Excited-state positronium formation from positron–atomic-hydrogen collisions

C. R. Mandal, Mita Mandal, and S. C. Mukherjee
Department of Theoretical Physics, Indian Association for the Cultivation of Science, Jadavpur, Calcutta 700 032, India
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Positronium formation into ground and $n=2$ levels has been studied in collisions of positrons with atomic hydrogen in the framework of an approximation called the boundary-corrected continuum-intermediate-state (BCCIS) approximation in the energy range of 0.08–2 keV. The conventional continuum-intermediate-state approximation does not satisfy the correct boundary condition. It has been shown that, with a suitable choice of the distorting potential, the boundary condition may be satisfied with a proper account of the intermediate continuum states. It has also been shown that the BCCIS approximation leads to the same transition amplitude as may be derived using the Vainshtein-Presnyakov-Sobelman approximation. The results obtained here are found to be in good agreement when compared with other theoretical results.

I. INTRODUCTION

Because of technological advancements, intense beams of positrons in a wide range of energies are now becoming available. As a consequence, many experimental works were performed to study positron-atom collisions during the past decade. Positronium cross-section data for collisions of positrons with different atoms over a wide range of energies are now available from the experimental works of Charlton *et al.* [1], Diana *et al.* [2], Fromme *et al.* [3], and Fornari, Diana, and Coleman [4]. In addition to the motivation for understanding the large discrepancies in the existing experimental results, theoretical studies on positronium formation have an intrinsic scientific impetus for acquiring comparative knowledge of charge-transfer dynamics of light- and heavy-particle collisions. Most of the theoretical and experimental investigations reported so far have been reviewed by Humberston [5] and by Griffith [6]. However, the main emphasis in these review articles has been placed on the low-energy positron collisions with atoms and molecules.

At high energies both theoretical and experimental investigations on positron-atom collisions are quite limited. Investigations on positron-atom collisions in first-order approximations may be found in the work of Saha and Ray [7]. They have employed the first-order Born approximation (FBA) and the first-order exchange approximation (FOEA) to study positronium formation into arbitrary states in collisions of positrons with atomic hydrogen; they derived the n^{-3} law for the cross sections. Spurred by an expectation of considerable improvement in the results over the FBA in the Schrödinger representation, Straton [8] has calculated the differential and total cross sections of positronium formation in collisions of positrons with atomic hydrogen in first order in the Fock-Tani representation using the second quantization technique. However, the results so obtained do not show appreciable improvement over the conventional FBA results. In the course of their investigations on positron-atom collisions at high energies, McGuire and his collaborators [9–12] have studied the processes in the framework of the strong potential Born (SPB) approximation. In their calculations, they have accounted for the intermediate ground state of the target spectrum accompanied by Coulomb distortion and the off-shell Coulomb wave in the projectile spectrum. It is known that the off-shell Coulomb wave takes an account of the upper part of the bound states and the lower part of the continuum. Basu and Ghosh [13] have calculated the positronium-formation cross section into the $1s$, $2s$, and $2p$ states in collisions of positrons with atomic hydrogen in the second-order Born approximation. In their evaluation of the second-order Born amplitude, they have taken into account two real states $(1s,2s)$ and three pseudostates $(2\bar{p},3\bar{s},3\bar{d})$ as the intermediate states of the target spectrum. However, they have shown that their forward second-order amplitudes are convergent with these few intermediate states. For the same processes, Tripathi, Sinha, and Sil [14] have calculated the same cross sections in the framework of the eikonal approximation. In such a calculation, one effectively takes an account of the intermediate elastic scattering term only. Collisions of energetic positrons with atomic hydrogen and helium have been studied by Roberts [15] in the framework of the second-order Fadeev-Watson formalism. The essence of this method lies in the fact that the kernel of the integral equation is compact. However, for mathematical simplicity, he has made some peaking approximations in the evaluation of the transition amplitude. Positronium-formation cross sections in the intermediate-energy region have been studied very recently by Nahar [16] in the framework of the FBA and the distorted wave Born approximation (DWBA). This method was originally developed by Shakeshaft and Wadehra [17] and later applied by Nahar and Wadehra [18,19]. Results reported so far in the above theoretical approximations are at significant variance with each other in the case of col-

lisions of energetic positrons with ground-state atomic hydrogen. If we look at charge transfer as the target ionization averaged over final-state momentum distribution, it may be expected that the inclusion of target continuum intermediate states is essential in such studies. With this view, we are motivated to study charge-transfer reaction in $e^+ + H$ collisions in light of the continuum-intermediate-state (CIS) approximation. However, the conventional CIS approximation does not satisfy the proper boundary condition. To overcome this difficulty, we have chosen the distorting potential in the entrance channel in such a way that proper boundary conditions for the scattering wave function are satisfied. Another useful feature of this method lies in the fact that the perturbing potential with which the transition amplitude is calculated decreases faster than the Coulomb potential. Hereafter, we will refer to this as the boundary-corrected continuum-intermediate-state (BCCIS) approximation.

The organization of the paper is as follows. In Sec. II, the transition amplitude in the framework of the BCCIS approximation is derived and its relationship to the Vainshtein-Presnyakov-Sobelman (VPS) approximation is shown explicitly. Results obtained in the present investigation are discussed in comparison with other existing results in Sec. III. Finally, the paper ends with concluding remarks in Sec. IV. Atomic units are used unless otherwise specified.

II. THEORY

A collision diagram is shown in Fig. 1. The total Hamiltonian for the system may be written as

$$H = H_0 - \frac{1}{r_T} - \frac{1}{r_P} + \frac{1}{R} , \tag{1}$$

where

$$H_0 = -\frac{1}{2\mu_i}\nabla^2_{R_T} - \frac{1}{2a}\nabla^2_{r_T} \quad \text{(entrance channel)} , \tag{2a}$$

$$= -\frac{1}{2\mu_f}\nabla^2_{R_P} - \frac{1}{2b}\nabla^2_{r_P} \quad \text{(exit channel)} , \tag{2b}$$

and

$$\mu_i = \frac{m(m+M)}{2m+M}, \quad \mu_f = \frac{2mM}{2m+M},$$
$$a = \frac{mM}{m+M}, \quad b = \frac{m}{2} , \tag{3}$$

and where m and M are the masses of the electron or positron and the proton, respectively. The total Hamiltonian may separate in terms of the channel Hamiltonian as

$$H = H_i + V_i, \quad H_i = H_0 - \frac{1}{r_T}, \quad V_i = \frac{1}{R} - \frac{1}{r_P} \tag{4a}$$

$$H = H_f + V_f , \quad H_f = H_0 - \frac{1}{r_P}, \quad V_f = \frac{1}{R} - \frac{1}{r_T} \tag{4b}$$

and the channel wave functions satisfy the equations

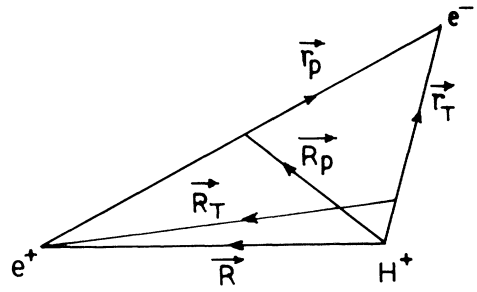

FIG. 1. Coordinate representation for the reaction $e^+ + H(1s) \rightarrow e^+ e^-(n1) + H^+$.

$$(E - H_i)\Psi_i = 0 , \quad (E - H_f)\Psi_f = 0 , \tag{5}$$

where

$$\Psi_i = \Phi_i(\mathbf{r}_T) e^{i\mathbf{k}_i \cdot \mathbf{R}_T}, \quad \Psi_f = \Phi_f(\mathbf{r}_p) e^{i\mathbf{k}_f \cdot \mathbf{R}_p} \tag{6a}$$

and

$$E = \frac{k_i^2}{2\mu_i} + \varepsilon_i \quad \text{(entrance channel)} \tag{6b}$$

$$= \frac{k_f^2}{2\mu_f} + \varepsilon_f \quad \text{(exit channel)} , \tag{6c}$$

where Φ_i (Φ_f), ε_i (ε_f), and $\mathbf{k}_i$ ($\mathbf{k}_f$) are, respectively, the initial (final) bound-state wave function, the initial (final) binding energy, and the initial (final) momenta of relative motion of the colliding systems.

A. Derivation of the transition amplitude in the BCCIS approximation

The prior form of the transition amplitude (with the first term only) in the formalism of Dodd and Greider [20] may be written in the framework of distorted theory as

$$T_{if}^{(-)} = \langle \Psi_f | \omega_f^{-*} [1 + g_x^- (V_f - W_f)]^* (V_i - W_i) \omega_i^+ | \Psi_i \rangle , \tag{7}$$

where the Möller operators ω_i^+ and ω_f^- and the propagator g_x^- are defined as

$$\omega_i^+ = 1 + \frac{1}{E - H_i - W_i + i\eta} W_i , \tag{8a}$$

$$\omega_f^- = 1 + \frac{1}{E - H_f - W_f - i\eta} W_f , \tag{8b}$$

$$g_x^- = \frac{1}{E - H + v_x - i\eta} , \tag{8c}$$

W_i (W_f) is the distorting potential in the initial (final) channel and v_x is a distorting potential in an intermediate channel, whose choice is restricted by the condition that it should contain no two-body potential occurring in V_i.

Now if we substitute

$$\omega_f^- | \Psi_f \rangle = | \chi_f^- \rangle \tag{9}$$

and

$$[1 + g_x^- (V_f - W_f)] | \chi_f^- \rangle = | \xi_f^- \rangle , \tag{10}$$

then $|\xi_f^-\rangle$ satisfies the equation [21] (in the limit $\eta\to 0$)

$$(E-H+v_x)|\xi_f^-\rangle=0 \tag{11}$$

provided that

$$v_x|\chi_f^-\rangle=0 . \tag{12}$$

Now writing $|\xi_f^-\rangle=|\Phi_f(\mathbf{r}_p)G^-\rangle$ and substituting in Eq. (11), we may find

$$\Phi_f(\mathbf{r}_p)\left[E-\varepsilon_f-H_0-\frac{1}{R}+\frac{1}{r_T}\right]G_f^- +\frac{1}{b}\nabla_{r_p}\Phi_f(\mathbf{r}_p)\cdot\nabla_{r_p}G_f^- +v_x\xi_f^-=0 . \tag{13}$$

Choosing $v_x\xi_f^-=-(1/b)\nabla_{r_p}\Phi_f(\mathbf{r}_p)\cdot\nabla_{r_p}G_f^-$ and on substitution in Eq. (13), we may find that G_f^- satisfies the differential equation

$$\left[\frac{k_f^2}{2\mu_f}+\frac{1}{2\mu_i}\nabla_{R_T}^2+\frac{1}{2a}\nabla_{r_T}^2+\frac{1}{r_T}-\frac{1}{R}\right]G_f^-=0 . \tag{14}$$

Now replacing $1/R$ by $1/R_T$ and looking for the proper boundary condition in the exit channel to our present problem, we may find the solution for G_f^- as

$$G_f^-=(b\mu_f)^{i\nu}|\Gamma(1+i\nu)|^2e^{i\mathbf{k}_f\cdot\mathbf{R}_p}\,{}_1F_1(i\nu;1;-ib(k_fR_T+\mathbf{k}_f\cdot\mathbf{R}_T))\,{}_1F_1(-i\nu;1;-ia(v_fr_T+\mathbf{v}_f\cdot\mathbf{r}_T)) , \tag{15}$$

where

$$\nu=\frac{1}{v_f},\quad \mathbf{v}_f=\frac{\mathbf{k}_f}{\mu_f} .$$

Since the incoming positron in the entrance channel interacts with a neutral atom, we choose $W_i=0$ (asymptotically) and we may find

$$(V_i-W_i)\omega_i^+|\Psi_i\rangle=V_i|\Psi_i\rangle . \tag{16}$$

So the transition amplitude given by Eq. (7) may be written explicitly as

$$T_{if}^{(-)}=(b\mu_f)^{i\nu}|\Gamma(1+i\nu)|^2\int d\mathbf{r}_T d\mathbf{R}_T e^{-i\mathbf{k}_f\cdot\mathbf{R}_p}\Phi_f^*(\mathbf{r}_p)\,{}_1F_1(-i\nu;1;ib(k_fR_T+\mathbf{k}_f\cdot\mathbf{R}_T)) \times{}_1F_1(i\nu;1;ia(v_fr_T+\mathbf{v}_f\cdot\mathbf{r}_T))\left[\frac{1}{R_T}-\frac{1}{r_p}\right]e^{i\mathbf{k}_i\cdot\mathbf{R}_T}\Phi_i(\mathbf{r}_T) . \tag{17}$$

In the case of the conventional CIS approximation [21], the choice of v_x is the same as is done here, but W_i is chosen as $1/R$ so that a Coulomb distortion is forcibly projected into the respective channel, whether it is intrinsic to the collisional system or not. A further high-energy approximation leads to the simplified form of the CIS approximation. Special care should be taken in choosing W_i so that proper boundary condition is satisfied in the entrance channel for the specific collisional problem under study.

B. Derivation of the transition amplitude in the VPS approximation

The exact transition amplitude (prior form) may be written as

$$T_{if}^{(-)}=\langle\Psi_f^-|V_i|\Psi_i\rangle , \tag{18}$$

where

$$(E-H)\Psi_f^-=0 . \tag{19}$$

In the VPS approximation [22], the exact wave function (Ψ_f^-) is approximated as

$$\Psi_f^-\simeq\Psi_f^{\mathrm{VPS}} . \tag{20}$$

Now we write

$$\Psi_f^{\mathrm{VPS}}=\Phi_f(\mathbf{r}_p)G_f^- , \tag{21}$$

where G_f^- satisfies the differential equation

$$\left[\frac{k_f^2}{2\mu_f}+\frac{1}{2\mu_i}\nabla_{R_T}^2+\frac{1}{2a}\nabla_{r_T}^2+\frac{1}{r_T}-\frac{1}{R_T}\right]G_f^- =\left[\frac{1}{R}-\frac{1}{R_T}-\frac{1}{b}\nabla_{r_p}\Phi_f(\mathbf{r}_p)\cdot\nabla_{r_p}\right]G_f^- . \tag{22}$$

Now neglecting the right-hand side of Eq. (22), we arrive at Eq. (14). With the solution for G_f^- and Ψ_f^{VPS}, it is trivial to show that the transition amplitudes are the same in both formalisms.

The transition amplitude given by Eq. (17) is evaluated in the exact same way as in our earlier investigation [23]. Excited states are generated by parametric differentiations. However, in the present investigation an added difficulty has arisen due to symmetric values of the projectile and target nuclear charges, which makes the evaluation of the hypergeometric function in the final expression more cumbersome and more computer time consuming.

III. RESULTS AND DISCUSSIONS

The computed results for positronium formation into the $1s$, $2s$, and $2p$ states in the case of positrons with

atomic hydrogen are given in Tables I–III together with other existing theoretical results. The total cross section has been calculated by applying n^{-3} law from $n \geq 3$ given by the relation

$$\sigma_{\text{tot}} = \sigma_{1s} + 1.616(\sigma_{2s} + \sigma_{2p}) . \quad (23)$$

Total-cross-section results are reported in Table IV and are compared in Fig. 2 with other results that are also calculated by Eq. (23). All comparisons are drawn only with existing theoretical results due to the nonavailability of any experimental results. As a check to our computer program, we have reproduced all first-order Born approximation (FBA) results [7] by setting the Sommerfeld parameter (ν) equal to zero in our calculation.

The cross-section results for positronium formation into the ground state are given in Table I. For a comparative study, we have also included the theoretical results of Tripathi, Sinha, and Sil [14], Nahar [16], Basu and Ghosh [13], Deb, McGuire, and Sil [11], and Roberts [15]. From the table, it is evident that our calculated results at intermediate energies differ by roughly a factor of 2 from all other results except those of Roberts [15]. With increasing energy, agreement is quite reasonable, within 15%. Capture cross-section results in the $2s$ state are given in Table II. We find from the table that our results agree quite well with those of Basu and Ghosh [13] and with the results of Nahar [16] at 200 and 500 eV, respectively. Contribution from the $2s$ state in the results of Tripathi, Sinha, and Sil [14] decreases quite fast with increasing energy in comparison to our calculated results. Good agreement is found with the results of Roberts [15] at high energies. Table III contains the results of the capture cross section in the $2p$ state. In the energy range of 80–500 eV, our calculated results are roughly half of those results obtained by Nahar [16], by Basu and Ghosh [13], by Deb [12], and also by Roberts [15]. With increasing energy, our calculated results differ significantly from those of Deb [12] and Roberts [15]. Good agreement is obtained with the results of Tripathi, Sinha, and Sil at 200 and 500 eV only. Total-cross-section results are shown in Table IV and are also compared in Fig. 2. Due to the nonavailability of any $2s$ results in the formalism of McGuire, Sil, and Deb [9], we are unable to compare them either in the table or in the figure. From Table IV and Fig. 2, we find that our calculated results for the total cross sections agree quite well with those of Tripathi, Sinha, and Sil [14] over the entire energy region. However, contributions from different shells and subshells differ appreciably between these two sets of data. Our results differ by roughly a factor of 1.5 from those of Basu and Ghosh [13] and Nahar [16]. The FBA results are larger than our calculated results over the entire region but less than the results obtained by Basu and Ghosh [13] and Nahar [16]. In this respect, the results obtained by Roberts [15] are reasonably high over the entire region. This may be due to the fact that the peaking approximation in a second-order calculation may not be reliable. Noted differences among the different sets of results may be attributed to the fact that the inclusion of intermediate states differs in different sets of results. They are also far from satisfactory completion, particularly for light particle collisions.

Differential cross-section results at 200 and 2000 eV are shown in Figs. 3 and 4, respectively. In each figure, the structures of the differential cross sections for positronium formation into the $1s$, $2s$, and $2p$ states are drawn together. From Fig. 3 we find that the minimum occurs at the same angle of approximately 35° for both cases of the capture into the $1s$ and $2s$ states, but no such minimum occurs in the curve for the $2p$ state. These minima may be attributed to the fact that the contributions from the attractive and repulsive parts of the potential interfere destructively, while such a situation does

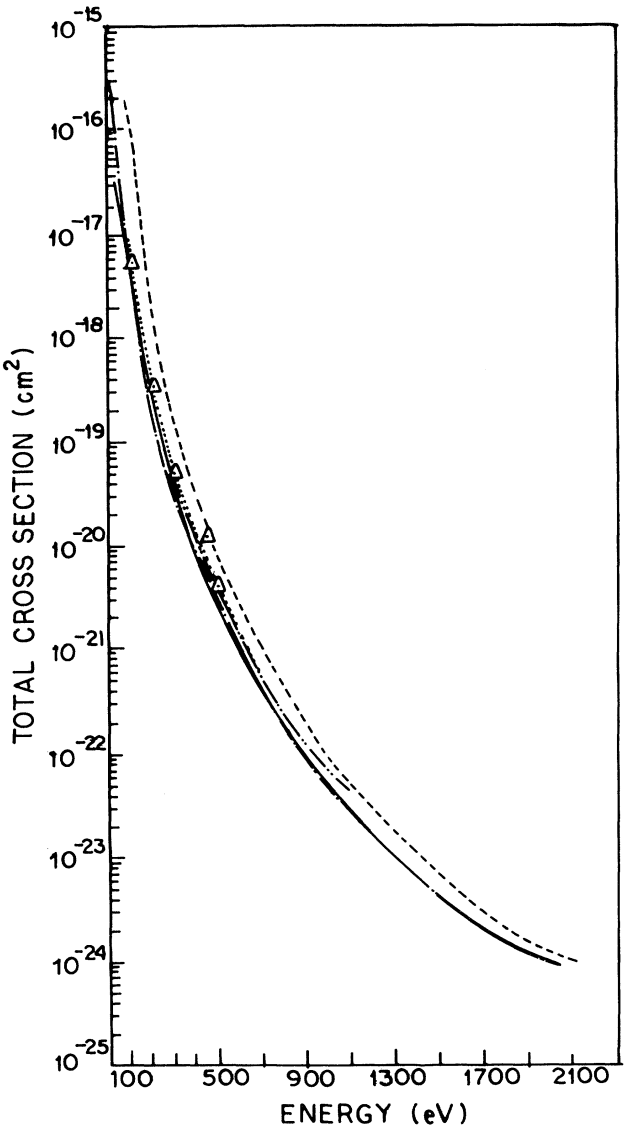

FIG. 2. Total-cross-section results for positronium formation in $e^+ + H(1s)$ collision. Theoretical results: ——, present results; — — —, results of Roberts (Ref. [15]), —·—·—, Glauber-Eikonal results of Tripathi, Sinha, and Sil (Ref. [14]); — — — —, first-order Born results; · · · ·, results of Basu and Ghosh (Ref. [11]); Δ, results of Nahar (Ref. [16]).

TABLE I. Positronium-formation cross section (in 10^{-16} cm^2) into the ground state; σ_{FBA}, first-order Born results; σ_{TSS}, results of Tripathi, Sinha, and Sil (Ref. [14]); σ_{BG}, results of Basu and Ghosh (Ref. [13]); σ_{DMS}, results of Deb, McGuire, and Sil (Ref. [10]) σ_R, results of Roberts (Ref. [15]); σ_N, results of Nahar (Ref. [16]); and σ_p, present results. Numbers in square brackets are powers of 10.

Energy (eV)	σ_{FBA}	σ_{TSS}	σ_N	σ_{BG}	σ_{DMS}	σ_R	σ_P
80	9.06[−2]	8.09[−2]		1.16[−1]			5.94[−2]
100	3.96[−2]	3.42[−2]	4.61[−2]	4.64[−2]	3.97[−2]	1.06	2.82[−2]
200	2.11[−3]	1.67[−3]	2.79[−3]	2.75[−3]	2.11[−3]	1.09[−2]	1.63[−3]
500	2.41[−5]	1.67[−5]	3.56[−5]	3.38[−5]	2.02[−5]	5.64[−5]	1.61[−5]
1000	5.68[−7]	3.82[−7]			4.08[−7]	6.84[−7]	3.50[−7]
2000	1.14[−8]	7.52[−9]			7.58[−9]	8.98[−9]	6.56[−9]

TABLE II. Positronium-formation cross section (in 10^{-16} cm^2) into $2s$ state; notations are the same as in Table I.

Energy (eV)	σ_{FBA}	σ_{TSS}	σ_N	σ_{BG}	σ_R	σ_P
80	1.36[−2]	1.27[−2]		2.22[−2]		1.49[−2]
100	6.05[−3]	5.35[−3]	6.69[−3]	1.09[−2]	1.40[−1]	7.59[−3]
200	3.18[−4]	2.46[−4]	3.81[−4]	4.46[−4]	2.60[−3]	4.59[−4]
500	3.26[−6]	2.26[−6]	4.59[−6]	4.70[−6]	8.07[−6]	4.58[−6]
1000	7.51[−8]	4.98[−8]			9.59[−8]	9.97[−8]
2000	1.49[−9]	9.59[−10]			1.21[−9]	1.94[−9]

TABLE III. Positronium-formation cross section (in 10^{-16} cm^2) into the $2p$ state; notations are the same as in Table I, except σ_D indicates the results of Deb (Ref. [12]).

Energy (eV)	σ_{FBA}	σ_{TSS}	σ_N	σ_{BG}	σ_D	σ_R	σ_P
80	4.40[−3]	3.00[−3]		5.29[−3]			1.98[−3]
100	1.67[−3]	1.03[−3]	1.37[−3]	1.93[−3]	1.29[−3]	3.49[−2]	7.75[−4]
200	4.62[−5]	2.52[−5]	4.84[−5]	5.46[−5]	4.46[−5]	5.55[−4]	2.47[−5]
500	1.93[−7]	9.68[−8]	2.82[−7]	3.06[−7]	2.60[−7]	2.48[−6]	1.41[−7]
1000	2.20[−9]	1.08[−9]			4.67[−9]	4.24[−8]	2.33[−9]
2000	2.16[−11]	1.06[−11]			1.28[−10]	7.41[−10]	3.47[−11]

TABLE IV. Total cross section (in 10^{-16} cm^2) for positronium formation in the $e^+ + H(1s)$ collision; notations follow Table I.

Energy (eV)	σ_{FBA}	σ_{TSS}	σ_N	σ_{BG}	σ_R	σ_P
80	1.19[−1]	1.06[−1]		1.60[−1]		8.67[−2]
100	5.21[−2]	4.45[−2]	5.94[−2]	6.71[−2]	1.35	4.17[−2]
200	2.70[−3]	2.11[−3]	3.50[−3]	3.56[−3]	1.60[−2]	2.41[−3]
500	2.97[−5]	2.05[−5]	4.34[−5]	4.19[−5]	7.35[−5]	2.37[−5]
1000	6.93[−7]	4.65[−7]			9.07[−7]	5.15[−7]
2000	1.38[−8]	9.06[−9]			1.21[−8]	9.75[−9]

not happen for odd angular momentum states at intermediate energy. this observation is along the same lines as previous calculations [24–26]. However, we find a second flat secondary minimum around 105° for the 2*s* state only. At large angles, the curves for the 1*s* and 2*p* states have sharp fall-off in comparison to the 2*s* state. Differential-cross-section results for the 1*s*, 2*s*, and 2*p* states at 2000 eV are shown in Fig. 4. In this case the minima occur for all the states at the same angle of approximately 32°. Here, the minima for the 1*s* and 2*s* states are sharper than the previous cases at 200 eV. In the case of the 2*s* state, a secondary but well-defined minimum is also found with a forward shift occurring at 72°. However, large-angle behavior of our differential cross-section results is different from the findings of Tripathi, Sinha, and Sil [14] and Basu and Ghosh [13]. The accounting of Coulomb distortion and the inclusion of target continuum states may be the reason for this difference.

It is well known [27] that the inclusion of the intermediate continuum states is very important to account for proper descriptions of the charge-transfer reactions at high energies. In addition, it has been well discussed by Bransden and Dewangan [28] that the boundary conditions should be satisfied in order to obtain accurate theoretical results for these reactions. The present theoretical method of calculation is embodied with these essential requirements and as such is expected to give

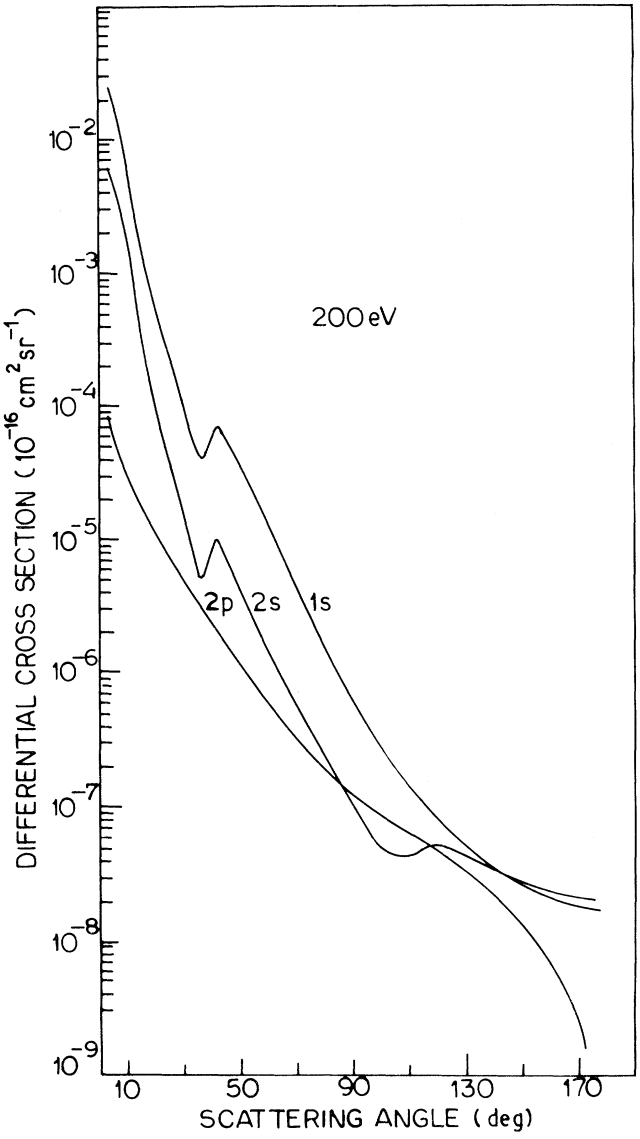

FIG. 3. Present computed results of differential cross section (in 10^{-16} cm^2 sr^{-1}) for positronium formation in $e^+ + H(1s)$ collision at 200 eV.

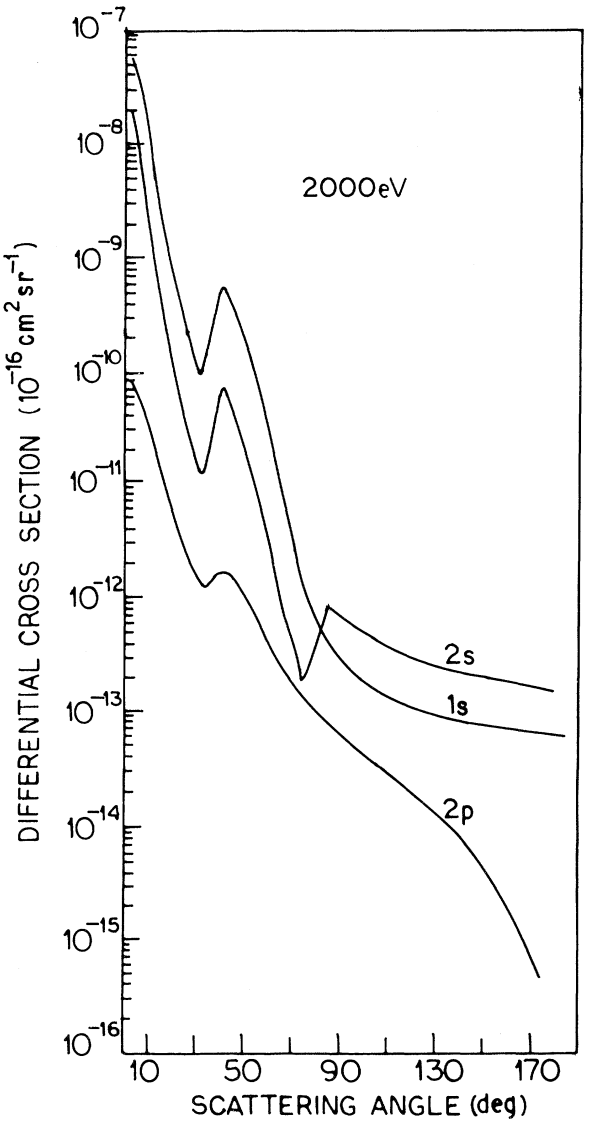

FIG. 4. Present computed results of differential cross section (in 10^{-16} cm^2 sr^{-1}) for positronium formation in $e^+ + H(1s)$ collision at 2000 eV.

more-reliable results. Unfortunately, no experimental results are available to make a quantitive assessment on all the theoretical approaches.

IV. CONCLUSION

The boundary-corrected continuum-intermediate-state (BCCIS) approximation is an intermediate theory between the continuum-intermediate-state (CIS) approximation and the continuum-distorted-wave (CDW) approximation. Although it is not a second-order theory, second-order effects are intrinsically embodied in it. By applying this theory to a positron-hydrogen collision system, the results obtained are reasonably good. Noted discrepancies in the results of positronium-formation cross sections in collisions of positrons with atomic hydrogen may only be resolved by experimental observations and more-elaborate theoretical investigations.

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