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Studies on ionization and excitation processes in Ps–Li scattering

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Abstract. Three different types of ionization and excitation processes are studied in detail for the scattering of positronium (Ps) by the simplest alkali atom (Li) using a Coulomb–Born approximation for ionization and first-Born approximation for excitation. This is the first work where orthogonalized Coulomb wave is used to represent the ionized electron for Ps–Li scattering using a single-electron and a three-electron prescription of the target. Li is chosen to minimize the effect of intrinsic correlation among the target atomic electrons so that it can extract the basic physics more accurately. All the possible Coulomb interactions are considered exactly. Comparative studies of different cross-sections using two different representations of the target provide us the informations to enrich our ideas about the system and the important role of core electrons.

Keywords. Ionization; positronium; Coulomb–Born; continuum; Coulomb wave function; core electrons.

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1. Introduction

Ionization is a very important reaction process in positronium (Ps)–atom scattering [1], but very little attention [2–8] is given to study such a process. Three different types of ionization in Ps–atom scattering are discussed in the literature [2–7]. Recently, UCL group reported an experimental measurement [8] of Ps-ionization cross-section for Ps–He system. Ionization processes start just above the corresponding thresholds. In the energy region near zero and below the threshold of excitation, elastic scattering is the only active process. The energy region close to the thresholds of ionization are highly complicated due to many different excitation and ionization channels in a very close energy gap. The effect of exchange and the dipole polarizability, e.g. van der Waals interaction are important at this region [9–11]. However, at a relatively higher energy region, both the effects are almost negligible [9–12]. In recent years some attention is given to the studies involving Ps [12,13] and Ps–atom scattering [2–11,14–18], but most of them are confined to study the elastic scattering using various methodologies [9–11,15–19]. To study

such processes, one has to deal with composite particles in the initial channel and in ionization, several charged particles in the final channel.

Different approximations may be used to find the scattering amplitudes. The first-Born approximation (FBA) is the simplest one where a plane wave is used to represent the scattered particle as well as the incident particle. It can be considered as a valid approximation because the projectile Ps is a neutral system and at the same time the static Coulomb interactions vanish in Ps–atomic systems due to coincidence of charge and mass centers in Ps. The validity and usefulness of FBA to describe Ps–atom scattering is well-understood from our previous studies [9,10]. However, the ionized electron is not free. Attractive Coulomb interaction from the core of parent nucleus has influence on it. So the free particle solution of Schrödinger equation which is a plane wave is not suitable to represent it. To consider this effect, we have used continuum Coulomb wave function for the ionized electron and this approximation is named as Coulomb–Born approximation (CBA) following Geltman [20]. To reduce the errors due to dynamical effect of nuclear screening [21], an effective charge of unity is introduced for the Li^+ core in the Coulomb wave function since both the electrons present in the core are s-electrons and with a spherical charge distribution. Asymptotically the ionized positron and electron of Ps will move with equal velocities away from their common center of mass. The problem is challenging due to the fact that it is very difficult to perform analytical calculation involving Ps due to the presence of ${}_1F_1$ term in the Coulomb wave function and the complex atomic system makes the problem more complicated.

Li is the simplest alkali atomic target with a valence electron outside the closed atomic core containing two electrons. We have treated this system as a one-electron hydrogen-like system in model I and a three-electron system with a determinantal wave function in the frozen core approximation in model II. Both the atoms are considered at ground states in the incident channel. In the present framework, we take into account the Ps excitations as $\mathrm{Ps}(1s \rightarrow nl)$ for $l+1 \leq n \leq 6$ with $l = 1, 3, 5$. The matrix elements for which the parities of initial and final Ps states are similar, vanish. Target channels which are taken into consideration are: $\mathrm{Li}(2s \rightarrow 2s)$, $\mathrm{Li}(2s \rightarrow 2p)$. Li orbitals are taken from [22].

The CBA theory of ionization in Ps–atom scattering was first introduced by the present author [4,5] on Ps–He system [4]. Later, the same theory was extended [5] for Ps–H, Ps–He and Ps–Li systems. In Ps–H system [5,6], the Coulomb wave functions used to represent the ionized electrons are orthogonal to the corresponding parent atomic states as both are hydrogen-like systems. But for Ps–He and Ps–Li systems, it is not so. In our previous article [7] we have introduced an orthogonalized Coulomb-wave to represent the target atomic continuum state for the first time in Ps–He system. Our Ps-ionization results for Ps–He system are in very close agreement with the measured values by the UCL group [8] and the coupled-pseudostate approximation theory by Belfast group (1999) [8]. We also reported a few more results for Ps–Li system [7] using our old-code with a single electron approximation for the target. In the present article we have introduced the orthogonality criteria to the target-continuum electron wave function using a Schmidt orthogonalization procedure previously used by Ehrhardt *et al* and Ray *et al* for electron impact ionization of helium [23]. To test the degree of validity of our single-electron approximation to represent the target, a three-electron wave

function considering the antisymmetry of the target system in a determinantal form has been incorporated for the first time in the present study associated with the orthogonalization of Coulomb wave.

The orthonormalized Coulomb wave functions $\phi^{(i)}_{\mathbf{k}'}$ and $\phi^{(ii)}_{\mathbf{k}'}$ corresponding to single-electron and three-electron models respectively can be written as

$$|\phi^{(i)}_{\mathbf{k}'}(\mathbf{r})\rangle = \{|\chi^-_{\mathbf{k}'}(\mathbf{r})\rangle - \langle\phi_{2s}(\mathbf{r}')|\chi^-_{\mathbf{k}'}(\mathbf{r}')\rangle|\phi_{2s}(\mathbf{r})\rangle\},$$

$$\begin{aligned}|\phi^{(ii)}_{\mathbf{k}'}(\mathbf{r})\rangle = \{&|\chi^-_{\mathbf{k}'}(\mathbf{r})\rangle - \langle\phi_{1s}(\mathbf{r}')|\chi^-_{\mathbf{k}'}(\mathbf{r}')\rangle|\phi_{1s}(\mathbf{r})\rangle \\ &-\langle\phi_{2s}(\mathbf{r}')|\chi^-_{\mathbf{k}'}(\mathbf{r}')\rangle|\phi_{2s}(\mathbf{r})\rangle\}.\end{aligned}$$

ϕ_{1s} and ϕ_{2s} represent respectively the 1s and 2s orbitals of atomic lithium. The asymptotic form of the hydrogen-like Coulomb wave function is

$$\chi^-_{\mathbf{k}}(\mathbf{r}) = 2\pi^{-3/2}\mathrm{e}^{-\gamma\pi/2}\Gamma(1-i\gamma)\mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}}{}_1F_1[i\gamma, 1, -i(kr+\mathbf{k}\cdot\mathbf{r})],$$

where $\gamma = -Z'/k$, Z' is the charge of the parent nucleus after ionization.

2. Theory

The ionization cross-sections are calculated using the following formulations:

(a) For ionization of projectile (Ps):

$$\sigma_{\mathrm{DIP}} = \frac{k_{\mathrm{f}}}{k_{\mathrm{i}}}\int \mathrm{d}\hat{\mathbf{k}}_{\mathrm{f}}\int \mathrm{d}\hat{\mathbf{k}}\int \mathrm{d}E_{\mathbf{k}}\sum_{n'l'}|f^{n'l'}_{\mathbf{k}}(\hat{\mathbf{k}}_{\mathrm{f}})|^2.$$

(b) For ionization of target (Li):

$$\sigma_{\mathrm{DIT}} = \frac{k_{\mathrm{f}}}{k_{\mathrm{i}}}\int \mathrm{d}\hat{\mathbf{k}}_{\mathrm{f}}\int \mathrm{d}\hat{\mathbf{k}}'\int \mathrm{d}E_{\mathbf{k}'}\sum_{nl}|f^{nl}_{\mathbf{k}'}(\hat{\mathbf{k}}_{\mathrm{f}})|^2.$$

(c) For ionization of both projectile and target:

$$\sigma_{\mathrm{DIB}} = \frac{k_{\mathrm{f}}}{k_{\mathrm{i}}}\int \mathrm{d}\hat{\mathbf{k}}_{\mathrm{f}}\int \mathrm{d}\hat{\mathbf{k}}'\int \mathrm{d}\hat{\mathbf{k}}\int \mathrm{d}E_{\mathbf{k}'}\int \mathrm{d}E_{\mathbf{k}}|f_{\mathbf{k}'\mathbf{k}}(\hat{\mathbf{k}}_{\mathrm{f}})|^2.$$

The corresponding scattering amplitudes in three-electron model are:

$$\begin{aligned}f^{n'l'}_{\mathbf{k}}(\hat{\mathbf{k}}_{\mathrm{f}}) = -\frac{1}{\pi}\int &\mathrm{e}^{-i\mathbf{k}_{\mathrm{f}}\cdot\mathbf{R}}\eta^*_{\mathbf{k}}(\boldsymbol{\rho})\Phi^*_{n'l'}\{\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3\}[V_{\mathrm{int}}] \\ &\times\mathrm{e}^{i\mathbf{k}_{\mathrm{i}}\cdot\mathbf{R}}\eta_{1s}(\boldsymbol{\rho})\Phi_G\{\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3\}\prod_{i=1}^{3}\mathrm{d}\mathbf{r}_{\mathrm{i}}\,\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{r},\end{aligned}$$

$$\begin{aligned}f^{nl}_{\mathbf{k}'}(\hat{\mathbf{k}}_{\mathrm{f}}) = -\frac{1}{\pi}\int &\mathrm{e}^{-i\mathbf{k}_{\mathrm{f}}\cdot\mathbf{R}}\eta^*_{nl}(\boldsymbol{\rho})\Phi^*_{\mathbf{k}'}\{\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3\}[V_{\mathrm{int}}] \\ &\times\mathrm{e}^{i\mathbf{k}_{\mathrm{i}}\cdot\mathbf{R}}\eta_{1s}(\boldsymbol{\rho})\Phi_G\{\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3\}\prod_{i=1}^{3}\mathrm{d}\mathbf{r}_{\mathrm{i}}\,\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{r},\end{aligned}$$

$$f_{\mathbf{k}'\mathbf{k}}(\hat{\mathbf{k}}_\mathrm{f}) = -\frac{1}{\pi}\int \mathrm{e}^{-i\mathbf{k}_\mathrm{f}\cdot\mathbf{R}}\eta^*_{\mathbf{k}}(\boldsymbol{\rho})\Phi^*_{\mathbf{k}'}\{\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3\}[V_\mathrm{int}]$$
$$\times \mathrm{e}^{i\mathbf{k}_\mathrm{i}\cdot\mathbf{R}}\eta_{1s}(\boldsymbol{\rho})\Phi_G\{\mathbf{r}_1,\mathrm{r}_2,\mathrm{r}_3\}\prod_{i=1}^{3}\mathrm{d}\mathbf{r}_\mathrm{i}\,\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{r}$$

with

$$\mathbf{R} = \frac{1}{2}(\mathbf{x}+\mathbf{r}),$$

$$\boldsymbol{\rho} = \mathbf{x}-\mathbf{r},$$

$\mathbf{x}$ and $\mathbf{r}$ are the coordinates of positron and electron in Ps, and $\mathbf{r}_i$; $i = 1$–3 are of target atomic electrons.

$$V_\mathrm{int} = \frac{Z}{|\mathbf{x}|} - \frac{Z}{|\mathbf{r}|} - \sum_{i=1}^{3}\frac{1}{|\mathbf{x}-\mathbf{r}_i|} + \sum_{i=1}^{3}\frac{1}{|\mathbf{r}-\mathbf{r}_i|},$$

where Z is the nuclear charge of the target atom.

Using the above substitution of $\boldsymbol{\rho}$ and $\mathbf{R}$ and the Jacobian coordinate transformation, the above scattering amplitudes can be separated into a Ps form-factor (I_Ps) and target form-factor (I_Li) like

$$I_\mathrm{Ps} = \int \eta^*_\mathrm{f}(\boldsymbol{\rho})\{\mathrm{e}^{-i\mathbf{q}\cdot\boldsymbol{\rho}/2} - \mathrm{e}^{i\mathbf{q}\cdot\boldsymbol{\rho}/2}\}\eta_\mathrm{i}(\boldsymbol{\rho})\mathrm{d}\boldsymbol{\rho}$$

and

$$I_\mathrm{Li} = \int \Phi^*_\mathrm{f}\left[Z - \sum_{k=1}^{3}\mathrm{e}^{i\mathbf{q}\cdot\mathbf{r}_\mathbf{k}}\right]\Phi_\mathrm{i}\prod_{k=1}^{3}\mathrm{d}\mathbf{r}_\mathbf{k}.$$

ϕ_i, ϕ_f and η_i, η_f represent respectively the initial and final state wave functions of target and Ps. The generic quantities k_f, k'_max, and k_max are evaluated from the conservation of energy condition given by

$$\frac{k_\mathrm{i}^2}{4} + E_\mathrm{i}^\mathrm{Li} + E_\mathrm{i}^\mathrm{Ps} = \frac{k_\mathrm{f}^2}{4} + E_\mathrm{f}^\mathrm{Li} + E_\mathrm{f}^\mathrm{Ps}.$$

where E_i^Ps, E_f^Ps and E_i^Li, E_f^Li represent respectively the initial and final state energies of Ps and Li; $\mathbf{k}_\mathrm{i}$ and $\mathbf{k}_\mathrm{f}$ are the initial and final momenta of the projectile. The Gauss–Legendré quadrature method is applied to carry on the numerical integrations.

3. Results and discussion

We present the cross-sections for three different kinds of ionization and excitation for all the important channels. The Ps-ionization cross-sections for different Li-transitions and Li-ionization cross-sections for different Ps-transitions are compared

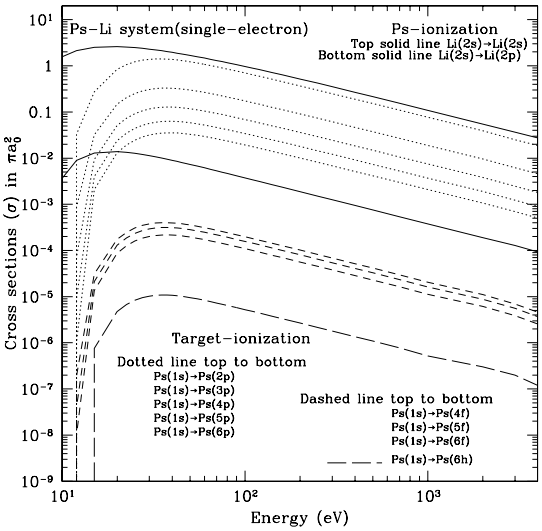

Figure 1. The ionization cross-sections for different target- and Ps-transitions in Ps–Li system in single-electron target.

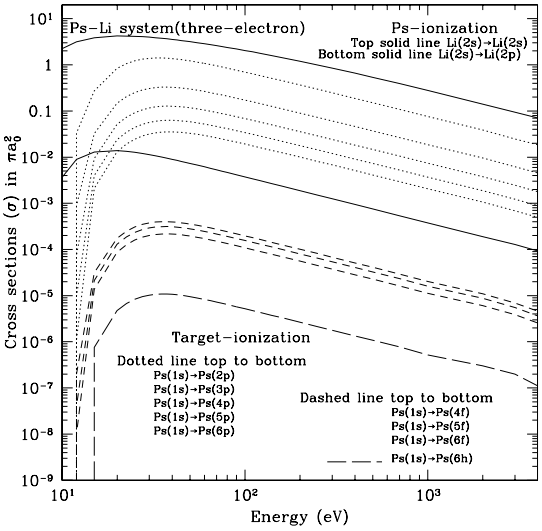

Figure 2. The ionization cross-sections for different target- and Ps-transitions in Ps–Li system in three-electron target.

for all the important channels in figures 1 and 2 using a hydrogen-like single-electron (model I) and a three-electron (model II) description of the target. Similarly in figures 3 and 4, all the important excitation cross-sections are compared using models I and II. The solid curves in figures 1 and 2, from top to bottom are

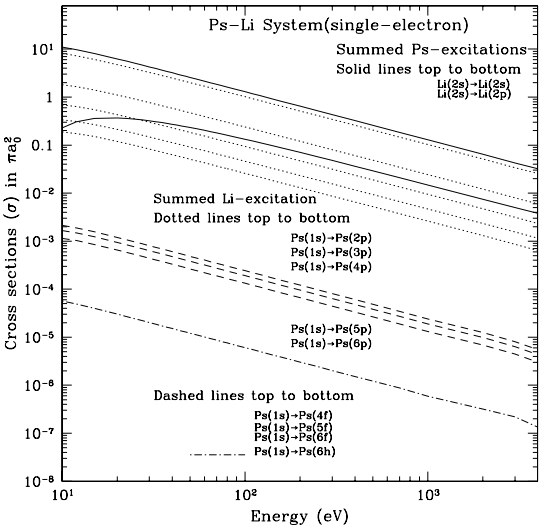

Figure 3. The excitation cross-sections for different target- and Ps-transitions in Ps–Li system in single-electron target.

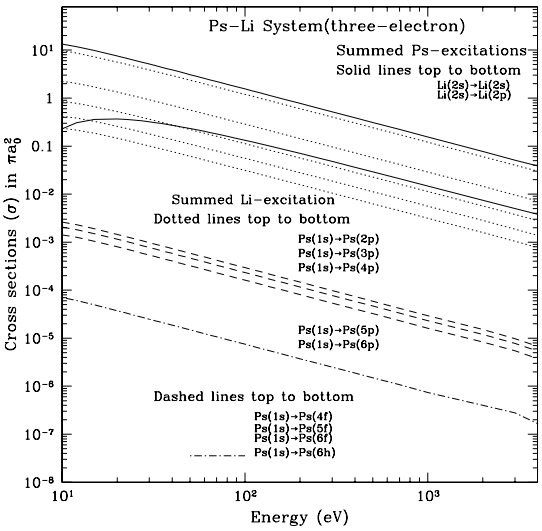

Figure 4. The excitation cross-sections for different target- and Ps-transitions in Ps–Li system in three-electron target.

representing the Ps-ionization cross-sections for target-transitions: Li($2s$) → Li($2s$), Li($2s$) → Li($2p$). Similarly the dotted curves from top to bottom represent the Li ionization cross-sections for Ps-transitions: Ps($1s$) → Ps(np), $n = 2$–6; the dashed curves from top to bottom are the same but for Ps-transitions: Ps($1s$) → Ps(nf),

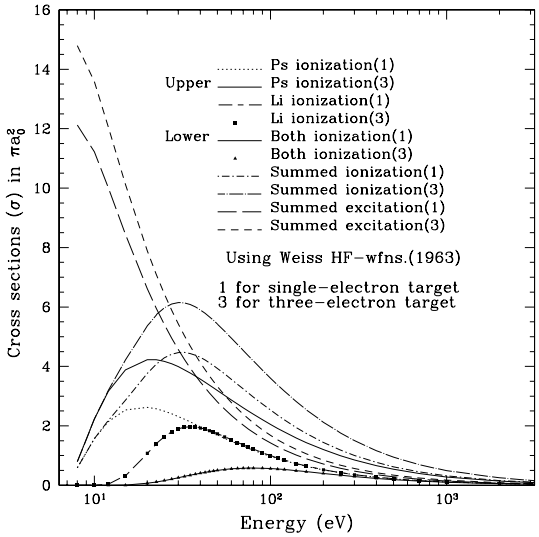

Figure 5. The comparison of the summed cross-sections for Ps–Li scattering in single-electron and three-electron targets against the Ps energy in eV.

$n = 4$–6 and the long dashed curve is displaying the Li-ionization cross-sections for $\mathrm{Ps}(1s) \rightarrow \mathrm{Ps}(6h)$. In an exactly similar fashion, all the excitation cross-sections are displayed in figures 3 and 4. By the word 'summed' we like to mean that the cross-sections are added for all the possible channels. The target elastic Ps-ionization and the target ionization channels with $\mathrm{Ps}(1s) \rightarrow \mathrm{Ps}(np)$ transitions are found to be more important. It is also to be noted that the contribution for a particular Ps-transition or a particular Li-transition is always greater than similar immediate higher one. The slow rate of falling of ionization and excitation cross-sections with the rise of incident energy indicate the importance of excitation as well as ionization processes for a very wide energy range.

In figure 5, we have compared our summed ionization cross-sections for Li-ionization, the summed ionization cross-sections for Ps-ionization, the both-ionization cross-sections, the summed or total ionization cross-sections and the summed excitation cross-sections using models I and II respectively with the variation of the incident projectile energy. The big and small dashed dotted lines are the summed ionization cross-sections, the small and big dashed curves are the summed excitation cross-sections, the dotted and upper solid lines are the Ps-ionization cross-sections using models I and II respectively. The big and small dashed line and the lower solid line are displaying the Li-ionization and both-ionization cross-sections using model I. Similarly solid squares and solid triangles are the Li-ionization and both-ionization cross-sections using model II. All the ionization cross-sections have peaks. It is to be noted that the two different curves using models I and II almost coincided for summed Li-ionization and both-ionization. However, a difference in magnitude in summed ionization curves occurred using models I and II, is due to the difference in Ps-ionization curves using models I

and II. The target-ionization and both-ionization processes are almost insensitive to the choice of models I and II, but the Ps-ionization and more specifically, the target-elastic Ps-ionization is highly sensitive to the choice of target representation. Similar findings are observed in excitation cross-sections too. Obviously, three-electron prescription of the present target is more accurate. So the core electrons have an important role to control the reaction process and they are more active when valence electron keeps itself silent (target-elastic channel). On the other hand, if valence electron plays a role (target-inelastic channel) the core electrons remain almost silent. The magnitudes of the cross-sections for Ps-ionization and Li-ionization are competing in single-electron model but the both-ionization cross-sections are much lower in magnitude. So both-ionization is not so important in Ps–Li scattering and are in disagreement with the behaviour of Ps–H [5,6] and Ps–He [5,7] systems.

4. Conclusions

In conclusion, three different types of ionization in Ps–Li system, e.g. Ps-ionization, Li-ionization and ionization of both are studied thoroughly using orthogonalized Coulomb wave for the target-ionized electron in a single-electron and a three-electron prescription of the target, following an exact methodology in a CBA. Different excitation cross-sections are also studied thoroughly using FBA for all the important channels with both the choices of the target (models I and II). The present study indicates the importance of excitation, the Ps-ionization and Li-ionization in Ps–Li scattering up to a moderately high energy region ($\sim$1000 eV). At very low energies near the threshold, the contribution of excitation is far greater than ionization. The comparative studies of different ionization and excitation cross-sections using models I and II shown in figures 1–4 provide an estimate of the relative importance of different channels and help to conceive a reasonable insight to find basic physics. It is deduced from the comparative studies of the cross-sections using models I and II in figure 5 that the core electrons have an important role to influence the scattering processes and the impact is more on target-elastic channels in which the target-valence electron remains silent. So it is necessary to include the effect of core electrons if a single-electron approximation is used to represent the target alkali atom.

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