Electron capture from helium by photons

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ELECTRON CAPTURE FROM HELIUM BY PROTONS

by

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Summary

The problem of the elctron capture by fast charged particles passing through a gas is examined mathematically. The applications of theoretical techniques to simple capture processes are discussed, with emphasis on the scattering of protons by helium for which experimental results are more readily available.

The thesis begins with a discussion of the treatment by classical methods of the mechanism of the capture process. The revival of interest in the classical approach to the problem is mentioned. It is shown that the distinction between the classical and quantum treatments is not complete and that in the asymptotic energy region the two descriptions have features in common. This is followed by a short discussion on the general theory of scattering and the derivation of the formal expressions for the scattering amplitude. The Born series expansion of the scattering matrix is discussed and the convergence difficulty associated with the series is mentioned. The argument that the internucleon potential should not contribute to the probability of electron capture is mentioned and it is shown that this difficulty is eliminated in the impulse approximation. The impact parameter method is examined in detail and its equivalence with the wave formalism is mentioned. It is shown that the refined treatment of Bates (1958) removes the difficulties associated with the lack of orthogonality between the initial and final states and eliminates the apparent dependence on the internucleon term. The continuum distorted wave method is discussed and the similarity between its asymptotic form and that of the second Born approximation is mentioned.

The impact parameter method is used to calculate the cross sections for the following processes in the energy ranges indicated:

(i) $H^+ + He(1s^2) \rightarrow H(1s) + He^+(1s)$ 30keV - 10 MeV

(ii) $H^+ + He(1s^2) \rightarrow H(1s, 2s, 2p) + He^+(1s)$ 1 keV - 1MeV

The sensitivity of the calculated cross section with the choice of the ground state helium wave function is investigated by calculating the cross section for reaction (i) using three approximate wave functions. The results for the reactions (i) and (ii) are compared and the atomic expansion method is discussed. A brief description of the numerical methods used is given.

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CHAPTER ONE

Introduction

We shall consider mainly fast collisions, in which the velocity of the projectile is much greater than the orbital velocity of the captured electron.

1.1 Classical Methods

The first calculation on the charge exchange for an atomic process was made by Thomas (1927). In his model the exchange occurs by two successive two-body Rutherford scatterings. The electron is first scattered by the heavy incident particle towards the target nucleus and acquires the speed of the incident particle, which continues to move in its original trajectory. The angle of scattering is determined, by the conservation of energy and momentum, to be 60° in the laboratory frame. The electron is then scattered by the nucleus, so that it now moves, with the speed unaltered, in the same direction as the incident particle.

The classical cross section of Thomas has the high velocity dependence * v^{-11}, as for the second Born approximation (Drisko, 1955) and the impulse approximation (Bransden and Cheshire, 1963). The similarity between the classical and the quantum mechanical calculations is striking, but Cooke (1963) showed by using the uncertainty principle that the Thomas

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* Atomic units will be used throughout, unless otherwise stated. V = 1 corresponds to a proton velocity of $2.188.10^8$ cm/sec.

process cannot be a high energy classical limit. Recently, Bates and Mapleton (1966) have pointed out that, in the model of Thomas, the distribution function for the electrons of the target does not take into account the shell structure of the target atom and so overestimates the probability of finding an electron at small radial distances. Bates and Mapleton (1966) have introduced a modification to the calculations of Thomas and developed a classical theory for symmetrical resonance in slow encounters. The method is found to be very successful.

Since the development of the quantum theory little work was done on classical methods until Gryzinski (1959) showed that they could be used for a wide variety of processes. Recently, by making use of a high speed computer, Abrines and Percival (1966) calculated by means of the Monte Carlo method the cross section for the electron capture by protons in hydrogen for a few energies in the range 38 to 218 keV. The quantal system is represented by a macroscopic classical model, and the scattering is considered entirely in terms of classical statistical mechanics. The Newton's equations for the three-body motion of the electron and the two protons are solved by numerical integration for a number of orbits. The calculated cross sections are rather higher than the experimental data.

The asymptotic form of the classical cross section for $H^+ + H(1s) \rightarrow H(1s) + H^+$ has been examined by Bates and Mapleton (1965). Both the classical theory and quantum mechanics are found to show, if the protons are considered distinguishable, the same v^{-6} velocity dependence and to have almost the same constant of proportionality.

1.2 Formal Theory of Rearrangement Collisions.

The scattering amplitude for a rearrangement collision can be obtained most easily by the method of Lippman (1956). The formal expressions for the matrix element will be derived from the time-independent theory, but the same results would follow from the time-dependent theory. We consider the process

$$1 \; + \; (2 + 3) \; \longrightarrow \; (1 + 2) \; + \; 3, \qquad 1.1$$

in which an initial state, consisting of a particle (1) incident of an electron (2) bound to a core (3), is transformed into a final state, consisting of a bound state of particles (1 + 2) and a free particle (3). For simplicity, the particles are assumed to be non-identical and spinless.

Let $\underline{x}$ and $\underline{k}_x$ be the position and momentum vectors of (2) relative to (3), $\underline{\sigma}$ and $\underline{k}_i$ of (1) relative to the centre of mass of (2 + 3). The vectors appropriate to the initial configuration are $(\underline{x}, \underline{\sigma}, \underline{k}_x, \underline{k}_i)$. In a similar way, the vectors appropriate to the final configuration are given by $(\underline{s}, \underline{\rho}, \underline{k}_s, \underline{k}_f)$. The momentum vectors $\underline{k}_i$ and $\underline{k}_f$ are related to the initial and final velocities of relative motion, $\underline{v}_i$ and $\underline{v}_f$, by the equations

$$\underline{k}_i = \mu_i \underline{v}_i \; , \qquad \underline{k}_f = \mu_f \underline{v}_f \; , \qquad 1.2$$

where the reduced masses μ_i and μ_f are given by

$$\mu_i = \frac{M_1 (1 + M_3)}{1 + M_1 + M_3} \; , \qquad \mu_f = \frac{M_3 (1 + M_1)}{1 + M_1 + M_3} \; , \qquad 1.3$$

with M_i as the mass of particle i.

If ϕ_i is the eigenfunction of (2 + 3) and ϕ_f of (+ 2), then the initial and final unperturbed states of the system are described by

$$\Phi_i(E_i) = e^{i \underline{k}_i \cdot \underline{\sigma}} \phi_i(\underline{x}), \qquad 1.4$$

$$\Phi_f(E_f) = e^{i \underline{k}_f \cdot \underline{\rho}} \phi_f(\underline{s}). \qquad 1.5$$

These states belong to the complete sets of orthogonol states, Φ_n and Φ_m , which satisfy the Schrödinger equations

$$(H_i - E_n)\,\Phi_n(E_n) = 0, \qquad 1.6$$

$$(H_f - E_m)\,\Phi_m(E_m) = 0, \qquad 1.7$$

where $H_i = K + V_{23}$, $H_f = K + V_{12}$, K is the total kinetic energy operator, and V_{ij} is the Coulomb interaction between the particles i and j.

The total Hamiltonian H in the centre-of-mass system is

$$H = K + V_{12} + V_{13} + V_{23} \qquad 1.8$$

H can be written as $H = H_i + V_i = H_f + V_f$, V_i and V_f being the initial and final perturbing potentials

$$V_i = V_{12} + V_{13}, \qquad 1.9$$

$$V_f = V_{13} + V_{23}. \qquad 1.10$$

The Schrödinger equation for the complete system is

$$(H - E_i)\, \Psi_i^+ (E_i) = 0. \qquad 1.11$$

Ψ_i^+ is the outgoing wave function corresponding to an initial state Φ_i and outgoing waves which describe elastic scattering, inelastic scattering, and rearrangement processes. For capture into the final state f, it has the asymptotic form

$$\Psi_i^+ \underset{r \to \infty}{\sim} \Phi_i + \frac{f(\theta)}{\rho}\, \Phi_f \,, \qquad 1.12$$

with $\theta = \cos^{-1}(\underline{k}_i \cdot \underline{k}_f)$, and $f(\theta)$ as the scattering amplitude from the initial state Φ_i to the final state Φ_f.

The capture cross section is then given by

$$Q_{if} = 2\, \frac{v_f}{v_i} \int_{-1}^{1} |f_{if}(\theta)|^2\, d(\cos\theta). \qquad 1.13$$

To obtain $f(\theta)$ from Ψ_i^+, we first define the three-particle Green's functions

$$(E_i + i\varepsilon - H_i)^{-1} = \int dn\, \frac{|\Phi_n\rangle\langle\Phi_n|}{E_i + i\varepsilon - E_n}\,, \qquad 1.14$$

$$(E_i + i\varepsilon - H_f)^{-1} = \int dm\, \frac{|\Phi_m\rangle\langle\Phi_m|}{E_i + i\varepsilon - E_m}\,, \qquad 1.15$$

where ε is an arbitrary positive real quantity, and Φ_n and Φ_m satisfy (1.4) and (1.5). We denote the operators

$$G_i\,(E_i + i\varepsilon) \equiv (E_i + i\varepsilon - H_i)^{-1}\,, \qquad 1.16$$

$$G_f\,(E_i + i\varepsilon) \equiv (E_i + i\varepsilon - H_f)^{-1}\,, \qquad 1.17$$

$$G_o\,(E_i + i\varepsilon) \equiv (E_i + i\varepsilon - K)^{-1}\,, \tag{1.18}$$

$$G\,(E_i + i\varepsilon) \equiv (E_i + i\varepsilon - H)^{-1}\,, \tag{1.19}$$

From the theory of differential equations, Ψ_i^+ satisfies the equation

$$\Psi_i^+(E_i + i\varepsilon) = \Phi_i(E_i) + G_i V_i \Psi_i^+(E_i + i\varepsilon), \tag{1.20}$$

with

$$\Psi_i^+(E_i) = \lim_{\varepsilon \to 0^+} \Psi_i^+(E_i + i\varepsilon).$$

By operating on the equation (1.19) to the left and right by $(E_i + i\varepsilon - H_i)$, we find

$$G = G_i[1 + V_i G] = [1 + G V_i]G_i\,,$$

and similarly we obtain

$$G_i = G[1 - V_i G_i] = [1 - G_i V_i]G,$$

so that

$$G_i = [1 - G_i V_i]G = [1 - G_i V_i][1 + G V_i]G_i\,,$$

and hence

$$[1 - G_i V_i][1 + G V_i] = 1. \tag{1.21}$$

Using (1.20) and (1.21), we have

$$\Psi_i^+(E_i + i\varepsilon) = [1 + G(E_i + i\varepsilon)V_i]\Phi_i(E_i). \tag{1.22}$$

Operating on (1.17) first by $(E_i + i\varepsilon - H_i)$, then by G_f and rearranging, we obtain

$$[1 - G_f V_f][1 + G V_i] = 1 + G_f (V_i - V_f), \tag{1.23}$$

so that

$$[1 - G_f V_f]\Psi_i^+(E_i + i\varepsilon) = [1 + G_f(V_i - V_f)]\,\Phi_i(E_i). \tag{1.24}$$

The term on the right-hand side can be worked out to the simple form

$$\begin{aligned}[1 + G_f(V_i - V_f)]\Phi_i(E_i) &= \left[\frac{E_i + i\varepsilon - H_f + V_i - V_f}{E_i + i\varepsilon - H_f}\right]\Phi_i(E_i) \\ &= \left[\frac{E_i + i\varepsilon - H_i}{E_i + i\varepsilon - H_f}\right]\Phi_i(E_i) \\ &= \frac{i\varepsilon}{E_i + i\varepsilon - H_f}\,\Phi_i(E_i).\end{aligned} \tag{1.25}$$

The Schrödinger equation describing the rearrangement collision can then be written as

$$\Psi_i^+(E_i + i\varepsilon) = G_f(E_i + i\varepsilon)\left[i\varepsilon\Phi_i(E_i) + V_f\Psi_i^+(E_i + i\varepsilon)\right]. \tag{1.26}$$

The transition rate W_{if} for a rearrangement process depends only on the second term on the right-term side of (1.26); the first has no singularity and so vanishes as $\varepsilon \to 0^+$, except in the special case when the three particles are unbound both in the initial and final states. Using the spectral representation of

G_f (1.15), we find

$$\Psi_i^+(E_i+i\varepsilon) = \int dm \, \frac{|\Phi_m\rangle\langle\Phi_m|V_f|\Psi_i^+(E_i+i\varepsilon)\rangle}{E_i+i\varepsilon-E_m} \, . \qquad 1.27$$

Ψ_i^+ contains the time dependence exp $(iE_it - \varepsilon t)/\hbar$, so that

$$W_{if} \equiv \frac{\partial}{\partial t}\left|\langle\Phi_f|\Psi_i^+\rangle\right|^2 = \lim_{\varepsilon\to 0^+} \frac{2\varepsilon}{\hbar}\,\frac{|T_{if}|^2}{(E_i-E_f)^2+\varepsilon^2} \, , \qquad 1.28$$

where

$$T_{if} = \langle\Phi_f(E_f)|V_f|\Psi_i^+(E_i)\rangle \, . \qquad 1.29$$

Since

$$\lim_{\varepsilon\to 0^+}\left[\frac{\varepsilon}{x^2+\varepsilon^2}\right] = i\pi\,\delta(x) \, ,$$

we obtain

$$W_{if} = \delta(E_i-E_f)\,\frac{2\pi}{\hbar}\,|T_{if}|^2 \, . \qquad 1.30$$

The scattering amplitude $f_{if}(\theta)$ is related to T_{if} by the equation

$$f_{if}(\theta) = -\frac{\mu_f}{2\pi}\,T_{if} \, . \qquad 1.31$$

In a similar manner, the incoming wave solution Ψ_f^- can be written as

$$\Psi_f^-(E_f-i\varepsilon) = \Phi_f(E_f) + G_f(E_f-i\varepsilon)V_f\Psi_f^-(E_f-i\varepsilon) , \qquad 1.32$$

and the transition matrix T_{if} becomes

$$T_{if} = \langle\Psi_f^-(E_f)|V_i|\Phi_i(E_i)\rangle \, . \qquad 1.33$$

We now consider the scattering matrix, or simply the S-matrix. Let the channels of the process be denoted by α, β, γ, etc. We express Ψ_α^+ as a linear combinations of the Ψ_β^-

$$\Psi_\alpha^+ = \sum_\beta \Psi_\beta^- S_{\beta\alpha} . \tag{1.34}$$

From the orthogonality of the scattering states we obtain

$$S_{\beta\alpha} = \langle \Psi_\beta^- | \Psi_\alpha^+ \rangle . \tag{1.35}$$

This is the S-matrix. The importance of the S-matrix lies in the fact that it is unitary. By using (1.34) and (1.35), we find

$$\sum_\gamma S_{\gamma\alpha}^* S_{\gamma\beta} = \delta_{\alpha\beta} , \tag{1.36}$$

$$\sum_\gamma S_{\alpha\gamma} S_{\beta\gamma}^* = \delta_{\alpha\beta} , \tag{1.37}$$

and hence

$$S S^\dagger = S^\dagger S = 1 . \tag{1.38}$$

The unitary nature of the S-matrix has an important physical meaning ; it ensures the conservation of flux or probability in a collision.

The present proof for the unitarity of the S-matrix is unsatisfactory. It is based on the assumption that the wave functions in different channels are orthogonal to each other. This is not the case in rearrangement collisions, where the colliding particle and the collision products are composite fragments, so that the channels overlap. An alternative proof is given by Jauch and Marchand (1966) and it shows unitarity to be a direct consequence of the asymptotic conditions and nothing more.

1.3 The Born Series.

In any general theory of scattering it is not difficult to derive exact expressions for the transition matrix of any collision. It is in the actual calculations that the difficulty arises. In almost all cases it is impossible to obtain an exact solution for Ψ_i^+ or Ψ_f^- and, in practice, various methods are used to find approximate solutions. A frequently used approximation is that of Born, and it consists in iterating the integral equation.

We consider the series expansion of the operator

$$G \equiv (E_i + i\varepsilon - H)^{-1} = (E_i + i\varepsilon - H_i - V_i)^{-1}.$$

On using the operator identity

$$(A + B)^{-1} = A^{-1}\left[1 - B(A+B)^{-1}\right], \qquad 1.39$$

and setting

$$A \equiv (E_i + i\varepsilon - H_i), \quad B \equiv -V_i ,$$

we obtain

$$G = G_i + G_i V_i G. \qquad 1.40$$

As $G \approx G_i$, the series representation is given by

$$G = G_i + G_i V_i G_i + G_i V_i G_i V_i G_i + \ldots\ldots, \qquad 1.41$$

and in a similar procedure

$$G = G_0 + G_0(V_{12}+V_{13}+V_{23})G_0 + G_0(V_{12}+V_{13}+V_{23})G_0(V_{12}+V_{13}+V_{23})G_0 + \cdots \qquad 1.42$$

The transition matrix is

$$T_{if} = \langle \Phi_f | V_f | \Psi_i^+ \rangle ,$$

with

$$\Psi_i^+ = \left[1 + G V_i \right] \Phi_i ,$$

Using (1.41), we get the series

$$T_{if} = \langle \Phi_f | V_f | \Phi_i \rangle + \langle \Phi_f | V_f G_i V_i | \Phi_i \rangle + \langle \Phi_f | V_f G_i V_i G_i V_i | \Phi_i \rangle + \cdots \qquad 1.43$$

When only the first term in this expansion is retained, we obtain the first Born approximation, often simply referred to as the Born approximation. We denote it by

$$T_{if}^{B+} \equiv \langle \Phi_f | V_f | \Phi_i \rangle . \qquad 1.44$$

The alternative expression for T_{if},

$$T_{if} = \langle \Psi_f^- | V_i | \Phi_i \rangle ,$$

can be iterated in terms of G_f $(E_f - i\varepsilon)$ by a similar procedure. In this case, the first term in the series expansion is

$$T_{if}^{B-} \equiv \langle \Phi_f | V_i | \Phi_i \rangle . \qquad 1.45$$

The two forms of the Born approximation, $T_{if}^{B\pm}$, using the post and prior interactions respectively, are identical provided the wave functions Φ_i and Φ_f are exact. They give different values if either Φ_i or Φ_f is not exact; this is the source of the post-prior discrepancy and it is impossible on physical grounds to predict which interaction will give a better estimate of the transition matrix.

The terms beyond the first few in the series expansion of T_{if} are difficult to evaluate; they must be negligible if any calculation based on this series is to be valid. It is shown by Zemach and Klein (1958) that, except for sufficiently high energies, the series expansion of the Green's function diverges. Aaron, Amado and Lee (1961) have found that for a class of potentials, including the Coulomb potential, the Born series diverges. Their proof is not rigorous, but the result is probably correct. However, Dettman and Leibfried (1966) have re-examined the Born series and expressed the views that the commonly used arguments to prove its divergence for rearrangement collisions at all energies do not hold. They treated in detail the one-dimensional three-body collision with δ-function interactions and found that, in this particular case, the series converged. The proof is not rigorous and their conclusion is open to question.

The problem is also investigated in the framework of the distorted-wave formalism by Greider and Dodd (1966). In this case too, the iterative solution of the integral equation is found to diverge.

A general and rigorous mathematical proof that the ordinary or the distorted - wave Born model is or is not valid would be extremely valuable, but probably difficult to find. It may well be that for potentials of practical importance the series diverges, so that the validity of the application of the Born approximation to atomic collisions remains in doubt. Accurate results are however obtained for some processes form the first one or two terms in the Born series. The approximation often works much better than may be expected.

1.4 The Impulse Approximation.

Chew (1950) first attempted to formulate the scattering amplitude in terms of exact two-body matrix elements. The method rests on the assumption that, for the process

$$1 + (2+3) \longrightarrow (1+2) + 3,$$

if the velocity of 1 is much greater than the orbital velocity of electron 2 in the bound system (2 + 3), the struck particle 2 may be regarded as a free particle during the collision. The effects of the binding potential V_{23} can be neglected, although it determines the initial state Φ_i.

We define the two-body Møller operator W_{12}^{+} by

$$\omega_{12}^{+}\chi(\underline{k}_s,\underline{k}_f) = \left[1 + (E_{k_s} + E_{k_f} + i\varepsilon - K - V_{12})^{-1} V_{12}\right]\chi(\underline{k}_s,\underline{k}_f) \equiv \psi(\underline{k}_s,\underline{k}_f), \qquad 1.46$$

where the momentum vectors $\underline{k}_s$ and $\underline{k}_f$ are defined as in section (1.2), and $X(\underline{k}_s, k_f)$ is a plane wave.

$X(\underline{k}_s, \underline{k}_f)$ and $\psi(\underline{k}_s, \underline{k}_f)$ satisfy the Schrödinger equations

$$(K - E_{k_s} - E_{k_f})\chi(\underline{k}_s, \underline{k}_f) = 0, \qquad 1.47$$

$$(K + V_{12} - E_{k_s} - E_{k_f})\psi(\underline{k}_s, \underline{k}_f) = 0. \qquad 1.48$$

$X(\underline{k}_s, \underline{k}_f)$ is the plane wave function for the three particles when there is no interaction between them. $\psi(k_s, k_f)$ is the product of a wave function for scattering of 1 by 2 with the potential V_{12} and energy E_{ks}, and a plane wave describing the motion of 3, with energy E_{kf}, relative to the centre of mass of (2 + 3).

We define the Møller matrix Ω^+ by

$$\Omega^+ = 1 + GV_i, \qquad 1.49$$

so that from (1.22)

$$\Psi_i^+ = \Omega^+ \Phi_i, \qquad 1.50$$

and from (1.29)

$$T_{if} = \langle \Phi_f | V_f | \Omega^+ \Phi_i \rangle. \qquad 1.51$$

After some manipulation (Chew and Goldberger, 1952), Ω^+ can be written in the form

$$\Omega^+ = (\omega_{12}^+ + \omega_{13}^+ - 1) + G\left[V_{23}, (\omega_{12}^+ + \omega_{13}^+)\right]$$
$$+ G\left[V_{12}(\omega_{13}^+ - 1) + V_{13}(\omega_{12}^+ - 1)\right]. \qquad 1.52$$

The second term on the right-hand side of (1.52) vanishes on neglecting the binding potential V_{23}, in accordance with the impulse approximation. The third term represents successive scatterings of the incident particle by the potentials V_{12} and V_{13} ; these multiple - scattering effects are negligible for charge transfer collisions.

The transition matrix is then

$$T_{if}^{I} \simeq \langle \Phi_f | V_f (\omega_{12}^{+} + \omega_{13}^{+} - 1) | \Phi_i \rangle . \qquad 1.53$$

From the alternative expression of T_{if} in terms of Ψ_f^{-} , we find

$$T_{if}^{II} \simeq \langle \Phi_f | (\omega_{23}^{-} + \omega_{12}^{-} - 1) V_i | \Phi_i \rangle . \qquad 1.54$$

It is expected on physical grounds that the internuclear potential V_{13} cannot affect the electron capture cross section. Setting $\omega_{13}^{\pm} \simeq 1$, we obtain

$$T_{if}^{I} \simeq \langle \Phi_f | V_f | \omega_{12}^{+} \Phi_i \rangle , \qquad 1.55$$

$$T_{if}^{II} \simeq \langle \omega_{23}^{-} \Phi_f | V_i | \Phi_i \rangle . \qquad 1.56$$

It is evident from the assumptions used that the impulse approximation will be better the weaker are the interactions. Its application to the collision of a particle with a neutral atom is intuitively plausible, but it does not follow that the extension to processes involving interparticle Coulomb potentials is exactly valid

The present formulation of the impulse approximation in unsatisfactory, for the Coulomb potentials have only in part been eliminated by the use of two-body operators. Moreover, the two forms of the transition matrix, T^1_{if} and T_{if} of (1.55) and (1.56) respectively, are not automatacally identical, and this may introduce a 'post-prior' discrepancy. These defects have been overcome in the new formulation by Fadeev (1961a,b, 1963).

1.5 Impact Parameter Formulation

In all collisions between atomic systems containing heavy particles, the motions of the heavy particles are essentially unaltered by any electronic excitation or re-arrangements unless the energy of relative motion is very low (Bates and Boyd; 1962a, b,). It is then advantageous in describing these processes to treat the electronic motions by quantum mechanics but the motions of the heavy particles by classical mechanics. The formulation which follows is mainly due to Bates (1958).

Let $\underline{R}$ and $\underline{v}$ be the position vector and velocity, respectively, of particle 1 relative to 3, and $\underline{r}$ the position vector of the electron 2 relative to the mid-point of $\underline{R}$. We choose a co-ordinate system with the z- axis along the direction of motion, so that

$$\underline{R} = \underline{\rho} + \underline{v} t \ , \quad z = v t \ . \qquad 1.57$$

The time t is chosen such that at $t = 0$ the particles 1 and 3 have a minimum separation ρ, known as the "impact parameter" of the collision.

The electronic wave function Ψ for the complete system satisfies the time-dependent Schrodinger equation.

$$H \Psi(\underline{r},t) = i \frac{\partial}{\partial t} \Psi(\underline{r},t) \ , \qquad 1.58$$

with

$$H = -\frac{1}{2} \nabla_r^2 + V_{12} + V_{13} \ . \qquad 1.59$$

Ψ is expressed in the form of a series expansion of eigenfunctions; the set of basis functions is chosen so that each term in the expansion is a solution of (1.58) in the limit of infinite nuclear separation (Bates and McCarroll, 1958). We write

$$\begin{aligned}\Psi(\underline{r},t) = {} & a_i(t)\,\phi_i(\underline{r}+\tfrac{1}{2}\underline{R})\exp\{-i(\tfrac{1}{2}\underline{v}\cdot\underline{r}+\tfrac{1}{8}v^2t+\varepsilon_i t)\} \\ & + b_f(t)\,\phi_f(\underline{r}-\tfrac{1}{2}\underline{R})\exp\{i(\tfrac{1}{2}\underline{v}\cdot\underline{r}-\tfrac{1}{8}v^2t-\varepsilon_f t)\} \\ & + \chi(\underline{r},t). \qquad 1.60\end{aligned}$$

ϕ_i and ϕ_f are the wave functions of the bound states (2 + 3) and (1 + 2), respectively. χ (r,t) is orthogonal to the other two terms on the right-hand side of (1.60) and may be expanded in the alternative forms

$$\chi(\underline{r},t) = \sum_{n\neq i} a_n(t)\,\phi_n(\underline{r}+\tfrac{1}{2}\underline{R})\exp\{-i(\tfrac{1}{2}\underline{v}\cdot\underline{r}+\tfrac{1}{8}v^2t+\varepsilon_n t)\}, \qquad 1.61$$

and

$$\chi(\underline{r},t) = \sum_{m\neq f} b_m(t)\,\phi_m(\underline{r}-\tfrac{1}{2}\underline{R})\exp\{i(\tfrac{1}{2}\underline{v}\cdot\underline{r}-\tfrac{1}{8}v^2t-\varepsilon_m t)\}. \qquad 1.62$$

Continuum states may also be included in χ(r,t). In this section, for simplicity we consider two states only and set $\chi = 0$; this is equivalent to assuming that coupling through all states other than i and f are negligible.

The expansion coefficients $a_i(t)$ and $b_f(t)$ depend on ρ although this dependence is not indicated explicitly. The initial conditions are

$$a_i(-\infty) = 1 , \quad b_f(-\infty) = 0 . \qquad 1.63$$

The probability amplitude for electron capture from an initial state i to a final state f is then $b_f(+\infty)$. The probability of capture at a particular value of the impact parameter is $|b_f(+\infty)|^2$ and the total capture cross section is

$$Q_{if} = 2\int |b_f(+\infty)|^2 \rho \, d\rho . \qquad 1.64$$

Using (1.58) and (1.59), we obtain

$$i\left(\dot{a}_i + \dot{b}_f S_{if} e^{i\varepsilon_{if}t}\right) = a_i h_{ii} + b_f K_{if} e^{i\varepsilon_{if}t} , \qquad 1.65$$

$$i\left(\dot{a}_i S_{fi} e^{i\varepsilon_{fi}t} + \dot{b}_f\right) = a_i K_{fi} e^{i\varepsilon_{fi}t} + b_f h_{ff} , \qquad 1.66$$

where

$$\varepsilon_{if} = -\varepsilon_{fi} = \varepsilon_i - \varepsilon_f ,$$

$$S_{if}(t) = S^*_{fi}(t) = \int \phi_i^*(\underline{r}+\tfrac{1}{2}\underline{R})\,\phi_f(\underline{r}-\tfrac{1}{2}\underline{R})\,e^{i\underline{v}\cdot\underline{r}}\,d\underline{r} ,$$

$$K_{if}(t) = \int \phi_i^*(\underline{r}+\tfrac{1}{2}\underline{R})\,V_{23}\,\phi_f(\underline{r}-\tfrac{1}{2}\underline{R})\,e^{i\underline{v}\cdot\underline{r}}\,d\underline{r} , \qquad 1.67$$

$$K_{fi}(t) = \int \phi_f^*(\underline{r}-\tfrac{1}{2}\underline{R})\,V_{12}\,\phi_i(\underline{r}+\tfrac{1}{2}\underline{R})\,e^{-i\underline{v}\cdot\underline{r}}\,d\underline{r} ,$$

$$h_{ii}(t) = \int \phi_i^*(\underline{r}+\tfrac{1}{2}\underline{R})\,V_{12}\,\phi_i(\underline{r}+\tfrac{1}{2}\underline{R})\,d\underline{r} ;$$

$$h_{ff}(t) = \int \phi_f^*(\underline{r}-\tfrac{1}{2}\underline{R})\,V_{23}\,\phi_f(\underline{r}-\tfrac{1}{2}\underline{R})\,d\underline{r} .$$

The terms in (1.65) and (1.66) are rearranged to give

$$i(1-|S_{if}|^2)\dot{a}_i = a_i(h_{ii}-S_{if}K_{fi})+b_f(K_{if}-S_{if}h_{ff})e^{i\varepsilon_{if}t}, \qquad 1.68$$

$$i(1-|S_{if}|^2)\dot{b}_f = a_i(K_{fi}-S_{fi}h_{ii})e^{i\varepsilon_{fi}t}+b_f(h_{ff}-S_{fi}K_{if}). \qquad 1.69$$

By substituting

$$\alpha_i = \frac{h_{ii}-S_{if}K_{fi}}{1-|S_{if}|^2}, \qquad \beta_f = \frac{h_{ff}-S_{fi}K_{if}}{1-|S_{if}|^2}, \qquad 1.70$$

and

$$\overset{\circ}{a}_i = a_i \exp\left\{i\int_{-\infty}^{t}\alpha_i dt\right\}, \qquad \overset{\circ}{b}_f = b_f \exp\left\{i\int_{-\infty}^{t}\beta_f dt\right\}, \qquad 1.71$$

in (1.68)and (1.69), we obtain

$$\overset{\circ}{\dot{a}}_i = -i\overset{\circ}{b}_f\left[\frac{K_{if}-S_{if}h_{ff}}{1-|S_{if}|^2}\right]\exp\{i(\varepsilon_{if}+\delta_{if})\}, \qquad 1.72$$

$$\overset{\circ}{\dot{b}}_f = -i\overset{\circ}{a}_i\left[\frac{K_{fi}-S_{fi}h_{ii}}{1-|S_{if}|^2}\right]\exp\{-i(\varepsilon_{if}+\delta_{if})\}, \qquad 1.73$$

where

$$\delta_{if} = \int_{-\infty}^{t}(\alpha_i-\beta_f)dt \qquad 1.74$$

$$\simeq \int_{-\infty}^{t}(h_{ii}-h_{ff})dt \qquad 1.75$$

If we make the assumption

$$\overset{\circ}{a}_i(t) = 1, \qquad 1.76$$

which implies neglecting back-coupling from the final to the initial states, we obtain

$$|b_f(+\infty)| = |\overset{\circ}{b}_f(+\infty)| = \left|\int_{-\infty}^{t}M_{if}dt\right|, \qquad 1.77$$

where

$$M_{if} = \frac{K_{fi} - S_{fi} h_{ii}}{1 - |S_{if}|^2} \exp -i(\varepsilon_{if} t + \delta_{if}) \qquad 1.78$$

$$\simeq (K_{fi} - S_{fi} h_{ii}) \exp -i(\varepsilon_{if} t + \delta_{if}). \qquad 1.79$$

Since

$$\int \phi_f^*(\underline{r} - \tfrac{1}{2}\underline{R})\left[V_{12}(\underline{r} - \tfrac{1}{2}\underline{R}) + V_{13}(\underline{R})\right]\phi_i(\underline{r} + \tfrac{1}{2}\underline{R}) e^{i\underline{v}\cdot\underline{r}} d\underline{r} \qquad 1.80$$

$$= K_{fi} + V_{13}(\underline{R}) S_{fi} \;,$$

and

$$\int \phi_i^*(\underline{r} + \tfrac{1}{2}\underline{R})\left[V_{12}(\underline{r} - \tfrac{1}{2}\underline{R}) + V_{13}(\underline{R})\right]\phi_i(\underline{r} + \tfrac{1}{2}\underline{R}) d\underline{r}$$

$$= h_{ii} + V_{13}(\underline{R}) \;, \qquad 1.81$$

it is evident that M_{if} is independent of the internucleon potential V_{13}.

The phase term δ_{if} comes from the difference between the effects of the interaction of the colliding systems when in the initial state and when in the final state. Its inclusion in (1.72) and (1.73) allows for distortion. This is expected to be important for charge transfer processes because of the large contribution from close encounters (Bates and McCarroll, 1962).

In the case of symmetrical resonance, δ_{if} vanishes since the initial and final states are identical (Bates, 1958). Moreover, the equations (1.72) and (1.73) become sufficiently simple to be solved exactly and so allows completely for back-coupling from the final to the initial states (McCarroll, 1961).

The impact parameter methol satisfies the requirements of the detailed balancing (Bates, 1958 b; Green, 1965). In the work of Bates (1958 b) detailed balancing is proved for processes having small transition probabilities. Green (1965) considers the general case and shows that the impact parameter method satisfies detailed balancing even though only a finite number of states is included in the expansion set. We consider the expansion of Ψ

$$\Psi(c;t) = \sum_n a_n(c;t)\,\phi_n , \qquad 1.82$$

where the symbol C is used to distinguish solutions corresponding to different conditions, and ϕ_n is a set of orthonormal functions. Let

$$S_{kn} = \langle \phi_k | \phi_n \rangle , \qquad 1.83$$

$$H_{kn} = \left\langle \phi_k \middle| H - i\frac{\partial}{\partial t} \middle| \phi_n \right\rangle . \qquad 1.84$$

We take the z-axis to be in the direction of the incident particle. We define

$$\Psi_R(c;x,y,z,t) \equiv \Psi(c;x,y,-z,-t)^* , \qquad 1.85$$

so that

$$a_{R,n}(c;t) = \epsilon_n a_n(c;-t)^* , \qquad 1.86$$

where $\epsilon_n = \pm 1$. We define also two particular solutions $\Psi^{\pm}(k;t)$ which have the property that as $t \to \mp \infty$

$$\Psi^{\pm}(k;t) \longrightarrow \phi_k(x,y,z,t) . \qquad 1.87$$

The essential time-reversal relations are

$$S^*_{nm}(-t) = \epsilon_n \epsilon_m S_{nm}(t) , \qquad 1.88$$

$$H^*_{nm}(-t) = \epsilon_n \epsilon_m H_{nm}(t) . \qquad 1.89$$

We write

$$\begin{aligned} a^+_k(n;+\infty) &= \lim_{t \to -\infty} \langle \Psi^-(k;t) | \Psi^+(n;t) \rangle \\ &= \lim_{t \to +\infty} \langle \Psi^+_R(n;t) | \Psi^-_R(k;t) \rangle \\ &= \lim_{t \to +\infty} \langle \epsilon_n \Psi^-(n;t) | \epsilon_k \Psi^+(k;t) \rangle \\ &= \epsilon_n \epsilon_k a^+_n(k;+\infty) . \end{aligned} \qquad 1.90$$

The proof of the detailed balancing then follows.

Approximations corresponding to each of those described above can also be obtained in the wave formalism which allows for the non-orthogonality of the initial and final eigenfunctions (Bates, 1958). In the simple case where distortion and back-coupling are ignored, the matrix element is obtained by replacing V_f in T_{if} by the effective interaction

$$\frac{1}{1 - |S_{if}|^2} \left[V_{12}\left(I - \tfrac{1}{2}\underline{R}\right) - h_{ii} \right] .$$

These results can also be obtained by a variational method, using the functional

$$I = \int \Psi^{*} (H-E) \Psi \, d\tau .$$

Let $F_n(\underline{r})$ and $G_n(\underline{\rho})$ be the coefficients of the initial and final bound states in the two-state expansion of Ψ. The method consists in using the property that I is stationary under all independent variations of F_n and G_n that leave the asymptotic forms of F_n and G_n unaltered.

Bassel and Gerjuoy (1960) have used the operator formalism of Gell-Mann and Goldberger (1953) to derive the distorted wave approximation. This method gives similar results as that of Bates, but the $|S_{if}|^2$ term is now not obtained.
Let $\mathcal{V}_i(\underline{r})$ and $\mathcal{V}_f(\underline{\rho})$ be arbitrary short range potentials, and X_i and X_f be solutions of the equations

$$(K + V_{23} - \mathcal{V}_i(\underline{r}) - E_i) \chi_i(E_i) = 0, \qquad 1.91$$

$$(K + V_{12} - \mathcal{V}_f(\underline{\rho}) - E_f) \chi_f(E_f) = 0 .$$

Then the incoming wave solution is given by

$$\Psi_f^-(E_f) = \frac{1}{E_f - i\varepsilon - K - V_{23} + \mathcal{V}_i} \left[-i\varepsilon \chi_f^-(E_f) + (V_{13} + V_{12} + \mathcal{V}_i) \Psi_f^-(E_f) \right], \qquad 1.92$$

and hence the transition matrix is

$$T_{if} = \langle \Psi_f^- | V_{13} + V_{12} + \mathcal{V}_i | \chi_i^+ \rangle . \qquad 1.93$$

The method consists in substituting ν_i by h_{ii} and ν_f by h_{ff}, since any other choice would be inconsistentin the light of the derivation using the variational principle. The term containing the internucleon potential V_{13}' is of the order m/M and is thus negligible.

Sil (1960) has explicitly used a variational method to obtain a formalism equivalent to that of the impact parameter.

1.6 The Continuum Distorted Wave Method.

Cheshire (1963b, 1964b) has suggested a new approach to the distorted wave method and developed an approximation which has the virtue of including continuum intermediate states.

The initial and final states $\Phi_i(t)$ and $\Phi_f(t)$, which satisfy the equations

$$\left(\frac{1}{2}\nabla_r^2 + \frac{1}{x} + i\frac{\partial}{\partial t}\right)\Phi_i(t) = 0, \qquad 1.94$$

$$\left(\frac{1}{2}\nabla_r^2 + \frac{1}{s} + i\frac{\partial}{\partial t}\right)\Phi_f(t) = 0, \qquad 1.95$$

are given by

$$\Phi_i(t) = \phi_i(\underline{x})\exp\left\{-i\left(\frac{1}{2}\underline{v}\cdot\underline{r} + \frac{1}{8}v^2 t + \epsilon_i t\right)\right\}, \qquad 1.96$$

$$\Phi_f(t) = \phi_f(\underline{s})\exp\left\{i\left(\frac{1}{2}\underline{v}\cdot\underline{r} - \frac{1}{8}v^2 t - \epsilon_f t\right)\right\}. \qquad 1.97$$

The complete wave functions $\Psi_i(t)$ and $\Psi_f(t)$ are then written as

$$\Psi_i(t) = \Phi_i(t)\mathcal{L}_i(t),$$

$$\Psi_f(t) = \Phi_f(t)\mathcal{L}_f(t), \qquad 1.98$$

where $\mathcal{L}_i(t)$ and $\mathcal{L}_f(t)$ are solutions of the equations

$$\left(\frac{1}{2}\nabla_r^2 + \frac{1}{s} - \frac{1}{R} + i\frac{\partial}{\partial t} - \frac{i}{2}\underline{v}\cdot\nabla_r\right)\mathcal{L}_i = \frac{\underline{x}}{x}\cdot\nabla_r\mathcal{L}_i, \qquad 1.99$$

$$\left(\frac{1}{2}\nabla_r^2 + \frac{1}{x} - \frac{1}{R} + i\frac{\partial}{\partial t} + \frac{i}{2}\underline{v}\cdot\nabla_r\right)\mathcal{L}_f = \frac{\underline{s}}{s}\cdot\nabla_r\mathcal{L}_f, \qquad 1.100$$

and have the boundary conditions

$$\lim_{t\to-\infty} \mathcal{L}_i = \lim_{t\to+\infty} \mathcal{L}_f = 1 . \qquad 1.101$$

First order approximations to $\mathcal{L}_i$ and $\mathcal{L}_f$, denoted by $\mathcal{L}_i'$ and $\mathcal{L}_f'$, are obtained by neglecting the right-hand sides of (1.99) and (1,100). At high velocities $\mathcal{L}_i'$ and $\mathcal{L}_f'$ are expected to be good approximations to $\mathcal{L}_i$ and $\mathcal{L}_f$ respectively, over the regions which contribute to the scattering amplitude.

The transition amplitude based on $\Phi_i \mathcal{L}_i'$ and $\Phi_f \mathcal{L}_f'$ as distorted waves is then given by

$$T_{if} = -i \int_{-\infty}^{\infty} dt \int d\underline{r} \left[\Phi_f^{*} \mathcal{L}_f \, \Phi_i \frac{\underline{x}}{x} \cdot \nabla_r \mathcal{L}_i' \right] . \qquad 1.102$$

This formula is exact. But the method does not take back-coupling into account and is therefore expected to be valid only at energies above 25keV. The calculated cross sections for $H^+ + H(1s) \to H(1s) + H^+$ are very close to those obtained with the impulse approximation at energies between 80 keV and 1 MeV, but between 40 and 80 keV the results are nearer to the calculations of McCarroll. The asymptotic form of this method at high energies is exactly that of the second Born approximation.

CHAPTER TWO

Review of Existing Calculations

2.1 The First Born Approximation

It was shown earlier that the Born approximation could be expressed as

$$T_{if}^{B+} = \langle \Phi_f | V_{13} + V_{23} | \Phi_i \rangle \,, \tag{2.1}$$

$$T_{if}^{B-} = \langle \Phi_f | V_{13} + V_{12} | \Phi_i \rangle \,. \tag{2.2}$$

Oppenheimer (1928) and Brinkman and Kramers (1930) argued that the internucleon potential V_{13} should not contribute to the probability of an electronic transition. This can be considered in the following way. At the energies the approximation may be valid (for incident protons the energy is much greater than 25keV) the relative velocity of the heavy incident and target nucleons is much greater than the orbital velocity of the electron. Any electron excitation or capture causes negligible change in the relative momentum of the nucleons, which therefore move in straight line trajectories. It is then evident that the potential V_{13} cannot affect the cross section. [This result might not be valid when there is a large contribution to the scattering amplitude from very close encounters (Fennema, 1963).]

The first detailed calculations for the process

$$H^+ + H(1s) \longrightarrow H(1s) + H^+ \tag{2.3}$$

were made by Brinkman and Kramers (1930). The first Born approximation was used, but the internucleon term V_{13} in it was neglected. We shall refer to the approximation when V_{13} is neglected as the Brinkman-Kramers approximation, and when V_{13} is retained as the Born approximation.

For the process (2.3) the Brinkman-Kramers cross section, in units of (πa_0^2), is given by

$$Q_{BK} = \frac{2^8}{5(1+v^2/4)^5 v^2}, \qquad 2.4$$

where v is the velocity of the incident proton in atomic units, so that the incident energy is $E = 24.97\ v^2$ keV. The cross sections for capture into excited states have been determined by Bates and McCarroll (1962).

Bransden, Dalgarno and King (1954) used the Brinkman-Kramers approximation to make the first calculations for the process

$$H^+ + He(1s^2) \longrightarrow H(nl) + He^+(1s). \qquad 2.5$$

The simple variational wave function for the belium atom,

$$\phi(\underline{r}_1, \underline{r}_2) = \frac{\alpha^3}{\pi} \exp\left\{-\alpha(r_1 + \underline{r}_2)\right\} \qquad \alpha = 1.6875, \qquad 2.6$$

is used, so that the post-prior descrepancy is present. Since it is impossible to know which interaction will give a better result, the prior interaction is used as it contains fewer terms than the post. Bransden, Dalgarno and King (1954) calculated $Q_{BK}(1s^2|n\ell,1s)$ $(n\ell=1s,2s,2p)$ and estimated $Q_B(1s^2|1s,1s)$, but the Born matrix was evaluted approximately to reduce the computational difficulties encountered. Comparison with the available experimental data up to 200 keV shows that Q_{BK} is too large and that Q_B agrees better with experiment.

It is expected on physical grounds that the internucleon potential V_{13} should not affect the probability of an electronic transition. However, Bates and Dalgarno (1952) and Jackson and Schiff (1953) independently argued that the neglect of the term V_{13} in the transition matrix element was unjustified. The initial and final wave functions Φ_i and Φ_f, respectively, are not eigenfunctions of the same Hamiltonian. There is thus a lack of orthogonality between Φ_i and Φ_f; this defect accounts for the large value of Q_{BK}. Since V_{13} is of the same magnitude but of opposite sign as the remaining potential term in T^B_{if}, the inclusion of V_{13} in the matrix element may correct the over estimate in the Brinkman-Kramers approximation.

Mapleton (1961a) has used the Born approximation to make extensive calculations on the process

$$H^+ + He(1s^2) \longrightarrow H(n\ell) + He^+(n'\ell') \qquad 2.7$$

in the energy range 7 keV to 1 MeV. He calculated the partial cross sections for capture into the 1s, 2s, 2p, 3s, 3p, or 3d states of hydrogen, leaving the residual heliumion in one of the 1.s, 2s, or 2p states. Since the inexact helium wave function (2.6) is used, different values are obtained for cross sections using the initial and final interactions. The post-prior discrepancy rises to a factor of almost 4 for $Q_B(1s^2|1s,2p)$ at 1 MeV, but it is not serious if the heliumion is left unexcited. Mapleton (1961) has also used the n^{-3} rule of Oppenheimer (1928) to evaluate the total cross section

$$Q_B(1s^2|\Sigma\,\Sigma) = \sum_{n\ell,n'\ell'} Q_B(1s^2|n\ell,n'\ell'), \qquad 2.8$$

and has found that the post-prior discrepancy for the total cross section never exceeds 20%.

The results of Mapleton (1961) for $Q_B(1s^2|1s,1s)$ are roughly 2.5 times larger than the values obtained by Bransden, Dalgarno and King (1954). In Figs. 1 and 2 , the mean of the post and prior total cross sections are compared with the experimental values of Stier and Barnett (1956), Barnett and Reynolds (1958), and Allison (1958). The agreement is generally good, but at high energies the theoretical curve falls too rapidly.

Another calculation for $Q_B(1s^2|1s,1s)$ was made by Mapleton (1963a), using now the Hylleraas six-parameter wave function for helium

$$\phi(\underline{r}_1,\underline{r}_2) = N\Big[1 + c_1|\underline{r}_1-\underline{r}_2| + c_2(r_1-r_2)^2 + c_3(r_1+r_2) + c_4(r_1+r_2)^2 + c_5|\underline{r}_1-\underline{r}_2|^2\Big]\exp\{-\alpha(r_1+\underline{r}_2)\}, \qquad 2.9$$

where C_i are variationally determined constants. It was pointed out by Bates and McCarroll (1962) that the simple variational helium wave function (2.6) underestimated the high momentum components and it was thought that the use of an improved wave function would provide more accurate results at high energies. In the new calculations of Mapleton (1963), the post-prior discrepancy is reduced to about 1%, but the final results are not in better agreement with experimental data. However, the Brinkman-Kramers cross section for the same process shows significant change at high energies. Although the old and new Q_{BK} agree within 4% at 1MeV, the new values of Q_{BK} at 10 MeV exceeds the old value by 47%.

Mapleton (1962) has also calculated the ratio $R = Q_B/Q_{BK}$, as a function of energy, for electron capture by protons in hydrogen and in helium. The ratio is roughly the same for both processes; for example, at 25 keV R(H) = 0.196 and R(He) = 0.128, while at 1MeV R(H) = 0.337 and R(He) = 0.271. Mapleton (1962) suggested that this similarity in the ratio could be maintained for electron capture from a more complex atom and that this relation could be used to estimate Q_B from Q_{BK}.

The high energy behaviour of the Born approximation for the electron capture by protons in hydrogen has been investigated by Jackson and Schiff (1953) and Mapleton (1964a). Both Q_B and Q_{BK} have the velocity dependence V^{-12}, and

$$Q_B \sim 0.661\, Q_{BK}. \qquad 2.10$$

This V^{-12} dependence comes from the contribution to the cross section of scattering in forward direction. There is also the contribution of scattering in the backward direction; this has the asymptotic form V^{-6} and is ultimately the dominant contribution.

In the capture process in the forward direction, the electron is 'picked up' by the incident proton, which is essentially undeflected. On the other hand, capture in the backward direction occurs when the incident proton makes a violent collision with the target proton, ejecting it from the atom and taking its place.

Mapleton (1964b) has investigated the asymptotic forms of the cross sections in the Born approximation and the distorted wave method for the resonance process $H^+ + H(1s) \rightarrow H(1s) + H^+$. If the protons are considered distinguishable, both methods give the V^{-6} dependence; but if the protons are considered indistinguishable, the cross section is not defined, because the contribution in the backward direction interferes with the direct scattering amplitude. These features have also been found in the impulse approximation (Coleman and McDowell,1964).

For nonresonant capture the situation is different; there is no significant contribution from the backward direction, and the Born cross section behaves ultimately as V^{-12}. Thus, in the electron capture by protons in helium, both the Born approximation and the distorted wave method are found to have the same asymptotic form as the Brinkman-Kramers approximation (Mapleton, 1964b).

2.2. The Second Born Approximation.

The large unphysical contribution from the internucleon term in the first Born approximation shows that this approximation is unsatisfactory and that the apparent agreement with experiment may be coincidental. It is important then to consider also the higher terms in the Born series. Unfortunately, these terms are difficult to evaluate; so far it is impossible to calculate even the second term in the series. However, Drisko (1955) has examined the high energy behaviour of the second Born approximation, in which the first two terms in the series are retained, for the process

$$H^+ + H(1s) \longrightarrow H(1s) + H^+ . \qquad 2.11$$

From (1.29) and (1.42), the second Born approximation can be written as

$$T_{if}^{B_2} = \langle \Phi_f | V_f + V_f G_0 V_i | \Phi_i \rangle , \qquad 2.12$$

where G_0 is the free particle Greens function.

Let ϵ_f be the energy of the bound system (1 + 2) in the ground state H(1s), $\underline{x}$ the position vector of 2 relative to 3, and $\underline{s}$ of 2 relative to 1. If M is the mass of proton and 1 of electron, we set

$$\mu = \frac{M(1+M)}{1+2M} , \quad a = \frac{M}{1+M} ,$$
$$\underline{\alpha} = \underline{k}_f - a\underline{k}_i , \quad \underline{\beta} = \underline{k}_i - a\underline{k}_f . \qquad 2.13$$

We define the Fourier transforms

$$g_i(\underline{k}) = \int e^{i\underline{k}\cdot\underline{x}}\,\phi_i(\underline{x})\,d\underline{x},$$
$$g_f(\underline{k}) = \int e^{-i\underline{k}\cdot\underline{s}}\,\phi_f^{*}(\underline{s})\,d\underline{s}\,. \qquad 2.14$$

G_o can be represented explicitly as

$$G_o = (2\pi)^{-6}\int d\underline{q}\,d\underline{q}'\;\frac{\exp i\{\underline{q}'\cdot(\underline{\rho}-\underline{\rho}')+\underline{q}\cdot(\underline{s}-\underline{s}')\}}{-k^2/2\mu+\epsilon_f+i\varepsilon-q^2/2a-q'^2/2\mu} \qquad 2.15$$

$$= (2\pi)^{-6}\int d\underline{q}\,d\underline{k}\;\frac{\exp i\{(\underline{k}_f-\underline{k})\cdot(\underline{\rho}-\underline{\rho}')+\underline{q}\cdot(\underline{s}-\underline{s}')\}}{-k^2/2\mu+\epsilon_f+i\varepsilon+(\underline{\beta}+\frac{1}{a}\underline{\alpha})\cdot\underline{k}-q^2/2a} \qquad 2.16$$

where $\underline{q}' = \underline{k}_f - \underline{k}$

Using (2.12) and (2.14), we find

$$\langle\Phi_f|\,V_f\,G_oV_i\,|\Phi_i\rangle$$
$$= 4\cdot(2\pi)^{-4}\int d\underline{q}\,d\underline{k}\left[-\frac{k^2}{2\mu}+\epsilon_f+\left(\underline{\beta}+\frac{1}{a}\underline{\alpha}\right)\cdot\underline{k}-\frac{q^2}{2a}+i\varepsilon\right]^{-1} I(\underline{q},\underline{k}), \qquad 2.17$$

where

$$I(\underline{q},\underline{k}) = \mathfrak{g}(V_{13},V_{12})+\mathfrak{g}(V_{13},V_{13})+\mathfrak{g}(V_{23},V_{12})+\mathfrak{g}(V_{23},V_{13}), \qquad 2.18$$

with

$$\mathfrak{g}(V_{13},V_{12}) = k^{-2}(a\underline{k}+\underline{\beta}+\underline{q})^{-2}\,g_i(\underline{k}-\underline{\alpha})\,g_f(-a\underline{k}-\underline{q}), \qquad 2.19$$

$$\mathfrak{g}(V_{13},V_{13}) = -k^{-2}(a\underline{k}+\underline{\beta}+\underline{q})^{-2}\,g_i\left(\tfrac{1}{1+M}\underline{k}-\underline{q}-\underline{\alpha}-\underline{\beta}\right)g_f(-a\underline{k}-\underline{q}), \qquad 2.20$$

$$\mathfrak{g}(V_{23},V_{12}) = k^{-2}(a\underline{k}+\underline{\beta}+\underline{q})^{-2}\,g_i\left(\tfrac{1}{1+M}\underline{k}-\underline{q}-\underline{\alpha}-\underline{\beta}\right)g_f\left(\tfrac{1}{1+M}\underline{k}-\underline{q}\right), \qquad 2.21$$

$$\mathfrak{g}(V_{23},V_{13}) = -k^{-2}(a\underline{k}+\underline{\beta}+\underline{q})^{-2}\,g_i(\underline{k}-\underline{\alpha})\,g_f\left(\frac{1}{1+M}\underline{k}-\underline{q}\right). \qquad 2.22$$

The term $g\,(V_{13}, V_{12})$ has a maximum at $\underline{k} = \underline{\alpha}$ and $\underline{q} = \frac{1}{1+M}\,\underline{k}$, so that at high energies we find

$$g(V_{13}, V_{12}) \simeq -\frac{1}{\alpha^2(\underline{\alpha}+\underline{\beta})^2}\, g_i(\underline{k}-\underline{\alpha})\, g_f(-a\underline{k}-\underline{q}), \qquad 2.23$$

$$\langle \Phi_f | V_{13} G_0 V_{12} | \Phi_i \rangle \simeq -\frac{32}{\alpha^2(\underline{\alpha}+\underline{\beta})^4}\,. \qquad 2.24$$

Similarly, we obtain

$$\langle \Phi_f | V_{23} G_0 V_{13} | \Phi_i \rangle \simeq -\frac{32}{\alpha^2(\underline{\alpha}+\underline{\beta})^4}, \qquad 2.25$$

$$\langle \Phi_f | V_{13} | \Phi_i \rangle \simeq \frac{64}{\alpha^2(\underline{\alpha}+\underline{\beta})^4}, \qquad 2.26$$

so that in the high energy limit

$$\langle \Phi_f | V_{13} + V_{13} G_0 V_{12} + V_{23} G_0 V_{13} | \Phi_i \rangle = 0\,. \qquad 2.27$$

Drisko also shows that the term which describes the internucleon interaction twice, $(V_{13}\ G_0\ V_{13})$, decreases faster than the Brinkman- Kramers term and the term corresponding to a double scattering of the electron, first by V_{23} and then by V_{13}. At sufficiently high energies, the last term in (2.27) is given by

$$\langle \Phi_f | V_{23} G_0 V_{12} | \Phi_i \rangle \simeq \frac{16\pi}{\alpha^2(v^2/2-\alpha^2/2+i4v)}\,. \qquad 2.28$$

In the high velocity limit, the second Born approximation becomes

$$Q^{B_2} \sim \frac{1}{4\pi v^2}\int_{-v^2/4}^{\infty}\left[-\frac{32\pi}{(1+\alpha^2)^3}+\frac{16\pi}{\alpha^2(v^2/2-\alpha^2/2+i4v)}\right]^2 d(\alpha^2) \qquad 2.29$$

$$= \left\{0{\cdot}2946 + \frac{5\pi v}{2^{12}}\right\} Q_{BK}\,. \qquad 2.30$$

Drisko (1955) estimated that the inclusion of the third term in the Born series would give

$$Q^{B_3} \sim \left\{ 0\cdot 319 + \frac{5\pi v}{2^{12}} \right\} Q_{BK} \,. \qquad 2.31$$

2.3 The Impulse Approximation.

Pradhan (1957) first showed that the impulse approximation would be very useful for treating the charge transfer in fast atomic collisions. He considered the process

$$H^{+} + H(1s) \longrightarrow H(1s) + H^{+} \qquad 2.32$$

and found the initial and final wave functions to be orthogonal to each other in the limit $m_e/M_p = 0$, thus showing the cross section to be independent of the internucleon potential.

Detailed calculations on the same process have since also been made by McDowell (1961), Cheshire (1963a), and Pradhan and Tripathy (1963).

In the impulse approximation, the scattering amplitude may be written in either of the forms (Pradhan, 1957; McDowell, 1961)

$$T_{if}^{I} = \langle \Phi_f | V_f | \omega_{12}^{+} \Phi_i \rangle \,, \qquad 2.33$$

$$T_{if}^{II} = \langle \omega_{23}^{-} \Phi_f | V_i | \Phi_i \rangle \,. \qquad 2.34$$

Pradhan (1957) and Pradhan and Tripathy (1963) calculated T_{if}^{I} by replacing V_f with the incorrect V_{12}, so that the matrix element now involves a double scattering by the incident proton. McDowell (1961) used the correct form of V_f in T^{I}_{if} but, to ease the numerical computations, he used an approximation in the momentum distribution of the unperturbed hydrogen atom.

Let the position andmomentum vectors appropriate to the final configuration be denoted by ($\underline{s}$, $\underline{\rho}$, $\underline{k}_s$, $\underline{k}_f$), as defined in section (1.2). The wave function which describes the unperturbed initial state of the system in momentum space is

$$\langle \underline{k}_s, \underline{k}_f | \Phi_i \rangle = (2\pi)^{-3} \int d\underline{s}\, d\underline{\rho}\, \Phi_i \exp\{-i(\underline{k}_s \cdot \underline{s} + \underline{k}_f \cdot \underline{\rho})\} \cdot \qquad 2.35$$

On using (1.4), we find

$$\langle \underline{k}_s, \underline{k}_f | \Phi_i \rangle = (2\pi)^{-3} \int d\underline{s}\, d\underline{\rho}\; \phi_i(\underline{x}) \exp\{-i(\underline{k}_s \cdot \underline{s} + \underline{k}_f \cdot \underline{\rho} - \underline{k}_i \cdot \underline{r})\}$$

$$= \delta(\underline{k}_s - a\underline{k}_f + \underline{k}_i)(2\pi)^{3/2} g_i\left((a - \tfrac{1}{a})\underline{k}_i - \tfrac{1}{a}\underline{k}_s\right)$$

$$= (2\pi)^{3/2} \delta(\underline{k}_s - a\underline{k}_f + \underline{k}_i) g_i\left(\underline{\alpha} + \tfrac{1}{a}(\underline{k}_s + \underline{\beta})\right), \qquad 2.36$$

where

$$g_i(\underline{k}) = (2\pi)^{-3/2} \int d\underline{x}\; \phi_i(\underline{x}) e^{i\underline{k} \cdot \underline{x}}. \qquad 2.37$$

To find $\omega^{+}_{12} \Phi_i$ we insert a complete set of plane waves between ω^{+}_{12} and Φ_i , so that

$$\omega^{+}_{12} \Phi_i = \int \omega^{+}_{12} | \underline{k}_s, \underline{k}_f \rangle \langle \underline{k}_s, \underline{k}_f | \Phi_i \rangle\, d\underline{k}_s\, d\underline{k}_f$$

$$= (2\pi)^{-3} \int e^{i\underline{k}_f \cdot \underline{\rho}}\, \psi_{\underline{k}_s}(\underline{s}) \langle \underline{k}_s, \underline{k}_f | \Phi_i \rangle\, d\underline{k}_s\, d\underline{k}_f \cdot \qquad 2.38$$

On using (2.36) and (2.38), we obtain

$$\omega_{12}^{+}\Phi_i = (2\pi)^{-3/2}\int\delta(\underline{k}_s - a\underline{k}_f + \underline{k}_i)e^{i\underline{k}_f\cdot\underline{\rho}}\psi_{\underline{k}_s}(\underline{s})\,g_i\left(\underline{\alpha}+\frac{1}{a}(\underline{k}_s+\underline{\beta})\right)d\underline{k}_s\,d\underline{k}_f$$

$$= (2\pi)^{-3/2}e^{i\frac{1}{a}\underline{k}_i\cdot\underline{\rho}}\int d\underline{k}\,e^{i\frac{1}{a}\underline{k}\cdot\underline{\rho}}\psi_{\underline{k}}^{+}(\underline{s})\,g_i\left(\underline{\alpha}+\frac{1}{a}(\underline{k}+\underline{\beta})\right), \qquad 2.39$$

where $\psi_{\underline{k}}(\underline{s})$ is the Coulomb function

$$\psi_{\underline{k}}(\underline{s}) = e^{-\pi\nu/2}\Gamma(1+i\nu)e^{i\underline{k}\cdot\underline{s}}\,{}_1F_1(-i\nu;1;iks - i\underline{k}\cdot\underline{s}), \qquad 2.40$$

with

$$\nu = -a/k\,. \qquad 2.41$$

From (2.33) we find

$$T_{if}^{I} = (2\pi)^{-3/2}a^{-3}\int d\underline{k}\,d\underline{s}\,d\underline{\rho}\,e^{-i\underline{k}_f\cdot\underline{\rho}}\phi_f(\underline{s})V_f\,e^{i\frac{1}{a}(\underline{k}_i+\underline{k})\cdot\underline{\rho}}\psi_{\underline{k}}(\underline{s})$$

$$\times\, g_i\left(\underline{\alpha}+\frac{1}{a}(\underline{k}+\underline{\beta})\right), \qquad 2.42$$

where $$V_f = |\underline{\rho} - (1-a)\underline{s}|^{-1} - |\underline{\rho} + a\underline{s}|^{-1}. \qquad 2.43$$

After integrating over $\underline{s}$ amd $\underline{\rho}$, we have

$$T_{if}^{I} = \sqrt{\frac{2}{\pi}}\cdot\frac{1}{a}\int d\underline{k}\,\frac{g_i\left(\underline{\alpha}+\frac{1}{a}(\underline{k}+\underline{\beta})\right)}{(\underline{k}+\underline{\beta})^2}\cdot\left[\mathfrak{g}_f\left(\underline{k};\frac{1}{M}(\underline{k}+\underline{\beta})\right) - \mathfrak{g}_f(\underline{k},-\underline{k}-\underline{\beta})\right], \qquad 2.44$$

where $$\mathfrak{g}_f(\underline{k},\underline{\Lambda}) = \int\phi_f^{*}(\underline{s})\,\psi_{\underline{k}}(\underline{s})\,e^{i\underline{\Lambda}\cdot\underline{s}}\,d\underline{s}\,. \qquad 2.45$$

The first term in the bracket of (2.44) comes from the internucleon potential V_{13}. In the limit $\frac{1}{M} = 0$ it vanishes since $\mathfrak{g}(\underline{k},o) = 0$, as $\phi_f(\underline{s})$ and $\psi_{\underline{k}}(\underline{s})$ are different eigenfunctions of the same Hamiltonian (Pradhan, 1957).

The high velocity limit of the impulse approximation has been investigated by Bransden and Cheshire (1963), who considered for simplicity the process $H^+ + H(1s) \rightarrow H(1s) + H^+$. Since $\frac{1}{M_p} \rightarrow 0$,

$$T_{if}^{I}(1s,1s) = -\sqrt{\frac{2}{\pi}} \cdot \frac{i}{a} \int d\underline{k}\, \frac{g_{1s}\left(\underline{\alpha} + \frac{1}{a}(\underline{k}+\underline{\beta})\right)}{(\underline{k}+\underline{\beta})^2}\, \mathscr{g}_{1s}(\underline{k}, -\underline{k}-\underline{\beta}). \qquad 2.46$$

$\mathscr{g}_{1s}(\underline{k},-\underline{k}-\underline{\beta})$ is a slowly varying function while $g_{1s}\left(\underline{\alpha} + \frac{1}{a}(\underline{k} + \underline{\beta})\right)$ is strongly peaked about $\underline{k} = -(\underline{\beta} + a\underline{\alpha}) = a\underline{v}$, so that at high velocities

$$T_{if}^{I} \simeq -\sqrt{\frac{2}{\pi}} \cdot \frac{i}{a}\, \mathscr{g}(a\underline{v}, a\underline{\alpha}) \int d\underline{k}\, \frac{g_{1s}\left(\underline{\alpha} + \frac{1}{a}(\underline{k}+\underline{\beta})\right)}{(\underline{k}+\underline{\beta})^2}. \qquad 2.47$$

After integrating over $\underline{k}$ and taking the limit $\frac{1}{M_p} \rightarrow 0$, we find

$$T_{if}^{I} \sim -4\sqrt{\pi}\, \mathscr{g}(\underline{v}, \underline{\alpha})\, (1+\alpha^2)^{-1}, \qquad 2.48$$

so that the cross section in the high velocity limit is given by

$$Q_i^{I}(1s,1s) \sim \left(0{\cdot}2946 + \frac{5\pi v}{2^{11}}\right) Q_B(1s,1s). \qquad 2.49$$

This is similar to the high energy behaviour of the second Born approximation. However, in (2.49) the second term, which ultimately dominates the cross section, is larger by a factor 2.

Bransden and Cheshire (1963) have applied the impulse approximation to the process

$$H^+ + He(1s^2) \longrightarrow H(1s) + He^+(1s). \qquad 2.50$$

The simple variational wave function of (2.6) for the helium atom is used.

Let 1, 3, 2, and 4 denote the incident proton, the helium nucleus, the captured electron, and the passive electron, respectively. The transition matrix for the capture of the electron 2 from an initial state i to a final state f can be written as

$$ {}^{I}T^{+}_{if} = \langle \Phi_f | V_{13}+V_{23}+V_{14}+V_{24} | (\omega^{+}_{13}+\omega^{+}_{12}+\omega^{+}_{14}-2)\Phi_i \rangle \; , \qquad 2.51 $$

$$ {}^{I}T^{-}_{if} = \langle \Phi_f (\omega^{-}_{13}+\omega^{-}_{23}+\omega^{-}_{14}+\omega^{-}_{24}-3) | V_{12}+V_{13}+V_{14} | \Phi_i \rangle \, . \qquad 2.52 $$

The interaction between the proton and the helium nucleus is expected to have a negligible effect on the transition probability, so that we can set $\omega^{\pm}_{13} = 1$. The interaction between the proton and the passive electron 4 is also expected to be unimportant and we write $\omega^{\pm}_{14} = 1$. The equation (2.51) then becomes

$$ {}^{I}T^{+}_{if} = \langle \Phi_f | V_{13}+V_{23}+V_{14}+V_{24} | \omega^{+}_{13}\Phi_i \rangle \, . \qquad 2.53 $$

In the matrix element ${}^{I}T^{-}_{if}$ of (2.52) the operator ω^{-}_{34} describes the distortion of the wave function by the electron-electron interaction. This term is difficult to evaluate, but an approximate value of ${}^{I}T^{-}_{if}$ is obtained by setting $\omega^{-}_{24} = 1$ and modifying the remaining term ω^{-}_{23} such that $\omega^{-}_{23}\, X_{\underline{k}}\,(23)$ is the scattering function for the captured electron in a 'screened'

Coulomb field of charge Z = 1.6875, instead of Z = 2. The matrix element ${}^{I}T^{-}_{if}$ is then

$$ {}^{I}T^{-}_{if} = {}^{I}T^{-}_{if}(Z = 1\cdot6875) = \langle \Phi_f \omega^{-}_{23} | V_{12} + V_{13} + V_{14} | \Phi_i \rangle . \qquad 2.54 $$

The momentum transfer of the passive electron 4 is neglected, so that the initial and final unperturbed wave functions are

$$ \begin{aligned} \Phi_i &= \psi_i(\underline{x}, \underline{t})\, e^{i \underline{k}_i \cdot \underline{\sigma}} , \\ \Phi_f &= \chi_f(\underline{t})\, \phi_f(\underline{s})\, e^{i \underline{k}_f \cdot \underline{\rho}} , \end{aligned} \qquad 2.55 $$

where $\psi_i(\underline{x},\underline{t})$ is the ground state helium wave function, $\phi_f(\underline{s})$ the hydrogen ground state function, and $X_f(\underline{t})$ the ground state function of the helium ion. The neglect of the momentum transfer of the passive electron simplifies considerably the evaluation of the matrix elements and was used previously by Bransden, Dalgarno and King (1954). To check the error introduced in the calculation of ${}^{I}Q_{1s}(1s^2|1s,1s)$ by this approximation, Bransden and Cheshire (1963) evaluated $Q^{B}_{if}(1s^2|1s,1s)$ using the approximation and compared them with the results of Mapleton (1961a), who did not use this approximation. The agreement is better than 2% above 100 keV.

The cross section ${}^{I}Q(1s^2|1s,1s)$ is calculated from both ${}^{I}T^{+}_{if}$ and ${}^{I}T^{-}_{if}$. However, the term from ω^{-}_{34} is difficult to evaluate exactly, so that the results obtained from ${}^{I}T^{-}_{if}$ are not considered to be reliable and below 400 keV the post-prior discrepancy is serious.

In Figs 1 and 2 the results of ${}^{I}Q^{+}(1s^2|\Sigma,\Sigma)$, which includes a correction for capture into excited states, are compared with the experimental measurements and with the Born approximation calculations of Mapleton (1961a). The agreement is good in the range 50 keV to 700 keV, but above this energy both $Q^{B}(1s^2|\Sigma,\Sigma)$ and ${}^{I}Q^{+}(1s^2|\Sigma,\Sigma)$ seem to be too small.

Although the Born and the impulse approximations give very similar total cross sections, they do not predict the same angular distributions. Both show strong peaks in the forward direction. But in the Born approximation the distribution has a large angle tail; this is unphysical and comes entirely from the internucleon potential.

Another unsatisfactory feature of the Born approximation is that as the impact parameter tends to zero the probabality of capture diverges and violates unitarity badly, (Schiff, 1954). Bransden and Cheshire (1963) evaluated the probability at 70.3 keV and 703 keV, using the impulse approximation, and found that it never exceeded unity.

The impulse approximation describes the capture process fairly well at high energies. It fails at low energies because it does not take into account 'back-coupling' from the initial to the final states and so violates unitary.

2.4 The Impact Parameter Method.

McCarroll (1961) has used the two-state approximation in the impact parameter formatism to evaluate the cross section for the process

$$H^{+} + H(1s) \rightarrow H(1s) + H^{+} \qquad 2.56$$

in the energy range 0.1 keV to 1 MeV. This work has been extended to capture into the 2s and 2p states by McElroy (1963). The results confirm that above 25 keV back-coupling is not important, but at low energies it greatly reduces the cross section and , if neglected, the calculated probability of charge transfer may exceed unity.

Distortion has no effect on the symmetrical resonance process (2.56), as was pointed out in section (1.5), but it is expected to be important for an asymmetrical reaction. The calculations of McCarroll and McElroy (1962) on

$$H(1s) + He^{2+} \rightarrow H^{+} + He^{+}(1s) \qquad 2.57$$

show that distortion increases the cross section considerably at moderate energies, because the Coulomb repulsion reduces the separation between the initial and final potential surfaces. It has an extremely marked effect for capture into excited states over the energy range 25 to 80 keV (McElroy, 1963). For the process

$$H(1s) + He^{2+} \rightarrow H^{+} + He^{+}(2s, 2p) , \qquad 2.58$$

if allowance is made for distortion the cross section tends to zero as the energy of relative motion is decreased indefinitely, but if no allowance is made the cross section tends to infinity.

Lovell and McElroy (1965) have formulated a four - state approximation for the collision process between the proton and hydrogen atom. The method consists in retaining four terms in the expansion of Ψ in (1.60). Their calculations over the range 1 to 50 keV show that the two - state approximation is accurate for capture into the ground state over this energy region, but unsatisfactory for the capture into the 2s state at energies below 25 keV, when the extra channels represented in the wave function become important. It would seem from these results that, under the conditions when the (2s) hydrogen states are important, the (2p) states would also be important, requiring a six - state approximation.

Recently, Wilets and Gallaher (1966) have made calculations on the $H^+ + H$ scattering, using an expansion which includes 1s, 2s, and 2p states, and in some calculations 3s and 3p states. The results for excitation and for capture into the 2p state are smaller by a factor of 2 than the experimental data. The inclusion of the 3s and 3p states does not change the 1s and 2p cross sections, but the 2s cross sections are affected, particularly at 9 keV.

The two - state Bates approximation is used by Green, Stanley and Chiang (1965) for calculations on the process

$$H^+ + He(1s^2) \longrightarrow H(1s) + He^+(1s). \qquad 2.59$$

The helium wave function employed is of the open shell type (Eckart, 1930),

$$\psi(r_1, r_2) = N\left[\exp\left(-\alpha r_1 - \beta r_2\right) + \exp\left(-\alpha r_2 - \beta r_1\right)\right] \qquad 2.60$$

where α and β are variationally determined constants. Since this wave function is approximate, to satisfy detailed balancing the equations corresponding to (1.72) and (1.73) are derived by requiring that the internal helium wave function satisfies only the expression

$$\langle \psi(r_1, r_2) | H(He) - \varepsilon | \psi(r_1, r_2) \rangle = 0 , \qquad 2.61$$

where H is the Hamiltonian of the helium atom and ε the variationally determined energy for this wave function.

The calculations of Green, Stanley and Chiang (1965) are given in Table 1. The results confirm that distortion and back-coupling are very important below 30 keV and that the cross section becomes increasingly sensitive to distortion as the energy is decreased. In Table 2 the calculated cross section is compared with the experimental measurement, which includes capture into excited states and excitation and so is expected [on the basis of the Born approximation calculations of Mapleton (1961a)] to be about 15 - 20% above the calculated values. Comparison shows that the calculated cross section is, in fact, roughly equal to the experimental value over the energy range 15 to 100 keV. Above 100 keV the calculated cross section is clearly too large; at 400 keV it is nearly twice the experimental measurement. On the low energy side of the cross section maximum (at about 25 keV), the agreement with experiment is poor; the theoretical cross section is too large by about 50% at 6.25 keV, and too small by a factor of 14 at 1 keV.

CHAPTER THREE

3 Present Calculations.

Introduction.

The impact parameter method is used for calculations on the electron capture by protons in helium. The first part deals with the capture into the ground state and with the sensitivity of the calculated cross section with the choice of the helium wave function. This is followed by an investigation using the coupling of the 1s, 2s, and 2p states of hydrogen.

3.1 The Two-State Approximation.

We consider the process

$$H^+ + He(1s^2) \longrightarrow H(1s) + He^+(1s). \qquad 3.1$$

The relative velocity $\underline{v}$ between the proton and the nucleus of the helium atom is assumed to remain constant during the collision. This condition is satisfied unless $\underline{v}$ is extremely low. Bates and Boyd (1962b) have used the actual classical orbit of the projectile in the short range field presented by the neutral target system to calculate the effect of departure from rectilinear motion on cross sections determined within first-order approximations. The effect is found to be negligible at energies above a few electron volts.

Let $\underline{R}$ be the postition vector of the incident proton p relative to the nucleus n of the helium atom. We choose a co-ordinate system with the z-axis along the direction of motion, so that

$$\underline{R} = \underline{\rho} + \underline{v}t \quad , \quad z = vt \quad , \qquad 3.2$$

where ρ is the impact parameter and the time t is chosen such that at $t = 0$ p and n are at their closest distance of approach. The origin 0 is chosen to be at the mid-point of $\underline{R}$. Let $\underline{r}_i$, $\underline{r}_{pi}$, and $\underline{r}_{ni}$ denote the position vectors of the electron i relative to 0, p, and n, respectively.

We consider the electron 1 to be captured and the electron 2 as 'passive' during the collision. The two-state approximation for the electronic wave function of the system is then given by

$$\Psi(\underline{r}_1, \underline{r}_2, t) = a_0(t)\Psi_0(\underline{r}_1, \underline{r}_2, t) + a_1(t)\Psi_1(\underline{r}_1, \underline{r}_2, t), \qquad 3.3$$

where a_0 (t) and a_1 (t) are time-dependent coefficients corresponding to the initial and final states Ψ_0 and Ψ_1. If ϕ_1 $(\underline{r}_{p1})$ is the wave function and η_1 the binding energy of H(1s), $\psi(\underline{r}_{p2})$ and μ_0 of He$^+$ (1s), and $X(\underline{r}_{n1}, \underline{r}_{n2})$ and ε_0 of He (1s^2), we write

$$\Psi_0(\underline{r}_1, \underline{r}_2, t) = X(\underline{r}_{n1}, \underline{r}_{n2}) \exp\left[-i\left\{\varepsilon_0 t + v^2 t + \tfrac{1}{2}\underline{v}\cdot(\underline{r}_1 + \underline{r}_2)\right\}\right], \qquad 3.4$$

$$\Psi_1(\underline{r}_1, \underline{r}_2, t) = \phi_1(\underline{r}_{p1})\psi(\underline{r}_{n2}) \exp\left[-i\left\{(\eta_1 + \mu_0)t + v^2 t + \tfrac{1}{2}\underline{v}\cdot(-\underline{r}_1 + \underline{r}_2)\right\}\right]. \qquad 3.5$$

The inclusion on the right-hand sides of (3.4) and (3.5) of the terms containing the velocity $\underline{v}$ allows for the translational motion of the electron, according to the nucleus it is attached in the limit of infinite internucleon separation (Bates and McCarroll, 1958).

The total Hamiltonian of the electronic system is

$$H = -\frac{1}{2}\nabla^2_{r_1} - \frac{1}{2}\nabla^2_{r_2} + V_{p1} + V_{p2} + V_{n1} + V_{n2} + V_{12}, \qquad 3.6$$

where the kinetic energy operators are given by

$$\nabla^2_{r_1} = \nabla^2_{r_{n1}} + \nabla_{r_{n1}}\cdot\nabla_R + \frac{1}{4}\nabla^2_R = \nabla^2_{r_{p1}} - \nabla_{r_{p1}}\cdot\nabla_R + \frac{1}{4}\nabla^2_R, \qquad 3.7$$

$$\nabla^2_{r_2} = \nabla^2_{r_{n2}} + \nabla_{r_{n2}}\cdot\nabla_R + \frac{1}{4}\nabla^2_R, \qquad 3.8$$

V_{pi} and V_{ni} are the interactions on the electron i by p and n, respectively, and V_{12} is the electron-electron interaction.

The wave functions $\phi_1(\underline{r}_{p1})$ and $\psi(\underline{r}_{n2})$ satisfy the equations

$$\left(-\frac{1}{2}\nabla^2_{r_{p1}} + V_{p1} - \eta_0\right)\phi_1(\underline{r}_{p1}) = 0, \qquad 3.9a$$

$$\left(-\frac{1}{2}\nabla^2_{r_{n2}} + V_{n2} - \mu_1\right)\psi(\underline{r}_{n2}) = 0. \qquad 3.9b$$

As $\chi(\underline{r}_{n1}, \underline{r}_{n2})$ may not be an exact wave function for He(1s^2) we use the condition

$$\int \chi(\underline{r}_{n1},\underline{r}_{n2})\left[-\frac{1}{2}\nabla^2_{r_{n1}} - \frac{1}{2}\nabla^2_{r_{n2}} + V_{n1} + V_{n2} + V_{12} - \epsilon_0\right]\chi(\underline{r}_{n1},\underline{r}_{n2})\,d\tau = 0, \qquad 3.10$$

where ε_0 is determined variationally.

The time-dependent Schrödinger equation is

$$H\,\Psi(\underline{r}_1,\underline{r}_2,t) = i\frac{\partial}{\partial t}\,\Psi(\underline{r}_1,\underline{r}_2,t). \qquad 3.11$$

The equations corresponding to (1.64) are

$$\begin{aligned}
&\varepsilon_{01} = -\varepsilon_{10} = \varepsilon_0-\mu_0-\eta_1,\\
&S_{01}(t)=S_{10}^{*}(t) = \int \chi^{*}(\underline{r}_{n1},\underline{r}_{n2})\,\phi_1(\underline{r}_{p1})\psi(\underline{r}_{n2})\,e^{i\underline{v}\cdot\underline{r}_1}e^{i\varepsilon_{01}t}\,d\underline{r}_1 d\underline{r}_2,\\
&A_{00}(t) = \int \chi^{*}(\underline{r}_{n1},\underline{r}_{n2})\left[V_{p1}+V_{p2}\right]\chi(\underline{r}_{n1},\underline{r}_{n2})\,d\underline{r}_1 d\underline{r}_2,\\
&B_{11}(t) = \int \phi_1^{*}(\underline{r}_{p1})\psi^{*}(\underline{r}_{n2})\left[V_{p2}+V_{n1}+V_{12}\right]\phi_1(\underline{r}_{p1})\psi(\underline{r}_{n2})\,d\underline{r}_1 d\underline{r}_2,\\
&K_{01}(t) = \int e^{i\underline{v}\cdot\underline{r}_1}e^{i\varepsilon_{01}t}\chi^{*}(\underline{r}_{n1},\underline{r}_{n2})\left[V_{p2}+V_{n1}+V_{12}\right]\\
&\qquad\qquad\times\,\phi_1(\underline{r}_{p1})\psi(\underline{r}_{n2})\,d\underline{r}_1 d\underline{r}_2, \qquad\qquad 3.12\\
&K_{10}(t) = \int e^{-i\underline{v}\cdot\underline{r}_1}e^{i\varepsilon_{10}t}\phi_1^{*}(\underline{r}_{p1})\psi^{*}(\underline{r}_{n2})\\
&\qquad\qquad\times\left[-\tfrac{1}{2}\nabla^2_{r_{n1}}-\tfrac{1}{2}\nabla^2_{r_{n2}}+V_{p1}+V_{p2}+V_{n1}+V_{n2}+V_{12}-\varepsilon_0\right]\chi(\underline{r}_{n1},\underline{r}_{n2})\,d\underline{r}_1 d\underline{r}_2.
\end{aligned}$$

We write

$$\alpha_0 = \frac{A_{00}-S_{01}K_{10}}{1-|S_{01}|^2}, \qquad \alpha_1 = \frac{B_{11}-S_{10}K_{01}}{1-|S_{01}|^2}, \qquad 3.13$$

$$\delta_{01} = \int_{-\infty}^{\infty}(\alpha_0-\alpha_1)\,dt, \qquad 3.14$$

so that the equations corresponding to (1.64) and (1.65) are

$${}^{\circ}\dot{a}_0 = -i\,{}^{\circ}a_1\left[\frac{K_{01}-S_{01}B_{11}}{1-|S_{01}|^2}\right]\exp\left[i(\varepsilon_{01}+\delta_{01})\right], \qquad 3.15$$

$${}^{\circ}\dot{a}_1 = -i\,{}^{\circ}a_0\left[\frac{K_{10}-S_{10}A_{00}}{1-|S_{01}|^2}\right]\exp\left[-i(\varepsilon_{01}+\delta_{01})\right]. \qquad 3.16$$

The coefficients a_o (t) and a_1 (t) are time-dependent and have the initial conditions

$$a_0(-\infty) = 1 \quad , \quad a_1(-\infty) = 0 . \qquad 317$$

The cross section for the capture of the first electron is

$$\sigma = 2\int |a_1(+\infty)|^2 \rho \, d\rho \, , \qquad 3.18$$

so that the coupled equations (3.15) and (3.16) must be solved to evaluate a_1 $(+\infty)$.

The wave functions ϕ_1 $(\underline{r}_{p1})$ and $\psi(\underline{r}_{n2})$ are given explicitly as

$$\phi_1(\underline{r}) = \frac{1}{\pi} e^{-r} \, , \ \eta_1 = -\frac{1}{2} \, , \qquad 3.19$$

$$\psi(\underline{r}) = \sqrt{\frac{8}{\pi}} e^{-2r} \, , \ \mu_0 = -2 \, . \qquad 3.20$$

It is difficult to obtain an exact helium ground-state wave function because of the electron-electron interaction. We have mentioned earlier the suggestion that the use of an improved wave function than the simple variational function (2.5) might give more accurate results. Accordingly, the calculations are performed by using three approximate ground-state helium wave functions :

1. The simple variational function

$$\chi^{(1)} = \frac{N}{\pi} \exp\{-\alpha(r_1 + r_2)\} \, ,$$

$$\alpha = 1\cdot6875 \, , N = \alpha^3 \, , \varepsilon_0 = -2\cdot8475 \, ; \qquad 3.21$$

2. The separable three-parameter function of Green et al. (1954)

$$\chi^{(2)} = \frac{N}{\pi}\left[\exp(-\alpha r_1) + c\exp(-\beta r_1)\right]\left[\exp(-\alpha r_2) + c\exp(-\beta r_2)\right],$$

$$\alpha = 1{\cdot}455\,799\ ,\ \beta = 2\alpha\ ,\ c = 0{\cdot}6\ , \qquad 3.22$$

$$N = \left[2\left\{\frac{1}{\alpha^3\beta^3} + \frac{64}{(\alpha+\beta)^6}\right\}\right]^{-1/2},\ \epsilon_0 = -2{\cdot}861\,67\ ;$$

3. The open shell function of Eckart (1930)

$$\chi^{(3)} = \frac{N}{\pi}\left[\exp(-\alpha r_1)\exp(-\beta r_2) + \exp(-\beta r_1)\exp(-\alpha r_2)\right], \qquad 3.23$$

$$\alpha = 2{\cdot}1832\ ,\ \beta = 1{\cdot}1885\ ,\ N = 2{\cdot}202\,908\ ,\ \epsilon_0 = -2{\cdot}8757.$$

In each the parameters are determined variationally. Coulson and Neilson (1961) have examined the accuracy of several approximations to the ground state helium function by calculating the mean electron-electron separation (r_{12}) for each approximation. The simple function $X^{(1)}$ gives the smallest value of (r_{12}), and the function $X^{(3)}$ is found to be a rather good approximation to the accurate six-parameter Hylleraas function, which gives the largest value of (r_{12}).

The methods for evaluating the integrals in (3.12) are outlined in Appendices A and B. The integrals using the simple helium wave function $X^{(1)}$ are listed inAppendix C; those using $X^{(2)}$ and $X^{(3)}$ can be easily obtained also.

The results of the calculation are shown in Table 2, together with those of Green et al. (1965) and with the results of experiments, which measure the cross section for capture summed over all final states. It is seen that the maximum difference between the results of the present calculation is less than 5% in the energy range 30 keV to 1 MeV, and about 10% at 10 MeV. This difference is not confined to the total cross section, but extends to the differential cross sections, expressed as a function of the impact parameter. On the basis of the Born approximation calculations of Mapleton (1961a), it is expected that for comparison with experimental values the calculated cross sections have to be increased by a factor of up to 30% to allow for capture into excited states. It is then evident that the considerable disagreement with experiment is not substantially improved by employing the refined wave functions $X^{(2)}$ and $X^{(3)}$ rather than the simple function $X^{(1)}$.

This lack of sensitivity is in accord with the work of Mapleton (1963), who found that the Born approximation cross sections calculated with the simple function $X^{(1)}$ and with a six-parameter Hylleraas function did not differ by more than 5 to 15% up to 1 MeV.

Comparison between the present results with those of Green et al. (1965) shows that the agreement is very close at 400 keV and to within 10% at 30 keV. The small differences one attributed to the effect of the electron exchange in the final state employed by Green et al. (1965). In their work the final state wave function Ψ_1 is symmetrized in the co-ordinates of the two electrons, which are in a singlet spin state. Since the initial state wave function Ψ_0 is symmetric this procedure does not alter the coupling terms between the initial and final terms in (3.15) and (3.16), but it allows for electron exchange to first order in that part of the wave function describing elastic scattering of H by He^+ in the final state. First-order exchange calculations are often misleading, so that in the present work an unsymmetrical final-state wave function is used. The effect of the exchange decreases with increasing velocity, as expected, and it is not very important at the energies under consideration.

3.2 The Four - State Approximation.

It was seen earlier that the two - state approximation of Bates, while giving fairly good results in the intermediate energy range 30 - 100 keV, shows considerable disagreement with experiment at low and high energies. The experiments measure however the cross sections for capture summed over all final states. It is then natural, by taking also into account the work of Lovell and McElroy (1965) on the effect of coupling in collisions between fast protons and hydrogen atoms, to ask whether the inclusion of excited states in the expansion of the complete wave function would improve the agreement of the theory with experiment.

At the range of energies under consideration all channels are open, and this would suggest the need to consider an infinite number of discrete states. However, the energy levels of the excited states of hydrogen are lower than those of the helium ion, so that in a second-order approximation the excited states of hydrogen should be considered first.

In the present calculations we consider the capture into the 1s, 2s, and 2p states of hydrogen, leaving the helium ion in the ground state :

$$H^{+} + He(1s^{2}) \longrightarrow H(1s,2s,2p) + He^{+}(1s). \qquad 3.24$$

We use the same set of co-ordinates as in section (3.1), and we choose the plane of collision, which contains the proton and the helium nucleus, to be the x - z plane. It is then seen that, if the 2p states of hydrogen are represented by the functions $\phi_H\ (2p_x)$, $\phi_H\ (2p_y)$, and $\phi_H\ (2p_z)$, the contribution from the state $\phi_H\ (2p_y)$ vanishes.

We write

$$\Psi(\underline{r}_1, \underline{r}_2, t) = \sum_{i=0}^{4} a_i(t)\, \Psi_i\, (\underline{r}_1, \underline{r}_2, t)\,, \qquad 3.25$$

where

$$\Psi_0(\underline{r}_1, \underline{r}_2, t) = X(\underline{r}_{n1}, \underline{r}_{n2})\, \exp\left[-i\left\{\varepsilon_0 t + v^2 t + \tfrac{1}{2}\underline{v}\cdot(\underline{r}_1 + \underline{r}_2)\right\}\right], \qquad 3.26$$

$$\underset{i \neq 0}{\Psi_i}(\underline{r}_1, \underline{r}_2, t) = \phi_i(\underline{r}_{p1})\, \psi(\underline{r}_{n2})\, \exp\left[-i\left\{(\eta_i + \mu_0)t + v^2 t + \tfrac{1}{2}\underline{v}\cdot(-\underline{r}_1 + \underline{r}_2)\right\}\right]. \qquad 3.27$$

The subscript i = 1, 2, 3, 4 corresponds to the 1s, 2s, $2p_x$, and $2p_z$ states of hydrogen, respectively. The explicit forms of these states are :

$$\begin{aligned}
\phi_1\,(1s) &= \frac{1}{\sqrt{\pi}}\, e^{-r} & \eta_1 &= -\tfrac{1}{2}\,, \\
\phi_2\,(2s) &= \frac{1}{4\sqrt{2\pi}}\,(2-r)\, e^{-\frac{1}{2}r} & \eta_2 &= -\tfrac{1}{8}\,, \\
\phi_3\,(2p_x) &= \frac{1}{4\sqrt{2\pi}}\, x\, e^{-\frac{1}{2}r} & \eta_3 &= -\tfrac{1}{8}\,, \\
\phi_4\,(2p_z) &= \frac{1}{4\sqrt{2\pi}}\, z\, e^{-\frac{1}{2}r} & \eta_4 &= -\tfrac{1}{8}\,:
\end{aligned} \qquad 3.28$$

The function $X(\underline{r}_{n1}, \underline{r}_{n2})$ is the simple helium wave function (3.21), $\psi(\underline{r}_{n2})$ is the wave function of the helium ion in the ground state and is given explicitly in (3.20).

The time-dependent Schrodinger equation can be written as

$$\left(H - i\frac{\partial}{\partial t}\right)\sum_{i=0}^{4} a_i(t)\Psi_i(\underline{r}_1,\underline{r}_2,t) = 0 \;. \qquad 3.29$$

By using the equations

$$\left\langle \Psi_j^{*}(\underline{r}_1,\underline{r}_2,t)\right| H - i\frac{\partial}{\partial t}\left|\sum_{i=0}^{4} a_i(t)\Psi_i(\underline{r}_1,\underline{r}_2,t)\right\rangle = 0 \qquad 3.30$$

$$j = 0,1,2,3,4 \,,$$

we obtain a set of coupled differential equations in the matrix form

$$i\left|\begin{matrix} 1 & S_{o1} & S_{o2} & S_{o3} & S_{o4} \\ S_{1o} & 1 & 0 & 0 & 0 \\ S_{2o} & 0 & 1 & 0 & 0 \\ S_{3o} & 0 & 0 & 1 & 0 \\ S_{4o} & 0 & 0 & 0 & 1 \end{matrix}\right|\left|\begin{matrix} \dot{a}_o \\ \dot{a}_1 \\ \dot{a}_2 \\ \dot{a}_3 \\ \dot{a}_4 \end{matrix}\right| = \left|\begin{matrix} A_{oo} & K_{o1} & K_{o2} & K_{o3} & K_{o4} \\ K_{1o} & B_{11} & B_{12} & B_{13} & B_{14} \\ K_{2o} & B_{21} & B_{22} & B_{23} & B_{24} \\ K_{3o} & B_{31} & B_{32} & B_{33} & B_{34} \\ K_{4o} & B_{41} & B_{42} & B_{43} & B_{44} \end{matrix}\right|\left|\begin{matrix} a_o \\ a_1 \\ a_2 \\ a_3 \\ a_4 \end{matrix}\right| \qquad 3.31$$

where

$$\varepsilon_{oi} = (\varepsilon_o - \eta_i - \mu_o) \qquad\qquad i,j = 1,2,3,4,$$

$$S_{oi}(t) = S_{io}^{*}(t) = \int e^{i\underline{v}\cdot\underline{r}_1} e^{i\varepsilon_{oi}t}\chi(\underline{r}_{n1},\underline{r}_{n2})\phi_i(\underline{r}_{p1})\psi(\underline{r}_{n2})d\underline{r}_1 d\underline{r}_2, \qquad 3.32$$

$$A_{oo}(t) = \int \chi^{*}(\underline{r}_{n1},\underline{r}_{n2})\Big[V_{p1}+V_{p2}\Big]\chi(\underline{r}_{n1},\underline{r}_{n2})d\underline{r}_1 d\underline{r}_2 \,,$$

$$B_{ij}(t) = B_{ji}^{*}(t) = \int e^{i(\eta_i-\eta_j)t}\phi_i^{*}(\underline{r}_{p1})\psi^{*}(\underline{r}_{n2})\Big[V_{p2}+V_{n1}+V_{12}\Big]\phi_j(\underline{r}_{p1})\psi(\underline{r}_{n2})d\underline{r}_1 d\underline{r}_2 \,,$$

$$K_{oi}(t) = \int e^{i\underline{v}\cdot\underline{r}_1} e^{i\varepsilon_{oi}t}\chi(\underline{r}_{n1},\underline{r}_{n2})\Big[V_{p2}+V_{n1}+V_{12}\Big]\phi_i(\underline{r}_{p1})\psi(\underline{r}_{n2})d\underline{r}_1 d\underline{r}_2,$$

$$K_{io}(t) = \int e^{-i\underline{v}\cdot\underline{r}_1} e^{-i\varepsilon_{oi}t}\phi_i^{*}(\underline{r}_{p1})\psi^{*}(\underline{r}_{n2})$$

$$\Big[-\tfrac{1}{2}\nabla_{r_{n1}}^{2} - \tfrac{1}{2}\nabla_{r_{n2}}^{2} + V_{p1}+V_{p2}+V_{n1}+V_{n2}+V_{12}-\varepsilon_o\Big]\chi(\underline{r}_{n1},\underline{r}_{n2})d\underline{r}_1 d\underline{r}_2 \,.$$

The coefficients $a_i(t)$ are time-dependent and have the initial conditions

$$a_0(-\infty) = 1 \quad , \quad \underset{i \neq 0}{a_i}(-\infty) = 0 \ . \qquad 3.33$$

The cross section for the capture into the state i of hydrogen is then

$$\sigma_i = 2\int |a_i(+\infty)|^2 \rho \, d\rho \qquad i = 1, 2, 3, 4 \ . \qquad 3.34$$

The integrals in (3.32) have the time reversal relations

$$\begin{aligned} S_{0i}^*(-t) &= \epsilon_i S_{0i}(t) \ , \quad K_{0i}^*(-t) = \epsilon_i K_{0i}(t) \ , \\ K_{i0}^*(-t) &= \epsilon_i K_{i0}(t) \ , \quad A_{00}^*(-t) = A_{00}(t) \ , \qquad 3.35 \\ B_{ij}^*(-t) &= \epsilon_i \epsilon_j B_{ij}(t) \ , \end{aligned}$$

where

$$i, j = 1, 2, 3, 4 \qquad \underset{i,j \neq 4}{\epsilon_{i,j}} = 1 \qquad \epsilon_4 = -1 \ .$$

It them, follows, by using the proof of Green outlined in section (1.5), that the equation (3.31) satisfies the requirements of detailed balancing.

The methods for evaluating the integrals in (3.31) are given in Appendices A and B. These integrals are listed in Appendix D.

In Figs. 1 and 2 the present results for the total capture into the 1s, 2s, and 2p states of hydrogen are compared with the Born approximation and the impulse approximation calculations, and with the experimental data of Hasted (1955), Stier and Barnett (1956), Barnett and Reynolds (1958), and Allision (1958). It is seen that the presen t calculation shows quite good agreement with experiment in the energy range 25 to 100 keV.

At high energies the decrease of the calculated cross section with energy appears to be too small. A similar discrepancy occurs on the low energy of the cross section maximum (about 25 KeV), but at lower energies the theoretical cross sections become smaller than the available measurements (Hasted, 1955) by a factor of 5 at 1 KeV. It is expected of course that for low velocity collisions the expansion based on atomic wave functions is no longer appropriate and that the expansion using molecular eigenfunctions, formed by the colliding system at fixed internuclear separation, may be used.

In Fig. 3 the results for the capture into the 1s state are compared with the results using the two-state expansion. It is seen that at energies above 30 KeV the coupling due to the 2s and 2p states has little effect on the calculated cross section for capture into the ground state. The present results are appreciably greater than those of Green et al. (1965) at low energies, by a factor of 2 at 1 KeV. These differences are partly attributed to the use of a symmetrized final state wave function in the work of Green et al. and this has the effect of allowing for ellectron exchange. The inclusion of electron to first order does not usually give better results, as was pointed out in section (3. 1). It s effect in this system is quite unimportant at energies above 30 KeV, but it is expected to be appreciable at low energies.

Experimental cross sections for the partial captures into the 2s and 2p states of hydrogen are availabe unfortunately for the small energy range 5 to 40 KeV only. Fig. 4 shows the experimental data, the present results and the Born approximation calculations of Mapleton (1961) for the capture into the 2s state. It is seen that the present results agree quite well with the measurements of Jaecks et al. (1965) and Andreev et al. (1966), but those of Colli et al. (1962) are larger by a factor of up to 6. In Fig. 5 the present calculations for the capture into the 2p state are compared with the Born approximation calculations of Mapleton (1961) and with the experimental data. It is seen that the present results show quite good agreement with the measurements of De Heer et al. (1963), but those of Pretzer et al. (1963) and Andreev et al. (1966) one smaller by a factor of about 2.

An alternative way of comparing the theory with the experiment is to consider the theoretical predictions and the measurements for the capture probability for a fixed value of the product ΘT of the scattering angle and the incident proton energy. To a good approximation constant ΘT corresponds to a constant distance of closest approach and to a constant impact parameter. It is seen in Fig. 9 that the agreement with experiment for the capture over all final states is good at high energies, but poor at low energies. The positions of the maxima and minima are predicted quite well by the theory, but the theoretical capture probability is grossly in error at low energies.

Fig. 10 shows the present results for the probability of capture into the 1s state and those of Green (1966) for $\Theta T = 20$. The agreement is good at high energies. At low energies the results of Green are appreciably smaller; this may be partly attributed to the effect of electron exchange in his calculations, as we have pointed out earlier.

The calculations on the probability of capture into the 2s and 2p states for $\theta T = 20$ are shown in Figs. 11 and 12, respectively. Dose and Mayer (1966) have reported recently their measurements on the probability of capture into 2s state at a scattering angle of 2.2° in the enrgy range 4.5 to 60 KeV.

Comparision between the results given in Figs. 1 and 2 and those in Fig. 3 shows that the inclusion of the excited states of hydrogen in the expansion method does not alter appreciably the calculated cross section. This would suggest that the considerable disagreement with experiment would not be substantially improved by employing an expansion based on several discrete states rather than the lowest two-state approximation. Taking also into account the result of calculations in the impulse approximation, to reduce the calculated cross section substantially, it would seem necessary to represent the continuum intermediate states in some way.

CHAPTER FOUR

4.1 Numerical Methods

The evaluation of the cross section using the expansion methods of Bates involves a triple integration over x, the time t, and the impact parameter ρ. We shall consider mainly the numerical methods employed in the calculations using the four-state approximation. The calculations using the two-state approximation are easier to perform, but similar techniques can be applied.

We consider first the evaluation of the matrix elements in (3.32). The most difficult terms to calculate are those which relate the initial to the final states : S_{oi}, S_{io}, K_{oi} and K_{io}. Expressions for these matrix elements are of the forms:

$$
\begin{aligned}
I_1 &= e^{-i\frac{v^2}{2}t}\int_0^1 x^n(1-x)^m\left[\frac{R}{\Delta^2}+\frac{1}{\Delta^3}\right]e^{-R\Delta}e^{iv^2tx}\,dx,\\
I_2 &= e^{-i\frac{v^2}{2}t}\int_0^1 x^n(1-x)^m\left[\frac{R^2}{\Delta^3}+\frac{3R}{\Delta^4}+\frac{3}{\Delta^5}\right]e^{-R\Delta}e^{iv^2tx}\,dx,\\
I_3 &= e^{-i\frac{v^2}{2}t}\int_0^1 x^n(1-x)^m\left[\frac{R^3}{\Delta^4}+\frac{6R^2}{\Delta^5}+\frac{15R}{\Delta^6}+\frac{15}{\Delta^7}\right]e^{-R\Delta}e^{iv^2tx}\,dx,
\end{aligned}
\qquad 4.1
$$

where

$$\Delta^2 = \lambda^2 x + (1-x)(\mu^2 + x v^2) \quad \text{and} \quad n, m \geqslant 0.$$

These functions depend on the proton velocity v and they oscillate rapidly for large values of v. Analysis of these terms shows that for a given value of v, the main contributions come from values of x near the ends of the range of integration. It is therefore convenient to divide the range of integration over x into three sections : $0 \leqslant x \leqslant 0{\cdot}15$, $0{\cdot}15 \leqslant x \leqslant 0{\cdot}85$, .

and $0.85 \leqslant x \leqslant 1$. The integration for each section is performed by means of the Gaussian interpolation method. At 30 KeV the number of Gaussian points used for these three ranges of integration are 14, 7, and 5, respectively, to obtain an accuracy of better than 1 part in 10^5. The integrands oscillate repidly as v increases, so that at high energies more Gaussian points are required in order to achieve the same accuracy; at 1 MeV the number of points used are 20, 20, and 10, respectively.

The time-reversal relations of the matrix elements in (3.31) are exploited to find the values of these terms at time +t from those at -t.

The coupled differential equations of (3.31) can be written compactly in the form

$$i \; S \dot{a} = K a , \qquad 4.2$$

where S and K are matrices and a is a column vector. Since S, K, and a are complex functions of time it is convenient to define

$$\begin{aligned} S &= S' + i S'' , \\ K &= K' + i K'' , \\ a &= a' + i a'' , \end{aligned} \qquad 4.3$$

in which S', S", K', K", a' and a" are real. The equation (4.2) can then be written as

$$\begin{vmatrix} S' & -S'' \\ S'' & S' \end{vmatrix} \begin{vmatrix} \dot{a}' \\ \dot{a}'' \end{vmatrix} = \begin{vmatrix} K'' & K' \\ -K' & K'' \end{vmatrix} \begin{vmatrix} a' \\ a'' \end{vmatrix} , \qquad 4.4$$

which is of the form

$${}^{o}S\,{}^{o}\dot{a} = {}^{o}K\,{}^{o}a\,, \qquad 4.5$$

To solve (4.5) we need to find first the inverse ${}^{o}S^{-1}\,{}^{o}K$, , so that

$${}^{o}\dot{a} = ({}^{o}S^{-1}\,{}^{o}K)\,{}^{o}a\,. \qquad 4.6$$

The Kutta-Merson method (Fox, 1962) is used to solve the coupled differential equations of (4.6). This method is reported to be more efficient than the commonly used Runge-Kutta method. It provides a check on the accuracy during the integration and it alters automatically the step size at every stage of the integration to give the accuracy required.

The range of integration over t depends clearly on the velocity of the incident proton. It is found that, if R_{max} is the maximum internucleon distance, $R_{max} = 16$ provides a good range of integration for the convergence of the terms in (4.6). The Chebyshev is used to obtain the interpolation points of $({}^{o}S^{-1}\,{}^{o}K)$ at every value of t during the integration. The range of integration over t, $|t_{max}|$, is divided into two parts t_{max} to $\frac{1}{2}t_{max}$, and $\frac{1}{2}t_{max}$ to 0. It is found that for these two ranges by using 10 and 15 Chebyshev points, respectively, an accuracy of better than 1 part in 3×10^3 is obtained at 30 KeV. At 1 MeV the number of points required are 15 and 25, respectively.

Since by definition the probability never exceeds unity, this condition provides a useful check on the calculations. Moreover, detailed balancing is checked for each of the two-state reactions of (3.24).

In the equation (3.31) the matrix elements S_{oi}, S_{io}, K_{io}, and K_{oi} contain the exponential function $e^{-R\lambda}$ and so decrease rapidly to zero as R increases. The other terms, A_{oo} and B_{ij}, are the Coulomb terms and they have the asymtotic forms of R^{-1}, $R^{-2}\, e^{i\varepsilon_{ij}t}$, and R^{-2}, etc. It is then evident that significant couplings of the amplitudes can occur even at the large interpolation distances, so that it is important to extrapolate the amplitudes $a_i(+t_{max})$ to find $a_i(+\infty)$. The common diagonal term R^{-1}_{max} causes only a change in the phase and so does not affect the capture amplitude. The term $e^{i\varepsilon_{ij}t}R^{-2}_{max}$ does not give any appreciable contribution, and the terms which decrease faster than R^{-2}_{max} can be neglected. There is however significant coupling between the 2s and 2p states due to the R^{-2}_{max} term. Analysis shows that the extrapolation correction is given by

$$a_{2s}(+\infty) = a_{2s}(+t_{max})\cos(-3/v^2 t_{max}) - i a_{2p_z}(+t_{max})\sin(-3/v^2 t_{max}),$$

$$a_{2p_z}(+\infty) = a_{2p_z}(+t_{max})\cos(-3/v^2 t_{max}) - i a_{2s}(+t_{max})\sin(-3/v^2 t_{max}). \qquad 4.7$$

The final integration over the impact parameter is done by using the Gaussian extrapolation method. An 8-point Gaussian method is usually adequate for energies above 30 KeV, but at lower energies the range of integration is sub-divided and the Gaussian method is applied to each sub-division. It is estimated that the overall accuracy is better than 5% for the total and the 1s capture cross sections, and 10% for the cross sections for captures into 2s and 2p states of hydrogen.

4.2 Conclusion

The present calculations indicate that the inclusion of more discrete states in the expansion method of Bates would not improve the considerable disagreement with experiment at high energies. If this can be confirmed, it would suggest that the method is inadequate because it does not take continuum transitions into account, whereas the results of the second Born and the impulse approximations indicate that ultimately continuum intermediate states play an important part in the capture process.

However, little experimental work is done on the electron capture by protons in helium at high energies and the measurements of Barnett and Reynolds (1958) only are available. Further investigation, both theoretical and experimental, is desirable.

Appendix A

Evaluation of the integrals

$$I_1 = \int e^{-\lambda r_{n1}} e^{-\mu r_{p1}} e^{i\underline{v}\cdot\underline{r}_1} \, d\underline{r}_1 , \qquad \mathrm{A}\cdot 1$$

$$I_2 = \int r_{p1} e^{-\lambda r_{n1}} e^{-\mu r_{p1}} e^{i\underline{v}\cdot\underline{r}_1} \, d\underline{r}_1 , \qquad \mathrm{A}\cdot 2$$

$$I_3 = \int x_{p1} e^{-\lambda r_{n1}} e^{-\mu r_{p1}} e^{i\underline{v}\cdot\underline{r}_1} \, d\underline{r}_1 , \qquad \mathrm{A}\cdot 3$$

$$I_4 = \int \frac{e^{-\lambda r_{n1}}}{r_{n1}} e^{-\mu r_{p1}} e^{i\underline{v}\cdot\underline{r}_1} \, d\underline{r}_1 , \qquad \mathrm{A}\cdot 4$$

$$I_5 = \int e^{-\lambda r_{n1}} \frac{e^{-\mu r_{p1}}}{r_{p1}} e^{i\underline{v}\cdot\underline{r}_1} \, d\underline{r}_1 , \qquad \mathrm{A}\cdot 5$$

Let O be the mid-point of R , $\underline{R}_A \equiv \overrightarrow{OA}$, $\underline{R}_B \equiv \overrightarrow{OB}$,

so that

$$\underline{R} = -\underline{R}_B + \underline{R}_A , \quad \underline{r}_{p1} = \underline{r}_1 - \underline{R}_A , \quad \underline{r}_{n1} = \underline{r}_1 - \underline{R}_B .$$

Using the Fourier transforms

$$e^{-\lambda r} = \frac{1}{\pi^2} \int \frac{\lambda}{(\lambda^2+q^2)^2} e^{i\underline{q}\cdot\underline{r}} \, d\underline{q} , \qquad \mathrm{A}\cdot 6$$

$$\frac{e^{-\lambda r}}{r} = \frac{1}{2\pi^2} \int \frac{1}{(\lambda^2+q^2)} e^{i\underline{q}\cdot\underline{r}} \, d\underline{q} , \qquad \mathrm{A}\cdot 7$$

we can write

$$I_1 = \frac{1}{\pi^4}\int d\underline{r}_1 \int d\underline{q}_1 \int d\underline{q}_2 \, \frac{\lambda}{(\lambda^2+q_1^2)^2} \, \frac{\mu}{(\mu^2+q_2^2)^2} \exp i\left\{\underline{q}_1\cdot\underline{r}_{n1} + \underline{q}_2\cdot\underline{r}_{p1} + \underline{v}\cdot\underline{r}_1\right\}. \qquad \text{A}\cdot 8$$

The integration over $d\underline{r}_1$ is easily performed to give

$$\int d\underline{r}_1 \longrightarrow (2\pi)^3 \, \delta(\underline{q}_1 + \underline{q}_2 + \underline{v}) \exp -i\left\{\underline{q}_2\cdot\underline{R}_A + \underline{q}_1\cdot\underline{R}_B\right\}, \qquad \text{A}\cdot 9$$

and on integrating over $d\underline{q}_2$ we have

$$I_1 = \frac{2}{\pi} e^{i\underline{v}\cdot\underline{R}_A} \int d\underline{q}_1 \, \frac{4\lambda\mu \, e^{i\underline{q}_1\cdot\underline{R}}}{(\lambda^2+q_1^2)^2(|\underline{v}+\underline{q}_1|^2+\mu^2)^2}$$

$$= \frac{2}{\pi} e^{i\underline{v}\cdot\underline{R}_A} \frac{\partial}{\partial\lambda}\frac{\partial}{\partial\mu} \mathcal{J} \, , \qquad \text{A}\cdot 10$$

where

$$\mathcal{J} = \int d\underline{q}_1 \, \frac{e^{i\underline{q}_1\cdot\underline{R}}}{(\lambda^2+q_1^2)(|\underline{v}+\underline{q}_1|^2+\mu^2)} \, . \qquad \text{A}\cdot 11$$

Using the formula (Feynman, 1949)

$$\frac{1}{ab} = \int_0^1 \frac{1}{[ax+b(1-x)]^2} \, dx \, , \qquad \text{A}\cdot 12$$

with the substitutions

$$\underline{p} = \underline{q}_1 + \underline{v}\,(1-x) \, ,$$

$$\Delta^2 = \lambda^2 x + (1-x)\mu^2 + x(1-x)v^2, \qquad A\cdot 13$$

we write

$$g = \int_0^1 dx \int d\underline{p} \; \frac{\exp(i\,\underline{p}\cdot\underline{R})\exp\{-i\,\underline{v}\cdot\underline{R}(1-x)\}}{(p^2+\Delta^2)^2}. \qquad A\cdot 14$$

By making use of the standard integral

$$\int \frac{\exp(i\,\underline{p}\cdot\underline{R})}{(p^2+\Delta^2)^2}\, d\underline{p} = \frac{\pi^2}{\Delta} e^{-R\Delta}, \qquad A\cdot 15$$

we get

$$g = \pi^2 \int_0^1 dx \; \exp\left[-i\,\underline{v}\cdot\underline{R}(1-x) - R\Delta\right]\cdot\frac{1}{\Delta} \qquad A\cdot 16$$

so that

$$I_1 = 2\pi\lambda\mu e^{i\underline{v}\cdot\underline{R}_A} \int_0^1 \left[\frac{R^2}{\Delta^3} + \frac{3R}{\Delta^4} + \frac{3}{\Delta^3}\right] x(1-x) e^{-R\Delta} e^{-i\underline{v}\cdot\underline{R}(1-x)} dx, \qquad A\cdot 1$$

with

$\underline{v} \cdot \underline{R} = v^2t$ and $\underline{v} \cdot \underline{R} = \frac{1}{2}v^2t.$

The integrals I_2 and I_3 are evaluated by using the transformations

$$I_2 = -\frac{\partial}{\partial\mu} I_1, \qquad A\cdot 18$$

$$I_3 = -\frac{\partial}{\partial\mu}\left[\frac{1}{\mu}\frac{\partial}{\partial A_x}\right] I_1, \qquad A\cdot 19$$

where (A_x, A_y, A_z) are the position co-ordinates of p relative to O.

$$I_4 = 2\pi\mu e^{i\underline{v}\cdot\underline{R}_A}\int_0^1\left[\frac{R}{\Delta^2}+\frac{1}{\Delta^3}\right](1-x)e^{-R\Delta}e^{-i\underline{v}\cdot\underline{R}(1-x)}dx, \qquad A\cdot 20$$

$$I_5 = 2\pi\lambda e^{i\underline{v}\cdot\underline{R}_A}\int_0^1\left[\frac{R}{\Delta^2}+\frac{1}{\Delta^3}\right]x\, e^{-R\Delta}e^{-i\underline{v}\cdot\underline{R}(1-x)}dx, \qquad A\cdot 21$$

We shall use $I(\lambda,\mu,n,m,\ell)$ to denote

$$I(\lambda,\mu,n,m,3) = 2\lambda^n\mu^m e^{-i\frac{\underline{v}^2}{2}t}\int_0^1 x^n(1-x)^m\left[\frac{R}{\Delta^2}+\frac{1}{\Delta^3}\right]e^{-R\Delta}e^{iv^2tx}dx,$$

$$I(\lambda,\mu,n,m,5) = 2\lambda^n\mu^m e^{-i\frac{\underline{v}^2}{2}t}\int_0^1 x^n(1-x)^m\left[\frac{R^2}{\Delta^3}+\frac{3R}{\Delta^4}+\frac{3}{\Delta^5}\right]e^{-R\Delta}e^{iv^2tx}dx, \qquad A\cdot 2$$

$$I(\lambda,\mu,n,m,7) = 2\lambda^n\mu^m e^{-i\frac{\underline{v}^2}{2}t}\int_0^1 x^n(1-x)^m\left[\frac{R^3}{\Delta^4}+\frac{6R^2}{\Delta^5}+\frac{15R}{\Delta^6}+\frac{15}{\Delta^7}\right]e^{-R\Delta}e^{iv^2tx}dx.$$

Appendix B

Evaluation of the integrals

$$I_1 = \int r^n e^{-\lambda r} \frac{e^{-\mu|\underline{r}-\underline{R}|}}{|\underline{r}-\underline{R}|} Y_\ell^m(\theta_1,\phi_1)\, d\underline{r}, \qquad \text{B-1}$$

$$I_2 = \int r^n e^{-\lambda r} e^{-\mu|\underline{r}-\underline{R}|} Y_\ell^m(\theta_1,\phi_1)\, d\underline{r}, \qquad \text{B-2}$$

$$I_3 = \int r^n \frac{e^{-\lambda r}}{|\underline{r}-\underline{R}|} Y_\ell^m(\theta_1,\phi_1)\, d\underline{r}\, . \qquad \text{B-3}$$

We use the expansion series (Watson, 1958)

$$\frac{e^{-\mu|\underline{r}-\underline{R}|}}{|\underline{r}-\underline{R}|} = \sum_{\ell=0}^{\infty} \frac{(2\ell+1)\ K_{\ell+\frac{1}{2}}(\mu R)\ I_{\ell+1/2}(\mu r)\ P_\ell(\cos\theta)}{\sqrt{R}\qquad\qquad \sqrt{r}}\ , \qquad r \leq R \qquad \cos\theta = \frac{\underline{r}\cdot\underline{R}}{Rr}$$

where

$$K_{\ell+1/2}(\mu R) = \sqrt{\frac{\pi}{2\mu R}}\ e^{-\mu R} \sum_{n=0}^{\ell} \frac{(\ell+n)!}{n!\,(\ell-n)!\,(2\mu R)^n}\ ,$$

$$I_{\ell+1/2}(\mu r) = \frac{1}{\sqrt{2\pi\mu r}} \left[e^{\mu r} \sum_{n=0}^{\ell} \frac{(-)^n\,(\ell+n)!}{n!\,(\ell-n)!\,(2\mu r)^n} + (-)^{\ell+1} e^{-\mu r} \sum_{n=0}^{\ell} \frac{(\ell+n)!}{n!\,(\ell-n)!\,(2\mu r)^n} \right];$$

$$P_\ell(\cos\theta) = \frac{4\pi}{(2\ell+1)} \sum_{m=-\ell}^{\ell} Y_\ell^{m*}(\theta_2,\phi_2)\, Y_\ell^m(\theta_1,\phi_1)\, ; \qquad \text{B-4}$$

and the standard formula

$$\frac{1}{|\underline{r}-\underline{R}|} = \frac{1}{r}\sum_{l=0}^{\infty}\left(\frac{R}{r}\right)^{l} P_l(\cos\theta) \qquad r \geqslant R$$

$$= \frac{1}{R}\sum_{l=0}^{\infty}\left(\frac{r}{R}\right)^{l} P_l(\cos\theta) \qquad r \leqslant R \quad , \qquad B\cdot 5$$

where

$$\cos\theta = \cos\theta_1\cos\theta_2 + \sin\theta_1\sin\theta_2\cos(\phi_1-\phi_2)$$

and

(θ_1,ϕ_1) and (θ_2,ϕ_2) are the polar angles of $\underline{r}$ and $\underline{R}$. The integrals I_1 and I_3 can then be evaluated easily for definite values of n, m, and l. The integral I_2 is calculated in the same way after expressing it as

$$I_2 = -\frac{\partial}{\partial\mu} I_1 . \qquad B\cdot 6$$

The integrals will be listed in the forms of $f(n,\lambda,l)$ and $F(n,\lambda,\mu,l)$, where

$$f(n,\lambda,l)\,Y_l^m(\theta_2,\phi_2) = \frac{1}{4\pi}\int r^n \frac{e^{-\lambda r}}{|\underline{r}-\underline{R}|} Y_l^m(\theta_1,\phi_1)\,d\underline{r} ,$$

$$F(n,\lambda,\mu,l)\,Y_l^m(\theta_2,\phi_2) = \frac{1}{4\pi}\int r^n \frac{e^{-\mu|\underline{r}-\underline{R}|}}{|\underline{r}-\underline{R}|} e^{-\lambda r}\left[2+\frac{1}{|\underline{r}-\underline{R}|}\right] Y_l^m(\theta_1,\phi_1)\,d\underline{r} . \qquad B\cdot 7$$

We also denote

$$g_0 = 2\left[\left(1+\frac{1}{2R}\right)e^{-4R} - \frac{1}{2R}\right], \qquad \text{B-8}$$

$$g_1 = \frac{2}{R} - \left(2+\alpha+\frac{2}{R}\right)e^{-(2+\alpha)R}. \qquad \text{B-9}$$

List of Integrals $f(n, \lambda, \ell)$

(i) $f(0,\lambda,0) = \frac{1}{\lambda^2}\left[\frac{2}{R\lambda} - \left(1+\frac{2}{R\lambda}\right)e^{-R\lambda}\right].$

(ii) $f(1,\lambda,0) = \frac{1}{\lambda^2}\left[\frac{6}{R\lambda^2} - \left(R+\frac{4}{\lambda}+\frac{6}{R\lambda^2}\right)e^{-R\lambda}\right].$

(iii) $f(1,\lambda,1) = \frac{1}{3\lambda^2}\left[\frac{24}{R^2\lambda^3} - \left(3R+\frac{12}{\lambda}+\frac{24}{R\lambda^2}+\frac{24}{R^2\lambda^3}\right)e^{-R\lambda}\right].$

(iv) $f(2,\lambda,0) = \frac{1}{\lambda^2}\left[\frac{24}{R\lambda^3} - \left(R^2+\frac{6R}{\lambda}+\frac{18}{\lambda^2}+\frac{24}{R\lambda^3}\right)e^{-R\lambda}\right].$

(v) $f(2,\lambda,1) = \frac{1}{\lambda^2}\left[\frac{40}{R^2\lambda^4} - \left(R^2+\frac{6R}{\lambda}+\frac{20}{\lambda^2}+\frac{40}{R\lambda^3}+\frac{40}{R^2\lambda^4}\right)e^{-R\lambda}\right].$

(vi) $f(2,\lambda,2) = \frac{1}{\lambda^2}\left[\frac{144}{R^3\lambda^5} - \left(R^2+\frac{6R}{\lambda}+\frac{24}{\lambda^2}+\frac{72}{R\lambda^3}+\frac{144}{R^2\lambda^4}+\frac{144}{R^3\lambda^5}\right)e^{-R\lambda}\right].$

List of Integrals $F(n, \lambda, \mu, l)$ $\qquad \delta \equiv (\mu^2-\lambda^2)$

$$\text{(i)} \quad F(0,\lambda,\mu,0) = \frac{2}{\delta}\left[\frac{1}{2} + \frac{2\mu}{\delta} - \frac{\lambda}{R\delta}\left(1+\frac{8\mu}{\delta}\right)\right]e^{-\lambda R}$$

$$+ \frac{2\lambda}{\delta^2}\left[2 + \frac{1}{R}\left(1+\frac{8\mu}{\delta}\right)\right]e^{-\mu R}$$

$$\text{(ii)} \quad F(1,\lambda,\mu,0) = \frac{2}{\delta}\Big[R\left(\frac{1}{2}+\frac{2\mu}{\delta}\right) - \frac{2\lambda}{\delta}\left(1+\frac{8\mu}{\delta}\right)$$

$$+ \frac{1}{R\delta^2}\left((\mu^2+3\lambda^2) + \frac{8\mu^3+40\mu\lambda^2}{\delta}\right)\Big]e^{-\lambda R}$$

$$- \frac{2}{\delta^3}\left[2(\mu^2+3\lambda^2) + \frac{1}{R}\left(\mu^2+3\lambda^2 + \frac{8\mu^3+40\mu\lambda^2}{\delta}\right)\right]e^{-\mu R}$$

$$\text{(iii)} \quad F(1,\lambda,\mu,1) = 2\Big[R\left(\frac{1}{2\delta}+\frac{2\mu}{\delta^2}\right) - \left(\frac{2\lambda}{\delta^2}+\frac{16\mu\lambda}{\delta^3}\right)$$

$$+ \frac{1}{R}\left(\frac{4\lambda^2}{\delta^3}+\frac{48\mu\lambda^2}{\delta^4}\right) + \frac{1}{R^2}\left(\frac{4\lambda}{\delta^3}+\frac{48\mu\lambda}{\delta^4}\right)\Big]e^{-\lambda R}$$

$$- 2\left[\frac{8\mu\lambda}{\delta^3} + \frac{1}{R}\left(\frac{4\mu\lambda}{\delta^3}+\frac{48\mu^2\lambda}{\delta^4}\right) + \frac{1}{R^2}\left(\frac{4\lambda}{\delta^3}+\frac{48\mu\lambda}{\delta^4}\right)\right]e^{-\mu R}$$

$$\text{(iv)} \quad F(2,\lambda,\mu,0) = 2\Big[\frac{R^2}{\delta}\left(\frac{1}{2}+\frac{2\mu}{\delta}\right) - \frac{3\lambda R}{\delta^2}\left(1+\frac{8\mu}{\delta}\right) + \frac{3}{\delta^3}\left(\mu^2+3\lambda^2+\frac{8\mu^3+40\mu\lambda^2}{\delta}\right)$$

$$- \frac{12\lambda}{R\delta^4}\left(\mu^2+\lambda^2 + \frac{4\mu(3\mu^2+5\lambda^2)}{\delta}\right)\Big]e^{-\lambda R}$$

$$+ \frac{24\lambda}{\delta^4}\left[2(\mu^2+\lambda^2) + \frac{1}{R}\left(4\mu\frac{(3\mu^2+5\lambda^2)}{\delta} + \mu^2+\lambda^2\right)\right]e^{-\mu R}$$

(v)

$$\begin{aligned} F(2,\lambda,\mu,1) = 2\Big[& \frac{R^2}{\delta}\left(\frac{1}{2}+\frac{2\mu}{\delta}\right)-\frac{3\lambda R}{\delta^2}\left(1+\frac{8\mu}{\delta}\right)+\frac{2}{\delta^3}\left(\mu^2+5\lambda^2+\frac{8\mu(\mu^2+8\lambda^2)}{\delta}\right) \\ & -\frac{4\lambda}{R\delta^4}\left(\mu^2+5\lambda^2+\frac{12\mu(\mu^2+7\lambda^2)}{\delta}\right) \\ & -\frac{4}{R^2\delta^4}\left(\mu^2+5\lambda^2+\frac{12\mu(\mu^2+7\lambda^2)}{\delta}\right)\Big]e^{-\lambda R} \\ +2\Big[& \frac{8\mu(\mu^2+5\lambda^2)}{\delta^4}+\frac{4\mu}{R\delta^4}\left(\mu^2+5\lambda^2+\frac{12\mu(\mu^2+7\lambda^2)}{\delta}\right) \\ & +\frac{4}{R^2\delta^4}\left(\mu^2+5\lambda^2+\frac{12\mu(\mu^2+7\lambda^2)}{\delta}\right)\Big]e^{-\mu R} \end{aligned}$$

(vi)

$$\begin{aligned} F(2,\lambda,\mu,2) = 2\Big[& R^2\left(\frac{1}{2\delta}+\frac{2\mu}{\delta^2}\right)-R\left(\frac{3\lambda}{\delta^2}+\frac{24\mu\lambda}{\delta^3}\right)+\left(\frac{12\lambda^2}{\delta^3}+\frac{144\mu\lambda^2}{\delta^4}\right) \\ & +\frac{1}{R}\left(\frac{12\lambda(\mu^2-3\lambda^2)}{\delta^4}+\frac{48\mu\lambda(3\mu^2-11\lambda^2)}{\delta^5}\right) \\ & -\frac{1}{R^2}\left(\frac{72\lambda^2}{\delta^4}+\frac{1152\mu\lambda^2}{\delta^5}\right)-\frac{1}{R^3}\left(\frac{72\lambda}{\delta^4}+\frac{1152\mu\lambda}{\delta^5}\right)\Big]e^{-\lambda R} \\ +2\Big[& \frac{48\mu^2\lambda}{\delta^4}+\frac{1}{R}\left(\frac{24\mu^2\lambda}{\delta^4}+\frac{48\mu\lambda(9\mu^2-\lambda^2)}{\delta^5}\right) \\ & +\frac{1}{R^2}\left(\frac{72\mu\lambda}{\delta^4}+\frac{1152\mu^2\lambda}{\delta^5}\right)+\frac{1}{R^3}\left(\frac{72\lambda}{\delta^4}+\frac{1152\mu\lambda}{\delta^5}\right)\Big]e^{-\mu R} \end{aligned}$$

Appendix C

List of integrals for $H^+ + He(1s^2) \rightarrow H(1s) + He^+(1s)$, using the helium wave (3.21)

$$c_1 \equiv \frac{8\sqrt{2}\alpha^3}{(2+\alpha)^3} e^{i\varepsilon_{01}t} \quad , \quad a \equiv 2(\alpha^2+\varepsilon_0) + (2-\alpha)(2+\alpha).$$

$$S_{01} = 2c_1 I(\alpha,1,1,1,5). \qquad C.1$$

$$A_{00} = 2\left(\alpha+\frac{1}{R}\right)e^{-2\alpha R} - \frac{2}{R}. \qquad C.2$$

$$B_{11} = g_0 - 4f(0,2,0) - 4F(0,2,4,0). \qquad C.3$$

$$K_{01} = -c_1\Big[g_1 \cdot I(\alpha,1,1,1,5) + 2I(\alpha,1,0,1,3)$$

$$+ (2+\alpha)I(2+2\alpha,1,1,1,5) + 2I(2+2\alpha,1,0,1,3)\Big]. \qquad C.4$$

$$K_{10} \equiv K_{01}^{*} + k_{10}$$

$$k_{10} = -c_1\Big[a I(\alpha,1,1,1,5) - 2\alpha I(\alpha,1,0,1,3) + 2I(\alpha,1,1,0,3)\Big]. \qquad C.5$$

Appendix D

List of integrals for H^+ + $He(1s^2) \rightarrow H(1s, 2s, 2p\quad) + He^+(1s)$, using the helium wave function (3.21).

The integrals h_{00}, h_{11}, S_{01}, K_{01} and K_{11} are given in Appendix C.

$$c_2 \equiv \frac{4\alpha^3}{(2+\alpha)^3} e^{i\varepsilon_{02}t}, \quad a \equiv 2(\alpha^2+\varepsilon_0) + (2-\alpha)(2+\alpha), \quad b \equiv \frac{1}{\sqrt{2}} e^{-i\frac{3}{8}t}$$

$$S_{02} = c_2 \left[4\, I(\alpha, 0{\cdot}5, 1, 1, 5) - I(\alpha, 0{\cdot}5, 1, 2, 7)\right] \qquad D\cdot 1$$

$$S_{03} = 2\rho\, c_2\, I(\alpha, 0{\cdot}5, 1, 2, 5) \qquad D\cdot 2$$

$$S_{04} = 2c_2 \left[vt\, I(\alpha, 0{\cdot}5, 1, 2, 5) - \frac{iv}{\alpha} I(\alpha, 0{\cdot}5, 2, 2, 7)\right] \qquad D\cdot 3$$

$$\begin{aligned} B_{12} = -b\Big[& 2f(0, 1{\cdot}5, 0) - f(1, 1{\cdot}5, 0) \\ & + 2F(0, 1{\cdot}5, 4, 0) - F(1, 1{\cdot}5, 4, 0)\Big] \end{aligned} \qquad D\cdot 4$$

$$B_{13} = -b\left[f(1, 1{\cdot}5, 1) + F(1, 1{\cdot}5, 4, 1)\right] \frac{\rho}{R} \qquad D\cdot 5$$

$$B_{14} = -b\left[f(1, 1{\cdot}5, 1) + F(1, 1{\cdot}5, 4, 1)\right] \frac{vt}{R} \qquad D\cdot 6$$

$$B_{22} = \mathcal{J}_0 - \frac{1}{2} f(0,1,0) + \frac{1}{2} f(1,1,0) - \frac{1}{8} f(2,1,0)$$

$$- \frac{1}{2} F(0,1,4,0) + \frac{1}{2} F(1,1,4,0) - \frac{1}{8} F(2,1,4,0) \qquad \text{D.7}$$

$$B_{23} = \frac{\rho}{8R} \Big[2f(1,1,1) - f(2,1,1) + 2F(1,1,4,1) - F(2,1,4,1) \Big] \qquad \text{D.8}$$

$$B_{24} = \frac{vt}{8R} \Big[2f(1,1,1) - f(2,1,1) + 2F(1,1,4,1) - F(2,1,4,1) \Big] \qquad \text{D.9}$$

$$B_{33} = \mathcal{J}_0 - \frac{1}{24} \Big[f(2,1,0) - f(2,1,2) + F(2,1,4,0) - F(2,1,4,2) \Big]$$

$$- \frac{\rho^2}{8R^2} \Big[f(2,1,2) + F(2,1,4,2) \Big] \qquad \text{D.10}$$

$$B_{34} = - \frac{\rho v t}{8R^2} \Big[f(2,1,2) + F(2,1,4,2) \Big] \qquad \text{D.11}$$

$$B_{44} = \mathcal{J}_0 - \frac{1}{24} \Big[f(2,1,0) + F(2,1,4,0) \Big]$$

$$+ \left(\frac{\rho^2}{8R^2} - \frac{1}{12} \right) \Big[f(2,1,2) + F(2,1,4,2) \Big] \qquad \text{D.12}$$

$$K_{02} = - c_2 \Big[2 \mathcal{J}_1 \cdot I(\alpha, 0.5, 1, 1, 5) + 4 I(\alpha, 0.5, 0, 1, 3)$$

$$+ (4 + 2\alpha) I(2+2\alpha, 0.5, 1, 1, 5) + 4 I(2+2\alpha, 0.5, 0, 1, 3)$$

$$- \frac{1}{2} \mathcal{J}_1 \cdot I(\alpha, 0.5, 1, 2, 7) - I(\alpha, 0.5, 0, 2, 5)$$

$$- \left(1 + \frac{\alpha}{2}\right) I(2+2\alpha, 0.5, 1, 2, 7) - I(2+2\alpha, 0.5, 0, 2, 5) \Big] \qquad \text{D.13}$$

$$K_{03} = -c_2\rho\Big[g_1 \cdot I(\alpha,0{\cdot}5,1,2,5) + 2I(\alpha,0{\cdot}5,0,2,3)$$

$$+(2+\alpha)I(2+2\alpha,0{\cdot}5,1,2,5)+2I(2+2\alpha,0{\cdot}5,0,2,3)\Big] \qquad \text{D}\cdot 14$$

$$K_{04} = -c_2 v t\Big[g_1 \cdot I(\alpha,0{\cdot}5,1,2,5) + 2I(\alpha,0{\cdot}5,0,2,3)$$

$$+(2+\alpha)I(2+2\alpha,0{\cdot}5,1,2,5)+2I(2+2\alpha,0{\cdot}5,0,2,3)\Big]$$

$$+ic_2 v\Big[\frac{1}{\alpha}g_1 \cdot I(\alpha,0{\cdot}5,2,2,7) + \frac{2}{\alpha}I(\alpha,0{\cdot}5,1,2,5)$$

$$+\frac{(2+\alpha)}{(2+2\alpha)}I(2+2\alpha,0{\cdot}5,2,2,7)+\frac{1}{(1+\alpha)}I(2+2\alpha,0{\cdot}5,1,2,5)\Big] \qquad \text{D}\cdot 15$$

$$K_{i0} \equiv K_{0i}^{*} + k_{i0} \qquad i = 1,2,3,4 .$$

$$k_{20} = -c_2\Big[2aI(\alpha,0{\cdot}5,1,1,5) - 4\alpha I(\alpha,0{\cdot}5,0,1,3) + 2I(\alpha,0{\cdot}5,1,0,3)$$

$$-\frac{a}{2}I(\alpha,0{\cdot}5,1,2,7)+\alpha I(\alpha,0{\cdot}5,0,2,5)-I(\alpha,0{\cdot}5,1,1,5)\Big]^{*} \qquad \text{D}\cdot 16$$

$$k_{30} = -c_2\rho\Big[aI(\alpha,0{\cdot}5,1,2,5) - 2\alpha I(\alpha,0{\cdot}5,0,2,3)+2I(\alpha,0{\cdot}5,1,1,3)\Big]^{*} \qquad \text{D}\cdot 17$$

$$k_{40} = -c_2 v t\Big[aI(\alpha,0{\cdot}5,1,2,5) - 2\alpha I(\alpha,0{\cdot}5,0,2,3)+2I(\alpha,0{\cdot}5,1,1,3)\Big]^{*}$$

$$+ic_2 v\Big[\frac{1}{\alpha}I(\alpha,0{\cdot}5,2,2,7)-2I(\alpha,0{\cdot}5,1,2,5)+\frac{2}{\alpha}I(\alpha,0{\cdot}5,2,1,5)\Big]^{*} \qquad \text{D}\cdot 18$$

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FIGURE LEGENDS

FIG. 1 & 2

Total cross sections for the reaction $H^+ + He(1s^2) \rightarrow H + He^+$.

Curve 1 : Born approximation (Mapleton, 1961)

Curve 2 : Impulse approximation (Bransden and Cheshire, 1963)

Curve 3 : Present calculations $H^+ + He(1s^2) \rightarrow H(1s, 2s, 2p) + He^+(1s)$

X : Experimental points (Allison, 1958. Barnett and Reynolds, 1958)

FIG. 3

Cross sections for the capture into the state H (1s)

Curve : Present calculations $H^+ + He(1s) \rightarrow H(1s, 2s, 2p) + He^+(1s$

Results of Green et al (1965)

\+ Results of Bransden et al (1966)

& + are calculated for $H^+ + He^2(1s) \rightarrow H(1s) + He^+(1s)$

FIG. 4

Cross sections for the capture into the state H(2s)

Curve 1 : Average of the post and prior cross sections in the Born approximation (Mapleton, 1961).

$H^+ + He(1s^2) \rightarrow H(2s) + He^+(1s)$

Curve 2 : Present calculations $H^+ + He(1s^2) \rightarrow H(1s, 2s, 2p) + He^+(1s$

Experimental points $H^+ + He(1s^2) \rightarrow H(2s) + He^+$

⊙ Colli et al (1962)

x Jaecks et al (1965) ; Andreev et al (1966)

FIG. 5

Cross section for the capture into the state H(2p)

Curve 1 : Average of the post and prior cross sections in the Born approximation (Mapleton, 1961)

$H^{+} + He(1s^{2}) \rightarrow H(2p) + He^{+}(1s)$

Curve 2 : Present calculations $H^{+} + He(1s^{2}) \rightarrow H(1s, 2s, 2p) + He^{+}(1s)$

Experimental Points X = Andreev et al (1966) ; Pretzer et al (1963)

θ = de Heer et al (1963)

$H^{+} + He(1s^{2}) \rightarrow H(2p) + He^{+}$

FIG. 6

Probability x impact parameter for capture into H(1s)

$H^{+} + He(1s^{2}) \rightarrow H(1s, 2s, 2p) + He^{+}(1s)$

Normalisation Facter is:-

N = $1{\cdot}37 \times 10^{2}$ at 1 keV, N = $2{\cdot}94$ at 6.25 keV,

N = $1{\cdot}35$ at 30.2 keV, N = $1{\cdot}48 \times 10^{4}$ at 1 MeV

FIG. 7

Probability x impact parameter for capture into H(2s)

$H^{+} + He(1s^{2}) \rightarrow H(1s, 2s, 2p) + He^{+}(1s)$

Normalisation Factor is:-

N = $4{\cdot}65 \times 10^{3}$ at keV, N = $1{\cdot}25 \times 10^{2}$ at 6.25 keV,

N = $3{\cdot}92 \times 10$ at 30.2 keV, N = $1{\cdot}23 \times 10^{5}$ at 1 MeV.

FIG. 8

Probability x impact parameter for capture into H(2p)

$H^{+} + He(1s^{2}) \rightarrow H(1s, 2s, 2p) + He^{+}(1s)$

Normalisation Factor is:-

N = $1{\cdot}46 \times 10^{3}$ at 1keV, N = $3{\cdot}81 \times 10$ at 6.25 keV,

N = $4{\cdot}45 \times 10$ at 30.2 keV, N = $7{\cdot}90 \times 10^{6}$ at 1 MeV.

FIG. 9

Total capture probability

Present work $H^+ + He(1s^2) \rightarrow H(1s, 2s, 2p) + He^+(1s)$

Experimental results (Helbig et al., 1964) $H^+ + He(1s^2) \rightarrow H + He^+$

FIG. 10

Probability for capture into H(1s)

Curve 1 : Results of Green (1966)

$H^+ + He(1s^2) \rightarrow H(1s) + He^+(1s)$

Curve 2 : Present calculations

$H^+ + He(1s^2) \rightarrow H(1s, 2s, 2p) + He^+(1s)$

FIG. 11

Probability for capture into H(2s)

$H^+ + He(1s^2) \rightarrow H(1s, 2s, 2p) + He^+(1s)$

x : Corresponding experimental point of Dose and Meyer (1966) at $\theta T = 20$.

FIG. 12

Probability for capture into H(2p)

$H^+ + He(1s^2) \rightarrow H(1s, 2s, 2p) + He^+(1s)$

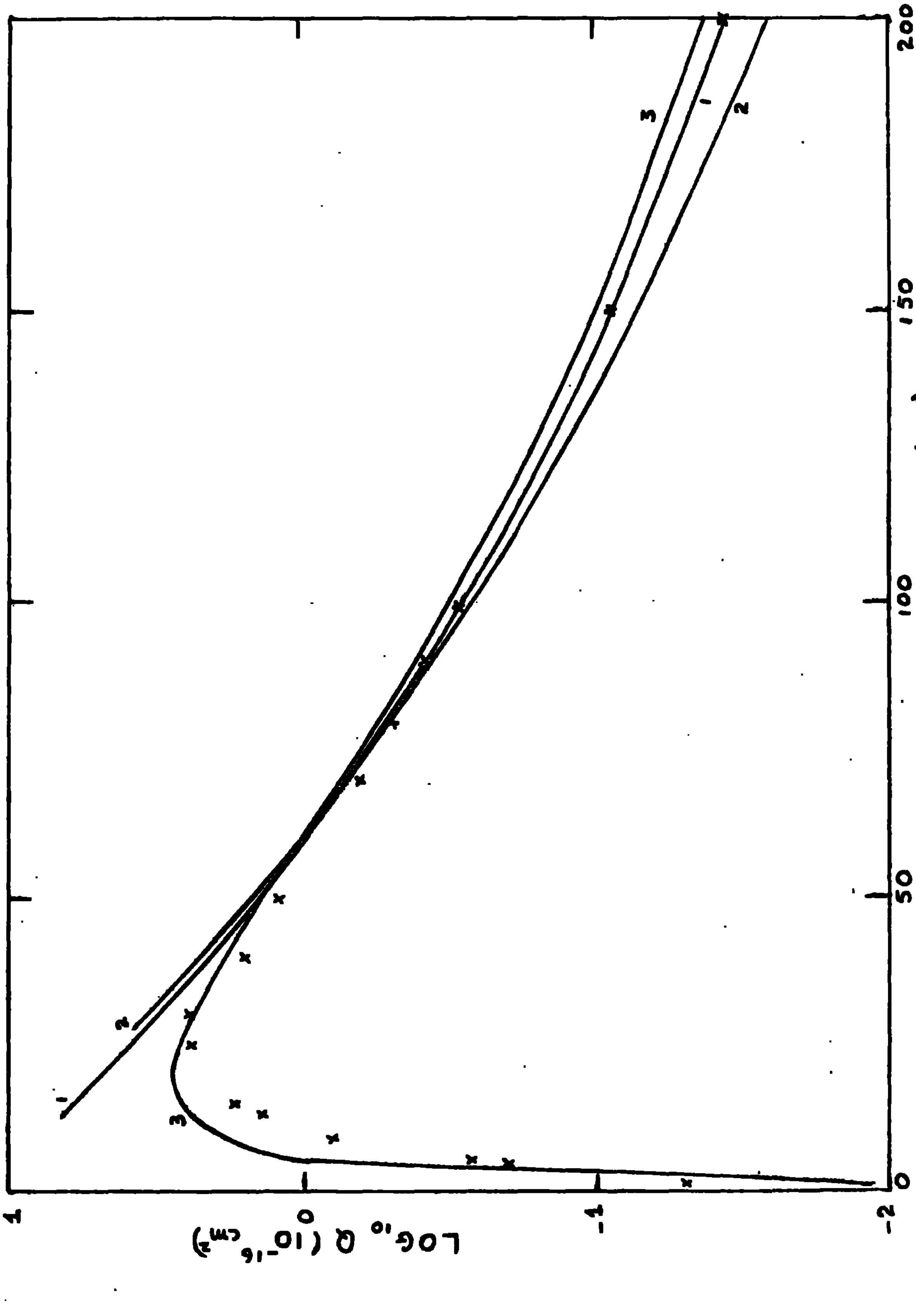

1
0
-1
-2
LOG₁₀ Q (10⁻¹⁶ cm²)
0
50
100
150
200
INCIDENT PROTON ENERGY (keV)
1
2
3
3
1
2

FIG. 1

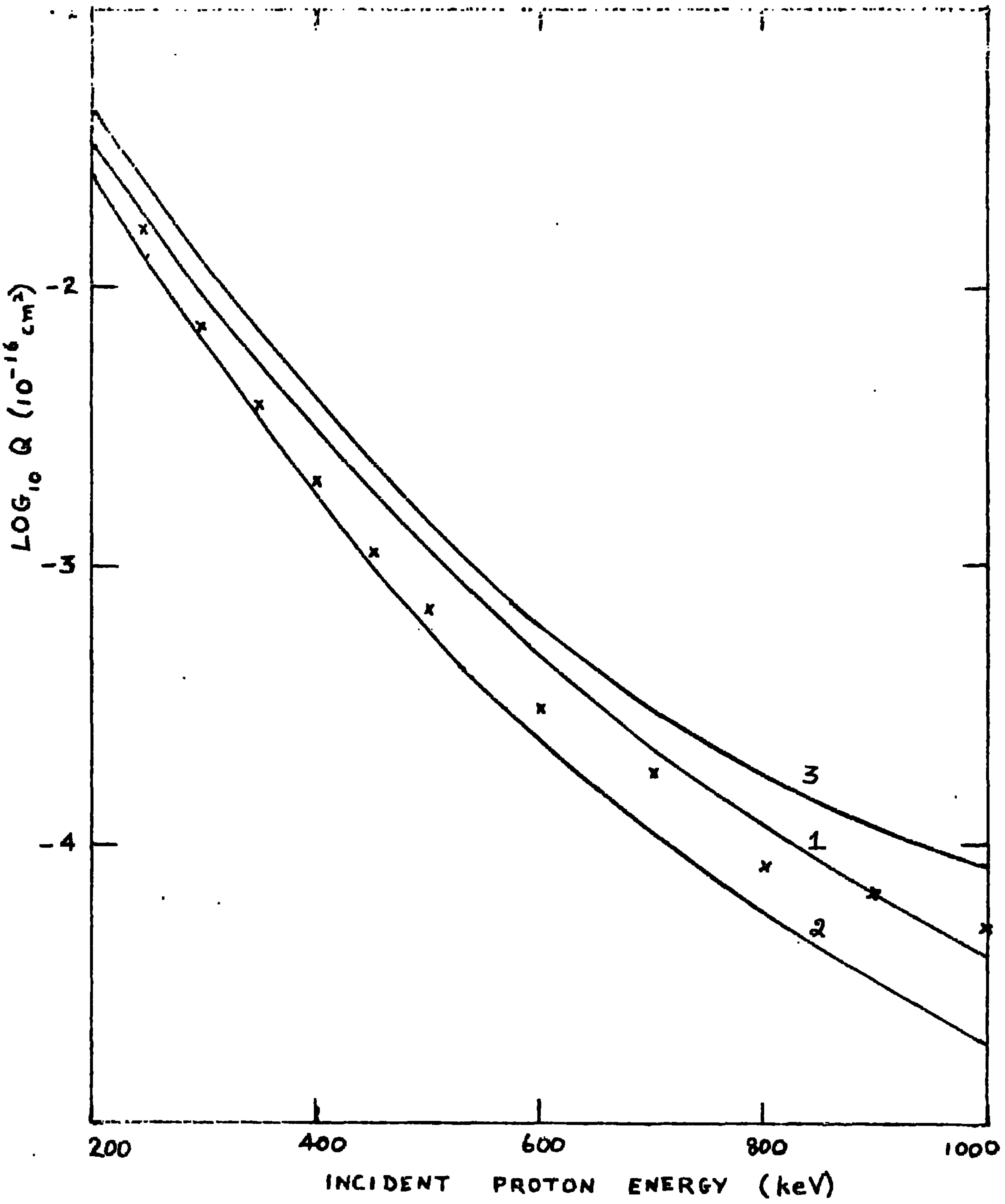

LOG$_{10}$ Q (10^{-16} cm^2)
-2
-3
-4
3
1
2
200
400
600
800
1000
INCIDENT PROTON ENERGY (keV)

FIG. 2

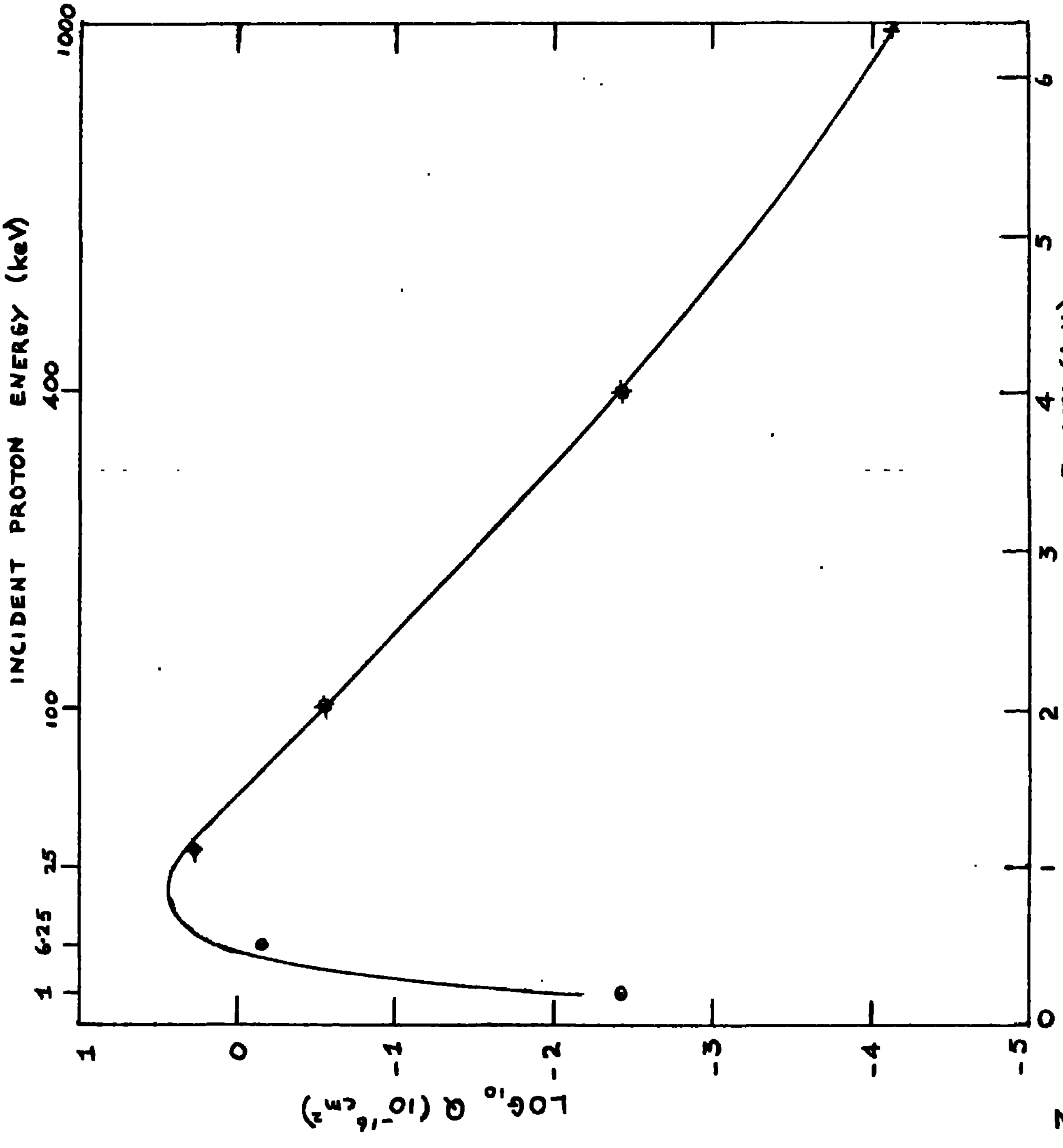

INCIDENT PROTON ENERGY (keV)
1
6·25
25
100
400
1000
INCIDENT PROTON VELOCITY (A·U·)
0
1
2
3
4
5
6
LOG10 Q (10^-16 cm^2)
1
0
-1
-2
-3
-4
-5

FIG. 3

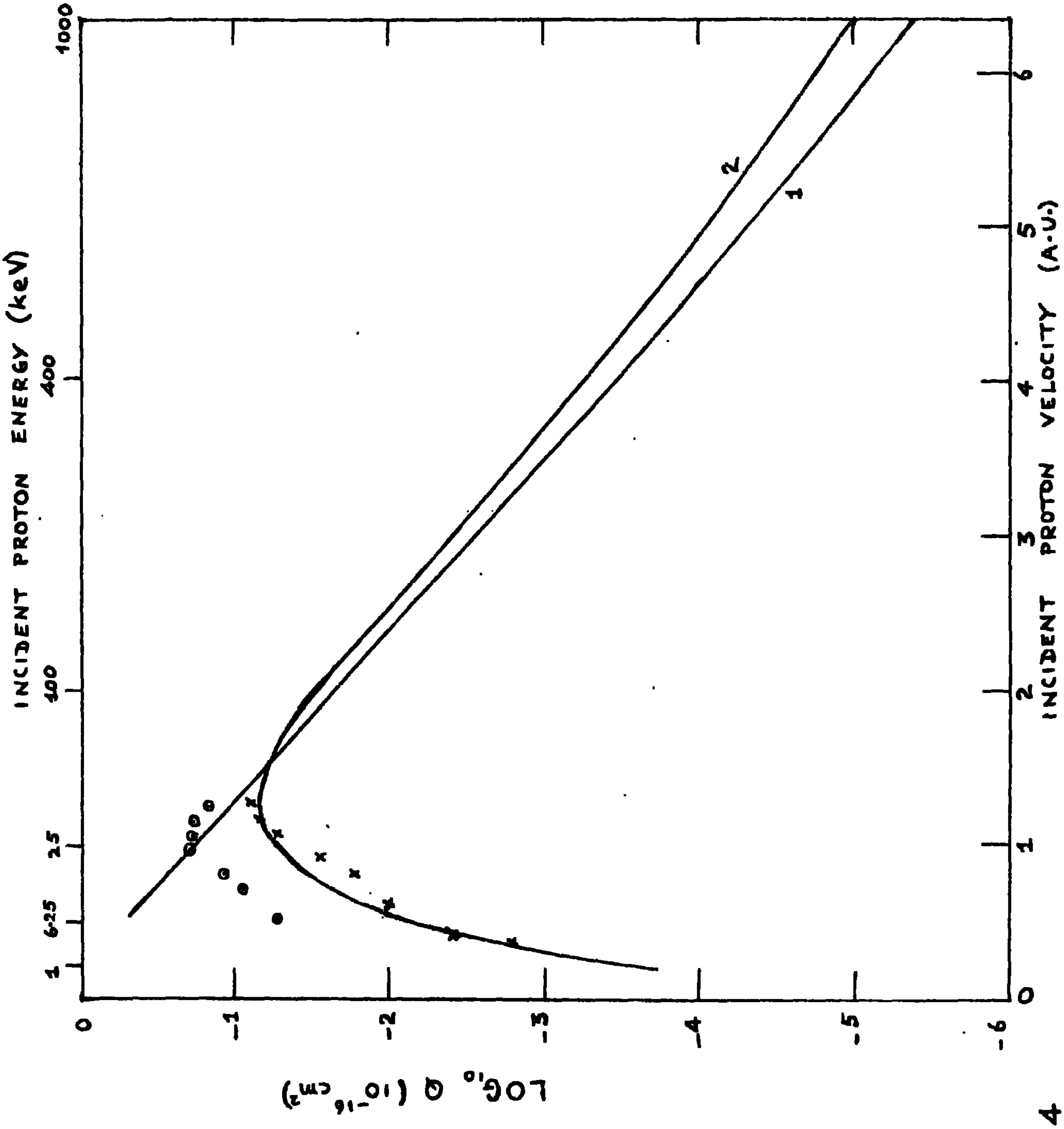

INCIDENT PROTON ENERGY (keV)
1
6.25
25
100
400
1000
INCIDENT PROTON VELOCITY (A.U.)
0
1
2
3
4
5
6
LOG_{10} Q (10^{-16} cm^2)
0
-1
-2
-3
-4
-5
-6
1
2

FIG. 4

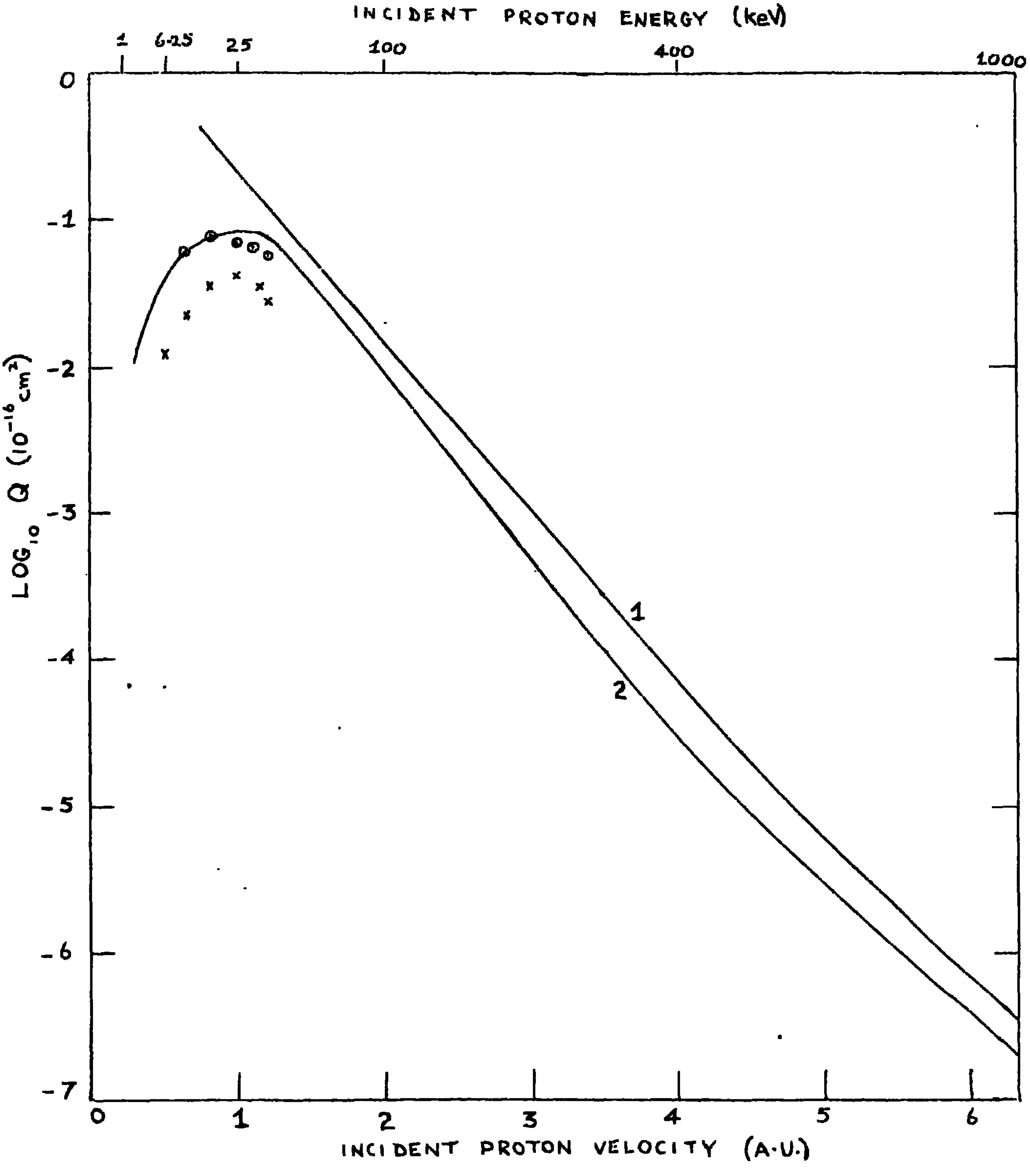

INCIDENT PROTON ENERGY (keV)
1
6.25
25
100
400
1000
0
-1
-2
-3
-4
-5
-6
-7
LOG$_{10}$ Q (10^{-16}cm^2)
1
2
0
1
2
3
4
5
6
INCIDENT PROTON VELOCITY (A.U.)

FIG. 5

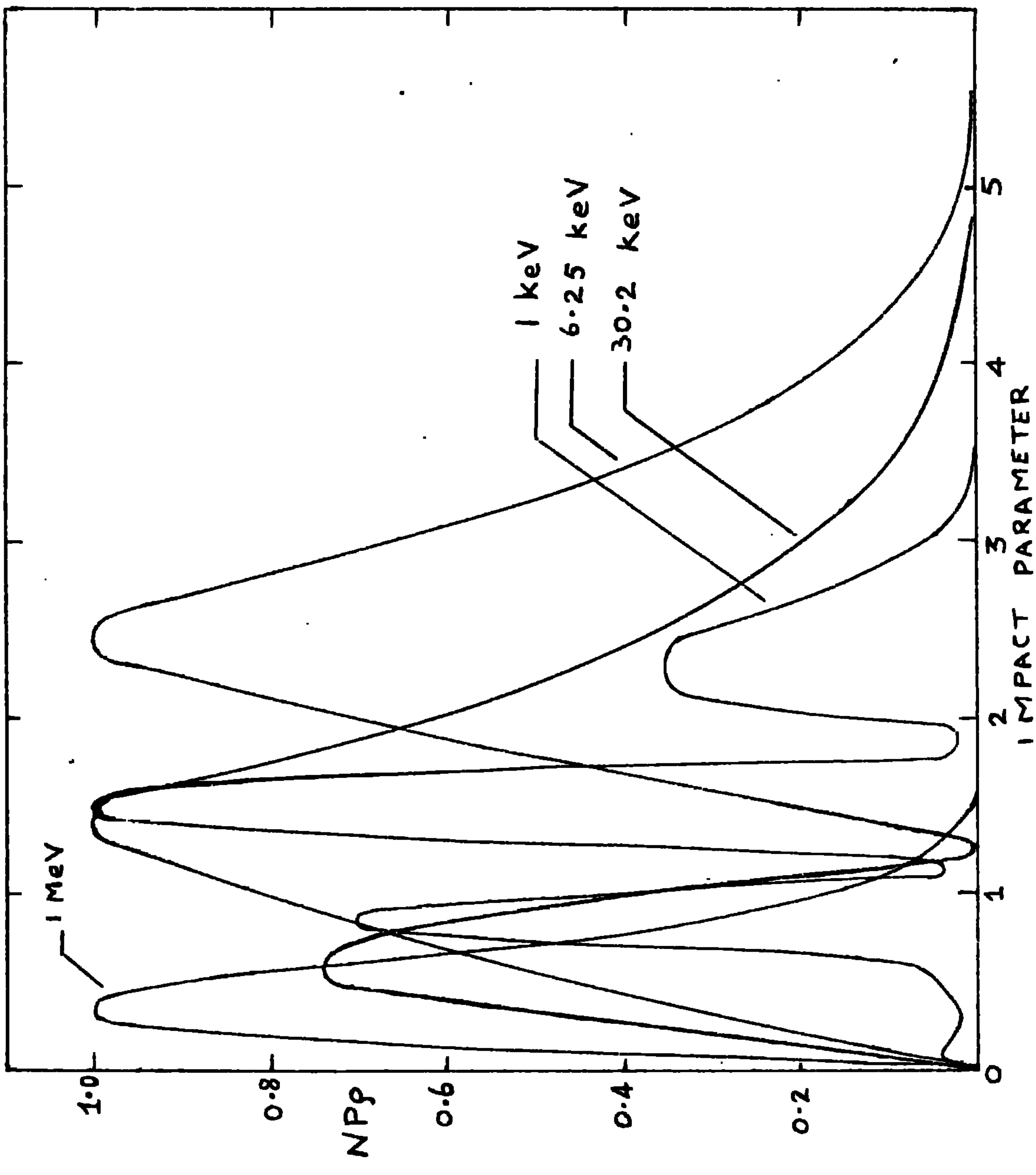

1 MeV
1 keV
6·25 keV
30·2 keV
NPρ
1·0
0·8
0·6
0·4
0·2
0
1
2
3
4
5
IMPACT PARAMETER

FIG. 6

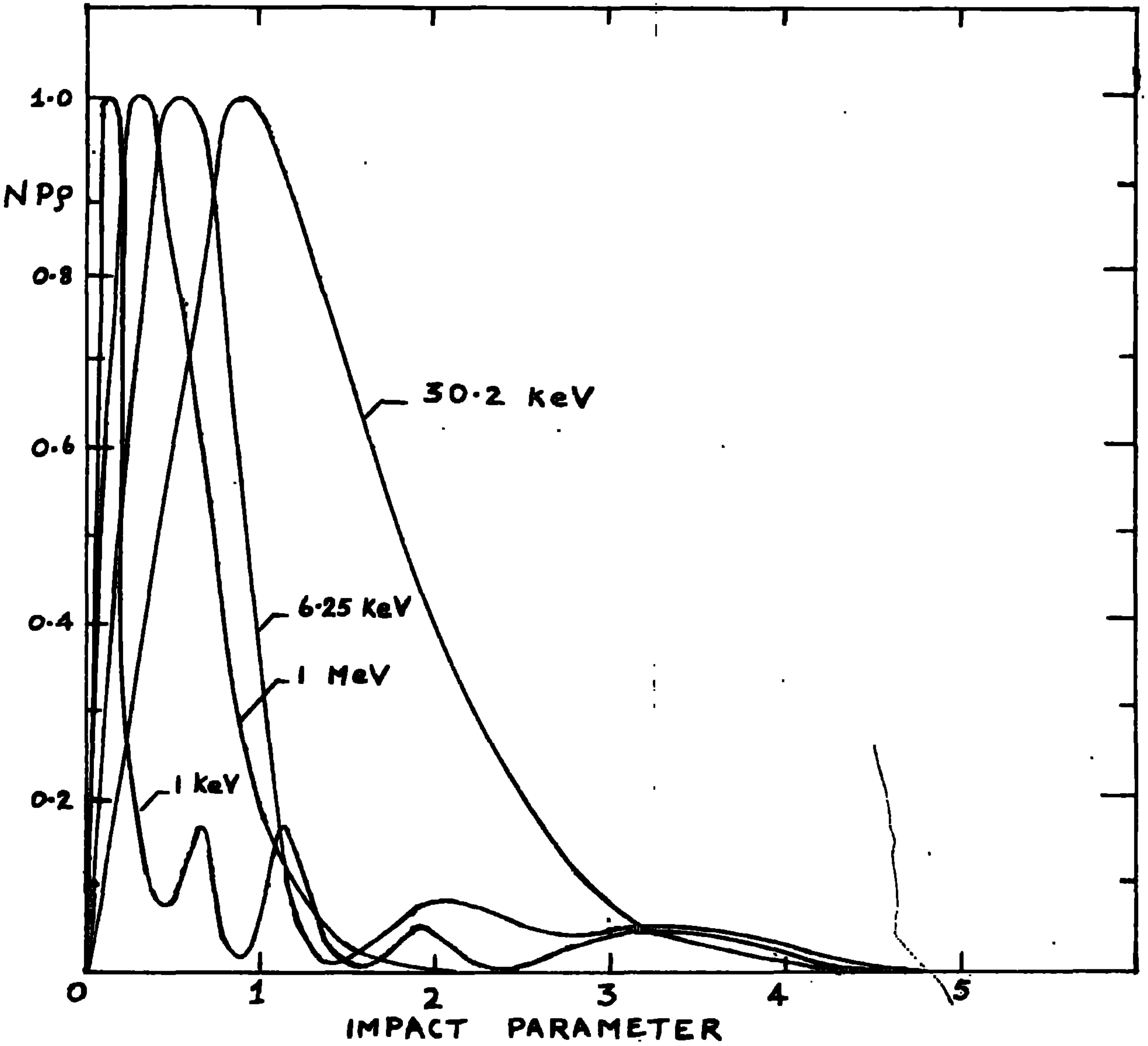
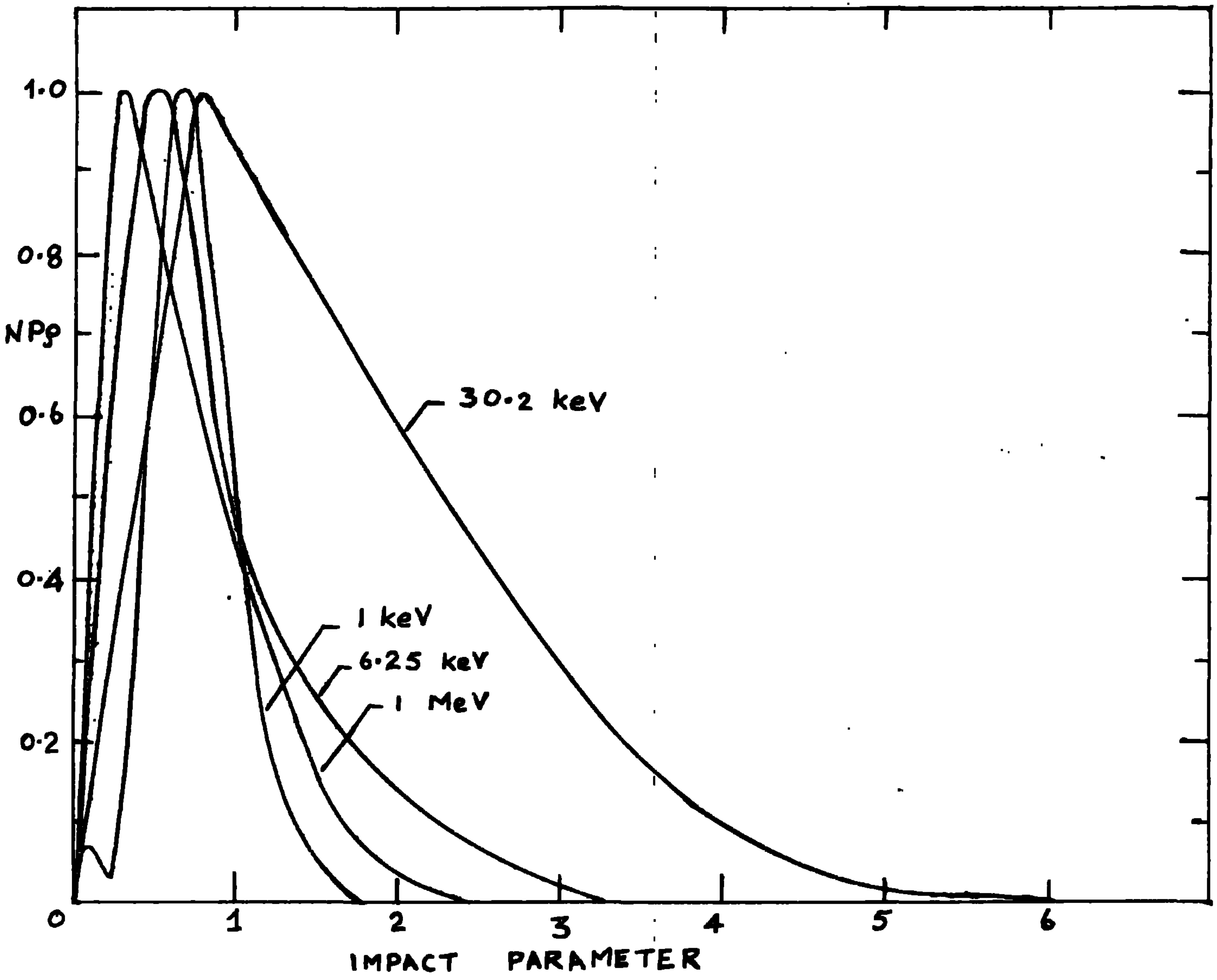

NPρ
1·0
0·8
0·6
0·4
0·2
0
1
2
3
4
5
IMPACT PARAMETER
30·2 keV
6·25 KeV
1 MeV
1 keV

FIG. 7


1·0
0·8
NPρ
0·6
0·4
0·2
0
1
2
3
4
5
6
IMPACT PARAMETER
30·2 keV
1 keV
6·25 keV
1 MeV

FIG· 8

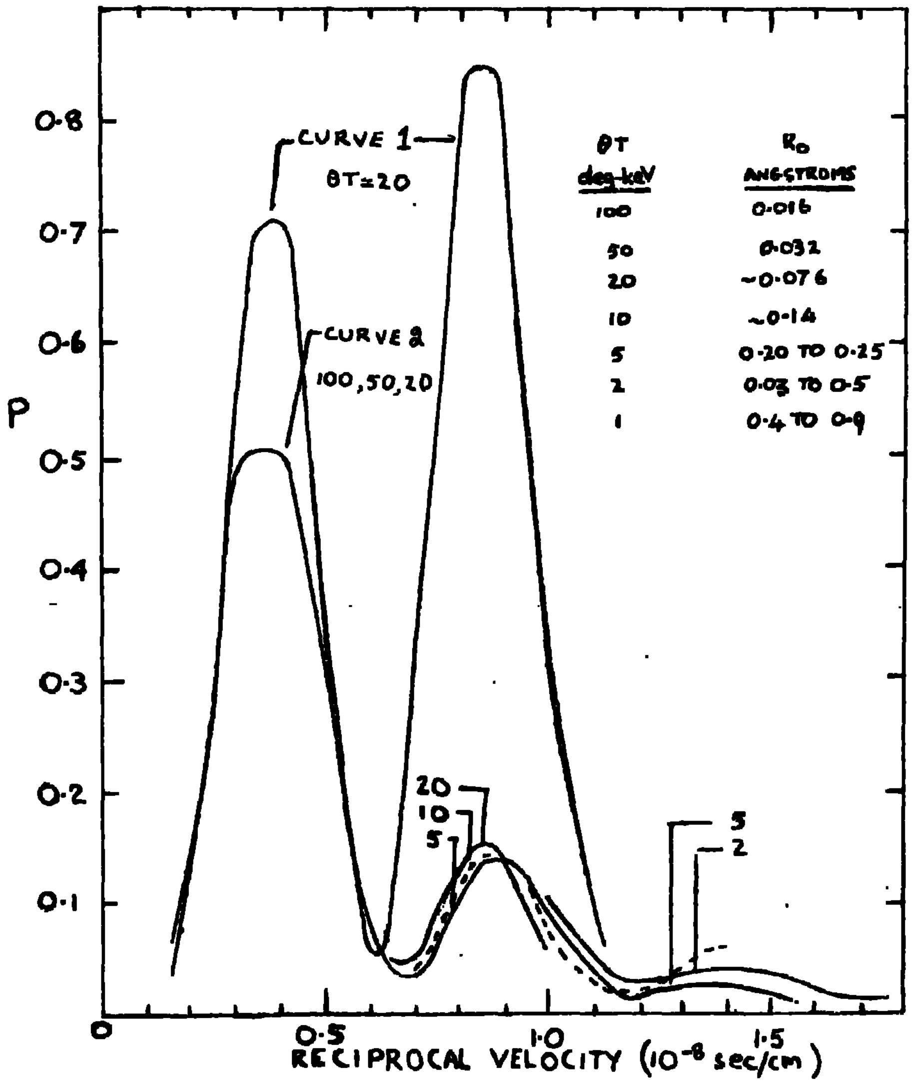

CURVE 1
θT=20
CURVE 2
100,50,20
θT deg-keV
R₀ ANGSTROMS
100 0·016
50 0·032
20 ~0·076
10 ~0·14
5 0·20 TO 0·25
2 0·03 TO 0·5
1 0·4 TO 0·9
20
10
5
5
2
P
0·1
0·2
0·3
0·4
0·5
0·6
0·7
0·8
0
0·5
1·0
1·5
RECIPROCAL VELOCITY (10⁻⁸ sec/cm)

FIG 9

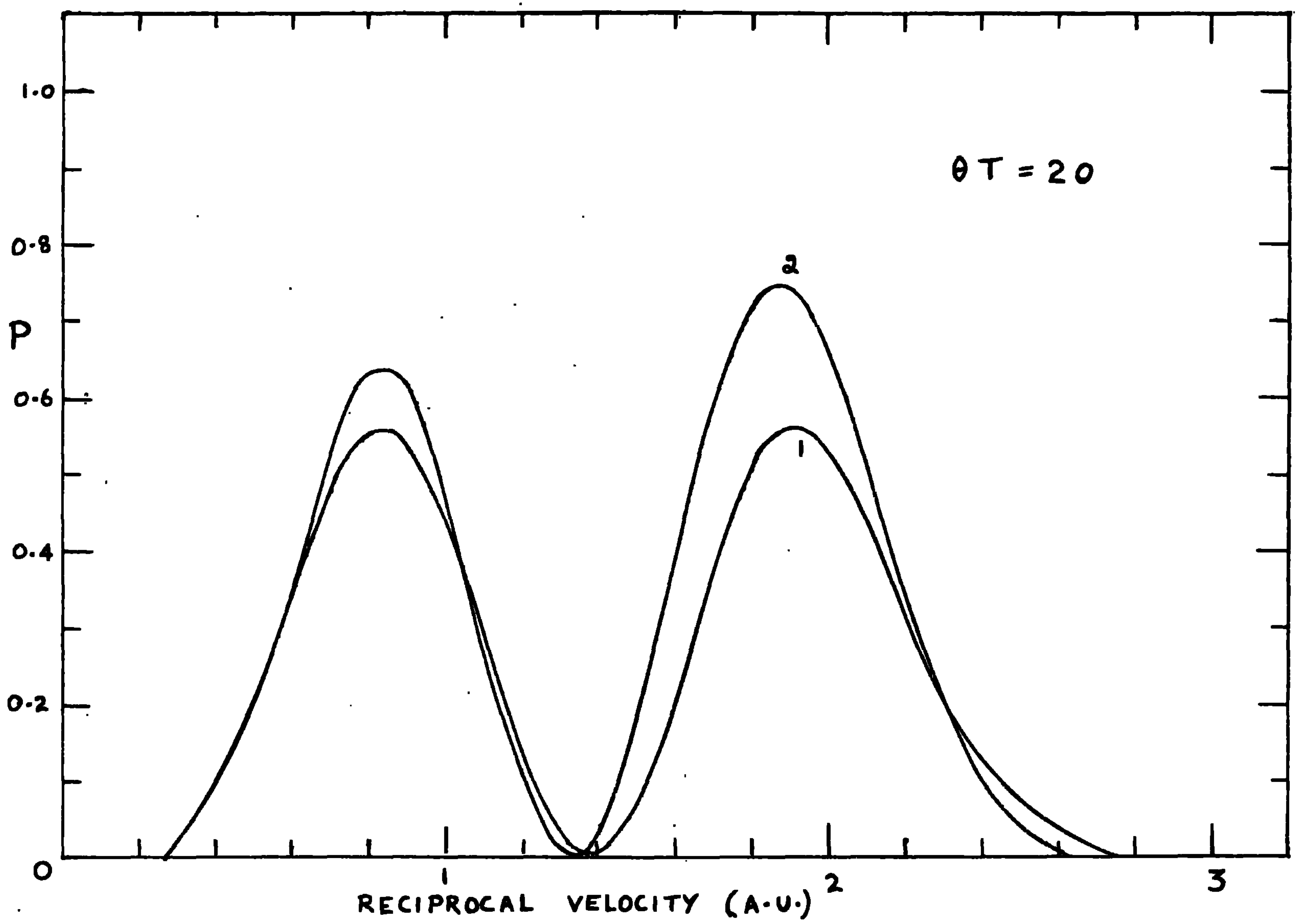


FIG. 10

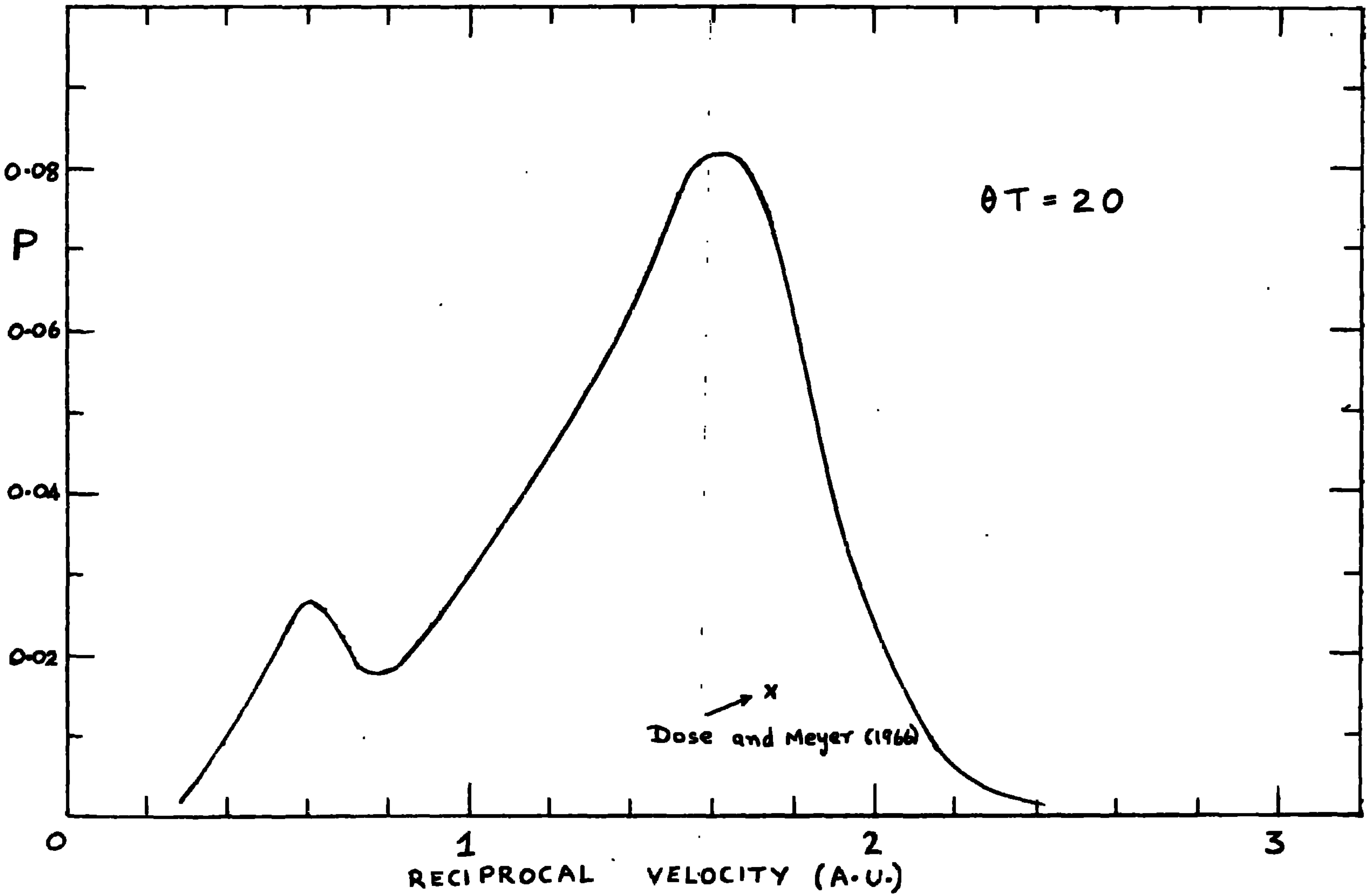

θT = 20
P
0·08
0·06
0·04
0·02
0
1
2
3
RECIPROCAL VELOCITY (A.U.)
x
Dose and Meyer (1966)

FIG. 11

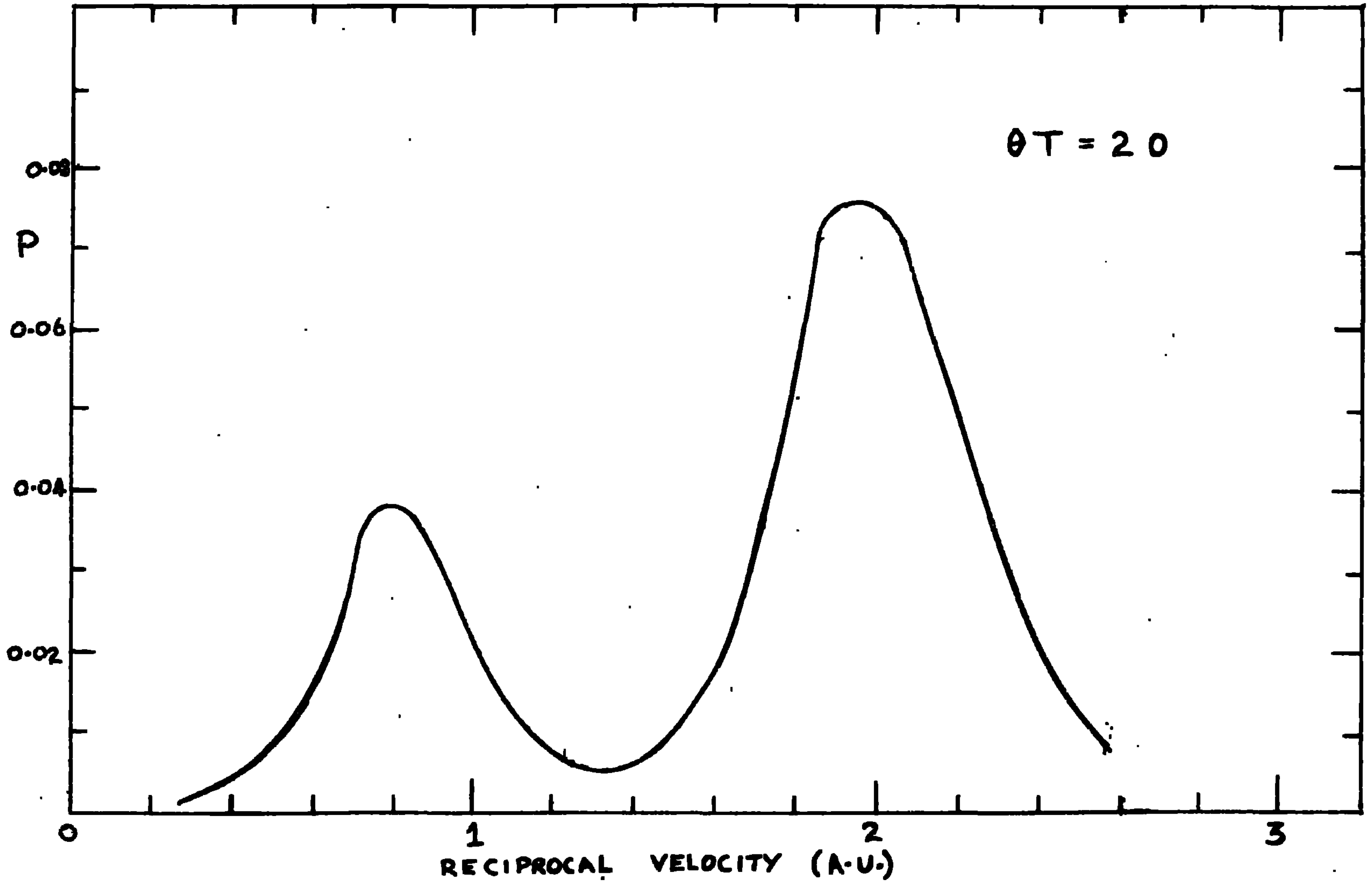


FIG. 12

TABLE 1.

Cross Sections for $H^+ + He\ (1s^2) \longrightarrow H(1s) + He^+\ (1s)$, calculated by Green, Stanley, and Chiang (1965).

Proton Energy (KeV)	Cross Sections (10^{-16} cm^2) (1)	(2)	(3)	(4)
1	7.852, - 1	5.862, - 3	1.815, - 1	3.553, - 3
6.25	4.571	1.025	1.95	7.48, - 1
30.2	2.393	2.274	2.015	1.916
100	2.666, - 1	2.897, - 1	2.553, - 1	2.756, - 1
400	3.412, - 3	3.543, - 1		

(1) Calculated with distortion and probability conservation neglected; (2) calculated with only probability conservation neglected; (3) Calculated with only distortion neglected; (4) calculated with both distortion and probability conservation takin into account.

TABLE 2.

Cross sections for $H^+ + He\ (1s^2) \longrightarrow H(1s) + He^+(1s)$.

Proton Energy (KeV)	Cross Sections (10^{-16} cm^2)				
	(1)	(2)	(3)	(4)	(5)
1				3.55, - 3	5.0, - 2 (a)
6.25				7.48, - 1	5.6, - 1 at7keV (b)
30.2	2.19	2.14	2.02	1.92	1.95 (b)
100	2.90, - 1	2.93, - 1	2.85, - 1	2.76, - 1	3.0, - 1 (b)
400	3.66, - 3	3.66, - 3	3.51, - 3	3.54, - 3	2.0, - 3 (c)
1,000	7.4, - 5		7.1, - 5		5.0, - 5 (c)
10,000	3.1, - 10		3.4, - 10		(1.2 ± 0.4),-10 (d)

(1) Calculated with simple helium wave function $X^{(1)}$; (2) calculated with helium wave function $X^{(2)}$ of Green et al. 1954; (3) calculated with helium wave function $X^{(3)}$ of Eckart 1930; (4) results of Green et al. 1965; (5) experimental total cross sections. (a) Hasted 1955; (b) Stier and Barnett 1956; (c) Barnett and Reynolds 1958; (d) Berkner et al. 1965, University of California Rep. UCRL - 16054 (this experiment employed 21 MeV deuterons).

(1), (2) and (3) are present calculations.

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