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Exponential correlated basis in Schwinger variational principle for positronium formation in hydrogen

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Abstract. An exponential correlated basis set is tested within the framework of multi-channel Schwinger variational principle in the momentum space. It is found that inclusion of only the positron-electron correlation in the basis set is enough to obtain accurate results for all significant partial waves for ground state positronium formation in positron-hydrogen collisions at low and intermediate energies (6.856–75 eV). Results are in conformity with other accurate variational and non-variational calculations as well as observed data available in the literature.

PACS. 34.85.+x Positron scattering – 36.10.Dr Positronium, muonium, muonic atoms and molecules

1 Introduction

Recently elastic positron collisions from hydrogen atoms was successfully studied within the framework of Schwinger variational principle by using an exponential correlated basis [1,2]. In this paper, a similar type of basis is tested for positronium (Ps) formation in positron-hydrogen collisions which is a fundamental rearrangement collision process in a perfect three-body scattering system.

Since the pioneering work of Massey and Mohr in 1954 [3], this process has been studied by a variety of methods with various degrees of sophistication and significant advancement has been made over the years [4–19]. In recent years the problem of Ps formation in positron-hydrogen collisions has been investigated theoretically with renewed interest. This interest has been stimulated by the availability of experimental data of total reaction cross section and Ps formation cross section for e^+-hydrogen collisions [20,21]. It is also of interest to fully understand one of the simplest quantum mechanical rearrangement collision processes.

At the low energy region there exist several variational and non-variational calculations for this process. Mention may be made of Kohn-Hulthen variational calculation of Stein and Sternlicht [4], Humberston [5] and Brown and Humberston [6], Harris-Nesbet algebraic method of Kuang and Gien [7], algebraic 'enlarged six-pseudostate', calculation of Gien [8], 21-state close-coupling calculation of Mitroy [15], Schwinger variational calculation of Roy and Mandal [17] and Kar and Mandal [19]. Although these calculations, except those of [19], are limited to a few partial waves, the results of these calculations for ground state Ps formation at low incident energies agree nicely among one another and probably these are the most accurate results available in this energy region.

Significantly less attention has been paid to obtain results of comparable accuracy at the intermediate energies. For intermediate energies of positron impact, particular mention may be made of the calculations using the impulse approximation [9], the distorted-wave approximations [10–12], Fock-Tani field-theoretic equations [13], the R-matrix method [14], the coupled 33-state method [18], the 28-state close coupling approximation method [15] and the two-center convergent close-coupling approach of Bray and Kadyrov [16].

Though a few non-variational results are known to be available in the literature, there is still a scarcity of variational calculations at the intermediate energy region. In order to fulfill this goal, we have made an endeavour in the present calculation to obtain mainly an accurate estimate of Ps formation cross section (both total and differential) at the intermediate energy regime. While doing so, we have also tested the accuracy of the present method at the low incident energies where there are a large number of accurate calculations (both variational and non-variational) to compare with.

Of late, the multi-channel Schwinger's variational method has been used in the momentum space to study the scattering of positrons by hydrogen atoms [17,19]. In these works, inverse type correlation functions of the form

$$\frac{1}{(a+br_{12})^{m_0-\frac{1}{2}}} \quad \text{and} \quad \frac{1}{(a+br_{12}+cr_1)^{m_0-\frac{1}{2}}} \qquad (1)$$

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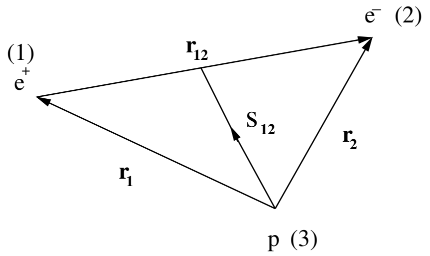

Fig. 1. Coordinate representation of positron-hydrogen system.

have been utilized with respect to the coordinate system as depicted in Figure 1 in the discrete basis set. Definitive results have been obtained for ground state Ps formation up to 150 eV of incident positron energy for all significant partial waves using only 12 terms in the basis set. These results are in conformity with other accurate theoretical calculations [5,6,8] as well as experimental observations [20].

In this paper, our main objective is to establish that accurate results for all partial waves at low as well as intermediate energies for Ps formation in positron-hydrogen collisions can easily and elegantly be obtained using a small discrete basis set within the framework of the SVP which, since its inception by Schwinger [22], has been widely utilised successfully in atomic, molecular and nuclear physics [1,23–35] (and further references given in [1]). Analysing the optimised non-linear variational parameters in the basis set we make some important conclusive remarks about the physical attributes of the Ps formation mechanism. Our investigation endeavours to perform reliable predictions of the scattering parameters such as the scattering amplitudes for all significant partial-waves and total cross sections.

The plan of the paper is as follows. In Section 2 we discuss the underlying theory of choosing the basis set. Section 3 is devoted to the discussions of the results as obtained by the present calculation. Finally in Section 4 we make our concluding remarks.

2 Theory

We choose correlated basis functions as follows:

$$u_m(\vec{r}_1,\vec{r}_2) = (-1)^{m-1}\xi_m(\vec{r}_1,\vec{r}_2)\Phi_i(\vec{r}_1,\vec{r}_2),\ m = 1,2,3,... \tag{2}$$

$$v_n(\vec{r}_1,\vec{r}_2) = (-1)^{n-1}\xi_n(\vec{r}_1,\vec{r}_2)\Phi_f(\vec{r}_{12},\vec{s}_{12}),\ n = 1,2,3,... \tag{3}$$

where the same correlation function $\xi_m(\vec{r}_1,\vec{r}_2)$ is chosen for both the incident (e^+ + H) direct and the final (Ps + H^+) rearrangement channels:

$$\xi_m(\vec{r}_1,\vec{r}_2) = e^{-\alpha_m r_1-\beta_m r_2-\gamma_m r_{12}}, \tag{4}$$

with $\alpha_{2m} = p$, $\alpha_{2m-1} = 0$, and β_m, γ_m, p, are non-linear variational parameters to be optimised. Here Φ_i, Φ_f are plane-wave states in the initial and final states respectively, which are given by equations (6) and (7).

We have used the Schwinger variational amplitude in the momentum space as obtained by Kar and Mandal [19]:

$$[A^{(L)}_{fi}(k_f,k_i)] = \sum_{m,n}\sum_{p,q} A^{(L)}_{fm}(k_f,k_i) {D^{(L)(pq)}_{mn}}^{-1} A^{(L)}_{ni}(k_f,k_i) \tag{5}$$

which is a function of the scattering energies for any partial wave L. Here $A^{(L)}_{fm}(k_f,k_i)$, $A^{(L)}_{ni}(k_f,k_i)$ are the input two-body amplitudes and ${D^{(L)(pq)}_{mn}}^{-1}$ are the inverse matrix elements of the double-scattering matrix $D^{(L)(pq)}_{mn}$. The evaluation of the relevant amplitudes is shown in Appendix. These are obtained in closed analytic forms.

The largest value of m and n used in equation (5) is 4. The correlated basis functions u_m, v_n, along with ξ_m, ξ_n, are not orthogonalised, they are square-integrable. Indeed they satisfy the large-distance behaviour as is expected of the scattering functions because of the presence of the plane-wave states Φ_i, Φ_f in them. In fact, this choice of basis functions has made our application of the SVP quite distinctive from other applications in nuclear, atomic and molecular physics.

The applicability of the present method will not be jeopardized for large values of m, n so long as the choices of the nonlinear exponents α_j, β_j, γ_j are distinct ($j = m,n$; $m,n = 1,2,...,N$). No two rows or columns of the double scattering matrix D will ever be the same to make it singular. This has been carefully ensured in all of our calculations using SVP.

Further, the method of optimization of the nonlinear variational parameters in the present and earlier SVP calculations is quite different from the conventional variational methods. While conventional variational calculations increase the number of basis functions to hundred of terms using a single set values of the variational parameters, we have changed these nonlinear variational exponents keeping the size of the basis set fixed ($N = 4,6,8$ or 10) to attain convergence. We have endeavoured and succeeded in determining the best possible set of β_j, γ_j for stationary Schwinger amplitudes over a range of the variational parameter, p. This poor man's method works wonderfully for the accurate determination of the scattering parameters in positron-atom collisions and is easily manageable even on a IBM-compatible Pentium IV PC.

For the present calculation we have set $\beta_m = 0$. Optimization of the scattering amplitude can then be achieved very conveniently by varying the other non-linear variational parameters. It was found that only γ_m had significant contribution compared to other two parameters. It may be a manifestation of the small number of terms in basis expansion. We can physically explain the reasons behind such a nature of the dependence on parameters in our basis as follows.

The basic interaction responsible for a transition in the internal state of the atom is the positron-electron correlation. In other words, if the positron-electron interaction is turned off, the internal state of the atom will remain unaltered. The only effect of the positron-proton interaction is to deflect the incident positron. Since the mass of the proton is very large compared to that of the positron and the electron (1836:1), this deflection is of appreciable measure for low incident positron energy and consequently indirectly influences the internal structure of the atom. But with the increase in the incident positron energies this effect gradually slows down and hardly affects the probability of transition of the internal state of the atom in the intermediate and high energies. Thus $\beta_m = 0$ in our calculation signifies that the change in the electronic coordinate is largely due to the positron-electron correlation. As the positron and the bound electron are very much lighter than the proton, the positron comes very near to the electron, binds with the electron and goes away.

One of the highlights of our present calculation is that, only four terms of the exponential basis function are required to predict accurate amplitudes and cross sections for all significant partial-waves at incident energies in the range 6.8558–75 eV. This has been made possible by the existence of infinite order position-electron correlation in the exponent of the basis set. The beauty of the exponential basis set is that the exponential function properly combines each power of r_{12} to produce essentially exact positron-electron correlation. We noticed similar effect while constructing normal two-electron bound state wave function for helium and its isoelectronic sequence [36]. In that case we observed that the exponential trial functions were better than inverse type trial functions in the sense that the exponential basis set yields better results with in less number of terms than with the inverse type functions.

3 Results and discussion

We have evaluated the stationary scattering amplitude (5) using correlated basis functions (2) and have optimised the non-linear variational parameters p and γ_m, $m = 1, 2, 3, 4$ generating random numbers using Monte-Carlo optimization technique. One of the interesting points of our calculation is the technique for optimizing the non-linear variational parameters p and γ_m, $m = 1, 2, 3, 4$. For a given value of the variational parameters γ_m, $m = 1, 2, 3, 4$ p is varied within a certain finite range, say, $[0.0, 2.0]$ to seek the stationary values of $[A^{(L)}_{fi}(k_f, k_i)]$. We have set $\gamma_1 = \gamma_2$ and $\gamma_3 = \gamma_4$ in conformity with the choice of α_m to have a hold over the process of optimization. It has been further found that if digits after the decimal point of the variational parameters $\gamma_3 = \gamma_4$ are put one unit lower than the digits after the decimal point of the variational parameters $\gamma_1 = \gamma_2$ a systematic method makes the optimization process convenient. Of course, there are other stray values of the variational parameters which optimize the amplitude $[A^{(L)}_{fi}(k_f, k_i)]$ to essentially obtain the same number.

It has been found that the stationary amplitudes are remarkably stable for each partial wave. These, along with the corresponding variational parameters are shown in Table 2 for the partial-waves $l = 0, 2, 5$ at the incident positron energies 9.826 eV and 25 eV respectively. In Figure 2 we have plotted γ_1 as a function of energy for S-wave. This figure shows that γ_1 first increases a little bit and then decreases systematically with higher energies as expected. This fact is an important information regarding the relation of positron-electron correlation with Ps formation.

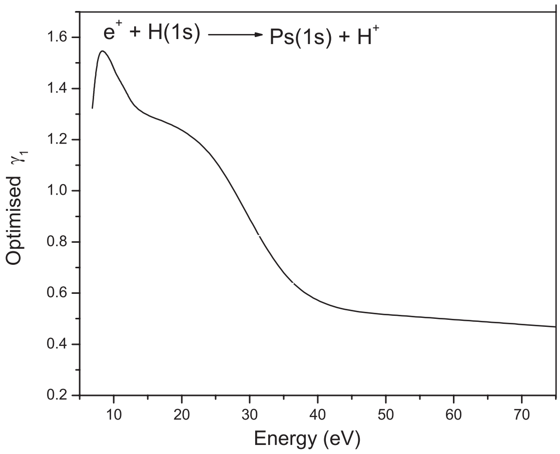

Fig. 2. Variation of optimised γ_1 with energy (eV) for S-wave.

3.1 Positronium formation in the Ore gap (6.8–10.2 eV)

We have obtained results for the ground state Ps formation cross section at low-energies of positron impact in the Ore gap for S-, P-, D- and higher partial-waves up to $L = 14$. These values are highly accurate and compare nicely with those obtained by the Kohn-Hulthen variational methods [5,6] for S-, P-, D- waves as well as Schwinger variational method [19] for all partial-waves. In Table 1 we display our results along with those available in the literature [5–8,15]. The present values are in satisfactory agreement with the Harris-Nesbet algebraic method calculation of Kuang and Gien [7], algebraic 'enlarged six-pseudo-state' calculation of Gien [8], 21-state close-coupling calculation of Mitroy [15], etc.

This may fairly lead to the conclusion that the problem of Ps formation in positron-hydrogen collisions is considered to be solved in the Ore gap to a fair degree of accuracy.

3.2 Positronium formation beyond Ore gap

We have presented in Table 3 our present results along with the findings of Kar and Mandal [19] for the positron energy beyond Ore gap. There are no significant differences in the results obtained by using two different basis sets. The over-all close agreement between these Schwinger variational calculations and other theoretical methods emphasizes further the accuracy of the present findings.

Table 1. Partial-wave ground-state Ps formation cross sections (in units of πa_0^2) for positron-hydrogen scattering at energies in the Ore gap. The numbers in square brackets indicate powers of 10.

k_i (a.u.)	0.71	0.75	0.8	0.85
$l = 0$				
Present	0.416[−2]	0.443[−2]	0.492[−2]	0.579[−2]
Variational (a)	0.41[−2]	0.44[−2]	0.49[−2]	0.58[−2]
Harris-Nesbet (b)	0.404[−2]	0.441[−2]	0.493[−2]	0.549[−2]
Algebraic E6PS (c)	0.404[−2]	0.426[−2]	0.480[−2]	0.550[−2]
21-state (d)	0.405[−2]	0.427[−2]	0.472[−2]	0.560[−2]
$l = 1$				
Present	0.268[−1]	0.367	0.475	0.566
Variational (a)	0.27[−1]	0.365	0.482	0.561
Harris-Nesbet (b)	0.267[−1]	0.367	0.483	0.565
Algebraic E6PS (c)	0.267[−1]	0.366	0.483	0.564
21-state (d)	0.266[−1]	0.366	0.483	0.563
$l = 2$				
Present	0.624[−3]	0.336	0.828	1.058
Variational (a)	0.62[−3]	0.335	0.812	1.057
Harris-Nesbet (b)	0.683[−3]	0.320	0.862	1.162
Algebraic E6PS (c)	0.683[−3]	0.321	0.860	1.158
21-state (d)	0.682[−3]	0.320	0.859	1.158
$l = 3$				
Present	0.468[−5]	0.356[−1]	0.272	0.597
Variational (e)	0.444[−5]	0.355[−1]	0.272	0.593
Harris-Nesbet (b)	0.500[−5]	0.354[−1]	0.271	0.596
Algebraic E6PS (c)	0.445[−5]	0.357[−1]	0.271	0.595
21-state (d)	0.44[−5]	0.356[−1]	0.270	0.596
$l = 4$				
Present		0.205[−2]	0.543[−1]	0.203
Variational (e)		0.202[−2]	0.556[−1]	0.201
$l = 5$				
Present		0.562[−4]	0.453[−2]	0.256[−1]
Variational (e)		0.725[−4]	0.431[−2]	0.231[−1]
Total cross section				
Present	0.316[−1]	0.744	1.639	2.458
Variational (e)	0.315[−1]	0.741	1.631	2.449
Harris-Nesbet (b)	0.315[−1]	0.729	1.666	2.499
Algebraic E6PS (c)	0.314[−1]	0.730	1.663	2.492
21-state (d)	0.313[−1]	0.728	1.660	2.49

(a) Variational calculation, Humberston [5], Brown and Humberston [6]; (b) Harris-Nesbet algebraic method, Kuang and Gien [7]; (c) Algebraic 'enlarged six-pseudostate', Gien [8]; (d) 21-state close-coupling, Mitroy [15]; (e) Schwinger variational, Kar and Mandal [19].

3.3 Comparison with experiment

In Figure 3, we display the total cross section for ground-state Ps formation in positron-hydrogen collisions as predicted by the present calculations, the Schwinger variational calculations of Kar and Mandal [19], the 33-state calculation of Kernoghan et al. [18], the observed data of Zhou et al. [20] and Weber et al. [21] in the energy-range 6.8–75.0 eV. There is good accord between both the Schwinger results and the 33-state calculation [18] over the whole energy region for which results are available. Though the observed data of Weber et al. are a little bit higher than our results, the data of Zhou et al. are in favourable agreement with our theoretical predictions in shape and magnitudes at all energies. As a matter of fact the observed data of Zhou et al. are found consistently to be in better agreement with theory. In the words of Zhou et al. [20], '...we expect our "This work" results to be the most reliable indicators of the actual Q_{Ps}... It is very encouraging to see the very good agreement of the present Q_{Ps} measurements with the recent coupled 33-state calculation of Kernoghan et al. [...] and the 21-state close-coupling approximation calculation of Mitroy [...] and with the most of the other theoretical calculations [...]'.

Inclusion of excited-state contributions though small will however enhance the present values to a certain extent. It is to be noted that the figure for total cross

Table 2. The steady range of amplitudes and cross sections for the incident positron energy 9.826 eV and 25 eV respectively. The numbers in square brackets indicate powers of 10.

$E = 9.826$ eV				$E = 25$ eV			
$l = 0$							
$(\gamma_1 = \gamma_2 = 1.4955,\ \gamma_3 = \gamma_4 = 1.3844)$				$(\gamma_1 = \gamma_2 = 1.2264,\ \gamma_3 = \gamma_4 = 1.1153)$			
	amplitude		cross		amplitude		cross
p	real	imaginary	section	p	real	imaginary	section
1.0	0.457[−1]	0.213[−2]	0.0058	1.0	0.402[−1]	−0.568[−3]	0.0018
1.1	0.457[−1]	0.213[−2]	0.0058	1.1	0.402[−1]	−0.570[−3]	0.0018
1.2	0.457[−1]	0.213[−2]	0.0058	1.2	0.402[−1]	−0.571[−3]	0.0018
1.3	0.457[−1]	0.212[−2]	0.0058	1.3	0.402[−1]	−0.573[−3]	0.0018
1.4	0.457[−1]	0.212[−2]	0.0058	1.4	0.402[−1]	−0.574[−3]	0.0018
1.5	0.457[−1]	0.212[−2]	0.0058	1.5	0.402[−1]	−0.576[−3]	0.0018
$l = 2$							
$(\gamma_1 = \gamma_2 = 0.3567,\ \gamma_3 = \gamma_4 = 0.2456)$				$(\gamma_1 = \gamma_2 = 0.5135,\ \gamma_3 = \gamma_4 = 0.4024)$			
	amplitude		cross		amplitude		cross
p	real	imaginary	section	p	real	imaginary	section
0.7	0.277	0.100[−1]	1.058	0.7	0.3501	0.142[−1]	0.668
0.8	0.276	0.101[−1]	1.058	0.8	0.3501	0.142[−1]	0.669
0.9	0.276	0.101[−1]	1.058	0.9	0.3501	0.142[−1]	0.669
1.0	0.276	0.101[−1]	1.058	1.0	0.3501	0.143[−1]	0.669
1.1	0.276	0.101[−1]	1.058	1.1	0.3501	0.142[−1]	0.669
1.2	0.276	0.100[−1]	1.058	1.2	0.3501	0.142[−1]	0.669
$l = 5$							
$(\gamma_1 = \gamma_2 = 0.1612,\ \gamma_3 = \gamma_4 = 0.0501)$				$(\gamma_1 = \gamma_2 = 0.4408,\ \gamma_3 = \gamma_4 = 0.3297)$			
	amplitude		cross		amplitude		cross
p	real	imaginary	section	p	real	imaginary	section
1.0	0.290[−1]	0.306[−2]	0.0256	0.6	0.1324	0.182[−2]	0.2099
1.1	0.290[−1]	0.322[−2]	0.0257	0.7	0.1324	0.182[−2]	0.2099
1.2	0.290[−1]	0.326[−2]	0.0257	0.8	0.1324	0.182[−2]	0.2099
1.3	0.291[−1]	0.351[−2]	0.0257	0.9	0.1324	0.182[−2]	0.2099
1.4	0.291[−1]	0.356[−2]	0.0258	1.0	0.1324	0.182[−2]	0.2099
1.5	0.291[−1]	0.341[−2]	0.0256	1.1	0.1324	0.182[−2]	0.2100

section, Figure 3, resembles to the figure for the correlation parameter γ_1, Figure 2.

4 Conclusions

Multi-channel Schwinger's variational principle has conveniently and elegantly been used in momentum space to study the Ps formation in positron-hydrogen scattering at low and intermediately energies. Our expression of the scattering amplitude is simple and easy to interpret. In the absence of any minimum principle the method uses the stationary property of the scattering amplitude. So the choice of the basis set should be judicious in order to incorporate the essential features of the underlying system.

Our present study of ground state Ps formation in positron-hydrogen collisions uses an exponential correlated discrete basis set in both the elastic and rearrangement channels. Inclusion of only the positron-electron correlation in the basis set for Schwinger variational principle is enough to obtain accurate results for ground state Ps formation in positron-hydrogen collisions.

Appendix A: Evaluation of two-body amplitudes for Ps formation in positron-hydrogen collisions

In what follows we have used the basis set (2) to calculate the two-body amplitudes defined in Section 2 of this paper. We show how these amplitudes are obtained in closed forms for an efficient evaluation.

In coordinate representation (Fig. 1), we have

$$\Phi_i(\vec{r}_1, \vec{r}_2) = e^{i\vec{k}_i\cdot\vec{r}_1}\phi_i(\vec{r}_2) \tag{6}$$

$$\Phi_f(\vec{r}_{12}, \vec{s}_{12}) = e^{i\vec{k}_f\cdot\vec{s}_{12}}\eta_f(\vec{r}_{12}) \tag{7}$$

where $(\phi_i(\vec{r}_2), \eta_f(\vec{r}_{12}))$ denote (H, Ps) bound-states and $(h\vec{k}_i, h\vec{k}_f)$, the momenta of the incident positron and outgoing Ps, respectively. For ground state Ps formation in positron-H collisions, we have:

$$\phi_i(\vec{r}_2) = N_i e^{-\lambda_i r_2}, \tag{8}$$

$$\eta_f(\vec{r}_{12}) = N_f e^{-\lambda_f r_{12}}, \tag{9}$$

where $N_i = \sqrt{\frac{\lambda_i^3}{\pi}}$, $N_f = \sqrt{\frac{\lambda_f^3}{\pi}}$, $\lambda_f = \frac{\lambda_i}{2}$, $\lambda_i = \frac{1}{a_0}$ (a.u.).

Table 3. The present partial-wave contributions to the ground-state Ps formation cross sections (in units of πa_0^2) in positron-hydrogen collisions at energies in the energy range 10.2–75 eV. The numbers in square brackets indicate powers of 10.

		Energy (eV)						
l		10.2	12.0	13.6	25.0	35.0	50.0	75.0
0	a	0.0064	0.0072	0.0084	0.0018	0.0004	0.0032	0.0009
	b	0.0064	0.0075	0.0084				
1	a	0.6082	0.6696	0.6545	0.1678	0.726[−1]	0.492[−1]	0.177[−1]
	b	0.606	0.674	0.652				
2	a	1.0953	1.3690	1.3583	0.6690	0.2054	0.857[−1]	0.239[−1]
	b	1.102	1.352	1.377				
3	a	0.6386	0.6605	0.6406	0.4980	0.2367	0.904[−1]	0.282[−1]
	b	0.633	0.664	0.718				
4	a	0.2455	0.3803	0.4071	0.3779	0.2292	0.829[−1]	0.227[−1]
	b	0.243	0.383	0.404				
5	a	0.387[−1]	0.1348	0.1876	0.2099	0.1464	0.777[−1]	0.184[−1]
	b	0.374[−1]	0.132	0.190				
6	a	0.433[−2]	0.217[−1]	0.394[−1]	0.1020	0.785[−1]	0.430[−1]	0.171[−1]
	b	0.440[−2]	0.217[−1]	0.384[−1]				
7	a	0.513[−3]	0.327[−2]	0.701[−2]	0.431[−1]	0.419[−1]	0.284[−1]	0.122[−1]
	b	0.509[−3]	0.355[−2]	0.864[−2]				
8	a	0.658[−4]	0.505[−3]	0.132[−2]	0.177[−1]	0.202[−1]	0.133[−1]	0.109[−1]
	b	0.705[−4]	0.589[−3]	0.183[−2]				
9	a		0.828[−4]	0.246[−3]	0.570[−2]	0.938[−2]	0.721[−2]	0.549[−2]
10	a			0.450[−4]	0.275[−2]	0.409[−2]	0.367[−2]	0.264[−2]
11	a				0.939[−3]	0.160[−2]	0.191[−2]	0.126[−2]
12	a				0.320[−3]	0.724[−3]	0.891[−3]	0.509[−3]
13	a				0.106[−3]	0.322[−3]	0.415[−3]	0.203[−3]
14	a				0.339[−4]	0.122[−3]	0.181[−3]	0.796[−4]
Total	a	2.6377	3.2468	3.3046	2.0972	1.0477	0.4880	0.1622
Total	b	2.636	3.239	3.399				

a: Present results, b: Schwinger's variational results of Kar and Mandal [19].

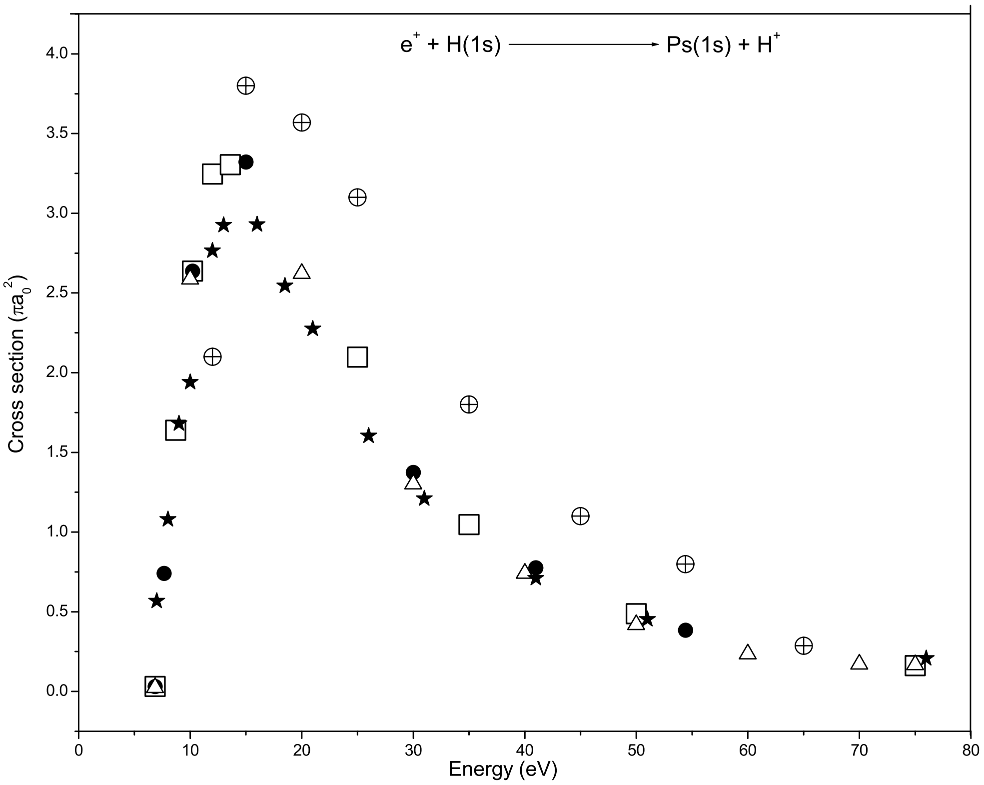

Fig. 3. Total Ps formation cross section (πa_0^2) as a function of energy (eV) in the energy range 6.8557–75 eV for the reaction $e^+ + H(1s) \rightarrow P(1s) + H^+$. (□) Present result; (●) Schwinger variational result of Kar and Mandal [19]; (△) 33-state approximation of Kernoghan et al. [18]; (★) experimental data of Zhou et al. [20]; (⊕) experimental data of Weber et al. [21].

A.1 $\mathbf{A_{nm}(\vec{k}_f, \vec{k}_i)}$

The amplitude $A_{nm}(\vec{k}_f, \vec{k}_i)$ is thus obtained as:

$$
\begin{aligned}
A_{nm}(\vec{k}_f, \vec{k}_i) &= \left(-\frac{\mu_f}{2\pi}\right) \langle v_n | V_f | u_m \rangle \\
&= \left(-\frac{\mu_f}{2\pi}\right) \int v_n^* V_f u_m d\vec{r}_1 d\vec{r}_2 \qquad (10)
\end{aligned}
$$

which on using the expression for v_n^*, u_m and $V_f = 1/r_1 - 1/r_2$ becomes

$$
\begin{aligned}
A_{nm}(\vec{k}_f, \vec{k}_i) &= \left(-\frac{\mu_f}{2\pi}\right) (-1)^{n+m-2} N_i N_f^* \\
&\times \int e^{i\vec{v}_1\cdot\vec{r}_1 + i\vec{v}_2\cdot\vec{r}_2 - \alpha_{nm} r_1 - \beta_{nm} r_2 - \gamma_{nm} r_{12}} \left(\frac{1}{r_1} - \frac{1}{r_2}\right) d\vec{r}_1 d\vec{r}_2 \\
&= \left(-\frac{\mu_f}{2\pi}\right) (-1)^{n+m-2} N_i N_f^* \left[I_1 - I_2\right] \quad \text{(say)} \qquad (11)
\end{aligned}
$$

where $\alpha_{nm} = \alpha_n + \alpha_m$, $\beta_{nm} = \beta_n + \beta_m + \lambda_i$, $\gamma_{nm} = \gamma_n + \gamma_m + \lambda_f$, $\vec{v}_1 = \vec{k}_i - \frac{\vec{k}_f}{2}$ and $\vec{v}_2 = -\frac{\vec{k}_f}{2}$.

Now taking Fourier integral transforms for functions of the form $\exp(-\lambda r)/r$, $\exp(-\lambda r)$:

$$
\exp(-\lambda r)/r = \frac{1}{2\pi^2} \int \frac{e^{i\vec{p}\cdot\vec{r}}}{p^2 + \lambda^2} d\vec{p} \qquad (12)
$$

$$
\exp(-\lambda r) = \frac{\lambda}{\pi^2} \int \frac{e^{i\vec{p}\cdot\vec{r}}}{(p^2 + \lambda^2)^2} d\vec{p} \qquad (13)
$$

and utilised the δ-function properties, such as,

$$
\begin{aligned}
\int e^{i(\vec{q} - \vec{\Delta})\cdot\vec{r}} f(\vec{q}) d\vec{q} d\vec{r} &= (2\pi)^3 \int \delta(\vec{q} - \vec{\Delta}) f(\vec{q}) d\vec{q} \\
&= (2\pi)^3 f(\vec{\Delta}). \qquad (14)
\end{aligned}
$$

we get

$$
\begin{aligned}
I_1 &= \int e^{i\vec{v}_1\cdot\vec{r}_1 + i\vec{v}_2\cdot\vec{r}_2 - \alpha_{nm} r_1 - \beta_{nm} r_2 - \gamma_{nm} r_{12}} \frac{1}{r_1} d\vec{r}_1 d\vec{r}_2 \\
&= 32 \beta_{nm} \gamma_{nm} \\
&\times \int \frac{d\vec{p}}{(p^2 + \alpha_{nm}^2)(|\vec{p} + \vec{v}_1 + \vec{v}_2|^2 + \beta_{nm}^2)^2 (|\vec{p} + \vec{v}_1|^2 + \gamma_{nm}^2)^2} \\
&= 32\pi^2 \beta_{nm} \gamma_{nm} L_{122}(\alpha_{nm}; \vec{\Delta}_1, \beta_{nm}; \vec{\Delta}_2, \gamma_{nm}) \qquad (15)
\end{aligned}
$$

where we have used the Dalitz's integral as defined by relation

$$
\begin{aligned}
L_{lmn}(\delta; \vec{v_1}, \lambda_1; \vec{v_2}, \lambda_2) &= \frac{1}{\pi^2} \\
&\times \int \frac{d\vec{p}}{(p^2 + \delta^2)^l (|\vec{p} - \vec{v_1}|^2 + \lambda_1^2)^m (|\vec{p} - \vec{v_2}|^2 + \lambda_2^2)^n} \qquad (16)
\end{aligned}
$$

and set $\vec{\Delta}_1 = \vec{v}_1 + \vec{v}_2 = \vec{k}_i - \vec{k}_f$; $\vec{\Delta}_2 = \vec{v}_1 = \vec{k}_i - \frac{\vec{k}_i}{2}$. Our simple prescription to evaluate such Dalitz's integral effectively and efficiently has been described in [12].

In a similar fashion we obtain

$$
\begin{aligned}
I_2 &= \int e^{i\vec{v}_1\cdot\vec{r}_1 + i\vec{v}_2\cdot\vec{r}_2 - \alpha_{nm} r_1 - \beta_{nm} r_2 - \gamma_{nm} r_{12}} \frac{1}{r_2} d\vec{r}_1 d\vec{r}_2 \\
&= 32 \beta_{nm} \gamma_{nm} \\
&\times \int \frac{d\vec{p}}{(p^2 + \alpha_{nm}^2)(|\vec{p} + \vec{v}_1 + \vec{v}_2|^2 + \beta_{nm}^2)^2 (|\vec{p} + \vec{v}_1|^2 + \gamma_{nm}^2)^2} \\
&= 32\pi^2 \alpha_{nm} \gamma_{nm} L_{212}(\alpha_{nm}; \vec{\Delta}_1, \beta_{nm}; \vec{\Delta}_2, \gamma_{nm}). \qquad (17)
\end{aligned}
$$

Using the expressions (15) and (17) of I_1 and I_2 in the expression (11) of $A_{nm}(\vec{k}_f, \vec{k}_i)$ we finally obtain

$$
\begin{aligned}
A_{nm}(\vec{k}_f, \vec{k}_i) = C \Big[&\beta_{nm} L_{122}(\alpha_{nm}; \vec{\Delta}_1, \beta_{nm}; \vec{\Delta}_2, \gamma_{nm}) \\
&- \alpha_{nm} L_{212}(\alpha_{nm}; \vec{\Delta}_1, \beta_{nm}; \vec{\Delta}_2, \gamma_{nm}) \Big] \qquad (18)
\end{aligned}
$$

where $C = \left(-\frac{\mu_f}{2\pi}\right) (-1)^{n+m} N_i N_f^* 32\pi^2 \gamma_{nm}$.

A.2 $\mathbf{A_{ni}(\vec{k}_f, \vec{k}_i)}$

The amplitude $A_{ni}(\vec{k}_f, \vec{k}_i)$ is given by:

$$
\begin{aligned}
A_{ni}(\vec{k}_f, \vec{k}_i) &= \left(-\frac{\mu_f}{2\pi}\right) \langle v_n | V_f | \phi_i \rangle \\
&= \left(-\frac{\mu_f}{2\pi}\right) \int v_n^* V_f \varPhi_i d\vec{r}_1 d\vec{r}_2 \qquad (19)
\end{aligned}
$$

which on using the expression for v_n^*, $\varPhi_i$ and $V_f = 1/r_1 - 1/r_2$ becomes

$$
\begin{aligned}
A_{nm}(\vec{k}_f, \vec{k}_i) &= \left(-\frac{\mu_f}{2\pi}\right) (-1)^{n-1} N_i N_f^* \\
&\times \int e^{i\vec{v}_1\cdot\vec{r}_1 + i\vec{v}_2\cdot\vec{r}_2 - \alpha_n r_1 - \beta_1 r_2 - \gamma_1 r_{12}} \left(\frac{1}{r_1} - \frac{1}{r_2}\right) d\vec{r}_1 d\vec{r}_2 \\
&= \left(-\frac{\mu_f}{2\pi}\right) (-1)^{n-1} N_i N_f^* \left[I_1 - I_2\right] \qquad \text{(say)} \quad (20)
\end{aligned}
$$

where $\beta_1 = \beta_n + \lambda_i$, $\gamma_1 = \gamma_n + \lambda_f$, $\vec{v}_1 = \vec{k}_i - \frac{\vec{k}_f}{2}$ and $\vec{v}_2 = -\frac{\vec{k}_f}{2}$.

Applying the same technique as above we get

$$
\begin{aligned}
A_{ni}(\vec{k}_f, \vec{k}_i) = C_1 \Big[&\beta_1 L_{122}(\alpha_n; \vec{\Delta}_1, \beta_1; \vec{\Delta}_2, \gamma_1) \\
&- \alpha_n L_{212}(\alpha_n; \vec{\Delta}_1, \beta_1; \vec{\Delta}_2, \gamma_1) \Big] \qquad (21)
\end{aligned}
$$

where $C_1 = \left(-\frac{\mu_f}{2\pi}\right) (-1)^{n-1} N_i N_f^* 32\pi^2 \gamma_1$.

A.3 $\mathbf{A_{fm}(\vec{k}_f, \vec{k}_i)}$

As in previous two cases the $A_{fm}(\vec{k}_f, \vec{k}_i)$ amplitude can be obtained as:

$$
\begin{aligned}
A_{fm}(\vec{k}_f, \vec{k}_i) = C_2 \Big[&\beta_2 L_{122}(\alpha_m; \vec{\Delta}_1, \beta_2; \vec{\Delta}_2, \gamma_2) \\
&- \alpha_m L_{212}(\alpha_m; \vec{\Delta}_1, \beta_2; \vec{\Delta}_2, \gamma_2) \Big] \qquad (22)
\end{aligned}
$$

where $C_2 = \left(-\frac{\mu_f}{2\pi}\right)(-1)^{m-1} N_i.N_f^* 32\pi^2\gamma_2$, $\beta_2 = \beta_m + \lambda_i$, $\gamma_2 = \gamma_m + \lambda_f$, $\vec{v}_1 = \vec{k}_i - \frac{\vec{k}_f}{2}$ and $\vec{v}_2 = -\frac{\vec{k}_f}{2}$.

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