# Theoretical studies of certain atomic collisions.

## 1. Electron loss from H$^-$ in H and ionization of lithium by fast protons and electrons.

## 11. Transport properties of an ionized gas.

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# ABSTRACT.

General formulations of the quantal theory of collisions between two atomic systems are available and the relevant sections are summarized in Chapter I. The results of Born can then be applied in Chapter II to the problem of electron loss from fast $H^-$ passing through its parent gas at impact energies lying between 2.5 kev and 10 Mev. The sensitivity of the cross sections for which either of the resultant H atoms is excited to the 2p state, to the choice of bound and free wave functions is examined and the total loss cross section is compared with data on electron loss in $H_2$ and H. The same theory is used in Chapter III to study the excitation and ionization of Lithium by fast electron and proton impact at incident energies up to 1 kev and 1 Mev respectively. The ionization cross sections obtained using Seaton's method (1959) yield comparision material, and the excitation calculations are tested for sensitivity to choice of orbital parameters.

In Chapter IV the rather different methods used for treating slow collisions between electrons and positive ions are employed to gain information on the diffusion and viscosity cross sections and hence on the transport coefficients, in particular the electrical and thermal conductivities. Various numerical and analytical approximations are obtained for these quantities, in the ranges $10^{4}$°K – $10^{7}$°K and $10^{8}$ – $10^{18}$ per $cm^{3}$ of temperature and electron number density respectively It is shown that the electrical conductivity passes through

a maximum at a temperature which is possibly in the laboratory range for high number densities. The numerical results are summarized in a series of tables.

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# CHAPTER I.

## Applications of the theory of atomic collisions.

1.1 The present state of atomic physics makes it very desirable to obtain detailed information on the magnitude and energy variation of the cross sections for many atomic processes. General formulations of the problems connected with the collision of two atomic systems, at least one of which has a detailed structure, are available (c.f. Mott and Massey 1949, Massey 1956) while an alternative approach, developed by Gelmann, Goldberger and their co-workers, has been reviewed by DeWitt (1955). This thesis will deal with the application of these results to three different cases. Of these, 'Electron loss from fast negative ions of atomic hydrogen passing through atomic hydrogen' and the 'Ionization of Lithium atoms by fast protons and electrons' require the same mathematical approach, namely, the use of Born's approximation. The third problem, the calculation of the transport coefficients of an ionized gas, is shown to be dependent on slow collisions between electrons and positive ions and must be treated by rather different methods.

In this first chapter we shall summarize the mathematical formulation of these first two problems in terms of Born's approximation and introduce some results which are of use in the third problem. More detailed accounts of these proceedures are given in the references cited above.

For the sake of simplicity, we shall start by considering the scattering of a monoenergetic beam of electrons by a fixed, spherically symmetric centre of force. It will become apparent that this problem is closely connected with the diffusion problem of Chapter **IV**.

Taking the origin of coordinates at the centre of force and choosing the $z$-axis $(\theta=0)$ along the direction of incidence of the electron beam, which we suppose to have flux density $N$ and velocity $v$, we wish to determine the number of electrons that are contained in some solid angle $d\omega=d(\cos\theta)d\phi$ about the direction $(\theta,\phi)$, at a large distance from the scattering centre. We observe that the number of atoms crossing an area $dS$ perpendicular to $(\theta,\phi)$ at distance $r$ from the origin will be proportional to $dS$, and inversely proportional to $r^2$. This quantity will also be directly proportional to the original flux $N$ across unit area perpendicular to the initial direction and so may be expressed as

$$N\,I(\theta)\,d\omega \qquad \ldots\ldots\ldots\ldots \quad (1)$$

$I(\theta)\,d\omega$ obviously having areal dimensions. This is called the differential cross section for scattering through an angle $\theta$ into solid angle $d\omega$. We can then define the total cross section for scattering by a centre of force of electrons with velocity $v$ , as

$$Q(v) = 2\pi\int_0^\pi I(\theta)\sin\theta\, d\theta \qquad \text{..........} \; (2)$$

since $V(r)$ the scattering potential, is independent of the asimuthal angle $\phi$ . Suppose that we now attempt to calculate $Q(v)$ classically: then as is well known, we do not get a finite result unless $V(r)=0$ for all $r$ greater than some finite $r_0$ . Quantum mechanically however, we can proceed as follows: we restrict $V(r)$ to have the form

$$r V(r) \rightarrow 0 \quad \text{as } r \rightarrow \infty \qquad \text{..........} \; (3)$$

and represent the electron beam by a plane wave $e^{ikz}$, along the $z$- axis, towards negative $z$ , where the beam flux is now $v$ electrons per unit area per unit time. The outgoing wave will have an $e^{ikz}$ component and also one due to scattering; we may write this as

$$\psi \sim e^{ikz} + \frac{1}{r} f(\theta) e^{ikr} \qquad \text{..........} \; (4)$$

for large $r$ . Since the flux of electrons across $dS$ at $(r,\theta,\phi)$ is by (4)

$$v r^{-2} |f(\theta)|^2 dS \qquad \text{..........} \; (5)$$

unit incident flux is $|f(\theta)|^2 d\omega$ .

Thus,

$$|f(\theta)|^2 = I(\theta) \qquad \text{..........} \ (6)$$

Hence we can determine the differential and total cross sections, if we can solve the relevant Schrodinger equation for $f(\theta)$. That is, we require the solutions of the equation

$$\nabla^2\psi + \frac{2m}{\hbar^2}\left(E - V(r)\right)\psi = 0 \qquad \text{..........} (7)$$

where $E > 0$, which satisfy the boundary conditions $\psi(0)=0$, and equation (4) above. It is convenient to rewrite equation (7) in the form

$$\nabla^2\psi + \left(k^2 - U(r)\right)\psi = 0 \qquad \text{..........} \ (8)$$

and since $\psi$ must be symmetrical about the $z$-axis, we may expand $\psi$ in the form

$$\psi = \frac{1}{r}\sum_{n=0}^{\infty}\psi_n(r)P_n(\cos\theta) \qquad \text{..........} \ (9)$$

On substitution in equation (8) this yields

$$\frac{d^2}{dr^2}\psi_n + \left[k^2 - U(r) - \frac{n(n+1)}{r^2}\right]\psi_n = 0 \qquad \text{..........} \ (10)$$

Also, we may expand $e^{ikr\cos\theta}$ in the form

$$e^{ikr\cos\theta} = \sum_n i^n(2n+1)j_n(kr)P_n(\cos\theta) \qquad \text{..........} \ (11)$$

where

$$j_n(x) = \left(\frac{\pi}{2x}\right)^{1/2} J_{n+1/2}(x) \qquad \text{.......... (12)}$$

$$\sim x^{-1}\sin(x - \tfrac{1}{2}n\pi) \qquad \text{.......... (13)}$$

for large $x$

is a spherical Bessel function of order n.

Therefore equations (9), (12), (13) are consistent if

$$\psi_n \sim i^n(2n+1)k^{-1}\sin(kr - \tfrac{1}{2}n\pi) + a_n e^{ikr} \qquad \text{.......... (14)}$$

so then we must have

$$f(\theta) = \sum_n a_n P_n(\cos\theta) \qquad \text{.......... (15)}$$

and it remains to determine the coefficients $a_n$.

Equation (10) has a solution $\psi_n$ with asymptotic form

$$\psi_n \sim r\{\lambda j_n(kr) + \mu j_{-n}(kr)\} \qquad \text{.......... (16)}$$

provided that $rU(r) \to 0$ as $r \to \infty$, $j_{-n}(x)$ being the spherical Bessel function of order -n, and satisfying

$$j_{-n}(x) \sim \frac{1}{x}(-1)^n\cos(x - \tfrac{1}{2}n\pi) \qquad \text{.......... (17)}$$

Hence it is apparent that

$$\psi_n \sim b_n\sin(kr - \tfrac{1}{2}n\pi + \eta_n) \qquad \text{.......... (18)}$$

where the phase shift is given by

$$\tan \eta_n = (-1)^n \frac{\mu}{\lambda} \qquad \text{..........} \; (19)$$

The evaluation of the coefficients is carried out by a comparision of equations (9), (14), (18). These relations yield

$$a_n = (e^{2i\eta_n}-1)(2n+1)/2ik \qquad \text{..........} \; (20)$$

$$b_n = (2n+1)\, i^n e^{i\eta_n}/k \qquad \text{..........} \; (21)$$

and the expansion for $f(\theta)$ then becomes

$$f(\theta) = \frac{1}{2ik}\sum_{n=0}^{\infty}(2n+1)(e^{2i\eta_n}-1)P_n(\cos\theta) \qquad \text{...........} (22)$$

The following result for the total cross section $Q$, can then be easily derived,

$$Q = \frac{4\pi}{k^2}\sum_{n=0}^{\infty}(2n+1)\sin^2\eta_n \qquad \text{..........} \; (23)$$

a formula first introduced by Faxen and Holtsmark (1927).

1.2 It is convenient to introduce here the expressions for the diffusion and viscosity cross sections $Q_D$ and $Q_\eta$ respectively, relevant to the study of the conductivity of an ionized gas pursued in a later chapter. These are defined by

$$Q_D = 2\pi\int_0^{\pi}(1-\cos\theta)\, I(\theta)\sin\theta\, d\theta \qquad \text{.........} \; (24)$$

$$Q_\eta = 2\pi \int_0^\pi \sin^3\theta \, I(\theta)\, d\theta \qquad \text{.......... (25)}$$

c.f. equation (1). We can express these in terms of the phase shifts as follows:-

$$Q_D = \frac{\pi}{2k^2}\int_0^\pi \left| \sum_{n=0}^{\infty} (2n+1)(e^{2i\eta_n}-1) P_n(\cos\theta) \right|^2 (1-\cos\theta)\, d(\cos\theta) \qquad \text{.......... (26)}$$

$$= \frac{\pi}{2k^2} \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} (2n+1)(2m+1)(e^{2i\eta_n}-1)(e^{-2i\eta_m}-1) \int_{-1}^{+1} (1-\mu) P_m(\mu) P_n(\mu)\, d\mu$$

$$= \frac{\pi}{k^2}\sum_{n=0}^{\infty} (2n+1)\left| e^{2i\eta_n}-1 \right|^2 - \frac{2\pi}{k^2}\sum_{n=0}^{\infty} (n+1)(e^{2i\eta_n}-1)(e^{-2i\eta_{n+1}}-1) - \frac{2\pi}{k^2}\sum_{n=0}^{\infty} n(e^{-2i\eta_{n-1}}-1)(e^{2i\eta_n}-1)$$

$$= \frac{\pi}{k^2}\sum_{n=0}^{\infty} (n+1)(e^{2i\eta_n}-1)(e^{-2i\eta_n}-e^{-2i\eta_{n+1}}) + \frac{2\pi}{k^2}\sum_{n=0}^{\infty} n(e^{2i\eta_n}-1)(e^{-2i\eta_n}-e^{-2i\eta_{n-1}})$$

$$= \frac{\pi}{k^2}\sum_{n=0}^{\infty} (n+1)\left| e^{2i\eta_n} - e^{2i\eta_{n+1}} \right|^2$$

$$= \frac{4\pi}{k^2}\sum_{n=0}^{\infty} (n+1)\sin^2(\eta_n - \eta_{n+1})$$

$$\text{.......... (27)}$$

and similarly,

$$Q_\eta = \frac{2\pi}{k^2}\sum_{n=0}^{\infty} (n+1)\sin^2(\eta_n - \eta_{n+2})\left\{\frac{n+2}{n+3/2}\right\} \qquad \text{.......... (28)}$$

2.1 An approximate expression for the differential cross section $|f(\theta)|^2 d\omega$ may be obtained if we suppose that the effect of the potential $V(r)$ is small and this is certainly true for $V(r) >> E$ i.e. for a fast collision.

Writing equation (8) in the form

$$\nabla^2\psi + k^2\psi = U\psi \qquad \text{..........} \; (29)$$

and using the method of Green's function, (c.f. 2.3 and Mott and Massey 1949) we have

$$\psi(\underline{r}) = \psi_0(\underline{r}) - \frac{1}{4\pi}\int \frac{U(r')\psi(r')\,e^{ik|\underline{r}-\underline{r}'|}}{|\underline{r}-\underline{r}'|}\,d\underline{s}' \qquad \text{..........} \; (30)$$

where $\psi_0(\underline{r})$ is a solution of the equation

$$\nabla^2\psi + k^2\psi = 0 \qquad \text{..........} \; (31)$$

the right hand side of equation (29) having been treated as a known function.

Born's approximation is then derived by substituting a plane wave $e^{ikz}$ for $\psi_n$ in the integral in (30), (the exact solution for $U = 0$) giving

$$\psi(r,\theta) = e^{ikz} - \frac{1}{4\pi}\int \frac{U(r')e^{ikz'}e^{ik|\underline{r}-\underline{r}'|}}{|\underline{r}-\underline{r}'|}\,d\underline{s}' \qquad \text{..........} \; (32)$$

For large values of $r$, $\psi(r,\theta)$ has the asymptotic form (4), and comparision with equation (32), yields the following approximate expression for $f(\theta)$,

$$f^B(\theta) = -\frac{1}{4\pi}\int e^{ik(\underline{n}_0-\underline{n})\cdot\underline{r}'}\,U(r')\,d\underline{s}' \qquad \text{..........} \; (33)$$

where $\underline{n}_0, \underline{n}$ are unit vectors in the directions of incidence and of scattering.

Writing $\underline{K} = k(\underline{n}_0 - \underline{n})$ and noting that we may take $\underline{K} \cdot \underline{r}' = \cos\theta$, we may perform the necessary integrations over the solid angles and obtain an alternative form to (33) for $f^B(\theta)$, which will be of greater practical use, namely,

$$f^B(\theta) = -\frac{2m}{\hbar^2}\int V(r)\frac{\sin Kr}{Kr}\, r^2\, dr \qquad \text{.......... (34)}$$

2.2 It is of interest to see how the Born approximation may also be derived from first order time dependent perturbation theory. The wave equation for the system is

$$\mathcal{H}\Psi = i\hbar\frac{\partial\Psi}{\partial t} \qquad \text{.......... (35)}$$

$\Psi$ being the complete wave function describing the motion. We shall suppose that the Hamiltonian $\mathcal{H}$ approximates to a time independent Hamiltonian $\mathcal{H}_0$ for which the Schrödinger equation can be solved and treat the time dependence as a relatively small effect accounted for by introducing the perturbation $\lambda\mathcal{H}'$. The unperturbed eigenfunctions $\Psi^0$ satisfy the equation

$$\mathcal{H}_0\Psi^0 = i\hbar\frac{\partial\Psi^0}{\partial t} \qquad \text{.......... (36)}$$

and are of the form

$$\Psi_n^0 = \psi_n^0 e^{-\frac{i}{\hbar}E_n t} \qquad \text{.......... (37)}$$

These functions form a complete set and we may therefore write

$$\Psi = \sum_n c_n(t)\Psi_n^{\circ} \qquad \text{..........} \quad (38)$$

Substitution of expression (38) for $\Psi$ into equation (35), and simplifying, yields

$$\lambda \sum_n c_n \mathcal{H}'\Psi_n^{\circ} = i\hbar \sum_n \frac{dc_n}{dt}\Psi_n^{\circ} \qquad \text{...........} \quad (39)$$

We now multiply both sides of (39) by $\Psi_m^{\circ *}$ and perform the integration over coordinate space, so that we finally obtain

$$\frac{dc_m}{dt} = -\frac{i\lambda}{\hbar}\sum_n c_n \int \Psi_m^{\circ *}\mathcal{H}'\Psi_n^{\circ}\, d\tau \qquad \text{...........} \quad (40)$$

$$= -\frac{i\lambda}{\hbar}\sum_n c_n H_{mn} e^{i\nu_{mn}t} \qquad \text{..........} \quad (41)$$

where $H_{mn}$ is the matrix element of the perturbation and

$$\hbar\nu_{mn} = E_m - E_n \qquad \text{..........} \quad (42)$$

Expansion of the coefficients $c_n(t)$ in terms of powers of $\lambda$ in what is assumed to be an analytic series for $0 \leq \lambda \leq 1$, and substitution in (41) gives

$$\frac{dc_m^{(0)}}{dt} = 0 \ ; \ \frac{dc_m^{(s)}}{dt} = -\frac{i}{\hbar}\sum_n c_n^{(s)} e^{i\nu_{mn}t}, \ s = 0, 1, 2, \ldots \qquad \text{..........} \quad (43)$$

$$c_n = c_n^{(0)} + c_n^{(1)}\lambda + c_n^{(2)}\lambda^2 + c_n^{(3)}\lambda^3 + \ldots\ldots$$

on equating the coefficients of $\lambda^s$.

If we make the assumption that the system is in a definite unperturbed energy state at the time of application of the perturbation, we may write

$$c_m^{(0)} = \delta_{ml} \qquad \ldots\ldots\ldots\ldots (44)$$

Restricting ourselves to a first order perturbation, integration of the appropriate equation in (43) leads to

$$c_m^{(1)}(t) = -\frac{i}{\hbar}\int_{-\infty}^{t} H_{ml}(t')\, e^{i\nu_{ml}t'}\, dt' \qquad \ldots\ldots\ldots\ldots (45)$$

Thus the probability of finding the system in a state $m$ at time $t$ is given by

$$|c_m^{(1)}(t)|^2 = \frac{4\,|H_{ml}|^2 \sin^2 \frac{1}{2}\nu_{mn} t}{\hbar^2 \nu_{ml}^2}$$

and if we assume that the perturbation $H_{ml}$ operates only between the times $0$ and $t$ and is independent of time in this range. The transition probabilities from the initial state $l$ to one of almost equal energy can then be written as

$$W = t^{-1}\int |c_m^{(1)}(t)|^2 \rho(m)\, dE_m \qquad \ldots\ldots\ldots\ldots (46)$$

$\rho(m)$ being defined as the density of final states such that $\rho(m)\,dE_m$ is the number of these states in the energy range $dE_m$. Equation (46) reduces to

$$W = \frac{2\pi}{\hbar}\,|H_{ml}|^2 \rho(m) \qquad \ldots\ldots\ldots\ldots (47)$$

when it is realized that $H_{ml}$, $\rho(m)$ are slowly varying and that they may be withdrawn from under the integral sign. We may now derive Born's approximation directly, by considering the motion of an electron in a volume $\Omega$ under the influence of a perturbing potential $V(r)$ and allocating to it the initial and final wave functions

$$\psi_l = \frac{1}{\sqrt{\Omega}} e^{ik\underline{n}_0\cdot\underline{r}} \qquad \text{.......... (48)}$$

$$\psi_m = \frac{1}{\sqrt{\Omega}} e^{ik\underline{n}\cdot\underline{r}} \qquad \text{.......... (49)}$$

The density of final energy states, $\rho(m)$, may be expressed as

$$\rho(m) = \frac{\Omega p^2}{h^3} \frac{dp}{dE_m} \, d\omega \qquad \text{.......... (50)}$$

where $d\omega$ is an element of solid angle about the direction of scattering $\underline{n}$ and $p$ is the electron momentum. Also since

$$W = \frac{v}{\Omega} I(\theta) \, d\omega \qquad \text{.......... (51)}$$

$v$ being the electron velocity, we finally obtain,

$$I(\theta) = \frac{4\pi^2 m^2}{h^4} \left| \int V(r') e^{ik(\underline{n}_0 - \underline{n})\cdot\underline{r}'} d\underline{v}' \right|^2 \qquad \text{.......... (52)}$$

which it will be noticed, is equivalent to (33).

2.3 It is convenient here to derive an expression for the phase shifts $\eta_n$ using the variational principle and the integral equation formulation of the problem. We will first consider briefly a method of solution of the more general differential equation

$$\left[ \underline{\mu} - m_0 \right] \psi(\underline{r}) = f(\underline{r}) \qquad \text{..........} \quad (53)$$

where $\underline{\mu}$ is a hermitian operator of which $\psi_m$, $m$ are complete sets of eigenvalues and eigenfunctions respectively, and $f(\underline{r})$ is a known function of $\underline{r}$. It can then be easily shown that $\psi(\underline{r})$ may be written in the form (see Schiff 1955)

$$\psi(\underline{r}) = \int G_{m_0}(r|r') f(\underline{r}') \, d\underline{r}' \qquad \text{..........} \quad (54)$$

where $G_{m_0}(r|r')$ is referred to as Green's function for the system. Substitution of (54) in (53) then immediately yields

$$\left[ \underline{\mu} - m_0 \right] G_{m_0}(r|r') = \delta(\underline{r} - \underline{r}') \qquad \text{..........} \quad (55)$$

We shall now apply this method to the specific equation

$$\frac{d^2\psi_n}{dr^2} + \left[ k^2 - \frac{n(n+1)}{r^2} \right] \psi_n = U(r)\psi_n \qquad \text{..........} \quad (56)$$

and we shall assume that the right hand side of (56) is a known function of $\underline{r}$. In accordance with equation (54) we may then write down the general solution for $\psi_n$

$$\psi_n(r) = Akr\, j_n(kr) - \frac{1}{4\pi} \int_0^\infty G_n(r|r') U(r') \psi_n(r') \, dr' \qquad \text{..........} \quad (57)$$

where $A$ is a constant and $G_k(r|r')$ satisfies

$$\left[\frac{d^2}{dr^2} + k^2 - \frac{n(n+1)}{r^2}\right] G_k(r|r') = \delta(r-r') \qquad \text{..........} \quad (58)$$

Bearing in mind that $\psi_n(r)$ must satisfy the appropriate boundary conditions

$$\psi_n(0) = 0$$

$$\psi_n \sim b_n \sin(kr - \tfrac{1}{2}n\pi + \eta_n) \qquad \text{..........} \quad (59)$$

we see that the choice of Green's functions consistent with (59) is given by

$$G_k(r|r') = -krr' \begin{cases} j_n(kr)\, n_n(kr') & r \leq r' \\ j_n(kr')\, n_n(kr) & r \geq r' \end{cases} \qquad \text{..........} \quad (60)$$

where the function $j_n(x)$ has already been defined in equations (12) and (13) and $n_n(x)$ is a spherical Neumann function of order n defined by

$$n_n(x) = \left(\frac{\pi}{2x}\right)^{1/2} N_{n+1/2}(x) \qquad \text{..........} \quad (61)$$

$$\sim -x^{-1}\cos(x - \tfrac{1}{2}n\pi) \qquad \text{..........} \quad (62)$$

for large $x$

(57) now becomes more explicitly,

$$\psi_n(r) = Akr\, j_n(kr) + \frac{kr}{4\pi}\int_0^r n_n(kr)\, r'\, j_n(kr')\, U(r')\, \psi_n(r')\, dr'$$

$$+ \frac{kr}{4\pi}\int_r^\infty j_n(kr)\, r'\, n_n(kr')\, U(r')\, \psi_n(r')\, dr' \qquad \text{..........} \quad (63)$$

which fulfils the conditions (59) if

$$\tan\eta_n = \frac{1}{A}\int_0^\infty j_n(kr')\,U(r')\,\Psi_n(r')\,r'\,dr' \qquad \text{..........} \quad (64)$$

We can now eliminate $A$ between equations (63), (64) and obtain a variational integral for $\cot\eta_n$ by multiplying both sides of the resulting equation by $kU(r)\Psi_n(r)$ and performing an integration over the variable $\underline{r}$ ,

$$[\cot\eta_n] = \frac{k\int_0^\infty U\Psi_n^2\,dr + \frac{1}{4\pi}\int_0^\infty\int_0^\infty \Psi_n(r)\,U(r)\,G_k(r|r')\,U(r')\,\Psi_n(r')\,dr'\,dr}{\left[\int_0^\infty krj_n\,U\,\Psi_n\,dr\right]^2} \qquad \text{..........} \quad (65)$$

which on making use of (60) may be simplified to

$$[\cot\eta_n] = \frac{k\int_0^\infty U\Psi_n^2\,dr - 2\int_0^\infty krn_n(kr)\,U(r)\,\Psi_n(r)\int_0^r kr'j_n(kr')\,U(r')\,\Psi_n(r')\,dr'\,dr}{\left[\int_0^\infty krj_n\,U\,\Psi_n\,dr\right]^2}$$

$$\text{....} \quad (66)$$

The Born approximation to the phase shift may be obtained immediately by inserting the incident wave $krj_n(kr)$ as a trial wave function and neglecting the second term of the numerator which is of higher order in $U(r)$ than the first. However a considerably better approximation is often acquired by the retention of the second term, i.e.

$$[\cot\eta_n] \simeq \cot\eta_n^B\left\{1 - \frac{2\int_0^\infty (krn_n)\,U(krj_n)\int_0^r (kr'j_n)^2\,U\,dr'\,dr}{k\int_0^\infty U(krj_n)^2\,dr}\right\} \quad \text{..} \quad (67)$$

where $\eta_n^B$ is the Born approximation phase shift.

2.4 On the other hand, when $V(r)>E$ i.e. $k<<1$, we may apply an approximation due to Jefferys (1926) for the phase shift $\eta_n$. We require the solution of equation (10) which may be written in the alternative form

$$\left\{\frac{d^2}{dr^2}+F(r)\right\}\psi_n=0 \qquad \text{..........} \; (68)$$

where

$$F(r)=k^2-U(r)-\frac{n(n+1)}{r^2} \qquad \text{..........} \; (69)$$

If we write $\psi_n = Ae^{i\beta}$ , and substitute into equation (68) we obtain

$$A''+2iA'\beta'+i\beta''A-\beta'^2A+FA=0 \qquad \text{..........} \; (70)$$

where dashes denote differentiation w.r.t. $r$. As a first approximation we may set $\beta'^2=F(r)$ which gives

$$\beta=\int[F(r)]^{1/2}dr \qquad \text{..........} \; (71)$$

so that if $F(r)$ is nearly constant over the range considered

$$\beta=[F(r)]^{1/2}r+\text{const} \qquad \text{..........} \; (72)$$

It follows that to this approximation $A$ is constant and hence that

$$A''<<A'F^{1/2}<<AF \qquad \text{..........} \; (73)$$

Thus a second evaluation of $A$ is derived from

$$2A'\beta'+\beta''A=0$$

giving $$A=\text{const}\,[F(r)]^{-1/4} \qquad \text{...........} \; (74)$$

and we may write

$$\psi_n = \left[F(r)\right]^{-1/4} \exp\left\{ \pm i \int^r \left[F(r)\right]^{1/2} dr \right. \qquad \text{.......... (75)}$$

Now $F(r)$ has a single zero between zero and infinity at $r=r_0$ say. The solution above will clearly be exponential for $r<r_0$ since in this region $F(r)<0$ and for $r>r_0$ it will be an oscillating function. Since $\psi_n(0)=0$ is a necessary condition, $\psi_n$ must decrease exponentially for $r<r_0$ and hence the appropriate approximation valid for $r>r_0$ must be

$$\psi_n \simeq F^{-1/4} \sin\left[\tfrac{1}{4}\pi + \int_{r_0}^{r} F^{1/2} dr\right] \qquad \text{........... (76)}$$

The asymptotic form of $\psi_n$ for large $r$ is

$$\text{const.} \sin\left[\tfrac{1}{4}\pi + \int_{r_0}^{\infty} \left\{F^{1/2} - k\right\} dr + k(r-r_0)\right] \qquad \text{........... (77)}$$

which must be consistent with the alternative form (18), so the phase shift $\eta_n$, to the required approximation, is

$$\eta_n = \tfrac{1}{4}\pi + \tfrac{1}{2}n\pi - kr_0 + \int_{r_0}^{\infty} \left\{F^{1/2} - k\right\} dr \qquad \text{.......... (78)}$$

or in an equivalent form

$$\eta_n = \int^{\infty} \left\{ k^2 - U(r) - \frac{n(n+1)}{r^2} \right\}^{1/2} dr - \int^{\infty} \left\{ k^2 - \frac{n(n+1)}{r^2} \right\}^{1/2} dr \qquad \text{.......... (79)}$$

where in both integrals the lower limits are given by the zero of the respective integrands. Later in 1937, Langer introduced a modification to this formula replacing the factor $n(n+1)$ by $(n+\frac{1}{2})^2$. This is accomplished by making the substitutions $\rho = e^r$ and $\psi_n r^{-1/2} = \phi_n$ and then obtaining an approximation similar to (76) for $\phi_n$. Writing the expression for the phase shift in its modified form

$$\eta_n = -\int^{\infty}\left(k^2 - \frac{(n+\frac{1}{2})^2}{r^2}\right)^{1/2} dr + \int^{\infty}\left(k^2 - U(r) - \frac{(n+\frac{1}{2})^2}{r^2}\right)^{1/2} dr \qquad \text{.... (80)}$$

we may expand the second integrand for large n and (80) yields

$$\eta_n = \int^{\infty}\left(k^2 - \frac{(n+\frac{1}{2})^2}{r^2}\right)^{1/2}\left\{1 - \frac{U(r)}{2\left(k^2 - \frac{(n+\frac{1}{2})^2}{r^2}\right)}\right\} dr - \int^{\infty}\left(k^2 - \frac{(n+\frac{1}{2})^2}{r^2}\right)^{1/2} dr \qquad \text{.... (81)}$$

$$= -\frac{1}{2k}\int^{\infty}\frac{r\,U(r)}{\sqrt{r^2 - p^2}}\, dr \qquad \text{.......... (82)}$$

where $p$, the impact parameter is given by

$$p = \frac{n+\frac{1}{2}}{k} \qquad \text{.......... (83)}$$

The expression (82) will prove to be of use in the evaluation of certain diffusion cross sections when at low temperatures ($\sim 10^3\,{}^\circ K$) Born's approximation is no longer valid. (See Chapter IV )

3.1 We have now to consider the more general theory applicable to collision phenomena in which there is an appreciable reaction between the incident particle and the scattering centre, which is now assumed to have structure. In the treatment of this problem it is necessary to distinquish between direct inelastic collisions in which there is direct exchange of energy between the relative translational motion and the internal motions of the colliding systems and the rearrangement collisions which result in a redistribution of electrons and nuclei. We shall only discuss here the former type of collision, as we take no account of exchange in the specific problems to be considered, but an account of rearrangement processes can be found in Mott and Massey (loc: cit:)

Firstly, in order to illustrate the general method employed, we shall consider the simplest type of collision, that of electrons scattered by hydrogen atoms resulting in the excitation of the atom to the nth state. In a manner exactly analogous to that used to define the differential cross section for an elastic collision, we shall call $I_n(\theta)\,d\omega$ the differential cross section for scattering into a solid angle $d\omega$ after having excited the atom to its nth state and the total cross section is then given by integration over all solid angles, so that

$$Q_{on} = \int_0^{2\pi}\int_0^{\pi} I_{on}(\theta,\phi)\sin\theta\,d\theta\,d\phi \qquad \text{..........} \; (84)$$

Neglecting the very small spin orbital interaction, the wave equation for the whole system may be written as

$$\left[\frac{\hbar^2}{2m}(\nabla_1^2+\nabla_2^2)+E+\frac{e^2}{r_1}+\frac{e^2}{r_2}-\frac{e^2}{r_{12}}\right]\Phi(1,2)=0 \qquad \text{.......} \; (85)$$

where the suffices 1,2 refer to incident and atomic electrons respectively and $E$ is the aggregate of the energy of the atomic electron in its ground state and the kinetic energy of the incident electron. The wave function $\Phi(1,2)$ may of course be represented as

$$\Phi(1,2) = \Omega(\sigma_1,\sigma_2)\,\Psi(\underline{r}_1,\underline{r}_2) \quad \text{..........} \quad (86)$$

where $\Omega$ depends only on the spin coordinates and $\Psi$ is merely a function of position. If the indistinguishability of the electrons is ignored, we may assume $\Omega$ to have the form

$$\delta(s_1|\sigma_1)\,\delta(s_2|\sigma_2) \quad \text{..........} \quad (87)$$

where $s_1, s_2$ are spin quantum numbers and the delta function is such that

$$\begin{aligned} \delta(s|\sigma) &= 0 \quad \text{for } \sigma \neq s \\ \delta(s|\sigma) &= 1 \quad \text{for } \sigma = s \end{aligned} \quad \text{..........} \quad (88)$$

$s_1, s_2$ being able to take either of the two values $\alpha, \beta$ and remaining unaltered throughout the encounter.

The function $\Psi(\underline{r}_1,\underline{r}_2)$ may be expanded in terms of the complete set of eigenfunctions $\psi_n(\underline{r}_2)$ of the hydrogen atom, thus

$$\Psi(\underline{r}_1,\underline{r}_2) = \sum_n \psi_n(\underline{r}_2)F_n(\underline{r}_1) \quad \text{..........} \quad (89)$$

where the summation is taken over all discrete values, and also includes integration over the continuum.
The wave functions $\psi_n(\underline{r})$ satisfy the equation

$$\left(\frac{\hbar^2}{2m}\nabla^2 + E_n + \frac{e^2}{r}\right)\psi_n = 0 \quad \text{..........} \quad (90)$$

and so substituting (89) in (85) and making use of (90),

$$\sum_n \psi_n(\mathbf{r}_2)\left\{\frac{\hbar^2}{2m}\nabla^2+E-E_n\right\}F_n(\mathbf{r}_1) = e^2\left(\frac{1}{r_{12}}-\frac{1}{r_1}\right)\Psi(\mathbf{r}_1,\mathbf{r}_2) \quad \ldots\ldots (91)$$

Multiplication of both sides of equation (91) by $\psi_n^*(\mathbf{r}_2)$ and integration over the coordinate $\mathbf{r}_2$ , yields

$$\left\{\frac{\hbar^2}{2m}\nabla_1^2+E-E_n\right\}F_n(\mathbf{r}_1) = \int\left(\frac{e^2}{r_{12}}-\frac{e^2}{r_1}\right)\Psi(\mathbf{r}_1,\mathbf{r}_2)\psi_n^*(\mathbf{r}_2)\,d\tau_2 \quad \ldots\ldots (92)$$

and in an alternative form

$$\left\{\frac{\hbar^2}{2m}\nabla_1^2+E-E_n-V_{nn}\right\}F_n(\mathbf{r}_1) = \sum_{m\neq n} V_{mn}(\mathbf{r}_1)\,F_m(\mathbf{r}_1) \quad \ldots\ldots (93)$$

where

$$V_{mn}(\mathbf{r}_1) = \int\left(\frac{1}{r_{12}}-\frac{1}{r_1}\right)\psi_m(\mathbf{r}_2)\psi_n^*(\mathbf{r}_2)\,d\tau_2 \quad \ldots\ldots (94)$$

$$= \int \frac{1}{r_{12}}\psi_m(\mathbf{r}_2)\psi_n^*(\mathbf{r}_2)\,d\tau_2 \text{ for } m\neq n \quad \ldots\ldots (95)$$

$\psi_m(\mathbf{r})$ and $\psi_n(\mathbf{r})$ being orthogonal.

It is obviously impossible to solve the infinite set of coupled differential equations (93) as they stand, but if the energy of the relative translational motion is large compared with the internal motion of the hydrogen atom i.e. the collision is said to be fast, we may make certain assumptions which lead to Born's approximation. These are

(1) that $V_{nn}(\mathbf{r}_1)$ in equation (93) may be neglected. (It can easily be seen from (94) that it is small for nearly all $r_{12}$, the small values of $r_{12}$ only occurring for a very

short time.)

(2) that the terms $V_{mn}(r_1)F_m(r_1)$ on the right hand side of (93) can be neglected for $V_{mn}(r_1)F_m(r_1) \neq V_{on}(r_1)F_o(r_1)$ (this is equivalent to assuming the atom is excited directly to its $n^{th}$ state and doesn't occupy any intermediate levels.)

These conditions also imply that $F_o(r_1)$ is undisturbed by the interaction and can therefore be represented by a plane wave. The equations (93) are then reduced to

$$\left\{\frac{\hbar^2}{2m} + E - E_n\right\}F_n(\underline{r}_1) = \int \frac{1}{r_{12}}\psi_o(\underline{r}_2)\psi_n^*(\underline{r}_2)\exp\{i\underline{k}_i\cdot\underline{r}_1\}\,d\underline{\tau}_2 \quad .... (96)$$

where the vectors $\underline{k}_i$, $\underline{k}_f$ are in the direction of the incident and scattered waves respectively and have magnitudes given by

$$\underline{k}_i = \frac{m\underline{v}_i}{\hbar} \quad ; \quad \underline{k}_f = \frac{m\underline{v}_f}{\hbar} \quad .... (97)$$

$v_i$ and $v_f$ being the initial and final velocities of the colliding systems. The solution of (96) we require must have asymptotic form

$$\frac{1}{r_1}\exp\{ik_i r_1\}f_{on}(\theta,\phi) \quad ............(98)$$

and it is easily deduced that

$$f_{on}(\theta,\phi) = -\frac{1}{4\pi}\iint\frac{\exp\{i(\underline{k}_i-\underline{k}_f)\cdot\underline{r}_1'\}}{|\underline{r}_1'-\underline{r}_2|}\psi_o(\underline{r}_2)\psi_n^*(\underline{r}_2)\,d\underline{\tau}_1'\,d\underline{\tau}_2 \quad ... (99)$$

(c.f. equation (33) ) The differential cross section $I_{on}(\theta,\phi)\,d\omega$ is given by

$$I_{on}(\theta,\phi)\,d\omega = \frac{k_f}{k_i}\left|f_{on}(\theta,\phi)\right|^2 d\omega \quad ........... (100)$$

which yields an expression for the total cross section on substitution in equation (84). It is most convenient to evaluate this using momentum variables instead of angular coordinates, so we let

$$\underline{k}_i - \underline{k}_f = \underline{K} \qquad \dots\dots\dots\dots (101)$$

and we them obtain

$$Q_{0n} = \frac{8}{\varkappa_i^2}\int_{K_{min}}^{K_{max}} |J|^2 K^{-3} dK \quad (\pi a_0^2) \qquad \dots\dots\dots\dots (102)$$

where

$$|J| = \left|\int \exp\{i\underline{K}.\underline{r}\}\psi_0(r)\psi_n^*(r)\,d\underline{r}\right| \qquad \dots\dots\dots\dots (103)$$

The limits of integration are given by

$$K_{max} = k_i + k_f \quad ; \quad K_{min} = k_i - k_f \qquad \dots\dots\dots\dots (104)$$

while the quantity of energy $\varkappa_i^2$ is given by

$$\varkappa_i^2 = \frac{\frac{1}{2}mv_i^2}{I_H} \qquad \dots\dots\dots\dots (105)$$

where $I_H$ is the ionization potential of hydrogen.

3.2. It now remains to generalize these results to the collision of any two atomic systems $A$ and $B$. The motion of the whole system may be described in terms of the coordinates of the centre of mass, the relative motion of the centres of mass of the two bodies and the motion of the individual electrons relative to their nuclei. The first of these is not necessary to the solution of the problem and may be separated out. The wave equation them takes the form

$$\left[\frac{\hbar^2}{2\mu}\nabla_r^2 - H_a(\underline{r}_a) - H_b(\underline{r}_b) + E + \frac{1}{2}\mu v_i^2 - V(\underline{r}, \underline{r}_a, \underline{r}_b)\right]\Psi = 0 \quad \dots\dots (106)$$

where $\mu$ is the reduced mass of the system; i.e. if $M_a$ and $M_b$ are the masses of the twp colliding bodies

$$\mu = \frac{M_a M_b}{M_a + M_b} \qquad \text{..........} \quad (107)$$

$H_a(r_a)$ and $H_b(r_b)$ are the Hamiltonians of the unperturbed atoms and $V(r, r_a, r_b)$ denotes the interaction potential. $E_n$ is the sum of the eigenenergies $E_n^a$, $E_n^b$ of the systems $A$ and $B$ and the wave function $\psi_n(r_a, r_b)$ of the complete system at infinite separation therefore satisfies

$$\left\{ H_a(r_a) + H_b(r_b) - E_n \right\} \psi_n(r_a, r_b) = 0 \qquad \text{...........} \quad (108)$$

The wave function $\Psi(r, r_a, r_b)$ may be expanded in terms of the complete set of eigenfunctions $\psi_n(r_a, r_b)$, so we may write

$$\Psi(r, r_a, r_b) = \sum_n F_n(r)\, \psi_n(r_a, r_b) \qquad \text{..........} \quad (109)$$

(c.f. equation (89)). Proceeding in a precisely similar way to before, we obtain an expression for the total cross section, of the form (84), where we now have

$$k_i = \frac{\mu \underline{v}_i}{\hbar} \quad ; \quad k_f = \frac{\mu \underline{v}_f}{\hbar} \qquad \text{..........} \quad (110)$$

and

$$|J| = \left| \int \exp\{ i\underline{K} . \underline{R} \} V(\underline{r}, \underline{r}_a, \underline{r}_b)\, \psi_0(\underline{r}_a, \underline{r}_b)\, \psi_n^*(\underline{r}_a, \underline{r}_b)\, d\underline{s}\, d\underline{r}_a\, d\underline{s}_b \right| \text{..........} \quad (111)$$

$K_{max}$, $K_{min}$ and $g_i^2$ are as given in equations (104), (105).

3.3 Lastly, we deduce the approximate formulae for $K_{max}$, $K_{min}$ which will be employed in the following problems involving electron and proton impact. In the latter case we may take

$$K_{max} \doteq 2k_i \sim \infty \qquad \text{..........} \quad (112)$$

and also

$$k_i^2 - k_f^2 = \frac{\mu^2}{\hbar^2}\left( v_i^2 - v_f^2 \right) \qquad \text{..........} \quad (113)$$

which yields the approximate formula

$$2k_i(k_i - k_f) = \frac{2\mu}{\hbar^2}\Delta E \quad \text{or,} \quad K_{min} = \frac{\Delta E}{2g_i} \qquad \text{..........} \quad (114)$$

where $\Delta E$ is the difference between the initial and final energies of the system measured in rydbergs. For electron impact we must derive more accurate formulae for $K_{max}$ and $K_{min}$. The upper limit of integration may be taken as $2k_i$, and employing equation (113) again

$$(2k_i - K_{min})K_{min} = \frac{2\mu}{\hbar^2}\Delta E$$

or

$$K_{min}^2 - 2k_i K_{min} + \frac{2\mu}{\hbar^2}\Delta E = 0 \qquad \text{..........} \; (115)$$

Solving this quadratic equation in $K_{min}$ and selecting the solution appropriate to a minimal value, we have,

$$K_{min} = k_i - k_i\left\{1 - \frac{\Delta E}{k_i\gamma_i}\right\}^{1/2} \qquad \text{..........} \; (116)$$

which becomes on expanding in a polynomial and neglecting all powers of $\frac{\Delta E}{\gamma_i}$ higher than the second,

$$K_{min} = \frac{\Delta E}{2\gamma_i}\left\{1 + \frac{m\Delta E}{4\mu\gamma_i^2}\right\} \qquad \text{..........} \; (117)$$

This formula is then sufficiently accurate to reproduce the marked threshold which is characteristic of all cross sections involving electron impact.

# CHAPTER II.

## Electron loss from fast $H^-$ in $H$.

1. In recent years a detailed theoretical study of heavy particle atomic collisions involving various combinations of atoms and positive ions has been carried out by Bates and his colleagues. Bates and Dalgarno have summarized this work and compiled a bibliography of the relevant experimental data up to 1955 (Bates and Dalgarno 1956 ).

In a theoretical treatment of such collisions it is necessary to divide them into two groups; those in which the relative collisional velocity of the two atomic systems is great compared with the internal velocities of the systems and those where they are of the same order of magnitude. In the former case Born's approximation appears to be adequate, a belief based on the correlation of the available experimental and theoretical data on processes involving $H$ , $He$, and their positive ions. We For example, there is good agreement between theoretical (Bates and Williams 1957) and experimental data on electron loss from fast hydrogen atoms passing through Helium and good agreement is also found when the target gas is molecular hydrogen and the cross sections are expressed per gas atom. (Bates and Griffing 1955, Stier and Barnett 1956) Further information of interest is given by a discussion of stopping power of $H_2$ for protons by Dalgarno and Griffing(1955).

In almost all cases however, other approximations have to be introduced which necessarily lead to an added element of uncertainty in the final results: the atomic wave functions are seldom exact, (although they may be known to a reasonably accurate approximation) and molecular structure may be disregarded. Also some cases of the greatest theoretical simplicity prove to be the most difficult from the experimental standpoint; for instance, perhaps the best test of the Born Approximation would be the ionization of atomic hydrogen by fast protons, i.e. the process

$$H^+ + H(1s) \rightarrow H^+ + H^+ + e \qquad \text{..........} \; (1)$$

since no approximations other than that of Born are introduced into the theoretical study, but until recently, (c.f. Fite et al 1958 ) there had been no hope of performing such an experiment owing to the difficulty of producing a reasonably pure beam of atomic hydrogen. The analogous process involving molecular hydrogen, may produce a free electron in two ways

$$H^+ + H_2({}^1\Sigma_g) \rightarrow H^+ + H_2^+ + e \qquad \text{..........} (2)$$

or

$$H^+ + H_2({}^1\Sigma_g) \rightarrow H^+ + H^+ + H + e \qquad \text{.........} \; (3)$$

sothat a measurement of the ejected electron current does not necessarily refer totally to process (2). Also the possibility of exchange makes a measurement of the

$H_2^+$ current equally ambiguous. However triple coincidence measurements of $H^+$, $H_2^+$ and $e$ are now being carried out by McDowell, McDaniel and Martin 1959 (Private communication) which should give some accurate information on process (2). A comparision of the present best available experimental data on the process is given by Afrosimov, Il'in and Federenko (1958) and is compared with the earlier work by McClure (1959). Averages of their measurements of slow $H_2^+$ and slow electrons may be compared with the theoretical data of Bates and Griffing (1953) on the assumption that $H_2 \triangleq 2H$ . The agreement is excellent both in absolute magnitude and variation of the cross section with energy.

In theoretical studies of collisions involving negative ions there are added complexities. Greater precision in the wave functions is required to describe adequately the ground state properties than is necessary for the corresponding isoelectronic neutral atom or positive ion, due to the low value of the detachment energy. Further, the wave functions describing an electron moving in the field of a neutral atom, which may be in an excited state, are less well known than those of an electron in a Coulomb field.

The present state of negative ion physics has been reviewed by Massey (1950) Loeb (1955) and Branscomb (1957). Bethe and Saltpeter (1957) give a detailed discussion of possible wave functions for the ground state of $H^-$ , and the formation of $H^-$ has been discussed by these authers and also by Donahue and Hushfar (1959).

Here we are mainly concerned with the collision properties of these negative ions. Very little work has been done on fast negative ion collisions although Sida (1955) has used Born's approximation to calculate the electron loss cross section for fast $H^-$ in $He$, in which both the resultant species are left in their ground states, i.e.

$$H^-(1s^2) + He(1s^2) \rightarrow H(1s) + e + He(1s^2) \qquad \text{..........} \ (4)$$

It is known that while a Hylleraas (1929) wave function describes the Helium atom in its ground state reasonably well, it gives a rather crude picture of the isoelectronic $H^-$ ion, so that these results are in only moderate agreement with the experimental data of Hasted (1952). It is difficult therefore in such a case to separate the effects of making Born's approximation from those due to the wave functions, since the errors may be of the same order of magnitude. The following results we obtain on the analogous loss process in atomic hydrogen would make a reinvestigation of process (4), using improved wave functions, of considerable value.

We consider the processes

$$H^-(1s^2) + H(1s) \rightarrow H(nl) + H(n'l') + e \qquad \text{..........} \ (5)$$

in which the electron moves, after the collision, in the field of an hydrogen atom in the $nl^{th}$ state. The sum of these processes gives $\sigma_{-1,0}$, the total electron loss cross section for fast $H^-$ in $H$;

$$\sigma_{-1,0} = \sum_{nl} \sum_{n'l'} Q(1s; 1s^2 \rightarrow n'l'; nl, c) \qquad \text{..........} \ (6)$$

where the summations are over the discrete states of the hydrogen atoms and $Q(1s;1s^2 \rightarrow n'l';nl,c)$ is the cross section for process (5). Until recently, there has been no direct comparision data available on processes (5) but several experimental groups have measured $\sigma_{-1,0}$ with molecular hydrogen as the target gas and Allison has reviewed the relevant material. (Allison 1958). During the course of this work however, Fite and his co-workers (Fite 1959, Private communication and Report of the 10th Annual National Gaseous Electronic Conference, Washington D.C. 1959) began experiments to measure $\sigma_{-1,0}$ for atomic hydrogen and their results have now been published (Hummer et al 1960). The energy range considered unfortunately only slightly overlaps ours, being below that where one might expect the Born approximation to be reliable.

The wave function of an electron moving in the field of $H(nl)$ which is required in connection with (4) is also of considerable interest in other processes, namely that of slow elastic scattering of electrons by hydrogen atoms and the photodetachment cross sections for $H^-$, which are of great astrophysical interest in connection with the opacity of the solar atmosphere.

In the remainder of the chapter we calculate $Q(1s;1s^2 \rightarrow n'l';nl,c)$ for various values of $n'l'$ and $nl$ and various choices of wave function, estimate $\sigma_{-1,0}$ and determine the sensitivity of negative ion cross sections to choice of wave function. Born's approximation is used throughout, possible exchange processes being neglected.

2.1 In this paragraph we describe the theory required for the cross sections $Q(1s;1s^2\rightarrow n'l';\varkappa l,e)$ . The differential cross section for the ejection of one of the $H^-$ electrons into the solid angle $d\omega$ having momentum lying between $\underline{\varkappa}$ and $\underline{\varkappa}+\delta\underline{\varkappa}$ may, according to the Born approximation (c.f. Chapter I § 3) be written as

$$I(K,\varkappa)dK\,d\varkappa = \frac{8\pi^3M^2}{h^4k_i^2}|L(K,\varkappa)|^2K\,dK\,d\varkappa \quad ............(7)$$

where $\underline{k}_i$, $\underline{k}_f$ are the initial and final momentum vectors and the vector $\underline{K}$ is defined by

$$\underline{K} = \underline{k}_i - \underline{k}_f = k_i\underline{n}_0 - k_f\underline{n}_1 \quad ...........(8)$$

$\underline{n}_0$, $\underline{n}_1$ being unit vectors in directions $\underline{k}_i$ and $\underline{k}_f$ respectively. $M$ is the reduced mass of the system, $h$ is Planck's constant and the matrix element $|L(K,\varkappa)|^2$ is given by

$$|L(K,\varkappa)| = \left|\iiiint \Psi_i^*\Psi_f V(\underline{R},\underline{\rho}_1,\underline{r}_2,\underline{r}_3)e^{i\underline{K}\cdot\underline{R}}d\underline{R}\,d\underline{\rho}_1\,d\underline{r}_2\,d\underline{r}_3\right| \quad .......(9)$$

where $\Psi_i$, $\Psi_f$ are the initial and final wave functions of the whole colliding system, $\underline{R}$ is the internuclear distance, $\underline{\rho}_1$ is the position vector of the target particles' electron with respect to its nucleus and $\underline{r}_2$ and $\underline{r}_3$ are the position vectors of the $H^-$ electrons with respect to the nucleus of the ion. The interaction potential $V(\underline{R},\underline{\rho}_1,\underline{r}_2,\underline{r}_3)$ may be written in the form

$$V(\underline{R},\underline{\rho}_1,\underline{r}_2,\underline{r}_3) = e^2\left[\frac{1}{R} - \frac{1}{|\underline{R}-\underline{\rho}_1|} - \frac{1}{|\underline{R}+\underline{r}_2|} - \frac{1}{|\underline{R}+\underline{r}_3|} + \frac{1}{|\underline{R}+\underline{r}_2-\underline{\rho}_1|} + \frac{1}{|\underline{R}+\underline{r}_3-\underline{\rho}_1|}\right] \quad ..........(10)$$

so that by making use of Bethe's formula (Bethe 1930)

$$\int \frac{e^{i\underline{K}\cdot\underline{r}}}{|\underline{r}-\underline{r}'|}\,d\underline{r}' = \frac{4\pi}{K^2}e^{i\underline{K}\cdot\underline{r}} \qquad \ldots\ldots\ldots\ldots (11)$$

we may perform the integration over $\underline{R}$ - space (the initial and final wave functions being independent of the internuclear distance) and (9) reduces to

$$|L(K,k)| = \frac{4\pi e^2}{K^2}\left|\iiint \Psi_i^{*}\Psi_f\left(1-e^{i\underline{K}\cdot\underline{\rho}_1}\right)\left(1-e^{-i\underline{K}\cdot\underline{r}_2}-e^{-i\underline{K}\cdot\underline{r}_3}\right)d\underline{\rho}_1\,d\underline{r}_2\,d\underline{r}_3\right| \ldots\ldots\ldots (12)$$

2.2 In order to proceed further with the evaluation of the matrix element $L(K,k)$, we must choose suitable wave functions $\Psi_i, \Psi_f$ to describe the motion. We neglect the possibility of exchange between the electrons of the incident and target particles and we suppose that after the collision the target atom is left in the $n'l'$ state while the residual $H$ atom is in the $nl$ state, both particles being assumed to be initially in their ground states. We therefore without loss of accuracy write the space parts as

$$\Psi_i = \psi(1s,\rho_1)\,\psi_i(H^-)$$

$$\Psi_f = \psi(n'l',\rho_1)\,\psi_f(H^-) \qquad \ldots\ldots\ldots\ldots (13)$$

Also since the total wave function must be antisymmetric with respect to the interchange of like particles and also the spin part must be antisymmetric, (the only known bound state of $H^-$ being the $(1s)^2\,{}^1S_0$ state) the space part must be symmetric in $r_2$ and $r_3$, and hence we choose a suitably normalized $H^-$ wave function of the form

$$\psi_i(H^-) = N_i\{\psi(\alpha, r_2)\psi(\beta, r_3) + \psi(\alpha, r_3)\psi(\beta, r_2) \quad \ldots\ldots\ldots \quad (14)$$

where $\psi(\alpha, r)$ is the wave function of a hydrogen atom in the $(1s)$ state with effective nuclear charge $\alpha$ and $N_i$ is a normalization constant. If we adopt a similar form for $\psi_f(H^-)$ given by

$$\psi_f(H^-) = N_f\{\psi(nl, r_2)\psi(k, r_3) + \psi(nl, r_3)\psi(k, r_2)\} \quad \ldots\ldots\ldots \quad (15)$$

$\psi(k, r_2)$ being the free wave function of the ejected electrons with momentum $\hbar k$, we may write equation (12) in the form

$$|L(n'l'; nl, c)| = \frac{8\pi^2 e^2}{K^2} N_i N_f \left| (a_1 a_4 + a_2 a_3 - a_1 x_4 - a_2 x_3 - a_3 x_2 - a_4 x_1)(a_1' - x_1') \right| \quad \ldots \quad (16)$$

The integrals $a_i$, $x_i$ $(i = 1, 2, 3, 4)$ are defined by

$$\begin{aligned} x_1(\alpha, K) &= \int \psi(1s, \alpha)\psi(nl, 1) e^{i\mathbf{K}\cdot\mathbf{r}} d\mathbf{r} \quad ; \quad x_2 = x_1(\beta, K) \\ x_3(\alpha, K) &= \int \psi(1s, \alpha)\psi(k) e^{i\mathbf{K}\cdot\mathbf{r}} d\mathbf{r} \quad ; \quad x_4 = x_3(\beta, K) \qquad \ldots \quad (17) \\ a_i(\alpha) &= x_i(\alpha, 0) \qquad ; \quad x_i' = x_i(1, K) \end{aligned}$$

We now restrict ourselves to an evaluation of the cross section for the cases in which $n'l'$ and $nl$ can each take the values $1s$ or $2p$ since it is clear that these transitions will make the major contribution to the total cross section $\sigma_{-1,0}$. It is obvious that for exact wave functions the term $(a_1 a_4 + a_2 a_3)$ in equation (16) should vanish; however with the approximate forms employed for $\psi(k)$ it does so only if $l \neq 0$.

It will be noticed that the matrix element is separable in the coordinates of the target and incident systems and hence the cross section $Q(1s; 1s^2 \rightarrow n'l'; nl, c)$ for the process may be written as

$$Q(1s;1s^2 \to n'l';nl,\epsilon) = \frac{2}{k_i^2}\iiint |\mathcal{F}(1s^2 \to nl,\epsilon)|^2 |G(1s \to n'l')|^2 K^{-3}\, dK\, dk\, d\omega \quad (\pi a_0^2) \qquad \text{.....} \; (18)$$

where

$$\mathcal{F}(1s^2 \to nl,\epsilon) = a_1 a_4 + a_2 a_3 + a_1 x_4 + a_2 x_3 + a_3 x_2 + a_4 x_1$$
$$G(1s \to n'l') = a_1{}' - x_1{}' \qquad \text{.....} \; (19)$$

all quantities being in atomic units. The unit of energy is defined by

$$k_i^2 = \frac{\frac{1}{2} m v_i^2}{I_H} \qquad \text{..........} \; (20)$$

where $m$ is the electronic mass and $I_H$ is the ionization potential of hydrogen such that $E_i(\text{kev}) \simeq 25.0\, k_i^2$.

3.1 It is important that we should now discuss the choice of $H^-$ and free electron wave functions. $H^-$ is isoelectronic with $He$, so the success of a simple variational wave function of the form (14) for $He$ (when $\psi(\alpha,r), \psi(\beta,r)$ are taken to be hydrogenic with effective nuclear charge $\alpha = \beta$ ) makes it an obvious first choice for the ground state of $H^-$. Hylleraas (1929) gives the following values for the ground state of $He$ using such a wave function,

$$E_{calc} = -2.848 \text{ a.u.} \qquad ; \quad E_{observ} = -2.9037226 \text{ a.u.}$$

which is not unsatisfactory. However for $H^-$

$$E_{calc} = -0.473 \text{ a.u.} \quad ; \; E_{observ} = -0.5276 \text{ a.u.} \qquad \text{.........} \; (21)$$

which is less good. On calculating the 1st ionization potential (detachment energy ) for $He$ we find

$$x_{calc} = 0.8475 \text{ a.u.} \quad ; \; x_{observ} = 0.9035 \text{ a.u.} \qquad \text{.........} \; (22)$$

which is 12% in error, but for $H^-$

$$x_{calc} = -0.0273 \text{ a.u.} \; ; \; x_{observ} = +0.0272 \text{ a.u.} \qquad \ldots\ldots\ldots \; (23)$$

and therefore the simple one parameter hydrogenic variational function is totally unsatisfactory in representing the ground state of $H^-$, at least at small distances from the nucleus, since it predicts an unstable ion.

Initial improvements in the $H^-$ gronnd state wave functions were made in a series of papers by Chandrasekhar and his collaborators (Chandrasekhar 1944 a,b; Chandrasekhar and Breen 1946; Chandrasekhar and Munch 1946) in which they described computations of the photoionization cross section as a function of photon frequency, $a\nu$, and the total absorption with successively more elaborate wave functions. In particular, Chandrasekhar and Breen used

$$\Psi_i(H^-)_2 = N_i\left\{e^{-\alpha r_1-\beta r_2}+e^{-\alpha r_2-\beta r_1}\right\} \qquad \ldots\ldots\ldots\ldots \; (24)$$

and a wave function of the form

$$\Psi_i(H^-)_3 = N_i^1\,\Psi_i(H^-)_2\,(1+\gamma r_{12})$$

which takes explicit account of the electron-electron repulsion was suggested by Chandrasekhar (1944). These functions yield attachment energies

$$x_2 = 0.0133 \text{ a.u.} \quad ; \quad x_3 = 0.02592 \text{ a.u.}$$

$$x_{observ} = 0.0272 \text{ a.u.}$$

which is quite satisfactory and very definitely a great improvement on the values (23). Another three parameter function due to Bethe (1929) is

$$\Psi_i(H^-)_4 = N_i'' e^{-\alpha(r_1+r_2)}\left[1+\beta r_{12}+\gamma(r_1-r_2)^2\right]$$

giving $x_4 = 0{\cdot}0253$ au. The functions with explicit dependence on $r_{12}$ are unsatisfactory for our purposes since they spoil the separability of the coordinates and give rise to excessively complicated analysis. Highly accurate $H^-$ ground state functions have recently been developed by Herzberg, Hylleraas, Kinoshita and others in connection with the study of fine structure of the He spectra. (c.f. Bethe and Saltpeter 1957). They are too complicated for general use in collision problems, although they are practicable for the simpler calculations involved in photdetachment studies. (Smith and Burch, 1959) General discussions of the significance of absorption by $H^-$ in the solar photosphere may be found in Massey (1950) or Aller (1953).

The Chandrasekhar and Breen function (24) gives both an acceptable attachment energy and fairly reliable values of $a_\gamma$, so that it would be a good representation not only in regions close to the nucleus, which contribute strongly to $x_2$, but also in distant regions which are more heavily weighted in calculations of $a_\gamma$. We therefore use the expression (24) as our most refined wave function with the parameters $\alpha = 1{\cdot}04$, $\beta = 0{\cdot}2808$ Chandrasekhar 1944). Dalgarno and McDowell (1956a) have used this function in a calculation of $H^-$, $H$ slow charge exchange and their results are in close agreement with the experimental data of Hummer et al (1960), over the range where their theory is valid. Also, their calculated $H_2^-$ interaction energies are in excellent agreement with the more elaborate calculations of Fischer-Hjalmers (1959, Private Communication) which take account of configuration interaction. We shall make use of (24) with $\alpha = \beta$, to simplify our calculations in certain cases and suppose the ratio of the magnitudes of the matrix element to be independent of the transition considered. This is unjustifiable a priori and extra calculations would be needed to provide such justification. While the assumption that an improvement in the bound wave function merely acts as a scale factor is probably not true in general, for the class of transitions

$$Q(1s; 1s^2 \rightarrow n'l'; nl, c)$$

with $l \neq 0$, the simplification in the matrix element due to the orthogonality of the atomic orbitals makes this a reasonable supposition. We have therefore calculated the cross section $Q(1s; 1s^2 \rightarrow 1s; 2p, c)$ with both $\psi_i(H^-)_1$ and $\psi_1(H^-)_2$ but employed only the former wave function for the other transitions.

3.2 Finally, we must choose a suitable wave function for the free electron. On the basis of previous calculations of the energy distribution of ejected electrons from ionizing collisions (Bates and Griffing 1953; Bates et al, 1957), or from simple considerations of conservation of energy and momentum, it is certain that the great majority of the detached electrons will have energies of only a few ev. They will therefore tend to remain in the neighbourhood of the parent atom for an appreciable proportion of the collision time and may be described by a wave function essentially independent of the target system owing to the fast relative collisional velocity. Since we shall evaluate only those cross sections for which $nl$ is either $1s$ or $2p$ we shall require wave functions for a slow electron in the field of a hydrogen atom in the $1s$ or $2p$ states. Consider first the system $\{H(1s)+e\}$ : the static field of the hydrogen atom in the $1s$ state is

$$V_{1s}(r) = \left(1+\frac{1}{r}\right)e^{-2r}$$

which falls off exponentially. If $\underline{k}$ , the momentum (in atomic units) of the ejected electron is not too small, it will rapidly pass out of the range of this field and behave as a completely free electron. We may therefore adopt as a first approximation

$$\psi_1(\underline{k}) = \frac{k}{(2\pi)^{3/2}}e^{i\underline{k}.\underline{r}} \qquad \ldots\ldots\ldots\ldots (25)$$

which is the wave function of a free particle with momentum between $\underline{k}$ and $\underline{k}+\delta\underline{k}$ normalized such that

$$\int d\omega\int\psi(\underline{k})\psi(\underline{k}')d\underline{k} = \delta(\underline{k}-\underline{k}') \qquad \ldots\ldots\ldots\ldots (26)$$

This function is not orthogonal to the initial hydrogenic $1s$ orbitals of the $H^-$ system, so its use will not ensure the orthogonality of $\Psi_i(H^-)$ and $\Psi_f(H^-)$ .

A second, rather better approximation is obtained by solving the Schrödinger equation for an electron in the static field of a hydrogen atom in the $nl$ state, i.e. making the one body approximation (Mott and Massey 1949). Thus we take $\Psi_2(\underline{k})$ to be given by

$$\Psi_2(\underline{k}) = \frac{k^{1/2} g_0(r)}{(2\pi)^{3/2} c r} \qquad \ldots\ldots\ldots\ldots (27)$$

where $g_0(r)$ is that solution of the differential equation

$$\left\{ \frac{d^2}{dr^2} + k^2 - 2V_0(r) \right\} g_0(r) = 0 \qquad \ldots\ldots\ldots\ldots (28)$$

where

$$V_0(r) = \int |\Psi(nl, \underline{r}')|^2 \left\{ -\frac{1}{r} + \frac{1}{|\underline{r} - \underline{r}'|} \right\} d\underline{r}' \qquad \ldots\ldots\ldots\ldots (29)$$

which satisfies the boumdary conditions

$$g_0(0) = 0 \quad ; \; g_0(r) \sim \frac{c \sin kr}{k^{1/2}} \text{ for large } r \qquad \ldots\ldots\ldots\ldots (30)$$

This solution only takes into account the $s$- wave of the continuum, but as for $nl = 2p$ only the $s$- wave contributes, the use of (27) is no restriction.

A more refined variational $s$-wave function has been developed by Khashaba and Massey (1958) for the motion of an electron in the field of $H(2p)$ which we may apply to the solving of all processes of the type

$$H(1s) + H^-(1s^2) \rightarrow H(n'l') + H(2p) + e \qquad \ldots\ldots\ldots\ldots (31)$$

It may be written in the form

$$\Psi_3(\underline{k}) = \frac{k}{(2\pi)^{3/2}} \left\{ \frac{\sin kr}{kr} \left(1 + d e^{-r}\right) + c\left(1 - e^{-r}\right) \frac{\cos kr}{kr} \right\} \qquad \ldots\ldots\ldots (32)$$

where $c$ and $d$ are variationally determined parameters. As these parameters are only tabulated at four points a graphical interpolation was carried out for other values of $k$, so the results obtained cannot be regarded as very accurate, especially as $c$ and $d$ exhibit rapid variation with increasing $k$.

We shall now consider processes of the type

$$H(1s) + H^-(1s^2) \rightarrow H(2p) + H(nl) + e \qquad \ldots\ldots\ldots\ldots(33)$$

It is unecessary to examine the effect of the two parameter $H^-$ wave function on the cross section as this is dwelt with in the arguments above and so it remains to consider the consequences of refining the free wave function. We have taken the case in which nl = 1s and the problem then resolves itself into finding a suitable free wave to describe the motion of an electron in the field of H(1s). As there is no closed form for the total cross section, we limit ourselves to the contribution from the s- and p-waves of the continuum and it is unlikely that the higher order partial waves will make a noticeable difference at the low values of the momentum $\hbar k$ which are of importance. Calculations of the s-wave scattering of electrons by hydrogen atoms have steadily increased in accuracy in the last thirty years. (c.f. Bransden, Dalgarno, John and Seaton, 1958, hereafter referred to as BDJS, and the included references.) In a general note on Hulthen's (1944) method, Huang selects as his trial wave function one of the form

$$r\psi(k) = f(r)\sin kr + g(r)\cos kr \qquad \ldots\ldots\ldots\ldots(34)$$

where $f(r)$, $g(r)$ are subject to the conditions

$$f(0) \text{ finite} \quad ; \quad \lim_{r\to\infty} f(r) = 1$$

$$g(0) = 0 \quad ; \quad \lim_{r\to\infty} g(r) = \lambda = \tan\eta \qquad \ldots\ldots\ldots\ldots(35)$$

and $\eta$ is the phase shift. Massey and Moiseiwitsch (1951) have used this form of $\psi(k)$ for their calculations on the exchange approximation in the symmetric and antisymmetric cases and find that good agreement is obtained with results from numerical integrations of the exchange equation for $k = 0$ in the latter case, while there is only fair agreement in the former. BDJS have made variational calculations of the phases for both the s- and p-wave scattering of electrons by hydrogen atoms with full allowances for exchange and investigations of the effects of polarization. For the s-wave scattering they have adopted, at all energies, a wave function of the form

$$\psi_4(k;s) = \frac{1}{r(2\pi)^{3/2}}\left[\sin kr + a_0(1-e^{-2r})\cos kr + bkre^{-r}\right] \qquad \ldots\ldots\ldots\ldots(36)$$

where $a_0 = \tan\eta_0$ , $\eta_0$ is the phase shift and b is a variational parameter, which had previously been shown, by Seaton (1957), to be a great improvement on that of Massey and Moiseiwitsch for small $k$ , due to the addition of an exponential term and led to closer agreement with the numerical integrations for the symmetric case. We have therefore used the form (36) as our function for the symmetric s-wave scattering.

The previous calculations on p-wave scattering had been restricted to the one body approximation (Chandrasekhar and Breen 1946). BDJS, after investigating several forms of trial wave function, finally chose

$$\Psi_4(\underline{k};p) = \frac{1}{r(2\pi)^{3/2}}\left\{ j_1(kr) - a_1\left[1-e^{-2kr}\right]^3 y_1(kr) + b_1(kr)^2 e^{-3kr}\right\} \qquad \ldots\ldots\ldots\ldots(37)$$

where

$$j_1(x) = \left(\frac{\pi x}{2}\right)^{\frac{1}{2}} J_{3/2}(x) \quad ; \quad y_1(x) = \left(\frac{\pi x}{2}\right)^{\frac{1}{2}} J_{-3/2}(x)$$

which had been used

The expression (37) for $\Psi_4(\underline{k},p)$ yields a value of $a_1$ by both the Hulthen and Kohn (1948) methods which is extremely close to the exact value of 0.1120. Brackmann et al (1958) have made some absolute measurements of the elastic scattering cross section of electrons by hydrogen atoms and they compare their results with those of Massey and Moiseiwitsch and BDJS. It appears that if we assume

a) that the p-wave partial cross section $Q_1$ is negligible compared with the s-wave partial cross section $Q_0$, or

b) that we take into consideration $Q_1$ and that the value of BDJS is correct, then there is some indication that the BDJS calculations are more consistent with experiment.

We have therefore finally adopted for $\Psi_4(k)$ a function which is the sum of the s- and p-waves given by BDJS.

4.1 In this section we evaluate all the necessary integrals $x_i$ which we shall need to evaluate the total cross sections for the various approximations to the free wave function. Firstly for the cross section $Q(1s;1s^2\rightarrow 1s;2p,C)$ we need $x_1$ with $nl=2p$, which is easily calculated, i.e.

$$x_1(2p) = \int \psi(1s,\alpha)\psi(2p,1)e^{i\underline{K}.\underline{r}}d\underline{r} \qquad \ldots\ldots\ldots \; (38)$$

$$= \frac{\alpha^{3/2}}{4\sqrt{2\pi}}\int r e^{-(\alpha+1/2)r}e^{iKr\mu}\mu \, d\underline{r}$$

on putting $\mu=\cos\theta$. Integrating over $\phi$

$$x_1(2p) = \frac{\alpha^{3/2}}{2\sqrt{2}}\int_0^\infty\int_{-1}^{+1} r^3 e^{-(\alpha+1/2)r+iKr\mu}\mu \, dr \, d\mu$$

an elementary integral. We obtain

$$x_1(2p) = \frac{2^{5/2}\alpha^{3/2}iK\delta}{(\delta^2+K^2)^3} \; ; \; \delta=\alpha+1/2 \qquad \ldots\ldots\ldots\ldots \; (39)$$

with a similar expression for the case $nl=1s$. The corresponding $a_i$ integrals $a_1(1s)$ and $a_1(2p)$ can then be deduced immediately by letting $K\rightarrow 0$. The only other distinct $x_i$ integral which need be considered is $x_3$, in the case where $\psi_K$ may be expanded in the form

$$\psi_K = \sum_l (2l+1)i^l e^{-i\eta_l}f_l(r)P_l(\cos\theta) \qquad \ldots\ldots\ldots\ldots \; (40)$$

We now neglect all scattering except that due to the $s$- and $p$- waves which are given by equations (36), (37). Therefore

$$x_3 \doteq \int\psi(1s,\alpha)\psi_4(\underline{K};s)e^{i\underline{K}.\underline{r}}d\underline{r} +$$

$$3iP_1(\cos\theta')\int\psi(1s,\alpha)\psi_4(\underline{K};p)e^{i\underline{K}.\underline{r}}d\underline{r} \qquad \ldots\ldots\ldots\ldots \; (41)$$

Let us consider first the $s$-wave scattering ;

$$\int \psi(K,\alpha)\,\Psi_4(\underline{k};s)\,e^{i\underline{k}.\underline{r}}\,d\underline{r}$$

$$= \frac{2^{1/2}\alpha^{3/2}}{\pi K}\int_0^\infty e^{-\alpha r}\sin Kr\left[\sin kr + a_0\cos kr\,(1-e^{-2r})\right]dr \qquad \ldots\ldots (42)$$

on expanding $e^{i\underline{k}.\underline{r}}$ in partial waves. This expression becomes, on expressing the products of the trigonometrical functions as sums of other similar functions

$$= \frac{\alpha^{3/2}}{\sqrt{2}\pi K}\int_0^\infty e^{-\alpha r}\left\{\cos(\overline{K-k}\,r) - \cos(\overline{K+k}\,r)\right\}dr + \frac{\alpha^{3/2}a_0}{\sqrt{2}\pi K}\int_0^\infty e^{-\alpha r}(1-e^{-2r})\left\{\sin(\overline{K+k}\,r) + \sin(\overline{K-k}\,r)\right\}dr$$

$$= \frac{\alpha^{3/2}}{\sqrt{2}\pi K}\left[\frac{\alpha}{\alpha^2+(K-k)^2} - \frac{\alpha}{\alpha^2+(K+k)^2}\right] + \frac{\alpha^{3/2}a_0}{\sqrt{2}\pi K}\left[\frac{(K+k)}{\alpha^2+(K+k)^2} + \frac{(K-k)}{\alpha^2+(K-k)^2} - \frac{(K+k)}{(\alpha+2)^2+(K+k)^2} - \frac{(K-k)}{(\alpha+2)^2+(K-k)^2}\right]$$

$$= \frac{2^{3/2}\alpha^{5/2}k}{\pi}\left[\left\{\alpha^2+(K-k)^2\right\}^{-1}\left\{\alpha^2+(K+k)^2\right\}^{-1}\right]$$

$$+ \frac{\sqrt{2}\alpha^{3/2}a_0}{\pi}\Big[(\alpha^2+K^2-k^2)\left\{\alpha^2+(K+k)^2\right\}^{-1}\left\{\alpha^2+(K-k)^2\right\}^{-1}$$

$$- \left\{(\alpha+2)^2+K^2-k^2\right\}\left\{(\alpha+2)^2+(K+k)^2\right\}^{-1}\left\{(\alpha+2)^2+(K-k)^2\right\}^{-1}\Big] \ldots (43)$$

The second integral in (41) is of the form

$$-9\cos\chi.\frac{\alpha^{3/2}}{\sqrt{2\pi}}\int_0^\infty\int_{-1}^{+1} re^{-\alpha r}\left(\frac{\pi}{2Kr}\right)^{1/2}J_{3/2}(Kr)\,P_1^{\,2}(\cos\theta)\ \times$$

$$\left[\left(\frac{\pi kr}{2}\right)^{1/2}J_{3/2}(kr) - a_1(1-e^{-2kr})^3\left(\frac{\pi kr}{2}\right)^{1/2}I_{3/2}(kr) + bk^2r^2e^{-3kr}\right]dr\,d(\cos\theta)$$

$$\ldots (44)$$

on substituting for $P_1(\cos\theta')$, using the Legendre polynomial addition theorem

$$P_1(\cos\theta') = P_1(\cos\chi)P_1(\cos\theta) + P_1{}'(\cos\chi)P_1{}'(\cos\theta)\cos(\phi-\psi) \ldots\ldots (45)$$

and integrating over $\phi$ . The relevant coordinate system is shown in figure 9, the scattered electron being ejected into solid angle $d\omega = d(\cos\chi)d\psi$. The integration over $\theta$ is now easily performed and (44) becomes

$$-\frac{3\sqrt{2}\alpha^{3/2}}{\pi}\cos\chi\Bigg[\frac{\pi}{2}\left(\frac{\mathcal{K}}{K}\right)^{1/2}\int_0^\infty re^{-\alpha r}J_{3/2}(Kr)J_{3/2}(\mathcal{K}r)\,dr \;-$$
$$\frac{\pi}{2}\left(\frac{\mathcal{K}}{K}\right)^{1/2}a_1\int_0^\infty re^{-\alpha r}\left(1-e^{-2\mathcal{K}r}\right)^3J_{3/2}(Kr)J_{-3/2}(\mathcal{K}r)\,dr$$
$$+\,b\mathcal{K}^2\left(\frac{\pi}{2K}\right)^{1/2}\int_0^\infty r^{5/2}e^{-(\alpha+3\mathcal{K})r}J_{3/2}(Kr)\,dr\Bigg] \qquad \ldots (46)$$

The first of the integrals within the square brackets may be readily evaluated (see Watson, The Theory of Bessel Functions 1944) who obtains

$$\int_0^\infty e^{-at}J_\nu(bt)J_\nu(ct)\,dt = \frac{1}{\pi\sqrt{bc}}Q_{\nu-1/2}\left(\frac{a^2+b^2+c^2}{2bc}\right) \qquad \ldots. (47)$$

so that

$$\int_0^\infty te^{-at}J_\nu(bt)J_\nu(ct)\,dt = -\frac{1}{\pi\sqrt{bc}}\frac{\partial}{\partial a}\left\{Q_{\nu-1/2}\left(\frac{a^2+b^2+c^2}{2bc}\right)\right\} \qquad \ldots. (48)$$

The above author also gives the result (P.386)

$$\int_0^\infty e^{-at}J_\nu(bt)t^{\nu+1}\,dt = \frac{2a.(2b)^\nu\,\Gamma(\nu+3/2)}{(a^2+b^2)^{\nu+3/2}\sqrt{\pi}} \qquad \ldots. (49)$$

from which we can immediately evaluate the third integral in (46). It now remains to calculate integrals of the type

$$I(\alpha) = \int_0^\infty re^{-\alpha r}J_{3/2}(Kr)J_{-3/2}(\mathcal{K}r)\,dr \qquad \ldots.. (50)$$

which becomes

$$I(\alpha) = \int_0^\infty \frac{-2}{\pi\sqrt{K\kappa}} e^{-\alpha r}\Big[-\cos Kr \sin \kappa r + \frac{\sin Kr \sin \kappa r}{Kr} - \frac{\cos Kr \cos \kappa r}{\kappa r} + \frac{\sin Kr \cos \kappa r}{K\kappa r^2}\Big] \quad ..(51)$$

$$= \frac{1}{\pi\sqrt{K\kappa}}\int_0^\infty e^{-\alpha r}\left\{\sin(\overline{K+\kappa}\,r) + \sin(\overline{\kappa - K}\,r)\right\}dr + \frac{2\alpha}{\pi(K\kappa)^{3/2}}\int_0^\infty \frac{\cos \kappa r \sin Kr}{r} e^{-\alpha r} dr - \frac{1}{\kappa}$$

on substituting for the Bessel functions and integrating the third term of (51) by parts. Therefore we finally obtain,

$$I(\alpha) = \frac{2}{\pi\sqrt{K\kappa}}\left\{\frac{\kappa(\alpha^2 - K^2 + \kappa^2)}{[\alpha^2 + (K+\kappa)^2][\alpha^2 + (K-\kappa)^2]} + \frac{\alpha}{2K\kappa}\tan^{-1}\frac{2\alpha K}{\alpha^2 + \kappa^2 - K^2}\right\} \quad ..(52)$$

and

$$x_3 = \frac{2^{3/2}\alpha^{5/2}\kappa}{\pi}\left\{[\alpha^2 + (K+\kappa)^2]^{-1}[\alpha^2 + (K-\kappa)^2]^{-1} + \frac{3\cos\chi}{4K^2\kappa^2}\left[Q_0(y) + \frac{y}{1+y^2}\right]\right\}$$

$$+ \frac{\alpha^{3/2}a_0}{\sqrt{2}\,\pi K}\left\{\frac{(K+\kappa)}{\alpha^2 + (K+\kappa)^2} + \frac{(K-\kappa)}{\alpha^2 + (K-\kappa)^2} - \frac{(K+\kappa)}{(\alpha+2)^2 + (K+\kappa)^2} - \frac{(K-\kappa)}{(\alpha+2)^2 + (K-\kappa)^2}\right\}$$

$$- \frac{2^{7/2}.\,3\alpha^{3/2}\,b\cos\chi}{\pi} \cdot \frac{K\kappa^2(\alpha + 3\kappa)}{[K^2 + (\alpha+3\kappa)^2]^3}$$

$$+ \frac{3}{\sqrt{2}}\alpha^{3/2}\cos\chi\left(\frac{\kappa}{K}\right)^{1/2} a_1\left\{I(\alpha) - 3I(\alpha+2\kappa) + 3I(\alpha+4\kappa) - I(\alpha+6\kappa)\right\} \quad ..(53)$$

The result for the contribution to $x_3$ from the $s$- and $p$-waves of the continuum when the free electron is represented by a plane wave is then easily obtained from (53) by letting the parameters $a_0$, $a_1$, $b$ tend to zero. Further, the value for both plane and modified free waves of $a_4$ also readily appears on letting $K \to 0$ in this equation, although in practice $q_4$ was worked out separately and was then available as a check on the calculation of $x_4$.

4.2 The necessary $a_i$ integrals must now be evaluated. When making the one body approximation to the free wave for cross sections of the type (31), we need to evaluate an $a_3$ integral of the form

$$a_3 = \frac{k^{1/2}}{(2\pi)^{3/2} e} \int \frac{\psi(1s,\alpha)}{r} g_0(r)\, d\mathbf{r} \qquad \text{......} \quad (54)$$

$$= \frac{\sqrt{2}\, k^{1/2} \alpha^{3/2}}{\pi e} \int_0^\infty r e^{-\alpha r} g_0(r)\, dr \qquad \text{......} \quad (55)$$

To do this, we must first solve equation (28) for $g_0(r)$. Evaluating $V_0(r)$ from (29), (28) becomes

$$\left\{\frac{d^2}{dr^2} + k^2 - \frac{24}{r^3} + 2e^{-r}\left[\frac{r^2}{8} + \frac{3r}{4} + \frac{11}{4} + \frac{7}{r} + \frac{12}{r^2} + \frac{12}{r^3}\right]\right\} g_0(r) = 0 \qquad \text{..} \quad (56)$$

which for small $r$ reduces approximately to

$$\left\{\frac{d^2}{dr^2} + k^2 + \frac{2}{r} - \frac{1}{2}\right\} g_0(r) = 0 \qquad \text{.....} \quad (57)$$

An expansion, $g_0 = \sum_n a_n r^n$ is used to solve (57) for small $r$ and to initiate an iteration process by which we tabulated values for $g_0(r)$ for $r$ ranging from 0·01 to 10·2, the method used being that of Fox and Goodwin (1949) who give the formula

$$\left(1+\tfrac{1}{12}h^2 f_1\right)y_1 = \left(2-\tfrac{5}{6}h^2 f_0\right)y_0 - \left(1+\tfrac{1}{12}h^2 f_{-1}\right)y_{-1} + \Delta$$

$$\Delta = \left(-\frac{1}{240}\delta^6 + \frac{13}{15120}\delta^8 - \cdots\right)y_0 \qquad \text{.......} \quad (58)$$

for solving the second order differential equation

$$y'' + fy = 0 \qquad \text{..........} \quad (59)$$

The normalization constant $C$ was calculated by a method due to Strömgren (c.f. Bates and Seaton 1949). It can be easily verified that (59) is satisfied by

$$y = Cz^{1/2}\sin\left[\phi(r)\right] \qquad \ldots\ldots\ldots \quad (60)$$

where $z$ which represents $\frac{d\phi}{dr}$ is given by

$$z^2 = f + z^{1/2}\frac{d^2}{dr^2}\left(z^{-1/2}\right) \qquad \ldots\ldots\ldots \quad (61)$$

This equation may be solved by iteration and since the convergence is extremely rapid, we only needed to replace $z$ by $\lambda^{1/2}$ in the second term. Now, choosing two radial distances $r_1$ and $r_2$ and introducing

$$a_1 = z_1^{1/2}y(r_1) \quad ; \quad a_2 = z_2^{1/2}y(r_2)$$
$$\alpha = \frac{1}{2}\int_{r_1}^{r_2} z\,dr \qquad \ldots\ldots\ldots \quad (62)$$

it can be readily shown that

$$C = \frac{1}{2}\left\{(a_1+a_2)^2\sec^2\alpha + (a_1-a_2)^2\operatorname{cosec}^2\alpha\right\}^{1/2} \qquad \ldots\ldots\ldots \quad (63)$$

Finally, we wish to estimate $a_3$ when the free wave has the form (32),

$$a_3 = \int \frac{\alpha^{3/2}}{\sqrt{\pi}}e^{-\alpha r}\frac{k}{(2\pi)^{3/2}}\left\{\frac{\sin kr}{kr}(1+de^{-r}) + c(1-e^{-r})\frac{\cos kr}{kr}\right\}d\mathbf{r}$$

$$= \frac{2^{1/2}\alpha^{3/2}}{\pi}\int_0^\infty re^{-\alpha r}\left\{\sin kr(1+de^{-r}) + c(1-e^{-r})\cos kr\right\}dr \qquad \ldots\ldots \quad (64)$$

on integration over the angular variables. All the integrals involved are well known, so $a_3$ becomes

$$a_3 = \frac{2^{1/2}\alpha^{7/2}}{\pi}\left[\frac{2k\alpha}{(\alpha^2+k^2)^2} + \frac{2k(\alpha+1)d}{[(\alpha+1)^2+k^2]^2} + \frac{c(\alpha^2-k^2)}{(\alpha^2+k^2)^2} - \frac{c\left[(\alpha+1)^2-k^2\right]}{[(\alpha+1)^2+k^2]^2}\right] \qquad \ldots \quad (65)$$

by setting the parameters $c$, $d$ equal to zero in (65) we obtain the value of $a_3$ for the plane wave approximation to $\psi(\varkappa)$ i.e.

$$a_3 = \frac{2^{3/2}\alpha^{5/2}K}{\pi(\alpha^2+K^2)^2} \qquad \text{.... (66)}$$

5. The evaluation of the matrix element $\int |\mathcal{J}(1s^2 \to nl, c)|^2 d\omega$ is trivial in the case $nl = 2p$, since in all the cases considered the integrand is independent of $\omega$, however when $nl = 1s$, we see that the matrix element may be written in the form

$$\int |\mathcal{J}(1s^2 \to nl, c)|^2 d\omega = \int (A + B\cos\chi)^2 d(\cos\chi)\, d\omega \qquad \text{...... (67)}$$

where $A$, $B$ are functions of $K$, $\varkappa$, so that

$$\int |\mathcal{J}(1s^2 \to nl, c)|^2 d\omega = 4\pi\left(A^2 + \tfrac{1}{3}B^2\right) \qquad \text{...... (68)}$$

The final integrations over $K$, $\varkappa$ where then carried out numerically for all cases. The upper limits of the integrations over $K$ and $\varkappa$ were taken to be infinity and it was sufficient to evaluate $K_{min}$ from the formula

$$K_{min} \doteq \frac{\Delta E + \varkappa^2}{2k_i}$$

(c.f. Chapter I) and to take $\varkappa_{min} = 0$.

6. At sufficiently high energies it is permissible to take $K_{max}$ as infinite and $K_{min}$ as zero in each term of the summation for $\sigma_{-1,0}$. Bates and Griffing (1954) have pointed out that it is often possible by application of the Bethe sum rule (Bethe 1930) or some variant of it, to sum such a series under these conditions. An approximate asymptotic expression for $\sigma_{-1,0}$ may be obtained by supposing that the

target hydrogen atom is left either in the ground or state; i.e.

$$\sigma_{-1,0} = \sum_{n'l'=1s,2p} \sum_{nl} Q(1s;1s^2 \rightarrow n'l';nl,c) \qquad \text{.......} \ (69)$$

Consider the case when $\alpha = \beta$ for simplicity,

$$\sigma_{-1,0} = \frac{2^5\pi}{g_i^2}\int_0^\infty\int_0^\infty \sum_{n'l'=1s,2p} |a_1' - x_1'|^2 \sum_{nl} |a_1 a_3 - a_1 x_3 - a_3 x_1|^2 K^{-3}\, dK\, d\mathcal{K} \qquad \text{.......} \ (70)$$

on carrying out the integration over the angles of ejection. Now $a_1(1s \rightarrow nl) = 0$ if $nl \neq ns$ and of the non zero terms only $a_1(1s\text{-}1s)$ will be large: thus (69) becomes

$$\sigma_{-1,0} \doteq \frac{2^5\pi}{g_i^2}\int_0^\infty\int_0^\infty \left[|G(1s\rightarrow 1s)|^2 + |G(1s\rightarrow 2p)|^2\right] |a_3|^2$$

$$\times \left[\sum_{nl} |x_1(nl)|^2 - |x_1(1s)|^2\right] K^{-3}\, dK\, d\mathcal{K}$$

$$+ Q(1s;1s^2 \rightarrow 1s;1s,c) + Q(1s;1s^2 \rightarrow 2p;1s,c) \qquad \text{.......} \ (71)$$

It is easily shown that

$$\sum_{nl} |x_1(nl)|^2 = 1 \qquad \text{.........} \ (72)$$

so we obtain, knowing $Q(1s;1s^2 \rightarrow 1s \text{ or } 2p;1s,c)$

$$\sigma_{-1,0} = \frac{2^5\pi}{g_i^2}\iint |a_3|^2 \left\{|G(1s\rightarrow 1s)|^2 + |G(1s\rightarrow 2p)|^2\right\}\left\{1 - |x_1(1s)|^2\right\} K^{-3}\, dK\, d\mathcal{K} + B/g_i^2 \qquad \text{...} \ (73)$$

where $B$ is a constant and (73) is readily evaluated when $\psi_1(\underline{\mathcal{K}})$ is used, to yield

$$\sigma_{-1,0} \sim \frac{41.36}{g_i^2} \quad (\pi a_0^2) \qquad \text{...........} (74)$$

7. While the cross sections are of primary interest, it is often important to know the distribution of the ejected electrons with respect to momentum and the fraction of those having energy in excess of some fixed amount, since

these quantities determine the resultant average gas temperature and the possibility of the occurence of secondary processes. It is clear that collisional detachment of electrons from slow $H^-$ by hydrogen atoms could be of considerable importance in the solar photosphere through its effect on the $H^-$ number density. Further, the energy, which is equivalent to the temperature of the ejected electrons will be of interest in computing the effect of collisional detachment as a cooling mechanism in magnetic fields. The first of these quantities, the momentum differential cross section, $Q(1s;1s^2 \to n'l';nl,c|\kappa^2;E_i)$ being the cross section for ejection of an electron in the specified transition with energy between $\kappa^2$, $\kappa^2+d\kappa^2$ rydbergs from an incident particle of energy $E_i$, arises as an intermediate step in our cross section calaulation. The fraction of electrons having energy greater than $\kappa_0^2$ rydbergs, after a transition $1s \to n'l'; 1s^2 \to nl, c$ is given by

$$\mathcal{F}(\kappa^2;E_i) = \frac{\int_{\kappa^2}^{\infty} Q(1s;1s^2 \to n'l';nl,c|\kappa^2,E_i)\,d\kappa^2}{\int_0^{\infty} Q(1s;1s^2 \to n'l';nl,c|\kappa^2,E_i)\,d\kappa^2} \qquad \text{.... (75)}$$

(c.f. Bates and Griffing 1953)

8.1. In this paragraph we discuss our results on the processes of the type

$$H(1s) + H^-(1s^2) \to H(1s) + H(nl) + e \qquad \text{........ (76)}$$

We considered in most detail that for which $nl = 2p$ since this leads to a helpful simplification in the matrix element, and to begin with, investigated the effect of improving the initial $H^-$ function using $\Psi_i(H^-)_1(\alpha=\beta)$ and $\Psi_i(H^-)_2\ (\alpha\neq\beta)$ the free wave function being taken as $\psi_1(\mathbf{k})$ for simplicity. The cross sections at all energies appear to be very sensitive to such changes, at least as regards absolute magnitude, the improved two parameter wave function increasing them by a order of magnitude. Almost all of this increase comes from small values of $K$ (forward scattering) and since the variational parameters enter as $N_\alpha^2(\alpha^2+K^2)^{-6}$ and $N_\beta^2(\beta^2+K^2)^{-6}$ where $\alpha=1{\cdot}04$ and $\beta=0{\cdot}2808$, $K$ being small, a large increase in the magnitude of $Q$ is to be expected, even allowing for the differing normalization factors $N_\alpha$ and $N_\beta$. Clearly this effect will be almost independent of the transition considered. It may be however, that inclusion of an $r_{12}$ term in the ionic wave function would not further increase the cross section.

Now consider the effect of modifying the free wave function, noting that for $nl=2p$ these two effects are independent. We have used both $\psi_1(\mathbf{k})$, a plane wave, $\psi_2(\mathbf{k})$ a s- wave one body solution and $\psi_3(\mathbf{k})$ the Khashaba-Massey variational function for an electron in the field of $H(2p)$. As the energy of impact increases, we had expected the mean ejection energy to increase also and the effects of distortion to become less important. Figure (1) where we display the results for these three cases shows that this is not the case: the distribution in energy of the ejected electrons seems to be nearly independent of impact energy and the obvious importance of distortion suggests that

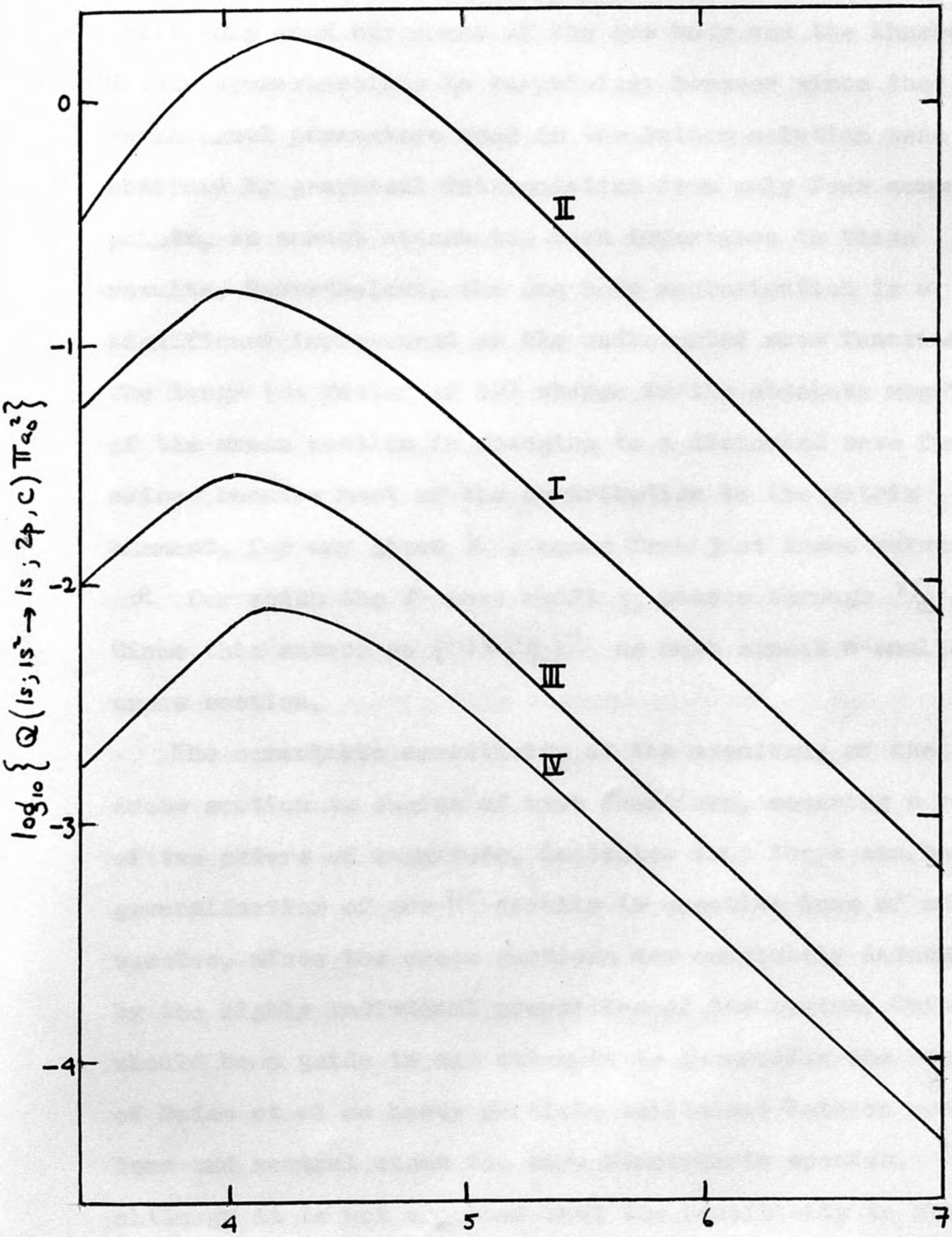

0
-1
-2
-3
-4
$\log_{10}\{Q(1s;1s^2 \rightarrow 1s;2p,C)\,\pi a_0^2\}$
II
I
III
IV
4
5
6
7
$\log_{10}\{E_i(\mathrm{ev})\}$

Figure 1.

nearly all these electrons are slow. (c.f. § 3.2). The relatively good agreement of the one body and the Khashaba-Massey approximations is surprising: however since the variational parameters used in the latter solution were obtained by graphical interpolation from only four computed points, we cannot attach too much importance to these results. Nevertheless, the one body approximation is a significant improvement on the undistorted wave function. The large ($\hat{=}$ factor of 10) change in the absolute magnitude of the cross section in changing to a distorted wave function arises because most of the contribution to the matrix element, for any given $K$, comes from just these values of $k$ for which the $s$- wave shift $\eta_0$ passes through $\pi/2$. Since this enters as $(1+\tan^2\eta_0)^{-1}$ we must expect a smaller cross section.

The remarkable sensitivity of the magnitude of the cross section to choice of wave functions, covering a range of two orders of magnitude, indicates that there can be no generalization of our $H^-$ results to negative ions of other species, since the cross sections are completely determined by the highly individual properties of the system. This should be a guide in any attempts to generalize the results of Bates et al on heavy particle collisions between positive ions and neutral atoms to, say, atmospheric species, although it is not expected that the sensitivity to choice wave function will be nearly as great in these cases.

By what can only be regarded as a fortunate coincidence at this stage, the effects of improving the bound and free wave functions are opposite in sign and similar in magnitude. We therefore felt justified, for other transitions of this class, in adopting the simplest wave functions. While the absolute magnitude of the cross section must be uncertain by perhaps as much as a factor of five, the relative magnitudes of the different cross sections of this group should be quite accurate.

We now deal with the other group of transitions in which $nl = 1s$ and consider in detail the transition

$$H(1s) + H^-(1s^2) \rightarrow H(2p) + H(1s) + e \qquad \ldots\ldots\ldots\ldots (77)$$

The corresponding cross section being $Q(1s;1s^2 \rightarrow 2p;1s,c)$, we evaluate this using a single parameter bound $H^-$ function $\psi_i(H^-)_1$, but using both a plane wave $\psi_1(\underline{k})$ and the BDJS function $\psi_4(\underline{k})$, taking into account both the $s$- and $p$- waves. As in the previous case, the variational parameters of the BDJS function are available only for a few values of $k$ and these differ according to whether the $s$- or $p$-wave is being considered. We computed the $s$-wave contribution to $\int |f(1s^2 \rightarrow 1s,c)|^2 d\omega$ for $k = 0.1(0.1)0.4$ and extrapolated to $k=0.5$ for each value of $K$, to compare it with the $p$-wave contribution evaluated for $k=0.5$ and $1.0$. These results were summed and are compared with the corresponding plane wave results in figure (2). Because $\eta_0$, the symmetric $s$- wave shift again passes through $\frac{\pi}{2}$ in the range of $k$ of interest the $\{1+\tan^2\eta_0\}^{-1}$ factor reduces the BDJS $s$- wave contribution by about a factor of seven at all $K$. However the $p$- wave contribution

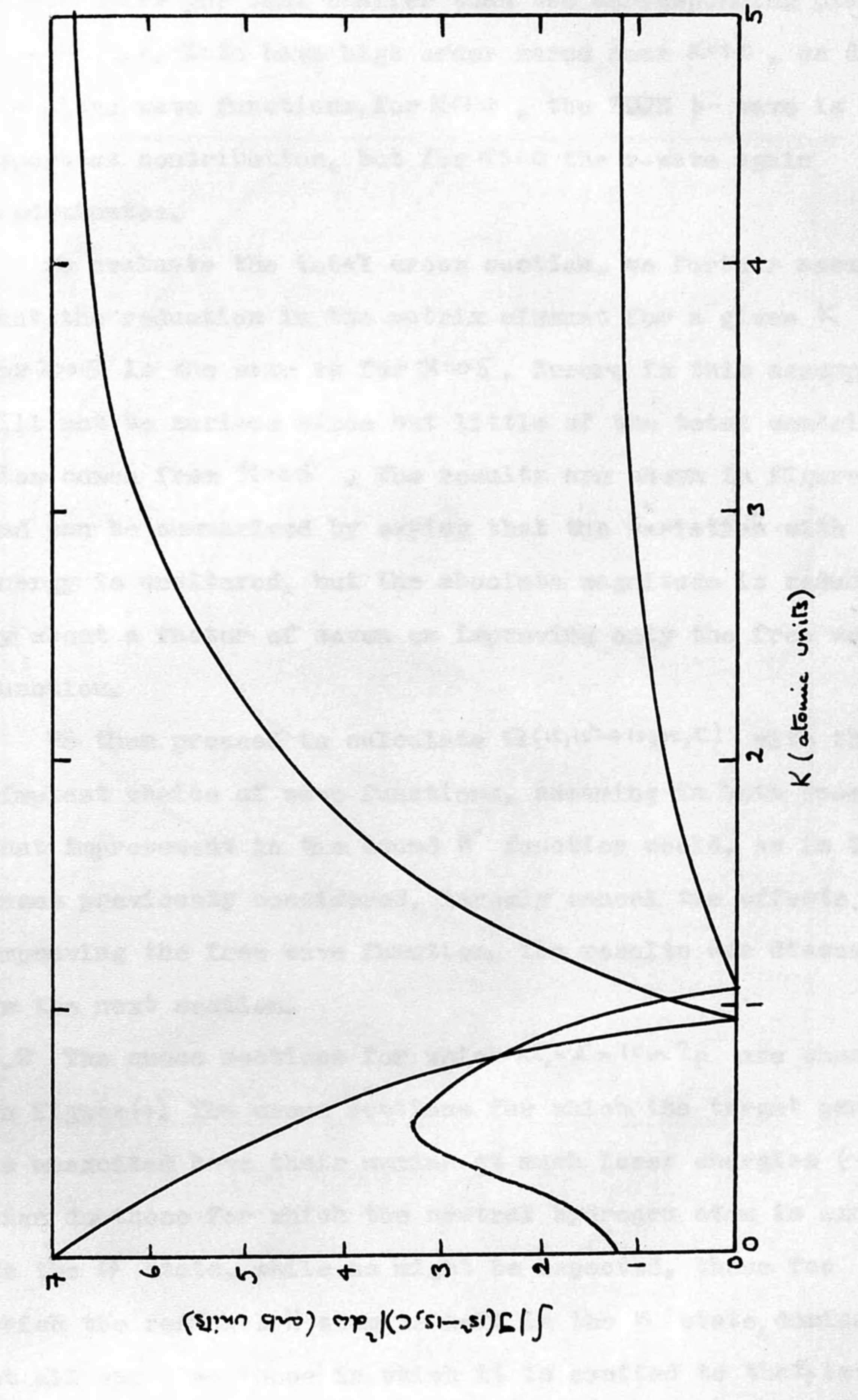

$\int |J(1s^2 \to 1s,c)|^2 d\omega$ (arb units)
7
6
5
4
3
2
1
0
0
1
2
3
4
5
K (atomic units)

Figure 2.

is only a few per cent smaller than the corresponding plane wave result. Both have high order zeros near $K=1.0$, as do the plane wave functions. For $K<1.0$, the BDJS $p$-wave is the important contribution, but for $K>1.0$ the $s$-wave again predominates.

To evaluate the total cross section, we further assume that the reduction in the matrix element for a given $K$ for $K>0.5$ is the same as for $K=0.5$. Errors in this assumption will not be serious since but little of the total contribution comes from $K>0.5$. The results are shown in figure (3), and can be summarized by saying that the variation with energy is unaltered, but the absolute magnitude is reduced by about a factor of seven on improving only the free wave function.

We then proceed to calculate $Q(1s;1s^2 \rightarrow 1s;1s,C)$ with the simplest choice of wave functions, assuming in both cases that improvement in the bound $H^-$ function would, as in the cases previously considered, largely cancel the effects of improving the free wave function. The results are discussed in the next section.

8.2 The cross sections for which $nl, n'l' = 1s$ or $2p$ are shown in figure (4). The cross sections for which the target particle is unexcited have their maxima at much lower energies ($\sim 10^4$ ev) than do those for which the neutral hydrogen atom is excited to the $2p$ state, while as might be expected, those for which the residual $H$ atom is left in the $1s$ state, dominate at all energies those in which it is excited to the $2p$ level.

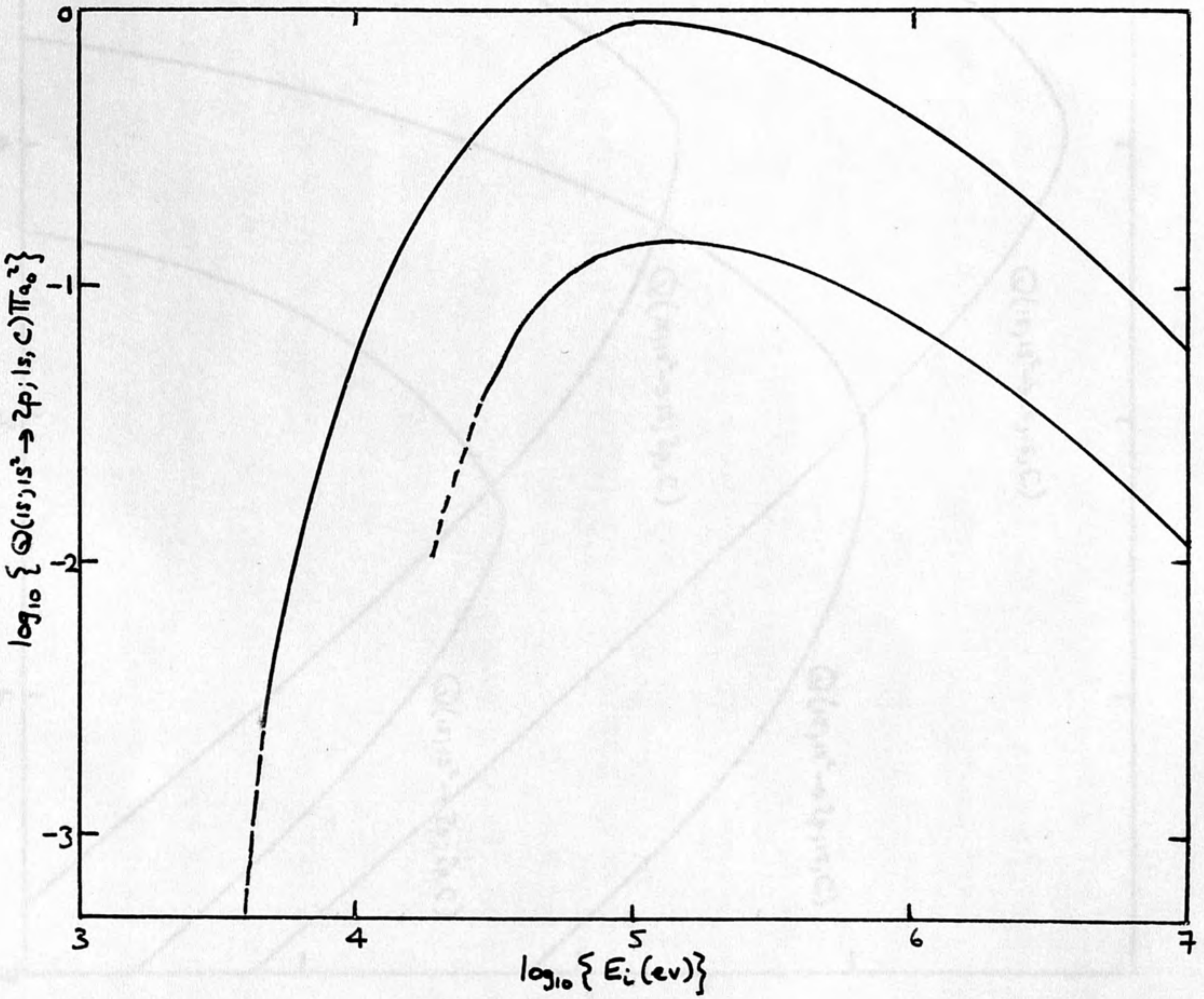


Figure 3.

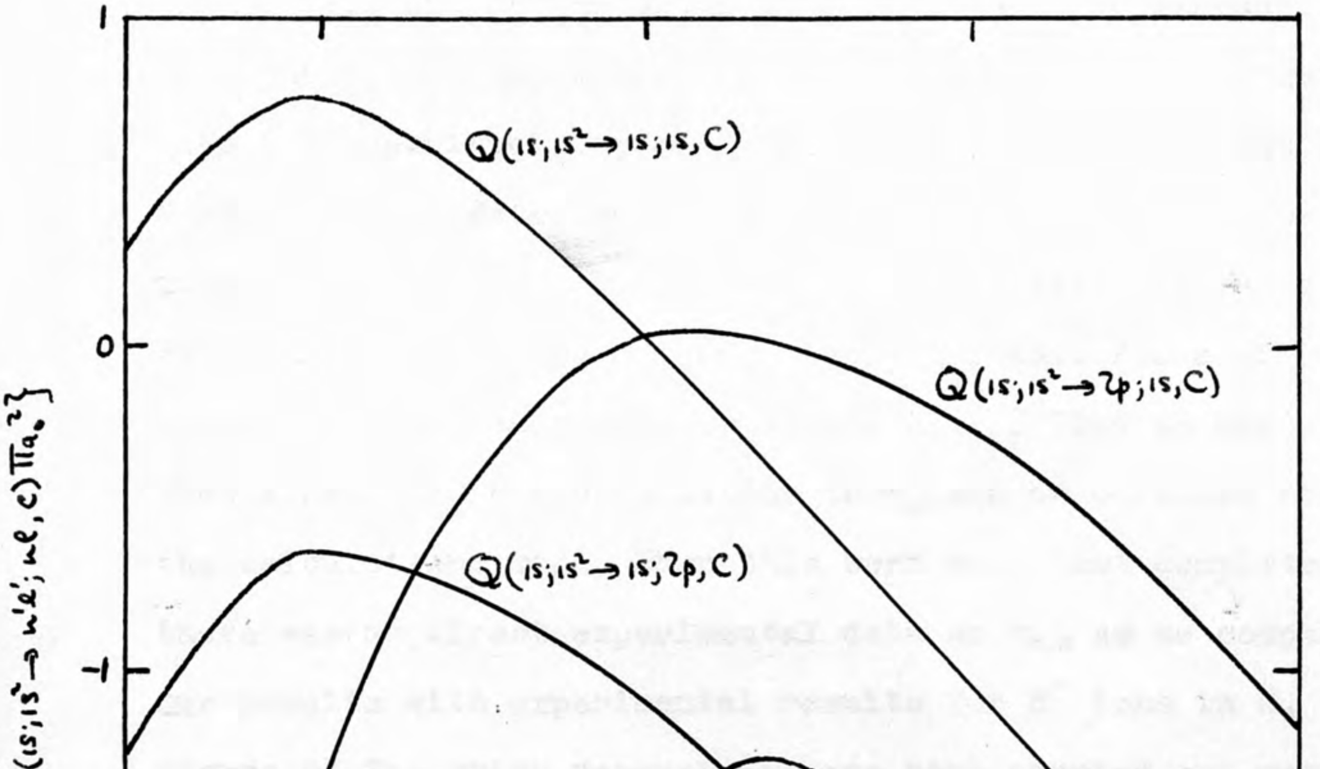

$Q(1s;1s^2 \rightarrow 1s;1s,C)$
$Q(1s;1s^2 \rightarrow 2p;1s,C)$
$Q(1s;1s^2 \rightarrow 1s;2p,C)$
$Q(1s;1s^2 \rightarrow 2p;2p,C)$
$\log_{10}\{Q(1s;1s^2 \rightarrow n'l';nl,C)\pi a_0^2\}$
$\log_{10}\{E_i(ev)\}$
1
0
-1
-2
-3
4
5
6
7

Figure 4.

It is noticeable that although the simple ionization cross section dominates at lower energies, that for $n'l' = 2p$ becomes increasingly important at high energies resulting in a much slower fall off of the total cross section with energy than might have been expected. Further, work carried out previously on collisions involving positive ions and neutral atoms of H and He (c.f. Bates and Dalgarno 1956) suggest that for given $l$ and $l'$, $\Delta l' \neq \pm 1$ the cross sections fall off rapidly with increasing $n$ and $n'$ and conversely, that for a given $n$ and $n'$ they decrease quickly with $l$ or $l'$. Thus we may suppose that a reasonable approximation to $\sigma_{-1,0}$ can be obtained from the calculations made. When this work was first completed, there was no direct experimental data on $\sigma_{-1,0}$ so we compared our results with experimental results for $H^-$ ions in $H_2$ (see figure 5) for which several authors have carried out measurements. (Whittier 1954; Stier and Barnett 1956; Rose, Connor and Bastide 1958). The results of Whittier lie some 20% higher at the maximum than those of Stier and Barnett and it should be noted that the experiments of the latter workers do not distinguish between $\sigma_{-1,0}$ and $\sigma_{-1,+1}$ double electron loss. However, since it is unlikely that the double capture process takes place, this is neglected. Our theoretical results point to $\sigma_{-1,+1}$ for $H^-$ in H being negligible. The agreement between experiment and theory is surprisingly good considering the approximations made, but in fact it is very doubtful if it is as good as it appears to be. Born's approximation fails at

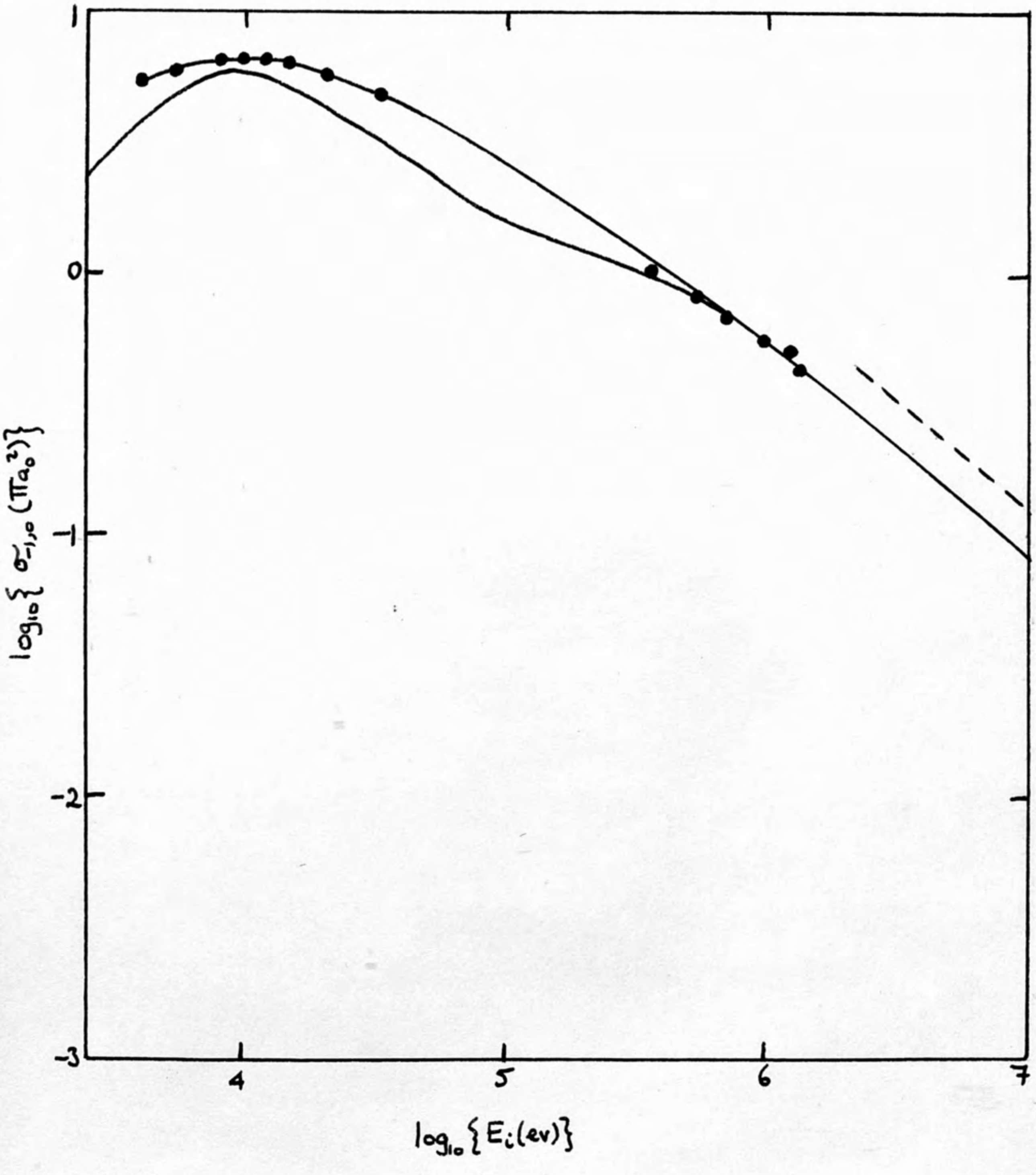


Figure 5.

low energies and would be expected to considerably over estimate in this region. It is therefore probable that in fact $\sigma_{-1,0}$ should be rather increased at all energies. In figure ( 8 ) we compare our results with data obtained by Hummer et al (1960) using atomic hydrogen and this indicates that we may well be right in this supposition as it can be seen that our curve lies about a factor of two below the experimental one at the peak (10 kev). It is of course difficult to estimate the error caused by the lack of orthogonality of the initial and final wave functions in the case of $nl=1s$ which dominates, but it is likely that the errors to which the Born approximation are at least as large. The dotted line in figure ( 5 ) represents the approximate asymptotic form for $\sigma_{-1,0}$ as obtained in § 6.

It is of interest to note the significance of the difference in the cross section involving atomic hydrogen as opposed to that for molecular hydrogen. While there are sound theoretical reasons for supposing that $H_2$ is approximately equivalent to two hydrogen atoms for bombardment by $H^+$, this is not so for $H^-$ which is, in contrast, a very diffuse system and indeed the non equivalence has been argued by Gerjuoy (1958).

The energy distribution of the ejected electrons is of interest in secondary prosesses. Figure ( 6 ) shows the variation of $\log_{10}\{Q(1s;1s^2\to 2p;1s,c\,|\,\kappa^2,E_i)\}$ as a function of $\kappa$ for

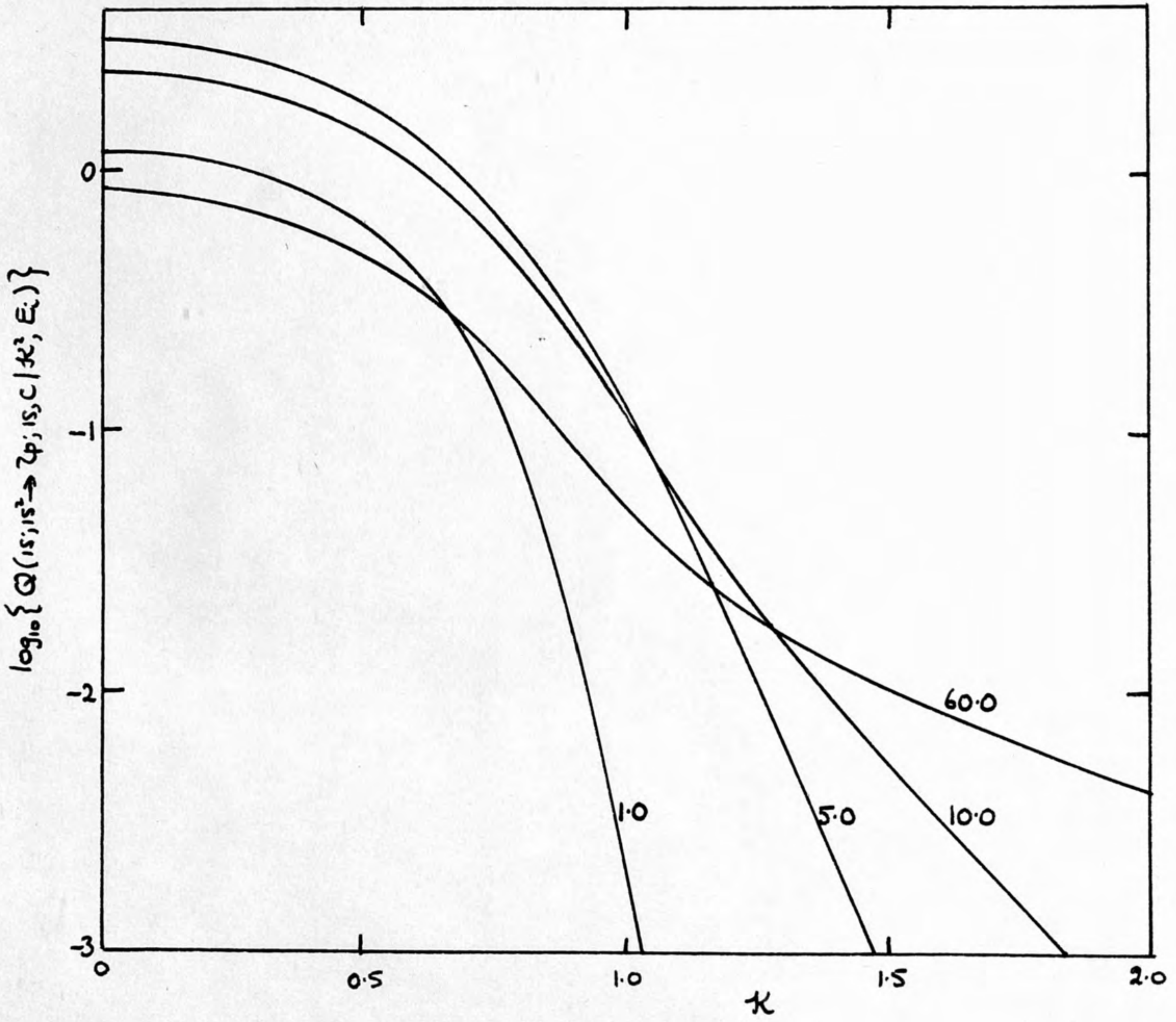

$\log_{10}\{Q(1s;1s^2 \rightarrow 2p;1s,c \mid \kappa^2; E_i)\}$
0
-1
-2
-3
0
0.5
1.0
1.5
2.0
$\kappa$
60.0
1.0
5.0
10.0

Figure 6.

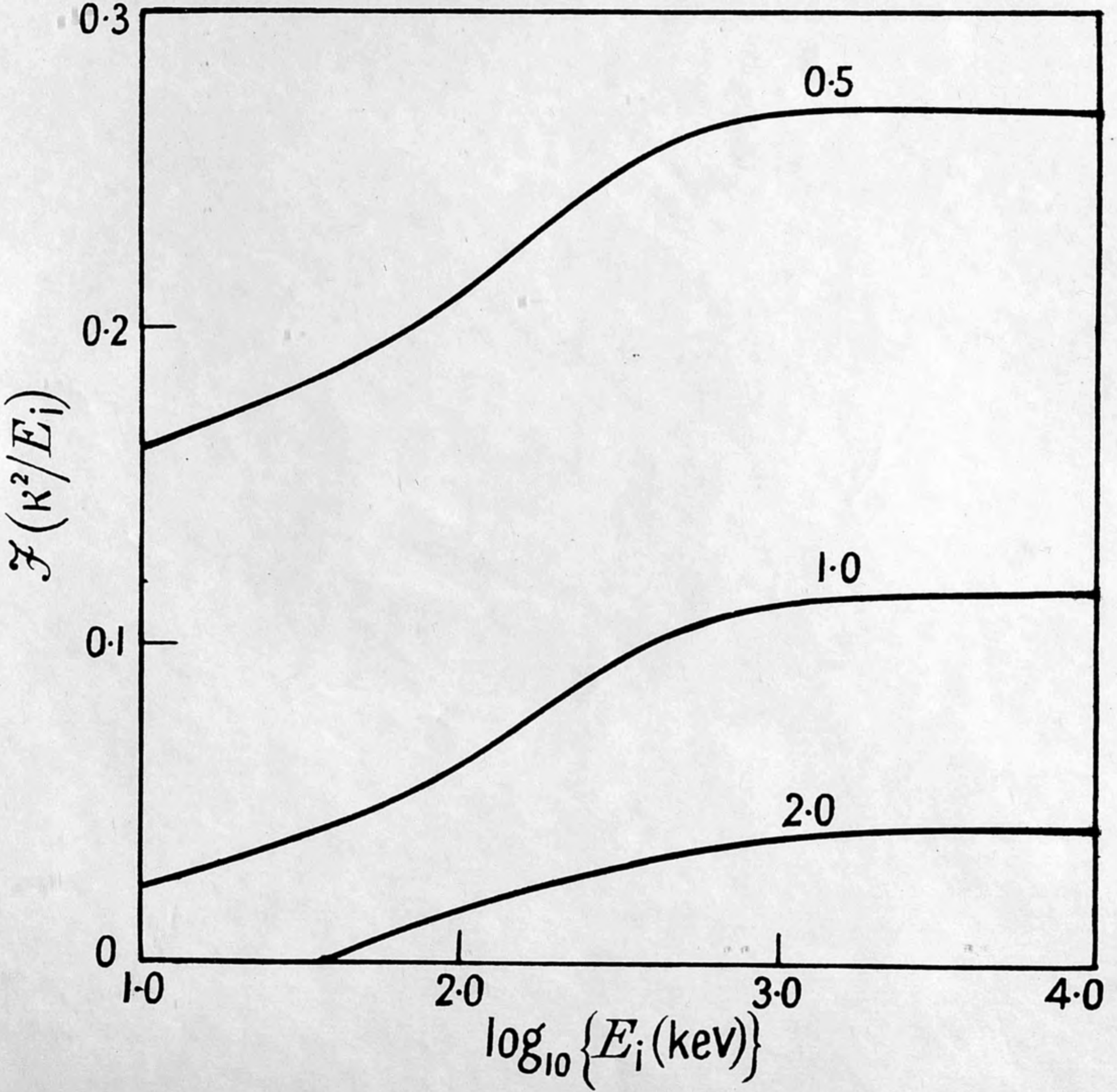

0·3
0·2
0·1
0
$\mathcal{F}(\kappa^2/E_i)$
0·5
1·0
2·0
1·0
2·0
3·0
4·0
$\log_{10}\{E_i(\text{kev})\}$

Figure 7.

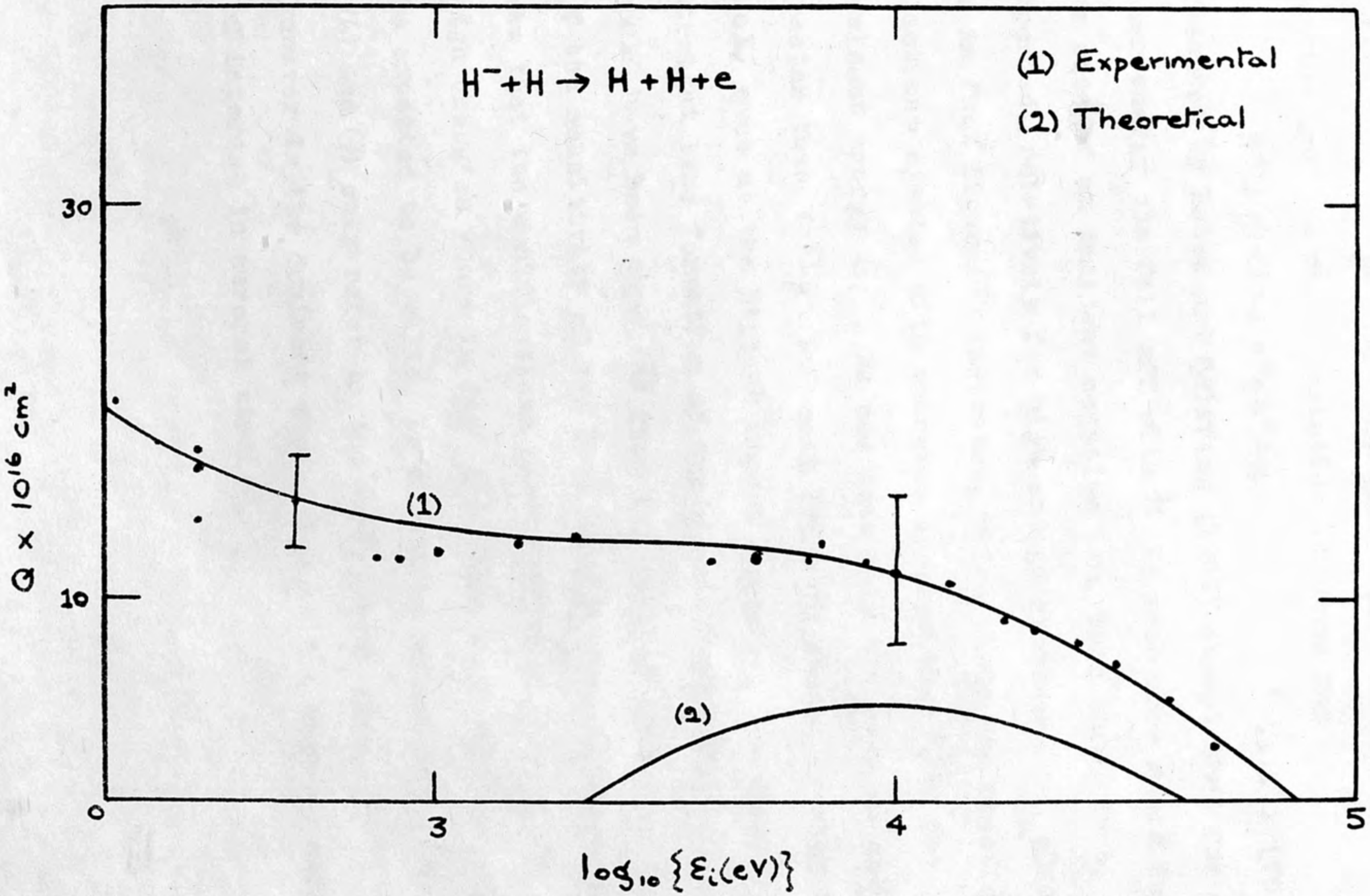

$H^- + H \rightarrow H + H + e$
(1) Experimental
(2) Theoretical
(1)
(2)
30
10
0
3
4
5
$Q \times 10^{16}\ cm^2$
$\log_{10}\{\varepsilon_i(eV)\}$

Figure 8.

certain incident particle energies. These curves exhibit the same general characteristics as those for

$$H^+ + H(1s) \rightarrow H^+ + H^+ + e \qquad \ldots\ldots \quad (78)$$

presented by Bates and Griffing (1953) except that for any given energy the fall off with $\kappa$ is much more rapid for the case of an incident negative ion. This shows that, as expected, relatively few high energy electrons are ejected, as in fact figure (7) indicates, which plots the fraction of electrons ejected with energies greater than $\kappa_0^2 I_H$ for incident energy $E_i$. We see that only 25% have an energy greater than $0{\cdot}5 I_H$ and only 12% with energy greater than $1{\cdot}0 I_H$ even at the highest impact energies. The essentially straight line formation of the curves for $\log\{E_i(ev)\} > 3{\cdot}0$ ev could have been expected from the earlier investigations of the sensitivity of the free wave functions, where we saw that the modifications persisted in their effects at high energies where in fact the plane wave function could be expected to be valid. It should be noted that figures (6) and (7) only refer to the $n'l' = 2p$, $nl = 1s$ case, which however is the dominant transition at the high energies of interest in auroral studies.

# CHAPTER III.

## The excitation and ionization of Lithium by electron and proton impact.

1. Born's approximation has been widely applied in the last thirty years to the problem of the theoretical evaluation of cross sections for the elastic and inelastic scattering of electrons by light atoms. However there is little experimental or theoretical data available on the ionization of atoms by fast impact except in the cases of H, He. Bates et al (1950) give a general discussion of the accuracy of the Born approximation and a comparision of theoretical and experimental results for excitation and ionization by electron impact. Much more recently it has realized that in fact there are only very minor differences between the analyses required for the theoretical calculations of the scattering of protons and electrons by atoms. For sufficiently high impact velocities, the only difference occurs as an alteration in the scale of incident energies, but as we approach the threshold, other factors become important. (For a brief survey of heavy particle collisions involving H, He see Chapter II and included references.) Bates and Griffing (1953) studied the ionization of Hydrogen by protons and Fite and Brackmann (1958) have published experimental and theoretical data relating to electron impact in which they get good agreement with the Born approximation at energies above 140 ev. Smith (1930)

studied the ionization cross sections of Helium, neon and argon experimentally and comparision data for Helium has been provided by Massey and Mohr (1933), Massey (1956) and Erskine (1954) who improved the agreement by obtaining the radial function for the p-wave by integrating the wave equation numerically. The simultaneous excitation and ionization of Helium by electron and proton impact has been treated by Dalgarno and McDowell (1956b) using a coulomb wave function for the ejected electron with a screening parameter chosen to fit the one body solution for three different momenta. Mapleton (1958) has also treated these processes, examining the choice of effective charges. For Lithium, Wu and Yu have studied double excitation and simultaneous excitation and ionization using however, only a plane wave for the ejected electron. The dearth of results of this type is probably due to the fact that even for the two electron atom, there are difficulties in choosing suitable and mutually orthogonal atomic orbitals, in taking account of the possible double transitions giving rise to the required final state and in estimating the contribution to the cross section from autoionization. Also for all elements with atomic number greater than two, the possibilities of inner shell ionization have to be considered. For auroral studies it would be very useful to have reliable ionization cross sections for proton impact on $O_2$ and $N_2$ , O and N but any theoretical treatment of these would be extremely lengthy and difficult. Laboratory studies of these cross sections are now being undertaken at

Georgia Tech at proton energies up to 1 Mev. It therefore seemed desirable to make a study of the ionization of Lithium, the simplest atom with a valence electron outside a closed shell, as a beginning in providing some theoretical comparision data. Also in order to throw some light on the probable contributions from such processes as simultaneous excitation and ionization, autoionization and inner shell ionization, we evaluate the cross sections for the excitations to the ($1s^2\ 2p$) ($1s2s2p$), ($1s\ 2s^2$) states from proton and electron impact in part repeating the calculations of Wu and Yu (1944), and paying particular attention to the choice of orbital parameters and the wave functions employed.

2.1 In this paragraph we formulate the necessary theory for the excitation cross sections and we suppose that initially the Lithium atom is in its ground state. $Q(1s^2, 2s \rightarrow nl, n'l', n''l'')$ is the cross section for the process in which the atom is excited to the $(nl\ n'l'\ n''l'')$ state. Born's approximation to the cross section is employed in which incident and scattered particles are described by plane waves; this is a valid assumption for fast collisions as the effect of distortion of these waves by the target atom must be small. The total cross section $Q$ for the excitation of an atom from a state i to a state f by proton or electron impact is given by (c.f. Mott and Massey, 1949)

$$Q(1s^2, 2s \rightarrow nl, n'l', n''l'') = \frac{8\pi^3\mu^2 e^4}{h^4 k_i^2} \iint_{K_{min}}^{K_{max}} |L(\underline{K}, t)|^2 K\, dK\, d\omega \quad \ldots\ldots\ldots\ldots (1)$$

where the symbols have their usual meanings. The matrix element $L(\underline{K},t)$ is obtained from the equation

$$L(\underline{K},t) = \iiiint \Psi_i^*(\underline{r}_1,\underline{r}_2,\underline{r}_3)\,\Psi_f(\underline{r}_1,\underline{r}_2,\underline{r}_3)\exp\{i\underline{K}\cdot\underline{R}\}$$

$$\times\; V(\underline{R},\underline{r}_1,\underline{r}_2,\underline{r}_3)\,d\underline{s}_1\,d\underline{s}_2\,d\underline{s}_3\,d\underline{R} \qquad \ldots\ldots\ldots\ldots(2)$$

in which $\Psi_i$ and $\Psi_f$ are as before, the initial and final wave functions of the whole system, $\underline{R}$ is the separation of the target and incident particles and $\underline{r}_1,\underline{r}_2,\underline{r}_3$ are the position vectors of the atomic electrons. $V(\underline{R},\underline{r}_1,\underline{r}_2,\underline{r}_3)$, the interaction potential may be written as

$$V(\underline{R},\underline{r}_1,\underline{r}_2,\underline{r}_3) = \mp\frac{3}{R} \pm \sum_{i=1}^{3}\frac{1}{|\underline{R}-\underline{r}_i|} \qquad \ldots\ldots\ldots\ldots(3)$$

Equation (2) is easily simplified by making use of (3) and integrating over $\underline{R}$ -space so that (2) becomes

$$L(\underline{K},t) = \frac{4\pi}{K^2}\iiint \Psi_i^*\Psi_f\left(\mp 3 \pm \sum_{i=1}^{3} e^{i\underline{K}\cdot\underline{r}_i}\right)d\underline{s}_1\,d\underline{s}_2\,d\underline{s}_3$$

$$= \frac{4\pi}{K^2}\iiint \Psi_i^*\Psi_f \sum_{i=1}^{3} e^{i\underline{K}\cdot\underline{r}_i}\,d\underline{s}_1\,d\underline{s}_2\,d\underline{s}_3 \qquad \ldots\ldots\ldots\ldots(4)$$

if we assume that the initial and final total wave functions are orthogonal. It now remains to select a suitable form for $\Psi_i$ and $\Psi_f$. In the following calculations determinantal wave functions are adopted, i.e. properly antisymmetrized combinations of normalized single electron wave functions. It should be noted here that it is possible to run into difficulty with this choice, as $e^{i\underline{K}\cdot\underline{r}_i}$ is a one electron operator so that if we choose atomic orbitals which are all members of the same complete set (i.e. orthogonal) the matrix element is identically zero. The ideal solution should be to arrange it so that while the individual orbitals are not orthogonal the integral $\int \Psi_i^* \Psi_f \, d\tau$ is zero. We cannot do this in all cases, but in the following analysis we assume that this is so. (However c.f. § 3 on results.) Following Wu and Yu we therefore adopt the wave functions

$$1s : \quad \psi = \frac{\alpha^{3/2}}{\sqrt{\pi}} e^{-\alpha r} \qquad \text{..........(5)}$$

$$2s : \quad \psi = \left\{ \frac{3\beta^5}{\pi(\alpha^2-\alpha\beta+\beta^2)} \right\}^{\frac{1}{2}} \left(1 - \frac{\alpha+\beta}{3} r\right) e^{-\beta r} \qquad \text{..........(6)}$$

$$2p : \quad \psi = \left(\frac{\delta^5}{\pi}\right)^{\frac{1}{2}} r e^{-\delta r} \cos\theta \qquad \text{..........(7)}$$

for the states indicated. A more accurate wave function describing the 2s electron in its ground state is given by Wilson (1933),

$$\psi = N_{2s}\left(\xi r e^{-\eta r} - e^{-\zeta r}\right) \qquad \text{..........(8)}$$

where $N_{2s}$ is a normalization factor and $\xi, \eta, \zeta$ are variational parameters. This function as it stands, suffers from the disadvantage that it is not orthogonal to the 1s ground state wave function, however this is not an insuperable difficulty, as a factor $\lambda e^{-\alpha r}$ may be added, in which $\lambda$ has an appropriate value, without altering the value of the determinant as a whole. We therefore adopt as an alternative 2s wave function

$$\psi = \gamma\left(\xi r e^{-\eta r} - e^{-\zeta r} + \lambda e^{-\alpha r}\right) \qquad \text{..........(9)}$$

and this is also used in some of the calculations to investigate the sensitivity of the cross sections to the choice of wave function. In addition to the parameter values obtained by Wu and Yu, we employ Slater values (Slater 1930) to find how much influence thse have on the magnitude of the cross section. The three transitions from the ground state to the 1s 2s 2p; $1s^2 2p$; $1s\ 2s^2$ states are selected for investigation as being probably the most dominant transitions. There is not necessarily a unique determinantal description of these states and we must determine a linear combination of the possible representative determinants which are eigenfunctions of all operators of a set of commuting angular momenta. (c.f. Eyring, Walter and Kimball 1944.) The appropriate determinants representing the states $1s^2 2s$; $1s^2 2p$; $1s\ 2s^2$ are respectively

$$D_1 = |\psi(1s)\alpha \quad \psi(1s)\beta \quad \psi(2s)\alpha| \qquad \ldots\ldots\ldots\ldots(10)$$

$$D_2 = |\psi(1s)\alpha \quad \psi(1s)\beta \quad \psi(2p)\alpha| \qquad \ldots\ldots\ldots\ldots(11)$$

$$D_3 = |\psi(1s)\alpha \quad \psi(2s)\beta \quad \psi(2s)\alpha| \qquad \ldots\ldots\ldots\ldots(12)$$

where $\alpha$ and $\beta$ are the spin functions and the determinants are given by the functions lying on the leading diagonal. Excitation to the state 1s 2s 2p involves the possibility of a double transition and it is found that the appropriate determinant is of the form

$$D = \frac{1}{\sqrt{6}} |D_4 + D_5 - 2D_6| \qquad \ldots\ldots\ldots\ldots(13)$$

where

$$D_4 = |\psi(1s)\alpha \quad \psi(2s)\alpha \quad \psi(2p)\beta| \qquad \ldots\ldots\ldots\ldots(14)$$

$$D_5 = |\psi(1s)\alpha \quad \psi(2s)\beta \quad \psi(2p)\alpha| \qquad \ldots\ldots\ldots\ldots(15)$$

$$D_6 = \left| \psi(1s)\beta \quad \psi(2s)\alpha \quad \psi(2p)\alpha \right| \qquad \ldots\ldots\ldots\ldots(16)$$

In the adoption of the determinant (14) our procedure differs from that of Wu and Yu in that for this transition they carry out two separate calculations, since this state may be attained either by inner shell excitation or by the double transition 2s→2p, 1s→2s. The substitution in equations (1), (2) of the selected forms for $\Psi_i$ and $\Psi_f$ then yields the following expressions for the three indicated cross sections

$$Q(1s^2,2s \rightarrow 1s^2,2p) = \frac{8}{k_i^2}\int |J(2s-2p)|^2 K^{-3}\,dK \;(\pi a_0^2) \qquad \ldots\ldots\ldots\ldots(17)$$

$$Q(1s^2,2s \rightarrow 1s,2s,2p) = \frac{12}{k_i^2}\int |J(1s-2p)|^2 K^{-3}\,dK \;(\pi a_0^2) \qquad \ldots\ldots\ldots\ldots(18)$$

$$Q(1s^2,2s \rightarrow 1s,2s^2) = \frac{8}{k_i^2}\int |J(1s-2s)|^2 K^{-3}\,dK \;(\pi a_0^2) \qquad \ldots\ldots\ldots\ldots(19)$$

where

$$|J(2s-2p)| = \left|\int \psi_i(2s)\,\psi_f(2p)\,e^{i\underline{K}\cdot\underline{r}}\,d\tau\right| \qquad \ldots\ldots\ldots\ldots(20)$$

and

$$k_i^2 = \frac{\frac{1}{2}mv_i^2}{I_H} \qquad \ldots\ldots\ldots\ldots(21)$$

the subscripts i and f denoting the initial and final functions. m, $I_H$ are the electronic mass and the ionization potential of hydrogen respectively. The integrals (17)-(19) can be readily evaluated analytically with the exception of (17) when the wave function (9) is employed, where it is easier to obtain them by a numerical method. These comparatively simple expressions have been obtained by assuming that the initial and final total wave functions are orthogonal which is in fact not necessarily true since in these functions we do not use the same parameters for a given electronic state.

2.2 We now pass on to the problem of the ionization of Lithium. A structureless particle of momentum $\hbar \underline{k}_i = \mu \underline{v}_i$ (in the system of coordinates referred to the centre of mass) is incident on a Lithium atom in its ground state. It is scattered through an angle $\theta$ and the 2s electron is ejected with momentum $\hbar \underline{t}$ into solid angle $d\omega$ about the direction $(\chi, \psi)$. Although we only consider simple ionization, we may assume that this process is the major contributor to the total ionization cross section, (c.f. § 3). In the case of electron impact there is a possibility of exchange, which however we do not take into account and Born's approximation is applied so that the relevant cross section $Q(1s^2, 2s \to nl, n'l', C)$ is given by

$$Q(1s^2, 2s \to nl, n'l', C) = \frac{8\pi^3 \mu^2 e^4}{h^4 k_i^2} \iint_{K_{min}}^{K_{max}} |L(\underline{K}, \underline{t})|^2 K\, dK\, d\underline{t}\, d\omega \qquad \text{..........(22)}$$

(c.f. equation (1)). The matrix element $L(\underline{K}, \underline{t})$ takes the form (2) and the initial and final wave functions are chosen to have the form (10) where in the latter case the 2s orbital is replaced by a function $\psi_{\underline{t}}^{-*}(r, z)$ which is a coulomb function describing an outgoing electron in the field of a positive charge ze. It will be noticed that $\Psi_f$ is a wave function which represents a singlet state only, of the final system, which is correct since for simp simple ionization only a final singlet state is possible. Substituting for $\Psi_i$ and $\Psi_f$ in $L(\underline{K}, \underline{t})$ it is a lengthy but fairly elementary matter to perform the necessary integrations over the spin variables and the separation $\underline{R}$ and obtain the simplified form

$$L(\underline{K},t) = \pm \frac{4\pi e^2}{K^2}\int \Phi(2s,r)\, e^{i\underline{K}.\underline{r}}\, \psi_{\underline{t}}^{-*}(\underline{r},z)\, d\underline{r} \quad \text{..........}(23)$$

where $\phi(2s)$ is given by (6) and where the two assumptions have been made that

(1) the 1s orbital of $Li^+$ is orthogonal to the 2s orbital of Li

(2) the function $\psi_{\underline{t}}^{-}(\underline{r},z)$ is orthogonal to the 1s and 2s orbitals of Li.

These conditions are all necessary if the initial and final total wave functions are to be orthogonal, but in our choice of orbitals condition (2) is not always satisfied, which gives rise to some difficulty in assessing the results. (1) is always satisfied, since if $\gamma$ is the effective nuclear charge for $Li^+(1s^2)$ a reasonable first approximation is to take $\alpha = \gamma = 2.694$ as we do. If $\alpha$ is not assumed equal to $\gamma$ an extra term appears in the matrix element which may be thought of as taking some account of inner shell ionization, which however is fairly improbable compared with the detachment of the 2s electron. In this case a variational calculation readily shows that the best value for $\gamma$ is given by

$$\gamma = 3 - 5/16 = 2.6875 \quad \text{(Eckhart 1930)} \quad \text{..........}(24)$$

which differs very little from the value of $\alpha$. From the work on the excitation cross sections and their sensitivity to choice of parameter, it seems unlikely that a difference of 0.0065 in $\gamma$ could make any significant difference to the magnitude of the cross section. It has not been considered worthwhile therefore to calculate the cross section for $\alpha \neq \gamma$ whem considering the extra labour involved. Condition (2) is a much more difficult one to satisfy. The most important contribution to the cross section should be from transitions to the p-wave in which case (2) is automatically satisfied for any value of z. However when the full expression is used difficulties arise. If we take $z = \alpha$ we can satisfy the first requirement but not the second. Physically, the nucleus will be well screened by the inner electrons from the ejected electron and $z = \beta$ or $z = 1.0$ is a better choice. However then neither of the conditions (2) can be satisfied and it is difficult to decide whether the advantages of satisfying the orthogonalization conditions outweigh those derived from physical considerations. (c.f. § 3 on results however.) In principle it is possible to form a linear combination of $\psi_t^{-*}(\beta, r)$, $\psi(1s, \alpha)$, $\phi(2s, \beta)$ which completely satisfies (2) and retains the correct asymptotic form, but this would lead to great complexit of algebra and it would be as simple to perform a Hartree-Fock solution for the ejected electrom. Writing then

$$\psi_t^-(\underline{r}, z) = \frac{t}{(2\pi)^{3/2}} e^{\pi z/2t} \Gamma\left(1 - \frac{iz}{t}\right) e^{i\underline{k}.\underline{r}} F\left(\frac{iz}{t}, 1, -itr - i\underline{t}.\underline{r}\right) \qquad \text{..........(25)}$$

where the normalization is such that

$$\int d\omega \int \underline{\Psi}_{\underline{t}}^{-*} \underline{\Psi}_{\underline{t}'}^{-} d\underline{1} = \delta(\underline{t}' - \underline{t}) \qquad \text{..........(26)}$$

straight forward but somewhat tedious analysis yields

$$Q(E_i) = \frac{2^8\beta^5 z}{5\epsilon\,\gamma_i^2}\int_0^{K_{max}}\int_{K_{min}}^{K_{max}} F(t,K)\exp\left\{-\frac{2z}{t}\arctan\frac{2\beta t}{\beta^2+K^2-t^2}\right\}$$
$$\times\left(1-e^{-\frac{2\pi z}{t}}\right)^{-1}(c^2+d^2)^{-4}(a^2-b^2)^{-5}t^{-3}K^{-3}\,dt\,dK \quad (\pi a_0^2) \qquad \ldots\ldots\ldots\ldots(27)$$

where

$$a=\beta^2+K^2+t^2\,;\; b=2Kt\,;\; c=\beta^2+K^2-t^2\,;\; d=2\beta t$$
$$\epsilon = \alpha^2-\alpha\beta+\beta^2 \qquad \ldots\ldots\ldots\ldots(28)$$

As we expect the contribution from the transitions to the p-wave of the continuum to be by far the greatest at all energies appreciably above the threshold, we also calculated $Q(E_i)$ using

$$\Psi_t^-(z;\,p\text{ wave}) = \frac{i\cos\delta}{6\pi}\left\{\frac{tz(t^2+z^2)}{1-e^{-2\pi z/t}}\right\}^{\frac{1}{2}} r e^{itr}\,{}_1F_1\left(2+\frac{iz}{t},4,2itr\right) \qquad \ldots\ldots\ldots\ldots(29)$$

retaining the normalization (26) and putting $\hat{\underline{t}}.\hat{\underline{r}}=\cos\delta$. The analysis is now somewhat simplified and the expression for $Q(E_i)$ becomes

$$Q_p(E_i) = \frac{8\beta^5 z}{\gamma_i^2}\iint\frac{(t^2+z^2)}{t^7K^7}\left(1-e^{-2\pi z/t}\right)^{-1}\exp\left\{-\frac{2z}{t}\arctan\frac{2\beta t}{\beta^2+K^2-t^2}\right\}$$
$$\times\left\{(\phi_1+\psi_2)\cos\Theta+(\phi_2-\psi_1)\sin\Theta\right\}^2 dK\,dt \quad (\pi a_0^2) \qquad \ldots\ldots\ldots\ldots(30)$$

the quantities $\phi_1$, $\phi_2$, $\psi_1$, $\psi_2$, $\Theta$, $F(t,K)$, being given in an Appendix. The expression $\{(\phi_1+\psi_2)\cos\Theta+(\phi_2-\psi_1)\sin\Theta\}$ when computed proved to largely cancel out at small values of $K$ so a power series expansion was developed by a numerical method, the leading term being $K^{+3}$. This of course verifies that the cross section has the right fall off at high energies since small $K$ implies large incident energy.

An alternative method of estimating the ionization cross section has been given by Seaton (1959). The approximation of Bethe (1930) gives

$$Q(E) = \frac{I_H}{\pi \alpha E}\int_0^{E-I} \frac{a(W)}{(I+W)} \log_e\left(\frac{4E\tau}{I+W}\right) dW \qquad \text{..........(31)}$$

where $I$ is the ionization potential, $E$ is the incident energy and $W$ that of the ejected electron. $a(W)$ is the photoionization cross section at an energy $W$. Then if we assume that for two atoms A and B the following relation holds,

$$\frac{a_A(I_A x)}{a_A(0)} = \frac{a_B(I_B x)}{a_B(0)} \qquad \text{..........(32)}$$

(31) and (32) give

$$\frac{I_A Q_A(I_A \epsilon)}{a_A(0)} = \frac{I_B Q_B(I_B \epsilon)}{a_B(0)} \qquad \text{..........(33)}$$

The Bethe approximation is most accurate at high energies and the relation (32) holds quite well for $\frac{a_{Ne}}{a_0}$ and $\frac{a_{Ne}}{a_N}$. In this particular case we compared Lithium with Helium since it is best to choose as a comparision species one whose outer electrons have the same orbital angular momentum. We used the results of Smith (1930), Erskine (1954), Massey (1956) on the ionization of helium together with the photoionization cross sections

$$a_{Li}(0) = 3.7 \times 10^{-18}\ \text{cm}^2 \ ; \qquad a_{He}(0) = 7.48 \times 10^{-18}\ \text{cm}^2 \qquad \text{..........(34)}$$

(see Bates 1946, Wheeler 1933, Ditchburn 1956.)

3.1 The results for the three excitation cross sections for proton and electron impact are displayed in figures 9-14. It will be noticed that the cross section $Q(1s^2 2s \rightarrow 1s^2 2p)$ dominates at all energies and that there is a much slower fall off with increasing impact energy, than is the case for either of the other two collisions considered. Reference to Table XII shows that in this case the parametric values are such that the neglect of the first integral term in equation (4) can be of no significance. It also indicates that there are no extra terms in the second integral which have been neglected. It would seem therefore that the cross sections obtained for this transition should be more accurate than those for the other tansitions, since to obtain equation (18), although $\Psi_i$ and $\Psi_f$ are orthogonal, certain terms have been ignored and in the case of the transition to 1s,2s$^2$ , the integral $\int \Psi_i^* \Psi_f \, d\tau$ makes a finite contribution. It is however difficult to assess the relative accuracy of the results since the Born approximation gives rise to an over estimation at the peak and the errors are most likely to be serious for optically allowed transitions. (Mott and Massey (1949). In figure (13) the cross sections for the excitation to the 1s$^2$ 2p level by electron impact are displayed. Wu and Yu's results are compared with those obtained by using wave functions (7), (9) with the parameter values 0.525, 0.65 for $\delta$ the former value giving the Slater orbital. An increase in $\delta$ leads to a downwards displacement of the cross section curve, but as we suppose that curve (3) provides the best approximation to the cross section, since for (3) the most accurate wave functions have been used, the Slater orbital gives a better approximation than do the orbitals used by Wu and Yu. All the curves have the same asymptotic fall off with energy and (1) and (3) differ by a factor of six at the peak. The corresponding cross sections for proton impact are shown in figure (10) and exhibit the same general features. Figures (9) and (12) show the results obtained for the cross section $Q(1s^2,2s \rightarrow 1s,2s,2p)$ for incident protons and electrons respectively. The curves (2) approximate very closely to (1) and the difference of a factor 1.2 is due to the fact that although the same wave functions have been used, we have made use of the form (13) for the final wave function. The curves (1) have been obtained by the addition of Wu and Yu's two sets of results. Finally, figures (11) and (14) compare the various results obtained for $Q(1s^2,2s \rightarrow 1s,2s^2)$ with the functions and parameters indicated. This is an optically forbidden transition and it will be noticed that the cross section is a factor $10^{-5}$ less than that of $Q(1s^2,2s \rightarrow 1s^2,2p)$ at the peak. In all cases the Slater orbitals give very reasonable agreement with results using variational parameters, especially for $Q(1s^2,2s \rightarrow 1s,2s,2p)$. It should be noted that a log-log scale is used and that the units of incident energy are electron volts, with the cross sections in units of $\pi a_0^2$.

3.2 The ionization cross sections were readily computed from the results given in § 3.2, and the expressions for $K_{min}$, $K_{max}$ are given in Chapter I § 3.3. The electron impact results are shown in figure (16) as computed from equations (30) and (33) with z put equal to $\alpha$ and 1.0. The choice $z = \alpha$ was made initially following the arguments of Arthurs and Moiseiwitsch (1958) which they showed should give the correct form at small values of r where most of the contribution to the matrix element probably arises. This choice is hard to justify on purely

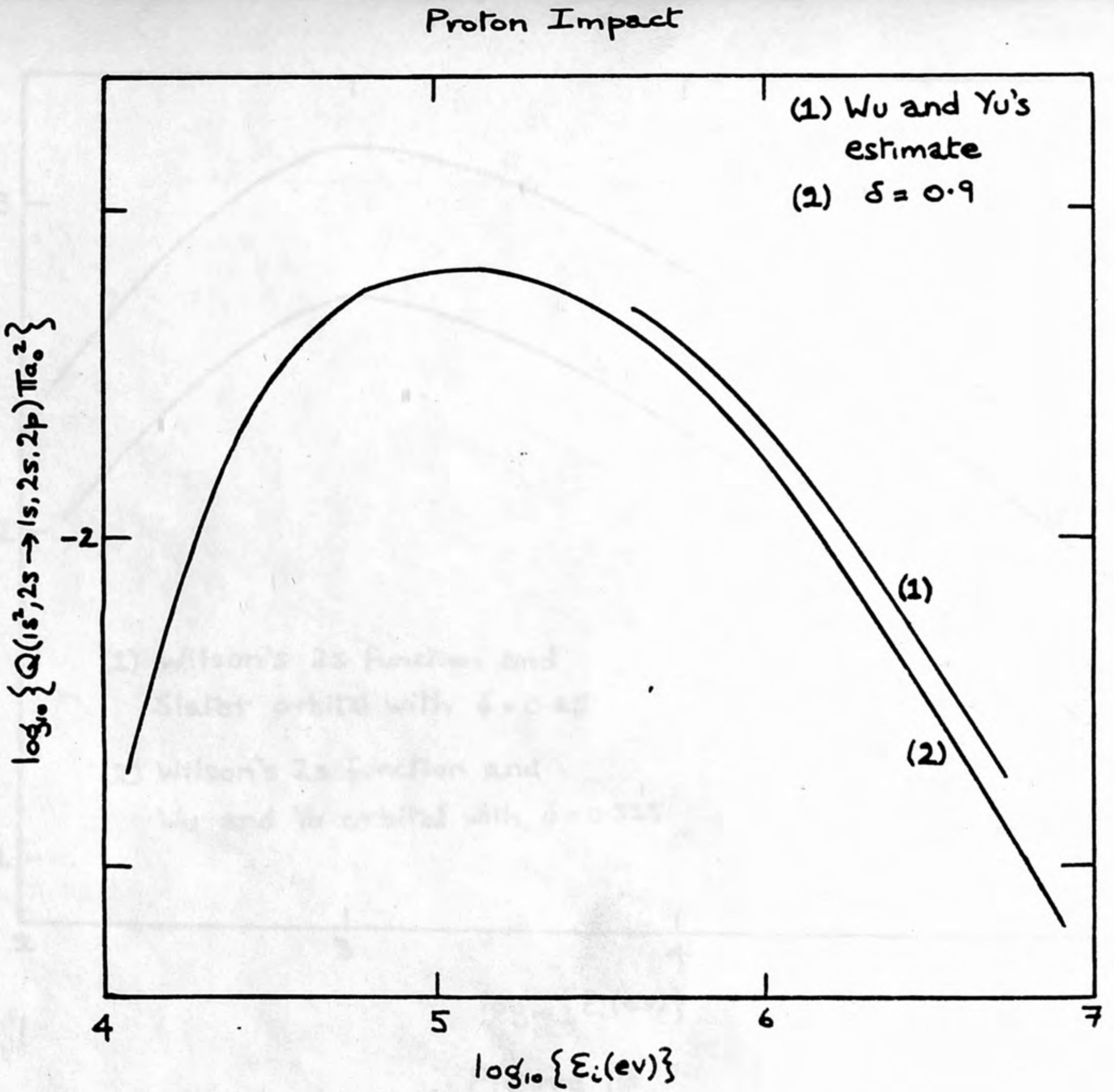
Proton Impact
(1) Wu and Yu's estimate
(2) $\delta = 0.9$
(1)
(2)
-2
4
5
6
7
$\log_{10}\{Q(1s^2,2s \rightarrow 1s,2s,2p)\pi a_0^2\}$
$\log_{10}\{E_i(ev)\}$

Figure 9

Proton Impact

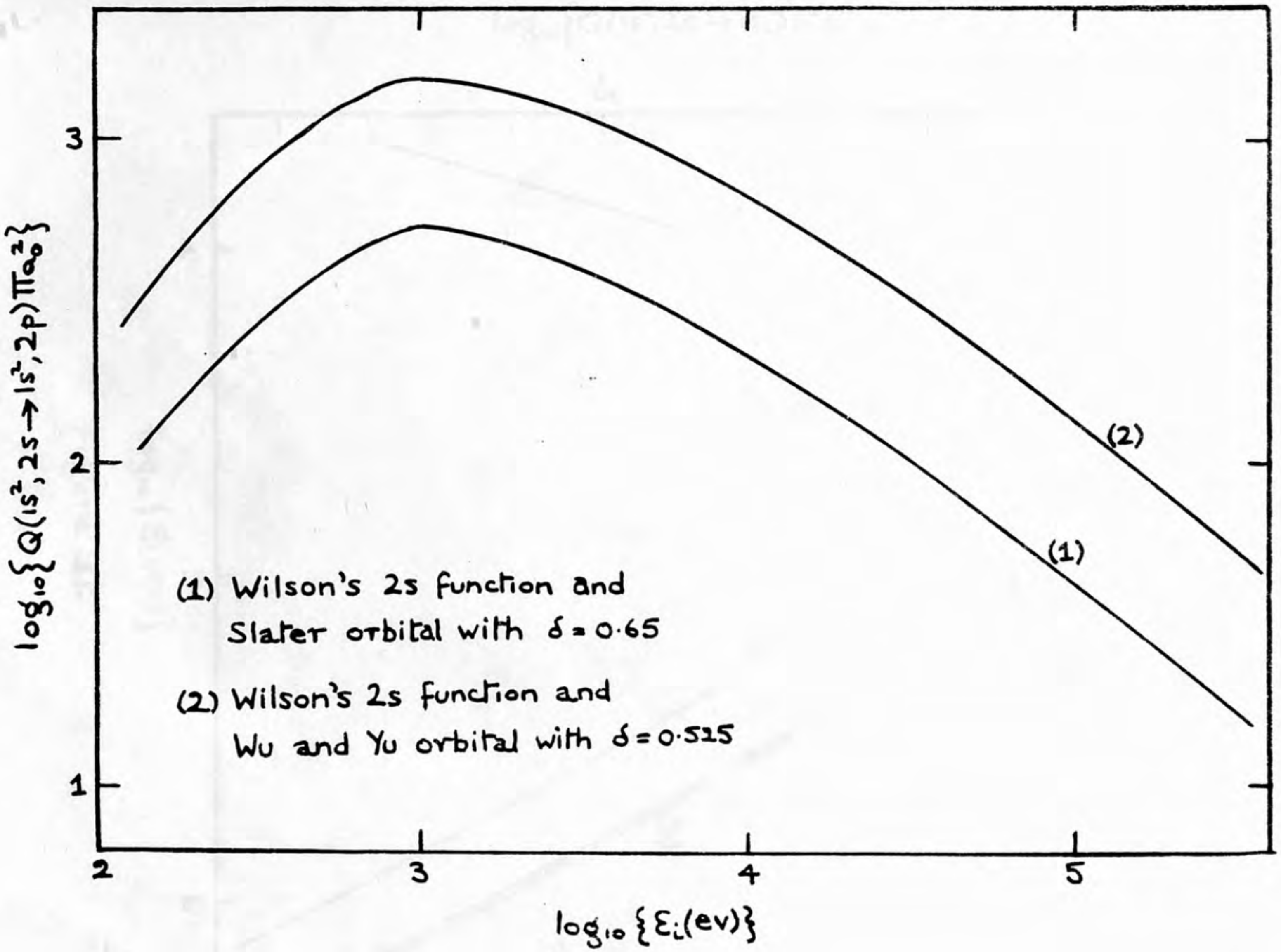


Figure 10

Proton Impact

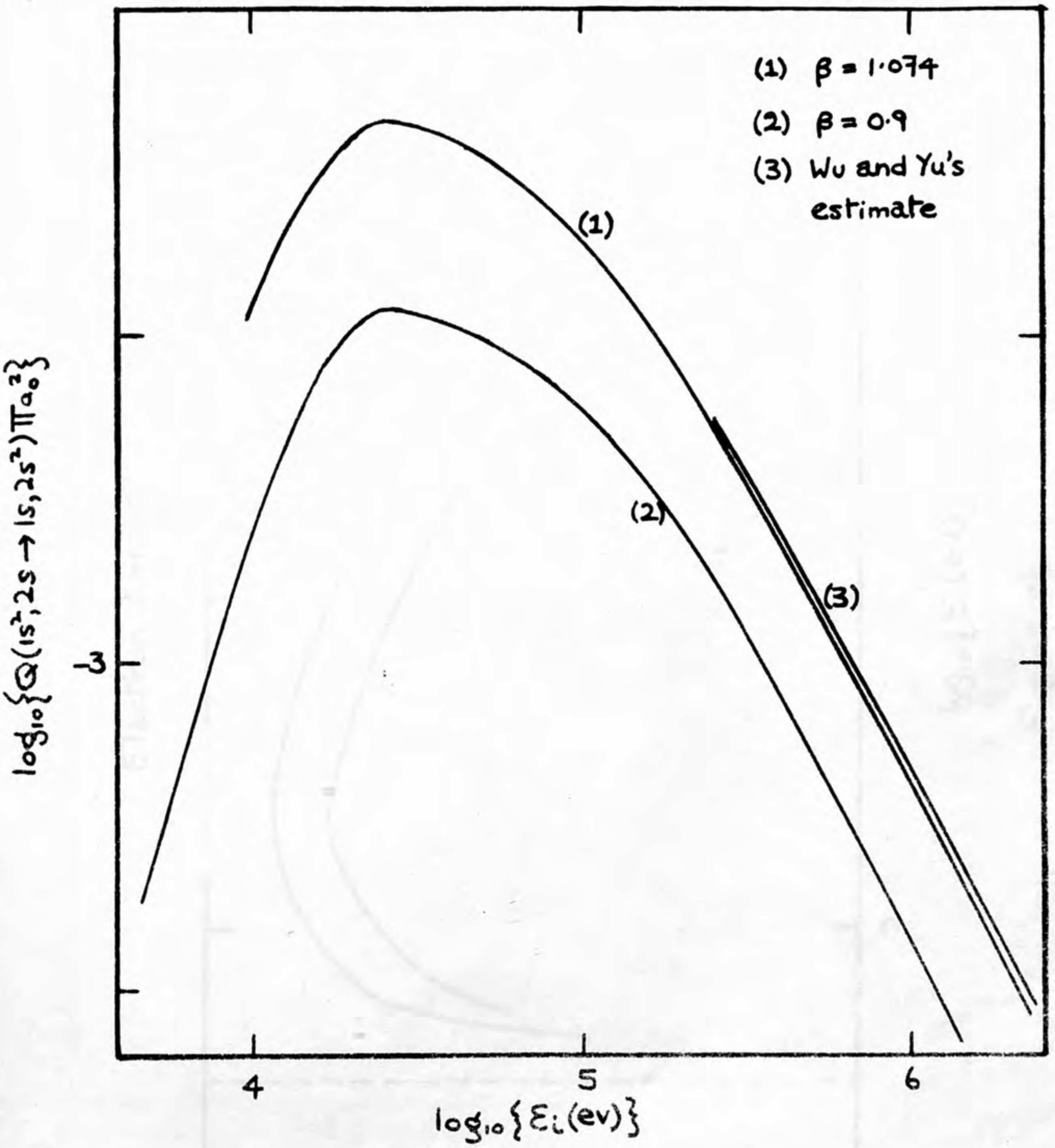


Figure 31

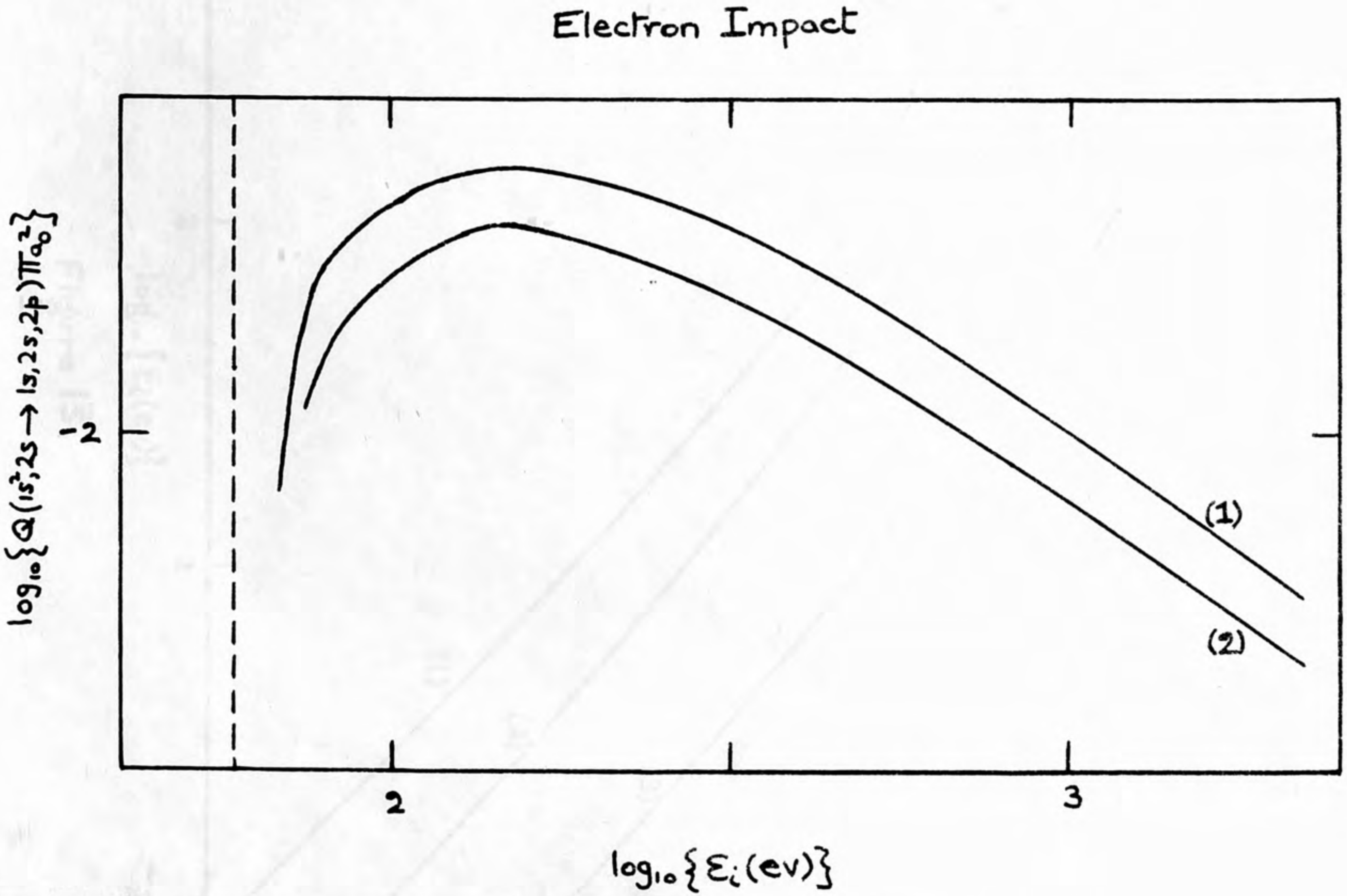

Electron Impact
$\log_{10}\{Q(1s^2 2s \rightarrow 1s,2s,2p)\pi a_0^2\}$
-2
2
3
$\log_{10}\{E_i(ev)\}$
(1)
(2)

Figure 12

Electron Impact

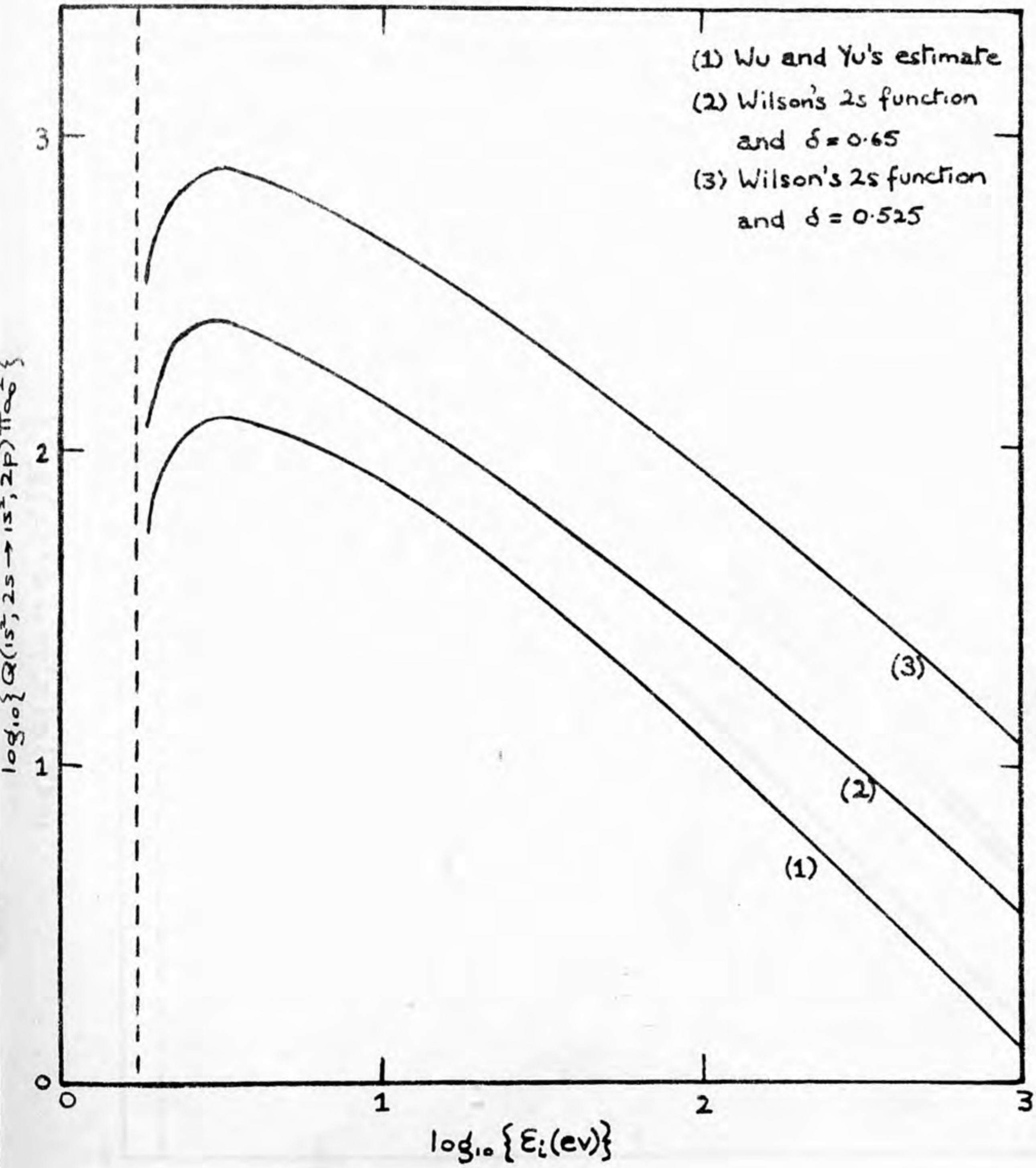


Figure 13

Electron Impact

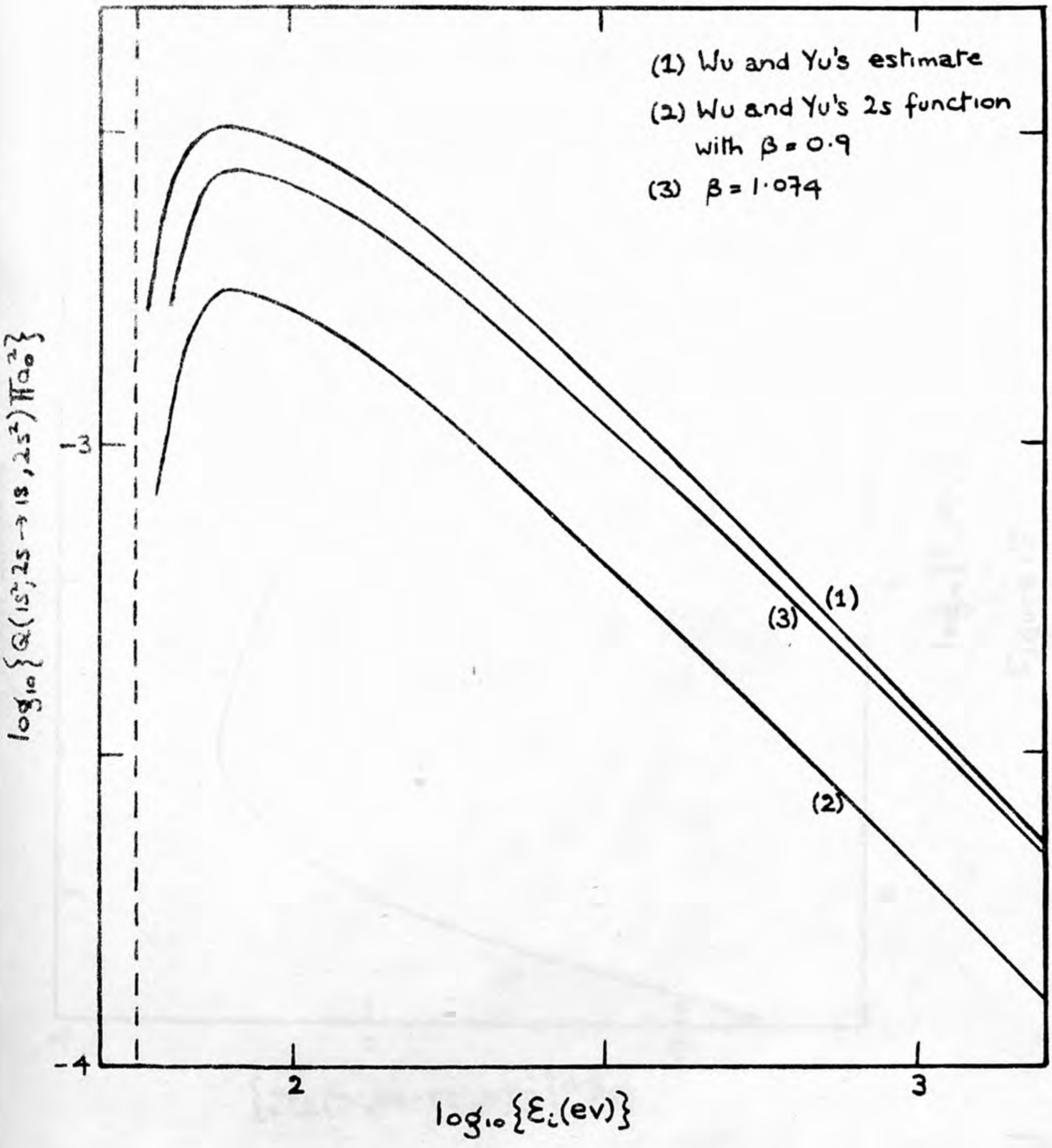
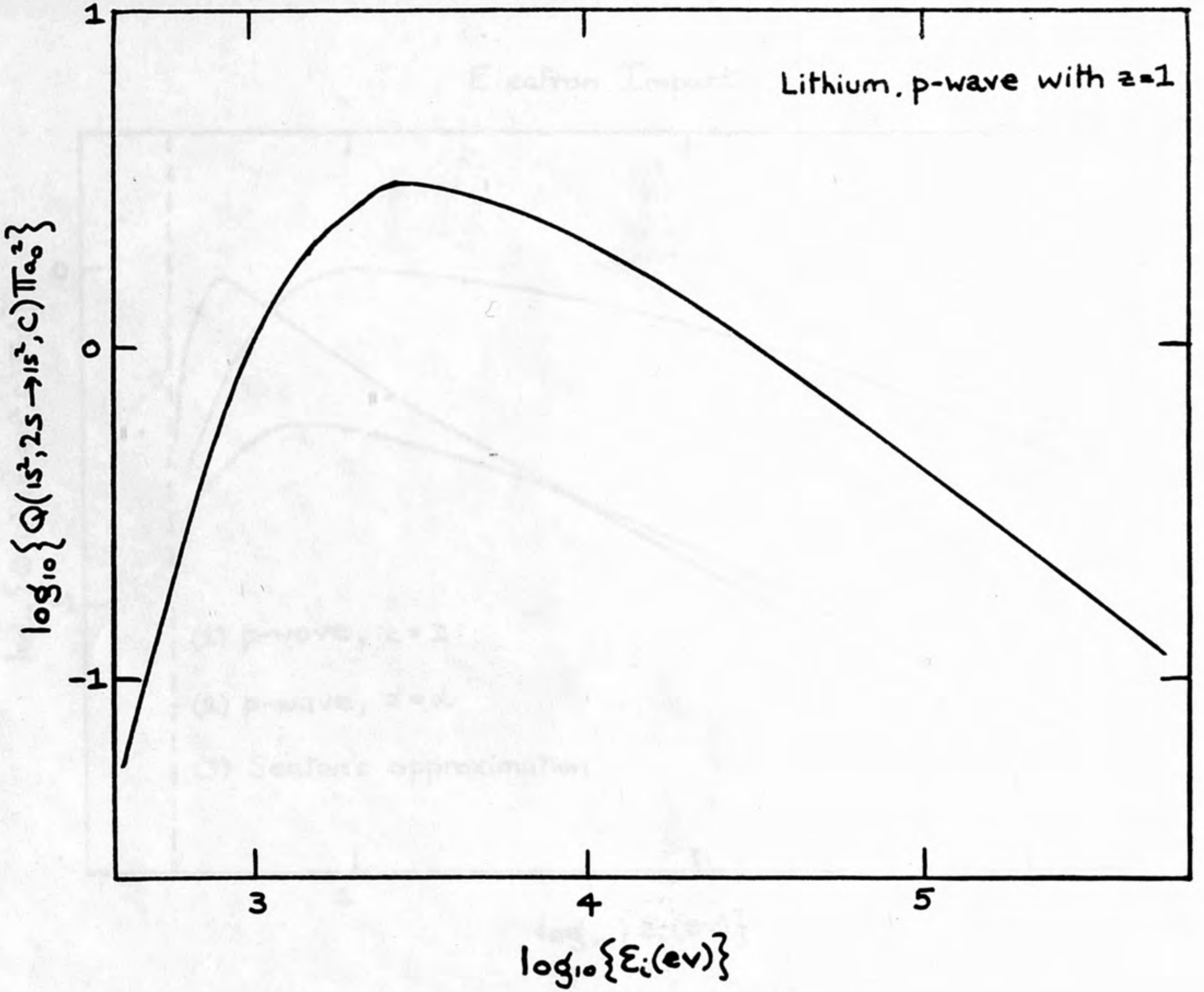


Figure 14



Proton Impact

Figure 15

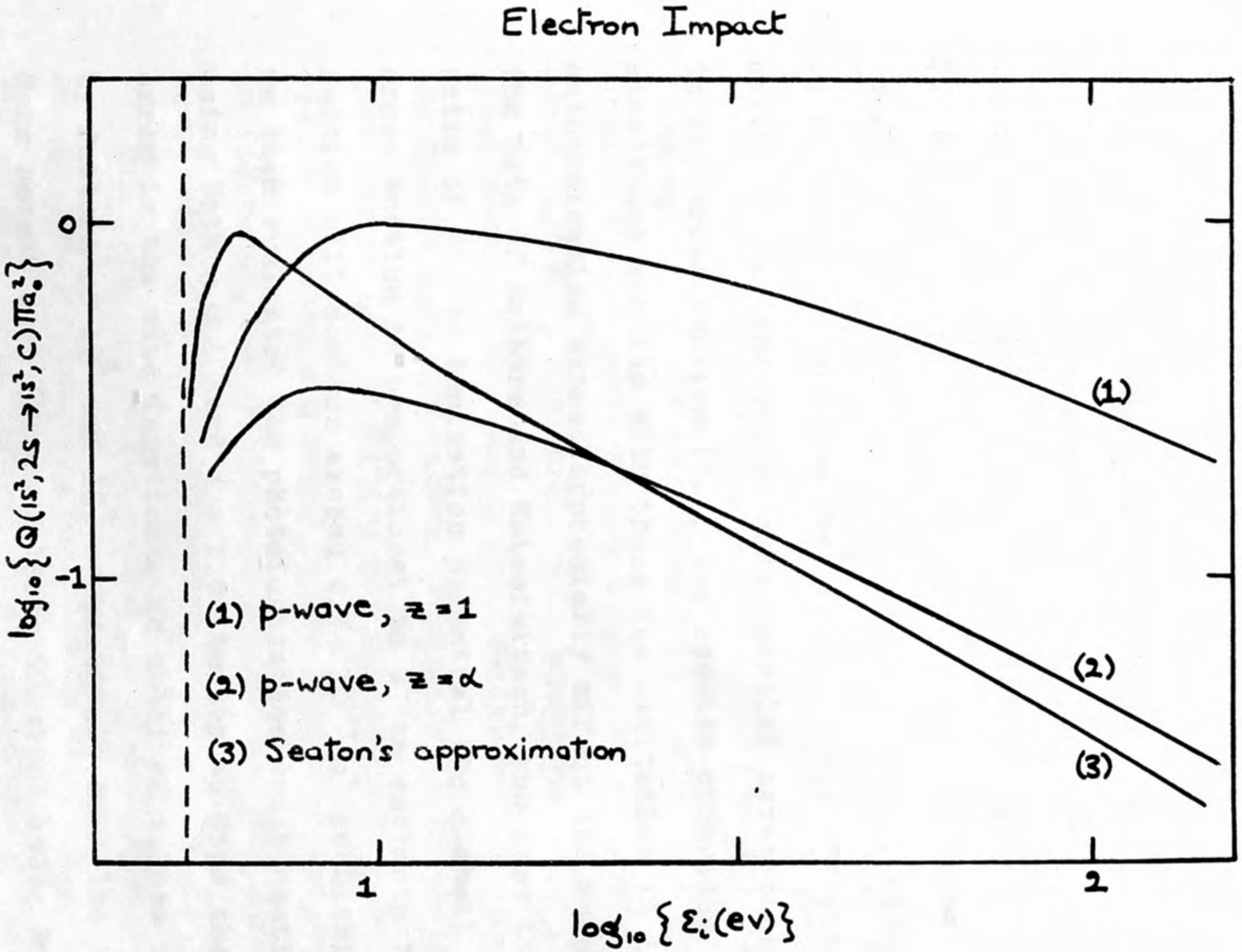

Electron Impact
0
-1
1
2
$\log_{10}\{Q(1s^2,2s \rightarrow 1s^2,C)\pi a_0^2\}$
$\log_{10}\{\varepsilon_i(ev)\}$
(1)
(2)
(3)
(1) p-wave, z = 1
(2) p-wave, z = α
(3) Seaton's approximation

Figure 16

physical grounds however and $z = 1.0$ should be much better at least at large r where there will be almost total screening. For $z = \alpha$ the p-wave results agree very well with those of equation (33) except near threshold, where (33) is not reliable as it is based on an expansion of powers of $\kappa$ and where the contribution from the s-wave might be expected to be the most important. If on the other hand we take $z = 1.0$, we have a cross section which is larger at all energies and exceeds that for $z = \alpha$ by a factor of 6.4 at 100ev. This does not agree nearly so well with Seaton's curve but in all cases there appears to be approximately the same rate of fall off with energy. It is unlikely that the higher order partial waves contribute much to the cross section (c.f. the results on proton impact.) and also comparing these results with those for excitation it is obvious that autoionization cannot appreciably affect the magnitudes. From the data of Arthurs and Moiseiwitsch, who show that at a given ratio of $E_i$ to ionization potential the k-shell ionization cross section is proportional to $z^2$ we estimate that the cross section will nowhere exceed $4.5 \times 10^{-20}$ cm$^2$ in Lithium. However we then evaluated the photoionization cross section at threshol using both $z = \alpha$ and $z = 1.0$ to try to find the probable error in the wave functions. We obtained values which differed by factors of $10^3$ and $10^2$ respectively from the value $3.7 \times 10^{-18}$ More recent work (Stewart 1954; Tunstead 1953; Burgess and Seaton 1960) suggests that the photoionization cross section is rather less, of the order of $1.2 - 2.5 \times 10^{-18}$ cm$^2$, in which case the curve obtained from (33) should be adjusted accordingly, but this does not alter the fact that both $z = \alpha$ and $z = 1.0$ both give very poor values for $a_{Li}(0)$. Later it was found that $a_{Li}(0)$ varied by as much as $10^5$ according to choice of z which would seem to make it a very difficult task to choose a value for z. It would be possible to select z so that $a_{Li}(0)$ had the value $2.5 \times 10^{-18}$ say, but there would be no physical basis for this choice. In retrospect, it would seem to be rather better to carry out a Hartree-Fock calculation for the ejected electron in the field of $Li^+(1s^2)$.

Turning now to proton impact cross sections calculated from formulae (27) and (30) displayed in figure(17) there is close agreement in the region where Born's approximation is of uncertain validity, but equation (27) breaks down at higher energies due to the nonorthogonality of $\psi_{\underline{k}}^-(\underline{r}, z)$ and $\phi(2s)$ causing a divergence of the curves. An expansion of $e^{i\underline{K}\cdot\underline{r}}$ in powers of $K$, for small $K$, shows that $|L(1s^2\text{-}C)|$ is not quite independent of the energy and remains a function of $t$ so that the matrix element does not vanish. Therefore it is probable that the lower curve (p-wave) gives the better result for $z = \alpha$. The result of putting $z = 1.0$ in the p-wave approximation is seen in figure(15). The maximum occurs at the same energy but is increased by a factor of seven.

The fraction of the number of ejected electrons which have energy greater than $t^2 I_H$ has already been defined in Chapter II and we display in figure(18) our results for Lithium under proton impact. At high energies more than 30% of these electrons have energy greater than 13.6 ev in close agreement with the results of Bates and Griffing for the ejection of a 1s electron from hydrogen but only about half as many as for 2p electrons (Bates, McDowell and Omholt 1957).

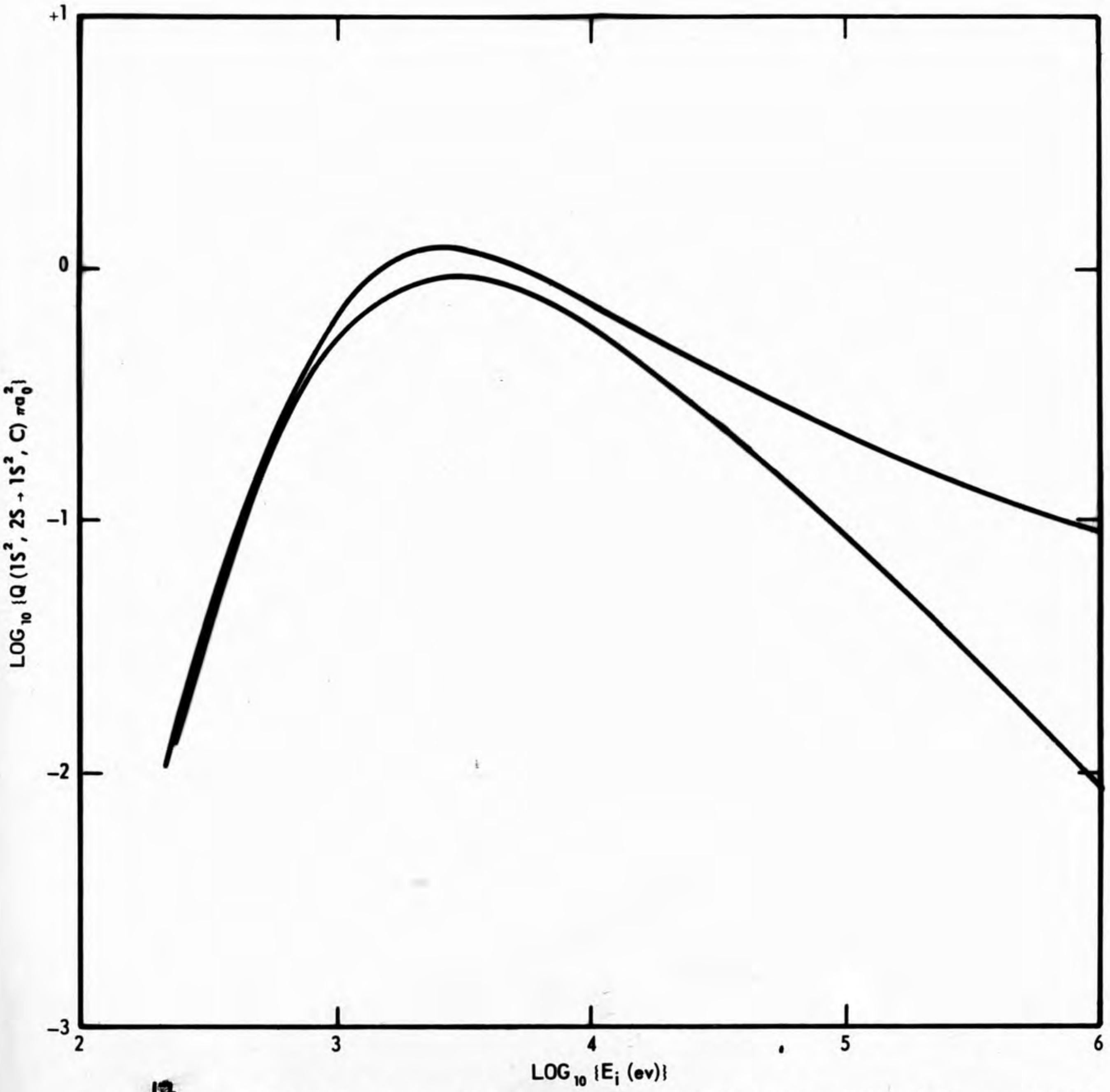


FIGURE ~~11~~ 17. IONIZATION OF LITHIUM BY PROTON IMPACT. LOWER CURVE p-WAVE BORN, $\alpha = z$; UPPER CURVE EQUATION 10, $\alpha = z$.

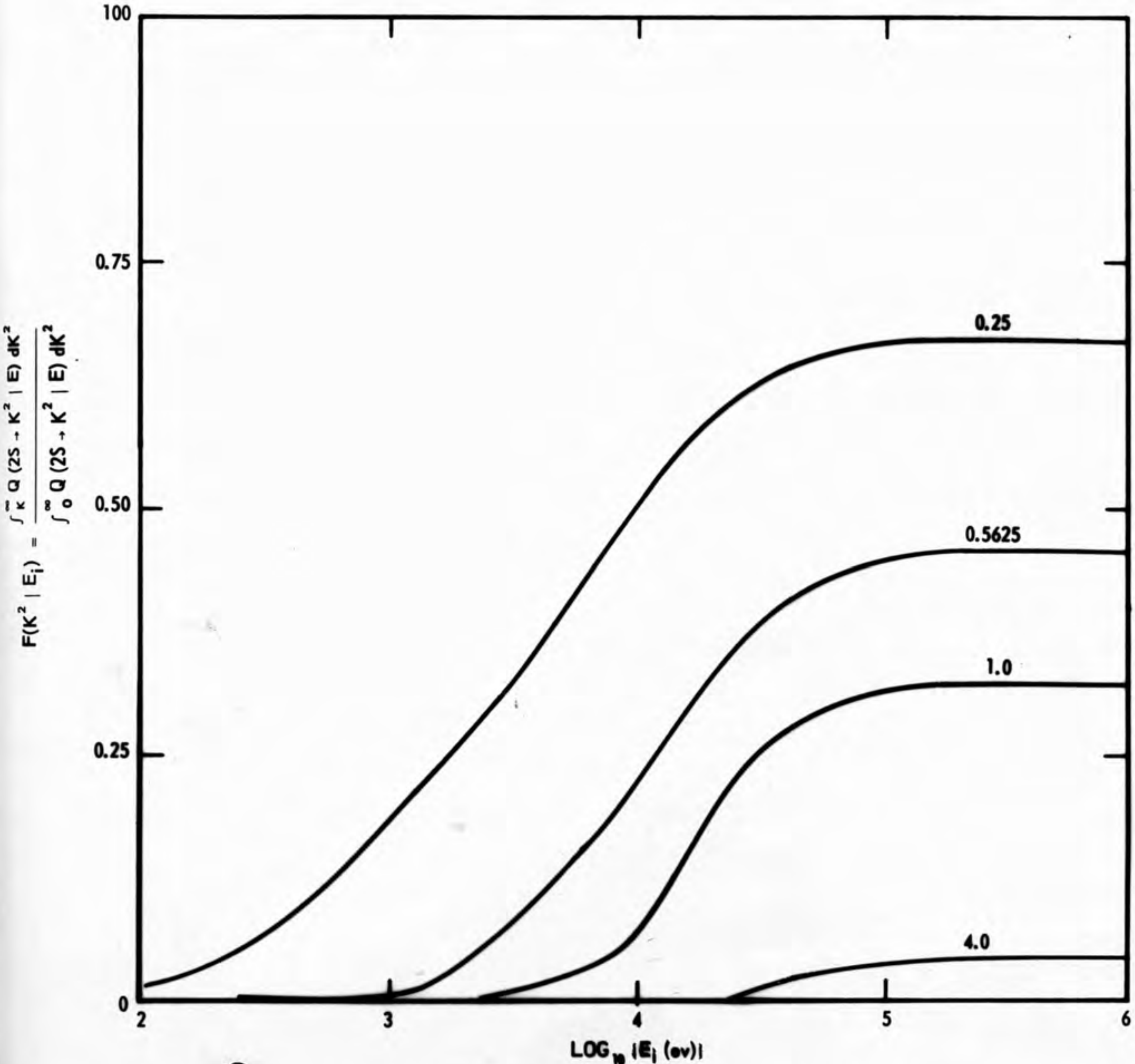


FIGURE 18 IONIZATION OF LITHIUM BY PROTON IMPACT. FRACTION OF ELECTRONS EJECTED WITH ENERGY GREATER THAN $K^2 I_H$. (NUMBERS ON CURVES GIVE VALUE OF $K^2$)

# CHAPTER IV.

## The transport properties of a fully ionized gas. A quantal study of diffusion and viscosity cross sections for a screened coulomb potential.

1. It has become clear, in recent years, that most of the matter in the observable universe occurs in the form of an ionized gas or plasma. The physics of plasmas is now in a state of rapid development, but the conditions of greatest astrophysical interest, namely high electron density and high kinetic temperature, are difficult to deal with experimentally. The relevant parameters, electron number density $n_e$ , and electron temperature $T_e$ (and the corresponding quantities for each species of ion present) are not readily observable directly. However it is possible, in principle, to deduce considerable infor information about them from measurements of the macroscopic properties of the plasma, in particular, the transport properties commonly known as the electrical conductivity $\sigma$ and the thermal conductivity $\lambda$ . Calculations of the variation of these quantities with $T_e$ and $n_e$ for a gas in local thermodynamic equilibrium, have been made by a number of authors from a classical point of view. (Cowling 1945; Landshoff 1949; Spitzer and Harm 1953; Spitzer et al 1950; Liboff 1959; Sodha and Varshni 1958;) The results of these various approaches are consistent and

results of these various approaches are consistent and

where it is possible to verify them experimentally, (Sakuntala, von Engel and Fowler (1960)), are of the correct order of magnitude.

The primary purpose of this present study is to point out that quantum mechanical effects should be taken into consideration and to calculate these effects as accurately as possible. It has been customary to apply the analysis of Debye and Hückel (originally developed for an electrolyte) to describe the ion-electron and electron-electron interactions in a plasma. This method employs a screened coulomb potential or some slight modification thereof. This potential leads to closed forms for the phase shifts and cross sections in many of the approximations normally adopted in studies of atomic and nuclear collision phenomena and also it is possible to calculate exact phase shifts for this potential by numerical integration of the relevant scattering equation. Thus a secondary purpose of the present work is to investigate the reliability of the various approximations in calculating phase shifts and cross sections for a Yukawa (or screened coulomb) potential.

2.1 Firstly, we shall derive the Maxwell-Boltzmann equation for a simple gas in any state. (there is no essential difference for a gas mixture) We define a distribution function $f(\underset{\sim}{r},\underset{\sim}{\omega},t)$, a function of position, velocity and time, which is such that at time $t$ the probable number of particles which are occupying the volume element defined by the vectors $\underline{r}$, $\underline{r}+d\underline{r}$ and have velocities in the range given by $(\underline{\omega}, \underline{\omega}+d\underline{\omega})$ is

$$f(\underline{r}, \underline{\omega}, t)\, d\underline{\omega}\, d\underline{r} \qquad \ldots\ldots\ldots (1)$$

We shall now suppose that each particle is subject to an external force $\underline{F}$ per unit mass, which is a function of $\underline{r}, t$ only and consider what happens to the system between the times $t$ and $t+dt$. In time $dt$ the velocity $\underline{\omega}$ of a particle will change to $\underline{\omega}+\underline{F}\,dt$, provided it has not undergone any collisions in this time and the position vector will have changed to $\underline{r}+\underline{\omega}\,dt$. Thus after a time $dt$, the particles which originally occupied the ranges $(\underline{r}, \underline{r}+d\underline{r})$, $(\underline{\omega}, \underline{\omega}+d\underline{\omega})$ now occupy the volume $(\underline{r}+\underline{\omega}\,dt, \underline{r}+\underline{\omega}\,dt+d\underline{r})$ and have velocities lying within the range $(\underline{\omega}+\underline{F}\,dt, \underline{\omega}+\underline{F}\,dt+d\underline{\omega})$. The probable number in this set is therefore given by

$$f(\underline{r}+\underline{\omega}\,dt, \underline{\omega}+\underline{F}\,dt, t+dt)\, d\underline{\omega}\, d\underline{r} \qquad \ldots\ldots\ldots (2)$$

according to the definition (1). However if we now take into consideration the changes in the spatial and velocity distribution due to collisions so that some original members of the set are 'lost' and others are gained, the net gain of particles to the final group must be $\left(\frac{\partial f}{\partial t}\right)_{coll} d\underline{\omega}\, d\underline{r}\, dt$ where $\left(\frac{\partial f}{\partial t}\right)_{coll}$ denotes the rate of change of the distribution function $f$ due to collisions. Thus we must have

$$f(\underline{r}+\underline{\omega}\,dt, \underline{\omega}+\underline{F}\,dt, t+dt)\, d\underline{\omega}\, d\underline{r} - f(\underline{r}, \underline{\omega}, t)\, d\underline{\omega}\, d\underline{r} = \left(\frac{\partial f}{\partial t}\right)_{coll} d\underline{\omega}\, d\underline{r}\, dt \qquad \ldots\ldots\ldots (3)$$

so that

$$\left(\frac{\partial f}{\partial t}\right)_{coll} = \frac{f(\underline{r}+\underline{\omega}\,dt, \underline{\omega}+\underline{F}\,dt, t+dt) - f(\underline{r}, \underline{\omega}, t)}{(t+dt) - t}$$

which in the limit as $dt \to 0$ becomes

$$\left(\frac{\partial f}{\partial t}\right)_{coll} = \frac{\partial f}{\partial t} + \underline{\omega} . \nabla_r f + \underline{F} . \nabla_\omega f \qquad .........(4)$$

where $\nabla_k f$ denotes the gradient of $f$ in $\underline{k}$-space. If there are no collisions then equation (4) represents Liouville's theorem applied to $f$, which is, in this case, constant along a dynamical trajectory for a conservative system. Equation (4) as it stands, is called the Maxwell-Boltzmann equation.

2.2 We will now give briefly the formulation of the Fokker-Planck equation derived from a consideration of a particle describing Brownian motion and under the influence of an external field of force. (For a general account of stochastic problems in physics see Chandrasekhar (1943)). In the theory of Brownian motion it is usual to start with the generalized form of Langevin's equation

$$\frac{d\underline{\omega}}{dt} = -\beta\underline{\omega} + \underline{A}(t) + \underline{F}(\underline{r},t) \qquad .........(5)$$

where $\beta$ is called the coefficient of dynamical friction which it is assumed is governed by Stokes' law and may be expressed in terms of the viscosity. This equation (5) makes the basic assumption that the motion may be split up into two parts a systematic part and a fluctuating part $\underline{A}(t)$ which is representative of the Brownian motion. We assume that the Brownian movement can be idealized as a Markoff process and the function $f(\underline{r},\underline{\omega},t+\Delta t)$ in phase space at time $t+\Delta t$ can then be derived from $f(\underline{r},\underline{\omega},t)$ using

$$f(\underline{r},\underline{\omega},t+\Delta t) = \iint f(\underline{r}-\Delta\underline{r},\underline{\omega}-\Delta\underline{\omega},t)\,\Psi(\underline{r}-\Delta\underline{r},\underline{\omega}-\Delta\underline{\omega};\Delta\underline{r},\Delta\underline{\omega})\,d(\Delta\underline{r})\,d(\Delta\underline{\omega}) \quad ....(6)$$

where $\Psi$ is such that

$$\Psi(\underline{r},\underline{\omega};\Delta\underline{r},\Delta\underline{\omega}) = \psi(\underline{r},\underline{\omega};\Delta\underline{\omega})\,\delta(\Delta\underline{r}-\underline{\omega}\Delta t) \qquad \text{..........(7)}$$

$\psi(\underline{r},\underline{\omega};\Delta\underline{\omega})$ being the transition probability in the velocity space and $\delta$ denoting Dirac's delta function. We can then integrate over $\Delta\underline{r}$ and write (6) in the form

$$f(\underline{r}+\underline{\omega}\Delta t,\underline{\omega},t+\Delta t) = \int f(\underline{r},\underline{\omega}-\Delta\underline{\omega},t)\,\psi(\underline{r},\underline{\omega}-\Delta\underline{\omega};\Delta\underline{\omega})\,d(\Delta\underline{\omega}) \qquad \text{.........(8)}$$

If the functions under the integral sign are now expanded in the form of a Taylor series and we neglect terms of the order of $(\Delta t)^2$ we have (see Chandrasekhar 1943)

$$O(\Delta t^2) + \left(\left(\frac{\partial f}{\partial t}\right)_{coll} + \underline{\omega}\cdot\nabla_r f\right)\Delta t = -\sum_i \frac{\partial}{\partial\omega_i}\left(f\langle\Delta\omega_i\rangle\right) + \frac{1}{2}\sum_{i,j}\frac{\partial^2}{\partial\omega_i{}^2}\left(f\langle\Delta\omega_i\,\Delta\omega_j\rangle\right)$$
$$+\ O\left(\langle\Delta\omega_i\,\Delta\omega_j\,\Delta\omega_k\rangle\right) \qquad \text{.........(9)}$$

where $\langle x\rangle$ denotes the average mean value of $x$ . This in the limit of $\Delta t\to 0$ becomes after substituting for the transition probability

$$\left(\frac{\partial f}{\partial t}\right)_{coll} + \underline{\omega}\cdot\nabla_r f + \underline{F}\cdot\nabla_\omega f = \beta\,\nabla_\omega\cdot(f\underline{\omega}) + q\,\nabla^2_\omega f \qquad \text{.........(10)}$$

where $q = \frac{\beta k T}{m}$.

It is interesting also to derive the diffusion equation as a special case of (10). We may rewrite (10) as

$$\left(\frac{\partial f}{\partial t}\right)_{coll} = \beta\left(\nabla_\omega - \frac{1}{\beta}\nabla_r\right)\cdot\left(f\underline{\omega} + \frac{q}{\beta}\nabla_\omega f - \frac{1}{\beta}\underline{F}f + \frac{q}{\beta^2}\nabla_r f\right) + \nabla_r\cdot\left(\frac{q}{\beta^2}\nabla_r f - \frac{1}{\beta}\underline{F}f\right) \text{...(11)}$$

and if we integrate (11) along the line

$$\underline{r} + \frac{1}{\beta}\underline{\omega} = \text{constant} = r_0 \qquad \text{.........(12)}$$

from $u=-\infty$ to $u=+\infty$, we have

$$\left(\frac{\partial}{\partial t}\right)_{coll}\int_{\underline{r}+\frac{1}{\beta}\underline{u}=r_0} f\,d\omega = \int_{\underline{r}+\frac{1}{\beta}\underline{u}=r_0}\nabla_r\cdot\left(\frac{q}{\beta^2}\nabla_r f - \frac{1}{\beta}\underline{F}f\right)d\underline{\omega} \qquad \text{.........(13)}$$

We now assume

a) that $F(\underline{r},t)$ does not change appreciably over distances of the order of $\left(\frac{q}{\beta^3}\right)^{1/2}$

b) that a maxwellian distribution of velocities is established after a time $\Delta t >> \beta^{-1}$ , the time of relaxation.

These assumptions enable us to write, $n(\underline{r},t)$ being the particle density

$$f(\underline{r},\underline{\omega},t) \simeq \left(\frac{m}{2\pi kT}\right)^{3/2} \exp\left(-\frac{m|\underline{\omega}|^2}{2kT}\right) \cdot n(\underline{r},t) \qquad \ldots\ldots\ldots(14)$$

so that (13) becomes

$$\left(\frac{\partial n}{\partial t}\right)_{coll} \simeq \Delta_{r_0} \cdot \left\{\frac{q}{\beta^2} \nabla_{r_0} n(\underline{r}_0) - \frac{1}{\beta} E(\underline{r}_0,t) n(\underline{r}_0)\right\} \qquad \ldots\ldots\ldots(15)$$

which generalizes to

$$\left(\frac{\partial n}{\partial t}\right)_{coll} = D \nabla_r^2 n \quad ; \; D = \frac{q}{\beta^2} \qquad \ldots\ldots\ldots(16)$$

in the case of zero external field. Thus we derive a link between the Fokker-Planck formalism based on the Langevin equation and the well known 'diffusion equation' which can be easily established on macroscopic grounds by considering the amount crossing a certain area in a certain time. The value of $D$ may be determined from

$$D = \frac{\langle \bar{r}^2 \rangle}{6t} \qquad \ldots\ldots\ldots(17)$$

where $\langle \bar{r}^2 \rangle$ denotes the average of all the mean free paths and (17) is the value of $D$ as determined when considering diffusion as a problem of a large number of random flights. To complete this introduction to the theory of gas motion and the phenomenon of diffusion it should be mentioned that Spitzer (1956) considers the diffusion coefficients $\langle \Delta\omega_k \rangle, \langle (\Delta\omega_k)^2 \rangle, \langle (\Delta\omega)^2 \rangle \langle (\Delta\omega_j)^2 \rangle$ which occur in the Fokker-Planck equation (9), where essentially represents Chandrasekhar's coefficient of dynamical friction $\beta$ and $D$ arises as a combination of all of Spitzers expressions.

(c.f. Chandrasekhar 1943 equation (247)).

3. We consider a fully ionized gas, composed of $n_e$ electrons and $n_i$ ions per cm$^3$ , at kinetic temperatures $T_e$ and $T_i$ respectively. For simplicity we assume that $T_e = T_i$ everywhere, and for the present we ignore the presence of magnetic fields. The mass motion of the plasma may be described by the Boltzmann equation

$$\frac{\partial f_i}{\partial t} + (\underline{v}_i \cdot \nabla) f_i + (\underline{a}_i \cdot \nabla_{\underline{v}}) f_i = \sum_j \left(\frac{\partial f_i}{\partial t}\right)_{coll_{ij}} \qquad \ldots\ldots\ldots(18)$$

for the velocity distribution function $f$ of the i$^{th}$ species $\underline{v}_i$ and $\underline{a}_i$ being the corresponding particle velocity and acceleration. The collision term appearing on the r.h.s. may be written

$$\left(\frac{\partial f}{\partial t}\right)_{coll_{ij}} = \iiint (f_i' f_j' - f_i f_j)\, \omega\, p\, dp\, d\Theta\, d\underline{v}_j \qquad \ldots\ldots\ldots(19)$$

in which primes denote the final values of $f_i$ and $f_j$ , $|\underline{\omega}| = |\underline{v}_i - \underline{v}_j|$ $p$ is the impact parameter and $\Theta$ is the angle between the orbital plane and that containing $\underline{v}_i$ and $\underline{v}_j$ before the collision. Such a representation implies that only two-body interactions are considered and these are supposed to affect the 'test particle' successively. Since the interactions to be considered are of much longer range than the nearest neighbour distance it would be preferable to include many body interactions in the collision term. This leads us to the alternative treatment of the problem as a stochastic process; i.e. we may replace (18) by a Fokker-Planck equation (Spitzer et al 1950; Spitzer and Harm 1953) which in turn implies the replacement of the collision term by one of the form $\sum_k r_{ik}$ where $r_{ik}$ is the displacement of the $i^{th}$ particle due to its interaction with the $k^{th}$. Such a theory neglects close encounters and treats all the interactions as simultaneous. Ideally, we should solve this equation and apply a correction for close encounters; however as Grad (1958) has pointed out, what one actually does is to neglect all but two-body encounters and treat these as simultaneous. The resultant expressions are then just those occurring in our earlier formulation, at least to the dominant terms. This accounts for the close agreement between the results of Landshoff (1949) and Cowling (1945) who used the Boltzmann approach and Spitzer and Harm (1953) who worked from a Fokker-Planck equation. A substantially similar argument was developed in another connection by Furry and Pitkanen (1951) who treated the problem of a small concentration of one gas diffusing through another in the case of zero external field. Using the diffusion equation (16), their results for $D_{ij}$ were identical with those of the $2^{nd}$ approximation of Chapman and Cowling (1952).

4. The adoption of a screened coulomb potential to represent the interaction of ions and electrons, or of like species, in a plasma has been justified by several authors, since Persico (1926) first investigated the problem. Following Liboff (1959) we consider a test charge in an otherwise neutral plasma. Defining the partial pressure of the $i^{th}$ charged species by

$$p_i = \frac{\rho_i}{e_i} k T_i \qquad \text{.......(20)}$$

where $i=1$ for electrons and $i=2$ for ions, $\rho_i$ is the charge density of the $i^{th}$ kind and $e_i$ the charge in e.s.u. on a particle of this species, we have then

$$\nabla p_i = \rho_i \underline{E} \qquad \text{........(21)}$$

where $\underline{E}$ is the electric field intensity. Further,

$$\nabla\cdot\underline{E} = 4\pi\left[\sum_i \rho_i + e_1\delta(r)\right] \qquad \text{........(22)}$$

is Poisson's equation for a test charge $e_1$ at the origin. From (20)

$$\nabla p_i = \frac{kT_i}{e_i}\nabla\rho_i = \rho_i\underline{E} \qquad \text{........(23)}$$

and therefore

$$\nabla\rho = \underline{E}\sum_i \frac{e_i\rho_i}{kT_i} \qquad \text{........(24)}$$

Taking the divergence of both sides,

$$\nabla^2\rho = (\nabla\cdot\underline{E})\sum_i \frac{e_i\rho_i}{kT_i} + \underline{E}\cdot\sum_i\frac{e_i\nabla\rho_i}{kT_i} \qquad \text{........(25)}$$

the last term being of order $E^2$. Linearizing,

$$\nabla^2\rho = (\nabla\cdot\underline{E})\sum_i\frac{e_i\rho_i}{kT_i} \qquad \text{........(26)}$$

and using (22)

$$\nabla^2\rho = \left\{\sum_i\frac{4\pi e_i\rho_i}{kT_i}\right\}\left\{\rho + e_1\delta(r)\right\}$$

$$= h_D^{-2}\left\{\rho + e_1\delta(r)\right\} \qquad \text{........(27)}$$

where the Debye length, $h_D$, is given by

$$h_D^{-2} = \sum_{i=1}^{2}\frac{4\pi e_i\rho_i}{kT_i} = \sum_{i=1}^{2}\frac{4\pi n_i e^2}{kT_i}$$

$$= \frac{8\pi n_e e^2}{kT_e} \qquad \text{........(28)}$$

by our earlier assumptions, so that

$$h_D = \left[\frac{kT_e}{8\pi n_e e^2}\right]^{1/2} \qquad \text{........(29)}$$

Now solving (27)

$$\rho = -\frac{e_1}{4\pi h_D^2} \cdot \frac{1}{r} e^{-r/h_D} \qquad \text{.........(30)}$$

which corresponds to an electrostatic potential

$$V(r) = \frac{e_1}{r} \exp\left\{-r/h_D\right\} \qquad \text{.........(31)}$$

for the total charge distribution. Clearly (31) will only be a reliable description of the interaction provided we are in the region outside the nearest neighbour distance. One should really adopt

$$V(r) = \frac{e_1}{r} \quad (r < n^{-1/3}) \qquad \text{.........(32)}$$

However we have

$$h_D \doteqdot 3 \cdot 5 \left(\frac{T_e}{n_e}\right)^{1/2} \text{cms} \qquad \text{.........(33)}$$

so that $h_D \gg n_e^{-1/3}$ if and only if

$$\sqrt{T} > 0 \cdot 3 n_e^{1/6} \qquad \text{.........(34)}$$

thus if $n_e < 10^{12}$ we require only that $T > 10^{3}$°K and if $n_e < 10^{18}$, $T > 10^{4}$°K, for our potential (31) to be a very adequate representation even at small $r$. Several authors have argued that a Debye-Hückel analysis cannot be applied to a plasma and that the electric field and potential should be obtained from a microfield analysis of the type performed by Holtsmark (1919). For example, Theimer and Hoffmann (1958,1959) argue as do Theimer and Gentry (Private communication) that in the Boltzmann equation approach only close two body'collisions' are considered (which is incorrect) while in the Fokker-Planck approach of Spitzer and his co-workers only distant encounters are considered (although they suppose many body interactions included). The Fokker-Planck approach they maintain, considers successive random collisions, but at the high temperatures and densities prevalent in a plasma the collision time $t \sim (p/v)$ is much longer than the randomization time $\tau \sim \frac{1}{n_e}$, so the so the collisions cannot be regarded as successive. (However this neglects Grads' point that a linearized Fokker-Planck analysis is really equivalent to a Boltzmann type formulation with all the two body interactions occurring simultaneously). Theimer and Gentry represent the local microfield at a point in the plasma as a superposition of shielded coulomb fields for each charge present in the plasma. This representation is equivalent to supposing that there exists a cloud of randomly distributed virtual particles each giving a field of the form (31), but which do not interact among themselves. The resulting energy density is shown to be the self energy of the true charges minus half the Debye-Hückel interaction energy. Theimer and Gentry now consider a test particle $A$ at a distance $r_m$ from some other particle $B$, where $r_m < n^{-1/3}$ and suppose $A$ sees only the interaction with $B$. It has been then assumed that for $r > r_m$ one has nearest neighbour zones of other test particles $B'$, which are completely shielded from one another. Then $A$ lies in a coulomb field cut off at $r = n^{-1/3}$. This seems to be merely a definition of their potential however, not an argument for a cut-off at $n^{-1/3}$. Given this, they then calaulate an effective plasma potential and fit it by an expression of the form

$$V(r) = \frac{e_1}{r}\exp(-ar)\cos(br) \qquad \ldots\ldots\ldots(35)$$

with $a \simeq b \simeq n_e^{+1/3}$. In another section of this paper we investigate this form of potential and show that given $a$, it leads to scattering properties closely similar to that of (31). The numerical results for the cross sections given by Theimer and Hoffmann show such large discrepancies from earlier work (Spitzer 1956) only because of the adoption of $n_e^{-1/3}$ as a cut off rather than $h_D$. The numerical analysis of Theimer and his colleagues has also been critized by Ecker and Muller (1959) on the grounds that the number of particles inside the Debye region $\delta$, must satisfy $\delta \gg 1$.

5.1 Application of the classical analysis of Chapman and Cowling to (18) yields expressions for the electrical and thermal conductivity correct to the second order. We introduce the collision integrals

$$\Omega_s^{(\ell)} = \left(\frac{2\pi kT}{\mu}\right)^{1/2}\int_0^\infty e^{-\gamma^2}\gamma^{2s+3}\phi_{12}^{(\ell)}(v)\,d\gamma \qquad \text{.........(36)}$$

in which

$$\gamma = \left(\frac{\mu}{2kT}\right)^{1/2} v \qquad \text{.........(37)}$$

$\mu$ is the reduced mass and $v$ the relative velocity of the colliding systems, $k$ is Boltzmann's constant and $T$ the absolute temperature. The function $\phi_{12}^{(\ell)}(v)$ is a collision cross section defined by

$$\phi_{12}^{(\ell)}(v) = 2\pi\int_0^\infty (1-\cos^\ell\theta)\,p\,dp \qquad \text{.........(38)}$$

the scattering angle being $\theta$. We may write (38) in terms of the scattering amplitude $f(\theta)$ instead of the impact parameter

$p$ , as

$$\phi_{12}^{(\ell)}(v) = 2\pi \int_0^{\pi} (1-\cos^{\ell}\theta)\, |f(\theta)|^2 \, d(\cos\theta) \qquad \text{.........(39)}$$

In terms of these functions (36) the second approximation to the electrical conductivity is given by

$$\sigma = \frac{n_i e^2 (n_i+n_j)}{n_j kT} \left[D_{ij}\right]_2 \qquad \text{.........(40)}$$

where $e$ is the electronic charge and $[D_{ij}]_2$ the second approximation to the diffusion coefficient,

$$\left[D_{ij}\right]_2 = \frac{3\rho kT}{16(n_i+n_j)\mu \Omega_1^{(1)}} \left[1+\epsilon_0\right] \qquad \text{.........(41)}$$

$\epsilon_0$ being a small correction term, which for $m_i << m_j$ is

$$\epsilon_0 = \frac{-\left[5\Omega_1^{(1)} - 2\Omega_2^{(1)}\right]^2}{4\left\{\left[\Omega_2^{(1)}\right]^2 - \Omega_3^{(1)}\Omega_1^{(1)}\right\}} \qquad \text{.........(42)}$$

Similarly, to the same approximation the thermal conductivity is given by

$$\lambda = \frac{1{\cdot}6875\, C_v\, kT}{\Omega_{(2)}^{(2)}} \qquad \text{.........(43)}$$

5.2 It is clear from equations (40) - (43), that the only $\Omega_s^{(\ell)}$ integrals appearing in either the electrical or thermal conductivity are those with $\ell=1$ or $\ell=2$ and hence by (38) only two $\phi_{12}^{(\ell)}(v)$ functions occur in the analysis. These functions $\phi_{12}^{(1)}$ and $\phi_{12}^{(2)}$ are well known in atomic collision theory as the diffusion and viscosity cross sections $Q_D$ and $Q_\eta$ , defined by

$$\phi_{12}^{(1)}(v) = Q_D(v) = 2\pi \int_0^{\infty} (1-\cos\theta)\, p\, dp \qquad \text{.........(44)}$$

$$\phi_{12}^{(2)}(v) = Q_\eta(v) = 2\pi \int_0^{\infty} \sin^2\theta\, p\, dp \qquad \text{.........(45)}$$

They can be expressed in terms of the scattering amplitudes for the potential $V(r)$

$$Q_D(v) = 2\pi \int_0^{\pi} (1-\cos\theta) |f(\theta)|^2 d(\cos\theta) \qquad \text{..........(46)}$$

$$Q_\eta(v) = 2\pi \int_0^{\pi} \sin^2\theta \, |f(\theta)|^2 d(\cos\theta) \qquad \text{..........(47)}$$

Clearly $Q_\eta(v)$ gives more weight to scattering at $\frac{\pi}{2}$ and $Q_D(v)$ to scattering in the forward direction, than does the usual elastic scattering cross section $Q_{el}$. Provided the scattering centre is not of the same nature as the scattered particle it is an elementary matter to express both cross sections in terms of the scattering phase shifts $\eta_l$ (c.f. Chapter I §1.1) for $V(r)$. In terms of these phase shifts the relevant cross sections become (Chapter I §1.2)

$$Q_D(k^2) = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (l+1) \sin^2(\eta_l - \eta_{l+1}) \qquad \text{.........(48)}$$

$$Q_\eta(k^2) = \frac{2\pi}{k^2} \sum_{l=0}^{\infty} \frac{(l+1)(l+2)}{(l+3/2)} \sin^2(\eta_l - \eta_{l+2}) \qquad \text{.........(49)}$$

Here, we have employed quantal methods to derive $Q_D$ and $Q_\eta$. However most earlier workers have used classical mechanics to evaluate these quantities. Perisco (1926) used a coulomb potential for $r<r_0$ and a Debye screened coulomb potential for $r>r_0$, with $r_0$ such that $V(r_0)=\frac{kT}{e_1}$. Cowling (1945) and Spitzer's group use a coulomb potential with a cut off at either $n_e^{-1/3}$ or $h_D$ ; Liboff (1959) adopts the same potential as we do, while Theimer and Hoffmann (1958;1959) use a potential of the form (35) but with $b \simeq a = n_e^{+1/3}$ and using the quantum mechanical Born Approximation rather than a classical model. Were the potential a pure coulomb potential to all $r$, then a classical approach would be valid. Unfortunately the cross sections would then diverge at all energies and no physically meaningful result would be obtained. This was realised by Marshak (1941), who used uncertainty principle arguments to reject the classical approach for all $\theta <$ some $\theta_0$ and chooses the corresponding impact parameter $p_M$ as a cut-off. The long range nature of the interaction however means that much of the contribution to $Q_D$ and $Q_\eta$ arises form just this diffraction region. Landshoff (1949) in addition neglects scattering through angles $\theta \simeq \pi$ but retains a classical approximation elsewhere. On the other hand while Theimer and Hoffmann use a quantal model, their improper choice of $n_e^{-1/3}$ as screening parameter and failure to investigate the validity of the Born approximation is unsatisfactory.

The classical model of Spitzer retains only the leading term in a series expansion of the integrand of the scattering integral and yields

$$Q_D = 4 p_0^2 \log(\alpha p_0)$$

$$Q_\eta = 8 p_0^2 \log(\alpha p_0) \qquad \text{..........(50)}$$

where $\alpha = h_D^{-1}$ and $p_0$ is the classical distance of closest approach,

$$p_0 = \frac{e_1 e_2}{\mu v^2} \qquad \text{..........(51)}$$

Liboff's work shows that the adoption of a screened coulomb potential, but retention of a classical approach, yields the same result to the dominant log term. We have retabulated Spitzer's results for comparision purposes, his table using a mean value of $p_0$ averaged over all test particles.

Before going on to discuss the detailed evaluation of phase shifts and cross sections the uncertainty principle arguments referred to above indicate that for our potential (31) a classical description of the scattering is valid for all $\theta > \theta_0$ where

$$\theta_0 \sim \frac{1}{k h_D} \simeq \frac{3\times10^{-7}}{T} n_e^{1/2} \text{ radians} \qquad \ldots\ldots\ldots(52)$$

while Born's approximation is valid for all $\theta < \theta_0$. Thus Jeffery's approximation to the quantal phase shifts might be expected to be good for $\theta_0$ small, i.e. high $T$ and low $n_e$, while Born's would be the better approximation for high $n_e$ and low $T$. Similarly for the Theimer and Hoffmann potential (35) taking

$$a \simeq b \simeq 0{\cdot}63\, n^{-1/3} \text{ cms} \qquad \ldots\ldots\ldots\ldots(53)$$

we find

$$\theta_0 \sim \frac{5\times10^{-6}\, n^{1/3}}{T^{1/2}} \text{ radians} \qquad \ldots\ldots\ldots\ldots(54)$$

leading to similar conclusions. Thus Born's approximation will be best just in that range where they do not apply it.

6. The form

$$\frac{d^2}{dr^2} g_\ell(r) + \left[k^2 - 2\mu V(r) - \frac{\ell(\ell+1)}{r^2}\right] g_\ell(r) = 0$$

in which we have written the scattering equation is not very satisfactory for a numerical integration since as $r \to 0$

$$g_\ell(r) \to r^\ell$$

and as we shall be interested in large $\ell$ ($\ell \gg 1$), accuracy is lost from the beginning. However, the solution can be expressed in closed form (Mott and Massey 1949) if $\alpha = 0$ in terms of a product of $r^\ell$ times a hypergeometric function. We therefore put

$$y_\ell(r) = r^\ell g_\ell(r) \qquad \ldots\ldots\ldots\ldots(55)$$

so that $y_\ell(r)$ satisfies

$$y_\ell'' + \frac{2(\ell+1)}{r} y_\ell' + \left\{k^2 + \frac{A}{r} e^{-\alpha r}\right\} y_\ell = 0 \qquad \ldots\ldots\ldots\ldots(56)$$

subject to the boundary conditions

$$y_\ell(0) = 1\cdot 0 \quad ; \quad y_\ell(r) \sim A r^{-\ell} \sin(kr - \tfrac{1}{2}\ell\pi + \eta_\ell) \qquad \ldots\ldots\ldots\ldots(57)$$

and

$$\begin{aligned} A &= -1 \quad \text{(election - election interaction)} \\ A &= +z \quad \text{(election-nucleus of charge z)} \end{aligned} \qquad \ldots\ldots\ldots\ldots(58)$$

Starting values are derived from a power series solution about $r = 0$, for a potential of the form (31),

$$y_\ell(r) \xrightarrow[r \to 0]{} 1 - \frac{A}{(\ell+1)} r + \frac{A^2 - \frac{1}{2}(\ell+1)(k^2 - 2A\alpha)}{(\ell+1)(2\ell+3)} r^2$$

$$- \frac{\left[A^3 - \frac{1}{2}A(3\ell+4)(k^2-2A\alpha) + \frac{1}{2}(\ell+1)(2\ell+3)A\alpha^2\right] r^3}{3(\ell+1)(\ell+2)(2\ell+3)}$$

$$+ r^4 \frac{\left[(\ell+1)(\ell+2)(2\ell+3)A\alpha^3 + (4\ell+7)(2\ell+3)A^2\alpha^2 - 2(3\ell+5)A^2(k^2-2A\alpha) + 2A^4 + \frac{3}{2}(\ell+1)(\ell+2)(k^2-2A\alpha)^2\right]}{12(2\ell+5)(2\ell+3)(\ell+1)(\ell+2)} \qquad \ldots\ldots\ldots\ldots(59)$$

which reduces to the usual hypergeometric function as $\alpha \to 0$. Details of the lengthy numerical proceedures and the programming of the Univac 1101 are given in §8. It is sufficient to say here, that for any $r > \alpha^{-1}$

$$y_l(r) = A r^{-(l+1)} \left\{ j_l(kr) \cos\eta_l - y_l(kr) \sin\eta_l \right\} \qquad \text{..........(60)}$$

where $j_l(x)$ and $y_l(x)$ are spherical Bessel functions of half integral order. Then if a zero of the solution occurs at $r = r_0$,

$$\eta_l = \arctan\left\{ \frac{j_l(kr_0)}{y_l(kr_0)} \right\} \qquad \text{..........(61)}$$

Let $\eta_l^{(i)}$ be the resultant approximation to $\eta_l$ at the $i^{th}$ zero of the solution and $\eta_{l+1}^{(i)}$ the corresponding approximation to $\eta_{l+1}$. Then $\Delta\eta_l^{(i)} = \eta_l^{(i)} - \eta_{l+1}^{(i)}$ is almost independent of i for large i ($i > 20$ say) and provides the required exact solution.

6.2 When the phase shift $\eta_l \ll 1$, it is easily shown that

$$\tan\eta_l \doteq \eta_l^B = 2k\mu \int_0^\infty r^2 V(r) \left[ j_l(kr) \right]^2 dr \qquad \text{..........(62)}$$

where $j_l(kr)$ is the $l^{th}$ order spherical Bessel function of the $1^{st}$ kind. Therefore using the interaction (31),

$$\eta_l^B = -\mu\pi \int_0^\infty e^{-\alpha r} \left[ J_{l+\frac{1}{2}}(kr) \right]^2 dr \qquad \text{..........(63)}$$

which may be readily evaluated to give

$$\eta_l^B = -\frac{\mu}{k} Q_l \left\{ 1 + \frac{\alpha^2}{2k^2} \right\} \qquad \text{..........(64)}$$

This is known as the $1^{st}$ Born approximation to the phase shift, since if one replaces $(e^{2i\eta_l} - 1)$ in the Faxén-Holtsmark formula for the elastic scattering cross section by $2i\eta_\ell$, we obtain, on summation, the usual Born approximation to $Q_{el}$. When $\ell$ is large (Hobson 1931),

$$Q_\ell\left\{1+\frac{\alpha^2}{2k^2}\right\} \xrightarrow[\ell\to\infty]{} \left(\frac{\pi}{\ell}\right)^{\frac{1}{2}} \exp\left\{-(\ell+1)\frac{\alpha}{k}\right\}\left(\frac{k}{2\alpha}\right)^{\frac{1}{2}} \qquad \text{..........(65)}$$

so introducing the impact parameter $p$,

$$p = \frac{\ell+\frac{1}{2}}{k} \qquad \text{..........(66)}$$

$\eta_\ell$ becomes

$$\eta_\ell^{B} = -\frac{\mu}{k}\left(\frac{\pi p}{2\alpha}\right)^{\frac{1}{2}} e^{-\alpha p} \qquad \text{..........(67)}$$

and is monotonic decreasing with $\ell$ increasing.

63 In Chapter I§2.4 we use a method due to Jefferys, (1926), to obtain an expression for $\eta_\ell$ when there is only a weak interaction, i.e.

$$\eta_\ell = -\frac{\mu}{k}\int_{p}^{\infty} \frac{r V(r)\, dr}{\sqrt{r^2-p^2}} \qquad \text{..........(68)}$$

which is for our form of potential,

$$\eta_\ell = -\frac{\mu}{k}\int_{p}^{\infty} \frac{e^{-\alpha r}}{\sqrt{r^2-p^2}}\, dr \qquad \text{..........(69)}$$

Differentiating both sides w.r.t. $\alpha$,

$$\frac{\partial\eta_\ell}{\partial\alpha} = +\frac{\mu}{k}\int_{p}^{\infty} \frac{r e^{-\alpha r}}{\sqrt{r^2-p^2}}\, dr \qquad \text{..........(70)}$$

The integral on the right hand side is a standard Laplace transform (Erdelyi et al 1954), yielding

$$\frac{\partial\eta_\ell}{\partial\alpha} = \frac{\mu}{k}\, p\, K_1(\alpha p) \qquad \text{..........(71)}$$

But now we can write

$$K_1(\alpha p) = -\frac{1}{p}\frac{\partial}{\partial\alpha}\left\{K_0(\alpha p)\right\} \qquad \text{..........(72)}$$

where $K_0(x)$ and $K_1(x)$ are zeroth and first order modified Bessel functions of the second kind. Hence

$$\eta_\ell^{MM} = -\frac{\mu}{k}K_0(\alpha p) \qquad \text{..........(73)}$$

and as $\ell \to \infty$ so does $p$ (for fixed $k$) and

$$\eta_\ell^{MM} \to -\frac{\mu}{k}\left(\frac{\pi p}{2\alpha}\right)^{\frac{1}{2}} e^{-\alpha p} \qquad \text{..........(74)}$$

which is an identical result to that obtained from the Born approximation in the same limit, (c.f. equation (67)). This equality also holds for the potential $V(r) = Ae^{-\alpha r}$ and is conjectured to be a general property of the potentials of the form $V(r) = Ar^n e^{-\alpha r}$ $(n=0, \pm 1, \ldots)$. We shall also be interested in the modified screened coulomb potential adopted by Theimer and Hoffman. Using the Massey-Mohr approximation it yields

$$\eta_\ell^{MM}(T\text{-}H) = \mathcal{R}\left(\frac{\mu}{k}K_0\left[\sqrt{2}\alpha p e^{-i\pi/4}\right]\right) \qquad \text{..........(75)}$$

6.4 When variational methods were first introduced in atomic collision theory by Hulthen (1944; 1948), he illustrated his methods by applying them to a screened coulomb potential, the angular momentum being zero. He considers the differential equation

$$\left.\begin{aligned} &\frac{d^2\phi}{dx^2} + \left\{k^2 + v(x)\right\}\phi = 0 \\ &0 \leq x \leq +\infty \;;\; k > 0 \;;\; \phi(0) = 0 \;;\; \phi(\infty) \text{ finite} \end{aligned}\right\} \text{..........(76)}$$

and $v(x)$ is assumed continuous except perhaps at $x=0$ where the usual conditions apply. If we suppose $xv(x)\to 0$ as $x\to\infty$ and define

$$L[\psi] = \int_0^\infty \psi\,\mathcal{L}\,\psi\,dx \qquad \text{..........(77)}$$

$$\mathcal{L} = \frac{d^2}{dx^2} + k^2 + v(x)$$

and consider varied functions $\phi + \delta\phi = \phi^t$

$$\begin{aligned} \phi(x) &\xrightarrow[x\to\infty]{} \sin(kx+\eta) \\ \phi^t(x) &\xrightarrow[x\to\infty]{} \sin(kx+\eta+\delta\eta) \end{aligned} \qquad \text{..........(78)}$$

then it is easily shown that if $\delta\phi=0$ at $x=0$

$$\delta\phi \xrightarrow[x\to\infty]{} \cos(kx+\eta)\,\delta\eta \qquad \text{..........(79)}$$

and so

$$\delta L = -k\,\delta\eta \qquad \text{..........(80)}$$

So that varying $\phi$ in such a way that $L\equiv 0$ is always fulfilled, we have a stationary phase

$$\delta\eta = 0 \qquad \text{..........(81)}$$

Now introduce $y(x)$

$$\left.\begin{aligned} \phi(x) &= \sin(kx+\eta) - \sin\eta\cdot y(x) \\ \text{so that}\quad y(0) &= 1 \qquad y(\infty) = 0 \end{aligned}\right\} \qquad \text{..........(82)}$$

and using (76)

$$y'' + k^2 y + v(x)y = v(x)\left\{\cos kx + \cot\eta\,\sin kx\right\} \qquad \text{..........(83)}$$

we note that a solution of (83) can satisfy the conditions on $y$ for only one value of $\eta$ . Equation (83) is the Euler equation of a certain variational problem. Put

$$J = \int_0^\infty F(x,y,y')\,dx \qquad \text{..........(84)}$$

with

$$F(x,y,y') = -y'^2 + k^2y^2 + v(x)(\cos kx - y)^2 \qquad \text{..........(85)}$$

and require $J$ to be stationary subject to

$$N = \int G(x,y)\,dx = \text{const} \qquad \text{..........(86)}$$

with

$$G(x,y) = v(x)\sin kx\,(\cos kx - y) \qquad \text{..........(87)}$$

which yields (83), Multiplying (83) by $\{\cos kx - y\}$ and integrating

$$J + \lambda N = 0 \qquad (\lambda = \cot\eta) \qquad \text{..........(88)}$$

Now the true solution $\phi$ satisfies

$$\sin\eta = \frac{1}{k}\int_0^\infty \sin kx\; v(x)\,\phi(x)\,dx \qquad \text{..........(89)}$$

and introducing (82) for $\phi(x)$ we obtain

$$N = k(1 - \eta^B\cot\eta) \qquad \text{..........(90)}$$

where $\eta^B$ is the Born phase shift. This can fairly readily be generalized to non-zero angular momentum. Now choose a trial function

$$y^t = y_0 + \sum_1^n c_\nu y_\nu \qquad \text{..........(91)}$$

where the $c_\nu$ are variable parameters. Then if $J$ is to be stationary with $N$ constant

$$\delta J + 2\lambda \delta N = 0 \qquad \text{..........(92)}$$

yields the set of coupled equations

$$N = \text{const} \; ; \; \frac{\partial J}{\partial c_\nu} + 2\lambda \frac{\partial N}{\partial c_\nu} = 0 \quad (\nu = 1, 2 \ldots n) \qquad \text{..........(93)}$$

In Hulthen's paper this is applied to the potential

$$v(x) = b\frac{e^{-x}}{x} \qquad (\ell = 0) \qquad \text{..........(94)}$$

with a trial function

$$y(x) = e^{-x} + (1 - e^{-x}) \sum_1^n c_\nu e^{-\nu x} \qquad \text{..........(95)}$$

and $\eta_0$ is tabulated for $0 \leq k \leq 1.0$ and b=1.5 and 1.6, n being either 1,2 or 3. The method is lengthy and was therefore not used here.

6.5 A variational principle for the phase shift has been given by Morse and Feshbach (1953) which is due to Schwinger. We consider the differential equation

$$\left.\begin{aligned} &\frac{d^2 u_\ell}{dr^2} + \left\{k^2 - \frac{\ell(\ell+1)}{r^2} - \lambda U(r)\right\} u_\ell = 0 \\ &u_\ell(0) = 0 \qquad u_\ell(r) \sim \sin(kr - \tfrac{1}{2}\ell\pi + \eta_\ell) \end{aligned}\right\} \qquad \text{..........(96)}$$

see Chapter I § 2.3 and obtain the form

$$\cot\eta_\ell \simeq \cot\eta_\ell^B \left\{ 1 - \frac{2}{k} \cot\eta_\ell^B \int_0^\infty (kry_\ell) U(krj_\ell) \int_0^r (kr' j_\ell)^2 U(r') \, dr' dr \right. \qquad \text{..........(97)}$$

for the phase shift. For our choice of potential this may be evaluated as follows. Consider the integral

$$I = \int_0^{kr} x e^{-\beta x}\left[j_\ell(x)\right]^2 dx = \frac{\pi}{2}\int_0^{kr} e^{-\beta x}\left[J_{\ell+\frac{1}{2}}(x)\right]^2 dx \qquad \text{..........(98)}$$

with $\beta = \frac{\alpha}{k}$ and introduce the expansion, Watson(1944)

$$\left[J_{\ell+\frac{1}{2}}(x)\right]^2 = \sum_{m=0}^{\infty} \frac{(-1)^m\,\Gamma(2\ell+2m+2)\,\left(\frac{x}{2}\right)^{2\ell+2m+1}}{m!\,\Gamma(2\ell+m+2)\left\{\Gamma(\ell+m+\frac{3}{2})\right\}^2} \qquad \text{..........(99)}$$

so we have

$$I = \frac{\pi}{2}\sum_{m=0}^{\infty}\frac{(-1)^m\,\Gamma(2\ell+2m+2)}{m!\,\Gamma(2\ell+m+2)\left\{\Gamma(\ell+m+\frac{3}{2})\right\}^2}\int_0^{kr}\left(\frac{x}{2}\right)^{2\ell+2m+1} e^{-\beta x}\,dx \qquad \text{..........(100)}$$

Now the incomplete $\gamma$ function is defined as (Erdelyi et al 1953)

$$\int_0^{\alpha r} y^{2\ell+2m+1} e^{-y}\,dy = \gamma(2\ell+2m+2\,;\alpha r) \qquad \text{..........(101)}$$

so $I$ becomes on putting $y = \beta x$

$$I = \pi\sum_{m=0}^{\infty}\frac{(-1)^m\,\Gamma(2\ell+2m+2)\,\gamma(2\ell+2m+2);\alpha r)}{m!\,\Gamma(2\ell+m+2)\left\{\Gamma(\ell+m+\frac{3}{2})\right\}^2(2\beta)^{2\ell+2m+2}} \qquad \text{..........(102)}$$

Substitute (102) in (97) and simplify

$$\cot\eta_\ell = \cot\eta_\ell^B\left\{1 - \frac{4\pi\mu^2}{k}\cot\eta_\ell^B\int_0^{\infty} J_{\ell+\frac{1}{2}}(x)\,Y_{\ell+\frac{1}{2}}(x)\,e^{-\beta x}\,I(\beta)\,dx\right\} \qquad \text{..........(103)}$$

We can then again expand the product of Bessel functions

$$J_{\ell m} = \int_0^{\infty} e^{-\beta x} J_{\ell+\frac{1}{2}}(x)\,Y_{\ell+\frac{1}{2}}(x)\,\gamma(2\ell+2m+2\,;\beta x)\,dx \qquad \text{..........(104)}$$

and using (102) we have

$$\cot\eta_\ell = \cot\eta_\ell^{B}\left\{1-\frac{4\pi^2\mu^2}{k}\cot\eta_\ell^{B}\sum_{m=0}^{\infty}\frac{(-1)^m\,\Gamma(2\ell+2m+2)\,J_{\ell m}}{m!\,(2\beta)^{2\ell+2m+2}\,\Gamma(2\ell+m+2)\left\{\Gamma(\ell+m+\frac{3}{2})\right\}^2}\right\} \quad .(105)$$

while

$$J_{\ell m} = \sum_{p=0}^{\infty}\frac{(-1)^p(2p)!}{(p!)^2\,\Gamma(\ell+\frac{3}{2}+p)\,\Gamma(p-\ell+\frac{1}{2})}\,\frac{1}{\beta}\cdot\frac{1}{(2\beta)^{2p}}\int_0^\infty y^{2p}e^{-y}\,\gamma(2\ell+2m+2;y)\,dy \quad .(106)$$

The integrals in this expression can be put in the form of hypergeometric functions, (Erdelyi et al 1954)

$$J_{\ell m} = \sum_{p=0}^{\infty}\frac{2(-1)^p(2p)!\qquad\Gamma(2\ell+2m+2p+3)}{(2\beta)^{p+1}(p!)^2\,\Gamma(\ell+\frac{3}{2}+p)\,\Gamma(p-\ell+\frac{1}{2})\,(2\ell+2m+2)\,2^{2\ell+2m+2p+3}}$$

$$\times\ {}_2F_1\left(1,\,2\ell+2m+2p+3,\,2\ell+2m+3,\,\tfrac{1}{2}\right) \qquad ..(107)$$

Introducing this in (105) we have finally,

$$\cot\eta_\ell = \cot\eta_\ell^{B}\left\{1-\frac{4\pi^2\mu^2}{k}\cot\eta_\ell^{B}\sum_{m=0}^{\infty}\sum_{p=0}^{\infty}\frac{(-1)^{m+p}(2p)!\,\Gamma(2\,\overline{\ell+m+1})}{m!\,(p!)^2(2\beta)^{2\ell+2m+p+3}}\right.$$

$$\left.\times\frac{\Gamma(2\ell+2m+2p+3)(2\ell+2m+2)^{-1}\,{}_2F_1(1,2\ell+2m+2p+3,2\ell+2m+3,\frac{1}{2})}{\Gamma(2\ell+m+2)\left\{\Gamma(\ell+m+\frac{3}{2})\right\}^2\Gamma(\ell+\frac{3}{2}+p)\,\Gamma(p-\ell+\frac{1}{2})\,4^{\ell+m+p+1}}\right\} \quad ..(108)$$

The double summation is a function of $\ell$, the angular momentum and $\beta=\frac{\alpha}{k}$ only, so we can write,

$$\cot\eta_\ell = \cot\eta_\ell^{B}\left\{1-\frac{4\pi^2\mu^2}{k}\cot\eta_\ell^{B}\,\mathcal{F}(\ell,\beta)\right\} \qquad ..........(109)$$

and evaluate $\mathcal{F}(\ell,\beta)$ as a function of $\beta$, given $\ell$. Here,

$$\beta=\frac{\alpha}{k}=\Theta_0=\frac{3\times10^{-7}n_e^{1/2}}{T} \qquad ..........(110)$$

which appeared previously as the angle below which the Born approximation to the scattering amplitudes was valid. For the range of $n_e$ and $T_e$ of interest in the present work, the convergence of $\mathcal{H}(\ell,\beta)$ is very slow. However for a short range nuclear screened coulomb potential at high centre of mass energies equation (109) should provide an excellent approximation. A further discussion will be given elsewhere.

7.1 In evaluating the cross sections, it should in principle, be most accurate to use the exact values of $\Delta\eta_\ell = \eta_\ell - \eta_{\ell+1}$ and $\Delta^{(2)}\eta_\ell = \eta_\ell - \eta_{\ell+2}$ as obtained in § 6.1 equations (48),(49). However available computer time restricted such computations to $\ell<10$ for a limited number of values of $T$ and $n_e$. We can estimate the number of phases giving an appreciable contribution to the sum, by noting that at an impact parameter equal to the Debye length, the relevant angular momentum is

$$\ell \simeq k h_D \doteq \frac{1}{\beta} \doteq \frac{3\times10^6 T(^\circ K)}{\sqrt{n_e}} \qquad \text{..........(111)}$$

so that for $T=10^4$ and $n_e=10^{18}$, $\ell\sim 30$, while for $T=10^7$ and $n_e=10^8$ $\ell\sim3\times10^9$. However for $T<10^6$ and $n_e=10^{18}$, $T<10^5$, $n_e=10^{16}$, and $T=10^4$, $n_e=10^{14}$ less than 3000 phases enter and it proved practical to evaluate the summations using the Born approximation (64) for $\eta_\ell$. The results ar are displayed in Table I and should be more accurate than the results from any of the other approximate methods,

7.2 We now turn to the Massey- Mohr approximation to the cross sections and it is clear from 7.1 that a large number of phases enter the expressions for $Q_D$ and $Q_\eta$. However for

$l>>1$, $\Delta\eta_l$ and $\Delta^{(2)}\eta_l$ are slowly varying quantities and it should be possible to replace the summation by an integration without appreciable loss of accuracy. Introducing the impact parameter $p$, and noting that for $k$ not too small,

$$\Delta\eta_l \simeq \xi(p) = -\frac{1}{k}\frac{\partial\eta(p)}{\partial p} \qquad \text{..........(112)}$$

we can write equation (48) as

$$Q_D = 4\pi\int_0^\infty p\sin^2\xi(p)\,dp \qquad \text{..........(113)}$$

Since from (72) we have

$$\eta(p) = -\frac{\mu}{k}K_0(\alpha p) \qquad \text{..........(114)}$$

$\xi(p)$ becomes

$$\xi(p) = \frac{\mu\alpha}{k^2}K_1(\alpha p) \qquad \text{..........(115)}$$

$K_1(x)$ being a 1st order modified Bessel function of the second kind. From its known properties, $\xi(p)$ is monotonic decreasing, hence there exists some $\bar{p}$ such that $\xi(p) < \frac{\pi}{2}$, $p > \bar{p}$ while for $p < \bar{p}$, $\sin^2\xi(p)$ oscillates rapidly and may be replaced by its average value. Thus

$$Q_D = \bar{p}^2 + 4\int_{\bar{p}}^\infty p\sin^2\xi(p)\,dp \quad (\pi a_0^2) \qquad \text{..........(116)}$$

where

$$\frac{\mu\alpha}{k^2}K_1(\alpha\bar{p}) = \frac{\pi}{2} \qquad \text{..........(117)}$$

defines $\bar{p}$. In the range of $T$, $n_e$ of interest $\alpha\bar{p} << 1$, so $K_1(\alpha\bar{p}) \simeq (\alpha\bar{p})^{-1}$, hence (117) becomes

$$\bar{p} = \frac{2\mu}{\pi k^2} = \frac{1}{\pi E} = \frac{2p_0}{\pi} \qquad \text{..........(118)}$$

where $p_0$ is Spitzers' classical distance of closest approach. It is now necessary to solve (116) and 117) numerically: however in the limit $T \to \infty$ $(\alpha\bar{p} \to 0)$ it can be shown that they reduce to the classical results of Spitzer (1956) and Liboff (1959). We first note that if for $p > \bar{p}$ we replace $\sin^2 \xi(p)$ by $\xi^2(p)$ the errors will be less than 5%, then

$$Q_D = \bar{p}^2 + \frac{4\mu^2\alpha^2}{k^4} \int_{\bar{p}}^{\infty} p \left[K_1(\alpha p)\right]^2 dp \qquad \text{..........(119)}$$

the integral being of standard Lommel form (Gray et al 1931). Evaluating it we have

$$Q_D = \bar{p}^2 + \frac{2\mu^2\alpha^2\bar{p}^2}{k^4} \left\{\left[K_1'(\alpha\bar{p})\right]^2 - \left(1 + \frac{1}{(\alpha\bar{p})^2}\right)\left[K_1(\alpha\bar{p})\right]^2\right\} \qquad \text{.........(120)}$$

primes indicating differentiation w.r.t. $\bar{p}$ . Put

$$\beta^2 = \frac{\mu^2\alpha^2}{k^4} \quad ; \quad y = \alpha\bar{p} \qquad \text{..........(121)}$$

and use the relation

$$\left[K_1'(y)\right]^2 = \frac{1}{y^2} K_1^2(y) + \frac{2}{y} K_1(y) K_0(y) + K_0^2(y) \qquad \text{..........(122)}$$

the dashes now indicating differentiation w.r.t. $y$ . Then

$$Q_D = \bar{p}^2 \left\{1 + 2\beta^2\left[K_0^2(y) - K_1^2(y) + \frac{2}{y} K_1(y) K_0(y)\right]\right\} \qquad \text{..........(123)}$$

Since $y << 1$,

$$\left.\begin{aligned} K_1(y) &\simeq \frac{1}{y} + \frac{1}{2} y \left\{\log \tfrac{1}{2} y - \tfrac{1}{2} + \gamma\right\} + O(y^3) \\ K_0(y) &\simeq -(\gamma + \log \tfrac{1}{2} y)(1 + \tfrac{1}{4} y^2) + \tfrac{1}{4} y^2 + O(y^4) \end{aligned}\right\} \qquad \text{..........(124)}$$

and putting these expansions in (123) we have

$$Q_D = \bar{p}^2 \left\{ 1 - \frac{2}{\bar{p}^2} \left( \frac{\mu}{k^2} \right)^2 \left[ 2\gamma + 1 + 2 \log \tfrac{1}{2} y \right] \right\} + O\left(\bar{p}^{-4}\right) \quad \ldots\ldots\ldots(125)$$

where $\gamma$ is Euler's constant. Expressing this in terms of $p_0$,

$$Q_D = 4 p_0^2 \left\{ \log \frac{\alpha p_0}{\pi} - 0.98 \right\} \quad \ldots\ldots\ldots\ldots(126)$$

which would be identical to Liboff's result if we had chosen $\bar{p}$ ; $\xi(\bar{p}) = 1$ rather than $\frac{\pi}{2}$ , but differs from Liboff's only in a small correction term. An identical treatment of $Q_\eta$ is possible.

It is of interest to apply the method described above, to the Theimer-Hoffman potential (35). We have again

$$Q_D = \bar{p}^2 + \int_{\bar{p}}^{p_0} p \sin^2 \xi(p)\, dp \quad (\pi a_0^2) \quad \ldots\ldots\ldots\ldots(127)$$

where in this case

$$\xi(p) = \frac{\mu}{2k^2} \left\{ \bar{a} K_1(\bar{a} p) + a K_1(a p) \right\} \quad \ldots\ldots\ldots\ldots(128)$$

in which

$$a = \alpha + ib \quad \ldots\ldots\ldots\ldots(129)$$

and a bar indicates a complex conjugate. Putting $y = ap$ and noting that (McLachlan 1934)

$$\overline{K_1(z)} = K_1(\bar{z}) \quad \ldots\ldots\ldots\ldots(130)$$

while since $b \triangleq \alpha$

$$a = \sqrt{2}\, \alpha\, e^{-i\pi/4} \quad \ldots\ldots\ldots\ldots(131)$$

we have

$$\bar{a}K_1(\bar{z}) + aK_1(z) = 2\alpha\left[\mathrm{ker}_1(\sqrt{2}z) + \mathrm{kei}_1(\sqrt{2}z)\right] \quad \text{..........}(132)$$

in terms of the modified Kelvin functions of the 1st order and both kinds, hence

$$Q_D^{T.H.} = \bar{p}^2 + 4\int_{\bar{p}}^{\infty} p\sin^2\left\{\alpha p_0\left[\mathrm{ker}_1(\sqrt{2}\alpha p) + \mathrm{kei}_1(\sqrt{2}\alpha p)\right]\right\}dp \quad \text{........}(133)$$

while in this case $\bar{p}$ is such that

$$\frac{\mu}{2k^2}\left[\bar{a}\cdot\frac{1}{\bar{\alpha}p} + a.\frac{1}{\alpha p}\right] \simeq \frac{\pi}{2} \quad \text{..........}(134)$$

giving $\bar{p} = \frac{2\mu}{\pi k^2}$ as before. Expansion of the Kelvin functions for small argument yields the limiting form

$$Q_D \simeq 4p_0^2\left\{\frac{1}{2}\log\left[\frac{p_0^2}{\pi^2}(\alpha^2+b^2)\right] - 0{\cdot}98\right\} \quad \text{..........}(135)$$

in agreement with (126). Thus, at high temperatures the classical result of Spitzer agrees with the semiclassical BWKJ result and which is unaffected if we modify the potential by multiplying it by a $\cos(r/h_D)$ term. The superimposed oscillation is so slow that it is entirely dominated by the rapid exponential variation.

7.3 Born's approximation to the scattering amplitude for a central potential $V(r)$ is represented by

$$f(\theta) \simeq -\frac{\mu}{2\pi k^2}\int e^{i\underline{K}\cdot\underline{r}}V(r)ds = f^B(\theta) \quad \text{..........}(136)$$

where $\underline{K} = \underline{k}_i - \underline{k}_f$ and yields for the simple potential (31)

$$f^B(\theta) = \frac{2\mu}{\alpha^2+k^2} \quad \text{..........}(137)$$

so that the cross sections become

$$Q_D^{\,B} = \frac{2\mu^2}{k^4}\left[\log\left(1+\frac{4k^2}{\alpha^2}\right) - \frac{4k^2}{\alpha^2+4k^2}\right] \quad \ldots\ldots\ldots\ldots(138)$$

and

$$Q_\eta^{\,B} = \frac{2\mu^2}{k^6}\left[(2k^2-\alpha^2)\log\left(1+\frac{4k^2}{\alpha^2}\right) - 4k^2\right] \quad \ldots\ldots\ldots\ldots(139)$$

Theimer and Hoffman have obtained the equivalent expressions for their potential (35), which in our notation become

$$f^{\,B}(\theta)_{T-H} = \frac{2\mu k^2}{(4\alpha^4+k^4)} \quad \ldots\ldots\ldots\ldots(140)$$

and

$$Q_D^{\,B}(T.H.) = \frac{\mu^2}{k^4}\left[\log\left(1+\frac{4k^4}{\alpha^4}\right) - \frac{4k^4}{\alpha^4+4k^4}\right] \quad \ldots\ldots\ldots\ldots(141)$$

$$Q_\eta^{\,B}(T.H.) = \frac{2\mu^2}{k^4}\left[\log\left(1+\frac{4k^4}{\alpha^4}\right) - 3 + \frac{3\alpha^2}{2k^2}\tan^{-1}\frac{2k^2}{\alpha^2}\right] \ldots\ldots\ldots\ldots(142)$$

Introducing atomic units, we have

$$k^2 = 6{\cdot}362\times10^{-6}\,T\,(^\circ K) \;\; ; \;\; \alpha = 7{\cdot}67_0\times10^{-10}\left(\frac{n_e}{T}\right)^{1/2} \quad \ldots\ldots\ldots\ldots(143)$$

so that

$$Q_D^{B} \triangleq 4{\cdot}5\times10^{10}\,T^{-2}\left[\log\left(1+\frac{4{\cdot}54\times10^{13}}{n_e}T^2\right)\right]\pi a_0^2 \ldots\ldots\ldots\ldots(144)$$

and

$$\begin{aligned} Q_\eta^{B} \triangleq 6{\cdot}76\times10^{15}\,T^{-3}\Big[&\left(1{\cdot}33\times10^{-5}\,T - 5{\cdot}88\times10^{-19}\frac{n_e}{T}\right) \\ &\times\log\left(1+\frac{4{\cdot}54\times10^{13}}{n_e}T^2\right) - 2{\cdot}67.10^{-5}\,T\Big]\,\pi a_0^2 \end{aligned} \quad \ldots\ldots\ldots\ldots(145)$$

The results are given in tables II-V and are discussed in §8.

7.4 Since most digital computers used in scientific calculations have well developed matrix inversion programmes included in their library of subroutines, for the sake of completeness we have investigated how we might use this approach to calculate $\eta_\ell$ for a screened coulomb potential. Writing the scattering equation as

$$\left\{ \frac{d^2}{dx^2} + k^2 - \frac{\ell(\ell+1)}{x^2} \right\} f(x) = F(x) \qquad ..........(146)$$

with

$$F(x) = G(x) f(x) \ ; \ G(x) = -\frac{2\mu}{x} e^{-\alpha x} \qquad .........((147)$$

and imposing the conditions

$$\begin{aligned} &F(x) \to 0 \quad \text{as} \quad x \to \infty \\ &f(0) = 0 \ ; \ f(x) \sim B\left\{ \cos\eta_\ell \cdot j_\ell(kx) - \sin\eta_\ell \cdot y_\ell(kx) \right\} \end{aligned} \qquad ..........(148)$$

we can transform (146) into the integral equation

$$f(x) = kx\, j_\ell(kx) + \int_0^\infty K_\ell(x,x')\, G(x')\, f(x')\, dx' \qquad ..........(149)$$

The kernel $K(x,x')$ is given by

$$\begin{aligned} K_\ell(x,x') &= (-1)^\ell k\, j_\ell(kx)\, y_\ell(kx')\, xx' \quad (x \leq x') \\ &= (-1)^\ell k\, y_\ell(kx)\, j_\ell(kx')\, xx' \quad (x \geq x') \end{aligned} \qquad ..........(150)$$

Then

$$\tan\eta_\ell = -\int_0^\infty x'\, j_\ell(kx')\, F(x')\, dx' \qquad ..........(151)$$

Adopting a proceedure analogous to that of Fraser (1959), (who dealt with the $\ell=0$ case ), if $x_i, x_j$ are two specific values of $x$ in $(0,\infty)$ we define the matrix elements

$$L_{ij}^{(\ell)} = K_\ell(x_i, x_j') \; ; \; V_j = G(x_j) \; ; \; f_j = f(x_j) \qquad \ldots\ldots\ldots\ldots(152)$$

and write the integral in (149) as

$$\int_0^\infty K_\ell(x,x')\,G(x')\,f(x')\,dx' = \sum_{j=1}^{N} B_j L_{ij}^{(\ell)} V_j f_j \qquad \ldots\ldots\ldots\ldots(153)$$

where the $B_j$ are weight factors in a numerical integration proceedure. Writing $j_\ell(kx_i) = j_{\ell i}$ , we obtain a set of $N$ by $N$ matrix elements

$$\sum_{j=1}^{N} \left\{ \delta_{ij} - B_j L_{ij}^{(\ell)} V_j \right\} f_j = kx_i j_{\ell i} \quad (i = 1 \ldots N) \qquad \ldots\ldots\ldots\ldots(154)$$

to which a standard proceedure of solution may be applied; then knowing $f(x_i)$, we have

$$\tan\eta_\ell = -\sum_{i=1}^{N} x_i j_{\ell i} V(x_i) f(x_i) \qquad \ldots\ldots\ldots\ldots(155)$$

Computer time available did not allow us to evaluate the using this formulation.

8. In this paragraph we give the numerical proceedures and then discuss the results. It was originally hoped that it would be possible to compute exact phase shifts for a screened coulomb potential for a wide range of $\ell$ , $T$ and $n_e$ . At sufficiently large $r$ the scattering equation has asymptotic form $A\sin(kr - \frac{1}{2}\ell\pi + \eta_\ell)$ , so it goes through a loop where $kr$ changes by $2\pi$ , i.e.

$$\Delta r = \frac{2\pi}{k} \simeq \frac{2.5 \times 10^3}{\sqrt{T}}\; a_0 \qquad \ldots\ldots\ldots\ldots(156)$$

Now for an accurate numerical integration, we should like to have at least twenty points per loop. The asymptotic region may be supposed reached when $r$ is of the order of $h_D$

$$h_D \simeq 1.3\times10^{9}\left(\frac{T}{n_e}\right)^{\frac{1}{2}} \text{ atomic units} \qquad \text{..........(157)}$$

so the number of steps required in the integration is of the or order of

$$N \simeq \frac{10^{7}T}{\sqrt{n_e}} \qquad \text{..........(158)}$$

Thus even for the most extreme conditions considered ($T=10^4$, $n_e=10^{18}$) at least 1000 steps were required.(In practice we had to go four times as far to get adequate convergence.) For $T=10^7$ and $n_e=10^{18}$ we need approximately $10^5$ steps. This immediately restricted application of the direct numerical integration to the ranges

$$T = 5\times10^{3},\ 10^{4} \text{ and } 5\times10^{4}\ {}^{\circ}K$$
$$n_e = 10^{18} \text{ and } 10^{16}$$

The asymptotic form $\sin(kr - \frac{1}{2}\ell\pi + \eta_\ell)$ is only valid if $(\ell+\frac{1}{2})^2/kr << 1$ since it is obtained by representing the Bessel functions by the leading term in their asymptotic expansion. For the above ranges of $T$ and $n_e$ this sufficed only for $\ell \leq 5.0$, while for $\ell > 5.0$ we have, at the i$^{th}$ zero of the solution

$$\eta_\ell^{(i)} = \tan^{-1}\left\{\frac{J_{\ell+1/2}(kr_0^{(i)})}{Y_{\ell+1/2}(kr_0^{(i)})}\right\} \qquad \text{.........(159)}$$

that is we require the half-integer order Bessel functions of large order and argument. The iterative proceedure used in calculating these led to unacceptable truncation errors if $\ell \geq 10$, so in no case did we attempt to evaluate $\Delta\eta_\ell$ for $\ell \geq 10$. The differential equation was solved on the Univac Era 1101 computer at Georgia Institute of Technology by Dr. M.R.C. McDowell who has very kindly supplied the following description of the programming. The basic differential equation was put in the form (56); the solution was then started by using the series expansion (59) at r = 0.00(0.01)0.02 and the method of Fox and Goodwin (1949) employed to continue the solution. Writing (56) as

$$y'' + 2fy' + gy = 0$$
$$f = \frac{(\ell+1)}{r} \quad ; \quad g = k^2 + \frac{A}{r}e^{-\alpha r} \qquad \text{...........(160)}$$

and letting $y_{-1}(r_{-1}), y_0(r_0), y_1(r_1)$, be three successive points of the solution, at intervals $h = r_1 - r_0 = r_0 - r_{-1}$, we have

$$y_1 = \left\{(2-h^2 g_0)y_0 - (1-hf_0)y_{-1} + \Delta_0\right\}/(1+hf_0) \qquad \text{...........(161)}$$

with

$$\Delta_0 = \left[\left(\frac{1}{12}\delta^4 - \frac{1}{90}\delta^6 + \dots\right)y_0 + 2\mu\left(\frac{1}{6}\delta^3 - \frac{1}{30}\delta^5 + \dots\right)hf_0y_0\right] \qquad \text{...........(162)}$$

This gives $y_1$ in terms of the two known points $y_0$, $y_{-1}$. We continued the solution for 18 points at interval $h_1 = h$, without the $\Delta_0$ term. $\Delta_0$ was then evaluated for all except the first and last three of these points, in terms of the central differences $\delta^n$, and corrected values $y_m^{(1)}$ (m = 3,....15) obtained. These in turn were used to obtain $y_m^{(2)}$ (m = 3,....15) and so on until convergence to seven significant figures was obtained. The interval was then doubled (if $r_{max} < \alpha$) and $y_{14}^{(j)}$, $y_{15}^{(j)}$ used as starting values for the next set of points. As soon as r exceeded $\alpha^{-1}$, each set of 18 points was started on the drum and examined for a change of sign. A six point Lagrangian interpolation then gave the value of $r$, $r^{(i)}$, at which the $i^{th}$ zero occurred and the corresponding phase shift $\eta_\ell$ was calculated. There was no convergence of $\eta_\ell^{(i)}$ as $i \to \infty$ ; however $\Delta\eta_\ell^{(i)} = \eta_\ell^{(i)} - \eta_{\ell+1}^{(i)}$ which was the quantity of interest , converged rapidly and appeared reliable to at least three significant figures. The required Bessel functions were obtained via the usual iterative proceedure,

$$J_{\nu-1}(z) + J_{\nu+1}(z) = 2\nu z^{-1} J_\nu(z) \qquad \text{...........(163)}$$

beginning with

$$J_{\frac{1}{2}}(z) = \left(\frac{2}{\pi z}\right)^{\frac{1}{2}} \sin z \quad ; \quad J_{-\frac{1}{2}}(z) = \left(\frac{2}{\pi z}\right)^{\frac{1}{2}} \cos z \qquad \text{...........(164)}$$

Tables of $\sin z$ and $\cos z$ for 0(0.001)1.000 and 1.0(1.0)400.0 to 12 significant figures were stored on the drum; $kr_0^{(i)}$ was then rounded off to six significant figures to obtain $\sin kr_0^{(i)}$ and $\cos kr_0^{(i)}$ using the formulae for sin(A+B),cos(A+B). The proceedure was tested by reproducing large portions of the W.P.A. tables ($z$ =1.0(0.1)20.0)and appeared entirely satisfactory for $\nu \leq 21/2$. A flow chart for the entire calculation is shown in Figures (19) and (20)

None of the other computations were of comparable difficulty. In calculating the Born approximation phase shifts, $Q_\ell\left(1 + \frac{\alpha^2}{2k^2}\right)$ was obtained from a recurrence relation. It is believed the resulting values are reliable to four significant figures for $\ell \leq 4500$. The Massey-Mohr phase shifts and the expression for $\xi(p)$ involved calculating $K_0(x)$ and $K_1(x)$ over a wide range of the

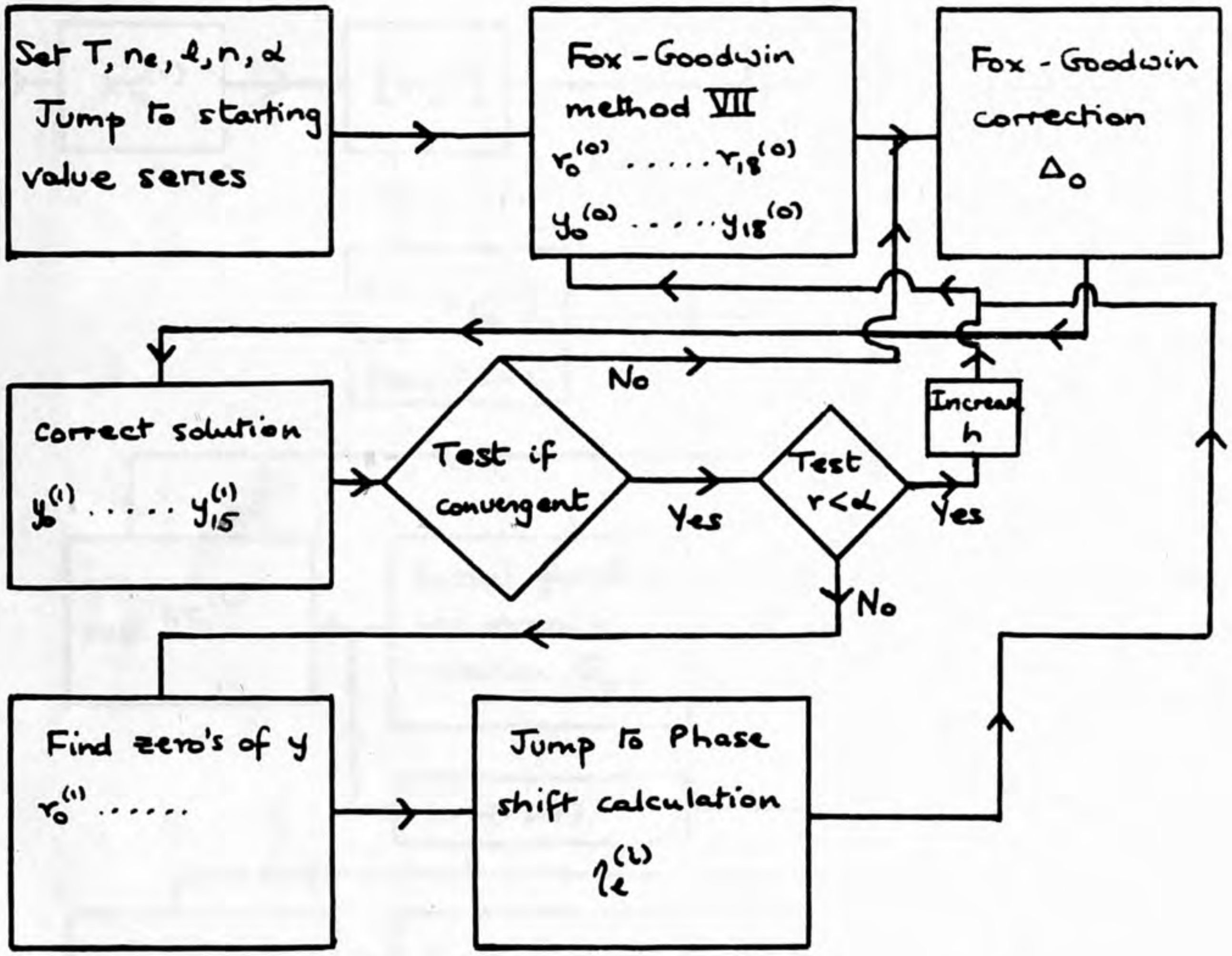


Figure 19 Flow chart for solution of equation (58).

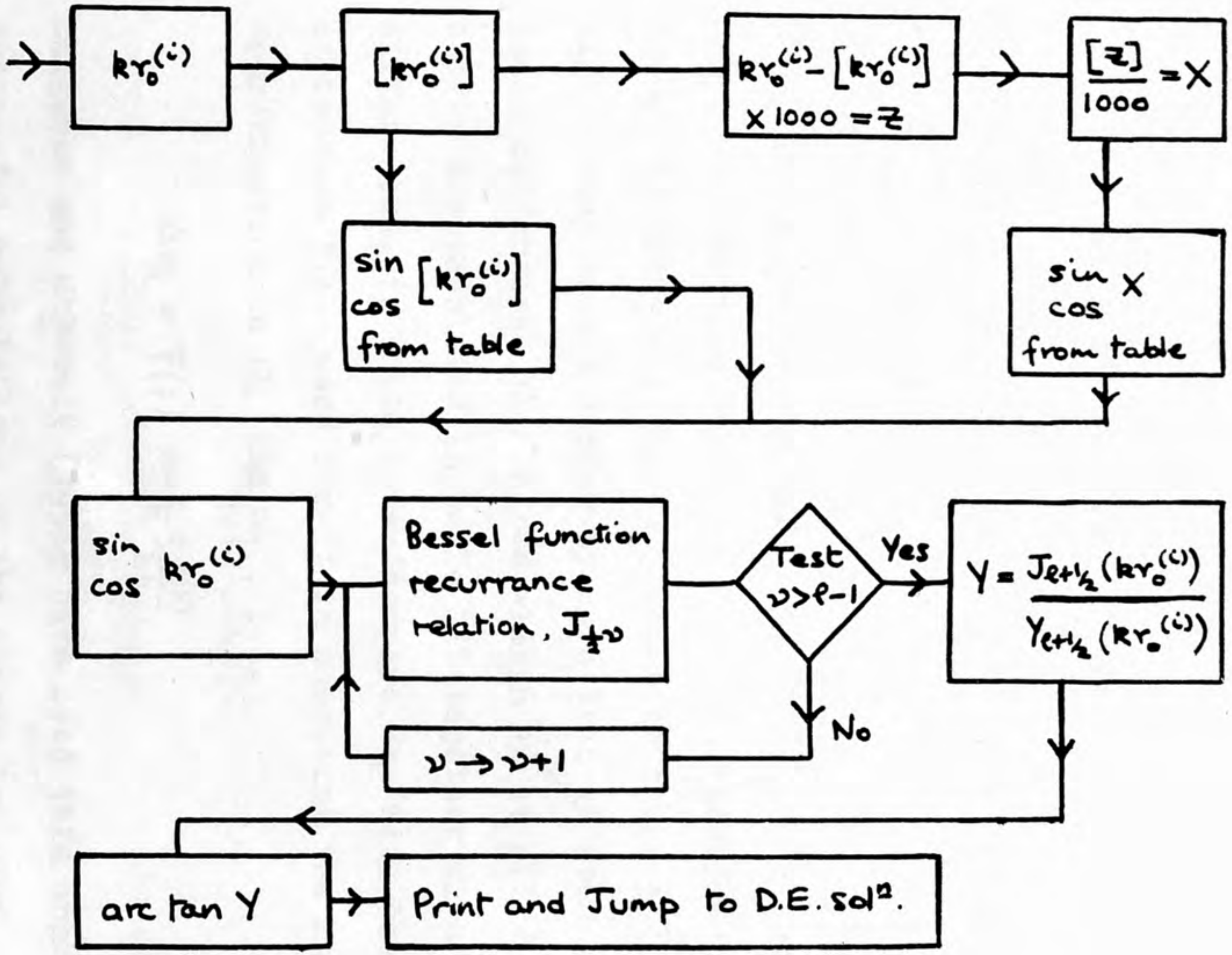


Figure 20 Phase Shift Calculation.

argument. The series expansions were used for $x \leq 20.0$ and the asymptotic form beyond this, check values being taken from the standard British Association tables. The Massey-Mohr approximation to $Q_D$ and $Q_\eta$, equation (116), was then evaluated using both a Weddle formula and Gauss' method. The values of $Q_D$ and $Q_\eta$ reported in tables IA and IB were computed directly, using the programme written for the Born approximation phase shifts as a subroutine and stopping arbitarily when $\ell = 4500$. The typically slow convergence of the $\ell^{th}$ order partial sum is shown in table IC and illustrates the extreme range of the potential.

Turning now to the calculations of phase shift differences $\Delta\eta_\ell$, we find that while the Born and Massey-Mohr approximations to $\eta_\ell$ do not always agree (except at large $\ell$), for low $T$ and high $n_e$ they do not differ by more than 1% even at $\ell = 1$, while their differences $\Delta\eta_\ell$ agree within 1% at all $\ell$. Some phase shifts are tabulated in table XII together with the corresponding differences. In table XI we compare $\Delta\eta_\ell$ with the approximate expression $\xi(p)$ used for it in computing the Massey-Mohr approximation to $Q_D$ and $Q_\eta$, i.e.

$$\Delta\eta_\ell \doteq \xi(p) = -\frac{1}{k}\frac{\partial\eta(p)}{\partial p} \qquad \text{..........(165)}$$

Dalgarno and McDowell (1956a) have used this approximation in their successful calculations of the charge transfer cross section for $H^-$ in H, but it was not at that time possible to subject it to a direct test. We find that for $\ell \geq 30$ (all $T$ and $n_e$) the error involved is less than 1% and for large $\ell$ is usually less than 0.5%. It is therefore an adequate approximation, since except at very low energies, most of the contribution to $Q_D$ and $Q_\eta$ arises from $\ell >> 30$.

We have computed "exact" values of $\Delta\eta^\ell$ by numerical integration of the differential equation, for $n_e = 10^{18}$, $V(r) = -\frac{1}{r}e^{-\alpha r}$ (electron-proton gas) and $T = 5 \times 10^3$, $10^4$ and $5 \times 10^4$ °K and the results are shown in table IX, together with the corresponding Born and Massey-Mohr values. The exact $\Delta\eta_\ell$ are always less than the approximate values for $\ell = 0,1,2,3$ but cross over near $\ell = 3$ and remain larger for all $\ell$ up tp 10. The limited data available suggests that they lie 10% above the approximate values. This would have the effect of increasing the "best" values of the cross sections as displayed in table I by perhaps 20%; we must therefore regard these values as uncertain by this amount. The exact phases vary sm smoothly with $\log T$ and with $n_e$. We note that both the Massey-Mohr and Born and also the variational approximations to $\eta_\ell$ and $\Delta\eta_\ell$ are of the form

$$\Delta\eta_\ell = z_1 z_2 f(\alpha, r, k) \qquad \text{..........(165)}$$

while the cross sections are also proportional to $z_1$ and $z_2$, the measures of the charges on the two interacting particles. This implies that to the Born or Massey-Mohr approximation the values of $Q_D$ and $Q_\eta$ for an electron-electron interaction, or for an electron-proton interaction differ only by the reduced mass factor. This is no longer true if the sum over the phase shifts is used, nor if exact phase shifts are considered.

We have calculated $Q_D$ and $Q_\eta$ in several different ways: the "best" values are probably those already discussed, which were obtained from equations (48) and (49) using (64) for $\eta_\ell$. The recurrence relation used in obtaining $Q_\ell(x)$ led to increasing error in $\eta_\ell^B$ as $\ell$ increased. However a calculation has been carried out which gives $\eta_\ell^B$ correct to 4 significant figures for $\ell \leq 4500$. The results (table IA) for $Q_D$ are in close agreement with the Massey-Mohr approximation for $T < 10^5$ °K, as expected. They are perhaps 10% or 15% larger confirming that the result of the classical approximation underestimates the cross sections for small $T$ and large $n_e$. The relation $Q_\eta \doteq 2Q_D$ is satisfied only at high temperatures $T > 10^5$ °H; at the lowest $T$ considered ($5 \times 10^3$ °K) we have more nearly $Q_\eta \doteq \frac{3}{2} Q_D$. For the other values considered we have used Spitzer's result (50) (but with $p_0$ and not $\bar{p}_0$), the Massey-Mohr (113) and the Born approximations (138) and (139) for $5 \times 10^3 \leq T \leq 10^7$ °K and $n_e = 10^3 (10^2) 10^{18}$ per cm$^3$. Tables II and IV give the Born approximation results, while in tables III and V, the same approximation is applied to the Theimer-Hoffman potential. In tables VII and VIII we give the ratio of these Born and Massey-Mohr approximations for $Q_D$ to the Spitzer values. It can be seen that the classical approximation is in general excellent. In the range of $T$ and $n_e$ studied, it never differs by more than 20% from either the Massey-Mohr or Born values. Liboff, in a private communication, has suggested that when $\theta_0$ is small, the classical is the best approximation from uncertainty principle arguments. However Spitzer's result represents only the leading term in an expansion, whereas the Born includes all the terms. Also the contribution from $\theta < \theta_c$ need not be small when $\theta_0$ is small. The Born approximation is certainly valid for $n_e \geq 10^{16}$, at all $T$, but even for $n_e \leq 10^{16}$ it may still be preferable to the classical approximation because it retains all terms in the collision integral. Similarly, at sufficiently high $T$ and low $n_e$ the Massey-Mohr approximation reduces to the classical expression, (at least when the log term is properly dominant.) However at lower temperatures, where the log term is of the same order as some of the others, the Massey-Mohr includes all these and as we observe (c.f. § 9) it has a very different behaviour as $(\frac{T}{n_e}) \to 0$. Quantal effects will become more important as $n_e$ increases and $T$ decreases and we feel that the Massey-Mohr values should be an improvement on the classical values for $n_e > 10^{14}$ and

$n_e$ increases and T decreases and we feel the Massey-Mohr values should be an improvement on the classical values for $n_e > 10^{19}$ and $T < 10^5$ °K. Since the Massey-Mohr values of $\Delta\eta_\ell$ are in closely agreement with the Born values, the difference between the tabulated Massey-Mohr values of $Q_D$ and those given in table IA must be entirely due to the replacement of the summation by an integration and the averaging proceedure for $p < \bar{p}$. The values in table IA should be the better. In table VI we also show some values of $\bar{p}$ for interatomic potentials; $\bar{p}^2$ is a good approximation to the integral from 0 to $\bar{p}$ in $Q_D$ since almost all the cross section arises from $p > \bar{p}$.

9. It is of interest to examine the behaviour of the cross sections as $T \to \infty$. If we write

$$k^2 = aT \quad ; \quad h_D = \frac{1}{b}\left(\frac{T}{n_e}\right)^{\frac{1}{2}} \qquad \text{..........(167)}$$

then Spitzer's result becomes

$$Q_D^{\text{SPITZER}} \xrightarrow[T\to\infty]{} \frac{2}{a^2T^2}\log\left\{\left(\frac{a}{b}\right)^2\frac{T^3}{n_e}\right\} \qquad \text{..........(168)}$$

as does our Massey-Mohr result. On the other hand the Born approximation yields

$$Q_D^{\text{BORN}} \xrightarrow[T\to\infty]{} \frac{2}{a^2T^2}\log\left\{\left(\frac{4a}{b^2}\right)\frac{T^2}{n_e}\right\} \qquad \text{..........(169)}$$

Letting $\Lambda_B$ be the argument of the logarithm in (169) and $\Lambda_S$ that of (168), we have

$$\Lambda_S = \frac{aT}{4}\Lambda_B \simeq 1{\cdot}5.10^{-6}\,T\,\Lambda_B \qquad \text{..........(170)}$$

so that the classical value will always exceed the Born if $T > 7\times10^5$ °K. Marshak's (1941) quantum correction as given by Spitzer is

$$\Lambda_M = 9\times10^{-4}\,T^{1/2}\,\Lambda_B \quad (T > 1{\cdot}5\,10^6\,{}^\circ K) \qquad \text{..........}(171)$$

so that the Born will still be less than the corrected classical value in this range. However the main result of interest is that all the approximations agree in predicting that

$$Q_D \underset{T\to\infty}{\sim} \frac{A}{T^2}\log(BT) \qquad \text{..........}(172)$$

where $A$ and $B$ are constants, for a given $n_e$, and hence that to the same order the electrical conductivity $\sigma$ behaves as

$$\sigma \underset{T\to\infty}{\rightarrow} \text{const}\ T^{3/2}/\log_e\Lambda \qquad \text{..........}(173)$$

In particular Spitzer (1956) gives

$$\sigma \sim \frac{1{\cdot}5\times10^{-4}\,T^{3/2}}{\log_e\Lambda_S} \qquad \text{..........}(174)$$

our result simply replacing $\Lambda_S$ by $\Lambda_B$ in (174).

In the limit in which $\left(\frac{I}{n_e}\right)\to 0$, Spitzer's analysis breaks down, since the logarithmic term is no longer the leading term in his equation 5-12. We adopt the Massey-Mohr formulation in this region; $Q_D$ is given by equations (115-117) and we note that as $\left(\frac{I}{n_e}\right)\to 0$, $\alpha\bar{p}\to\infty$, so that we may replace the Bessel functions in the expression for $\xi(p)$ by their asymptotic forms,

$$Q_D = \bar{p}^2 + 4\int_{\bar{p}}^{\infty} p\sin^2\left\{\left(\frac{\pi\alpha}{2k^4p}\right)^{\frac{1}{2}} e^{-\alpha p}\right\} dp \qquad \text{..........}(175)$$

$$\doteq \bar{p}^2 + 4\left(\frac{\pi\alpha}{2k^4}\right)\int_{\bar{p}}^{\infty} e^{-2\alpha p}\,dp$$

so that

$$Q_D \doteq \bar{p}^2 \left\{ 1 + \frac{\pi^2}{2\alpha \bar{p}} \right\} \qquad \text{..........(176)}$$

Using (117), $\bar{p}$ is given by the transcendental equation

$$\bar{p} = \frac{2\alpha p_0^2}{\pi} e^{-2\alpha \bar{p}} \qquad \text{..........(177)}$$

and substituting this in (176)

$$Q_D \doteq \frac{4\alpha^2 p_0^4}{\pi^2} e^{-4\alpha \bar{p}} \qquad \text{..........(178)}$$

We now take logarithms

$$\log \bar{p} + 2\alpha \bar{p} = \log\left(\frac{c}{E^2}\right) \qquad \text{..........(179)}$$

and since $\log \bar{p} << 2\alpha \bar{p}$ for $\alpha \bar{p} \to \infty$, we have

$$\bar{p} \doteq \frac{1}{2\alpha} \log\left(\frac{c}{E^2}\right) \qquad \text{..........(180)}$$

with $c = \frac{2\alpha}{\pi}$. Hence,

$$Q_D \to \frac{1}{4\alpha^2} \left\{ \log\left(\frac{2\alpha}{\pi E^2}\right) \right\}^2 \text{ as } \left(\frac{T}{n_e}\right) \to 0 \qquad \text{.........(181)}$$

From (29), $\alpha$ is proportional to $\frac{1}{\sqrt{T}}$, so

$$Q_D \xrightarrow[T \to 0]{} \frac{1}{4} T \log^2 \{ C T^{-2} \} \qquad \text{..........(182)}$$

where $C$ is a constant for a given $n_e$. Then (182) implies

$$\gamma \sim T^{-3/2} / \log^2 \frac{1}{T} \text{ as } \left(\frac{T}{n_e}\right) \to 0 \qquad \text{..........(183)}$$

Equation (183) will be valid provided $\alpha \bar{p} >> 1$, or for $\bar{p} >> h_D$; this gives $(T/n_e) < 10^{-14}$. While this criterion is never satisfied in the laboratory, it may well be in some regions of astrophysical interest. Further, it indicates that $J(T)$ tends to zero at both low and high temperatures and must therefore pass through a maximum at some intermediate temperature $T_0$ , which for high number densities is probably in the laboratory range.

10. In equations (40) and (43) we have given expressions for the electrical and thermal conductivity in terms of integrals involving the cross sections $Q_D$ and $Q_\eta$ . These may be regarded evaluated analytically if we adopt the Born approximation expressions for these cross sections, § 7.3 equations (138) and (139). Since for $T \geq 10^5\,{}^\circ K$, Born's approximation gives $Q_\eta \doteq 2Q_D$ we may write

$$\phi_{12}^{(2)}(v) \doteq 2\phi_{12}^{(1)}(v) \qquad \text{..........(184)}$$

and

$$\phi_{12}^{(1)}(v) \doteq \frac{2\mu^2}{k^4} \log \frac{4k^2}{\alpha^2} \qquad \text{..........(185)}$$

Then the collision integral of interest is $\Omega_s^{(1)}$ with $s = 1, 2$ or $3$,

$$\Omega_s^{(1)} = 2\mu\sqrt{\pi}\, b^{2s+3} \int_0^\infty x^{2s-1} e^{-b^2x^2} \log \frac{4x^2}{\alpha^2}\, dx \qquad \text{..........(186)}$$

in which

$$b = (2\mu k'T)^{-1/2} \qquad \text{..........(187)}$$

where $k'$ is Boltzmann's constant. The integral in (186) is a standard Laplace transform. Setting,

$$y = \frac{4x^2}{\alpha^2} \quad ; \quad \delta = \frac{b^2\alpha^2}{4} \qquad \text{..........(188)}$$

we have

$$\Omega_s^{(1)} = \frac{\mu\sqrt{\pi}\, b^{2s+3}\alpha^{2s}}{4^s}\int_0^\infty y^{s-1} e^{-\delta y} \log y \, dy \qquad \dots\dots\dots\dots(189)$$

where

$$\int_0^\infty y^t e^{-\delta y} \log y \, dy = \frac{t!}{\delta^{t+1}}\left[1 + \tfrac{1}{2} + \cdots \tfrac{1}{t} - \log \gamma\delta\right] \qquad \dots\dots\dots\dots(190)$$

and hence

$$\Omega_s^{(1)} = \mu\sqrt{\pi}\, b^3 (s-1)!\left[1 + \tfrac{1}{2} + \cdots\cdots \tfrac{1}{s-1} - \log \gamma\delta\right] \qquad \dots\dots\dots\dots(191)$$

where $\gamma$ is Euler's constant, For s=1,2, or 3, we have

$$\begin{aligned}
\Omega_1^{(1)} &= -\mu\sqrt{\pi}\, b^3 \log(\gamma\delta) \\
\Omega_2^{(1)} &= \mu\sqrt{\pi}\, b^3 \left[1 - \log(\gamma\delta)\right] \\
\Omega_3^{(1)} &= 2\mu\sqrt{\pi}\, b^3 \left[\tfrac{3}{2} - \log(\gamma\delta)\right] \\
\Omega_2^{(2)} &= 2\mu\sqrt{\pi}\, b^3 \left[1 - \log(\gamma\delta)\right]
\end{aligned} \qquad \dots\dots\dots\dots(192)$$

Immediately then the thermal conductivity is given by

$$\lambda = \frac{1{\cdot}6875 \; kT\, C_v}{2\mu\sqrt{\pi}\, b^3\left[1 - \log(\gamma\delta)\right]} \qquad \dots\dots\dots\dots(193)$$

The second order correction $\epsilon_0$ to the diffusion coefficient is

$$\epsilon_0 = \frac{(2 + 3\log(\gamma\delta))^2}{4(\log^2(\gamma\delta) - \log(\gamma\delta) - 1)} \qquad \dots\dots\dots\dots(194)$$

and

$$1 + \epsilon_0 = \frac{\log(\gamma\delta)\left[13\log(\gamma\delta) + 8\right]}{4(\log^2(\gamma\delta) - \log(\gamma\delta) - 1)} \qquad \dots\dots\dots\dots(195)$$

so that substitution of this expression in (40) and (41) yields

$$\mathcal{J} = \frac{3e^2}{64\sqrt{\pi}\,b^3\mu^2}\left\{\frac{13\log(\gamma\delta)+8}{1+\log(\gamma\delta)-\log^2(\gamma\delta)}\right\} \qquad \text{..........(196)}$$

A similar result may be derived using Spitzer's classical formulation; the first order value for $\mathcal{J}$ is

$$\mathcal{J}_0 = \frac{3e^2}{32\sqrt{\pi}\,b^3\mu^2\log(\gamma\alpha b^2)}$$

$$= \frac{3e^2}{32\sqrt{\pi}\,b^3\mu^2\log\left(\frac{\alpha}{k^2}\right)^{-1}} \qquad \text{...........(197)}$$

whereas our first order value for $\mathcal{J}$ is

$$\mathcal{J}_0 = \frac{3e^2}{16\sqrt{\pi}\,b^3\mu^2\log\left(\frac{\alpha^2}{4k^2}\right)^{-1}}$$

$$\doteq \frac{3e^2}{32\sqrt{\pi}\,b^3\mu^2\log\left(\frac{\alpha}{2k}\right)^{-1}} \qquad \text{..........(198)}$$

Since $(1+\epsilon_0)$ is very closely independent of $T$ and $n_e$ in the ranges of interest,(For $10^5 \leq T \leq 10^{70}$K, $10^{12} \leq n_e \leq 10^{18}$ , $\log_e(\gamma\delta)$ lies between 24.6 and 70.7, so $(1+\epsilon_0) \doteq 3.42$) * See note on next page we differ only in the argument of the logarithmic term from Landshoff and Spitzer. We have, to Born's approximation

$$\mathcal{J}_B = 1.5 \times 10^{-13}\left[\log_e \frac{2h_D}{\sqrt{p_0}}\right]^{-1} T^{3/2} \text{ e.m.u.} \qquad \text{..........(199)}$$

whereas the classical approximation to $Q_D$ and $Q_\eta$ yields

$$\sigma_c = 1.5 \times 10^{-13} \left[ \log_e \frac{h_D}{p_0} \right]^{-1} T^{3/2} \text{ e.m.u.} \qquad \text{..........(200)}$$

in the case where the ionic charge is unity. Our value for the conductivity is smaller than Spitzer's value for $T < 10^5$ °K and larger for $T > 10^6$ °K, although the differences are of the second order. However neither the Born nor the classical approximation to the cross sections is valid for $T < 10^5$ °K and the Massey-Mohr result should be preferable in this range. Writing as in equation (181)

$$Q_D \to \frac{1}{4\alpha^2} \left\{ \log \left( \frac{2\alpha}{\pi\epsilon^2} \right) \right\}^2 \quad \text{as} \left( \frac{T}{h_e} \right) \to 0$$

we have in terms of $k$ ,

$$Q_D \to \frac{k' T}{32 \pi h_e e^2} \left\{ \log \left( \frac{2\alpha}{\pi k^2} \right) \right\}^2 \qquad \text{...........(201)}$$

and in place of equation (186) we have an integral of the form

$$\int_0^\infty e^{-py} y^{s+1} \left[ \log y \right]^2 dy \qquad \text{..........(202)}$$

which we were unable to evaluate in terms of known functions.

* This implies that $\epsilon_0 \doteq 2.4$, which is inconsistent with the definition of $\epsilon_0$ as a second order correction term. It is not clear how this discrepancy arises as the analysis seems to be correct.

## TABLE IA.

$Q_D$ calculated using the Born approximation to the phase shifts. The summation formulae are cut off at $\ell = 4500$.

| $T$ °K<br>$n_e$ | $5 \times 10^3$ | $10^4$ | $5 \times 10^4$ | $10^5$ |
|---|---|---|---|---|
| $10^{18}$ | 5452 | 2328 | 188.4 | 57.36 |
| $10^{16}$ | 14,012 | 4570 | 263 | – |
| $10^{14}$ | 22,991 | – | – | – |

## TABLE IB.

$Q_\eta$ calculated using the Born approximation to the phase shifts, with $\ell \leq 4500$.

| $T$ °K<br>$n_e$ | $5 \times 10^3$ | $10^4$ | $5 \times 10^4$ | $10^5$ |
|---|---|---|---|---|
| $10^{18}$ | 6914 | 3306 | 314.1 | 99.37 |
| $10^{16}$ | 22,733 | 7693 | 493.8 | – |
| $10^{14}$ | 40,506 | – | – | – |

## TABLE IC.

Partial sums $Q' = \sum_{\ell=0}^{\ell'} (\ell+1) \sin^2 \Delta\eta_{\ell}^{B}$ at $n_e = 10^{18}$, $T = 5 \times 10^4$ °K.

| $\ell'$ | $\Delta\eta_{\ell'}^{B}$ | $Q'(\ell')$ | $\ell'$ | $\Delta\eta_{\ell'}$ | $Q'(\ell')$ |
|---|---|---|---|---|---|
| 0 | 1.7728 | 0.9597 | 91 | 1.5625(2) | 12.4056 |
| 1 | 0.8862 | 2.1599 | 92 | 1.5400(2) | 12.4274 |
| 2 | 0.5906 | 3.0901 | 93 | 1.5180(2) | 12.4488 |
| 3 | 0.4427 | 3.8241 | 94 | 1.4864(2) | 12.4700 |
| 4 | 0.3539 | 4.4247 | 95 | 1.4753(2) | 12.4906 |
| 5 | 0.2947 | 4.9311 | 96 | 1.4546(2) | 12.5109 |
| 6 | 0.2524 | 5.3676 | 97 | 1.4344(2) | 12.5308 |
| 7 | 0.2207 | 5.7509 | 98 | 1.4145(2) | 12.5504 |
| 8 | 0.1960 | 6.0921 | 99 | 1.3951(2) | 12.5698 |
|  |  |  | 100 | 1.3760(2) | 12.5886 |
|  |  |  | 3000 | 1.204 (4) | 13.482 |

## TABLE II.

The Born approximation to $Q_D$ for a screened coulomb potential.

| $n_e \backslash T^\circ K$ | $10^5$ | $2.5\times10^5$ | $5\times10^5$ | $7.5\times10^5$ | $10^6$ | $5\times10^6$ | $10^7$ |
|---|---|---|---|---|---|---|---|
| $10^{18}$ | 54.14 | 9.98 | 2.75 | 1.28 | 7.49(1) | 3.57(2) | 9.56(3) |
| $10^{16}$ | 74.9 | 13.3 | 3.57 | 1.65 | 9.56(1) | 4.40(2) | 1.16(2) |
| $10^{14}$ | 95.6 | 16.6 | 4.40 | 2.02 | 1.16 | 5.23(2) | 1.37(2) |
| $10^{12}$ | 116.4 | 19.9 | 5.23 | 2.39 | 1.37 | 6.06(2) | 1.58(2) |

## TABLE III.

The Born approximation to $Q_D$ for a Theimer-Hoffman potential.

| $n_e \backslash T^\circ K$ | $10^5$ | $2.5\times10^5$ | $5\times10^5$ | $7.5\times10^5$ | $10^6$ | $5\times10^6$ | $10^7$ |
|---|---|---|---|---|---|---|---|
| $10^{18}$ | 53.19 | 9.84 | 2.71 | 1.27 | 7.4(1) | 3.54(2) | 9.47(3) |
| $10^{16}$ | 74.00 | 13.16 | 3.54 | 1.64 | 9.47(1) | 4.37(2) | 1.15(2) |
| $10^{14}$ | 94.72 | 16.47 | 4.37 | 2.01 | 1.15 | 5.20(2) | 1.36(2) |
| $10^{12}$ | 115.4 | 19.79 | 5.20 | 2.37 | 1.36 | 6.03(2) | 1.57(2) |

## TABLE IV.

Born approximation to $Q_\eta$ for a screened coulomb potential.

| $n_e \backslash T^\circ K$ | $10^5$ | $2.5\times10^5$ | $5\times10^5$ | $7.5\times10^5$ | $10^6$ | $5\times10^6$ | $10^7$ |
|---|---|---|---|---|---|---|---|
| $10^{18}$ | 99.27 | 18.51 | 5.13 | 2.41 | 1.41 | 6.79(2) | 1.82(2) |
| $10^{16}$ | 140.8 | 25.16 | 6.79 | 3.15 | 1.82 | 8.44(2) | 2.24(2) |
| $10^{14}$ | 182.2 | 31.78 | 8.44 | 3.88 | 2.24 | 1.01(1) | 2.65(2) |
| $10^{12}$ | 223.7 | 38.41 | 10.10 | 4.62 | 2.65 | 1.18(1) | 3.07(2) |

## TABLE V.

Born approximation to $Q_\eta$ for a Theimer-Hoffman potential.

| $n_e$ \ T°K | $10^5$ | $2.5\times10^5$ | $5\times10^5$ | $7.5\times10^5$ | $10^6$ | $5\times10^6$ | $10^7$ |
|---|---|---|---|---|---|---|---|
| $10^{18}$ | 97.47 | 18.25 | 5.06 | 2.38 | 1.39 | 6.72(2) | 1.80(2) |
| $10^{16}$ | 139.0 | 24.90 | 6.72 | 3.12 | 1.80 | 8.38(2) | 2.22(2) |
| $10^{14}$ | 180.4 | 31.54 | 8.38 | 3.85 | 2.22 | 1.00(1) | 2.63(2) |
| $10^{12}$ | 221.9 | 38.17 | 10.04 | 4.59 | 2.63 | 1.17(1) | 3.05(2) |

## TABLE VI.

Massey-Mohr approximation to $Q_D$ for a screened coulomb potential.

| $n_e$ \ T°K | $10^4$ | $2.5\times10^4$ | $5\times10^4$ | $7.5\times10^4$ | $10^5$ | $5\times10^5$ | $10^6$ | $5\times10^6$ |
|---|---|---|---|---|---|---|---|---|
| $10^{18}$ | 1961 | 526.8 | 172.8 | 87.57 | 53.58 | 3.118 | 8.837(1) | 4.429(2) |
| $10^{16}$ | 4188 | 891.6 | 264.2 | 128.2 | 76.41 | 4.018 | 1.103 | 5.082(2) |
| $10^{14}$ | 6493 | 1257 | 355.1 | 168.4 | 98.95 | 4.812 | 1.264 | - |
| $10^{12}$ | 8769 | 1616 | 442.4 | 806.0 | 119.1 | 5.190 | - | - |
| $10^{10}$ | 10,958 | 1931 | 506.4 | 227.9 | 129.4 | - | - | - |
| $10^{8}$ | 12,594 | 2073 | 520.3 | 232.0 | - | - | - | - |
| $\bar{p}$ | 8.00 | 4.00 | 2.001 | 1.334 | 1.001 | 2.001(1) | 1.00(1) | 2.00(2) |

### TABLE VII.

Ratio of Spitzer's classical approximation to the Born approximation for $Q_D$.

| $n_e \backslash T\,^{\circ}K$ | $10^5$ | $5\times10^5$ | $10^6$ | $5\times10^6$ | $10^7$ |
|---|---|---|---|---|---|
| $10^{18}$ | 1.076 | 0.9518 | 0.9188 | 0.8657 | 0.8491 |
| $10^{16}$ | 1.053 | 0.9627 | 0.9353 | 0.8881 | 0.8709 |
| $10^{14}$ | 1.041 | 0.9693 | 0.9463 | 0.9038 | 0.8899 |
| $10^{12}$ | - | 0.9741 | 0.9541 | 0.9162 | 0.9029 |
| $10^{10}$ | - | - | 0.9600 | 0.9255 | 0.9132 |
| $10^{8}$ | - | - | - | 0.9313 | 0.9215 |

### TABLE VIII.

Ratio of Spitzer's classical approximation to the Massey-Mohr approximation for $Q_D$.

| $n_e \backslash T\,^{\circ}K$ | $10^4$ | $5\times10^4$ | $10^5$ | $5\times10^5$ | $10^6$ |
|---|---|---|---|---|---|
| $10^{18}$ | 0.9378 | 0.9648 | 0.9740 | 0.9886 | 0.9911 |
| $10^{16}$ | 0.9592 | 0.9785 | 0.9826 | 0.9887 | 0.9895 |
| $10^{14}$ | 0.9779 | 0.9833 | 0.9846 | 0.9670 | - |
| $10^{12}$ | 0.9835 | 0.9788 | 0.9667 | - | - |
| $10^{10}$ | 0.9788 | 0.9326 | - | - | - |
| $10^{8}$ | 0.9353 | 0.8208 | - | - | - |

## TABLE IX.

Exact, Massey-Mohr and Born values of $\Delta\eta_\ell$ for $n_e = 10^{18}$, at $T = 5\times10^3$, $10^4$ and $5\times10^4$ °K.

| $\ell$ | $\Delta\eta_\ell^{Exact}$ | $\Delta\eta_\ell^{B}$ | $\Delta\eta_\ell^{MM}$ | |
|---|---|---|---|---|
| 1 | 1.1248 | 1.9697 | 2.0132 | |
| 2 | 0.9800 | 1.3049 | 1.3204 | |
| 3 | 0.8371 | 0.9511 | 0.9761 | |
| 4 | 0.7890 | 0.7699 | 0.7720 | |
| 5 | 0.6537 | 0.6351 | 0.6372 | $10^4$ °K |
| 6 | 0.5560 | 0.5384 | 0.5390 | |
| 7 | 0.4916 | 0.4655 | 0.4654 | |
| 8 | 0.4390 | 0.4086 | 0.4010 | |
| 9 | 0.3950 | 0.3628 | 0.3632 | |
| 10 | - | 0.3250 | 0.3201 | |
| 1 | 1.317 | 2.7465 | - | |
| 2 | 1.191 | 1.7961 | - | |
| 3 | 1.129 | 1.3165 | - | $5\times10^3$ °K |
| 4 | 1.008 | 1.0261 | - | |
| 5 | 0.862 | 0.8308 | - | |
| 6 | 0.757 | 0.6905 | - | |
| 1 | 0.726 | 0.8862 | 0.909 | |
| 2 | 0.534 | 0.5906 | 0.600 | |
| 3 | 0.452 | 0.4427 | 0.451 | $5\times10^4$ °K |
| 4 | 0.364 | 0.3539 | 0.351 | |
| 5 | 0.304 | 0.2947 | 0.295 | |
| 6 | 0.262 | 0.2524 | 0.245 | |

## TABLE X.

Massey-Mohr approximation to $\Delta\eta_\ell$ compared with $\zeta(p)$ for $T = 10^6$ °K, $n_e = 10^{18}$.

| $\ell$ | $\Delta\eta_\ell$ | $\zeta(p)$ | % error |
|---|---|---|---|
| 1 | 2.025(1) | 2.848(1) | 40.7 |
| 5 | 6.623(2) | 7.290(2) | 10.1 |
| 10 | 3.607(2) | 3.788(2) | 5.0 |
| 20 | 1.888(2) | 1.937(2) | 2.5 |
| 60 | 6.494(3) | 6.544(3) | 0.76 |
| 100 | 3.917(3) | 3.939(3) | 0.54 |
| 300 | 1.300(3) | 1.306(3) | 0.45 |
| 1000 | 3.626(4) | 3.630(4) | 0.11 |

## TABLE XI.

Born and Massey-Mohr values of $\eta_\ell$, $\Delta\eta_\ell$ at $T = 5\times10^4$, $n_e = 10^{18}$.

| $\ell$ | $\eta_\ell^{MM}$ | $\eta_\ell^{B}$ | $\Delta\eta_\ell^{MM}$ | $\Delta\eta_\ell^{B}$ |
|---|---|---|---|---|
| 1 | 8.539 | 8.519 | 0.909 | 0.886 |
| 2 | 7.630 | 7.633 | 0.600 | 0.591 |
| 3 | 7.034 | 7.043 | 0.451 | 0.443 |
| 4 | 6.582 | 6.600 | 0.351 | 0.354 |
| 5 | 6.233 | 6.246 | 0.295 | 0.295 |
| 6 | 5.938 | 5.951 | 0.253 | 0.252 |
| 7 | 5.685 | 5.699 | 0.225 | 0.221 |
| 8 | 5.460 | 5.478 | - | - |

## TABLE XII

Ground state $1s^2,2s$

$\alpha = 2.694$ ; $\beta = 0.764$ Wu and Yu.

$\sqrt{\pi}\gamma = 0.37$ ; $\xi = 1.35$ ; $\eta = 0.67$ ; $\zeta = 1.5$ ; $\lambda = -2.8$ Wilson.

Excited state $1s^2,2p$

$\alpha = 2.694$ ; $\delta = 0.525$ Wu and Yu.

$\alpha = 2.7$ ; $\delta = 0.65$ Slater.

Excited state $1s,2s^2$

$\alpha = 3.027$ ; $\beta = 1.074$ Wu and Yu.

$\alpha = 3.00$ ; $\beta = 0.9$ Slater.

Excited state $1s,2s,2p$

$\alpha = 3.00$ ; $\beta = 1.11$ ; $\delta = 0.877$ Wu and Yu.

$\alpha = 3.00$ ; $\beta = 0.9$ ; $\delta = 0.9$ Slater.

## APPENDIX.

The function $F(t,K)$ introduced in equation (27) is given by

$$
\begin{aligned}
F(t,K) = {} & 3(5a^4+10a^2b^2+b^4)(f_1^2+f_4^2) \\
& + 12ab(5a^2+3b^2)(f_1f_2+f_4f_5) \\
& + (5a^4+38a^2b^2+5b^4)(f_2^2+2f_1f_3+2f_4f_6+f_5^2) \\
& + 12ab(5b^2+3a^2)(f_2f_3+f_5f_6) \\
& + 3(5b^4+10a^2b^2+a^4)(f_3^2+f_6^2)
\end{aligned}
\qquad \text{..........(A1)}
$$

in which

$$
\begin{aligned}
f_1 &= at(c^2+d^2)g_1-\delta g_5 & f_2 &= t(ag_2-bg_1)(c^2+d^2)-\delta g_6 \\
f_3 &= -tb(c^2+d^2)g_2-\delta g_7 & f_4 &= at(c^2+d^2)g_3-\delta g_8 \\
f_5 &= t(ag_4-bg_3)-\delta g_9 & f_6 &= -tb(c^2+d^2)g_4-\delta g_{10}
\end{aligned}
\qquad \text{..........(A2)}
$$

where

$$
\begin{aligned}
g_1 &= za(tc-\beta d)+\beta t(c^2+d^2) \\
g_2 &= zb(\beta d-tc) \quad ; \quad g_4 = -zb(\beta c+td) \\
g_3 &= za(\beta c+td)-z\beta(c^2+d^2) \\
g_5 &= a^2y_1+ay_2+2\beta^2(c^2+d^2)^2(2t^2-z^2) \\
g_6 &= -2aby_1-by_2 \quad ; \quad g_7 = b^2y_1 \\
g_8 &= a^2y_3+ay_4-6zt\beta^2(c^2+d^2)^2 \\
g_9 &= -2aby_3-by_4 \quad ; \quad g_{10} = b^2y_3
\end{aligned}
\qquad \text{..........(A3)}
$$

and

$$y_1 = 4zt\left\{\beta t(c^2-d^2) - cd(\beta^2-t^2)\right\} - 2z^2\left\{(\beta^2-t^2)(c^2-d^2) + 4\beta tcd\right\} + ztd(c^2+d^2)$$

$$y_2 = 4z\beta(c^2+d^2)\left\{z(\beta c+td) - t(\beta d-tc)\right\} - t^2(c^2+d^2)^2$$

$$y_3 = 4z^2\left\{\beta t(c^2-d^2) - cd(\beta^2-t^2)\right\} + 2zt\left\{(\beta^2-t^2)(c^2-d^2) + 4\beta tcd\right\} - ztc(c^2+d^2)$$

$$y_4 = 4z\beta(c^2+d^2)\left\{t(\beta c+td) + z(\beta d-tc)\right\} + tz(c^2+d^2)^2$$

$$\ldots\ldots\ldots\ldots(A4)$$

The expressions $\textcircled{H}$ , $\phi_1$ , $\Phi_2$ , $\Psi_1$ , $\Psi_2$, can be written as

$$\textcircled{H} = \frac{z}{t}\log_e\left|\frac{\beta - it - ik}{\beta + it - ik}\right| \qquad \ldots\ldots\ldots\ldots(A5)$$

and

$$\Phi_1 = 8Kt^4(t^2+z^2)^{-1}(c^2+d^2)^{-1}\left[(\beta-z)c + 2\beta(t^2+\beta z)\right]$$

$$\Phi_2 = 2\delta'\left\{\beta(c^2+d^2)^{-2}(c^2-d^2+4ct^2)(a^2+b^2) - 2a(t^2+z^2)^{-1}(c^2+d^2)^{-1}\right.$$
$$\left.(2\beta dt^2 + zct^2 + 2\beta z^2c + 2\beta z^2t^2) + z^{-1}(3\beta z + zt^2)\right\}$$

$$\Psi_1 = 4t^2(t^2+z^2)^{-1}\left\{a(c^2+d^2)^{-1}\left[c(t^2+\beta z) - 2\beta t^2(\beta-z)\right] - \beta z^{-1}(t^2+z^2)\right\}$$

$$\Psi_2 = 8t^2K\delta'(c^2+d^2)^{-2}\left\{a(c^2-d^2-4\beta^2c) - (t+z)^{-1}(a^2-b^2)(z^2c-d^2-2\beta zt^2-4\beta z^2)\right\}$$

$$\delta' = \frac{1}{3}(\alpha+\beta) \qquad \ldots\ldots\ldots\ldots(A6)$$

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# Electron Loss from Fast Negative Ions of Atomic Hydrogen passing through Atomic Hydrogen

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

$$\mathrm{H(1s)+H^-(1s^2)\to H(1s\ or\ 2p)+H(1s\ or\ 2p)+e}$$

at impact energies between 2·5 kev and 10 Mev. The sensitivity of the cross section of the process

$$\mathrm{H(1s)+H^-(1s^2)\to H(1s)+H(2p)+e}$$

to the choice of bound and free $\mathrm{H^-}$ wave function is examined, as is that of the process

$$\mathrm{H(1s)+H^-(1s^2)\to H(2p)+H(1s)+e}$$

to the choice of free $\mathrm{H^-}$ wave function. The electron loss cross section $\sigma_{-1,0}$ is approximated by a sum rule, for the simplest choice of wave function. The results are compared with those of Allison for $\mathrm{H^-}$ electron loss in $\mathrm{H_2}$. The energy distribution of ejected electrons at high impact energies is also given.

## § 1. INTRODUCTION

IN recent years a detailed theoretical study of fast collision processes involving hydrogen and helium atoms and positive ions, has been carried out by Bates and his colleagues using Born's approximation (see Bates and Dalgarno 1956 for a brief summary of this work up to that date, Boyd, Moiseiwitsch and Stewart 1957, Bates and Williams 1957).

Considerable interest is attached to comparable studies of processes involving the negative ion of atomic hydrogen $\mathrm{H^-}$. Electron loss cross sections for fast $\mathrm{H^-}$ in He to Born's approximation have been published by Sida (1955). In this paper we investigate the simplest of such processes, single electron loss from fast $\mathrm{H^-}$ in H. Since the negative ion is a much more diffuse system than the corresponding neutral atom, one would expect the cross sections for these processes to be more sensitive to choice of atomic wave functions than the atom–atom and atom–positive ion collisions previously studied. We therefore employ a variety of wave functions in some of the calculations, to investigate this sensitivity.

There are no available experimental data in the magnitude of the electron loss cross section, though measurements are now being undertaken elsewhere. However, Allison (1958) has recently reviewed the results for $\mathrm{H^-}$ electron loss in molecular hydrogen. Preliminary data on the atomic case (Branscomb and Fite 1959, private communication) suggest that the cross sections are closely similar, near their maximum.

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## § 2. THEORY

We consider a collision between a fast H$^-$ ion and a hydrogen atom. Both systems are initially in their ground states; an electron is ejected from the negative ion only and each of the residual atoms may be left in any discrete state. Born's approximation is employed, exchange being neglected. The electron loss cross section $\sigma_{-1,0}$ may be expressed as

$$\sigma_{-1,0}=\sum_{n'l'}{}' \sum_{nl}{}' Q(1\mathrm{s}\,;1\mathrm{s}^2\rightarrow n'l'\,;nl,\,\mathrm{C}) \qquad \ldots\ldots(1)$$

the dashes on the summations indicating that only discrete terms are to be included. Here $Q(1\mathrm{s}\,;1\mathrm{s}^2\rightarrow n'l'\,;nl,\,\mathrm{C})$ is the cross section for the process

$$\mathrm{H}(1\mathrm{s})+\mathrm{H}^-(1\mathrm{s}^2)\rightarrow\mathrm{H}(n'l')+\mathrm{H}(nl)+\mathrm{e}. \qquad \ldots\ldots(2)$$

This cross section is given by (Mott and Massey 1949)

$$Q(1\mathrm{s}\,;1\mathrm{s}^2\rightarrow n'l'\,;nl,\,\mathrm{C})=\frac{8\pi^3\mu^2e^4}{h^4k_\mathrm{i}^2}\int\int_0^{\kappa_\mathrm{max}}\int_{\kappa_\mathrm{min}}^{\kappa_\mathrm{max}}|L(n'l'\,;\,nl,\,\mathrm{C})|^2K\,dK\,d\kappa\,d\omega \qquad \ldots\ldots(3)$$

the ejected electron having momentum $\hbar\boldsymbol{\kappa}$, lying in the solid angle $d\omega$ about the direction $(\chi,\psi)$. The momentum of relative motion is $\hbar\mathbf{K}$,

$$\mathbf{K}=\mathbf{k}_\mathrm{i}-\mathbf{k}_\mathrm{f}\,;\;\mathbf{k}_\mathrm{i}=\frac{\mu\mathbf{v}_\mathrm{i}}{\hbar}\,;\;\mathbf{k}_\mathrm{f}=\frac{\mu\mathbf{v}_\mathrm{f}}{\hbar} \qquad \ldots\ldots(4)$$

where $\mu$ is the reduced mass of the system, $\mathbf{v}_\mathrm{i}$ and $\mathbf{v}_\mathrm{f}$ are the initial and final relative velocities and the $z$ axis is taken along $\mathbf{K}$.

The matrix element $L(n'l'\,;\,nl,\,\mathrm{C})$ is

$$L(n'l'\,;\,nl,\,\mathrm{C})=\int\int\int\int\Psi_\mathrm{i}{}^*(\boldsymbol{\rho}_1,\mathbf{r}_2,\mathbf{r}_3)\,\Psi_\mathrm{f}(\boldsymbol{\rho}_1,\mathbf{r}_2,\mathbf{r}_3)\exp\{i\mathbf{K}\,.\,\mathbf{R}\}$$
$$\times V(\mathbf{R},\boldsymbol{\rho}_1,\mathbf{r}_2,\mathbf{r}_3)\,d\boldsymbol{\rho}_1d\mathbf{r}_2d\mathbf{r}_3d\mathbf{R}, \qquad \ldots\ldots(5)$$

in which $\Psi_\mathrm{i}$ and $\Psi_\mathrm{f}$ are the initial and final wave functions of the whole system, $\mathbf{R}$ is the internuclear separation, $\boldsymbol{\rho}_1$ is the position vector of the target particles' electron with respect to its nucleus; $\mathbf{r}_2$ and $\mathbf{r}_3$ are the position vectors of the H$^-$ electrons with respect to the nucleus of the ion; and $V(\mathbf{R},\boldsymbol{\rho}_1,\mathbf{r}_2,\mathbf{r}_3)$ is the interaction potential, which may be written in the form

$$V(\mathbf{R},\boldsymbol{\rho}_1,\mathbf{r}_2,\mathbf{r}_3)=\frac{1}{R}-\frac{1}{|\mathbf{R}-\boldsymbol{\rho}_1|}-\frac{1}{|\mathbf{R}+\mathbf{r}_2|}-\frac{1}{|\mathbf{R}+\mathbf{r}_3|}$$
$$+\frac{1}{|\mathbf{R}+\mathbf{r}_2-\boldsymbol{\rho}_1|}+\frac{1}{|\mathbf{R}+\mathbf{r}_3-\boldsymbol{\rho}_1|}. \qquad \ldots\ldots(6)$$

Integration over $\mathbf{R}$-space yields

$$Q(1\mathrm{s}\,;1\mathrm{s}^2\rightarrow n'l'\,;\,nl,\,\mathrm{C})=\frac{2}{\mathscr{S}_\mathrm{i}{}^2}\int\int_0^{\kappa_\mathrm{max}}\int_{\kappa_\mathrm{min}}^{\kappa_\mathrm{max}}$$
$$\times\mathscr{I}(1\mathrm{s}^2\rightarrow nl,\,\mathrm{C})|^2|G(1\mathrm{s}\rightarrow n'l')|^2K^{-3}dK\,d\kappa\,d\omega, \qquad \ldots\ldots(7)$$

all quantities being in atomic units. The integral $\mathscr{I}(1\mathrm{s}^2\rightarrow nl,\,\mathrm{C})$ depends only on the initial and final states of the H$^-$ ion; similarly the integral $G(1\mathrm{s}\rightarrow n'l')$ depends only on those of the target H atom. Both may be evaluated analytically, by elementary methods.

The unit of energy is defined by

$$\mathscr{S}_\mathrm{i}{}^2=mv_\mathrm{i}^2/2I_\mathrm{H} \qquad \ldots\ldots(8)$$

where $I_\mathrm{H}$ is the ionization potential of atomic hydrogen and $m$ is the electronic mass.

## § 3. Sensitivity of the Cross Sections to choice of Wave Functions

The wave functions are written as products of atom and ion wave functions, a valid approximation at large **R**. We put

$$\Psi_{\mathrm{i,f}}=\psi(n'l'\,;\boldsymbol{\rho}_1)\psi_{\mathrm{i,f}}(\mathrm{H}^-) \qquad \ldots\ldots(9)$$

where $\psi(n'l', \boldsymbol{\rho}_1)$ is the wave function of a hydrogen atom in the $n'l'$ state, and

$$\left.\begin{aligned}\psi_{\mathrm{i}}(\mathrm{H}^-)&=N_{\mathrm{i}}\{\psi(\alpha, \mathbf{r}_2)\psi(\beta, \mathbf{r}_3)+\psi(\alpha, \mathbf{r}_3)\psi(\beta, \mathbf{r}_2)\}\\ \psi_{\mathrm{f}}(\mathrm{H}^-)&=N_{\mathrm{f}}\{\psi(nl, \mathbf{r}_2)\psi_\kappa(\mathbf{r}_3)+\psi(nl, \mathbf{r}_3)\psi_\kappa(\mathbf{r}_2)\}.\end{aligned}\right\} \qquad \ldots\ldots(10)$$

Consider first the initial H⁻ wave function. Studies of the binding energy, attachment energy, and other properties of H⁻ (cf. Bethe and Salpeter 1957) suggest that a good wave function must take explicit account of the electrons mutual repulsion. This leads to great analytical complexity and was not adopted. If $\psi(\alpha, \mathbf{r})$ and $\psi(\beta, \mathbf{r})$ are taken to be hydrogenic 1s orbitals with effective nuclear charges $\alpha$ and $\beta$, then a variational calculation of the binding energy yields $\alpha=1{\cdot}04$, $\beta=0{\cdot}2808$ and gives a close approximation to the attachment energy (Chandrasekhar 1944). This wave function has also been used in calculations of the photo detachment cross section (Chandrasekhar and Breen 1946) and of symmetric (H⁻, H) charge transfer (Dalgarno and McDowell 1956, Branscomb, Fite, Stebbings and Hummer 1959, to be published) and gives good agreement with the experimental data in both cases. We have used it to calculate the cross section of the process

$$\mathrm{H(1s)}+\mathrm{H}^-(1\mathrm{s}^2)\rightarrow\mathrm{H(1s)}+\mathrm{H(2p)}+\mathrm{e} \qquad \ldots\ldots(11)$$

in which the matrix element is greatly simplified by orthogonality of the atomic orbitals. Its use with any but the simplest free electron wave function, or in other processes, led to prohibitively lengthy calculations. We therefore adopted the simple hydrogenic wave function with $\alpha=\beta=0{\cdot}6875$ for the remainder of our work, using (11) as a scaling process. It should be remarked that the success of a wave function in predicting the binding energy implies only that it is accurate in regions near the nucleus, and is in itself no criterion of its value in collision problems, in which the electron density distribution over a wide range of radial distances may be important.

The ejected electron moves in the field of a hydrogen atom in the *nl* state. Since this field falls off exponentially it would appear a reasonable first approximation to represent the free electron by a plane wave

$$\psi_1(\boldsymbol{\kappa})=\frac{\kappa}{(2\pi)^{3/2}}\,\mathrm{e}^{i\boldsymbol{\kappa}\cdot\mathbf{r}} \qquad \ldots\ldots(12)$$

where we have normalized $\psi(\boldsymbol{\kappa})$ according to

$$\int d\omega\int\psi(\boldsymbol{\kappa})\psi(\boldsymbol{\kappa}')d\boldsymbol{\kappa}=\delta(\kappa'-\kappa). \qquad \ldots\ldots(13)$$

It should be noted that the resulting H⁻ wave function is not orthogonal to the ground state wave function. A better approximation would be to use the one-body approximation (Mott and Massey 1949), that is, to solve the Schrödinger equation for an electron in the static field of a hydrogen atom in the *nl* state,

$$\psi_2(\boldsymbol{\kappa})=\frac{\kappa^{1/2}g_0(r)}{(2\pi)^{3/2}Cr} \qquad \ldots\ldots(14)$$

where $g_0(r)$ is the solution bounded at the origin and having asymptotic form

$$g_0(r) \sim \frac{\sin \kappa r}{\kappa^{1/2}} \qquad \ldots\ldots(15)$$

of the equation

$$\left\{\frac{d^2}{dr^2} + \kappa^2 - 2V_0(r)\right\} g_0(r) = 0 \qquad \ldots\ldots(16)$$

in which

$$V_0(r) = \int |\psi(nl)|^2 \left\{\frac{1}{r_2} - \frac{1}{|\mathbf{r}_2 - \mathbf{r}_3|}\right\} d\mathbf{r}_3, \qquad \ldots\ldots(17)$$

the normalization of $g_0(r)$ being carried out by the method of Strömgren (cf. Bates and Seaton 1949). The resulting wave function represents the s-wave of the continuum only.

We considered the two sets of processes

$$\mathrm{H(1s)} + \mathrm{H^-(1s^2)} \rightarrow \mathrm{H}(n'l') + \mathrm{H(1s)} + \mathrm{e} \qquad \ldots\ldots(18)$$

and

$$\mathrm{H(1s)} + \mathrm{H^-(1s^2)} \rightarrow \mathrm{H}(n'l') + \mathrm{H(2p)} + \mathrm{e}. \qquad \ldots\ldots(19)$$

For the second of these, process (19), only the s-wave of the continuum contributes, so the use of (14) is no limitation. A more refined variational wave function for an electron in the field of H(2p) has been developed by Khashaba and Massey (1958). It may be written in the form

$$\psi_3(\boldsymbol{\kappa}) = \frac{\kappa}{(2\pi)^{3/2}} \left\{\frac{\sin \kappa r}{\kappa r}(1 + d\mathrm{e}^{-r}) + c(1 - \mathrm{e}^{-r})\frac{\cos \kappa r}{\kappa r}\right\}, \qquad \ldots\ldots(20)$$

where $c$ and $d$ are variationally determined parameters. These parameters vary rapidly with $\kappa$ and are only tabulated at four points. They were interpolated graphically for other values of $\kappa$. The results obtained cannot therefore be regarded as very accurate.

We have calculated the cross section for (19) taking $n'l' = 1\mathrm{s}$ with each of $\psi_1(\boldsymbol{\kappa})$, $\psi_2(\boldsymbol{\kappa})$ and $\psi_3(\boldsymbol{\kappa})$ and with $\psi_1(\boldsymbol{\kappa})$ used both a one parameter and a two parameter bound wave function. The results are displayed in figure 1. As might be expected the two parameter bound wave function, which portrays the ion as a very diffuse system, yields a cross section an order of magnitude larger than does the one parameter approximation. Almost all of the effect arises from small values of $\kappa$; the term in the integration over $\kappa$ involving $\beta = 0{\cdot}2808$ is much larger for $\kappa < 1{\cdot}0$ than is the corresponding term in the one parameter approximation involving $\alpha = 0{\cdot}6875$, even when allowance is made for the much smaller normalizing factor. The result of improving the free electron wave function is surprising in that the one body approximation compares quite favourably with that of Khashaba and Massey. Both reduce the cross section considerably, the latter by an order of magnitude, and this is true at all impact energies considered.[†] (It might have been supposed that distortion would only be important at low impact energies, since at high energies more of the contribution to the cross section comes from large values of $\kappa$ for which the plane wave representation should be valid.) The energy variation of the cross section is not, of course, sensitive to the choice of wave function. The corrections to its magnitude occasioned by

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[†] The behaviour is controlled by the normalizing factor which is very small in the region of $\kappa$ of interest, since the s-wave phase shift becomes quite large. Cancellation is also significant.

improvements in the bound wave function are opposite in sense but, perhaps fortuitously, of the same magnitude as are those due to improvement of the free electron wave function. It is clear that the behaviour shown in figure 1 is typical of all processes of type (19), since the term in the matrix element involving $n'l'$ acts primarily as a scale factor. The remaining calculations on these processes may therefore be greatly simplified by adopting $\psi_1(\kappa)$ and the one parameter bound wave function. The relative magnitudes of the cross sections for the processes considered should be quite accurate, and their absolute values should not be greatly in error.

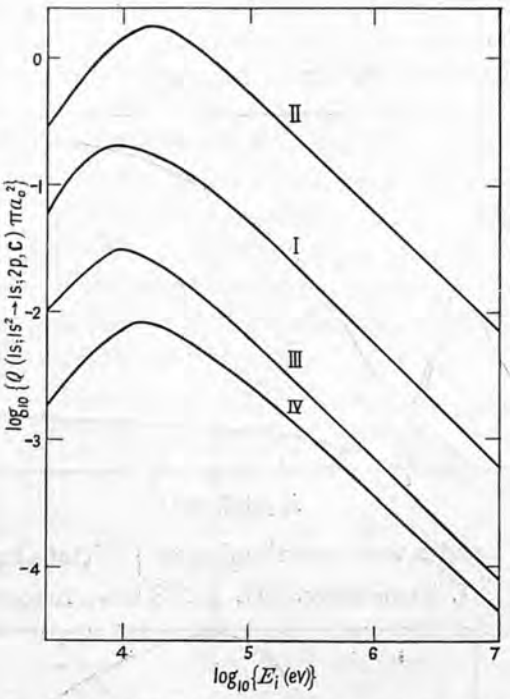

Figure 1. Cross section $Q(1s;\ 1s^2 \rightarrow 1s;\ 2p,\ C)$ computed on Born's approximation.
I. One parameter bound, plane wave free electron.
II. Two parameter bound, plane wave free electron.
III. One parameter bound, one-body free electron.
IV. One parameter bound, Khashaba–Massey free electron.

We consider now processes of type (18), and again employ $\psi_1(\kappa)$ as a first approximation, together with the simple one parameter bound wave function. In the absence of a closed form for the total cross section we restrict ourselves to a consideration of the s and p waves of the continuum. The neglect of higher partial waves is unlikely to be serious at the low values of $\kappa$ which are of importance.

Much effort has been spent on obtaining improved s-waves for an electron outside a hydrogen atom in the ground state (cf. Bransden, Dalgarno, John and Seaton 1958, hereafter referred to as BDJS) and recently the above authors have obtained a variationally determined p-wave. Their results seem in better agreement with the experimental evidence on slow elastic scattering than do any others (Brackmann, Fite and Neynaber 1958). We have therefore adopted their wave functions for the symmetric exchange case,

$$\psi_4(\boldsymbol{\kappa};\mathrm{s}) = \frac{1}{(2\pi)^{3/2}r}\left\{\sin\kappa r + a_0{}^{+(t)}\{1-\mathrm{e}^{-2r}\}\cos\kappa r + b\kappa r\,\mathrm{e}^{-r}\right\} \quad \ldots\ldots(21)$$

in which $\eta_0{}^+ = \tan a_0{}^{+(t)}$ is the s-wave phase shift and $b$ is a variational parameter. For the p-wave BDJS adopt

$$\psi_4(\boldsymbol{\varkappa}, \mathrm{p}) = \frac{1}{(2\pi)^{3/2} r}\{\mathrm{j}_1(\kappa r) - a_1{}^{(t)}[1-\mathrm{e}^{-2\kappa r}]^3 \mathrm{y}_1(\kappa r) + b_1(\kappa r)^2 \mathrm{e}^{-3\kappa r}\} \quad \ldots\ldots (22)$$

where

$$\mathrm{j}_1(x) = \left(\frac{\pi x}{2}\right)^{1/2} \mathrm{J}_{3/2}(x); \quad \mathrm{y}_1(x) = \left(\frac{\pi x}{2}\right)^{1/2} \mathrm{J}_{-3/2}(x) \quad \ldots\ldots (23)$$

while $a_1{}^{(t)}$ and $b_1$ are variational parameters.

The s-wave function (21) was used for $\kappa = 0{\cdot}1(0{\cdot}1)0{\cdot}4$ to calculate $|\mathscr{I}(1\mathrm{s}^2 \rightarrow 1\mathrm{s}, \mathrm{C})|^2$ and the results compared with those obtained using the s-component of the plane wave. The general behaviour of the matrix element, as a function of $K$ and $\kappa$ was but little changed; however, it is multiplied by a normalizing factor of $1/[1+a_0{}^{+(t)^2}]$. In the region of interest $\eta_0{}^+$ passes through $\pi/2$ and $a_0{}^{+(t)}$ becomes very large. Thus over the whole range of $\kappa$ considered, the s-wave contribution to the matrix element is decreased by about a factor of seven. The results were extrapolated to $\kappa = 0{\cdot}5$ in order to compare them with the p-wave contribution, which was evaluated for $\kappa = 0{\cdot}5$ and $\kappa = 1{\cdot}0$. The general behaviour is the same in both cases, the modified p-wave being about

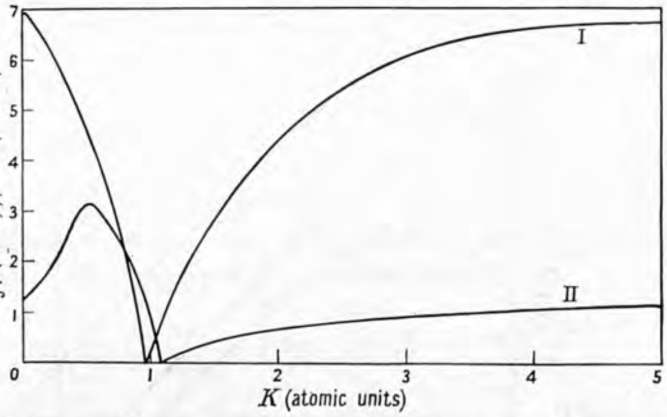

Figure 2. The s and p wave contribution to $\int|\mathscr{I}(1\mathrm{s}^2 \rightarrow 1\mathrm{s}, \mathrm{C})|^2\, d\omega$ for $\kappa = 0{\cdot}5$. I. Plane wave. II. BDJS wave function.

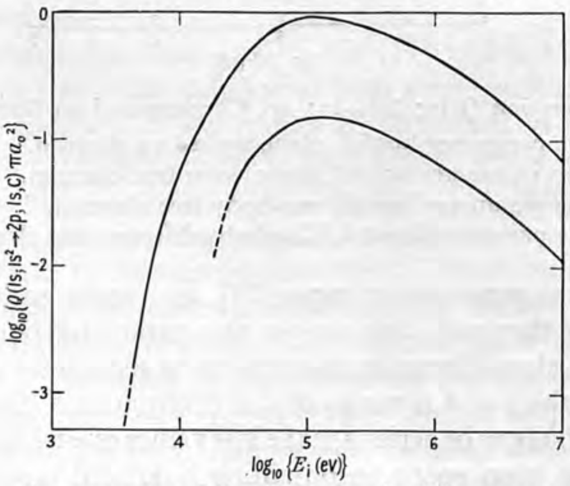

Figure 3. Cross section $Q(1\mathrm{s};\ 1\mathrm{s}^2 \rightarrow 2\mathrm{p};\ 1\mathrm{s}, \mathrm{C})$: upper curve, plane wave for free electron; lower curve, BDJS wave function.

10% less than the p component of the plane wave. The p-wave contribution is but a small fraction of the s-wave contribution in the plane wave case, except in the region near $K=1{\cdot}0$ where they both have a zero and here it is always smaller than the s-wave. However, in the BDJS case the s-wave contribution is greatly reduced while that of the p-wave is scarcely altered and hence dominates at small $K$, giving a sharp maximum in the matrix element near $K=0{\cdot}5$ (cf. figure 2). The total cross section was then calculated on the assumption that the matrix element was decreased in the same ratio (for a given $K$) for $\kappa>0{\cdot}5$ as for $\kappa=0{\cdot}5$. Errors in this assumption are unlikely to be serious since there is only a small contribution to $Q$ from large $\kappa$. The results are shown in figure 3 for $n'l'=2$p.

## § 5. Electron Loss Cross Sections

It is unlikely that the effect of improving the bound wave function for processes of type (18) will be significantly different from that in processes of type (19); that is, they will be slightly larger but of opposite sign to the corrections obtained by modifying the free wave function. Hence the cross sections calculated for processes of type (18) using the one parameter bound and plane wave free wave functions should be correct, relative to each other and to the similar results for processes of type (19), and their absolute magnitudes should be fairly good, perhaps to within a factor of five.

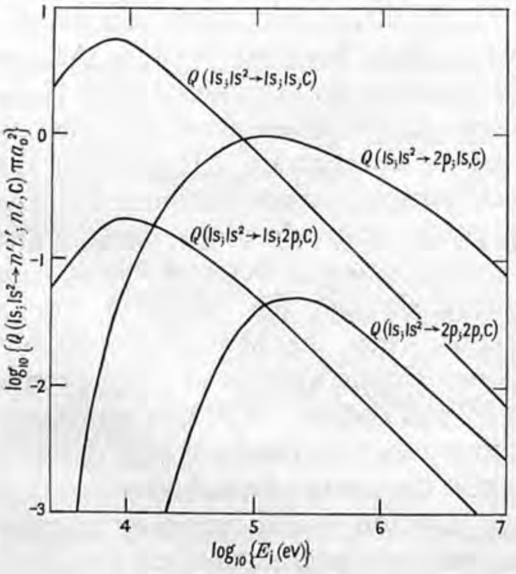

Figure 4. Born approximation cross sections for the processes $H(1s)+H^-(1s^2)\to H(1s \text{ or } 2p)+H(1s \text{ or } 2p)+e$ computed using a one parameter bound wave function and a plane wave for the free electron.

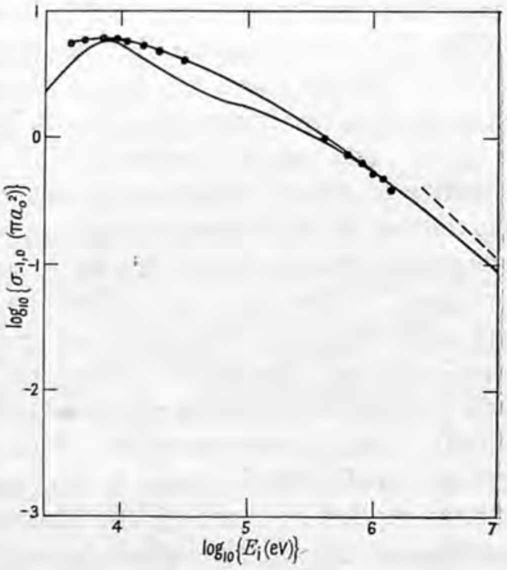

Figure 5. Electron loss cross section $\sigma_{-1,0}$ for H⁻ ions in H. The upper curve is drawn through the experimental points (cf. Allison 1958). The lower curve gives the computed values. The broken line to the right represents the approximate asymptotic result. The experimental results of Whittier (1954) lie some 20% higher at 4 kev.

These cross sections, for $nl=1$s and 2p, are shown in figure 4. The cross sections for which the target particle is unexcited have their maxima at much lower energies than do those in which it is left in a 2p state. This results in a much slower fall off of $\sigma_{-1,0}$ with increasing impact energy than would otherwise be expected. Further, for any given $n'l'$ the major contribution comes from single transitions of the $H^-$ ion, that is, from electron loss without excitation of the residual atom.

The cross sections shown in figure 4 should make the most significant contribution to $\sigma_{-1,0}$ at all energies. Previous work on $H^{+,0}$ collisions with H and He (cf. Bates and Dalgarno 1956) indicates that at any given energy the Born approximation cross sections for any given $l$ or $l'$ fall off rapidly with increasing $n$ or $n'$; and conversely for any given $n$ or $n'$ and $\Delta l$ or $\Delta l' \neq \pm 1$, they fall off rapidly with increasing $l$ or $l'$. The sum of the cross sections for processes (18) and (19) with $n'l' = 1s$ or $2p$ is displayed as $\sigma_{-1,0}$ in figure 5. It is possible to get an approximate asymptotic representation of $\sigma_{-1,0}$ by ignoring the contribution (which should be small) from processes in which the target atom is left in states other than 1s or 2p; that is

$$\sigma_{-1,0} \simeq \sum_{nl} \{Q(1s\,;1s^2 \rightarrow 1s\,; nl,\, C) + Q(1s\,;1s^2 \rightarrow 2p\,; nl,\, C)\}. \quad \ldots\ldots (24)$$

(This summation includes an integration over the continuum and so takes account of double electron loss $\sigma_{-1,+1}$.) Using a sum rule technique this can be evaluated to yield

$$\sigma_{-1,0} \sim \frac{42 \cdot 16}{\mathscr{S}_1^2} (\pi a_0^2). \qquad \ldots\ldots (25)$$

There are no direct experimental data on $\sigma_{-1,0}$. Several authors have however presented results on $\sigma_{-1,0}$ for $H^-$ ions in $H_2$ (Whittier 1954, Stier and Barnett 1956, Rose, Connor and Bastide 1958) which have been reviewed by Allison (1958). While there are sound theoretical reasons for supposing that $H_2$ is equivalent to two hydrogen atoms for collisions with $H^+$, this is not so for collisions with $H^-$, and indeed Gerjuoy (1958) has argued the contrary. However in the absence of direct experimental data the comparison is made in figure 5. The agreement is surprisingly good, in view of the approximations made. The theoretical results should not be in error by more than a factor of five at high energies. They are much less trustworthy, through the failure of Born's approximation, near the maximum cross section, where they should considerably over-estimate. Preliminary data obtained with atomic hydrogen by Branscomb and Fite indicate a cross section of between 5·0 and 10·0 $\pi a_0^2$ at 5000 ev remaining steady to much lower energies. This may imply that our results at high energies are too small; which would in turn imply that the use of a bound wave function taking explicit account of the electronic interaction would increase the cross sections even more than does the replacement of the one parameter by the two parameter approximation. Further discussion must await the detailed experimental results.

The energy distribution of the ejected electrons is of interest in connection with secondary processes. In figure 6 we show the variation of

$$\log_{10}\{Q(1s\,;1s^2 \rightarrow 2p\,; 1s,\, C|\kappa^2,\, E_1)\}$$

as a function of $\kappa$ for some selected incident particle energies. This is such that $Q(1s\,;1s^2 \rightarrow 2p\,;1s,\, C|\kappa^2,\, E_1)d\kappa^2$ is the cross section for the process in which $n'l' \rightarrow 2p\,; nl \rightarrow 1s$ and an electron is ejected with energy between $\kappa^2$ and $\kappa^2 + d\kappa^2$ times $I_H$, by an incident particle of energy $E_1$. These curves show the same general behaviour as do those presented for

$$H^+ + H(1s) \rightarrow H^+ + H^+ + e \qquad \ldots\ldots (26)$$

by Bates and Griffing (1953), but a very much faster fall off at any given energy. That is, there are relatively few high energy electrons ejected: this picture is substantiated by the data on $\mathscr{F}(\kappa^2|E_{\rm i})$, the fraction of electrons ejected with energy greater than $\kappa^2 I_{\rm H}$ at incident energy $E_{\rm i}$, which are displayed in figure 7. Only 25% of the electrons have energies greater than $0{\cdot}5 I_{\rm H}$ and only 10% have energies exceeding one $I_{\rm H}$, even at the highest impact energies. While figures 6 and 7 only refer to the $n'l' = 2$p, $nl = 1$s case, this is dominant at the high energies of interest in auroral studies.

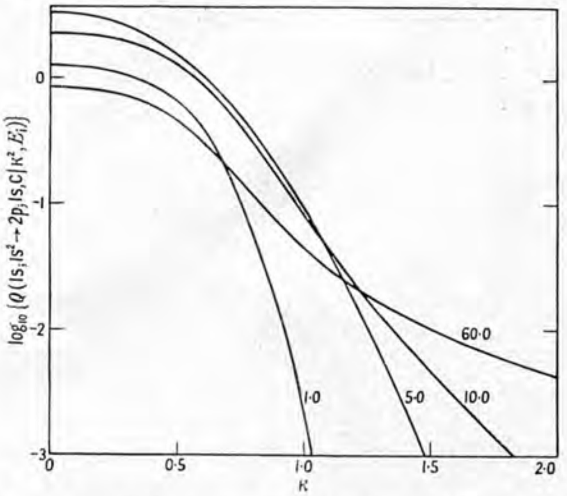

Figure 6. The energy distribution of the ejected electrons. The numbers on the curves give the energy of the incident particle in units of $\mathscr{S}_{\rm i}^2$.

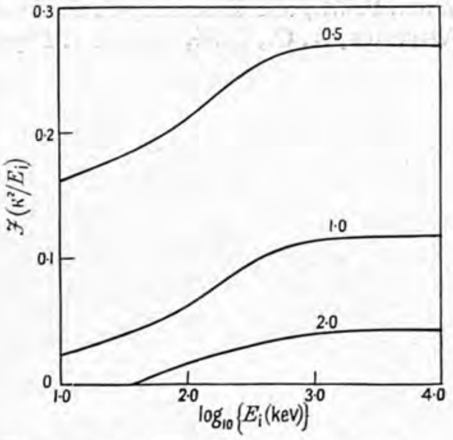

Figure 7. The fraction of ejected electrons which have energy greater than $\kappa^2 I_{\rm H}$. The numbers on the curves give the relevant values of $\kappa^2$.

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