

## Electron scattering from hydrogen atoms at intermediate energies: integrated cross sections to $n = 3$ levels

B R Odgers, M P Scott and P G Burke

Department of Applied Mathematics and Theoretical Physics, The Queen's University of Belfast, Belfast BT7 1NN, UK

Received 7 March 1994

**Abstract.** A modified version of the IERM approach is applied to electron scattering from hydrogen atoms at intermediate energies to evaluate integrated cross sections for the  $n = 2$  to  $n = 3$  transitions. Results are compared with earlier work which overestimates these cross sections due to the omission of continuum channels. These results have important applications in astrophysics.

### 1. Introduction

Electron impact excitation of atomic hydrogen at low energies has been the subject of numerous theoretical and experimental studies over many years, but until recently, very little was known about scattering at intermediate energies. At these energies an infinite number of channels are open and any accurate model must allow for loss of flux into these channels. One method which does allow for this loss of flux is the intermediate energy  $R$ -matrix (IERM) approach first introduced by Burke *et al* (1987). This theory was applied successfully to electron scattering from atomic hydrogen with excitation to the  $n = 2$  levels by Scott *et al* (1989) and Scholz *et al* (1991). Other results which have given accurate results at intermediate energies include those of Bray and Stelbovics (1992) which use a close coupling formalism in which the target states are expanded in an orthogonal  $L^2$  Laguerre basis.

More recently a modified version of the IERM approach has been applied to the study of electron–hydrogen-atom scattering with excitation to the  $n = 3$  levels by Scott *et al* (1993). Transitions from the  $n = 1$  levels to the  $n = 2$  and  $n = 3$  levels have also been investigated by Callaway and Unnikrishnan (1993) using a coupled pseudostate approach and by Aggarwal *et al* (1991) using a 15-state  $R$ -matrix calculation. The calculation of Aggarwal *et al* only retains bound hydrogen orbitals in the atomic electron basis and hence does not allow for loss of flux into the continuum channels. This leads to significant disagreements between the results of Aggarwal *et al* and the results of Scott *et al* and Callaway *et al* which are in good agreement with experimental measurements of Mahan *et al* (1976).

In this paper, we extend the calculation of Scott *et al* to obtain integrated cross sections for electron scattering from atomic hydrogen for the  $n = 2$  to  $n = 3$  transitions. Results for these transitions are important for modelling the observed  $n = 3 \rightarrow 2$  and  $n = 3 \rightarrow 1$  lines present in many laboratory and astrophysical plasmas.

In section 2 we give details of the IERM approach used in this work, while in section 3 we describe our present calculation. In section 4 we compare our results with those of Aggarwal *et al* (1991), which are the only other theoretical results currently available.

## 2. Theory

The intermediate  $R$ -matrix method (IERM) was first introduced by Burke *et al* (1987). In this approach the two-electron wavefunction  $\Psi_E^{LS\pi}(r_1, r_2)$  is expanded in the  $R$ -matrix inner region in terms of an energy-independent basis  $\Theta_k^{LS\pi}(r_1, r_2)$

$$\Psi_E^{LS\pi}(r_1, r_2) = \sum_k A_{Ek}^{LS\pi} \Theta_k^{LS\pi}(r_1, r_2). \quad (1)$$

The  $R$ -matrix basis states  $\Theta_k^{LS\pi}(r_1, r_2)$  are given by

$$\Theta_k^{LS\pi}(r_1, r_2) = [1 + (-1)^S P_{12}] \sum_{n_1 n_2}^{n_{\max}} \sum_{l_1 l_2}^{l_{\max}} r_1^{-1} u_{n_1 l_1}(r_1) r_2^{-1} u_{n_2 l_2}(r_2) \mathcal{Y}_{l_1 l_2 L M_L}(\hat{r}_1, \hat{r}_2) \alpha_{n_1 l_1 n_2 l_2 k}^{LS\pi} \quad (2)$$

The angular functions  $\mathcal{Y}_{l_1 l_2 L M_L}(\hat{r}_1, \hat{r}_2)$  are eigenfunctions of  $L^2, l_1^2, l_2^2$  and the  $\alpha_{n_1 l_1 n_2 l_2 k}^{LS\pi}$  are expansion coefficients which are chosen to diagonalize the two-electron Hamiltonian in the internal region;  $L$  and  $S$  are the total orbital and spin angular momenta respectively of the two-electron system and  $\pi$  is the parity;  $l_1$  and  $l_2$  are the orbital angular momenta of the scattered and atomic electrons and  $P_{12}$  is the antisymmetry space exchange operator. The basis functions  $u_{nl}(r)$  which are used to describe the radial motion of the scattered and target electrons are made up of bound hydrogen orbitals and members of a complete set of continuum orbitals whose radial functions are solutions of the differential equation

$$\left( \frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + V(r) + k_{nl}^2 \right) u_{nl}(r) = \sum_{n'=1}^{n_{\text{bound}}} \lambda_{nn'} \mu_{n'}(r) \quad (3)$$

with boundary conditions

$$u_{nl}(0) = 0 \quad du_{nl}(r)/dr|_{r=a} = 0 \quad (4)$$

where  $a$  is the radius of the internal region,  $n_{\text{bound}}$  is the number of bound hydrogen orbitals with angular momentum  $l$  and  $\lambda_{nn'}$  are Lagrange multipliers, included to ensure that the continuum functions are orthogonal to the bound hydrogen orbitals. The potential  $V(r)$  was taken as  $2Z/r$ . Any possible inadequacy in this  $R$ -matrix basis set and consequent loss of accuracy in the resulting  $R$ -matrices will arise from limiting  $l_{\max}$ , the maximum value of  $l_1$  and  $l_2$ . Inadequacies introduced by the truncation of  $n_{\max}$  are taken into account by the Buttle correction (Buttle 1967) to the diagonal elements of the  $R$ -matrix. The feature of these internal region basis states which makes them suitable for application to intermediate energy scattering and sets them apart from the standard  $R$ -matrix theory is that the same basis is used to describe the motion of both the scattered electron and atomic electron. As a result, most of the products  $u_{n_1 l_1}(r_1) u_{n_2 l_2}(r_2)$  are such that both  $u_{n_1 l_1}(r_1)$  and  $u_{n_2 l_2}(r_2)$  are continuum orbitals. Terms of this type, which are not included in the standard  $R$ -matrix basis states, allow for loss of flux into highly excited and ionizing channels. Their inclusion therefore enables information on the intermediate energy collision to be obtained. If we want to extend the calculation of Scott *et al* (1989) and Scholz *et al* (1991) to include the  $n=3$  levels

it is necessary to increase the  $R$ -matrix boundary from 25 au to 38 au to completely envelope the  $n=3$  bound hydrogen orbitals. Consequently,  $n_{\max}$  must be increased from 30 to around 40 if we wish to calculate cross sections in the same energy range. This increase in the number of one electron basis functions leads to an increase in the size of the Hamiltonian matrix from around 3000 to around 5000. It is clear that the computational difficulties raised by this increase in  $n_{\max}$  are too great for efficient evaluation of the  $n=3$  problem.

A modified IERM approach was proposed by Scott and Burke (1993) in an attempt to overcome the above problem. As we can see from equation (2), in the original IERM approach the  $R$ -matrix basis states were constructed from products of one-electron functions made up of bound hydrogen orbitals and members of a complete set of continuum orbitals. The large number of  $R$ -matrix basis states arose because the same number of one-electron functions was being used to describe the motion of both the scattered and atomic electron. It was shown by Scott and Burke that it is possible to reduce the size of the atomic electron basis, and hence the number of two-electron basis functions, and still get converged results. We define the  $R$ -matrix basis states for each partial wave symmetry as

$$\Theta_k^{LS\pi}(r_1, r_2) = [1 + (-1)^S P_{12}] \sum_{n_1}^{n_{1\max}} \sum_{n_2}^{n_{2\max}} \sum_{l_1}^{l_{1\max}} \sum_{l_2}^{l_{2\max}} r_1^{-1} u_{n_1 l_1}(r_1) r_2^{-1} u_{n_2 l_2}(r_2) \\ \times \mathcal{Y}_{l_1 l_2 L M_L}(\hat{r}_1, \hat{r}_2) \alpha_{n_1 l_1 n_2 l_2 k}^{LS\pi} \quad (5)$$

where  $n_{1\max}$  is the maximum  $n$  value for the angular momentum  $l_1$  of the one-electron basis functions describing the motion of the scattering electron and  $n_{2\max}$  is the maximum  $n$  value for the angular momentum  $l_2$  of the one-electron basis functions describing the motion of the atomic electron. Scott and Burke (1993) showed that converged results could be obtained for transitions involving the  $n=3$  levels by taking  $n_{2\max}$  as 12. This reduction in  $n_{2\max}$  reduces the size of the Hamiltonian matrix to around 3000.

Diagonalization of the energy-independent Hamiltonian matrix within the  $\Theta_k^{LS\pi}$  basis yields the eigenvalues  $E_k$  and eigenvectors  $\alpha_k$  from which the reduced width surface amplitudes  $\omega_{ik}$  and eventually the energy dependent  $R$ -matrix may be evaluated. The  $K$ -matrices are evaluated by matching the Buttle corrected  $R$ -matrices from the internal and external regions at the  $R$ -matrix boundary. The external region problem is solved using the asymptotic package of Noble and Nesbet (1984). In the previous IERM calculations only the physical hydrogen states were retained in the atomic electron basis in the external region (in this case 1s, 2s, 2p, 3s, 3p, 3d). The inclusion of the continuum-continuum terms in the expansion of the wavefunction in the internal region gives rise to pseudoresonance features at intermediate energies in the physical  $T$ -matrix if these continuum channels are not also explicitly included in the external region. These pseudoresonances were removed in previous IERM calculations by energy averaging the  $T$ -matrix elements over these resonances using an averaging procedure proposed by Burke *et al* (1981). It was shown by Scholz (1991) that the pseudoresonance features could also be eliminated by explicitly including the extra pseudochannels in the external region as well as in the internal region. It was shown that, while it was necessary to retain coupling in the external region amongst the physical channels and between the physical channels and pseudochannels, it was possible to neglect coupling amongst the pseudochannels. This allowed the continuum-continuum terms included in the internal region to be 'matched' to channels involved in the external region calculation.

### 3. The calculation

The calculation was divided into two parts—the solution of the internal region problem ( $r \leq a$ ) and the solution of the external region problem ( $r \geq a$ ).

The internal region calculation was also divided into two parts. First, for partial waves with total orbital angular momentum  $L \leq 13$  we used the exchange form of the modified IERM approach introduced by Scott and Burke (1993). The  $R$ -matrix boundary was set to 38 au to accommodate the  $n=3$  bound states required for this calculation. The atomic electron basis used in this modified approach consisted of six physical atomic basis states (1s, 2s, 2p, 3s, 3p, 3d) plus a number of pseudostates. In these calculations we have taken  $n_{2\max} = 12$  which was found to be sufficient to obtain converged results for transitions involving the  $n=3$  levels (Scott and Burke 1993).  $l_{2\max}$  was set to 3 and  $l_{1\max}$  to  $L + l_{2\max}$  for each  $L$ . In order to obtain converged results for scattering

Table 1. Basis for the reduced IERM calculation.

1s	2s	3s	$\overline{4s}$	$\overline{5s}$	...	...	$\overline{12s}$	13s	...	...	35s
	2p	3p	$\overline{4p}$	$\overline{5p}$	...	...	$\overline{12p}$	13p	...	...	35p
		3d	$\overline{4d}$	$\overline{5d}$	...	...	$\overline{12d}$	13d	...	...	35d
			$\overline{4f}$	$\overline{5f}$	...	...	$\overline{12f}$	13f	...	...	35f

electron energies up to 2.5 Ryd. it was necessary to set  $n_{1\max}$  to 35. Table 1 shows the one-electron basis functions used in the calculation. The 'bars' represent numerical continuum orbitals which are included in both the atomic electron and scattered electron bases. The additional continuum orbitals in the scattered electron basis are represented in italics.

For partial waves with total orbital angular momentum  $L$  such that  $14 \leq L \leq 40$  a non-exchange version of the IERM code was used. As  $L$  increases the coupling between the channels decreases and it is possible to reduce the value of  $n_{2\max}$ . However, as  $L$ , and hence  $l_{1\max}$ , increases it is necessary to increase  $n_{1\max}$  slightly to ensure convergence of the scattering electron basis.

Integrated cross sections were evaluated by summing the contributions from all partial waves up to  $L=40$ . For  $41 \leq L \leq \infty$  a geometric series was assumed. This contribution was found to be less than 1% of the total. As in the work of Scholz (1991) small oscillations were still present in the cross section which were smoothed using a simple Chebyshev-series least-squares fit.

### 4. Results

In figures 1 and 2 we present our results for the integrated cross section for  $n=2$  to  $n=3$  transitions for atomic hydrogen. Previous calculations by Scott *et al* (1993) using the reduced IERM approach show that convergence for the transitions for  $n=1$  to  $n=3$  levels for atomic hydrogen was achieved by  $L=13$ . This is not so for the  $n=2$  to  $n=3$  transitions. The contribution for  $L > 13$  is quite large for some of the optically allowed transitions, especially for the 2p–3d transition which increases by about 50%, while the 2s–3s transition only increases by about 1%. Table 2 contains more information on the contributions to the  $n=2$  to  $n=3$  transitions for  $L \leq 13$  and  $L > 13$ .

Due to the difficulty in measuring these cross sections experimentally, there are no experimental data with which to compare our results. The results of Aggarwal *et al*

Table 2. Breakdown of total cross section for  $n=2$  to  $n=3$  transitions in units of  $\pi a_0^2$ .

Transition	$E=1.1$ Ryd		$E=1.3$ Ryd		$E=1.5$ Ryd		$E=1.69$ Ryd		$E=1.96$ Ryd	
	$L \leq 13$	$L > 13$	$L \leq 13$	$L > 13$	$L \leq 13$	$L > 13$	$L \leq 13$	$L > 13$	$L \leq 13$	$L > 13$
2s-3s	3.0710	0.0117	3.2392	0.1475	2.9677	0.3152	2.5870	0.4189	2.0873	0.4764
2s-3p	6.9464	0.0730	6.0884	1.0728	5.3686	2.5689	4.6700	3.8827	3.7177	5.1723
2s-3d	9.8388	0.2555	9.8519	0.8708	8.8241	2.0253	7.8205	2.6725	6.4457	3.2562
2p-3s	0.9603	0.0027	0.5364	0.0306	0.4058	0.0706	0.3310	0.1048	0.2560	0.1372
2p-3p	5.2310	0.0264	4.4894	0.2591	3.7685	0.5019	3.1872	0.6550	2.5194	0.7657
2p-3d	16.2664	0.0854	16.4327	2.0842	15.1567	4.8736	13.6788	7.1811	11.4937	9.6167

Table 3. Total cross section for the  $n=1$  to  $n=3$  and  $n=2$  to  $n=3$  transitions in units of  $\pi a_0^2$ .

Transition	$E=1.1$ Ryd		$E=1.3$ Ryd		$E=1.5$ Ryd		$E=1.69$ Ryd		$E=1.96$ Ryd		$E=2.2$ Ryd		$E=2.4$ Ryd	
	$L \leq 13$	$L > 13$	$L \leq 13$	$L > 13$	$L \leq 13$	$L > 13$	$L \leq 13$	$L > 13$	$L \leq 13$	$L > 13$	$L \leq 13$	$L > 13$	$L \leq 13$	$L > 13$
1s-3s	0.9603	0.0117	0.5364	0.0306	0.4058	0.0706	0.3310	0.1048	0.2560	0.1372	0.2208	0.1910	0.1910	0.1910
1s-3p	5.2310	0.0730	4.4894	0.2591	3.7685	0.5019	3.1872	0.6550	2.5194	0.7657	2.0866	1.8395	1.8395	1.8395
1s-3d	16.2664	0.0854	16.4327	2.0842	15.1567	4.8736	13.6788	7.1811	11.4937	9.6167	9.7647	8.6221	8.6221	8.6221
2s-3s	3.0827	0.0027	3.3868	0.0306	3.2829	0.0706	3.0060	0.1048	2.5637	0.1372	2.2476	2.0316	2.0316	2.0316
2s-3p	7.0194	0.2555	7.1612	0.8708	7.9375	2.0253	8.5527	2.6725	8.8900	3.2562	8.8176	8.6114	8.6114	8.6114
2s-3d	10.0943	0.0264	10.7228	0.2591	10.8494	0.5019	10.4931	0.6550	9.7019	0.7657	8.9232	8.2832	8.2832	8.2832
2p-3s	0.9630	0.0027	0.5670	0.0306	0.4764	0.0706	0.4358	0.1048	0.3932	0.1372	0.3726	0.3476	0.3476	0.3476
2p-3p	5.2574	0.0264	4.7485	0.2591	4.2704	0.5019	3.8422	0.6550	3.2851	0.7657	2.8613	2.5844	2.5844	2.5844
2p-3d	16.3518	0.0854	18.5169	2.0842	20.0302	4.8736	20.8599	7.1811	21.1105	9.6167	20.6199	19.9238	19.9238	19.9238

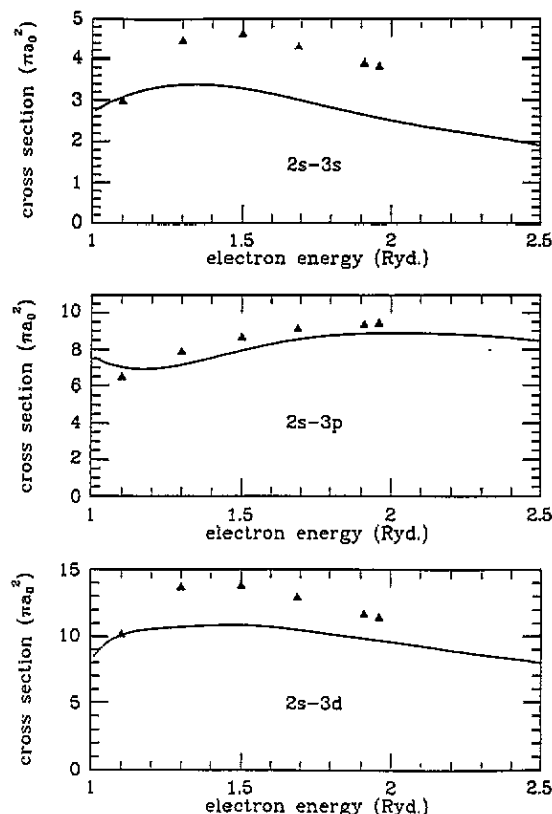


Figure 1.  $e^- + H$  integrated cross sections in units of  $\pi a_0^2$  for (a) 2s-3s, (b) 2s-3p and (c) 2s-3d transitions. Full curve, present reduced IERM results;  $\blacktriangle$ , 15-state *R*-matrix results of Aggarwal *et al* (1991).

(1991) are the only other theoretical results to date and these are also shown in figures 1 and 2. The 15-state close coupling calculation of Aggarwal *et al*, which retains the target states 1s, 2s, ..., 5g in a close coupling expansion, does not include loss of flux into the continuum channels. This omission explains why the results of Aggarwal *et al* differ significantly from the current IERM data. The results of Aggarwal *et al* for the 2s-3s, 2p-3s and 2p-3p are all about 35% greater than the current results while the corresponding results for the 2s-3p cross section are only about 7% greater than ours. As expected the results for the  $n=2$  to  $n=3$  transitions of Aggarwal *et al* are in better agreement with the current IERM results than the results for the  $n=1$  to  $n=3$  transitions. As the coupling between the  $n=2$  and  $n=3$  states is stronger than the coupling between the  $n=1$  and  $n=3$  states the effect of omitted states in the former case is relatively smaller. In table 3 we give the results for integrated cross sections for the  $n=1$  to  $n=3$  and  $n=2$  to  $n=3$  transitions for specified scattered electron energies in the range 1 Ryd to 2.5 Ryd.

## 5. Conclusion

In this paper we have reported the values of total integrated cross sections for atomic hydrogen for the  $n=1$  to  $n=3$  and  $n=2$  to  $n=3$  transitions. The results have been

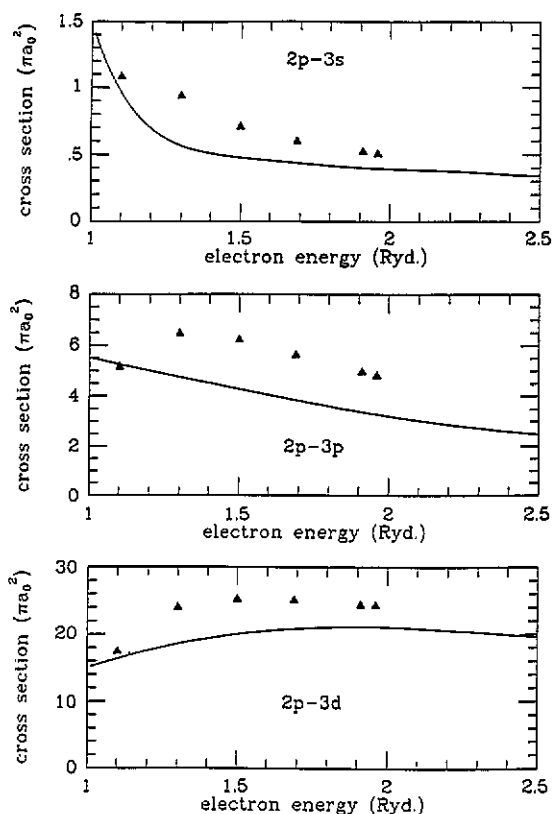


Figure 2.  $e^- + H$  integrated cross sections in units of  $\pi a_0^2$  for (a) 2p-3s, (b) 2p-3p and (c) 2p-3d transitions. Full curve, present reduced IERM results;  $\blacktriangle$ , 15-state  $R$ -matrix results of Aggarwal *et al* (1991).

obtained using a modified version of the IERM approach of Burke *et al* (1987). For the  $n=1$  results (previously reported by Scott *et al* (1993)) we obtain good agreement with the theoretical work of Callaway *et al* (1993) and with the experimental results of Mahan *et al* (1976). The only data available for comparison with the  $n=2$  to  $n=3$  results are the 15-state close-coupling data of Aggarwal *et al* (1991). These results are significantly higher than ours as they did not allow for the continuum channels. In future papers we shall report calculations for differential cross sections and other parameters for the  $n=1$  and  $n=2$  to  $n=3$  transitions of hydrogen which are of importance in applications and experiments.

### Acknowledgments

This work was supported by a grant from the SERC and by EC grant no ERB CHRX CT920013. One of us (BRO) gratefully acknowledges receipt of a post-graduate studentship from the Department of Education for Northern Ireland.

## References

- Aggarwal K M, Berrington K A, Burke P G, Kingston A E and Pathak A 1991 *J. Phys. B: At. Mol. Opt. Phys.* **24** 1385-410
- Bray I and Stelbovics A 1992 *Phys. Rev. A* **46** 6995-7011
- Burke P G, Berrington K A and Sukumar C V 1981 *J. Phys. B: At. Mol. Phys.* **14** 289-305
- Burke P G, Noble C J and Scott M P 1987 *Proc. R. Soc. A* **410** 289-310
- Buttle P J A 1967 *Phys. Rev.* **160** 719-29
- Callaway J and Unnikrishnan K 1993 *J. Phys. B: At. Mol. Opt. Phys.* **26** L419-23
- Mahan A H, Gallagher H and Smith S J 1976 *Phys. Rev. A* **13** 156-66
- Noble C J and Nesbet R K 1984 *Comput. Phys. Commun.* **33** 399-411
- Scholz T T 1991 *J. Phys. B: At. Mol. Opt. Phys.* **24** 2127-46
- Scholz T T, Walters H R J, Burke P G and Scott M P 1991 *J. Phys. B: At. Mol. Opt. Phys.* **24** 2097-126
- Scott M P and Burke P G 1993 *J. Phys. B: At. Mol. Opt. Phys.* **26** L191-5
- Scott M P, Odgers B R and Burke P G 1993 *J. Phys. B: At. Mol. Opt. Phys.* **26** L827-30
- Scott M P, Scholz T T, Walters H R J and Burke P G 1989 *J. Phys. B: At. Mol. Opt. Phys.* **22** 3055-77