, the parameters α_1 , α_2 and α are given below

$$\alpha_1 = \frac{1}{p_1}$$
 for $\overline{q} = \overline{p}_1$, $\alpha_2 = \frac{1}{p_2}$ for $\overline{q} = \overline{p}_2$ and $\alpha = -\frac{1}{p}$ for $\overline{q} = \overline{p}$.

For the normalization constant $\mathcal{N}(\bar{p}_1, \bar{p}_2)$ of equation (9) has been calculated numerically. Now applying above equations, we get,

$$T_{\mathcal{F}i} = \mathcal{N}(\bar{\mathbf{p}}_1, \bar{\mathbf{p}}_2)[T_{\mathcal{B}} + T_{\mathcal{B}'} + T_i - 2T_{P\mathcal{B}}]$$
(9)
where

$$T_{\mathcal{B}} = \langle \Phi_{\overline{p}_1}^{(-)}(\bar{r}_1) e^{i\overline{p}_2 \cdot \bar{r}_2} | V_i | \Phi_i(\bar{r}_1, \bar{r}_2) \rangle$$

$$\tag{10}$$

$$T_{\mathcal{B}'} = \langle \Phi_{p2}^{(-)}(\overline{r_2}) e^{i\overline{p}_1.\overline{r}_1} | V_i | \Phi_i(\overline{r}_1, \overline{r}_2) \rangle$$
(11)

$$T_{i} = \langle \Phi_{\overline{p}}^{(-)}(\overline{r}) e^{i.\overline{p}.\overline{R}} | V_{i} | \Phi_{i}(\overline{r}_{1}, \overline{r}_{2}) \rangle$$
(12)

$$T_{P\mathcal{B}} = \langle e^{i\bar{p}_1.\bar{r}_1 + i\bar{p}_2.\bar{r}_2} | V_i | \Phi_i(\bar{r}_1, \bar{r}_2) \rangle$$
(13)



Here equation (10) is called first Born term.

The first-born equations for hydrogenic 3s-state estimation are,

$$\begin{split} \mathsf{T}_{\mathcal{B}} &= \frac{1}{162\sqrt{6}\pi^2} \left\langle \Phi_{p_1}^{(-)}(\vec{r}_1) \mathrm{e}^{\mathrm{i}\overline{p}_2.\vec{r}_2} \left| \frac{1}{r_{12}} - \frac{1}{r_2} \right| \mathrm{e}^{\mathrm{i}.\overline{p}_1.\overline{r}_2} (27 - 18r_1 + 2r_1^2) \mathrm{e}^{-\lambda_1.r_1} \right\rangle \\ &= \frac{1}{162\sqrt{6}\pi^2} \int \Phi_{p_1}^{(-)*}(\vec{r}_1) \mathrm{e}^{-\mathrm{i}.\overline{p}_2.\vec{r}_2} (\frac{1}{r_{12}} - \frac{1}{r_2}) \mathrm{e}^{\mathrm{i}.\overline{p}_1.\vec{r}_2} (27 - 18r_1 + 2r_1^2) \mathrm{e}^{-\lambda_1.r_1} \mathrm{d}^3 r_1 \mathrm{d}^3 r_2 \\ &= \frac{1}{162\sqrt{6}\pi^2} \int \Phi_{p_1}^{(-)*}(\vec{r}_1) \mathrm{e}^{-\mathrm{i}.\overline{p}_2.\vec{r}_2} \frac{27}{r_{12}} \cdot \mathrm{e}^{\mathrm{i}.\overline{p}_1.\vec{r}_2} \cdot \mathrm{e}^{-\lambda_1.r_1} \mathrm{d}^3 r_1 \mathrm{d}^3 r_2 \\ &- \frac{1}{162\sqrt{6}\pi^2} \int \Phi_{p_1}^{(-)*}(\vec{r}_1) \mathrm{e}^{-\mathrm{i}.\overline{p}_2.\vec{r}_2} \frac{1}{r_{12}} 18r_1 \cdot \mathrm{e}^{\mathrm{i}.\overline{p}_1.\vec{r}_2} \cdot \mathrm{e}^{-\lambda_1.r_1} \mathrm{d}^3 r_1 \mathrm{d}^3 r_2 \\ &+ \frac{1}{162\sqrt{6}\pi^2} \int \Phi_{p_1}^{(-)*}(\vec{r}_1) \mathrm{e}^{-\mathrm{i}.\overline{p}_2.\vec{r}_2} \frac{1}{r_{12}} 2r_1^2 \cdot \mathrm{e}^{\mathrm{i}.\overline{p}_1.\vec{r}_2} \cdot \mathrm{e}^{-\lambda_1.r_1} \mathrm{d}^3 r_1 \mathrm{d}^3 r_2 \\ &- \frac{1}{162\sqrt{6}\pi^2} \int \Phi_{p_1}^{(-)*}(\vec{r}_1) \mathrm{e}^{-\mathrm{i}.\overline{p}_2.\vec{r}_2} \frac{1}{r_{12}} 2r_1^2 \cdot \mathrm{e}^{\mathrm{i}.\overline{p}_1.\vec{r}_2} \cdot \mathrm{e}^{-\lambda_1.r_1} \mathrm{d}^3 r_1 \mathrm{d}^3 r_2 \\ &+ \frac{1}{162\sqrt{6}\pi^2} \int \Phi_{p_1}^{(-)*}(\vec{r}_1) \mathrm{e}^{-\mathrm{i}.\overline{p}_2.\vec{r}_2} \frac{1}{r_{2}} \cdot 27 \cdot \mathrm{e}^{\mathrm{i}.\overline{p}_1.\vec{r}_2} \cdot \mathrm{e}^{-\lambda_1.r_1} \mathrm{d}^3 r_1 \mathrm{d}^3 r_2 \\ &+ \frac{1}{162\sqrt{6}\pi^2} \int \Phi_{p_1}^{(-)*}(\vec{r}_1) \mathrm{e}^{-\mathrm{i}.\overline{p}_2.\vec{r}_2} \frac{1}{r_2} \cdot 27 \cdot \mathrm{e}^{\mathrm{i}.\overline{p}_1.\vec{r}_2} \cdot \mathrm{e}^{-\lambda_1.r_1} \mathrm{d}^3 r_1 \mathrm{d}^3 r_2 \\ &+ \frac{1}{162\sqrt{6}\pi^2} \int \Phi_{p_1}^{(-)*}(\vec{r}_1) \mathrm{e}^{-\mathrm{i}.\overline{p}_2.\vec{r}_2} \frac{1}{r_2} \cdot 18r_1 \cdot \mathrm{e}^{\mathrm{i}.\overline{p}_1.\vec{r}_2} \cdot \mathrm{e}^{-\lambda_1.r_1} \mathrm{d}^3 r_1 \mathrm{d}^3 r_2 \\ &+ \frac{1}{162\sqrt{6}\pi^2} \int \Phi_{p_1}^{(-)*}(\vec{r}_1) \mathrm{e}^{-\mathrm{i}.\overline{p}_2.\vec{r}_2} \frac{1}{r_2} \cdot 2r_1^2 \cdot \mathrm{e}^{\mathrm{i}.\overline{p}_1.\vec{r}_2} \cdot \mathrm{e}^{-\lambda_1.r_1} \mathrm{d}^3 r_1 \mathrm{d}^3 r_2 \\ &+ \frac{1}{162\sqrt{6}\pi^2} \int \Phi_{p_1}^{(-)*}(\vec{r}_1) \mathrm{e}^{-\mathrm{i}.\overline{p}_2.\vec{r}_2} \frac{1}{r_2} \cdot 2r_1^2 \cdot \mathrm{e}^{\mathrm{i}.\overline{p}_1.\vec{r}_2} \cdot \mathrm{e}^{-\lambda_1.r_1} \mathrm{d}^3 r_1 \mathrm{d}^3 r_2 \\ &+ \frac{1}{162\sqrt{6}\pi^2} \int \Phi_{p_1}^{(-)*}(\vec{r}_1) \mathrm{e}^{-\mathrm{i}.\overline{p}_2.\vec{r}_2} \mathrm{e}^{\mathrm{i}.\overline{p}_1.\vec{r}_2} \mathrm{e}^{\mathrm{i}.\overline{p}_1.\vec{r}_2} \mathrm{e}^{-\lambda_1.r_1} \mathrm{d}^3 r_1 \mathrm{d}^3 r_2 \\ &+ \frac{1}{162\sqrt{6}\pi^2} \int \Phi_{p_1}^{(-)*}(\vec{r}_1) \mathrm{e}^{\mathrm{i}.\overline{p}_2.\vec{r}_2}$$

where

$$\begin{split} \mathsf{T} \mathscr{b}_{1} &= -\frac{18}{162\sqrt{6}\pi^{2}} \int \varphi_{\overline{P}_{1}}^{(-)^{*}}(\bar{r}_{1}) \exp(-\mathrm{i}\overline{\mathsf{P}}_{2}.\bar{r}_{2}) \left(\frac{r_{1}}{r_{12}}\right) \exp(\mathrm{i}\overline{\mathsf{P}}_{1}.\bar{r}_{2}) \exp(-\lambda_{1}r_{1}) \mathrm{d}^{3}r_{1} \mathrm{d}^{3}r_{2} \\ \mathsf{T} \mathscr{b}_{2} &= \frac{18}{162\sqrt{6}\pi^{2}} \int \varphi_{\overline{\mathsf{P}}_{1}}^{(-)^{*}}(\bar{r}_{1}) \exp(-\mathrm{i}\overline{\mathsf{P}}_{2}.\bar{r}_{2}) \left(\frac{r_{1}}{r_{2}}\right) \exp(\mathrm{i}\overline{\mathsf{P}}_{1}.\bar{r}_{2}) \exp(-\lambda_{1}r_{1}) \mathrm{d}^{3}r_{1} \mathrm{d}^{3}r_{2} \\ \mathsf{T} \mathscr{b}_{3} &= -\frac{27}{162\sqrt{6}\pi^{2}} \int \varphi_{\overline{\mathsf{P}}_{1}}^{(-)^{*}}(\bar{r}_{1}) \exp(-\mathrm{i}\overline{\mathsf{P}}_{2}.\bar{r}_{2}) \left(\frac{1}{r_{2}}\right) \exp(\mathrm{i}\overline{\mathsf{P}}_{1}.\bar{r}_{2}) \exp(-\lambda_{1}r_{1}) \mathrm{d}^{3}r_{1} \mathrm{d}^{3}r_{2} \\ \mathsf{T} \mathscr{b}_{4} &= \frac{27}{162\sqrt{6}\pi^{2}} \int \varphi_{\overline{\mathsf{P}}_{1}}^{(-)^{*}}(\bar{r}_{1}) \exp(-\mathrm{i}\overline{\mathsf{P}}_{2}.\bar{r}_{2}) \left(\frac{1}{r_{12}}\right) \exp(\mathrm{i}\overline{\mathsf{P}}_{1}.\bar{r}_{2}) \exp(-\lambda_{1}r_{1}) \mathrm{d}^{3}r_{1} \mathrm{d}^{3}r_{2} \\ \mathsf{T} \mathscr{b}_{5} &= \frac{2}{162\sqrt{6}\pi^{2}} \int \varphi_{\overline{\mathsf{P}}_{1}}^{(-)^{*}}(\bar{r}_{1}) \exp(-\mathrm{i}\overline{\mathsf{P}}_{2}.\bar{r}_{2}) \left(\frac{r_{1}^{2}}{r_{12}}\right) \exp(\mathrm{i}\overline{\mathsf{P}}_{1}.\bar{r}_{2}) \exp(-\lambda_{1}r_{1}) \mathrm{d}^{3}r_{1} \mathrm{d}^{3}r_{2} \\ \mathsf{T} \mathscr{b}_{6} &= \frac{2}{162\sqrt{6}\pi^{2}} \int \varphi_{\overline{\mathsf{P}}_{1}}^{(-)^{*}}(\bar{r}_{1}) \exp(-\mathrm{i}\overline{\mathsf{P}}_{2}.\bar{r}_{2}) \left(\frac{r_{1}^{2}}{r_{12}}\right) \exp(\mathrm{i}\overline{\mathsf{P}}_{1}.\bar{r}_{2}) \exp(-\lambda_{1}r_{1}) \mathrm{d}^{3}r_{1} \mathrm{d}^{3}r_{2} \\ \mathsf{T} \mathscr{b}_{6} &= \frac{2}{162\sqrt{6}\pi^{2}} \int \varphi_{\overline{\mathsf{P}}_{1}}^{(-)^{*}}(\bar{r}_{1}) \exp(-\mathrm{i}\overline{\mathsf{P}}_{2}.\bar{r}_{2}) \left(\frac{r_{1}^{2}}{r_{12}}\right) \exp(\mathrm{i}\overline{\mathsf{P}}_{1}.\bar{r}_{2}) \exp(-\lambda_{1}r_{1}) \mathrm{d}^{3}r_{1} \mathrm{d}^{3}r_{2} \\ \mathsf{T} \mathscr{b}_{6} &= \frac{2}{162\sqrt{6}\pi^{2}} \int \varphi_{\overline{\mathsf{P}}_{1}}^{(-)^{*}}(\bar{r}_{1}) \exp(-\mathrm{i}\overline{\mathsf{P}}_{2}.\bar{r}_{2}) \left(\frac{r_{1}^{2}}{r_{2}}\right) \exp(\mathrm{i}\overline{\mathsf{P}}_{1}.\bar{r}_{2}) \exp(-\lambda_{1}r_{1}) \mathrm{d}^{3}r_{1} \mathrm{d}^{3}r_{2} \end{aligned}$$

In a similar way we can write the first-born equations for hydrogenic 2S-state as,

$$\begin{split} \mathsf{T}_{\mathcal{B}} &= \frac{1}{16\pi^2} \left\langle \Phi_{\overline{p}_1}^{(-)}(\bar{r_1}) \mathrm{e}^{\mathrm{i}\overline{p}_2.\bar{r}_2} \left| \frac{1}{r_{12}} - \frac{1}{r_2} \right| \mathrm{e}^{\mathrm{i}.\overline{p}_1.\overline{r}_2} (2 - r_1) \mathrm{e}^{-\lambda_1.r_1} \right\rangle \\ &= \frac{1}{16\pi^2} \int \Phi_{p_1}^{(-)*}(\bar{r_1}) \mathrm{e}^{-\mathrm{i}.\overline{p}_2.\bar{r}_2} (\frac{1}{r_{12}} - \frac{1}{r_2}) \mathrm{e}^{\mathrm{i}.\overline{p}_1.\bar{r}_2} (2 - r_1) \mathrm{e}^{-\lambda_1.r_1} \mathrm{d}^3 r_1 \mathrm{d}^3 r_2 \\ &= \frac{1}{16\pi^2} \int \Phi_{p_1}^{(-)*}(\bar{r_1}) \mathrm{e}^{-\mathrm{i}.\overline{p}_2.\bar{r}_2} \frac{1}{r_{12}} \cdot 2 \mathrm{e}^{\mathrm{i}.\overline{p}_1.\bar{r}_2} \cdot \mathrm{e}^{-\lambda_1.r_1} \mathrm{d}^3 r_1 \mathrm{d}^3 r_2 \\ &- \frac{1}{16\pi^2} \int \Phi_{p_1}^{(-)*}(\bar{r_1}) \mathrm{e}^{-\mathrm{i}.\overline{p}_2.\bar{r}_2} \frac{1}{r_{12}} 2 \cdot \mathrm{e}^{\mathrm{i}.\overline{p}_1.\bar{r}_2} \cdot \mathrm{e}^{-\lambda_1.r_1} \mathrm{d}^3 r_1 \mathrm{d}^3 r_2 \\ &- \frac{1}{16\pi^2} \int \Phi_{p_1}^{(-)*}(\bar{r_1}) \mathrm{e}^{-\mathrm{i}.\overline{p}_2.\bar{r}_2} \frac{1}{r_{12}} r_1 \cdot \mathrm{e}^{\mathrm{i}.\overline{p}_1.\bar{r}_2} \cdot \mathrm{e}^{-\lambda_1.r_1} \mathrm{d}^3 r_1 \mathrm{d}^3 r_2 \\ &+ \frac{1}{16\pi^2} \int \Phi_{p_1}^{(-)*}(\bar{r_1}) \mathrm{e}^{-\mathrm{i}.\overline{p}_2.\bar{r}_2} \frac{1}{r_2} \cdot r_1 \cdot \mathrm{e}^{\mathrm{i}.\overline{p}_1.\bar{r}_2} \cdot \mathrm{e}^{-\lambda_1.r_1} \mathrm{d}^3 r_1 \mathrm{d}^3 r_2 \end{split}$$

 $T_{\mathcal{B}} = T \mathscr{b}_1 + T \mathscr{b}_2 + T \mathscr{b}_3 + T \mathscr{b}_4$



where

$$\begin{split} \mathsf{T} \mathscr{b}_{1} &= \ \frac{1}{16\pi^{2}} \int \varphi_{p_{1}}^{(-)*}(\bar{\mathscr{r}}_{1}) \mathsf{e}^{-\mathrm{i}.\bar{p}_{2}.\bar{\mathscr{r}}_{2}} \frac{1}{r_{12}} \cdot 2\mathsf{e}^{\mathrm{i}.\bar{p}_{1}.\bar{\mathscr{r}}_{2}} \cdot \mathsf{e}^{-\lambda_{1}.r_{1}} \mathsf{d}^{3} \mathscr{r}_{1} \mathsf{d}^{3} \mathscr{r}_{2} \\ \mathsf{T} \mathscr{b}_{2} &= \ -\frac{1}{16\pi^{2}} \int \varphi_{p_{1}}^{(-)*}(\bar{\mathscr{r}}_{1}) \mathsf{e}^{-\mathrm{i}.\bar{p}_{2}.\bar{\mathscr{r}}_{2}} \frac{1}{r_{12}} 2 \cdot \mathsf{e}^{\mathrm{i}.\bar{p}_{1}.\bar{\mathscr{r}}_{2}} \cdot \mathsf{e}^{-\lambda_{1}.r_{1}} \mathsf{d}^{3} \mathscr{r}_{1} \mathsf{d}^{3} \mathscr{r}_{2} \\ \mathsf{T} \mathscr{b}_{3} &= \ -\frac{1}{16\pi^{2}} \int \varphi_{p_{1}}^{(-)*}(\bar{\mathscr{r}}_{1}) \mathsf{e}^{-\mathrm{i}.\bar{p}_{2}.\bar{\mathscr{r}}_{2}} \frac{1}{r_{12}} \mathscr{r}_{1} \cdot \mathsf{e}^{\mathrm{i}.\bar{p}_{1}.\bar{\mathscr{r}}_{2}} \cdot \mathsf{e}^{-\lambda_{1}.r_{1}} \mathsf{d}^{3} \mathscr{r}_{1} \mathsf{d}^{3} \mathscr{r}_{2} \\ \mathsf{T} \mathscr{b}_{4} &= \ \frac{1}{16\pi^{2}} \int \varphi_{p_{1}}^{(-)*}(\bar{\mathscr{r}}_{1}) \mathsf{e}^{-\mathrm{i}.\bar{p}_{2}.\bar{\mathscr{r}}_{2}} \frac{1}{r_{2}} \cdot \mathscr{r}_{1} \cdot \mathsf{e}^{\mathrm{i}.\bar{p}_{1}.\bar{\mathscr{r}}_{2}} \cdot \mathsf{e}^{-\lambda_{1}.r_{1}} \mathsf{d}^{3} \mathscr{r}_{1} \mathsf{d}^{3} \mathscr{r}_{2} \end{split}$$

After analytical calculations using Lewis's integral [20], Using computer programming language, we have quantitatively calculated the Born equation. The first-Born triple differential cross sections is finally calculated by

$$\frac{\mathrm{d}^{3}\sigma}{\mathrm{d}\Omega_{1}\mathrm{d}\Omega_{2}\mathrm{d}E_{1}} = \frac{\mathrm{p}_{1}\mathrm{p}_{2}}{\mathrm{p}_{i}} |\mathrm{T}_{\mathcal{F}i}|^{2}$$
(14)

Here E_1 is the energy of the ejected electron.

3. Result & Discussion:

In this segment we explore the comparison of ionization of atomic hydrogen at metastable 3S-state TDCS and metastable 2S-state DDCS by electrons. Comparing the DDCS for the 2S metastable state with the TDCS for the 3S ground state reveals the influence of the initial electronic configuration on the ionization process. The higher-energy orbital in the 2S state is expected to lead to different angular and energy distributions for the ejected electron compared to the ground state. Additionally, including the momentum information in TDCS offers a more complete picture of the momentum transfer between the colliding particles.

The first-Born triple differential cross sections (TDCS) for the ionization process with incident energy $E_i = 250 \text{ eV}$, here the ejected angles (θ_1) varies and the scattered angles (θ_2) are fixed. The ejected angle θ_1 varies from 0[°] to 360[°]. Hydrogenic 3S-state [26] and the 2S-state results of [25] are presented here for comparison. Then we compare the TDCS of 2S-state and 3S-state with the first-born 2S-state DDCS [28]. We consider $\phi = 0^{°}$ as recoil region and $\phi = 180^{°}$ as binary region of the present calculations.

In the first-Born result we presented the triple differential cross sections (TDCS) for the ionization of metastable 3S- state hydrogen atoms and double differential cross section (DDCS) by electrons for the incident energy $E_i = 250$ eV, ejected electron energy $E_1 = 5$ eV for the scattering angles θ_2 existing in the given figures.

Table 1: The ionization of atomic hydrogen atoms through electron impact at the metastable 3S-state is investigated using triple differential cross sections (TDCS). The results show that the emission angle θ_1 for incident energy is 250eV, the scattering angle is $\theta_2=9^0$ and the ejected electron energy is $E_1=5eV$. Here B1(3S): 3S-state first Born TDCS results; B1(2S): 2S-state first Born TDCS results; $B_1(2S)$: 2S-state first Born TDCS results.

Ejected	B1(2S)	B1(3S)	B1(2S)
angles(θ_1)			DDCS
0	3.8461	5.6175	0.01359
36	2.6382	3.8662	0.02075



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72	2.2079	3.2424	0/00147
108	3.2756	4.7899	0.00359
144	3.6140	5.2803	0.01676
180	2.3431	3.4386	0.00007
216	2.3873	3.5025	0.02361
252	3.6768	5.3713	0.00037
288	3.1916	4.6682	0.00010
324	2.1905	3.2172	0.00019
360	2.7073	3.9663	0

It is noted that the table above displays by accounting for the remaining ion's momentum, TDCS offers a more comprehensive view of the ionization process than DDCS. The TDCS values for the 3S-state (B1(3S)) are consistently higher than those for the 2S-state (B1(2S)) at corresponding ejected angles (θ 1). This indicates that the ionization probability is higher for the 3S-state compared to the 2S-state under the given conditions. The 2S-state DDCS data (B1'(2S)) show a substantial variation in magnitude and physical interpretation between the triple and double differential cross sections (TDCS) for the 2S and 3S states compared to the TDCS values for both states. For the 3S-state (B1(3S)), the TDCS values show a peak around θ 1 = 0 and θ 1 = 144 degrees, indicating higher probabilities of electron ejection at these angles.

The 3S-state has the lowest TDCS values at $\theta 1 = 72$ degrees and $\theta 1 = 324$ degrees, indicating less advantageous angles for electron ejection.

The DDCS data (B1'(2S)) show large peaks at $\theta 1 = 36$ degrees and $\theta 1 = 216$ degrees, with more fluctuation and lower values overall. The extremely low results at other angles, like $\theta 1 = 72$ degrees and $\theta 1 = 324$ degrees, show that there is virtually little chance of ionization at these angles. The TDCS value for the 3S-state is 5.6175 for $\theta 1 = 0$ degrees, but it is 3.8461 for the 2S-state, indicating a distinct preference for ionization in the 3S-state.

The TDCS of the 3S-state at $\theta 1 = 180$ degrees is 3.4386, while that of the 2S-state is 2.3431, indicating once more the higher ionization probability of the 3S-state at this angle. The difference between TDCS and DDCS magnitudes is shown by the extremely low (0.00007) DDCS findings at $\theta 1 = 180$ degrees.

The data in Table 1 shows that the higher TDCS values for the 3S-state across most ejection angles indicate that the ionization of hydrogen atoms by electron impact is more likely in the metastable 3S-state than in the 2S-state. Furthermore, even though they are smaller, the DDCS values offer additional insight into the ionization process by highlighting the significance of angle and energy in predicting the probability of electron ejection.

Conclusion

An extremely intriguing element of the current investigation is shown. The table demonstrates how the outcomes of TDCS and DDCS are remarkably different from one another. In contrast, two TDCS results of the 3S-state and the 2S-state first Born result showed good agreement. The current computation is based on Das and Seal's multiple scattering theory, which makes a substantial addition to the understanding of hydrogenic metastable 3S-state and 2S-state ionization issues. Additional theories and experimental research in the relevant subject will be required for the evaluation of the current efforts. This thorough comparison improves our knowledge of the dynamics of atomic hydrogen ionization, especially in various metastable states and under certain circumstances.



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Department of Mathematics, Chittagong University of Engineering and Technology Chittagong-4349, Bangladesh.

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