

ON THE EVALUATION OF ELASTIC AND
INELASTIC COLLISION FREQUENCIES
FOR HYDROGENIC-LIKE PLASMAS

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September, 1967

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COLLISION FREQUENCIES FOR HYDROGENIC-LIKE PLASMAS

by

E. L. BYDDER

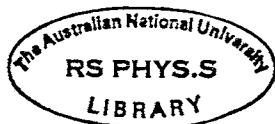
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SUMMARY

Detailed calculations of the generalised collision frequencies for the principal elastic, excitation, ionisation, and charge exchange collisions in the formation of a hydrogenic plasma are given. A modified form of Born's approximation is used for the differential cross sections, and approximations corresponding to a high temperature gas are used. The results enable certain sets of 13-moment equations describing the plasma formations to be completed.

1. Introduction

Recently methods have been devised to enable full account to be taken of inelastic as well as elastic collision processes in the application of Grad's 13-moment equations to partially ionised gases (Bydder,¹ Bydder and Liley²). The resulting collision integrals are expressed in terms of certain generalised collision "frequencies" (but including a number density factor), $\Omega^{\mu,\nu}(r)$, which are similar to functions $\Omega^{\nu}(r)$ used by Chapman and Cowling³ for elastic collisions. The final forms of these collision terms are, however, of little practical value without the associated Ω 's being determined explicitly through the use of the relevant collision differential cross sections. In the limiting case of elastic collisions there are only five such parameters involved, and these have already been obtained for many different types of interactions (e.g. reference 3). However, since the $\Omega^{\mu,\nu}(r)$ are peculiar to references 1 and 2, obviously no other equivalent calculations have been carried out for the inelastic case. For this reason the following more general calculations have been made, essentially completing the equations of reference 2 and also of a paper to be published (Bydder and Liley⁴), for a particular form of hydrogenic plasma.

In general there are 20 Ω 's to be determined for each particle type present. Therefore at first sight the task is a formidable one. However, as will be seen, reasonable and inter-related expressions can be obtained for certain specific cases. In this report the $\Omega^{\mu,\nu}(r)$ are obtained explicitly for processes applicable to the formation of a laboratory hydrogenic-like plasma.

In attempting to follow the collision processes during the development of a fully ionised plasma from molecular hydrogen, collisions involving (Goodyear and Von Engel⁵) H_2 , H , H_2^* , H^* , H_2^+ , H^+ and electrons should be taken into account. Because of the large number of possible types of collisions between these particles, a simplified model, restricted to H , H^* , H^+ and electrons, is considered. In all probability this is a realistic model for sufficiently high initial temperatures, and in general should give results suitable for comparison with experiment. Unfortunately, even for this simple case, the relevant expressions for the Ω 's are not particularly amenable to integration, and in certain cases various approximations are necessary. Generally speaking, relatively exact expressions can be obtained for elastic collisions (Chapman and Cowling, loc cit, and also Appendix C), the major approximations

applying to the inelastic processes. These approximations are such that the Ω 's tend to be inaccurate near the threshold energy, which is unfortunate, but they do lead to reasonably accurate results for appreciably higher energies.

The $\Omega_{jk,i}^{\mu,\nu}(\tau)$ are defined in references 1, 2 and 4 by

$$\Omega_{jk,i}^{\mu,\nu}(\tau) = \pi^{\frac{1}{2}} \int_{Y_0}^{\infty} e^{-Y^2} Y^{2r+2} \phi_{jk,i}(\mu,\nu) dY$$

where $\phi_{jk,i}(\mu,\nu)$ is given by

$$\phi_{jk,i}(\mu,\nu) = \int (1 - \lambda^{\mu} \cos^{\nu} \chi) g \sigma \sin \chi d\chi$$

In these formulae, $\underline{Y} = \delta \underline{g}$, \underline{g} being the

relative velocity of the colliding particles, and $\sigma \sin \chi d\chi d\epsilon \equiv \sigma d\Omega$ is the differential cross section for the collision between particles of types j, k involving particles of type i . The remaining parameters, also defined in references 1, 2 and 4, are given as they subsequently occur in this report. For convenience, however, the following may be listed:

\underline{g} is the relative velocity of the colliding particles j, k before the collision;

\underline{g}' is the relative velocity of the particles j', k' produced in the collision;

$\lambda = |\underline{g}'| / |\underline{g}|$ (see also Appendix B);

$\Delta_{jk}(\underline{\Psi}_i) = \underline{\Psi}_i \delta_{ij'} + \underline{\Psi}_i \delta_{ik'} - \underline{\Psi}_i \delta_{ij} - \underline{\Psi}_i \delta_{ik}$,
where $\underline{\Psi}_i$ is some function of the particle parameters, and the δ_{ij} are ordinary Kronecker deltas;

$\Delta \mathcal{E}$ is the kinetic energy "gain" in the collision.

Since there are not suitable analytical expressions for the differential (or for that matter, total) cross sections for all of the processes being considered, two main approaches are possible. The first would be to obtain empirical relations for the differential cross section for each process, in the relevant energy range, based on the use of accurate calculations and experimental results. Unfortunately there are relatively few accurate calculations for the differential cross sections, and fewer experimental results. More data is available on total cross sections, and empirical relations for the differential cross sections which integrate to the known total values could have been chosen. This would, however, be particularly tedious. The second approach is to use a consistent mathematical approximation for theoretical evaluations of the differential cross sections, for example, the Born approximation or certain modifications of this approximation. It is the latter approach which is used in the subsequent calculations. It must be stated, however, that the inverse fifth power law and other such classical models provide a much better description of certain of the elastic collisions than any form of the Born approximation. Ω 's calculated for such classical cross sections are given in Chapman and Cowling,³ and for convenience these calculations are briefly summarised in Appendix C. For the present report, the Born approximation has been applied to all collisions, being multiplied by a numerical factor to produce "reasonable" approximations to the total cross sections in the energy range 0 - 100 ev. The detailed derivation of the various cases and a comparison with known values of total cross section is given in Appendix A.

For notational convenience, $q^2/4\pi\epsilon_0$ is replaced by e^2 where q is the electron charge, and ϵ_0 is the free-space permittivity (rationalised mks units being used). Except where otherwise designated, $d\Omega$ is the solid angle into which the asymptotic relative velocity \underline{g} of the colliding particles is deflected with polar angle χ ; m_r is the reduced mass of the colliding particles; \hbar is Planck's constant divided by 2π ; and \underline{k} is the (reduced) wave vector of the colliding particles, given by \underline{p}/\hbar . \underline{p} is the reduced momentum $m_r \underline{g}$. Finally, a_0 is the Bohr radius, and the change in wave vector in a collision, \underline{K} , is defined by

$$(1) \quad \underline{K} = \underline{k}_f - \underline{k}_0 ,$$

\underline{k}_0 and \underline{k}_f being the wave vectors before and after the collision. The moduli of these wave vectors, k_0 and k_f (the wave numbers), are of course equal for elastic collisions. The differential cross sections given in the following sub-sections are derived in Appendix A, and include the "correction" factors.

2.1 Elastic Collisions Between Electrons

The differential cross section for these Coulomb collisions is

$$(2) \quad \sigma d\Omega = \frac{m_r^2 e^4}{4 \hbar^4 k_0^4} \operatorname{cosec}^4 \chi/2 d\Omega$$

with $\chi \gg \chi_0$. χ_0 is the Debye cut-off angle (see Appendix A).

2.2 Elastic Collisions Between Electrons and Hydrogen Atoms

The adjusted Born differential cross section is

$$(3) \quad \sigma d\Omega = \frac{(0.45) 4 m_r^2 e^4 a_0^4 (K^2 a_0^2 + 8)^2}{\hbar^4 (K^2 a_0^2 + 4)^4} d\Omega$$

2.3 Elastic Collisions Between Electrons and Protons

This Coulomb differential cross section has the same form as (2)

$$(4) \quad \sigma d\Omega = \frac{m_r^2 e^4 \operatorname{cosec}^4 \chi/2}{4 \hbar^4 k_0^4} d\Omega$$

with $\chi \gg \chi_0$ (Debye cut-off).

2.4 Elastic Collisions Between Hydrogen Atoms

The adjusted Born cross section is

$$(5) \quad \sigma d\Omega = \frac{(2.0 \times 10^{-2}) 4 m_r^2 e^4 a_0^8 K^4 (a_0^2 K^2 + 8)^4}{\hbar^4 (a_0^2 K^2 + 4)^8} d\Omega$$

2.5 Elastic Collisions Between Hydrogen Atoms and Protons

Of the same general form as (3), the differential cross section is

$$(6) \quad \sigma d\Omega = \frac{(2.0 \times 10^{-2}) 4 m_r^2 e^4 a_0^4 (K^2 a_0^2 + 8)^2 d\Omega}{\hbar^4 (K^2 a_0^2 + 4)^4} .$$

2.6 Elastic Collisions Between Protons

Formally the same as (2) and (4),

$$(7) \quad \sigma d\Omega = \frac{m_r^2 e^4 \operatorname{cosec}^4 \chi / 2 d\Omega}{4 \hbar^4 k_0^4}$$

with $\chi \gg \chi_0$ (Debye cut-off).

2.7 1s - 2p Excitation Collisions Between Electrons and Hydrogen Atoms

The adjusted Born approximation gives

$$(8) \quad \sigma d\Omega = \frac{(.45) 3^2 2^{15} k_f m_r^2 a_0^2 e^4 d\Omega}{k_0 \hbar^4 K^2 (4 a_0^2 K^2 + 9)^6}$$

2.8 Ionisation Collisions Between Electrons and Hydrogen Atoms

A simplified form of the Born approximation used for this case

gives

$$(9) \quad \sigma d\Omega_1 d\Omega_2 dk = \frac{(.14 \times 10^{-3}) 2^6 \pi a_0^2 m_r^2 e^4 k_f k d\Omega_1 d\Omega_2 dk}{\hbar^4 k_0 K^4 (a_0^2 K^2 + 1)^4}$$

where $d\Omega_1$ is the solid angle into which the incident electron is scattered (with wave vector \underline{k}_f), and $d\Omega_2$ the solid angle into which the atomic electron is ejected with wave vector \underline{k} . Details are given in Appendix A.

2.9 Charge Exchange Collisions Between Hydrogen Atoms and Protons

A simplified Born approximation gives

$$(10) \quad \sigma d\Omega = \frac{(2.1 \times 10^{-2}) 2^8 m_r^2 e^4 a_0^4}{\hbar^4 (K^2 a_0^2 + 1)^6} d\Omega$$

where, for this case, $\underline{K} = \underline{k}_0 + \underline{k}_f$.

3. Evaluation of the ϕ 's

3.1 Elastic Collisions

The general $\phi(\mu, \nu)$ defined previously are simplified for elastic collisions, since $\lambda = 1$. Hence the $\phi(\mu, \nu)$ are independent of μ :

$$(11) \quad \phi(\mu, \nu) = \int (1 - \cos^{\nu} \chi) g \sigma \sin \chi d\chi \\ \equiv \phi(\nu),$$

and these $\phi(\nu)$ are the same as those used by Chapman and Cowling.³

(a) Electron-electron collisions

These results are given in reference 3.

$$(12) \quad \phi_{ee}(1) = \int_{\chi_0}^{\pi} \frac{(1 - \cos \chi) e^4 g \operatorname{cosec}^4 \chi / 2 \sin \chi d\chi}{4 m_r^2 g^4} = \frac{e^4 \log(1 + \Lambda_{ee}^2)}{m_r^2 g^3},$$

where

$$(13) \quad \Lambda_{ee} = \lambda_D g^2 m_r / e^2$$

(λ_D being the Debye length). Similarly,

$$(14) \quad \phi_{ee}(2) = \frac{2 e^4}{m_r g^3} \left(\log(1 + \Lambda_{ee}^2) - \frac{\Lambda_{ee}^2}{1 + \Lambda_{ee}^2} \right) \sim 2 \phi_{ee}(1),$$

since Λ_{ee} is large.

(b) Electron-hydrogen atom collisions

According to (3),

$$(15) \quad \phi_{ea}(1) = \int_0^\pi \frac{(1 - \cos \chi) g (\cdot 45) 4 m_r^2 e^4 a_0^4 (K^2 a_0^2 + 8)^2 \sin \chi d\chi}{\hbar^4 (K^2 a_0^2 + 4)^4}.$$

Since for elastic collisions

$$(16) \quad K^2 = 2 k_0^2 (1 - \cos \chi),$$

using the substitution $y = 1 - \cos \chi$, after some manipulation the result is

$$(17) \quad \phi_{ea}(1) = \frac{(\cdot 45) 4 m_r^2 e^4 a_0^4 g}{\hbar^4 q^2} \left(\log \frac{q+2}{2} + \frac{q^3 - 6q^2 - 24q}{6(q+2)^3} \right)$$

$$\text{where } q^2 = 2 k_0^2 a_0^2 = 2 m_r^2 g^2 a_0^2 / \hbar^2.$$

Similarly

$$(18) \quad \phi_{ea}(2) = \int_0^\pi \frac{(1 - \cos^2 \chi) g (\cdot 45) 4 m_r^2 e^4 a_0^4 (K^2 a_0^2 + 8)^2 \sin \chi d\chi}{\hbar^4 (4 + K^2 a_0^2)^4}$$

$$= 2 \phi_{ea}(1) - \frac{(\cdot 45) 4 m_r^2 e^4 a_0^4 g (6q + 16)}{3 \hbar^4 (q + 2)^3}.$$

Alternatively, for the same collisions considered according to an inverse power force law, the $\phi_{ea}(v)$ are essentially given in Appendix C.

(c) Electron-proton collisions

These collisions give the same expressions as for electron-electron collisions.

$$(19) \quad \phi_{ep}(1) = \frac{e^4}{m_r^2 g^3} \log(1 + \Lambda_{ep}^2),$$

$$(20) \quad \phi_{ep}(2) = \frac{2e^4}{m_r^2 g^3} \left(\log(1 + \Lambda_{ep}^2) - \frac{\Lambda_{ep}^2}{1 + \Lambda_{ep}^2} \right) \sim 2\phi_{ep}(1),$$

where $\Lambda_{ep} = \lambda_0 g^2 m_r / e^2$.

(d) Hydrogen atom-hydrogen atom collisions

Using equation (5)

$$(21) \quad \phi_{aa}(1) = \int_0^\pi \frac{(1 - \cos \chi) g (2 \times 10^{-2})^4 m_r^2 e^4 a_0^8 K^4 (a_0^2 K^2 + 8)^4 \sin \chi d\chi}{\hbar^4 (a_0^2 K^2 + 4)^8}$$

On substituting for K^2 (from (16)) the part of (21) to be integrated is

$$(22) \quad I = \int_0^\pi \frac{(1 - \cos \chi)^3 (p - q \cos \chi)^4 \sin \chi d\chi}{(r - q \cos \chi)^8}$$

where $q = 2k_0^2 a_0^2$, $p = q + 8$, $r = q + 4$.

Elementary application of standard integrals provides the result:

$$(23) \quad I = \frac{1}{q^4} \left[\frac{24576}{7(qy+4)^7} - \frac{143360}{6(qy+4)^6} - \frac{3072}{5(qy+4)^5} - \frac{768}{4(qy+4)^4} + \frac{192}{3(qy+4)^3} + \frac{216}{2(qy+4)^2} - \frac{4}{(qy+4)} + \log(qy+4) \right]_0^2,$$

the limits being on y . For the greater part of the energy range being considered,

$q \gg 1$; taking this into account, the approximation

$$(24) \quad I = \frac{1}{q^4} \log \frac{q+2}{2}$$

will be used. In this case,

$$(25) \quad \phi_{aa}(1) = \frac{g (2 \times 10^{-2})^4 m_r^2 e^4 k_0^4 a_0^8 \log \frac{q+2}{2}}{\hbar^4 q^4}.$$

Similarly, with the same approximation,

$$(26) \quad \phi_{aa}(2) = \frac{g(2 \times 10^{-2}) 32 m_r^2 e^4 k_0^4 a_0^8 \log \frac{q+2}{2}}{\hbar^4 q^4} \\ = 2 \phi_{aa}(1).$$

Again, possibly better alternative results, based on inverse power force laws, are given in reference 3 (see also Appendix C).

(e) Hydrogen atom-proton collisions

Using the differential cross section (6), for this case

$$(27) \quad \phi_{ap}(1) = \int_0^\pi \frac{(1 - \cos \chi) g(2 \times 10^{-2}) 4 m_r^2 e^4 a_0^4 (K^2 a_0^2 + 8)^2 \sin \chi d\chi}{\hbar^4 (K^2 a_0^2 + 4)^4}.$$

The integration is similar to the previous cases. Taking $q = 2 k_0^2 a_0^2 \gg 1$,

$$(28) \quad \phi_{ap}(1) = \frac{(2 \times 10^{-2}) 4 g m_r^2 e^4 a_0^4 \log \frac{q+2}{2}}{\hbar^4 q^2}.$$

Again, it may be shown that

$$(29) \quad \phi_{ap}(2) = \frac{(2 \times 10^{-2}) 8 g m_r^2 e^4 a_0^4 \log \frac{q+2}{2}}{\hbar^4 q^2} \\ = 2 \phi_{ap}(1).$$

(As mentioned with certain other cases, reference may also be made to Chapman and Cowling³.)

(f) Proton-proton collisions

The calculation for this case is formally the same as for electron-electron collisions, the results being

$$(30) \quad \phi_{pp}(1) = \frac{e^4}{m_r^2 g^3} \log(1 + \Lambda_{pp}^2)$$

where $\Lambda_{pp} = \lambda_0 g^2 m_r / e^2$; and similarly,

$$(31) \quad \phi_{pp}(2) = \frac{2 e^4}{m_r^2 g^3} \left(\log(1 + \Lambda_{pp}^2) - \frac{\Lambda_{pp}^2}{1 + \Lambda_{pp}^2} \right) \sim 2 \phi_{pp}(1).$$

3.2 Inelastic Collisions

For inelastic collisions involving particles j, k colliding to produce particles j', k' ,

$$(32) \quad \lambda^2 = \frac{m_j m_k}{m_{j'} m_{k'}} - \frac{2 (m_j + m_k) \Delta \mathcal{E}}{m_{j'} m_{k'} g^2}.$$

Therefore it is necessary to use the general form for the ϕ 's which, from the Introduction, is

$$(33) \quad \phi(\mu, \nu) = \int_0^\pi (1 - \lambda^\mu \cos^\nu \chi) g \sigma \sin \chi \, d\chi.$$

For excitation collisions where the nature of the colliding particles does not change (the energy being carried away by photons, for example), the following ϕ 's are required to evaluate the collision terms: $\phi(-\infty, 0)$, $\phi(1, 1)$, $\phi(2, 0)$ and $\phi(2, 2)$. In more general inelastic collisions it is also necessary to calculate $\phi(3, 1)$.

(a) Electron-hydrogen atom 1s - 2p excitation collisions

Using the differential cross section (8),

$$(34) \quad \phi(\mu, \nu) = \int_0^\pi \frac{(1 - \lambda^\mu \cos^\nu \chi) g (4.5) 3^2 2^{15} k_f m_r^2 e^4 a_0^2 \sin \chi \, d\chi}{\hbar^4 k_0 K^2 (4K^2 a_0^2 + 9)^6}$$

and since

$$(35) \quad K^2 = k_o^2 + k_f^2 - 2k_o k_f \cos \chi,$$

ignoring the constant terms in (34), this becomes

$$(36) \quad I(\mu, \nu) = \int_0^\pi \frac{(1 - \lambda^\mu \cos^\nu \chi) \sin \chi d\chi}{(p - q \cos \chi)(r - s \cos \chi)^6}$$

where

$$(37) \quad \begin{aligned} p &= k_o^2 + k_f^2 ; & q &= 2k_o k_f ; & r &= 9 + 4a_o^2(k_o^2 + k_f^2) ; \\ s &= 8a_o^2 k_o k_f ; & t &= ps - qr = -18k_o k_f ; \\ r \pm s &= 9 + 4a_o^2(k_o \pm k_f)^2 . \end{aligned}$$

Using the substitution $y = r - s \cos \chi$,

$$(38) \quad I(\mu, \nu) = \int_{r-s}^{r+s} \frac{(1 - \lambda^\mu [r/s - y/s]^\nu) dy}{(t + qy) y^6}$$

and it follows that $I(\mu, \nu)$ can be expressed in terms of integrals P , Q and R , where (since ν takes the values 0, 1 and 2):

$$(39) \quad P = \int_{r-s}^{r+s} \frac{dy}{(t + qy) y^6} ,$$

$$(40) \quad Q = \int_{r-s}^{r+s} \frac{dy}{(t + qy) y^5} ,$$

$$(41) \quad R = \int_{r-s}^{r+s} \frac{dy}{(t + qy) y^4} .$$

These integrals are readily evaluated. Considering (39), it is found that

$$(42) \quad P = \frac{1}{t^6} \left[-\frac{1}{5} \left(\frac{t+qy}{y} \right)^5 + \frac{5}{4} \left(\frac{t+qy}{y} \right)^4 q - \frac{10}{3} \left(\frac{t+qy}{y} \right)^3 q^2 + \frac{10}{2} \left(\frac{t+qy}{y} \right)^2 q^3 - 5 \left(\frac{t+qy}{y} \right) q^4 + q^5 \log \left(\frac{t+qy}{y} \right) \right]_{r-s}^{r+s}$$

After inserting the limits of integration in the general term

$$\left[q^{5-n} \left(\frac{t+qy}{y} \right)^n \right]_{r-s}^{r+s} \quad \text{and substituting for } r+s \quad \text{and } r-s \quad ,$$

except near threshold it is found that this can be approximated by

$$(43) \quad \left[q^{5-n} \left(\frac{t+qy}{y} \right)^n \right]_{r-s}^{r+s} \sim q^5 = (2k_0 k_f)^5 .$$

Similarly, considering the term in (42) involving the logarithm, away from the threshold,

$$(44) \quad \left[q^5 \log \left(\frac{t+qy}{y} \right) \right]_{r-s}^{r+s} \sim q^5 \log \frac{9}{4a_0^2 (k_0 - k_f)^2}$$

On the other hand, near threshold, it is found that both of these terms (43) and (44) are of the same order. From a physical point of view, it is the near threshold region that is usually of particular importance despite the small total cross section, since during the excitation and ionisation stages the mean particle energies are within this region. However, it is only with the simplification achieved by discarding all terms in (42) except the logarithm term that a comprehensible form for the Ω 's can be obtained. In this case, the integral (42) becomes

$$(45) \quad P = \frac{q^5}{t^6} \log \frac{9}{4a_0^2 (k_0 - k_f)^2} \\ = \frac{1}{3^{1/2} k_0 k_f} \log \frac{3}{2a_0 (k_0 - k_f)} \quad ,$$

while similar approximations in calculating Q , R give

$$(46) \quad Q = 9P \quad ,$$

$$(47) \quad R = 81P \quad .$$

Taking the relevant particular values of ν ,

$$(48) \quad I(\mu, 0) = (1 - \lambda^\mu)P$$

$$I(\mu, 1) = (1 - \lambda^\mu r/s)P + (\lambda^\mu/s)Q$$

$$I(\mu, 2) = (1 - \lambda^\mu r^2/s)P + (2\lambda^\mu r/s^2)Q - (\lambda^\mu/s^2)R .$$

Writing

$$(49) \quad A = (.45) 3^2 2^{15} g m_r^2 k_f e^4 a_0^2 / \hbar^4 k_0$$

and using (46), (47), the ϕ 's become

$$(50) \quad \phi(\mu, 0) = A(1 - \lambda^\mu)P$$

$$(51) \quad \phi(\mu, 1) = A(1 - \lambda^\mu \frac{k_0^2 + k_f^2}{2k_0 k_f})P$$

$$(52) \quad \phi(\mu, 2) = A(1 - \lambda^\mu (\frac{k_0^2 + k_f^2}{2k_0 k_f})^2)P .$$

Again it is necessary to make assumptions corresponding to a non-threshold region. Since for the excitation collisions being considered,

$$(53) \quad \lambda^2 = 1 - 2\Delta E/m_r g^2 = 1 - 2m_r \Delta E/\hbar^2 k_0^2 \quad ,$$

$$(54) \quad \lambda \sim 1 - m_r \Delta E/\hbar^2 k_0^2 \equiv \alpha/k_0^2 \quad .$$

Also from the energy conservation (since $\Delta \mathcal{E}$ is the excitation energy)

$$(55) \quad k_0^2 = k_f^2 + 2m_r \Delta \mathcal{E} / \hbar^2 ;$$

$$k_0^2 + k_f^2 = 2k_0^2 - 2m_r \Delta \mathcal{E} / \hbar^2 = 2\alpha ;$$

$$k_f \sim \alpha / k_0 .$$

Using these relations in equations (50 to (52), giving the ϕ 's, it follows that

$$(56) \quad \phi(-\infty, 0) = AP ,$$

$$(57) \quad \phi(1, 1) = A(1 - \frac{2\alpha}{2\alpha} \lambda) P$$

$$\sim (m_r \Delta \mathcal{E} / \hbar^2 k_0^2) AP ,$$

$$(58) \quad \phi(2, 2) = A(1 - (\frac{2\alpha}{2\alpha})^2 \lambda^2) P = (2m_r \Delta \mathcal{E} / \hbar^2 k_0^2) AP$$

$$= 2 \phi(1, 1) ,$$

$$(59) \quad \phi(2, 0) = A(1 - \lambda^2) P$$

$$= \phi(2, 2) ,$$

$$= 2 \phi(1, 1) .$$

Hence for the Ω 's the following relationships apply:

$$(60) \quad \Omega^{2,2}(r) = \Omega^{2,0}(r) = 2 \Omega^{1,1}(r) .$$

Again, using (55) in (45), AP simplifies to

$$(61) \quad AP = \frac{(.45) 2^{15} g m_r^2 e^4 a_0^2}{3^{10} \hbar^4 k_0^2} \log \left(\frac{3 \hbar^2 k_0^2}{2 m_r \Delta \mathcal{E}} \right) .$$

Equations (56) to (59) enable the ϕ 's to be expressed in terms of (61).

(b) Electron-hydrogen atom ionising collisions

An ionisation collision is essentially an encounter in which the atomic electron is excited to the continuum state. For this reason, for the incident electron scattered in the collision, the process may be treated as excitation with variable $\Delta \mathcal{E}$. On the other hand, owing to the stripping of the atom and the production of new particles, for the atom, the proton produced, and the atomic electron ejected, the collisions need to be considered in more detail. To some extent the physics of these collisions is contained within certain δ -functions used in references 1, 2 and 4; nevertheless the Ω 's must be calculated for each different particle type for which the 13-moment equations are required. In general, for each particle considered, the $\Delta \mathcal{E}$ are different, and the λ 's must be expressed in terms of these for integration over the range of $\Delta \mathcal{E}$.

Let $d\Omega_1$ be the solid angle into which the incident electron (with incident (reduced) wave vector \underline{k}_0) is scattered with wave vector \underline{k}_f , and $d\Omega_2$ the solid angle into which the atomic electron is ejected with wave vector \underline{k} . It is shown in Appendix A that it is satisfactory to refer all these parameters to a frame moving with the centre of mass of the two colliding particles. The subscripts e_1 , e_2 , a , p will refer respectively to the scattered electron, atomic electron, atom, and proton produced. For the collision dynamics (but not the general equations for the electron component) the scattered and atomic electrons are treated separately.

(i) Scattered electron, e_1

Using equation (33) and the differential cross section (9), (χ being the polar angle of \underline{k}_f with respect to \underline{k}_0)

$$(62) \quad \phi_{e_1, a, e_1}(\mu, \nu) = \frac{\int (1 - \lambda_{e_1}^{\mu} \cos^{\nu} \chi) g(1.4 \times 10^{-3}) 2^6 \pi m_r^2 e^4 a_0^2 k_f k \sin \chi d\chi d\Omega_2 d\mathcal{K}}{\hbar^4 k_0 K^4 (a_0^2 K^2 + 1)^4}$$

where

$$(63) \quad K^2 = k_o^2 + k_f^2 - 2 k_o k_f \cos \chi .$$

It is almost impossible to calculate the Ω 's from (62) as such; however, by approximating the term $(a_o^2 K^2 + 1)^4$ in the denominator by $(a_o^2 k_o^2 + 1)^4$, it becomes possible to evaluate the sequence of integrals required to obtain the Ω 's. Although by no means an accurate approximation, the K^4 term, also in the denominator, nullifies the effect of this approximation.

From the conservation of energy, it follows that

$$(64) \quad k_o^2 = k_f^2 + \kappa^2 + 2 m_r I / \hbar^2$$

where I is the ionisation energy of the atom. Integration over $d\Omega_2$ yields a factor 4π . The limits of integration over χ are $(0, \pi)$, while from (64) the limits on κ are $(0, (k_o^2 - 2m_r I / \hbar^2)^{1/2})$. The equation (62) becomes

$$(65) \quad \phi_{ea,ei}(\mu, \nu) = \frac{4\pi(-14 \times 10^{-3}) 2^0 \pi g m_r^2 a_o^2 e^4}{\hbar^4 k_o (a_o^2 k_o^2 + 1)^4} J_1(\mu, \nu)$$

where

$$(66) \quad J_1(\mu, \nu) = \int_0^\pi \int_0^{(k_o^2 - 2m_r I / \hbar^2)^{1/2}} \frac{(1 - \lambda^\mu \cos^\nu \chi) k_f \sin \chi dx \kappa d\kappa}{(k_o^2 + k_f^2 - 2 k_o k_f \cos \chi)^2} ,$$

this being evaluated in Appendix B. For this case, λ is given by

$$(67) \quad \lambda^2 = 1 - (\kappa^2 + 2 m_r I / \hbar^2) / k_o^2 .$$

Using the values from this appendix for the appropriate (μ, ν) , on putting

$$(68) \quad \alpha^2 = k_o^2 - 2 m_r I / \hbar^2$$

and

$$(69) \quad A = \frac{(-14 \times 10^{-3}) 2^6 \pi g a_0^2 m_r^2 e^4 4 \pi}{\hbar^4 k_0 (a_0^2 k_0^2 + 1)^4} \cdot \frac{2 \alpha^3}{3 (2 m_r / \hbar^2)^2} ,$$

the results are:

$$(70) \quad \phi_{ea,e_i}(-\infty, 0) = A ,$$

$$(71) \quad \phi_{ea,e_i}(1, 1) = A \left(1 - \frac{k_0^2 + \alpha^2}{6 k_0^2} \right) ,$$

$$(72) \quad \phi_{ea,e_i}(2, 2) = A \left(1 - \frac{(k_0^2 + \alpha^2)^2}{4 k_0^4} \right) ,$$

$$(73) \quad \phi_{ea,e_i}(2, 0) = A \left(1 - \frac{3 \alpha^2}{5 k_0^2} \right) ,$$

$$(74) \quad \phi_{ea,e_i}(3, 1) = A \left(1 - \frac{3 \alpha^2 (k_0^2 + \alpha^2)}{10 k_0^4} \right) .$$

Finally, $2 m_r \Gamma / \hbar^2$ is neglected compared with k_0^2 in the parenthesised terms after substituting for α from (59). (Again this corresponds to an approximation valid away from threshold. However, apart from being consistent with previous approximations taken, this type of approximation in the present calculations is necessary to obtain workable results.) The results then become

$$(75) \quad \phi_{ea,e_i}(1, 1) = \frac{2}{3} \phi_{ea,e_i}(-\infty, 0) ,$$

$$(76) \quad \phi_{ea,e_i}(2, 2) = \frac{2 m_r \Gamma}{\hbar^2 k_0^2} \phi_{ea,e_i}(-\infty, 0) ,$$

$$(77) \quad \phi_{ea,e_i}(2, 0) = \frac{2}{5} \phi_{ea,e_i}(-\infty, 0) ,$$

$$(78) \quad \phi_{ea,e_i}(3, 1) = \frac{2}{5} \phi_{ea,e_i}(-\infty, 0) .$$

(ii) The atomic electron, e_2

Similarly to (62), but for this case with χ being the polar angle of \underline{k} with respect to \underline{k}_0 , and χ_1 the deflection angle of \underline{k}_f ,

$$(79) \quad \Phi_{e_1, e_2}(\mu, \nu) = \int (1 - \lambda^\mu \cos^\nu \chi) g (-14 \times 10^{-3}) \pi m_r^2 e^4 2^6 a_0^2 \\ \times \frac{k_f k \sin \chi d\chi d\Omega_1 dk}{\hbar^4 k_0 K^4 (a_0^2 K^2 + 1)^4}$$

where now K^2 is in terms of χ_1 (being defined in fact from the differential cross section):

$$(80) \quad K^2 = k_0^2 + k_f^2 - 2 k_0 k_f \cos \chi_1 .$$

For this case (Appendix B)

$$(81) \quad \lambda^2 = 1 - (k_0^2 - k^2) / k_0^2 .$$

Integration over χ is straightforward, owing to the cross sectional independence of this angle. Defining

$$(82) \quad J_2(\mu, \nu) = \int_0^\pi (1 - \lambda^\mu \cos^\nu \chi) \sin \chi d\chi ,$$

elementary integration gives

$$(83) \quad J_2(\mu, \nu) = 2 - \lambda^\mu (1 + (-1)^\nu) / (\nu + 1) .$$

Integration of (79) over the solid angle $d\Omega_1$ involves only terms in M where

$$(84) \quad M = \int \frac{\sin \chi_1 d\chi_1 d\epsilon_1}{K^4 (a_0^2 K^2 + 1)^4} .$$

As in the previous case, the term $(a_0^2 K^2 + 1)^4$ is replaced by $(a_0^2 k_0^2 + 1)$. Integration over the azimuthal angle gives 2π , and with the above approximation, integration over χ_1 may be effected, giving

$$(85) \quad M = 4\pi / ((a_0^2 k_0^2 + 1)^4 (k_0^2 - k_f^2)^2)$$

Returning to (79), $\phi(\mu, \nu)$ becomes

$$(86) \quad \phi_{e\alpha, e_2}(\mu, \nu) = \int_0^\alpha \frac{\pi m_r^2 M J_2(\mu, \nu) g(-14 \times 10^{-3}) 2^6 a_0^2 k_f \kappa d\kappa}{\hbar^4 k_0} \\ = \frac{4\pi B}{(a_0^2 k_0^2 + 1)^4} L(\mu, \nu)$$

where

$$(87) \quad B = \frac{(-14 \times 10^{-3}) 2^6 a_0^2 \pi m_r^2 e^4}{\hbar^4 k_0}$$

α is defined by (68) and $L(\mu, \nu)$ is calculated in Appendix B. Taking the values of $L(\mu, \nu)$ from this Appendix, and since A , already defined by (69), is

$$(88) \quad A = \frac{4\pi B}{(a_0^2 k_0^2 + 1)^4} \cdot \frac{2\alpha^3}{3(2m_r I / \hbar^2)^2},$$

the $\phi(\mu, \nu)$ are given by

$$(89) \quad \phi_{e\alpha, e_2}(-\infty, 0) = A,$$

$$(90) \quad \phi_{e\alpha, e_2}(1, 1) = A,$$

$$(91) \quad \phi_{e\alpha, e_2}(2, 2) = \left(\frac{2}{3} + \frac{\alpha^2}{5k_0^2}\right),$$

$$(92) \quad \phi_{e_a, e_2}(2, 0) = \frac{3}{5} \frac{\alpha^2}{k_0^2} A ,$$

$$(93) \quad \phi_{e_a, e_2}(3, 1) = A .$$

Since

$$(94) \quad \left(\frac{2}{3} + \frac{\alpha^2}{5 k_0^2} \right) \sim \frac{13}{15} ,$$

the $\phi(\mu, \nu)$ may be expressed as follows in terms of $\phi(-\infty, 0)$:

$$(95) \quad \phi_{e_a, e_2}(1, 1) = \phi_{e_a}(-\infty, 0) ,$$

$$(96) \quad \phi_{e_a, e_2}(2, 2) = \frac{13}{15} \phi_{e_a}(-\infty, 0) ,$$

$$(97) \quad \phi_{e_a, e_2}(2, 0) = \frac{3}{5} \frac{\alpha^2}{k_0^2} \phi_{e_a}(-\infty, 0) \sim \frac{3}{5} \phi_{e_a}(-\infty, 0) ,$$

$$(98) \quad \phi_{e_a, e_2}(3, 1) = \phi_{e_a}(-\infty, 0) .$$

In any case it is obvious from (33) that $\phi_{e_a}(-\infty, 0)$ is simply the total cross section for the collision multiplied by $g/2\pi$ and therefore for all particles involved in a particular (inelastic) collision, the $\phi(-\infty, 0)$ are identical. Thus (89) is identical with (70).

(iii) The atoms

In the part of Appendix B dealing with the calculation of the λ 's it was pointed out that for atoms as a particle type in this type of ionising collision, the only Ω 's involved are the $\Omega^{-\infty, 0}(\mathbf{r})$, which are independent of λ . Hence for the atoms,

$$(99) \quad \phi_{e_a, a}(-\infty, 0) = \int g \sigma \sin \chi \, d\chi = \frac{\int g (1.4 \times 10^{-3}) 2^8 \pi^2 a_0^2 m_r^2 k_f K e^4 \sin \chi \, d\chi \, d\chi}{\hbar^4 k_0 K^4 (a_0^2 K^2 + 1)^4}$$

where $\chi = \cos^{-1}((-k_0) \cdot (-k_f) / k_0 k_f) = \chi_1$.

Again replacing $(a_0^2 k^2 + 1)^4$ by $(a_0^2 k_0^2 + 1)^4$, since on differentiating (63),

$$(100) \quad \sin \chi, d\chi = K dK / k_0 k_f,$$

$$(101) \quad \phi_{ea}(-\infty, 0) = C \int \frac{\kappa d\kappa dK}{K^3}$$

where

$$(102) \quad C = \frac{g (\cdot 14 \times 10^{-3}) m_r^2 e^4 2^8 \pi^2 a_0^2}{\hbar^4 k_0^2 (a_0^2 k_0^2 + 1)^4}.$$

The upper and lower limits on K are $k_0 \pm k_f$. Using (64) and (68),

$$(103) \quad k_f^2 = \alpha^2 - \kappa^2,$$

and therefore, on integrating over K

$$(104) \quad \phi_{ea}(-\infty, 0) = \int_0^\alpha \frac{\kappa d\kappa 2 k_0 k_f}{(k_0^2 - k_f^2)^2} \sim \int_0^\alpha \frac{\kappa d\kappa (\alpha^2 - \kappa^2)^{\frac{1}{2}} k_0}{(2 m_r I / \hbar^2)^2}.$$

The remaining integration is straightforward also:

$$(105) \quad \phi_{ea}(-\infty, 0) = \frac{2}{3} \frac{C k_0 \alpha^3}{(2 m_r I / \hbar^2)^2}.$$

It is apparent on comparing (105) with (70), for example, that the $\phi_{ea}(-\infty, 0)$ obtained for the different cases are equal; this suggests that the different approximations made are consistent.

(iv) The protons

As discussed in Appendix B the Ω 's for the protons produced in the ionising collisions are readily obtained from those for the atoms. In particular, when terms of order $\frac{m_e}{m_a}$ are neglected, the Ω 's are the same for the protons as for the atoms. There is, therefore, no need to calculate the particular $\phi_{ea}(\mu, \nu)$ for these protons.

(c) Charge exchange collisions

As discussed in Appendix A, only resonant charge exchange collisions are considered. These charge exchange collisions are elastic in the sense that there is no kinetic energy absorbed in the collision, although in the strict sense of a change in the nature of the colliding particles the collisions are inelastic. Nevertheless, the most convenient way of considering this case is to calculate the $\Delta_{jk}(\psi_i)$ and hence the ϕ 's for the ψ -functions of the atom (or proton) present after the collision minus the ψ -functions of the atom (or proton), involving the other nucleus, before the collision. From this point of view, the collision is elastic, with differential cross section (10).

Since $\delta(1) = \delta(2) = 0$ for elastic collisions, there is no need to consider $\phi(-\infty, 0)$, while $\phi(2, 0) = 0$ and $\phi(3, 1) = \phi(1, 1) = \phi(1)$ say. Also let $\phi(2, 2) = \phi(2)$; then

$$(106) \quad \phi(\nu) = D \int_0^\pi \frac{(1 - \cos^\nu \chi) \sin \chi \, d\chi}{(a_0^2 K^2 + 1)^6}$$

where

$$(107) \quad D = \frac{(2.1 \times 10^{-2}) g m_r^2 a_0^4 z^8 e^4}{\hbar^4}.$$

Substituting for K^2 (defined for equation (10))

$$(108) \quad \phi_{ap}(\nu) = D \int_0^\pi \frac{(1 - \cos^\nu \chi) \sin \chi \, d\chi}{(1 + 2 k_0^2 a_0^2 (1 + \cos \chi))^6}$$

from which is obtained

$$(109) \quad \phi_{ap}(1,1) = D \left(\frac{1}{10 k_0^2 a_0^2} - \frac{1}{10 k_0^2 a_0^2} + \frac{1}{16 k_0^4 a_0^4} \right) \\ = D / 16 k_0^4 a_0^4 ,$$

$$(110) \quad \phi_{ap}(2) = D \left(\frac{1}{10 k_0^2 a_0^2} + \frac{1}{10 k_0^2 a_0^2} \right) \\ = D / 5 k_0^2 a_0^2 .$$

For these calculations, it has been assumed that $k_0^2 a_0^2 \gg 1$.

4. Evaluation of the Ω 's

The Ω 's, defined in the introduction and references 1, 2 and 4, are essentially the result of integrating the ϕ 's over the impact velocity. Restating the definition, (where $\gamma^2 = m_j m_f / 2 k (m_j T_k + m_k T_j)$)

$$(111) \quad \Omega_{jk,i}^{\mu,\nu}(r) = \pi^{\frac{1}{2}} \int_{Y_0}^{\infty} e^{-Y^2} Y^{2r+2} \phi_{jk,i}(\mu,\nu) dY$$

where $\underline{Y} = \gamma \underline{g}$, or since $\hbar \underline{k}_0 = m_r \underline{g}$, $\underline{Y} = \gamma \hbar \underline{k}_0 / m_r$.

Y_0 is the threshold value of Y for a particular collision. Thus for elastic collisions Y_0 is zero, while for a collision with excitation energy $\Delta \xi_0$,

$$(112) \quad Y_0^2 = 2 \gamma^2 \Delta \xi_0 / m_r .$$

This is taken account of, in a sense, in the ϕ 's, in that being functions of the differential cross section, below the threshold energy they take the value zero. However, the approximate cross sections used are not zero for all energies below the collision threshold, and it is necessary to specify the particular lower limit as in (112).

4.1 Elastic Collisions

For these collisions, with the Ω 's as with the ϕ 's, the definitions are formally the same as those given by Chapman and Cowling.³ The results for Coulomb collisions are given below are in fact the same as in reference 3; however, as already mentioned, the use of "adjusted" Born approximations for the differential cross sections for other elastic collisions leads to different results from those of reference 3 based on inverse power force laws. Since $\phi(\mu, \nu) \equiv \phi(\nu)$ for elastic collisions, it is evident that

$$(113) \quad \Omega_{jk,i}^{\mu, \nu}(r) \equiv \Omega_{jk}^{\nu}(r)$$

(using this equation to define $\Omega_{jk}^{\nu}(r)$).

(a) Electron-electron collisions

Equation (12) for $\phi(1)$, with (111) gives

$$(114) \quad \Omega_{ee}^1(r) = \pi^{\frac{1}{2}} \int_0^{\infty} \frac{e^{-Y^2} Y^{2r+2} e^4 \delta^3 \log(1 + \Lambda_{ee}^2) dY}{m_r^2 Y^3} .$$

Although Λ_{ee} is a function of Y , owing to its occurrence only in the logarithmic term, it is generally adequate to replace it by an "averaged" value (Liley⁶), regarding it as constant for the purposes of integration. In this case the integral is easily reduced to an expression involving the factorial function:

$$(115) \quad \Omega_{ee}^1(r) = \pi^{\frac{1}{2}} \delta^3 e^4 \log(\Lambda_{ee}^2) \Gamma(r) / 2 m_r^2 .$$

Similarly, since $\phi_{ee}^{(2)} = 2 \phi_{ee}^{(1)}$,

$$(116) \quad \Omega_{ee}^2(r) = 2 \Omega_{ee}^1(r) .$$

The "averaged" value of Λ_{ee} is

$$(117) \quad \Lambda_{ee} = 3kT_e \lambda_D / e^2 = 3(kT_e)^{3/2} / (e^2 (4\pi n_e e^2)^{1/2}),$$

where λ_D is the Debye length.

(b) Electron-hydrogen atom collisions

Using equation (17) for $\phi(1)$ gives

$$(118) \quad \Omega'_{ea}(r) = \pi^{1/2} \int_0^\infty \frac{e^{-Y^2} Y^{2r+2} (.45) 4 m_r^2 e^4 a_0^4 g dY}{\hbar^4 (2 k_0^2 a_0^2)^2} \\ \times \left(\log(a_0^2 k_0^2 + 1) + \frac{(2 a_0^2 k_0^2)^3 - 6(2 a_0^2 k_0^2)^2 - 24(2 a_0^2 k_0^2)}{6(2 a_0^2 k_0^2 + 2)^3} \right).$$

Retaining only the logarithm term, this equation becomes

$$(119) \quad \Omega'_{ea}(r) = \pi^{1/2} (.45) \frac{e^4 \gamma^3}{m_r^2} \int_0^\infty e^{-Y^2} Y^{2r-1} \log\left(1 + \frac{a_0^2 m_r^2}{\gamma^2 \hbar^2} Y^2\right) dY.$$

For the various τ , the following expressions for the $\Omega'(r)$ are obtained:

$$(120) \quad \Omega'_{ea}(1) = \frac{\pi^{1/2} (.45) e^4 \gamma^3}{m_r^2} \frac{1}{2} (-e^{1/b} \text{Ei}(-1/b)),$$

$$(121) \quad \Omega'_{ea}(2) = \frac{\pi^{1/2} (.45) e^4 \gamma^3}{m_r^2} \frac{1}{2} \left(1 + \frac{1-b}{b} e^{1/b} \text{Ei}(-1/b)\right),$$

$$(122) \quad \Omega'_{ea}(3) = \frac{\pi^{1/2} (.45) e^4 \gamma^3}{m_r^2} \frac{1}{2} \left(3 - \frac{1}{b} + \frac{(-2b^2 + 2b - 1)}{b^2} e^{1/b} \text{Ei}(-1/b)\right).$$

$Ei(-1/b)$ is the exponential-integral function (Gradshteyn and Ryzhik⁴), and the argument b is given by

$$(123) \quad b = \alpha_0^2 m_r^2 / \gamma^2 \hbar^2 .$$

The similar approximation of discarding terms other than the logarithm term in $\phi_{ea}(\lambda)$ (equation (18)) gives

$$(124) \quad \phi_{ea}(\lambda) = 2 \phi_{ea}(\lambda)$$

and therefore

$$(125) \quad \Omega_{ea}^2(r) = 2 \Omega_{ea}^1(r) .$$

(c) Electron-proton collisions

The calculation of the Ω 's is formally the same as for electron-electron collisions. The results are

$$(126) \quad \Omega_{ep}^1(r) = \pi^{1/2} \gamma^3 e^4 \log(1 + \Lambda_{ep}^2) \Gamma(r) / 2 m_r^2 ;$$

$$\Omega_{ep}^2(r) = 2 \Omega_{ep}^1(r) ,$$

where in this case Λ_{ep} is given by

$$(127) \quad \Lambda_{ep} = \frac{3}{2} \lambda_D \left(\frac{\alpha_e + \alpha_p}{\alpha_e \alpha_p} \right) m_r / e^2$$

$$\approx \frac{3 (k T_e)^{3/2}}{e^2 (4 \pi n_e e^2)^{1/2}} .$$

(d) Hydrogen atom-hydrogen atom collisions

The relevant $\phi(\nu)$ are given in (25), (26). Using (25) for

$\phi(1)$, $\Omega'_{aa}(r)$ is the integral

$$(128) \quad \Omega'_{aa}(r) = \frac{(2 \times 10^{-2}) \delta^3 e^4 \pi^{1/2}}{m_r^2} \int_0^\infty e^{-Y^2} Y^{2r-1} \log(1+bY^2) dY,$$

where $b = m_r^2 a_0^2 / \hbar^2 \delta^2$ as before.

From the results involving similar integrals for the electron-hydrogen atom collisions, in the same notation, the $\Omega'(r)$ become

$$(129) \quad \Omega'_{aa}(1) = \frac{(2 \times 10^{-2}) \delta^3 e^4 \pi^{1/2}}{m_r^2} \frac{1}{2} (-e^{1/b} \text{Ei}(-1/b))$$

$$(130) \quad \Omega'_{aa}(2) = \frac{(2 \times 10^{-2}) \delta^3 e^4 \pi^{1/2}}{m_r^2} \frac{1}{2} \left(1 + \frac{1-b}{b} e^{1/b} \text{Ei}(-1/b)\right)$$

$$(131) \quad \Omega'_{aa}(3) = \frac{(2 \times 10^{-2}) \delta^3 e^4 \pi^{1/2}}{m_r^2} \frac{1}{2} \left(3 - \frac{1}{b} + \frac{(-2b^2 + 2b - 1)}{b^2} e^{1/b} \text{Ei}(-1/b)\right).$$

Again, since $\phi_{aa}(2) = 2\phi_{aa}(1)$ it follows that

$$(132) \quad \Omega_{aa}^2(r) = 2\Omega'_{aa}(1).$$

(e) Hydrogen atom-proton collisions

From the equation (28) for $\phi_{ap}(1)$

$$(133) \quad \Omega'_{ap}(r) = \frac{(2 \times 10^{-2}) e^4 \delta^3 \pi^{1/2}}{m_r^2} \int_0^\infty e^{-Y^2} Y^{2r-1} \log(1+bY^2) dY$$

with b as in (123). The integrals have the same form as for the previous cases involving atoms, being expressible in terms of the exponential-integral functions.

The results are

$$(134) \quad \Omega'_{ap}(1) = \frac{(2 \times 10^{-2}) e^4 \gamma^3 \pi^{1/2}}{m_r^2} \frac{1}{2} (-e^{1/b} \text{Ei}(-1/b)),$$

$$(135) \quad \Omega'_{ap}(2) = \frac{(2 \times 10^{-2}) e^4 \gamma^3 \pi^{1/2}}{m_r^2} \frac{1}{2} \left(1 + \frac{1-b}{b} e^{1/b} \text{Ei}(-1/b) \right),$$

$$(136) \quad \Omega'_{ap}(3) = \frac{(2 \times 10^{-2}) e^4 \gamma^3 \pi^{1/2}}{m_r^2} \frac{1}{2} \left(3 - \frac{1}{b} + \frac{(-2b^2 + 2b - 1)}{b^2} e^{1/b} \text{Ei}(-1/b) \right).$$

Again, since $\phi_{ap}(2) = 2\phi_{ap}(1)$, it follows that

$$(137) \quad \Omega^2_{ap}(r) = 2 \Omega^1_{ap}(r).$$

(f) Proton-proton collisions

Formally the same as for electron-electron collisions and electron-proton collisions, the results are

$$(138) \quad \Omega'_{pp}(r) = \pi^{1/2} \gamma^3 e^4 \log(1 + \mathcal{L}^2_{pp}) T(r) / 2 m_r^2$$

$$(139) \quad \Omega^2_{pp}(r) = 2 \Omega^1_{pp}(r).$$

For these collisions, however,

$$(140) \quad \mathcal{L}_{pp} = 3 \lambda_D m_r / \alpha_p e^2 = (3 k T_p / e^2) (k T_e / 4 \pi n_e e^2)^{1/2}.$$

4.2 Electron-Hydrogen Atom 1s - 2p Excitation Collisions

The $\Omega_{ea}^{\mu,\nu}(\mathbf{r})$, given by (111) are functions of, amongst other variables, the lower limit of integration $Y_0 = (2\delta^2 \Delta \mathcal{E}_0 / m_r)^{1/2}$. Since δ is a function of the temperature, the $\Omega^{\mu,\nu}(\mathbf{r})$ will essentially be functions of the electron and atom temperatures. As will be seen, in general the $\Omega^{\mu,\nu}(\mathbf{r})$ can only be reduced to expressions in terms of incomplete Gamma functions, which in this case are dimensionless functions of the temperatures. The incomplete Gamma functions are, however, tabulated functions, and in certain extreme cases they can be written in terms of analytical functions. The following Ω 's are required: $\Omega^{-\infty,0}(\mathbf{r})$, $\Omega^{1,1}(\mathbf{r})$, $\Omega^{2,2}(\mathbf{r})$, $\Omega^{2,0}(\mathbf{r})$, with $\mathbf{r} = 0, 1, 2, 3$; but since relations (60) express $\Omega^{2,2}(\mathbf{r})$ and $\Omega^{2,0}(\mathbf{r})$ in terms of $\Omega^{1,1}(\mathbf{r})$, it is only necessary to evaluate $\Omega^{-\infty,0}(\mathbf{r})$ and $\Omega^{1,1}(\mathbf{r})$, for these value of \mathbf{r} .

The calculation of $\Omega_{ea}^{-\infty,0}(\mathbf{r})$ involves using (56) for $\phi_{ea}(-\infty,0)$.

This gives

$$(141) \quad \Omega^{-\infty,0}(\mathbf{r}) = \frac{(.45)e^4 2^{15} a_0^2 \delta \pi^{1/2}}{3^{10} \hbar^2} \int_{Y_0}^{\infty} e^{-Y^2} Y^{2r+1} \log(bY) dY$$

where b has the value $3\hbar/2a_0\delta\Delta\mathcal{E}_0$ (bearing no relation to the term b , defined in (123)).

Consider the function $I(\mathbf{r}, Y_0)$ defined by

$$(142) \quad I(\mathbf{r}, Y_0) = \int_{Y_0}^{\infty} e^{-Y^2} Y^{2r+1} \log(bY) dY.$$

A change of variable yields

$$(143) \quad I(\mathbf{r}, Y_0) = \frac{1}{4} \int_{Y_0^2}^{\infty} e^{-x} x^r \log(b^2 x) dx,$$

and this can be integrated by parts for the various values of r . Let $\Gamma(r, z)$ be an incomplete Gamma function, defined by

$$(144) \quad \Gamma(r, z) = \int_z^{\infty} e^{-x} x^{r-1} dx .$$

(Some authors define the incomplete Gamma function in the inverse way, that is, by $(\Gamma(r) - \Gamma(r, z))$ in the above notation, but the definition (144) is more suitable for the purposes of this report) Provided $z > 0$, the $\Gamma(r, z)$ are defined for all r .

In terms of these functions (144), integration of (143) gives

$$(145) \quad I(0, Y_0) = \frac{1}{4} \left(e^{-Y_0^2} \log b^2 Y_0^2 + \Gamma(0, Y_0^2) \right),$$

$$(146) \quad I(1, Y_0) = \frac{1}{4} \left(e^{-Y_0^2} (Y_0^2 + 1) \log b^2 Y_0^2 + \Gamma(1, Y_0^2) + \Gamma(0, Y_0^2) \right),$$

$$(147) \quad I(2, Y_0) = \frac{1}{4} \left(e^{-Y_0^2} (Y_0^4 + 2Y_0^2 + 2) \log b^2 Y_0^2 + \Gamma(2, Y_0^2) \right. \\ \left. + 2\Gamma(1, Y_0^2) + 2\Gamma(0, Y_0^2) \right),$$

$$(148) \quad I(3, Y_0) = \frac{1}{4} \left(e^{-Y_0^2} (Y_0^6 + 3Y_0^4 + 6Y_0^2 + 6) \log b^2 Y_0^2 + \Gamma(3, Y_0^2) \right. \\ \left. + 3\Gamma(2, Y_0^2) + 6\Gamma(1, Y_0^2) + 6\Gamma(0, Y_0^2) \right) .$$

It is evident that the $\Omega_{ea}^{-\infty, 0}(r)$ are obtained using these results for $I(r, Y_0)$ in equation (141), that is,

$$(149) \quad \Omega_{ea}^{-\infty, 0}(r) = \frac{(.45) e^4 2^{15} a_0^2 \delta \pi^{1/2}}{3^{10} \hbar^2} I(r, Y_0) .$$

The $\Omega_{ea}^{1,1}(r)$ are calculated using equation (57) for $\phi_{ea}(1,1)$.

This gives

$$(150) \quad \Omega_{ea}^{1,1}(r) = \frac{(-.45)\pi^{1/2} e^4 2^{15} a_0^2 m_r \Delta \xi_0 \gamma^3}{3^{10} m_r^2 \hbar^2} \int_{Y_0}^{\infty} e^{-Y^2} Y^{2r-1} \log(bY) dY$$

where again $b = 3\gamma\hbar/2a_0\Delta\xi_0$. It follows from this equation that the $\Omega^{1,1}(r)$ can also be expressed in terms of the $I(r, Y_0)$, defined in (142), and hence in terms of the incomplete Gamma functions. In particular,

$$(151) \quad \Omega_{ea}^{1,1}(r) = \frac{(-.45)\pi^{1/2} e^4 2^{15} a_0^2 m_r \gamma^3 \Delta \xi_0}{3^{10} m_r^2 \hbar^2} I(r-1, Y_0).$$

The integral $I(-1, Y_0)$, not previously given, has the value

$$(152) \quad I(-1, Y_0) = \frac{1}{4} \left(\Gamma(0, Y_0^2) \log b^2 + \int_{Y_0^2}^{\infty} \frac{e^{-x} \log x}{x} dx \right).$$

The last integral on the right hand side of (152) exists for $Y_0^2 > 0$; being of a similar nature to the incomplete Gamma functions, it may also readily be evaluated numerically.

Finally, the remaining Ω 's are related to (149) and (151) by

$$(153) \quad \Omega_{ea}^{2,2}(r) = 2 \Omega_{ea}^{1,1}(r)$$

$$(154) \quad \Omega_{ea}^{2,0}(r) = 2 \Omega_{ea}^{1,1}(r).$$

4.3 Electron-Hydrogen Atom Ionisation Collisions

For these collisions the Ω 's are defined by (111). The lower limit of integration is given by $Y_0 = (2\gamma^2 I/m_r)^{1/2}$ where I is the ionisation energy. As with excitation collisions, since γ is a function of the electron and atom temperatures, the Ω 's are also functions of these temperatures. When

$T_a / T_e \ll m_a / m_e$, then $\gamma^2 \sim \alpha_e = m_e / 2kT_e$, in which case the Ω 's are simply functions of the electron temperature. This also applies to the excitation collisions of course. For each of the particles (incident electron, atom, atomic electron, and proton produced), the following Ω 's are required: $\Omega^{-\infty, 0}(\mathbf{r})$, $\Omega^{1,1}(\mathbf{r})$, $\Omega^{2,2}(\mathbf{r})$, $\Omega^{2,0}(\mathbf{r})$, $\Omega^{3,1}(\mathbf{r})$ with \mathbf{r} taking the values 0, 1, 2, and 3. Fortunately, it is not necessary to calculate all 80 Ω 's. As shown in Appendix B, the Ω 's for the protons are essentially equal to the Ω 's for the atoms. Furthermore, for the individual particles, relations have been given between various $\phi(\mu, \nu)$, enabling many Ω 's to be expressed in terms of others.

In particular it has been shown that for the incident electron, all $\phi_{ea, e_1}(\mu, \nu)$ can be expressed in terms of $\phi_{ea, e_1}(-\infty, 0)$ or $\phi_{ea, e_1}(2, 2)$; for the atomic electron, all $\phi_{ea, e_2}(\mu, \nu)$ can be expressed in terms of $\phi_{ea, e_2}(-\infty, 0)$ and for the protons and atoms, the only $\phi(\mu, \nu)$ involved is $\phi_{ea}(-\infty, 0)$; and finally that the $\phi_{ea, i}(-\infty, 0)$ are equal for all particles involved in a particular collision. The general form of $\Omega^{(\mu, \nu)}(\mathbf{r})$ being given in equation (111), it is evident that it is a function of $\phi(\mu, \nu)$, γ_0 , and certain other constants of the collision. Therefore all particles in the collision have the same $\Omega^{-\infty, 0}(\mathbf{r})$. It follows that for the ionisation collisions, only 8 of the Ω 's need be calculated, namely $\Omega_{ea}^{-\infty, 0}(\mathbf{r})$ and $\Omega_{ea, e_1}^{2, 2}(\mathbf{r})$ with $\mathbf{r} = 0, 1, 2$ and 3 .

Since

$$(155) \quad \gamma_0^2 = 2\gamma^2 I / m_r,$$

using this relation and also those after (111),

$$(156) \quad k_0^2 - 2m_r I / \hbar^2 = m_r^2 (\gamma^2 - \gamma_0^2) / \gamma^2 \hbar^2$$

$$a_0^2 k_0^2 + 1 = a_0^2 m_r^2 (\gamma^2 + \gamma_1^2) / \gamma^2 \hbar^2$$

where $Y_1^2 = \delta^2 \hbar^2 / m_r^2 a_0^2$, and, like Y_0 , is a constant of the collision. With $\phi_{ea}(-\infty, 0)$, given in equation (70) for example, from (111),

$$(157) \quad \Omega_{ea}^{-\infty, 0}(r) = \frac{(.14 \times 10^{-3}) \pi^{1/2} \hbar^2 2^9 \pi^2 \delta^5 e^4}{3 a_0^6 m_r^4 (2 m_r I / \hbar^2)^2} I(r; Y_0, Y_1)$$

where $I(r; Y_0, Y_1)$ is defined by

$$(158) \quad I(r; Y_0, Y_1) = \int_{Y_0}^{\infty} \frac{e^{-Y^2} Y^{2r+2} (Y^2 - Y_0^2)^{3/2}}{(Y^2 + Y_1^2)^4} dY .$$

$I(r; Y_0, Y_1)$ may be reduced on making appropriate approximations, or it may be numerically evaluated. As discussed previously, $I(r; Y_0, Y_1)$ is essentially a function of the electron temperature.

Similarly, using equation (72) for $\phi_{ea, e_i}^{2, 2}$, it may be verified that

$$(159) \quad \Omega_{ea, e_i}^{2, 2}(r) = \frac{(.14 \times 10^{-3}) \pi^{1/2} \hbar^2 e^4 2^{10} \pi^2 \delta^7 m_r I}{3 m_r^6 a_0^6 (2 m_r I / \hbar^2)^2} I(r-1; Y_0, Y_1),$$

$I(r; Y_0, Y_1)$ being again given by (158).

Finally, using equations (70) to (78), (95) to (98), and (105), the set of 48 Ω 's for the collision (as already mentioned, 32 of the Ω 's associated with the atom and proton particle types need not be considered), in terms of the 8 independent Ω 's are as follows. For convenience, $\Omega_{ea}^{-\infty, 0}(r)$ and $\Omega_{ea, e_i}^{2, 2}(r)$ are also repeated.

$$(160) \quad \Omega_{ea}^{-\infty, 0}(r) = \frac{(.14 \times 10^{-3}) \hbar^2 e^4 \pi^{5/2} 2^9 \delta^5}{3 a_0^6 m_r^4 (2 m_r I / \hbar^2)^2} I(r; Y_0, Y_1)$$

with $I(r; Y_0, Y_1)$ defined in equation (158),

$$(161) \quad \Omega_{ea, e_1}^{1,1}(r) = \frac{2}{3} \Omega_{ea}^{-\infty, 0}(r)$$

$$(162) \quad \Omega_{ea, e_1}^{2,0}(r) = \frac{2}{5} \Omega_{ea}^{-\infty, 0}(r)$$

$$(163) \quad \Omega_{ea, e_1}^{3,1}(r) = \frac{2}{5} \Omega_{ea}^{-\infty, 0}(r)$$

$$(164) \quad \Omega_{ea, e_1}^{2,2}(r) = \frac{(\cdot 14 \times 10^{-3}) \pi^{5/2} \hbar^2 e^4 z^{10} \gamma^7 m_r I}{3 m_r^6 a_0^6 (2 m_r I / \hbar^2)^2} I(r-1; Y_0, Y_1)$$

$$(165) \quad \Omega_{ea, e_2}^{1,1}(r) = \Omega_{ea}^{-\infty, 0}(r)$$

$$(166) \quad \Omega_{ea, e_2}^{2,2}(r) = \frac{13}{15} \Omega_{ea}^{-\infty, 0}(r)$$

$$(167) \quad \Omega_{ea, e_2}^{2,0}(r) = \Omega_{ea}^{-\infty, 0}(r)$$

$$(168) \quad \Omega_{ea, e_2}^{3,1}(r) = \Omega_{ea}^{-\infty, 0}(r)$$

$$(169) \quad \Omega_{ea, a}^{-\infty, 0}(r) = \Omega_{ea}^{-\infty, 0}(r)$$

$$(170) \quad \Omega_{ea, p}^{-\infty, 0}(r) = \Omega_{ea}^{-\infty, 0}(r) .$$

4.4 Hydrogen Atom-Proton Charge Exchange Collisions

The nature of the charge exchange collisions has already been discussed. The $\phi_{ap}(\mu, \nu)$ are given by (109) and (110), being independent of μ , while the Ω 's required are $\Omega_1(r)$, $\Omega_2(r)$ with $r = 1, 2$ and 3 . Using (109) and since the collisions are essentially elastic, from (111),

$$(171) \quad \Omega_{ap}^1(r) = \frac{(2 \cdot 1 \times 10^{-2}) z^4 e^4 \gamma^3 \pi^{1/2}}{2 m_r^2} \Gamma(r)$$

Similarly with $\phi_{ap}(z)$ given by (110), it follows that

$$(172) \quad \Omega_{ap}^2(r) = \frac{(2.1 \times 10^{-2}) 2^8 e^4 a_0^2 \delta}{10 \hbar^2} \Gamma(r+1) \quad .$$

The Differential Cross SectionsA1.1 The Born Approximation

In this Appendix, quantum-mechanical expressions are obtained for the differential cross sections for certain processes involving electrons, hydrogen atoms and protons, which are required to calculate the ϕ 's and Ω 's. A Born type of approximation has been chosen to give analytical expressions for the differential cross section, and a numerical adjustment factor is included which is selected to obtain a "reasonable" approximation to the known total cross sections in the energy range 0 - 100 ev.

Proceeding formally, consider a collision involving atomic particles j and k referred to a frame moving with the centre of mass. Suppose that $\underline{r}_j, \underline{r}_k$ represent the electron position vectors of the particles relative to their respective nuclei (these being zero of course if the particles are electrons), and \underline{r} the inter-nuclear distance, with $V(\underline{r}, \underline{r}_j, \underline{r}_k)$ the interaction potential. $\mathcal{H}_j(\underline{r}_j)$, $\mathcal{H}_k(\underline{r}_k)$ are the internal (unperturbed) Hamiltonians of the two particles, referred to their respective nuclei, \underline{g}_{jk} is the initial asymptotic relative velocity, and $\Psi(\underline{r}, \underline{r}_j, \underline{r}_k)$ is the complete wave function for both particles. The Schrodinger equation for the system is

$$(A1) \left[\frac{\hbar^2}{2m_r} \frac{\partial^2}{\partial \underline{r}^2} - \mathcal{H}_j - \mathcal{H}_k + \frac{1}{2} m_r g_{jk}^2 + E_0 - V \right] \Psi = 0$$

where $m_r = m_j m_k / (m_j + m_k)$ is the reduced mass, and E_0 the unperturbed ground state energy of the system associated with \mathcal{H}_j and \mathcal{H}_k . The term $\frac{1}{2} m_r g_{jk}^2$ is the asymptotic kinetic energy of the system.

Neglecting the possibility of electron exchange, Ψ can be expanded as

$$(A2) \Psi(\underline{r}, \underline{r}_j, \underline{r}_k) = \left(\sum_q + \int \right) \psi_q(\underline{r}_j, \underline{r}_k) F_q(\underline{r})$$

where $\Psi_q(\underline{r}_j, \underline{r}_k)$ is the set of all possible $\phi_q(\underline{r}_j) \phi_q(\underline{r}_k)$ which are eigenfunctions for the particles j and k . $F_q(\underline{r})$ is essentially a scattering function, to be determined by solving the Schrodinger equation. $E_q = E_{q,j} + E_{q,k}$ is the sum of the eigenvalues of the two particles corresponding to the eigenfunctions $\phi_q(\underline{r}_j)$ and $\phi_q(\underline{r}_k)$. The summation is over discrete states and the integration over continuum states. Substituting this expansion in the Schrodinger equation (A1) gives

$$(A3) \left(\sum_q + \int \right) \Psi_q(\underline{r}_j, \underline{r}_k) \left[\frac{\hbar^2}{2m_r} \frac{\partial^2}{\partial \underline{r}^2} + \frac{1}{2} m_r g_{jk}^2 + E_0 - E_q \right] F_q(\underline{r}) = V(\underline{r}, \underline{r}_j, \underline{r}_k) \underline{\Psi}(\underline{r}, \underline{r}_j, \underline{r}_k) .$$

Multiplying (A1) by $\Psi_q^*(\underline{r}_j, \underline{r}_k) d\underline{r}_j d\underline{r}_k$ and integrating, this becomes

$$(A4) \left[\frac{\hbar^2}{2m_r} \frac{\partial^2}{\partial \underline{r}^2} + \frac{1}{2} m_r g_{jk}^2 + E_0 - E_q \right] F_q(\underline{r}) = \int V(\underline{r}, \underline{r}_j, \underline{r}_k) \underline{\Psi}(\underline{r}, \underline{r}_j, \underline{r}_k) \Psi_q^*(\underline{r}_j, \underline{r}_k) d\underline{r}_j d\underline{r}_k .$$

$F_0(\underline{r})$ represents the sum of an incident and a scattered wave, while $F_q(\underline{r})$ ($q \neq 0$) must represent scattered waves only. Hence the respective asymptotic forms can be shown to be (Mott and Massey⁸):

$$(A5) F_0 \sim e^{i\mathbf{k}_0 \cdot \underline{r}} + \frac{1}{r} e^{i\mathbf{k}_f(0) \cdot \underline{r}} f_0(\chi, \epsilon)$$

$$(A6) F_q \sim \frac{1}{r} e^{i\mathbf{k}_f(q) \cdot \underline{r}} f_q(\chi, \epsilon)$$

where \mathbf{k}_0 is the (reduced) incident wave vector such that the reduced momentum \underline{p} , is given by $\hbar \mathbf{k}_0$. Similarly $\mathbf{k}_f(q)$ is the reduced wave vector of the scattered particle for the state q . Then the scattered current density for

the q^{th} state of excitation is

$$(A7) \quad \frac{\hbar \underline{k}_f(q)}{m_r} \left| \frac{1}{r} e^{i \underline{k}_f(q) \cdot \underline{r}} f_q(\chi, \epsilon) \right|^2 = \frac{\hbar \underline{k}_f(q)}{m_r r^2} |f_q(\chi, \epsilon)|^2 .$$

The differential cross section for the deflection of the final wave vector, $\underline{k}_f(q)$, into a solid angle $(\Omega, \Omega + d\Omega)$ with excitation state q is the ratio of the scattered current per unit solid angle about Ω to the incident current density, giving

$$(A8) \quad \sigma_q d\Omega = \frac{k_f}{k_0} |f_q(\chi, \epsilon)|^2 d\Omega .$$

Subject to the plane wave Born approximation,

$$(A9) \quad \underline{\Psi} = e^{i \underline{k}_0 \cdot \underline{r}} \psi_0(\underline{r}_j, \underline{r}_k) .$$

Substituting this expression for $\underline{\Psi}$ in the right hand side of (A4), this equation becomes

$$(A10) \quad \left[\frac{\hbar^2}{2m_r} \frac{\partial^2}{\partial \underline{r}^2} + \frac{\hbar^2 k_f^2(q)}{2m_r} \right] F_q(\underline{r}) \\ = \int V(\underline{r}, \underline{r}_j, \underline{r}_k) e^{i \underline{k}_0 \cdot \underline{r}} \psi_0(\underline{r}_j, \underline{r}_k) \psi_q^*(\underline{r}_j, \underline{r}_k) d\underline{r}_j d\underline{r}_k$$

with asymptotic solution

$$(A11) \quad F_q(\underline{r}) = \frac{1}{r} e^{i \underline{k}_f(q) \cdot \underline{r}} \frac{m_r}{2\pi \hbar^2} \int V e^{i \underline{k} \cdot \underline{r}} \psi_0 \psi_q^* d\underline{r}_j d\underline{r}_k$$

or

$$(A12) \quad f_q(\chi, \epsilon) = \frac{m_r}{2\pi \hbar^2} \int V e^{i \underline{k} \cdot \underline{r}} \psi_0 \psi_q^* d\underline{r}_j d\underline{r}_k d\underline{r} .$$

In these equations, $\underline{K} = \underline{k}_0 - \underline{k}_f(q)$; $k_f^2 = \frac{m r^2 g_{jk}^2}{\hbar^2} + \frac{2 m r (E_0 - E_q)}{\hbar^2}$.

In the case of excitation to the continuum level, Ψ_q is the wave function whose matrix element, taken with the ground state wave function and interaction potential, gives the probability of a particular direction and energy of the atomic electron (as well as the direction and energy of the scattered particle). With the Hamiltonians $\mathcal{H}_j(\underline{r}_j)$, $\mathcal{H}_k(\underline{r}_k)$ of the electrons of the particles j and k referred to their respective centres of mass, the eigenfunctions $\phi_q(\underline{r}_j)$, $\phi_q(\underline{r}_k)$, grouped under the term Ψ_q , therefore relate the continuum state electron parameters to the centre of mass of the particle, say k , from which it was displaced. Consequently the angle and energy of the ejected electron is not referred to the centre of mass of the system j and k , but to particle k . In order to use the differential cross sections in the centre of mass system, it becomes necessary to convert these parameters to this system. Bearing this in mind, the above results give, formally, for ionisation (with \underline{k} the atomic electron wave vector):

$$(A13) \quad \sigma d\Omega_1 d\Omega_2 d\kappa = \frac{k_f}{k_0} \left| f(\chi_1, \epsilon_1, \chi_2, \epsilon_2, \kappa) \right|^2 d\Omega_1 d\Omega_2 d\kappa$$

where the subscripts $1, 2$ refer to the scattered (incident) particle and the atomic (ejected) electron, respectively.

Regarding the frames of reference, the differential cross section as obtained above has to be transformed to the frame moving with the centre of mass of the colliding particles (which will be called the "c. m. frame"). It is also necessary to obtain an expression for the internal energy of the "composite" particle produced in the collision, as noted previously. The types of collisions being considered are those in which one of the colliding particles, say j , is scattered, while the other particle, say k , on collision breaks up into two "sub-particles", r and s . The form (A13) of the differential cross section refers the angle and velocity of to the c. m. frame, but (owing to the reference frame of the Hamiltonians) it refers

the velocities and solid angles of \mathbf{r} and \mathbf{s} to a frame moving with their centre of mass (the " \mathbf{k} " frame). Using \underline{v} , χ and Ω to denote velocities, angles and solid angles in the c.m. frame, and \underline{u} , Θ and ω velocities, angles, and solid angles in the " \mathbf{k} " frame, the problem is to express \underline{u}_r , \underline{u}_s , ω_r and ω_s in terms of Ω and \underline{v} . Clearly,

$$(A14) \quad m_j \underline{v}_j + m_k \underline{v}_k = 0 \quad \text{or} \quad \underline{v}_k = -\frac{m_j}{m_k} \underline{v}_j .$$

Then

$$(A15) \quad \underline{v}_r = \underline{u}_r + \underline{v}_k = \underline{u}_r - \frac{m_j}{m_k} \underline{v}_j ,$$

$$\underline{v}_s = \underline{u}_s - \frac{m_j}{m_k} \underline{v}_j .$$

The azimuthal angle, that is the angle with the plane of the collision, is the same for both frames. Hence the elements of solid angle in the two frames are respectively $d\Omega = \sin \chi d\chi d\epsilon$ and $d\omega = \sin \Theta d\Theta d\epsilon$. Taking components of velocity of (A15) in a cartesian frame gives

$$(A16) \quad v_{rx} = v_r \cos \chi_r = u_r \cos \Theta_r - \frac{m_j}{m_k} v_j \cos \chi_j$$

$$v_{ry} = v_r \sin \chi_r = u_r \sin \Theta_r - \frac{m_j}{m_k} v_j \sin \chi_j .$$

From these relations it follows that

$$(A17) \quad u_r^2 = v_r^2 + \left(\frac{m_j}{m_k}\right)^2 v_j^2 + 2 v_j v_r \frac{m_j}{m_k} \cos(\chi_j - \chi_r)$$

$$(A18) \quad u_s^2 = v_s^2 + \left(\frac{m_j}{m_k}\right)^2 v_j^2 + 2 v_j v_s \frac{m_j}{m_k} \cos(\chi_j - \chi_s)$$

$$(A19) \quad \sin \Theta_r = \frac{v_r \sin \chi_r + (m_j/m_k) v_j \sin \chi_j}{(v_r^2 + (m_j/m_k)^2 v_j^2 + 2 v_r v_j (m_j/m_k) \cos(\chi_j - \chi_r))^{1/2}}$$

$$(A20) \quad \sin \theta_s = \frac{v_s \sin \chi_s + (m_j/m_k) v_j \sin \chi_j}{(v_s^2 + (m_j/m_k)^2 v_j^2 + 2 v_s v_j (m_j/m_k) \cos(\chi_j - \chi_s))^{1/2}} .$$

When j is an electron and k an atom, on neglecting $\frac{m_e}{m_a}$ compared with unity, the c. m. and " k " frames become identical, as would be expected.

The $\Delta \mathcal{E}$ term is discussed in references 1, 2 and 4. Essentially it is the sum of the ionisation energy and the internal kinetic energy of the composite "particle". Suppose of three particles, q , s and t , q and s form a composite "particle", then for this case

$$(A21) \quad \Delta \mathcal{E} = I + \frac{1}{2} \frac{m_q m_s}{m_q + m_s} (\underline{v}_q - \underline{v}_s)^2 .$$

This is given later (in Appendix B) for the particular case of electron-hydrogen atom ionising collisions.

A1.2 The Born Differential Cross Sections

A1.2.1 Elastic Collisions

a. Electron-electron collisions

With the neglect of the electron spin, the classical method, the Born approximation, and the exact partial wave calculation all yield the well known Coulomb collision result for the differential cross section:

$$(A22) \quad \sigma d\Omega = \frac{m_r^2 e^4 \operatorname{cosec}^4 \chi/2}{4 \hbar^4 k_0^4} d\Omega .$$

Since the nature of the collision terms in the moment equations involves treating the colliding particles as distinguishable (when they are identical), it is doubtful whether it would be adequate to take account of exchange effects purely in the differential cross section. Although the energy range 0 - 100 eV is that in which exchange effects make their greatest contribution to the cross sections, they are not considered in this report.

b. Electron-hydrogen atom collisions

Using (A8), (A12) with the ground state wave functions for hydrogen, since the interaction potential is

$$(A23) \quad V = e^2 \left(\frac{1}{r} - \frac{1}{|\underline{r} - \underline{r}_1|} \right)$$

where \underline{r}_1 is the atomic electron position vector with respect to the nucleus, the Born differential cross section is

$$(A24) \quad \sigma d\Omega = \frac{4 a_0^4 m_r^2 e^4 (a_0^2 K^2 + 8)^2}{\hbar^4 (a_0^2 K^2 + 4)^4} d\Omega .$$

In this equation (as defined previously), $K^2 = (\underline{k}_0 - \underline{k}_f)^2 = 2k_0^2(1 - \cos\chi)$.

c. Electron-proton collisions

The Coulomb result applies for this case, the differential cross section being

$$(A25) \quad \sigma d\Omega = \frac{m_r^2 e^4 \operatorname{cosec}^4 \chi/2}{4 \hbar^4 k_0^4} d\Omega .$$

d. Hydrogen atom-hydrogen atom collisions

Using \underline{r}_1 , \underline{r}_2 for the position vectors of the atomic electrons referred to their respective nuclei, and \underline{r} for the internuclear distance, the interaction potential is

$$(A26) \quad V = e^2 \left(-\frac{1}{r} + \frac{1}{|\underline{r} - \underline{r}_1|} + \frac{1}{|\underline{r} + \underline{r}_2|} - \frac{1}{|\underline{r} + \underline{r}_2 - \underline{r}_1|} \right) .$$

The colliding atoms are regarded as distinguishable, in which case, using the ground state wave functions, from (A8) and (A12), the differential cross section for these

collisions is

$$(A27) \quad \sigma d\Omega = \frac{4 m_r^2 e^4 a_0^8 K^4 (a_0^2 K^2 + 8)^4}{\hbar^4 (a_0^2 K^2 + 4)^8} d\Omega .$$

e. Hydrogen atom-proton collisions

Apart from the difference in the reduced masses, these collisions are identical with the electron-hydrogen atom collisions, of case (b). The differential cross section is

$$(A28) \quad \sigma d\Omega = \frac{4 m_r^2 e^4 a_0^4 (a_0^2 K^2 + 8)^2}{\hbar^4 (a_0^2 K^2 + 4)^4} d\Omega .$$

f. Proton-proton collisions

These Coulomb collisions are formally the same as case (a). The differential cross section is therefore

$$(A29) \quad \sigma d\Omega = \frac{m_r^2 e^4 \operatorname{cosec}^4 \chi/2}{4 \hbar^4 k_0^4} d\Omega .$$

A2.2.2 Inelastic Collisions

It is reasonable to suppose that in an inelastic collision with an atom, owing to the screening effect of the atomic electron, atoms will have a smaller cross section than protons. Again, using the Born approximation, an estimate of the relative magnitudes of the cross sections of protons and electrons in inelastic collisions with atoms can be obtained as follows (Bates and Griffing⁹). Let $Q_e(E), Q_p(E)$ be total cross sections for a given electron or proton energy E respectively. Then if $\Delta \mathcal{E}$ is the kinetic energy defect in the collision the Born approximation gives

$$(A30) \quad Q_e(\gamma E) = \frac{1}{8} \left[Q_p(m_p E/m_e) - \left(\frac{\Delta \mathcal{E}}{4E} \right)^2 Q_p(m_p \Delta \mathcal{E}/16 m_e E) \right]$$

where

$$(A31) \quad \gamma = (1 + \Delta E/4E)^2 \sim 1 + \Delta E/2E$$

and m_e , m_p are the electron and proton masses. Very approximately, this gives

$$(A32) \quad Q_p(E) = \gamma Q_e(\gamma m_e E/m_p).$$

According to (A32), then, the proton-atom cross section for a given incident energy is of the same order as the electron-atom cross section for an incident energy m_e/m_p of the proton energy. Since for low energies the electron cross section is small, the proton-atom cross section (and the atom-atom cross section also) will be very small in the energy range 0 - 100 ev. It is reasonable, therefore, to neglect protons and atoms as inelastic collision projectiles for the calculations of the report.

a. Electron-hydrogen atom 1s-2p excitation collisions

The only excitation process that will be considered is 1s-2p excitation, this process having a much larger total cross section than that to any other level from the ground state. The interaction potential is given in (A23). Using the ground state hydrogen atom wave function and the $2p(m=0)$ wave function in (A11) to calculate $f(1s-2p)$, from (A8) the differential cross section is

$$(A33) \quad \sigma d\Omega = \frac{k_f 3^2 2^{15} m_r^2 a_0^2}{k_0 \hbar^4 K^2 (9 + 4 a_0^2 K^2)^6} d\Omega.$$

b. Electron-hydrogen atom ionising collisions

For these collisions, using the exact continuum wave function (Mott and Massey,⁸ p 233) in the calculation of the Born approximation for the differential cross section leads to an exceedingly complicated expression. Let $d\Omega_1$ be the solid angle into which the incoming electron is scattered; $d\Omega_2$ the solid angle into which the atomic electron is ejected with wave vector \mathbf{k} ; and

$\underline{k} = \underline{k}_o - \underline{k}_f$, \underline{k}_o , \underline{k}_f being initial and final wave vectors of the incident electron, as before. Then the differential cross section for this collision is

$$(A34) \quad \sigma d\Omega_1 d\Omega_2 d\kappa = \frac{2^8 m_f^2 a_o^4 e^4 k_f \kappa e^{-\frac{2}{\kappa a_o} \tan^{-1} \left(\frac{2 \kappa a_o}{1 + a_o^2 (K^2 - \kappa^2)} \right)}}{4 \pi^2 \hbar^4 \pi k_o K^2 (a_o^2 (K^2 + \kappa^2 - 2 K \kappa \cos \delta) + 1)^4} \\ \times \frac{(a_o^2 (K - \kappa \cos \delta)^2 + \cos^2 \delta) d\Omega_1 d\Omega_2 d\kappa}{(1 - e^{-\frac{2\pi}{\kappa a_o}}) ((1 - \kappa^2 a_o^2 + K^2 a_o^2)^2 + 4 \kappa^2 a_o^2)} .$$

In this equation, δ is the angle between K and κ . $d\Omega_1$ and κ are in fact referred to a frame moving with the centre of mass of the atom after the collision, but it is apparent from equations (A17) to (A20) that the error involved in taking these variables as referred to the c. m. for the collision is only of order m_e/m_a .

However, it is obvious that this expression (A34) is unsuitable for calculation of the ϕ 's and Ω 's, where successive integrations over functions involving the differential cross section are necessary. Even when this differential cross section is averaged over the solid angle of ejection of the atomic electron, the resulting expression is too complicated to be used in evaluating the Ω 's.

The problem may, however, be approached in a simpler way. The main reason for the complicated form of (A34) is the complex nature of the continuum wave function for the hydrogen atomic electron. It is therefore reasonable to consider replacing it by a plane wave function, in a similar manner to that in which the relevant Born approximation was obtained by using a plane wave (A9) in equation (A10). Such a plane wave is

$$(A35) \quad \phi_i = e^{i \underline{\kappa} \cdot \underline{r}_i} ,$$

\underline{r}_i being the position vector of the atomic electron relative to the c. m. (But, similarly to the Born approximation being valid for large energies of the incident electron, so this approximation is actually valid only for high energies of the ejected electron.)

The appropriate normalising factor is not entirely clear, but to obtain the correct form of the differential cross section, $\phi_i \phi_i^* d\mathbf{k}$ should represent a probability density of particles with wave numbers \mathbf{k} in the range $(\mathbf{k}, \mathbf{k} + d\mathbf{k})$, and so have dimensions (volume)⁻¹. A comparison of the final form obtained, using this wave function, with (A34), obtained by using the correct wave function, suggests that the correct form for ϕ_i is

$$(A36) \quad \phi_i = (\mathbf{k}/a_0)^{1/2} e^{i\mathbf{k}\cdot\mathbf{r}_i}.$$

The use of an adjusting factor with the total cross section obtained using this wave function will mean that the neglect of numerical factors is of no consequence. With (A36) for the final wave function and the normal ground state hydrogen wave function as the initial wave function, the Born approximation, equation (A13), may be used to calculate $f(\mathbf{k})$. From (A8) the differential cross section is found to be

$$(A37) \quad \sigma d\Omega_1 d\Omega_2 d\mathbf{k} = \frac{2^6 \pi a_0^2 m_r^2 e^4 k_f \mathbf{k} d\Omega_1 d\Omega_2 d\mathbf{k}}{\hbar^4 k_0 K^4 (a_0^2 (K^2 - \mathbf{k}^2) + 1)^4}.$$

In general, $|\underline{K}| \gg |\underline{k}|$ and therefore it is convenient to simplify (A37) to

$$(A38) \quad \sigma d\Omega_1 d\Omega_2 d\mathbf{k} = \frac{2^6 \pi a_0^2 m_r^2 e^4 k_f \mathbf{k} d\Omega_1 d\Omega_2 d\mathbf{k}}{\hbar^4 k_0 K^4 (a_0^2 K^2 + 1)^4}.$$

Again, since $\hbar^2 \mathbf{k}^2 = 2m_r E_{\mathbf{k}}$, (A37) is easily rearranged to give the probability of ejection of the atomic electron in the energy range $(E_{\mathbf{k}}, E_{\mathbf{k}} + dE_{\mathbf{k}})$.

c. Proton-hydrogen atom charge exchange collisions

Resonant charge exchange, where the electron energy relative to the nucleus is the same for the final "atoms" as for the initial "atoms", is in general the only type of charge exchange collision with an appreciable cross

section. This can occur between hydrogen atoms and protons. It has been shown (Bates¹⁰) that the correct interaction potential for such collisions is not the simple "post" or "prior" interaction (identical for the symmetrical proton hydrogen atom system), but a much more complicated function. Furthermore, in calculating the collision cross section, account should be taken of the change in translational motion of the electron that accompanies the jump between the nuclei. However, in order to achieve reasonable analytical expressions, both of these considerations will be ignored, it being assumed that the inclusion of a numerical adjustment factor will bring the Born calculation under these simplifications to an acceptable approximation for this process.

The "prior" interaction potential is

$$(A39) \quad V = e^2 \left(\frac{1}{|\underline{r} + \underline{r}_1|} - \frac{1}{r} \right)$$

where \underline{r} is the internuclear separation, and \underline{r}_1 the position vector of the electron relative to the nucleus that it has before collision. The Born approximation for this case gives

$$(A40) \quad f = \frac{m_r}{2\pi \hbar^2} \int V e^{i\underline{k} \cdot \underline{r}} \psi_0(\underline{r}_1) \psi_f^*(\underline{r}_1) d\underline{r} d\underline{r}_1,$$

but, somewhat differently from the previous cases, \underline{k}_0 is the (reduced) wave vector of the incident nucleus, \underline{k}_f the wave vector of the "scattered" nucleus; ψ_0 , ψ_f are the wave functions of the electron in the initial and final atoms; and also

$$(A41) \quad \underline{K} = \underline{k}_0 + \underline{k}_f ; \quad K^2 = 2 k_0^2 (1 + \cos \chi).$$

Using ground state hydrogen atom wave functions for ψ_0 , ψ_f to obtain f , the differential cross section follows from (A8):

$$(A42) \quad \sigma \, d\Omega = \frac{2^8 m_r^2 e^4 a_0^4}{\hbar^4 (a_0^2 K^2 + 1)^6} d\Omega \quad .$$

A1.3 The Total Cross Sections

In this section, the expressions obtained for the differential cross sections in the previous section are integrated over the scattering angles to obtain the total collision cross sections as a function of incident energy and other parameters. These total cross sections are compared with experimental results or exact numerical calculations to give a numerical adjustment factor. This factor is used to bring the "Born" approximations into reasonable agreement with the probable cross sections in a region for which the plane wave assumption is entirely inadequate. However since the energy range of interest is limited, the approximations are considered sufficient to be used in the calculations of the Ω 's to obtain an estimate of the collision terms in the moment equations for the formation of a plasma. As discussed previously, it is likely that certain classical approximations better describe the non-Coulomb elastic collisions involved.

A1.3.1 Elastic Collisions

- a. Coulomb collisions (electron-electron, electron-proton proton-proton)

With Coulomb collisions the integral of the differential cross section diverges. For this reason the well known Debye cut-off is introduced, the Debye length representing a distance from a particle beyond which the electrostatic shielding of the other particles is "complete". Usually put forward as an upper limit on an impact parameter, it may equally well be expressed as a minimum angle of deflection in a collision.

Since the details of Coulomb collisions are discussed in many books, only the bare facts need be given. In terms of an impact parameter b , the scattering angle χ is

$$(A43) \quad \chi = 2 \sin^{-1} \left(1 / (1 + \Lambda^2)^{1/2} \right)$$

where

$$(A44) \quad \Lambda = m_r b g^2 / e^2 .$$

The Debye length, λ_D , being

$$(A45) \quad \lambda_D = \left(\frac{k T_e}{4 \pi n_e e^2} \right)^{1/2} ,$$

it follows at once that the minimum deflection χ_0 is given by (A43) on taking $\Lambda = \Lambda_{jk}$ where

$$(A46) \quad \Lambda_{jk} = \lambda_D m_r g_{jk}^2 / e^2 = \left(\frac{k T_e}{4 \pi n_e e^2} \right)^{1/2} m_r g_{jk}^2 / e^2 .$$

The total cross section, in terms of χ_0 , is

$$(A47) \quad \sigma_T = \frac{2 \pi m_r^2 e^4}{4 \hbar^4 k_0^4} \left(\frac{8}{\chi_0^2} \right) .$$

No correction factors are required for this well known result.

b. Electron-hydrogen atom collisions

Since $K^2 = 2 k_0^2 (1 - \cos \chi)$, on differentiating,

$$(A48) \quad K dK = k_0^2 \sin \chi d\chi .$$

The upper and lower limits of integration over K become $2k_0$ and 0 . Using the differential cross section (A24), with the substitution (A48) the total cross section is

$$\begin{aligned}
 \text{(A49)} \quad \sigma_T &= \int_0^{2k_0} \int_0^{2\pi} \frac{4a_0^4 m_r^2 e^4 (a_0^2 K^2 + 8)^2 K dK d\epsilon}{\hbar^4 k_0^2 (a_0^2 K^2 + 4)^4} \\
 &= \frac{\pi m_r^2 e^4 a_0^2 (7k_0^6 a_0^6 + 18k_0^4 a_0^4 + 12k_0^2 a_0^2)}{3\hbar^4 k_0^2 (1 + a_0^2 k_0^2)^3} .
 \end{aligned}$$

c. Hydrogen atom-hydrogen atom collisions

Using (A48) in the differential cross section (A27), the application of standard integrals gives the total cross section:

$$\begin{aligned}
 \text{(A50)} \quad \sigma_T &= \frac{8\pi m_r^2 e^4 a_0^2}{\hbar^4 k_0^2 (1 + a_0^2 k_0^2)^7} \left(\frac{33}{140} k_0^{14} a_0^{14} + \frac{7}{5} k_0^{12} a_0^{12} + \frac{16}{5} k_0^{10} a_0^{10} \right. \\
 &\quad \left. + \frac{10}{3} k_0^8 a_0^8 + \frac{4}{3} k_0^6 a_0^6 \right) .
 \end{aligned}$$

d. Hydrogen atom-proton collisions

This is algebraically the same result as for electron-hydrogen atom collisions:

$$\text{(A51)} \quad \sigma_T = \frac{\pi m_r^2 e^4 a_0^2 (7k_0^6 a_0^6 + 18k_0^4 a_0^4 + 12k_0^2 a_0^2)}{3\hbar^4 k_0^2 (1 + k_0^2 a_0^2)^3} .$$

A1.3.2 Inelastic Collisions

Since

$$\text{(A52)} \quad K^2 = k_0^2 + k_f^2 - 2k_0 k_f \cos \chi ,$$

differentiation yields

$$\text{(A53)} \quad K dK = k_0 k_f \sin \chi d\chi .$$

The limits of integration with respect to K are $k_0 \pm k_f$; from the energy equation for the type of collision being considered,

$$(A54) \quad k_0^2 = k_f^2 + \frac{2 m_r \Delta \mathcal{E}}{\hbar^2}$$

giving

$$(A55) \quad k_f = \left(k_0^2 - \frac{2 m_r \Delta \mathcal{E}}{\hbar^2} \right)^{1/2} \sim k_0 \left(1 - \frac{m_r \Delta \mathcal{E}}{\hbar^2 k_0^2} \right),$$

where $\Delta \mathcal{E}$ is the energy transferred inelastically to the atom. The upper and lower limits of K are taken as $2 k_0$ and $m_r \Delta \mathcal{E} / \hbar^2 k_0$, respectively. The approximate limits cannot be expected to be reasonable near the threshold energy, and they are therefore "over-ruled" in this region by taking $\sigma_T = 0$ at threshold.

a. Electron-hydrogen atom 1s-2p excitation

For these collisions $\Delta \mathcal{E}$ is the (discrete) excitation energy (10.2 eV). From (A33) and using (A53) the total cross section is

$$(A56) \quad \sigma_T = \int_{\frac{m_r \Delta \mathcal{E}}{\hbar^2 k_0}}^{2 k_0} \int_0^{2\pi} \frac{k_f m_r^2 e^4 3^2 2^{15} a_0^2 K dK}{k_f k_0^2 \hbar^4 K^2 (9 + 4 K^2 a_0^2)^6} \\ \sim \frac{2^{17} \pi m_r^2 e^4 a_0^2}{9^5 \hbar^4 k_0^2} \log \frac{3 \hbar^2 k_0}{a_0 m_r \Delta \mathcal{E}}$$

for sufficiently large k_0 .

b. Electron-hydrogen atom ionisation collisions

With ionisation collisions, in equation (A54), $\Delta \mathcal{E}$ becomes

$$(A57) \quad \Delta \mathcal{E} = I + \hbar^2 k^2 / 2 m_e$$

where m_e is the mass of the ejected electron, and I is the ionisation energy. For this case the upper and lower limits on K are more conveniently written as $2k_0$ and $(Im_r/\hbar^2 k_0 + \mathcal{K}^2/2k_0)$. The limits of integration over χ are 0 and $(k_0^2 - \frac{2mI}{\hbar^2})^{1/2} \equiv \alpha$. From (A38) and using (A53) the total cross section is given by

$$(A58) \quad \sigma_T = \int_0^\alpha \int_{k_0 - k_f}^{k_0 + k_f} \int_0^{2\pi} \frac{k_f K m_r^2 e^4 2^6 \pi a_0^2 \mathcal{K} d\mathcal{K} d\epsilon d\Omega_2}{k_f \hbar^4 k_0^2 K^4 (a_0^2 K^2 + 1)^4}$$

where $d\Omega_2$ is the solid angle of the ejected electron. With k_0 sufficiently large,

$$(A59) \quad (k_0 + k_f)a_0 \sim 2k_0 a_0 - \frac{a_0}{k_0} \left(\frac{m_e I}{\hbar^2} + \frac{\mathcal{K}^2}{2} \right) \gg 1 ;$$

$$(k_0 - k_f)a_0 \sim \frac{a_0}{k_0} \left(\frac{m_e I}{\hbar^2} + \frac{\mathcal{K}^2}{2} \right) \ll 1 .$$

Using these approximations (invalid near threshold), the result is

$$(A60) \quad \sigma_T = \frac{m_e^2 e^4 2^9 \pi^3 a_0^2}{\hbar^4} \left(\hbar^2/2m_e I - 1/k_0^2 \right)$$

(since, on neglecting the term m_e/m_a compared with unity, the reduced mass, m_r , is equal to the electron mass, m_e).

c. Charge exchange collisions

As discussed earlier for this case, K^2 is given by

$2k_0^2(1 + \cos\chi)$ and therefore

$$(A61) \quad \sin\chi d\chi = -K dK / k_0^2 .$$

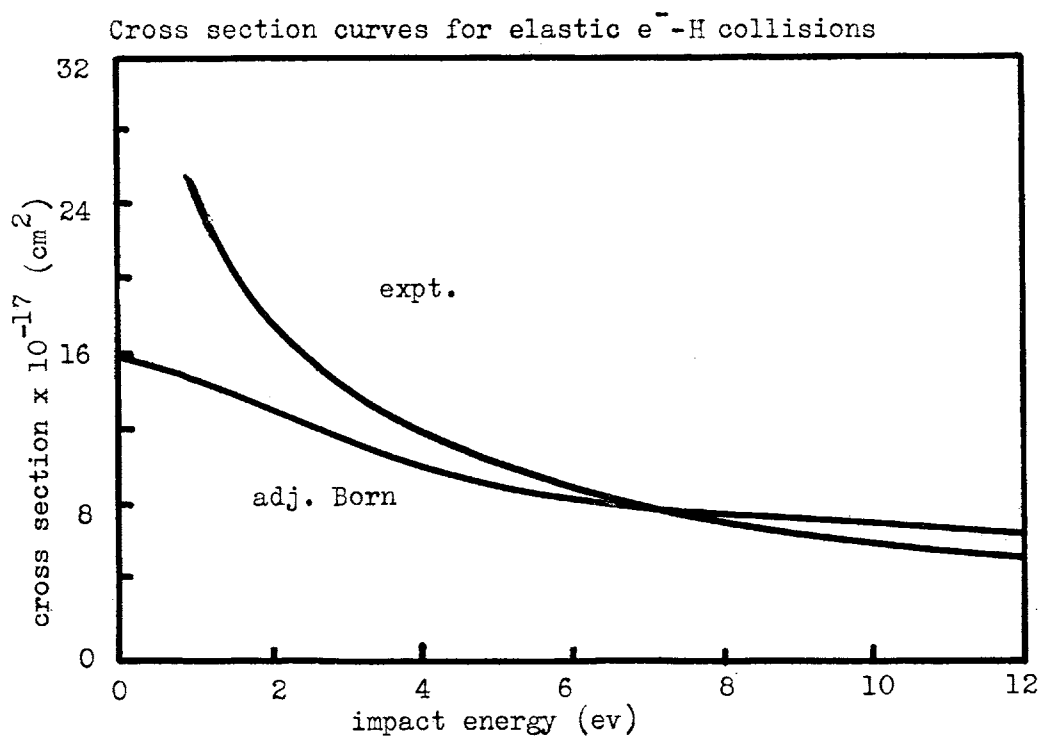
This collision being effectively elastic, using this relation in (A42) and integrating over K with limits 0, $2k_0$ gives the total cross section. For k_0 large (owing to the large reduced mass in this collision), the result is

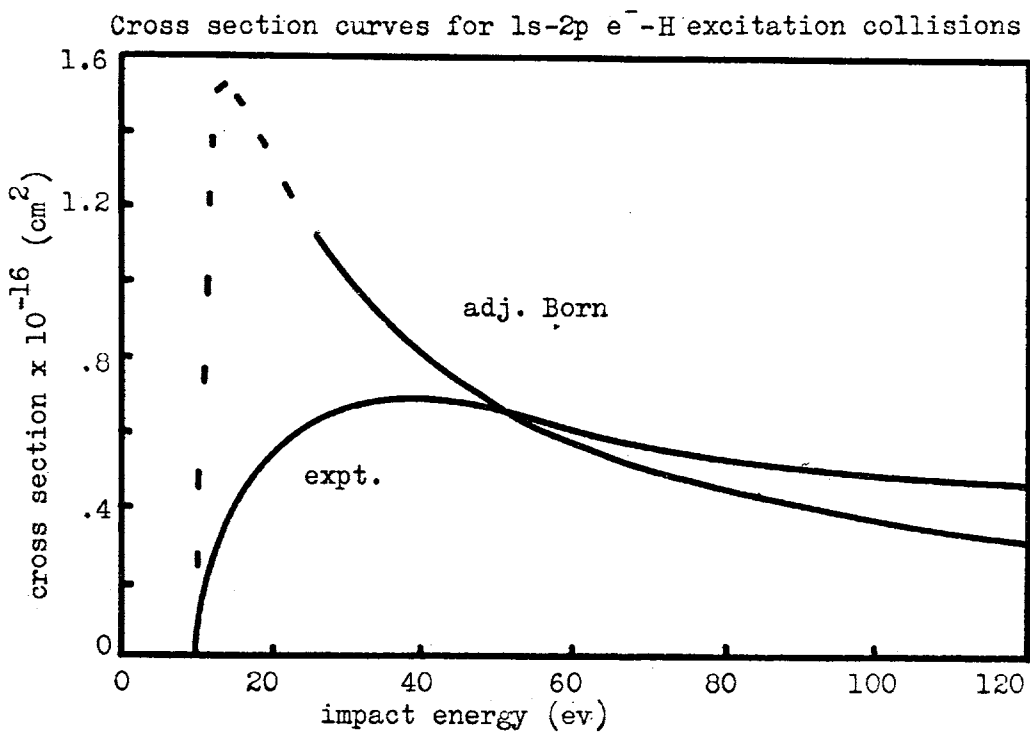
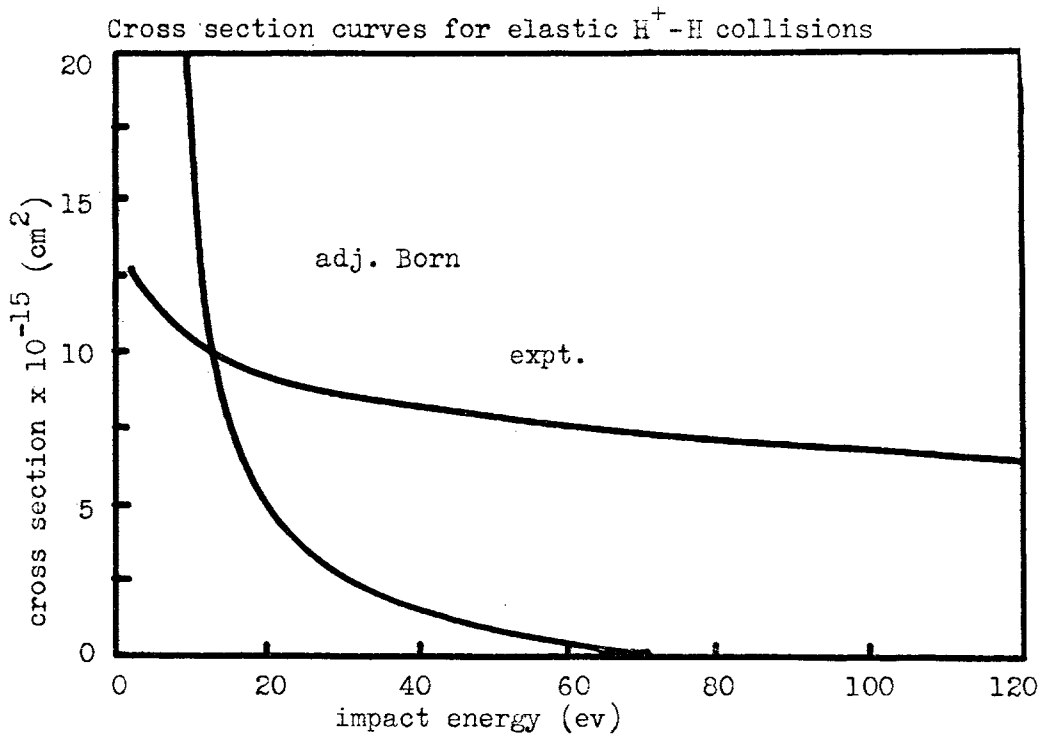
$$(A62) \quad \sigma_T = \frac{\pi m_r^2 e^4 2^9 a_0^2}{5 \hbar^4 k_0^2}$$

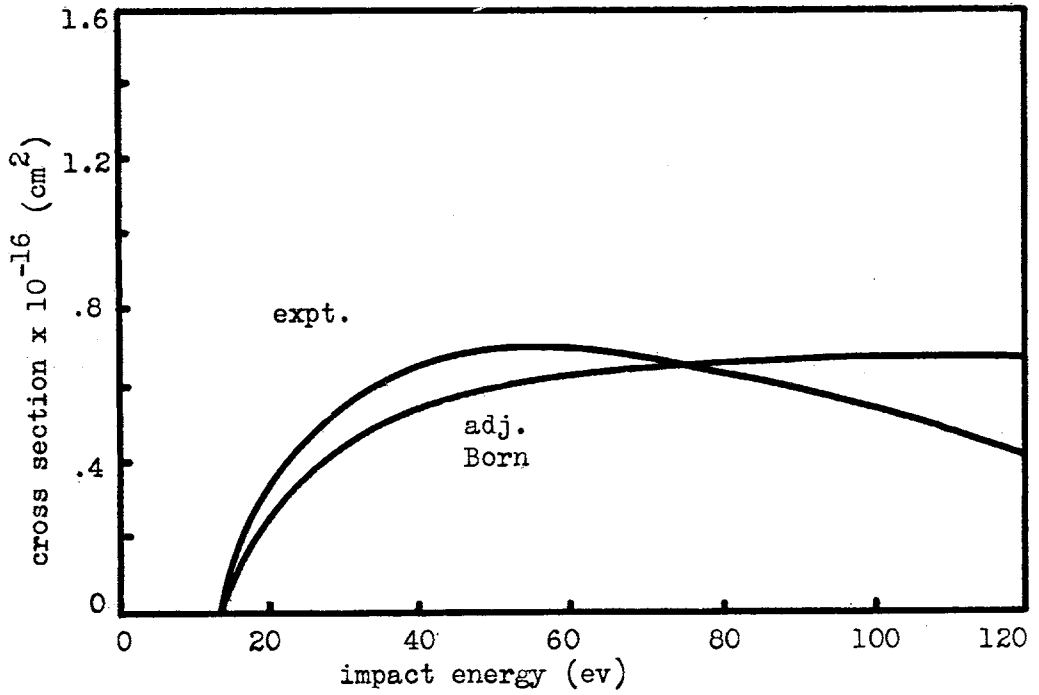
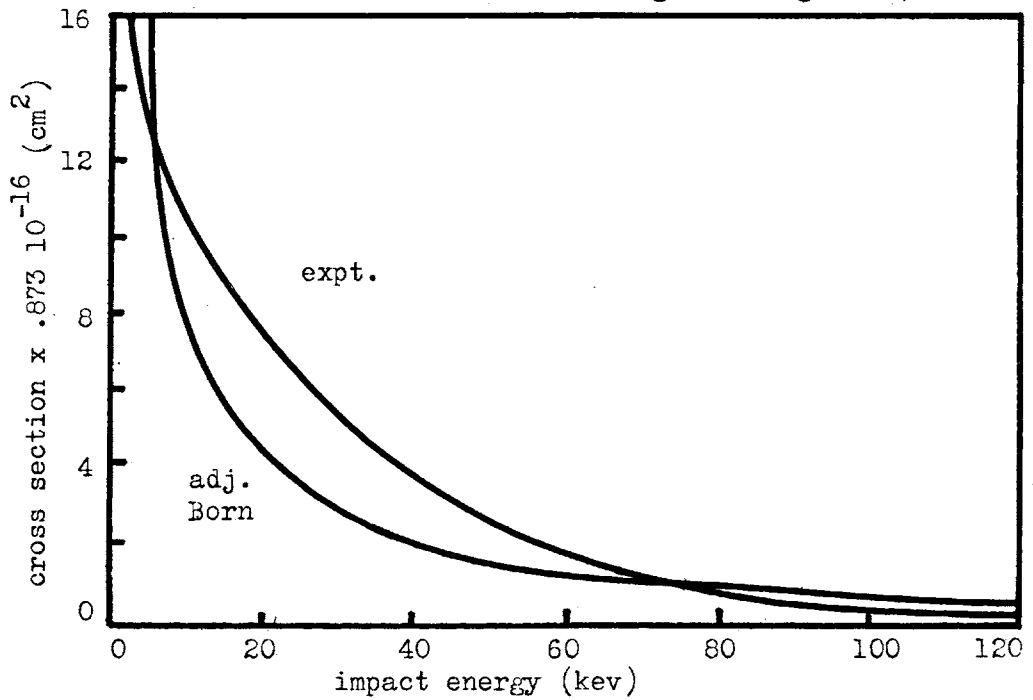
A1.3.3 Comparison with Known Values of Cross Sections

Since the Coulomb calculations are exact (apart from neglect of exchange) these are not discussed. For all of the other cases considered except elastic hydrogen atom-hydrogen atom collisions (for which no data appears to be available, perhaps owing to the problem of recombination to form molecular hydrogen), curves showing a comparison of numerically adjusted Born-type total cross sections with known values are given. Most of the "known" data is taken from Barnett, Ray and Thompson.¹¹ The charge exchange cross sections are from Bates.¹²

The numerical factors which the calculated Born-type total cross sections have been multiplied by to give the results in the figures are as follows:





Cross section curves for e^- -H ionisation collisionsCross section curves for H^+ -H charge exchange collisions

- a. Electron-hydrogen atom elastic collisions.
Born calculation multiplied by 0.45.
- b. Hydrogen atom-proton elastic collisions.
Born calculation multiplied by 2.0×10^{-2} .
- c. Hydrogen atom-hydrogen atom elastic collisions.
No comparison with "known" results being possible,
the same factor as with (b) above is taken: 2.0×10^{-2} .
- d. Electron-hydrogen atom 1s-2p excitation.
Born calculation multiplied by 0.45.
- e. Electron-hydrogen atom ionisation.
Born calculation (simplified) multiplied by 0.14×10^{-3} .
- f. Hydrogen atom-proton charge exchange.
Born calculation (simplified) multiplied by 2.1×10^{-2} .

Subsidiary Relations for Electron-Hydrogen
Atom Ionisation Collisions

B1. The λ 's and $\Delta \mathcal{E}$'s

In considering the dynamics of inelastic binary collisions, the λ 's are defined by

$$(B1) \quad \lambda^2 = m_j m_k / m_{j'} m_{k'} - 2 m_0 \Delta \mathcal{E} / m_{j'} m_{k'} g^2$$

where $\Delta \mathcal{E}$ is the apparent kinetic energy loss in the collision. For an ionisation collision for example, $\Delta \mathcal{E}$ is the sum of the ionisation energy and the change in internal energy of the particles j' , k' compared with j , k . With the particular ionisation collisions being considered, considerable simplification is achieved by neglecting terms of order m_e/m_a compared with unity; it has been shown in Appendix A that this permits the frame of reference for all differential cross section parameters to be taken as the c.m. frame. This is not necessarily so for the "composite" particle internal energies, however.

a. The incident electron, e_1

For the collision dynamics of this particle, the two "particles" after the collision are the incident (and scattered) electron, and the proton + atomic electron system. The apparent energy loss in the collision, $\Delta \mathcal{E}$, is, quite simply,

$$(B2) \quad \Delta \mathcal{E} = I + \hbar^2 \mathcal{K}^2 / 2 m_r .$$

The last term in (B2) being the internal kinetic energy of the proton + electron system; as before \mathcal{K} is the wave vector of the atomic electron, and m_e/m_a is neglected compared with unity. I is the ionisation energy. Using (B1), λ is given by

$$(B3) \quad \lambda^2 = 1 - (2I + \hbar^2 \mathcal{K}^2 / m_r) / m_r g^2 .$$

b. The Atomic Electron, e_2

Corresponding to this particle being one of the particles after the collision, the remaining "particle" is the system proton + incident electron. In the c. m. system, this latter "particle" has internal energy $\hbar^2 k_0^2 / 2m_r$ (neglecting terms of order m_e / m_a). The apparent energy loss is therefore

$$(B4) \quad \Delta \mathcal{E} = I + \hbar^2 k_f^2 / 2m_r .$$

From this it follows that

$$(B5) \quad \lambda^2 = 1 - (2I + \hbar^2 k_f^2 / m_r) / m_r g^2 .$$

c. The Proton, p

The composite "particle" after this collision is the system of the two electrons. In the c. m. system, the respective velocities of the scattered and atomic electrons are $\hbar \underline{k}_f / m_e$ and $\hbar \underline{k} / m_e$. The internal kinetic energy relative to their centre of mass is therefore $\frac{m_e}{4} (\hbar / m_e)^2 (\underline{k}_f - \underline{k})^2$, and so

$$(B6) \quad \Delta \mathcal{E} = I + \frac{\hbar^2}{4m_e} (\underline{k}_f - \underline{k})^2 .$$

Therefore

$$(B7) \quad \lambda^2 = 1 - 2 \left(I + \frac{\hbar^2}{4m_e} (k_f^2 + k^2 - 2\underline{k}_f \cdot \underline{k}) \right) / m_r g^2 .$$

In general, away from threshold $|\underline{k}| \ll |\underline{k}_f|$, and so in this region it is possible to write

$$(B8) \quad \lambda^2 = 1 - 2 \left(I + \frac{\hbar^2 k_f^2}{4m_e} \right) / m_r g^2 .$$

d. The atom, a

This particle is not present after the collision, and therefore, using the δ -functions defined in refs. 1, 2, it may be verified that the collision integrals for the atoms only involve $\Omega^{-\infty,0}(r)$. Since by definition these Ω 's are independent of λ , they are also independent of ΔE . The ΔE , however, are implicit in the integration of the differential cross section over all possible energies of the ejected electron in the calculation of the Ω 's for this case.

It is worthwhile noting that, with the neglect of terms of order m_e / m_a , there is a simple relationship between the Ω 's for the atoms and those for the protons in an ionisation collision. This may be seen by considering the δ -functions (refs. 1, 2) and neglecting all terms of order m_e / m_a . It can also be seen in another simple way. Neglect of terms involving the electron mass is equivalent to regarding the collision as an event which strips the electron from the atom, forming a proton with the same mass and velocity as that of the atom before the collision. In the notation of reference 2, this means that

$$(B9) \quad \Delta_{ea}(\psi_p) = \psi_p' = -\psi_a.$$

Since only the $\Omega^{-\infty,0}(r)$ are involved, it follows that (the δ -functions containing the sign relevant to (B9)):

$$(B10) \quad \Omega_{ea,p}^{-\infty,0}(r) = \Omega_{ea,a}^{-\infty,0}(r).$$

B2. Integrals Occurring in the Calculation of the ϕ 's and Ω 's

a. The Integral $J_1(\mu, \nu)$

Consider

$$(B11) \quad J_1(\mu, \nu) = \int_0^\pi \int_0^{\left(k_0^2 - 2m_r I / \hbar^2\right)^{1/2}} \frac{(1 - \lambda^{2\nu} \cos^2 \chi) k_f k \sin \chi \, d\chi \, dk}{(k_0^2 + k_f^2 - 2k_0 k_f \cos \chi)^2},$$

with

$$(B12) \quad \lambda^2 = 1 - 2\left(I + \frac{\hbar^2 k^2}{2m_e}\right) m_r / \hbar^2 k_0^2.$$

This integral (B11) occurs for the case of an ionisation collision where the particle being considered is the incident (and scattered) electron. Conservation of energy in the collision gives

$$(B13) \quad \frac{\hbar^2 k_0^2}{2m_r} = I + \frac{\hbar^2 k_f^2}{2m_r} + \frac{\hbar^2 k^2}{2m_r}$$

and since $m_e \sim m_r$ the reduced mass for the collision, it follows from (B11) that

$$(B14) \quad \lambda^2 = k_f^2 / k_0^2.$$

The following values of $J_1(\mu, \nu)$ are required: $(-\infty, 0)$, $(1, 1)$, $(2, 2)$, $(2, 0)$, $(3, 1)$.

i. Integration over χ

In equation (B11), integration over χ is readily effected with the use of a substitution of the form $x = \cos \chi$. This gives

$$(B15) \quad J_1(\mu, \nu) = \int_0^{\left(k_0^2 - 2m_r I / \hbar^2\right)^{1/2}} \left(2 / (k_0^2 - k_f^2)^2 - \lambda^{2\nu} I(\nu)\right) k_f k \, dk$$

where

$$(B16) \quad I(0) = 2 / (k_0^2 - k_f^2)^2$$

$$(B17) \quad I(1) = \frac{1}{4 k_0^2 k_f^2} \left(2 \log \frac{k_0^2 - k_f^2}{k_0^2 + k_f^2} + 4 k_0 k_f \frac{(k_0^2 + k_f^2)}{(k_0^2 - k_f^2)^2} \right)$$

$$(B18) \quad I(2) = \frac{2}{4 k_0^2 k_f^2} \left(1 + \left(\frac{k_0^2 + k_f^2}{k_0^2 - k_f^2} \right)^2 + \frac{k_0^2 + k_f^2}{k_0 k_f} \log \frac{k_0^2 - k_f^2}{k_0^2 + k_f^2} \right).$$

Ignoring the logarithm term and, in addition, retaining only the terms which are largest away from the threshold, these formulae are represented by

$$(B19) \quad I(\nu) = \frac{2 (k_0^2 + k_f^2)^\nu}{(k_0^2 - k_f^2)^2 (2 k_0 k_f)^\nu}.$$

Accordingly, $J_1(\mu, \nu)$ becomes

$$(B20) \quad J_1(\mu, \nu) = \int_0^{\left(k_0^2 - 2m_r I / \hbar^2 \right)^{1/2}} \frac{2}{(k_0^2 - k_f^2)^2} \left(1 - \lambda^\mu \frac{(k_0^2 + k_f^2)^\nu}{(2 k_0 k_f)^\nu} \right) k k_f dk.$$

ii. Integration over k

Using α as defined previously, i.e.

$$(B21) \quad \alpha^2 = k_0^2 - 2m_r I / \hbar^2,$$

k_f and λ are

$$(B22) \quad k_f^2 = \alpha^2 - k^2$$

$$\lambda^2 = (\alpha^2 - k^2) / k_0^2.$$

From equation (B20), $J_1(\mu, \nu)$ can be written as

$$(B23) \quad J_1(\mu, \nu) = P(\mu, \nu) - Q(\mu, \nu)$$

where

$$(B24) \quad P(\mu, \nu) = \int_0^\alpha \frac{2 k_f k dk}{(k_o^2 - k_f^2)^2}$$

$$(B25) \quad Q(\mu, \nu) = \int_0^\alpha \frac{2 k_f k dk}{(k_o^2 - k_f^2)^2} \lambda^\mu \frac{(k_o^2 + k_f^2)^\nu}{(2 k_o k_f)^\nu} .$$

In general, for ionisation collisions of this type, the atomic electrons are ejected with low energy. In view of this, the error introduced by replacing the terms

$$(B26) \quad (k_o^2 - k_f^2)^2 = (k^2 + 2 m_r I / \hbar^2)^2$$

in the denominator by $(2 m_r I / \hbar^2)^2$ is not unduly large. This simplification gives

$$(B27) \quad P(\mu, \nu) = \int_0^\alpha \frac{2 (\alpha^2 - k^2)^{1/2} k dk}{(2 m_r I / \hbar^2)^2} = \frac{2 \alpha^3}{3 (2 m_r I / \hbar^2)^2} .$$

Again, in calculating $Q(\mu, \nu)$, in the term involving $(k_o^2 + k_f^2)$, k^2 is neglected so that

$$(B28) \quad \begin{aligned} k_o^2 + k_f^2 &= 2 k_o^2 - 2 m_r I / \hbar^2 - k^2 \\ &\sim 2 k_o^2 - 2 m_r I / \hbar^2 \\ &= k_o^2 + \alpha^2 . \end{aligned}$$

In this case,

$$(B29) \quad Q(\mu, \nu) = \frac{2 (k_o^2 + \alpha^2)^\nu}{(2 m_r I / \hbar^2)^2 2^\nu k_o^{\mu+\nu}} \int_0^\alpha (\alpha^2 - k^2)^{\frac{\mu-\nu+1}{2}} k dk ,$$

$$= \frac{2 (k_0^2 + \alpha^2)^\nu}{(2m_r I / \hbar^2)^2 2^\nu k_0^{\mu+\nu}} S(\mu, \nu)$$

where the $S(\mu, \nu)$ are given by

$$(B30) \quad S(-\infty, 0) = 0$$

$$S(1, 1) = S(2, 2) = \alpha^3 / 3$$

$$S(3, 1) = S(2, 0) = \alpha^5 / 5 .$$

Finally, therefore,

$$(B31) \quad J_1(-\infty, 0) = \frac{2 \alpha^3}{3 (2m_r I / \hbar^2)^2}$$

$$(B32) \quad J_1(1, 1) = \frac{2 \alpha^3}{3 (2m_r I / \hbar^2)^2} \left(1 - \frac{(k_0^2 + \alpha^2)}{2 k_0^2} \right)$$

$$(B33) \quad J_1(2, 2) = \frac{2 \alpha^3}{3 (2m_r I / \hbar^2)^2} \left(1 - \frac{(k_0^2 + \alpha^2)^2}{4 k_0^4} \right)$$

$$(B34) \quad J_1(2, 0) = \frac{2 \alpha^3}{3 (2m_r I / \hbar^2)^2} \left(1 - \frac{3 \alpha^2}{5 k_0^2} \right)$$

$$(B35) \quad J_1(3, 1) = \frac{2 \alpha^3}{3 (2m_r I / \hbar^2)^2} \left(1 - \frac{3 \alpha^2 (k_0^2 + \alpha^2)}{10 k_0^4} \right) .$$

b. The Integral $L(\mu, \nu)$

Consider

$$(B36) \quad L(\mu, \nu) = \int_0^{(k_0^2 - 2m_r I / \hbar^2)^{1/2}} \frac{k_f k dk}{(2m_r I / \hbar^2 + k^2)^2} \left(2 - \lambda^\mu \frac{(1 + (-1)^\nu)}{\nu + 1} \right) .$$

This integral arises when the particle being considered is the ejected atomic electron. For this case,

$$(B37) \quad \lambda^2 = 1 - (k_0^2 - \kappa^2)/k_0^2, \quad ,$$

the notation being as previously used in this section. (B36) is conveniently separated into two parts, the first being independent of (μ, ν) . Taking

$$(B38) \quad L(\mu, \nu) = W + X(\mu, \nu),$$

$$(B39) \quad W = 2 \int_0^\alpha \frac{\kappa (\alpha^2 - \kappa^2)^{1/2} d\kappa}{(2m_r \bar{I}/\hbar^2 + \kappa^2)^2},$$

with α as in (B21). Although it is possible to evaluate the integral in this form (B39), usable expressions for calculating the Ω 's are only obtained if the denominator is replaced by $(2m_r \bar{I}/\hbar^2)^2$ as in earlier integrals of this section. With this substitution, W is easily obtained:

$$(B40) \quad W = \frac{2\alpha^3}{3(2m_r \bar{I}/\hbar^2)^2}.$$

The second part of integral (B36), with (B38) and using (B37), is

$$(B41) \quad X(\mu, \nu) = - \int_0^\alpha \frac{\lambda^\mu (1 + (-1)^\nu) k_f \kappa d\kappa}{(\nu + 1)(2m_r \bar{I}/\hbar^2)^2} \\ \sim - \int_0^\alpha \left(1 - \frac{k_0^2 - \kappa^2}{k_0^2}\right)^{\mu/2} \frac{(1 + (-1)^\nu) k_f \kappa d\kappa}{(\nu + 1)(2m_r \bar{I}/\hbar^2)^2}.$$

For the individual cases,

$$(B42) \quad X(-\infty, 0) = X(1, 1) = X(3, 1) = 0$$

while

$$(B43) \quad X(2,2) = - \int_0^{\alpha} \frac{2 k_f k dk}{3(2m_r I / \hbar^2)^2} \left(1 - \frac{k_0^2 - k^2}{k_0^2} \right)$$

and this becomes

$$(B44) \quad X(2,2) = - \frac{2}{3(2m_r I / \hbar^2)^2} \left(\frac{\alpha^3}{3} - \frac{\alpha^5}{5k_0^2} \right),$$

while lastly,

$$(B45) \quad X(2,0) = - \int_0^{\alpha} \frac{2 k_f k dk}{(2m_r I / \hbar^2)^2} \left(1 - \frac{k_0^2 - k^2}{k_0^2} \right) = 3 X(2,2).$$

Using (B38), $L(\mu, \nu)$ has the values

$$(B46) \quad L(3,1) = L(1,1) = L(-\infty, 0) = \frac{2\alpha^3}{3(2m_r I / \hbar^2)^2}$$

$$(B47) \quad L(2,2) = \frac{2\alpha^3}{3(2m_r I / \hbar^2)^2} \left(\frac{2}{3} + \frac{\alpha^2}{5k_0^2} \right)$$

$$(B48) \quad L(2,0) = \frac{2\alpha^3}{3(2m_r I / \hbar^2)^2} \frac{3\alpha^2}{5k_0^2} .$$

Inverse Power and Attractive-Repulsive Type Interactions

For the sake of completeness, and to provide a comparison with the Born-type calculations presented in this report, the inverse power and attractive-repulsive type interaction classical calculations of the Ω 's for elastic collisions are given. These are as discussed by Chapman and Cowling,³ and this Appendix is a summary of the relevant parts of their tenth chapter.

C1. Inverse Power Repulsive Force

Let P be the force between two molecules of masses m_j , m_k at a distance r , satisfying the relation

$$(C1) \quad P = \mathcal{K}_{jk} / r^\nu.$$

By considering the equations of motion of the two particles, it may readily be shown that, in polar coordinates (r, θ) ,

$$(C2) \quad r^2 \dot{\theta} = \text{const.}, = gb$$

$$(C3) \quad \frac{1}{2} (\dot{r}^2 + r^2 \dot{\theta}^2) + m_0 \mathcal{K}_{jk} / m_j m_k (\nu-1) r^{\nu-1} = \text{const.}, = \frac{1}{2} g^2.$$

b is the impact parameter of the collision, such that

$$(C4) \quad \sigma \sin \chi \, d\chi = b \, db$$

Writing

$$(C5) \quad v = b/r$$

$$v_0 = b \left(m_j m_k g^2 / m_0 \mathcal{K}_{jk} \right)^{\frac{1}{\nu-1}},$$

at the apse of the orbit

$$(C6) \quad 1 - v^2 - \frac{2}{v-1} \left(\frac{v}{v_0} \right)^{v-1} = 0.$$

Let v_{00} denote the real positive root of (C6); then from the geometry of the collision it is apparent that the angle between the asymptotes is twice the value of Θ corresponding to $v = v_{00}$, and therefore χ has the value

$$(C7) \quad \chi = \pi - 2 \int_0^{v_{00}} \left(1 - v^2 - \frac{2}{v-1} \left(\frac{v}{v_0} \right)^{v-1} \right)^{-\frac{1}{2}} dv.$$

Using (C7), $\phi_{jk}(\ell)$ can be transformed as follows:

$$(C8) \quad \begin{aligned} \phi_{jk}(\ell) &= \int_0^\pi (1 - \cos^\ell \chi) g \sigma \sin \chi d\chi \\ &= \left(\frac{m_0 k_{jk}}{m_j m_k} \right)^{\frac{2}{v-1}} g \frac{v-5}{v-1} \int_0^\infty (1 - \cos^\ell \chi) v_0 dv_0 \\ &\equiv \left(\frac{m_0 k_{jk}}{m_j m_k} \right)^{\frac{2}{v-1}} g \frac{v-5}{v-1} A_\ell(v), \end{aligned}$$

with $A_\ell(v)$ a pure number depending only on ℓ and v , and tabulated for certain values of ℓ and v in Chapman and Cowling.

Using this expression for $\phi(\ell)$, $\Omega^\ell(r)$ is readily evaluated.

Since

$$(C9) \quad \Omega_{jk}^\ell(r) = \pi^{1/2} \int_0^\infty e^{-Y^2} Y^{2r+2} \phi_{jk}(\ell) dY,$$

it follows that

$$(C10) \quad \Omega_{jk}^\ell(r) = \frac{\pi^{1/2} A_\ell(v) k_{jk}^{\frac{2}{v-1}} (2kT)^{\frac{v-5}{2(v-1)}} \Gamma(r+2 - \frac{2}{v-1})}{2(m_j m_k / m_0)^{1/2}}.$$

C2. Attractive-Repulsive Interaction

The forces between several types of molecules can be well approximated to by an equation of the form

$$(C11) \quad P = \mathcal{K}_{jk} / r^\nu - \mathcal{K}'_{jk} / r^{\nu'}$$

(where the force P is taken as positive when repulsive, and $\nu > \nu'$).

Using a similar method to that indicated above, it may be shown that the angle χ is given by

$$(C12) \quad \chi = \pi - 2 \int_0^{\nu_{00}} \left(1 - \nu^2 - \frac{2}{\nu-1} \left(\frac{\nu}{\nu_0} \right)^{\nu-1} + \frac{2}{\nu'-1} \left(\frac{\nu}{\nu'_0} \right)^{\nu'-1} \right)^{-1/2} d\nu$$

where

$$(C13) \quad \nu_0 = b (m_j m_k g^2 / m_0 \mathcal{K}_{jk})^{1/(\nu-1)}$$

$$\nu'_0 = b (m_j m_k g^2 / m_0 \mathcal{K}'_{jk})^{1/(\nu'-1)}$$

and ν_{00} is the (least) positive root of the equation

$$(C14) \quad 1 - \nu^2 - \frac{2}{\nu-1} \left(\frac{\nu}{\nu_0} \right)^{\nu-1} + \frac{2}{\nu'-1} \left(\frac{\nu}{\nu'_0} \right)^{\nu'-1} = 0.$$

The evaluation of $\phi(\ell)$ and $\Omega^\ell(r)$ are, for this potential, somewhat difficult in the general case. If, however, the attractive part of the field is weak, fairly simple approximations can be made. When \mathcal{K}'_{jk} is small, χ can be written approximately as

$$(C15) \quad \chi = \chi_0 + \chi_1 \mathcal{K}'_{jk} / T \frac{\nu-\nu'}{\nu-1}$$

where T is a mean temperature of the colliding particle types, and χ_0 is the value of χ obtained when only the repulsive part of the interaction force is considered. Using this approximation (C15),

$$(C16) \quad \phi_{jk}^l(\ell) \sim \int_0^\pi \left(1 - \cos^\ell(\chi_0 + \chi, \kappa_{jk}' / T \frac{v-v'}{v-1}) \right) g \sigma \sin \chi_0 d\chi_0 \\ = (\phi_{jk}^l(\ell))_0 \left(1 + \beta(\ell) / T \frac{v-v'}{v-1} \right),$$

where $(\phi_{jk}^l(\ell))_0$ is identical with the $\phi_{jk}^l(\ell)$ of the previous case, and $\beta(\ell)$ is independent of T . Hence finally,

$$(C17) \quad \Omega_{jk}^l(r) = (\Omega_{jk}^l(r))_0 \left(1 + s_{jk}(\ell, r) / T \frac{v-v'}{v-1} \right)$$

where $(\Omega_{jk}^l(r))_0$ is identical with the corresponding $\Omega_{jk}^l(r)$ of the previous part of this Appendix. $s_{jk}(\ell, r)$ is a function of $\ell, r, \kappa_{jk}, \kappa_{jk}', v$ and v' , and is tabulated (in a component form) for the Sutherland and Lennard-Jones molecular models in reference 3.

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