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Model Potential Approach for Positronium Impact Ionization of Alkali Atoms

Research Article

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Abstract. Positronium impact target ionization processes of alkali atoms are investigated in the frame work of model potential formalism and using the Coulomb distorted eikonal approximation. Alkali atoms are visualised as one electron species and to take the effect of the core electrons, the valence electron is assumed to move in the field of a model potential. Interesting qualitative features are noted both in the ejected electron and scattered Ps distributions in triple differential as well as double differential levels of the collision cross sections.

Keywords. Positronium; ionization; Model potential; Coulomb distorted eikonal approximation

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1. Introduction

Alkali atoms as targets in atomic collisions have been considered in a large number of experimental and theoretical studies over the years, as they can be addressed both theoretically and experimentally relatively easily such that detailed comparison is possible [1]. Again collisions with alkali-metal atoms are of interest for application in the design of laser systems in VUV regime [2] and for diagnostics of (fusion) plasmas and their impurities [3, 4]. Further, from the theoretical point of view, the shell structure of alkalis are interesting in the sense that the quasi-one electron models of the loosely bound outermost electron and a stationary effective potential due to frozen inner shell electrons are the appealing features of the alkali atoms involved in collision processes. On the other hand, use of positronium as the projectile becomes interesting as new experimental techniques and theoretical methods are enabling increasingly stringent tests of the understanding of basic atomic and molecular collision phenomena as well as of fundamental antiparticle-matter interactions. In this paper a comparative study of Ps impact ionization of two alkali atoms are performed. Such collision processes find interest as the targets are alkali atoms having simple structures, low ionization potentials and large polarizabilities where as the projectile being the simplest particle-antiparticle system.

From the theoretical perspective, single ionization process by Ps impact, even of the simplest hydrogenic target is a bit difficult task [5] as it becomes a four body problem. The complexity mainly arises due to the internal degrees of freedom of the projectile Ps which must be taken into account. However the direct Coulomb interaction between the Ps and the atomic target is very much smaller as compared to that arising from the electron exchange effect between them [6]. 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. Therefore, our main task is to develop suitable mathematical tools necessary for solving the many body Schrodinger equation that appears in this particular single ionization process. Various approximation models like close coupling [7–9], R-matrix theory [10, 11], different variational methods [12–14] were developed for solving the Ps impact elastic and inelastic scattering processes. From such investigations one can make a comparative study of the different theoretical models with relative merits and demerits and their agreements with the available experimental data. The suitability of different mathematical models depends on the collision partners, particular collisional channel and on the energy regime concerned. *Close coupling* (CC) methods are proved to be quite successful in the lower incident energy regime while the CDW models are supposed to be more suitable with reasonable accuracy at comparatively moderate and higher incident energies for which the CC methods become increasingly difficult with energies to compute with.

The recent experimental and theoretical results of Brawley et al. [15] show that the total cross sections of atoms with Ps as projectile is unexpectedly close to that of a bare electron projectile moving at the same velocity. These findings motivated us to study theoretically the target ionization process of alkali atoms by Ps impact and to compare the results with the corresponding electron impact ionization results. The present model is based on the frame work of *Coulomb Modified Distorted Wave Approximation* (CMDA). We have calculated both the *triple differential cross sections* (TDCS) and the double differential cross sections (DDCS) and have tried to compare the findings with the existing theoretical and experimental results [16–18] of electron impact ionization of Na atom.

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 occurring in the transition matrix elements which are quite difficult and time consuming. The present study of target ionization (by Ps impact) is different from that of the 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 ejected electron distributions as the TDCS of the ejected electron varies with both the energy and the angle of the scattered Ps. The inclusion of the exchange effect between the projectile electron and the target electron in the final channel would lead to formidable difficulties in the present prescription.

The present problem addresses the theoretical study of the dynamics of target inelastic process, e.g., single ionization of the target (Na, K, Rb and Cs atom), both being initially in their ground states.

$$e^+e(1s)+X(1s)\to e^+e(1s)+X^++e\,, \tag{1}$$

where X = Na,K,Rb,Cs.

Since both the composite bodies interact in the initial channel, theoretical prescription is difficult and as such one has to resort to some simplifying assumptions to circumvent the mathematical complexity. The present calculation is performed in the framework of post collisional Coulomb Distorted Eikonal Approximation taking account of the proper asymptotic boundary condition of the ejected electron in final channel, which is one of the most important criteria for a reliable estimate of the ionization cross-sections.

2. Theory

The prior form of the ionization amplitude for the aforesaid process (1) is given as:

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

The initial asymptotic wave function ψ_i in equation (2) is chosen as

$$\psi_i=\phi_{Ps}(|\vec{r}_1-\vec{r}_2|)e^{i\vec{k}_i\cdot\vec{R}}\phi_T(\vec{r}_3)\,. \tag{3a}$$

where $\vec{R}=(\vec{r}_1+\vec{r}_2)/2$ 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

$$\phi_{Ps}(|\vec{r}_1-\vec{r}_2|)=N_{1s}\exp(-\lambda_i r_{12}) \tag{3b}$$

with $N_{1s}=\lambda_i^{3/2}/\sqrt{\pi}$ and $\lambda_i=1/2$. The ground state wave function of the target alkali atoms is chosen in the form of a simple hydrogenic orbital as

$$\phi_T(r_3)=N_T\exp(-\lambda_T r_3)\,. \tag{4}$$

The value of λ_T is taken from the work of Hart and Goodfriend [19] and $N_T=\dfrac{\lambda_T^{\frac{3}{2}}}{\sqrt{\pi}}$.

The complexity of working with many electron atom have prevailed over in different theoretical investigation [20–25] by considering the model potential [26, 27], where the effect of the core electrons have not been considered explicitly. The model potential of the alkali atoms initiates the multi-electron core interaction with the single valence electron by an analytic modification of the Coulomb potential. In the present calculation V_i is the initial channel perturbation not diagonalized in the initial state is chosen as model potential following the work of Schweizer et al. [28] given by

$$V_i = \frac{1}{r_1} - \frac{1}{r_2} - \frac{1}{r_{13}} + \frac{1}{r_{23}} + \frac{N}{r_1}\exp(-a_1 r_1) - \frac{N}{r_2}\exp(-a_1 r_2) + a_2\exp(-a_3 r_1) - a_2\exp(-a_3 r_2) \tag{5}$$

where $\vec{r}_1$, $\vec{r}_2$ and $\vec{r}_3$ in eqn. (2) are the position vectors of the positron and the electron of the Ps and the bound electron of the target atom (Na, K, Rb and Cs) respectively, with respect to the target nucleus; N = 10 and 18 for Na and K respectively and $\mu_f = 2$. The values of a_1, a_2 and a_3 are taken from the work of Schweizer *et al.* [28].

Here, $\vec{r}_{13} = \vec{r}_1 - \vec{r}_3$ and $\vec{r}_{23} = \vec{r}_2 - \vec{r}_3$.

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

$$(H - E)\Psi^{\pm} = 0, \tag{6}$$

where the full Hamiltonian of the system is given by,

$$H = -\frac{\nabla_R^2}{2\mu_i} - \frac{\nabla_{12}^2}{2\mu_{ps}} - \frac{\nabla_3^2}{2} - \frac{1}{r_{12}} + \frac{Z_t}{r_1} - \frac{Z_t}{r_2} - \frac{Z_t}{r_3} - \frac{1}{r_{13}} + \frac{1}{r_{23}} + \frac{N}{r_1}\exp(-a_1 r_1)$$
$$- \frac{N}{r_2}\exp(-a_1 r_2) + a_2\exp(-a_3 r_1) - a_2\exp(-a_3 r_2),$$

where μ_i and μ_{Ps} are 2 and 1/2, respectively.

In the present work we have adopted the prior version of the transition matrix (eqn.) which is supposed to be more suitable for an ionization process [29–32]. Equation (6) 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)) involving two bound particles (Ps) and one continuum particle is approximated by the following ansatz in the framework of Coulomb-eikonal approximation [31–34]:

$$\Psi_f^-(\vec{r}_1, \vec{r}_2, \vec{r}_3) = N_{1s}\exp\left(-\lambda_f r_{12}\right) N_3 (2\pi)^{-3/2} e^{i\vec{k}_3\cdot\vec{r}_3}\, {}_1F_1(-i\alpha_3, 1, -i(k_3 r_3 + \vec{k}_3\cdot\vec{r}_3))$$
$$e^{i\vec{k}_f\cdot\vec{R}}\exp\left\{ i\eta_f \int_z^{\infty}\left(\frac{1}{r_1} - \frac{1}{r_2}\right) dz' \right\}, \tag{7}$$

where $N_3 = \exp\left(\frac{\pi\alpha_3}{2}\right)\Gamma(1 - i\alpha_3)$ with $\alpha_3 = -\frac{1}{k_3}$,$\eta_f = \frac{1}{k_f}$; and $\lambda_f = \lambda_i = 1/2$; since the Ps remains in the ground state in final channel.

$\vec{k}_3$ and $\vec{k}_f$ are the final momentum of the ejected electron and the positronium respectively. Equation (7) 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. (7). Since in the final channel the ejected electron from the target is in the long range Coulomb field of the residual target ion (Na^+, K^+, Rb^+, Cs^+), this interaction is incorporated in eqn. (7). 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)–(7), we obtain the target ionization amplitude (direct) for the process (1) as

$$\begin{aligned} T_{if}^{direct} \equiv & -\frac{\mu_f}{2\pi}\iiint N_3^* N_T (2\pi)^{-3/2} \exp(-\lambda_T \vec{r}_3) e^{i\vec{k}_i\cdot\vec{R}} (N_{1s})^2 \exp(-\lambda r_{12}) \\ & \Big(\frac{z_t}{r_1} - \frac{z_t}{r_2} - \frac{1}{r_{13}} + \frac{1}{r_{23}} + \frac{N}{r_1}\exp(-a_1 r_1) \\ & -\frac{N}{r_2}\exp(-a_1 r_2) + a_2 \exp(-a_3 r_1) - a_2 \exp(-a_3 r_2)\Big) \\ & e^{-i\vec{k}_3\cdot\vec{r}_3} e^{-i\vec{k}_f\cdot\vec{R}} (r_1+z_1)^{i\eta_f} (r_2+z_2)^{-i\eta_f} {}_1F_1(i\alpha_3, 1, i(k_3 r_3 + \vec{k}_3\cdot\vec{r}_3)) d\vec{r}_1 d\vec{r}_2 d\vec{r}_3, \end{aligned} \tag{8}$$

where $\lambda = \lambda_i + \lambda_f$. After much analytical reduction [35–39] the target ionization amplitudes T_{if} in equation (8) is finally reduced to a three dimensional numerical integral. The *triple differential cross sections* (TDCS) [36] is given by

$$\frac{d^3\sigma}{dE_3 d\Omega_f d\Omega_3} = \frac{k_f k_3}{k_i} |T_{if}|^2 \tag{9}$$

and the *double differential cross sections* (DDCS) i.e., $\frac{d^2\sigma}{dE_3 d\Omega_f}$ are obtained by integrating over the solid angle $d\Omega_3$.

It may be mentioned in this context that 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.

3. Results and Discussion

The TDCS and the DDCS results are computed for target ionization of the alkali atoms, Na, K, Rb and Cs by Ps impact. For the single ionization, the threshold energy is determined by E_{th}=$E^{1s}_{(Na,K,Rb,Cs)}$. 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_f and ϕ_3 can assume values $0^0$and 180^0. In this work we have adopted $\phi_f = \phi_3 = 0^0$ for asymmetric geometry.

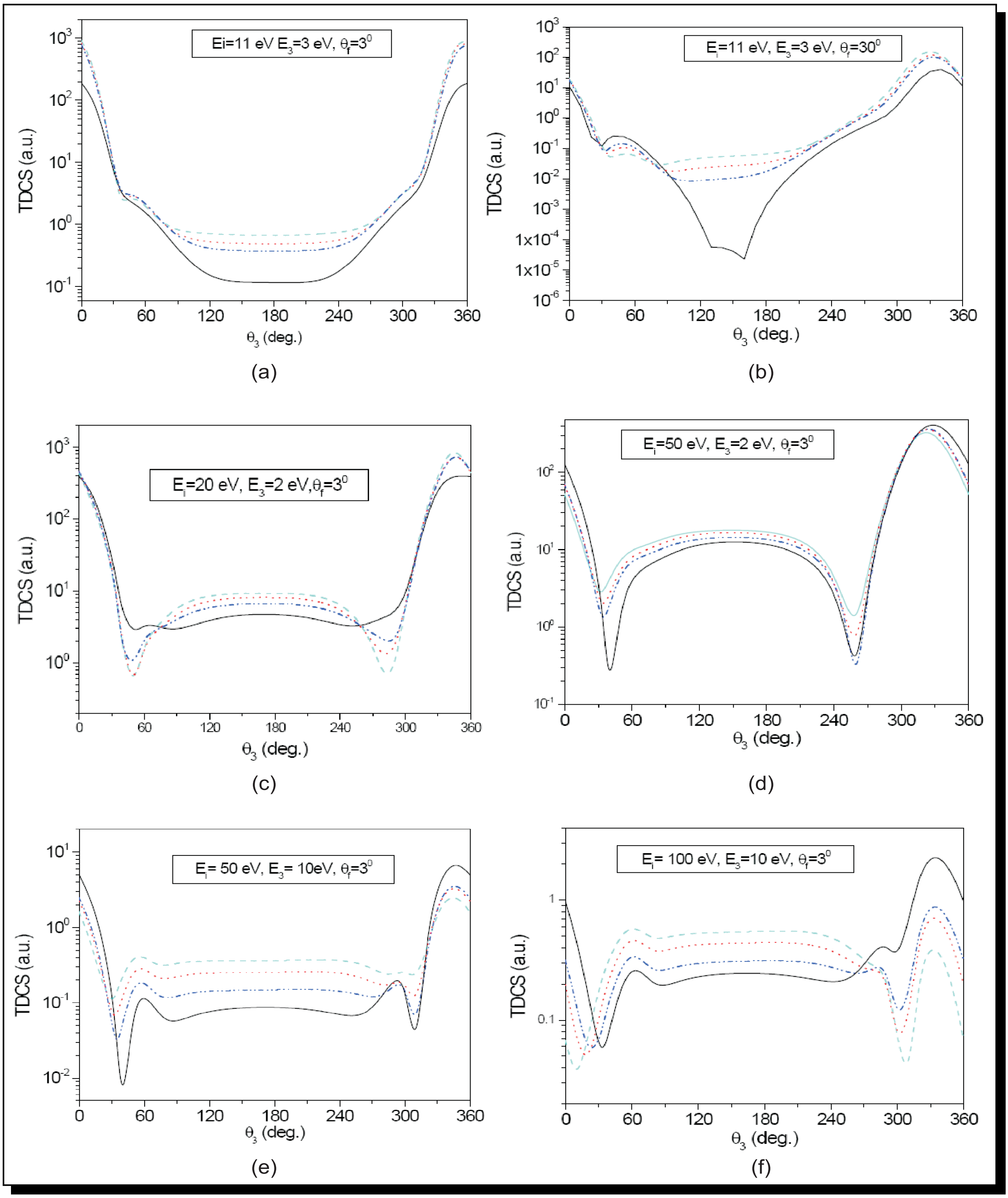

Figure 1. Triple differential cross section for Ps impact ionization of Sodium, Potassium, Rubidium and Caesium in the coplanar ($\emptyset_3 = \emptyset_f = 0^0$) asymmetric geometry. The solid curve represents the TDCS for Sodium, the dashed dot curve represents Potassium, dotted curve represents Rubidium and dashed curve represents Caesium. In Figure 1a, incident energy ($E_i = 11$ eV and ejected electron energy $E_3 = 3$ eV $\theta_f = 3^0$, in Figure 1 $E_i = 11$ eV, $E_3 = 3$ eV b $\theta_f = 30^0$. In Figure 1c $E_i = 20$ eV, $E_3 = 2$ eV, $\theta_f = 3^0$, in Figure 1d $E_i = 50$ eV, $E_3 = 2$ eV, $\theta_f = 3^0$. Figure 1d and Figure 1e depict the kinematics $E_i = 50$ eV, $E_3 = 10$ eV, $\theta_f = 3^0$ and $E_i = 100$ eV, $E_3 = 10$ eV, $\theta_f = 3^0$, respectively.

Figure 1 exhibit the angular distributions (TDCS in atomic unit (a.u.)) of the ejected electron (θ_3) for the atoms Na, K, Rb and Cs. For the TDCS shown in Figure 1a, incident energy (E_i) is kept fixed at 11 eV, ejected electron energy (E_3) is taken 3 eV, and the scattering angle of the incident Ps ($\theta_f =$) is 3°. The TDCS curves for all these atoms exhibit similar nature, i.e., a peak at extreme forward. In this kinematics the TDCS for Rb and Cs atoms exhibit much higher values than Na and K atoms. It is clear from Figure 1b, where θ_f is 30°, the extreme forward peak moves slightly followed by a shoulder like structure. The TDCS value is lower for higher scattering angle as expected. For higher scattering angle, Na and K atoms behave differently from Rb and Cs in either sides of 180°.

TDCS for higher incident energy in Figures 1c and 1d, shows forward peak with some associated hump like structures in recoil side. The overall TDCS values for all these atoms however decreases with higher incident energy. When the incident energy is increased further, keeping fixed emission energy of the electron, as in Figures 1e and 1f, the hump like structure disappears and shoulder like structures appear in both sides of the forward peak. It is evident from all Figures 1a to 1e that for higher incident energy the TDCS of Na dominates over K, Rb and Cs atoms.

To compare the findings of Ps impact ionization with that of electron, TDCS of Na atom with respect to the Ps scattering angles are depicted in Figure 2a-f, for different emission angle of the electron for a particular incident energy 11.138 eV [18]. It is clear from the figures, that for lower scattering angle, forward ejection is preferred. Again, for this particular incident energy, velocity matching between the electron and the Ps dominates merely on the equal energy sharing between them. The solid curve in Figure 2 represents velocity matching kinematics between the ejected electron and the scattered positronium. It should also be pointed out here that the mass of the Ps being double to that of the electron, we have considered the Ps ejected energy to be twice the ejected energy of the electron to keep pace between the ejected electron and the Ps in the velocity space. Comparison between electron and Ps impact ionization shows that for smaller values of the scattering angle, the Ps impact ionization takes over the electron impact ionization where as for higher scattering angle, the electron impact ionization dominates over the Ps one.

We have compared the TDCS for both equal velocity and equal energy sharing between the ejected electron and the scattered positronium for Na atom. The solid curve in Figure 3 represents velocity matching kinematics between the ejected electron and the scattered positronium. It should also be pointed out here that the mass of the Ps being double to that of the electron, we have considered the Ps ejected energy to be twice the ejected energy of the electron to keep pace between the ejected electron and the Ps in the velocity space.

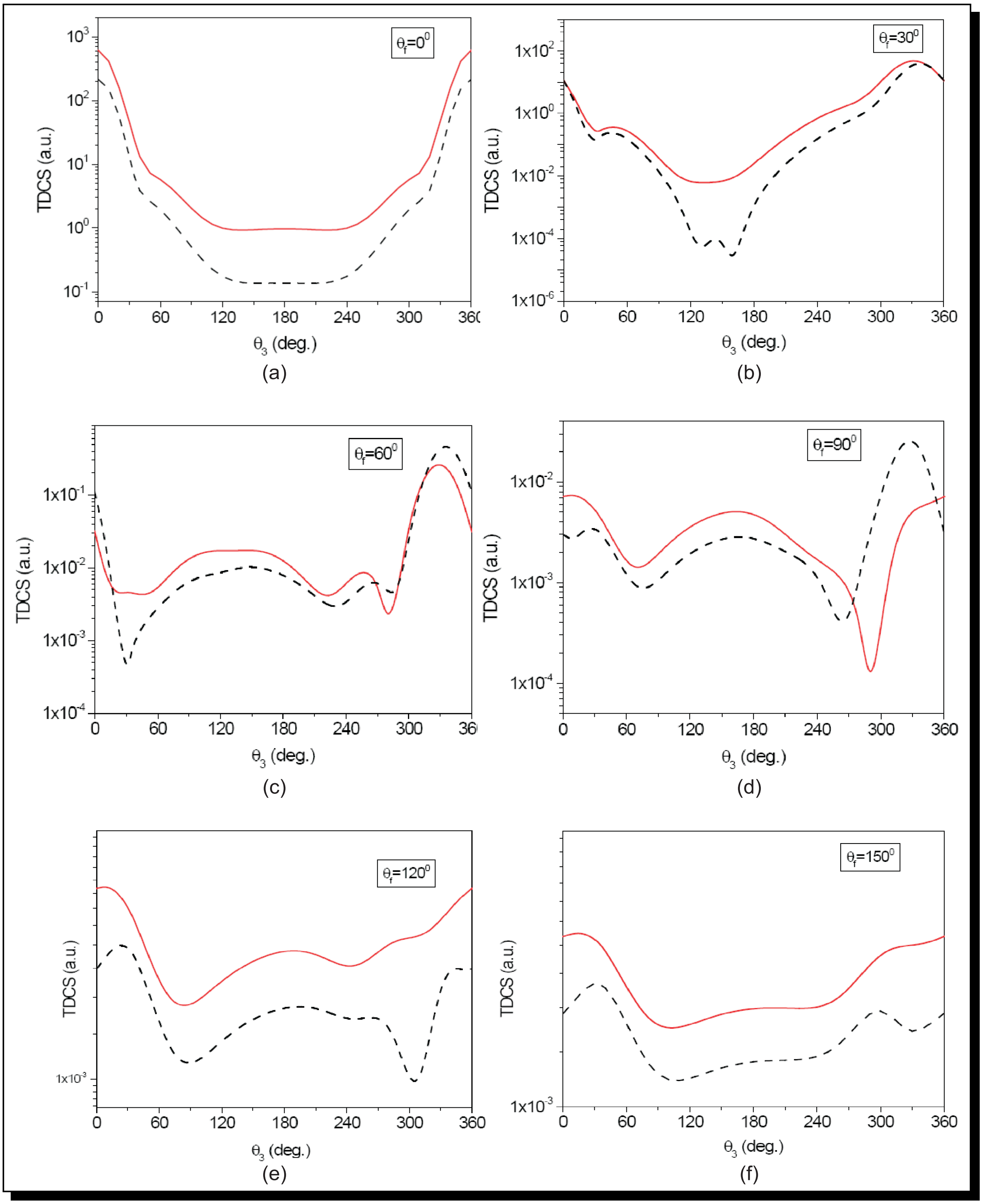

Figure 2. Triple differential cross section for Ps impact ionization of Sodium for different values of scattering angle at an incident energy 11.138 eV in the coplanar asymmetric geometry ($\phi_3 = \phi_f = 0^0$). The dashed curve represents equal energy sharing ($E_3 = E_f = 3$ eV) and the solid curve represents for equal velocity of the ejected electron and scattered positronium ($E_3 = 2$ eV, $E_f = 4$ eV).

Figure 3 illustrates the Ps impact fully differential cross sections in the symmetric geometry ($\theta_3 = -\theta_f$) [16]. The figures reveal that for symmetric kinematics extreme forward ejection of electron is preferred for the energy regime considered here. For higher incident energy (35.138 eV; Figure 3a), this peak moves to higher angle but having lesser magnitude. Again, it shows that at lower incident energy, velocity matching (Figure 3b) between the electron and Ps is more preferred where as for higher incident energy equal energy sharing between them (Figure 3a) predominates. The TDCS of electron impact ionization of Na [16] for equal energy sharing in symmetric geometry shows a prominent binary peak for different incident energy, where as in this case the forward maxima falls sharply from 0° angle, shows prominent deviation from electron impact ionization. However the peak structure occurs for Ps impact ionization at higher incident energy behave similarly as that for electron impact.

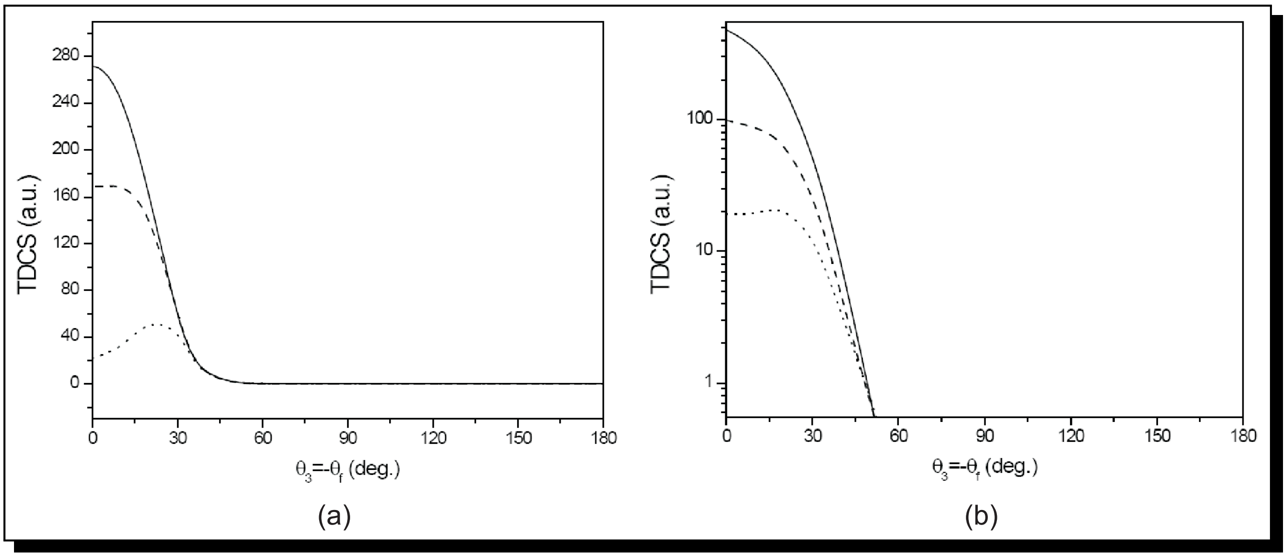

Figure 3. Triple differential cross section for Ps impact ionization of Sodium in the coplanar symmetric geometry ($\theta_3 = -\theta_f$). In Figure 3 solid curve represents $E_i = 15.138$ eV, dashed line is for $E_i = 25.138$ eV and the dotted line presents $E_i = 35.138$ eV. Figure 3a represents equal energy sharing kinematics i.e., $E_3 = E_f = 5$ eV (solid curve), dashed curve ($E_3 = E_f = 10$ eV), dotted curve ($E_3 = E_f = 15$ eV). Figure 3b represents velocity matching kinematics: solid curve ($E_3 = 3.33$, $E_f = 6.66$ eV), dashed curve ($E_3 = 6.66$, $E_f = 13.34$ eV) and Dotted curve represents the kinematics $E_i = 10$ eV, $E_f = 20$ eV.

The next Figure 4a to Figure 4d exhibit the double differential cross sections (DDCS) with respect to the scattered Ps angle (θ_f) for the Ps-Na, K and Cs system. Figure 4a, Figure 4b depict the Ps distributions for the fixed incident energy 25 eV where as Figure 4c and Figure 4d represents the DDCS for 45 eV, keeping the ejected electron energy fixed at 5 eV (Figure 4a, Figure 4c) and 10 eV (Figure 4b, Figure 4d), respectively. It is revealed that the DDCS distributions for Sodium, Potassium and Caesium are similar in nature though the magnitude differs depending on the kinematics. From Figures 4a and Figure 4b it is evident that asymmetric energy sharing between Ps and the ejected electron is more favoured than equal energy sharing among them.

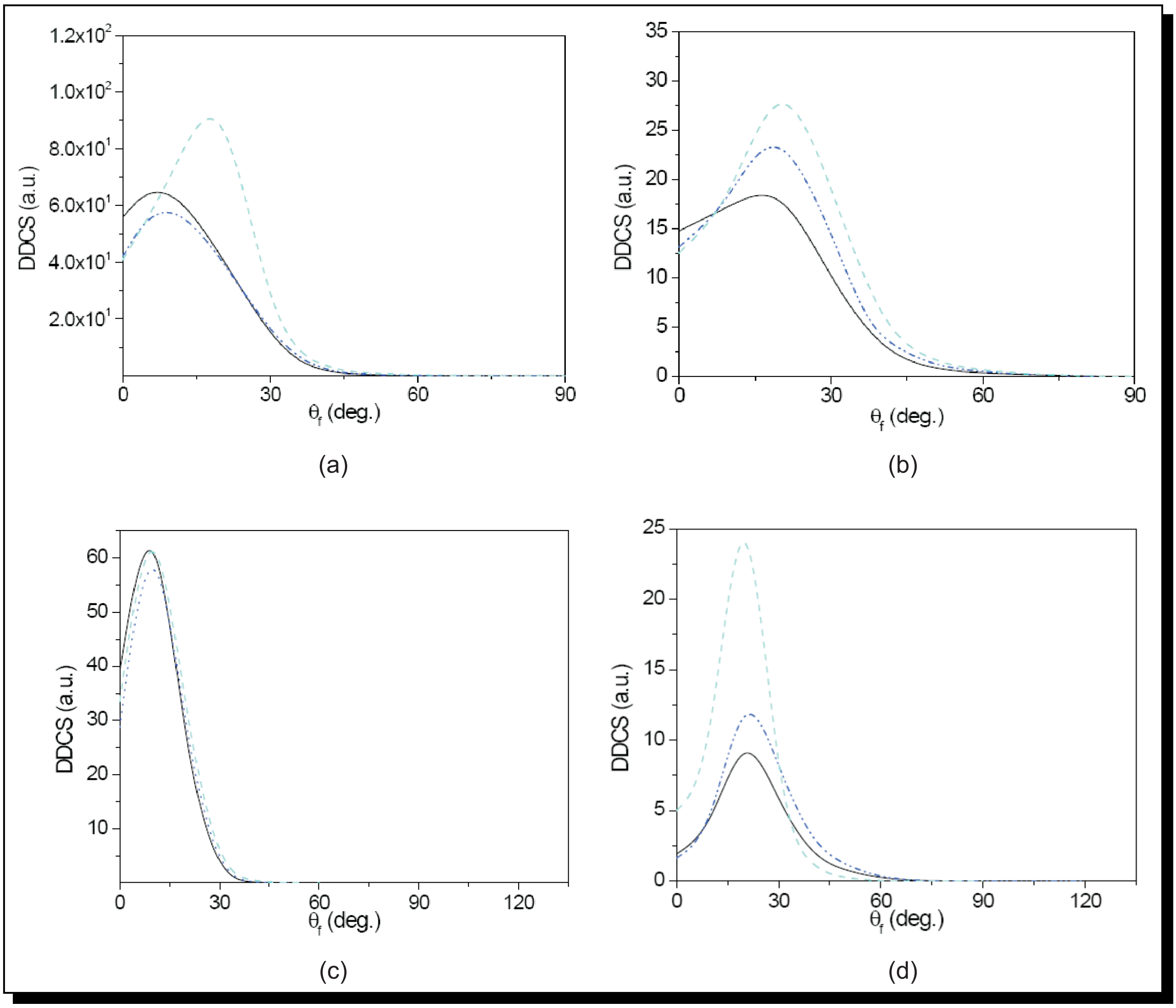

Figure 4. Double differential cross section for Ps impact ionization of Sodium (solid curve), Potassium (dash dotted curve) and Caesium (dashed curve) for different asymmetric kinematics. In Figure 4a, $E_i = 25$ eV, $E_3 = 5$ eV, in Figure 4b, $E_i = 25$ eV, $E_3 = 10$ eV in Figure 4c $E_i = 45$ eV, $E_3 = 5$ eV and in Figure 4d $E_i = 45$ eV, $E_3 = 10$ eV.

4. Conclusion

(1) Though qualitative similarities between the electron and the positronium impact ionization of the alkali atom (Na) are revealed for particular kinematics (higher incident energy), in conformity with experiment [15], mainly for low incident energy, both qualitative and quantitative discrepancies are prominent between the TDCS of two colliding particles.

(2) Study of both the Equal energy sharing and the probability of velocity matching between the scattered projectile and ejected particle, shows velocity matching kinematics is preferred than the equal energy sharing though the incident energy and the collision geometry also other two major prevailing factors.

(3) The DDCS with respect to the scattered Ps angle shows similar qualitative behaviour for the alkali atoms Sodium, Potassium and Caesium. Regarding the magnitude of the DDCS, it can be inferred that for lower ejection energy Na dominates while for higher ejection energy Cs takes precedence.

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Competing Interests

The author declares that he has no competing interests.

Authors' Contributions

The author wrote, read and approved the final manuscript.

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