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Research Article

4F and 5F Excitations of Atomic Hydrogen by Electron Impact

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Abstract. The excitation cross-sections of the 4F and 5F states of atomic hydrogen by electron impact have been calculated at incident energies 1.00 to 42.25 Ry, using the hybrid theory, which is variationally correct. The present calculation is a single-channel or a distorted wave calculation. Partial waves ranged from $L = 3$ to 14 to obtain converged results. Excitations of higher states are needed for diagnostics of the solar and astrophysical plasmas. They are also needed to model plasma in fusion research, because they indicate the possibility that a state will be excited to a higher state when colliding with another state. Transition rates to the lower states can be measured by observing decays of the excited states.

Keywords. Hybrid theory, Excitation cross-sections

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1. Introduction

Excitation of atoms and ions has applications in various fields like photochemistry, creating fluorescence, in laser field, solar, astrophysics, and fusion research etc. Gryziński [8] carried out calculations of excitation and ionization of atoms, molecules, and ions using classical theory, obtaining cross-sections within a factor of 2 or 3 compared to the experimental results. However, cross-sections for excitations to $2S$ [4] state of atomic hydrogen calculated using the hybrid theory [5] agreed well with those obtained using the close-coupling and R-matrix formalisms. Later, excitations to P [3] and D [6] states were also calculated using the same formalism. This formalism is variationally correct and gives bounds on the phase shifts. They are always lower than the exact results, approaching the exact results as the basis in the calculation is increased. Also, cross-sections obtained using this approach for photo detachment and photoionization agree well with those obtained using the close-coupling and R-matrix formalisms. These two approaches provide accurate results for most processes. The hybrid theory has also been applied to calculate Feshbach resonances [2]. The excited states are important because of the emission and absorption of light in atomic hydrogen. The transition rates can be measured when the excited states decay to the lower states and compared to the theoretical rates [1]. The incident electron loses 0.9375 Ry in exciting the 4F state of angular momentum $l_t = 3$. It loses 0.96 Ry in exciting the 5F state. Therefore, the incident $\vec{l}_i = \vec{l}_t + \vec{l}_f$, where $\vec{l}_f$ is the outgoing angular momentum, and the minimum $\vec{l}_i$ is equal to 3 for exciting the hydrogen atom to 4F and 5F states by electron impact. We use Rydberg units: energy in Rydberg = 13.605 eV and length in Bohr radius a_0. Therefore, cross-sections are in a_0^2. We give in Table 1 the cross-sections for incident momentum for exciting the 4F and 5F states and in Table 2 we give the convergence with respect to the incident angular momentum for $k_i = 6$ for the 4F and 5F states, the highest momentum used in the calculation is 6.5, the incident energy = 42.25 Ryd. We find that cross-sections are well converged by $L = 14$.

2. Theory and Calculations

Using the Lippman-Schwinger equation [9], the scattering wave function is given by

$$\Psi(r) = \exp(i\vec{k}\cdot\vec{r}) + T\frac{e^{ikr}}{r}. \tag{2.1}$$

In eq. (2.1), $k = k_i$ is the incident momentum and T is the transition matrix describing excitation, it is a function of the momentum k_f of the outgoing electron. The transition matrix is given by

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

In eq. (2.2), the interaction potential V is defined as

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

In eq. (2.3),

$$r_{12} = |\vec{r}_1 - \vec{r}_2|.$$

Ψ_i is the initial state wave function which is given by

$$\Psi_i = (u(\vec{r}_1)\Phi^{\text{pol}}(\vec{r}_1,\vec{r}_2) + \text{exchange})/\sqrt{2}. \tag{2.4}$$

In eq. (2.4), $u(\vec{r}_1)$ represents the scattering function and $\Phi^{\text{pol}}(\vec{r}_1,\vec{r}_2)$ is the target wave function when it is polarized by the incident electron, producing a change in energy equal to $-\frac{\alpha E^2}{2}$, where E is the electric field produced by the incident electron, and α is the polarizability of the target. The polarized target function (Temkin [13]) is given by

$$\Phi^{\text{pol}}(\vec{r}_1,\vec{r}_2) = \phi_0(\vec{r}_2) - \frac{\chi(r_1)}{r_1^2}u_{1s\to p}(r_2)\frac{\cos(\theta_{12}}{\sqrt{Z\pi}}. \tag{2.5}$$

Here,

$$u_{1s\to p}(r_2)=e^{-zr_2}(0.5Zr_2^2+r_2) \tag{2.6}$$

and $\chi(r_1)$ is a cutoff function which can be chosen in various ways. We choose a smooth cutoff function given by Shertzer and Temkin [12], and it is given as

$$\chi(r_1)=\frac{\int_0^{r_1} d\vec{r}_2\phi_0(\vec{r}_2)u_{1s\to p}(r_2)}{\int_0^{\infty} d\vec{r}_2\phi_0(\vec{r}_2)u_{1s\to p}(r_2)}. \tag{2.7}$$

This gives

$$\chi(r_1)=1-e^{-2Zr_1}\left(\frac{(Zr_1)^4}{3}+\frac{4}{3}(Zr_1)^3+2(Zr_1)^2+2Zr_1+1\right). \tag{2.8}$$

The advantage of this function is that the polarization of the target takes place whether the incident particle is outside or inside the orbit of the target electron. It is indicated in [13] that the second term in eq. (2.5) is proportional to $\frac{1}{r_1^2}$. Therefore, it is necessary to have a cut-off function. This function can be chosen of any suitable form as indicated in [4,5,12,13]. The target ground state wave function is

$$\emptyset_0(r_2)=\sqrt{\frac{Z^3}{\pi}e^{-Zr_2}}, \tag{2.9}$$

where Z is the charge of the nucleus, equal to 1.0 for a hydrogen atom. The scattering function has a plane wave normalization (Edmonds [7]), given by

$$\sqrt{4\pi(2L+1)}. \tag{2.10}$$

Therefore, the scattering function has the form

$$u(\vec{r}_1)=\sqrt{4\pi(2L+1)}\frac{u(r_1)}{r_1}Y_{L0}(\theta_1,\varphi_1). \tag{2.11}$$

Y_{L0}, the spherical harmonics, is a function of the angular momentum L, depending on polar angles θ_1 and φ_1. The function $u(0)=0$, and

$$u((r_1)=\frac{\sin\left(kr_1+\eta-\frac{L\pi}{2}\right)}{kr_1},\quad \text{for } r_1\to\infty. \tag{2.12}$$

In eq. (2.12), η is the phase shift. The scattering function is obtained from

$$\int d\vec{r}_2 d\Omega_1 Y_{L0}(\Omega_1)\Phi^{\text{pol}}(\vec{r}_1,\vec{r}_2)|H-E|\Psi_i=0. \tag{2.13}$$

$E=E_{\text{target}}+k^2$ is the total energy and H is the Hamiltonian of the system:

$$H=-\nabla_1^2-\nabla_2^2-\frac{2Z}{r_1}-\frac{2Z}{r_2}+\frac{2}{r_{12}}. \tag{2.14}$$

Distances r_1 and r_2 are the distances of the incident electron and target electron from the nucleus, and $r_{12}=|\vec{r}_1-\vec{r}_2|$. The nucleus is supposed to be fixed so that recoil can be neglected. The expression for the cross section is given by

$$\sigma(a_0^2)=\frac{k_f}{k_{f_i}}\int |T_{fi}|^2 d\Omega. \tag{2.15}$$

In eq. (2.15), k_i and k_f are the momenta of the incident electron and of the outgoing electron. The matrix T_{fi} is the matrix of equation (2.2) between the initial and the final state. The final state consists of the 4F or 5F state and the plane wave of momentum k_f (cf. [7, eq. (5.8.3)]).

The excitation cross-sections are given in Table 1. It is noticed that the 5F excitation cross-sections are lower than the 4F excitation cross-sections in the beginning. In both cases, there is a minimum at $k = 1.3$, and then they increase up to $k = 6.0$. After that they decrease as the incident energy increases. We indicate in Table 2 the convergence of the cross-sections at $k = 6$ as the angular momentum L increases. We find cross-sections have converged by $L = 14$.

Table 1. Excitation cross-sections (a_0^2)

k	Excitation to 4F	Excitation to 5F
0.97	14.463	
1.00	2.6658	1.5999
1.10	1.1845	0.8515
1.20	0.3396	0.3193
1.30	0.1879	0.2317
1.40	0.2173	0.3085
1.50	0.3089	0.4404
1.60	0.4225	0.5976
1.90	0.7263	1.0711
2.00	0.9116	1.2305
2.50	1.4795	1.9718
3.00	1.9662	2.5779
3.50	2.3224	3.0250
4.00	2.6153	4.3291
5.00	2.8223	3.6396
6.00	2.8684	3.6858
6.50	2.8488	3.6541

Table 2. Convergence of cross-sections (a_0^2) at incident momentum $k = 6.0$ with the angular momentum L(maximum) $= Lm$

Lm	Excitation to 4F state	Excitation to 5F state
3	1.9662	2.5139
4	2.5746	3.3000
5	2.7684	3.5536
6	2.8330	3.6394
7	2.8555	3.6695
8	2.8635	3.6805
9	2.8665	3.6846
10	2.8677	3.6847
11	2.8681	3.6854
12	2.8683	3.6857
13	2.8684	3.6858
14	2.8684	3.6858

The cross-sections have been calculated using the noniterative method (Omidvar [10]) for the scattering of the electron from the ground state of the hydrogen atom. The iterative method is described in [4].

3. Conclusions

Using the hybrid theory, we have calculated excitation cross-sections by electron impact to the $n = 4$ and 5 with $l = 3$ states for incident energy in the range 1 to 42.25 Ry. Fourteen angular momenta have been used for most incident energies to obtain converged cross-sections. Decays to lower states can provide information about transition rates and compared with the theoretical results [1]. Calculations were carried out using the computers of the Heliophysics Science Division. Quadruple precision was used. Therefore, results in tables are expected to have four figure accuracy. We expect that the accuracy of cross-sections given in Table 1 have four figure accuracy.

The method of *Polarized Orbitals* (POM) (Temkin [13]) is not a variational correct method. The accuracy of this method can be judged by comparing the singlet S and triplet S phase shifts for electron-hydrogen scattering. Using POM, phase shifts are 0.947 and 1.815 for $k = 0.7$, respectively. Using the R-matrix approach (Scholz *et al.* [11]) which provides accurate results, phase shifts are 0.925 and 1.780. This indicates an accuracy of POM equal to 0.022 for the singlet state and 0.035 for the triplet state. We can conclude that the accuracy of POM is of the order of 0.03. However, the present formalism is variationally correct. Therefore, accuracy is better in the present method.

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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