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High-energy cross sections for electron excitations of excited hydrogen atoms in which the principal quantum number is changed by 1

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Abstract. At large impact energies E the cross section Q for the electron excitation from the n, l state of hydrogen to the n', l' state may be written in the form $QE = A \log E + B$. The first Born approximation is used to calculate these A's and B's for all transitions with $n = 1, 2, 3, 4, 5$ and 6 and with $n' = n+1$. The A's and B's associated with the main optically allowed transitions (i.e. $l' = l+1$) are largest. However, for small values of l we find that in calculating the B's we must take account of all other transitions, besides the main optically allowed transitions, for the sum total effect of these minor transitions is almost as large as that of the main optically allowed transitions. These minor transitions can be neglected in calculating the A's for the average cross section from one energy level to another but they increase the B's for the average cross sections by about 25%.

1. Introduction

The cross sections for the excitation of the excited states of hydrogen by electron impacts are of great importance in plasma and stellar physics.

Some quantum-mechanical calculations on these cross sections have been carried out using the first Born approximation. For example, the work of Boyd (1958) and McCrea and McKirgan (1960) can be used to obtain cross sections for all electron excitations from the first excited state of hydrogen. McCoyd, Milford and Wahl (1960) have also used the first Born approximation to calculate cross sections for all transitions from the levels with principal quantum number $n = 3$ to the levels with principal quantum number $n' = 4$. The cross sections for the main optically allowed transitions (i.e. $l' = l+1$) have been calculated for transitions from state $n = 4$ to $n' = 5$ (Fisher, Milford and Pomilla 1960) and from $n = 5$ to $n' = 6$ (Milford, Morrissey and Scanlon 1960). The cross sections for two of the main optically allowed transitions have also been calculated for $n = 10$ to $n' = 11$ (McCoyd and Milford 1963).

In order to obtain more information about these electron excitation cross sections we extend the work of Milford, and calculate the cross sections for electron excitation for all transitions from the levels $n = 4$ to $n' = 5$, from $n = 5$ to $n' = 6$ and from $n = 6$ to $n' = 7$.

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2. Calculations

Using the first Born approximation (Mott and Massey 1952), it can be shown (McCoyd, Milford and Wahl 1960) that the cross section for electron excitation from the state of atomic hydrogen with principal quantum number n and azimuthal quantum number l to the state with principal quantum number n' ($n' > n$) and azimuthal quantum number l' can be written in the form†

$$Q_{n,l;n',l'}(E) = \frac{1}{E}\sum_{r=-1}^{x} a_r I^r_{2(n+n')} \tag{1}$$

where E is the energy of the incident electron, x is a certain integer, a_r is a constant which depends on n, l, n' and l' but which is independent of E and where

$$I_q^r = \int_{\gamma_1}^{\gamma_2} \gamma^r(1+\gamma^2)^{-q}d\gamma \tag{2}$$

with γ_1 and γ_2 given by

$$\gamma_1\gamma_2 = \frac{n'-n}{n'+n} \qquad \text{and} \qquad (2E)^{1/2} = \frac{(\gamma_1+\gamma_2)(n'+n)}{2nn'}. \tag{3}$$

In order to calculate $Q_{n,l;n',l'}(E)$ we must first obtain the a_r's, using the method given by McCoyd, Milford and Wahl (1960), and then evaluate the I_q^r's at each value of the incident electron energy.

If the energy of the incident electron is large the labour of the computation is greatly reduced, for we find that if E is large

$$I_q^{-1} = \frac{1}{2}\left[\ln E + \ln\left\{8\left(\frac{nn'}{n-n'}\right)^2\right\} - \sum_{v=1}^{q-1}\frac{1}{v}\right] \tag{4}$$

and

$$I_q^r(r > -1) = \frac{\{\frac{1}{2}(r-1)\}!\,\{q-\frac{1}{2}(r+3)\}!}{2(q-1)!} \tag{5}$$

and hence we can write

$$Q_{n,l;n',l'}(E) = A_{n,l;n',l'}\frac{\log E}{E} + \frac{B_{n,l;n',l'}}{E}. \tag{6}$$

When the a_r's are known, for given values of n, l, n' and l', we can employ (1), (4), (5) and (6) to obtain $A_{n,l;n',l'}$ and $B_{n,l;n',l'}$. These may then be used in (6) to calculate the cross section at any high incident electron energy.

The work of Milford shows that cross sections can be written in the form (6) almost down to the maximum in cross sections. Since it is unlikely that the first Born approximation is accurate to such low energies (Somerville 1963), we only calculate the constants $A_{n,l;n',l'}$ and $B_{n,l;n',l'}$, as they will provide all of the useful information that can be obtained from the first Born approximation. The present cross sections should not be used at such low energies.

For our computations we constructed a machine programme which used the procedure of Milford to calculate the a_r's. In actual practice we found that if we started with eight significant figures we could obtain reliable cross sections for $n \leqslant 3$. However, when we started with sixteen significant figures we could obtain reliable cross sections for $n \leqslant 6$.

† Throughout this discussion we will give energies in atomic units, 1 atomic unit = 27·21 ev and cross sections in units of πa_0^2.

Table 1. The constant $A_{n,l;n+1,l'}$ appearing in expression (6) for the cross section for electron excitation from the n, l state of hydrogen to the $n+1, l'$ state

n / l'	1	2		3		4		5		6	
l	$l+1$	$l-1$	$l+1$	$l-1$	$l+1$	$l-1$	$l+1$	$l-1$	$l+1$	$l-1$	$l+1$
0	$2{\cdot}55554^{0}$†	—	$1{\cdot}44189^{1}$	—	$4{\cdot}59191^{1}$	—	$1{\cdot}11374^{2}$	—	$2{\cdot}28997^{2}$	—	$4{\cdot}20723^{2}$
1		$4{\cdot}50592^{-1}$	$2{\cdot}30703^{1}$	$3{\cdot}05520^{0}$	$5{\cdot}85731^{1}$	$1{\cdot}08286^{1}$	$1{\cdot}24706^{2}$	$2{\cdot}80850^{1}$	$2{\cdot}35367^{2}$	$6{\cdot}03713^{1}$	$4{\cdot}06969^{2}$
2				$1{\cdot}04130^{0}$	$9{\cdot}63946^{1}$	$5{\cdot}69443^{0}$	$1{\cdot}82210^{2}$	$1{\cdot}80842^{1}$	$3{\cdot}18127^{2}$	$4{\cdot}39129^{1}$	$5{\cdot}20489^{2}$
3						$1{\cdot}81571^{0}$	$2{\cdot}75450^{2}$	$8{\cdot}77006^{0}$	$4{\cdot}46642^{2}$	$2{\cdot}58364^{1}$	$6{\cdot}93502^{2}$
4								$2{\cdot}77910^{0}$	$6{\cdot}31615^{2}$	$1{\cdot}23757^{1}$	$9{\cdot}32362^{2}$
5										$3{\cdot}93300^{0}$	$1{\cdot}25469^{3}$

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

The values of $A_{n,l;n',l'}$ and $B_{n,l;n',l'}$ which we calculated for $n = 1, 2, 3, 4, 5$ and 6 and $n' = n+1$ are given in tables 1 and 2. Where possible the results were compared with the work of Milford, and in all cases the agreement was better than the number of figures tabulated.

Table 2. The constant $B_{n,l;n',l'}$ appearing in expression (6) for the cross section for electron excitation from the n, l state of hydrogen to the $n+1, l'$ state

(i) $n = 1; n' = 2$

$l \backslash l'$	0	1
0	$2{\cdot}21972^{-1}$	$1{\cdot}31230^{0}$

(ii) $n = 2; n' = 3$

$l \backslash l'$	0	1	2
0	$2{\cdot}65802^{0}$	$1{\cdot}24800^{1}$	$8{\cdot}39713^{0}$
1	$3{\cdot}99941^{-1}$	$2{\cdot}91037^{0}$	$2{\cdot}76432^{1}$

(iii) $n = 3; n' = 4$

$l \backslash l'$	0	1	2	3
0	$1{\cdot}14427^{1}$	$5{\cdot}18870^{1}$	$2{\cdot}33809^{1}$	$1{\cdot}19064^{1}$
1	$3{\cdot}46909^{0}$	$1{\cdot}35409^{1}$	$7{\cdot}70677^{1}$	$2{\cdot}63303^{1}$
2	$2{\cdot}72100^{-1}$	$1{\cdot}82684^{0}$	$1{\cdot}08504^{1}$	$1{\cdot}52264^{2}$

(iv) $n = 4; n' = 5$

$l \backslash l'$	0	1	2	3	4
0	$3{\cdot}27418^{1}$	$1{\cdot}48805^{2}$	$5{\cdot}12764^{1}$	$2{\cdot}76470^{1}$	$1{\cdot}42129^{1}$
1	$1{\cdot}44799^{1}$	$3{\cdot}95509^{1}$	$1{\cdot}83237^{2}$	$5{\cdot}75453^{1}$	$2{\cdot}26898^{1}$
2	$1{\cdot}25238^{0}$	$9{\cdot}65680^{0}$	$3{\cdot}58115^{1}$	$2{\cdot}93579^{2}$	$6{\cdot}48213^{1}$
3	$1{\cdot}60877^{-1}$	$7{\cdot}93109^{-1}$	$4{\cdot}38471^{0}$	$2{\cdot}74820^{1}$	$5{\cdot}09245^{2}$

(v) $n = 5; n' = 6$

$l \backslash l'$	0	1	2	3	4	5
0	$7{\cdot}47736^{1}$	$3{\cdot}44407^{2}$	$9{\cdot}84044^{1}$	$5{\cdot}12649^{1}$	$3{\cdot}25064^{1}$	$1{\cdot}45208^{1}$
1	$4{\cdot}22280^{1}$	$9{\cdot}10958^{1}$	$3{\cdot}79400^{2}$	$1{\cdot}04112^{2}$	$4{\cdot}98231^{1}$	$2{\cdot}01424^{1}$
2	$3{\cdot}63720^{0}$	$3{\cdot}17967^{1}$	$8{\cdot}53129^{1}$	$5{\cdot}41502^{2}$	$1{\cdot}28822^{2}$	$3{\cdot}99612^{1}$
3	$6{\cdot}05328^{-1}$	$3{\cdot}02747^{0}$	$1{\cdot}86000^{1}$	$7{\cdot}66019^{1}$	$8{\cdot}22874^{2}$	$1{\cdot}32265^{2}$
4	$1{\cdot}14981^{-1}$	$4{\cdot}57102^{-1}$	$1{\cdot}48878^{0}$	$8{\cdot}33281^{0}$	$5{\cdot}62514^{1}$	$1{\cdot}29880^{3}$

(vi) $n = 6; n' = 7$

$l \backslash l'$	0	1	2	3	4	5	6
0	$1{\cdot}47928^{2}$	$6{\cdot}92065^{2}$	$1{\cdot}72206^{2}$	$8{\cdot}59996^{1}$	$5{\cdot}68581^{1}$	$3{\cdot}46845^{1}$	$1{\cdot}32525^{1}$
1	$9{\cdot}92057^{1}$	$1{\cdot}80895^{2}$	$7{\cdot}07734^{2}$	$1{\cdot}72442^{2}$	$8{\cdot}53084^{1}$	$4{\cdot}68249^{1}$	$1{\cdot}69645^{1}$
2	$8{\cdot}36260^{0}$	$8{\cdot}10660^{1}$	$1{\cdot}71737^{2}$	$9{\cdot}37578^{2}$	$2{\cdot}11372^{2}$	$8{\cdot}68963^{1}$	$2{\cdot}82289^{1}$
3	$1{\cdot}55052^{0}$	$7{\cdot}85936^{0}$	$5{\cdot}34176^{1}$	$1{\cdot}61558^{2}$	$1{\cdot}31514^{3}$	$2{\cdot}51876^{2}$	$6{\cdot}41741^{1}$
4	$3{\cdot}83122^{-1}$	$1{\cdot}53046^{0}$	$5{\cdot}06942^{0}$	$3{\cdot}11448^{1}$	$1{\cdot}42283^{2}$	$1{\cdot}89371^{3}$	$2{\cdot}37325^{2}$
5	$8{\cdot}84758^{-2}$	$3{\cdot}19471^{-1}$	$8{\cdot}02989^{-1}$	$2{\cdot}40646^{0}$	$1{\cdot}38540^{1}$	$1{\cdot}00674^{2}$	$2{\cdot}79159^{3}$

We have also a useful independent check on the $A_{n,l;n',l'}$, for if $f_{n,l;n',l'}$ is the oscillator strength for the transition and $E_n - E_{n'}$ is the difference in the energy of the levels then

$$A_{n,l;n',l'} = \frac{2{\cdot}30259\, f_{n,l;n',l'}}{E_n - E_{n'}}. \tag{7}$$

The values of $f_{n,l;n',l'}$ have been tabulated to six significant figures by Green *et al.* (1957) and we find that if $n \leqslant 5$ our calculations agree with these oscillator strengths to six significant figures. For $n = 6$ our values also agree with these f values to six significant figures if $l > 2$, but for $l = 2$ the oscillator strengths give $A_{6,2;7,1} = 4{\cdot}38926(1)$ and $A_{6,2;7,3} = 5{\cdot}20493(2)$, for $l = 1$, $A_{6,1;7,0} = 6{\cdot}04372(1)$ and $A_{6,1;7,2} = 4{\cdot}07050(2)$ and for $l = 0$, $A_{6,0;7,1} = 4{\cdot}20900(2)$. The maximum error is 0·1%.

The accuracy of the B's is similar to that of the A's. If $n \leqslant 5$ the results should be accurate to the number of figures given, for $n = 6$ with $l > 2$ the results should be accurate to six figures also, but for $n = 6$ with $l \leqslant 2$ the results are not so accurate. Since there is some cancellation in the calculation of the B's from the a_r's we should expect that these B's are in general less accurate than the A's.

3. Discussion of results

It is well known that for optically forbidden transitions the cross sections for electron excitations fall off as $1/E$, when E is large, and so if $l' \neq l \pm 1$ we have $A_{n,l;n',l'} = 0$. From table 1 we see that $A_{n,l;n',l+1} > A_{n,l;n',l-1}$; this is particularly true for the larger values of l where the A's are greatest. In most physical problems, however, we are not interested in the individual cross sections from one degenerate level to another degenerate level, since, if electron collision processes are important, the degenerate levels are usually populated according to their statistical weights. Under these circumstances we require the average cross section for transitions between the two energy levels. This is defined by

$$Q_{n;n'}(E) = \frac{1}{n^2} \sum_{l'=0}^{n'-1} \sum_{l=0}^{n-1} (2l+1) Q_{n,l;n',l'}(E). \tag{8}$$

At large incident electron energies

$$Q_{n;n'}(E) = A_{n;n'} \frac{\log E}{E} + \frac{B_{n;n'}}{E} \tag{9}$$

where $A_{n;n'}$ and $B_{n;n'}$ are defined in a similar way to $Q_{n;n'}(E)$. The $A_{n;n'}$'s and $B_{n;n'}$'s for $n = 1, 2, 3, 4, 5$ and 6 and $n' = n+1$ were calculated from tables 1 and 2. They are tabulated in table 3 with the ratios $B_{n;n'}/A_{n;n'}$.

Table 3. The constants $A_{n;n+1}$ and $B_{n;n+1}$ appearing in expression (9) for the average value of the cross sections for electron excitation from the states of hydrogen with principal quantum number n to the states with principal quantum number $n+1$

n	$A_{n;n+1}$	$B_{n;n+1}$	$B_{n;n+1}/A_{n;n+1}$
1	2·55554	1·53427	0·600370
2	21·2454	29·0989	1·36966
3	79·7759	142·879	1·79100
4	212·398	440·454	2·07372
5	463·914	1059·93	2·28476
6	889·655	2182·12	2·45277

Table 4. The ratios of constants $A_{n;n+1}$ and $B_{n;n+1}$ appearing in expression (9) calculated by considering only the main optically allowed transitions to those calculated by considering all transitions

n	$\dfrac{A_{n;n+1}(l' = l+1 \text{ transitions})}{A_{n;n+1}(\text{all transitions})}$	$\dfrac{B_{n;n+1}(l' = l+1 \text{ transitions})}{B_{n;n+1}(\text{all transitions})}$
1	1·00000	0·855324
2	0·984093	0·819700
3	0·979983	0·812197
4	0·978323	0·813242
5	0·977489	0·816636
6	0·977014	0·820557

We can also calculate the $A_{n;n'}$'s from the average value of the oscillator strengths. These agreed with the tabulated values to six places except for $n = 6$, which gives $A_{6;7} = 889{\cdot}670$.

In table 4 we have tabulated the ratios of the values of the $A_{n;n'}$'s obtained by considering only the main optically allowed transitions ($l' = l+1$) to the values obtained by considering all transitions. A similar ratio for the B's is also tabulated. The ratios for the A's shows that when calculating $A_{n;n'}$ we need only consider the main optically allowed transitions.

The general pattern of the $B_{n,l;n',l'}$'s in table 2 is very similar to that of the $A_{n,l;n',l'}$'s. We find that the B's associated with the main optically allowed transitions ($l' = l+1$) are largest and that these B's increase with n and l. However, if we consider states with small l values we find that we must take account of other transitions besides the main optically allowed transitions, for the sum total effect of these transitions $\Sigma_{l' \neq l+1} Q_{n,l;n+1,l'}$ is almost as large as that of the main optically allowed transitions. In general, we are not interested in the individual cross section but in the average cross section (8). The average values $B_{n;n'}$ of the $B_{n,l;n',l'}$'s are defined by (9) and are given in table 3. They should be accurate to the number of figures given, except $B_{6;7}$ which, like $A_{6,7}$, should be accurate to 2 or 3 in the fifth figure.

In table 4 we tabulate the ratios of the values of the $B_{n;n'}$'s obtained by considering only the main optically allowed transitions ($l' = l+1$) to the values obtained by considering all transitions. This shows that, like the $A_{n;n'}$'s, the main optically allowed transitions provide the major contribution to the average values of the $B_{n,l;n',l'}$'s. However, in calculating the $B_{n;n'}$'s a neglect of all other transitions would lead to an error of about 25%.

In order to obtain further information about the first Born cross sections for electron excitation, McCoyd and Milford (1963) calculated the $A_{n,l;n',l'}$'s and $B_{n,l;n',l'}$'s for two of the main optically allowed transition cross sections, $Q_{10,0;11,1}$ and $Q_{10,9;11,10}$ for transitions from the state $n = 10$ to the state $n' = 11$. They used these with the results for $n \leqslant 5$ to interpolate graphically for the A's and B's for all optically allowed transitions. A comparison of their results with the present results for $n = 6$, and a similar but less accurate unpublished set for $n = 7$, shows that the interpolation is reliable to the accuracy given by McCoyd and Milford (1963). Unfortunately, in their interpolation they only considered the main optically allowed transitions and so for small l's, where other transitions give large $B_{n,l;n',l'}$'s, the interpolated values are not very useful.

Saraph (1964) has also used the dipole approximation to obtain the average value of the cross sections for all $n \rightarrow n+1$ transitions. Comparison of these cross sections with the present data showed that, for $n = 4$, 5 and 6, Saraph's $B_{n;n'}$ values were in error by about 25%.

Since the present calculations are accurate to six figures it should be possible to use them to extrapolate to higher values of n. We found that if we took

$$A_{n;n+1} = 0{\cdot}439766n^4 + 1{\cdot}310233n^3 + 1{\cdot}064710n^2 - 0{\cdot}267944n \qquad (10)$$

where the constants were determined by $A_{3;4}$, $A_{4;5}$, $A_{5;6}$ and $A_{6;7}$, then we could reproduce $A_{1;2}$ to 0·3% and $A_{19;20}$ to 0·04%. We also found that the leading term in (10) agreed to better than 4% with the value calculated directly from the variation of $A_{n;n+1}$ for large n given by Menzel and Pekeris (1935). This suggests that (10) will reproduce $A_{n;n+1}$ quite accurately for all values of n.

To obtain an expression for $B_{n;n+1}$ we considered the ratio $B_{n;n+1}/A_{n;n+1}$; this is given in table 3. We found that this could be best fitted by

$$\frac{B_{n;n+1}}{A_{n;n+1}} = 1{\cdot}175618 + 1{\cdot}809321 \log n - \frac{0{\cdot}828495}{n} + \frac{0{\cdot}254505}{n^2}. \qquad (11)$$

Here we determined the constants from $B_{2;3}$, $B_{3;4}$, $B_{4;5}$ and $B_{5;6}$ as we felt that the $B_{6;7}$ was only accurate to 2 or 3 in the fifth figure. This equation gave $B_{1;2}$ to 0·2% and $B_{6;7}$ to 0·01%, which is as accurate as our calculation $B_{6;7}$. We should not, however, expect that this expression for $B_{n;n+1}$ is as accurate as the expression given for $A_{n;n+1}$.

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