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Ionization of positronium (Ps) in collision with atoms

Hasi Ray [1]

Institute for Plasma Research, Bhat, Gandhinagar 382428, Gujrat, India

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ABSTRACT

Ps ionization in Ps–atom scattering is of fundamental importance. The singly differential cross sections (SDCS) provides more accurate information to test a theory than integrated or total ionization cross section since the averaging over one parameter is not required. We evaluate the SDCS for Ps-ionization with respect to the longitudinal energy distribution of the break-up positron and electron in Ps–H and Ps–He scattering and compare them with the recently available experimental and theoretical data.

The fragmentation of positronium (Ps) is a process which helps to understand the mechanism of Ps and atom/molecule scattering [1–13]. Recently, the experimental group at University College of London (UCL) lead by G. Laricchia has measured [4–6] the singly-differential Ps-ionization cross sections with respect to the longitudinal energy distribution of the break-up positron in Ps and He collision which motivated the present study. The number of papers which deal Ps-fragmentation is extremely limited [2–20]. Only a very few experimental data [4–6] on Ps-ionization in Ps–He scattering is available in the literature. The fragmentation or ionization or break-up of Ps starts only at 6.8 eV.

We study collision of Ps with atom. The kind of calculation is a bit difficult and challenging due to presence of many charge centers. In such a system of a Ps and an atom, the exchange between the Ps-electron and the atomic-electron is highly important and sensitive at lower incident energies, and it is an effect of fundamental interest. We calculate the singly (energy) differential cross sections for Ps-ionization in Ps–H and Ps–He scattering using the Coulomb–Born–Oppenheimer approximation (CBOA) and the Coulomb–Born approximation (CBA); both the theories were introduced by Ray [2,3,15–19] to calculate the integrated cross sections. The differential cross section is more informative than integrated cross section since it relaxes the averaging over a coordinate system e.g. angular or energy distribution. In the present case the averaging over energy distribution of the break-up positron and/or electron is relieved.

The scattering amplitudes can be expressed in post and prior forms, both will provide the same results if the system wave functions are exact [21]. We use the post form of the scattering amplitude; in this expression $\langle \Psi_f | v_f | \Psi_i^+ \rangle$ (following conventional notation), the incident channel wave function is treated as a plane wave as in first Born approximation (FBA). Since the projectile is a neutral system, the present plane wave approximation for the incident Ps may not introduce an error. In addition the first order effect due to polarizability is absent in such system. So it is nearly accurate which is evident from the comparison of FBA and the close coupling approximation (CCA) results of our earlier calculation [22,23]. Only at very low energies, the FBA and CCA elastic cross sections differ in Ps–H [22] and Ps–Li [23] systems. The break-up electron is treated as a Coulomb wave. As the incident Ps is a composite system of a positron and an electron, we treat the moving Ps as having a center of mass (c.m.) motion with momenta $\mathbf{k}_i$ and $\mathbf{k}_f$ in the initial and final channels respectively, and a relative motion of electron with respect to positron; the c.m. motion is represented by a plane wave.

A few words regarding the target He wave function is useful. The accuracy of the present calculation again depends on the accuracy of the ground state He atomic wave function. We used the

E-mail address: hasi_ray@yahoo.com.

[1] Present address: S-407, Flat No. 6, B.P. Township, Kolkata 700094, India.

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first kind of wave function prescribed by Winter [24]. This wave function is not correlated. A correlated wave function for the target atomic He would be more useful for better accuracy, but it complicates our calculation further. It should be a good task to use a correlated wave function to tackle the present problem.

The singly energy differential cross section (SDCS) for the break-up of Ps in Ps and atom scattering is defined [10] as

$$\frac{d\sigma}{dE} = \int d\hat{\mathbf{k}}_p \int d\hat{\mathbf{k}}_e \frac{d^3\sigma}{d\hat{\mathbf{k}}_p\, d\hat{\mathbf{k}}_e\, dE} \tag{1}$$

where $\mathbf{k}_p$, $\mathbf{k}_e$ are the momenta of the break-up positron and electron respectively and E is the sum of the kinetic energies of break-up positron and electron after ionization.

In inelastic collisions, only the energy conservation is true. If v_p, v_e represent respectively the speeds (i.e. magnitudes of the velocities) of break-up positron and electron from Ps, ϵ_{Ps} is the ionization potential of Ps, then the energy conservation relation

$$E = E_i - \epsilon_{\text{Ps}} = \frac{1}{2}v_p^2 + \frac{1}{2}v_e^2 \tag{2a}$$

$$= v_f^2 + \frac{1}{4}v^2 \tag{2b}$$

should be fulfilled if the incident energy is E_i; v_f is the magnitude of the c.m. velocity of fragmented Ps and v is the magnitude of relative velocity of the break-up electron with respect to the break-up positron in the final channel after ionization.

The momentum transfer $\mathbf{Q}$ is defined as $\mathbf{Q} = \mathbf{k}_i - \mathbf{k}_f$, so that

$$Q^2 = k_i^2 + k_f^2 - 2k_i k_f \cos\theta \tag{3}$$

if θ is the scattering angle and $\mathbf{k}_i$, $\mathbf{k}_f$ are initial and final momenta. According to our definition, the SDCS is defined as

$$\frac{d\sigma}{dE_{\mathbf{k}}} = \int d\hat{\mathbf{k}}_f \int d\hat{\mathbf{k}} \frac{d^3\sigma}{d\hat{\mathbf{k}}_f\, d\hat{\mathbf{k}}\, dE_{\mathbf{k}}}. \tag{4}$$

Again

$$\mathbf{k}_p = \mathbf{k}_f - \frac{1}{2}\mathbf{k}, \tag{5a}$$

$$\mathbf{k}_e = \mathbf{k}_f + \frac{1}{2}\mathbf{k} \tag{5b}$$

which gives $d\mathbf{k}_p = d\mathbf{k}_f$ if we make $\mathbf{k}$ unaltered and $d\mathbf{k}_e = \frac{1}{2}d\mathbf{k}$ if we make $\mathbf{k}_f$ unaltered. It is obvious that $dE_{\mathbf{k}} = k\,dk$ and $\int dE_k = \int dE$.

If the longitudinal energy of break-up positron is E_{pl} and it makes an angle θ_p with $\mathbf{k}_i$, then

$$E_p = \frac{1}{2}v_p^2 = \frac{E_{pl}}{\cos^2\theta_p} \tag{6a}$$

and

$$v_e^2 = 2\left(E_i - \epsilon_{\text{Ps}} - \frac{E_{pl}}{\cos^2\theta_p}\right). \tag{6b}$$

The magnitude of relative velocity (i.e. relative speed) of break-up electron with respect to break-up positron can be defined as

$$v = v_e - v_p, \tag{7a}$$

$$v^2 = v_p^2 + v_e^2 - 2v_p v_e = 4k^2 \tag{7b}$$

and

$$v_f^2 = E_i - \epsilon_{\text{Ps}} - \frac{1}{4}v^2 = \frac{1}{4}k_f^2. \tag{7c}$$

If the longitudinal energy of break-up electron is E_{el} and it makes an angle θ_e with $\mathbf{k}_i$, then

$$E_e = \frac{1}{2}v_e^2 = \frac{E_{el}}{\cos^2\theta_e} \tag{8a}$$

and

$$v_p^2 = 2\left(E_i - \epsilon_{\text{Ps}} - \frac{E_{el}}{\cos^2\theta_e}\right). \tag{8b}$$

The triply differential cross sections (TDCS) for the break-up of Ps in Ps–H and Ps–He scatterings are defined as

$$\frac{d^3\sigma}{d\mathbf{k}_f\, d\hat{\hat{\mathbf{k}}}\, dE_{\mathbf{k}}} = \frac{k_f k}{k_i}\left\{\frac{1}{4}|F_k + G_k|^2 + \frac{3}{4}|F_k - G_k|^2\right\}, \tag{9a}$$

$$\frac{d^3\sigma}{d\mathbf{k}_f\, d\hat{\hat{\mathbf{k}}}\, dE_{\mathbf{k}}} = \frac{k_f k}{k_i}\left|F_{\mathbf{k}}^{\text{He}} - G_{\mathbf{k}}^{\text{He}}\right|^2 \tag{9b}$$

where F_k, G_k represent respectively the direct and exchange matrix elements for Ps–H scattering; $F_{\mathbf{k}}^{\text{He}}$, $G_{\mathbf{k}}^{\text{He}}$ represent respectively the direct and exchange matrix elements for Ps–He scattering. These are defined as

$$F_{\mathbf{k}}^{\text{He}}(\hat{\mathbf{k}}_f) = -\frac{1}{\pi}\int e^{-i\mathbf{k}_f\cdot\mathbf{R}_1}\eta_{\mathbf{k}}^*(\boldsymbol{\rho}_1)\Phi_f^*\{\mathbf{r}_2,\mathbf{r}_3\}\left[V_{\text{He}}^F\right] \times e^{i\mathbf{k}_i\cdot\mathbf{R}_1}\eta_{1s}(\boldsymbol{\rho}_1)\Phi_i\{\mathbf{r}_2,\mathbf{r}_3\}\,d\mathbf{x}\,d\mathbf{r}_1\,d\mathbf{r}_2\,d\mathbf{r}_3, \tag{10a}$$

$$G_{\mathbf{k}}^{\text{He}}(\hat{\mathbf{k}}_f) = -\frac{1}{\pi}\int e^{-i\mathbf{k}_f\cdot\mathbf{R}_2}\eta_{\mathbf{k}}^*(\boldsymbol{\rho}_2)\Phi_f^*\{\mathbf{r}_1,\mathbf{r}_3\}\left[V_{\text{He}}^G\right] \times e^{i\mathbf{k}_i\cdot\mathbf{R}_1}\eta_{1s}(\boldsymbol{\rho}_1)\Phi_i\{\mathbf{r}_2,\mathbf{r}_3\}\,d\mathbf{x}\,d\mathbf{r}_1\,d\mathbf{r}_2\,d\mathbf{r}_3 \tag{10b}$$

with

$$V_{\text{He}}^F = \frac{Z}{|\mathbf{x}|} - \frac{Z}{|\mathbf{r}_1|} - \frac{1}{|\mathbf{x}-\mathbf{r}_2|} + \frac{1}{|\mathbf{r}_1-\mathbf{r}_2|} - \frac{1}{|\mathbf{x}-\mathbf{r}_3|} + \frac{1}{|\mathbf{r}_1-\mathbf{r}_3|} \tag{11a}$$

and

$$V_{\text{He}}^G = \frac{Z}{|\mathbf{x}|} - \frac{Z}{|\mathbf{r}_2|} - \frac{1}{|\mathbf{x}-\mathbf{r}_1|} + \frac{1}{|\mathbf{r}_2-\mathbf{r}_1|} - \frac{1}{|\mathbf{x}-\mathbf{r}_3|} + \frac{1}{|\mathbf{r}_2-\mathbf{r}_3|} \tag{11b}$$

with $\mathbf{R}_j = \frac{1}{2}(\mathbf{x}+\mathbf{r}_j)$ and $\boldsymbol{\rho}_j = (\mathbf{x}-\mathbf{r}_j)$; $j = 1, 2$. Here, $\mathbf{x}$ is the coordinate of positron in Ps, and $\mathbf{r}_j$; $j = 1$ to 3 are those of electrons in Ps and He respectively in the incident channel with respect to the center of mass of the system. Functions η and Φ indicate the wave functions of Ps and He, respectively. Subscript 'i' identifies the incident channel, whereas 'f' represents the final channel. Accordingly $\mathbf{k}_i$ and $\mathbf{k}_f$ are the momenta of the projectile in the initial and final channels respectively. Z is the nuclear charge of the target helium atom. The target atomic wave functions are considered at ground states in both the incident and final channels. If we remove the third electron from the Ps–He system which is represented by the position coordinate $\mathbf{r}_3$, the expressions (10a), (10b), (11a), (11b) should fit to Ps–H system. The continuum Coulomb wave function $\eta_{\mathbf{k}}$ is chosen from Ref. [3] which is orthogonal to the ground state Ps wave function.

In Figs. 1(a) and 1(b), we present the SDCS results for Ps–H scattering with respect to the longitudinal energy distribution of the break-up positron and electron at the incident energies 33 eV and 60 eV using CBOA (i.e. with exchange) and CBA (i.e. without exchange). For the Ps–H system, there is no experimental data and no reported theoretical data. Figs. 2(a) and 2(b) display the present SDCS data for Ps–He system with respect to the longitudinal energy distribution of break-up positron and electron respectively with the recently available corresponding experimental [5,6] and theoretical [10,11,20] data at the incident energies 33 eV and 60 eV. In Fig. 3, we displays the data at the incident energy 100 eV; here is no experimental data. We compare our data using both the CBOA and the CBA with the corresponding impulse approximation (IA) data of Starrett et al. [20] in this figure. It is to be noted that the area under the SDCS curves for e^+ and e^- are always equal. So