A NEW APPROACH TO UTILIZING TWO-STATE APPROXIMATION IN HYDROGEN FORMATION THROUGH LANDING PROTON ON POSITRONIUM: A COMPUTATIONAL INVESTIGATION AND STUDY

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Abstract

Despite the fact that any laboratory data on the antihydrogen formation by landing antiproton on the positronium atom, as a three-body charge-transfer reaction, at energies being appropriate for high-precision spectroscopy of antimatter has not been reported yet, some measurements of charge-conjugation reaction have been performed. This reaction is the hydrogen formation by landing proton on positronium. In this study, the two-state approximation is utilized for the charge-transfer process in the proton-positronium collisional system. Through this method, the non-orthogonality of initial and final states, and its contribution to the angular distribution of partial cross sections are considered. The state-to-state partial cross sections for the transition from the ground state of positronium to the ground state and some excited states of hydrogen are reported; furthermore, finally, the total cross sections are provided.

1. Introduction

Currently, as regards the theoretical and applied physics, one of the fascinating

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subjects is the study of matter-antimatter symmetries in the world. As the detection and investigation of hydrogen atom’s properties such as spectral lines have revolutionized physicists’ perception of matter, and considerably helped the quantum mechanics theory to be discovered and developed, the detection and investigation of antihydrogen atom can also pave the way for defining antimatter’s properties and fundamental laws of physics [1-3]. For instance, the spectroscopies conducted on hydrogen atom indicate that the excited state $2s$ is a metastable state with the lifetime $0.14\text{s}$. Such lifetime causes the half width of spectral line of transition $1s - 2s$ to considerably narrow. Regarding this half width is about one hertz, and such radiation’s frequency is of order $2.5 \times 10^{15}$, this transition can be employed to perform high-precision spectroscopies with accuracy $1/10^{15}$. If the two-photon transition $1s - 2s$ in antihydrogen atom is precisely measured, the antihydrogen Rydberg constant (the anti-Rydberg) can be accurately determined. Based on the CPT theorem, these two constants should be equal. The precise comparison between these two constants can be an important criterion for accepting or rejecting this theorem [4, 5]. Another property of hydrogen atom is that it is stable in no-material media which this stability makes preparations for conducting precise spectroscopies. However, it is essential to form the antihydrogen at low velocities in order that the Doppler effect on the first-order approximation can be neglected. In addition, to trap and detect the antihydrogen in the magnetic traps, it should be formed at very low temperatures about $1\text{K}$. Finally, since creating completely-no-material media is currently impossible, we should adequately produce antihydrogen to perform exact tests on the antimatter [1-5].

Various methods of forming antihydrogen are proposed and carried out in CERN [6-9] and Fermilab [10]. In one of the studies conducted in CERN [6], the antihydrogen atoms are produced through landing relativistic antiprotons with energies of the order $2\text{GeV}$ on the hydrogen atoms in a gas target, and through three-body charge-transfer reaction. Due to the slight amount and extremely high velocity of these achieved antihydrogen atoms, they are not appropriate to perform spectroscopy tests. In another test, by trapping antiprotons and combining them with cold positrons, the cold antihydrogen is produced [7]. Recently, through trapping $5\text{MeV}$ antiprotons in the Penning-Ioffe trap, a considerable amount of cold antihydrogen has been produced [9]. Another proposed method of producing antihydrogen is to land the antiproton on the positronium atom at low and non-
relativistic energies. Because of having large cross section, such interaction is appropriate for producing a substantial number of slow antihydrogen atoms. However, owing to the empirical limitations of slowing down antiproton by accelerators, the possibility of performing such test has not been hitherto provided, and the plans for providing such possibility are being developed. As a result of these empirical limitations, a few measurements of charge-conjugation reaction have been carried out instead of directly measuring the above reaction [11]. In these tests, the hydrogen is produced through landing the proton on the positronium atom, and its production’s total cross section is measured at three specific energies which this measurement is not very rich in statistical terms. Various theoretical studies of such reaction have been conducted [12-15]. Since this reaction is a three-body equation, its precise solution is impossible and the methods utilized to define it are approximate [16-18]. The theoretical investigation of electron-transfer process in ion-atom collisions in the framework of classical physics and through proposing a two-stage process called Thomas has been carried out by Thomas [19, 20]. In the Thomas process, the electron is scattered first by the projectile and then by the target ion in the final direction of the projectile; and since its (electron) velocity equals the projectile velocity and its (electron) charge is opposite the projectile charge, it is absorbed into the projectile. Afterwards, by means of quantum studies, Drisko demonstrated that the Thomas double process is equivalent to the second-order term of Born series [21, 22]. According to the Bohr’s correspondence principle, the limit-state quantum results should be consistent with the classical results. Therefore, at extremely high energies, it is expected that the Thomas double-scattering process will be the dominant process; consequently, the second-order Born term will be the most effective factor in the scattering amplitude. Nowadays, in the three-body scattering theory, there are lots of approximate methods whose scope of application is limited to a special range of incident energy. In this study, the two-state approximation [23, 24] is employed to compute the partial and total cross sections of hydrogen formation in the proton-positronium collision. In the second section, we describe the theoretical basis of formulation, and calculate the intended reactions. Finally, in the third section, we discuss the computations’ results.

2. The Theoretical basis and Calculations

We consider a three-body collision in which the projectile $P$ lands on a bound pair consisting of the target ion $T$ and the active electron $e$. The $M_P$, $M_T$ and $m$, ...
respectively, symbolize the mass of these particles. If the projectile’s energy is sufficient, various events could occur during such collision. The electron abstraction by projectile is one of these events, i.e., \( P + (T + e)^* \rightarrow T + (P + e)^* \). The wave function of the bound subsystem is the Hamiltonian eigenfunction \( h_i \) in the initial channel and the Hamiltonian eigenfunction \( h_f \) in the final channel:

\[
h_i \phi_i(r_T) = \varepsilon_i \phi_i(r_T); \quad h_i = -\frac{1}{2\mu_i} \nabla^2_{r_T} + V_{T_e},
\]

\[
h_f \phi_f(r_P) = \varepsilon_f \phi_f(r_P); \quad h_f = -\frac{1}{2\mu_f} \nabla^2_{r_P} + V_{P_e}.
\]

where \( \varepsilon_i \) and \( \varepsilon_f \) are, respectively, the electron energy in the initial and final bound states, \( \phi_i(r_T) \) and \( \phi_f(r_P) \) are, respectively, the eigenfunctions delineating the electron state in these channels, the vectors \( r_T \) and \( r_P \) are the vector of electron position in relation to \( T \) and \( P \), and finally, \( V_{T_e} \) and \( V_{P_e} \) are the potentials of two-body interaction between electron and the ions of target and projectile. We consider these interactions as Coulomb interactions. The reduced masses of bound subsystems in the initial and final channels are, respectively, indicated by \( \mu_i \) and \( \mu_f \). The initial and final perturbing potentials equal \( V_i = V_{PT} + V_{P_e} \) and \( V_f = V_{PT} + V_{T_e} \), respectively. The Hamiltonian of the total three-body system can be written as one of these forms: \( H = H_i + V_i \) or \( H = H_f + V_f \), where

\[
H_i = -\frac{1}{2\nu_i} \nabla^2_{r_T} + h_i + V_i, \quad H_f = -\frac{1}{2\nu_f} \nabla^2_{r_P} + h_f + V_f.
\]

\( R_T \) and \( R_P \) are the position vectors of the ions \( T \) and \( P \) in relation to the mass center of the bound subsystems \( (T + e) \) and \( (P + e) \); \( \nu_i \) and \( \nu_f \) are the corresponding reduced masses in the initial and final channels:

\[
\nu_i = M_p (M_T + m) / (M_p + M_T + m), \quad \nu_f = M_T (M_p + m) / (M_p + M_T + m).
\]

If it is assumed that the total of system is a two-state system whose states can be indicated by kets \( |i\rangle \) and \( |f\rangle \) in the corresponding Hilbert space, through
normalizing the free particle’s wave function as \( \langle r | \bar{k} \rangle = (2\pi)^{-3/2} \exp(i\bar{k} \cdot r) \), these states can be shown in the position space as the following forms:

\[
\langle \mathbf{R}_f, \mathbf{r}_f | \uparrow \rangle = (2\pi)^{-3/2} \phi_\uparrow(\mathbf{r}_f) \exp(i\mathbf{K}_i \cdot \mathbf{R}_f), \\
\langle \mathbf{R}_f, \mathbf{r}_f | \downarrow \rangle = (2\pi)^{-3/2} \phi_\downarrow(\mathbf{r}_f) \exp(i\mathbf{K}_f \cdot \mathbf{R}_f),
\]

(4)

where \( \mathbf{K}_i \) and \( \mathbf{K}_f \) are the wave vectors of incident and scattered particles, respectively. We consider their propagation as the free-particle propagation. The states indicated in equation (4) fulfill the Schrödinger equations

\[
i E_i \langle i | H | i \rangle + \epsilon_i, \quad E_f = \frac{1}{2v_f} K_f^2 + \epsilon_f.
\]

(5)

In the two-state approximation, the system’s total state is considered as a linear superposition of these eigenstates:

\[
|\psi\rangle = a(t) \exp(-iE_i t)|i\rangle + b(t) \exp(-iE_f t)|f\rangle
\]

(6)

which must satisfy the Schrödinger equation \( H|\psi\rangle = i\hbar \partial|\psi\rangle / \partial t \). Inputting this wave function to the Schrödinger equation, multiplying the equation’s both sides by \( |i\rangle \) and \( |f\rangle \), and doing some mathematical calculations lead to the two coupled equations below:

\[
i(1 - |\langle f | i\rangle|^2) a(t) = (\langle i | V | i \rangle - \langle f | V | i \rangle \langle i | f \rangle) a(t) + (\langle i | V | f \rangle - \langle f | V | f \rangle \langle i | f \rangle) b(t) e^{i(E_i - E_f) t},
\]

\[
i(1 - |\langle f | i\rangle|^2) b(t) = (\langle f | V | i \rangle - \langle i | V | f \rangle \langle i | f \rangle) a(t) e^{i(E_i - E_f) t} + (\langle f | V | f \rangle - \langle i | V | f \rangle \langle i | f \rangle) b(t).
\]

(7)

The initial conditions governing on this complex of equations are that, at initial times before the collision, the system is in the initial state, i.e., \( |a(\infty)\rangle = 1 \) and \( |b(\infty)\rangle = 0 \). The solution to the above coupled equations is achieved according to the time-dependent perturbation theory under the above initial conditions. Through
inserting the zero-order solution for amplitudes $a = 1$ and $b = 0$, the first-order transition matrix for transiting from the initial state $|i\rangle$ to the final state $|f\rangle$ is obtained as follows:

$$T_{fi} = \frac{\langle f|V|i\rangle - \langle i|V_f|i\rangle \langle f|V_f\rangle}{1 - |\langle f|V_f\rangle|^2}. \quad (8)$$

The wave function’s Fourier transform is considered as

$$\phi(k) = \int \phi(r) \exp(-i k \cdot r) dr. \quad (9)$$

Therefore, the system’s asymptotic states in the linear-momentum space are as the forms below:

$$\langle k, K|i\rangle = (2\pi)^{-3/2} \phi_i(k) \delta(K - K_i),$$

$$\langle k, K|f\rangle = (2\pi)^{-3/2} \phi_f(k) \delta(K - K_f). \quad (10)$$

Through calculating the initial and final states in the momentum space, inputting the momentum closure equation between brackets, inserting the wave functions into the integrand, and removing the three-dimensional Dirac delta functions appeared in the obtained expression, the overlap of integrals between the initial and final states, $\langle f|i\rangle$, can be computed as the following form:

$$\langle f|i\rangle = (2\pi)^{-3} \phi_f^*(K) \phi_i(-J). \quad (11)$$

where $J$ and $K$ are, respectively, the momenta transferred to the ions of target and projectile during the collision. Also, through inputting a complete ensemble of momenta, utilizing an appropriate Jacobi coordinates, applying equation 1, calculating the integrals appeared on the Dirac delta functions, and some mathematical simplifications, the Born first-order transition amplitude, $\langle f|V|i\rangle$, can be written as follows:

$$\langle f|V|i\rangle = -\frac{(2\pi)^{-3}}{2\mu_f}(K^2 - 2\mu_f e_f) \phi_f^*(K) \phi_i(-J) + (2\pi)^{-6}$$

$$\times \int d\kappa \phi_f^*(K - \kappa) \phi_i(-\kappa - J) V_{TF}(\kappa). \quad (12)$$

Considering that the interaction between all the particles is the Coulomb interaction,
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the Fourier transform of Coulomb repulsive potential \(1/r\) can be substituted for \(V_{PT}(k)\), i.e., \(V_{PT}(k) = 4\pi/k^2\). The expected value of perturbing potential in the initial channel in the initial state of the system or the transition matrix \(\langle i|V_i|i\rangle\) can be written as the integral form below:

\[
\langle i|V_i|i\rangle = \int dR V_{PT}(R) + \int dR d\tau_i V_{PT}(\tau_i) \phi_i(\tau_i) |^2,
\]

\[
\text{where } r_p = r_T + R, \text{ and the vector } R \text{ denotes the position vector of } P \text{ in relation to } T. \text{ Through inserting the two-body Coulomb attractive and repulsive potentials, and the positronium atom’s ground-state wave function, } \phi_{100}(r_T) = \frac{1}{2\sqrt{2\pi}} \exp\left(-r/2\right), \text{ into the above equation, we obtain}
\]

\[
\langle i|V_i|i\rangle = (2\pi)^{-\frac{3}{2}} \left[ \int \frac{dR}{R} - \frac{1}{8\pi} \int \frac{dR d\tau_i}{|R + \tau_i|} \exp\left(-r/2\right) \right].
\]

Subsequently, by computing different parts of the integral, we will have

\[
\langle i|V_i|i\rangle = \frac{1}{16\pi^3} \int \frac{dR}{R} \int_0^\infty (r_T - R) r_T \exp\left(-r_T\right) dr_T = \frac{1}{\pi^2}.
\]

Consequently, the expected value of the initial perturbation potential in the total system’s initial state equals \(\frac{1}{\pi^2}\) for the process below:

\[
H^+ + Ps(100) \rightarrow H(nlm) + e^+.
\]

Regarding the normalization of plane wave, the incident particles’ flux equals \(j_i = (2\pi)^{-\frac{3}{2}} K_i/v_i\). The density of final states per energy unit can also be computed as the following form:

\[
d\rho_f = \frac{K_f^2 d\Omega}{dE_f} = v_f K_f d\Omega.
\]

By employing the above equation, the probability rate of the transition to final states will be equal to \(2\pi |T_{fi}|^2 d\rho = 2\pi v_f K_f |T_{fi}|^2 d\Omega\). Through defining the partial cross section as the ratio of the transition probability rate per spatial angular unit to the
incident particles’ flux, we have

\[
\left( \frac{d\sigma}{d\Omega} \right)_{C.M.} = (2\pi)^2 \nu_i \nu_f \left( \frac{K_f}{K_i} \right) |T_{fi}|^2. \tag{18}
\]

For the rearrangement process of the transition from the positronium atom’s ground state to the hydrogen atom’s ground or excited state, i.e., the transition \(1s \rightarrow nlm\), the transition matrix can be written as follows:

\[
T_{nlm} = \frac{1}{2\pi^2} \int d^3k \frac{\phi_{nlm}^*(k + K)\phi_{100}(k - J) - \left( \frac{K^2}{2\mu_f} - \varepsilon_f + \frac{1}{\pi^2} \right) \phi_{nlm}^*(K)\phi_{100}(-J)}{(2\pi)^3[1 - |\phi_{nlm}(K)\phi_{100}(-J)|/(2\pi)^3]^2}. \tag{19}
\]

If we consider the transition \(1s \rightarrow 1s\), the integral term of equation (19) can be analytically calculated by the equation below:

\[
I = 8\pi\sqrt{2} \int \frac{d^3k}{k^2} \frac{1}{(k^2 + 2k \cdot J + J^2 + 1)^2} \frac{1}{(k^2 - 2k \cdot J + J^2 + 1/4)^2}. \tag{20}
\]

Through the Feynman integral

\[
\frac{1}{ab} = \int_0^1 \frac{dt}{[at + b(1 - t)]^2} \tag{21}
\]

and the successive differentiations with respect to \(a\) and \(b\), we obtain

\[
\frac{1}{a^m b^n} = \frac{(m + n - 1)!}{(m - 1)! (n - 1)!} \int_0^1 \frac{t^{m-1}(1-t)^{n-1} dt}{[at + b(1 - t)]^{m+n}}. \tag{22}
\]

Particularly for \(m = n = 2\), we have

\[
\frac{1}{a^2 b^2} = 6 \int_0^1 \frac{t(1-t) dt}{[at + b(1 - t)]^4}. \tag{23}
\]

By applying equation (23) to equation (20), it can be written as

\[
I = 8\pi\sqrt{2} \left( 6 \int_0^1 dt (1-t) \int \frac{d^3k}{k^2} \frac{1}{(k^2 + 1v \cdot k + x)^4} \right). \tag{24}
\]
where \( \mathbf{v} = (\mathbf{K} + \mathbf{J}) t - \mathbf{J}, \ x = \frac{1}{2} (K^2 + 1)(t + 1) \), and both of them are the function of \( t \). Now by means of the integral equality

\[
\int \frac{d\mathbf{k}}{k^2 (k^2 + 2v \cdot \mathbf{k} + x)^2} = \frac{\pi^2}{x\sqrt{x - v^2}}
\]

and twice differentiating its both sides with respect to \( x \), the three-dimensional inner integral of equation (24) is calculated. Through inputting the result to equation (24), three one-dimensional integrals of \( t \) are achieved:

\[
I = 8\pi^2 \sqrt{2} \int_0^1 dt (1 - t) \left( \frac{3}{4x(x - v^2)^{3/2}} + \frac{2}{x^2(x - v^2)^{3/2}} + \frac{2}{x^3(x - v^2)^{3/2}} \right).
\]

These one-dimensional integrals can be easily and analytically computed as well. For the other transitions, the analytic solution to the integral \( I \) is impossible, and we have to numerically compute it. Herein, the nine-point Gauss-Legendre quadrature is exploited to calculate the integrals related to the excited transitions.

### 3. Results and Discussion

In this section, a number of results are presented. Figures 1a and 1b indicate the partial cross section of hydrogen formation in the proton-positronium collision in the ground state and the electron transition to the states \( 1s, 2s \), and \( 2p \) of the formed hydrogen for the incident energies 30keV and 150keV, respectively. The cross sections are calculated in the framework of three-body system’s mass center, and the angular range is considered between 0 and 180°.

Through investigating Figures 1a and 1b, it can be observed that the angular distributions of cross section for all the states have an approximately similar shape, but different magnitudes. As expected, the ground-state transition is the dominant transition, and the transition to the excited states is smaller than to the ground state. Increasing the energy decreases the partial cross section. In the same cross sections computed for the proton-hydrogen collision using the two state approximation, a dip is observed in the cross section in the forward angles. This case is due to the fact that the two terms appeared in the numerator of equation (19) that result from two potentials with opposite signs neutralize each other’s effect. This dip in the cross section is nonphysical since the empirical measurements do not indicate such dip. As
can be seen in Figure 1, this dip in the hydrogen-formation cross section is not observed.

Figure 2a illustrates that the cross section related to the excited states $3s$, $3p$, and $3d$ is very smaller than the ground-state transition, and practically, their effect on the total cross section can be neglected. However, these cross sections have also maximum in the forward angles, and decline with increasing the scattering angle. Moreover, these partial cross sections decrease with raising the incident energy. In Figure 2b, the cross section of the transition to the final orbits corresponding to the principal quantum numbers $(n = 1, 2, 3)$ are compared with each other and with the sum of them. As can be seen, the ground-state transition dominates the other transitions, and the Oppenheimer simple rule $1/n^3$ is approximately established such that the equations $\sigma_2 = \sigma_1/8$ and $\sigma_3 = \sigma_1/27$ are approximately established in all the angles so that the total cross section of the transition to the all final bound states can be computed by $\sigma_t = \sigma_1 \sum_{n=1}^{\infty} l/n^3 = 1.20206 \sigma_1$. Therefore in any angle, the ground-state transition approximately comprises 83% of the hydrogen-formation total cross section in that angle.

In Figures 3a and 3b, using the two-state approximation (TSA), the hydrogen-formation total cross section in the proton-positronium collision is calculated for the transitions $1s - 2s$ and $1s - 2p$, respectively. The obtained results are compared with the similar results derived from the first order Born approximation (FBA) and the Eikonal approximation [25]. As many theoretical computations indicate, for the average- and high-energy regions, these approximations are appropriate for describing the charge-transfer process in three-body collisions as far as the Thomas double scattering does not become significant. Figure 3a demonstrates that, for the transition $1s - 2s$ and at low energies, the results achieved using the two-state approximation are higher than the two other approximations’ results; however, as the energy rises, these results decline, and the high energies coincide with the cross sections obtained by the first Born approximation. This coincidence is due to the fact that, in equation (19), as the energy increases, the denominator approaches the one. As can be observed in Figure 3b, for the transition $1s - 2p$, the values of TSA’s results are between the values of two other approximations’ results. However, as the energy rises, these values approach the results of FBA, and finally, coincide with them.
In Figure 4, the TSA’s results are extrapolated to the lower energies, and compared with few empirical results reported for the three-body interaction. Although the reported empirical data is not considerable in terms of number, the comparison indicates that the computations’ results are consistent with the laboratory data.

4. Conclusion

In this study, the two-state approximation is employed to compute the partial and total cross sections of hydrogen formation in the ground-state proton-positronium collision. Also, this approximation is exploited for the average- and high-energy regions, and for the electron transition to the ground state and some excited states of hydrogen atom. Through this method, the non-orthogonality of initial and final states of the system, its impact on the angular distribution of partial cross sections, and its effect on the total cross sections are investigated. In fact, the two-state approximation can be considered as a type of correction in the first Born approximation. The same as the first Born approximation, the two-state approximation can be applied at the average and high energies. At extremely high energies that the Thomas double scattering process is dominant, either the first Born approximation or the two-state approximation are not valid, and the second-order terms applying the effect of Thomas process on the scattering must be added to them. In the two-state approximation’s valid region, its results are compared with the other calculations’ results and available laboratory results. This comparison indicates a good consistence.

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References

Figure 1. The partial cross section of hydrogen formation in the ground state $1s$ and excited states $2s$ and $2p$ in the ground-state proton-positronium collision for the incident energies: (a) 30 keV; (b) 150 keV.
Figure 2. The partial cross section of hydrogen formation (a) in the excited states 3s, 3p, and 3d for the incident energy 150 keV; (b) the comparison of the cross sections of the transition to the principal quantum orbits $n = 1, 2, 3$, and the sum of them at the same energy.
Figure 3. The hydrogen-formation total cross section for the transitions: (a) $1s \rightarrow 2s$ and (b) $1s \rightarrow 2p$ that are computed using the two-state approximation, and compared with the results of the first Born and Eikonal approximations.
Figure 4. The comparison between the TSA’s results and the available laboratory data.