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Research Article

# Ionization of the 1*S* and *nS* States of the Atomic Hydrogen by Positron and Electron Impacts

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**Abstract.** The ionizations of the $1S$ and $nS$ states of the atomic hydrogen have been carried out using the hybrid theory, which is variationally correct and has been obtained by modifying the method of polarized orbitals. Earlier, we calculated cross sections of exciting the higher states from the ground state, and cross sections of photoabsorption. Now, we apply the same approach to the ionization of states. The distortion of the orbit is considered due to the incident positron or electron. The distortion takes place whether the incident particle is outside or inside the orbit. Temkin considered distortion of the target electron only when the incident particle is outside the orbit of the target. However, there is no simple way to consider distortion of $nS$ states of atomic hydrogen. The cross sections are calculated by considering the distortion in the initial state as well as in the final state only in the $1S$ state and are compared with the previous calculations and the experimental results. The present cross sections have a maximum at an energy which is the same as the incident energy in the experimental results.

**Keywords.** Positron and electron impact ionization of the $1S$ and $nS$ states of atomic hydrogen, Polarizability

**PACS.** 34.kw



## 1. Introduction

Using quantum mechanics and relativity, Dirac [1] in 1928 formulated the relativistic wave equation, which helped him to predict an antiparticle, called positron, of electron of spin $\frac{\hbar}{2}$. Positrons, produced by the collision of cosmic rays in a cloud chamber, were detected experimentally by Anderson [3] in 1932. This was an important discovery of the 20th century.

Formation of antihydrogen by positronium impact on antiproton has been studied. Mills [10] observed the positronium ion and by photodetachment created a positronium atom. The positronium annihilation has been used to study Fermi surface in a single crystal. The annihilations of positrons with electrons resulting in 0.511 MeV gamma rays in the galaxy have been studied, providing important information about the solar atmosphere [12]. Positrons are used in the PET scan (Positron Emission Tomography) to detect cancer in the human body. We have used the hybrid theory [4] to calculate positronim formation, positron and electron annihilation cross sections, and to study elastic scattering. We have used the same formulation to calculate electron-hydrogenic systems elastic scattering phase shifts, photo absorptions cross sections of two-electron systems, and their recombination [5]. The previous calculations of various processes are mentioned to indicate that the hybrid theory is a useful formulation and provides accurate results. Now, we apply the same formulation to study ionization of atomic hydrogen by positrons and electrons impacts. Ionization of hydrogen atoms has been of interest for a long time. Attempts have been made to derive the threshold law. In 1953, Wannier [17] derivation indicated that the cross section at threshold is $\sigma \propto E^{1.1268}$, where $E$ is the excess energy after ionization of the hydrogen atom. For positron impact, derivation by Klar [9] gave $\sigma \propto E^{2.65}$. However, it has not been possible to derive the proportionality coefficient. Temkin [16] made several attempts.

## 2. Calculations

We describe first ionization by positron impact. Ionization of the $1S$ state of the hydrogen atom is indicate by

$$e^+ + H(1S) \to e^+ + p + e^- . \tag{2.1}$$

Cross section for ionization is given by

$$\sigma = \frac{k_f}{k_i}\int |T_{f_i}|^2 d\Omega, \tag{2.2}$$

where $k_i$ and $k_f$ are the initial and final momenta of the positron and $T_{f_i}$ is the matrix element given by

$$T_{f_i} = -\frac{1}{4\pi}\left\langle \psi_f \left| \frac{2Z}{r_1} - \frac{2}{r_{12}} \right| \psi_i \right\rangle . \tag{2.3}$$

In the above equation, $\psi_i$ and $\psi_f$ are the initial and final state wave functions.

$Z = 1$ is the nuclear charge, $r_1$ and $r_2$ are position coordinates of the incident positron and target electron, and $r_{12} = |\vec{r_1} - \vec{r_2}|$. The initial wave function is given by

$$\psi_i(r_1, r_2) = u(\vec{r_1})\phi^{\text{pol}}(r_1, r_2), \tag{2.4}$$

$\phi^{\text{pol}}(r_1, r_2)$ is the target function which represents the distortion of the ground state wave function $\phi(r_2)$ due to the incident positron and is given [15] by $\phi^{\text{pol}}$, as indicated below

$$\phi^{\text{pol}}(r_1, r_2) = \left[\phi(\vec{r_2}) + \frac{\chi(r_1)}{r_1^2} e^{-Zr_2}(0.5Z r_2^2 + r_2)\cos(\theta_{12})/\sqrt{\pi Z}\right]. \tag{2.5}$$

In the electron-hydrogen scattering, the sign before the second term is negative [15] instead of positive sign. The fact that the sign is positive in the positron-hydrogen scattering can be verified by going through the derivation given in reference [15].

$\chi(r_1)$ is the cutoff function which can be chosen in various forms. We chose the one introduced by Shertzer and Temkin [13] and is given by

$$\chi(r_1) = 1 - e^{-2Zr_1}\left(\frac{r_1^4}{3} + \frac{4r_1^3}{3} + 2r_1^2 + 2r_1 + 1\right). \tag{2.6}$$

The scattering function $u(\overrightarrow{r_1}) = \frac{u(r_1)}{r_1} Y_{L0}(\Omega_1)$ is obtained by solving the equation

$$\langle \phi^{\text{pol}}(r_1, r_2)|H - E|u(\overrightarrow{r_1})\phi^{\text{pol}}(r_1, r_2)\rangle = 0. \tag{2.7}$$

The function (2.6) results in an attractive polarization potential $\alpha(r_1)/r_1^4$ in the equation for the continuum function $u$, where $\alpha(r_1)$ is the dipole polarizability equal to 4.5 $a_0^3$ for for the ground state of the hydrogen atom when $r_1$ is tending to infinity. We assume that after ionization, positron and electron share the remaining energy equally. The same is the case when there are 2 electrons in the final state. We have

$$k_f^2 + k_e^2 = k_i^2 - 1.0, \tag{2.8}$$

where 1.0 Ryd is the binding energy of the 1$S$ state.

The final state wave function is given by

$$\psi_f(\overrightarrow{r_1}, \overrightarrow{r_2}) = e^{\overrightarrow{k_f \cdot\cdot r_1}} FC(k_e, \overrightarrow{r_2}), \tag{2.9}$$

where $e^{\overrightarrow{k_f \cdot\cdot r_1}}$ is a plane wave function [7] having an expansion given by

$$4\pi(i)^l Y_{lm}(\widehat{k}_f) Y_{lm}(\Omega_1). \tag{2.10}$$

$FC((k_e, \overrightarrow{r_2})$ is the Coulomb function given by

$$\frac{FC(r_2)}{(k_e, r_2)} Y(\Omega_2). \tag{2.11}$$

These functions, at various $r_2$ are obtained from the Handbook [2]. The cross sections at various energies are given in Table 1. Incident partial waves up to 5 are usually required to obtain converged results, as shown in Table 2.

## 3. Positrons and Electron Cross Sections

We have calculated ionization of the 1$S$ state by positron impact. The cross sections are given in Table 1. We find there is a maximum of the cross sections at an incident energy of 1.25 Ryd. Convergence with respect to partial waves is given in Table 2.

**Table 1.** Ionization cross sections of 1$S$ state by a positron impact (units are $10^{-16}$ cm$^2$) at various incident energies (Ryd)

| $k_i^2$ | Cross sections | $k_i^2$ | Cross sections |
|---|---|---|---|
| 1.20 | 0.4160 | 1.60 | 0.1630 |
| 1.25 | 0.6716 | 2.00 | 0.7557(−1) |
| 1.30 | 0.3224 | 3.00 | 0.1629(−1) |
| 1.40 | 0.2539 | 4.00 | 0.5601(−2) |
| 1.50 | 0.2021 | 5.00 | 0.2303(−2) |

**Table 2.** Converge of cross sections of $1S$ state (units are $10^{-16}$ cm$^2$) by positron impact of at incident energy of 5 Ryd with a partial wave $L$

| L | Cross sections |
|---|---|
| 0 | 0.9896(−3) |
| 1 | 0.9547(−3) |
| 2 | 0.3397(−3) |
| 3 | 0.1830(−4) |
| 4 | 0.3723(−6) |
| 5 | 0.3828(−8) |

In Table 3, phase shifts of positron-hydrogen are given at two incident energies, 1.2 and 1.4 (Ryd). Phase shifts increase in the beginning and then decrease as $L$ increases.

**Table 3.** Phase shifts for positron-hydrogen scattering at two energies, 1.2 and 1.4 (Ryd) for various partial waves

| L | $k_i^2 = 1.2$ | $k_i^2 = 1.4$ |
|---|---|---|
| 0 | −3.813(−1) | −4.002(−2) |
| 1 | −3.340(−2) | −4.890(−2) |
| 2 | 2.945(−2) | 2.457(−2) |
| 3 | 2.765(−2) | 2.799(−2) |
| 4 | 1.808(−2) | 1.965(−2) |
| 5 | 1.118(−2) | 1.259(−2) |

## 4. Ionization of excited states

In Table 4, we give ionization cross sections of excited states due to the positron impact. As indicated earlier, the distortion of the excited states has not been considered. It is a nontrivial problem to define a suitable wave function as a simple expression given equation (2.5) for the ground state (cf. reference [6] for details).

**Table 4.** Ionization cross sections ($a_0^2$) of the exited states of hydrogen by positron impact

| | Cross sections | | | |
|---|---|---|---|---|
| $k_i^2$ | $1S$ | $2S$ | $3S$ | $4S$ |
| 0.49 | | 4.1883 | 1686.4690 | |
| 1.20 | 1.4864 | 0.3213 | 57.6382 | 0.5499(−1) |
| 1.40 | 0.9072 | 0.2006 | 29.4576 | 0.6827(−2) |
| 2.00 | 0.2701 | 0.5120(−1) | 4.1531 | 0.6933(−3) |
| 3.00 | 0.5822(−1) | 0.8941(−2) | 0.5112 | 0.1096(−2) |
| 4.00 | 0.2001(−1) | 0.2605(−2) | 0.4792(−1) | 0.2495(−3) |
| 5.00 | 0.8229(−2)) | 0.1321(−2) | 0.2439(−1) | 0.2775(−4) |

There is an experiment on the ionization of atomic hydrogen by Spicher *et al*. [14]. The present results indicate a maximum in the cross sections at 1.25 Ryd which agrees with the maximum given in [14], Figure 3. However, their result includes the contributions of the electron-impact ionization as well as proton-impact ionization. To compare the calculated results with those of [14], we calculated cross sections due to the electron impact. In Table 3, we give total cross sections.

Position of the calculated maximum of the cross sections agrees with the position of their observed cross section. They give results in a figure. It is difficult to make a quantitative comparison. Ghosh *et al*. [8] have calculated ionization cross sections. The present results are very much like their results. However, we cannot compare their results with the present results because they have a negative sign in the $\phi^{\rm pol}(r_1,r_2)$ in eq. (2.5) while it should be positive for positrons. Also, they have not given any details about the initial state: Does it include distortion of the target? In Table 4, phase shifts of positron-hydrogen are given at incident energies.

Ionization cross sections of the excited states of the atomic hydrogen by positron impact have been carried out and compared with the cross sections of the ground state. After the ionization, the electron and proton are in the Coulomb field exactly as in the ionization of the ground state. The present cross sections, given in Table 4, are found to be higher than the cross sections for the ground state. The cross sections tend to increase near the threshold. However, no concise expression like eq. (2.5) is available for the distortion of the excited states [6]. Therefore, no distortion has been included in the initial and final states.

## 5. Electron Impact Ionization

We describe changes required in the above formulation to calculate electron impact ionization cross sections. The matrix element is given by

$$T_{f_i} = -\frac{1}{4\pi}\left\langle \psi_f \left| -\frac{2Z}{r_1} + \frac{2}{r_{12}} \right| \psi_i \right\rangle. \tag{5.1}$$

In eq. (2.5), the plus sign before $\chi(r_1)$ should be changed to a minus sign. The initial wave function is given by

$$\psi((r_1,r_2) = \frac{1}{\sqrt{2}}[u(\overrightarrow{r_1})\phi^{\rm pol}(r_1,r_2) \pm (1 \leftrightarrow 2)]. \tag{5.2}$$

We include an exchange of identical particles in eq. (5.2). In the above equation, the plus sign refers to the singlet states while the minus sign refers to the triplet states. The rest of the formulation remains the same. In Table 5, we give the electron impact cross sections. These cross sections increase and then decrease as the incident energy increases.

In Table 6, we give the total ionization cross sections due to the positron and electron impact total ionization cross sections. Electron impact cross sections are given in Table 7.

The present results indicate a maximum in the cross sections at 1.25 Ryd which agrees with [14, Figure 3], indicating the maximum. Their results include the contributions of the electron-impact ionization as well as proton-impact ionization. Position of the calculated maximum of the cross sections at 1.25 Ryd = 17 eV agrees with the position at 20 eV of their observed maximum cross section. However, the calculated cross section at 17 eV is 3.7 $10^{-16}$ cm$^2$, while the observed value is 1.5 $10^{-16}$ cm$^2$. Perhaps there is contamination due to hydrogen molecules. They give results in a figure. It is difficult to make a quantitative comparison. The present calculation includes exchange and the distortion in the initial as well in the final

**Table 5.** Electron impact ionization cross sections (units are $10^{-16}$ cm$^2$) at various incident energies (Ryd)

| $k_i^2$ | Cross sections | $k_i^2$ | Cross Sections |
|---|---|---|---|
| 1.20 | 1.3479 | 1.60 | 0.3712 |
| 1.25 | 2.9976 | 2.00 | 0.1396 |
| 1.30 | 2.6911 | 3.00 | 0.1339 |
| 1.40 | 0.5122 | 4.00 | 0.1439 |
| 1.50 | 0.6307 | 5.00 | 0.1675(−1) |

**Table 6.** Positron and electron ionization impacts cross sections (units are $10^{-16}$ cm$^2$) at various incident energies (Ryd)

| $k_i^2$ | Cross sections | $k_i^2$ | Cross sections |
|---|---|---|---|
| 1.20 | 1.7639 | 1.60 | 0.5342 |
| 1.25 | 3.6696 | 2.00 | 0.2151 |
| 1.30 | 3.0135 | 3.00 | 0.1502 |
| 1.40 | 0.7661 | 4.00 | 0.1495 |
| 1.50 | 0.8322 | 5.00 | 0.1905(−1) |

**Table 7.** Ionization cross sections ($a_0^2$) of the exited states of hydrogen by electron impact

| $k_i^2$ | $1S$ | $2S$ |
|---|---|---|
| 1.20 | 1.4864 | 0.1297(−1) |
| 1.40 | 0.9072 | 0.1831 |
| 2.00 | 0.2701 | 0.7438(−1) |
| 3.00 | 0.5822(−1) | 0.2858(−1) |
| 4.00 | 0.2001(−1) | 0.2115(−2) |
| 5.00 | 0.8229(−2) | 0.7991(−3) |

state. Ghosh *et al*. [8] have calculated ionization cross sections. The present results are very much like their results. However, we cannot compare their results with the present results because they have a negative sign in the $\phi^{\mathrm{pol}}(r_1, r_2)$ in eq. (2.5) while it should be positive. Also, they have not given any details about the initial state: Does it include distortion of the target? In Table 7, we give cross sections for ionizing the $1S$ and $2S$ states. Experimental results of ionization of the $2S$ by electron impact could not be found.

## 6. Conclusions

We have used the hybrid theory to calculate positron-impact and electron-impact ionization cross sections of the $1S$ state of the atomic hydrogen. The distortion of the orbit of the target is considered in the initial state as well as in the final state. In Table 6, we give the total cross sections. The experimental results include the positron-impact as well as the electron-impact cross sections. The present results appear to compare well qualitatively with the curve of the experimental results. We find that the calculated cross sections are higher than the experimental results. It would have been helpful if numerical results were given instead of a curve. The present formulation has been used to calculate ionization of higher states. The present formulation can be used to calculate ionization cross sections of various states of hydrogenic ions. Calculations were carried out in quadruple precision using the noniterative method [11], and they were carried out using computer of the Heliophysics Science Division.

## Appendix

For a positron impact ionization, using eq. (2.9) and eq. (2.10), we can write the first term of eq. (2.3) in the form

$$T_1 = -\frac{2Z}{4\pi}\left\langle \psi_f \left| \frac{1}{r_1} \right| \psi_i \right\rangle, \tag{A.1}$$

$$= -2Z(-i)^L (sum5)(sumC) Y_{L0}(\widehat{k}_f), \tag{A.2}$$

where

$$sum5 = \int_0^\infty dr_1 j_L(k_f r_1) u(r_1), \tag{A.3}$$

$$sumC = 2z^{1.5} \int_0^\infty r_2 dr_2 FC(r_2) e^{-Zr_2}, \tag{A.4}$$

$$T_2 = \frac{1}{4\pi}\left\langle \psi_f \left| -\frac{1}{r_{12}} \right| \psi_i \right\rangle, \tag{A.5}$$

$$T_2 = T_{22} + T_{22}^{\text{pol}}, \tag{A.6}$$

$$T_{22} = 4Z^{1.5} Y_{L0}(\widehat{k}_f) \int_0^\infty r_1 dr_1 j_L(k_f r_1) Ex8(r_1), \tag{A.7}$$

where

$$Ex8(r_1) = \int_0^\infty r_2 dr_2 \frac{FC(r_2)}{r_>} e^{-Zr_2}, \tag{A.8}$$

$$T_{22}^{\text{pol}} = \frac{4}{3}\frac{1}{\sqrt{Z}} Y_{L0}(\widehat{k}_f)(sum5p), \tag{A.9}$$

$$sum5p = \int_0^\infty r_1 dr_1 j_L(k_f r_1) \frac{\chi(r_1)}{r_1^2} u(r_1) Ex88(r_1), \tag{A.10}$$

where

$$Ex88(r_1) = \int_0^\infty FC(r_2) \frac{r_<^L}{r_>^{L+1}} e^{-Zr_2}\left(\frac{Z}{2} r_2^2 + r_2\right). \tag{A.11}$$

### Competing Interests

The author declares that he has no competing interests.

### Authors' Contributions

The author wrote, read and approved the final manuscript.

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