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Research Article

Excitations of the 4F and 5F States of Atomic Hydrogen by Positron Impact

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Abstract. The excitation cross sections of the 4F and 5F states of atomic hydrogen by positron impact have been calculated at low incident energies (from 1.00 to 4.41 Ry), using the variational polarized method, also called the hybrid theory. Partial waves ranged from $L = 3$ to 20 to obtain converged cross sections. The importance of the long-range interaction in the threshold region is discussed. A comparison of S, P, D, and F cross sections is given. These cross sections are needed because of cascades from higher states to the S state when the cross sections of the S state in hydrogen are measured or in diagnostics of solar and astrophysical observations. The phase shifts at low energies are also given.

Keywords. Hybrid theory, Excitation cross sections, Phase shifts

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1. Introduction

Dirac [6] in 1928, using the concepts of the relativity theory and quantum mechanics, formulated the relativistic equation of an electron. He predicted a positive particle, proton, as an antiparticle of an electron. At that time, electrons and protons were the only particles known. Hermann Weyl showed from the symmetry considerations that this antiparticle must have the same mass as an electron. Later, this particle came to be known as a positron, which was discovered in cosmic rays by Anderson [1] in 1933. Positrons and electrons form positronium atoms which annihilate giving a 511 keV gamma ray line with a width of 1.6 keV. This line originates from the center of the galaxy and has been observed. Positrons have been discovered in the Sun, stars, and in the interstellar medium (Gopalswamy [8]). They also contribute to the opacity of the atmosphere of the Sun (Bhatia and Pesnell [5]). They have been used in medicine called PET (*Positron Emission Tomography*) scan. The scan is used to monitor and treat a verity of conditions of diseases in the body. Positrons have been used to detect defects in metal surfaces. Mills [9] produced positronium ions and then by photodetachment created positronium atoms, which are like hydrogen atoms. We use Ry units: length is in the Bohr radius a_0 and energy is in Rydberg = 13.605 eV. Throughout $a(-b)$ implies $a \times 10^{-b}$.

2. Theory and Calculations

Earlier, we studied various processes involving positrons. Among such processes are scattering, annihilation, excitation etc. We used the hybrid theory, also called variational polarized orbital method (Bhatia [3]) which includes both short-range and long-range correlations and is variationally correct, i.e., the calculated phase shifts have lower bonds to the exact phase shifts. We have calculated cross sections for the excitation of S, P, and D states (Bhatia [4]). Now, we extend the same method to calculate cross sections for the excitation of the $n = 4$ and 5, and $l = 3$ states. The method for calculating has been described in various publications. However, for completeness and clarity, we briefly describe this method. The excitation cross section from the initial state 'i' to the final state 'f' is given by

$$\sigma_{fi} = \frac{k_f}{k_i} \int |T_{fi}|^2 d\Omega. \tag{2.1}$$

In the above expression k_i and k_f are the initial and final momenta and the transition matrix T_{fi} given by

$$T_{fi} = -\left(\frac{1}{4\pi}\right) \langle \Psi_f | V | \Psi_i \rangle. \tag{2.2}$$

The transition involves a potential given by

$$V = \frac{2Z}{r_1} - \frac{2}{r_{12}}, \tag{2.3}$$

where r_1 is the distance of the incident positron from the nucleus, which is assumed to be of infinite mass so that the recoil can be neglected, $r_{12} = |\vec{r}_1 - \vec{r}_2|$ is the positron-electron distance, and Z is the nuclear charge. The initial state wave function is given by

$$\Psi_i = u(\vec{r}_1)\Phi^{pol}(\vec{r}_1, \vec{r}_2), \tag{2.4}$$

In the above, $u(\vec{r}_1)$ represents the scattering function and $\Phi^{pol}(\vec{r}_1, \vec{r}_2)$ is the target wave function when the target is polarized due to the incident positron which produces a change in energy equal to $-0.5\alpha E^2$, where α is the polarizability of the target and E is the electric field produced by the incident positron. The polarized target function (Temkin and Lamkin [12]) is given by

$$\Phi^{pol}(\vec{r}_1, \vec{r}_2) = \varnothing_0(\vec{r}_2) + \frac{\chi(r_1)}{r_1^2} u(r_2) \frac{\cos(\theta_{12})}{\sqrt{Z\pi}}. \tag{2.5}$$

In the above, $\chi(r_1)$ is a smooth cutoff function (Shertzer and Temkin [11]), given by

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

The function $u(r_2)$ is given by

$$u(r_2) = e^{-Zr_2}(0.5Zr_2^2 + r_2). \tag{2.7}$$

The unperturbed target function is given by

$$\emptyset_0(\vec{r}_2) = \sqrt{\frac{Z^3}{\pi}} e^{-Zr_2}. \tag{2.8}$$

The scattering function has a wave plane normalization (Edmonds [7]), given by

$$\sqrt{4\pi(2L+1)}. \tag{2.9}$$

Including the normalization, we can write the scattering function in the form

$$u(\vec{r}_1) = \sqrt{4\pi(2L+1)}\frac{u(r_1)}{r_1} Y_{L0}(\theta_1, \emptyset_1). \tag{2.10}$$

The spherical harmonics Y_{L0}, a function of the angular momentum L, depends upon the spherical polar angles θ_1 and $\emptyset_1$. The scattering function $u(r_1)$ is obtained from the functional involving the Schrodinger equation

$$\int d(\vec{r}_2)\Omega_1 Y_{L0}(\Omega_1)\Phi^{pol}|H - E|\Psi_i = 0. \tag{2.11}$$

In the above equation, $E = E_{target} + k_i^2$ is the total energy and H is the Hamiltonian of the system:

$$H = -\nabla_1^2 - \nabla_2^2 + \frac{2Z}{r_1} - \frac{2Z}{r_2} - \frac{2}{r_{12}}. \tag{2.12}$$

The resulting differential equation is solved by a non-iterative method (Omidvar [10]). The final wave function is given by

$$\psi_f(\vec{r}_1, \vec{r}_2) = \phi_{nf}(\vec{r}_2) e^{i\vec{k}_f \vec{r}_1}. \tag{2.13}$$

In the above equation, $\phi_{nf}(\vec{r}_2)$ represent the target wave function in the excited state nF, $n = 4$, and 5 while $l = 3$.

3. Results

In Table 1, we give the excitation cross sections for exciting nF states by positron impact.

Table 1. Cross sections $\sigma(\pi a_0^2) \times 10^3$ for exciting nf states

k_i	$n = 4$	$n = 5$
1.0	0.197	0.151
1.1	0.525	0.280
1.2	0.297	0.290
1.3	0.261	0.281
1.4	0.236	0.274
1.5	0.204	0.276
1.6	0.195	0.281
1.7	0.184	0.277
1.8	0.171	0.232
1.9	0.207	0.365
2.0	0.215	0.380
2.1	0.227	0.414

We find that the cross sections are significant. Perhaps $l = 4$ excitation cross sections would be still significant. In Table 2, we show the convergence with respect to the angular momentum L for $k_i = 1.6$ for $n = 4$ as well as or $n = 5$ excitation cross sections.

Table 2. Convergence with respect to L

L(max)	$n = 4$	$n = 5$
3	0.869(−4)	0.197(−3)
4	0.914(−4)	0.207(−3)
5	0.963(−4)	0.212(−3)
6	0.107(−3)	0.221(−3)
7	0.124(−3)	0.235(−3)
8	0.144(−3)	0.249(−3)
9	0.162(−3)	0.262(−3)
10	0.176(−3)	0.273(−3)
11	0.188(−3)	0.281(−3)
12	0.195(−3)	0.786(−5)

In Table 3, we give the total excitation cross sections of nS, nP, nD and nf states.

Table 3

k_i	Cross sections for exciting nS, nP, and nD states	Cross sections including $4f$ and $5f$ states
1.0	1.91	1.9103
1.1	2.26	2.2608
1.2	2.35	**2.3506**
1.4	2.38	2.3805
1.5	2.23	2.2305
1.6	2.20	2.2005
1.8	2.02	2.0204
2.0	1.83	1.8306

In Table 4, we give phase shifts for a few incident momenta and angular momenta.
In Table 4, phase shifts (radians) at a few values of the incident momenta.

Table 4

k_i	$L = 3$	$L = 4$	$L = 5$
0.5	1.007(−2)	4.831(−3)	2.645(−3)
1.0	2.419(−2)	1.547(−2)	9.525(−2)
1.5	1.896(−2)	1.984(−2)	1.560(−2)
2.0	8.612(−4)	1.395(−2)	1.589(−2)

4. Conclusions

We have calculated excitation cross section, at low incident positron energies, of the $4F$ and $5F$ states of atomic hydrogen, using the hybrid theory. We find these cross sections have significant values. Earlier, we have calculated excitation cross sections of nS, nP, and nD states. These cross sections were found to be much larger than the present cross sections. Wigner [13] has pointed out the importance of long-range forces near the threshold. We have included such forces throughout the calculation. Decay to the lower states can be observed, and the observed transition rates can be compared with those given in Bethe and Salpeter [2].

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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