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A simple Model for Positronium Formation in Positron – Hydrogen Atom Collisions

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Abstract. We report calculations of total positronium Ps(1s)-formation cross section for positron scattering by ground-state atomic hydrogen in the energy range of Ps-formation threshold of 6.8 eV to 120 eV. For the description of the process of electron capture to the bound state of the projectile the Oppenheimer–Brinkman–Kramers approximation has been used. The values of the total cross section obtained from this simple quantum-mechanical model are in qualitative agreement with the experimental results.

Keywords: positron, positronium formation, total cross section
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1. Introduction

Positrons, since their discovery, have been extensively used as probes in different branches of physics as reviewed in 1982 by Ghosh et al. [1] and more recently by Drachman [2]. During the past few years great progress has been achieved in the experimental and theoretical study of positron–atom collisions. When a positron collides with, for example, a hydrogen atom the following processes are possible:

Elastic scattering	$e^+ + H(1s) \rightarrow e^+ + H(1s)$,
Excitation	$e^+ + H(1s) \rightarrow e^+ + H(nlm)$,
Ionization	$e^+ + H(1s) \rightarrow e^+ + e^- + p$,
Annihilation	$e^+ + H(1s) \rightarrow p + \gamma$,
Positronium formation	$e^+ + H(1s) \rightarrow Ps(nlm) + p$.

Experimentally, positron–atom collisions are difficult to study because of the low intensity of available positrons beams. Positrons emerge usually from radioactive

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Na^{22} or Co^{58} sources with energies of a few hundred keV. To obtain a monoenergetic beam with energy of a few eV, moderation is required with consequent loss of flux. On the theoretical side the advances have been associated with the development of coupled-channel methods for positron–hydrogen atom collisions as reviewed by Walters et al. [3]. The first quantum-mechanical theory of inelastic collisions of fast charged particles with atoms has been established by Bethe [4] in 1930. This theory is based on the first Born approximation (B1), and has been applied at the first time in 1954 by Massey and Mohr [5] for positronium (Ps) formation in positron–hydrogen collision. In spite of the fact, that more sophisticated methods [6–8] give more accurate results for the total Ps-formation cross section, the Bethe theory has the advantage of following analytical expressions for the elastic scattering, excitation, ionization and the positronium-formation cross sections. The annihilation process cannot be treated in this model, because it is significant only at very low impact energies of the positron, where the Born approximation cannot be applied. In this paper we present application of first order Oppenheimer–Brinkman–Kramers approximation (OBK1), which is the simplified version of the B1 approximation, to study positronium formation in positron scattering by ground state atomic hydrogen. In Section 2 a brief description of the model of positronium formation and the method of calculation will be outlined. The details for evaluating the transition matrix, the differential and the total cross sections are considered in Section 3. The results are discussed and compared with other calculations and experimental data of Zhou et al. [9] and Weber et al. [10] in Section 4.

2. The Model of Positronium Formation

Positronium formation in positron–hydrogen collisions is a three-body charge rearrangement process in which an electron of mass m and charge q_e is transferred from a bound orbital centered on the proton to a bound orbital around the moving positron. The positronium is a very light H like atom of mass $2m$ and reduced mass $m/2$. The threshold for Ps formation is at an energy of $E_{\rm th} = 0.5R_\infty$ (R_∞ is the Rydberg constant in eV) below the ionization potential of the atom. For hydrogen this threshold is at 6.8 eV. Various theories have been applied to this problem as reviewed in a recent paper by Walters [3]. In our model the Hamilton operator for the reaction

$$\mathrm{e}^+ + \mathrm{H(1s)} \rightarrow \mathrm{Ps(1s)} + \mathrm{p} \tag{1}$$

has two equivalent forms. In the incident channel

$$H = -\frac{\hbar^2}{2m}\boldsymbol{\nabla}_{\boldsymbol{r}}^2 + h_i + V_i \equiv H_i + V_i,$$

$$h_i = -\frac{\hbar^2}{2m}\boldsymbol{\nabla}_{\boldsymbol{x}}^2 - \frac{e^2}{x}, \quad V_i = \frac{e^2}{r} - \frac{e^2}{|\boldsymbol{r}-\boldsymbol{x}|}, \tag{2}$$

here $e^2 = q_e^2/4\pi\epsilon_0$, $\boldsymbol{x}$ denotes the coordinates of the orbital electron, and $\boldsymbol{r}$ those of the incident positron, measured from the the position of the nucleus, assumed fixed. In Eq. (2) h_i is the Hamiltonian of the hydrogen atom and the positron–hydrogen interaction is described by V_i. After the positronium having been formed it is more appropriate to use the following positronium coordinates

$$\boldsymbol{s} = \boldsymbol{r} - \boldsymbol{x}, \quad \boldsymbol{R} = \frac{1}{2}(\boldsymbol{r} + \boldsymbol{x}), \tag{3}$$

where $\boldsymbol{R}$ is the center-of-mass vector of the positronium relative to the proton and $\boldsymbol{s}$ denotes the positronium internal coordinates. The splitting of the Hamiltonian (2) in the the rearranged channel is

$$\begin{aligned} H &= -\frac{\hbar^2}{4m}\boldsymbol{\nabla}^2_{\boldsymbol{R}} + h_f + V_f \equiv H_f + V_f, \\ h_f &= -\frac{\hbar^2}{m}\boldsymbol{\nabla}^2_{\boldsymbol{s}} - \frac{e^2}{s}, \qquad V_f = \frac{e^2}{\left|\boldsymbol{R} + \frac{1}{2}\boldsymbol{s}\right|} - \frac{e^2}{\left|\boldsymbol{R} - \frac{1}{2}\boldsymbol{s}\right|}, \end{aligned} \tag{4}$$

where h_f is the Hamiltonian of the positronium. The initial ϕ_i and final ϕ_f states of the colliding system in the incoming and outcoming channels can be given as eigenfunctions

$$\mathcal{H}^{\infty}_{i,f}\ \phi_{i,f} = E_{i,f}\phi_{i,f} \tag{5}$$

of the

$$\begin{aligned} \mathcal{H}^{\infty}_{i} &= \lim_{r\to\infty,\ x\,\text{finite}} H = -\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2_{\boldsymbol{r}} + h_i = H_i, \\ \mathcal{H}^{\infty}_{f} &= \lim_{R\to\infty,\ s\,\text{finite}} H = -\frac{\hbar^2}{4m}\boldsymbol{\nabla}^2_{\boldsymbol{R}} + h_f = H_f \end{aligned} \tag{6}$$

asymptotic Hamiltonians. Since, the perturbation potentials V_i and V_f are of short range, so that the relative motion will be described by simple plane waves $e^{\mathrm{i}\boldsymbol{k}\boldsymbol{r}}$ and $e^{\mathrm{i}\boldsymbol{\kappa}\boldsymbol{R}}$, respectively, in the initial and final arrangements. Taking into account, that

$$h_{i,f}\varphi_{i,f} = \epsilon_{i,f}\varphi_{i,f}, \tag{7}$$

where $\epsilon_i = -R_\infty$ and $\epsilon_f = -0.5R_\infty$ are the ground-state binding energies of the hydrogen and positronium, respectively, the wave function in the incoming channel can be written as

$$\phi_i(\boldsymbol{x}, \boldsymbol{r}) = \varphi_i(\boldsymbol{x})\exp(\mathrm{i}\boldsymbol{k}\boldsymbol{r}) = \frac{1}{\sqrt{\pi \mathrm{a}_0^3}}\exp(-x/a_0)\exp(\mathrm{i}\boldsymbol{k}\boldsymbol{r}). \tag{8}$$

Here a_0 is the Bohr radius, $\boldsymbol{k}$ is the wave number of the incident positron relative to the target nucleus. After collisions, when the positronium is at large distant from the proton, the final state of the system in the outgoing Ps(1s) channel is given by

$$\phi_f(\boldsymbol{s}, \boldsymbol{R}) = \varphi_f(\boldsymbol{s})\exp(\mathrm{i}\boldsymbol{\kappa}\boldsymbol{R}) = \frac{1}{\sqrt{\pi \mathrm{a}^3}}\exp(-s/a)\exp(\mathrm{i}\boldsymbol{\kappa}\boldsymbol{R}), \tag{9}$$

where $a = 2a_0$ and $\boldsymbol{\kappa}$ is the wave number of the center-of-mass motion of the ground state positronium with respect to the nucleus. The total energy of the process (1)

$$E_i = \frac{\hbar^2 k_i^2}{2m} + \epsilon_i = \frac{\hbar^2 k_f^2}{4m} + \epsilon_f = E_f, \tag{10}$$

where $\boldsymbol{k}_i = \boldsymbol{k}$ and $\boldsymbol{k}_f = \boldsymbol{\kappa}$. In this method, the initial and final electronic states are assumed to be undistorted atomic eigenstates φ_i and φ_f of target and projectile, respectively. Moreover, we note that the function ϕ_i is an eigenfunction of the channel Hamiltonian H_i whereas the function ϕ_f is an eigenfunction of a different channel Hamiltonian H_f. Therefore their orthogonality is not ensured. What matters is that the two states are orthogonal when the distance between projectile and target goes to infinity when we can define the initial and final states in the collision. This is ensured by the exponential decay of bound wave functions. This asymptotic orthogonality is necessary for the following formulation of the theory. The differential cross section for the capture and scattering into solid angle $\mathrm{d}\Omega_f$ of $\boldsymbol{\kappa}$ for process (1) is

$$\frac{\mathrm{d}\sigma_{fi}(E_i)}{\mathrm{d}\Omega_f} = \frac{m^2}{2\pi^2\hbar^4}\frac{\kappa}{k}|T_{fi}(E_i)|^2, \tag{11}$$

where the transition matrix T is determined by the interaction of the projectile and the target. $\Omega_f \equiv (\Theta_f, \Phi_f)$ are the polar angles of $\boldsymbol{\kappa}$ with respect to $\boldsymbol{k}$ as axis. The total cross section can be obtained integrating Eq. (11) over $\mathrm{d}\Omega_f$:

$$\sigma_{fi}(E_i) = \frac{m^2}{2\pi^2\hbar^4}\frac{\kappa}{k}\int |T_{fi}(E_i)|^2 \mathrm{d}\Omega_f. \tag{12}$$

For example, in the first Born approximation the transition matrix can be written as

$$T_{fi}^{\mathrm{B1}}(E_i) = \langle \phi_i(E_i)\,|V_i|\,\phi_f(E_f)\rangle\,. \tag{13}$$

3. Calculation of the Cross Sections

The transition matrix can be calculated in the B1 approximation using Eq. (13) with the expressions (8) and (9) for the initial and the final states, and Eq. (2) for the interaction between the incident positron and the hydrogen atom. Massey and Mohr [5] determined the total cross section in this way. The initial and final states are not orthogonal, thus the contribution of the positron–proton interaction to the transition matrix does not vanish automatically. This difficulty does not occur in the B1 approximation for excitation or ionization, because in that case the initial and final states are orthogonal. It is interesting to note that this inconsistency does not happen in the boundary corrected Born approximation: it was shown that if Coulomb boundary corrected states are used this interaction causes only a phase

factor in the transition amplitude, which does not contribute to the total cross section [11]. The result of the B1 approximation is identical with the first Coulomb boundary corrected Born approximation for symmetric charge transfer collision, such as (1). In the present treatment we will use the plane-wave OBK1 approximation which is obtained by neglecting the residual positron–proton interaction term in the perturbation potential V_i. The OBK1 approximation provides a poorer description of the experimental data than the B1 approximation. This fact demonstrate the importance of Coulomb boundary corrected states. Using this simplified model the integrations can be performed analytically as follows. The expressions of the transition matrix (13)

$$T_{fi}^{\mathrm{OBK1}} = \frac{e^2}{\pi\sqrt{8}a_0^3}\int\int \exp\Big(-\mathrm{i}\boldsymbol{\kappa R}\Big)\exp\Big(-\frac{s}{2a_0}\Big)\exp\Big(\mathrm{i}\boldsymbol{kr}\Big)\times \\ \times\exp\Big(-\frac{x}{a_0}\Big)\Big(-\frac{1}{s}\Big)\mathrm{d}^3\boldsymbol{r}\mathrm{d}^3\boldsymbol{x} \tag{14}$$

can be written in the form

$$T_{fi}^{\mathrm{OBK1}} = -\frac{e^2}{\pi\sqrt{8}a_0^3}\int \exp\Big(-\mathrm{i}\boldsymbol{\lambda s}\Big)\frac{1}{s}\exp\Big(-\frac{s}{2a_0}\Big)\mathrm{d}^3\boldsymbol{s}\times \\ \times\int\exp\Big(-\mathrm{i}\boldsymbol{qx}\Big)\exp\Big(-\frac{x}{a_0}\Big)\mathrm{d}^3\boldsymbol{x}, \tag{15}$$

where the momentum transfer vector $\boldsymbol{q} = \boldsymbol{\kappa} - \boldsymbol{k}$ and the wave vector $\boldsymbol{\lambda} = \boldsymbol{\kappa}/2 - \boldsymbol{k}$ have been introduced. The integrations in Eq. (15) can be performed easily, and from Eq. (11) we obtain the differential cross section

$$\frac{\mathrm{d}\sigma_{\mathrm{Ps}}}{\mathrm{d}\Omega} = \frac{2^8a_0^2}{\pi^2}\frac{\kappa}{k}\frac{1}{\left(1+q^2a_0^2\right)^6}. \tag{16}$$

It seems from Eq. (16), that a peak appears in the differential cross section based on T_{fi}^{OBK1} at forward scattering angle $\Theta = 0^\circ$. The total cross section given by Eq. (12) can be calculated in the following way. Taking into account that $\mathrm{d}\Omega = 2\pi\sin\Theta\mathrm{d}\Theta$, where Θ is the scattering angle, and for given positron energy (i.e. for given k)

$$q^2 = \left(\boldsymbol{\kappa} - \boldsymbol{k}\right)^2 = \kappa^2 + k^2 - 2\kappa k\cos\Theta, \tag{17}$$

implies $q\mathrm{d}q = k\kappa\sin\Theta\mathrm{d}\Theta$, we obtain

$$\mathrm{d}\Omega = \frac{2\pi}{k\kappa}\mathrm{d}q, \tag{18}$$

and

$$\sigma_{\mathrm{Ps}} = \int\limits_{4\pi}\frac{\mathrm{d}\sigma_{\mathrm{Ps}}}{\mathrm{d}\Omega}\mathrm{d}\Omega = \int\limits_{|\kappa-k|}^{\kappa+k}\frac{\mathrm{d}\sigma_{\mathrm{Ps}}}{\mathrm{d}\Omega}\frac{2\pi q}{k\kappa}\mathrm{d}q. \tag{19}$$

Using Eq. (16) the result of the integration for the total cross section of the Ps(1s) formation is:

$$\sigma_{\rm Ps} = \frac{2^{10}a_0^2}{5\pi}\frac{\xi}{\zeta}\frac{1}{\Big[\big((\xi-\zeta)^2+1\big)\big((\xi+\zeta)^2+1\big)\Big]^5}\Big[5\xi^8+20\xi^6(3\zeta^2+1)+$$

$$+2\xi^4(63\zeta^4+70\zeta^2+15)+20\xi^2(3\zeta^2+1)(\zeta^2+1)^2+5(\zeta^2+1)^4\Big], \qquad (20)$$

where

$$\xi = \kappa a_0, \qquad \zeta = k a_0. \qquad (21)$$

Formula (20) can be evaluated approximately for high projectile energy E as well as for the positronium-formation threshold $E_{\rm th}$ and we obtain:

$$\sigma_{\rm Ps}(E\to\infty) \approx \frac{1189\cdot 2^{21/2}}{5\pi a_0^{10}}\frac{1}{k^{12}} \propto v_{\rm p}^{-12}, \qquad \sigma_{\rm Ps}(E\to E_{\rm th}) = 0. \qquad (22)$$

In the B1 approximation, as already pointed out for large projectile velocities $v_{\rm p}$, the charge changing cross sections decreases asymptotically as $v_{\rm p}^{-12}$ or E^{-6}, see Shakeshaft [12]. This dramatic dependence on velocity occurs because the overlap in momentum space between the initial and final electron wave function diminishes very fast as the relative velocity increases. It follows from relation (22) that the applied OBK1 approximation gives back the $v_{\rm p}^{-12}$ asymptotic behavior of the total cross section. Our calculation predict the cross section maximum $\sigma_{\rm Ps} = 5.359 \cdot 10^{-16}$ cm^2 at $E = 10.184$ eV. These values can be calculated only numerically from Eq. (20).

4. Results and Discussion

In Fig. 1 the calculated total Ps-formation cross section is compared with the experimental results of Zhou et al. [9] along with prior measurements of Weber et al. [10] and several theoretical values [5–8, 13] as a function of the positron energy. The measured $\sigma_{\rm Ps}$'s and most of the calculated values follow a rather smooth, bell-like, structureless curve. Both theory and experiment exhibit a broadly similar energy dependence, i.e. $\sigma_{\rm Ps}$ increases rapidly from the Ps-formation threshold energy before peaking and falling as a function of $E^{-\gamma}$. It is obvious that the total cross section for Ps formation is dominated by capture into 1s state. Because of the probability of capture process is the largest when the projectile velocity $v_{\rm p}$ is near to orbital velocity of ground state electron $v_{\rm e}$ in the hydrogen atom, thus the peak in the total cross section appears approximately at $v_{\rm p} \approx v_{\rm e}$ or $E \approx R_\infty$. The B1 approximation calculations of Massey and Mohr [5] and the Fock–Tani calculations of Straton [13] predict cross sections which peak at an energy 3 eV lower than the measurements

and with magnitudes greater by about 35% and 50%, respectively. The accurate Kohn variational calculations of Brown and Humberston [6] are restricted to low incident energies, but Weber et al. [10] note that the extrapolation of these predictions to higher energies does not appear inconsistent with the size and energy location of observed maximum in $\sigma_{\rm Ps}$. The $\sigma_{\rm Ps}$ values measured by Zhou et al. [9] are reasonably consistent with the prior experimental result [10] and are in very good agreement with the coupled 33-state calculation of Kernoghan et al. [7] and with the 28-state close-coupling approximation by Mitroy [8] (except at energies below the Ps-formation threshold).

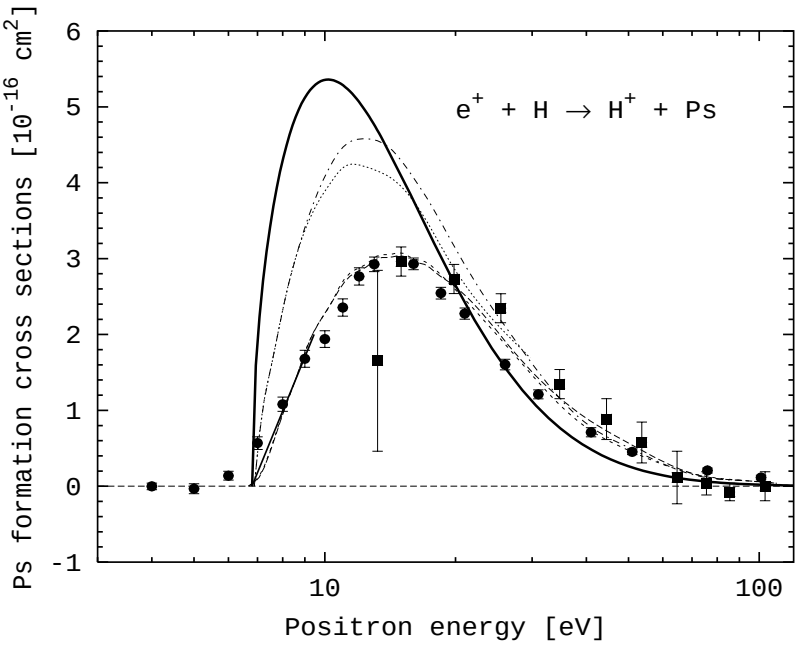

Fig. 1. Positronium-formation cross sections for e^+–H scattering. *Theory*: thick solid line, present work; dotted curve, Massey and Mohr [5]; thin solid line, Brown and Humberston [6]; short broken curve, Kernoghan et al. [7]; long broken curve, Mitroy [8]; full curve with dots, Straton [13]. *Experiment*: circles, Zhou et al. [9]; squares, Weber et al. [10].

Compared to the accurate calculations of Kernoghan et al. [7] and Mitroy [8], our calculated cross sections increase more rapidly close to the positronium-formation threshold. The OBK1 model predicts 70% larger value for the maximum of the cross section and 4 eV lower projectile energy for the position of the maximum.

This discrepancy is due to the fact such low energy processes cannot be treated satisfactory by first-order perturbation theory. Furthermore, the OBK1 approximation has a serious shortcoming. The wave functions in entrance and exit channels do not satisfy the correct asymptotic Coulomb boundary conditions. Indeed, the long-range nature of the Coulomb interaction does not allow one to use unperturbed atomic wave functions even at finite separations. However, the obtained cross sections are close to the measured data of Zhou et al. [9] in the intermediate collision energy range (between 20 eV and 30 eV).

For proton–hydrogen collision it is shown that Thomas-type double scattering mechanism is the dominant process at high energies in the case of electron capture [12]. The second order Born approximation which was applied to describe this process gives a v_{p}^{-11} asymptotic velocity dependence of the double scattering cross section σ_{DS}. In contrast, the OBK1 cross section σ_{OBK1} varies as v_{p}^{-12}. Form the different velocity dependence it comes that σ_{DS} dominates over σ_{OBK1} above a certain projectile energy. In Fig. 1 a similar effect can be observed for positron–hydrogen collision. The values of the σ_{Ps} cross section are less than the cross sections calculated within the higher order approximations and the measured data of Zhou et al. [9] at high impact energies. Although not accurate, our elementary treatment gives a qualitative, but at the same time analytical description of the electron rearrangement process in the positron–hydrogen collision, resulting Ps formation.

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