Journal of Atomic, Molecular, Condensate & Nano Physics
Vol. 3, No. 2, pp. 105–113, 2016
ISSN 2349-2716 (online); 2349-6088 (print)
Published by RGN Publications

http://www.rgnpublications.com

A Comparative Study of Ionization of Hydrogenic Ions by Positronium Impact

Research Article

D. Ghosh[1,*] and C. Sinha[2]

[1] *Department of Physics, Michael Madhusudan Memorial College, Durgapur, Burdwan, India*
[2] *Department of Theoretical Physics, Indian Association for the Cultivation of Science, Kolkata 700032, India*
***Corresponding author:** dipalighoshwb@gmail.com

Abstract. A comparative study of target ionization processes of Hydrogenic ions by Positronium impact are investigated. Calculations are performed using the Coulomb distorted eikonal approximation. Interesting qualitative features are noted both in the scattered Ps and the ejected electron distributions in triple differential as well as double differential cross sections. The Ps impact ionization of three hydrogenic ions shows some distinct variation from the electron impact ionization.

Keywords. Antimatter; Positronium

PACS. 13.85.Hd

Received: February 15, 2015 **Accepted:** January 3, 2016

1. Introduction

The present work concerns a comparative study of single ionization of some ionic (hydrogenic) targets, e.g., He^+, Li^{++} and Be^{+++}. For this particular target ionization process we have considered positronium (Ps) as the projectile because, being the bound state of electron and its antimatter positron, Ps has a zero-static interaction due to the coincidence of its centre of charge and centre of mass in contrast to conventional atoms.

From the theoretical point of view, single ionization process by Ps impact even of the simplest hydrogenic target is a bit difficult task as it becomes a four body problem. The complexity mainly arises due to the internal degrees of freedom of the projectile Ps (unlike the electron or the positron impact) that must be taken into account. However the direct Coulomb interaction

between the Ps and the atomic or ionic target is very much weakened as compared to that arising from the electron exchange effect between them [1]. Again the calculation of this exchange process is rather difficult since it involves electron swapping between two different centres, the target and the Ps though the electron exchange effect seems to be not the main driving force for the target ionization process.

The present investigation is mainly motivated by the experimental results of Laricchia et al. [2], where they have observed electron like scattering of the Ps atom. According to their experimental as well as theoretical (close coupling) results, the Ps total cross sections is unexpectedly close to that of a bare electron, moving at the same velocity. This finding created interest to study theoretically the target ionization process by Ps impact and to compare the results with the corresponding electron impact ionization results. Hydrogenic ions being the simplest ions (He^+, Li^{++} and Be^{+++}) are chosen as the target for the initial work. We have calculated the *Triple differential cross sections* (TDCS) and the *Double differential cross sections* (DDCS) at different incident energies and with different kinematics to compare the collision cross sections of these targets in view of the Ps impact ionization.

The basic difference between the electron impact and the Ps impact ionization lies in the fact that in the latter case, both the projectile and the target are composite objects having an internal structure and as such the dynamics demands evaluation of multicenter integrals in the transition matrix elements which are quite difficult and time consuming. The present target ionization (by Ps impact) is different from the pure single ionization of the target atom/ion by positron or electron impact and as such the present TDCS additionally carries the information about the influence of the Ps on the target electron distributions. Further, consideration of the exchange effect between the projectile electron and the target electron in the final channel arises formidable difficulties to solve the problem in the present prescription.

2. Theory

The present problem addresses the theoretical study of the dynamics of target inelastic process, e.g., single ionization of the target (He^+ ion, Li^{++} ion and Be^{+++} ion), all the ions being initially in their ground states.

$$e^+ e + X(1s) \rightarrow e^+ e(1s) + X^+ + e \tag{2.1}$$

where $X = He^+, Li^{++}, Be^{+++}$.

The prior form of the ionization amplitude for the aforesaid process (2.1) is given as:

$$T_{if}^{prior} = -\frac{\mu_f}{2\pi} \langle \Psi_f^-(\vec{r}_1, \vec{r}_2, \vec{r}_3) | V_i | \psi_i(\vec{r}_1, \vec{r}_2, \vec{r}_3) \rangle \tag{2.2}$$

V_i is the initial channel perturbation not diagonalized in the initial state, given by,

$$V_i = \frac{z_t}{r_1} - \frac{z_t}{r_2} - \frac{1}{r_{13}} + \frac{1}{r_{23}} \tag{2.3}$$

$\vec{r}_1$, $\vec{r}_2$ and $\vec{r}_3$ in eqn. (2.2) are the position vectors of the positron and the electron of the Ps and the bound electron of the target ion (He^+, Li^{++}, Be^{+++}) respectively, with respect to the target nucleus;

Z_t (= 2,3,4) is the charge of the target nucleus and $\vec{r}_{13} = \vec{r}_1 - \vec{r}_3$, $\vec{r}_{23} = \vec{r}_2 - \vec{r}_3$.

The wave-function Ψ_f^- satisfy the outgoing wave boundary condition. The corresponding Schrodinger equation is given by,

$$(H - E)\Psi^{\pm} = 0 \tag{2.4}$$

where the full Hamiltonian of the system is given by,

$$H = -\frac{\nabla_R^2}{2\mu_i} - \frac{\nabla_{12}^2}{2\mu_{ps}} - \frac{\nabla_3^2}{2} - \frac{1}{r_{12}} + \frac{Z_t}{r_1} - \frac{Z_t}{r_2} - \frac{Z_t}{r_3} - \frac{1}{r_{13}} + \frac{1}{r_{23}} \tag{2.5}$$

The initial asymptotic wave function ψ_i in equation (2.2) is chosen as

$$\psi_i = \phi_{Ps}(|\vec{r}_1 - \vec{r}_2|)e^{i\vec{k}_i\cdot\vec{R}}\phi_T(\vec{r}_3) \tag{2.6a}$$

where $\vec{R} = \frac{(\vec{r}_1+\vec{r}_2)}{2}$ and k_i is the initial momentum of the Ps atom with respect to the target nucleus. The ground state wave function of the Ps atom

$$\phi_{Ps}(|\vec{r}_1 - \vec{r}_2|) = N_{1s}\exp(-\lambda_i r_{12}) \tag{2.6b}$$

with $N_{1s} = \lambda_i^{\frac{3}{2}}/\sqrt{\pi}$ and $\lambda_i = \frac{1}{2}$. The ground state wave function of the target hydrogenic ion is given as

$$\phi_T(r_3) = N_T\exp(-\lambda_T r_3) \tag{2.7}$$

where $\lambda_T = 2,3,4$ and $N_T = \frac{\lambda_T^{\frac{3}{2}}}{\sqrt{\pi}}$.

In the present work we have adopted the prior version of the transition matrix (eqn. (2.2)) which is supposed to be more suitable for an ionization process [3–6]. Equation (2.4) concerning a four body problem could not be solved exactly and as such one has to resort to some simplifying assumptions. The final state wave function Ψ_f^- (eqn. (2.2)) involving two bound particles (Ps) and one continuum particle is approximated by the following ansatz in the framework of Coulomb-Eikonal approximation [5–8]:

$$\Psi_f^-(\vec{r}_1,\vec{r}_2,\vec{r}_3) = N_{1s}\exp(-\lambda_f r_{12})(2\pi)^{-\frac{3}{2}}N_3 e^{i\vec{k}_3\cdot\vec{r}_3}N_f e^{i\vec{k}_f\cdot\vec{R}}(r_1+z_1)^{i\eta_f}(r_2+z_2)^{-i\eta_f}$$
$$ {}_1F_1(-i\alpha_3, 1, -i(k_3 r_3 + \vec{k}_3\cdot\vec{r}_3)) \tag{2.8}$$

where $\lambda_i = \lambda_f = \frac{1}{2}$, $N_3 = \exp\left(\frac{\pi\alpha_3}{2}\right)\Gamma(1 - i\alpha_3)$ with $\alpha_3 = -\frac{Z_t}{k_3}$, $\eta_f = \frac{Z_t}{k_f}$.

Equation (2.8) satisfies the incoming wave boundary condition which is one of the essential criteria for a reliable estimate of an ionization process.

The two centre effect on the electron of the Ps due to its parent ion (e^+) and the screened target ion is implicit in eqn. (2.8). Since in the final channel the ejected electron from the target is in the long range Coulomb field of the residual target ion (He^{++}, Li^{+++} and Be^{++++}), this interaction is incorporated in eqn.(2.8). The justification of the present ansatz for the approximate wave function (Ψ_f^-) can be given as follows. The confluent hypergeometric function (${}_1F_1$) arises because of the continuum wave function of the ejected electron in the field of its parent target ion. The strong interactions between the target nucleus and the two components of the incident particle (e and e^+ of Ps) are taken into account by the two eikonal factors in the final channel. In order to avoid the complexity in the analytical calculations, we have neglected the higher order interactions between the e^+/e of the Ps and the target electron and have

mainly concentrated on the ionization of the target; this interaction being considered through the perturbation interaction in the initial channel.

In view of equations (2.2)-(2.8), we obtain the target ionization amplitude (direct) for the process (2.1) as

$$T_{if}^{direct} \equiv -\frac{\mu_f}{2\pi}\iiint N_3^* N_T (2\pi)^{-\frac{3}{2}} \exp(-\lambda_T \vec{r}_3) e^{i\vec{k}_i\cdot\vec{R}} N_{1s}^2 \exp(-(\lambda_i+\lambda_f) r_{12})$$
$$\left(\frac{z_t}{r_1} - \frac{z_t}{r_2} - \frac{1}{r_{13}} + \frac{1}{r_{23}}\right) e^{-i\vec{k}_3\cdot\vec{r}_3} e^{-i\vec{k}_f\cdot\vec{R}}$$
$$(r_1+z_1)^{i\eta_f} (r_2+z_2)^{-i\eta_f}\, {}_1F_1(i\alpha_3, 1, i(k_3 r_3 + \vec{k}_3\cdot\vec{r}_3)) d\vec{r}_1\, d\vec{r}_2\, d\vec{r}_3 \tag{2.9}$$

After much analytical reduction [9–11] the target ionization amplitudes T_{if} in equation (2.9) is finally reduced to a three dimensional numerical integral. The triple differential cross sections (TDCS) [12] is given by

$$\frac{d^3\sigma}{dE_3 d\Omega_f d\Omega_3} = \frac{k_f k_3}{k_i} |T_{if}|^2 \tag{2.10}$$

Due to the principle of detailed balance, the transition amplitude obtained from the post and prior forms should in principle, be the same if the exact scattering wave function in the initial or final channel (Ψ_i^+, Ψ_f^-) could be used, which for a four body problem is a formidable task. In the case of approximate wave functions, the afore said two forms might not lead to identical results giving rise to some post-prior discrepancy. However, in the case of simple First Born Approximation (FBA) where the initial or final scattering states are represented by the corresponding asymptotic wave functions, there should not be any post-prior discrepancy. In the present model, the full scattering wave functions are different in the post and prior versions and as such the corresponding results might differ to some extent. However as mentioned before, for the ionization process, the prior form is supposed to be [4, 6] more suitable than the post one.

3. Results and Discussion

The TDCS and the DDCS results are computed for Ps impact target ionization of He^+, Li^{++} and Be^{+++}. For the single ionization, the threshold energy is determined by $E_{th} = E^{1s}_{(He^+, Li^{++}, Be^{+++})}$. Since the present study is made in coplanar geometry, i.e., $\vec{k}_i$, $\vec{k}_f$ and $\vec{k}_3$ all being in the same plane, the azimuthal angles ϕ_i, ϕ_f and ϕ_3 can assume values 0°and 180°.

Figures 1 and 2 exhibit the angular distributions (TDCS) of the ejected electron (θ_3) for the singly charged helium ion (He^+) and doubly charged lithium ion (Li^{++}) target respectively in atomic unit (a.u.) for different scattering angles of the incident Ps ($\theta_f = 2°, 4°$), keeping the ejected electron energy (E_3) fixed at 10 eV and the incident energy (E_i) at 750 eV. The same TDCS having similar kinematics for triply charged Beryllium ion (Be^{+++}) is demonstrated in Figure 2 as inset. As may be noted from the Figures 1 and 2, the double peak structure becomes prominent for increasing ionic charge of the target i.e. for $Li^{++}$and Be^{+++} ion. For all these target ions cross sections get diminished for larger scattering angle of positron. Like the electron impact TDCS of the ejected electron, here also, the binary peak is more prominent than the recoil one and the main contribution comes out from the binary side.

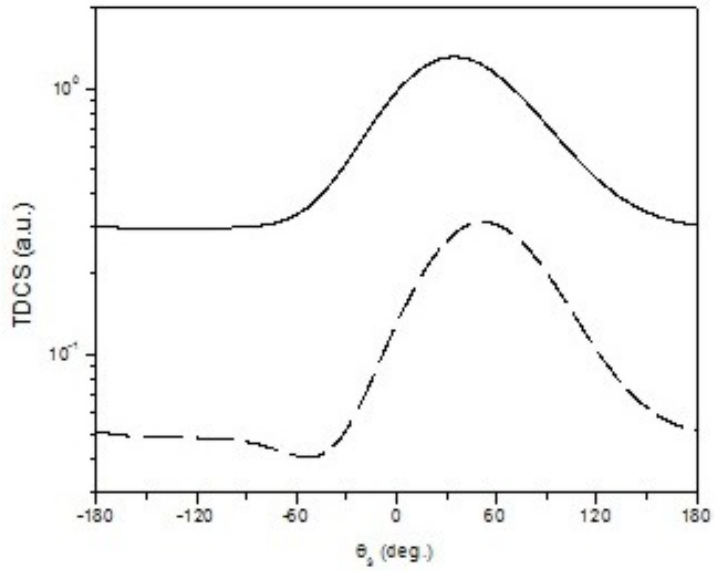

Figure 1. The triple differential cross sections (TDCS) for Ps-He^{+} system against the ejected electron angle (θ_3) for different values of ejected Ps atom angle (θ_f), keeping fixed ejected energy ($E_3 = 10$ eV). The incident energy is fixed at 750 eV. The solid curve represents $\theta_f = 2°$, dashed curve is for $\theta_f = 4°$.

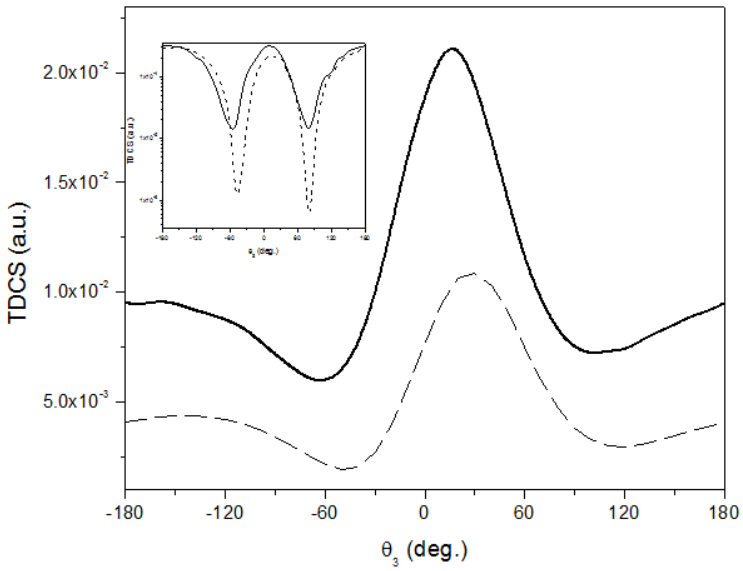

Figure 2. Similar distribution and kinematics for Ps-Li^{++} system. Inset curve represents Ps-Be^{++} system.

Figures 3 and 4 demonstrates TDCS for two different kinematics corresponding to the three different target ions. Figure 3 represents the ejected electron distribution for the incident energy $E_i = 1500$ eV, and Figure 4 represents the same distribution for $E_i = 2000$ eV, keeping the ejected electron energy ($E_3 = 10$ eV) same for both the kinematics. Comparing Figures 3 and 4, it can be inferred that for the Li^{++} and Be^{+++} target, the binary peak gets sharper

than that for the He^+ target though the overall distribution has larger cross sections for the latter. Figures 3 and 4 reveal that for same kinematics the recoil peak gets more pronounced for Be^{+++} and Li^{++} ion than He^+ ion target. Since the recoil peak is mainly governed by the electron-target nucleus interaction, the large recoil peak for the target having higher Z, may be qualitatively explained by the stronger elastic scattering from the nucleus [12].

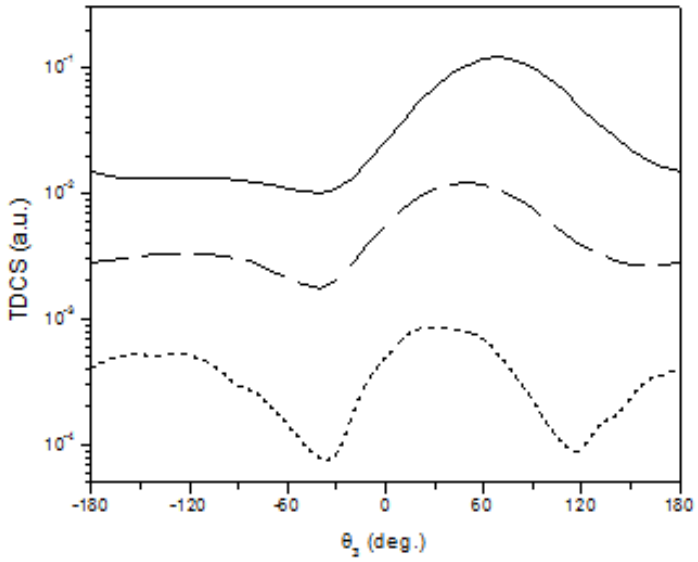

Figure 3. The triple differential cross sections (TDCS) for Ps-He^+ system (solid curve), for Ps-Li^{++} system (dashed curve) and for Ps-Be^{+++} system (dotted curve) against the ejected electron angle (θ_3) for $E_i = 1500$ eV, $E_3 = 10$ eV and $\theta_f = 4°$.

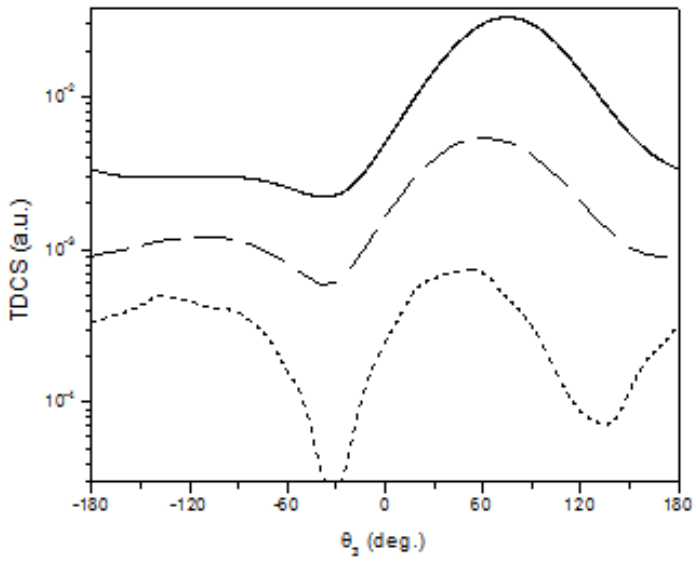

Figure 4. Same as in Figure 3 but for $E_i = 2500$ eV, $E_3 = 10$ eV and $\theta_f = 4°$.

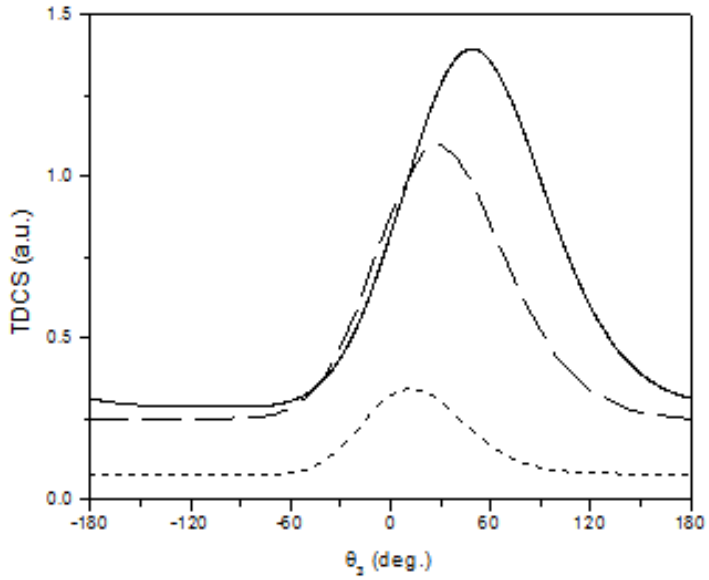

Figure 5. (color online) The triple differential cross sections (TDCS) for different incident energy for Ps-He^+ system. The ejected energy is fixed at 10 eV and $\theta_f = 2°$. The incident energies are 300 eV (dotted curve), 600 eV (dashed curve) and 1200 eV (solid curve) respectively.

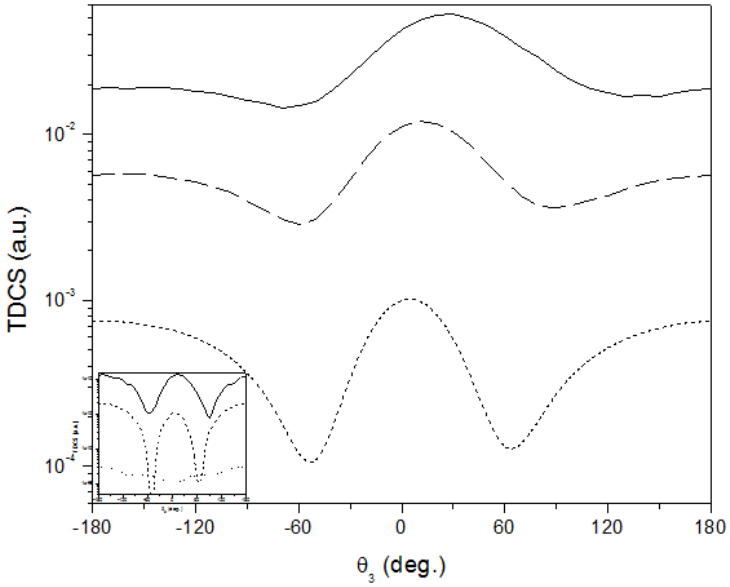

Figure 6. Same as in Figure 5 but for Ps-Li^{++} system. The inset of Figure 6 represents Ps-Be^{+++} system.

Figures 5 and 6 demonstrate the present TDCS of the ejected electron (θ_3) corresponding to the He^+ and Li^{++} (inset Be^{+++}) target respectively for different incident energy of incident positronium. Figure 6 (E_i = 300 eV, 600 eV, 1200 eV; E_3 = 10 eV for $\theta_f = 2°$) reveals the clear evidence of a double peak structure that becomes more pronounced for lower value of incident energy (E_i = 300 eV, 600 eV). This could probably be due to double scattering effect (scattering

from two centres) of the ejected electron from the Ps projectile as was noted in the charge transfer problems at relatively high incident energies [13, 14]. Whereas, for the same kinematics He^+ target does not show any prominent double peak structure (Figure 5). It is also noted that for the same kinematics, the TDCS decreases for higher value of the target charge Z, as expected physically. In comparison to Figure 5, we find that the recoil peak structure gets more prominent for the Be^{+++} target. This is again due to stronger elastic scattering of the electron from the residual target nucleus (Be^{++++}) than from the target nucleus He^{++}. Another point to be noted from these two figures is that, with increasing incident energy the TDCS increases whereas the fact is reverse for the target ionization by electron impact. The difference in the nature of TDCS may arise from the fact that in the present case the projectile being the neutral one, does not produce any effective interaction with the ejected electron which is responsible to decrease the TDCS at higher incident energy up to the considered incident energy regime.

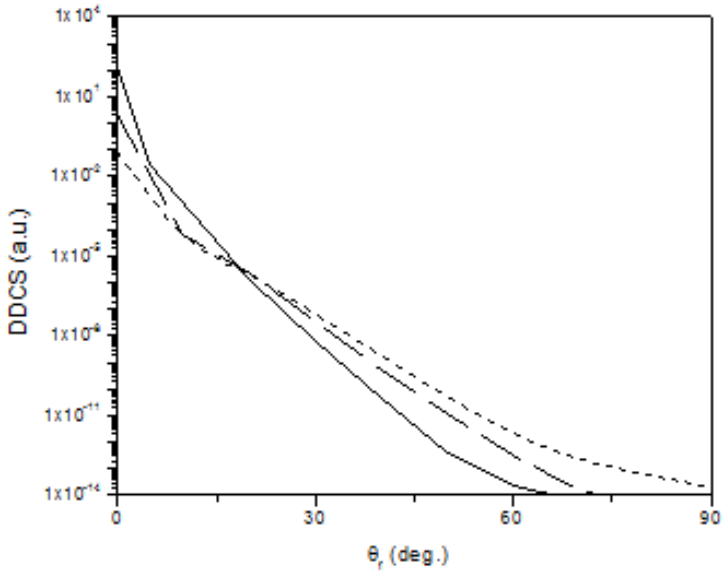

Figure 7. DDCS against the ejected Ps angle (θ_f) for different incident energy keeping ejected electron energy fixed at $E_3 = 10$ eV and incident energy $E_i = 2000$ eV, Ps-He^+ system (solid curve), Ps-Li^{++} system (dashed curve), Ps-Be^{+++} system (dotted curve

Figure 7 demonstrates the double differential cross sections (DDCS) with respect to the scattered Ps angle (θ_f) for the Ps-He^+, Ps-Li^{++} and Ps-Be^{+++} systems. This figure depicts the Ps distributions at an incident energy 2000 eV keeping the ejected electron energy fixed at 10 eV. Here the solid curve represents He^+ target, dashed curve represents Li^{++} target and the dotted on represents DDCS for Be^{+++} ion. From the figure it is clear that the maximum of DDCS distribution is higher for He^+ target than the rest targets though after more or less 20° of the scattered angle DDCS for Li^{++} and Be^{+++} gets larger than He^+ ion.

4. Conclusion

In the present study it is found that with increasing incident energy the TDCS increases whereas the fact is reverse for the target ionization by electron impact. The difference in the nature of TDCS may arise from the fact that in the present case the projectile being the neutral one, does not produce any effective interaction with the ejected electron up to the incident energy regime which is responsible to decrease the TDCS at higher incident energy. On the contrary, Like the electron impact TDCS of the ejected electron, here also, the binary peak is more prominent than the recoil one and the main contribution comes out from the binary side though, the large recoil peak at lower energy (vide inset of Figure 3) for the ionic targets may be qualitatively explained by the stronger elastic scattering from the nucleus since the recoil peak is mainly governed by the electron-target nucleus interaction.

Acknowledgment

UGC Minor Research Project PSW-026/13-14 dated 18-3-2014.

Competing Interests

The authors declare that they have no competing interests.

Authors' Contributions

All the authors contributed significantly in writing this article. The authors read and approved the final manuscript.

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