

## Elastic scattering of electrons by atomic hydrogen at intermediate energies

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**Abstract.** The elastic scattering of atomic hydrogen is calculated using the  $R$ -matrix method. Total and differential cross sections are reported in the intermediate-energy region and excellent agreement is found with the experimental measurements of Callaway and Williams. Some calculations were also made at low energies where good agreement was obtained with the experimental measurements of Williams and with the accurate variational calculations of Schwartz and Armstead. Momentum transfer and spin-flip cross sections are also calculated.

### 1. Introduction

The elastic scattering of electrons by ground-state hydrogen atoms is one of the simplest processes in atomic physics. It has been studied extensively both theoretically (Schwartz 1961, Armstead 1968, Winters *et al* 1974, Williams 1975a, Callaway and Williams 1975, Byron and Joachain 1977, Bransden and McDowell 1978, Ermolaev and Walters 1979) and experimentally (Teubner *et al* 1974, Lloyd *et al* 1974, Williams 1975a, b, van Wingerden *et al* 1977). In an earlier paper (Fon *et al* 1978) we used the  $1s\text{--}\overline{2p}$  pseudostate approximation of Burke *et al* (1969) to calculate the differential and total cross sections for elastic scattering of electrons by hydrogen atoms for electron impact energies from 1 to 200 eV. These results were in good agreement with experimental data over a wide range of energies. However, the  $\overline{2p}$  state has an unphysical threshold at 11.4 eV (0.84 Ryd) which gives rise to unreliable results close to this threshold. The  $1s\text{--}\overline{2p}$  approximation is also unable to take account of the effect of the resonances which lie just below the  $n = 2$  threshold.

In this paper we improve on our earlier calculations by carrying out an  $R$ -matrix calculation (Burke *et al* 1971) which retains the lowest three atomic states  $1s$ ,  $2s$ ,  $2p$  and in addition includes three pseudostates. A small number of calculations are also carried out including six pseudostates with pseudothresholds at different energies. Both of these calculations give the resonance structure below the  $n = 2$  threshold, but in this region our calculations are not expected to be too accurate as there are insufficient correlation terms in our total wavefunction expansion.

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## 2. Basic theory

### 2.1. The atomic eigenstates and the pseudostates

The  $R$ -matrix method has been described in detail elsewhere (Burke and Robb 1975). In this work on the elastic scattering of electrons by the 1s state of hydrogen we retain only the lowest three atomic eigenstates (1s, 2s, 2p) but in addition three pseudostates ( $\overline{3s}$ ,  $\overline{3p}$ ,  $\overline{3d}$ ) are also included. Both the atomic and pseudo-orbitals are expanded in the following form

$$P_{nl}(r) = \sum_i c_i r^{p_i} \exp(-\xi_i r) \quad (1)$$

where the  $c_i$ ,  $p_i$  and  $\xi_i$  coefficients used in the present calculations are displayed in table 1.

**Table 1.** The atomic and pseudo-orbital coefficients for the six-state  $R$ -matrix calculation.

Orbitals	$p_i$	$c_i$	$\xi_i$	Energy (au)	$P_{nl}(r = 22.5 \text{ au})$	Threshold (Ryd)
1s	1	1.0	1.0	-0.5	$8 \times 10^{-8}$	0
2s	1	1.0	0.5	-0.125	$-2 \times 10^{-3}$	0.75
	2	-1.732 0508	0.5			
$\overline{3s}$	1	2.463 4593	0.6143	0.1	$2 \times 10^{-3}$	1.2
	2	-5.801 4995	0.6143			
	3	3.713 3916	0.6143			
$\overline{2p}$	2	1.0	0.5	-0.125	$1 \times 10^{-3}$	0.75
$\overline{3p}$	2	2.442 3778	0.6910	0.1	$4 \times 10^{-4}$	1.2
	3	-2.305 7233	0.6910			
$\overline{3d}$	3	1.0	0.8911	0.1	$6 \times 10^{-6}$	1.2

The pseudo-orbitals ( $\overline{3s}$ ,  $\overline{3p}$ ,  $\overline{3d}$ ) are generated subject to the following constraints:

- (i) the atomic orbitals (1s, 2s, 2p) and pseudo-orbitals form an orthogonal set;
- (ii) the coupling between the ground state and the p states must give almost the full dipole polarisability of the ground state;
- (iii) all pseudo-orbitals must have a similar range to the  $n = 2$  hydrogen orbitals;
- (iv) the  $n = 3$  pseudostates ( $\overline{3s}$ ,  $\overline{3p}$ ,  $\overline{3d}$ ) are made degenerate to avoid difficulties with the solution in the asymptotic region.

The method of generating these pseudo-orbitals is described by Burke and Mitchell (1973).

Table 1 also gives the threshold energies of the states. It is seen that the  $\overline{3s}$ ,  $\overline{3p}$  and  $\overline{3d}$  states all have threshold at 1.2 Ryd. In the scattering calculation this threshold gives rise to unphysical effects for an electron energy in the region of 1.2 Ryd. To obtain accurate results in the region of 1.2 Ryd we carried out a more complex calculation using six pseudostates ( $\overline{3s'}$ ,  $\overline{3p'}$ ,  $\overline{3d'}$ ,  $\overline{4s'}$ ,  $\overline{4p'}$ ,  $\overline{4d'}$ ). These orbitals were chosen using the constraints (i)–(iv) above and are given in table 2. The pseudothresholds for this calculation are at 1.0, 1.946, 2.051 and 2.512 Ryd, and so we should obtain accurate results in the region of 1.2 Ryd.

**Table 2.** The atomic and pseudo-orbital coefficients for the nine-state  $R$ -matrix calculation.

Orbitals	$p_i$	$c_i$	$\xi_i$	Energy (au)	$P_{nl}$ ( $r = 22.5$ au)	Threshold (Ryd)
1s	1	1.0	1.0	-0.5	$8 \times 10^{-8}$	0
2s	1	1.0	0.5	-0.125	$-2 \times 10^{-3}$	0.75
	2	-1.732 0508	0.5			
$\overline{3s}$	1	0.548 2045	0.6981	0.0	$2 \times 10^{-3}$	1.0
	2	1.090 3341	0.6981			
	3	-5.345 0118	0.6981			
	4	4.090 2087	0.6981			
$\overline{4s}$	1	4.040 5305	0.6981	0.75592	$-2 \times 10^{-3}$	2.512
	2	-12.353 3507	0.6981			
	3	14.526 6456	0.6981			
	4	-6.195 6252	0.6981			
2p	2	1.0	0.5	-0.125	$1 \times 10^{-3}$	0.75
$\overline{3p}$	2	-0.066 3992	0.753	0.0	$5 \times 10^{-4}$	1.0
	3	2.839 3187	0.753			
	4	-2.883 5426	0.753			
$\overline{4p}$	2	4.549 8012	0.753	0.52546	$1 \times 10^{-3}$	2.051
	3	-8.360 2480	0.753			
	4	4.372 3044	0.753			
$\overline{3d}$	3	-0.440 3721	0.9187	0.0	$1 \times 10^{-3}$	1.0
	4	1.399 7355	0.9187			
$\overline{4d}$	3	2.793 9349	0.9187	0.47268	$1 \times 10^{-3}$	1.946
	4	-2.457 7918	0.9187			

## 2.2. The collision wavefunction

The continuum orbitals (Burke and Robb 1975) are obtained by solving the radial equation

$$\left( \frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + V(r) + k_i^2 \right) U_i(r) = \sum_j \lambda_{ij} P_j(r) \quad (2)$$

where

$$U_i(0) = 0 \quad \frac{a}{U_i(a)} \frac{dU_i}{dr} \Big|_{r=a} = 0 \quad (3)$$

and the  $\lambda_{ij}$  are Lagrange undetermined multipliers which ensure that

$$\int_0^a U_i P_j dr = 0 \quad (4)$$

for all orbitals of the same angular symmetry. In addition  $V(r)$  is taken to be the ground-state frozen-core potential and  $a = 22.5$  au. This ensures that all bound orbitals are negligible for  $r > a$ . In the calculation reported here twenty continuum orbitals were retained for the  $R$ -matrix six-state calculation, and the highest partial wave considered was  $L = 7$ . In the case of the nine-state calculation only 13 continuum orbitals were retained and the highest partial wave considered was  $L = 5$ .

The total wavefunction in the internal region is then expanded in terms of the  $R$ -matrix basis

$$\Psi_k = \mathcal{A} \sum_{ij} a_{ijk} \Phi_i U_j + \sum_j b_{jk} \phi_j. \quad (5)$$

The  $\Phi_i$  are channel functions formed from the atomic eigenstates and pseudostates and the angular and spin functions for the scattered electron. The  $\phi_j$  are two-electron correlation functions and are included for completeness. The coefficients  $a_{ijk}$  and  $b_{jk}$  are obtained by diagonalising the electron-hydrogen-atom Hamiltonian in this basis

$$\langle \Psi_k | H | \Psi_{k'} \rangle = E_k \delta_{kk'} \quad (6)$$

where the integrals are carried out over the internal region.

### 2.3. Calculation of differential and total cross sections

The differential cross section for elastic scattering is defined (in units of  $a_0^2 \text{ sr}^{-1}$ ) by

$$\sigma(\theta) = \frac{d\sigma(\theta)}{d\Omega} = \frac{1}{2(2S_i + 1)} \sum_S (2S + 1) |f_{(\theta)}^S|^2 \quad (7)$$

where  $S = 0$  and  $S = 1$  correspond to the singlet and triplet amplitudes. If  $T^{SL}$  denotes the elastic scattering matrix element of the  $T$  matrix for a given  $S$  and  $L$  then in (7) the scattering amplitude

$$f^S(\theta) = \frac{-i}{2k} \sum_L (2L + 1) P_L(\cos \theta) T^{SL} \quad (8)$$

where  $k$  is the wavenumber of the incident electron.

The spin-flip cross section is given by

$$\sigma_{\text{SF}}(\theta) = \frac{1}{4} |f^1 - f^0|^2 = |g(\theta)|^2 \quad (9)$$

where  $g(\theta)$  is the exchange amplitude. While the total cross section is given by

$$Q_{\text{Elast}} = 2\pi \int_0^\pi \sigma(\theta) \sin \theta \, d\theta \quad (10)$$

and the momentum transfer cross section by

$$Q_{\text{MT}} = 2\pi \int_0^\pi \sigma(\theta) (1 - \cos \theta) \sin \theta \, d\theta. \quad (11)$$

In evaluating (8) we followed a procedure similar to that adopted by Fon *et al* (1978) in their  $1s\text{-}\overline{2p}$  calculations. For  $0 \leq L \leq 7$  the  $T$ -matrix elements were obtained from the  $R$ -matrix calculation described above. At the electron energies considered here the  $T$ -matrix elements obtained from the  $R$ -matrix and  $1s\text{-}\overline{2p}$  calculations were in good agreement at  $L = 7$ , hence for  $8 \leq L \leq 24$  the  $T$ -matrix elements were taken from the non-exchange  $1s\text{-}\overline{2p}$  calculations of Fon *et al* (1978) and for large  $L$  ( $L \geq 25$ ) the  $T$  matrices were given to sufficient accuracy by

$$T_L = -2(\tan \eta_L)^2 + 2i(\tan \eta_L) \quad (12)$$

where

$$\tan \eta_L = \frac{\pi \alpha k^2}{(2L+3)(2L+1)(2L-1)} \quad (13)$$

with  $\alpha$  equal to the hydrogen ground-state polarisability (O'Malley *et al* 1961).

### 3. Results and discussion

#### 3.1. Phaseshifts at low energies

The present six-state  $R$ -matrix calculations of singlet and triplet phaseshifts for S and P waves are given in table 3 and are compared with the  $1s\text{-}\overline{2p}$  calculations of Fon *et al* (1978) and the accurate variational calculations of Schwartz (1961) and Armstead (1968). It is clear that the present six-state calculations are significantly better than the  $1s\text{-}\overline{2p}$  results, the improvement being most marked at  $k^2 = 0.64$  with  $L = 0$  and  $S = 0$ , where the  $^1S$  resonance below the  $n = 2$  threshold is affecting the phase.

**Table 3.** Singlet ( $S = 0$ ) and triplet ( $S = 1$ ) partial phaseshifts (rad).

$k^2$	0.36		0.49		0.64	
	$S = 0$	$S = 1$	$S = 0$	$S = 1$	$S = 0$	$S = 1$
$L = 0$						
(a)	1.041	1.933	0.930	1.780	0.886	1.643
(b)	1.022	1.932	0.911	1.779	0.867	1.643
(c)	0.959	1.930	0.829	1.776	0.734	1.639
$L = 1$						
(a)	-0.009	0.341	-0.013	0.393	-0.004	0.427
(b)	-0.013	0.340	-0.018	0.390	-0.011	0.425
(c)	-0.020	0.331	-0.025	0.384	-0.020	0.418

(a) Variational calculation (Schwartz 1961, Armstead 1968).

(b)  $R$ -matrix six-state calculation (present).

(c) Close-coupling  $1s\text{-}\overline{2p}$  calculation (Fon *et al* 1978).

#### 3.2. Total elastic and momentum transfer cross sections

The present results for the total elastic scattering cross section (10) are given in table 4. The results of the six-state  $R$ -matrix calculations are given at all energies except at  $k^2 = 1.21$  which is too close to the pseudostate threshold ( $k^2 = 1.2$ ) to give reliable results. To obtain accurate results in this energy region calculations were also carried out using the  $R$ -matrix method with nine states. The nine-state results should be reliable at  $k^2 = 1.21$  and should be more accurate than the six-state result at  $k^2 = 1.44$ . For comparison purposes we also carried out nine-state calculations at  $k^2 = 0.81$  and 2.25. At these energies, the six- and nine-state results differ by only 1% and this is probably a good indication of the accuracy of the six-state results at these energies.

At low impact energies the six-state results are compared with calculations of the total cross section obtained by Fon *et al* (1978) using the accurate variational phaseshifts for the S, P and D waves with  $1s\text{-}\overline{2p}$  results for the higher partial waves. The present six-state results agree with these accurate results to about 0.5%.

**Table 4.** Cross sections for total elastic scattering in units of  $\pi a_0^2$ .

$k^2(a_0^{-1})$	$E$ (eV)	(a)	(b)	(c)
0.36	4.90	12.21		12.27
0.49	6.66	9.953		10.01
0.64	8.70	8.167		8.205
0.81	11.0	6.487	6.553	
0.8836	12.0	5.906		
1.0	13.6	5.152		
1.21	16.5	—	4.237	
1.44	19.6	3.409	3.513	
2.25	30.6	2.003	2.026	
3.675	50.0	1.050		

(a) *R*-matrix six-state calculation.(b) *R*-matrix nine-state calculation.(c) Calculations using accurate variational phaseshifts for s, p and d waves and  $1s-2\bar{p}$  for higher partial waves (Fon *et al* 1978).

In table 5 we give the six-state *R*-matrix calculations for the momentum transfer cross section (11). As for the total cross section, we also give nine-state results for  $k^2 = 1.21$  and  $k^2 = 1.44$ , the nine-state result at  $k^2 = 1.44$  should be more reliable than the six-state result. At  $k^2 = 0.81$  and  $k^2 = 2.25$  the six- and nine-state results differ by approximately 0.2% and 2.2% respectively and this should be a good indication of the accuracy of these calculations.

**Table 5.** Momentum transfer cross sections ( $\pi a_0^2$ ) using *R*-matrix (a) six-state and (b) nine-state calculations.

$E$ (eV)	$\sigma_{MT}(\pi a_0^2)$						
	11.02	12.02	13.6	16.5	19.6	30.6	50
(a)	4.326	3.740	3.056	—	1.646	0.745	0.303
(b)	4.333			2.207	1.657	0.729	

### 3.3. Differential cross sections

For low electron energies, below the first excitation threshold, accurate differential cross sections for elastic scattering of hydrogen have already been given by Fon *et al* (1978). In table 6 we give the results of our six-state *R*-matrix calculations. Results are not given in the electron energy region near the pseudostate threshold (1.2 Ryd). However, in table 7 we present our nine-state *R*-matrix results for electron energies of 1.21 and 1.44 Ryd. For comparison purposes we also give our nine-state results at 0.81 and 2.25 Ryd. The difference of less than 3%, between our six- and nine-state results at these energies, is a good indication of the accuracy of our results.

There have been several recent measurements of the elastic differential cross section (Teubner *et al* 1974, Lloyd *et al* 1974, Williams 1975a, b, Callaway and Williams

**Table 6.** Differential cross section ( $a_0^2 \text{ sr}^{-1}$ ) for elastic scattering from hydrogen using  $R$ -matrix six-state calculation.

$\theta(\text{deg}) \backslash E(\text{eV})$	11.02	12.02	13.6	30.6	50.0
0	9.671	9.763	9.767	9.871	8.574
5	8.467	8.492	8.399	7.692	5.914
10	7.271	7.242	7.060	5.625	3.825
20	5.378	5.267	4.985	2.950	1.694
30	4.000	3.835	3.526	1.628	8.678 <sup>-1</sup>
40	2.998	2.817	2.524	9.771 <sup>-1</sup>	4.910 <sup>-1</sup>
50	2.278	2.100	1.842	6.335 <sup>-1</sup>	3.009 <sup>-1</sup>
60	1.762	1.596	1.380	4.368 <sup>-1</sup>	1.975 <sup>-1</sup>
70	1.396	1.247	1.067	3.166 <sup>-1</sup>	1.355 <sup>-1</sup>
80	1.143	1.008	8.549 <sup>-1</sup>	2.402 <sup>-1</sup>	9.621 <sup>-2</sup>
90	9.763 <sup>-1</sup> †	8.410 <sup>-1</sup>	7.160 <sup>-1</sup>	1.889 <sup>-1</sup>	7.121 <sup>-2</sup>
100	8.792 <sup>-1</sup>	7.607 <sup>-1</sup>	6.303 <sup>-1</sup>	1.524 <sup>-1</sup>	5.535 <sup>-2</sup>
110	8.378 <sup>-1</sup>	7.182 <sup>-1</sup>	5.846 <sup>-1</sup>	1.258 <sup>-1</sup>	4.457 <sup>-2</sup>
120	8.414 <sup>-1</sup>	7.135 <sup>-1</sup>	5.685 <sup>-1</sup>	1.075 <sup>-1</sup>	3.693 <sup>-2</sup>
130	8.789 <sup>-1</sup>	7.364 <sup>-1</sup>	5.735 <sup>-1</sup>	9.617 <sup>-2</sup>	3.168 <sup>-2</sup>
140	9.370 <sup>-1</sup>	7.767 <sup>-1</sup>	5.921 <sup>-1</sup>	8.946 <sup>-2</sup>	2.835 <sup>-2</sup>
150	1.003	8.232 <sup>-1</sup>	6.164 <sup>-1</sup>	8.485 <sup>-2</sup>	2.601 <sup>-2</sup>
160	1.062	8.649 <sup>-1</sup>	6.396 <sup>-1</sup>	8.107 <sup>-2</sup>	2.419 <sup>-2</sup>
170	1.103	8.939 <sup>-1</sup>	6.560 <sup>-1</sup>	7.824 <sup>-2</sup>	2.313 <sup>-2</sup>
180	1.117	9.039 <sup>-1</sup>	6.617 <sup>-1</sup>	7.717 <sup>-2</sup>	2.283 <sup>-2</sup>

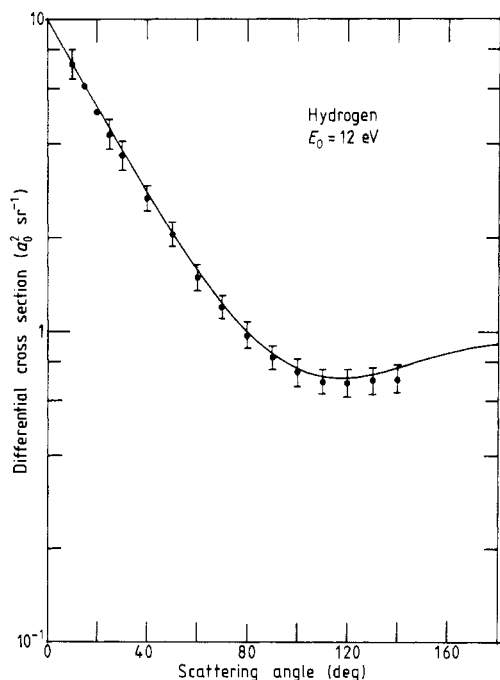
† The superscript denotes the power of 10 by which the number should be multiplied.

**Table 7.** Differential cross section ( $a_0^2 \text{ sr}^{-1}$ ) for elastic scattering from hydrogen using  $R$ -matrix nine-state calculation.

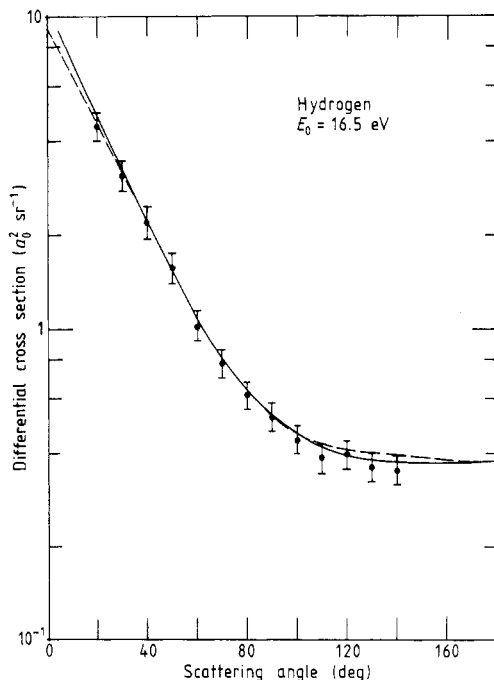
$\theta(\text{deg}) \backslash E(\text{eV})$	11.02	16.5	19.6	30.6
0	9.942	1.042 <sup>1</sup>	1.048 <sup>1</sup>	9.960
5	8.710	8.728	8.717	7.774
10	7.485	7.185	6.992	5.707
20	5.525	4.800	4.403	3.031
30	4.085	3.192	2.767	1.698
40	3.045	2.151	1.783	1.028
50	2.301	1.492	1.203	6.592 <sup>-1</sup>
60	1.774	1.077	8.553 <sup>-1</sup>	4.385 <sup>-1</sup>
70	1.403	8.124 <sup>-1</sup>	6.392 <sup>-1</sup>	3.031 <sup>-1</sup>
80	1.147	6.414 <sup>-1</sup>	4.992 <sup>-1</sup>	2.216 <sup>-1</sup>
90	9.774 <sup>-1</sup> †	5.303 <sup>-1</sup>	4.060 <sup>-1</sup>	1.733 <sup>-1</sup>
100	8.767 <sup>-1</sup>	4.603 <sup>-1</sup>	3.433 <sup>-1</sup>	1.424 <sup>-1</sup>
110	8.324 <sup>-1</sup>	4.189 <sup>-1</sup>	3.022 <sup>-1</sup>	1.205 <sup>-1</sup>
120	8.342 <sup>-1</sup>	3.964 <sup>-1</sup>	2.768 <sup>-1</sup>	1.051 <sup>-1</sup>
130	8.721 <sup>-1</sup>	3.853 <sup>-1</sup>	2.629 <sup>-1</sup>	9.499 <sup>-2</sup>
140	9.335 <sup>-1</sup>	3.807 <sup>-1</sup>	2.578 <sup>-1</sup>	8.853 <sup>-2</sup>
150	1.005	3.789 <sup>-1</sup>	2.588 <sup>-1</sup>	8.364 <sup>-2</sup>
160	1.071	3.782 <sup>-1</sup>	2.633 <sup>-1</sup>	7.942 <sup>-2</sup>
170	1.117	3.782 <sup>-1</sup>	2.679 <sup>-1</sup>	7.632 <sup>-2</sup>
180	1.133	3.782 <sup>-1</sup>	2.697 <sup>-1</sup>	7.514 <sup>-2</sup>

† The superscript denotes the power of 10 by which the number should be multiplied.

1975). In figures 1–5 we compare the present  $R$ -matrix calculations with the experimental results given by Callaway and Williams (1975). For electron energies of 12, 16.5 and 30 eV (figures 1, 2 and 4) there is excellent agreement between our theory and experiment; the theoretical curve always lies between the experimental error bars. At 50 eV (figure 5) our theory and experiment are also in excellent agreement for  $\theta \geq 40^\circ$ , at smaller angles our results lie slightly outside the experimental errors bars. The greatest difference between our theory and experiment is at 20 eV (figure 3); however, even in this case the calculated results lie only slightly outside the experimental error bars.



**Figure 1.** Differential cross section ( $a_0^2 \text{ sr}^{-1}$ ) at 12 eV. Theory: —, present  $R$ -matrix six-state calculation. Experiment: ●, Callaway and Williams (1975).

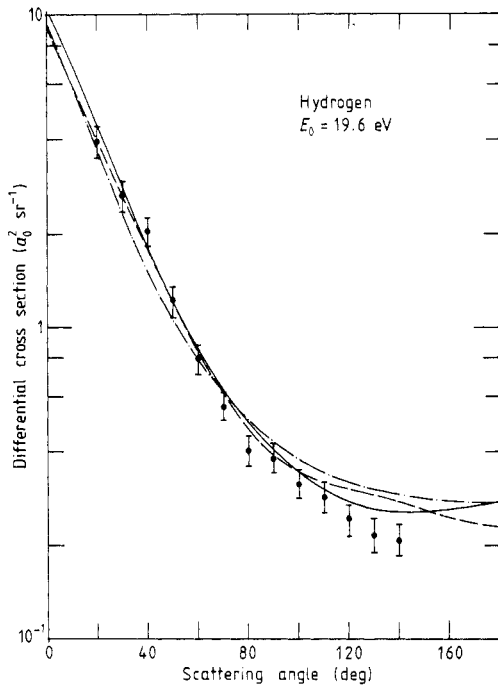


**Figure 2.** Differential cross section ( $a_0^2 \text{ sr}^{-1}$ ) at 16.5 eV. Theory: —, present  $R$ -matrix nine-state calculation; —, calculation of Callaway and Williams (1975). Experiment: ●, Callaway and Williams (1975).

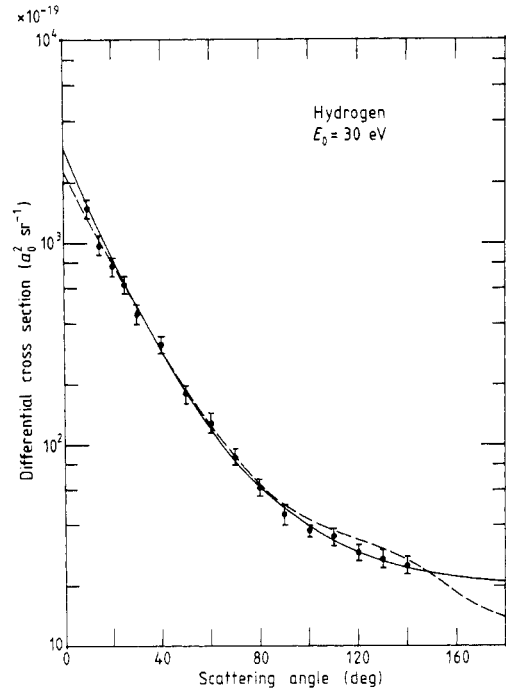
Figures 2, 3 and 4 also compare our results and the experimental results with the calculations of Callaway and Williams (1975). Our results are in only slightly better agreement with the experiments than their calculations. The only real difference in the two calculations arises at small- and large-angle scattering. At large-angle scattering the calculations of Callaway and Williams (1975) have a slight oscillation. Fon *et al* (1978) have shown that this can be attributed to using the asymptotic expression (13) for low values of  $L$ .

In order to assess the accuracy of the results of the  $1s\text{--}\overline{2p}$  pseudostate approximation (Fon *et al* 1978) we have plotted the  $1s\text{--}\overline{2p}$  results of 20 and 50 eV on figures 3 and 5 respectively. We see that at both energies the  $1s\text{--}\overline{2p}$  approximation underestimates at low angles but overestimates at large angles.





**Figure 3.** Differential cross section ( $a_0^2 \text{ sr}^{-1}$ ) at 20 eV. Theory: —, present  $R$ -matrix nine-state calculation; — · —,  $1s-2p$  calculation of Fon *et al* (1978); — — calculation of Callaway and Williams (1975). Experiment: ●, Callaway and Williams (1975).



**Figure 4.** Differential cross sections ( $10^{-19} \text{ cm}^2 \text{ sr}^{-1}$ ) at 30 eV. Theory: —, present  $R$ -matrix nine-state calculation; — · —, calculation of Callaway and Williams (1975). Experiment: ●, Callaway and Williams (1975).

### 3.4. Spin-flip cross section

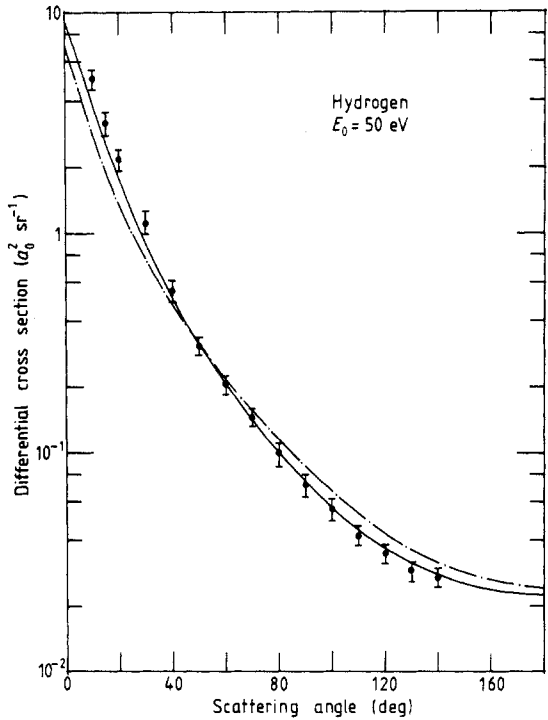
We have also calculated

$$R = \frac{|g(\theta)|^2}{\sigma(\theta)} \quad (14)$$

the ratio of the spin-flip cross section (9) to the differential cross section  $\sigma(\theta)$  (7). This ratio is calculated in table 8. The difference between the nine-state and six-state results at 11 and 30 eV would suggest that at low energies the results have an accuracy of about 5% but at high energies the error in this ratio may be approximately 15%.

## 4. Conclusion

The present results show that the six-state  $R$ -matrix calculation for elastic scattering of electrons by hydrogen atoms gives very good results for both total and differential cross sections. These six-state results, in conjunction with the nine-state  $R$ -matrix results, cover a wide energy range and are in good agreement with the accurate variational results at low energies. There is also excellent agreement between these calculations and the measured differential cross sections.



**Figure 5.** Differential cross sections ( $a_0^2 \text{ sr}^{-1}$ ) at 50 eV. Theory: —, present  $R$ -matrix six-state calculation; - - -,  $1s\text{-}2p$  calculation (Fon *et al* 1978). Experiment:  $\bullet$ , Williams (1975b).

**Table 8.**  $R(|g|^2/\sigma)$  for elastic scattering from hydrogen using  $R$ -matrix (a) six-state and (b) nine-state calculations.

Angle (deg)	$E(\text{eV})$		11.02	16.5	19.6	30.6		50
	(a)	(b)	(b)	(b)	(a)	(b)	(a)	
0	$3.925^{-2}$	$3.744^{-2}$	$2.537^{-2}$	$1.881^{-2}$	$1.310^{-2}$	$1.237^{-2}$	$1.584^{-2}$	
5	$4.461^{-2}$	$4.252^{-2}$	$3.015^{-2}$	$2.252^{-2}$	$1.671^{-2}$	$1.577^{-2}$	$2.248^{-2}$	
10	$5.113^{-2}$	$4.874^{-2}$	$3.608^{-2}$	$2.770^{-2}$	$2.247^{-2}$	$2.118^{-2}$	$3.262^{-2}$	
20	$6.491^{-2}$	$6.214^{-2}$	$5.092^{-2}$	$4.171^{-2}$	$3.986^{-2}$	$3.762^{-2}$	$5.794^{-2}$	
30	$7.865^{-2}$	$7.593^{-2}$	$6.955^{-2}$	$6.084^{-2}$	$6.367^{-2}$	$6.063^{-2}$	$7.948^{-2}$	
40	$9.064^{-2}$	$8.842^{-2}$	$9.070^{-2}$	$8.355^{-2}$	$8.842^{-2}$	$8.627^{-2}$	$9.350^{-2}$	
50	$9.932^{-2}$	$9.784^{-2}$	$1.119^{-1}$	$1.058^{-1}$	$1.080^{-1}$	$1.101^{-1}$	$1.011^{-1}$	
60	$1.042^{-1}$	$1.034^{-1}$	$1.306^{-1}$	$1.232^{-1}$	$1.187^{-1}$	$1.285^{-1}$	$1.038^{-1}$	
70	$1.078^{-1}$	$1.068^{-1}$	$1.462^{-1}$	$1.336^{-1}$	$1.206^{-1}$	$1.398^{-1}$	$1.030^{-1}$	
80	$1.146^{-1}$	$1.137^{-1}$	$1.615^{-1}$	$1.386^{-1}$	$1.183^{-1}$	$1.461^{-1}$	$1.000^{-1}$	
90	$1.355^{-1}$	$1.335^{-1}$	$1.812^{-1}$	$1.436^{-1}$	$1.179^{-1}$	$1.515^{-1}$	$9.621^{-2}$	
100	$1.796^{-1}$	$1.763^{-1}$	$2.096^{-1}$	$1.571^{-1}$	$1.230^{-1}$	$1.577^{-1}$	$9.135^{-2}$	
110	$2.499^{-1}$	$2.455^{-1}$	$2.483^{-1}$	$1.880^{-1}$	$1.351^{-1}$	$1.636^{-1}$	$8.411^{-2}$	
120	$3.390^{-1}$	$3.339^{-1}$	$2.952^{-1}$	$2.398^{-1}$	$1.554^{-1}$	$1.703^{-1}$	$7.560^{-2}$	
130	$4.326^{-1}$	$4.265^{-1}$	$3.463^{-1}$	$3.071^{-1}$	$1.828^{-1}$	$1.801^{-1}$	$7.057^{-2}$	
140	$5.173^{-1}$	$5.089^{-1}$	$3.969^{-1}$	$3.784^{-1}$	$2.120^{-1}$	$1.939^{-1}$	$7.168^{-2}$	
150	$5.850^{-1}$	$5.731^{-1}$	$4.426^{-1}$	$4.422^{-1}$	$2.379^{-1}$	$2.102^{-1}$	$7.490^{-2}$	
160	$6.331^{-1}$	$6.172^{-1}$	$4.791^{-1}$	$4.905^{-1}$	$2.590^{-1}$	$2.276^{-1}$	$7.316^{-2}$	
170	$6.616^{-1}$	$6.425^{-1}$	$5.026^{-1}$	$5.198^{-1}$	$2.739^{-1}$	$2.422^{-1}$	$6.638^{-2}$	
180	$6.711^{-1}$	$6.508^{-1}$	$5.108^{-1}$	$5.296^{-1}$	$2.795^{-1}$	$2.482^{-1}$	$6.255^{-2}$	

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