

Electron impact induced transitions between the $n = 1, 2, 3$ levels of atomic hydrogen at low energies

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Abstract. An algebraic variational close-coupling code is used to evaluate electron impact excitation cross sections between the $n = 1, 2$ and 3 levels of atomic hydrogen at energies up to the $n = 4$ threshold. Results are obtained in a six-state basis and with a much larger basis (14 to 18 states). Comparisons are made with earlier six-state calculations. The results from the best basis are significantly lower than the previous six-state calculations for the $2l-3l'$ cross sections: in particular for $2p-3d$ they are more than a factor of two lower close to the $n = 3$ threshold. The total $n = 2$ to $n = 3$ cross section is 76% lower than that of Burke and co-workers at our lowest energy. The positions and widths of the Feshbach resonances for $L = 0, 1$, in general, agree well with those of Ho. There is a broad shape resonance (3S) just above the $n = 3$ threshold.

1. Introduction

There has been little published work on excitation of atomic hydrogen by slow electrons in the energy range just above the $n = 3$ threshold. Six-state close-coupling calculations were reported by Burke *et al* (1967) and further details are available in Ormonde *et al* (1969). Ho (1979) has recently used a rotated-coordinates method to investigate the positions and widths of the resonances between the $n = 3$ and $n = 4$ thresholds. Earlier work (Ho 1977, Morgan *et al* 1977) showed good agreement between the complex rotation method and many channel close-coupling for the positions and widths of resonances between the $n = 2$ and $n = 3$ thresholds. The first aim of the present paper is to extend this comparison to the $n = 4$ threshold. There are no published measurements.

The total cross sections for all $nl \rightarrow n'l'$ transitions ($n, n' \in (1, 2, 3)$) are required for astrophysical and plasma applications. These are usually taken to be the six-state close-coupling values, over the energy range where these are available, while $n \rightarrow n'$ cross sections are often represented by a semi-empirical formula due to Johnson (1972). We have recently shown (Hata *et al* 1980) that both the six-state close-coupling and Johnson's results (which agree well) are in error by almost a factor of two for the $n = 2$ to $n = 3$ transition just above the $n = 3$ threshold ($k_1^2 = 0.90$ Ryd). We shall show that our results agree well with six-state results for $n = 1 \rightarrow n = 3$, while the Johnson formula is

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again in error by almost a factor of two at $k_1^2 = 0.90$. (Here k_1^2 is the incident electron's energy in rydbergs, when the target is in its ground state.)

Burgess and his colleagues have claimed on the basis of observations on laser pumped atomic hydrogen plasmas (Burgess *et al* 1978, 1980) that the rate coefficients obtained from Johnson's formula for transitions out of the $n = 2$ level are much too large. The observations cover the electron temperature range 0.41 to 1.0 eV, while the energy difference of the $n = 2$ and $n = 3$ states is 1.9 eV. We have therefore recalculated the cross sections of interest in the energy range $0.90 \leq k_1^2 \leq 0.93$.

In § 2 we summarise our model, a detailed description being given elsewhere (Morgan 1980), and in § 3 present our results on the resonance structures. We then (§ 4) compare the present results for some individual $nl-n'l'$ transitions with our own six-state calculations and the earlier six-state results, giving a table of our final values at eight energies. Finally (§ 5) we present summed $n-n'$ cross sections and discuss briefly some implications of our results.

2. Theoretical model

We have used the algebraic variational close-coupling code of Morgan (1980). The total wavefunction may be written, in a usual notation

$$\Psi_{\Gamma_i}(\mathbf{x}_1, \mathbf{x}_2) = \mathcal{A} \sum_i \psi(\Gamma_i, \mathbf{x}_1, \hat{\mathbf{x}}_2) F_{ij}(r_2) \quad (2.1)$$

where \mathbf{x}_1 denotes the space and spin coordinates of particle 1, $\hat{\mathbf{x}}_2$ the spin and angular coordinates of particle 2, and r_2 its radial coordinate. We assume the centre-of-mass motion has been separated out. The wavefunction is written in the coupled representation in which $\Gamma_i = \{L_i, S_i, \Pi, L_A, S_A, l_i \gamma_i\}$ denotes the set of conserved quantum numbers in channel i . If Γ_i is the initial channel, then the function F_{ij} describes the scattering in channel Γ_i . It may be written

$$r F_{ij}(r) = \sum_l (\alpha_{jl}^{(0)} f_{li}^{(0)}(r) + \alpha_{jl}^{(1)} f_{ji}^{(1)}(r)) + \sum_{\mu} C_{ij}^{(\mu)} \eta_{i\mu}(r) \quad (2.2)$$

where the first bracket contains sinusoidal functions while the $\eta_{i\mu}$ are quadratically integrable functions, which we refer to as correlation functions. Thus, we may rewrite (2.2) as

$$\Psi_{\Gamma_i}(\mathbf{x}_1, \mathbf{x}_2) = \mathcal{A} \sum_l \sum_{s=0}^1 \alpha_{jl}^{(s)} \sum_i \psi(\Gamma_i, \mathbf{x}_1, \hat{\mathbf{x}}_2) f_{li}^{(s)}(r_2) + \sum_{\nu} C_{j\nu} \Phi_{\nu} \quad (2.3)$$

where

$$\Phi_{\nu} = \mathcal{A} \psi(\Gamma_i, \mathbf{x}_1, \hat{\mathbf{x}}_2) \eta_{i\nu}(r_2) \quad (2.4)$$

is a two-electron quadratically integrable part of Ψ_{Γ_i} . This is of the same form as equation (6) of Berrington *et al* (1975). However, in their R -matrix calculations they must include all the orbitals used in constructing the $\psi(\Gamma_i, \mathbf{x}_1, \hat{\mathbf{x}}_2)$ in their Φ_{ν} whereas our choice is unrestricted.

Our model is prescribed by

- (i) choosing a set of exact target functions to be included explicitly,
- (ii) choosing a set of pseudo-states to represent those states not included in (i),

(iii) choosing a set of correlation functions to represent the non-sinusoidal character of the scattering functions when the incident electron is 'inside' the atom. These also represent two-electron correlations through the Φ_{ν} , though not necessarily all of these.

Since we wish to investigate resonances between the $n = 3$ and $n = 4$ thresholds, it is appropriate to take (i) as all the $n = 1, 2, 3, 4$ target states. We do not incur any penalties by adding pseudo-states whose thresholds lie above the $n = 4$ threshold, provided we restrict the incident energy to lie below this threshold; i.e. we do not have to deal with pseudo-resonances in the present case.

The final model chosen depends on incident energy k_1^2 and total orbital angular momentum L , for reasons to be discussed below. However it may be summarised by giving the number of states of each orbital angular momentum included and the number and type of correlation term. The states, number and type of correlation terms used for each L are set out in table 1. The states and pseudo-states are obtained by diagonalising the one-electron Hamiltonian on a basis of Slater-type orbitals,

$$\psi(r) = r^{n_j} \exp(-\alpha_j r) \quad (2.5)$$

where n_j and α_j are given in table 2.

Table 1.

	L			
	0	1	2	3+
ns	4	4	4	4
$\bar{n}\bar{s}$	3	2	1	1
np	3	3	3	3
$\bar{n}\bar{p}$	2	2	2	2
nd	2	2	2	2
$\bar{n}\bar{d}$	1	1	1	1
nf	1	1	1	1
$\bar{n}\bar{f}$	1	1	—	—
$\bar{n}\bar{g}$	1	—	—	—
Total	18	16	14	14
Correlation terms				
Type A	9	10	—	—
Type B	—	—	12	—

In the above nl is the number of exact, and $\bar{n}\bar{l}$ of pseudo-states, of each l included in the basis for each total orbital angular momentum L .

We found we could obtain close, but not exact, representations of the $n = 4$ states, using only the eighteen orbitals given in table 2, rather than the full twenty linearly independent terms strictly required. Comparisons were made of the 18-term and 20-term basis results at selected angular momentum and energies and showed no significant differences. We therefore adopted the simpler basis for the main calculations.

Two different sets of correlation functions were used, both of the above form (2.5). For $L = 0, 1, 2$ we found it better to use fixed n_j and α_j in a geometric sequence

Table 2. Parameters for Slater orbitals for each l .

$l=0$	n_i	0	0	1	0	1	2	0
	α_j	1.0	0.5	0.5	0.3333	0.3333	0.3333	0.2
1	n_i	1	1	1	2	1		
	α_j	1.0	0.5	0.3333	0.3333	0.2		
2	n_i	2	2	2	2			
	α_j	0.5	0.3333	0.2				
3	n_i	3	3					
	α_j	0.5	0.25					
4		$n=4$		$\alpha_1=0.4$				

(Callaway and Wooten 1974) the parameters being given in table 3, while for $L > 2$ more rapid convergence and improved stability were obtained with fixed α_j and integer n_j ($\alpha_j = 1.20$; $j = 0, \dots, 11$); see Morgan (1980) for a discussion of the choice for e^- , He^+ . We refer to the variable α case as type A, fixed α as type B.

Table 3. Exponents for type A correlation functions: $n_j = 0$.

	1	2	3	4	5	6	7	8	9	10
ζ_i ($L=0, 1$)	4.0	2.5	1.5	0.9	0.6	0.4	0.2	0.1	0.05	—
ζ_j ($L=2$)	1.5	0.90	0.6	0.4	0.2	0.15	0.1	0.06	0.04	0.03

To ensure that the function F_{ij} is regular at the origin we choose the $f_i^{(s)}$ to be linear combinations of functions of the form

$$g_i^{(s)} = (1 - e^{-\gamma r})^{l_i+1} \begin{cases} \sin \\ \cos \end{cases} (k_i r) \quad s = 1, 2 \quad (2.6)$$

where i runs over all open channels.

For most purposes we followed Callaway *et al* (1974) in choosing $\gamma = 1.2$. However for channels in which k_j^2 is small and $l_j \gg 1$ the angular momentum barrier forces F_{ij} to be small and non-oscillatory for all r less than the classical turning point,

$$r_c \approx k_j^{-1} [l_j(l_j + 1)]^{1/2} \quad (2.7)$$

and we choose γ in such cases, so that

$$[1 - \exp(-\gamma r_c)]^{l_M+1} \approx 0.99 \quad (2.8)$$

where l_M is the highest projectile orbital angular momentum in any channel.

For $L = 2$ we compared the results obtained using the 16-term basis and the 18-term basis at $k_1^2 = 0.90$ and found the former adequate. A similar comparison allowed us to adopt a 14-term basis for $L \geq 3$. The choice of type of correlation term is not crucial. In table 4 we compare our six-state calculations for $L = 2$ at $k_1^2 = 0.90$ using both types of correlation function. Results are given for the $2l-3l'$ transitions only. There are small differences, the largest being about 10%, comparable with the differences obtained for a given set using different variational methods. The total $L = 2$ contribution to the 2-3 transition is however stable to change of correlation to better than 4%. It is clear that

Table 4. Six-state calculations for $L = 2$ at $k_1^2 = 0.90$. Partial cross sections in units of πa_0^2 .

		Partial cross sections (πa_0^2)	
		Type A	Type B
2s-3s	S	0.3308	0.3061
	T	0.0087	0.0079
2s-3p	S	1.0710	1.0748
	T	0.2983	0.2999
2s-3d	S	1.2729	1.2760
	T	0.2614	0.2604
2p-3s	S	0.3756	0.3655
	T	0.2620	0.2840
2p-3p	S	0.5859	0.5879
	T	0.6358	0.6557
2p-3d	S	1.0038	0.9954
	T	0.7055	0.6726
Total 2-3		6.552	6.787

provided we can be content with this (10%) level of accuracy for the partial cross sections, there is no particular reason to choose set A rather than set B for this L . For higher L the effects of correlation extend to larger r as the angular momentum barrier moves out, and it is easier to span the space between the 'edge of the atom' and this barrier with type B terms than with type A, for the same number of terms.

Our results for individual partial-wave contributions to individual transitions are converged, in general, to better than 10%. As an example we take the $L = 3$ contributions to the $2l-3l'$ group at $k_1^2 = 0.90$ (table 5): here again the total $L = 3$ contribution to the 2-3 transition is much more accurate, being stable to better than 0.5%. We have found (for $L = 0, 1$) that adding one or two more correlation terms does not affect resonance positions, but as with the cases just discussed, resonance widths are not converged to better than 10%. For the best basis used the bound-bound matrix contains over 4×10^4 elements, and a limit on the number of correlation terms that can be used is imposed in practice by the size of this matrix, and loss of accuracy due to linear dependence. In the energy range of interest here, below the $n = 4$ threshold there are no pseudo-resonances of finite width.

Table 5. The effect of including an extra type B correlation term on the $L = 3$ partial cross sections at $k_1^2 = 0.90$, in πa_0^2 .

	12 terms	13 terms
2s-3s	0.289	0.318
2s-3p	0.366	0.419
2s-3d	0.312	0.301
2p-2s	0.347	0.325
2p-3p	0.478	0.462
2p-3d	1.123	1.086
Total 2-3	2.915	2.911

3. Resonance positions and widths

We have investigated resonance structure in the $L = 0$ and $L = 1$ contributions, from just above the $n = 3$ to just below the $n = 4$ thresholds.

As with the $n = 2$ threshold, there is a shape resonance close to threshold. We find this to be a 3S and it is seen in the triplet contribution to the $3s \rightarrow 3p, 3d$ channels. It is due to the angular momentum barrier in the $3p$ and $3d$ channels; there is a short-range repulsive interaction and a strong long-range dipole attractive interaction. The interaction constant for the dipole term is much larger than for $n = 2$, so it is not clear whether such a resonance exists above the $n = 2$ threshold. Taylor and Burke (1967) found a 1P shape resonance above that threshold, but we have been unable to resolve any $^{1,3}P$ shape resonances above the $n = 3$ threshold. Ho (1979) uses a complex rotation method and can only obtain the Feshbach resonances, so did not find this shape resonance. The effect of this resonance on the $1s-3d$ 3S cross section is shown in figure 1.

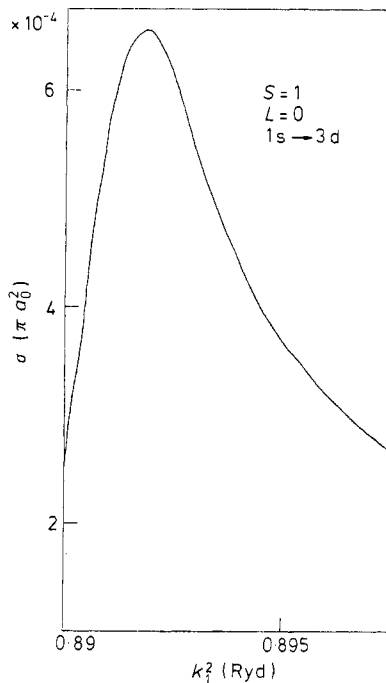


Figure 1. The 3S shape resonance at $k_1^2 = 0.8907$ in the $1s-3d$ cross section. Only the $L = 0$ contribution to the cross section is shown.

3.1. Feshbach resonances ($L = 0, 1$)

For $L = 0$ there are two series of resonances. Decoupling the asymptotic radial equations and writing them as

$$\left(\frac{d^2}{dr^2} - \frac{\Lambda_l}{r^2} + k^2 \right) G(r) = 0 \quad (3.1)$$

we find two negative eigenvalues

$$\Lambda_{01} = -33.32 \quad \Lambda_{02} = -5.34 \quad (3.2)$$

and both values satisfy $\Lambda_{0i} < -\frac{1}{4}$ (Landau and Lifshitz 1959), but it is not possible to assign the calculated resonances to either eigenvalue in an unambiguous way. For $L = 1$ there are three such negative eigenvalues

$$\Lambda_{11} = -32.05 \quad \Lambda_{12} = -18.46 \quad \Lambda_{13} = -3.86. \quad (3.3)$$

Our resonance positions, which are stable to four figures, and widths (which may be uncertain by $\pm 10\%$) are compared in table 6 with the results of Ho (1979). We obtain our positions and widths by fitting Fano profiles on the assumption of isolated resonances. Our model uses an inner region ($r \leq R_0$) in which exchange and coupling between the open and closed channels is included. Exchange is omitted for $r > R_0$, and while we could in principle include these couplings, numerical difficulties in obtaining asymptotic solutions when the closed $n = 4$ channels are included, made it impractical (cf Morgan 1980).

Table 6. Resonance positions and widths (rydbergs), in $L = 0$ and $L = 1$.

	This paper		Ho (1979)	
	E_r	Γ_r	E_r	Γ_r
³ S	0.8907	0.0043	—	—
¹ S	0.9218	0.0029	0.9208	0.0019
¹ S	0.930	<0.001	0.93057	0.00175
¹ S	0.934	0.0010	—	—
³ S	0.9320	0.00005	—	—
¹ P	0.9265	0.0033	0.9256	0.0021
¹ P	0.9359	0.0006	—	—
³ P	0.9220	0.0032	0.9214	0.0022
³ P	—	—	0.9314	0.0013
³ P	0.9343	0.0011	—	—

In consequence we find the widths are sensitive to the choice of R_0 . Our positions agree with Ho's to within 9×10^{-4} Ryd, except for the second ³P resonance where we may miss a very weak resonance near 0.9314: however, we see very narrow resonances in the ¹S and ³S scattering. The energy spectrum of the resonances is shown in figure 2, and it is immediately apparent that the structure is very closely analogous to that of the lowest bound states of helium. This allows us to identify the configurations responsible tentatively. Starting with the $(3l, kl')$ configuration we can interpret the first and third ¹S resonances as $(4s)^2$ and $(4s5s)$ which are both strong. The weak ¹S resonance at $k_1^2 = 0.930$ probably belongs to the Λ_{02} sequence; its configuration is uncertain, but may be $(4p5p)$. The lowest ³S is the shape resonance, and the higher one $(4s5s)$. We then interpret our P resonances as $(4s4p)$ and $(4s5p)$ configurations in both singlet and triplet. It would then follow that the exchange energies were

$$\Delta E_{4s,5s} \approx 0.0020$$

$$\Delta E_{4s,4p} \approx 0.0045$$

$$\Delta E_{4s,5p} \approx 0.0016.$$

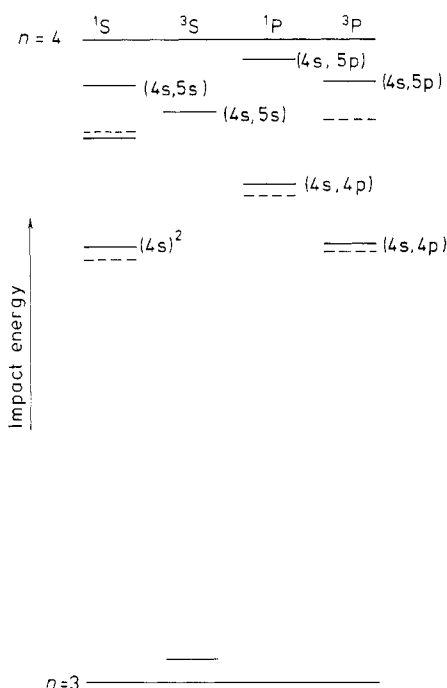


Figure 2. The energy spectrum of the resonances between the $n = 3$ and $n = 4$ thresholds. The full lines indicate our results, the broken lines those of Ho (1979). Tentative assignments ($nl, n'l'$) are shown.

A further interesting feature is that, for the first time, we see the same resonance in different transitions. In particular the lowest 1S resonance $(4s)^2\ ^1S$ is seen in the $n = 1$ to $n = 3$ transition and in the $n = 2$ to $n = 3$ transition (figure 3). The parameters of the resonance are given in table 6.

4. Cross sections for $nl \rightarrow n'l'$ transitions

We do not consider the $1s \rightarrow 2l$ transitions in this paper; these have previously been investigated using algebraic variational close-coupling methods by Callaway and his collaborators (Callaway *et al* 1977) and our results agree with theirs in the energy range under consideration.

4.1. $1s \rightarrow 3l$ transitions

First, we briefly compare our six-state calculations with the six-state results of Burke *et al* (1967) and both of these with the results obtained with the full basis (table 7). Only one parity is involved, that of the entrance channel.

Our full basis results are slightly smaller than those of either six-state calculation, the six-state results of Ormonde *et al* (1969) being slightly larger than our own: however the cross section for this transition at this energy is well represented in a six-state calculation. The triplet contribution is very small, in all models. The total

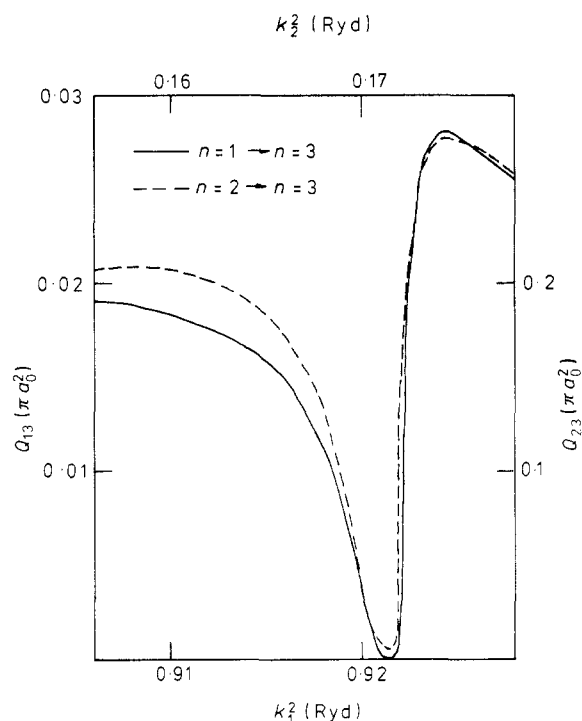


Figure 3. The lowest $1S$ resonance in the $n = 2$ to $n = 3$ transition compared with the same resonance in the $n = 1$ to $n = 3$ transition at the corresponding incident energies.

Table 7. Comparison of six-state and eighteen-state $L = 0$ contributions to $1s \rightarrow 3l$ cross sections at $k_1^2 = 0.90$ (in πa_0^2), summed over spins.

	Our six-state	Ormonde <i>et al</i> (1969)	Full basis
$1s \rightarrow 3s$	0.0068	0.0074	0.0065
$1s \rightarrow 3p$	0.0092	0.0099	0.0085
$1s \rightarrow 3d$	0.0032	0.0034	0.0030
Total $n = 1$ to $n = 3$	0.0192	0.0207	0.0180

$1s \rightarrow 3l$ ($l = 0, 1, 2$) cross sections, summed over spin and total orbital angular momentum, are presented in table 8, where they are compared at two energies with the previous six-state values (Burke *et al* 1967). The partial-wave expansion has effectively converged, in our energy range, by $L = 6$.

Our full basis calculations for $1s \rightarrow 3s, 3d$ agree well with those of Burke *et al* (1967) at $k_1^2 = 0.90$ though we are 8% lower for $1s \rightarrow 3p$. There are larger discrepancies between our results and those of Burke *et al* at $k_1^2 = 0.93$, especially for $1s \rightarrow 3d$, where we are 35% lower. In our model, the $3d$ state can couple strongly with $4p$ and higher p pseudo-states and with $4f$ and higher f pseudo-states. At $k_1^2 = 0.93$ we would expect to see resonance effects from the $n = 4$ threshold at $k_1^2 = 0.9375$.

Table 8. Total $1s \rightarrow 3l$ ($l = 0, 1, 2$) cross sections in πa_0^2 : (a) this paper, (b) Burke *et al* (1967).

k_1^2		$1s \rightarrow 3s$	$1s \rightarrow 3p$	$1s \rightarrow 3d$
0.900	(a)	0.0321	0.0575	0.0331
	(b)	0.032	0.062	0.034
0.905	(a)	0.0383	0.0625	0.0317
0.910	(a)	0.0413	0.0644	0.0324
0.915	(a)	0.0377	0.0686	0.0330
0.920	(a)	0.0240	0.0474	0.0287
0.925	(a)	0.0506	0.0726	0.0360
0.930	(a)	0.0495	0.0856	0.0415
	(b)	0.055	0.097	0.056

4.2. $2l \rightarrow 3l'$ transitions

First, we make some comparisons between our six-state values and those of Ormonde *et al* (1967). The dominant contributions at $k_1^2 = 0.90$ are from $L = 1$ and $L = 2$, and are compared in table 9, which also gives our full basis results. In each case we have summed over singlet and triplet contributions. For $L = 1$ the two sets of six-state results agree well except for $2p \rightarrow 3d$ where the difference is about 10%. However, the six-state results can be very different from those obtained with the full basis. For example, the $2s \rightarrow 3d$ cross section is then reduced by about a factor of three. The total $L = 1$ contribution to $n = 2$ to $n = 3$ transitions agrees within 3% for the two six-state calculations, but is decreased by 25% on going to our best basis. For $L \geq 2$ Ormonde *et*

Table 9. The $L = 1$ and $L = 2$ contributions to the $2l \rightarrow 3l'$ cross sections at $k_1^2 = 0.15$, in πa_0^2 . (a) This paper, six-state; (b) Ormonde *et al* (1969), six-state; (c) this paper, best basis.

	$L = 1$		
	(a)	(b)	(c)
2s-3s	4.98	4.88	3.97
2s-3p	1.95	1.98	2.19
2s-3d	1.10	1.05	0.317
2p-3s	0.0722	0.0685	0.213
2p-3p	1.376	1.379	1.277
2p-3d	1.908	2.129	1.343
Total $L = 1$	4.525	4.662	3.743
	$L = 2$		
	(a)	(b)	(c)
2s-3s	0.314	0.878	0.116
2s-3p	1.375	1.442	1.280
2s-3d	1.536	1.700	2.344
2p-3s	0.650	0.652	0.701
2p-3p	1.878	2.590	1.708
2p-3d	3.048	5.148	2.187
Total $L = 2$	4.988	7.297	4.382

The totals are averaged over initial states.

al (1969) and also Burke *et al* (1967) neglected exchange couplings between channels involving an $n = 2$ and an $n = 3$ state. Our six-state values show that this is a reasonable approximation for s-p transitions only, but can be very poor otherwise. For example, for the 2s-3s transition it induces an error of almost a factor of three. This is probably because there is no long-range coupling in this case, and exchange is relatively more important. Again, going to a large basis gives significant changes: the 2s-3s contribution decreasing by almost a factor of three from our six-state result, and by more than a factor of seven from the Ormonde *et al* value. Comparing the $L = 2$ contribution with the total $n = 2 \rightarrow n = 3$ cross section in various approximations we see that Burke *et al*'s six-state value is about 50% higher than ours, but our full basis result is within 5% of our six-state result.

For the 2-3 transitions there are contributions from both parities. For channels with parity $(-1)^{L+1}$ our results are in strong disagreement for all L with those of Ormonde *et al*, almost certainly due to their neglect of some exchange couplings (table 10). The relevant transitions are 2p-3p and 2p-3d, for $L \geq 1$. In the earlier six-state calculations these contribute almost 40% of the total Q_{23} at $k_1^2 = 0.90$, whereas we find that they contribute less than 15% in both our six-state and best basis calculations (which agree well). This is the most important reason for the fact that our total Q_{23} cross section is so much lower than the previous values (see § 5 below).

Table 10. The contributions from selected L , summed over spins, to the 2-3 cross section from channels with $(-1)^{L+1}$ parity, at $k_2^2 = 0.15$ Ryd, in units of πa_0^2 .

		Six-state	Full basis	Ormonde <i>et al</i> (1969)
$L = 1$	(a)	0.5915	0.5739	1.6666
	(b)	0.3744	0.3739	1.2465
$L = 2$	(a)	0.6343	0.5177	0.7669
	(b)	1.3796	0.9089	2.6750
$L = 3$	(a)	0.4965	0.3588	1.4834
	(b)	0.8605	0.6301	2.6421
$L = 4$	(a)	0.0331	0.0267	0.0143
	(b)	0.0980	0.0863	0.0444

(a) 2p-3p transition.

(b) 2p-3d transition.

Our best basis results for $2 \rightarrow 3$ transitions summed over L , S and π are given, for each of the six transitions, in table 11, but these do not fully account for resonance effects, no detailed search for resonances having been made for $L > 1$. For an initial 2s state, the 3s and 3p cross sections are larger than that for 2s-3d near the $n = 3$ threshold, but away from threshold 2s-3p is always largest. For atoms initially in the 2p state the 2p-3d cross section is largest throughout this energy range, while 2p-3s remains relatively small. In the latter case the singlet contribution is small relative to the triplet for $k_2^2 > 0.16$, but in the former both are of comparable magnitude throughout. In table 11 we give the six-state values of Burke *et al* (1967) at the two energies for which they are available. The biggest discrepancy occurs for 2p-3d where, as previously remarked, the $(-1)^L$ parity contributions, which are much reduced when all exchange terms are retained, make a large contribution. In so far as any conclusion can be drawn from two

Table 11. Calculated cross sections for the $2l-3l'$ transitions in πa_0^2 . The effects of resonances for $L > 1$ are not included explicitly. The six-state values of Burke *et al* (1967) are shown in brackets.

k_2^2	2s-3s	2s-3p	2s-3d
0.150	5.009 (6.93)	5.309 (5.69)	3.840 (4.47)
0.155	5.461	6.641	3.902
0.160	5.357	7.523	4.517
0.165	5.117	7.994	5.085
0.170	3.722	6.389	5.304
0.175	5.025	8.929	7.000
0.180	4.430 (7.82)	9.309 (11.94)	8.339 (9.58)
	2p-3s	2p-3p	2p-3d
0.150	1.516 (1.48)	5.215 (8.86)	6.089 (13.30)
0.155	1.816	5.964	7.318
0.160	2.187	6.746	8.577
0.165	2.089	7.441	9.513
0.170	1.819	6.828	10.427
0.175	2.975	6.749	10.467
0.180	2.847 (3.08)	7.681 (10.69)	11.180 (17.26)

points, the difference between our results and the six-state results for $2p \rightarrow 3d$ decreases rapidly with increasing impact energy, so the six values given by Burke *et al* at energies $0.21 \leq k_2^2 \leq 0.35$ may be relatively reliable. Burke *et al*'s suggestion that omission of the $n = 4$ states would be less important for the $2 \rightarrow 3$ transition than for $1 \rightarrow 3$ is not correct.

Calculations for transitions involving the $n = 4$ states would require inclusion of all $n = 5$ states in the basis and would be difficult.

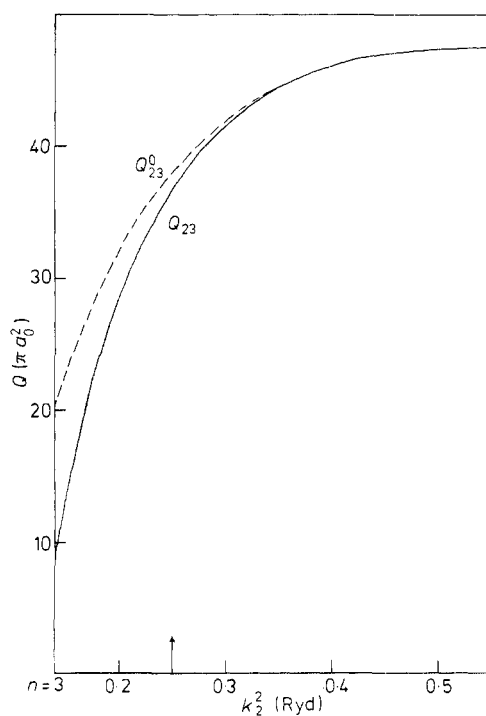
5. Total $n-n'$ cross sections

Our results, summed over S , L , π and over individual transitions, for the $n-n'$ cross sections are given in table 12. Our results for Q_{12} are close to those obtained in an earlier model by Callaway *et al* (1975), who give results at 0.90. They obtain values of 0.166 and 0.356 respectively for Q_{1s-2s} and Q_{1s-2p} summed up to $L = 3$, whereas we obtain 0.171 and 0.3954 respectively, which are 16% and 11% higher than the large-basis results. In each case for Q_{13} and Q_{23} we compare with the six-state results of Burke *et al* (1967) at $k_1^2 = 0.90$, 0.93 and with Johnson's semi-empirical formula (Johnson 1972). The results for $n = 2$ to $n = 3$ have been discussed in more detail elsewhere (Hata *et al* 1980). They lie 70% lower than the old six-state results at $k_2^2 = 0.15$ but this decrease becomes less significant with increasing energy, being only 36% at our highest energy.

The effect on the 2-3 rate coefficient will be small, unless the maximum of the electron energy distribution is close to the threshold energy; even then the change will

Table 12. Total n - n' excitation cross sections in πa_0^2 .

k_1^2	This paper	Burke <i>et al</i> (1967)	Johnson (1972)
$n = 1 \rightarrow n = 3$			
0.90	0.123	0.128	0.068
0.905	0.133		0.069
0.910	0.138		0.070
0.915	0.139		0.071
0.920	0.100		0.072
0.925	0.159		0.073
0.930	0.177	0.208	0.074
$n = 2 \rightarrow n = 3$			
0.90	13.1	22.1	23.0
0.905	15.3		24.1
0.910	17.5		25.2
0.915	18.8		26.2
0.920	18.2		27.2
0.925	20.4		28.1
0.930	22.4	30.6	29.1

**Figure 4.** Johnson's cross section $Q_{23}^{(0)}$ and our modified result $Q_{23} = (1 - A e^{-\beta u}) Q_{23}^{(0)}$, (see text) with $A = 18.25$ and $\beta = 3.47$. An arrow indicates the ionisation threshold. The cross section is in units of πa_0^2 .

be small if the electron energy distribution is Maxwellian. We have adjusted Johnson's formulae to agree with our results at $k_2^2 = 0.15$ and 0.18 by inserting a factor $(1 - A e^{-\beta u})$, $u = \Delta E/E$ (see Hata *et al* 1980), and the new estimate of Q_{23} is compared with the original Johnson values in figure 4. There is no significant difference for $k_2^2 > 0.35$.

These simple estimates of the rate coefficient do not explicitly include the effects of the resonances. We find no resonance broader than 50 meV, and although there will be many narrow resonances below the $n = 4$ and higher thresholds, we suspect that their effect on the rate coefficient will be small, provided the width of the electron energy distribution is appreciably greater than 50 meV.

Our values of Q_{13} are significantly lower (18%) than those of Burke *et al* (1967) at the higher of the two energies where comparison is possible. This is primarily due to the effects of coupling to the $n = 4$ states. Johnson's formula is poor throughout the energy range, its predictions being between a factor of two and a factor of three lower. In view of the direct relevance of the results to both laboratory and astrophysical plasmas (Hata *et al* 1980, Burgess *et al* 1978, 1980) a direct measurement of Q_{13} would be of considerable interest.

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References

- Berrington K A, Burke P G and Sinfaiam A L 1975 *J. Phys. B: Atom. Molec. Phys.* **3** 1459–73
 Burgess D D, Kolbe G and Ward J M 1978 *J. Phys. B: Atom. Molec. Phys.* **11** 2765–78
 Burgess D D, Myerscough V P, Skinner C H and Ward J M 1980 *J. Phys. B: Atom. Molec. Phys.* **13** 1675–702
 Burke P G, Ormonde S and Whitaker W 1967 *Proc. Phys. Soc.* **92** 319–35
 Callaway J and Wooten J W 1974 *Phys. Rev. A* **9** 1924–31
 Hata J, Morgan L A and McDowell M R C 1980 *J. Phys. B: Atom. Molec. Phys.* **13** L347–52
 Ho Y K 1977 *J. Phys. B: Atom. Molec. Phys.* **10** L373–7
 — 1979 *J. Phys. B: Atom. Molec. Phys.* **12** L543–6
 Johnson L C 1972 *Astrophys. J.* **174** 227–36
 Landau L D and Lifshitz E M 1959 *Quantum Mechanics* (London: Pergamon) § 35
 Morgan L A 1979 *J. Phys. B: Atom. Molec. Phys.* **12** L735–8
 — 1980 *J. Phys. B: Atom. Molec. Phys.* **13** 3703–15
 Morgan L A, McDowell M R C and Callaway J 1977 *J. Phys. B: Atom. Molec. Phys.* **10** 3297–305
 Ormonde S, Whitaker W, Huebner W and Burke P G 1969 *Technical Report* No AFWL-TR-67-10 vol 1
 Taylor A J and Burke P G 1967 *Proc. Phys. Soc.* **92** 336–44