Differential cross sections for elastic and inelastic positronium-hydrogen-atom scattering

Sadhan K. Adhikari

_Instituto de Física Teórica, Universidade Estadual Paulista 01.405-900 São Paulo, São Paulo, Brazil_

(March 31, 2022)

Abstract

We report results of differential cross sections for elastic scattering, target-elastic Ps excitations and target-inelastic excitation of hydrogen in a five-state coupled-channel model allowing for Ps(1s)H(2s,2p) and Ps(2s,2p)H(1s) excitations using a recently proposed time-reversal-symmetric regularized electron-exchange model potential. The present model yields a singlet Ps-H S-wave resonance at 4.01 eV of width 0.15 eV and a P-wave resonance at 5.08 eV of width 0.004 eV. We also study the effect of the inclusion of the excited Ps and H states on the convergence of the coupled-channel scheme.

_PACS Number(s): 34.10.+x, 36.10.Dr_
Lately, there have been great interest in the experimental [1–4] and theoretical [5–7] studies of ortho positronium (Ps) atom scattering from different neutral atomic and molecular targets. We suggested a time-reversal symmetric regularized nonlocal electron-exchange model potential [8] and used it in the study of total cross section of Ps scattering by H [9], He [9,10], Li [11], Ne [12], Ar [12] and H$_2$ [13]. Our results were in agreement with experimental total cross section [12], specially at low energies for He, Ne, Ar and H$_2$. Among all Ps-atom systems, the positronium-hydrogen (Ps-H) system is the simplest and is of fundamental interest.

In our first studies on Ps-H system we calculated the partial cross sections, low-energy phase shifts, scattering lengths and effective ranges and S-wave singlet resonance and binding energies using a regularized model-exchange potential [9,10]. This potential has a parameter which allows for small variations of the scattering observables at low energies. The results for scattering at high energies is insensitive to the variation of this parameter. At medium and high energies the cross sections of the present model reduce to [14] the first Born cross sections with Oppenheimer exchange potential [15]. The present model is made to reproduce simultaneously the accurate variational estimates for the singlet S-wave resonance [16] and Ps-H binding energies [17]. The agreement of the calculated singlet resonance and binding energies with the variational estimates assures of the realistic nature of the regularized exchange potential [8]. Hence, for the sake of completeness a study of the differential cross sections for Ps-H scattering with the regularized electron-exchange potential seems worthwhile.

In this paper we present a theoretical study of Ps-H scattering employing a five-state model allowing for excitation of both Ps and H atoms using the regularized model exchange potential mentioned above. We calculate the differential cross sections for quenching in addition to those for different elastic and inelastic transitions. We also report the energies and widths of the singlet Ps-H resonances in different partial waves.

The theory for the coupled-channel study of Ps-H scattering with the regularized model potential has already appeared in the literature [8–10]. It is worthwhile to quote the relevant working equations here. We solve the following Lippmann-Schwinger scattering integral
equation in momentum space

\[ f_{\mu'\nu'\mu\nu}(k',k) = B_{\mu'\nu'\mu\nu}(k',k) \]

\[ - \sum_{\mu'\nu'} \int \frac{dk''}{2\pi^2} \frac{B_{\mu'\nu'\mu''\nu''}(k',k) f_{\mu''\nu''\mu\nu}(k'',k)}{k''^2/4 - k''^2/4 + i0} \]

(1)

where the singlet (+) and triplet (−) “Born” amplitudes, \( B^{\pm} \), are given by \( B^{\pm}_{\mu'\nu'\mu\nu}(k',k) = g^{D}_{\mu'\nu'\mu\nu}(k',k) \pm g^{E}_{\mu'\nu'\mu\nu}(k',k) \), where \( g^D \) and \( g^E \) represent the direct and exchange Born amplitudes and the \( f^{\pm} \) are the singlet and triplet scattering amplitudes, respectively. The quantum states are labeled by the indices \( \mu\nu \), \( \mu \) referring to the hydrogen atom and \( \nu \) to the Ps atom. The variables \( k, k', k'' \) etc denote the appropriate momentum states; \( k_{\mu''\nu''} \) is the on-shell relative momentum of Ps with respect to H in the channel \( \mu''\nu'' \). We use units \( \hbar = m = 1 \) where \( m \) is the electron mass. The differential cross section is defined by

\[ \frac{d\sigma}{d\Omega}_{\mu'\nu'\mu\nu} = \frac{k'}{4k} \left[ |f_{\mu'\nu'\mu\nu}(k',k)|^2 + 3|f_{\mu'\nu'\mu\nu}(k',k)|^2 \right] \]

(2)

and the quenching cross section that describes conversion from ortho- to para-positronium is defined by

\[ \frac{d\sigma}{d\Omega}_{\mu'\nu'\mu\nu}^{\text{quen}} = \frac{k'}{16k} \left| f_{\mu'\nu'\mu\nu}(k',k) - f_{\mu'\nu'\mu\nu}(k',k) \right|^2 . \]

(3)

The Ps-H direct Born amplitude is given by [18]

\[ g^{D}_{\mu'\nu'\mu\nu}(k_f,k_i) = \frac{4}{Q^2} \int \phi^*_{\mu'}(r) \left[ 1 - \exp(iQ\cdot r) \right] \phi_{\mu}(r) dr \]

\[ \times \int \chi^*_{\nu'}(t) 2i \sin(Q\cdot t/2) \chi_{\nu}(t) dt. \]

(4)

The Ps-H model exchange (Born) amplitude is a generalization of the electron-hydrogen model exchange potential of ref. [19] and is given by [10]

\[ g^{E}_{\mu'\nu'\mu\nu}(k_f,k_i) = \frac{4(-1)^{l+l'}}{D} \int \phi^*_{\mu'}(r) \exp(iQ\cdot r) \phi_{\mu}(r) dr \]

\[ \times \int \chi^*_{\nu'}(t) \exp(iQ\cdot t/2) \chi_{\nu}(t) dt \]

(5)

with

\[ D = (k_f^2 + k_i^2)/8 + C^2[(\alpha_{\mu}^2 + \alpha_{\nu}^2)/2 + (\beta_{\nu}^2 + \beta_{\nu}^2)/2] \]

(6)
where \( l \) and \( l' \) are the angular momenta of the initial and final Ps states, the initial and final Ps momenta are \( \mathbf{k}_i \) and \( \mathbf{k}_f \), \( Q = \mathbf{k}_i - \mathbf{k}_f \), \( \alpha_{\mu}^2 / 2 \) and \( \alpha_{\mu'}^2 / 2 \), and \( \beta_{\nu}^2 \) and \( \beta_{\nu'}^2 \) are the binding energies of the initial and final states of H and Ps in atomic units, respectively, and \( C \) is the only parameter of the potential. Normally, the parameter \( C \) is taken to be unity which leads to reasonably good result. However, it can be varied slightly from unity to get a precise fit to a low-energy observable. This variation of \( C \) has no effect on the scattering observables at high energies and the model exchange potential reduces to the Born-Oppenheimer exchange potential \([14]\) at high energies.

After a partial-wave projection, the singlet (+) and triplet (−) scattering equations \([1]\) are solved by the method of matrix inversion. The maximum number of partial waves included in the solution of the integral equation is 100 and the contribution of the higher partial waves is included in the first Born approximation. This procedure provides convergence of the partial-wave scheme.

In the present study we use the value \( C = 0.785 \) throughout the present investigation, as in a recent study \([10]\). Interestingly enough, with this value of \( C \), the five-state model produces a singlet S-wave Ps-H binding energy of 1.05 eV and resonance energy of 4.01 eV with width 0.15 eV. This binding energy is consistent with both the accurate variational estimate of 1.067 eV \([17]\) and experimental result of 1.1 ± 0.2 eV \([20]\). Whereas the present resonance energy is essentially identical to the recent variational study of 4.0058 eV, the agreement of the present width of 0.15 eV with the variational estimate of 0.0952 eV is only fair \([16]\). The 22-Ps-state R-matrix calculation \([5]\) yielded a S-wave resonance energy of 4.55 eV with width 0.084 eV. The present model with \( C = 0.785 \) yielded a P-wave resonance at 5.08 eV with width 0.004 eV. Variational calculation for the P-wave resonance \([21]\) yielded a energy of 4.285 eV with width 0.0435 eV, whereas the 22-Ps-state R-matrix calculation yielded 4.88 eV and 0.058 eV for these quantities, respectively.

Here we present results of Ps-H scattering using a five-state model that includes the following states: Ps(1s)H(1s), Ps(2s)H(1s), Ps(2p)H(1s), Ps(1s)H(2s) and Ps(1s)H(2p). The truncated model that includes the first \( n \) states of this set will be termed the \( n \)-state model. The Born terms for the simultaneous excitation of both H and Ps atoms are found to be
small and will not be considered here in the coupled-channel scheme. We calculate the elastic Ps(1s)H(1s) differential cross section and inelastic differential cross sections to Ps(2s)H(1s), Ps(2p)H(1s), Ps(1s)H(2s) and Ps(1s)H(2p) states. In addition we calculate the differential quenching cross section for elastic scattering.

In order to show the general trend of the result, we performed calculations at the following incident positronium energies: 20, 30, 40, 60, and 100 eV. We exhibit the differential cross sections for elastic scattering and differential quenching cross sections for elastic scattering at these energies in Figs. 1 and 2, respectively. In Figs. 3 – 6 we exhibit the inelastic cross sections for transition to Ps(2s)H(1s), Ps(2p)H(1s), Ps(1s)H(2s) and Ps(1s)H(2p) states at 20, 30, 40, 60, and 100 eV. From all these figures we find that, as expected, the differential cross section is more isotropic at low energies where only the low partial waves contribute to the cross sections. At higher energies more and more partial waves are needed to achieve convergence and the differential cross sections are more anisotropic.

As Ps is highly polarizable compared to H, Ps-excitation cross sections are larger than corresponding H-excitation cross sections and Ps excitations are expected to play a more important role in Ps-H scattering compared to H excitations. However, it is interesting to investigate the effect of the inclusion of H and Ps states on the dominating inelastic Ps cross sections at low and medium energies. At high energies such effect is small and the different cross sections tend to the corresponding first Born approximation cross sections with the the Oppenheimer exchange potential \([14,15]\). Hence, in addition to just reporting the differential cross sections we also study the effect of including more states in the expansion scheme to the dominating Ps(1s,2s,2p) partial cross sections. We make this study on the partial cross sections at different energies which we show in Table I. From the table we see how the elastic cross sections change with the inclusion of more Ps functions in the basis set. However, the inclusion of basis functions corresponding to higher excitations of H states have less influence on the convergence. Such small change of partial cross sections as in Table I will contribute to a small difference in the corresponding differential cross sections which will be unobservable in a plot on a logarithmic scale as in Figs. 1 – 6. Hence we do not exhibit the corresponding differential cross sections here.
Table 1: Ps-H partial cross sections in units of $\pi a_0^2$ at different positronium energies using different basis functions

| E (eV) | 1-St | 2-St | 3-St | 4-St | 5-St | Ps(2s) | Ps(2s) | Ps(2s) | Ps(2s) | Ps(2p) | Ps(2p) | Ps(2p) |
|-------|------|------|------|------|------|--------|--------|--------|--------|--------|--------|--------|
| 0.1   | 24.18| 22.91| 21.52| 20.73| 19.84| 0.117  | 0.115  | 0.118  | 0.120  | 1.68   | 1.74   | 1.72   |
| 5     | 7.28 | 7.24 | 5.51 | 5.47 | 5.29 | 0.078  | 0.074  | 0.070  | 0.069  | 0.83   | 0.83   | 0.82   |
| 10    | 3.97 | 3.74 | 2.80 | 2.90 | 2.50 | 0.078  | 0.074  | 0.070  | 0.069  | 0.83   | 0.83   | 0.82   |
| 20    | 1.41 | 1.37 | 1.20 | 1.18 | 1.18 | 0.078  | 0.074  | 0.070  | 0.069  | 0.83   | 0.83   | 0.82   |

To summarize, we have performed a five-state coupled-channel calculation of Ps-H scattering at medium energies using a regularized time-reversal symmetric electron-exchange model potential recently suggested by us and successfully used in other Ps scattering problems. The present model yields a singlet Ps-H S-wave resonance at 4.01 eV of width 0.15 eV and a P-wave resonance at 5.08 eV of width 0.004 eV. We present results for differential cross sections at several incident Ps energies between 20 eV to 100 eV for elastic scattering. Differential cross sections of quenching scattering are also reported in addition to those for elastic and inelastic excitation to Ps(2s,2p)H(1s) and Ps(1s)H(2s,2p) states. The effect of including the H states in the coupled-channel scheme on the elastic and Ps-excitation cross sections is found to be small.

The work is supported in part by the Conselho Nacional de Desenvolvimento - Científico e Tecnológico, Fundação de Amparo à Pesquisa do Estado de São Paulo, and Financiadora de Estudos e Projetos of Brazil.
REFERENCES

[1] A. J. Garner, G. Laricchia, and A. Özen, J. Phys. B 29, 5961 (1996); Zafar, G. Laricchia, M. Charlton, and A. Garner, Phys. Rev. Lett. 76, 1595 (1996); A. J. Garner and G. Laricchia, Can. J. Phys. 74, 518 (1996); A. J. Garner, A. Özen, and G. Laricchia, Nucl. Instrum. & Methods Phys. Res. B 143, 155 (1998).

[2] M. Skalsey, J. J. Engbrecht, R. K. Bithell, R. S. Vallery, and D. W. Gidley, Phys. Rev. Lett. 80, 3727 (1998).

[3] Y. Nagashima, T. Hyodo, K. Fujiwara, and A. Ichimura, J. Phys. B 31, 329 (1998).

[4] H. H. Andersen, E. A. G. Armour, J. W. Humberston, and G. Laricchia, Nucl. Instrum. & Methods Phys. Res. B 143, U10 (1998).

[5] C. P. Campbell, M. T. McAlinden, F. G. R. S. MacDonald, and H. R. J. Walters, Phys. Rev. Lett. 80, 5097 (1998).

[6] H. Ray, J. Phys. B 32, 5681 (1999).

[7] M. I. Barker and B. H. Bransden, J. Phys. B 1, 1109 (1968); 2, 730 (1969); S. Hara and P. A. Fraser, J. Phys. B 8, L472 (1975).

[8] S. K. Adhikari, Phys. Rev. A 62, 062708 (2000); P. K. Biswas and S. K. Adhikari, ibid. 59, 363 (1999).

[9] S. K. Adhikari and P. K. Biswas, Phys. Rev. A 59, 2058 (1999).

[10] P. K. Biswas and S. K. Adhikari, Chem. Phys. Lett. 317, 129 (2000).

[11] P. K. Biswas, Phys. Rev. A 61, 012502 (2000).

[12] S. K. Adhikari, P. K. Biswas, and R. A. Sultanov, Phys. Rev. A 59, 4829 (1999).

[13] P. K. Biswas and S. K. Adhikari, J. Phys. B 31, L737 (1998); 31, L315 (1998); 33, 1575 (2000).

[14] S. K. Adhikari and P. Mandal, J. Phys. B 33, L761 (2000).
[15] J. R. Oppenheimer, Phys. Rev. 32, 361 (1928).

[16] Y. K. Ho, Phys. Rev. A 17, 1675 (1978); Z.-C. Yan and Y. K. Ho, Phys. Rev. A 59, 2697 (1999).

[17] Z.-C. Yan and Y. K. Ho, Phys. Rev. A 60, 5098 (1999); A. M. Frolov and V. H. Smith, Jr., ibid. 55, 2662 (1997); N. Jiang and D. M. Schrader, Mat. Sc. Forum 255-2, 312 (1997).

[18] P. K. Biswas and A. S. Ghosh, Phys. Lett. A 223, 173 (1996).

[19] M. R. H. Rudge, Proc. Phys. Soc. London 86, 763 (1965).

[20] D. M. Schrader, F. M. Jacobson, N. P. Frandsen, and U. Mikkelsen, Phys. Rev. Lett. 69, 57 (1992).

[21] Y. K. Ho and Z.-C. Yan, J. Phys. B 31, L877 (1998); Z.-C. Yan and Y. K. Ho, Phys. Rev. A 57, R2270 (1998).
**Figure Caption:**

1. Differential cross section (in units of $a_0^2$) for elastic Ps-H scattering at the following incident Ps energies: 20 eV (dashed-dotted line), 30 eV (dashed-double-dotted line), 40 eV (dashed-triple-dotted line), 60 (dashed line), and 100 eV (full line).

2. Differential quenching cross section (in units of $a_0^2$) for elastic Ps-H scattering at the following incident Ps energies: 20 eV (dashed-dotted line), 30 eV (dashed-double-dotted line), 40 eV (dashed-triple-dotted line), 60 (dashed line), and 100 eV (full line).

3. Differential cross section (in units of $a_0^2$) for inelastic Ps-H scattering to Ps(2s)H(1s) state at the following incident Ps energies: 20 eV (dashed-dotted line), 30 eV (dashed-double-dotted line), 40 eV (dashed-triple-dotted line), 60 (dashed line), and 100 eV (full line).

4. Differential cross section (in units of $a_0^2$) for inelastic Ps-H scattering to Ps(2p)H(1s) state at the following incident Ps energies: 20 eV (dashed-dotted line), 30 eV (dashed-double-dotted line), 40 eV (dashed-triple-dotted line), 60 (dashed line), and 100 eV (full line).

5. Differential cross section (in units of $a_0^2$) for inelastic Ps-H scattering to Ps(1s)H(2s) state at the following incident Ps energies: 20 eV (dashed-dotted line), 30 eV (dashed-double-dotted line), 40 eV (dashed-triple-dotted line), 60 (dashed line), and 100 eV (full line).

6. Differential cross section (in units of $a_0^2$) for inelastic Ps-H scattering to Ps(1s)H(2p) state at the following incident Ps energies: 20 eV (dashed-dotted line), 30 eV (dashed-double-dotted line), 40 eV (dashed-triple-dotted line), 60 (dashed line), and 100 eV (full line).
Fig 1
Fig 2

Scattering angle (degree)

Differential cross section (units of $a_0^2$)

20 eV
30 eV
40 eV
60 eV
100 eV
Fig 3

Differential cross section (units of $a_0^2$)

Scattering angle (degree)

20 eV
30 eV
40 eV
60 eV
100 eV
Fig 4
Fig 5
Fig 6

Differential cross section (units of $a_0^2$) vs. Scattering angle (degree) for various energies: 20 eV, 30 eV, 40 eV, 60 eV, and 100 eV.