Cross Sections for Charge-Exchange Reactions of the Type $H^+ + H(n_1 l_1 m_1) \rightarrow H(n_2 l_2 m_2) + H^+$

ROBERT M. MAY AND J. G. LODGE
The Daily Telegraph Theoretical Department, School of Physics, University of Sydney, Sydney, Australia
(Received 22 June 1964; revised manuscript received 4 August 1964)

We consider charge-exchange reactions of the general type $H^+ + H(n_1 l_1 m_1) \rightarrow H(n_2 l_2 m_2) + H^+$, and use some recently derived sum rules to get comparatively simple closed expressions for the cross section. Calculations are performed in the Born approximation. We consider all excited target H atoms with $n_1 \geq 2$ and all (appropriate) $l_1 \leq 3$; we average over m_1. We evaluate the total cross section for formation of final states with given principal quantum number n_2; i.e., we sum over l_2 and m_2. These results may be easily modified to include the case where the target atoms are H-like alkali atoms.

1. INTRODUCTION

THERE is considerable current interest[1–3] in the production of highly excited neutral atoms for injection into plasma devices, by means of charge-exchange reactions of the type

$$H^+ + H(n_1 l_1 m_1) \rightarrow H(n_2 l_2 m_2) + H^+ \qquad (1)$$

(n, l and m are the usual H-atom quantum numbers). The initial H atom is usually taken to be in the ground state ($n_1 = 1$); however, it has been suggested by various people[4,5] that the cross section for forming highly excited final states could be enhanced by use of mildly excited H atoms ($n_1 = 2$ or 3) or by H-like alkali atoms [e.g., Li ($2s$) which is similar to H ($2s$)]. This possibility has been explored experimentally by Futch and Damm[4] and theoretically by Hiskes and Mittleman[5] (HM).

An essential ingredient of any theoretical investigation of the production of highly excited neutrals by the reaction (1) is a knowledge of the appropriate cross section, $\sigma(n_1 l_1 m_1 | n_2 l_2 m_2)$. As has been pointed out by many authors, this cross section is not the only relevant quantity: the rate of loss of highly excited neutral atoms by collisions and by spontaneous and stimulated decay is also of relevance in determining the equilibrium fraction of highly excited atoms in the outgoing beam. In the present paper we limit our attention to an evaluation of the charge-exchange cross sections only.

The cross section for the reaction (1) when the target is in the ground state ($n_1 = 1$) is known for arbitrary n_2 and l_2,[3,6] and will not concern us here. Previous calculations for the cross section when the target atom is not in the ground state are due to HM, who use a computer to find the cross section for transitions from the initial states $2s$ and $6s$ to all final s states ($l_2 = 0$). Using the central field approximation, these results may be applied to the case where the target atoms are Li ($2s$) and Cs ($6s$).

In the present work, we use some recently derived sum rules for the H-atom wave functions[7] to get comparatively simple expressions for the charge-exchange cross sections, in closed form. We consider all initial states with $n_1 \geqslant 2$, and all (appropriate) $l_1 \leqslant 3$ (we average over m_1). For a given initial state we evaluate the total cross section for formation of final states with given n_2; that is, we sum over l_2 and m_2 for a given n_2. We call the resultant cross section $\sigma(\langle n_1 l_1 \rangle | n_2)$. At high incident proton energies the $l_2 = 0$ term dominates this sum, but around those energies at which the cross section has its maximum the states $l_2 = 1$ and 2 (included in our results but not in HM) contribute significantly. This point is discussed further in Sec. 4.

In Sec. 2, $\sigma(\langle n_1 l_1 \rangle | n_2)$ is calculated for the cases $n_1 = 2$ ($l_1 = 0$, 1) and $n_1 = 3$ ($l_1 = 0$, 1, 2). The results are exact in Born approximation. In Sec. 3, we calculate $\sigma(\langle n_1 l_1 \rangle | n_2)$ for $n_1 \geqslant 4$: In this section we employ an approximation which is exact up to terms of relative order n_1^{-2}.

In Sec. 4, the results are discussed briefly. Their relevance to $\sigma(\langle n_1 l_1 \rangle | n_2)$ for the alkali metals (Li, Na, K, etc.) is shown explicitly.

Our calculations are performed in Born approximation: the usual criterion of validity is that the speed v of the incident proton relative to the target should be greater than the initial electron speed. Defining the dimensionless speed p:

$$p = \hbar v / e^2, \qquad (2)$$

we conclude that our calculations are to be taken seriously provided $p > 1/n_1$ [i.e., energy $> (25/n_1^2)$ keV]. This point is discussed further in Ref. 3.

2. CROSS SECTIONS FOR $n_1 = 2, 3$

The cross section for charge-exchange reactions of the type described by Eq. (1) is well known in Born approximation (see, for example, Ref. 6). In the limit

[1] D. R. Sweetman, Nucl. Fusion Suppl. **1**, 279 (1962).
[2] S. N. Kaplan, G. A. Paulikas, and R. V. Pyle, Phys. Rev. Letters **9**, 347 (1962).
[3] S. T. Butler, R. M. May, and I. D. S. Johnston, Phys. Letters **10**, 281 (1964).
[4] A. H. Futch and C. C. Damm, Nucl. Fusion **3**, 124 (1963).
[5] J. R. Hiskes and M. H. Mittleman, University of California Radiation Laboratory Report No. UCRL-9969, 1962, p. 128 (unpublished); hereafter referred to as HM.
[6] D. R. Bates and A. Dalgarno, Proc. Phys. Soc. (London) **A66**, 972 (1953).
[7] R. M. May, Phys. Rev. **136**, A669 (1964).

of infinite proton mass we can write[3,6]

$$\sigma(n_1l_1m_1|n_2l_2m_2)$$

$$=(2\pi p)^{-2}\int_{-\infty}^{+\infty}\int dq_x dq_y |f_1(\mathbf{q})|^2|g_2(\mathbf{Q})|^2. \quad (3)$$

$f_1(\mathbf{q})$ is the Fourier transform of the initial H-atom wave function, and $g_2(\mathbf{Q})$ that of the final wave function multiplied by r^{-1}. The proton has been taken incident along the z axis so that we can write

$$q^2+\lambda^2n_1^{-2}=Q^2+\lambda^2n_2^{-2}=q_x^2+q_y^2+\lambda^2\beta, \quad (4)$$

with $\beta(p,n_1,n_2)$ defined by

$$\beta(p,n_1,n_2)=(1/4p^2)\{p^4+2p^2(n_1^{-2}+n_2^{-2}) +(n_1^{-2}-n_2^{-2})^2\}. \quad (5)$$

λ is the inverse Bohr radius, $\lambda\equiv 1/a_0$.

For the sum over final-state matrix elements we can use the *exact* sum rule[7]

$$\sum_{l=0}^{n-1}\sum_{m=-l}^{l}|g_{nlm}(\mathbf{Q})|^2=\frac{2^4\pi\lambda^3}{n^3}\frac{1}{(Q^2+\lambda^2n^{-2})^2}. \quad (6)$$

Use of a similar result for $f(\mathbf{q})$ leads to a simple result for the cross section (exact in Born approximation) provided we may average over l_1 and m_1 for a given target. This result is presented elsewhere.[7] For alkali H-like atoms as the target (e.g., Li in Ref. 4), this average is not likely to be the experimentally relevant quantity, because for a given n_1 the s state will in general lie lower than the p and d states with the consequence that we need the cross section for individual values of l_1.

We now evaluate the charge-exchange cross section $\sigma(\langle n_1l_1\rangle|n_2)$ defined in the introduction; that is,

$$\sigma(\langle n_1l_1\rangle|n_2)$$

$$\equiv\frac{1}{2l_1+1}\sum_{m_1=-l_1}^{l_1}\sum_{l_2=0}^{n_2-1}\sum_{m_2=-l_2}^{l_2}\sigma(n_1l_1m_1|n_2l_2m_2). \quad (7)$$

For $n_1=2$ ($l_1=0$, 1) and $n_1=3$ ($l_1=0$, 1, 2,) we substitute the exact Fourier transform,[8] $f_1(\mathbf{q})$, for the relevant H-atom wave functions into Eq. (3). Use of (4) and (6) enables the resulting integrals to be performed simply.

The ensuing expressions for the charge-exchange cross sections are exact in Born approximation, and may be conveniently written

$$\sigma(\langle n_1l_1\rangle|n_2)=(\pi a_0^2/p^2n_2^3)F(n_1,l_1,\beta), \quad (8)$$

with $\beta(p,n_1,n_2)$ defined by (5), and

$$F(2,0,\beta)=\frac{32}{5\beta^5}\left\{1-\frac{5}{6\beta}+\frac{5}{28\beta^2}\right\}, \quad (9)$$

$$F(2,1,\beta)=\frac{16}{9\beta^6}\left\{1-\frac{3}{14\beta}\right\}, \quad (10)$$

$$F(3,0,\beta)=\frac{256}{135\beta^5}\left\{1-\frac{80}{81\beta}+\frac{1760}{5103\beta^2} -\frac{320}{6561\beta^3}+\frac{1280}{531\,441\beta^4}\right\}, \quad (11)$$

$$F(3,1,\beta)=\frac{4096}{6561\beta^6}\left\{1-\frac{10}{21\beta}+\frac{2}{27\beta^2}-\frac{8}{2187\beta^3}\right\}, \quad (12)$$

$$F(3,2,\beta)=\frac{32\,768}{688\,905\beta^7}\left\{1-\frac{7}{36\beta}+\frac{7}{729\beta^2}\right\}. \quad (13)$$

If we are interested in forming highly excited final states, then $n_2\gg 1$, and β may be taken approximately independent of n_2:

$$\beta(p,n_1,n_2\gg 1)\approx\{(p^2+n_1^{-2})/2p\}^2. \quad (14)$$

The F factors then become independent of n_2, and the cross sections may be written in the form

$$\sigma(\langle n_1l_1\rangle|n_2)=\frac{\pi a_0^2}{p^2n_2^3}F(p,n_1,l_1)\left\{1+O\frac{1}{n_2^2}\right\}. \quad (15)$$

3. CROSS SECTIONS FOR $n_1\geqslant 4$

For $n_1\geqslant 4$, an exact evaluation of the fourier transform of the initial H-atom wave function becomes cumbersome. We may instead use the approximate result[9]

$$\frac{1}{2l+1}\sum_{m=-l}^{l}|f(\mathbf{q})|^2=\frac{2^6\pi\lambda^5}{n^3}\cdot\frac{1}{q^8}\cdot\left\{j_l\left(\frac{2\lambda}{q}\right)\right\}^2 \cdot\left\{\prod_{i=0}^{l}\left(1-\frac{i^2}{n^2}\right)\right\}\left\{1+O\frac{\lambda^2}{n^2q^2}\right\}. \quad (16)$$

Substituting (16) into (3) leads to the cross section

$$\sigma(\langle n_1l_1\rangle|n_2)=\frac{2^8}{5p^2n_1^3n_2^3\alpha^5}I_{l_1}(\alpha)\left\{1+O\frac{1}{n_1^2}\right\}, \quad (17)$$

[8] This Fourier transform can be obtained straightforwardly. Alternatively, the quantity

$$\sum_{m_1=-l_1}^{l_1}|f_1(\mathbf{q})|^2$$

can be read off from the sum rule (22) of Ref. 7, using the appropriate low-order Gegenbauer polynomials for $n_1=2$ and 3.

[9] This result follows as the limiting case of the sum rule (22) of Ref. 7. A similar result is derived in detail by R. M. May, Nucl. Fusion 4, No. 3 (1964), and is used (Ref. 3) to discuss the fractional contributions of the various l_2 states in the particular case $n_1=1$.

where α is the appropriate limiting form of β:

$$\alpha=\{(p^2+n_2^{-2})/2p\}^2 \tag{18}$$

$$\approx p^2/4 \quad \text{for} \quad n_2\gg 1. \tag{19}$$

The I_l functions are given by the integral

$$I_l(\alpha)=5\int_1^\infty \frac{ds}{s^6}\{j_l(2s^{-1/2}\alpha^{-1/2})\}^2. \tag{20}$$

With the aid of the power series for the square on a Bessel function,[10] we can write

$$I_l(\alpha)=\sum_{i=0}^{\infty}\frac{(-1)^i(4/\alpha)^{i+l}}{i!(i+2l+1)!}\frac{(2i+2l)!!}{(2i+2l+1)!!}\frac{5}{(5+l+i)}. \tag{21}$$

These functions are tabulated for various values of α and $l=0, 1, 2, 3$ in Table I.

TABLE I. $I_l(\alpha)$ defined by Eq. (21).

α \ l	0	1	2	3
0.25	0.022	0.046	0.043	0.043
0.31	0.009	0.084	0.091	0.032
0.39	0.018	0.128	0.084	0.021
0.50	0.055	0.163	0.071	0.013
1.0	0.287	0.181	0.030	0.003
1.2	0.362	0.171	0.023	0.002
1.5	0.451	0.154	0.016	0.001
2.0	0.557	0.130	0.010	...
3.0	0.682	0.097	0.005	...
4.0	0.752	0.078	0.003	...
6.0	0.828	0.055	0.001	...
$\gg 1$	$1-O(\alpha^{-1})$	$10/(27\alpha)$	$O(\alpha^{-2})$	$O(\alpha^{-3})$

Equation (17) in conjunction with Table I thus gives an excellent approximation to $\sigma(\langle n_1 l_1\rangle|n_2)$ for all $n_1\gtrsim 4$.

4. DISCUSSION

In Secs. 2 and 3 we have found the cross sections for the reaction (1), where the target H atom is in the excited state with quantum numbers n_1 and l_1. As observed by HM, such expressions can be used to get approximate cross sections when the target atom is a ground-state alkali metal (n_1=principal quantum number for the "free" electron; $l_1=0$). In this case, the initial electronic wave functions are taken to be as for the appropriate H-atom case with an effective nuclear charge Z due to the imperfect screening by the inner electrons.[11]

It is a straightforward matter to include Z in the wave functions which generate $f_1(\mathbf{q})$ in Eq. (3). The resulting Eqs. (8) and (17) for the cross sections must be modified firstly, by a multplicative factor Z^{-5}, and secondly, by replacing the definition of β in Eq. (8) [see Eq. (5)] by

$$\beta(p,n_1,n_2)\equiv\frac{1}{4p^2Z^2}\{p^4+2p^2(Z^2n_1^{-2}+n_2^{-2}) + (Z^2n_1^{-2}-n_2^{-2})^2\} \tag{22}$$

and similarly replacing the definition of α in Eq. (17) [see Eq. (18)] by

$$\alpha\equiv\{(p^2+n_2^{-2})/2pZ\}^2. \tag{23}$$

The Born approximation should now be valid providing $p>Z/n_1$.

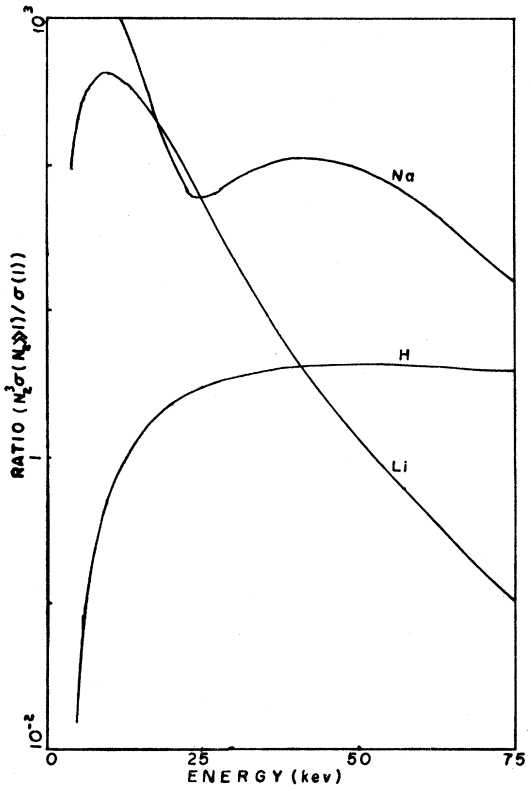

FIG. 1. Charge-exchange cross sections for forming highly excited H atoms, $n_2\gg 1$ (as a ratio to $n_2^{-3}\times$cross section for forming ground-state H atoms) as a function of incident proton energy. Target atoms are H($1s$), Li($2s$), Na($3s$).

In Fig. 1 we display our results by plotting the charge-exchange cross section for forming highly excited H atoms ($n_2\gg 1$) from targets of Li ($2s$) or Na ($3s$) atoms: this cross section is proportional to n_2^{-3} [see Eq. (15)]. This cross section is displayed as a ratio to the corresponding one for forming ground state H atoms ($n_2=1$): the ratio is plotted as a function of incident proton energy. (The corresponding ratio for a ground-state H-atom target is given for comparison.)

We recall that our results for a given n_2 are obtained by summing over *all* angular momentum quantum

[10] G. N. Watson, *Theory of Bessel Functions* (Cambridge University Press, New York, 1952), p. 147.

[11] Calculations for Z may be made using the self-consistent-field approximation. See J. C. Slater, *Quantum Theory of Atomic Structure* (McGraw-Hill Book Company, Inc., New York, 1960), Chap. 9, p. 210.

numbers l_2 and m_2: on the other hand, HM calculate for $l_2=0$ only. When the target consists of ground-state H atoms, the difference between the two calculations is known[3,9]: At high incident proton energies ($p\gg1$) only the $l_2=0$ term contributes significantly to the sum, and both calculations give the same result; in the neighborhood of the resonance for forming highly excited final states ($p\sim1$) the $l_2=0$ term contributes only 28% of the cross section. When the target atoms have $n_1\neq1$, we expect a similar result to hold: Comparison between the present results and those of HM for Li bears out this expectation. At incident proton energies of 25 keV, the cross section for forming final states with $n_2=10$ contains 80% $l_2=0$ contributions; at $6\frac{1}{4}$ keV (in the neighborhood of the maximum) it contains 35% $l_2=0$ terms.

Finally, we emphasize again that the cross section for forming highly excited states by charge-exchange reactions of the general type (1) is only one ingredient in a calculation of the equilibrium fraction of excited neutrals in the outgoing beam. It is also necessary to know the cross sections for all processes which disrupt the atoms, and these are not all available. (In particular, the total cross section for ionization of H atoms by collision with alkali atoms is necessary: this quantity does not seem to be known, nor is it easy to calculate.)

ACKNOWLEDGMENTS

Our thanks are due to Professor S. T. Butler, and Professor C. N. Watson-Munro for stimulating discussions, and to Professor H. Messel for the excellent facilities provided. This work was supported in part by the Nuclear Research Foundation within the University of Sydney. One of us (J.G.L.) is the holder of a C.S.I.R.O. Senior Post-Graduate Studentship.

PHYSICAL REVIEW VOLUME 137, NUMBER 3A 1 FEBRUARY 1965

Stark Effect of the Hyperfine Structure of Cesium-133†

J. D. FEICHTNER, M. E. HOOVER,* AND M. MIZUSHIMA
Department of Physics and Astrophysics, University of Colorado, Boulder, Colorado
(Received 27 January 1964; revised manuscript received 9 September 1964)

The change $\Delta(\mathcal{E})$ in transition frequency of the $(F=4, M_F=0)\leftrightarrow(F=3, M_F=0)$ transition of the ground state of Cs^{133} as a result of the application of an external electric field $\mathcal{E}$ has been calculated theoretically. The effects of differences in the ground-state wave functions due to the hyperfine interaction have been included, as well as differences in energy denominators due to hyperfine structure. The calculation gives $\Delta(\mathcal{E})=-1.9\times10^{-6}(1\pm0.1)\mathcal{E}^2$ cps, which is to be compared with the experimental value of $-2.29\times10^{-6}(1\pm0.03)\mathcal{E}^2$ cps, where $\mathcal{E}$ is in V/cm.

I. INTRODUCTION

IN 1957, Haun and Zacharias[1] measured the change $\Delta(\mathcal{E})$ of the transition frequency of the $(F=4, M_F=0)\leftrightarrow(F=3, M_F=0)$ transition in the ground state of Cs^{133} in an electric field $\mathcal{E}$. They found $\Delta(\mathcal{E})=-2.29\times10^{-6}(1\pm0.03)\mathcal{E}^2$ cps, where $\mathcal{E}$ is the electric field in V/cm. These authors made an order-of-magnitude calculation of this effect, using perturbation theory and assuming that only the $6p$ levels were mixed with the ground state. As a further approximation, they neglected the hyperfine structure of the $6p$ levels and found theoretically $\Delta(\mathcal{E})\approx-0.82\times10^{-6}\mathcal{E}^2$ cps. Schwartz[2] attempted a complete calculation of this Stark effect including the wave function differences between $F=4$ and $F=3$ states, but the attempt was unsuccessful owing to lack of values for some of the matrix elements. Recently Anderson[3] completed a more accurate calculation, omitting the difference in wave functions and assuming an average value for the energy of the fine structure terms. Anderson's result, $\Delta(\mathcal{E})=-2.67\times10^{-6}\times\mathcal{E}^2$ cps,[4] is much closer to the experimental result.

Recently, some theoretical calculations of cesium wave functions have been published[5-7] as have revised experimental values for the polarizability of the cesium atom.[8,9] In the following calculation of the Stark shift, we use the new wave functions and polarizability values, and in addition we take into account the mixing of the ground state $F=4$ and $F=3$ wave functions with the

† Supported by National Bureau of Standards, Boulder Laboratories, and National Science Foundation.
* Permanent address: Goshen College, Goshen, Indiana.
[1] R. D. Haun and J. R. Zacharias, Phys. Rev. **107**, 107 (1957).
[2] Indicated as a private communication in Ref. 1.
[3] L. W. Anderson, Nuovo Cimento **22**, 936 (1961).
[4] Here we have substituted the more recent polarizability data of Ref. 8.
[5] P. M. Stone, Los Alamos Report No. LA-2886, UC-34, Physics TID-4500 (19th ed.), 1963 (unpublished). Available from Office of Technical Services, U. S. Department of Commerce, Washington 25, D. C.
[6] P. M. Stone, Phys. Rev. **127**, 1151 (1962).
[7] P. M. Stone, Los Alamos Report No. LA-2625, Physics, TID-4500 (16th ed.), 1961 (unpublished). Available from Office of Technical Services, U. S. Department of Commerce, Washington 25, D. C.
[8] G. E. Chamberlain and J. C. Zorn, Phys. Rev. **129**, 677 (1963).
[9] A. Salop, E. Pollack, and B. Bederson, Phys. Rev. **124**, 1431 (1961).