# Inelastic Collisions between Heavy Particles I: Excitation and Ionization of Hydrogen Atoms in Fast Encounters with Protons and with other Hydrogen Atoms

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Abstract. Born's approximation is used to calculate the cross sections of the following processes:

 $H^+(\text{or }H(1s)) + H(1s) \rightarrow H^+(\text{or }H(1s)) + H(2s, 2p, 3s, 3p, 3d \text{ or }C),$  where C represents the continuum. The results are presented mainly in graphical form. In the case of the ionizing collisions the energy distribution of the ejected electrons is also given.

### § 1. Introduction

HOUGH inelastic collisions between heavy particles are of importance in aurorae and in many other phenomena few detailed calculations on them have been performed. The present paper is devoted to the investigation of some of the simpler of such collisions:

$$H^+ + H(1s) \rightarrow H^+ + H(2s, 2p, 3s, 3p \text{ or } 3d),$$
 .....(1)  
 $H(1s) + H(1s) \rightarrow H(1s) + H(2s, 2p, 3s, 3p \text{ or } 3d),$  .....(2)  
 $H^+ + H(1s) \rightarrow H^+ + H^+ + e,$  .....(3)  
 $H(1s) + H(1s) \rightarrow H(1s) + H^+ + e.$  .....(4)

Born's approximation is used, no account being taken of exchange. Results for relatively low impact energies are included to enable the range of validity of the approximation to be assessed should proper comparison data become available. This range is still very uncertain. Charge transfer between hydrogen atoms and protons has recently been studied (cf. Bates and Dalgarno 1952, Dalgarno and Yadav 1953, Jackson and Schiff 1953) and for it Born's approximation appears to be quite satisfactory when the energy of the incident particle is above about 25 kev; but the process is of course dissimilar from those under discussion.

## § 2. Theory

- 2.1. Consider an encounter between the atomic system A, comprised of a nucleus of charge  $Z_a e$  and an electron, and another atomic system B, comprised either of a bare nucleus of charge  $Z_b e$ , or of such a nucleus and an electron. These two cases can be treated together, the symbols for corresponding quantities being distinguished, when this is necessary, by superscripts + and  $\pm$  (as in eqns. (9) and (10) below). According to the simple Born approximation
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(cf. Mott and Massey 1949) the cross section associated with the reaction in which A is excited from state p to state q, B remaining unchanged, is

$$Q(\mathbf{p} \to \mathbf{q}) = \frac{8\pi^3 M^2}{K_p^2 h^4} \int_{K_{\min}}^{K_{\max}} |\mathcal{N}|^2 K dK \qquad \dots (5)$$

where h is Planck's constant, M is the reduced mass  $M_a M_b / (M_a + M_b)$ ;

$$\mathbf{K} = \mathbf{K}_{\mathbf{p}} - \mathbf{K}_{\mathbf{q}}, \qquad \dots (6)$$

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$$\mathbf{K}_{\mathbf{p}} = 2\pi M \mathbf{v}_{\mathbf{p}}/h, \qquad \mathbf{K}_{\mathbf{q}} = 2\pi M \mathbf{v}_{\mathbf{q}}/h; \qquad \dots (7)$$

v<sub>p</sub> and v<sub>q</sub> are the initial and final velocities of relative motion; and, assuming that at least one of the colliding systems is neutral,

$$\mathcal{N} = \int \int \chi_p(\mathbf{r}_a) \chi_q^*(\mathbf{r}_a) \exp(i\mathbf{R} \cdot \mathbf{K}) V(\mathbf{R}, \mathbf{r}_a) d\mathbf{r}_a d\mathbf{R}, \qquad \dots (8)$$

 $\chi_{p}(\mathbf{r}_{a})$  and  $\chi_{q}(\mathbf{r}_{a})$  being the wave functions of the electron bound to nucleus A, **R** being the relative position vector of the heavy particles, and  $V(\mathbf{R}, \mathbf{r_a})$  being the interaction potential. If B is a bare nucleus this interaction potential is

$$V^{+}(\mathbf{R}, \mathbf{r}_{\mathbf{a}}) = e^{2} \left[ \frac{Z_{\mathbf{a}} Z_{\mathbf{b}}}{R} - \frac{Z_{\mathbf{b}}}{|\mathbf{R} - \mathbf{r}_{\mathbf{a}}|} \right], \qquad \dots (9)$$

and if there is an electron of wave function  $\phi_{
m n}({f r}_{
m b})$  attached it is

$$V^{\pm}(\mathbf{R}, \mathbf{r}_{\mathbf{a}}) = e^2 \int \phi_n(\mathbf{r}_{\mathbf{b}}) \left[ \frac{Z_{\mathbf{a}} Z_{\mathbf{b}}}{R} - \frac{Z_{\mathbf{a}}}{|\mathbf{R} + \mathbf{r}_{\mathbf{b}}|} - \frac{Z_{\mathbf{b}}}{|\mathbf{R} - \mathbf{r}_{\mathbf{a}}|} + \frac{1}{|\mathbf{R} + \mathbf{r}_{\mathbf{b}} - \mathbf{r}_{\mathbf{a}}|} \right] \phi_n^*(\mathbf{r}_{\mathbf{b}}) d\mathbf{r}_{\mathbf{b}}. \dots (10)$$

The first two terms within the curly brackets of integral (10) give no contribution to  $\mathcal{N}$  owing to the fact that  $\chi_p$  and  $\chi_q$  are orthogonal. On neglecting them it may be seen that if  $\phi_n$  represents the 1s state (which is the only case which will be considered) then effectively

$$V^{\pm}(\mathbf{R}, \mathbf{r}_{a}) = -e^{2} \left[ \frac{Z_{b} - 1}{|\mathbf{R} - \mathbf{r}_{a}|} + \left\{ \frac{Z_{b}}{a_{0}} + \frac{1}{|\mathbf{R} - \mathbf{r}_{a}|} \right\} \exp\left( \frac{-2Z_{b}}{a_{0}} |\mathbf{R} - \mathbf{r}_{a}| \right) \right], \quad \dots (11)$$

where  $a_0$  is the radius of the first orbital of hydrogen. Substitution of (9) and (11) in (8) and application of the integration formula of Bethe (1930) yields

$$|\mathcal{N}^{+}| = \frac{4\pi e^{2}a_{0}^{2}}{t^{2}}Z_{b}|\mathcal{I}|, \qquad \dots (12)$$

$$|\mathcal{N}^{\pm}| = \frac{4\pi e^2 a_0^2}{t^2} Z_b \left\{ 1 - \frac{16Z_b^3}{(4Z_b^2 + t^2)^2} \right\} |\mathcal{I}|, \qquad \dots (13)$$

in which

$$\mathbf{t} = \mathbf{K} a_0 \qquad \dots \dots (14)$$

$$|\mathscr{I}| = \left| \int \chi_{\mathbf{p}}(\mathbf{r}_{\mathbf{a}}) \chi_{\mathbf{q}}^{*}(\mathbf{r}_{\mathbf{a}}) \exp(i\mathbf{t} \cdot \mathbf{r}_{\mathbf{a}}) d\mathbf{r}_{\mathbf{a}} \right|, \qquad \dots (15)$$

ra being now in atomic units. From (5) it hence follows that

$$Q^{+}(p \to q) = \left[ \frac{8Z_b^2}{s^2} \int_{t_{\min}}^{t_{\max}} |\mathscr{I}|^2 t^{-3} dt \right] \pi a_0^2 \qquad \dots (16)$$

(which is of course a standard result, cf. Mott and Massey 1949) and

$$Q^{\pm}(\mathbf{p} \to \mathbf{q}) = \left[ \frac{8Z_{b}^{2}}{s^{2}} \int_{t_{\min}}^{t_{\max}} |\mathcal{I}|^{2} t^{-3} \left\{ 1 - \frac{16Z_{b}^{3}}{(4Z_{b}^{2} + t^{2})^{2}} \right\}^{2} dt \right] \pi a_{0}^{2}, \quad \dots (17)$$

 $s^2 = \frac{1}{2} m v_p^2 / I_H$ where

 $I_{\rm H}$  being the ionization potential of hydrogen. If  $\Delta E({\rm p,\,q})$  is the difference between the energies of the two states in units of  $I_{\rm H}$ , then

$$t_{\min} = (K_{p} - K_{q})a_{0} \qquad \dots (19)$$

$$\simeq \frac{\Delta E(p, q)}{2s} \left[ 1 + \frac{m\Delta E(p, q)}{4Ms^{2}} \right] \qquad \dots (20)$$

since  $m\Delta E(\mathbf{p},\mathbf{q})/Ms^2$  is small compared with unity except in the region immediately above the threshold (where in any event Born's approximation is invalid). As is usual in the treatment of heavy particle collisions, it is sufficient to take  $t_{\rm max}$  as infinite. Comparison of (16) and (17) shows that if the energy of relative motion E is much less than  $[EZ_b^{1/2} + M\Delta E(\mathbf{p}, \mathbf{q})^2/16mZ_b^{3/2}]$  then  $Q^+(\mathbf{p} \to \mathbf{q}|E)$  and  $Q^\pm(\mathbf{p} \to \mathbf{q}|E)$  are approximately equal.

Before proceeding to the detailed calculations it may be noted from (15) that  $|\mathcal{I}|$  is a function of  $t/Z_a$  (or the more convenient equivalent  $t/\Delta E(p, q)^{1/2}$ ), so that the cross sections may be expressed in the form

$$Q^{+}(\mathbf{p} \to \mathbf{q} \mid E) = \{Z_{\mathbf{b}}^{2} / \Delta E(\mathbf{p}, \mathbf{q})^{2}\} f_{pq}(M\Delta E(\mathbf{p}, \mathbf{q}) / E) \qquad ..... (21)$$

$$Q^{\pm}(\mathbf{p} \to \mathbf{q} \mid E) = Q^{+}(\mathbf{p} \to \mathbf{q} \mid E) - \{1 / \Delta E(\mathbf{p}, \mathbf{q})^{2}\} [Z_{\mathbf{b}} g_{pq} \{M\Delta E(\mathbf{p}, \mathbf{q}) / E, \Delta E(\mathbf{p}, \mathbf{q}) / Z_{\mathbf{b}}^{2}\} - h_{pq} \{M\Delta E(\mathbf{p}, \mathbf{q}) / E, \Delta E(\mathbf{p}, \mathbf{q}) / E, \Delta E(\mathbf{p}, \mathbf{q}) / Z_{\mathbf{b}}^{2}\}] \qquad ..... (22)$$

where for any given pair of quantum numbers p and q the functions  $f_{pq}$ ,  $g_{pq}$  and  $h_{pq}$  depend only on the variables indicated and the region immediately above the threshold is again excluded. These scaling relations give the results which will be presented later a rather wider applicability than they would otherwise have.

2.2. For discrete transitions  $|\mathcal{I}|$  can be got from (15) by elementary methods. If  $t/Z_a$  is denoted by  $\tau$  then

$$\begin{split} |\mathscr{I}(1s \to 2s)| &= 2^{17/2}\tau^2/(4\tau^2 + 9)^3 \\ |\mathscr{I}(1s \to 2p)| &= 2^{15/2} \times 3\tau/(4\tau^2 + 9)^3 \\ |\mathscr{I}(1s \to 3s)| &= 2^4 \times 3^{7/2}(27\tau^2 + 16)\tau^2/(9\tau^2 + 16)^4 \\ |\mathscr{I}(1s \to 3p)| &= 2^{11/2} \times 3^3(27\tau^2 + 16)\tau/(9\tau^2 + 16)^4 \\ |\mathscr{I}(1s \to 3d)| &= 2^{17/2} \times 3^{7/2}\tau^2/(9\tau^2 + 16)^4 \end{split} \right\} . \qquad (23)$$

On substituting in (16) and (17) and resolving the integrands into partial fractions analytical expressions for the cross sections can readily be obtained. These have little interest and need not be displayed here: for they are, in general, cumbersome and, owing to very severe cancellation between the individual terms, are awkward to evaluate, so that except in a few instances it is easier to perform the necessary integrations numerically. However, in the case of slow collisions we may expand in powers of  $1/\tau$ , and if we retain only the leading term we get the following formulae in which the cross sections are in units of  $\pi a_0^2 (8.8 \times 10^{-17} \, \text{cm}^2)$ , the reduced mass is measured on the scale on which the proton mass is unity, and the energies of relative motion and excitation are in electron volts:

$$\begin{array}{l} Q(1s \rightarrow 2s) = 1 \cdot 3 \times 10^{-6} Z_{\rm b}{}^{2} E^{4} / M^{4} \Delta E(1s - 2s)^{6} \\ Q(1s \rightarrow 2p) = 7 \cdot 4 \times 10^{-9} Z_{\rm b}{}^{2} E^{5} / M^{5} \Delta E(1s - 2p)^{7} \\ Q(1s \rightarrow 3s) = 2 \cdot 0 \times 10^{-7} Z_{\rm b}{}^{2} E^{4} / M^{4} \Delta E(1s - 3s)^{6} \\ Q(1s \rightarrow 3p) = 1 \cdot 1 \times 10^{-9} Z_{\rm b}{}^{2} E^{5} / M^{5} \Delta E(1s - 3p)^{7} \\ Q(1s \rightarrow 3d) = 6 \cdot 1 \times 10^{-13} Z_{\rm b}{}^{2} E^{6} / M^{6} \Delta E(1s - 3d)^{8} \end{array}$$
 ..... (24)\*

\* The distinguishing superscripts are omitted since at the low energies concerned  $Q^+$  and  $Q^\pm$  are of almost equal magnitude. For some purposes it is convenient to replace E and M, respectively, by the energy and mass of the incident particle.

with 
$$\Delta E \ll E \ll \sim 100 \, M \Delta E$$
. .....(25)

To be sure the range of energies covered is not one over which the treatment can be expected to give reliable results; but it is to be noted that the formulae show that the Born approximation is successful in predicting the extremely rapid fall off in the cross section at low impact energies, and the other main features characteristic of near-adiabatic heavy particle collisions (cf. Bates and Massey, 1954).

2.3. In the calculations on transitions into the continuum the free wave function was taken as

$$\chi_{\kappa}(\mathbf{r}_{a}) = [Z_{a}\kappa^{1/2}[2\pi a_{0}\{1 - \exp((-2\pi/\kappa)\}^{1/2}\Gamma(1 - i/\kappa)]^{-1}]$$

$$\times \exp(iZ_{a}\kappa r_{a}/a_{0}) \int_{0}^{\infty} u^{-i/\kappa} \exp((-u)I_{0}([4iZ_{a}\kappa u(z_{a} + r_{a})/a_{0}]^{1/2}) du \dots (26)$$

where  $\varkappa$  denotes  $2\pi m v a_0/h Z_a$ , v is the velocity of ejection of the electron,  $z_a$  is its coordinate, with respect to nucleus A, along a line parallel to the direction of ejection, and  $I_0$  is the usual Bessel function (Sommerfeld 1931). The rather lengthy analysis involved in the integration of (15) is essentially the same as that described by Massey and Mohr (1933) in their work on ionization by electron collision. It is therefore only necessary to give the result:

$$|\mathscr{I}(1s \to \kappa)|^2 = \frac{2^8 \kappa \tau^2 (1 + 3\tau^2 + \kappa^2) \exp\left[(-2/\kappa) \tan^{-1}\left(2\kappa/(1 + \tau^2 - \kappa^2)\right)\right]}{3\left\{1 + (\tau - \kappa)^2\right\}^3 \left\{1 + (\tau + \kappa)^2\right\}^3 \left\{1 - \exp\left(-2\pi/\kappa\right)\right\}}. \quad \dots (27)$$

Substitution of this expression in (16) and (17) gives  $Q(1s \rightarrow \kappa)$ , which is such that  $Q(1s \rightarrow \kappa) d\kappa$  is the cross section of an ionizing collision in which the  $\kappa$  value of the liberated electron lies between  $\kappa$  and  $\kappa + d\kappa$ , all angles of ejection being included. The completion of the calculation must in general be carried out by numerical methods. If condition (25) is satisfied we can however obtain simple approximate formulae: thus, proceeding as in the case of excitation and using the same units, we find that the cross section associated with the ejection of an electron with energy between  $\epsilon$  and  $\epsilon + d\epsilon$  ev is

$$Q(1s \to \epsilon)d\epsilon = \{1.7 \times 10^{-6} Z_b^2 E^4 \Delta E(1s - c)^3 / M^4 [\Delta E(1s - c) + \epsilon]^{10} \} d\epsilon, \qquad \dots (28)$$

and so the total cross section,

$$\int_0^\infty Q(1s \to \epsilon) d\epsilon = 1.9 \times 10^{-7} Z_b^2 E^4 / M^4 \Delta E(1s - c)^6, \qquad \dots (29)$$

E being again the energy of relative motion and  $\Delta E(1s-c)$  being the ionization potential.

2.4. If the velocities of relative motion are the same, and are sufficiently high, the cross sections  $Q^+$  for proton-atom collisions are of course equal to the cross sections  $Q^-$  for the corresponding electron-atom collisions (cf. Mott and Massey 1949). It is worth noting that a more general relation between the two exists. The inequality of the cross sections at moderate and low velocities of relative motion arises because both  $t_{\rm max}$  and  $t_{\rm min}$  are different. Thus with protons  $t_{\rm max}$  is  $(M/m)\Delta E/t_{\rm min}$ , which enables the upper integration limit in (16) to be treated as infinite except for extremely slow collisions; but with electrons this

simplification only becomes valid at much higher velocities since here  $t_{\max}$  is  $\Delta E/t_{\min}$ . Again with protons (20) is a good approximation to (19), and indeed it is generally sufficient to take  $t_{\min}$  as  $\Delta E/2s$ ; but with electrons it is necessary to use the more accurate formula

$$(\Delta E + t_{\min}^2)/2t_{\min} = s, \qquad (t_{\min} \le \Delta E^{1/2}).$$
 (30)

Suppose now that in corresponding proton-atom and electron-atom collisions the energies  $E^+(x)$  and  $E^-(x)$  are such that  $t_{\min}$  in both cases is equal to x, and denote the cross sections at these energies by  $Q^+(E^+(x))$  and  $Q^-(E^-(x))$  respectively. From (16) and (18) it is apparent that we can write

$$Q^{+}(E^{+}(x)) = (M/m)w(x)/E^{+}(x) \qquad \dots (31)$$

and

$$Q^{-}(E^{-}(x)) = \{w(x) - w(\Delta E/x)\}/E^{-}(x), \quad (x \leq \Delta E^{1/2}), \quad \dots \quad (32)$$

where w is a function of only the variable indicated. Noting that

$$E^{-}(x) = (\gamma m/M)E^{+}(x), \qquad (E^{+}(x) \geqslant M\Delta E/4m) \qquad \dots (33)$$

with

$$\gamma = \left\{1 + \frac{M\Delta E}{4mE^+(x)}\right\}^2, \qquad \dots (34)$$

it may be seen from (31) and (32) that

$$Q^{-}(E^{-}(x)) = \gamma^{-1} \left\{ Q^{+}(E^{+}(x)) - \frac{E^{+}(y)}{E^{+}(x)} Q^{+}(E^{+}(y)) \right\}, \quad \dots (35)$$

where

$$E^+(y) = M^2 \Delta E^2 / 16m^2 E^+(x),$$
 .....(36)

which expresses the electron-atom cross section at energy  $E^-(x)$  in terms of the proton-atom cross sections at the related energies  $E^+(x)$  and  $E^+(y)$ . As the Born approximation has been evaluated for numerous electron-atom cross sections (cf. Bates, Fundaminsky, Leech and Massey 1950, Massey and Burhop 1952) the formula provides a useful check on the computation of the proton-atom cross sections. Clearly the electron-atom cross sections are smaller than the corresponding proton-atom cross sections.

2.5. Finally we will consider briefly the kinetic energy

$$T = (m/M_{\rm A})t^2 \qquad \dots (37)$$

given to a stationary atom suffering excitation or ionization. For a fixed impact energy the integrands in (16) and (17) fall off extremely rapidly as t increases beyond some value  $t_{\rm M}$  so that transitions in which T is more than several times

$$T_{\mathrm{M}} = (m/M_{\mathrm{A}})t_{\mathrm{M}}^{2} \qquad \dots (38)$$

are very rare. In any particular case  $t_{\rm M}$  can of course easily be found from the expression for the matrix element.

The general position is illustrated sufficiently by the 1s-2s and 1s-2p transitions of atomic hydrogen. If the incident particle is a proton it is immediately apparent from (16) and (23) that for both transitions  $t_M$  is simply

 $t_{\min}$ ; if the incident particle is a hydrogen atom it may be shown from (17) and (23) that for the 1s-2s transition

$$t_{\text{M}} = t_{\text{min}},$$
  $(t_{\text{min}} \ge 0.87_{7})$   
=  $0.87_{7},$   $(t_{\text{min}} \le 0.87_{7})$ 

and for the 1s-2p transition

$$t_{M} = t_{\min},$$
  $(t_{\min} \ge 0.57_{7})$   
=  $0.57_{7},$   $(t_{\min} \le 0.57_{7}).$ 

On substituting in (38) it is found that if  $\mathscr{E}$  is the energy of the incident hydrogen ion or atom in kev then according to the Born approximation

$$\begin{split} T_{\rm M} = & (0.026/\mathscr{E}) \, \mathrm{ev} & \begin{cases} \text{H+ ion impact, } 1\mathrm{s} - 2\mathrm{s, } 1\mathrm{s} - 2\mathrm{p \; transitions, } \; \mathrm{all} \; \mathscr{E} \\ \text{H atom impact, } 1\mathrm{s} - 2\mathrm{s \; transition, } \; \mathscr{E} \leqslant 4.6 \, \mathrm{kev} \\ \text{H atom impact, } 1\mathrm{s} - 2\mathrm{p \; transition, } \; \mathscr{E} \leqslant 10.5 \, \mathrm{kev} \end{cases} \\ = & 0.0057 \, \mathrm{ev} & \begin{cases} \text{H atom impact, } 1\mathrm{s} - 2\mathrm{s \; transition, } \; \mathscr{E} \geqslant 4.6 \, \mathrm{kev} \\ \text{H atom impact, } 1\mathrm{s} - 2\mathrm{p \; transition, } \; \mathscr{E} \geqslant 10.5 \, \mathrm{kev.} \end{cases} \end{split}$$

The kinetic energy transferred is thus minute. Qualitative verification of this well-known characteristic of inelastic collisions is provided by the recent experiments of Keene (1949).

## § 3. RESULTS

3.1. The cross sections associated with the processes mentioned in the introduction were computed from the formulae that have been given. Figures 1 to 6 show the values obtained. It should be noted that a log-log scale is used,

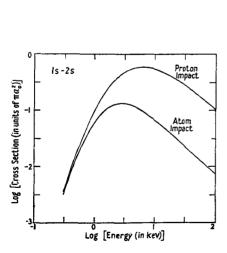


Fig. 1.  $H^++H(1s) \rightarrow H^++H(2s)$  and  $H(1s)+H(1s) \rightarrow H(1s)+H(2s)$ .

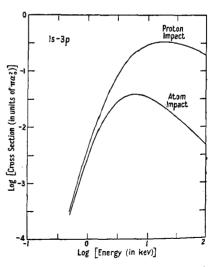


Fig. 4.  $H^++H(1s)\to H^++H(3p)$  and  $H(1s)+H(1s)\to H(1s)+H(3p)$ .

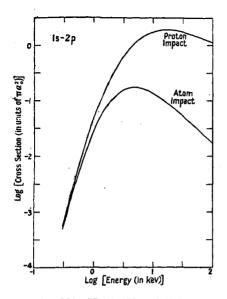


Fig. 2.  $H^++H(1s) \rightarrow H^++H(2p)$  and  $H(1s)+H(1s) \rightarrow H(1s)+H(2p)$ .

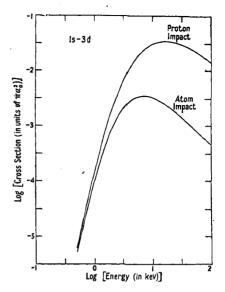


Fig. 5.  $H^++H(1s) \rightarrow H^++H(3d)$  and  $H(1s)+H(1s) \rightarrow H(1s)+H(3d)$ .

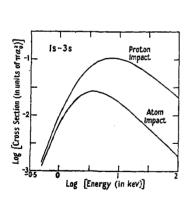


Fig. 3.  $H^++H(1s) \rightarrow H^++H(3s)$  and  $H(1s)+H(1s) \rightarrow H(1s)+H(3s)$ .

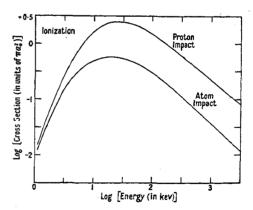


Fig. 6.  $H^++H(1s) \rightarrow H^++H^++e$  and  $H(1s)+H(1s) \rightarrow H(1s)+H^++e$ .

Figs. 1-6. Cross-section-energy curves.

and that the independent variable chosen is *not* E, the energy of relative motion, but is instead  $\mathscr{E}$ , the energy of the incident particle, the atom undergoing the transition being taken to be at rest. In the case of the excitations the results for energies above 100 kev (the upper limit in the figures) can most conveniently be

presented algebraically: thus by expanding in inverse powers of  $\mathscr E$  (which we measure in kev) we find that

$$\begin{array}{c} Q^{+}(1s \rightarrow 2s) = 11 \cdot 1 \, \mathscr{E}^{-1}\{1 - 7 \cdot 8 \, \mathscr{E}^{-1}\}, \\ Q^{\pm}(1s \rightarrow 2s) = 0 \cdot 721 \, \mathscr{E}^{-1}\{1 - 123 \, \mathscr{E}^{-8}\}, \\ Q^{+}(1s \rightarrow 2p) = 128 \, \mathscr{E}^{-1} \, \{\log \, \mathscr{E} - 1 \cdot 185 + 4 \cdot 1 \, \mathscr{E}^{-1}\}, \\ Q^{\pm}(1s \rightarrow 2p) = 1 \cdot 78 \, \mathscr{E}^{-1}\{1 - 48 \, \mathscr{E}^{-2}\}, \\ Q^{+}(1s \rightarrow 3s) = 2 \cdot 20 \, \mathscr{E}^{-1}\{1 - 7 \cdot 5 \, \mathscr{E}^{-1}\}, \\ Q^{\pm}(1s \rightarrow 3s) = 0 \cdot 186 \, \mathscr{E}^{-1}\{1 - 180 \, \mathscr{E}^{-8}\}, \\ Q^{+}(1s \rightarrow 3p) = 20 \cdot 5 \, \mathscr{E}^{-1}\{\log \, \mathscr{E} - 1 \cdot 104 + 2 \cdot 4 \, \mathscr{E}^{-1}\}, \\ Q^{\pm}(1s \rightarrow 3p) = 0 \cdot 478 \, \mathscr{E}^{-1}\{1 - 57 \, \mathscr{E}^{-2}\}, \\ Q^{+}(1s \rightarrow 3d) = 1 \cdot 69 \, \mathscr{E}^{-1}\{1 - 19 \cdot 4 \, \mathscr{E}^{-1} + 162 \, \mathscr{E}^{-2}\}, \\ Q^{\pm}(1s \rightarrow 3d) = 0 \cdot 0453 \, \mathscr{E}^{-1}\{1 - 1473 \, \mathscr{E}^{-8}\}, \end{array}$$

the unit of cross section being  $\pi a_0^2$  as usual. The final term in each of the expressions is very small, and is included mainly to demonstrate how rapidly the asymptotic form is approached.

On comparing a  $Q^+$  curve with the corresponding  $Q^\pm$  curve it will be observed that the former lies close to, but above, the latter at low energies, that its maximum is much larger and occurs at much higher energies, and that its final rate of fall off is the same for optically forbidden transitions but is slightly slower for optically allowed transitions. It will be noted also that the curves for each spectral series (such as  $1s \rightarrow ns$ ) are almost identical in shape, any one curve approximating to the preceding curve displaced downwards and to the right, the latter displacement being far greater than the difference between the excitation potentials.

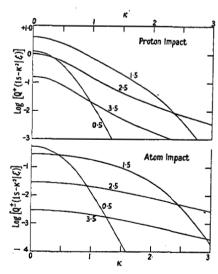


Fig. 7. Energy distribution of the ejected electrons. The upper set of curves refers to process (3) and the lower set to process (4). The numbers on the individual curves give the logarithm of the energy of the incident particle (expressed in kev).

In the case of ionization information is often required on the energy distribution of the ejected electrons. One convenient way of representing the distribution is by the function  $Q(1s \to \kappa^2 | \mathscr{E})$ , which is such that  $Q(1s \to \kappa^2 | \mathscr{E}) d\kappa^2$  is the cross section for a collision in which an incident particle of energy  $\mathscr{E}$  ejects an electron with energy between  $\kappa^2$  and  $\kappa^2 + d\kappa^2$  times the ionization potential.\* Figure 7 shows the variation of  $\log \{Q^+(1s \to \kappa^2 | \mathscr{E})\}$  and of  $\log \{Q^+(1s \to \kappa^2 | \mathscr{E})\}$  with  $\kappa$  for some selected impact energies. Attention is drawn to the rapidity of the fall off when  $\mathscr{E}$  is small, to the change in the form of the distribution as  $\mathscr{E}$  is increased, and to the great difference between the proton and atom cases when  $\mathscr{E}$  is large. It should perhaps be mentioned that the rather abrupt changes of slope which occur are real, and are associated with passage through the maximum of a curve of  $Q(1s \to \kappa^2 | \mathscr{E})$  plotted against  $\mathscr{E}$ .

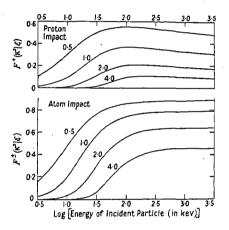


Fig. 8. Fraction of ejected electrons which have more than a certain amount of energy  $\kappa^2$ . The upper set of curves refers to process (3) and the lower set to process (4). The numbers on the individual curves give  $\kappa^2$  (expressed in units of  $I_{\rm H}$ , the ionization potential of hydrogen).

Instead of the actual energy distribution it is sometimes more useful to know

$$F(\kappa^2|\mathscr{E}) = \int_{\kappa^2}^{\infty} Q(1s \to \kappa^2|\mathscr{E}) d\kappa^2 / \int_{0}^{\infty} Q(1s \to \kappa^2|\mathscr{E}) d\kappa^2, \quad \dots (40)$$

that is the fraction of the ejected electrons which have energy greater than  $\kappa^2$  times the ionization potential. The results of some relevant calculations are displayed in fig. 8. As can be seen, F increases rapidly until  $\mathscr E$  is some 100 kev, and thereafter is approximately constant. The value of F on what may be called the plateau is quite large: thus when  $\kappa^2$  is unity, F is about 0.3 in the protoncase, and is about 0.8 in the atom case. This is of considerable interest in connection with aurorae.

- 3.2. Experimental work on collisions between heavy particles is extremely difficult as is evidenced by the contradictory results that have been reported
- \*For corresponding values of  $\mathscr E$  the energy of the incident particle and E the energy of relative motion we have of course that  $Q(1s \to \kappa^2 \mid \mathscr E)$  is equal to  $Q(1s \to \kappa \mid E)/2\kappa$  where  $Q(1s \to \kappa \mid E)$  is the function introduced in §2.3.

(cf. Massey and Burhop 1952). The only relevant data at present available refer to ionization, which is naturally simpler to study than is excitation.

Keene (1949) has conducted a careful investigation of the process

$$H^+ + H_2 \rightarrow H^+ + H_2^+ + e$$
 .....(41)

over an energy range of from 2 to 36 kev. The agreement with theory is rather poor: for example, the observed cross section at the upper limit of the energy range covered is  $1.5(\pm 0.2)\pi a_0^2$ , whereas the predicted cross section\* is  $3.4\pi a_0^2$ ; and again the observed cross section curve is still increasing steadily at this energy, whereas the predicted cross section curve is passing through its maximum. There is thus apparently a discrepancy of the type characteristic of the Born approximation (cf. Bates, Fundaminsky, Leech and Massey 1950). At an impact energy of 36 kev the velocity of the proton is about equal to the orbital velocity of the bound electrons, so it would not be surprising if the theory should prove to be inadequate. However, it would be premature to conclude that the error is as great as is indicated by Keene's experiments, for the charge transfer cross sections he obtained with the same apparatus are significantly different from those of some later workers (cf. Jackson and Schiff 1953).

By studying the passage of a beam of hydrogen atoms through hydrogen gas Bartels (1932), Montague (1951) and Ribe (1951) have determined the cross section associated with

$$H_2 + H \rightarrow H_2 + H^+ + e.$$
 .....(42)

Their results are mutually consistent, and when combined cover the 20 to 300 kev energy range. The calculated variation over this energy range (cf. fig. 6) is essentially identical with that observed. However, Born's approximation gives the absolute magnitude of the cross section for process (4) to be only half the measured cross section (per hydrogen atom).† Part of the difference may arise from the fact that a small fraction of the hydrogen atoms in the beam must have been in excited states, for judging from the work of Yavorsky (1945) on ionization by electron impact the cross section of excited atoms is very many times that of normal atoms. Another, and probably much more important, factor is that in the process studied in the laboratory the neutral molecule causing the transition is not necessarily left in the initial state but may itself be excited or ionized, so that process (4) represents only one of the possible reaction paths. Calculations on the contributions from simultaneous ionization and excitation and double ionization are in progress.

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\* In predicting the cross section one molecule was assumed to be equivalent to two atoms and scaling formula (21) was used to allow for the fact that the *vertical* ionization potential of molecular hydrogen is  $1 \cdot 2I_H$ .

† In contrast, the semi-classical treatment of Bohr (1948) gives a cross section which is about thrice too large. This treatment assumed that only close collisions are effective and that in these the ionizing effects of the individual particles constituting the perturbing atom or molecule are additive.

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