Scattering of protons from helium

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Abstract

The main work described in this thesis, is the original calculation of the excitation of helium by proton and of electron - capture process from helium by proton where the 2nd order potential introduced by Bransden & Coleman (1972) has been applied.

It begins with a discussion of the existing methods relevant to the present work and followed by the construction of a second - order potential. A critical survey of the previous work has also been presented and its relation to the present work and result is d iscussed.

The cross-sections for the following processes is calculated in the energy - range indicated

(i) $p + He(1S^2) \longrightarrow H^+(1S,2S,2p) + He(1S^2)$ 25 Kev - 500 Kev

(ii) $p + He(1S^2) \longrightarrow H\ (1S) + He^+(1S)$ 30 Kev - 10 Mev

The calculated cross - section along with existing results has also been presented and it is seen that the present method provides better results for the excitation process, but for the charge - exchange process, our results do not agree with the results of the experiment at high energies.

CONTENTS

CHAPTER 1

Introduction

This thesis is mainly concerned with the excitation and the charge exchange of helium by protons. Examples of these reactions are:-

$$p + He\ (1S^2) \longrightarrow p + He\ (1S^2) \quad (a)$$

$$p + He\ (1S^2) \longrightarrow p + He\ (1S,2S) \quad (b)$$

$$p + He\ (1S^2) \longrightarrow H(1S) + He^+\ (1S) \quad (c)$$

The reaction (a) is known as the elastic collision where there is no change of the internal energies of the particles in atoms and where the incident particle can be deflected through a certain angle. The reaction (b) is an excitation process where the particles in the atom may be excited to different energy levels and the reaction (c) is known as the electron capture or charge - exchange process where electron from one atom is exchanged to another ion during the collision. In electron capture either or both of the hydrogen atom and helium positive ion can be excited in the final state.

The present calculations are based on the paper written by Bransden & Coleman (1972) which we have applied to both the excitation and charge - exchange reactions given above and also to excitation of the 2^1P level of helium.

Before giving a description of that method, it is necessary to discuss some other methods which have been applied to the evaluation of the cross - sections for the reactions noted above. The methods we describe here both for Direct and Rearrangement collision.

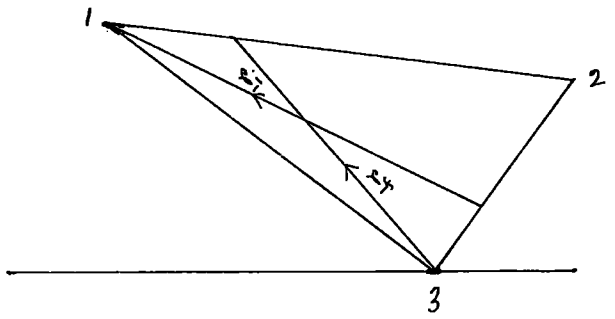


Figure 1.1

1.1 Derivation of the scattering amplitude

For the sake of simplicity, let us consider a three particle system in which the particle 1 is incident on an atom composed of an electron 2 and a nucleus 3. Then the reactions for the system for both Direct and Rearrangement cases will be given by

1 + (2 + 3) → 1 + (2 + 3) (a)

1 + (2 + 3) → 3 + (1 + 2) (b)

respectively. Our intention here, is to find an expression for scattering amplitude in both cases.

For Direct scattering, we know that the initial and final states consist of the free particle 1 moving relative to the bound particle (2 + 3). In the rearrangement system the initial state will be the same but the final state now consists of the free particle 3 and the bound particle (1 + 2). Let r_i, k_i be the position and momentum vectors of the incident particle 1 joining the centre of mass of (2 + 3) and R_1, p_1 be the position and the momentum vectors of the particle 2 and 3 in the initial state. Similarly we can define r_f, K_f, R_2, p_2 which are the necessary vectors represented by the final state. Also, we know, that the initial and

final momentum are related to $\underline{k}_i \simeq \mu_i \underline{v}_i$ and $\underline{k}_f = \mu_f \underline{v}_f$ where $\underline{v}_i$ and $\underline{v}_f$ are the initial and final velocities and μ_i and μ_f are the initial and final reduced masses respectively:

$$\mu_i = \frac{M_1(M_2+M_3)}{M_1+M_2+M_3} = \mu_f \qquad \text{(for Direct collision)}$$

$$\mu_i = \frac{M_1(M_2+M_3)}{M_1+M_2+M_3}, \qquad \mu_f = \frac{M_3(M_1+M_2)}{M_1+M_2+M_3} \qquad \text{(for Rearrangement collision)}$$

M_1, M_2, M_3 being the masses of the particles 1, 2 and 3 respectively.

Now the Schrodinger equation in the centre of mass system is

$$(H - E)\psi_i(\underline{R}_1, \underline{r}_i) = 0 \qquad (1\text{-}1)$$

where the Hamiltonian H can be expressed as

$$H = K + V_1 + V_2 + V_3$$

$$= -\frac{1}{2\mu_i}\nabla^2_{\underline{R}_1} - \frac{1}{2}\nabla^2_{\underline{r}_f} + V_1 + V_2 + V_3$$

$$\simeq -\frac{1}{2\mu_f}\nabla^2_{\underline{R}_2} - \frac{1}{2}\nabla^2_{\underline{r}_i} + V_1 + V_2 + V_3 \qquad (1\text{-}2)$$

K is the kinetic energy operator and the potential V_1 acts between particles 2 and 3, V_2 between particles 1 and 3, and V_3 between particles 2 and 1, and μ is the reduced mass. The boundary condition for the Direct collision

to be placed on ψ are that for, large $\underline{R}_1$, $\underline{r}_1$,

$$\psi \sim \sum_n \left[\delta_{no} e^{i\underline{k}_i \cdot \underline{r}_i} + \frac{f_n(\theta) e^{i\underline{k}_n \underline{r}_i}}{r_i} \right] \phi_n(\underline{R}_i) \qquad (1\text{-}3)$$

The first term in (1-3) represents the incident wave function and the 2nd term is the outgoing spherical wave describing the scattered particles and $f_n(\theta_1)$ is the scattering amplitude.

Since there is no incident wave function in the rearranged channel we require, when $\underline{R}_2$ & $\underline{r}_2$ are both large

$$\psi \sim \sum_m g_m(\theta_2) \frac{e^{i\underline{k}_f \underline{r}_f}}{r_f} \phi_m(\underline{R}_2) \qquad (1\text{-}4)$$

The differential cross - section for both direct and exchange scattering is determined by $|f_n(\theta_1)|^2$ or $|g_m(\theta_2)|^2$ respectively.

To obtain exact expressions for $f(\theta_1)$ and $g(\theta_2)$ we need the three - particles Green's function defined as

$$G_{1o}(E_i + i\epsilon) = (E_i + i\epsilon - H_o)^{-1}$$

$$G_{1i}(E_i + i\epsilon) = (E_i + i\epsilon - H_i)^{-1}$$

$$G_{1f}(E_f + i\epsilon) = (E_f + i\epsilon - H_f)^{-1}$$

$$G_1(E_i + i\epsilon) = (E_i + i\epsilon - H)^{-1}$$

where G_{1o}, G_{1i}, G_{1f}, G_1 are known as the free particle, the initial, the final and the full Green's function respectively, and $H_i = K + V_i$, $H_f = K + V_3$.

The solution of (1-1) is given by

$$\psi_i^{\pm} = \phi_i + G_i^{\pm} V_i \psi_i^{\pm} \qquad (1\text{-}5)$$

where (+) and (-) signs represents the outgoing and the incoming wave function respectively.

Using the exact defination of $G_i^{\pm}$, the equation (1-5) gives

$$\psi_i^{\pm} = \phi_i + \frac{1}{E_i \pm i\epsilon - H_i} V_i \psi_i^{\pm} \qquad (1\text{-}6)$$

Similarly, we get

$$\psi_f^{\pm} = \phi_f + \frac{1}{E_i \pm i\epsilon - H_f} V_f \psi_f^{\pm} \qquad (1\text{-}7)$$

Now, the scattering matrix is

$$S_{fi} = \langle \psi_f^- | \psi_i^+ \rangle$$

$$= \langle \psi_f^+ | \psi_i^+ \rangle + \langle \psi_f^- - \psi_i^+ | \psi_i^+ \rangle$$

$$= \delta_{fi} + \langle \phi_f | \left(\frac{1}{E_i - i\epsilon - H_f} - \frac{1}{E_i + i\epsilon - H_f} \right) V_f | \psi_i^+ \rangle$$

where

$$\langle \psi_f^+ | \psi_i^+ \rangle = \delta_{fi}$$

Since $(E_f - H_f)\psi = 0$ and $V_i = V_f$ we get

$$S_{fi} = \delta_{fi} - 2\pi i \, \delta(E_i - E_f) \langle \phi_f | V_f | \psi_i^+ \rangle \qquad (1\text{-}8)$$

where we have used the relation

$$\lim_{\epsilon \to 0} \frac{\epsilon}{\epsilon^2 + (E_i - E_f)^2} = \pi \delta(E_i - E_f)$$

The equation (1-8) is valid for the Direct collision reaction where $H = H_i + V_i = H_f + V_f$ and $V_i = V_f$

For the rearrangement collision, the conditions are that

$$H = H_i + V_i = H_f + V_f \text{ and } V_i \neq V_f$$

Therefore, by applying the formula

$$\frac{1}{P} = \frac{1}{Q} + \frac{1}{Q}(P - Q)\frac{1}{P} \qquad (1\text{-}9)$$

where $P = E_i + i\epsilon - H_i$

and $Q = E_i + i\epsilon - H_f$ and $E_i = E_f$.

we get

$$G_i^{\pm} = \frac{1}{E_i \pm i\epsilon - H_i}$$

$$= G_f^{\pm}\left[1 + (H_f - H_i)G_i^{\pm}\right]$$

$$= G_f^{\pm}\left[1 + (V_i - V_f)G_i^{\pm}\right] \qquad (1\text{-}10)$$

Substituting (1-10) into (1-5), we get

$$\psi_i^{\pm} = \phi_i + G_f^{\pm}\left[1 + (V_i - V_f)G_i^{\pm}\right]V_i\psi_i^{\pm}$$

$$\psi_i^{\pm} = \phi_i + G_f^{\pm}\left[(V_i - V_f)\phi_i + V_f\psi_i^{\pm}\right]$$

$$= \phi_i\left[1 + \frac{V_i - V_f}{E_i + i\epsilon - H_f}\right] + G_f^{\pm} V_f \psi_i^{\pm}$$

$$= \phi_i\left[\frac{E_i + i\epsilon - H_f + V_i - V_f}{E_i + i\epsilon - H_f}\right] + G_f^{\pm} V_f \psi_i^{\pm}$$

$$= \frac{i\epsilon\phi_i}{(E_i + i\epsilon - E_f)} + \frac{V_f\psi_i^{\pm}}{(E_i + i\epsilon - E_f)} \qquad (1\text{-}11)$$

where we have used $(E_f - H_f)\phi_f = 0$ and also $(E - H)\phi_i = 0$

The scattering matrix can now be obtained in the same way as above and we find again that

$$S_{fi} = \delta_{fi} - 2\pi i\,\delta(E_i - E_f)\langle\phi_f|V_f|\psi_i^{+}\rangle \qquad (1\text{-}12)$$

These relations were first proved by Lippman (1966) in the time independent theory. It is also applicable in the time dependent theory.

Equation (1-8) can be written as

$$S_{fi} = \delta_{fi} - 2\pi i\,\delta(E_i - E_f)T_{fi} \qquad (1\text{-}13)$$

where T_{fi} is known as the transition matrix from the initial state i to the final state f and is defined as

$$T_{fi} = \langle \phi_f | V_f | \psi_i^+ \rangle$$

$$= \langle \psi_f^- | V_f | \phi_i \rangle \qquad (1\text{-}14)$$

Equation (1-13) can be used to calculate the transition probability defined as

$$W_{fi} = \frac{\partial}{\partial t} | \langle \psi_f | \psi_i^+ \rangle |^2$$

$$= \frac{2\pi}{\hbar} | T_{fi} |^2 \delta(E_i - E_f) \qquad (1\text{-}15)$$

The required scattering amplitude is given by

$$f(\theta) = - \frac{\mu_f}{2\pi} W_{fi} \qquad (1\text{-}16)$$

and the total cross - section from the initial state i to the final state f is

$$Q_{if} = \frac{2\pi}{\hbar} \frac{\mu_f}{\mu_i} \int | f(\theta) |^2 d\Omega$$

$$= \frac{2\pi}{\hbar} \frac{\mu_f}{\mu_i} \int | T_{fi} |^2 d\Omega \qquad (1\text{-}17)$$

1.2 The Born Series

From the previous chapter we know that the transition probability from the initial state i for the final state f is

$$W_{fi} = \frac{2\pi}{\hbar} |T_{fi}|^2$$

where

$$T_{fi} = \langle \phi_f | V_f | \psi_i^{\pm} \rangle \qquad (1\text{-}18)$$

As it is very difficult to calculate the transition matrix keeping the exact expressions ψ_i^+ or ψ_i^-, various approximations have been introduced. One of them is the Born approximation which can be described as below. The Born approximation is expected to be valid for higher energies.

Also from equation (1-5), we find

$$\psi_i^{\pm} = \phi_i + G_i^{\pm} V_i \psi_i^{\pm}$$

$$= \phi_i + G_i^{\pm} V_i \phi_i$$

$$\therefore \psi_i (1 + G_i^{\pm} V_i) \phi_i \qquad (1\text{-}19)$$

Therefore

$$T_{fi} = \langle \phi_f | V_f | (1 + G_i^{\pm} V_i) \phi_i \rangle \qquad (1\text{-}20)$$

We also know from the previous section that

$$G_i^{\pm} = \frac{1}{E_i \pm i\epsilon - H}$$

$$= \frac{1}{E_i \pm i\epsilon - H_i - V_i}$$

$$= \frac{1}{(E_i \pm i\epsilon - H_i)\left(1 - \frac{V_i}{E_i \pm i\epsilon - H_i}\right)}$$

$$= G_i^{\pm}\,(1 - V_i G_i^{\pm})$$

$$= G_i^{\pm}\,(1 + V_i G_i^{\pm} + V_i G_i^{\pm} V_i G_i^{\pm} + \cdots\cdots) \qquad (1\text{-}21)$$

Similarly we can express $G^{\pm}$ in terms of $G_0^{\pm}$ which can be expressed as the series

$$G^{\pm} = G_0^{\pm}\,(1 + V_0 G_0^{\pm} + V_0 G_0^{\pm} V_0 G_0^{\pm} + \cdots\cdots) \qquad (1\text{-}22)$$

The equation (1-20) can be expressed either in terms of $G_i^{\pm}$ or $G_{i0}^{\pm}$ and we find

$$T_{fi} = \langle \phi_f | V_f | \phi_i \rangle + \langle \phi_f | V_f | G_i^{\pm} \phi_i \rangle + \langle \phi_f | V_f | V_i G_i^{\pm} \phi_i \rangle + \cdots \qquad (1\text{-}23)$$

$$= \langle \phi_f | V_f | \phi_i \rangle + \langle \phi_f | V_f | G_0^{\pm} \phi_i \rangle + \langle \phi_f | V_f | V_i G_0^{\pm} \phi_i \rangle + \cdots \qquad (1\text{-}24)$$

The series (1-23) and (1-24) are both known as Born Series. The first term of this series is known as the first Born approximation to the scattering amplitude. Similarly when we add the second term with the first term we obtain the second Born approximation. In the same way, we can define the third Born approximation, but for high energies it is believed that the third and the other terms of the Born Series can be neglected.

The convergence of the Born Series for potential scattering has been discussed by Kohn (1952), Jost and Pais (1951), Manning (1965), but the problems encountered in the three particle system are rather different. Recently Dettmann & Leibfried (1968), Rubin et al (1966, 1967) have concluded that the Born expansion for the three particle system with short range forces converges for all energies for both the Rearrangement and the Direct collisions. No proof of the Born series for particles interacting via the long range coulomb potential is available. The previous work based on this method for the Direct and the Rearrangement collision will be discussed in Chapter 3 and Chapter 5 respectively.

1.3 The Distorted wave approximation

The amplitude in the Born approximation is the matrix element of the interaction between the colliding systems taken between unperturbed wave - functions. It is possible to introduce a similar matrix element but taken with respect to wave - functions that are perturbed or 'distorted' in some predetermined fashion, this idea is the basis of the distortion method. In general the Born approximation cross-sections are too large at low energies and the distorted wave approximation is often quite effective in reducing the cross - sections for about the right order of magnitude. From equation (1-19), we find

$$\psi_i^+ = \phi_i + \frac{(H - H_i)}{E + i\epsilon - H}\phi_i \qquad (1\text{-}25)$$

and

$$\psi_f^- = \phi_f + \frac{(H - H_f)}{E + i\epsilon - H}\phi_f \qquad (1\text{-}26)$$

where $H = H_i + V_i = H_f + V_f$

Similarly, for some other Hamiltonian H', we get

$$\chi_i^+ = \phi_i + \frac{(H' - H_i)}{E + i\epsilon - H'}\phi_i \qquad (1\text{-}27)$$

$$\chi_f^- = \phi_f + \frac{(H' - H_f)}{E + i\epsilon - H'} \qquad (1\text{-}28)$$

Substituting (1-27) into (1-25), we find

$$\psi_i^+ = \chi_i^+ - \frac{(H' - H_i)\phi_i}{E + i\epsilon - H'} + \frac{(H - H_i)\phi_i}{E + i\epsilon - H} \qquad (1\text{-}29)$$

From (1-9), we see that

$$\frac{1}{E+i\epsilon-H'} = \frac{1}{E+i\epsilon-H}\left[1+\frac{(H'-H)}{E+i\epsilon-H'}\right] \qquad (1\text{-}30)$$

Therefore, (1-29) gives

$$\psi_i^+ = \chi_i^+ - \frac{(H'-H_i)\phi_i}{E+i\epsilon-H}\left[1+\frac{(H'-H)}{E+i\epsilon-H'}\right]+\frac{(H-H_i)\phi_i}{E+i\epsilon-H}$$

$$= \chi_i^+ + \frac{1}{E+i\epsilon-H}\left[(-H'+H_i+H-H_i)-\frac{(H'-H)(H'-H_i)}{E+i\epsilon-H'}\right]$$

$$= \chi_i^+ + \frac{(H-H')}{E+i\epsilon-H}\left[1+\frac{(H'-H_i)}{E+i\epsilon-H'}\right]\phi_i$$

$$= \chi_i^+ + \frac{(H-H')}{E+i\epsilon-H}\chi_i^+$$

(1-31)

Similarly,

$$\psi_f^- = \chi_f^- + \frac{H-H'}{E+i\epsilon-H}\chi_f^- \qquad (1\text{-}32)$$

Let

$$T_{fi} = \langle\phi_f|H-H_f|\psi_i^+\rangle = \langle\psi_f^-|H-H_i|\phi_i\rangle$$

$$T'_{fi} = \langle\phi_f|H'-H_f|\chi_i^+\rangle = \langle\chi_f^-|H'-H_i|\phi_i\rangle$$

Then

$$T_{fi} - T'_{fi}$$

$$= \langle \phi_f | H - H_f | \psi_i^+ \rangle - \langle \phi_f | H' - H_f | \chi_i^+ \rangle$$

$$= \langle \phi_f | H - H_f | \left(\chi_i^+ + \frac{(H - H')\chi_i^+}{E + i\epsilon - H} \right) \rangle - \langle \phi_f | H' - H_f | \chi_i^+ \rangle$$

$$= \langle \phi_f | H - H' | \chi_i^+ \rangle + \langle \phi_f | \frac{(H - H')(H - H_f)}{E + i\epsilon - H} | \chi_i^+ \rangle$$

$$= \langle \psi_f^- | H - H' | \chi_i^+ \rangle$$

Similarly,

$$T_{fi} - T'_{fi} = \langle \psi_f^- | H - H' | \chi_i^+ \rangle$$

Similarly

$$T_{fi} - T'_{fi} = \langle \chi_f^- | H - H' | \psi_i^+ \rangle$$

Therefore

$$\langle \psi_f^- | H - H' | \chi_i^+ \rangle = \langle \chi_f^- | H - H' | \psi_i^+ \rangle$$

Therefore

$$\begin{aligned} T_{fi} &= T'_{fi} + \langle \psi_f^- | H - H' | \chi_i^+ \rangle \\ &= T'_{fi} + \langle \chi_f^- | H - H' | \psi_i^+ \rangle \end{aligned} \qquad (1\text{-}33)$$

Suppose

$$H = H_i + U_i + W_i = H_f + U_f + W_f$$

where H_i and H_f are the initial and final unperturbed Hamiltonians respectively. U_i and U_f are arbitrary potentials respectively.

Writing $H = H' + W_i = H' + W_f$

where $H' = H_i + U_i = H_f + U_f$

from (1-33), we get

$$T_{fi} = \langle \phi_f | V_f - W_i | \chi_i^+ \rangle + \langle \psi_f^- | W_i | \chi_i^+ \rangle \qquad (1\text{-}34)$$

or $$T_{fi} = \langle \xi_f^- | V_i - W_f | \phi_i \rangle + \langle \xi_f^- | W_f | \psi_i^+ \rangle \qquad (1\text{-}35)$$

where to avoid confusion, the eigen functions of H' has been denoted by $\xi_f^{\pm}$. The Distorted Born approximation for T_{fi} is obtained by replacing ψ_i^+ by χ_i^+ in (1-35) i.e.

$$T_{fi} = \langle \xi_f^- | V_i - W_f | \phi_i \rangle + \langle \xi_f^- | W_f | \chi_i^+ \rangle \qquad (1\text{-}36)$$

Equations (1-34 and (1-36) are both known as the Distorted wave Born approximation, which is the first term in a Distorted wave Born Series.

1.4 The Impulse approximation

From the previous section, we know that the transition probabilities for the initial state i for the final state f can be defined as

$$T_{fi} = \langle \phi_f | V_f | \psi_i^+ \rangle \qquad (1\text{-}37)$$

Since the exact wavefunction ψ_i^+ is very difficult to calculate in a true three body approximation, the impulse approximation, has been introduced by Chew (1950) in which the three body wave function ψ_i^+ is replaced by a superposition of wave - functions relating to two particle scattering. This idea of Chew (1950), has been elaborated by Askin and Wick (1952) and Chew and Wick (1952). Also, at the same time, Chew and Goldberger (1952) extended the idea which is applicable to the Direct collision only. Prodhan (1957) first extended the method to the calculation of the charge - exchange process using a slightly different version of the impulse approximation. We present the formulation given by McDowell (1961) which is applicable for both Direct and Rearrangement processes.

We consider the system given in section (1.1).

From equation (1-19), we know that

$$\psi_i^+ = \Omega^+ \phi_i$$

where $\Omega^+ = 1 + G_1^+ V_i$

So the equation (1-37) can be written as

$$T_{fi} = \langle \phi_f | V_f | \Omega^+ \phi_i \rangle \qquad (1\text{-}38)$$

To obtain the impulse approximation we need to express the three-body Møller operators Ω^+ in terms of the two-body operators W_{ij}^+, which satisfies the equation.

$$W_{ij}^+(m)\chi_m = \left(1 + \frac{V_{ij}}{E_m - H_o - V_{ij} + i\epsilon}\right)\chi_m \qquad (1\text{-}39)$$

where V_{ij} is the interaction potential between the particle i and the particle j. The wave function χ_m satisfies the differential equation

$$(H_o - E_m)\chi_m = 0$$

and $\psi_m^+(ij)$ describes the motion under the potential V_{ij} alone,

$$(H_o + V_{ij})\psi_m^+(ij) = E_m\psi_m^+(ij)$$

which implies that $\psi_m^+(ij) = W_{ij}^+\chi_m$ (1-40)

Now $$G_1^+ = \frac{1}{E - H + i\epsilon}$$

So with the help of the formula (1-9) above we can express G_1^+ in the following form

$$G_1^+ = \frac{1}{(E_m - H_o - V_{ij} + i\epsilon)} + \frac{1}{(E_m - H + i\epsilon)}(E_m - H_o - V_{ij} + i\epsilon - E + H - i\epsilon) \times \frac{1}{(E_m - H_o - V_{ij} + i\epsilon)}$$

Operating both sides by V_{ij}, we get

$$G_1^+ V_{ij} = \frac{V_{ij}}{(E_m - H_o - V_{ij} + i\epsilon)} + \frac{V_{ij}}{(E_m - H + i\epsilon)}(E_m - H_o - V_{ij} - E + H) \times \frac{1}{(E_m - H_o - V_{ij} + i\epsilon)} V_{ij} \qquad (1\text{-}41)$$

From equation (1-39), we get

$$\frac{V_{ij}}{(E_m - H_o - V_{ij} + i\epsilon)} = W^{+}_{ij}(m) - 1$$

Therefore from equation (1-41) we find

$$G_1^{+} V_{ij} = (W^{+}_{ij}(m) - 1) + G_1^{+}[(E_m - E) + V_{12} + V_{13} + V_{23} - V_{ij}](W^{+}_{ij}(m) - 1) \qquad (1\text{-}42)$$

Let

$$(W^{+}_{ij}(m) - 1) = b^{+}_{ij}(m)$$

Then from (1-42), we get

$$G_1^{+} V_{ij} = b^{+}_{ij}(m) + G_1^{+}[(E_m - E) + V_{12} + V_{13} + V_{23} - V_{ij}] b^{+}_{ij}(m) \qquad (1\text{-}43)$$

Substituting (1-43) in (1-38), we now obtain

$$T_{if} = \langle \phi_f | V_f | (W^{+}_{13} + W^{+}_{12} - 1)\phi_i \rangle$$

$$+ \langle \phi_f | V_f | G_1^{+}[(V_{23}, (b^{+}_{13} + b^{+}_{12})]\phi_i \rangle$$

$$+ \langle \phi_f | V_f | G^{+}(V_{13} b^{+}_{12} + V_{12} b^{+}_{13})\phi_i \rangle \qquad (1\text{-}44)$$

The equation (1-44) is known as the impulse approximation which can be applied for both Direct and Rearrangement collision. This expression is much too complicated to be used in practical calculations and further approximation are made.

If the collision is rapid, the influence of the binding potential V_{23}, during the collision is small and can be

neglected. In addition at high energies it is reasonable to neglect the influence of multiple scattering in the 3rd term. The impulse approximation is then

$$T_{fi}^{IMP} = \langle \phi_f | V_f | (W_{13}^{+} + W_{12}^{+} - 1) \phi_i \rangle$$
$$= \langle \phi_f | V_f | \phi_i^{IMP} \rangle \qquad (1\text{-}45)$$

where

$$\phi_i^{IMP} = (W_{13}^{+} + W_{12}^{+} - 1) \phi_i$$

For the excitation process, the impulse approximation can be given as

$$T_{fi}^{IMP} = \langle \phi_f | V_{12} + V_{13} | (W_{12}^{+} + W_{13}^{+} - 1) \phi_i \rangle \qquad (1\text{-}46)$$

where

$$\phi_i = e^{i k_i \cdot \underline{r}_i} \chi_i(\underline{R}_1)$$

and

$$\phi_f = e^{i k_f \cdot \underline{r}_i} \chi_f(\underline{R}_1)$$

where $\underline{r}_i$ ~~and σ~~ is the centre of mass from the particle 1. In the case of heavy particle impact V_{12} cannot contribute for reasons to be explained. Therefore impulse approximation can be written in the simple form

$$T_{fi}^{IMP} = \langle \phi_f | V_{13} | W_{13}^{+} \phi_i \rangle \qquad (1\text{-}47)$$

where

$$W_{12}^{+} = 1$$

The equation (1-46) is known as the post form of the impulse approximation, because that contains the interaction potential V_f. We can also define the prior form of the impulse approximation, which is given by

$$T_{fi}^{-IMP} = \langle \phi_f^{-IMP} | V_i | \phi_i \rangle$$
$$= \langle (W_{13}^{-} + W_{12}^{-} - 1) \phi_f | V_i | \phi_f \rangle \qquad (1\text{-}48)$$

For excitation process, we get $V_i = V_f$ but for the rearrangement process V_i will be different from V_f. The application of the above method will be described in Chapters 3 and 5.

This method is defective in several respects. The potentials have only in part been eliminated by replacing them with two - body scattering amplitude, the initial and final interactions appear asymmetrically which may produce a post - prior discrepency. Both these difficulties can be overcome by using Fadeev's method (1961a, 1961b). A slightly different formulation of Fadeev's approach has been given by Lovelace (1964a), which is more approximate for three particle collision. In this case the initial and final states consists of a bound system and a free particle. These methods are discussed in the books by Bransden (1970) and McDowell and Coleman (1970).

1.5 The impact parameter method and the truncated eigen function method

A very great simplification can be made in the theory of the scattering of atoms by atoms or ions, because the wave-length associated with the relative motion of the colliding particles is usually very small compared with atomic dimension. The wave-length λ of a proton of mass M and velocity V is given by

$$\lambda\!\!\!^{-} = \frac{\lambda}{2\pi} = \frac{\hbar}{MV}$$

The reduced wave-length $\lambda\!\!\!^{-}$ is equal to the Bohr radius of the hydrogen atom a_0, when $V \approx 10^5$ cm sec^{-1}, which corresponds to a kinetic energy by less than $(\frac{1}{100})$ ev . For kinetic energies with which we are concerned, which extend from 1ev to several Mev, $\lambda\!\!\!^{-}$ is always much smaller than the range of interaction, which is certainly greater than a_0. Since the proton is the lightest projectile, for all other atom the inequality $\lambda\!\!\!^{-} << a_0$ will be satisfied. Under these short wave-length conditions, it is generally possible to define classical trajectories which are followed by the colliding atoms. For the trajectory to be well defined, it is also necessary for the uncertainty, $\Delta\theta$ in the angle of scattering to be small compared with θ . We have $\Delta\theta \approx \frac{\Delta p}{p}$, where Δp is the uncertainty in the transverse momentum transferred to an incident particle of momentum p. As the range of the interaction is of order a_0, $\Delta p \simeq \frac{\hbar}{a_0}$ and it follows that classical condition will apply if $\theta > \frac{\hbar}{pa_0}$. The critical angle $\frac{\hbar}{pa_0}$ is less than 1^0 for protons with energies of a few tens of electron volts, and is smaller still for other nuclei with the same energy. As experimental arrangements

exclude very small angles, this is not a practical limitation and the motion of colliding atoms can be described classically, except in certain circumstances, in which interference effects, arising from a difference in phase of the wave - function associated with different classical paths, are of importance. In contrast to the motion of the heavy particles, which can accurately taken to be classical, the electronic motion which is associated with discrete states must be described by quantum mechanics. (Bransden, 1972).

This approximation is a good approximation unless the impact energy is very low (Bates and Boyd, 1962a,b). Also in the impact parameter treatment the nuclear assumed to behave like classical particles and quantum perturbation theory is applied to determine the change of a transition from one electronic state to another.

Let us consider the impact parameter method for both direct and rearrangement collision. Let $\underline{R}$ be the position vector of the particle 1 relative to 3 and let $\underline{r}_1$, $\underline{r}_2$, $\underline{r}$ be the position vectors of the electron relative to 1, 3 and the centre of mass of $\underline{R}$ respectively. Let v be the relative velocity of the proton which remains constant and which is moving parallel to the z - axis. Let ρ be the perpendicular distance of the proton and the z axis which is known as the impact parameter and before collision the condition related to is $\underline{R} = \rho + vt$, $z = vt$ and $v \cdot \rho = 0$

The complete electronic wave - function $\psi(\underline{r},t)$ satisfies the time - dependent Schrodinger equation (in atomic units)

$$H\psi(\underline{r},t) = i \frac{\partial \psi(\underline{r},t)}{\partial t} \qquad (1\text{-}49)$$

where H is the hamiltonian as $H = -\frac{1}{2}\nabla_2^2 + V_{12} + V_{13} + V_{23}$ and V_{12}, V_{13} and V_{23} can be expressed by the help of coulomb potentials.

Now, we can expand $\psi(r,t)$ either in the form of

$$\sum_n a_n(t)\phi_n(r,t)\, e^{(-i\upsilon z/2 - i\upsilon^2 t/8 - i\alpha_p t)} \qquad (1\text{-}50)$$

or in the form of

$$\sum_m b_m(t)\phi_m(r,t)\, e^{(i\upsilon z/2 - i\upsilon^2 t/8 - i\beta_q t)} \qquad (1\text{-}51)$$

where the coefficients $a_n(t)$ and $b_m(t)$ are time - dependent function. ϕ_n and ϕ_m are the wave functions of the bound states before collision and after collision respectively.

From (1-50) and (1-51) we can calculate the coefficients $a_n(t)$ or $b_m(t)$ in the following way.

$$a_n(t) = \int \psi(r,t)\phi_n^*(r,t)\exp(i\upsilon z/2 + i\upsilon^2 t/8 + i\alpha_p t)$$

Similarly,

$$b_m(t) = \int \psi(r,t)\phi_m^*(r,t)\exp(-i\upsilon z/2 + i\upsilon^2 t/8 + i\beta_q t)$$

So the probability amplitude for finding the system either in the n'th level or in the m'th level can be obtained by $|a_n(+\infty)|^2$ or $|b_m(+\infty)|^2$ respectively.

Total cross - section can be obtained by using the following formula

$$\sigma = \int_0^\infty I\rho\, d\rho \quad 2\pi a_o^2 \qquad (1\text{-}52)$$

where I is $|a_n(+\infty)|^2$ or $|b_m(+\infty)|^2$ for the excitation or charge exchange process respectively.

The Variational Principle.

But to get the exact solution of (1-49) we can apply the variational principle, defined as

$$I = \int \psi^* \left(H - i\frac{\partial}{\partial t}\right) \psi \, d\tau$$

where ψ and ψ^* are the total wave functions which satisfies the boundary condition

$$\psi = \psi + \delta\psi \quad , \quad \psi^* = \psi^* + \delta\psi^* \quad \text{when } r \to \infty$$

which requires $\delta\psi(\underline{r}, t) = 0$

and $\delta\psi^*(\underline{r}, t) = 0$ as $t \to \pm\infty$

The trial function can be expressed as below

$$\psi(\underline{r}, t) = \sum_n a_n(t) \Phi_n(\underline{r}, t) \exp(-i v z/2 - i v^2 t/8 - i\alpha_p t)$$

$$+ \sum_m b_m(t) \Phi_m(\underline{r}, t) \exp(i v z/2 - i v^2 t/8 - i\beta_q t)$$

$$+ \gamma(\underline{r}, t) \qquad (1\text{-}53)$$

where $\gamma(\underline{r}, t)$ is a function which can be represented by the set of eigen functions with the nucleus 2 or 3, but neither the initial nor the final state is included in either set. Consequently $\gamma(\underline{r}, t)$ is orthogonal to $\phi_n(\underline{r}, t)$ and $\phi_m(\underline{r}, t)$ so that it has the expressions

$$\gamma(\underline{r}, t) = \sum_{p \neq i} a_p(t) \phi_p(\underline{r}, t) \exp(-i v z/2 - i v^2 t/8 - i\alpha_p t)$$

$$= \sum_{q \neq f} b_q(t) \phi_q(\underline{r}, t) \exp(i v z/2 - i v^2 t/8 - i\beta_q t) \qquad (1\text{-}54)$$

The equation (1-53) is very difficult to solve. So some other approximations must be used. We now, describe the two-state approximation following the method due to Bates (1958).

<u>The Two-state approximation.</u>

In this case only the initial and final states are included

in the trial wave-function. So the equation (1-53) reduces to

$$\psi(\underline{r},t) = a_i(t)\phi_i(\underline{r},t)\exp(-i\upsilon z/2 - i\upsilon^2 t/8 - i\alpha_i t) + b_f(t)\phi_f(\underline{r},t)\exp(i\upsilon z/2 - i\upsilon^2 t/8 - i\beta_f t) \qquad (1\text{-}55)$$

where $a_i(t)$ and $b_f(t)$ are the time-dependent coefficients in the initial and final states respectively. If we now set the initial condition $a_i(-\infty) = 1$ and $b_f(-\infty) = 0$, then the scattering amplitude from the initial state i to the final state f for the excitation or charge exchange process can be given either by $|a_i(+\infty)|^2$ or by $|b_f(+\infty)|^2$ which can easily be calculated by (1-55). Cross-section can be obtained after applying the formula (1-52). To get the coefficients a_i and b_f the following method has been used.

Substituting (1-55) into (1-49) and multiply both sides firstly by $\phi_i^*(\underline{r},t)\exp(i\upsilon z/2 + i\upsilon^2 t/8 + i\alpha_i t)$ and secondly by $\phi_f^*(\underline{r},t)\exp(-i\upsilon z/2 + i\upsilon^2 t/8 + i\beta_f t)$ and integrating overall the space, we get the following two sets of equation.

$$i(\dot{a}_i + \dot{b}_f S_{if}\exp(-i\epsilon_{fi}t)) = b_f K_{if}\exp(i\epsilon_{fi}t) + a_i h_{ii} \qquad (1\text{-}56)$$

and

$$i(\dot{b}_f + \dot{a}_i S_{fi}\exp(-i\epsilon_{if}t) = a_i K_{fi}\exp(-i\epsilon_{if}t) + b_f h_{ff} \qquad (1\text{-}57)$$

The other terms will be zero as they are orthogonal to each other, and where $\epsilon_{fi} = (\beta_f - \alpha_i)$. The matrix elements

S_{if}, S_{fi}, K_{if}, K_{fi}, h_{ii}, h_{ff} can be defined as

$$S_{if} = \int \phi_i^*(\underline{r}_1)\phi_f(\underline{r}_2)\, e^{i\upsilon z}\, d\tau$$

$$S_{fi} = \int \phi_f^*(\underline{r}_1)\, \phi_i(\underline{r}_2)\, e^{-i\upsilon z}\, d\tau$$

$$K_{fi} = \int \phi_f^*(\underline{r}_2)\, V_{13}\, \phi_i(\underline{r}_1)\, e^{-i\upsilon z}\, d\tau$$

$$K_{if} = \int \phi_i^*(\underline{r}_1)\, V_{12}\, \phi_f(\underline{r}_2)\, e^{i\upsilon z}\, d\tau$$

$$h_{ii} = \int \phi_i^*(\underline{r}_1)\, V_{12}\, \phi_i(\underline{r}_1)\, d\tau$$

$$h_{ff} = \int \phi_f^*(\underline{r}_2)\, V_{13}\, \phi_f(\underline{r}_2)\, d\tau$$

From (1-56) and (1-57), after rearranging, we get

$$\dot{a}_i(1 - |S_{if}|^2) = a_i(h_{ii} - S_{if}K_{fi}) + b_f(K_{if} - S_{if}h_{ff})\, e^{i\epsilon_{if}t} \qquad (1\text{-}58)$$

$$\dot{b}_f(1 - |S_{if}|^2) = a_i(K_{ii} - S_{fi}h_{ii})\, e^{i\epsilon_{fi}t} + b_f(h_{ff} - S_{fi}K_{if}) \qquad (1\text{-}59)$$

Again substituting

$$X_i = \frac{h_{ii} - S_{if}K_{fi}}{1 - |S_{if}|^2}$$

and

$$Y_f = \frac{h_{ff} - S_{fi}K_{fi}}{1 - |S_{if}|^2}$$

and also putting

$${}^{o}a_i = {}^{o}a_i \exp\left[-i\int_{-\infty}^{t} X_i\, dt\right]$$

and

$${}^{o}b_f = {}^{o}b_f \exp\left[-i\int_{-\infty}^{t} Y_f\, dt\right]$$

removes the secular terms of (1-58) and (1-59) giving

$$i\,{}^{o}\dot{a}_i = {}^{o}b_f\left[\frac{K_{if} - S_{if}h_{ff}}{1 - |S_{if}|^2}\right] e^{\left[-i(\beta_f - \alpha_i)t + i\delta_{if}\right]} \qquad (1\text{-}60)$$

$$i\,{}^{o}\dot{b}_f = {}^{o}a_i \left[\frac{K_{fi} - S_{fi}h_{ii}}{1 - |S_{if}|^2}\right] e^{[-i(\alpha_i - \beta_f) - i\delta_{if}]} \qquad (1\text{-}61)$$

where

$$\delta_{if} = \int_{-\infty}^{t} (X_i - Y_f)\,dt$$
$$\simeq \int_{-\infty}^{t} (h_{ii} - h_{ff})\,dt$$

Taking the relevant solution of (1-60) to be ${}^{o}a_i(t) = 1$ which implies the neglecting of back-coupling from the final state f to the initial state i and inserting this condition in (1-61), we get

$$|b_f(+\infty)| = |{}^{o}b_f(+\infty)| = \left|\int_{-\infty}^{\infty} M_{if}\,dt\right|$$

where

$$M_{if} = \frac{K_{fi} - S_{fi}h_{ii}}{1 - |S_{if}|^2} \exp\left[-i(\alpha_i - \beta_f) - i\delta_{if}\right]$$

$$\simeq (K_{fi} - S_{fi}h_{ii}) \exp\left[-i(\alpha_i - \beta_f) - i\delta_{if}\right]$$

In the case of symmetrical resonance (Bates, 1958), we get

$$i\,{}^{o}\dot{a}_i = M_{if}\,{}^{o}b_f$$

$$i\,{}^{o}\dot{b}_f = M_{if}\,{}^{o}a_i$$

where

$$M_{if} = \frac{K_{if} - S_{if}h_{ff}}{1 - |S_{if}|^2} = \frac{K_{fi} - S_{fi}h_{ii}}{1 - |S_{if}|^2}$$

where

$$\alpha_i = \beta_f \quad , \quad \delta_{if} = \delta_{fi}$$

which is a simple formula to be solved exactly and so allows completely for back - coupling from the final states to the initial states (McCarroll, 1961). The term δ_{if} is the difference between the effects of the interaction when in the initial state and when in the final state.

1.6 Many - state approximation.

To improve the accuracy of the results, calculations have also been done by taking more than two states for both Direct and Rearrangement collision - process. From equation (1-53) we have the trial function

$$\Psi(\underline{r},t) = \sum_n a_n(t)\,\phi_n(\underline{r},t)\,e^{(-i\underline{v}z/2 - iv^2t/8 - i\alpha_p t)}$$

$$+ \sum_m b_m(t)\,\phi_m(\underline{r},t)\,e^{(iv z/2 - iv^2t/8 - i\beta_q t)}$$

$$+ V(\underline{r},t)$$

This can be represented by the two-state approximation, where the initial and final state should be included and which we have shown in the previous section. But to get better accuracy we can add as many state we like if we are able to do computing. We shall talk about these methods in the section given below.

The Sturmian expansion.

Gallaher and Wilets (1968), have first introduced this approximation and applied this in the proton- hydrogen scattering problem. In the calculations they have expanded the electronic wave function in terms of travelling sturmian waves about each protonwith the Sturmian functions quantized about the interproton axis.

These basis states of the particle A is given by

$$U_K\left(\underline{A}\right) = \phi_K(\underline{r}_B, B')\exp(\pm iv z/2)\exp\left(-i(\epsilon_K + \tfrac{v^2}{8})t\right)$$

where

$$\phi_k(\underline{r}_i') = \left[S_{n\ell}(r_i')/r_i'\right] Y_{\ell m}(\theta_i', \phi_i')$$

Similarly we can define another wave-function with respect to the particle B.

and the Sturmian functions $S_k(r) = S_{nl}(r)$ satisfy the equation,

$$\left(-\frac{1}{2}\frac{d^2}{dr^2} + \frac{l(l+1)}{2r^2} - \frac{\alpha_K}{r}\right) S_k(r) = E_l S_k(r)$$

The Sturmian function $S_k(r)$ has been first introduced by Rotenberg (1962), who choosed $E_l = -\frac{1}{2}$, the ground state energy of the hydrogen atom. Gallaher and Wilets (1968) used $E_l = -\frac{1}{2(l+1)^2}$. The Sturmian function is similar to Schrödinger equation, but the energy E_l appears as a fixed parameter. It is the effective change of α_K which acts as an eigen value. The required boundary conditions of $S_k(r)$ is zero at the origin and decay at infinity. $\phi_K(r)$ form an infinite, discrete and complete set of states. Unlike the hydrogenic function, there is no continuum. Their Sturmian functions are explicitly given by scaled hydrogen function, as

$$S_k(r) = \alpha k^{\frac{1}{2}} R_K(\alpha_K r)$$

where $R_K(\alpha_K r)$. is the usual radial hydrogen function. The normalization is chosen such that $\langle k|k\rangle = 1$. In Rotenberg's sturmian set, only the 1S sturmian function coincides with the 1S hydrogenic function. ,But in the above case the Sturmian 1S, 2p 3d.....etc. coincides with the corresponding hydrogen wave - function ϕ_K. The Sturmian states are more compact than the hydrogenic states. This can be seen by noting that $\langle \hat{k}|\frac{1}{r}|\hat{k}\rangle = \frac{1}{n(l+1)}$ as compared with $\langle \hat{k}|\frac{1}{r}|\hat{k}\rangle = \frac{1}{n^2}$. The results obtained by using the method has been agreed with experimental result by Helbig and Everhart (1963) for 3^o scattering angle.

The Pseudo - state approximation.

The Sturmian expansion has certain difficulties. Firstly it does not represent the states when internuclear separation is very large. Secondly, it does not satisfy the bound - state except for the lowest value of ℓ . By Pseudo - state approximation, introduced by Cheshire et al (1970), the above difficulties have been removed. Cheshire et al (1970), have used the same Sturmian expansion for the hydrogenic 1S, 2S and 2p states but added some extra terms by

$$\phi_K(\underline{r}) = \exp(-\lambda_e \underline{r}) \left[\sum_j \alpha_j r^j \right] Y_{\ell,m}(\theta, \phi)$$

which is known as the orbital pseudo - state wave functions, where $Y_{\ell m}(\theta, \phi)$ are spherical harmonics, k and j are subscripts indicating the orbitals concerned, $i = \ell + 1$, $j \geq 1$, $K = \xi_j + \ell + m + 2$ and where the radial functions is given by

$$S_{ij}(r) = \exp(-\lambda_i r) \sum_{q=1}^{j+\xi-i} S(i,j,q)\, r^{q+i-2}$$

the parameters have been chosen in this way that these functions are orthogonal to the 1S, 2S and 2p hydrogenic states and to each other. In this way, they have managed to get the correct boundary conditions for 1S, 2S and 2p states and added some omitted terms for the charge - exchange and excitation process as well.

CHAPTER 2

Second-order potential

In chapter 1, we discussed the most important approximations which have been applied to heavy particle scattering. In this chapter, we give a brief description of the second - order potential, in the impact parameter formalism, first introduced by Bransden and Coleman (1972) which we have used for our calculations. In the many state approximation only a limited number of states can be included in the wave function To overcome this, a second-order potential matrix has been constructed where we try to account approximately for the infinite number of states and which can be evaluated in a closure approximation. The second-order potentials depend on a parameter which can be set so that the correct long - range effective potential is obtained in the entrance channel and the method combines the characteristics of close - coupling and polarized orbital methods.

2.1 General formalism

Let the nucleus A be located at the fixed origin of the co-ordinate system and let the incident particles B move with a constant velocity V along a line of distance ρ and parallel to z - axis which satisfies the condition $R = \rho + Vt$, before collision, where ρ is known as the impact parameter. Let the electronic wave - function $\psi(\underline{r}, t)$ can be defined as

$$\psi(\underline{r},t) = \sum_n a_n(t)\phi_n(\underline{r})e^{-i\epsilon_n t} \qquad (2\text{-}1)$$

where $a_n(t)$ is the coefficient dependent on t.

The initial unperturbed eigenfunction $\phi_n(\underline{r},t)$ satisfies

$$H_o \phi_n = \epsilon_n \phi_n \qquad (2\text{-}2)$$

for the target nucleus, where H_o is the Hamiltonian for the unperturbed atom and ϵ_n is the unperturbed energy.

Now, substituting (2-1) into the time - dependent Schrödinger equation (1-49) and using (2-2) and multiplying both sides by $\phi_n^*(\underline{r})\, e^{i\epsilon_n t}$, we get a set of coupled equations given by

$$i \frac{\partial}{\partial z} a_n(z) = \frac{1}{v} \sum_{m=o}^{\infty} a_m(z)\, V_{nm}(z)\, e^{i(\alpha_{mn} z)/v} \qquad (2\text{-}3)$$

where we have

$$z = vt \qquad (2\text{-}4)$$

and $$(\epsilon_m - \epsilon_n) = \alpha_{mn}$$

and V_{mn} can be expressed as

$$V_{nm} = \int \phi_n^*(r)\, V(\underline{r},t)\, \phi_m(r)\, dr \qquad (2\text{-}5)$$

which is known as the matrix interaction potential between the projectile and the target. Summation sign in (2-3) includes the integration over the continuum states. The equation (2-3), thus obtained, is an exact form of the Schrodinger equation and forms the cases of the truncated eigenfunction expansion.

The scattering amplitude can now be obtained by setting the Boundary conditions as below,

$$a_n(-\infty) = \delta_{no}$$

where o denotes the incident channel. The probability amplitude $a_n(+\infty)$ is then evaluated by using the equation (2-3) and integrating that from $-\infty$ to $+\infty$. The scattering amplitude is obtained by integrating $|a_n(+\infty)|^2$ over all values of the impact parameters, given by

$$\sigma = 2 \int_0^{\infty} \rho\, |a_n(+\infty)|^2\, d\rho\, \pi d_o^2 \qquad (2\text{-}6)$$

2.2 Second-order potential

In many problems it is expected that one or more states will be of particular importance in the expansion (2-1). For these states, labelled n = o, 1,...N, the corresponding equation (2-3) are retained without approximation, while for all states $n > N$, the equations (2-3) are modified so that only the potential terms coupling with states $n \leq N$ are retained

$$i\frac{\partial}{\partial z} a_n(z) = \frac{1}{v}\sum_{m=o}^{N} a_m(z) V_{nm}(z)\, e^{i(\alpha_{mn} z)/v} \qquad (2\text{-}7)$$

Solution of (2-7) is $n = N+1, N+2, \ldots\ldots$

$$a_n = \frac{1}{iv}\sum_{m=o}^{N}\int_{-\infty}^{z/v} a_m(z') V_{nm}(z')\, e^{i(\alpha_{mn} z')/v}$$

$$n > N \qquad (2\text{-}8)$$

By substituting (2-8) into (2-3), we obtain the final set of coupled integro-differential equations which is in the impact parameter formalism and which is given by

$$i\frac{\partial}{\partial z} a_n = \frac{1}{v}\sum_{m=o}^{N} a_m(z) V_{nm}(z)\, e^{i\alpha_{mn} z/v}$$

$$- \frac{1}{v^2}\sum_{m=o}^{N}\int_{-\infty}^{z/v} a_m(z') \sum_{j=N+1}^{\infty} V_{nj}(z)\, V_{jm}(z')$$

$$\times \exp\left[i(\epsilon_n - \epsilon_j)z/v + i(\epsilon_j - \epsilon_m)z'/v\right] dz'$$

$$\text{for} \qquad n \leq N \qquad (2\text{-}9)$$

The equation (2-9) can also be written as

$$i\frac{\partial}{\partial z}a_n = \frac{1}{v}\sum_{m=0}^{N} a_m(z)\,V_{nm}(z)\,e^{i\alpha_{mn}z/v} - \frac{i}{v^2}\int_{-\infty}^{z/v}\sum_{m=0}^{N} a_m(z')\,K_{nm}(z,z')\,dz' \qquad (2\text{-}10)$$

$$n = 0, 1, 2, \ldots N$$

where

$$K_{nm}(z,z') = \sum_{j=N+1}^{\infty} V_{nj}(z)\,V_{jm}(z')\,e^{i[(\epsilon_n-\epsilon_j)z/v + (\epsilon_j-\epsilon_m)z'/v]} \qquad (2\text{-}11)$$

The potential K_{nm} can be evaluated by using the closure approximation in which ϵ_n, the energy of the excitation of the target in the state n , is replaced by an effective average excitation energy $\bar{\epsilon}$. The closure relation

$$\sum_n \phi_n(\underline{r})\,\phi_n^*(\underline{r}') = \delta(\underline{r}-\underline{r}') \qquad (2\text{-}12)$$

can now be used to write K_{nm} in the form

$$K_{nm}(z,z') = e^{i[(\epsilon_n-\bar{\epsilon})z/v + (\bar{\epsilon}-\epsilon_m)z'/v]}\left[V_{nm}(z,z') - \sum_{j=0}^{N} V_{nj}(z)\,V_{jm}(z')\right] \qquad (2\text{-}13)$$

where $j \geq N+1$

where the potential $V_{nm}(z, z')$ can be defined as

$$V_{nm}(z,z') = \int \phi_n^*(\underline{r})\,V(\underline{r},z)\,V(\underline{r},z')\,\phi_m(\underline{r})\,d\underline{r} \qquad (2\text{-}14)$$

and can be expressed in a suitable form for the numerical calculation by using the technique given by Coleman (1970), described below in chapter 4.

The equation (2-13) can also be solved by substituting $\bar{\epsilon}'$ for $j > M$ where M = N + 1 and the exact energies of all lower levels are used, where $\bar{\epsilon}'$ is an new effective energy.

The amplitude for excitation to the state n, for $n > N$, is obtained by solving a modified version of the equation (2-3) which allows for 'distortion' in the final state, ie.

$$i\frac{\partial}{\partial z}a_n = \frac{1}{v}\sum_{m=0}^{N} a_m(z)V_{nm}(z)e^{i\alpha_{mn}z/v} + a_n V_{nn}(z) \qquad (2\text{-}15)$$

The solution of (2-10) and (2-15) is dependent on the boundary conditions given above.

2.3 The effective energy $\bar{\epsilon}$

In paper I (Bransden and Coleman, 1972) the effective energy $\bar{\epsilon}$ has been introduced to obtain the correct long range potential due to dipole polarizability. Also we know that should be fixed so that in adiabatic limit of the incident channel asymptotic behaviour can be obtained.

Using the adiabatic limit $v \to 0$, the term containing the kernel on the right hand side of equation (2-10) then reduces to

$$I = \int_{-\infty}^{z} dz' K_{nm}(z,z')\, a_n(z') \qquad (2\text{-}16)$$

$$= \int_{-\infty}^{z} K_{0,0}(z,z')\, a_0(z')\, dz' \qquad n=m=0 \qquad (2\text{-}17)$$

$$= \left[W(z,z')\, a_0(z')\right]_{-\infty}^{z} - \int_{-\infty}^{z} dz'\, W(z,z')\frac{\partial a}{\partial z} \qquad (2\text{-}18)$$

where $W(z,z') = \int K_{00}(z,z')\, dz'$

and $$K_{00}(z,z') = \sum_{j=N+1}^{\infty} V_{0j}(z)\, V_{j0}(z')\, e^{-i\bar{k}_n(z-z')/v} \qquad (2\text{-}19)$$

where $\bar{k}_n = \dfrac{(\epsilon_j - \epsilon_0)}{v}$

Velocity independent term is $\left[W(z,z')\right]_{-\infty}^{z}$

$$W(z,z') = \sum_{j=N+1}^{\infty} e^{-i\bar{k}_n z} V_{0j}(z) \int e^{i\bar{k}_n z'} V_{j0}(z')\, dz' \qquad (2\text{-}20)$$

$$= \sum_{j=N+1}^{\infty} V_{oj}(z)\, e^{-i\bar{k}_n z} \left\{ \frac{1}{i\bar{k}_n} e^{i\bar{k}_n z'} V_{jo}(z') - \int \frac{dz'}{i\bar{k}_n} e^{i\bar{k}_n z'} \frac{\partial}{\partial z} V_{jo}(z') \right\} \tag{2-21}$$

Therefore

$$\left[W(z,z') \right]_{-\infty}^{z} \sim \sum_{j=N+1}^{\infty} \frac{V_{oj}(z)\, V_{jo}(z)}{i\bar{k}_n} \tag{2-22}$$

$$\sim \sum_{j=N+1}^{\infty} \frac{|V_{oj}(z)|^2}{i(\epsilon_o - \epsilon_j)} \tag{2-23}$$

Therefore I can be written as

$$I = \int_{-\infty}^{z} K_{oo}(z,z')\, a_o(z') = V_{oo}^{P}\, a_o(z) \tag{2-24}$$

where

$$V_{oo}^{P} = \sum_{j=N+1}^{\infty} \frac{|V_{oj}(z)|^2}{(\epsilon_o - \epsilon_j)} \tag{2-25}$$

The adiabatic second-order potential is given by V^{pol}. Therefore, in the incident channel, the charged potential V_{oo}^{P} is

$$V_{oo}^{P} = V^{POL}(z) - \sum_{j=1}^{N} \frac{|V_{oj}(z)|^2}{(\epsilon_o - \epsilon_j)} \tag{2-26}$$

for N = 0, by castillejo et al (1960),

$$V_{oo}^{P} = -\frac{\alpha}{2z^4} \tag{2-27}$$

where α is the dipole polarizability. But in the closure approximation, we get

$$V_{oo}^{P}(z) = \sum_{j=N+1}^{\infty} \frac{|V_{oj}(z)|^2}{(\epsilon_o - \bar{\epsilon})} \tag{2-28}$$

for N = 0,

$$V_{oo}^{P}(z) = -\beta/2(\epsilon_o - \bar{\epsilon})z^4 \tag{2-29}$$

where β is easily evaluated. Thus $\bar{\epsilon}$ can be given by

$$\bar{\epsilon} = (\epsilon_o + \beta/\alpha) \tag{2-30}$$

which gives the correct asymptotic form in the adiabic limit in the entrance channel when $N \neq 0$, a similar procedure can be followed if the contribution to the dipole polarizability arising from those p states occurring explicitly in the coupled equations is taken into account.

CHAPTER 3

3. Earlier work on excitation

3.1 The Born approximation

From chapter 1, we know that the cross-section from the initial state i to the final state f is given by

$$Q_{if} = \frac{\mu^2}{2\pi} \frac{K_f}{K_i} |T_{fi}|^2 d\Omega \tag{3-1}$$

where μ is the reduced mass, K_i and K_f are the initial and final momenta and T_{fi} has been defined as

$$\begin{aligned} T_{fi} &= \langle \phi_f | V_i | \psi_i^+ \rangle \\ &= \langle \psi_f^- | V_i | \phi_i \rangle \end{aligned} \tag{3-2}$$

Since for the Direct collision $V_i = V_f$, and $\phi_i = e^{i K_i \cdot \underline{r}_i} \chi_i(\underline{R}_1)$

and $\phi_f = e^{i K_f \cdot \underline{r}_i} \chi_f(\underline{R}_1)$

The equation (3-2) is known as the Born approximation, which is very difficult to solve if we use the exact expressions of ψ_i^+ or ψ_i^-. To make the calculation a bit easier Bethe (1930) has expressed (3-2) in a simple form which is known as Bethe approximation, which is given by

$$I(\underline{r}_j) = \frac{4\pi}{P^2} \int e^{i \underline{P} \cdot \underline{r}_j} \chi_i(\underline{R}_1) \chi_f^*(\underline{R}_1) d\underline{R}_1 \tag{3-3}$$

The formula (3-3) has first been used by Bates and Griffling (1953) to calculate the cross-section of the following process $H^+ + H(1S) \longrightarrow H^+$ or $H(1S) + H(2S, 2p, 3S, 3p, 3d, c)$

where c means the continuum states. The same authors (1954) also calculated the cross-section for the following process as well.

$$H(1S) + H(1S) \longrightarrow H(2S \text{ or } 2p) + H(2S,2p,3S,3p,3d,c)$$

Pomilla and Milford (1966) have also done the calculations keeping the projectile and the target initially in the excited states for hydrogen atom. The experimental results for hydrogen are too low to be valid, because Born approximation can give good results only for higher energies.

The theoretical work on proton-helium scattering on excitation has previously been done by Moiseiwitsch and Stewart (1954), Bell (1961), Bell and Skinner (1962). Similarly the experimental works are available by Thomas and Bent (1967), Galliard (1966), Gabriel and Heddle (1960). Most recent and valuable work on First Born approximation on proton - helium collision has been done by Bell et al (1968c) who have obtained the generalized oscillator strengths for excitation of the ground state of helium using many parameter wave - functions. These are employed to obtain proper impact excitation cross-sections in the ? First Born approximation for the excitation from the ground state of atomic helium to n^1s = 2 to 7), (n^1p = 2 to 4) and 3^1D excited states and for the elastic scattering of protons. Their results have been compared with the experimental results available by Van Den Bos (1968b), Denis et al (1967). The results of Van Den Bos (1968b) are smaller than their results. The results of Bell et al (1968c) for 2^1s and 2^1p excitations of proton from helium has been predicted in table 2 and 3 respectively.

3.2 The Second Born approximation.

From chapter 1, we know that the Second Born approximation can be given by

$$T_{fi}^{B2} = T_{fi}^{B1} + \langle \phi_f | V_f G_i^+ V_i | \phi_i \rangle \qquad (3\text{-}4)$$

where T_{fi}^{B1} is the First Born approximation and the second term of the above series is given by

$$T_{fi}^{B2'} = 2 \sum_n \int\int e^{-i\underline{K}_f \cdot \underline{r}_i} V_{fn}(\underline{r}_i) \frac{e^{iK_n |\underline{r}_i - \underline{r}_i'|}}{|\underline{r}_i - \underline{r}_i'|} V_{ni} e^{i\underline{K}_i \cdot \underline{r}_i'} d\underline{r}_i \, d\underline{r}_i'$$

where $G_n^+ = \dfrac{e^{iK_n |\underline{r}_i - \underline{r}_i'|}}{|\underline{r}_i - \underline{r}_i'|}$ and $V_{nm} = \langle \chi_n | V | \chi_m \rangle$

Where the sum over n is over all the states of the target atom including continuum states.

As it is very difficult to calculate all the terms in the equation (3-5), Massey and Mohr (1934) have ignored the variation of K_n in the calculations on proton - hydrogen scattering. Instead of K_n they used K_i and evaluated the equations (3-5) with the help of closure approximation. But Kingston et al (1960) have solved it in a different way. In their case, they have taken all the 1S, 2S, 2p states and neglected the other terms. They also carried out the calculations on the proton - hydrogen collision problem. Their results are larger than the results obtained by First Born approximation. But when only 2S and 2p were retained, results are quite near to the distortion approximation. Similar calculations have also been done by Moisewtsch and Perrin (1965). Holt and Moisewitsch (1968) have done this calculation by taking both approaches given by Massey and Mohr (1934) and Kingston et al (1960). Holt et al (1971) also have applied the same method when they have calculated the

excitation of helium to the 2^1S and 2^1p states by electron and proton impact and results are available in table 2 and 3 respectively. Recently Wooling and McDowell (1972) have done some calculations on the excitation of electron from helium by applying various forms of the Second Born approximation.

3.3 Eigenfunction expansion method.

From chapter 2, we have

$$i\dot{a}_n(z) = \frac{1}{v}\sum_{m=0}^{\infty} a_m(z)\, V_{nm}(z)\, e^{i\alpha_{mn} z/v} \qquad (3\text{-}6)$$

where V_{nm} is the interaction potential and is defined as

$$V_{nm} = \int \phi_n^*(\underline{r})\, V(\underline{r}, z)\, \phi_m(\underline{r})\, d\tau$$

The equation (3-6) is equivalent to First Born approximation and is known as the Impact parameter First Born approximation or in short I.P.B. approximation. The cross - sections obtained by the application of this model are available in the papers written by Bates (1959), Bell (1961) and Bell and Skinner (1962), McDowell and Plutta (1966). Results of this approximation are very poor below 100 Kev.

Modification of I.P.B. method has been suggested by Bates (1959) and Mittleman (1961) which has been initially applied by Bates (1959).

Skinner (1962) and Bell and Skinner (1962) examined the transition

$$H^+ + H(1S) \longrightarrow H^+ + H(2p)$$

where they have obtained the coupling between the degenerate final sub-states $^2P_0$, $^2P_{\pm 1}$, and of direct coupling of these to the initial state, but not allowing the coupling for back - coupling or coupling to 2S. The resulting coupled first - order linear differential equation must be solved numerically. Their equation was of the form given below

$$i\vartheta \dot{a}_0 = a_0 V_{00}$$

$$i\vartheta \dot{a}_1 = a_0 V_{10} e^{i\beta z} + a_1 V_{11} + a_2 V_{12}$$

$$i\vartheta \dot{a}_2 = a_0 V_{20} e^{i\beta z} + a_1 V_{21} + a_2 V_{22}$$

where the coefficients a_K refers to the ground - state if K = 0, the $2p_0$ state if K = 1, and the $2p_{+1}$ state if K = 2, β is W_{01}/ϑ , $W_{01} = W_{02}$

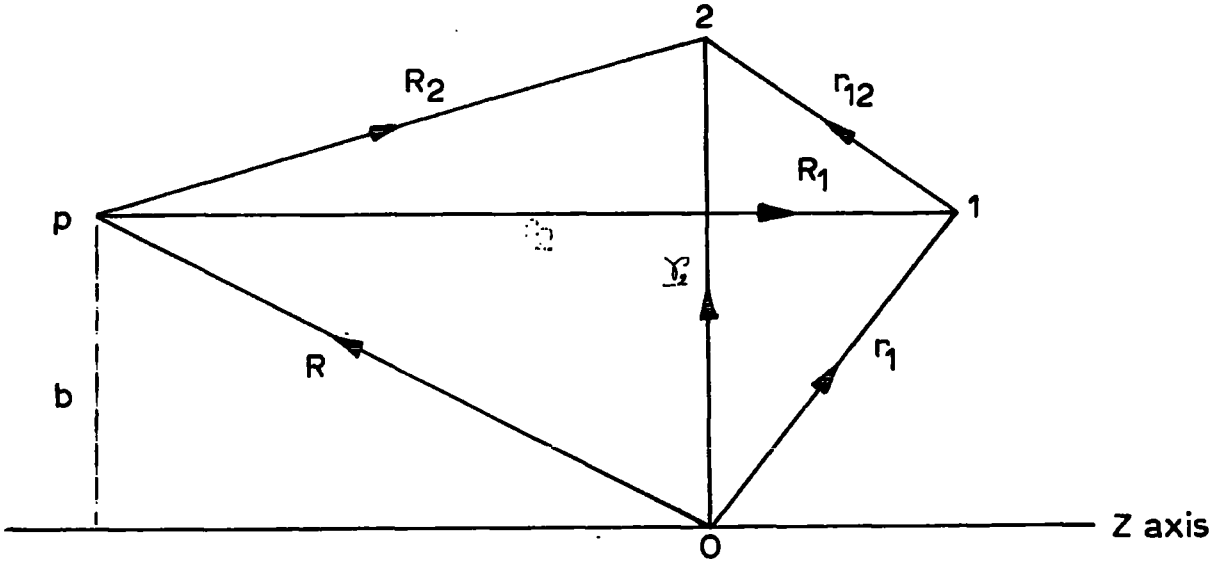
Also to solve the equation (3-6), a special class of perturbation method has first been introduced by Callaway and Bauer(1965) which has been applied on proton - hydrogen scattering process by Callaway and Dugan (1966). By this method they have calculated the 2S and 2p levels of hydrogen atom by slow protons (E $\lesssim$ 50 Kev) where they have neglected exchange and included $1S, 2S, 2p_0, 2p_{+1}$ states explicitly. Their results are three or more times larger than the experimental results given by Stebbings et al (1965), Gailly (1968). But their results for the 2p states has been agreed with Bell and Skinner (1962).

Most recent work on I.P.B. approximation has been given by Flannery (1970). The cross-sections are obtained for both the 2^1S and 2^1p excitation of helium by proton and electron impact and are shown in table 3 and 4 respectively.

CHAPTER 4

Present calculation on excitation

Introduction: In this chapter we calculate the cross - section for the elastic scattering and the 2^1S and 2^1p excitations of helium atom by proton impact keeping the helium atom initially in their ground state. The calculations have been performed using the truncated eigenfunction - expansion method, in the impact parameter formalism, introduced by Bransden and Coleman, 1972, which has successfully been used by Bransden et al (1972) and Sullivan et al (1972) to the scattering of electrons and protons from hydrogen atom. Recently, a paper has also been published on the electron - helium scattering by Berrington et al (1972).



Let p be the proton incident on the nucleus 0 which is fixed and has been taken as an origin. Let $\underline{R}$, $\underline{r}_1$, $\underline{r}_2$, $\underline{r}_{12}$, $\underline{R}_1$, $\underline{R}_2$ be the position vectors between the proton p and the nucleus 0, the nucleus 0 and the electron 1, the nucleus 0 and the electron 2, the electron 1 and the electron 2, the proton p and the electron 1, the proton p and the electron 2 respectively. Let V be the velocity along the direction of z - axis so that before collision, we have $\underline{R} = b + vt$, where $v.b = 0$ and b is the perpendicular distance between p and the z axis which is known as the impact parameter.

Total Hamiltonian is given by

$$H = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 + V_{01} + V_{02} + V_{12} + V_{p1} + V_{p2} + V_{op}$$

where we can define $V_{01}, V_{02}, V_{12}, V_{p1}, V_{p2}, V_{op}$ by the help of coulomb potentials.

So H can be written as

$$H = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - \frac{2}{r_1} - \frac{2}{r_2} - \frac{1}{R_1} - \frac{1}{R_2} + \frac{2}{R} + \frac{1}{r_{12}} \qquad (4\text{-}1)$$

The electronic wave - function $\psi(\underline{r}_1, \underline{r}_2, t)$ can be given by

$$\psi(\underline{r}_1, \underline{r}_2, t) = \sum_n a_n(t)\,\phi_n(\underline{r}_1, \underline{r}_2)\, e^{-i\epsilon_n t} \qquad (4\text{-}2)$$

$\phi_n(\underline{r}_1, \underline{r}_2)$ is known as the unperturbed helium wave function which satisfies the condition

$$H_e\,\phi_n(\underline{r}_1, \underline{r}_2) = \epsilon_n \phi_n(\underline{r}_1, \underline{r}_2) \qquad (4\text{-}3)$$

where ϵ_n and H_e represents the unperturbed eigen energy and the unperturbed hamiltonian for the helium atom in their ground state respectively.

Now, substituting (4-3) into the time - dependent Schrödiger equation (1-49) and following the procedure given in chapter

2, we get a set of coupled equations given below

$$i\frac{\partial a_n}{\partial z} = \frac{1}{v}\sum_{m=0}^{N} V_{nm}(z)\, a_m(z)\, e^{i(\epsilon_n - \epsilon_m)z/v} - \frac{i}{v^2}\int_{-\infty}^{z/v}\sum_{m=0}^{N} dz'\, K_{nm}(z,z')\, a_n(z') \qquad (4\text{-}4)$$

where V_{nm} and K_{nm} have been expressed in the same way as in chapter 2.

If we use N = 0 in equation (4-4), we get the one - channel equation only, which is given by

$$i\frac{\partial a_o}{\partial z} = \frac{1}{v} V_{oo}\, a_o(z) - \frac{i}{v^2}\int_{-\infty}^{z/v} dz'\, K_{oo}(z,z')\, a_o(z') \qquad (4\text{-}5)$$

For our present calculation we have included the back - couplings from 2^1S and 2^1p inelastic channel to the ground state for the elastic amplitude which is given by

$$i\frac{\partial}{\partial z} a_o = \frac{1}{v}\sum_{m=0,N} V_{om}(z)\, exp\{i(\epsilon_o - \epsilon_m)z/v\}\, a_o(z) - \frac{i}{v^2}\int_{-\infty}^{z/v} dz'\, K_{oo}(z,z')\, a_o(z') \qquad (4\text{-}6)$$

where N = 3.

where $K_{oo}(z,z')$ can be expressed by following the equation (2-12) given in chapter 2, where now, we are using n = m = o

Therefore

$$K_{oo}(z,z') = e^{i(\bar{\epsilon}-\epsilon_o)(z-z')/v}\left[V_{oo}(z,z') - V_{oo}(z)\,V_{oo}(z')\right] \tag{4-7}$$

$V_{oo}(z)$ and $V_{oo}(z')$ can be defined as in chapter 2, and we can express $V_{oo}(z,z')$ as below

$$V_{oo}(z,z') = \int d\underline{r}_1 \int d\underline{r}_2\, \psi_o^*(\underline{r}_1,\underline{r}_2)\left(\frac{2}{R} - \frac{1}{R_1} - \frac{1}{R_2}\right)\left(\frac{2}{R'} - \frac{1}{R_1'} - \frac{1}{R_2'}\right)\psi_o(\underline{r}_1,\underline{r}_2) \tag{4-8}$$

where $R = b + z$, $R' = b + z'$

and $z = v\,t$, $z' = v\,t'$

The equation (4-8) can now be expressed as

$$V_{oo}(z,z') = 2I_{R_1R_1'} + 2I_{R_1R_2'} + \frac{4}{RR'} I_1 I_2 - \frac{4}{R'} I_{R_1} - \frac{4}{R} I_{R_1'}$$

where

$$I_{R_1R_1'} = \int d\underline{r}_1 \,|u(\underline{r}_1)|^2 \frac{1}{|\underline{r}_1 - \underline{R}_1||\underline{r}_1 - \underline{R}_1'|} \int d\underline{r}_2\,|u(\underline{r}_2)|^2 \tag{4-9}$$

$$I_{R_1R_2'} = \int d\underline{r}_1\,|u(\underline{r}_1)|^2 \frac{1}{|\underline{r}_1 - \underline{R}|} \int d\underline{r}_2\,|u(\underline{r}_2)|^2 \frac{1}{|\underline{r}_2 - \underline{R}'|} \tag{4-10}$$

$$I_1 I_2 = \int d\underline{r}_1\,|u(\underline{r}_1)|^2 \int d\underline{r}_2\,|u(\underline{r}_2)|^2 \tag{4-11}$$

$$I_{R_1} = \int d\underline{r}_1\,|u(\underline{r}_1)|^2 \frac{1}{|\underline{r}_1 - \underline{R}|} \int d\underline{r}_2\,|u(\underline{r}_2)|^2 \tag{4-12}$$

$$I_{R_1'} = \int d\underline{r}_1\,|u(\underline{r}_1)|^2 \frac{1}{|\underline{r}_1 - \underline{R}'|} \int d\underline{r}_2\,|u(\underline{r}_2)|^2 \tag{4-13}$$

In the above equation we have used $\Psi(\underline{r}_1, \underline{r}_2) = U(\underline{r}_1)\, U(\underline{r}_2)$

Also we know that

$$\int d\underline{r}_1 |u(\underline{r}_1)|^2 \frac{1}{|\underline{r}_1 - \underline{R}|\,|\underline{r}_1 - \underline{R}'|} = \int d\underline{r}_2 |u(\underline{r}_2)|^2 \frac{1}{|\underline{r}_2 - \underline{R}|\,|\underline{r}_2 - \underline{R}'|}$$

$$\int d\underline{r}_1 |u(\underline{r}_1)|^2 = \int d\underline{r}_2 |u(\underline{r}_2)|^2$$

and

$$\int d\underline{r}_1 \frac{|u(\underline{r}_1)|^2}{|\underline{r}_1 - \underline{R}|} = \int d\underline{r}_2 \frac{|u(\underline{r}_2)|^2}{|\underline{r}_2 - \underline{R}|}$$

From the above equations, the equation (4-10) is very difficult to evaluate. But that has been done by employing the ~~numerical~~ technique given by Coleman (1970) which will be presented in Appendix C.

The inelastic amplitude has similarly been considered by taking all the direct couplings between the four channels (1^1S, 2^1S and the two independent magnetic sub - states of 2^1p), which is now

$$i \frac{\partial}{\partial z} a_n(z) = \frac{1}{v} \sum_{m=0,N} V_{nm}(z)\, e^{i\{(\epsilon_n - \epsilon_m) z/v\}} \qquad a_m(z) \qquad (4\text{-}14)$$

$n \neq o$

and $N = 3$.

Total cross-section has been calculated by employing the formula

$$Q(is, n) = 2 \int_0^\infty \frac{K_n}{K_o} |a_n(+\infty)|^2 b\, db \qquad \pi a_o^2 \qquad (4\text{-}15)$$

Flannery (1970) has solved the equation (4-14) for both elastic and inelastic cases for proton - helium collisions.

4.1 Calculations

For the 1^1S, 2^1S and 2^1p states the following Hartree - Fock function have been used and defined as in Flannery (1970)

$$\Psi_{1s}(\underline{r}_1, \underline{r}_2) = \frac{1.6966}{\pi} \{exp(-1.4r_1) + 0.799 \times exp(-2.61 r_1)\}$$

$$\times \{exp(-1.4r_2) + 0.799 \times exp(-2.61 r_2)\} \quad (4\text{-}16)$$

$$\Psi_{2s}(\underline{r}_1, \underline{r}_2) = \frac{N}{(1+\Delta^2)^{1/2}} [exp(-2r_2)\{exp(-\lambda r_1) - (cr_1) \times exp(-\mu r_1)\}$$

$$+ exp(-2r_1)\{exp(-\lambda r_2) - cr_2 \times exp(-\mu r_2)\}] \quad (4\text{-}17)$$

$$\Psi_{2p}(\underline{r}_1, \underline{r}_2) = \frac{0.3783}{\sqrt{\pi}} [r_1 \, exp\{-(0.485 r_1 + 2r_2) y_{1,m}(r_1)\}$$

$$+ r_2 \, exp\{-(0.485 r_2 + 2r_1) y_{1,m}(r_2)\}] \quad (4\text{-}18)$$

respectively. The equations (4-16), (4-17) and (4-18) was first introduced by Byron and Joachain (1966), Goldberg and Clogston (1939) and Cohen and McEachran (1967) respectively. The unknown values in the equation (4-17) is given by $\lambda = 1.1946$, $\mu = 0.4733$, $N = 0.70640$, $\Delta = 0.007322$ and $C = 0.26832$.

To solve equation (4-6) and (4-14) we applied the integro - differential equation for numerical calculations by a Hamming's method. Then, we have used Simpson's rule to integrate over the impact parameter b, to get the total cross - sections from equation (4-15). The measurement of Martin (1960) being used for the 2^1S and 2^1p excitation energies (0.7577

and 0.7799 a.u.). The values of the effective energy has been considered as below.

4.2 The average excited energy.

From chapter 2, we know that the average excitation energy is $-\frac{\alpha}{2r^4}$ and is very important for the long - range potential due to dipole polarizability of a neutral atom in the scattering process. From paper II and IV, we know that the effective energy can be replaced either by all the levels above the ground state which is equal to 1.14 or we can use the exact 2^1S and 2^1p energies and average the remaining energies which is equal to 1.34. In this calculation we have used the value of energy as 1.34.

Also from paper II and IV we notice that the variation of the effective energy has very little effects on the elastic cross-section in the one - channel approximation of equation (4-6) given above.

4.3 Elastic scattering of protons

Equations (4-6) and (4-14) have been solved with the full static coupling between 1^1S, 2^1S and 2^1p states where we have used the second - order term in the elastic channel. Total cross - section for the elastic channel has been calculated by using the formula (4-15). In table 1 our predictions for elastic scattering are shown, no experimental data or other calculated results are available for comparison.

4.4 The 2^1S excitation of helium by protons.

The total cross-section, evaluated with the full static coupling between the 1^1S, 2^1S and 2^1p states and the 2nd order term in the elastic channel, are shown in table 2 for the 2^1S excitations. These are compared with the First Born cross - sections (B1) of Bell et al (1968). The Second Born approximation (SB2) of Holt et al (1971), the results of a four - channel approximation of Flannery (1970). As there are no experimental data available we could not compare our results with any experimental result. Though we have included the 2nd order term yet our results are below Flannery (1970). But the present results are a little larger than the values of First Born and 2nd Born approximation at high energies. Figure (1) shows the effects of various approximation on the total cross - sections.

4.5 The 2^1p excitation of helium by protons.

Table 3 shows the results with full static coupling between the 1^1S, 2^1S, 2^1p states and the second - order term in the elastic channel. This is compared with the results using the four - channel approximation of Flannery (1970), the First Born approximation (B1) of Bell et al (1968), the second Born approximation (SB2) of Holt et al (1971). Here, also no experimental results are available. Figure (2) shows the effects of various approximation on the total cross - sections.

CHAPTER 5

Earlier work on charge - exchange.

5.1 Classical approximation

The first calculation on the capture process $H^+ + H(1S) \longrightarrow H(1S) + H^+$ was made by Thomas (1927). In his calculations he considered the above process as a two - body collision where the collision can occur firstly between the electron and the incident ion and secondly between the electron and the nucleus of the target. He found that the cross - section behaves like v^{-11} when the velocity V is very high. Drisko (1955) and Bransden and Cheshire (1963) have also obtained the same results for their calculations on the 2nd Born approximation and the Impulse approximation respectively. But Cook (1963) has shown by the uncertainty Principle that the Thomas model can not be in a high - energy limit. Using Monte Carlo's method Abrines and Percival (1964) have solved the Newtonians equations of three - body motion for two protons and an electron and have hence obtained the cross - section for capture H^+ - H(1S) collisions at a few impact energies. The modification of Thomas model was made by Bates and Mapleton (1965) where they found that predictions of the modified theory are in good accord with the experimental data. They also developed a simple classical theory for the symmetrical resonance capture in slow encounters.

5.2 The First Born approximation

From chapter 1, we know that the First Born approximation is given by

$$T_{fi} = \langle \phi_f | V_f | \phi_i \rangle \qquad (5\text{-}1)$$

where ϕ_i and ϕ_f are the initial and final wave functions, and V_f is the interaction, which we can express by the help of Coulomb potential.

Brinkman and Kramers (1930) and Oppenheimer (1928) have attempted to solve the equation (5-1) to get the cross - sections for the process $H^+ + H(1S) \rightarrow H(1S) + H^+$. But in their calculations they have considered only the electron - incident interaction and ignored the nuclear - nuclear interaction, as they have concluded that internuclear potential has very little contribution to charge - exchange cross - sections, which is arising for the non-orthogonality of $\phi_i(\underline{r}_1)$ and $\phi_f(\underline{r}_2)$. The calculated cross - section in the ground state capture has been given in units of πa_o^2 and is

$$Q_{OBK} = 2^8/5(1+v^2/4)v^2$$

where V is the velocity of the incident proton in atomic units that the incident energy $E = 24.97V^2$ Kev. But in the high energy limit the ground - state cross - sections behaves like

$$Q_{OBK} = 2^{18}/5\, v^{12}$$

and the capture into the n'th level has been found as

$$Q_{OBK} = Q_{OBK}(1S)/n^3$$

From this, Oppenheimer (1928) suggested that the capture cross - section into the n'th level is proportional to $1/n^3$. Their calculation approximately is four times higher than the

existing experimental results and still higher at lower energies. They calculated only the ground - state electron - capture cross - section and their procedure has since been followed by Saha and Basu (1945) and Takayyangi (1952). The cross - section for the excited states and many electron - systems has been calculated by Bates and McCarroll (1962), Omidvar (1967), Mapleton (1963, 1965, 1966, 1968), Nikolaev (1967).

But Bates and Dalgarno (1952) concluded that the internuclear potential should not be so small and negligible and so in their calculations they first included this term and carried out their calculations for the same process which we have mentioned above. Corinaldesi and Trainer (1952) and Jackson and Schiff (1954) also did the same calculations by using the Fourier's transform of Feynmann (1949).

The first calculations for the process

$$H^+ + He(1s^2) \rightarrow He^+(1s) + H(1s) \qquad (5\text{-}2)$$

have been done by Bransden, Dalgarno and King (1954) where they have obtained the simple ground - state helium wave function

$$\psi(\underline{r}_1, \underline{r}_2) = \frac{\lambda^3}{\pi} \exp[-\lambda(r_1 + r_2)] \qquad (5\text{-}3)$$

where $\lambda = 1.6875$

They calculated both $Q_{OBK}(1S^2/\ 1S,\ 1S)$ and $Q_B(1S^2/\ 1S,\ 1S)$ and they have found that the cross - section Q_{OBK} is larger than Q_B which agrees better with the experimental results. Here Q_{OBK} (given in page 52) means the Brinkman Kramer's cross - section and Q_B is the Born cross - section.

Detailed calculations for the above process (5-2) has been carried out by Mapleton (1961) who also obtained the same helium wave function (5-3), where he calculated both the post

and prior cross - sections for the cases (1S, 1S),(1S, 2p), (2S, 1S), (2S, 2p), (2p, 2S),(3S, 1S).

His results are 2.5 times greater than Bransden, Dalgarno and King (1954). But the mean value of his post and prior cross - sections have been compared with the existing experimental results done by Steir and Barnett (1956), Barnett and Reynolds (1958), Allisien (1958) and the agreement between them is quite close. Mapleton (1963), again, has done some calculations for the above - mentioned process (5-2) using the six - parameter helium wave function by Hyllerass and has also calculated the cross - section for the post and prior form wave function of helium. The calculated cross - sections have been improved by using more accurate wave - function from which we can conclude that for the large impact parameters we should use accurate wave function which can give the correct result for the high energies.

5.3 The Second - Born approximation

On the Second Born approximation, only Drisko (1955)'s work is available where he applied this method to calculate the cross - section for the proton - hydrogen cases.
We know, from chapter 1, the Second Born approximation, is given by

$$T_{fi}^{B2} = \langle \phi_f | V_f | \phi_i \rangle + \langle \phi_f | V_f G^+ V_i | \phi_i \rangle$$
$$= T_{fi}^{B} + \langle \phi_f | V_f G^+ V_i | \phi_i \rangle \qquad (5\text{-}4)$$

In equation (5-4) Drisko used free Green's function G_0 which is now

$$T_{fi}^{B2} = T_{fi}^{B} + \langle \phi_f | V_f G_0^+ V_i | \phi_i \rangle \qquad (5\text{-}5)$$

The equation (5-5) can be written as

$$T_{fi}^{B2} = T_{fi}^{B} + I(V_1, V_2) + I(V_2, V_2) + I(V_2, V_3) + I(V_1, V_3)$$
$$= T_{fi}^{B} + I(V, V) \qquad (5\text{-}6)$$

and G_0 can be defined with the help of configuration space,

$$G_0(\underline{r}_3, \underline{R}_3, \underline{r}_3', \underline{R}_3') = (2\pi)^{-6} \int dq_{v_3} \int dp_3 \frac{\exp\left[i\{\underline{q}_{v_3}\cdot(\underline{r}_3 - \underline{r}_3') + \underline{p}_3\cdot(\underline{R}_3 - \underline{R}_3')\}\right]}{\left[\frac{K_f^2}{2\mu_3} + E_B + i\epsilon - E_{q_{v_3}} - E_{p_3}\right]}$$

E_B is the kinetic energy of hydrogen in the ground state 1S and p_i and q_i are the momenta, μ_i and M_i are the reduced masses defined as

$$\mu_i = \frac{m_1 (m_2 + m_3)}{m_1 + m_2 + m_3}$$

and

$$M_i = \frac{m_2 m_3}{(m_2 + m_3)}$$

From Drisko, ~~the second part of~~ the equation (5-6) can be given by

$$4.(2\pi)^{-4}\int d\underline{q}\int d\underline{K}\left[-\frac{\underline{k}^2}{2\mu_3}+E_B+\left(\beta+\frac{1+M}{M}\alpha\right).k-\frac{1+M}{2M}q^2\right]^{-2} I(\underline{q},\underline{K})$$

where I($\underline{q}$, $\underline{k}$) has been represented by the 2nd part by (5-6).

The calculations of $I(V_1, V_2)$ etc. are available in the book written by McDowell & Coleman (1970) and also in the paper written by Bransden (1965).

Drisko neglected the term containing $1/M$ and found that

$T_{fi}^{B} + I(V_2, V_2) + I(V_2, V_3) = 0$

for the high energy cases. He also neglected the internuclear potential. So he was left only with the two equation , which was

$$T_{fi}^{B2} = T_{fi}^{BK} + I(V_1, V_3) \qquad (5\text{-}7)$$

The required cross - section of (5-7) now has been given by

$$Q^{B2} \sim (0.2996 + 5\pi V/2^{12})\, Q_{BK}$$

which is having the same V^{-11} dependence as Thomas (1927) had in his result. Drisko (1955) also added the 3rd term of the Born approximation given in chapter 1 and obtained the result as

$$Q^{B3} \sim (0.319 + 5\pi V/2^{12})\, Q_{BK}$$

which has also contained the same independence as before.

5.4 The Distorted wave approximation.

Bassel and Gerjuoy (1960) first attempted to calculate the cross - section for proton - hydrogen charge - exchange process where he adopted the distorted wave method. We know, that the exact transition for the above process from the initial state i to the final state f can be given by

$$T_{fi} = \langle \psi_f^- | V_i - W_f | \chi_i^+ \rangle \qquad (5\text{-}8)$$

The equation (5-8) can be altered for the distorted wave method which is given by

$$T_{fi}^{DWD} = \langle \xi_f^- | V_i - W_f | \chi_i^+ \rangle \qquad (5\text{-}9)$$

and which is known as the first - order distorted wave approximation.

In their calculations Bassel and Gerjuoy (1960) defined U_i and U_f as

$$U_i = \int d\underline{r} \, |\phi_i(\underline{r})|^2 V_i(\underline{r}, \rho)$$

$$U_f = \int d\underline{r} \, |\phi_f(\underline{r})|^2 V_f(\underline{r}, \rho)$$

which they have integrated for constant separation ρ . But instead of taking the distorted initial and final wave function they have obtained the undistorted initial and final wave function in their calculations. The equation was of the form given below

$$T_{fi}^{DWD} = T_{fi}^{B} + T_{fi}^{BG} \qquad (5\text{-}10)$$

Their calculated cross - section is very close to the First Born approximation.

Their method, since then has been followed by Grant and Shapiro (1965) where they have used the exact expressions for ξ_f^- and χ_i^+ . Here, they found that their result was quite near to Brinkman and Kramer's result. The details discussion

of this method are available in Bransden (1970) and McDowell and Coleman (1970).

5.5 The Impulse approximation

From chapter 1, we know that the impulse approximation for the prior and post can be given by

$$T_{fi}^{IMP} = \langle \phi_f | V_f (W_{13}^{+} + W_{12}^{+} - 1) \phi_i \rangle \qquad (5\text{-}11)$$

$$T_{fi}^{-IMP} = \langle (W_{13}^{+} + W_{12}^{+} - 1) \phi_f^{-} | V_i | \phi_i \rangle \qquad (5\text{-}12)$$

Also we have shown in chapter 1, that (5-11) or (5-12) can be reduced into

$$T_{fi}^{IMP} = \langle \phi_f | V_{13} | \phi_i \rangle$$

$$T_{fi}^{-IMP} = \langle \phi_f^{-} | V_{13} | \phi_i \rangle$$

This approximation has been applied by Pradhan (1957) to the capture process

$$H(1S) + P \rightarrow P + H(1S) \qquad (5\text{-}13)$$

where in the case of V_{13} he took V_{23}. This simplifies the analysis, but the resulting matrix no longer describes the collision under consideration (Bassel and Gerjuoy, 1960). The calculation on the above process (5-13) has also been carried out by Cheshire (1965) and McDowell (1961). McDowell (1961) has used the correct form of T_{fi}^{IMP} given in chapter 1, where he did his calculation simultaneously by including and excluding the V_{12} interaction.

This approximation has also been applied to proton - helium collision by Bransden and Cheshire (1963) where they have described the impulse approximation as

$$T_{fi}^{IMP} = \langle \phi_f | V_{12} + V_{23} + V_{14} + V_{34} | (W_{12}^{+} + W_{13}^{+} + W_{14}^{+} - 2) \phi_i \rangle \qquad (5\text{-}14)$$

In this case, the particle 1, incident on a helium atom in the ground state with nucleus 2 and electrons 2 and 3 captures (3) into the ground state by hydrogen leaving residual ion in the ground state.

The post form

$$T_{fi}^{-IMP} = \langle \phi_f | (W_{12}^{-} + W_{23}^{-} + W_{14}^{-} + W_{34}^{-} - 3) | V_{12} + V_{13} + V_{14} | \phi_i \rangle \qquad (5\text{-}15)$$

has also been considered.

Due to distortion they neglected V_{12} as well as W_{12}^{+}. Similarly they have neglected W_{14}^{+} in the same way and the equation (5-14) gives

$$T_{fi}^{IMP} = \langle \phi_f | V_{12} + V_{23} + V_{14} + V_{34} | W_{13}^{+} \phi_i \rangle \qquad (5\text{-}16)$$

In the post case the V_{34}^{-} term is known as the electron - electron interaction , which is very difficult to evaluate. So they have expressed

$$T_{fi}^{-IMP} = \langle W_{23}^{-} \phi_f | V_{12} + V_{13} + V_{14} | \phi_i \rangle \qquad (5\text{-}17)$$

The cross - sections have been calculated for both prior (5-16) and post (5-17) form, where they have obtained simple ground - state helium wave function. Their results are below the experimental results and has been shown in figure 17.

5.6 Atomic eigenfunction expansion method

Bates two - state method has first been used by McCarroll (1961) for the symmetrical resonance process

$$H^+ + H(1S) \rightarrow H(1S) + H^+$$

Later on, McCarroll and McElroy (1962) has extended the calculations for the non-resonance process

$$He^{2+} + H(1S) \longrightarrow H(1S) + H^+ \qquad (5\text{-}18)$$

McElroy (1963) has done calculations for the accidental resonant reaction

$$He^{2+} + H(1S) \rightarrow He^{+} \ (2S \text{ or } 2p) + H^+$$

and non-resonant reaction

$$H^+ + H(1S) \longrightarrow H(2S \text{ or } 2p) + H^+$$

Lovell & McElroy (1963) have followed the earlier work of McElroy (1963) and investigated the following process

$$H^+ + H(1S) \rightarrow H(1S) + H^+$$

$$H^+ + H(1S) \rightarrow H(2S) + H^+$$

$$H^+ + H(1S) \rightarrow H^+ + H(2S)$$

The above process (5-18) has later been extended by Wilets and Galleher (1966) where they included 1S, 2S and 2p states for their calculations. In some of their calculations they also included 3S and 3p states as well.

On proton - helium scattering, Green et al (1965) have also applied Bates two - state method, where they have used the open - shell function of Eckart (1930)

$$\phi(\underline{r}_1, \underline{r}_2) = N\left[\exp(-\alpha r_1)\exp(-\beta r_1) + \exp(-\alpha r_2)\exp(-\beta r_2)\right] \qquad (5\text{-}19)$$

for the ground - state helium wave - function. In equation

(5-19) N is the normalization factor and α and β are given by

$$\alpha = 2.1832, \quad \beta = 1.1885, \quad E = 2.8757.$$

The sensitivity of the helium wave - function has been investigated by Bransden and Sin Fai lam (1966) where they have done their calculations by employing equation (5-19) as well as two other wave - functions $\phi^{(1)}$ and $\phi^{(2)}$ given below.

$$\phi^{(1)} = \frac{N}{\alpha^3} e^{-\alpha(r_1 + r_2)} \tag{5-20}$$

where $\alpha = 1.6875$ and N is the normalization constant and

$$\phi^{(2)} = N\left[\exp(-\alpha r_1) + (c)\exp(-\beta r_1)\right] \times \left[\exp(-\alpha r_2) + (c)\exp(-\beta r_2)\right] \tag{5.21}$$

where

$$\alpha = 1.455799, \quad \beta = 2\alpha, \quad C = 0.6$$

$$\text{and } E = -2.86.$$

In each case parameters are determined variationally.
It has been shown by Shull and Lowdin (1966) and Green et al (1954) that both (5-19) and (5-21) are good approximation. But the calculated cross - sections of Bransden and Sin Fai lam (1966) for three different employed wave - functions shown above, do not vary from each other. So they have concluded that the simple helium wave - function is good enough for any further calculations.
Sin Fai lam (1967), has extended this work by the inclusion of the excited states (2^1S, 2^1p states) of hydrogen. But that did not agree very well with the experimental data. To compare with the experiment, the calculated cross - sections have to be increased by a factor of up to 30% to allow capture

into excited states (Mapleton, 1961).

CHAPTER 6

Present calculation on [illegible] charge - exchange

Introduction The two - state impact parameter method, first investigated by Bates (1958), has been used for the non - resonant charge - exchange reaction

$$p + He\ (1S^2) \longrightarrow H(1S) + He^+(1S)$$

which we have described in chapter 1. Our method, though based on the method of Bates (1958), has been modified by applying the 2nd order potential and using the closure approximation derived by Bransden and Coleman (1972). A short description of their method has also been given in chapter 2, which has successfully been used for the excitation process between proton or electron impact from hydrogen atom (Sullivan et al, 1972a, 1972b) as well as for electron impact from helium atom (Berrington et al, 1972).

We are considering the same co-ordinates in the X - Z plane as we did in chapter 4, where the total Hamiltonian is

$$H = -\tfrac{1}{2}\nabla_1^2 - \tfrac{1}{2}\nabla_2^2 - \frac{2}{r_1} - \frac{2}{r_2} - \frac{1}{R_1} - \frac{1}{R_2} + \frac{1}{r_{12}} + \frac{2}{R} \qquad (6\text{-}1)$$

and where $\underline{r}_1$, $\underline{r}_2$, $\underline{R}_1$, $\underline{R}_2$ and $\underline{R}$ have been defined.

Since, in this chapter, we are dealing with the reactions between proton and helium and especially the charge - exchange or electron - capture cases, we get

$$P + He\,(1S^2) \rightarrow H\,(1S) + He^+(1S) \qquad (6\text{-}2)$$

for which, before collision, we get

$$\psi_n(\underline{r}_1, \underline{r}_2, t) = \psi_n(\underline{r}_1, \underline{r}_2)\, e^{-i\epsilon_n t} \qquad (6\text{-}3)$$

and after collision,

$$\tilde{\omega}_{ij}(\underline{R}_1, \underline{r}_2, t) = \chi_{ij}(\underline{R}_1, \underline{r}_2)\, e^{-i(\mu_i + \eta_j + \frac{v^2}{2})t + i\underline{v}\cdot\underline{r}_1} \quad (6\text{-}4)$$

where ψ_n and χ_{ij} are the initial and final ~~Helium~~ wave - function respectively, ϵ_n is the binding energy of the helium wave - function before collision and $(\mu_i + \eta_j)$ be the binding energy of the wave - function $\chi_{ij}(\underline{R}_1, \underline{r}_2)$ which can be split into

$$\chi_{ij}(\underline{R}_1, \underline{r}_2) = \phi_i(\underline{R}_1)\,\phi_j(\underline{r}_2)$$

The wave - functions $\phi_i(\underline{R}_1)$ and $\phi_j(\underline{r}_2)$ are given explicitly as

$$\phi_i(\underline{R}_1) = \frac{1}{\sqrt{\pi}}\, e^{-\underline{R}_1} \quad (6\text{-}5)$$

and

$$\phi_j(\underline{r}_2) = \frac{\sqrt{8}}{\sqrt{\pi}}\, e^{-2\underline{r}_2} \quad (6\text{-}6)$$

and which satisfies the equations

$$\left(-\frac{1}{2}\nabla_1^2 - \frac{1}{R_1}\right)\phi_i(\underline{R}_1) = \mu_i\,\phi_i(\underline{R}_1)$$

and

$$\left(-\frac{1}{2}\nabla_2^2 + \frac{2}{r_2}\right)\phi_j(\underline{r}_2) = \eta_j\,\phi_j(\underline{r}_2)$$

The helium wave - function satisfies the equation

$$\int \psi_n^*(\underline{r}_1, \underline{r}_2)\left(-\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - \frac{2}{r_1} - \frac{2}{r_2} + \frac{1}{r_{12}}\right)\psi_n(\underline{r}_1, \underline{r}_2) = \epsilon_n \quad (6\text{-}7)$$

Now, we can employ the two - state approximation given by Bates (1958) where the initial and final state will be considered. Therefore

$$\psi(\underline{r}_1, \underline{r}_2, t) = \sum_n a_n(t)\, U_n(\underline{r}_1, \underline{r}_2, t) + \sum_{ij} b_{ij}(t)\, \tilde{\omega}_{ij}(\underline{R}_1, \underline{r}_2) \quad (6\text{-}8)$$

where Σ implies a sum over the discrete states and an integration over the continuum states.

Substituting (6-8) in the time - dependent Schrodinger equation (in atomic units)

$$H\Psi(\underline{r}_1, \underline{r}_2, t) = i \frac{\partial \Psi(\underline{r}_1, \underline{r}_2, t)}{\partial t} \tag{6-9}$$

and using all the conditions given above, we get a set of coupled equations, given by

$$i\dot{a}_n + i \sum_{ij} N_{n,ij} \dot{b}_{ij} = \sum_n H_{n,n'} a_{n'} + \sum_{ij} K_{n,ij} b_{ij} \tag{6-10}$$

$$i\dot{b}_{ij} + i \sum_n \bar{N}_{ij,n} \dot{a}_n = \sum_{ij} \overline{H_{ij,n}} b_n + \sum_n \overline{K_{ij,n}} \tag{6-11}$$

where $N_{n,ij}$, $H_{n,n'}$, $K_{n,ij}$, $\bar{N}_{ij,n}$, $\bar{H}_{ij,n}$, $\bar{K}_{ij,n}$ can be defined in the following way

$$N_{n,ij} = e^{iE^{(1)}_{n,ij}t} \int d\underline{r}_1 \int d\underline{r}_2 \, \psi_n(\underline{r}_1, \underline{r}_2) \chi_{ij}(\underline{R}_1, \underline{r}_2) e^{i\vartheta \cdot \underline{r}_1} \tag{6-12}$$

$$H_{n,n'} = e^{iE^{(2)}_{n,n'}t} \int d\underline{r}_1 \int d\underline{r}_2 \, \psi^*_n(\underline{r}_1, \underline{r}_2) \left(\frac{2}{R} - \frac{1}{R_1} - \frac{1}{R_2}\right) \psi_{n'}(\underline{r}_1, \underline{r}_2) \tag{6-13}$$

$$K_{n,ij} = e^{iE^{(1)}_{n,ij}t} \int d\underline{r}_1 \int d\underline{r}_2 \, \psi_n(\underline{r}_1, \underline{r}_2) \left(\frac{2}{R} - \frac{2}{r_1} - \frac{1}{R_2} + \frac{1}{r_{12}}\right) \times \left(\chi_{ij}(\underline{R}, \underline{r}_2) e^{i\vartheta \cdot \underline{r}_1}\right) \tag{6-14}$$

$$\overline{N_{ij,n}} = e^{-iE^{(1)}_{n,ij}t} \int d\underline{r}_1 \int d\underline{r}_2 \, \chi^*_{ij}(\underline{R}_1, \underline{r}_2) \psi_n(\underline{r}_1, \underline{r}_2) e^{-i\vartheta \cdot \underline{r}_1} \tag{6-15}$$

$$\overline{H_{ij,ij'}} = e^{iE_{ij,ij'}t} \int d\underline{r}_1 \int d\underline{r}_2 \, \chi^*_{ij'}(\underline{R}_1, \underline{r}_2)\left(-\frac{2}{r_1} - \frac{1}{R_2} + \frac{1}{r_{12}} + \frac{2}{R}\right)\chi_{ij}(\underline{R}_1, \underline{r}_2) \tag{6-16}$$

$$\overline{K_{ij,n}} = e^{-iE^{(1)}_{n,ij}t} \int d\underline{r}_1 \int d\underline{r}_2 \, \chi^*_{ij}(\underline{R}_1, \underline{r}_2)\,\psi_n(\underline{r}_1, \underline{r}_2)$$

$$\times \left(-\frac{1}{R_1} - \frac{1}{R_2} + \frac{2}{R}\right) e^{i\vartheta \cdot \underline{r}_1} \tag{6-17}$$

where

$$E^{(1)}_{n,ij} = (\epsilon_n - \epsilon_{ij}) \tag{6-18}$$

$$E^{(2)}_{n,n'} = (\epsilon_n - \epsilon_{n'}) \tag{6-19}$$

and

$$E_{ij,i'j'} = (\eta_i + \mu_j - \eta_{i'} - \mu_{j'}) \tag{6-20}$$

where the values of ϵ, η, μ can be given by

$$\epsilon = -2.84$$

$$\eta = -0.5$$

$$\mu = -0.2$$

respectively.

If we, now, consider, these equations for the case of $n \neq 0$, $i \neq 0$, $j \neq 0$, we can approximate (1) by retaining coupling to state $n = 0$, $i = 0$, $j = 0$ only and (2) by neglecting the diagonal terms.

Therefore, we get

$$i\dot{a}_n + i\sum_{ij} N_{n,ij}\dot{b}_{ij} = H_{n,o}a_o + K_{n,o}b_o \tag{6-21}$$

$$i\dot{b}_{ij} + i\sum_{n}\overline{N_{ij,n}}\,\dot{a}_n = \overline{H_{ij,o}}\,b_o + \overline{K_{ij,o}}\,a_o \qquad (6\text{-}22)$$

for $n \neq 0$, $i\,j \neq 0$.

For further approximation, we have used $b_{ij} \sim o$, if $ij \neq 0$

Then

$$i\dot{a}_n = H_{n,o}\,a_o + K_{n,o}\,b_o \qquad (6\text{-}23)$$

$$i\,a_n = \int_{-\infty}^{t'} dt' \{H_{n,o}(t')\,a_o(t') + K_{n,o}(t')\,b_o(t')\} \qquad (6\text{-}24)$$

and equations for $n = i \pm j = 0$ become

$$i\dot{a}_o + i\,N_{o,o}\,\dot{b}_o = H_{o,o}\,a_o + K_{o,o}\,b_o + \frac{1}{i}\sum_{n\neq o} H_{o,n} \times \int_{-\infty}^{t'} dt' \{H_{n,o}(t')\,a_o(t') + K_{n,o}(t')\,b_o(t')\} \qquad (6\text{-}25)$$

and also from (6-22), we get

$$i\dot{b}_o + i\overline{N_{o,o}}\,a_o = \overline{H_{o,o}}\,b_o + K_{o,o}\,a_o \qquad (6\text{-}26)$$

As in chapter 2 the potentials $H_{o,\,n}(t)\,H_{n,o}(t')$ and $H_{o,n}(t)\,K_{n,o}(t')$ are too complicated to evaluate exactly. Hence we have applied a further approximation called closure approximation as in chapter 2, and by the help of which we can write

$$H_{o,n}(t)\,H_{n,o}(t') = \left[H_{n,n}(t,t') - \sum_{j=o}^{N} H_{nj}(t)\,H_{jm}(t')\right] \times \exp(\epsilon_o - \bar{\epsilon})(t-t')$$

The other potential $H_{o,n}(t)K_{n,o}(t')$ has been dropped from our calculations.

Now substituting $n = 0$, equation(6-25) can be given by

$$i\dot{a}_o + iN_{o,o}\dot{b}_o = H_{o,o}a_o + k_{o,o}b_o + \frac{1}{i}\int_{-\infty}^{t'}\left[H_{o,o}(t,t') - \sum_{j=o}^{N} H_{oj}(t)\,H'_{jo}(t')\right]a_o(t') \times \exp(\epsilon_o - \bar{\epsilon})(t-t')\,dt' \qquad (6\text{-}27)$$

If we now take N = 0, the equation (6-27) gives

$$i\dot{a}_o + iN_{o,o}\dot{b}_o = H_{o,o}a_o + k_{o,o}b_o + \frac{1}{i}\int_{-\infty}^{t'}\left[H_{o,o}(t,t') - H_{o,o}(t)H_{o,o}(t')\right]a_o(t') \times \exp(\epsilon_o - \bar{\epsilon})(t-t')\,dt' \qquad (6\text{-}28)$$

where

The term $H_{o,o}(t, t')$ can be expressed like equation (4-9) defined in chapter 4 where $z = \vartheta t$ and $z' = \vartheta t'$ and can be solved in the same way as noted in chapter 4. In this case we have taken the values of the effective energy as 1.14, where we have applied the same condition given in chapter 4. The equation (6-26) and (6-28) has been solved by Hamming's method to get the time -dependent coefficients $a_o(t)$ and $b_o(t)$ with the initial boundary conditions $a_o(-\infty) = 1$ and $b_o(-\infty) = 0$

Total cross - section for charge - exchange from the initial state i to the final state f is now obtained by using the formula

$$Q_{if} = 2\pi a_o^2 \int_o^{\infty} \rho\,|b_f(+\infty)|^2\,d\rho \qquad (6\text{-}29)$$

where ρ is impact parameter.

Calculations

Calculations have been investigated for three different cases where we have used the one - parameter simple helium wave function given by

$$\psi(\underline{r}_1, \underline{r}_2) = \frac{N}{\pi}\, e^{-\alpha(r_1 + r_2)} \qquad (6\text{-}30)$$

where $N = \alpha^3$, $\alpha = 1.68$, $\epsilon_0 = -2.8472$.

Case A Distorted wave approximation (1)

In this case we have considered the coupling for initial state only and so the equation (6-26) and (6-28), mentioned above, can be given by

$$i\dot{a}_0 = H_{0,0}\, a_0 + \frac{1}{i}\int dt' \left[H_{0,0}(t,t') - H_{0,0}(t)\, H_{0,0}(t')\right] \times a_0(t') \exp(\bar{\epsilon} - \epsilon_0)(t-t') \tag{6-31}$$

$$i\dot{b}_0 = K_{0,0}\, a_0 \tag{6-32}$$

The cross - section of the charge - exchange can be calculated by using the formula (6-29) given above.

Case B. Distorted wave approximation (2)

The equations (6-26) and (6-28) can also be written in the following forms

$$i\dot{a}_0 = \frac{H_{0,0} - N_{0,0}\bar{K}_{0,0}}{1 - |N_{0,0}|^2} a_0 + \frac{K_{0,0} - N_{0,0}\bar{H}_{0,0}}{1 - |N_{0,0}|^2} b_0 - \frac{i}{1 - |N_{0,0}|^2} \int_{-\infty}^{t} \left[H_{0,0}(t,t') - H_{0,0}(t)\, H_{0,0}(t')\right] \times a_0(t') \exp(\epsilon_0 - \bar{\epsilon})(t-t')\, dt' \tag{6-33}$$

and

$$i\dot{b}_0 = \frac{\bar{H}_{0,0} - \bar{N}_{0,0} K_{0,0}}{1 - |N_{0,0}|^2} b_0 + \frac{\bar{K}_{0,0} - \bar{N}_{0,0} H_{0,0}}{1 - |N_{0,0}|^2} a_0 + \frac{i}{1 - |N_{0,0}|^2} \int_{-\infty}^{t} \left[H_{0,0}(t,t') - H_{0,0}(t)\, H_{0,0}(t')\right] \times a_0(t') \exp(\epsilon_0 - \bar{\epsilon})(t-t')\, dt' \tag{6-34}$$

In case B for elastic scattering we have used the formula (6-31), but for the charge - exchange case we have used

$$i\dot{b}_0 = \frac{\overline{H_{0,1,0}} - \overline{N_{0,1,0}}\,K_{0,1,0}}{1 - |N_{0,1,0}|^2}\, b_0 + \frac{\overline{K_{0,1,0}} - \overline{N_{0,1,0}}\,H_{0,1,0}}{1 - |N_{0,1,0}|^2}\, a_0$$

(6-35)

cross - sections have been calculated using the same formula (6-29).

Case C In this case we have used the formulas (6-33) and (6-34) as given above where the expressions for full couplings has been used and applied the same formula (6-29) to get the cross - sections.

The methods for evaluating the integrals (6-12), (6-13), (6-14), (6-15), (6-16), (6-17) will be shown in the appendices.

The results of the present calculations are shown for various proton energies in the table 4, together with the results of Bransden and Sin fai lam (1966), Green et al (1965), Mapleton (1961) and the results of the experiments which measure the total cross - sections for capture summed over all final states. To compare with the experiment the calculated cross - sections have to be increased by a factor of up to 30% to allow for capture into excited states (Mapleton, 1961).

Figures (3, 4, 5, 6), (7, 8, 9, 10), (11, 12, 13), show the present result for the probability of capture into the 1S state for various energies for Case A, Case B and Case C respectively.

Figure 14 shows the present results for Case A, Case B and Case C discussed above. Among these calculations we get better accuracy for Case C only which give quite good results

between 30 to 100 Kev when we compare them with the existing experimental results. For higher energies the Case C and Case B give larger results than Case A.

In figure (15) we are comparing the results for the present calculation for Case C with the experimental results. It is seen from figure 15 or table 4 that the results of the present calculations is nearly 30% larger than the experimental results at 500 Kev, nearly 50% larger at 1000 Kev, nearly 4 times larger at 10 Mev.

In figure 16 we have shown our calculated results for Case C as well as the existing theoretical results given by Green et al (1965) and Bransden and Sin fai lam (1966). The present results are very close to Green et al (1965). There are small differences between the results of the present calculation and Bransden and Sin fai lam (1966) at lower energies. But it is seen at once that the maximum differences between the results of the present and Bransden and Sin fai lam are 30% at higher energies.

Figure 17 shows the results of the present calculations for Case A and the results obtained by Mapleton (1961) and Bransden and Cheshire (1963). The present results do not agree with the results by Impulse approximation, but quite near to Mapleton's results at higher energies.

From the above interpretation of the present results it is seen that the considerable disagreement between theory and the experiment at higher energies is not substantially improved by employing the 2nd order potential in Bates two - state method.

CHAPTER 7

Numerical methods

In this chapter, we give a short description of our calculations involved in chapter 6, as the calculations in chapter 4 have also been done in the same way. From chapter 6, we get that the most difficult terms are $N_{0,0}$, $\bar{N}_{0,0}$, $K_{0,0}$, $\bar{K}_{0,0}$. The expression for the matrix elements are of the forms

$$I_1 = e^{-i\vartheta^2 t/2} \int_0^1 x^n (1-x)^m \left(\frac{R}{\Delta^2} + \frac{1}{\Delta^3}\right) e^{-R\Delta} e^{i\vartheta^2 t x} dx \qquad (7\text{-}1)$$

$$I_2 = e^{-i\vartheta^2 t/2} \int_0^1 x^n (1-x)^m \left(\frac{R^2}{\Delta^3} + \frac{3R}{\Delta^4} + \frac{3}{\Delta^5}\right) e^{-R\Delta} e^{i\vartheta^2 t x} dx \qquad (7\text{-}2)$$

where $$\Delta^2 = \lambda^2 x + (1-x)(\mu^2 + \vartheta^2 x) \qquad n, m \geq 0 \qquad (7\text{-}3)$$

The above functions depends on the proton velocity V and oscillates rapidly as V increases. To perform the integration, the integrals have been divided into three sections $0.0 \leq x \leq 0.15$, $0.15 \leq x \leq 0.85$, $0.85 \leq x \leq 1.0$ and then the calculations have been done by using the Gaussian interpolation method. At 30 Kev, the number of Gaussian points are 6 and for higher energies more points have been considered to get the same accuracy.

The matrix elements for the Case A, Case B and Case C have been solved by using Hamming's method described by Wilf and Ralston (1967) as given below.

Hamming's method

Hammings method is a modification of Milne's predictor - corrector method which has been used to solve the first order differential equation

$$\frac{dy}{dx} = F(x, y) \qquad (7\text{-}4)$$

with the given initial point $y(x_0) = y_0$. This method has two advantages, firstly it is a suitable fourth - order integration procedure that requires the evaluation of the right - hand side of the system only two times per step. Secondly at each step the calculation procedure gives an estimate for the local truncation error, thus procedure is able without a significant amount of calculation time, to choose and change the step - length h .

Let $X_n - 3$, $X_n - 2$, $X_n - 1$, X_n be the known values. Now results at points

$$X_{n+1} = X_n + h$$

are computed by the formulas below

Predictor:

$$P_{n+1} = y_{n-3} + \frac{4h}{3}\left[2y'_n - y'_{n-1} + 2y'_{n-2}\right] \qquad (7\text{-}5)$$

Modifier:

$$M_{n+1} = P_{n+1} - \frac{112}{121}(P_n - C_n) \qquad (7\text{-}6)$$

$$M'_{n+1} = F(x_{n+1}, y_{n+1}) \qquad (7\text{-}7)$$

Corrector:

$$C_{n+1} = \frac{1}{8}\left[9y_n - y_{n-2} + 3h\left(M'_{n+1} + 2y_n' - y_{n-1}'\right)\right] \tag{7-8}$$

Final value:

$$y_{n+1} = C_{n+1} + \frac{9}{121}\left(P_{n+1} - C_{n+1}\right) \tag{7-9}$$

where Y Y', P, M, M', and C are column vectors, and the truncation error can be given by

$$T_2 = \frac{9}{121}\left(C_{n+1} - P_{n+1}\right) \tag{7-10}$$

As this method is not self - starting, it is very important that the starting values should be as accurate as possible, because errors in these starting values may increase during computation. So to do this we have used Newton's interpolation formula using forward differences to get the required values Y_1, Y_2 and Y_3. For example, we have

$$y_1 = y_0 + \frac{h}{24}\left[9y_0' + 19y_1' - 5y_2' + y_3'\right] \tag{7-11}$$

$$y_2 = y_0 + \frac{h}{3}\left[y_0' + 4y_1' + y_2'\right] \tag{7-12}$$

$$y_3 = y_0 + \frac{3h}{8}\left(y_0' + 3y_1' + 3y_2' + y_3'\right) \tag{7-13}$$

To use these formulas we estimate the Y_1, Y_2 and Y_3 and calculate y_1', y_2', y_3' by using the differential equation and then calculate Y_1, Y_2, Y_3 using (7-11), (7-12), (7-13) respectively. Then we iterate until convergence. Also to start with we can set

$$P_n - C_n = 0 \tag{7-14}$$

Step - length can be doubled or halved in the following way. In our case we have set two errors $\alpha_1 = .0001$ and $\alpha_2 = .00001$ and adjustment can be done by the test value

$$\delta = \sum_{i=1}^{n} a_i (P_{i+1} - C_{i+1}) \qquad (7\text{-}15)$$

when $\delta > \alpha_1$, the step-length has been halved and following inter polation formulas have been used

$$y_{n-\frac{1}{2}} = \frac{1}{256}(80 y_n + 135 y_{n-1} + 40 y_{n-2} + y_{n-3}) + \frac{h}{256}(-15 y_n' + 90 y_{n-1}' + 15 y_{n-2}') \qquad (7\text{-}16)$$

$$y_{n-\frac{3}{2}} = \frac{1}{256}(12 y_n + 135 y_{n-1} + 108 y_{n-2} + y_{n-3}) + \frac{h}{256}(-3 y_n' - 54 y_{n-1}' + 27 y_{n-2}') \qquad (7\text{-}17)$$

Similarly, when $\delta < \alpha_2$, the step - length has been doubled.

The integrals in (6-31) etc. were evaluated by repeated application of Simpson's rule.

Total cross-sections have been calculated by applying the Simpson's rule as well.

CHAPTER 8

Conclusion

The main contribution, in this thesis, is the application of the 2nd - order potential for both excitation and charge - exchange processes.

In the case of excitation, as there is no experiment, we have compared our results with the existing theoretical results. It is found that the present results are in close agreement with other results above 100 Kev. At low energies, less than 100 Kev, our results are nearly 40% smaller than the results of Flannery where he did his calculations by taking 1S, 2S and 2p states of the target. It means that the coupling for the rearrangement channel is likely to have significant effect on the Direct excitation cross - sections at low energies and needs further investigation as indicated in paper II (Bransden et al, 1972).

But on the charge - exchange, experimental results are available and it is seen that the results obtained by including the 2nd order potential with the Bates two state method is not very satisfactory and gives a larger result than the experiment at high energies. It is now known that the formulation of the method (which we already presented in Chapter 6) is not consistent with the charge - exchange process. On the other hand, it provides better results for the Distorted wave method at high energies which is very close for the experimental results as well as the calculation of the first Born approximation. Among the theoretical

calculations on charge - exchange, only the results of first Born approximation give quite reliable results at high energies as compared to the experimental results. Like Born approximation, the results of the Distorted wave approximation do not agree with the experimental results at low energies.

For excitation process, we believe that our method should provide better results, as it did in the case of electron - helium cases shown in paper IV (Berrington et al, 1972) where some experimental results are available. But for charge exchange process that conclusion is not applicable as it is a complicated process where instead of one orbit we have taken two orbits. More refined work should be needed on this particular topic.

APPENDIX A

Evaluation of the integrals:

$$I_1 = \int e^{-\lambda r_1} e^{-\mu R_1} e^{i\upsilon \cdot r_1} \, dr_1 \qquad \text{(A-1)}$$

$$I_2 = \int \frac{e^{-\lambda r_1}}{r_1} e^{-\mu R_1} e^{i\upsilon \cdot r_1} \, dr_1 \qquad \text{(A-2)}$$

$$I_3 = \int e^{-\lambda r_1} \frac{e^{-\mu R_1}}{R_1} e^{i\upsilon \cdot r_1} \, dr_1 \qquad \text{(A-3)}$$

where $R_1 = r_1 - R$

To integrate I_1, we have to use the Fourier's transforms which is given by

$$e^{-\lambda r} = \frac{1}{\pi^2} \int \frac{\lambda}{(\lambda^2+q^2)^2} e^{iq \cdot r} \, dq \qquad \text{(A-4)}$$

$$\frac{e^{-\lambda r}}{r} = \frac{1}{2\pi^2} \int \frac{1}{(\lambda^2+q^2)} e^{iq \cdot r} \, dq \qquad \text{(A-5)}$$

Therefore

$$I_1 = \frac{\partial^2}{\partial\lambda\partial\mu} \frac{1}{4\pi^4} \int dr_1 \int dq_1 \int dq_2 \frac{1}{(\lambda^2+q_1^2)} \frac{1}{(\mu^2+q_2^2)} \qquad \text{(A-6)}$$

$$\times \exp\left[i \left(q_1 \cdot r_1 + q_2 (r_1 - R) + \upsilon \cdot r_1 \right) \right]$$

$$= \frac{\partial^2}{\partial\lambda\partial\mu}\ \frac{1}{4\pi^4}\int d\underline{q}_1\ \frac{1}{(\lambda^2+q_1^2)}\int d\underline{q}_2\ \frac{1}{(\mu^2+q_2^2)} \qquad \text{(A-7)}$$

$$\times \int d\underline{r}_1\ exp\left[\underline{q}_1\cdot\underline{r}_1 + \underline{q}_2\cdot(\underline{r}_1-\underline{R}) + \upsilon\cdot\underline{r}_1\right]$$

integrating over $\underline{r}_1$

$$I_1 = \frac{\partial^2}{\partial\lambda\partial\mu}\ \frac{1}{4\pi^4}\int d\underline{q}_1\ \frac{1}{(\lambda^2+q_1^2)}\int d\underline{q}_2\ \frac{1}{(\mu^2+q_2^2)}$$

$$\times (2\pi)^3\,\delta(\underline{q}_1+\underline{q}_2+\upsilon)\ exp\,(-i\underline{q}_2\cdot\underline{R}) \qquad \text{(A-8)}$$

$$= \frac{\partial^2}{\partial\lambda\partial\mu}\ \frac{2}{\pi}\int d\underline{q}_1\ \frac{1}{(\lambda^2+q_1^2)}\int d\underline{q}_2\ \frac{1}{(\mu^2+q_2^2)}$$

$$\times\ \delta(\underline{q}_1+\underline{q}_2+\upsilon)\ exp(-i\underline{q}_2\cdot\underline{R}) \qquad \text{(A-9)}$$

put $\underline{q}_2 = \underline{q}_1 + \upsilon$

$d\underline{q}_2 = d\underline{q}_1$

Integrating over $d\underline{q}_2$

$$I_1 = \frac{\partial^2}{\partial\lambda\partial\mu}\ \frac{2}{\pi}\int d\underline{q}_1\ \frac{1}{(\lambda^2+q_1^2)}\ \frac{e^{i(\underline{q}_1+\upsilon)\cdot\underline{R}}}{(\mu^2+(q_1+\upsilon)^2)} \qquad \text{(A-10)}$$

$$= \frac{\partial^2}{\partial\lambda\partial\mu}\ \frac{2}{\pi}\ e^{i\upsilon\cdot\underline{R}}\int d\underline{q}_1\ \frac{1}{(\lambda^2+q_1^2)}\ \frac{e^{i\underline{q}_1\cdot\underline{R}}}{(\mu^2+(\underline{q}_1+\upsilon)^2)} \qquad \text{(A-11)}$$

$$= \frac{2}{\pi}\ \frac{\partial^2}{\partial\lambda\partial\mu}\ e^{i\upsilon\cdot\underline{R}}\ I \qquad \text{(A-12)}$$

where

$$I = \int d\underline{q}_1 \; \frac{1}{(\lambda^2 + q_1^2)} \; \frac{e^{i\underline{q}_1 \cdot \underline{R}}}{(\mu^2 + (q_1 + v)^2)} \qquad \text{(A-13)}$$

To integrate I, we have used Feyman's formula,

Feyman, 1949

$$\frac{1}{ab} = \int_0^1 \frac{dx}{[ax + b(1-x)]^2} \qquad \text{(A-14)}$$

Therefore I gives

$$I = \int_0^1 dx \int d\underline{p} \; \frac{e^{i\underline{p}\cdot\underline{R}} \; e^{-iv\cdot\underline{R}(1-x)}}{[p^2 + \Delta^2]^2} \qquad \text{(A-15)}$$

where

$$\underline{p} = \underline{q}_1 + v(1-x) \qquad \text{(A-16)}$$

$$\Delta^2 = \lambda^2 x + (1-x)(1 + v^2 x) \qquad \text{(A-17)}$$

Since, we know

$$\int \frac{e^{i\underline{p}\cdot\underline{R}}}{(p^2 + \Delta^2)^2} = \frac{\pi^2}{\Delta} \; e^{-\Delta R} \qquad \text{(A-18)}$$

we get

$$I = \pi^2 \int_0^1 dx \; e^{-iv\cdot\underline{R}(1-x) - R\Delta} \; \frac{1}{\Delta} \qquad \text{(A-19)}$$

Therefore

$$I_1 = 2\pi \frac{\partial}{\partial\lambda}\frac{\partial}{\partial\mu} e^{i\vartheta\cdot\underline{R}} \int_0^1 dx \, \frac{1}{\Delta} \, e^{-i\vartheta\cdot\underline{R}(1-x)-R\Delta} \tag{A-20}$$

$$\frac{\partial\Delta}{\partial\lambda} = \frac{2\lambda x}{2\Delta} \tag{A-21}$$

$$\frac{\partial\Delta}{\partial\mu} = \frac{2\mu(1-x)}{2\Delta} \tag{A-22}$$

$$I_1 = 2\pi\lambda\mu \int_0^1 dx \, x(1-x) \, e^{i\vartheta\cdot\underline{R}x} \left(\frac{1}{\Delta}\frac{\partial}{\partial\Delta}\right)^2 \frac{1}{\Delta} \, e^{-R\Delta} \times e^{-R\Delta} \, e^{i\vartheta\cdot\underline{R}x} \tag{A-23}$$

$$I_2 = -2\pi\mu \int_0^1 x \, e^{i\vartheta\cdot\underline{R}x} \left(\frac{1}{\Delta}\frac{\partial}{\partial\Delta}\right) \frac{1}{\Delta} \, e^{-R\Delta} \times e^{i\vartheta\cdot\underline{R}x} \, dx \tag{A-24}$$

$$I_3 = -2\pi\lambda \int_0^1 (1-x) \, e^{i\vartheta\cdot\underline{R}x} \left(\frac{1}{\Delta}\frac{\partial}{\partial\Delta}\right) \frac{1}{\Delta} \, e^{-R\Delta} \times e^{i\vartheta\cdot\underline{R}} \, dx \tag{A-25}$$

Therefore

$$I_1 = 2\pi\lambda\mu \, e^{i\vartheta\cdot\underline{R}} \int_0^1 dx \, x(1-x) \left(\frac{3R}{\Delta^4} + \frac{3}{\Delta^5} + \frac{R^2}{\Delta^3}\right) \times \left(e^{-R\Delta} \cdot e^{i\vartheta\cdot\underline{R}x}\right) dx \tag{A-26}$$

Similarly,

$$I_2 = 2\pi\mu\, e^{i\vartheta\cdot\underline{R}} \int_0^1 (1-x)\left(\frac{R}{\Delta^2} + \frac{1}{\Delta^3}\right) e^{-R\Delta}\, e^{i\vartheta\cdot\underline{R}x}\, dx \qquad \text{(A-27)}$$

$$I_3 = 2\pi\lambda\, e^{i\vartheta\cdot\underline{R}} \int_0^1 x\left(\frac{R}{\Delta^2} + \frac{1}{\Delta^3}\right) e^{-R\Delta}\, e^{i\vartheta\cdot\underline{R}x}\, dx \qquad \text{(A-28)}$$

APPENDIX B

Evaluation of the integrals:

$$I_1 = \int r^n e^{-\lambda r} \frac{e^{-\mu|\underline{r}-\underline{R}|}}{|\underline{r}-\underline{R}|} \, d\underline{r} \tag{B-1}$$

$$I_2 = \int r^n e^{-\lambda r} e^{-\mu|\underline{r}-\underline{R}|} \, d\underline{r} \tag{B-2}$$

$$I_3 = \int r^n \frac{e^{-\lambda r}}{|\underline{r}-\underline{R}|} \, d\underline{r} \tag{B-3}$$

To solve I_1, I_2, I_3 the expansion series by Watson (1958) has been used

We know

$$\frac{e^{-\mu|\underline{r}-\underline{R}|}}{|\underline{r}-\underline{R}|} = \sum_{\ell=0}^{\infty} \frac{(2\ell+1) K_{\ell+\frac{1}{2}}(\mu R) I_{\ell+\frac{1}{2}}(\mu r) P_\ell(\cos\theta)}{\sqrt{r}\sqrt{R}} \tag{B-4}$$

where

$$r \leq R \,, \qquad \cos\theta = \frac{\underline{r}\cdot\underline{R}}{rR}$$

$$K_{\ell+\frac{1}{2}}(\mu R) = \sqrt{\frac{\pi}{2\mu R}} e^{-\mu R} \sum_{n=0}^{\infty} \frac{(\ell+n)!}{n!\,(\ell-n)!\,(2\mu R)^n} \tag{B-5}$$

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

$$\left. + (-)^{\ell+1} e^{-\mu r} \sum_{n=0}^{\ell} \frac{(\ell+n)!}{n!\,(\ell-n)!\,(2\mu r)^n} \right] \tag{B-6}$$

$$P_\ell(\cos\theta) = \frac{4\pi}{2\ell+1} \sum_{m=-\ell}^{\ell} Y_\ell^{m*}(\theta_2, \phi_2)\, Y_\ell^{m}(\theta_1, \phi_1) \qquad \text{(B-7)}$$

$$\frac{1}{|\underline{r} - \underline{R}|} = \frac{1}{r} \sum_{\ell=0}^{\infty} \left(\frac{R}{r}\right)^{\ell} P_\ell(\cos\theta) \qquad r \geq R \qquad \text{(B-8)}$$

$$= \frac{1}{R} \sum_{\ell=0}^{\infty} \left(\frac{r}{R}\right)^{\ell} P_\ell(\cos\theta) \qquad r \leq R \qquad \text{(B-9)}$$

where

$$\cos\theta = \cos\theta_1 \cos\theta_2 + \sin\theta_1 \sin\theta_2 \cos(\phi_1 - \phi_2) \qquad \text{(B-10)}$$

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

$$I_2 = -\frac{\partial}{\partial \mu} I_1 \qquad \text{(B-11)}$$

APPENDIX C

Elliptical integral for evaluation of the integral:

$$I(\underline{R},\underline{R}') = \int \frac{e^{-\alpha r}}{|\underline{r}-\underline{R}||\underline{r}-\underline{R}'|}\, d\underline{r} \qquad \text{(C-1)}$$

By following the method given by Coleman (1970), we can express I as

$$I(R,R') = \sum_{\ell=0}^{\infty} \frac{4\pi}{(2\ell+1)} P_\ell(\cos\theta) \int_0^\infty e^{-\alpha r} V_\ell(r,R) V_\ell(r,R') r^2 dr \qquad \text{(C-2)}$$

$$= 4\pi[A + NB + C]$$

where

$$V_\ell(r,R) = r^\ell / R^{\ell+1} \quad \text{if} \quad r < R$$

$$= R^\ell / r^{\ell+1} \quad \text{if} \quad r > R \qquad \text{(C-3)}$$

and

$$A = \sum_{\ell=0}^{\infty} \frac{1}{(2\ell+1)} P_\ell(\cos\theta) \frac{1}{(RR')^{\ell+1}} \int_0^{R'} e^{-\alpha r} r^{2\ell+2}\, dr \qquad \text{(C-4)}$$

$$B = \sum_{\ell=0}^{\infty} \frac{1}{(2\ell+1)} P_\ell(\cos\theta) \left(\frac{R'}{R}\right)^\ell \frac{1}{R} \qquad \text{(C-5)}$$

$$C = \sum_{\ell=0}^{\infty} \frac{1}{(2\ell+1)} P_\ell(\cos\theta) (RR')^\ell \int_R^\infty \frac{e^{-\alpha r}}{r^{2\ell}}\, dr \qquad \text{(C-6)}$$

$$N = \int_{R'}^{R} r\, e^{-\alpha r}\, dr = \left(\frac{\alpha R'+1}{\alpha^2} e^{-\alpha R'} - \frac{\alpha R+1}{\alpha^2} e^{-\alpha R}\right) \qquad \text{(C-7)}$$

Putting

$$r = R'y \quad , \quad r' = R' \longrightarrow y = 1$$

$$A = \sum_{l=0}^{\infty} \frac{1}{(2l+1)} R' \left(\frac{R'}{R}\right)^{l+1} \int_0^1 e^{-\alpha R' y} y^{2l+2} P_l(\cos\theta)\, dy \qquad (C\text{-}8)$$

$$= \int_0^1 e^{-\alpha R' y} \sum_{l=0}^{\infty} \frac{1}{(2l+1)} R' \left(\frac{R' y^2}{R}\right)^{l+1} P_l(\cos\theta)\, dy$$

Now

$$\sum_{l=0}^{\infty} t^l P_l(\cos\theta) = (1 - 2t\cos\theta + t^2)^{-\frac{1}{2}} \qquad |t| \le 1 \qquad (C\text{-}9)$$

Also

$$\sum_{l=0}^{\infty} \frac{Z^{l+\frac{1}{2}}}{l+\frac{1}{2}} P_l(\cos\theta) = \int_0^Z \frac{dt}{\sqrt{t}\,\sqrt{1 - 2t\cos\theta + t^2}} \qquad (C\text{-}10)$$

Put

$$Z = \frac{R'}{R} y^2$$

$$\sum_{l=0}^{\infty} \frac{1}{2l+1} R' \left(\frac{R' y^2}{R}\right)^{l+1} P_l(\cos\theta) = \frac{R'^{\frac{3}{2}} y}{z\sqrt{R}} \sum_{l=0}^{\infty} \frac{1}{l+\frac{1}{2}} R^{l+\frac{1}{2}} P_l(\cos\theta) \qquad (C\text{-}11)$$

Let

$$t = \frac{1 - \cos\psi}{1 + \cos\psi} \qquad (C\text{-}12)$$

$$\cos\psi = \frac{1-t}{1+t} \qquad (C\text{-}13)$$

then

$$t \to 0 \ , \ \psi \to 0$$

and

$$t = z \longrightarrow \psi = \phi = \cos^{-1}\left(\frac{1-z}{1+z}\right)$$

Also putting the values of t, we get

$$1 - 2t\cos\theta + t^2 = \frac{4(1 - k^2\sin^2\psi)}{(1 + \cos\psi)^2} \qquad \text{(C-14)}$$

where

$$k^2 = \tfrac{1}{2}(1 + \cos\theta) = \cos^2\frac{\theta}{2} \qquad \text{(C-15)}$$

$$\frac{dt}{d\psi} = \frac{2\sin\psi}{(1+\cos\psi)^2} \qquad \text{(C-16)}$$

$$t^{\frac{1}{2}} = \frac{\sin\psi}{1 + \cos\psi} \qquad \text{(C-17)}$$

$$\frac{dt}{\sqrt{t}} = \frac{2\,d\psi}{1 + \cos\psi} \qquad \text{(C-18)}$$

Therefore

$$\int_0^z \frac{dt}{\sqrt{t}\sqrt{1 - 2t\cos\theta + t^2}} = \int_0^{\phi} \frac{d\psi}{\sqrt{1 - k^2\sin^2\psi}} = F(\phi, k) \qquad \text{(C-19)}$$

$$A = \frac{R'}{2}\left(\frac{R'}{R}\right)^{\frac{1}{2}} \int_0^1 y\, e^{-\alpha R' y} F(\phi, k)\, dy \qquad \text{(C-20)}$$

$$\begin{aligned} B &= \frac{1}{2(RR')^{\frac{1}{2}}} \sum_{l=0}^{\infty} \frac{1}{(l+\frac{1}{2})} \left(\frac{R'}{R}\right)^{l+\frac{1}{2}} P_l(\cos\theta) \\ &= \frac{1}{2(RR')^{\frac{1}{2}}} \sum_{l=0}^{\infty} \frac{1}{(l+\frac{1}{2})} \left(\frac{R'}{R}\right)^{l+\frac{1}{2}} P_l(\cos\theta) \\ &= \frac{1}{2(RR')^{\frac{1}{2}}} \int_0^{z_1} \frac{dt}{(1 - 2t\cos\theta + t^2)^{\frac{1}{2}}} \\ &= \frac{1}{2(RR')^{\frac{1}{2}}} F(\phi_1, k) \end{aligned} \qquad \text{(C-21)}$$

where

$$\phi_1 = \cos^{-1} \frac{1 - z_1}{1 + z_1} \tag{C-22}$$

and $$z_1 = \frac{R'}{R}$$

$$C = \sum_{\ell=0}^{\infty} \frac{1}{2\ell+1} \frac{R'^{\ell}}{R^{\ell-1}} \int_1^{\infty} \frac{e^{-\alpha R' z}}{z^{2\ell}} P_\ell(\cos\theta)\, dz$$

$$= \sum_{\ell=0}^{\infty} \frac{1}{2\ell+1} P_\ell(\cos\theta) \frac{R'^{\ell}}{R^{\ell-1}} \int_1^{\infty} \frac{e^{-\alpha R' z}}{z^{2\ell}}\, dz$$

$$= \frac{R}{2} \left(\frac{R}{R'}\right)^{\frac{1}{2}} \int_1^{\infty} z\, e^{-\alpha R z} F(\phi_2, k)\, dz \tag{C-23}$$

where

$$\phi_2 = \frac{1 - z'}{1 + z'}, \quad z' = \frac{R'}{R z^2}$$

Therefore

$$I(R, R') = 2\pi \left[\frac{N F(\phi_1, k)}{(R R')^{1/2}} + \frac{R'^{3/2}}{\sqrt{R}} \int_0^1 y\, e^{-\alpha R' y} F(\phi, k)\, dy + \frac{R^{3/2}}{\sqrt{R'}} \int_1^{\infty} z\, e^{-\alpha R z} F(\phi_2, k)\, dz \right] \tag{C-24}$$

APPENDIX D

List of integrals for

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

$$V_{00}(R) = \langle \psi(1s) | V | \psi(1s) \rangle \qquad \text{(D-1)}$$

$$= 16 N_1 \left[J_0(2\alpha, R) + 2 c_1 J_0(\alpha+\beta, R) + c_1^2 J_1(2\beta, R) \right]$$

$$V_{10}(R) = \langle \psi(1s) | V | \psi(2s) \rangle$$

$$= 64 N_1 N_2 \Big[\{ J_0(\alpha+p, R) + c_1 J_0(\beta+p, R) \} A$$

$$+ B \{ 2 J_0(\alpha+\lambda, R) + c_2 J_1(\beta+\lambda, R) \qquad \text{(D-2)}$$

$$+ 2 c_1 J_0(\alpha+\mu, R) + c_1 c_2 J_1(\beta+\mu, R) \} \Big]$$

$$V_{22}(R) = \langle \psi(2s) | V | \psi(2s) \rangle$$

$$= 64 N_2^2 \Big[\frac{1}{(2p)^3} \{ 2 J_0(2\lambda, R) + 2 c_2 J_1(\lambda+\mu, R) + c_2^2 J_2(\mu+\mu, R)$$

$$+ \Big\{ \frac{2}{(2\lambda)^3} + \frac{12 c_2}{(\lambda+\mu)^4} + \frac{24 c_2^2}{(2\mu)^5} \Big\} J_0(2p, R) \qquad \text{(D-3)}$$

$$+ \Big\{ \frac{4}{(p+\lambda)^3} + \frac{6 c_2}{(p+\mu)^4} + \frac{12}{(p+\mu)^4} \Big\} J_0(p+\lambda, R)$$

$$+ \Big\{ \frac{c_2}{(p+\lambda)^3} + \frac{1}{(p+\lambda)^3} + \frac{6 c_2}{(p+\mu)^4} \Big\} J_1(p+\mu, R) \Big]$$

$$V_{13}(R) = \langle \Psi(1S) | V | \Psi(2P_0) \rangle$$

$$= 64 N_1 N_3 \sqrt{\pi}\; y_{1,0}(R) B \Big[L(\alpha+q, R) \qquad \text{(D-4)}$$

$$+ c_1 L(\beta+q, R) - \left(\frac{1}{(\alpha+q)^5} + \frac{c_1}{(\beta+q)^5} \right) \frac{8}{R^2} \Big]$$

Also

$$V_{13}(R) = \langle \Psi(1S) | V | \Psi(2P_{\pm 1}) \rangle \qquad \text{(D-5)}$$

$$= 64 N_1 N_3 \sqrt{\pi}\; y_{1,\pm 1}(R) B \Big[L(\alpha+q, R)$$

$$+ c_1 L(\beta+q, R) - \left(\frac{1}{(\alpha+q)^5} + \frac{c_1}{(\beta+q)^5} \right) \frac{8}{R^2} \Big]$$

$$V_{2P_0} V_{2P_0}(R) = \langle \Psi(2P_0) | V | \Psi(2P_0) \rangle \qquad \text{(D-6)}$$

$$= 16 N_3^2 \left[\frac{24\, J_0(2P, R)}{(2q)^5} + I_0 \right], \qquad m = 0$$

$$V_{2P_{\pm 1}, 2P_{\pm 1}}(R) = \langle \Psi(2P_{\pm 1}) | V | \Psi(2P_{\pm 1}) \rangle \qquad \text{(D-7)}$$

$$= 16 N_3^2 \left[\frac{24 J_0(2P, R)}{(2q)^5} + I_{\pm 1} \right]$$

where

$$J_0(Z, R) = \frac{1}{Z^3} \left(\frac{Z}{2} + \frac{1}{R} \right) e^{-ZR} \qquad \text{(D-8)}$$

$$J_1(Z, R) = \frac{1}{Z^4} \left[\left(\frac{6}{R} + 4Z + RZ^2 \right) e^{-ZR} \right] \qquad \text{(D-9)}$$

$$J_2(z,R) = \frac{1}{z^5}\left(R^2z^3 + 6Rz^2 + 18z + \frac{24}{R}\right)e^{-zR} \qquad \text{(D-10)}$$

$$L(z,R) = \frac{1}{z^5R^2}\left(R^3z^3 + 4z^2R^2 + 8zR + 8\right)e^{-zR} \qquad \text{(D-11)}$$

$$A = \left(\frac{2}{(\alpha+\lambda)^3} + \frac{6c_2}{(\alpha+\mu)^3} + \frac{2c_1}{(\beta+\lambda)^3} + \frac{6c_1c_2}{(\beta+\mu)^4}\right) \qquad \text{(D-12)}$$

$$B = \left(\frac{1}{(\alpha+p)^3} + \frac{c_1}{(\beta+p)^3}\right) \qquad \text{(D-13)}$$

$$Y_{1,0}(R) = \frac{\sqrt{3}}{\sqrt{4\pi}}\cos\theta \qquad \text{(D-14)}$$

$$Y_{1,\pm1}(R) = \frac{\sqrt{3}}{\sqrt{8\pi}}\sin\theta \qquad \text{(D-15)}$$

$$I_0 = \left(\frac{16\pi}{5}\right)^{\frac{1}{2}} Y_{2,0}(R)\left[\left(\frac{5R^2}{(2q)^2} + \frac{30R}{(2q)^3} + \frac{120}{(2q)^4} + \frac{360}{(2q)^5R} + \frac{720}{(2q)^5R^2} + \frac{720}{(2q)^7R^3}\right)e^{-2qR} - \frac{720}{(2q)^7R^3}\right] + Y_{0,0}(R)\sqrt{4\pi}\left[\frac{R^2}{(2q)^2} + \frac{6R}{(2q)^3} + \frac{18}{(2q)^4} + \frac{24}{(2q)^5R}\right]e^{-2qR} \qquad \text{(D-16)}$$

$$I_{\pm 1} = \frac{1}{2} Y_{0,0} \sqrt{4\pi} \left(\frac{R^2}{(2q)^2} + \frac{6R}{(2q)^3} + \frac{18}{(2q)^4} + \frac{24}{(2q)^5 R} \right) e^{-2qR}$$

$$+ \frac{1}{2} \frac{24}{R(2q)^5} - \frac{1}{2} \left(\frac{16\pi}{5} \right)^{\frac{1}{2}} Y_{2,0}(R) \left[\left(\frac{5R^2}{(2q)^2} \right. \right.$$

$$+ \frac{30R}{(2q)^3} + \frac{120}{(2q)^4} + \frac{360}{(2q)^4 R} + \frac{720}{(2q)^6 R^2}$$

$$\left. \left. + \frac{720}{(2q)^7 R^3} \right) e^{-2qR} - \frac{720}{(2q)^7 R^3} \right] \qquad \text{(D-17)}$$

where $$Y_{0,0}(R) = \frac{1}{\sqrt{4\pi}} \qquad \text{(D-18)}$$

$$Y_{2,0}(R) = \frac{\sqrt{5}}{4\sqrt{\pi}} \left(3\cos^2\theta - 1 \right) \qquad \text{(D-19)}$$

APPENDIX E

List of integrals for $H^+ + He(1s^2) \longrightarrow H(1s) + He^+(1s)$

$$H_{0,0} = 2\alpha e^{-2\alpha R}\left(1 + \frac{1}{\alpha R}\right) \qquad \text{(E-1)}$$

$$N_{0,0} = \frac{8\sqrt{8}}{(2+\alpha)^3}\,\bar{\bar{I}}_1(\alpha, R) \qquad \text{(E-2)}$$

$$\overline{N_{0,0}} = N^*_{0,0} \qquad \text{(E-3)}$$

$$\bar{H}_{0,0} = \left(\mu + \frac{1}{R}\right)e^{-2\mu R} + \left(\lambda + \frac{1}{R}\right)e^{-2\lambda R} + I_4 \qquad \text{(E-4)}$$

where

$$I_4 = -\frac{\lambda^3}{R(\lambda^2-\mu^2)^3}\Big[\lambda e^{-2\mu R}\{R\mu(\lambda^2-\mu^2) + (\lambda^2 - 3\mu^2)\}$$
$$+ \exp(-2\lambda R)\{R(\lambda^2-\mu^2)(2\mu^2-\lambda^2) \qquad \text{(E-5)}$$
$$- \lambda(\lambda^2 - 3\mu^2)\}\Big]$$

$$K_{0,0} = -\frac{4\sqrt{8}\,\alpha^3}{(2+\alpha)^3}\Big[I(\alpha)\cdot \bar{\bar{I}}_1(\alpha, R) \qquad \text{(E-6)}$$
$$+ 2\,\bar{\bar{I}}_2(\alpha, R) + (2+\alpha)\bar{\bar{I}}_1(2+2\alpha, R)$$
$$+ 2\,\bar{\bar{I}}_2(2+2\alpha, R)\Big]$$

where

$$I(\alpha) = \left[-\frac{2}{R} + \left(\alpha + 2 + \frac{2}{R}\right) e^{-(\alpha+2)R} \right] \tag{E-7}$$

$$\overline{K_{0,0}} = \frac{4\sqrt{8}\,\alpha^3}{(2+\alpha)^3} \left[\left\{ (\alpha+2)(\alpha-2) - (\alpha^2 + \epsilon_0) \right\} I_1(\alpha, R) \right.$$

$$\left. - 2\, I_3(\alpha, R) + 2\alpha\, I_2(\alpha, R) \right]$$

where

$$I_1(\alpha, R) = 2\alpha_1\, e^{\frac{-i v^2 t}{2}} \int_0^1 x(1-x) \left(\frac{3R}{\Delta^4} + \frac{3}{\Delta^5} + \frac{R^2}{\Delta^3} \right) e^{-\Delta R}\, e^{i v \cdot R x}\, dx$$

(E-8)

$$I_2(\alpha, R) = 2\, e^{\frac{-i v^2 t}{2}} \int_0^1 (1-x) \left(\frac{R}{\Delta^2} + \frac{1}{\Delta^3} \right) e^{-\Delta R}\, e^{i v \cdot R x}\, dx$$

(E-9)

$$I_3(\alpha, R) = 2\alpha\, e^{\frac{-i v^2 t}{2}} \int_0^1 x \left(\frac{R}{\Delta^2} + \frac{1}{\Delta^3} \right) e^{-\Delta R}\, e^{i v \cdot R x}\, dx$$

(E-10)

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Finally, I gratefully acknowledge the financial help from the County Council of Durham and British Council Authority during my final year which helped me to complete my studies in time.

Figure Captions

Figure 1. Total cross-sections for the 2^1S excitations of helium by proton impact.

Curve F1. Four channel coupling of Flannery (1970)

Curve P2. Our results for the four channel coupling with the second order potential.

Curve SB2. Second Born approximation (Holt et al, 1971a)

• First Born approximation (Bell et al, 1968)

⊙ Our results for the four channel coupling without the second - order potential.

Figure 2. Total cross-sections for the 2^1p excitations of helium by proton impact.

Curve F1, P2, SB2, • , ⊙ , are as in Figure 1.

Figure 3, Figure 4, Figure 5, Figure 6.
are the capture probabilities versus Impact parameter. The dots indicate the computed values. The Normalization factor N has the values 1.96 at 30.2 Kev, 8.362 at 100 Kev, 73.10 at 250 Kev, 1190.5 at 500 Kev respectively.

Figure 7, Figure 8, Figure 9, Figure 10.
are the capture probabilities versus Impact parameter. The dots indicate the computed values. The Normalization factor N has the values 1.73 at 30.2 Kev, 11.38 at 100 Kev, 119.08 at 250 Kev, respectively.

Figure 11, Figure 12, Figure 13.
are the capture probabilities versus Impact parameter. The dots indicate the computed values. The normalization factor N has the values 2.59 at 30 Kev, 12.8 at 100 Kev, 121.3 at 250 Kev, respectively.

Figure 14. Total capture cross-sections for helium atom by proton impact.

——— Present calculations (TC from Table 4)

• Present calculations (DW2 from Table 4)

△ Present calculations (DW1 from Table 4)

Figure 15. Total capture cross-sections for helium atom by proton impact.

——— Present calculations (TC from Table 4)

• Experimental results (Steir and Barrett, 1966, Barnett and Raynolds, 1958; Berkner et al, 1965).

Figure 16. Total capture cross-sections for helium atom by proton impact.

——— Present calculations (TC from Table 4)

△ Bransden et al (1966)

• Green et al (1965).

Figure 17. Total capture cross-sections for helium atom by proton impact.

——— Present calculations (DW1 from Table 4)

• First Born approximation (Mapleton, 1961)

△ Impulse approximation (Bransden & Cheshire, 1963).

Figure 18. Capture probabilities versus impact parameter for 30.2 Kev.

P ⟶ Present calculation

G ⟶ Green et al (1965)

BS ⟶ Bransden & Sin Fai lam (1966)

FIG. 1 .

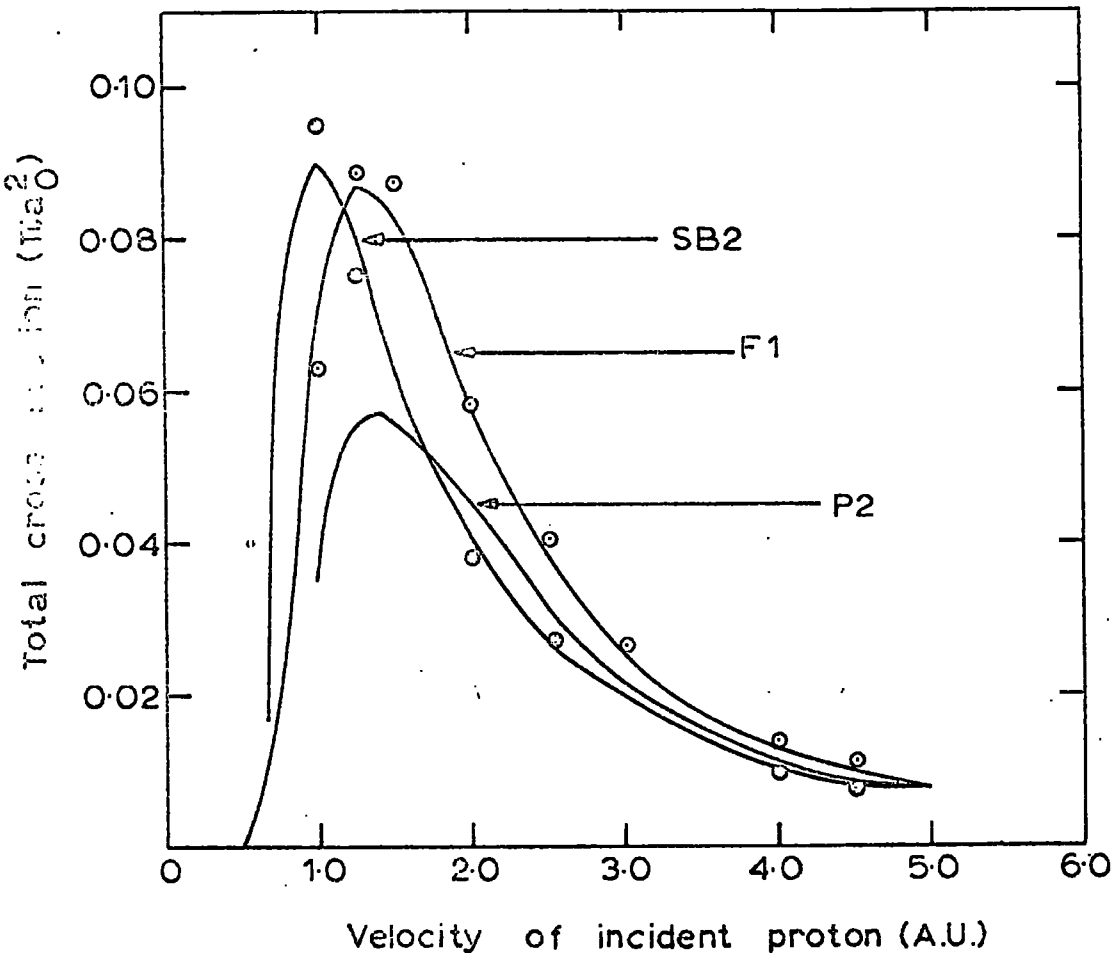
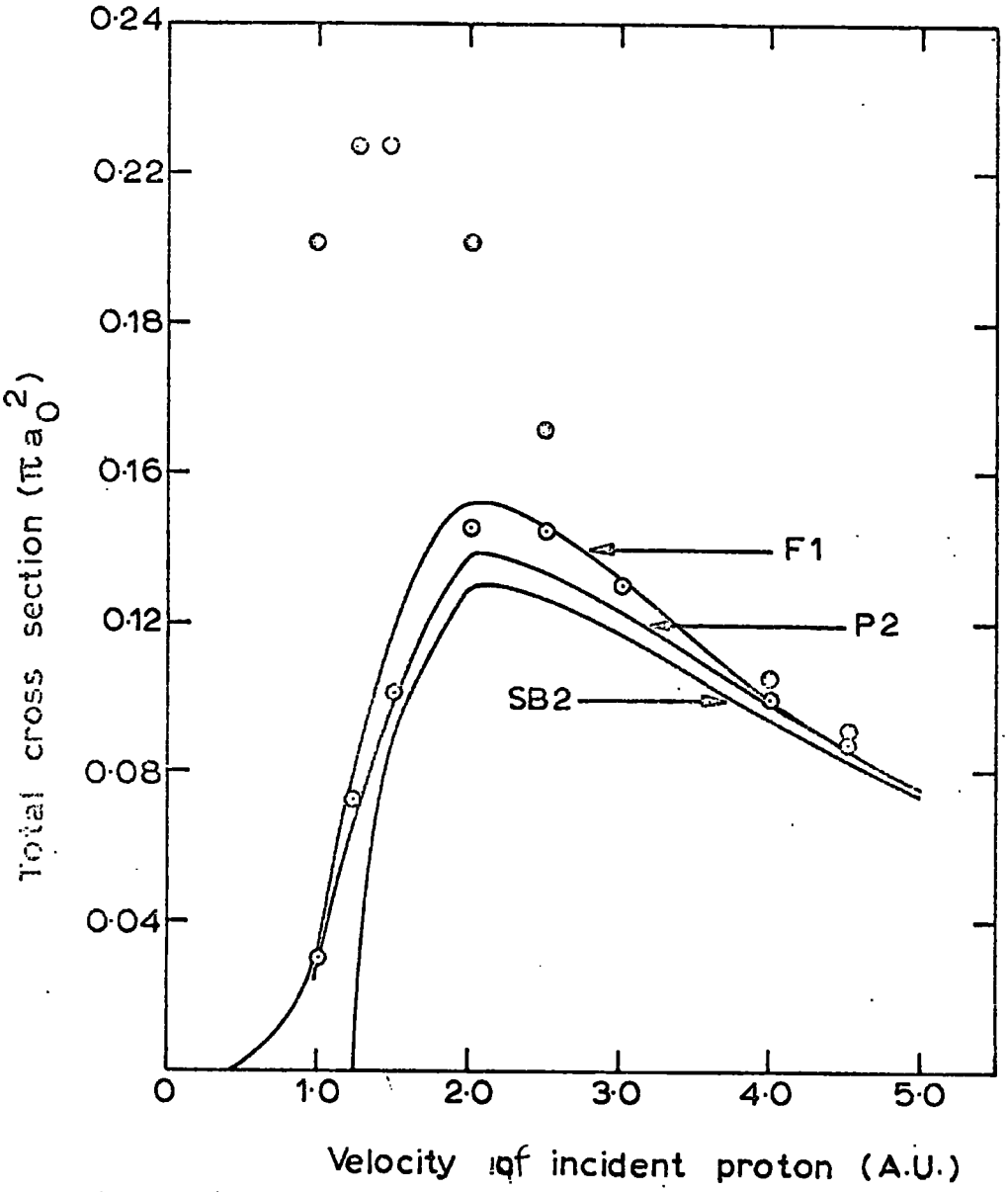

0·10
0·08
0·06
0·04
0·02
SB2
F1
P2
0
1·0
2·0
3·0
4·0
5·0
6·0
Velocity of incident proton (A.U.)

FIG. 2.


0·24
0·22
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0·16
0·12
0·08
0·04
0
1·0
2·0
3·0
4·0
5·0
Total cross section (πa_0^2)
Velocity of incident proton (A.U.)
F1
P2
SB2

FIG. 3.

E = 30 Kev (1)

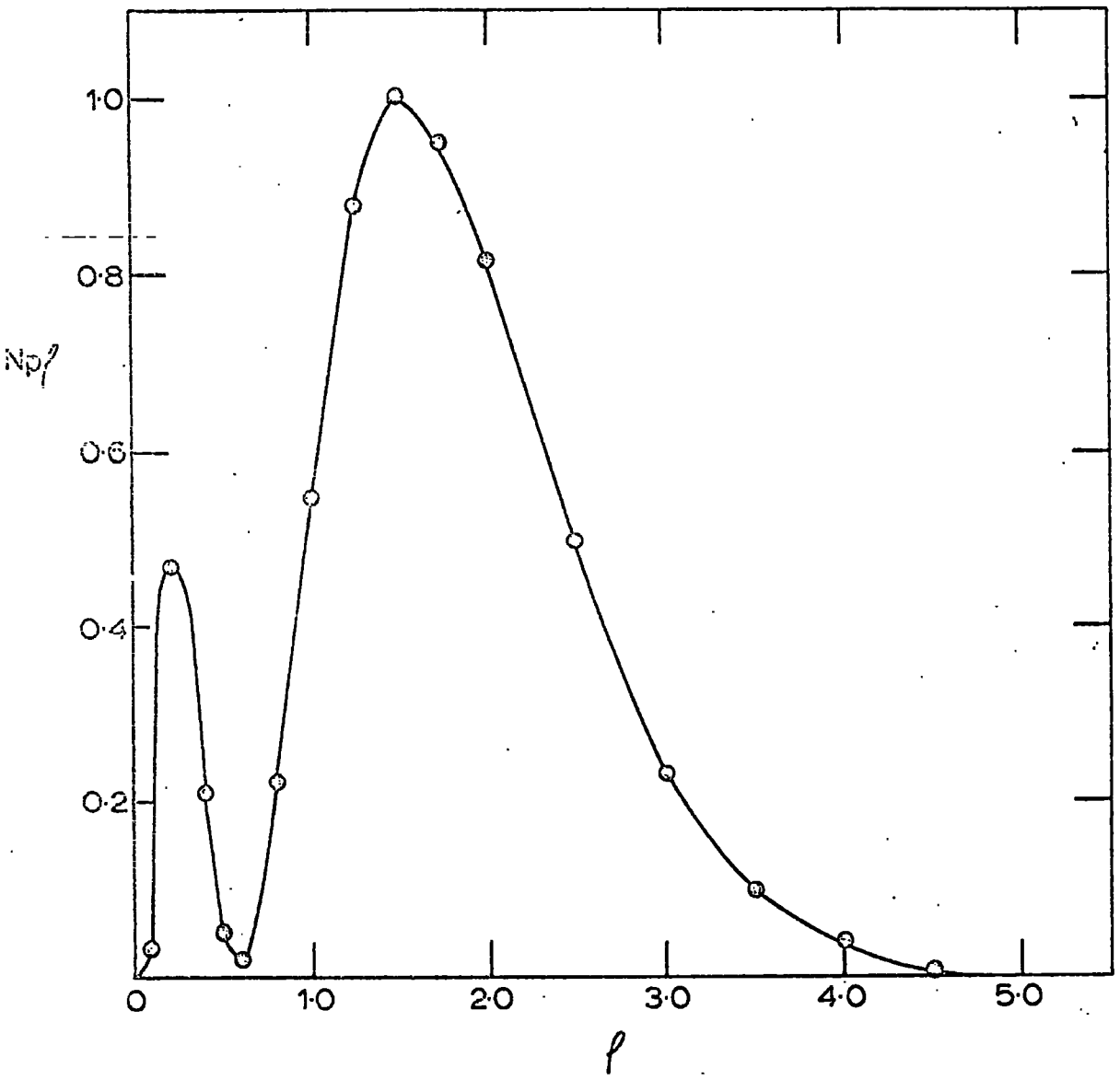

FIG. 4.

E = 100 Kev (1)

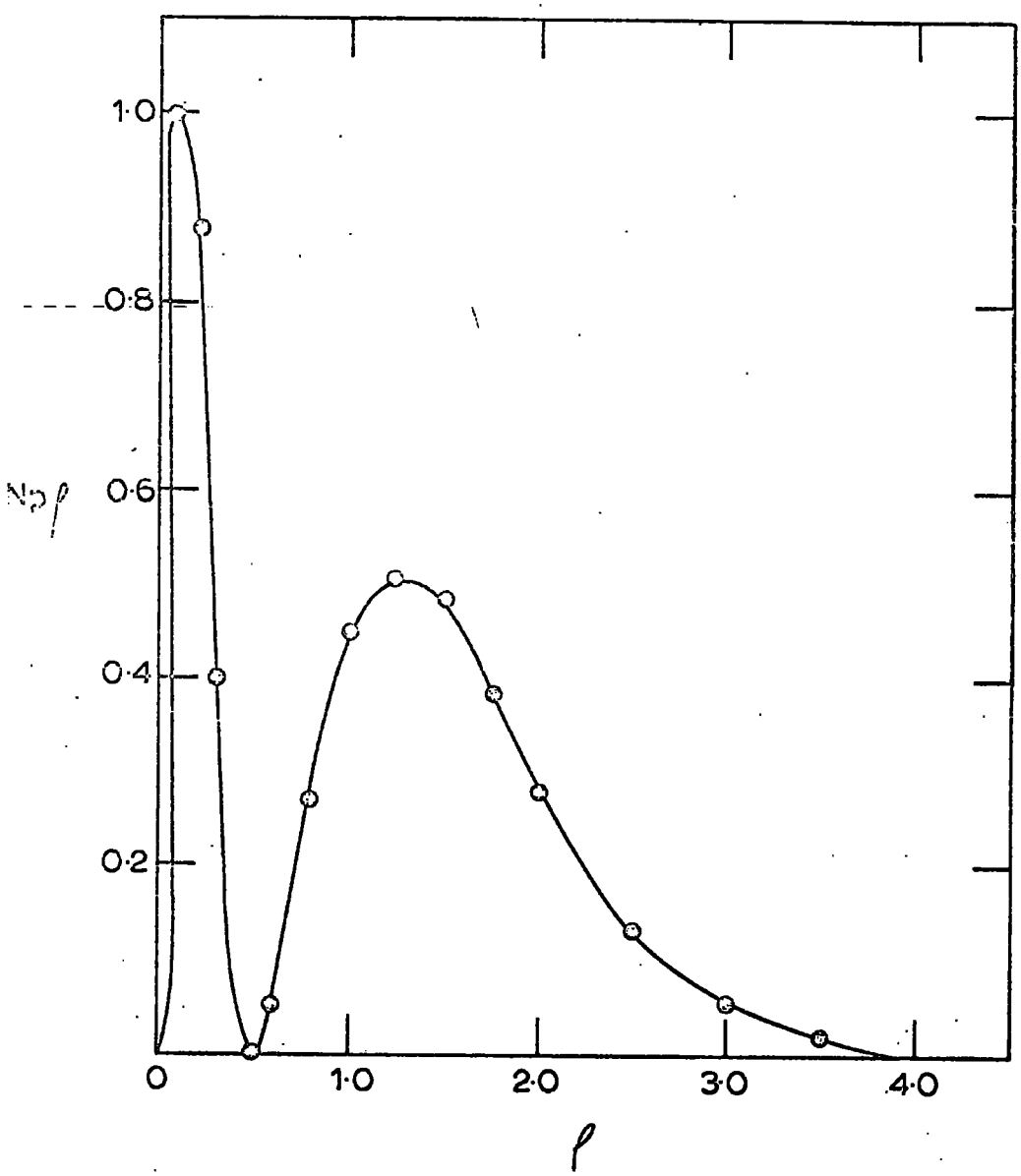

FIG. 5. E = 250 Kev (1)

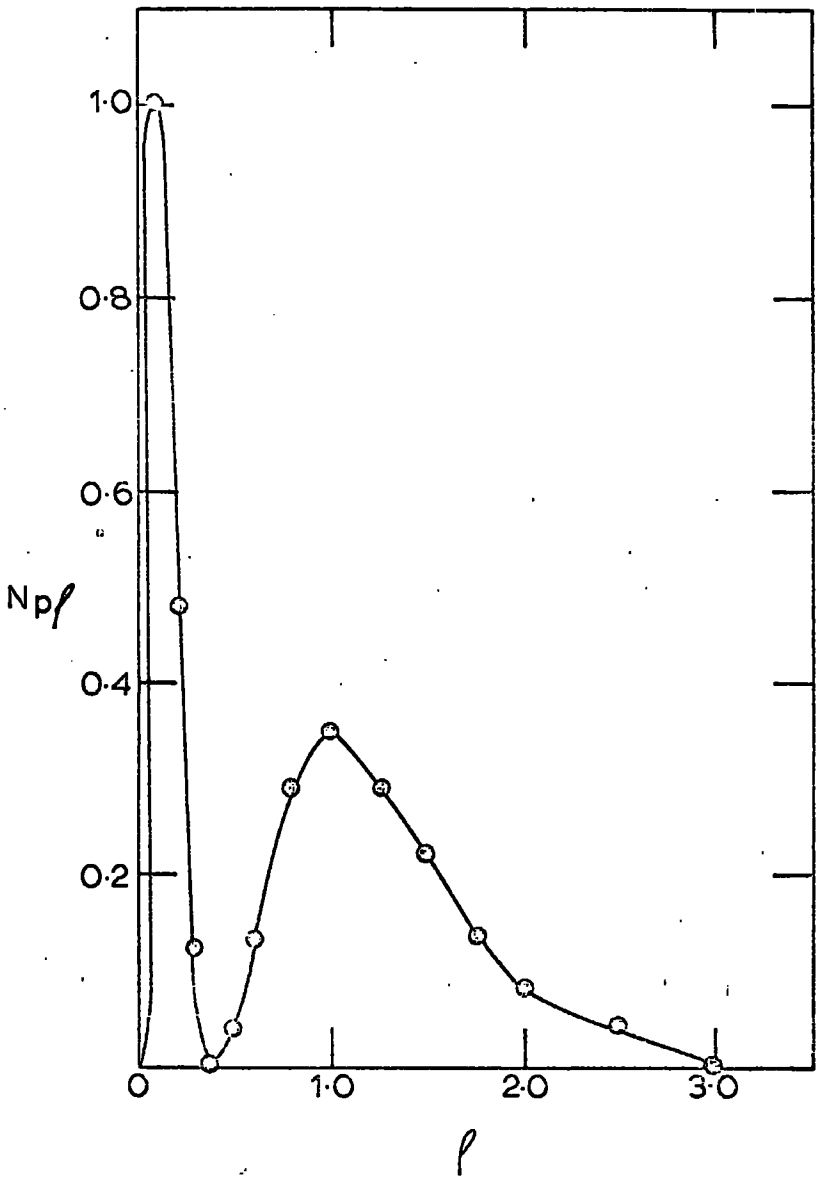

FIG. 6. E=500 Kev (1)

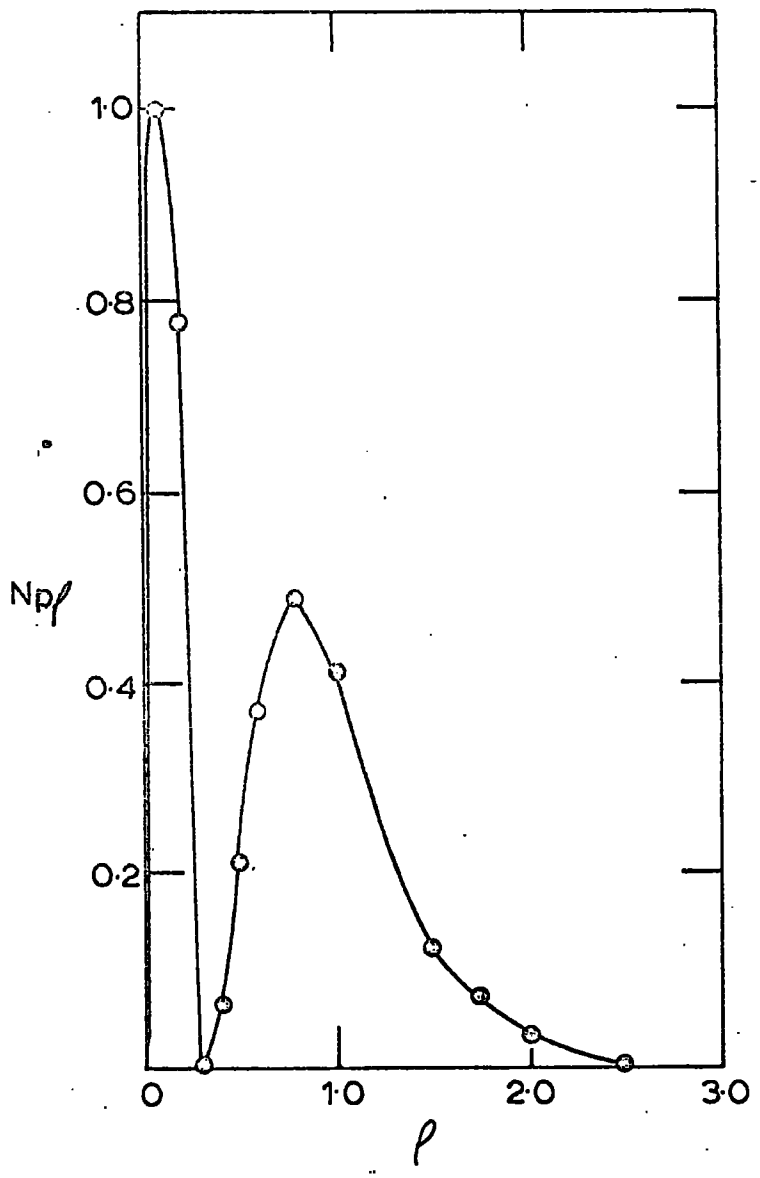

FIG. 7.

30·2 Kev (2)

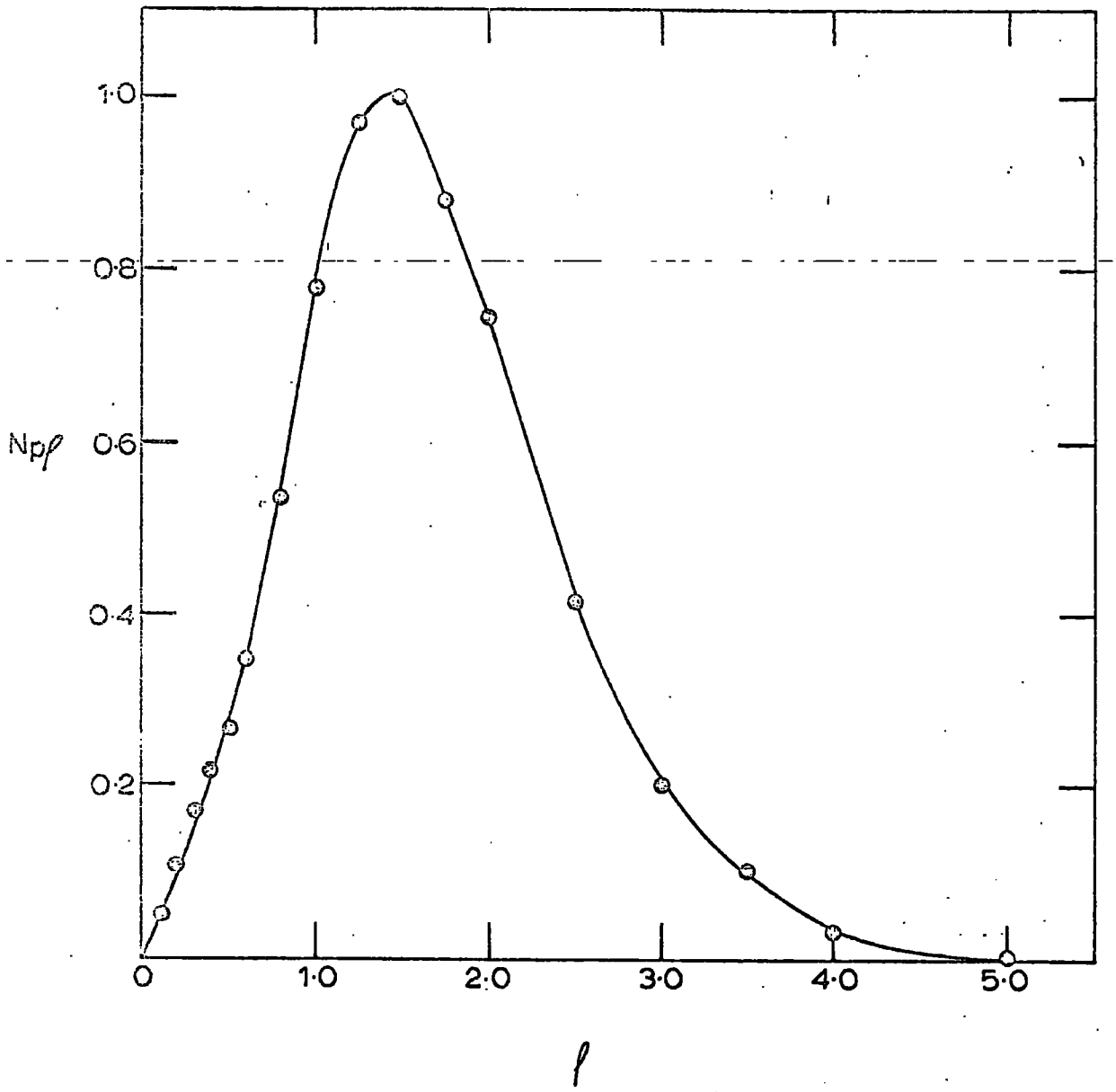

FIG. 8.

100 Kev (2)

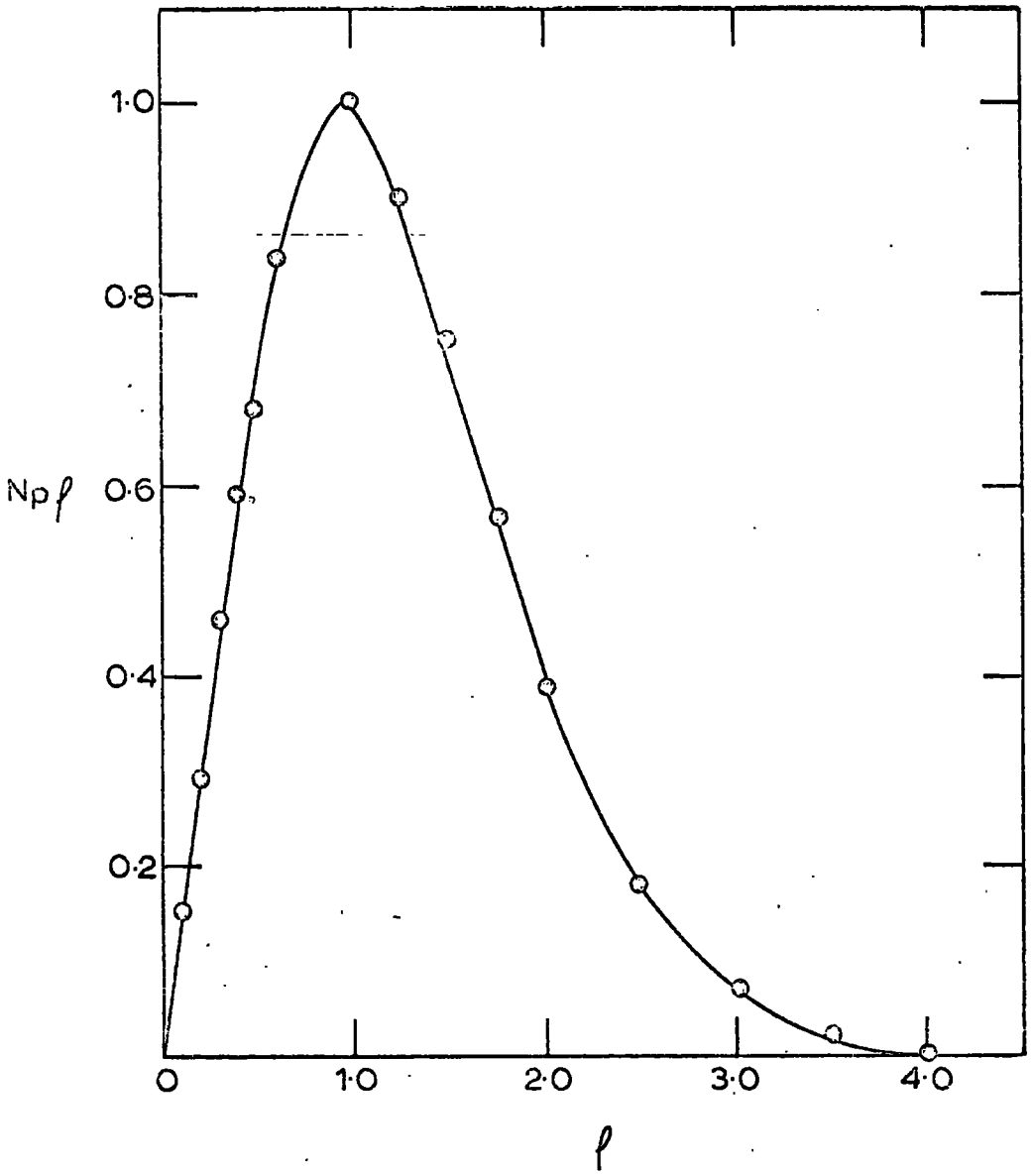

FIG. 9. E= 250 (2)

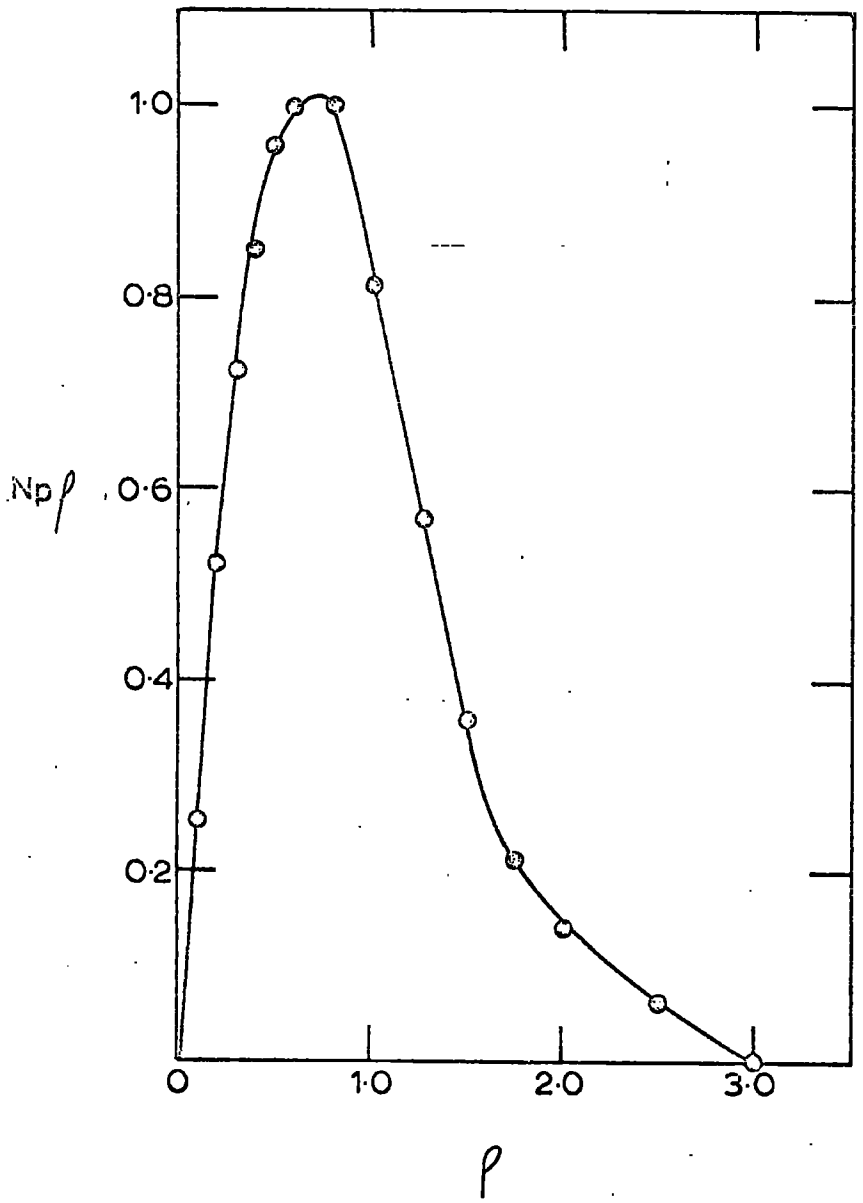

FIG.10.

E = 500 (2)

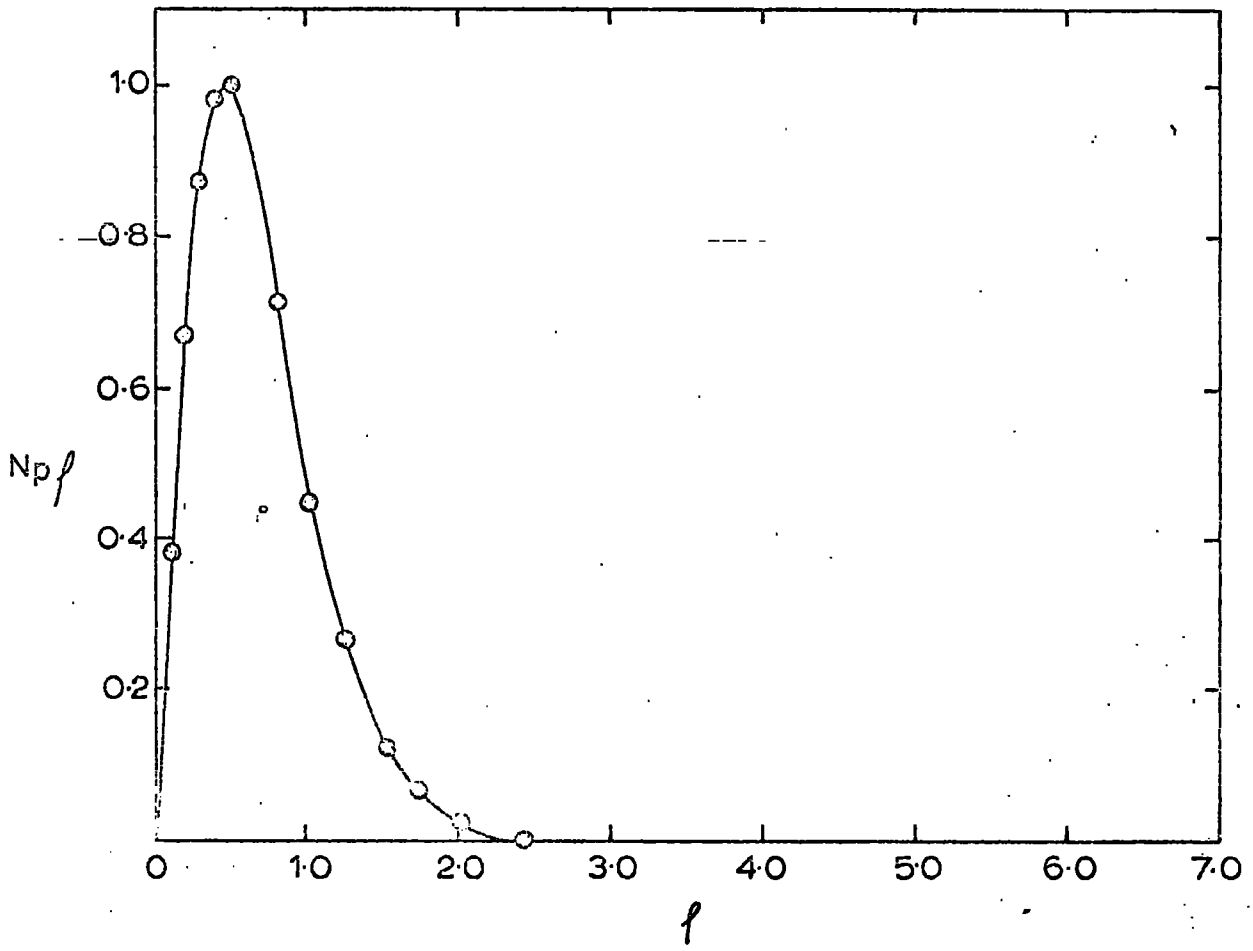

FIG.11.

E = 30 Kev. (3)

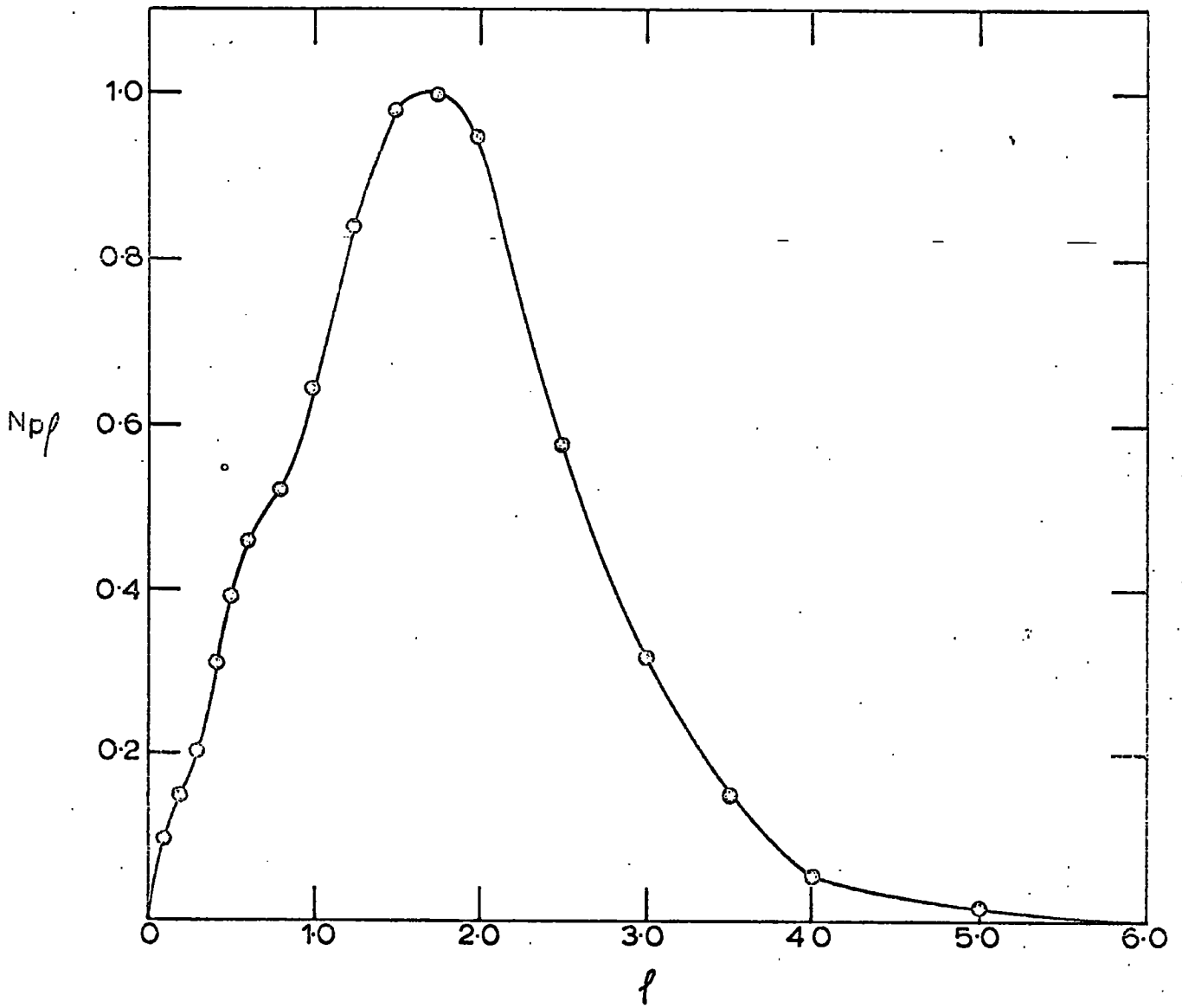

FIG.12.

E = 100 (3)

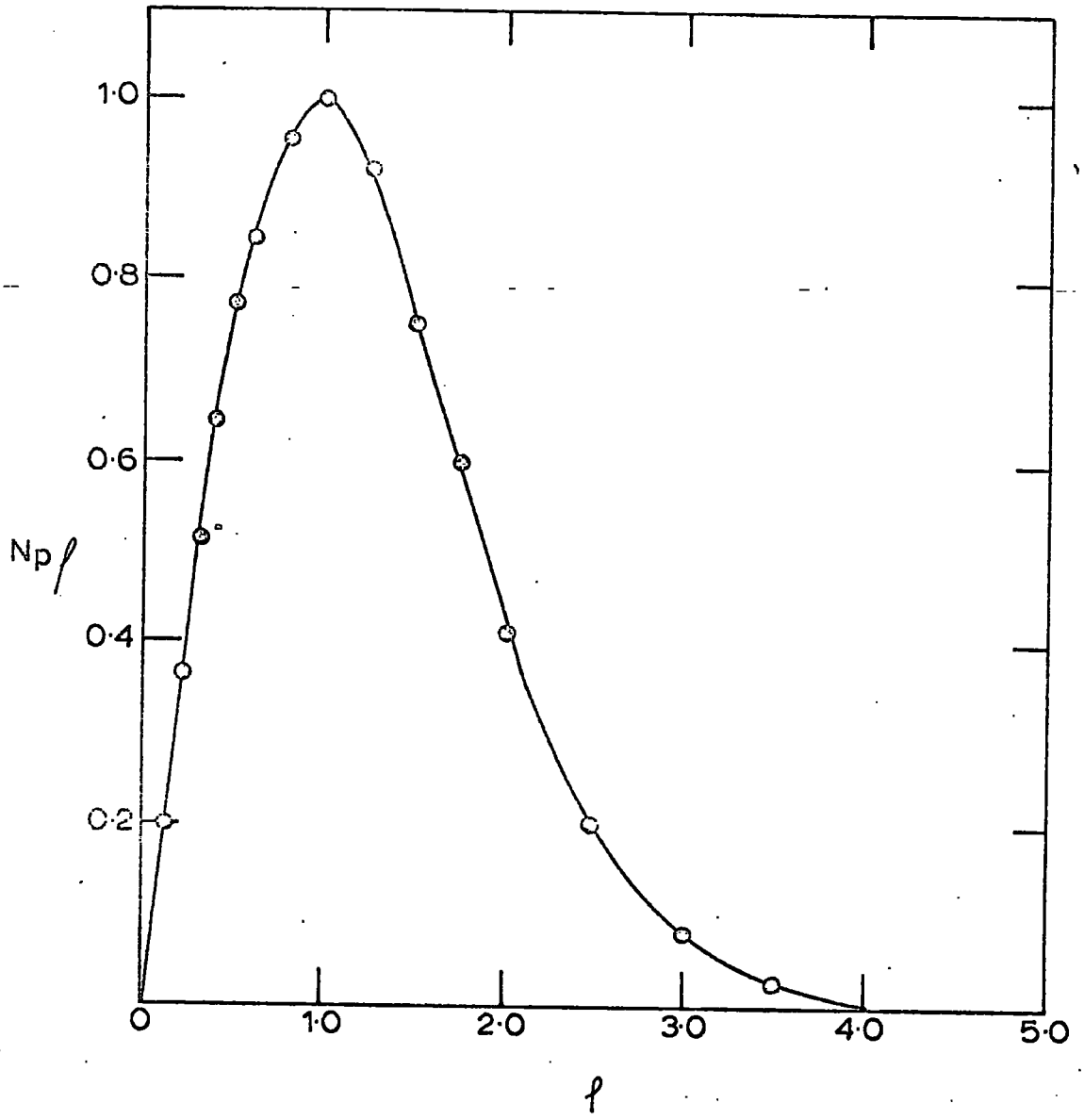

FIG.13.

E = 250 (3)

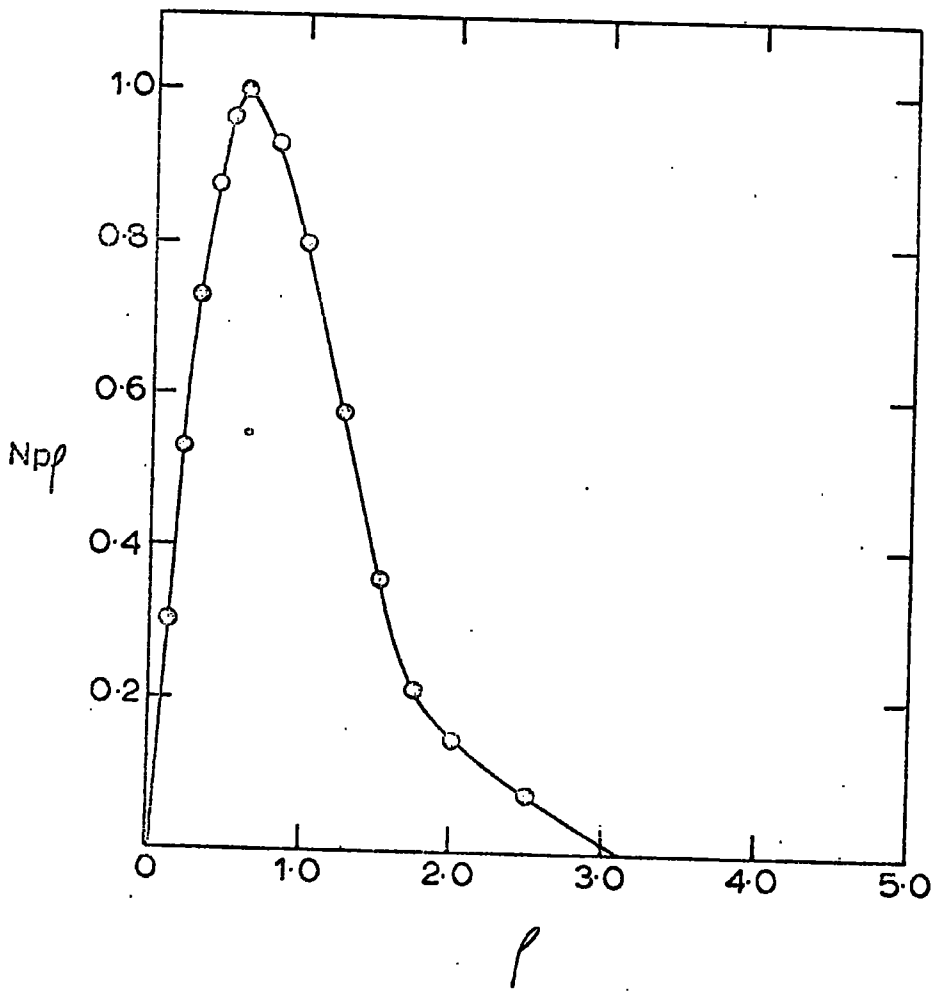

FIG.14. (A)

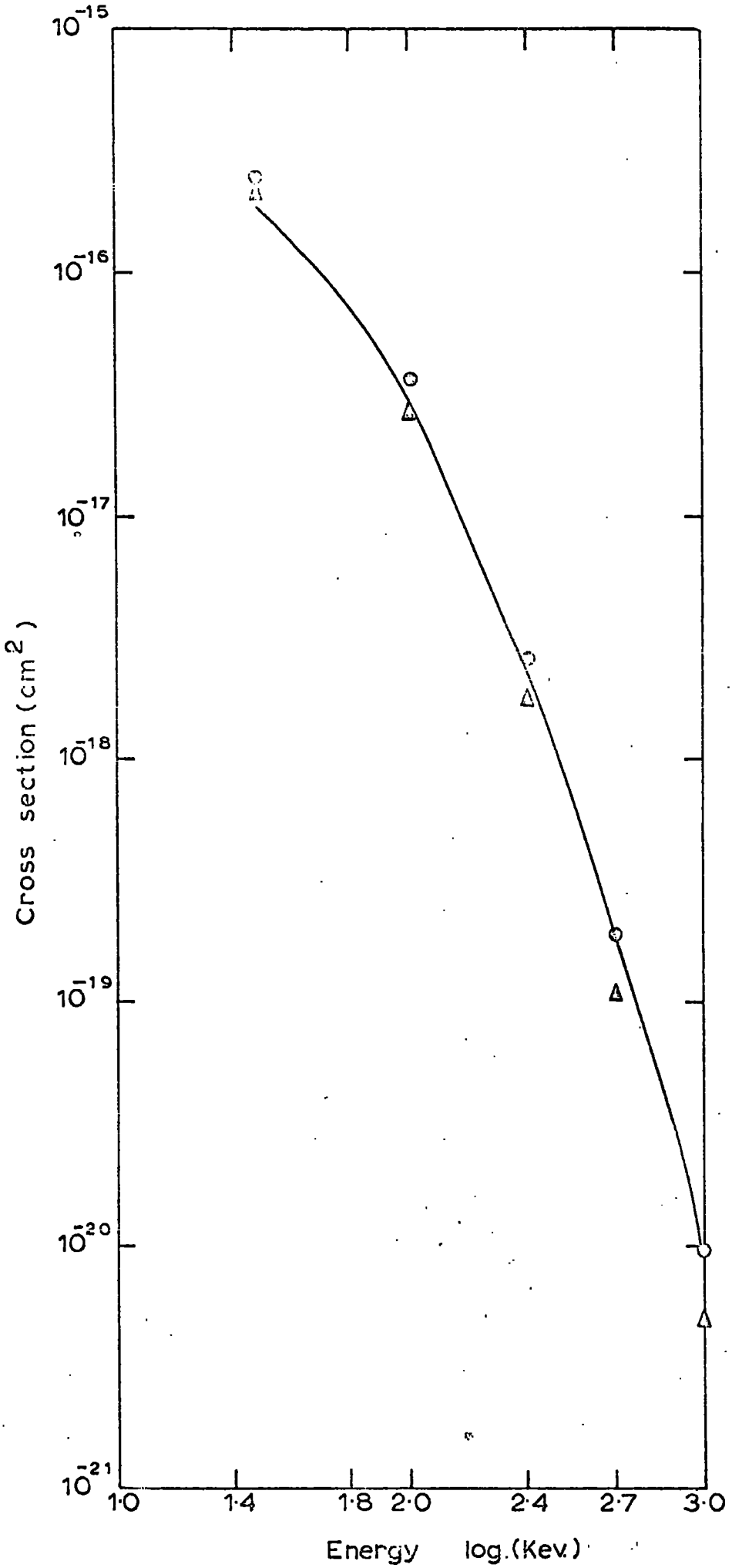
10^{-15}
10^{-16}
10^{-17}
10^{-18}
10^{-19}
10^{-20}
10^{-21}
Cross section (cm^2)
1·0
1·4
1·8
2·0
2·4
2·7
3·0
Energy log.(Kev.)

FIG.15. (B)

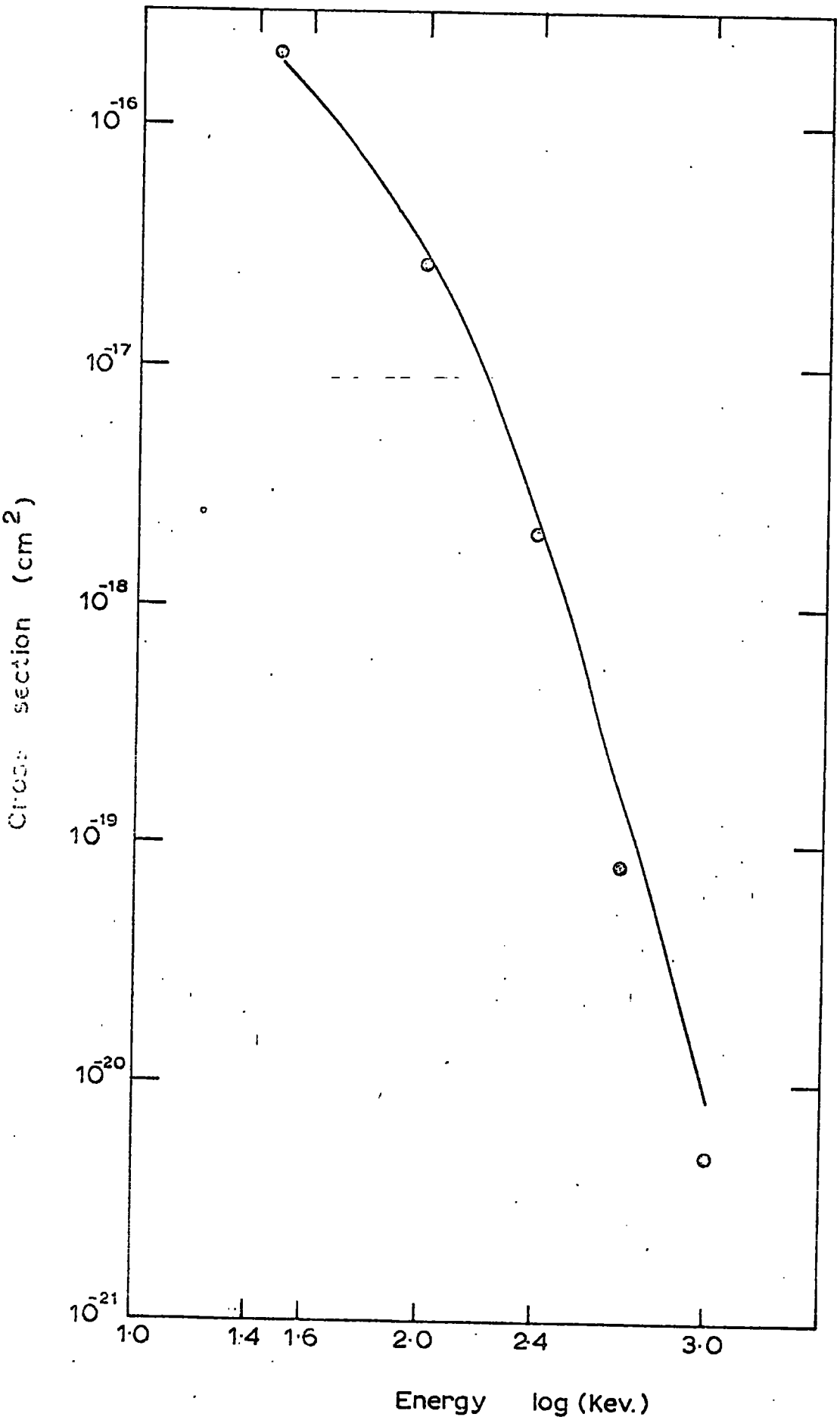
10^{-16}
10^{-17}
10^{-18}
10^{-19}
10^{-20}
10^{-21}
Cross section (cm^2)
1·0
1·4
1·6
2·0
2·4
3·0
Energy log (Kev.)

FIG.16. (C)

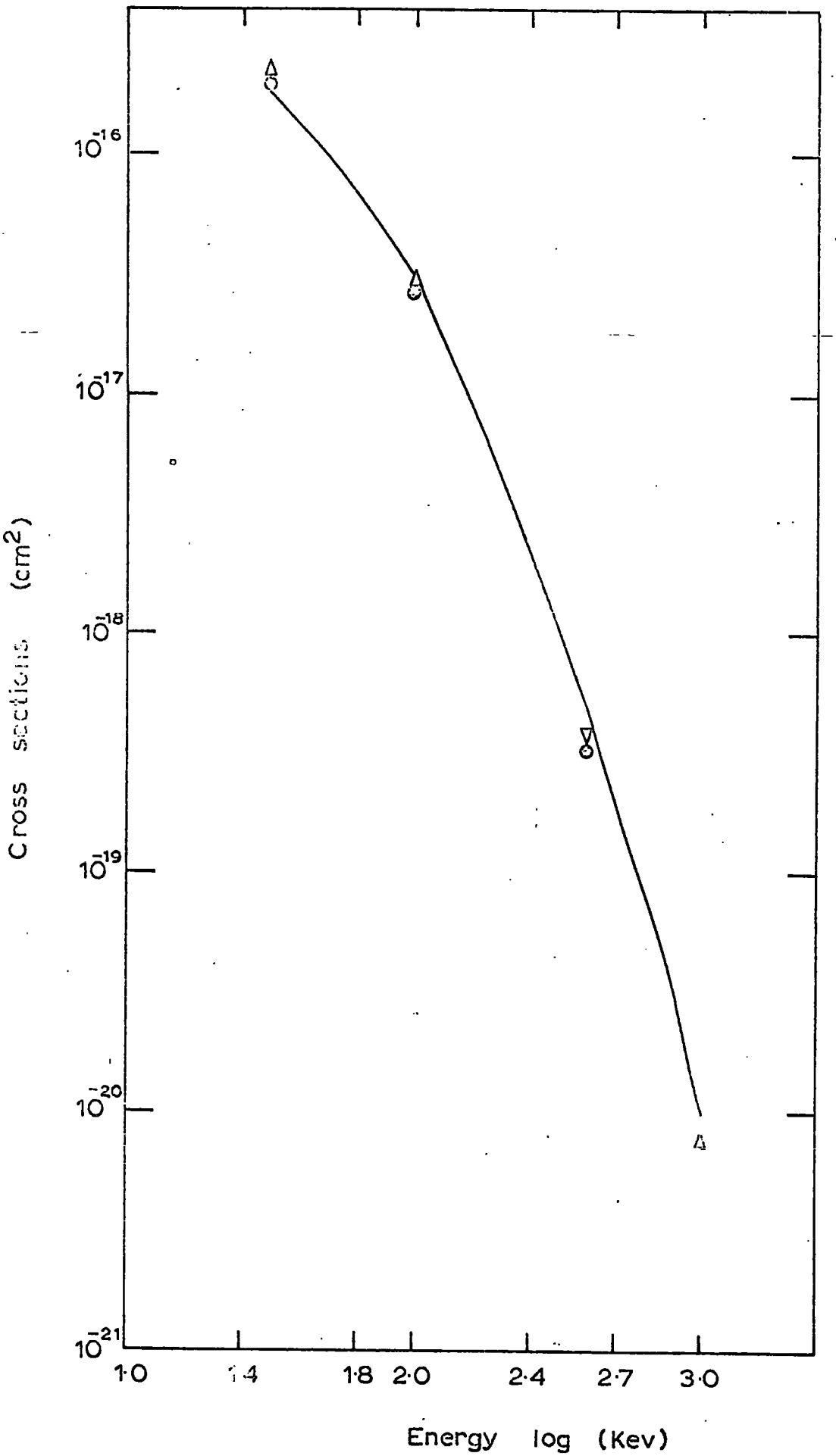
Cross sections (cm²)
10⁻¹⁶
10⁻¹⁷
10⁻¹⁸
10⁻¹⁹
10⁻²⁰
10⁻²¹
1·0
1·4
1·8
2·0
2·4
2·7
3·0
Energy log (Kev)

FIG.17. (D)

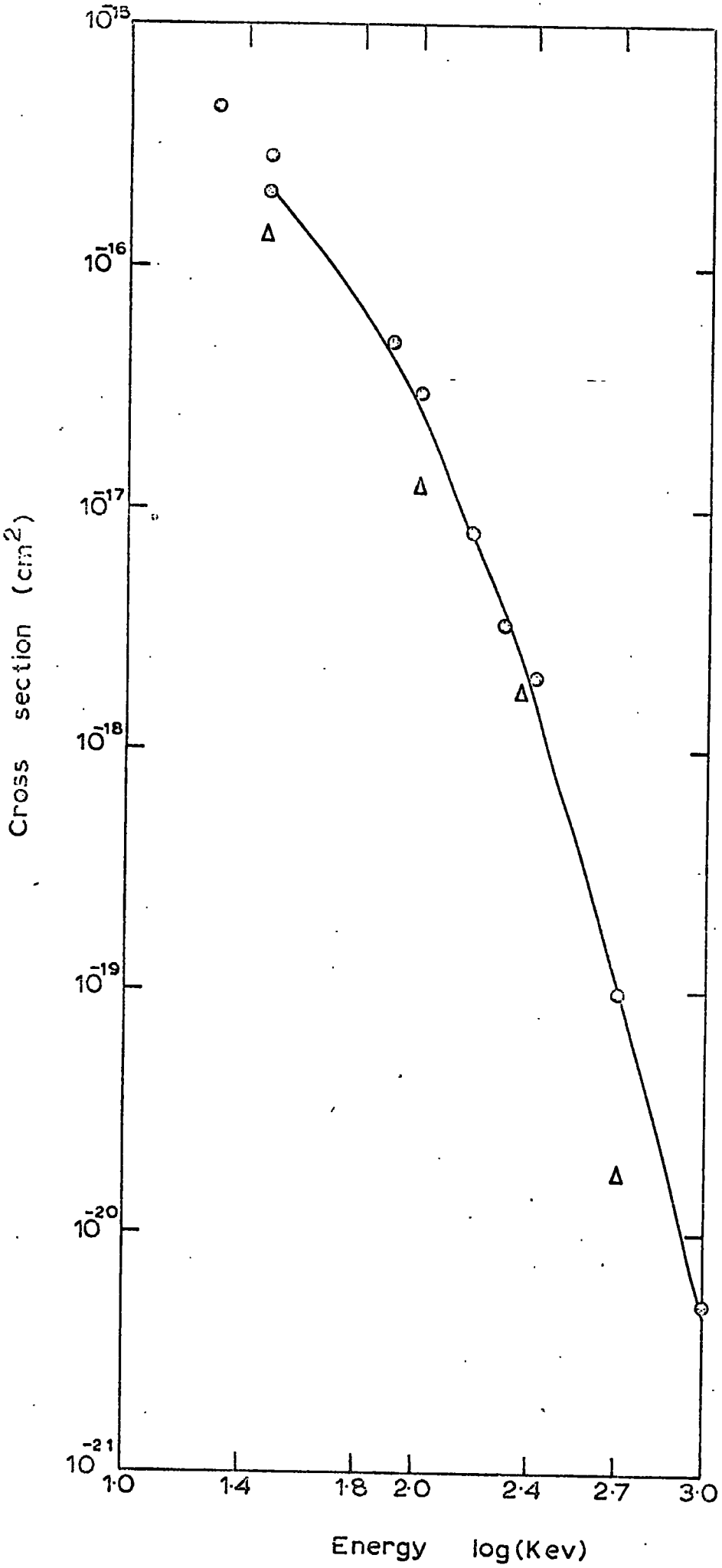
10^{-15}
10^{-16}
10^{-17}
10^{-18}
10^{-19}
10^{-20}
10^{-21}
Cross section (cm^2)
1·0
1·4
1·8
2·0
2·4
2·7
3·0
Energy log(Kev)

FIG.18.

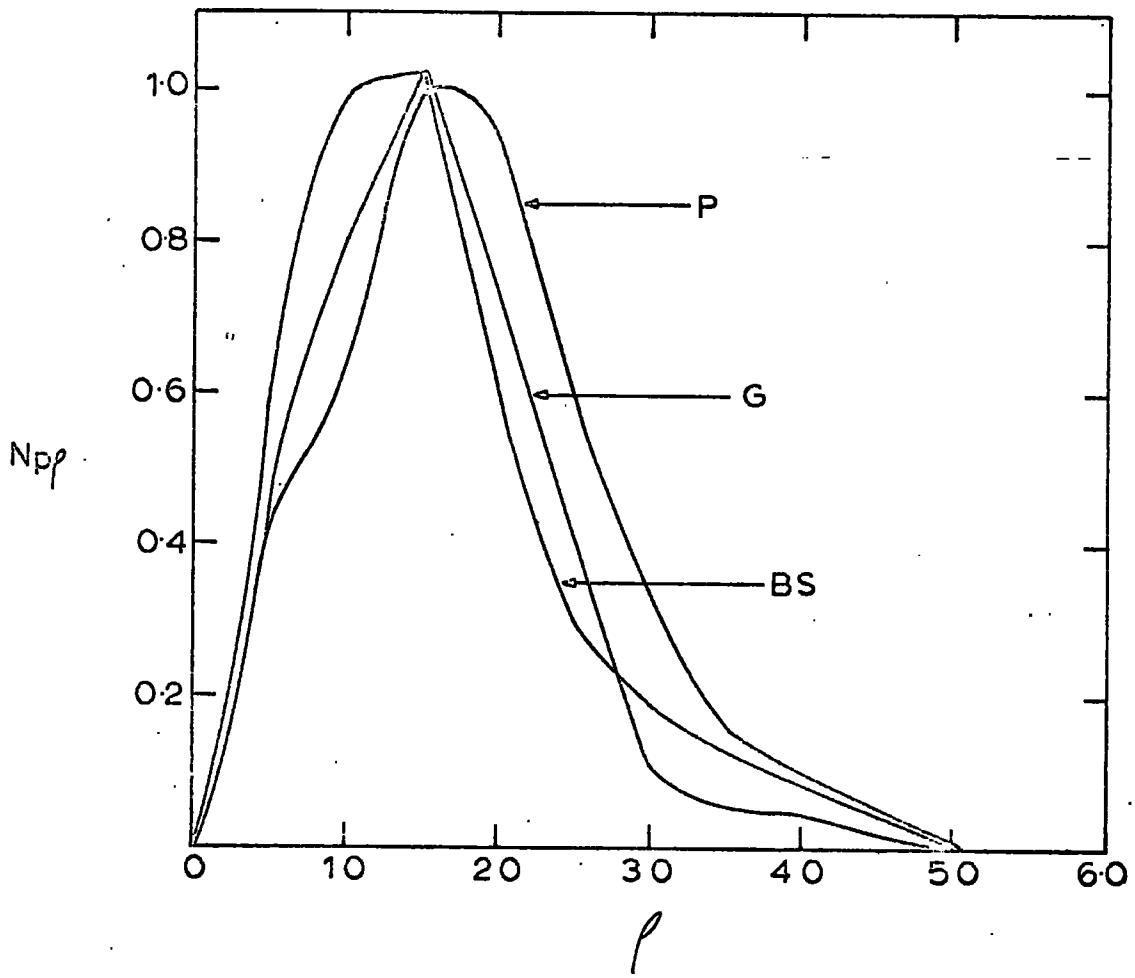

Table 1

Total cross-sections (in cm^2) for the elastic scattering of protons from helium.

Energy in Kev.	P1	P2	
25	1.026	0.9861	
30	0.9231	0.8292	
40	0.8062	0.7555	
100	0.5079	0.4803	
150	0.3945	0.3138	
225	0.2942	0.2509	
400	0.1836	0.1550	
500	0.1510	0.1424	

P1 Present calculations without the 2nd order potential

P2 Present calculations with the 2nd order potential

Table 2

Total cross-sections (in units of πa_o^2) for the 2^1S excitations of helium by protons.

Energy in Kev.	P1	P2	F1	B1	SB2
25	0.066	0.035	0.067	0.095	0.090
39	0.088	0.056	0.087	0.075	0.081
50	0.087	0.057			
100	0.058	0.046	0.058	0.038	0.041
150	0.040	0.031	0.038	0.027	0.026
225	0.026	0.021	0.025		0.020
400	0.014	0.011	0.014	0.010	0.010
500	0.011	0.009	0.010	0.008	

P1 Present calculations without the 2nd order potential.

P2 Present calculations with the 2nd order potential.

F1 Four-state approximation (Flannery, 1970)

B1 First Born approximation (Bell et al, 1968)

SB2 2nd. Born approximation (Holt et al, 1971).

Table 3

Total cross-sections (in units of πa_o^2)
for the 2^1p excitations of helium by protons.

Energy in Kev	P1	P2	F1	B1	SB2
25	0.030	0.025	0.037	0.204	
39	0.072	0.062	0.082	0.227	
50	0.090	0.090		0.228	
100	0.147	0.139	0.153	0.207	0.130
150	0.145	0.135	0.148	0.172	0.128
225	0.131	0.124	0.132		0.118
400	0.100	0.099	0.100	0.102	0.095
500	0.087	0.087	0.087	0.092	

P1 Present calculations without the 2nd order potential.

P2 Present calculation with the 2nd order potential.

F1 Four-state approximation (Flannery 1970).

B1 First Born approximation (Bell et al, 1968).

SB2 2nd Born approximation (Holt et al. 1971).

Table 4

Total cross-sections for electron capture by protons in helium

Cross - sections (10^{-16} cm^2)

Proton energy in Kev.	DW1	DW2	TC	BS	G	B1	Expt.
30	2.07	2.44	1.86	2.19	1.92	2.80	1.92 (a)
100	2.68^{-1}+	3.29^{-1}	3.06^{-1}	2.90^{-1}	2.76^{-1}	3.0^{-1}	2.76^{-1} (a)
250	1.73^{-2}	2.40^{-2}	2.35^{-2}			2.0^{-2}	2.0^{-2} (b)
500	1.06^{-3}	1.88^{-3}	1.88^{-3}			1.0^{-3}	8.0^{-4} (b)
1000	3.99^{-5}	9.38^{-5}	9.38^{-5}	7.4^{-5}		5.0^{-5}	5.0^{-5} (b)
10,000	1.57^{-10}		4.55^{-10}	3.1^{-10}			$(1.2 \pm 0.4)^{-10}$ (c)

\+ The superscript indicates the power 10 by which the number is to be multiplied.

DW1, DW2, TC are the present calculations following the case A, Case B, Case C in chapter 6.

BS results of Bransden et al (1966)

G results of Green et al (1965)

B1 First Born approximation (Mapleton, 1961)

Expt. Experimental results, (a) Steir & Barnett, 1966,

(b) Barnett & Raynolds, 1958.

(c) Barkner et al, 1965.

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