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LETTER TO THE EDITOR

Electron impact excitation of the $n=2$ to $n=3$ transition in atomic hydrogen near threshold

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Abstract. Algebraic variational method close-coupling calculations for electron impact excitation of the $n=2$ to $n=3$ transition in atomic hydrogen, using a large basis, are presented at energies below the $n=4$ threshold. Near the $n=3$ threshold the cross section is almost a factor of two lower than that predicted by Johnson. The results go some way towards resolving the discrepancy between Johnson's results and experiments on hydrogen plasmas. However, there is little effect on the rate coefficient at low temperatures ($\simeq 0{\cdot}8$ eV) on the assumption of a Maxwellian distribution.

Burgess *et al* (1978) have reported direct laser-based measurements of the collisional depopulation rate of the $n=2$ level of atomic hydrogen in a plasma. They concluded that they could not account for the observations if the cross sections and rate coefficients given by Johnson's semiempirical formulae (Johnson 1972) were correct. However, for the $n=2$ to $n=3$ transition Johnson's formulae are in excellent agreement with the best available theoretical results, namely, the six-state close-coupling calculation of Burke *et al* (1967), in the energy range $k_2^2=0{\cdot}15$ to $k_2^2=0{\cdot}35$. Here k_2^2 is the energy of the incident electron in rydbergs, measured from the $n=2$ threshold. Burgess *et al* (1978) state that 'in the temperature range studied (0·41 to 0·79 eV) Johnson's values for the 2–3 electron excitation and de-excitation rates are too high, probably by a factor exceeding five'. This temperature range corresponds to k_2^2 in the range 0·03–0·06, for the peak of the Maxwellian distribution, so that their remarks imply that the cross sections given by Johnson and by Burke *et al* are also as much as a factor of five high. Burgess *et al* (1980) studied a hydrogen plasma irradiated by high-intensity Hα, Hβ and Hγ. They find, for example, that 'the observed long-time enhancement in the laser fluorescence is much larger than theory for both Hα and Hβ' and 'the discrepancy suggests that the rates into $n=2$ are higher than predicted'; that is relative to those for $n=3$.

The rate coefficient for the 2–3 transition in atomic hydrogen is an important parameter for diagnostics in tokamaks. It is used to predict the number of ionisations by electron collision in terms of the observed number of Hα photons emitted per hydrogen atom inserted in the plasma (E Hinnov 1979, private communication). The conversion charts for this purpose given by Johnson and Hinnov (1972) are based on Johnson's

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(1972) cross sections and rate coefficients, and may be seriously in error if the suggestions of Burgess *et al* are correct.

We have therefore recalculated the cross section $Q_{23}(k_2^2)$ for this transition using the algebraic variational close-coupling code developed by Morgan (1980). For the present work the model adopted included the exact $n = 1$ to $n = 4$ target states together with a number of pseudostates with thresholds above the $n = 4$ threshold. The basis finally adopted is as follows:

$L = 0, 1$	(18/9)	7s–5p–3d–2f–1g
$L = 2$	(16/10)	6s–5p–3d–2f
$L = 3, 4, 5, 6$	(14/12 or 13)	5s–5p–3d–1f

where the first figure in brackets is the number of basis states and the second the number of correlation terms in each channel. The parameters of these basis states will be given in a subsequent publication (Hata *et al* 1980), where the resonance structures and cross sections for the individual $nl \to n'l'$ transitions will be reported.

We used from nine to thirteen correlation terms of the form $r^n\ e^{-\alpha r}$ (α constant) in each channel, the actual number, chosen to ensure adequate convergence, depending on L. To avoid the known anomalies in the Kohn, inverse Kohn and similar variational methods, we used Nesbet's RIAF method (Nesbet 1978).

Results were obtained at eight impact energies, in the range $0{\cdot}15 \leqslant k_2^2 \leqslant 0{\cdot}18$ Ryd, i.e. 2·04 to 2·45 eV. Numerical problems occur for $L > 3$ closer to threshold, though the partial-wave cross sections for $L = 0$, 1, 2 and 3 have been obtained at $k_2^2 = 0{\cdot}14$ Ryd.

None of these energies coincide with the position of any Feshbach resonance ($L = 0, 1$), but resonance structure for higher L has not been investigated. Our eigenphase sums are lower bounds in this energy range (below the $n = 4$ threshold) and enable us to conclude that our values for the total cross section have converged to about 10% with respect to the inclusion of further basis states or Slater-type-orbital correlation terms. Calculations at higher energies are in progress, but cannot be bounded in the same way.

To check our code we also carried out calculations in a six-state close-coupling model (1s–2s–2p–3s–3p–3d), which allows a direct comparison with the six-state calculations of Burke *et al* (1967). The results for $L = 1$ at $k_2^2 = 0{\cdot}15$ are given in table 1. The values given for Burke *et al*'s model are taken from the detailed tables (Ormonde *et al* 1969), for which we are indebted to Dr S Ormonde. These tables give full six-state results only for those channels with parity of the 1s L channel. As discussed below they approximate certain exchange terms in the opposite parity case. The agreement is satisfactory, though far from exact, except for the singlet contribution to 2s–3s. Here, however, our eighteen-state value of 0·0433 is in good agreement with our six-state value.

Part of the discrepancy may arise from the fact that Burke *et al* (1967) appear to have chosen to omit the exchange potentials coupling channels with $n = 2$ to channels with $n = 3$. This has serious effects for the odd-parity contributions, as shown in table 2. The effect of the approximation made by Burke *et al* is to considerably overestimate these contributions, apparently by more than a factor of three at $k_2^2 = 0{\cdot}15$.

A more detailed comparison with Burke *et al* (1967) is given in table 3, where it is clear that large discrepancies occur in the $L = 1, 2$ and 3 contributions to the 2p to $n = 3$

Table 1. Six-state close-coupling results for the even-parity contributions to individual $nl \to n'l'$ transitions at $k_2^2 = 0{\cdot}15$ Ryd (in πa_0^2).

		Present	Ormonde *et al* (1969)
2s–3s	S	0·0424	0·0287
	T	4·937	4·851
2s–3p	S	0·161	0·153
	T	1·787	1·827
2s–3d	S	0·0823	0·0844
	T	1·021	0·969
2p–3s	S	0·0484	0·0474
	T	0·0238	0·0211
2p–3p	S	0·3467	0·357
	T	1·030	1·023
2p–3d	S	0·300	0·297
	T	1·608	1·832

Table 2. Odd-parity contributions to the (*a*) 2p–3p and (*b*) 2p–3d transitions at $k_2^2 = 0{\cdot}15$, in πa_0^2: (i) our six-state calculation, (ii) our best calculation, (iii) Ormonde *et al* (1969), no 2–3 exchange. Singlet and triplet contributions have been added.

		(i)	(ii)	(iii)
$L=1$	*a*	0·592	0·574	1·667
	b	0·374	0·374	1·247
$L=2$	*a*	0·634	0·518	0·767
	b	1·38	0·909	2·675
$L=3$	*a*	0·497	0·359	1·483
	b	0·860	0·630	2·642
$L=4$	*a*	0·0331	0·027	0·014
	b	0·0980	0·086	0·044
Total $L \leqslant 4$		4·47	3·48	10·54

transitions. The total $n=2$ to $n=3$ cross section is $Q_{23} = \frac{1}{4}Q_{2s,n=3} + \frac{3}{4}Q_{2p,n=3}$. Our result for Q_{23} is almost a factor of two smaller than that of Burke *et al* (1967).

The main uncertainties in our calculation are given below.

(i) The contribution from $L>6$ is assumed to be unimportant at these energies.

(ii) The $L=5$ contribution is uncertain by ±20%. At these low energies the classical turning point r_c for $L=5$ is very large (>30 a_0) in the 3d $L-2$ and 3p $L-1$ channels, and consequently the scattering functions in those channels are of small amplitude inside r_c. We represent the scattering functions inside this sphere by

$$rF_{ij}(r) = \alpha_{ij}^{(0)} f_1(k_j, r) + \alpha_{ij}^{(1)} f_2(k_j, r) + \sum_\nu c_{j\nu}\eta_\nu(r) \tag{1}$$

where $[(\boldsymbol{\alpha}^{(0)})^{-1}\boldsymbol{\alpha}^{(1)}]_{ij} = K_{ij}$ (see Morgan 1980). Here

$$f_1(k, r) = (1-\mathrm{e}^{-\gamma r})^{l_j+1} \sin\theta(k, r) \tag{2}$$

$$f_2(k, r) = (1-\mathrm{e}^{-\gamma r})^{l_j+1} \cos\theta(k, r) \tag{3}$$

Table 3. Partial-wave contributions to 2s to $n=3$ and 2p to $n=3$ cross sections at $k_2^2=0{\cdot}15$, summed over singlet and triplet and parity (πa_0^2): (*a*) present results, (*b*) Ormonde *et al* (1969).

	2s		2p	
	(*a*)	(*b*)	(*a*)	(*b*)
$L=0$	0·388	0·520	0·192	0·182
1	6·470	7·924	3·782	6·499
2	3·740	4·002	4·595	8·390
3	0·764	0·774	2·370	6·247
4	2·554	3·367	1·715	2·169
5	0·199	0·491	0·165	0·326
6		0·011		0·009
$\sum_{L=0}^{6}$	14·1	17·1	12·8	23·8
	Weighted total Q_{23}			
	13·1			22·1

where

$$\theta(k, r) = (k_j r - \tfrac{1}{2} l_j \pi) \tag{4}$$

and the $\eta_\nu(r)$ are quadratically integrable. The cut-off parameter γ must be chosen to be small to produce the correct behaviour of $F_{ij}(r)$ inside r_c, and this causes computational problems in the case discussed.

(iii) There may be correlation effects which cannot be adequately represented with two-electron determinants constructed from Slater-type orbitals.

(iv) There is a broad ^{1}S shape resonance near $k_2^2 = 0{\cdot}14$ (Hata *et al* 1980) which may affect the value of the cross section close to threshold. Feshbach resonances for $L>1$ are not explicitly included.

However, none of these effects appears serious for the $n=1$ to $n=3$ cross section Q_{13}, where our values agree fairly well with those obtained by Burke *et al* (1967), but both are much larger than predicted by Johnson's formula (table 4).

Our final results for Q_{23} are given in table 5 where they are compared with the values of Burke *et al* (1967) at two energies, and with the predictions of Johnson's semi-empirical formula. Our result is 70% below Burke *et al* at the lowest energy, and 25% lower at $k_2^2=0{\cdot}18$. A graphical comparison of these results is shown in figure 1. The energy dependence is largely attributable to the change in the position of the centrifugal barrier with increasing L, and the increasing contribution from higher L as the energy

Table 4. Calculated values for $Q_{13}(\pi a_0^2)$.

	This paper	Burke *et al* (1967)	Johnson (1972)
$k_2^2=0{\cdot}15$	0·123	0·128	0·068
$k_2^2=0{\cdot}18$	0·177	0·208	0·074

Table 5. Calculated values of Q_{12} (πa_0^2).

K_2^2	Present	Johnson (1972)	Burke *et al* (1967)
0·15	13·1	23·0	22·1
0·155	15·3	24·1	—
0·160	17·5	25·2	—
0·165	18·8	26·2	—
0·170	18·2	27·2	—
0·175	20·4	28·1	—
0·180	22·4	29·0	30·6

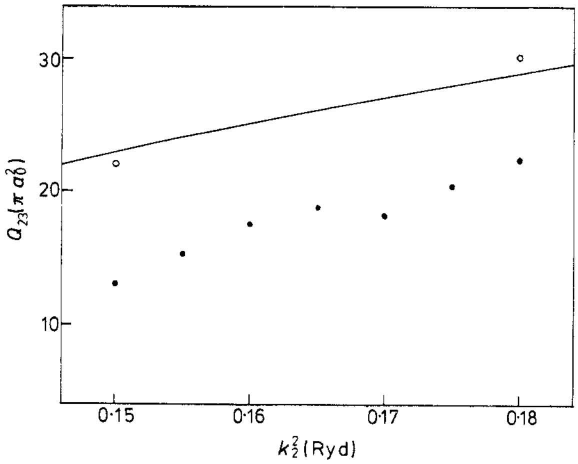

Figure 1. Total cross section for the $n = 2$ to $n = 3$ transition in atomic hydrogen, excited by electron impact (πa_0^2). The full curve is the Johnson semiempirical formula (1972), the open circles the six-state close-coupling result (Burke *et al* 1967) and the full circles the present results.

increases. There is some effect from Feshbach resonances in the $L = 0$ and 1 contributions, but these are narrow ($\Gamma \leqslant 0{\cdot}003$ for $L = 0, 1$); we have not calculated resonance profiles for $L > 1$, but we should not expect their inclusion to change our result significantly at the lower end of our energy range (i.e. just above the threshold) though there might be a significant effect very close to but below the $n = 4$ threshold.

Thus our conclusion must be that Burgess *et al*'s suggestion, that at temperatures below 0·80 eV cross sections based on Johnson's (1972) formula for the $n = 2$ to $n = 3$ transition are too high, is correct. We cannot lower the cross section by more than a factor of two on the basis of our calculation. It is more difficult to be sure about rate coefficients, from changes in cross section values over the narrow range of energies to which our results apply. We can attempt to estimate the rate coefficient, assuming a Maxwellian distribution of velocities, as follows.

Johnson's (1972) formula for the $n = 2$ to $n = 3$ transition may be written

$$Q_{23}^{(0)}(U) = \frac{14{\cdot}4}{U}(1 - \mathrm{e}^{-\alpha U})\left[A_{23}\left(\ln U + \frac{1}{2U}\right) + B_{23}\left(1 - \frac{1}{U}\right)\right]\pi a_0^2 \qquad (5)$$

where

$$U = 7{\cdot}2k_2^2 \tag{6}$$

and

$$A_{23} = 9{\cdot}226 \qquad B_{23} = 4{\cdot}4111 \qquad \alpha = 0{\cdot}363.$$

The values of A_{23}, B_{23} are primarily determined by the high-energy behaviour and α is introduced as a low-energy cut-off. We can fit our results to a variant of Johnson's formula by introducing an additional factor

$$Q'_{23} = f(U)Q_{23}^{(0)} \tag{7}$$

with

$$f = (1 - \gamma\, \mathrm{e}^{-\beta U}) \qquad \gamma = 18{\cdot}25 \qquad \beta = 3{\cdot}47 \tag{8}$$

which produces very little change outside the range of our data.

Johnson's (1972) cross section can be written

$$Q_{23}^{(0)} = (1 - \mathrm{e}^{-\alpha U})F(U) \tag{9}$$

and, hence, our modified result is

$$Q'_{23} = Q_{23}^{(0)} + \gamma[(1 - \mathrm{e}^{-\beta U}) - (1 - \mathrm{e}^{-(\beta+\alpha)U})]F(U) \tag{10}$$

so that we can readily compute the rate coefficient using equation (36) of Johnson's paper. At $T = 0{\cdot}79$ eV we find the rate coefficient using (10) is 0·93 times the value obtained using (5). The low rate coefficients apparently required at this temperature by Burgess *et al*'s experiments cannot be obtained from our cross sections unless the electron energy distribution in the plasma is non-Maxwellian. However, such a non-Maxwellian velocity distribution would not seem to account for all the discrepancies reported by Burgess *et al* (1978, 1980), particularly those involving rates into and out of the $n = 3$ state.

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