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Coulomb–Born–Oppenheimer approximation in Ps–H scattering

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Abstract. To improve the Coulomb–Born approximation (CBA) theory of ionization in positronium (Ps) and atom scattering, the effect of exchange is introduced. The nine-dimensional exchange amplitude for ionization of Ps in Ps–H scattering is reduced to a two-dimensional integral using the present Coulomb–Born–Oppenheimer approximation (CBOA). The methodology is extremely useful to evaluate ionization parameters for different target systems and for different types of ionization processes. It is then applied to evaluate the Ps-ionization cross-section and to estimate the effect of exchange on Ps-ionization in Ps–H system. We establish the importance of exchange at lower energy region.

Keywords. Positronium; ionization; exchange; electron-spin; continuum; Coulomb wave function.

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The importance of ionization in positronium (Ps) and atom scattering is discussed by Massey and Mohr [1]. It is only in recent years that this subject has started receiving attention [2–13]. A large number of theoretical studies are available in the literature to study the elastic and excitation processes using different coupled state methods, e.g. close-coupling approximation (CCA) [14–22], R-matrix theory [8–12], complex rotation stabilization method [23–26], different variational methods [27–32] in Ps–atom scattering and some other studies related to Ps [33–38]. Due to availability of low-energy Ps beams, different groups across the world have started experimental studies using the Ps beam [2,39–43]. Again a little attention is devoted to ionization [2], the only experimental result available in the literature is by the University College of London (UCL) group on Ps-ionization in Ps–He scattering.

Theoretically Ps–atom scattering is a highly difficult and challenging problem due to the composite structures of both the projectile and the target. Even the simplest system Ps–H involves four charge centers. In ionization, the problem is more complicated due to the presence of many charged particles in the final channel. The Coulomb–Born approximation (CBA) theory prescribed by Geltman [44] is highly successful [45] for ionization calculation at intermediate to high energy re-

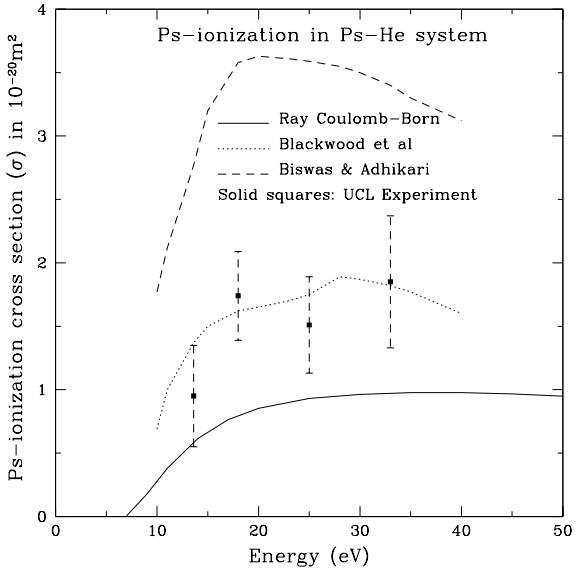

Figure 1. Comparison of Ps-ionization cross-sections [4] using CBA in Ps–He scattering with available theories and experiment [2].

gion. In that approximation, a Coulomb wave function [46] was used for the ionized electron to include the effect of Coulomb interaction of the parent nuclear charge on the ionized electron. The CBA theory was extended in Ps–atom scattering [3–7] by the present author. The CBA results [4] for Ps-ionization in Ps–He scattering are compared in figure 1 with the available experimental [2] and theoretical data obtained by using the first Born approximation (FBA) [13] and a coupled pseudostate R-matrix theory [8]. The comparison with experimental data indicated that some effects are not taken into account. The present work is an extension of that activity.

The Ps-ionization channel in Ps–atom scattering opens only at the incident Ps energy of 6.8 eV. In this energy region, the effect of exchange is highly important. The objective of the present work is to improve the CBA theory by including the effect of exchange and to get an estimate of exchange. But it is made difficult due to the large difference in system wave functions at the initial and final channels used to define the transition matrix element. The use of continuum Coulomb wave function for the ionized electron adds more rigor to the problem formulation due to the presence of a confluent hypergeometric function (${}_1F_1$) which contains a coupled co-ordinate at its argument.

The present study concerns Ps-fragmentation in Ps–H scattering. It includes the effect of exchange in a CBA [3–7]. It can be defined in a different way as if a Coulomb wave function is used for ionized electron in a Born–Oppenheimer approximation [47]. So it might not be a misnomer if we call the present theory as a Coulomb–Born–Oppenheimer approximation (CBOA). The CBA theory is one in which the moving Ps is treated as a plane wave and the ionized electron as a continuum Coulomb wave. From the physical point of view, the proposed CBOA is

a very good approximation to provide ionization data in Ps–atom scattering since Ps is such an atom which by itself is its antiatom [48] constituted by an elementary particle (electron) and its antiparticle (positron) with equal masses and charges. Since the charge and mass centers coincide, it can produce zero static potential in an interacting field and it itself is a neutral particle. So the free particle solution which is a plane wave, is sufficient to represent the dynamic motion of Ps in the initial channel or in the final channel; this is the qualitative definition of FBA.

The transition amplitude for scattering processes can be calculated using any of the form of post and prior interactions if the system wave functions are exact [49]. The general form of transition amplitude using post and prior forms are $\langle \Psi_{\rm f}|V_{\rm f}|\Psi_{\rm i}^{+}\rangle$ and $\langle \Psi_{\rm f}^{-}|V_{\rm i}|\Psi_{\rm i}\rangle$ respectively, following the conventional notations; $\Psi_{\rm i}^{+}$ and $\Psi_{\rm f}^{-}$ are the exact channel wave functions. In practice, it is very difficult to get an exact channel wave function for such a system, so we are forced to use an approximate form. According to our earlier experiences [50,51] and related studies [45], the post form can provide more reliable information about the scattering process than the prior form in the rearrangement channel using an approximate wave function. So in the present study we have chosen the post form. It seems to be due to the fact that it is more feasible to approximate the incident channel wave function in the asymptotic region by a free particle solution than the final channel wave function.

The Ps–H system contains two electrons. Due to their indistinguishability property electrons can interchange their positions, and the phenomenon is known as exchange. We consider their spins extrinsically. The two electron-spins can make a distribution of 1/4th possibility of forming a singlet state (combined spin = 0) and 3/4th possibility of forming a triplet state (combined spin = 1). Accordingly the space part of the system wave function should take a symmetric and an antisymmetric form to make the total wave function of the system an antisymmetric one. This is the advantage of a central potential. Obviously the angular integration of the spin part should be unity.

The triply-differential cross-section (TDCS) for the present ionization process is defined as

$$\frac{{\rm d}^3\sigma}{{\rm d}\hat{\mathbf{k}}_{\rm f}{\rm d}\hat{\mathbf{k}}\,{\rm d}E_{\mathbf{k}}} = \frac{k_{\rm f}}{k_{\rm i}}\left\{\frac{1}{4}|F_k+G_k|^2+\frac{3}{4}|F_k-G_k|^2\right\}, \tag{1}$$

if F_k and G_k are respectively the direct and exchange matrix elements considering space part only.

Accordingly the integrated or the total Ps-ionization cross-section (σ) can be expressed as

$$\sigma(E_{\rm i}) = \frac{k_{\rm f}}{k_{\rm i}}\int {\rm d}\hat{\mathbf{k}}_{\rm f}\int {\rm d}\hat{\mathbf{k}} \times \int {\rm d}E_{\mathbf{k}}\left[\frac{1}{4}F_{\mathbf{k}}(\hat{\mathbf{k}}_{\rm f})+G_{\mathbf{k}}(\hat{\mathbf{k}}_{\rm f})|^2+\frac{3}{4}|F_{\mathbf{k}}(\hat{\mathbf{k}}_{\rm f})-G_{\mathbf{k}}(\hat{\mathbf{k}}_{\rm f})|^2\right], \tag{2}$$

where

$$F_{\mathbf{k}}(\hat{\mathbf{k}}_{\rm f}) = -\frac{1}{\pi}\int {\rm e}^{-i\mathbf{k}_{\rm f}\cdot R_1}\eta_{\mathbf{k}}^{*}(\boldsymbol{\rho}_1)\Phi_{\rm f}^{*}\{\mathbf{r}_2\}[V_{\rm int}^{F}] \times {\rm e}^{i\mathbf{k}_{\rm i}\cdot R_1}\eta_{1s}(\boldsymbol{\rho}_1)\Phi_{\rm i}\{\mathbf{r}_2\}{\rm d}\mathbf{x}{\rm d}\mathbf{r}_1{\rm d}\mathbf{r}_2, \tag{3}$$

$$G_{\mathbf{k}}(\hat{\mathbf{k}}_{\rm f}) = -\frac{1}{\pi}\int \mathrm{e}^{-i\mathbf{k}_{\rm f}.R_2}\eta^*_{\mathbf{k}}(\boldsymbol{\rho}_2)\Phi^*_{\rm f}\{\mathbf{r}_1\}[V^G_{\rm int}] \times \mathrm{e}^{i\mathbf{k}_{\rm i}.R_1}\eta_{1s}(\boldsymbol{\rho}_1)\Phi_{\rm i}\{\mathbf{r}_2\}\mathrm{d}\mathbf{x}\mathrm{d}\mathbf{r}_1\mathrm{d}\mathbf{r}_2, \tag{4}$$

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 $\mathbf{r}_j$; $j = 1, 2$ are that of electrons in Ps and H 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 H. Subscript 'i' represents the incident channel, whereas 'f' represents the final channel. Accordingly $\mathbf{k}_{\rm i}$ and $\mathbf{k}_{\rm f}$ are the momenta of the projectile in the initial and final channels respectively.

$$V^F_{\rm int} = \frac{1}{|\mathbf{x}|} - \frac{1}{|\mathbf{r}_1|} - \frac{1}{|\mathbf{x}-\mathbf{r}_2|} + \frac{1}{|\mathbf{r}_1-\mathbf{r}_2|}, \tag{5}$$

$$V^G_{\rm int} = \frac{1}{|\mathbf{x}|} - \frac{1}{|\mathbf{r}_2|} - \frac{1}{|\mathbf{x}-\mathbf{r}_1|} + \frac{1}{|\mathbf{r}_1-\mathbf{r}_2|}. \tag{6}$$

Indices F and G indicate the direct and exchange channels respectively.

The asymptotic form of the Coulomb wave function $[\eta_{\mathbf{k}}(\boldsymbol{\rho})]$ is

$$\eta_{\mathbf{k}}(\boldsymbol{\rho}) = 2\pi^{-3/2}\mathrm{e}^{-\gamma\pi/2}\Gamma(1-i\gamma)\mathrm{e}^{i\mathbf{k}\cdot\rho}{}_1F_1[i\gamma, 1, -i(k\rho+\mathbf{k}\cdot\boldsymbol{\rho})], \tag{7}$$

where $\gamma = -Z'/k$, $Z'(=1$, in the present case) is the charge of parent nucleus after ionization. Further the continuum Coulomb wave function is orthogonal to the ground state positronium wave function.

The scattering amplitudes in both the direct and exchange channels for the simplest Ps–H system involve nine-dimensional integrals e.g. eqs (3) and (4). It consists of four interaction potential terms (see eqs (5) and (6)) of which the first two nuclear interaction terms are uncoupled and the other two terms, the electron–positron correlation and the electron–electron correlation are coupled. In addition there are coupled terms in the argument of ${}_1F_1$ function (eq. (7)). The initial state Ps wave function contains a coupled term in the exponential. In direct channel, the computation of the nine-dimensional scattering amplitude is a little bit simpler because of a symmetry in the system wave function in the initial and final channels which are already discussed in our previous articles [3–7]. Here we propose a methodology for evaluating the exchange amplitude and apply it to compute all the four interacting terms of the potential.

The mathematical steps followed are: (i) First the integrations over the incident channel positronium electron coordinate $\mathbf{r}_1$ are evaluated. (ii) In the second step a Jacobian coordinate transformation as $\mathbf{R}_2 = \frac{1}{2}(\mathbf{x}+\mathbf{r}_2)$ and $\boldsymbol{\rho}_2 = (\mathbf{x}-\mathbf{r}_2)$ is established. (iii) In the third step, $\mathbf{x}$ and $\mathbf{r}_2$ have been replaced in terms of $\boldsymbol{\rho}_2$ and $\mathbf{R}_2$. A very similar methodology is followed as used in our previous works [3–7] to simplify the rest with the help of Fourier transforms and Bethe integral-like standard formulations. Finally, the nine-dimensional integral expression of our Coulomb–Born exchange amplitude for the first three terms gets reduced to a simple two-dimensional integral as

$$
\begin{aligned}
G_{\mathbf{k}}^{1-3}(\hat{\mathbf{k}}_{\mathrm{f}}) = {} & 2\pi^{-1}\alpha_{\mathrm{i}}\beta_{\mathrm{f}}\mathrm{e}^{-\gamma\pi/2}\Gamma(1+i\gamma)\int_0^1 \mathrm{d}x\, x(1-x) \\
& \times \int_0^1 \mathrm{d}y y \left(\frac{1}{\mu_1}\frac{\partial}{\partial\mu_1}\right)^2 \frac{1}{\mu_1} \\
& \times \left[\beta_{\mathrm{i}}\left(\frac{1}{\mu_2}\frac{\partial}{\partial\mu_2}\right)^2 \frac{\{(\mathbf{k}+\mathbf{k}')^2-(k+i\mu_2)^2\}^{i\gamma}}{\{k'^2+\mu_2^2\}^{i\gamma+1}}\right. \\
& \left. -\mu_1\left(\frac{1}{\mu_3}\frac{\partial}{\partial\mu_3}\right)^2 \frac{\{(\mathbf{k}+\mathbf{k}'')^2-(k+i\mu_3)^2\}^{i\gamma}}{\{k''^2+\mu_3^2\}^{i\gamma+1}}\right] \\
& -2\pi^{-1}\alpha_{\mathrm{i}}\beta_{\mathrm{i}}\beta_{\mathrm{f}}\mathrm{e}^{-\gamma\pi/2}\Gamma(1+i\gamma)\int_0^1 \mathrm{d}x x \\
& \times \int_0^1 \mathrm{d}y\, y(1-y)\left(\frac{1}{\mu_1}\frac{\partial}{\partial\mu_1}\right) \\
& \times \left(\frac{1}{\mu_2}\frac{\partial}{\partial\mu_2}\right)^3 \left[\frac{\{(\mathbf{k}+\mathbf{k}')^2-(k+i\mu_2)^2\}^{i\gamma}}{\{k'^2+\mu_2^2\}^{i\gamma+1}}\right]. \qquad (8)
\end{aligned}
$$

Here

$$\mathbf{k}' = \frac{1}{2}(1+x)(1-y)\mathbf{k}_{\mathrm{i}} - \mathbf{k} - \left(\frac{1}{2}-y\right)\mathbf{k}_{\mathrm{f}}, \qquad (9a)$$

$$\mathbf{k}'' = \frac{1}{2}(1+x)y\mathbf{k}_{\mathrm{i}} - \mathbf{k} + \left(\frac{1}{2}-y\right)\mathbf{k}_{\mathrm{f}}, \qquad (9b)$$

$$\mu_1^2 = x\beta_{\mathrm{f}}^2 + (1-x)\alpha_{\mathrm{i}}^2 + \frac{1}{4}x(1-x)k_{\mathrm{i}}^2, \qquad (9c)$$

$$\mu_2^2 = y\beta_{\mathrm{i}}^2 + (1-y)\mu_1^2 + y(1-y)\left\{\frac{1}{2}(1+x)\mathbf{k}_{\mathrm{i}} - \mathbf{k}_{\mathrm{f}}\right\}^2, \qquad (9d)$$

$$\mu_3^2 = y\mu_1^2 + (1-y)\beta_{\mathrm{i}}^2 + y(1-y)\left\{\frac{1}{2}(1+x)\mathbf{k}_{\mathrm{i}} - \mathbf{k}_{\mathrm{f}}\right\}^2. \qquad (9e)$$

β_{i}, β_{f} and α_{i} are the screening parameters of the initial and final state H and the initial state Ps wave functions respectively.

However the fourth electron–electron correlation term takes a closed form as

$$
\begin{aligned}
G_{\mathbf{k}}^{4}(\hat{\mathbf{k}}_{\mathrm{f}}) = {} & \frac{32\beta_{\mathrm{i}}\beta_{\mathrm{f}}\mathrm{e}^{-\gamma\pi/2}\Gamma(1+i\gamma)}{\pi}\left(\frac{\partial}{\partial\beta_{\mathrm{f}}^2}\right)\left(\frac{\partial}{\partial\beta_{\mathrm{i}}^2}\right)\frac{1}{\sqrt{B^2-AG}} \\
& \times \log\left\{\frac{B+\sqrt{B^2-AG}}{B-\sqrt{B^2-AG}}\right\}\frac{\left\{\frac{1}{4}Q^2-(k+i\alpha_{\mathrm{i}})^2\right\}^{i\gamma}}{\left\{(\frac{1}{2}\mathbf{Q}-\mathbf{k})^2+\alpha_{\mathrm{i}}^2\right\}^{i\gamma+1}} \\
& \times \left\{\frac{\alpha_{\mathrm{i}}(i\gamma+1)}{\left(\frac{1}{2}\mathbf{Q}-\mathbf{k}\right)^2+\alpha_{\mathrm{i}}^2} - \frac{\gamma(k+i\alpha_{\mathrm{i}})}{\frac{1}{4}Q^2-(k+i\alpha_{\mathrm{i}})^2}\right\}, \qquad (10)
\end{aligned}
$$

where

$$B = \beta_{\rm f}\left\{\left(\mathbf{Q} - \frac{1}{2}\mathbf{k}_{\rm i}\right)^2 + \beta_{\rm i}^2\right\} + \beta_{\rm i}\left\{\frac{1}{4}\mathbf{k}_{\rm i}^2 + \beta_{\rm f}^2\right\}, \tag{11a}$$

$$AG = \left\{\left(\mathbf{Q} - \frac{1}{2}\mathbf{k}_{\rm i}\right)^2 + \beta_{\rm i}^2\right\}\left\{\frac{1}{4}\mathbf{k}_{\rm i}^2 + \beta_{\rm f}^2\right\}\{\mathbf{Q}^2 + (\beta_{\rm i} + \beta_{\rm f})^2\} \tag{11b}$$

and $\mathbf{Q} = \mathbf{k}_{\rm i} - \mathbf{k}_{\rm f}$.

To get a quantitative estimate of the effect of exchange at different energies, the detailed numerical calculations are performed after making all the differentiations of different terms in eqs (8) and (10). The formulation of total cross-section with exchange using the present scheme is a six-dimensional integral which was only a three-dimensional integral in CBA. All the integrations are performed using the algorithms for the standard numerical integration [50,51] and with the help of Gauss–Legendré quadratures. Our results for total Ps-ionization cross-section are displayed in figure 2. The solid line is our present total cross-section for Ps-ionization including the effect of exchange. The dotted one is the Ps-ionization cross-section [6] obtained using the CBA theory. The dashed curve displays the total Ps-ionization cross-sections of Belfast group [10] including the effect of exchange and using a 22-pseudostate coupled-channel method. The dashed–dotted curve is for the quenching cross-section obtained using our three-channel target-inelastic CCA [14]. It is plotted to get an idea about the probability of annihilation. Depending on the spin state of positron and electron, the Ps atom can exist in two different forms known as ortho (triplet) and para (singlet) Ps. The ortho Ps has

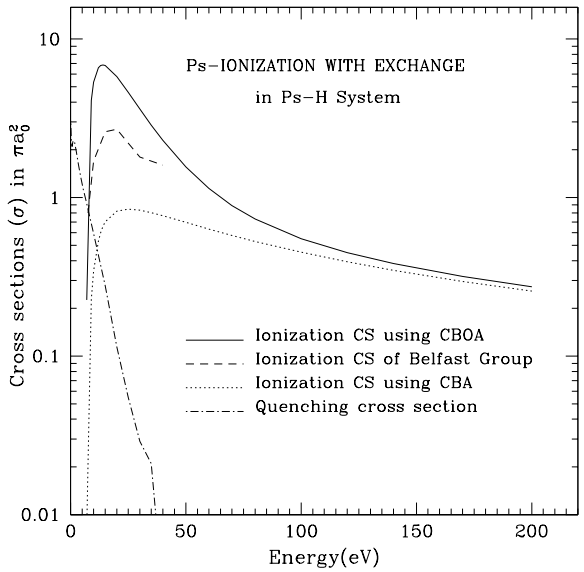

Figure 2. Comparison of Ps-ionization cross-sections with and without exchange in Ps–H scattering.

a life-time of $\sim 10^{-7}$ s and can take part in collision process. The para Ps has a life-time of $\sim 10^{-10}$ s which is a very short duration in comparison to collision time. It annihilates into two photons. The rate of annihilation of ortho Ps into three photons is $\sim 10^3$ times smaller than the rate of annihilation of para Ps into two photons. When elastic scattering, due to exchange of electrons, ortho Ps can be transformed into para Ps; the phenomenon is known as quenching. It is evident from the comparison that the quenching process is highly important at very low energies and below threshold of ionization. Above threshold, it is almost negligible with respect to ionization.

We have presented a complete treatment of exchange amplitude considering all the Coulomb interaction terms in the present CBOA scheme. The comparison of the present results with the existing CBA data [6] in figure 2 provides information that the effect of exchange is highly important at low energies and it has an appreciable effect up to a high incident energy region of more than 70 eV. These data are comparable to the results of Ps-ionization cross-sections reported by Belfast group with exchange [10] following R-matrix coupled-pseudostate formalism.

To conclude, we have successfully developed a methodology for calculating the exchange amplitude for Ps-ionization in Ps–atom scattering using a reliable Coulomb–Born–Oppenheimer approximation theory which enables us to reduce the nine-dimensional exchange amplitude to a two-dimesional integral form. It is a very useful tool for future advancement and to apply it for other ionization processes. Our ionization data are comparable with other existing theories. The importance of exchange at lower energy region is in agreement with other systems too. Theoretical data in an extended energy region using various theories and the experimental data are required for proper understanding of the physics.

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