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The Excitation of the 3*D* and 4*D* States of Atomic Hydrogen by Electron Impact

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Abstract: The excitation cross-sections of the 3*D* and 4*D* states of atomic hydrogen at low incident energies (from 0.90 to 5.00 Ry) were calculated using the variational polarized orbital method, which is also called the hybrid theory. Up to 12 partial waves (L = 2 to 13) were used to obtain converged cross-sections at high energies. The importance of the long-range forces near the threshold region and the behavior of the cross-sections in that region are indicated. The *S*, *P*, and *D* cross-sections are needed if the total excitation cross-sections are measured in addition to the elastic cross-sections. These cross-sections are also useful if the cascade from the *D* to the *P* to the *S* states is considered in the diagnostics of solar and astrophysical observations.

Keywords: electron impact excitation; variational polarized method; hybrid theory

1. Introduction

The variational polarized orbital method, also called the hybrid theory [1], is variationally correct and includes long-range and short-range correlations at the same time. This method was used to calculate scattering phase shifts, the excitation of the 2*S* and 2*P* states of a hydrogen atom at low incident electron energies, positron–hydrogen elastic scattering, the annihilation and formation of positrons, the resonances In, He and Li ions and the cross-sections of photo absorption and radiative attachments. This method, which requires fewer terms in the wave function, was used to obtain accurate results. The phase shifts obtained have lower bounds to the exact phase shifts. The results obtained using this method compare well with those obtained using the R-matrix formulation and the close-coupling approximation. The latter two approximations have been used extensively and are known to provide accurate results. The same method was applied to the excitation of the 3*D* and 4*D* states of atomic hydrogen. Cross-sections for the excitation of the 3*D* state are given in Table 1, and the convergence of cross-sections with an increasing angular momentum L is given in Table 2. Angular momenta of up to 12 (2 to 13) were used. It can be seen that the convergence is slow for the last few energies. It is not possible to calculate cross-sections for higher partial waves because of computer code limitations. We show cross-sections at various incident energies in Figure 1, which shows that there is one maximum and then the cross-sections decrease continuously. We use Rydberg units for energy and the Bohr radius a_0 for length; therefore, the cross-sections are in units of a_0^2.

Table 1. Excitation 3*D* cross-sections (a_0^2) at various incident energies E(Ry).

E	σ	*E*	σ	*E*	σ
0.90	0.351	1.05	0.511	2.00	0.1456
0.91	0.447	1.20	0.392	2.50	0.0859
0.92	0.503	1.30	0.340	3.00	0.0608

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Table 1. *Cont*.

E	σ	*E*	σ	*E*	σ
0.93	0.538	1.40	0.301	3.50	0.0484
0.94	0.558	1.45	0.288	4.00	0.0393
0.95	0.570	1.50	0.272	4.50	0.0320
1.00	0.558	1.70	0.145	5.00	0.0265

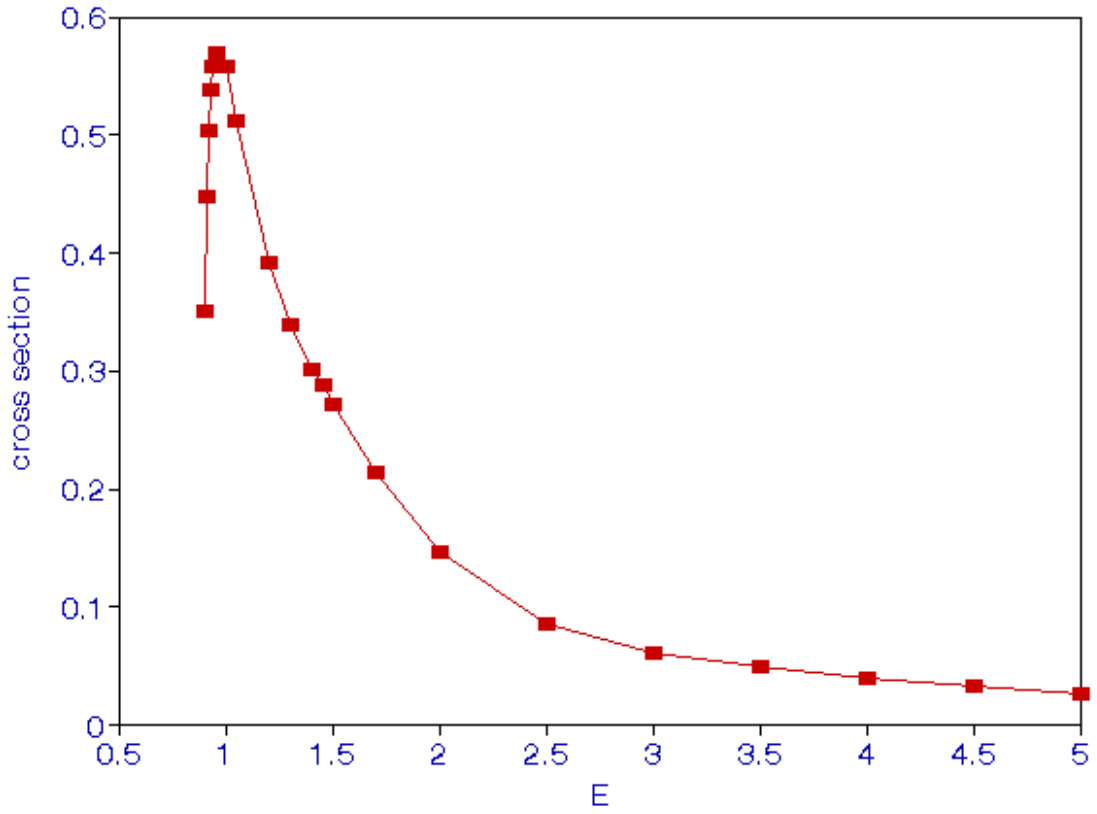

Figure 1. (Color online) The excitation 3*D* cross-sections (a_0^2) for the incident energies.

Table 2. The convergence of the cross-sections (a_0^2) with the maximum $L = Lm$.

Lm/*E*	1.50	2.00	2.50	3.00	3.50	4.00	4.50	5.00
2	0.0413	0.0100	0.0044	0.0024	0.0015	0.0011	0.0008	0.0007
3	0.2123	0.0745	0.0211	0.0048	0.0030	0.0019	0.0014	0.0011
4	0.2422	0.0975	0.0350	0.0129	0.0071	0.0047	0.0031	0.0022
5	0.2582	0.1154	0.0487	0.0223	0.0140	0.0089	0.0060	0.0042
6	0.2658	0.1279	0.0605	0.0317	0.0211	0.0142	0.0098	0.0069
7	0.2693	0.1358	0.0694	0.0399	0.0279	0.0196	0.0141	0.0101
8	0.2706	0.1404	0.0757	0.0464	0.0338	0.0247	0.0183	0.0136
9	0.2712	0.1429	0.0799	0.0522	0.0385	0.0290	0.0219	0.0170
10	0.2714	0.1443	0.0826	0.0556	0.0422	0.0326	0.0252	0.0200
11	0.2715	0.1450	0.0842	0.0580	0.0450	0.0355	0.0280	0.0226
12	0.2715	0.1454	0.0853	0.0596	0.0470	0.0377	0.0302	0.0247
13	0.2715	0.1456	0.0859	0.0608	0.0484	0.0393	0.0320	0.0265

The incident electron loses 0.8889 Ry of energy in exciting the 3*D* state and 0.9375 Ry in exciting the 4*D* state. The angular momentum changes by 2 units. Therefore, $\vec{L}_t = 2$ and $\vec{L}_i = \vec{L}_t + \vec{L}_f$.

There are calculations by Gumble [2] and by Morrison and Rudge [3]. It is stated in [2] that scattering amplitudes are correct to the first order. A comparison with the results given in Table 3 of Ref. [2] indicates that the cross-sections obtained in Ref. [2] are comparable to those obtained in the present calculations. However, they do not indicate convergence with respect to the incident angular momentum, as has been indicated in Table 2 for the present calculations.

Table 3. Excitation 4*D* cross-sections (a_0^2) at various incident energies E(Ry).

E	**σ**	***E***	**σ**	***E***	**σ**	***E***	**σ**
0.94	0.879	1.40	0.217	2.50	0.076	5.00	0.170
1.00	1.924	1.45	0.053	3.00	0.038		
1.05	1.335	1.50	0.085	3.50	0.022		
1.20	1.178	1.70	0.153	4.00	0.148		
1.30	0.033	2.00	0.148	4.50	0.115		

Similar calculations have been carried out for the excitation of the 4*D* state. The results are shown in Table 3.

We see two peaks at incident energies of 1.00 and 1.70 Ry in the excitation cross-sections of the 4*D* state; the cross-sections at these energies are 1.924 a_0^2 and 0.153 a_0^2. Gamble [2] does not provide cross-sections for excitation to the 4*D* state of the atomic hydrogen. Morris and Rudge [3] indicate cross-sections at very high energies in a figure, but it is very difficult to obtain any meaning numbers for a comparison with the cross-sections obtained via the present calculation.

A comparison of the excitation cross-sections to the 2*S*, 2*P* and 3*D* states shows that for the 2*P* state, the cross-sections are highest, as is indicated in Table 4 for a few incident energies. This is expected because 2*P* states represent dipole transitions.

Table 4. A comparison of cross-sections (a_0^2) for the 2*S*, 2*P* and 3*D* states.

E	**2*S* State**	**2*P* State**	**3*D* State**
1.05	8.406(-2)	11.366	0.511
1.20	7.332(-2)	7.062	0.392
1.50	8.580(-2)	3.418	0.272
2.00	6.946(-2)	2.230	0.146

2. Calculations

The variational polarized orbital method was used to calculate cross-sections for the excitation of the 3*D* and 4*D* states. The theory is given here for completeness, though it was indicated in previous publications. This is a distorted wave calculation because the two states 1*S* and 3*D* were treated separately, similar to the 1*S* and 4*D* states. The total cross-section from a state "*i*" to a state "*f*" is written as

$$6 = \frac{k_f}{k_i} \int |T_{fi}|^2 d'\Omega \tag{1}$$

Here k_i and k_f are the initial and final electron momenta, and T_{fi} is the matrix element for excitation from an initial state ψ_i to the final state ψ_f. The matrix element is given by the equation below:

$$T_{fi} = -(\frac{1}{4\pi}) < \psi_f | V | \psi_i > \tag{2}$$

The potential V is given by the equation below:

$$V = -\frac{2Z}{r_1} + \frac{2}{r_{12}} \tag{3}$$

In the above expression, Z is the charge of the nucleus, r_1 and r_2 are the distances of the incident electron and the target electron and $r_{12} = |\vec{r}_1 - \vec{r}_2|$. We assume that the nucleus is of infinite mass, i.e., the recoil of the nucleus can be neglected in the derivation of the equation of the scattering function $u(r)$. The initial scattering state wave function is given by the equation below:

$$\psi_i(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}}[u(\vec{r}_1)\Phi^{pol}(\vec{r}_1, \vec{r}_2) \pm (1 \leftrightarrow 2)] \tag{4}$$

Here, the plus sign refers to the singlet states, and the minus sign refers to the triplet states. The polarized wave function due to the perturbation of the ground state by the incident electron [4] is given by

$$\Phi^{pol}(\vec{r}_1, \vec{r}_2) = \phi_0(\vec{r}_2) - \frac{\chi_{St}(r_1)}{r_1^2} \frac{u_{1s\to 2p}(r_2)}{r_2} \frac{\cos(\theta_{12})}{\sqrt{Z\pi}} \tag{5}$$

The angle θ_{12} is the angle between $\vec{r}_1$ and $\vec{r}_2$. A smooth cutoff function, introduced by Shertzer and Temkin [5], is given below:

$$\chi_{ST}(r) = 1 - e^{-2Zr}((Zr)^4/3 + 4(Zr)^3/3 + 2(Zr)^2 + 2Zr + 1) \tag{6}$$

The function $u_{1s\to 2p}$ is given by

$$u_{1s\to 2p}(r_2) = e^{-Zr}(\frac{Z}{2}{r_2}^2 + r_2)\, r_2 \tag{7}$$

The target function is given by

$$\phi_0(r_2) = \sqrt{\frac{Z^3}{\pi}} e^{-Zr_2} \tag{8}$$

The scattering function $u(\vec{r}_1)$ is

$$u(\vec{r}_1) = a(L)\frac{u(r_1)}{r_1} Y_{L0}(\Omega_1) \tag{9}$$

The scattering function has a plane wave normalization given by

$$a(L) = \sqrt{4\pi(2L+1)} \tag{10}$$

The equation for $u(r_1)$ is obtained from the equation given below:

$$\left\langle Y_{L0}(\Omega_1)\Phi^{pol} | H - E | \Psi_i \right\rangle = 0 \tag{11}$$

The initial wave function is assumed to be exact, and the final state function has no exchange or polarization of the excited target. The final state is given by:

$$\psi_i(\vec{r}_1, \vec{r}_2) = e^{i\vec{k}_f \cdot \vec{r}_1} \phi_{3D}(r_2) Y_{2\mu}(\Omega_2) \tag{12}$$

We can write a similar equation for φ_{4D}. The excited state functions are given by

$$\varphi_{3d}(r_2) = \frac{2}{27}\left(\sqrt{\frac{2}{5}}\right) (Z/3)^{1.5} e^{-r_2/3} Y_{2\mu}(\Omega) \tag{13}$$

$$\varphi_{4d(r_2)=}\frac{(Z)^{3.5}}{384(5)^{0.5}} (r_2)^4 (6 - \frac{Z}{2} r_2) e^{-Zr_2/4} Y_{2\mu}(\Omega) \tag{14}$$

In the above target states, $\mu = -2, -1, 0, 1, 2$. The cross-section in units of a_0^2 is given by

$$\sigma(a_0^2) = \frac{k_f}{k_i} \int |T_{if}|^2 d\Omega_{k_f} \tag{15}$$

In Equation (12), the plane wave is given by

$$e^{i\vec{k}_i \cdot \vec{r}_1} = \sum_{lm} i^l j_l(k_f r_1) Y_{lm}(\Omega_1) Y^*_{lm}(\Omega_{k_f}) \tag{16}$$

Excitation cross-sections from 1*S* to 3*D* are given in Table 1 at various incident energies. The cross-section is at a maximum at $E = 0.95$, where its value is 0.570.

The excitation cross-section is given by

$$\sigma = \sigma_2 + \sigma_1 + \sigma_0 + \sigma_{-1} + \sigma_2 \tag{17}$$

Numerically, it can be seen that $\sigma_2 = \sigma_{-2}$ and $\sigma_1 = \sigma_{-1}$ as expected because of invariance under parity and because the forces involved are electromagnetic forces. In Figure 1, we show the excitation cross-sections. They go to zero as E goes to zero, as is clear from Equation (15).

Regarding long-range forces, Wigner [6] emphasized the importance of such forces in a threshold region, and they were included in the present calculation. Sadeghpour et al. [7] showed that in the threshold region, the cross-section is proportional to $1/\ln(k_f)$. The calculated cross-sections for the 3*D* state can be fitted to $-0.79214 - \frac{3.6714}{\ln(k_f)} - \frac{2.47116}{(\ln(k_f)^2}$. The fit to the calculated points, shown in Figure 2, is very good.

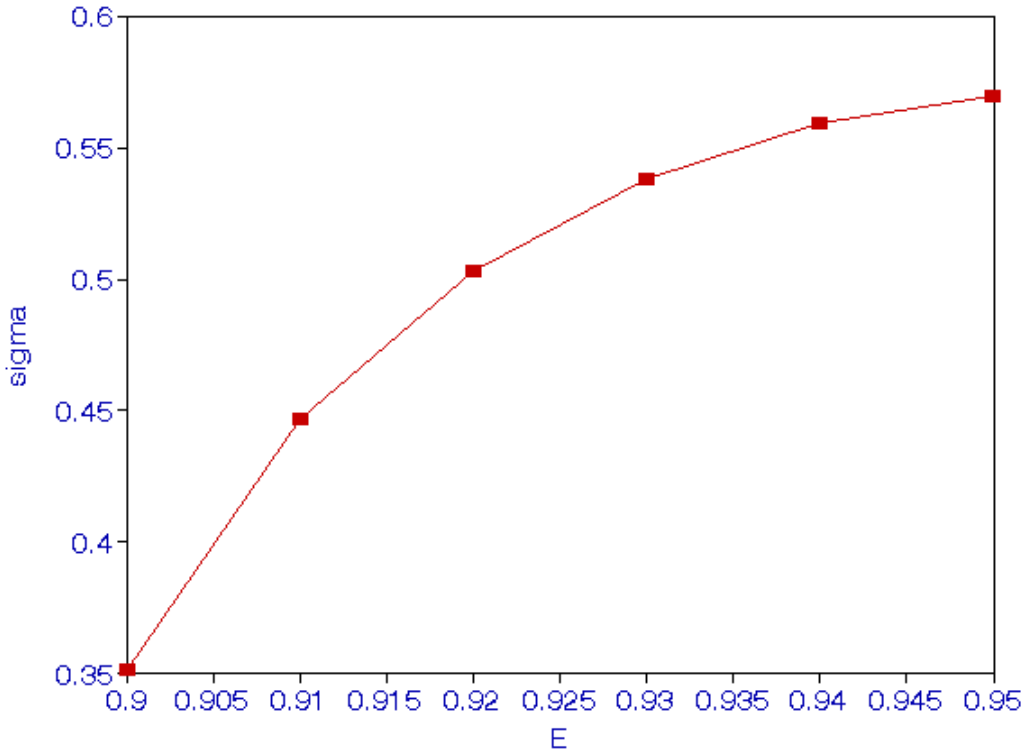

Figure 2. (Color online) Threshold behavior of 3*D* cross-sections vs. energy.

3. Conclusions

Calculations were carried out for the excitation of atomic hydrogen from the 1*S* state to the 3*D* and 4*D* states via electron impact in a distorted-wave approximation in the energy range from 0.90 to 5.00 Ry. The calculations were conducted using the distorted-wave approximation via the variational polarized orbital method. In the distorted approximation, the 1*S* and 3*D* channels and the 1*S* and 4*D* channels are assumed to be independent. Even though the close-coupling and *R*-matrix approaches provide improved results, they are harder to use and require too much computer time. Until now, there have been no such calculations for the excitation of *D* states. At present, these are the only fairly accurate results for excitation cross-sections for the 3*D* and 4*D* states. Elastic cross-sections are given in [8]. It is desirable to use another version of Equation (12) in which exchange and target polarization in the final state are included to indicate their importance in the final state. This would make the calculations more difficult to carry out. For comparison purposes, we only found the calculation by Gumble [2], which does not appear to be very accurate. Also, there are no experimental results for a comparison with the present 3*D* and 4*D* excitation cross-sections. Perhaps some experimentalists will be motivated to carry out experiments to determine the 3*D* and 4*D* excitation cross-sections of hydrogen. We have previously provided expressions given to calculate rate coefficients for 2*S* excitation cross-sections. The same can be used to calculate rate coefficients for the 3*D* and 4*D* states. There is a Born approximation [9] in terms of dipole and quadrupole polarizabilities to calculate phase shifts for higher partial waves. No such approximation is available for excitation cross-sections. Perhaps someone will be motivated to deduce such a formula.

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