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A theoretical study on wave function dependency of positronium impact collision cross sections

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Abstract

Triple Differential cross sections (TDCS) and double differential cross sections (DDCS) for single ionization of Sodium by Positronium impact are calculated using a frozen core approach within the frame work of Coulomb Distroted Eikonal Approximation (CDEA). TDCS and DDCS are presented within energy range 25 eV to 5000 eV for two different trial wave functions. In general, the DDCS evaluated from the two wave functions are found to differ by about ten to thousand times of magnitude. Comparison of the DDCS for two different wave functions reveals one possible source of the magnitude difference, i.e., the active electron's change of state due to the change in the orbital configuration.

Keywords: Coulomb Distorted Eikonal Approximation, Model Potential,

1. Introduction

The oldest known atom formed by the electron and its anti-particle positron is Positronium atom (Ps) [1], which can be regarded as the simplest purely leptonic electromagnetically bound system [2]. This short-lived atom has been the subject of widespread theoretical and experimental studies [2] since its discovery by Deutsch [3]. It has been used to explore a variety of fundamental phenomena associated with atomic physics, condensed matter physics, astrophysics, industrially important materials, living biological systems [4] etc. Being an atom composed of a particle-anti-particle pair, and a neutral one, Ps atom can penetrate deeper into the system than a charged particle, such as positron. It is necessary to understand how Ps atom interacts with other systems elastically and inelastically. Scattering processes involving Ps atoms is very much important in the investigations of solar processes [5].

In the present study, Sodium atom has been considered as the target while Positronium atom (Ps) as the projectile. From the theoretical point of view, the quasi-one electron model of the loosely bound outermost electron and a stationary effective potential due to frozen inner shell electrons is the appealing features of sodium atom. Thus, in this study sodium atom is treated as consisting of a positive core (Na^+) and a valence electron (e^-). The interaction of Na^+ and e^- is then approximated by a model potential [6, 7] and the calculation is performed with Coulomb Distorted Eikonal Approximation [8] (CDEA). In the present study complexity mainly arises due to the internal degrees of freedom of the projectile Ps which must be taken into account. The present triple differential cross sections (TDCS) additionally carry the information about the influence of the Ps atom on the target active electron wave function, which is studied considering two different wave functions of Na [9, 10].

Theory:

The present target ionization process is: $e^+e\,(1s) + \mathrm{Na}(1s) \rightarrow e^+e(1s) + Na^+ + e$ (1)

The prior form of the ionization amplitude for the above process is given as:

$$T_{if}(\vec{k}_i, \vec{k}_f, \vec{k}_3) = -\frac{\mu_f}{2\pi}\left\langle \Phi_f(\vec{r}_1, \vec{r}_2, \vec{r}_3) \left| V_i \right| \Phi_i(\vec{r}_1, \vec{r}_2, \vec{r}_3) \right\rangle \quad (2)$$

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

$$\Phi_i(\vec{r}_1, \vec{r}_2, \vec{r}_3) = \varphi^{Ps}(\vec{r}_{12})\, e^{i\vec{k}_i.\vec{R}}\, \varphi^{Na}(\vec{r}_3) \quad (3)$$

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

$$\varphi^{Ps}(r_{12}) = \frac{\lambda_{Ps}^{3/2}}{\sqrt{\pi}} \exp(-\lambda_{Ps} r_{12}) \quad (4)$$

where $\lambda_{ps} = 1/2$.

The ground state wave function of the target Sodium atom is chosen in the two forms. The first one is like a simple hydrogenic orbital as

$$\varphi_{1s}^{Na}(\vec{r}_3) = N_{Na} \exp(-\lambda_{Na} r_3) \quad (5a)$$

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where $N_{Na} = \frac{\lambda_{Na}^{\frac{3}{2}}}{\sqrt{\pi}}$, λ_{Na} being the bound state parameter of the Na atom , considered as a hydrogenic atom [9]. The second trial radial wave function for the active electron of the Na atom is chosen as

$$\varphi_{3s}^{Na}(\vec{r}_3) = \left(\frac{1}{4\pi}\right)^{1/2}\left[2(\lambda_{Na})^{3/2}e^{-\lambda_{Na}r_3} - 4\,(\lambda_{Na})^{5/2}r_3e^{-\lambda_{Na}r_3} + \frac{4}{3}(\lambda_{Na})^{7/2}e^{-\lambda_{Na}r_3}\ r_3^2\right] \quad (5b)$$

where $\lambda_{Na} = 0.36679$, is a variational parameter determined by optimizing the corresponding Rayleigh-quotient [10].

The complexity aroused when working with many electron atom have been passed up in different theoretical investigations [11- 16] by considering the model potential [17, 18], where the effect of the core electrons have not been considered explicitly. Here by an analytic modification of the Coulomb potential, the model potential of Na atom initiates the multi- electron core interaction with the single valence electron. In the present calculation V_i , the initial channel perturbation not diagonalized in the initial state is chosen as model potential following the work of Schweizer et al [6] given by,

$$V_i = \frac{1}{r_1} - \frac{1}{r_2} - \frac{1}{r_{13}} + \frac{1}{r_{23}} + \frac{N}{r_1}\ \exp\left(-a_1\, r_1\right) - \frac{N}{r_2}\ \exp\left(-a_1 r_2\right) + a_2\ \exp\left(-a_3\ r_1\right) - a_2\ \exp\left(-a_3 r_2\right) \quad (6)$$

$\vec{r}_1$, $\vec{r}_2$and $\vec{r}_3$in eqn.(2) are the position vectors of the positron, the electron of the Ps and the bound electron of the target atom (Na) respectively, with respect to the target nucleus; Here, $\vec{r}_{13} = \vec{r}_1 - \vec{r}_3$ and $\vec{r}_{23} = \vec{r}_2 - \vec{r}_3$, N= 10 for Na and μ_f=2. The model potential parameters are taken form the work of Sahoo et al [7] , where the values of variational parameters are. α (= 1.8321), β (= 1.0591) and γ (= 1.3162).

In this calculation the prior version of the transition matrix (eqn.(2)) is considered, which is quite suitable for an ionization process [19- 22]. This problem concerning a four body system, could not be solved exactly and thus some simplifying assumptions are taken. The final state wave function $\Phi_f(\vec{r}_1, \vec{r}_2, \vec{r}_3)$ (eqn.(2)) concerning two bound particles (Ps) and one continuum particle is approximated by the following ansatz in the framework of Coulomb – eikonal approximation [20- 23] :

$$\Phi_f(\vec{r}_1, \vec{r}_2, \vec{r}_3) = \varphi^{Ps}(\vec{r}_{12})e^{i\vec{k}_f.\vec{R}}N_3(2\pi)^{-3/2}e^{i\vec{k}_3.\vec{r}_3}\ {}_1F_1\left(-i\alpha_3, 1, -i\left(k_3r_3 + \vec{k}_3.\vec{r}_3\right)\right)\exp\left\{i\eta_f\int_z^\infty\left(\frac{1}{r_1}-\frac{1}{r_2}\right)dz'\right\} \quad (7)$$

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 corresponding Schrodinger equation is given by,

$$(H - E)\phi^{\pm} = 0 \quad (8)$$

where the full Hamiltonian of the system is given by,

$$H = -\frac{\nabla_R^2}{2\mu_i} - \frac{\nabla_{12}^2}{2\mu_{ps}} - \frac{\nabla_3^2}{2} - \frac{1}{r_{12}} + \frac{Z_t}{r_1} - \frac{Z_t}{r_2} - \frac{Z_t}{r_3} - \frac{1}{r_{13}} + \frac{1}{r_{23}} + \frac{N}{r_1}\ \exp\left(-a_1\, r_1\right) - \frac{N}{r_2}\ \exp\left(-a_1 r_2\right) + a_2\ \exp\left(-a_3 r_1\right) - a_2\ \exp\left(-a_3 r_2\right) \quad (9)$$

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

The strong interactions between the target nucleus and the two components of the incident particle (e & 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, the higher order interactions between the e^+ / e of the Ps and the target electron are neglected and mainly attention is given on the ionization of the target; this interaction being considered through the perturbative interaction in the initial channel.

In view of equations (2 – 7) , we obtain the target ionization amplitude (direct) for the process (1) as

$$T_{if}^{direct} = -\frac{\mu_f}{2\pi}\iint N_3^*\, N_{Na}(2\pi)^{-\frac{3}{2}}\exp(-\lambda_{Na}\vec{r}_3)\exp(i\vec{k}_i.\vec{R})N_{1s}^2\exp(-\lambda r_{12})$$

$$\left(\frac{Z_t}{r_1}-\frac{Z_t}{r_2}-\frac{1}{r_{13}}+\frac{1}{r_{23}}+\frac{N}{r_1}\exp(-a_1r_1)-\frac{N}{r_2}\exp(-a_1r_2)+a_2\exp(-a_3r_1)-a_2\exp(-a_3r_2)\right)\exp\left(-i\vec{k}_3.\vec{r}_3\right)\exp\left(-i\vec{k}_f.\vec{R}\right)(r_1+z_1)^{i\eta_f}(r_2+z_2)^{-i\eta_f}\ {}_1F_1\left(i\alpha_3,1,i\left(k_3r_3+\vec{k}_3.\vec{r}_3\right)\right)$$

$$d\vec{r}_1d\vec{r}_2d\vec{r}_3 \qquad (10)$$

Where $=\lambda_i+\lambda_f$. Following the equation (5b) target ionization amplitude becomes

$$T_{if}^{direct}=-\frac{\mu_f}{2\pi}\iiint N_3^*\left(\frac{1}{4\pi}\right)^{1/2}\left[2(\lambda_{Na})^{3/2}e^{-\lambda_{Na}r_3}-4(\lambda_{Na})^{5/2}r_3e^{-\lambda_{Na}r_3}+\frac{4}{3}(\lambda_{Na})^{7/2}e^{-\lambda_{Na}r_3}\ r_3^2\right]$$

$$\exp(i\vec{k}_i.\vec{R})N_{1s}^2\exp(-\lambda r_{12})$$

$$\left(\frac{Z_t}{r_1}-\frac{Z_t}{r_2}-\frac{1}{r_{13}}+\frac{1}{r_{23}}+\frac{N}{r_1}\exp(-a_1r_1)-\frac{N}{r_2}\exp(-a_1r_2)+a_2\exp(-a_3r_1)-a_2\exp(-a_3r_2)\right)\exp\left(-i\vec{k}_3.\vec{r}_3\right)\exp\left(-i\vec{k}_f.\vec{R}\right)(r_1+z_1)^{i\eta_f}(r_2+z_2)^{-i\eta_f}\ {}_1F_1\left(i\alpha_3,1,i\left(k_3r_3+\vec{k}_3.\vec{r}_3\right)\right)$$

$$d\vec{r}_1d\vec{r}_2d\vec{r}_3 \qquad (11)$$

After much analytical reduction [20- 23] the target ionization amplitudes T_{if} in equations (10) and (11) is finally reduced to a three dimensional numerical integral. The triple differential cross sections (TDCS) is given by

$$\frac{d^3\sigma}{dE_3d\Omega_fd\Omega_3}=\frac{k_fk_3}{k_i}\left|T_{if}\right|^2 \qquad (12)$$

and the DDCS, $\frac{d^2\sigma}{dE_3d\Omega_f}$ are obtained by integrating over the solid angle $d\Omega_3$.

RESULTS AND DISCUSSIONS

In the present work, the triple differential cross sections (TDCS) and the double differential cross sections (DDCS) of positronium impact ionization of Na are computed for two different wave functions of Na atom. For this ionization process, ground state (1S) positronium (Ps) have been considered. Since the present study is made in coplanar geometry, that is $\vec{k}_i\ \vec{k}_3$ and $\vec{k}_f$ are in the same plane, the azimuthal angles $\emptyset_i$, $\emptyset_3$ *and* $\emptyset_f$can assume values 0^0 and 180^0 .

Figure 1 displays TDCS in atomic unit (a.u.) of the ejected electron with scattering angle θ_3 for the present ionization process. To observe the variation of TDCS with incident energies for two studied wave functions (W.F.), different values of incident energies are chosen under same kinematics. From figure 1, it is clear that TDCSs are not only quantitatively dependent on the wave-functions, but a distinct qualitative difference is also noticed in the behavior of TDCS calculated with two different wave functions for both low and high incident energy regime.

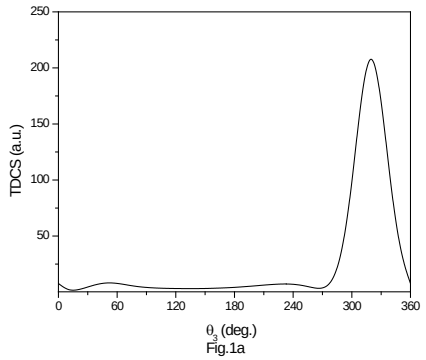

Fig.1a

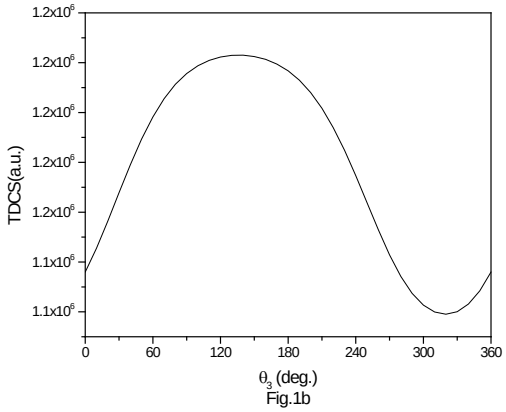

Fig.1b

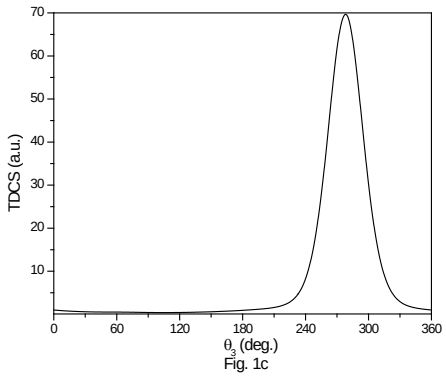

Fig. 1c

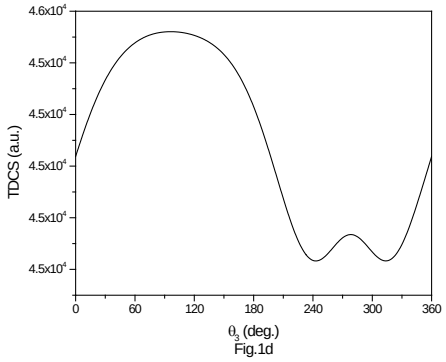

Fig.1d

Figures 1a to 1d represent TDCS against the ejected electron angle θ_3 for two different incident energies, with two different W.F. of Na atom. Figures 1a and 1b are plotted for incident energies (E_i) 50 eV, and figures 1c and 1d are plotted for E_i =500 eV. For all the case ejected energy of electron and scattered angle of Ps are kept fixed at 3 eV and 5^0 respectively. Figures 1a & 1c represent Hydrogenic W.F. and Figures 1b and 1d ground state (3s) W.F. of Na atom.

The measure of ejected energy is an important aspect for ionization process. Figures 2a and 2b exhibit the consequence of ejected electron energy for two different wave functions of Na atom, considered in the present collisional process. It is evident from this study that for both the wave functions, TDCS decreases with increase of ejected electron energy. Along with the magnitude of TDCS, a qualitative difference is also obvious in this figure

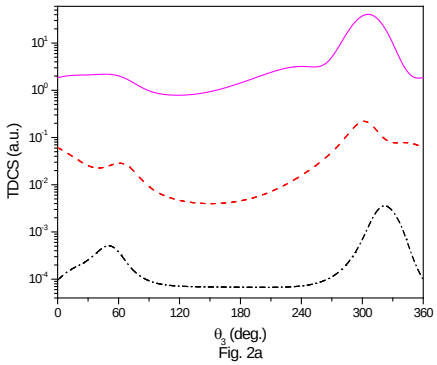

Fig. 2a

for the two different wave-functions. The TDCS is quite insensitive on the ejection angle for the ground state (3s) wave function where as noticeable changes are present in the TDCS for hydrogenic wave function of Na atom.

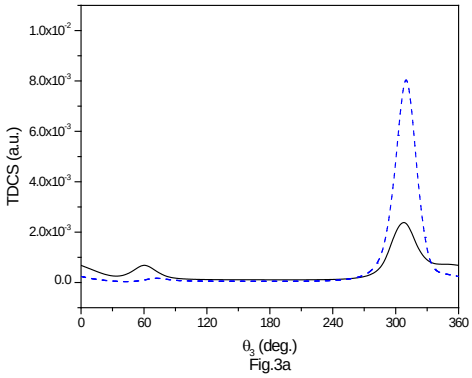

Fig.3a

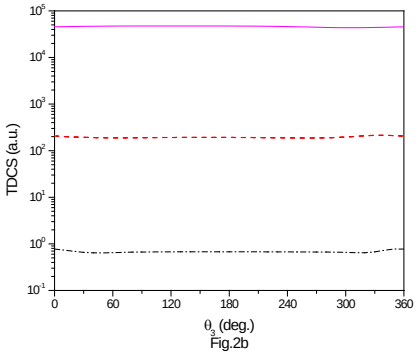

Fig.2b

Figures 2a and 2b represent TDCS against the ejected electron angle θ_3 for three different ejected energies, and two different W.F. of Na atom. All the curves in both the figures are plotted for incident energies (E_i) 100 eV. and scattered angle of Ps is 5^0 . Figure 2a and represent Hydrogenic W.F. and figure 2b represent ground state (3s) W.F. of Na atom. In the two figures ejected energy and of the electron are kept fixed at 5 eV (magenta curve), 20 eV (red curve) and 50 eV (black curve) respectively.

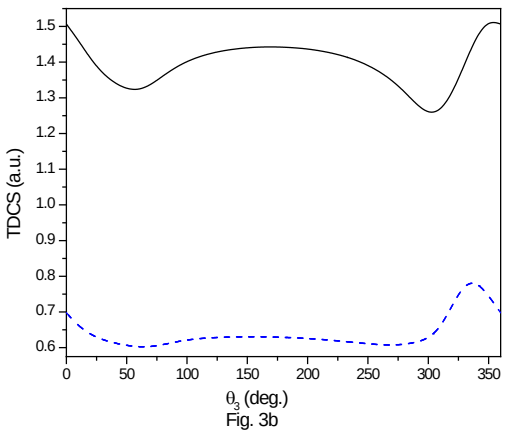

Fig. 3b

Figures 3a and 3b represent TDCS against the

ejected electron angle θ_3 for two different ejected angles (3^0, and 10^0), and two different W.F. of Na atom. All the curves in both the figures are plotted for incident energies (E_i) 150 eV. and ejected electron energy 50 eV . Figure3a represent Hydrogenic W.F. and figure 3b represent ground state (3s) W.F. of Na atom. In the two figures scattered Ps angle are kept fixed at 3^0 (black curve) and 10^0 (blue curve) respectively.

In the present collisional process, the dependency of the TDCS on the ejected electron angles are shown in figures 3a and 3b for both the hydrogenic and 3s wave function of Na atom. It is noted that the magnitude of TDCSs are more responsive with the ejection angle for 3s wave function than that of the hydrogenic one. Interestingly, for higher ejection angle the back-ward ejection is prominent in both the cases (blue dashed curve) while for lower ejection angle, presence of forward ejection along with the back ward ejection are clear in both cases though quantitative difference are there for two W.F. of Na.

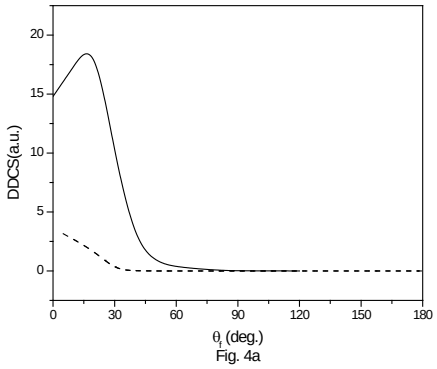

Fig. 4a

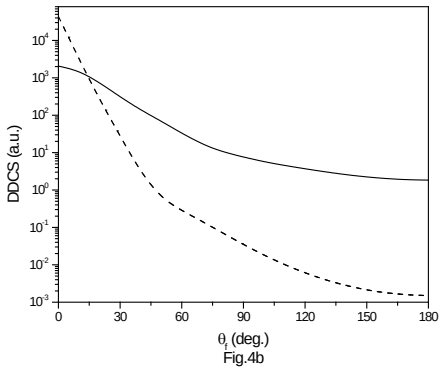

Fig.4b

Figures 4a and 4b represent DDCS against the scattered Ps angle θ_f for two different kinematics and two different W.F. of Na atom. The solid curves in both the figures represent for incident energies (E_i) 25 eV and ejected electron energy 10 eV and the dashed curves represent (E_i) 100 eV and ejected electron energy 10 eV. Figure 4a represent Hydrogenic W.F. and figure 4b represent ground state (3s) W.F. of Na atom.

The double differential cross sections (DDCS) against the scattered Ps angle has been plotted to observe the consequence of wave functions in Ps-Na collisional process. It is obvious that 3s W.F. results much more cross sections for same kinematics than that of hydrogenic W.F. of Na atom. Again, for the lower scattering angle, though the DDCS graph shows higher magnitude in both cases, it is noted that for same ejected electron energy (10 eV) 3s W.F. shows different qualitative behaviour than that for hydrogenic wave function.

Conclusions : The present work estimates the single ionization of Na atom by Ps impact for two different wave functions of Na atom. In the absence of any experimental data till now, it is difficult to put the two wave functions to the test. Since, for frozen core approximation, the outermost electron of the ground state Na atom is from 3s orbital, it seems the 3s W.F. is more authentic than that of the hydrogenic one, though only the experimental results can confirm the right choice of wave function for Positronium impact ionization of sodium atom.

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