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ORIGINAL PAPER

Asymptotic cross section and scaling law: positronium formation in Rydberg states in positron–hydrogen collisions

P Rej[1] **and A Ghoshal**[1,2]*

[1]Department of Mathematics, Burdwan University, Golapbag, Burdwan, West Bengal 713 104, India

[2]Department of Mathematics, Kazi Nazrul University, Nazrul Road, Asansol, West Bengal 713 340, India

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Abstract: Positronium formation in Rydberg states from the ground state of the hydrogen atom by positron impact has been studied within the framework of a distorted wave theory which includes static dipole polarization potential. The distorted wave scattering amplitude has been obtained in a closed form. A detailed investigation has been made on the differential and total cross sections in the energy range 25–300 eV of incident positron. It has been found that asymptotic cross sections for the positronium formation into different angular momentum states obey a simple law.

Keywords: Scaling law; Positronium; Rydberg state; Distorted wave theory

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1. Introduction

Formation of positronium (Ps) in highly excited states during collisions is of fundamental interest because of its important applications in diverse fields of physics, such as plasma physics [1–3], astrophysics [4–9], material science [10–14], chemical physics [14, 15], high energy physics [16, 17]. Positronium atoms are of particularly suitable to verify the prediction of quantum electrodynamics (QED). The annihilation of positronium has been a bench mark of bound state QED (BSQED) for many years. Positron annihilation are utilized most exclusively in the material science and chemical physics. Positronium has been known for a long time to exist in excited states and many experimental attempts have been made to study the properties of excited states of Ps with principle quantum number $n > 1$ [18–21]. Collision cross section data for various excited states are frequently required for plasma diagnostics and astrophysics. Moderately high excited states, such as $8 \le n \le 25$ are of practical importance from the point of view of laboratory production of hot plasmas [3]. Since atoms in ground state and low-lying excited states, such as $1 \le n \le 7$, are not significantly ionized, moderately excited atoms ($8 \le n \le 25$) being easily ionized are suitable for this purpose. Annihilation radiation observed in the solar flare, in the stellar atmospheres and in the interstellar space shows the formation of positronium atoms in different excited states in astrophysical environments [8, 9]. Furthermore, Rydberg states of positronium atom are used to produce antihydrogen in antimatter experiments [16, 17].

Positronium formation in positron–hydrogen collisions has been studied extensively with various degree of sophistication during the last five decades, both experimentally and theoretically [18–46] (and further references therein). But those studies are mostly concerned with the positronium formation in the ground state. The number of studies on positronium formation in excited states is very few; in particular positronium formation in *nlm* state is rare [42] and that study used a first-order calculation. It seems that carrying out sophisticated quantum mechanical calculations involving highly excited states becomes very complicated because of the presence of a large number of oscillations in the final bound state wavefunction. Recently, Ghoshal and Mandal [45] have investigated Ps formation in $n's$ state in $e^+ + \mathrm{H(ns)}$ collisions. But, calculation involving arbitrary *nlm* states is rather difficult than arbitrary *ns* states, because of the appearance of angular part in the former.

In this paper we focus our attention to investigate the reaction process:

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*Corresponding author, E-mail: arijit98@yahoo.com

$$e^+ + H(1s) \mapsto Ps(nlm) + p, \tag{1}$$

for arbitrary n, l and m. Our endeavour is to make a comprehensive study on the differential cross section and the total cross section.

We have extended the second order distorted wave theory put forward by Ghoshal and Mandal [46] in the momentum space to study the dynamics of the rearrangement process (Eq. (1)). In this theory the distortion potential in a particular channel has been approximated by the average (over internal motions) of perturbation of that particular channel over the bound states [28, 47]. This approximation works well for intermediate and high energies of incident positron. In the present work, we have modified the distorted wave formalism to take into account the effect of dipole polarization of the target atom into the distorted wave theory.

2. Theory and calculations

To describe the process given in Eq. (1), we use the center-of-mass coordinate system (as shown in Fig.1) in which the electron 3, initially bound to the target proton 2 of mass m_p, is finally captured by the incident positron 1. In this coordinate system the non-relativistic Hamiltonian (in a.u.) of the positron–hydrogen system, is given by

$$H = -\frac{1}{2m_i}\nabla^2_{R_1} - \frac{1}{2m_H}\nabla^2_{r_2} + \frac{1}{R_{12}} - \frac{1}{r_1} - \frac{1}{r_2}, \tag{2}$$

where $m_i = (m_p+1)/(m_p+2)$ and $m_H = m_p/(m_p+1)$. The Hamiltonian H can be written in terms of the channel Hamiltonians as

$$H = H_i + V_i = H_f + V_f$$

such that

$$H_i\Phi_i = E_i\Phi_i, \quad H_f\Phi_f = E_f\Phi_f,$$

where Φ_i, Φ_f are unperturbed initial and final states corresponding to the Hamiltonians

$$H_i = -\frac{1}{2m_i}\nabla^2_{R_1} - \frac{1}{2m_H}\nabla^2_{r_2} - \frac{1}{r_2}$$

and

$$H_f = -\frac{1}{2m_f}\nabla^2_{R_2} - \frac{1}{2m_{Ps}}\nabla^2_{r_1} - \frac{1}{r_1}$$

in the incident and final channel, respectively, with $m_f = 2m_p/(m_p+2), m_{Ps} = 1/2$ and the residual interactions $V_i = (1/R_{12} - 1/r_1)$ and $V_f = (1/R_{12} - 1/r_2)$ having energies E_i and E_f,

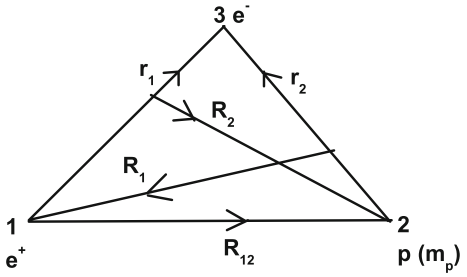

Fig. 1 Coordinate system used to describe positron–hydrogen system

$$E_\alpha = \frac{k_\alpha^2}{2m_\alpha} + \epsilon_\alpha \quad (\alpha = i,f).$$

Here (ϵ_i, ϵ_f), (k_i, k_f) are respectively, the eigen energies of bound states and positron momenta in the incident and final channels, whereas (m_i, m_f) are the reduced masses for the center of mass motion in the scattering system.

In the present investigation we use the partial wave distorted wave amplitude as obtained by Ghoshal and Mandal [46]:

$$A^{(L)}_{fi}(k_f, k_i) = g^{(L)}_B(k_f, k_i) + D^{(L)}_{fi}(k_f, k_i) \tag{3}$$

where $g^{(L)}_B(k_f, k_i)$ and $D^{(L)}_{fi}(k_f, k_i)$ are obtained as:

$$g^{(L)}_B(k_f, k_i) = \sqrt{k_i k_f}/2 \int_{-1}^{+1} [g_B(\vec{k}_f, \vec{k}_i)] P_L(\cos\theta) d(\cos\theta),$$

and

$$D^{(L)}_{fi}(k_f, k_i) = \sqrt{k_i k_f}/2 \int_{-1}^{+1} [D(\vec{k}_f, \vec{k}_i)] P_L(\cos\theta) d(\cos\theta),$$

in which the two-body amplitudes are given by

$$g_B(\vec{k}_f, \vec{k}_i) = \left(-\frac{m_f}{2\pi}\right)\langle\Phi_f|V_f|\Phi_i\rangle;$$
$$f_{f\gamma}(\vec{k}_f, \vec{k}_i) = \left(-\frac{m_\gamma}{2\pi}\right)\left\langle\Phi_f|V_f|\Phi''_\gamma\right\rangle;$$
$$\bar{f}_{\gamma i}(\vec{k}_f, \vec{k}_i) = \left(-\frac{m_i}{2\pi}\right)\left\langle\Phi''_\gamma|U_i|\Phi_i\right\rangle;$$

with the double scattering matrix elements

$$D_{fi}(\vec{k}_f, \vec{k}_i) = \frac{1}{(2\pi)^3}\sum_\gamma\left(-\frac{2\pi}{m_\gamma}\right)\int\frac{d\vec{k''}}{E - E''_\gamma + i\epsilon} f_{f\gamma}(\vec{k}_f, \vec{k''})\bar{f}_{\gamma i}(\vec{k''}, \vec{k}_i). \tag{4}$$

Here γ denotes the intermediate states of hydrogen atom. The distorted-wave amplitude $A^{(L)}_{fi}(k_f, k_i)$ is a function of the scattering energies for any partial wave L. In calculating $g^{(L)}_B$ and $D^{(L)}_{fi}$ we take ϕ_f to be zero, where ϕ_f is the azimuthal angle of $\vec{k}_f$ about $\vec{k}_i$ as $z-$ axis. In the present context this is no restriction. It corresponds to taking $\phi_p = 0$ in (Eq. (17)), where ϕ_p denotes the azimuthal angle of $\vec{p}$.

As proposed earlier, we choose the potentials U_i and U_f as:

$$U_i = \langle \phi_i | V_i | \phi_i \rangle \quad \text{and} \quad U_f = \langle \eta_f | V_f | \eta_f \rangle,$$

where ϕ_i, η_f are the bound state wave functions in the initial and final channel respectively and the integration is performed over the bound state coordinates. For $e^+ +$ H(1s)↦Ps(nlm) + p we have

$$U_i = \langle \phi_i | V_i | \phi_i \rangle = \langle \phi_{1s} | V_i | \phi_{1s} \rangle$$
$$U_f = \langle \eta_f | V_f | \eta_f \rangle = \langle \eta_{nlm} | V_f | \eta_{nlm} \rangle = 0,$$

where $V_i = (1/R_{12} - 1/r_1)$, $V_f = (1/R_{12} - 1/r_2)$. The unperturbed states in the incident and the final channel are given by

$$\Phi_i(\vec{r}_1, \vec{r}_2) = e^{i\vec{k}_i \cdot \vec{R}_1} \phi_i(\vec{r}_2) \quad \text{and} \quad \Phi_f(\vec{r}_1, \vec{r}_2) = e^{-i\vec{k}_f \cdot \vec{R}_2} \eta_f(\vec{r}_1).$$

$\phi_i(\vec{r}_2), \eta_f(\vec{r}_1)$ are the initial and final wave functions of H-atom and Ps-atom respectively, where i corresponds to $1s$, and f corresponds to nlm, $n = 2, 3, \ldots; l = 0, 1, 2, \ldots, n-1$; $m = -l, \ldots, +l$. It has been possible to obtain all two-body amplitudes in closed form and thus the distorted wave amplitude (Eq. (3)). Evaluation of the $1s \rightarrow nlm$ capture amplitude $g_B(\vec{k}_f, \vec{k}_i)$ is shown in the Appendix.

Here we have included only $\gamma = 1s$ intermediate state of hydrogen to evaluate the double scattering matrix elements (Eq. (4)). This makes a truncation of the contribution from transition to an intermediate excited state followed by super-elastic scattering from that state. Such a truncation does not affect the results too much at intermediate and high energies, because it has been observed from vast amount of collision calculations that the contribution from

Table 1 Partial wave contributions to the positronium formation cross sections (in units of πa_0^2) for the processes of $e^+ +$ H(1s) → Ps(nlm) + p

l	50 eV		100 eV		150 eV		200 eV		300 eV	
	(A)	(B)	(A)	(B)	(A)	(B)	(A)	(B)	(A)	(B)
0	0.3087[−2]	0.6591[−2]	0.2094[−3]	0.2322[−3]	0.4254[−4]	0.3110[−4]	0.1404[−4]	0.7402[−5]	0.2791[−5]	0.9395[−6]
1	0.1808[−2]	0.6817[−2]	0.8660[−4]	0.2445[−3]	0.1775[−4]	0.2539[−4]	0.5347[−5]	0.4680[−5]	0.8206[−6]	0.3917[−6]
2	0.1044[−1]	0.1813[−2]	0.6595[−3]	0.1170[−3]	0.1116[−3]	0.1580[−4]	0.2960[−4]	0.3358[−5]	0.4150[−5]	0.3238[−6]
3	0.1435[−1]	0.2010[−2]	0.1124[−2]	0.1331[−3]	0.1936[−3]	0.1834[−4]	0.5081[−4]	0.3951[−5]	0.6950[−5]	0.3928[−6]
4	0.1300[−1]	0.2713[−2]	0.1231[−2]	0.1775[−3]	0.2212[−3]	0.2398[−4]	0.5881[−4]	0.5087[−5]	0.8078[−5]	0.4959[−6]
5	0.9556[−2]	0.2829[−2]	0.1085[−2]	0.1982[−3]	0.2046[−3]	0.2698[−4]	0.5548[−4]	0.5716[−5]	0.7733[−5]	0.5537[−6]
6	0.6160[−2]	0.2402[−2]	0.8380[−3]	0.1871[−3]	0.1664[−3]	0.2609[−4]	0.4614[−4]	0.5575[−5]	0.6558[−5]	0.5428[−6]
7	0.3625[−2]	0.1770[−2]	0.5916[−3]	0.1566[−3]	0.1239[−3]	0.2257[−4]	0.3521[−4]	0.4890[−5]	0.5115[−5]	0.4815[−6]
8	0.1993[−2]	0.1185[−2]	0.3910[−3]	0.1201[−3]	0.8650[−4]	0.1797[−4]	0.2522[−4]	0.3961[−5]	0.3752[−5]	0.3958[−6]
9	0.1040[−2]	0.7358[−3]	0.2457[−3]	0.8604[−4]	0.5749[−4]	0.1342[−4]	0.1721[−4]	0.3015[−5]	0.2625[−5]	0.3066[−6]
10	0.5201[−3]	0.4340[−3]	0.1483[−3]	0.5857[−4]	0.3673[−4]	0.9542[−5]	0.1130[−4]	0.2187[−5]	0.1768[−5]	0.2266[−6]
11	0.2512[−3]	0.2447[−3]	0.8658[−4]	0.3821[−4]	0.2272[−4]	0.6510[−5]	0.7187[−5]	0.1524[−5]	0.1155[−5]	0.1612[−6]
12	0.1179[−3]	0.1343[−3]	0.4918[−4]	0.2412[−4]	0.1369[−4]	0.4299[−5]	0.4452[−5]	0.1029[−5]	0.7351[−6]	0.1110[−6]
13	0.5391[−4]	0.7168[−4]	0.2729[−4]	0.1479[−4]	0.8060[−5]	0.2759[−5]	0.2697[−5]	0.6750[−6]	0.4577[−6]	0.7443[−7]
σ	0.6601[−1]	0.2975[−1]	0.6774[−2]	0.1788[−2]	0.1307[−2]	0.2448[−3]	0.3635[−3]	0.5305[−4]	0.5269[−4]	0.5397[−5]
a:	0.6880[−1]	0.2530[−1]	0.6080[−2]	0.1170[−2]	0.1070[−2]	0.1430[−3]	0.2790[−3]	0.2870[−4]	0.3750[−4]	0.2630[−5]
b:	0.6440[−1]	0.2925[−1]	0.6870[−2]	0.1860[−2]			0.3600[−3]	0.5000[−4]		
c:	0.7076[−1]	0.1649[−1]	0.7610[−2]	0.1340[−2]	0.1510[−2]	0.2100[−3]	0.4300[−3]	0.5000[−4]	0.7000[−4]	0.1000[−4]
d:	0.5380[−1]	0.2610[−1]	0.5700[−2]	0.1900[−2]						
e:	0.7130[−1]	0.2760[−1]								
f:			0.8600[−2]	0.8800[−3]			0.5200[−3]	0.2800[−4]		
g:	0.4140[−1]	0.1660[−1]	0.5100[−2]	0.3000[−2]						
h:	0.6860[−1]		0.7270[−2]				0.3880[−3]			

Column (A) and Column (B) respectively stand for Ps(2s) and Ps(2p) formations. σ denotes the corresponding total excitation cross section obtained by summing up all significant partial wave contributions. The notation x[−y] stands for x $\times 10^{-y}$

a: The Glauber eikonal approximation of Tripathi et al. [26], b: analytical results of Sil et al. [29], c: distorted-wave Born approximation of Nahar [30], d: 33-state approximation of Kernoghan et al. [31] (data taken from graph within 5 % accuracy), e: 18-state approximation of Kernoghan et al. [32] (data taken from graph within 5 % accuracy), f: boundary-corrected continuum intermediate state (BCCIS) approximation Mandal et al. [38], g: convergent close-coupling approach of Kadyrov and Bray [40] (data taken from graph within 5 % accuracy), h: distorted wave approximation results of Nayek and Ghoshal [44]

Table 2 Partial wave contributions to the positronium formation cross sections (in units of πa_0^2) for the reaction $e^+ + H(1s) \rightarrow Ps(nlm) + p$ at 100 eV positron energy

l	Capture process						
	Ps(3s)	Ps(3p)	Ps(3d)	Ps(4p)	Ps(4d)	Ps(5p)	Ps(5d)
0	0.6390[−4]	0.8400[−4]	0.2021[−5]	0.3778[−4]	0.1351[−5]	0.1991[−4]	0.8367[−6]
1	0.2609[−4]	0.8829[−4]	0.3855[−5]	0.3968[−4]	0.2313[−5]	0.2090[−4]	0.1358[−5]
2	0.2006[−3]	0.4114[−4]	0.3985[−5]	0.1832[−4]	0.2393[−5]	0.9610[−5]	0.1405[−5]
3	0.3432[−3]	0.4663[−4]	0.2609[−5]	0.2073[−4]	0.1562[−5]	0.1086[−4]	0.9158[−6]
4	0.3769[−3]	0.6262[−4]	0.2092[−5]	0.2791[−4]	0.1249[−5]	0.1464[−4]	0.7316[−6]
5	0.3329[−3]	0.7033[−4]	0.1955[−5]	0.3140[−4]	0.1167[−5]	0.1649[−4]	0.6834[−6]
6	0.2577[−3]	0.6663[−4]	0.1895[−5]	0.2979[−4]	0.1132[−5]	0.1565[−4]	0.6634[−6]
7	0.1823[−3]	0.5589[−4]	0.1737[−5]	0.2501[−4]	0.1039[−5]	0.1315[−4]	0.6092[−6]
8	0.1207[−3]	0.4292[−4]	0.1482[−5]	0.1922[−4]	0.8881[−6]	0.1011[−4]	0.5208[−6]
9	0.7601[−4]	0.3080[−4]	0.1184[−5]	0.1380[−4]	0.7098[−6]	0.7255[−5]	0.4164[−6]
10	0.4596[−4]	0.2099[−4]	0.8921[−6]	0.9404[−5]	0.5351[−6]	0.4946[−5]	0.3140[−6]
11	0.2688[−4]	0.1370[−4]	0.6415[−6]	0.6140[−5]	0.3849[−6]	0.3230[−5]	0.2259[−6]
12	0.1530[−4]	0.8652[−5]	0.4429[−6]	0.3879[−5]	0.2658[−6]	0.2041[−5]	0.1560[−6]
13	0.8505[−5]	0.5307[−5]	0.2964[−6]	0.2380[−5]	0.1779[−6]	0.1252[−5]	0.1044[−6]
σ	0.2077[−2]	0.6379[−3]	0.2509[−4]	0.2854[−3]	0.1517[−4]	0.1500[−3]	0.8940[−5]

σ denotes the corresponding total cross section obtained by summing up all significant partial wave contributions. The notation x[−y] stands for x $\times 10^{-y}$

the ground state (1*s*) is most essential for the calculation of the scattering amplitude at intermediate and high energies. Thus, inclusion of only one intermediate state reduces the complexity of the problem without affecting the accuracy of the results much. However, effects of higher intermediate states can be compensated by taking into account the effect of the dipole polarization potential explicitly, which we do in the present work. It is well known that the hydrogen atom gets distorted by the slowly moving positron and the dominant long-range interaction is the polarization interaction. In the present work, we have incorporated the effect of the distortion of the target atom by means of the following polarization potential [48]:

$$V_{\text{pol}}(r) = -\frac{\alpha r^2}{2(r^2+d^2)^3}\,(\text{in a.u.}), \qquad (5)$$

where $\alpha = 4.5$ (a.u.) is the static dipole polarizability of the hydrogen atom and d is a variable parameter. The polarization potential (Eq. (5)) shows a minima at $r = d/\sqrt{2}$, and is, therefore, most attractive there. The parameter d is, then, approximately of the order of the size of the atom [48]. Inclusion of the polarization potential leads to a modification of two-body amplitudes, $f(\vec{k}_f, \vec{k}_i)$, in the elastic channel by $f(\vec{k}_f, \vec{k}_i) + f_{\text{pol}}(\vec{k}_f, \vec{k}_i)$, where $f_{\text{pol}}(\vec{k}_f, \vec{k}_i)$ is the amplitude due to the polarization potential (Eq. (5)). In other words, the elastic two-body amplitude is replaced by its polarized-Born counterpart. So it is expected that the inclusion of the effect of the dipole polarization potential explicitly will extend the applicability of the distorted wave theory towards further low energies, as well as to improve the accuracy of the results over previously reported results.

3. Results and discussion

In Table 1 we present the partial wave contributions to the Ps(2s) and Ps(2p) formation cross sections for different incident positron energies. This table also includes the results obtained by using some other methods, such as the Glauber eikonal approximation [26], analytical results [29], distorted wave Born approximation [30], 33-state approximation [31], 18-state approximation [32], boundary-corrected continuum intermediate state(BCCIS) approximation [38], convergent close-coupling approach [40] and distorted wave approximation results [44] . From this table we see that our distorted wave results are fairly accurate. Partial wave contributions to the positronium formation in various states are shown in Table 2 for 100 eV of incident positron energy. It is worthy to be mentioned here that for particular values of *n* and *l* we sum the contributions of all *m* degenerate states.

We present the differential cross sections for the positronium formation in some excited states in Fig. 2.

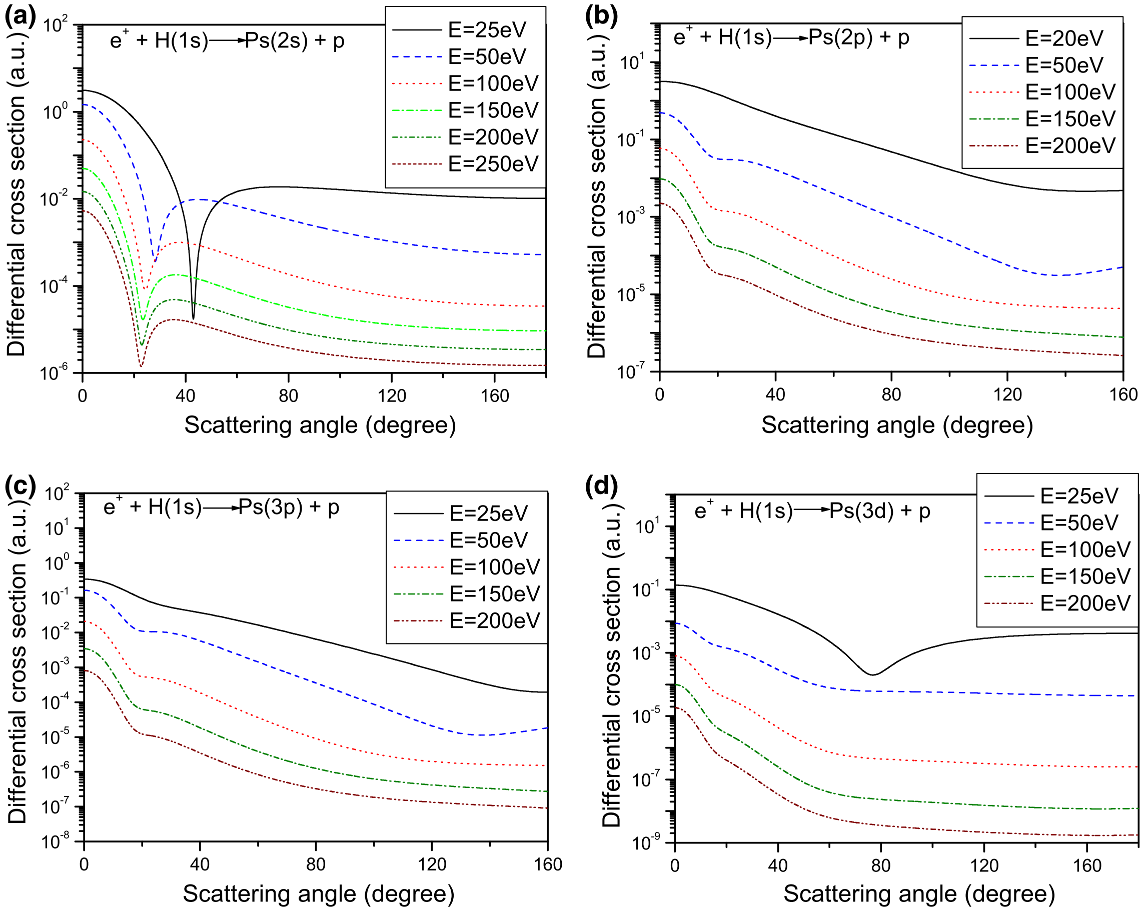

Fig. 2 Differential cross section (in a.u.) as a function of scattering angle (in degree) for positronium formation in (**a**) 2s state, (**b**) 2p state, (**c**) 3p state and (**d**) 3d state

From this figure we note that that the differential cross section for Ps(2s) formation exhibits a zero. With increasing incident energy the angular position of the zero slowly moves towards forward direction. The origin of this zero is due to the mutual cancelation of the contributions of the attractive and repulsive part of the interaction potential (i.e. due to the destructive interference between the two). This feature is common for the positronium formation in *s* states as can be seen from the surface plots in Fig. 3. While for the 2*p* state the curve falls almost monotonically as the angle increases without showing any structure, because for 2*p* state, as shown in Fig. 2, the sum of the contributions of all *m* degenerate states produces a swirl instead of a zero, so the 2*p* state does not exhibit such a minimum. This feature is also true for $l > 1$ states. Total cross sections for the positronium formation in various excited states at various incident energies are shown in Table 3 and Fig. 4. From Table 3 we note that cross section for the Ps formation in 4s state is greater than that of the 3d state. Similarly, cross section for the 5s state is greater than that of the 4f state, and so on.

3.1. Scaling law

It is observed that the Ps formation cross sections for different angular momentum states are scaled according to the law:

$$\sigma_{\mathrm{Ps(nl)}} = \frac{1}{n^3}\prod_{i=0}^{l}\left(1-\frac{i^2}{n^2}\right)\left(n_0^3\sigma_{\mathrm{Ps(n_0l)}}\right)_{n_0\to\infty}. \qquad (6)$$

The origin of such type of scaling law is due to the fact that $[f_{fi}(\vec{k}_f,\vec{k}_i)/(n^{-3}\prod_{i=0}^{l}(1-i^2/n^2))^{1/2}]$ remains more or less unchanged at moderate or high energies, the asymptotic cross section data can be used to obtain a reasonable estimate of the Ps formation cross sections for excited states with increase of the principal quantum number *n*. The values of the cross section obtained by using distorted-wave approximation and the scaling law (Eq. (6)) are shown in Table 4 at various incident positron energies ranging from 50 to 300 eV. From this table we notice that the results obtained by using scaling law (Eq. (6)) are in good accord with the results obtained by using distorted wave approximation. For higher values of *n* and *E* the

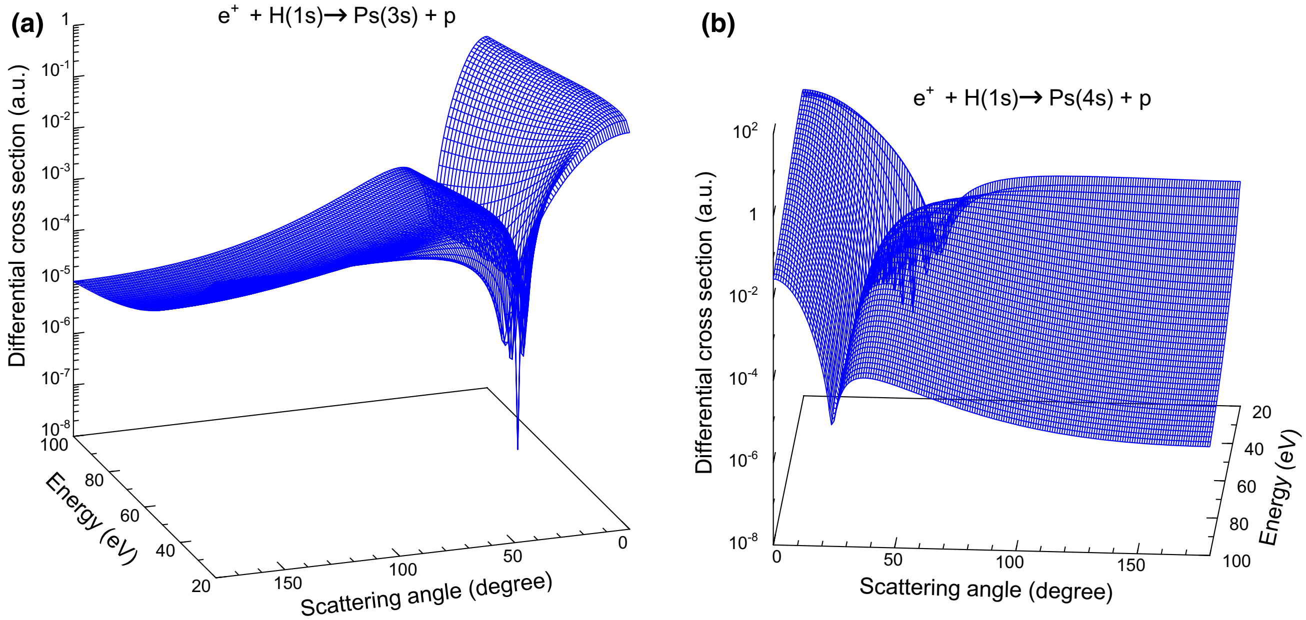

Fig. 3 Differential cross section (in a.u.) as a function of incident energy (in eV) and scattering angle (in degree) for (**a**) $e^+ + H(1s) \rightarrow Ps(3s) + p$ and (**b**) $e^+ + H(1s) \rightarrow Ps(4s) + p$

Table 3 Ps(nlm) formation cross section σ (in units of πa_0^2)

Ps state	E (in eV)						
	50	75	100	150	200	250	300
Ps(2s)	0.6601[−1]	0.1907[−1]	0.6774[−2]	0.1307[−2]	0.3635[−3]	0.1277[−3]	0.5269[−4]
(A):	0.6875[−1]		0.7291[−2]		0.3931[−3]		0.5638[−4]
Ps(2p)	0.2975[−1]	0.6350[−2]	0.1788[−2]	0.2448[−3]	0.5305[−4]	0.1534[−4]	0.5397[−5]
Ps(3s)	0.1990[−1]	0.5839[−2]	0.2077[−2]	0.3992[−3]	0.1106[−3]	0.3870[−4]	0.1593[−4]
(A):	0.2043[−1]		0.2177[−2]		0.1192[−3]		0.1811[−3]
Ps(3p)	0.1028[−1]	0.2252[−2]	0.6379[−3]	0.8742[−4]	0.1892[−4]	0.5462[−5]	0.1919[−5]
Ps(3d)	0.8226[−3]	0.1167[−3]	0.2509[−4]	0.2374[−5]	0.3950[−6]	0.9274[−7]	0.2752[−7]
Ps(4s)	0.8430[−2]	0.2490[−2]	0.8867[−3]	0.1702[−3]	0.4708[−4]	0.1646[−4]	0.6766[−5]
Ps(4p)	0.4525[−2]	0.1005[−2]	0.2854[−3]	0.3913[−4]	0.8466[−5]	0.2442[−5]	0.8578[−6]
Ps(5s)	0.4325[−2]	0.1281[−2]	0.4565[−3]	0.8758[−4]	0.2421[−4]	0.8458[−5]	0.3476[−5]
Ps(5p)	0.2357[−2]	0.5276[−3]	0.1500[−3]	0.2057[−4]	0.4450[−5]	0.1283[−5]	0.4506[−6]
Ps(5d)	0.2778[−3]	0.4189[−4]	0.8940[−5]	0.8389[−6]	0.1395[−6]	0.3276[−7]	0.9726[−8]
Ps(5f)	0.6955[−4]	0.3480[−5]	0.3399[−6]	0.1368[−7]	0.1524[−8]	0.2812[−9]	0.6969[−10]
Ps(6p)	0.1376[−2]	0.3094[−3]	0.8806[−4]	0.1207[−4]	0.2611[−5]	0.7530[−6]	0.2644[−6]

The notation x[−y] stands for x $\times 10^{-y}$

(A) distorted-wave approximation results of Ghoshal and Mandal [46]

agreement is quite good. However, at moderate energies the scaling law can still be applied to obtain cross section within limited accuracy. Even when n is not too large (say Eq. (4) or Eq. (5)) the scaling law can still be applied. Note that the scaling law (Eq. (6)) holds good for $(l/n) \ll 1$ so that $\prod_{i=0}^{l}(1 - i^2/n^2) \approx 1$. It is to be mentioned here that the $1/n^3$ scaling law for the cross section of positronium formation is also suggested earlier [31, 32, 42, 49]. Moreover, the asymptotic cross sections for the positron impact excitation of the hydrogen atom also obey a similar type of scaling law [50]. But in that case the scaling factor is slightly different.

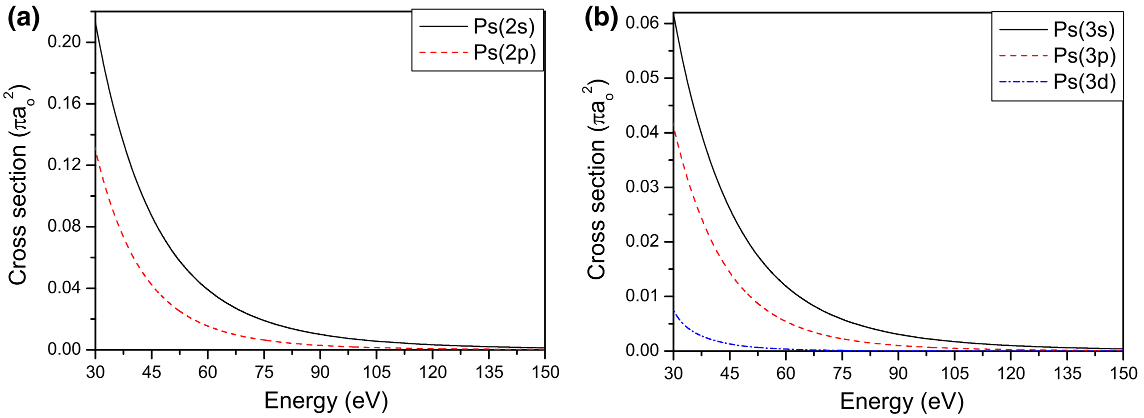

Fig. 4 Cross section (in πa_0^2) as a function of incident positron energy (in eV) for positronium formation in (**a**) $n = 2$ state and (**b**) $n = 3$ state

Table 4 Comparison of cross sections (in units of πa_0^2) calculated by using distorted wave theory and scaling law

E (eV)	*n*	6		8		10		12	
	l	(A)	(B)	(A)	(B)	(A)	(B)	(A)	(B)
50[a]	0	25.05723	25.28443	10.58731	10.66692	5.42542	5.46143	3.14136	3.16055
	1	13.75784	14.44812	5.85241	6.17149	3.00771	3.17787	1.74411	1.84472
	2	1.68067	1.60931	0.73310	0.72500	0.37974	0.38228	0.22093	0.22474
	3	0.50235	0.44103	0.25153	0.22767	0.13696	0.12712	0.08153	0.07699
	4	0.19668	0.18516	0.14181	0.12903	0.08946	0.08069	0.05748	0.05171
100[b]	0	26.49415	26.78631	11.20982	11.30048	5.74714	5.78584	3.32831	3.34829
	1	8.80598	9.43262	3.76682	4.02913	1.94091	2.07470	1.12708	1.20434
	2	0.55569	0.58502	0.25092	0.26355	0.13245	0.13897	0.07791	0.08170
	3	0.02565	0.02755	0.01377	0.01422	0.00783	0.00794	0.00479	0.00481
200[c]	0	14.04056	14.17787	5.93706	5.98129	3.04303	3.06242	1.76203	1.77223
	1	2.61139	2.80046	1.11697	1.19621	0.57552	0.61596	0.33420	0.35756
	2	0.08654	0.09110	0.03899	0.04104	0.02056	0.02164	0.01209	0.01272
	3	0.00111	0.00112	0.00057	0.00058	0.00032	0.00032	0.00019	0.00020
300[d]	0	20.14944	20.32322	8.51552	8.57386	4.36350	4.38981	2.52629	2.54040
	1	2.64401	2.83120	1.13063	1.20934	0.58248	0.62272	0.33822	0.36148
	2	0.06034	0.06349	0.02719	0.02860	0.01434	0.01508	0.00843	0.00887
	3	0.00051	0.00050	0.00026	0.00026	0.00015	0.00014	0.00009	0.00009

Column (A) corresponds to the cross sections calculated using distorted wave approximation. Column (B) corresponds to the cross sections calculated using the scaling law, $\sigma_{1s\rightarrow nl} = (1/n^3)\prod_{i=0}^{l}(1 - i^2/n^2)(n_0^3\sigma_{1s\rightarrow n_0 l})_{n_0\rightarrow\infty}$, as discussed in the text

[a] Cross section values are multiplied by 10^{+4}

[b] Cross section values are multiplied by 10^{+5}

[c] Cross section values are multiplied by 10^{+6}

[d] Cross section values are multiplied by 10^{+7}

4. Conclusions

The dynamics of the reaction: $e^+ + \mathrm{H(1s)} \mapsto \mathrm{Ps(nlm)} + \mathrm{p}$ has been investigated by using a distorted wave theory which includes the effect of static dipole polarizability explicitly. It has been possible to obtain the scattering amplitude by some straight-forward steps. We report reasonably accurate results for differential and total cross sections for the incident positron energy in the range 25–300 eV. Moreover, a simple law for obtaining asymptotic cross sections has been presented. We present sufficient analytical and numerical evidences for the sake of further theoretical and experimental works in this field.

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Appendix

Evaluation of the $1s \longrightarrow nlm$ capture amplitude $g_B(\vec{k}_f, \vec{k}_i)$.

The wave function of Ps atom in *nlm* state is given by

$$\begin{aligned}\eta_{nlm}(\vec{r}_1) &= R_{nl}(r_1) Y_{lm}(\theta_1, \phi_1)\\ &= \left\{ -\left[\left(\frac{2}{na_0}\right)^3 \frac{(n-l-1)!}{2n[(n+l)!]^3} \right]^{1/2} \right.\\ &\quad \left. \times\, e^{-\frac{r_1}{na_0}} \left(\frac{2}{na_0} r_1\right)^l L_{n+l}^{2l+1}\left(\frac{2}{na_0} r_1\right) \right\} Y_{lm}(\theta_1, \phi_1),\end{aligned} \tag{7}$$

where Y_{lm} denote the spherical harmonics, and L_{n+l}^{2l+1} denote the associated Laguerre polynomial of degree $(n+l)$ and order $(2l+1)$.

$1s \longrightarrow nlm$ capture amplitude $g_B(\vec{k}_f, \vec{k}_i)$ is given by

$$\begin{aligned}g_B(\vec{k}_f, \vec{k}_i) &= \left(-\frac{m_f}{2\pi}\right) \langle \Phi_f | V_f | \Phi_i \rangle\\ &= \left(-\frac{m_f}{2\pi}\right) \int e^{i[\vec{A}.\vec{r}_2 - \vec{B}.\vec{r}_1]} \eta^*_{nlm}(\vec{r}_1) \left[\frac{1}{R_{12}} - \frac{1}{r_2}\right] \phi_{1s}(\vec{r}_2) d\vec{r}_1 d\vec{r}_2\\ &= \left(-\frac{m_f}{2\pi}\right) [I_1 - I_2],\end{aligned} \tag{8}$$

where

$$\vec{A} = \frac{m_p}{m_p + 1} \vec{k}_i - \vec{k}_f, \quad \vec{B} = \vec{k}_i - \frac{\vec{k}_f}{2}$$

$$I_1 = \int e^{i[\vec{A} \cdot \vec{r}_2 - \vec{B} \cdot \vec{r}_1]} \eta^*_{nlm}(\vec{r}_1) \frac{1}{R_{12}} \phi_{1s}(\vec{r}_2) d\vec{r}_1 d\vec{r}_2, \tag{9}$$

$$I_2 = \int e^{i[\vec{A} \cdot \vec{r}_2 - \vec{B} \cdot \vec{r}_1]} \eta^*_{nlm}(\vec{r}_1) \frac{1}{r_2} \phi_{1s}(\vec{r}_2) d\vec{r}_1 d\vec{r}_2 \tag{10}$$

We first consider the integral I_1 which contains positron–proton interaction and hence rather difficult to evaluate. Taking Fourier transforms of the function $exp(-\lambda r)/r$ and then utilizing the $\delta-$function properties $\vec{r}_2$ integration can be carried our easily and we obtain

$$I_1 = -2\left(\frac{\gamma_1}{\pi}\right)^{3/2} \frac{\partial}{\partial \gamma_1} \int \frac{e^{i(\vec{s} - \vec{B}).\vec{r}_1}}{(|\vec{A} - \vec{s}|^2 + \gamma_1^2) s^2} \eta^*_{nlm}(\vec{r}_1) d\vec{r}_1 d\vec{s}. \tag{11}$$

where $\gamma_1 = 1/a_0$. Using integral representation of Feynman

$$\frac{1}{ab} = \int_0^1 \frac{dx}{[ax + b(1-x)]^2}$$

and setting $\lambda^2 = A^2 x(1-x) + \gamma_1^2 x$ we obtain

$$I_1 = -2\left(\frac{\gamma_1}{\pi}\right)^{3/2} \frac{\partial}{\partial \gamma_1} \int_0^1 dx e^{i(x\vec{A} - \vec{B}) \cdot \vec{r}_1} \eta^*_{nlm}(\vec{r}_1) d\vec{r}_1$$

$$\int \frac{e^{i(\vec{s} - x\vec{A}) \cdot \vec{r}_1}}{[|s - x\vec{A}|^2 + \lambda^2]^2} d\vec{s}$$

or,

$$I_1 = -2\pi^2 \left(\frac{\gamma_1}{\pi}\right)^{3/2} \frac{\partial}{\partial \gamma_1} \int_0^1 \frac{e^{i\vec{p} \cdot \vec{r}_1 - \lambda r_1}}{\lambda} \eta^*_{nlm}(\vec{r}_1) d\vec{r}_1 dx,$$

$$\vec{p} = x\vec{A} - \vec{B}$$

or,

$$I_1 = -2\pi^2 \left(\frac{\gamma_1}{\pi}\right)^{3/2} \frac{\partial}{\partial \lambda} \int_0^1 \frac{F}{\lambda} \left(\frac{\partial \lambda}{\partial \gamma_1}\right) dx$$

or,

$$I_1 = A_1 \left[\int_0^1 \frac{x}{\lambda^2} \frac{\partial}{\partial \lambda}(F) dx - \int_0^1 \frac{xF}{\lambda^3} dx \right], \tag{12}$$

where

$$A_1 = -2\pi^2 \gamma_1 \left(\frac{\gamma_1}{\pi}\right)^{3/2},$$

$$F = \int e^{i\vec{p} \cdot \vec{r}_1 - \lambda r_1} \eta^*_{nlm}(\vec{r}_1) d\vec{r}_1. \tag{13}$$

Using the expansion formula of plane wave in terms of spherical Bessel's function J_L, such as $exp(i\vec{p}.\vec{r}_1) = 4\pi \sum_{L,M} i^L j_L(pr_1) Y^*_{LM}(\hat{p}) Y_{LM}(\hat{r}_1)$, and then utilizing the orthogonal property of spherical harmonics Y_{LM} we obtain

$$\begin{aligned}F &= 4\pi i^l Y^*_{lm}(\hat{p}) N_{lm} \int_0^\infty j_l(pr_1) e^{-ar_1} L_{n+l}^{2l+1}(2\gamma_n r_1) r_1^{l+2} dr_1,\\ &\quad a = \lambda + \gamma_n \text{ and } \gamma_n = \frac{1}{na_0}.\end{aligned} \tag{14}$$

Now using the expansion formula of the associated Laguerre polynomial and a typical integral involving spherical Bessel function, such as

$$L_{n+l}^{2l+1}(x) = \sum_{i=0}^{n-l-1} (-1)^{i+1} \frac{[(n+l)!]^2}{(n-l-1-i)!(2l+1+k)!} \frac{x^i}{i!}$$

and

$$\int_0^\infty e^{-ax} j_l(bx) x^{l+1} dx = \frac{(2b)^l l!}{(a^2+b^2)^{l+1}}, (\mathrm{Re}(a) > |\mathrm{Im}(b)|), \tag{15}$$

we finally obtain

$$F = CY^*_{lm}(\hat{p}) \sum_{k=0}^{n-l-1} g(k) D(p,a,l+1,k+1), \tag{16}$$

where

$$D(x,y,l,m) = \frac{d^m}{dy^m}\left[\frac{1}{(x^2+y^2)^l}\right] \text{ and}$$

$$g(k) = \frac{(2\gamma_n)^k}{(n-l-1-k)!(2l+1+k)!k!}.$$

Substituting (Eq. (16)) into (Eq. (12)) we obtain

$$I_1 = A_1 C \sum_{k=0}^{n-l-1} g(k) \int_0^1 \frac{xY^*_{lm}(\hat{p})}{\lambda^2}\left[\frac{D(p,a,l+1,k+1)}{\lambda} - D(p,a,l+1,k+2)\right](2p)^l dx. \tag{17}$$

In the similar fashion the integral I_2 can be evaluated. The one-dimensional integration over [0, 1] appearing in integral (Eq. (17)) has been evaluated numerically by employing Gauss–Legendre quadrature formula. Note that the integral (Eq. (17)) has a fictitious singularity , which has been removed by taking a transformation of the form $x = z^2$.

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