# The high energy scattering of photons and alpha particles by hydrogen atoms

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# THE HIGH ENERGY SCATTERING OF PROTONS AND ALPHA PARTICLES BY HYDROGEN ATOMS

by

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# CONTENTS

PAGE

CHAPTER 5. IMPACT PARAMETER METHODS.

CHAPTER 6. SECOND ORDER METHODS.

CHAPTER 7. THE IMPULSE APPROXIMATION.

CHAPTER 8. RESULTS.

CHAPTER 9. THE HIGH ENERGY BEHAVIOUR OF ELECTRON CAPTURE CROSS SECTIONS.

# ABSTRACT

The major part of the thesis is concerned with the methods used to obtain approximate values of cross sections for rearrangement processes in which protons and alpha particles are scattered from hydrogen atoms.

Some of the relevant experiments are briefly described in Chapter 1 and time dependent scattering theory used in Chapter 2 to derive an exact depression for the cross section. Born expansions of the transition amplitude are introduced and in Chapter 3 some OBK and Born approximation calculations are discussed. Distorted wave, impact parameter and second order methods are considered in Chapters 4, 5 and 6, numerical results being given where possible. A new integral equation for the transition operator is obtained which has a connected kernal. The inhomogeneous term gives a modified first Born approximation to the transition amplitude.

The impulse approximation forms the subject of Chapters 7 and 8. A new derivation, due to Coleman, is given and calculations for the processes

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

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

$$\text{and}\quad He^{++} + H(1s) \rightarrow He^+\ (2p \text{ or } 3s) + H^+,$$

are described. The results are compared with those obtained by other workers. They are used to calculate the polarization of Lyman-alpha radiation emitted by 2p hydrogen atoms formed by capture and to investigate

the $n^{-3}$ rule by which estimates of total cross sections are often obtained.

The asymptotic form of the electron capture cross section as the velocity of the incident particle tends to infinity is discussed in Chapter 9. A brief survey is given of the forms predicted by the various theories described in previous chapters. The high energy form of the modified first Born approximation derived in Chapter 4 is then considered. It is found that, with the approximations made, it is the same as that of Drisko's Second Born approximation.

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Chapter 1.

# EXPERIMENTAL DETERMINATION OF ELECTRON CAPTURE CROSS SECTIONS

## 1) Introduction.

The cross section for a certain type of event in a given collision is equal to the number of events of this type per unit time per target divided by the flux of incident particles relative to the target.

Collisions in which one or more electrons are transferred from an ion A to an ion B are called charge exchange reactions. This thesis is concerned with the simplest charge exchange reaction, in which a structureless particle collides with a hydrogen atom and captures the electron. First, a brief account will be given of some of the experiments on such a system which have been performed in recent years.

Electron capture by protons in atomic hydrogen has been investigated by Fite, Brackmann and Snow (1958), Fite, Stebbings, Hummer and Brackmann (1960), Fite, Smith and Stebbings (1962), and Gilbody and Ryding (1966). More recently a different technique has been used by McClure (1966), Wittkower, Ryding and Gilbody (1966) and Bayfield (1968).

Fite, Smith and Stebbings (1962) have also measured cross sections for charge transfer between alpha-particles and atomic hydrogen.

## 2) Experiments involving crossed beams.

In the first group of experiments, an arbitrarily highly dissociated beam of hydrogen produced by thermal dissociation in a tungsten furnace was crossed in a vacuum region with a beam of fast protons, great care being taken to ensure that the whole proton beam passed through the beam of hydrogen. Measurements were made of the current of either the slow protons or the fast hydrogen atoms which were produced as a result of collisions involving charge transfer. They led to the determination of the ratio $Q_A/Q_M$, where $Q_A$, $Q_M$ are the cross sections for charge exchange in atomic and molecular hydrogen respectively. Absolute values of $Q_A$ were obtained using values of $Q_M$ given by Stier and Barnett (1956).

A difficulty with crossed beam experiments is that a large part of any signal is due to interactions between the proton beam and the background gas in the apparatus, since the density of this is greater than that of the hydrogen beam. For this reason it is customary to use a mechanical chopping wheel to modulate the hydrogen beam at a frequency of about 100 cps. Then, any signal due to such interactions is a d.c. signal whereas interactions between the proton and hydrogen beams give rise to a signal which occurs at the modulation frequency and in a specified phase.

In the experiments of Fite et al (1958, 1960), the two beams intersected midway between two plates mounted parallel to the plane of the beams. Slow protons, produced in the interaction region by the two processes of capture and ionization, were collected by applying an electric field across the plates. The contribution from ionization was determined by reversing the field and measuring the current of electrons. The ratio $Q_A/Q_M$ was obtained by comparing the slow ion signals when the beam from the furnace was mainly atomic and when it was entirely molecular.

The method was used to measure cross sections for incident proton energies in the range 400 ev - 40 kev.

At lower energies, the collecting field is sufficient to deflect the proton beam so the method must be modified. Fite et al (1962) arranged that the two beams should intersect at the centre of a cylindrical collector whose axis coincided with the direction of the proton beam. The slow ions produced were collected on the surface of the cylinder. The system was unable to distinguish between slow protons arising from charge transfer and those produced by ionization but, since the collecting cylinder almost totally enclosed the interaction region, it was assumed that the majority of electrons produced by ionizing collisions were also collected, so that the measured signal was due to capture alone. In this way cross sections were obtained for incident energies down to 20 ev.

The apparatus was also used to measure cross sections for charge transfer between $He^{++}$ ions and hydrogen atoms in the energy range 100 ev to 36 kev. These are the only available experimental results for this process.

For incident proton energies above 40 kev, the charge transfer cross section rapidly becomes too small for measurements of the slow ion current to yield accurate results. For this reason Gilbody and Ryding (1966) studied the fast beam instead. They used electrostatic deflection to separate the fast neutral atoms produced by charge transfer from the fast protons and measured the intensity of each beam separately. They obtained cross sections for incident proton energies in the range 38 - 130 kev.

At 40 kev where the data obtained by the two sets of workers overlaps, the result of Fite et al is approximately twice that of Gilbody and Ryding. The difference is not greatly in excess of the combined experimental error but has not been accounted for.

## 3) Single beam experiments.

As mentioned previously, one of the difficulties inherent in crossed beam experiments is the low density of the target gas and the consequent low signal/noise ratio. Two experiments have been performed recently which attempt to overcome this problem. In these, the proton beam is passed directly through a tungsten furnace, which provides an atomic hydrogen target of much greater thickness. However, accurate determination of the degree of dissociation of the hydrogen gas and the absolute density of the hydrogen atoms or molecules at any particular furnace temperature is then a very difficult problem. In both experiments, measurements were based on post collision charge analysis of the fast beam, as in the work of Gilbody and Ryding, and the quantity determined was the ratio $Q_A/Q_M$. Absolute values of $Q_A$ were then obtained using known values of $Q_M$.

McClure (1966) was the first to use this method, and obtained cross sections for incident energies between 2 and 117 kev. He obtained absolute values for the molecular cross section $Q_M$ which are in good agreement with the results of Stier and Barnett, and used them to determine absolute values of $Q_A$. His results are in agreement with those of Ryding and Gilbody in the ranges 38 - 42 kev and 80 - 120 kev but show a marked discrepancy around 50 kev. In the energy range 2 to 20 kev the results of Fite et al are greater than those of McClure by a factor of between

20% and 40%.

Using methods similar to those of McClure, Wittkower and others (1966) have attempted to resolve the discrepancy in previous experimental results at energies around 50 kev. They measured relative values of the ratio $Q_A/Q_M$ for various values of the incident proton energy. Absolute values of this ratio could not be obtained in their experiment. Instead, the relative values were normalised to the value obtained by McClure and by Gilbody and Ryding for an incident proton energy of 110 kev, an energy at which the two sets of data are in fairly good agreement. Absolute values for $Q_A$ were then obtained using Stier and Barnett's results for $Q_M$ and are in good agreement with the results of McClure. The result at 40 kev lies slightly above his but is still much too low to be consistent with that of Fite et al. For a comparison of the various experimental result see fig. 4 of Wittkower et al (1968).

## 4) Measurements of cross sections for capture into a specific state.

All the experiments so far discussed are concerned with the measurement of total capture cross sections, no attempt being made to calculate the cross section for capture into a particular level of the projectile.

Bayfield (1968) measured cross sections for the process

$$H^+ + H(1s) \longrightarrow H(2s) + H^+$$

for incident proton energies in the range 3 - 23 kev. A collimated proton beam was passed through a heated scattering cell containing hot argon or thermally dissociated hydrogen, and the fast collision products leaving the target were observed. Fast metastable atoms were detected by Stark-effect quenching in a d.c. electric field and subsequent observation of the resulting Lyman-alpha radiation. Measurements yielded values of the ratio $Q_H(2s)/Q_{Ar}(2s)$, where $Q_H$, $Q_{Ar}$ are the cross sections for proton - hydrogen, proton-argon collisions respectively. Bayfield also measured the energy dependence of the cross section $Q_{Ar}(2s)$. His results were normalised so that they agreed at one energy with absolute measurements of Jaecks et al (1965) and Andreev et al (1966). Absolute values of $Q_H(2s)$ could then be obtained.

Relative values of $Q_H(2s)$ in the energy range 40 - 200 kev were obtained by Ryding et al (1966) using a similar apparatus. Their measurements gave relative cross sections $Q_{H_2}(2s)$, $Q_{He}(2s)$ and values of the ratios $Q_H(2s)/Q_{H_2}(2s)$ and $Q_{H_2}(2s)/Q_{He}(2s)$. They used the value of $Q^B(2s)$ at 100 kev given by Mapleton (1962) to normalise their results. Gaily (1968b) suggested a better normalisation based on the absolute values of $Q_{He}(2s)$ given by Andreev et al (1966). He used these to normalise the values of $Q_{He}(2s)$ given by Ryding et al and used the resulting cross section values to calculate absolute values of $Q_H(2s)$.

Stebbings et al (1965) used a crossed beam technique to investigate Lyman-alpha production in proton-hydrogen collisions for incident proton energies in the range 600 ev to 30 kev. The processes which give rise to such radiation are

$$H^+ + H(1s) \longrightarrow H^+ + H(2p), \qquad (1.4.1)$$

$$H^+ + H(1s) \longrightarrow H(2p) + H^+. \qquad (1.4.2)$$

They are distinguishable because, in most collisions, momentum transfer between the colliding systems is very small. Thus, process (1) gives rise to excited atoms with thermal energies whereas those produced by process (2) have the same kinetic energy as the incident protons. The region of interaction of the two beams was viewed by an ultra-violet detection counter which could be rotated about the neutral beam axis in a plane containing the ion beam. On transit to the counter, the radiation passed through a molecular oxygen filter. This only transmits radiation whose wavelength lies in one of seven very narrow wavelength bands, one of which contains the Lyman-alpha wavelength (1215.7Å). For each value of the incident proton energy, the intensity, $I(\theta)$, of this radiation was measured at angles of $90^\circ$ and $54.5^\circ$ with respect to the proton beam. At the $90^\circ$ position, the counter axis was perpendicular to the plane containing the two beams and both excitation and capture contributed to the counter signal. However, at $54.5^\circ$, because of the velocity component of the projectiles along the viewing direction, the wavelength of the radiation resulting from capture was Doppler shifted by an amount sufficient to cause almost total attenuation in the oxygen cell, except at energies below 3 kev. Therefore, the signal obtained in this position was due almost entirely to direct excitation.

The cross section for either process is directly proportional to the total intensity of the emitted radiation and this can be obtained from the measurements made. Allowance was made for the polarization of the radiation arising from direct excitation but the capture radiation was assumed to be emitted isotropically. Absolute cross sections were obtained by using the same apparatus to measure Lyman-alpha production in electron-hydrogen collisions and normalizing to the e - H cross sections of Fite et al (1958, 1959).

They must be regarded with some caution for two reasons. Gaily (1968a) discovered that photoabsorption data for $O_2$ used by Stebbings et al were incorrect. At 5 kev, use of Gaily's measurements increases the cross section by about one sixth and the effect at higher energies is not yet known. Secondly, Gaily and Geballe have recently carried out an independent measurement of the cross section and preliminary results in the energy range 2 - 6 kev agree neither in shape nor in magnitude with those of Stebbings et al, disagreeing by a factor of ten at 6 kev. (Gaily and Geballe, 1968).

## Chapter 2.

# SCATTERING THEORY APPLIED TO ELECTRON CAPTURE

### 1) Introduction.

The remainder of this thesis is concerned with the theoretical determination of electron capture cross sections. Most of the work refers to collisions at high energies; that is, at energies such that the relative velocity of the colliding systems is greater than the orbital velocity of the active electron in its initial bound state. Atomic units are used except where the contrary is stated.

### 2) Basic notation.

Consider a rearrangement collision of the form

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

in which a structureless particle 1 of mass $M_1$ and charge $Z_1$ is incident on a bound system (2+3) and captures the electron 3. Particle 2 has mass $M_2$ and charge $Z_2$.

The position vectors of particles 1, 2, 3 with respect to some fixed origin 0 are $\underset{\sim}{r}_1, \underset{\sim}{r}_2, \underset{\sim}{r}_3$ and the relative position vectors of the three particles are denoted by $\underset{\sim}{r}, \underset{\sim}{x}, \underset{\sim}{R}$ where

$$\underset{\sim}{r} = \underset{\sim}{r}_3 - \underset{\sim}{r}_2 , \quad \underset{\sim}{x} = \underset{\sim}{r}_3 - \underset{\sim}{r}_1 , \quad \underset{\sim}{R} = \underset{\sim}{r}_1 - \underset{\sim}{r}_2 .$$

Let a,b be the reduced masses of the bound systems 1 + 3, 2 + 3 respectively.

$$a = \frac{M_1}{M_1 + 1} , \qquad b = \frac{M_2}{M_2 + 1} .$$

The complete Hamiltonian for the system may be written

$$H' = H_0' + V_{12} + V_{13} + V_{23}$$

where $V_{ij}$ denotes the interaction between particles i and j, and $H_0'$ is the kinetic energy operator

$$H_0' = -\frac{1}{2M_1}\nabla_1^2 - \frac{1}{2M_2}\nabla_2^2 - \frac{1}{2M_3}\nabla_3^2 .$$

It is convenient to consider the form taken by $H_0'$ in the centre of mass coordinate system. Let $\underline{R}_G$ be the position vector of the centre of mass of the three particles with respect to 0.

Then

$$\underline{R}_G = \frac{1}{M}\left(M_1\underline{r}_1 + M_2\underline{r}_2 + M_3\underline{r}_3\right),$$

where $M = M_1 + M_2 + 1$.

If $\underset{\sim}{s}$ is the position vector of particle 1 with respect to the centre of mass of system (2 + 3), and $\underset{\sim}{\rho}$ denotes the position vector of the centre of mass of (1 + 3) with respect to particle 2, then

$$\underset{\sim}{s} = b\underset{\sim}{r} - \underset{\sim}{x}, \qquad \underset{\sim}{\rho} = \underset{\sim}{r} - a\underset{\sim}{x} .$$

In the coordinate systems $(\underset{\sim}{r}, \underset{\sim}{s}, \underset{\sim}{R}_G)$ and $(\underset{\sim}{x}, \underset{\sim}{\rho}, \underset{\sim}{R}_G)$ the kinetic energy operator takes the forms

$$H_0' = -\frac{1}{2b}\nabla_r^2 - \frac{1}{2\mu_i}\nabla_s^2 - \frac{1}{2M}\nabla_{R_G}^2$$

$$= -\frac{1}{2a}\nabla_x^2 - \frac{1}{2\mu_f}\nabla_\rho^2 - \frac{1}{2M}\nabla_{R_G}^2 ,$$

where $\mu_i, \mu_f$ are the reduced masses of the initial and final systems,

$$\mu_i = \frac{M_1(M_2+1)}{M}, \qquad \mu_f = \frac{M_2(M_1+1)}{M}.$$

The potentials $V_{ij}$ are independent of $\underline{R}_G$ and consequently the motion of the centre of mass of the system may be separated out. In the rest of this thesis, the centre of mass frame of reference is used, in which the motion of the system is governed by the Hamiltonian

$$H = H_o + V_{12} + V_{13} + V_{23} = H_o + V,$$

where $H_o$ may be written in either of the forms

$$H_o = -\frac{1}{2\mu_i}\nabla_{\underset{\sim}{r}}^2 - \frac{1}{2b}\nabla_\rho^2 = \frac{1}{2\mu_f}\nabla_\rho^2 - \frac{1}{2a}\nabla_x^2 .$$

H can be split in several ways, two of which are

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

where

$$H_i = H_o + V_{23}, \quad H_f = H_o + V_{13}$$

$$V_i = V_{12} + V_{13}, \quad V_f = V_{12} + V_{23} .$$

3) Derivation of the expression for the cross section.

In the collision process there are three time intervals of interest. Two wave packets are prepared at some time in the remote past, one representing the initial state of the target system (2 + 3), and the other that of the projectile, particle 1. Because they are described by wave packets, the target and projectile can be localised in space, so it can be assumed that they are far apart and that there is no interaction between them. The interaction itself takes place during the second interval, and the observation of the collision products during the third. In the following work, the wave packet description will not be adopted. Instead, a special limiting process due to Goldberger and Watson (1964) will be applied to pure states.

The Schrödinger equation that describes the time development of the system in the absence of external influences is

$$i \frac{\partial \Psi(t)}{\partial t} = H \Psi(t) . \qquad (2.3.1)$$

If the wave function at time $t_0$ is known, then (1) may be integrated to give

$$\Psi(t) = e^{-iH(t-t_0)} \Psi(t_0) . \qquad (2.3.2)$$

If at time $t_0$ the target and projectile have not started to interact, then

$$\Psi(t_0) = e^{-iE_i t_0} \varphi_i ,$$

where $E_i$ is the centre of mass energy of the initial system and $\varphi_i$ satisfies the time independent equation

$$(H_i - E_i)\,\varphi_i = 0.$$

If $\underline{k}_i$ is the initial relative momentum of the colliding systems, then

$$\varphi_i = \exp(i\,\underline{k}_i\cdot\underline{r})\,\psi_i(\underline{r}), \qquad (2.3.3)$$

where $\psi_i(\underline{r})$ is the initial state of the bound system (2 + 3). If $\epsilon_i$ is the corresponding eigenenergy, $\psi_i(\underline{r})$ satisfies the equation

$$\left(-\frac{1}{2b}\nabla_r^2 + V_{23}(\underline{r}) - \epsilon_i\right)\psi_i(\underline{r}) = 0,$$

and

$$E_i = \frac{k_i^2}{2\mu_i} + \epsilon_i\,. \qquad (2.3.4)$$

It is convenient to suppose that the system is prepared in the initial state $\varphi_i$ at time $t_0 = -\infty$. Then, from (2)

$$\Psi(0) = \lim_{t_0\to-\infty} e^{iHt_0}\,e^{-iE_it_0}\,\varphi_i$$

if the limit can be defined. The following definition, due to Goldberger and Watson (1964), is adopted:

$$\lim_{t\to-\infty} f(t) = \lim_{\epsilon\to0+}\epsilon\int_{-\infty}^{0} e^{\epsilon t'} f(t')\,dt'. \qquad (2.3.5)$$

If the function f(t) possesses a limit in the ordinary sense as $t \to -\infty$, then this limit coincides with that given by (5). However, if f(t) is an oscillatory function, the above procedure provides the required damping of the oscillations.

Thus

$$\Psi(0) = \lim_{\epsilon \to 0+} \epsilon \int_{-\infty}^{0} e^{\epsilon t} e^{iHt} e^{-iE_i t} \varphi_i \, dt$$

$$= \lim_{\epsilon \to 0+} \frac{i\epsilon}{E_i - H + i\epsilon} \varphi_i .$$

It is usual to write

$$\Psi(0) \equiv \Psi_i^+ = \lim_{\epsilon \to 0+} \Psi_i^+(\epsilon) \qquad (2.3.6)$$

where

$$\Psi_i^+(\epsilon) = \frac{i\epsilon}{E_i - H + i\epsilon} \varphi_i .$$

Since $(H_i - E_i)\varphi_i = 0,$ this can be written

$$\Psi_i^+(\epsilon) = \varphi_i + \frac{1}{E_i - H + i\epsilon} V_i \varphi_i . \qquad (2.3.7)$$

Thus it can be seen that

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

i.e. $\Psi_i^+$ is an eigenfunction of H corresponding to energy $E_i$.

If A, B are any two operators for which the reciprocal operators $A^{-1}$, $B^{-1}$ are defined, then

$$A^{-1} = B^{-1} + B^{-1}(B - A)A^{-1}. \tag{2.3.8}$$

If

$$A = E_i - H + i\epsilon, \quad B = E_i - H_f + i\epsilon,$$

$$\frac{1}{E_i - H + i\epsilon} = \frac{1}{E_i - H_f + i\epsilon}\left(1 + V_f \frac{1}{E_i - H + i\epsilon}\right)$$

Therefore

$$\Psi_i^+(\epsilon) = \frac{i\epsilon\,\varphi_i}{E_i - H_f + i\epsilon} + \frac{1}{E_i - H_f + i\epsilon} V_f\,\Psi_i^+(\epsilon). \tag{2.3.9}$$

From (2) and (6) it can be seen that the Schrödinger picture wave function which describes, at time $t \geq 0$, the system which has evolved from the state $\varphi_i$ in the remote past is

$$\Psi(t) = \lim_{\epsilon \to 0+} \Psi^\epsilon(t),$$

where

$$\Psi^\epsilon(t) = e^{-iHt}\,\Psi_i^+(\epsilon).$$

The quantity of interest is the probability of finding such a system in the eigenstate $\varphi_f$ of the final unperturbed Hamiltonian $H_f$. If the corresponding eigenenergy is $E_f$, so that

$$(H_f - E_f)\,\varphi_f = 0,$$

this probability is

$$\left| \langle \varphi_f \, e^{-iE_f t} \mid \Psi(t) \rangle \right|^2 .$$

If $\underline{k}_f$ is the final relative momenta of the colliding systems, then

$$\varphi_f = \exp(i\underline{k}_f \cdot \underline{\rho}) \, \psi_f(\underline{x}) , \qquad (2.3.10)$$

where $\psi_f(\underline{x})$ is the final state of the bound system (1 + 3), and satisfies the equation

$$\left( - \frac{1}{2a} \nabla_x^2 + V_{13}(\underline{x}) - \epsilon_f \right) \psi_f(\underline{x}) = 0 ,$$

where

$$E_f = \frac{k_f^2}{2\mu_f} + \epsilon_f . \qquad (2.3.11)$$

Let

$$W_{if}^{\epsilon}(t) = \frac{d}{dt} \left| \langle \varphi_f \, e^{-iE_f t} \mid \Psi^{\epsilon}(t) \rangle \right|^2 .$$

Then the transition rate from state $\varphi_i$ to state $\varphi_f$ is

$$W_{if}(t) = \lim_{\epsilon \to 0} W_{if}^{\epsilon}(t) .$$

The limit $\epsilon \to 0+$ will not be taken until all the calculations have been performed, because, in fact $\left| \langle \varphi_f \, e^{-iE_f t} \mid \Psi(t) \rangle \right|^2$ is independent of time. Now

$$W_{if}^{\epsilon}(t) = W_{if}^{\epsilon}(0) + t \frac{d}{dt} W_{if}^{\epsilon}(0) + \cdots .$$

It can be shown (Goldberger and Watson, 1964), that

$$\lim_{\epsilon \to 0+} W_{if}^{\epsilon}(t) = \lim_{\epsilon \to 0+} W_{if}^{\epsilon}(0) .$$

Now,

$$W_{if}^{\epsilon}(0) = \frac{d}{dt} \left| \langle \varphi_f | e^{i(E_f - H)t} \Psi_i^{+}(\epsilon) \rangle \right|^2 \Bigg|_{t=0}$$

$$= i \langle \varphi_f | \Psi_i^{+}(\epsilon) \rangle \left( T_{if}^{+}(\epsilon) \right)^{*} + \text{c.c.} \qquad (2.3.12)$$

where $T_{if}^{+}(\epsilon) = \langle \varphi_f | V_f | \Psi_i^{+}(\epsilon) \rangle$, (2.3.13)

and c.c. denotes the complex conjugate of the first term.

From (9) and (13) it can be seen that

$$\langle \varphi_f | \Psi_i^{+}(\epsilon) \rangle = \frac{i\epsilon}{E_i - E_f + i\epsilon} \langle \varphi_f | \varphi_i \rangle + \frac{1}{E_i - E_f + i\epsilon} T_{if}^{+}(\epsilon).$$

Therefore (12) can be written

$$W_{if}^{\epsilon}(0) = \frac{-\epsilon}{(E_i - E_f)^2 + \epsilon^2} \left\{ (E_i - E_f)(A_{if} + A_{if}^{*}) - i\epsilon (A_{if} - A_{if}^{*}) \right\}$$

$$+ \frac{2\epsilon}{(E_i - E_f)^2 + \epsilon^2} \left| T_{if}^{+}(\epsilon) \right|^2, \qquad (2.3.14$$

where $A_{if} = \left\{ T_{if}^{+}(\epsilon) \right\}^{*} \langle \varphi_f | \varphi_i \rangle.$

$W_{if}(0)$ is the transition rate at time t = 0 for a transition from state i to state f. For the processes under consideration, the state f is a continuum state in the sense that particle 2 is free and $E_f > 0$, and therefore a quantity with more physical meaning is the transition rate to a group of states with energies centred about the energy $E_f$. Let the density of these states be $\rho(E_f)$ per unit solid angle. Then the transition rate from state $\varphi_i$ to one of the group of states with momentum vectors lying in the solid angle $d\Omega$ and energies in the range $E_f - \Delta E$

to $E_f + \Delta E$ is

$$\omega_{if}(0) = \lim_{\epsilon \to 0+} \int_{E_f - \Delta E}^{E_f + \Delta E} W_{if}^{\epsilon}(0)\, \rho(E)\, dE\, d\Omega . \qquad (2.3.15)$$

Using (14), (15) and the result

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

one obtains finally

$$\omega_{if}(0) = \begin{cases} 2\pi \rho(E_f)\, |T_{if}^{+}|^2\, d\Omega , & E_i = E_f \\ 0 , & E_i \neq E_f , \end{cases}$$

where $T_{if}^{+} = \langle \varphi_f | V_f | \Psi_i^{+} \rangle$ provided that $\varphi_f$, $\Psi_i^{+}$ represent states of the same energy. It can be shown that $\rho(E_f) = \mu_f k_f / 8\pi^3$, $k_f$ being the final relative momentum.

The number of incident particles per unit time which cause the required transition and are scattered into the solid angle $d\Omega$ is $N I(\Omega) d\Omega$, where $I(\Omega)$ is the differential scattering cross section and N is the incident flux. $\omega_{if}(0)$ is the transition rate when the incident flux is $k_i / \mu_i$.

Therefore,

$$I(\Omega) = \frac{\mu_i \mu_f}{4\pi^2} \frac{k_f}{k_i} |T_{if}^{+}|^2 .$$

The total cross-section for a transition from an initial state $\varphi_i$ to a final state $\varphi_f$ is

$$Q(if) = \frac{\mu_i \mu_f k_f}{4\pi^2 k_i} \int | T_{if}^{+} |^2 \, d\Omega \qquad (2.3.16)$$

By considering the time reversed system, and following a procedure similar to that outlined above, one obtains

$$I(\Omega) = \frac{\mu_i \mu_f k_f}{4\pi^2 k_i} | T_{if}^{-} |^2 ,$$

where

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

and

$$\Psi_f^{-} = \lim_{\epsilon \to 0+} \left( \varphi_f + \frac{1}{E_f - H - i\epsilon} V_f \varphi_f \right). \qquad (2.3.17)$$

It has been shown that transitions occur only between states of equal energy. In this case, $T_{if}^{+} = T_{if}^{-}$. Therefore, for scattering problems, the superscripts '+' and '-' can be omitted and $T_{if}$ can be written in two ways.

$$T_{if} = \langle \Psi_f^{-} | V_i | \varphi_i \rangle = \langle \varphi_f | V_f | \Psi_i^{+} \rangle . \qquad (2.3.18)$$

If spherical polar coordinates $(R, \theta, \varphi)$ are chosen with polar axis in the direction of the incident beam, and $| T_{if} |^2$ is independent of $\varphi$, then (16) may be written

$$Q(if) = \frac{\mu_i \mu_f k_f}{2\pi^2 k_i} \int_{-1}^{+1} | T_{if} |^2 \, d(\cos\theta) , \qquad (2.3.19)$$

($Q(if)$ being in units of $\pi a_0^2$).

It is sometimes convenient to express Q(if) in terms of an integral with respect to momentum transfer. If $\underline{p} = a\underline{k}_f - \underline{k}_i$ and $\underline{q} = b\underline{k}_i - \underline{k}_f$, then, using the relation $\cos\theta = \hat{\underline{k}}_i \cdot \hat{\underline{k}}_f$, (19) may be written

$$Q(if) = \frac{1}{4\pi^2 a v^2}\left(\frac{\mu_f}{\mu_i}\right)\int_{p^2_{min}}^{p^2_{max}} |T_{if}|^2 \, d(p^2) \qquad (2.3.20)$$

$$\text{———} = \frac{1}{4\pi^2 b v^2}\left(\frac{\mu_f}{\mu_i}\right)\int_{q^2_{min}}^{q^2_{max}} |T_{if}|^2 \, d(q^2), \qquad (2.3.21)$$

where $v = k_i/\mu_i$, and

$$p^2_{min} = (ak_f - k_i)^2, \qquad p^2_{max} = (ak_f + k_i)^2, \qquad (2.3.22)$$

$$q^2_{min} = (bk_i - k_f)^2, \qquad q^2_{max} = (bk_i + k_f)^2.$$

Since energy is conserved in the collision, (4) and (11) give

$$\frac{k_i^2}{2\mu_i} - \frac{k_f^2}{2\mu_f} = \epsilon_f - \epsilon_i = \Delta E, \qquad (2.3.23)$$

and $\Delta E$ is the energy defect for the process under consideration. If all energies are measured in Rydbergs, instead of atomic units, (23) becomes

$$\frac{k_i^2}{\mu_i} - \frac{k_f^2}{\mu_f} = \epsilon_f - \epsilon_i = \Delta E. \qquad (2.3.24)$$

If this equation is used to eliminate $k_f$ from (22), and terms of order $1/M$ are neglected, then

$$p_{min}^2 \simeq \frac{1}{4v^2}\left(v^2 + \Delta E\right)^2 .$$

Similarly, it can be shown that

$$p_{max}^2 \simeq 4v^2\left(\frac{M_1M_2}{M_1+M_2}\right)^2 - \left(\frac{2M_1M_2}{M_1+M_2}\right)\Delta E - \frac{(\Delta E)^2}{4v^2} .$$

For a resonant process, $\Delta E = 0$, and

$$p_{max}^2 \simeq 4v^2\left(\frac{M_1M_2}{M_1+M_2}\right)^2 .$$

In general, the value of $p_{max}^2$ is very large and no appreciable error is obtained by replacing the upper limit of integration in (20) by infinity. An exception occurs when $M_1 = M_2$ and it will be shown that in this case the exact expression for $p_{max}^2$ must be used.

The integration limits in (21) may easily be obtained using the relation

$$\frac{p^2}{a} - \frac{q^2}{b} = \frac{k_i^2}{\mu_i} - \frac{k_f^2}{\mu_f} = \Delta E, \qquad (2.3.25)$$

all energies being measured in Rydbergs.

## 4) The Born Series.

The total Green's function operators $G^{\pm}$ are given by

$$G^{\pm} = \lim_{\epsilon \to 0+} \frac{1}{E - H \pm i\epsilon} .$$

The initial and final state Green's functions $G_i^{\pm}$, $G_f^{\pm}$ and the free particle Green's functions $G_0^{\pm}$ are defined by similar expressions, i.e.

$$G_{i,f}^{\pm} = \lim_{\epsilon \to 0+} \frac{1}{E - H_{i,f} \pm i\epsilon} ,$$

$$G_0^{\pm} = \lim_{\epsilon \to 0+} \frac{1}{E - H_0 \pm i\epsilon} .$$

In terms of these operators, the wave function $\Psi_i^+$ defined by (2.3.6), (2.3.7) can be written

$$\Psi_i^+ = (1 + G^+ V_i)\, \varphi_i . \qquad (2.4.1)$$

Similarly, (2.3.17) may be written

$$\Psi_f^- = (1 + G^- V_f)\, \varphi_f .$$

Since

$$(1 - G_i^+ V_i)(1 + G^+ V_i) = 1 ,$$

$\Psi_i^+$ satisfies the integral equation

$$\Psi_i^+ = \varphi_i + G_i^+ V_i \Psi_i^+ .$$

The corresponding equation for $\Psi_f^-$ is

$$\Psi_f^- = \varphi_f + G_f^- V_f \Psi_f^- .$$

It was shown in §3 that the transition amplitude for a rearrangement collision is

$$T_{if} = \langle \varphi_f | V_f | \Psi_i^{+} \rangle \qquad (2.4.2)$$

$$= \langle \Psi_f^{-} | V_i | \varphi_i \rangle . \qquad (2.4.3)$$

Use of (1) gives

$$T_{if} = \langle \varphi_f | V_f ( 1 + \mathcal{G}^{+} V_i ) | \varphi_i \rangle . \qquad (2.4.4)$$

If a transition operator T is introduced, defined by the equation

$$T = V_f + V_f \mathcal{G}^{+} V_i , \qquad (2.4.5)$$

then (4) can be written

$$T_{if} = \langle \varphi_f | T | \varphi_i \rangle ,$$

although, since $\varphi_i$ and $\varphi_f$ are not eigenfunctions of the same Hamiltonian, $T_{if}$ is not a true matrix element of T.

Since

$$( 1 + \mathcal{G}^{+} V_i )( 1 - \mathcal{G}_i^{+} V_i ) = 1 ,$$

(5) is equivalent to the integral equation

$$T = V_f + T \mathcal{G}_i^{+} V_i . \qquad (2.4.6)$$

In the calculation of the cross section for any actual process, an approximate expression for $T_{if}$ must be used since, in general, tractable expressions for integrals involving the three body Green's function $G^+$ are not available. However, using the operator identity (2.3.8), several integral equations for $G^+$ can be obtained. For example,

$$\mathcal{G}^+ = \mathcal{G}_0^+ + \mathcal{G}^+ V \mathcal{G}_0^+ \qquad (2.4.7)$$

$$= \mathcal{G}_f^+ + \mathcal{G}^+ V_f \mathcal{G}_f^+ \qquad (2.4.8)$$

$$= \mathcal{G}_i^+ + \mathcal{G}^+ V_i \mathcal{G}_i^+ . \qquad (2.4.9)$$

Iteration of these equations gives series expansions of $G^+$ in terms of the simpler operators $\mathcal{G}_0^+, \mathcal{G}_f^+$ or $\mathcal{G}_i^+$. Various Born series for $T_{if}$ can be obtained by substituting these expansions in (4). For example, use of (7) and (8) gives

$$T_{if} = \langle \varphi_f | V_f | \varphi_i \rangle + \sum_{s=0}^{\infty} \langle \varphi_f | V_f (\mathcal{G}_0^+ V)^s \mathcal{G}_0^+ V_i | \varphi_i \rangle \qquad (2.4.10)$$

$$= \langle \varphi_f | V_f | \varphi_i \rangle + \sum_{s=1}^{\infty} \langle \varphi_f | V_f (\mathcal{G}_f^+ V_f)^s | \varphi_i \rangle \qquad (2.4.11)$$

The series derived from (9) is the same as that which would be obtained by iteration of (6). The substitution in (3) of any Born series for the Green's function $G^-$ gives further Born expansions of $T_{if}$. An approximate expression for the amplitude is obtained by retaining only a finite number of terms of any of these series. In practice, the number kept is generally one, or at most two, because of the difficulty of evaluating the individual terms. The first is either $\langle \varphi_f | V_f | \varphi_i \rangle$ or $\langle \varphi_f | V_i | \varphi_i \rangle$. These expressions are called the post and prior forms of the first Born approximation respectively, and are clearly obtained by replacing the exact wave functions $\Psi_i^+, \Psi_f^-$ in (2), (3) by the unperturbed functions $\varphi_i$, $\varphi_f$. If these functions are exact, then

$$\begin{aligned} T_{if}^{B} &= \langle \varphi_f | V_i | \varphi_i \rangle = \langle \varphi_f | H_i + V_i - H_i | \varphi_i \rangle \\ &= \langle \varphi_f | H_f + V_f - H_i | \varphi_i \rangle = \langle \varphi_f | V_f | \varphi_i \rangle, \end{aligned}$$

and the so-called "post-prior" discrepancy arises only when the exact unperturbed wave functions are not known.

In this thesis, the nth term on the right hand side of an equation such as (10) will be denoted by $T_{if}^{Bn}$ and will be called the nth Born term. The nth Born approximation to $T_{if}$ is obtained by taking the sum of the first n Born terms. Clearly Born terms, and hence Born approximations, of order higher than the first, are not uniquely defined.

In practical calculations, because of the difficulty of evaluating the higher order terms, the first Born approximation is widely used. Physical arguments suggest that when the velocity of the colliding systems is large, the interaction between them does not cause much distortion, so one might expect that

$$\lim_{V \to \infty} \left( T_{if} - T_{if}^{B} \right) = 0. \qquad (2.4.12)$$

However, although it is known that the Born series for two-body potential scattering always converges for energies greater than some finite value $E_o$, and that (12) holds, no similar statement can be made for collisions involving more than two particles. In fact, Aaron, Amado and Lee (1961) suggested that for a certain class of potentials, the Born series for $T_{if}$ diverges at all energies. Their argument was as follows.

They considered a model problem in which $V_{12} = 0$. Then (4) can be written

$$T_{if} = T_{if}^{B} + \langle \varphi_f | V_{23} | \underline{k}\,\underline{K}\rangle\langle \underline{k}\,\underline{K} | G^{+} | \underline{k}'\,\underline{K}'\rangle\langle \underline{k}'\,\underline{K}' | V_{13} | \varphi_i\rangle,$$

where an integration over the intermediate momenta is implied. They used the expansion

$$\langle \underline{k}\,\underline{K} | G^{+} | \underline{k}'\underline{K}'\rangle = \sum_{s=0}^{\infty} \langle \underline{k}\,\underline{K} | \{ G_0^{+} (V_{13} + V_{23}) \}^{s} G_0^{+} | \underline{k}'\,\underline{K}'\rangle \qquad (2.4.13)$$

and considered the subseries

$$S = \sum_{s=0}^{\infty} \langle \underline{k}\,\underline{K} | (G_0^{+} V_{13})^{s} G_0^{+} | \underline{k}'\,\underline{K}'\rangle,$$

which corresponds to particle 2 propagating freely while particles 1 and 3 interact via the potential $V_{13}$. They argued convincingly that divergence of the subseries S would imply divergence of the complete series defined by (13), since the potentials $V_{13}$ and $V_{23}$ are independent, and then showed that if $V_{13}$ can support a bound state and is such that its Fourier transform is negative definite, the subseries does diverge for some range of the intermediate momenta, no matter how high the total energy.

However, the significant question is whether the integrated series

$$\sum_{s=0}^{\infty} \langle \varphi_f | V_{23} ( G_0^{+} V_{13} )^{s} G_0^{+} V_{13} | \varphi_i \rangle$$

converges. Aaron, Amado and Lee suggested that divergence of S implied divergence of this series also. However, Dettman and Leibfried (1966) considered a problem in which $V_{13}$, $V_{23}$ were one-dimensional delta-function potentials and showed that although the subseries S does diverge, nevertheless the integrated series converges at sufficiently high incident energy. Since the delta function potential belongs to the class of potentials considered by Aaron, Amado and Lee, their suggestion must be regarded as untenable.

Although their work does not prove anything conclusive about the convergence of the Born series, it does emphasise an important point. If two particles interact via a potential $V_{ij}$ which can support bound states, then for some values of the energy of the two-body system, the series expansion of the two-body scattering operator will not converge, however weak be $V_{ij}$. The kernal of the integral equation (6) for the three-body scattering operator always contains terms which correspond to one particle propagating freely while the other two interact via a two-body potential. Iteration of this equation will therefore lead to a subseries of the above form. However, it should be possible to calculate the two-body amplitudes exactly without resorting to expansions. One of the ideas behind the impulse approximation discussed in Chapter 7 is the use of the sum of two-body scattering amplitudes to approximate to the three-body amplitude, rather than a series expansion of the form (10).

## Chapter 3.

## BORN APPROXIMATIONS

### 1) The OBK approximation

The first quantum mechanical calculations of electron capture cross sections were those of Oppenheimer (1928) and Brinkman-Kramers (1930) using a simplified version of the first Born approximation which will be referred to as the OBK approximation. They argued that the interaction $V_{12}$ between the heavy particles should not have much effect on the process and therefore took for the transition amplitude

$$T_{if}^{BK} = \langle \varphi_f | V_{23} | \varphi_i \rangle \equiv \langle \varphi_f | V_{13} | \varphi_i \rangle . \qquad (3.1.1)$$

It can be shown (see Ch. 5 § 2) that, in an exact calculation, the contribution to $T_{if}$ from $V_{12}$ is of order $^1/M$ and can be neglected, but this does not justify its omission in an approximate calculation.

If initially particles 2 and 3 are bound in state $\nu\lambda\mu$ and finally particles 1 and 3 are bound in state $nlm$, then

$$T_{if}^{BK} = - G_{nlm}^{*}(-\mathbf{p})\, g_{\nu\lambda\mu}(\mathbf{q}) ,$$

where

$$G_{nlm}(\mathbf{p}) = \int d\mathbf{x} \; e^{i\mathbf{p}\cdot\mathbf{x}} \, \psi_{nlm}(\mathbf{x}) ,$$

$$g_{nlm}(\mathbf{q}) = \int d\mathbf{r} \; \frac{Z_2}{r} \, e^{i\mathbf{q}\cdot\mathbf{r}} \, \psi_{\nu\lambda\mu}(\mathbf{r}) ,$$

and $Z_1, Z_2$ are the charges of particles 1 and 2. The hydrogenic wave function $\psi_{\nu\lambda\mu}(\underset{\sim}{r})$ satisfies the Schrödinger equation

$$\left(-\frac{1}{2b}\nabla^2 - \frac{Z_2}{r} + \frac{Z_2^2}{2\nu^2}\right)\psi_{\nu\lambda\mu}(\underset{\sim}{r}) = 0.$$

Multiplying through by $e^{i\underset{\sim}{q}\cdot\underset{\sim}{r}}$ and integrating with respect to $\underset{\sim}{r}$ gives

$$g_{\nu\lambda\mu}(\underset{\sim}{q}) = \frac{1}{2b}\left(q^2 + \frac{Z_2^2}{\nu^2}\right)G_{\nu\lambda\mu}(\underset{\sim}{q}).$$

If terms of order $^1/M$ are neglected compared with unity, it can be seen from (2.3.25) that

$$q^2 + \frac{Z_2^2}{\nu^2} = p^2 + \frac{Z_1^2}{n^2}.$$

Therefore,

$$T_{if}^{BK} = -\frac{1}{2}\left(p^2 + \frac{Z_1^2}{n^2}\right)G^*_{nlm}(-\underset{\sim}{p})\,G_{\nu\lambda\mu}(\underset{\sim}{q}) \tag{3.1.2}$$

and

$$Q^{BK}(\nu\lambda\mu - nlm) = \frac{1}{4\pi^2 v^2}\int_{p^2_{min}}^{p^2_{max}} |T_{if}^{BK}|^2 \, d(p^2). \tag{3.1.3}$$

The cross section for capture from an initial state $\nu\lambda$ to a final state $nl$ is obtained by averaging over values of $\mu$ and summing over $m$. With the change of variable

$$y = p^2 + \frac{Z_1^2}{n^2}, \tag{3.1.4}$$

the result can be written

$$Q^{BK}(\nu\lambda - nl) = \frac{1}{v^2}\,D(\nu\lambda - nl)\int_\beta^\infty F(\nu\lambda - nl)\,dy \tag{3.1.5}$$

where
$$\beta = \frac{1}{4\nu^2}\left[\nu^2 + \left(\frac{Z_2}{\nu} - \frac{Z_1}{n}\right)^2\right]\left[\nu^2 + \left(\frac{Z_2}{\nu} + \frac{Z_1}{n}\right)^2\right].$$

Values of $D(\nu\lambda - nl)$ and $F(\nu\lambda - nl)$ have been given for a large number of initial and final states by Bates and Dalgarno (1953) and, for the case $Z_1 = 1$, by Hiskes (1964). His expressions are written in terms of $y$ and the function $\mathfrak{z}$, defined by

$$\mathfrak{z} = \frac{1}{y}\left(y - 2b^2\right),$$

where $b = 1/n$. The corresponding results for arbitrary $Z_1$ are obtained simply by taking $b = Z_1/n$ in the definition of $\mathfrak{z}$. Examination of the functions D and F shows that, at high energies, only capture into s states is significant, as suggested by Oppenheimer (1928).

A much simpler expression than (5) can be obtained if only the principal quantum numbers, $\nu$, $n$, of the initial and final states are specified. Then,

$$Q^{BK}(\langle\nu\rangle - \langle n\rangle) = \frac{1}{\nu^2}\sum_{\lambda=0}^{\nu-1}\sum_{\mu=-\lambda}^{\lambda}\sum_{l=0}^{n-1}\sum_{m=-l}^{l} Q^{BK}(\nu\lambda\mu - nlm). \qquad (3.1.6)$$

May (1964) gave the following sum rule for Fourier transforms:-

$$\sum_{l=0}^{n-1}\sum_{m=-l}^{l}\left| g_{nlm}(p)\right|^2 = \frac{2^6\pi Z_1^5}{n^3 y^4}, \qquad (3.1.7)$$

where y is given by (4).

Combination of (2), (3), (6) and (7) gives

$$Q^{BK}(\langle\nu\rangle - \langle n\rangle) = \frac{2^{18}(Z_1Z_2)^5}{5\nu^5 n^3}\frac{\nu^8}{\left[\nu^2 + \left(\frac{Z_2}{\nu} - \frac{Z_1}{n}\right)^2\right]^5\left[\nu^2 + \left(\frac{Z_2}{\nu} + \frac{Z_1}{n}\right)^2\right]^5}. \qquad (3.1.8)$$

Thus if $\frac{Z_1^2}{n^2}$ can be neglected in comparison with $\frac{Z_2^2}{\nu^2}$,

$$Q^{BK}\left(\langle\nu\rangle-\langle n\rangle\right) \simeq \frac{2^{18}\,(Z_1 Z_2)^5\,v^8}{5\,\nu^5 n^3\left[v^2 + Z_2^2/\nu^2\right]^{10}} . \qquad (3.1.9)$$

For symmetric resonance processes ( $\Delta E = 0$ ), $\frac{Z_1^2}{n^2} = \frac{Z_2^2}{\nu^2}$ and the above approximation cannot be made. In general however, (9) will be valid for $n \gg 1$, in which case

$$Q^{BK}\left(\langle\nu\rangle - \langle n\rangle\right) \propto {}^{1}/{}_{n^3} . \qquad (3.1.10)$$

In the majority of calculations, the target is in its ground state, $\nu = 1$, and $Q^{BK}(n)$ will be written in place of $Q^{BK}(1s-\langle n\rangle)$ when no ambiguity can arise.

Using (9), an approximate value for the total cross section $Q^{BK}(\Sigma)$ for capture from the ground state of the target into any state of the projectile may be obtained.

$$Q^{BK}(\Sigma) \simeq \sum_{n=1}^{N-1} Q^{BK}(n) + \frac{2^{18}\,(Z_1 Z_2)^5\,v^8}{5\,(v^2+Z_2^2)^{10}} \sum_{n=N}^{\infty} \frac{1}{n^3} . \qquad (3.1.11)$$

Since

$$\sum_{n=N}^{\infty} \frac{1}{n^3} = \frac{1}{2N^2} + O\left(\frac{1}{N^3}\right) ,$$

$$Q^{BK}(\Sigma) \simeq \sum_{n=1}^{N-1} Q^{BK}(n) + \frac{N}{2}\, Q^{BK}(N) .$$

The total cross section may be calculated to any required degree of accuracy from this equation.

Equation (8) shows that

$$Q^{BK}(n) \underset{v \to \infty}{\sim} \frac{2^{18}(Z_1 Z_2)^5}{5v^{12}} \cdot \frac{1}{n^3} . \qquad (3.1.12)$$

The assumption that $Q^{BK}(n)$ is proportioned to $n^{-3}$ will be referred to as use of the $n^{-3}$ rule, and (10), (12) show that it is valid at all energies for $n >> 1$, and at high energies for all $n$. If it is assumed to hold at all energies for all values of $n$, (11) may be written

$$\begin{aligned} Q^{BK}(\Sigma) &\simeq Q^{BK}(1s) + Q^{BK}(2) \sum_{n=2}^{\infty} \frac{8}{n^3} \\ &\simeq Q^{BK}(1s) + 1.616\ Q^{BK}(2) . \qquad (3.1.13) \end{aligned}$$

Total OBK cross sections computed from (13) are compared with the results of various experiments in figs (8.2.4), (8.2.5) and are clearly much too large over the entire range of the measurements.

2) <u>The work of Tuan and Gerjouy</u>.

Before 1960 there were no experimentally determined capture cross sections, $Q_A$, for the process

$$H^+ + H \to H + H^+$$

for incident proton energies greater than about 10 kev. At higher energies it was usual to compare the theoretical predictions with the experimental cross section $Q_M$ for charge transfer from hydrogen molecules,

$$H^+ + H_2 \to H + H_2^+ .$$

The comparison was based on the assumption that if the incident proton velocity is large compared with the velocities of the bound electrons, then, for the purposes of charge transfer, one hydrogen molecule is equivalent to two hydrogen atoms so that

$$Q_A = \tfrac{1}{2}Q_M .$$

In 1960, Tuan and Gerjouy investigated the effect of the molecule on electron capture. They presented a simple treatment of the problem based on the OBK approximation and their results suggested that although the assumption

$$Q_A \simeq \tfrac{1}{2}Q_M$$

may be valid for incident energies below 400 kev, this is because of the cancellation of a number of molecular effects, not because such effects are themselves unimportant. In particular they found that

i) considerable interference occurs between the capture amplitudes from the two atomic centres in the molecule. This interference is constructive for capture into the ground state of $H_2^+$ at energies below 400 kev.

ii) high velocity electrons are more likely in the tightly bound $H_2$ molecule than in the H atom and there is more likelihood of the electron being captured if it has the same velocity as the incident proton.

iii) charge transfer in atomic hydrogen can equally well leave the electron in the gerade or ungerade state, whereas in molecular hydrogen transitions to ungerade states are extremely unlikely. This fact alone would tend to make

$$Q_A^{BK} = Q_M^{BK}$$

but $Q_M$ is increased relative to $Q_A$ by effects (i) and (ii).

Tuan and Gerjouy found that when $E < 400$ kev, $Q_A \simeq \frac{1}{2}Q_M$; for $E > 400$ kev, the interference becomes destructive and $\frac{1}{2}Q_M$ can be significantly less than $Q_A$ ; finally, as $v \rightarrow \infty$ , interference effects become negligible and

$$1.2 \leq \tfrac{1}{2}Q_M / Q_A \leq 1.4 ,$$

the value depending on the molecular wave function used.

Experimentally it has been found that, at energies below 40 kev, $Q_A$ as measured by Fite et al (1958, 1960) and $Q_M$ , measured by Stier and Barnett (1956) are of comparable magnitude; at higher energies (50 - 130 kev), $Q_A$ measured by Gilbody and Ryding is consistently less than $\frac{1}{2}Q_M$ of Stier and Barnett.

### 3) The First Born Approximation.

Bates and Dalgarno (1952) and Jackson and Schiff (1953) argued that although the potential $V_{12}$ should not affect the capture cross section in an exact calculation, it should be included when any approximation is used. Since $V_{12}$ and $V_{23}$ are of opposite sign, its inclusion will decrease the cross section.

The cross section in the first Born approximation is

$$Q^{B}(\nu\lambda - nl) = \frac{1}{4\pi^2 a v^2}\int_{p^2_{min}}^{p^2_{max}} \left| T_{if}^{BK} + I^{JS} \right|^2 d(p^2), \qquad (3.3.1)$$

where $T_{if}^{BK}$ is defined by (3.1.1) and $I^{JS}$, the contribution arising from the potential $V_{12}$ is

$$I^{JS} = \langle \varphi_f \mid V_{12} \mid \varphi_i \rangle .$$

It can be written (Jackson and Schiff, 1953)

$$I^{JS} = \frac{1}{2\pi^2}\int \frac{d\underline{t}}{t^2}\, G_{\nu\lambda}(\underline{q}-\underline{t})\, G^{*}_{nl}(-\underline{p}-\underline{t}). \qquad (3.3.2)$$

When the electron is captured from the ground state of the target into the ground state of the projectile, (2) takes the form

$$I^{JS} = \frac{32(ab)^{5/2}}{\pi}\int \frac{d\underline{t}}{t^2\left[a^2+(\underline{p}+\underline{t})^2\right]^2\left[b^2+(\underline{q}-\underline{t})^2\right]^2} .$$

This integral may be evaluated using a method due to Feynman.

For the symmetric resonance process

$$H^{+} + H(1s) \longrightarrow H(1s) + H^{+}, \qquad (3.3.3)$$

$a = b$, $p^2 = q^2$, $\Delta E = 0$, and the result is

$$I^{JS} = 32a^5\pi\left[\frac{1}{T^3}\left\{\frac{a}{\omega} + \frac{(\omega-4a^2)}{2\omega^{3/2}}\tan^{-1}\frac{\omega^{1/2}}{2a}\right\} + \frac{1}{T^2}\left\{\frac{2}{\omega^{3/2}}\tan^{-1}\frac{\omega^{1/2}}{2a} - \frac{4a}{\omega(\omega+4a^2)}\right\} + \frac{2}{Ta(\omega+4a^2)^2}\right] \qquad (3.3.4)$$

where $\omega = (\underline{p}+\underline{q})^2$, $T = a^2 + p^2$.

Using the definitions of $p$ and $q$, it can be shown that

$$\omega = -\frac{1}{a(M+1)^2}\,p^2 + a v^2,$$

where $k_i = \mu v$. If terms of order $1/M$ are neglected,

$$\omega = v^2, \quad p_{min}^2 = \frac{v^2}{4}, \quad p_{max}^2 \simeq \infty .$$

Using (4), together with (3.1.2), in (1), the cross section for the resonant process (3) can be written

$$Q^B = Q^{BK}\left[\frac{1}{192}\left(127 + \frac{56}{v^2} + \frac{32}{v^4}\right) - \frac{\tan^{-1}(v/2)}{48v}\left(83 + \frac{60}{v^2} + \frac{32}{v^4}\right) + \frac{\left(\tan^{-1}(v/2)\right)^2}{24v^2}\left(31 + \frac{32}{v^2} + \frac{16}{v^4}\right)\right]. \tag{3.3.5}$$

It follows that

$$Q^B \underset{v\to\infty}{\sim} 0.661\ Q^{BK} \tag{3.3.6}$$

Mapelton (1964) was the first to point out that this result is not in fact correct. The mistake arises from replacing the exact value of $p_{max}^2$, i.e. $M^2v^2$ by the approximate value of infinity. When $p = p_{max} = Mv$, $\omega = 0$, so it is the last term of (4) which provides the major contribution to the cross section at very high energies. The contribution from this term may be written

$$Q' = \frac{2^{10}a^7}{v^2}\int_{\frac{1}{4}v^2}^{M^2v^2}\frac{d(p^2)}{T^2\,(T')^4}, \tag{3.3.7}$$

where $T' = w + 4a^2$.

The integral may be evaluated to give

$$\frac{1}{a^5(4a+v^2+R^2)^5}\left[-\frac{T'}{T}+\frac{4R^2}{a}\ln\left|\frac{T'}{T}\right|+\frac{6R^4T}{aT'}+\frac{4R^6T^2}{2b^3(T')^2}+\frac{R^8T^3}{3a^4(T')^3}\right]_{\frac{1}{4}v^2}^{M^2v^2},$$

where $R = \frac{1}{M+1}$.

At high energies, the dominant term in this expression is the last one, and

$$Q' \underset{v\to\infty}{\sim} \frac{16}{3M^2}\cdot\frac{1}{v^6},$$

where $v^2$ is the energy of the incident proton measured in units of 25 kev. All other contributions to $Q^B$ tend to zero at least as fast as $v^{-12}$, so

$$Q^B \underset{v\to\infty}{\sim} \frac{16}{3M^2}\cdot\frac{1}{v^6}. \qquad (3.3.8)$$

This result has been derived here for the resonant capture process (3) but it can be shown that the important point is that $M_1 = M_2$, not that the energy defect is zero.

The previous discussion has ignored the fact that the incident proton and the target nucleus are indistinguishable. If hydrogen atoms are formed by capture in the backward direction, the ejected protons move in the direction of the incident beam, and cannot be separated from those particles which have been elastically scattered. Thus, for practical purposes, the cross section ceases to be defined at energies where the backward contribution is important.

For transitions other than capture into the ground state, the evaluation of $I^{JS}$ in closed form is extremely difficult. Jackson and Schiff used some numerical integration to obtain cross sections for capture into 2s and 2p. They showed that the ratio $Q^{B}(nl)/Q^{B}(1s)$ for nl = 2s, 2p was very similar to the corresponding ratio $Q^{BK}(nl)/Q^{BK}(1s$ They therefore postulated that the ratio $R = \frac{Q^{B}(nl)}{Q^{BK}(nl)}$ was almost independent of the final state and that Born cross sections could be obtained from the relationship

$$Q^{B}(nl) = \frac{Q^{B}(1s)}{Q^{BK}(1s)}\, Q^{BK}(nl). \qquad (3.3.9)$$

Using this expression, Bates and Dalgarno (1953) calculated cross sections for capture into final states

nl = 1s, 2s, 3s, 4s, 2p, 3p, 4p, 3d, 4d and 4f.

Mapleton (1962) calculated the ratio R for nl = 1s, 2s, 2p, 3s, 3p, 4s,5s His results, which are given in Table (1) show that it is in fact almost independent of the final state. Therefore the results of Bates and Dalgarno provide a good estimate of the true Born cross sections except at very low energies. Indeed, at energies above 150 kev their results are in good agreement with the exact values given by Mapleton.

The only experiments for capture into a single state of the projectile which are available for comparison purposes are those of Stebbings et al (1965) for the process

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

and of Bayfield (1968) and Ryding et al (1966) for the process

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

In order to compare theoretical predictions with the results of other experiments, some method of estimating the total cross section for capture into all excited states of the projectile must be found.

For the Born approximation, Jackson and Schiff used (9) for this purpose. They argued that since $Q^{BK}(n)$ is proportional to $n^{-3}$ at high energies, then so is $Q^{B}(n)$. They therefore took

$$\begin{aligned} Q^{B}(\Sigma) &= Q^{B}(1s)\left(1 + \frac{Q^{B}(2)}{Q^{B}(1s)} \sum_{n=2}^{\infty} \frac{8}{n^{3}}\right) \\ &\simeq Q^{B}(1s)\left(1 + 1.616\,\frac{Q^{B}(2)}{Q^{B}(1s)}\right). \end{aligned} \qquad (3.3.10)$$

However, fig (8.2.3) shows that the ratios $Q^{B}(n)\,/\,Q^{B}(1s)$ for $n = 2, 3$ approach their limiting value $n^{-3}$ very slowly as the energy increases and (10) considerably underestimates the true cross section at low and intermediate energies. A better estimate is obtained by using (9) to write

$$Q^{B}(\Sigma) = Q^{B}(1s) + \frac{Q^{B}(1s)}{Q^{BK}(1s)} \sum_{n=2}^{\infty} Q^{BK}(n).$$

Schiff (1954) used the first Born approximation to calculate cross sections for the processes

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

In fig (1), values of the ratio

$$R^{B}(2) = Q^{B}(2) / Q^{B}(1s)$$

taken from fig (3) of his paper are compared with the corresponding ratio given by the OBK approximation. At low energies the values given by the two approximations differ considerably. This is not surprising because for capture from the ground state of hydrogen into a state of $He^{+}$ with $n = 2$, the energy defect is zero, and the cross sections are very large at low energies. For proton impact on hydrogen in its ground state, the resonant transition is capture into the 1s state, and it is found that (9) provides a good estimate of the Born cross sections for all values of nl. Schiff therefore suggested that, for alpha particle impact, the following relation should be used in place of (9);

$$Q^{B}(n) = \frac{Q^{B}(2)}{Q^{BK}(2)} Q^{BK}(n) \; , \qquad n > 2.$$

Then the total capture cross section is

$$Q^{B}(\Sigma) = Q^{B}(1s) + Q^{B}(2) + \frac{Q^{B}(2)}{Q^{BK}(2)} \sum_{n=3}^{\infty} Q^{BK}(n).$$

Schiff was working before the sum rule of May was known, so used the $n^{-3}$

rule to evaluate $\sum_{n=3}^{\infty} Q^{BK}(n)$. From (3.1.8) it can be seen that $Q^{BK}(n)\,/\,Q^{BK}(2)$ varies considerably with energy before attaining its asymptotic value $\left(\frac{2}{n}\right)^3$, so Schiff wrote

$$Q^{B}(\Sigma) = Q^{B}(1s) + Q^{B}(2) + \frac{Q^{B}(2)}{Q^{BK}(2)}\, Q^{BK}(3) \sum_{n=3}^{\infty} \frac{27}{n^3}$$

$$\simeq Q^{B}(1s) + Q^{B}(2) + 2.1\, Q^{B}(2)\, \frac{Q^{BK}(3)}{Q^{BK}(2)} \,. \qquad (3.3.11)$$

## Table 3.3.1

The ratio $Q^B/Q^{BK}$ for $H^+ + H\,(1s) \rightarrow H(nl) + H^+$ obtained from the results of Mapleton (1962). E is the energy of the incident proton in kev.

| E<br>$nl$ | 63.24 | 112.46 | 200 | 355.6 | 632.4 | 1124.6 | 2000 |
|---|---|---|---|---|---|---|---|
| 1s | 0.162 | 0.190 | 0.228 | 0.274 | 0.327 | 0.382 | 0.431 |
| 2s | 0.145 | 0.170 | 0.210 | 0.261 | 0.317 | 0.375 | 0.430 |
| 3s | 0.144 | 0.167 | 0.207 | 0.259 | 0.315 | 0.375 | 0.427 |
| 4s | 0.144 | 0.166 | 0.207 | 0.258 | 0.316 | 0.373 | 0.425 |
| 5s | 0.144 | 0.165 | 0.206 | 0.258 | 0.316 | 0.375 | 0.426 |
| 2p | 0.146 | 0.181 | 0.227 | 0.278 | 0.333 | 0.385 | 0.433 |
| 3p | 0.139 | 0.173 | 0.221 | 0.274 | 0.330 | 0.384 | 0.424 |
| 2s+2p | 0.146 | 0.174 | 0.215 | 0.264 | 0.319 | 0.376 | 0.430 |
| 3s+3p | 0.141 | 0.170 | 0.212 | 0.262 | 0.324 | 0.375 | 0.427 |

## Table 3.3.2.

OBK cross sections, in units of $\pi a_0^2$, calculated by Mapleton (1962)

| Energy (kev) | Q(1s) | Q(2s) | Q(2p) | Q(3s) | Q(3p) |
|---|---|---|---|---|---|
| 63.24 | 1.75 | 3.04,-1 | 3.45,- 1 | 9.50,-2 | 1.20,- 1 |
| 112.5 | 2.63,-1 | 4.68,-2 | 3.28,- 2 | 1.48,-2 | 1.19,- 2 |
| 200 | 2.64,-2 | 4.42,-3 | 1.80,- 3 | 1.38,-3 | 6.57,- 4 |
| 355.6 | 1.84,-3 | 2.83,-4 | 6.58,- 5 | 8.72,-5 | 2.38,- 5 |
| 632.4 | 9.62,-5 | 1.38,-5 | 1.81,- 6 | 4.19,-6 | 6.48,- 7 |
| 1125 | 4.14,-6 | 5.62,-7 | 4.16,- 8 | 1.69,-7 | 1.48,- 8 |
| 2000 | 1.57,-7 | 2.06,-8 | 8.59,-10 | 6.16,-9 | 3.09,-10 |

## Table 3.3.3.

Born cross sections, in units of $\pi a_0^2$, calculated by Mapleton (1962)

| Energy (kev) | Q(1s) | Q(2s) | Q(2p) | Q(3s) | Q(3p) |
|---|---|---|---|---|---|
| 63.24 | 2.84,-1 | 4.42,-2 | 5.03,-2 | 1.37,-2 | 1.67, -2 |
| 112.5 | 5.00,-2 | 7.94,-3 | 5.93,-3 | 2.47,-3 | 2.07,- 3 |
| 200 | 6.01,-3 | 9.27,-4 | 4.08,-4 | 2.86,-4 | 1.45,- 4 |
| 355.6 | 5.04,-4 | 7.38,-5 | 1.83,-5 | 2.26,-5 | 6.52,- 6 |
| 632.4 | 3.15,-5 | 4.38,-6 | 6.02,-7 | 1.32,-6 | 2.14,- 7 |
| 1125 | 1.58,-6 | 2.11,-7 | 1.60,-8 | 6.33,-8 | 5.68,- 9 |
| 2000 | 6.77,-8 | 8.86,-9 | 3.72,-10 | 2.63,-9 | 1.31,-10 |

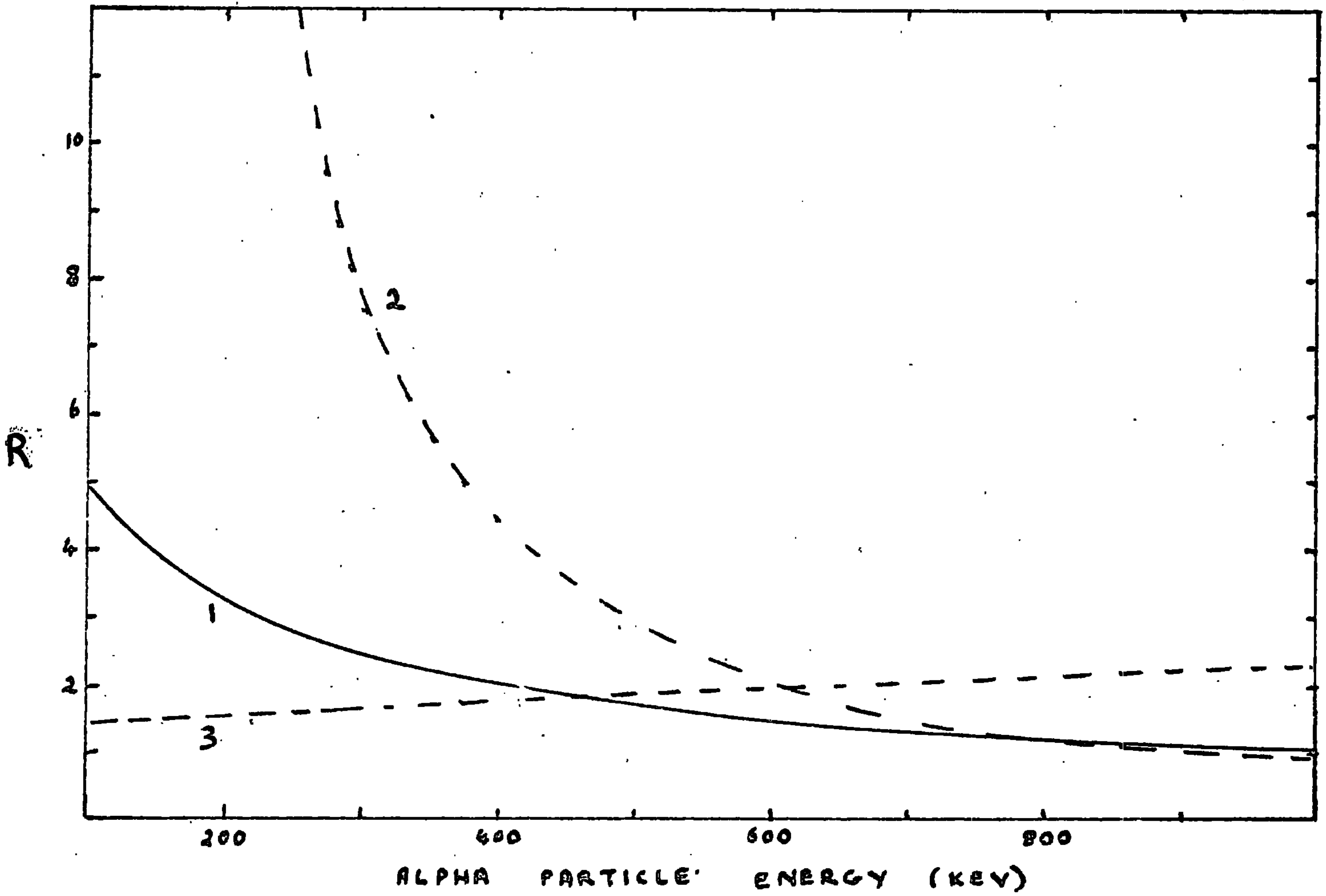


Fig 3.3.1. Cross section ratios for alpha particle impact.

Curve 1 ; $R_2^B = \frac{Q^B(2)}{Q^B(1s)}$ ; Curve 2; $R_2^{BK} = \frac{Q^{BK}(2)}{Q^{BK}(1s)}$

Curve 3 ; $R_3^{BK} = \frac{Q^{BK}(2)}{Q^{BK}(3)}$

4) Higher Born approximations.

No numerical calculations of capture cross sections have been carried out keeping more than one term of the Born series, but some work has been done on the high energy behaviour of the cross section. Drisko (1955) considered the process

$$H^{+} + H\,(1s) \rightarrow H\,(1s) + H^{+}.$$

He used the form of the Born series obtained by expanding the total Green's function $\mathcal{G}^{+}$ in terms of the free particle operator $\mathcal{G}_0^{+}$ (see (2.4.10)). The second Born term can then be written

$$T_{if}^{B2} = I(V_{12}, V_{12}) + I(V_{12}, V_{13}) + I(V_{23}, V_{12}) + I(V_{23}, V_{13}),$$

where $$I(U, V) \equiv \langle \varphi_f \,|\, U \mathcal{G}_0^{+} V \,|\, \varphi_i \rangle, \qquad (3.4.1)$$

and the third Born term is

$$T_{if}^{B3} = \langle \varphi_f \,|\, V_f \mathcal{G}_0^{+} V \mathcal{G}_0^{+} V_i \,|\, \varphi_i \rangle.$$

An excellent account of Drisko's work is available in the book by Coleman and McDowell (1969), and here only the results will be given. Drisko neglected terms of order $^1/_M$, and found that, at high energies,

$$I^{JS} + I(V_{23}, V_{12}) + I(V_{12}, V_{13}) \simeq 0,$$

so the Jackson-Schiff matrix element, which is so important in the first Born approximation is cancelled. He showed further that $I(V_{12}, V_{12})$

could be neglected compared with the other remaining terms so, in the second Born approximation, the internuclear potential plays no part (in the limit $1/M$ tends to zero). Thus,

$$T_{if}^{B} + T_{if}^{B2} \underset{v \to \infty}{\sim} T_{if}^{BK} + I(V_{23}, V_{13}),$$

where $v$ is the velocity of the incident particle, giving

$$Q^{B2} \underset{v \to \infty}{\sim} \left(0.2946 + \frac{5\pi v}{2^{12}}\right) Q^{BK}.$$

It can be shown that the $v^{-11}$ dependence comes entirely from the term $I(V_{23}, V_{13})$.

It is interesting to compare a classical calculation. The matrix element $I(V_{23}, V_{13})$ corresponds to two separate two-body collisions, the first between particles 1 and 3, and the second between 2 and 3. If 1, 2 and 3 are considered to be classical particles, the collisions can be treated using classical mechanics. The classical scattering angle is determined by the principles of conservation of energy and momentum and the additional requirements that, before either collision has taken place, particles 2 and 3 have zero relative velocity, and that finally 1 and 3 move together. These ideas were used by Thomas (1927) in his classical treatment of electron capture. He found that his cross section was of order $v^{-11}$ as $v$ tended to infinity.

Drisko also examined the third Born term $T_{if}^{B3}$. He ignored all terms involving $V_{12}$ and found that no new terms in $v^{-11}$ arise but the coefficient of $v^{-12}$ is altered. He estimated that

$$Q^{B3} \underset{v \to \infty}{\sim} \left(0.319 + \frac{5\pi v}{2^{12}}\right) Q^{BK}.$$

Drisko did not obtain the $v^{-6}$ dependence of Mapleton because when terms of order $^1/M$ are neglected, back scattering does not contribute to the cross section.

Mapleton (1967) considered the second Born term obtained by using the expansion of $\mathcal{G}^+$ in terms of $\mathcal{G}_f^+$ (see (2.4.10)). This gives

$$T_{if}^{B2} = \langle \varphi_f \mid V_f \mathcal{G}_f^+ V_i \mid \varphi_i \rangle .$$

His work indicates that the two forms of the second Born approximation predict the same high energy behaviour for the cross section, but, because of the approximations he was forced to make, the work cannot be regarded as conclusive. The difficulties he encountered are similar to those occurring in the analysis of Chapter 9.

## Chapter 4.

## DISTORTED WAVE APPROXIMATIONS.

### 1) Derivation of the transition amplitude.

The idea behind the distorted wave approach is to take exact account of the major part of the interaction potential so that the remainder may be regarded as a small perturbation. For example, suppose that the total Hamiltonian $H$ can be written

$$H = \hat{H} + \hat{V},$$

where $\hat{H}$ has the same kinetic energy terms as $H$, and that the transition amplitude for collisions governed by $\hat{H}$ can be obtained exactly. An expression for the difference between this and the required amplitude can be derived as follows.

It was shown in Chapter 2 that the exact amplitude for transitions governed by $H$ can be written

$$T_{if} = \langle \varphi_f | V_f | \Psi_i^+ \rangle = \langle \varphi_f | H - H_f | \Psi_i^+ \rangle, \qquad (4.1.1)$$

where $$\Psi_i^+ = \left( 1 + \frac{1}{E - H + i\epsilon} (H - H_i) \right) \varphi_i . \qquad (4.1.2)$$
(See (2.3.18), (2.4.1)).

Let $$\hat{T}_{if} = \langle \varphi_f | \hat{H} - H_f | \chi_i^+ \rangle,$$
where
$$\chi_i^+ = \varphi_i + \frac{1}{E - \hat{H} + i\epsilon} (\hat{H} - H_i) \varphi_i . \qquad (4.1.3)$$

Use of the operator identify (2.3.8) gives

$$\frac{1}{E - \hat{H} + i\epsilon} = \frac{1}{E - H + i\epsilon} \left( 1 + (H - \hat{H}) \frac{1}{E - \hat{H} + i\epsilon} \right). \qquad (4.1.4)$$

From (2), (3), (4), it can be shown that

$$\Psi_i^+ = \chi_i^+ + \frac{1}{E - H + i\epsilon} (H - \hat{H}) \chi_i^+ .$$

Then

$$T_{if} = \langle \varphi_f | H - H_f | \chi_i^+ \rangle + \langle \varphi_f | \left\{ 1 + (H - H_f) \frac{1}{E - H + i\epsilon} \right\} (H - \hat{H}) | \chi_i^+ \rangle$$

$$= \langle \varphi_f | \hat{H} - H_f | \chi_i^+ \rangle + \langle \Psi_f^- | H - \hat{H} | \chi_i^+ \rangle . \qquad (4.1.5)$$

where (2.3.17) has been used in the last step. Similarly, by starting from the alternative form of $T_{if}$, one obtains

$$T_{if} = \langle \chi_f^- | \hat{H} - H_i | \varphi_i \rangle + \langle \chi_f^- | H - \hat{H} | \Psi_i^+ \rangle . \qquad (4.1.6)$$

Now suppose that

$$\begin{aligned} H &= H_i + V_i &&= H_i + U_i + W_i \\ &= H_f + V_f &&= H_f + U_f + W_f , \end{aligned}$$

where $H_i, H_f$ are the initial and final unperturbed Hamiltonians of the system and the distorting potentials $U_i, U_f$ are such that $W_i, W_f$ fall off more rapidly than $r^{-1}$ as $r \to \infty$, but are otherwise arbitrary. First, take $\hat{H} = H_i + U_i$. Then (5) becomes

$$T_{if} = \langle \varphi_f | V_f - W_i | \chi_i^+ \rangle + \langle \Psi_f^- | W_i | \chi_i^+ \rangle , \qquad (4.1.7)$$

and from (3) it can be seen that

$$\chi_i^+ = \left( 1 + \frac{1}{E - H_i - U_i + i\epsilon} U_i \right) \varphi_i . \qquad (4.1.8)$$

Secondly, let $\hat{H} = H_f + U_f$, and denote the distorted wave functions by $\zeta_f^{\pm}$ to avoid confusion. Then (6) gives

$$T_{if} = \langle \zeta_f^- | V_i - W_f | \varphi_i \rangle + \langle \zeta_f^- | W_f | \Psi_i^+ \rangle , \qquad (4.1.9)$$

where

$$\zeta_f^- = \left( 1 + \frac{1}{E - H_f - U_f - i\epsilon} U_f \right) \varphi_f .$$

It is possible, by a suitable choice of the distorting potentials $U_i, U_f$ to simplify the exact expressions (7), (9) somewhat. For example, consider the term $\langle \varphi_f | V_f - W_i | \chi_i^+ \rangle$. Use of (3), with $\hat{H} = H_i + U_i$, and the relation

$$\langle \varphi_f | V_f | \varphi_i \rangle = \langle \varphi_f | V_i | \varphi_i \rangle$$

gives

$$\begin{aligned} \langle \varphi_f | V_f - W_i | \chi_i^+ \rangle &= \langle \varphi_f | (V_f - W_i) \left( 1 + \frac{1}{E - H_i - U_i + i\epsilon} U_i \right) | \varphi_i \rangle \\ &= \langle \varphi_f | \left( 1 + (V_f - W_i) \frac{1}{E - H_i - U_i + i\epsilon} \right) U_i | \varphi_i \rangle \\ &= i\epsilon \left( \langle \varphi_f | \chi_i^+ \rangle - \langle \varphi_f | \varphi_i \rangle \right). \end{aligned}$$

But $\langle \varphi_f | \varphi_i \rangle$ is finite if $\varphi_i \neq \varphi_f$, and therefore

$$\lim_{\epsilon \to 0+} \langle \varphi_f | V_f - W_i | \chi_i^+ \rangle = 0$$

provided that

$$\lim_{\epsilon \to 0+} i\epsilon \langle \varphi_f | \chi_i^+ \rangle = 0. \qquad (4.1.10)$$

If $U_i$ is chosen to depend only on the relative coordinate $\underline{r}$, then it cannot lead to rearrangement and condition (10) is satisfied. Similarly, if $U_f$ is chosen such that

$$\lim_{\epsilon \to 0+} i\epsilon \langle \zeta_f^- | \varphi_i \rangle = 0 \qquad (4.1.11)$$

then the first term of (9) vanishes. Thus, if conditions (10) and (11) are satisfied,

$$T_{if} = \langle \Psi_f^- | W_i | \chi_i^+ \rangle \qquad (4.1.12)$$

$$= \langle \zeta_f^- | W_f | \Psi_i^+ \rangle. \qquad (4.1.13)$$

It can be shown that the expressions obtained by replacing the exact wave functions $\Psi_f^-, \Psi_i^+$ by the distorted waves $\zeta_f^-, \chi_i^+$ are equal. They give the distorted wave Born approximation to $T_{if}$.

Thus

$$T_{if}^{DWB} = \langle \zeta_f^- \,|\, W_i \,|\, \chi_i^+ \rangle \tag{4.1.14}$$

$$= \langle \zeta_f^- \,|\, W_f \,|\, \chi_i^+ \rangle. \tag{4.1.15}$$

It was shown in Chapter 2 that (1) can be written

$$T_{if} = \langle \varphi_f \,|\, T \,|\, \varphi_i \rangle,$$

where the transition operator $T$ is defined by the equation

$$T = V_f + V_f \mathcal{G}^+ V_i$$

and satisfies the integral equation

$$T = V_f + T \mathcal{G}_i^+ V_i .$$

Similarly, a distorted wave operator $T^{DW}$ can be defined such that

$$T_{if} = \langle \zeta_f^- \,|\, W_f \,|\, \Psi_i^+ \rangle = \langle \zeta_f^- \,|\, T^{DW} \,|\, \chi_i^+ \rangle.$$

Since

$$\Psi_i^+ = (1 + \mathcal{G}^+ W_i)\, \chi_i^+,$$

it follows that

$$T^{DW} = W_f + W_f \mathcal{G}^+ W_i . \tag{4.1.16}$$

Furthermore, since

$$(1 + \mathcal{G}^+ W_i)\left(1 - \frac{1}{E - H_i - U_i + i\epsilon} W_i\right) = 1,$$

$T^{DW}$ satisfies the integral equation

$$T^{DW} = W_f + T^{DW} \frac{1}{E - H_i - U_i + i\epsilon} W_i . \tag{4.1.17}$$

Various distorted wave Born series may be obtained by expanding the operator $\mathcal{G}^+$ in (16) in terms of simpler operators. In each case, the first term will be

$$T_{if}^{DWB} = \langle \zeta_f^- | W_f | \chi_i^+ \rangle .$$

Greider and Dodd (1966) were the first to consider the convergence of such series. They pointed out that the same difficulties arise as in the case of undistorted waves because of the presence in the kernel of the integral equation (17) of terms corresponding to states where one particle propagates freely while the other two interact via a two-body potential.

In a later paper, Dodd and Greider (1966) proposed a method of removing the disconnected part of the kernel, thereby obtaining a new integral equation for $T^{DW}$. They introduced a completely arbitrary potential $V_x$, with the corresponding Green's function operator

$$g_x^+ = \frac{1}{E - H + V_x + i\epsilon} .$$

Use of the operator identity (2.3.8) gives

$$\mathcal{G}^+ = ( 1 + \mathcal{G}^+ V_x ) g_x^+ .$$

Using this relation, (16) may be written

$$T^{DW} = W_f + W_f g_x^+ W_i + W_f \mathcal{G}^+ V_x g_x^+ W_i .$$

But

$$W_f \mathcal{G}^+ = T^{DW} \frac{1}{E - H_i - U_i + i\epsilon} .$$

Therefore

$$T^{DW} = W_f + W_f g_x^+ W_i + T^{DW} \frac{1}{E - H_i - V_i + i\epsilon} V_x g_x^+ W_i . \qquad (4.1.18)$$

This equation has kernel $\frac{1}{E - H_i - U_i + i\epsilon} V_x g_x^+ W_i$, in which $V_x$ is completely arbitrary. If it is chosen so that it acts on any particle not affected by $W_i$, then the kernel is connected and iteration of (18) should provide a meaningful series of approximations to the scattering amplitude. The first approximation is

$$T_{if}^{I} = \langle \zeta_f^- | W_f + W_f g_x^+ W_i | \chi_i^+ \rangle . \qquad (4.1.19)$$

As an example, suppose that the distorting potential $U_i$ is zero. Then (18) becomes

$$T^{DW} = W_f + W_f g_x^+ V_i + T G_i^+ V_x g_x^+ V_i . \qquad (4.1.20)$$

Since $V_i = V_{12} + V_{13}$, the kernel of this equation can be split into two parts

$$K_2 = G_i^+ V_x g_x^+ V_{12} , \quad K_3 = G_i^+ V_x g_x^+ V_{13} ,$$

and both parts are made connected by the choice $V_x = V_{23}$. Then (19) becomes

$$T_{if}^{I} = \langle \zeta_f^- | W_f + W_f \frac{1}{E - H_0 - V_i + i\epsilon} V_i | \phi_i \rangle . \qquad (4.1.21)$$

The high energy behaviour of this matrix element is discussed in Chapter 9.

## 2) Applications of the distorted wave method to rearrangement collisions.

Bassel and Gerjouy (1960) were the first to use the distorted wave method for rearrangement collisions. They considered the reaction

$$H^+ + H\,(1s) \rightarrow H\,(1s) + H^+ , \qquad (4.2.1)$$

and chose for the distorting potential $U_i$ the average static interaction in the initial state,

$$U_i = \int d\underline{r} \; |\psi_i(\underline{r})|^2 \; V_i(\underline{r}, \underline{s}) .$$

This choice ensures that $U_i$ depends only on $\underline{s}$, and also means that the internuclear potential $V_{12}$ almost disappears from the potential $W_i = V_i - U_i$. The exact transition amplitude $T_{if}$ is given by (4.1.12) and the first order approximation by (4.1.14). The distorting potential $U_f$ occurring in the definition of the function $\zeta_f^-$ is completely arbitrary and was chosen to be

$$U_f = \int d\underline{x} \; |\psi_f(\underline{x})|^2 \; V_f(\underline{x}, \underline{\rho}) .$$

However, with these choices, (4.1.8), (4.1.10) cannot be solved exactly and Bassel and Gerjouy replaced the distorted waves $\chi_i^+$, $\zeta_f^-$ in (4.1.14) by the undistorted ones $\varphi_i$, $\varphi_f$, although they retained the potential $W_i = V_i - U_i$. However, $U_i$ appears in the equation just because distorted waves have been used and there is no justification for retaining it when they are replaced by plane waves. Thus, from a theoretical point of view, the Bassel-Gerjouy approximation is no more satisfactory than the OBk or Born ones. Cross sections for process (1), calculated from the matrix element

$$T_{if}^{BG} = \langle \varphi_f \,|\, V_i - U_i \,|\, \varphi_i \rangle$$

are given in table (1), labelled $Q^{BG}$.

Grant and Shapiro (1965) attempted to improve the method by using more exact expressions for $\chi_i^+$, $\zeta_f^-$. If the Green's function $(E - H_i - U_i + i\epsilon)^{-1}$ appearing in (4.1.8) is expanded in terms of $U_i$, then the first term in an iterative solution of the equation is

$$\chi_i^+ = (1 + G_i^+ U_i)\, \varphi_i .$$

Similarly, one obtains

$$\zeta_f^- = (1 + G_f^- U_f)\, \varphi_f .$$

These are the distorted wave functions used by Grant and Shapiro. Their transition amplitude is obtained by substituting in (4.1.14) and keeping only terms of first and second order in the potentials. Thus,

$$T_{if}^{GS} = T_{if}^{BG} + 2 \langle \varphi_f | V_f - U_f | G_i^+ U_i \varphi_i \rangle .$$

Results for process (1) obtained using this expression are given in table (1) denoted by $Q^{GS}$. It can be seen that $Q^{GS} > Q^{BG}$ at all energies.

In the work of both Bassel and Gerjouy, and Grant and Shapiro, some terms of order $^1/M$ were neglected, and it was found that

$$Q^{BG} \underset{V \to \infty}{\sim} Q^{BK} , \qquad Q^{GS} \underset{V \to \infty}{\sim} Q^{BK} .$$

Mapleton (1964) considered the high energy form of the cross section obtained by using $T_{if}^{BG}$, with the exact value of the potential $V_i - U_i$, not the value obtained by letting $^1/M$ tend to 0, and found that it was the same as that of $Q^B$.

A different form of distorted wave has been used by McCarroll and Salin (1967a) to discuss process (1). If the exact wave function is written

$$\Psi_i^+ = \psi_{1s}(\underline{r})\, \mathcal{G}(\underline{x}, \underline{\rho}),$$

it can be shown that $\mathcal{G}(\underline{x}, \underline{\rho})$ satisfies

$$\left( -\frac{1}{2\mu} \nabla_\rho^2 - \frac{1}{2b} \nabla_r^2 - \frac{1}{x} + \frac{1}{\rho} - E + \epsilon_i \right) \mathcal{G}(\underline{x}, \underline{\rho})$$

$$= \left( -\frac{1}{R} + \frac{1}{\rho} - \frac{1}{b} \underline{\nabla}_r \ln \psi_{1s} \cdot \underline{\nabla}_r \ln \mathcal{G} \right) \mathcal{G}(\underline{x}, \underline{\rho}). \qquad (4.2.2)$$

The distorted wave in the initial state was chosen to be

$$\chi_i^+ = \psi_{1s}(\underline{r})\, g_i(\underline{x}, \underline{\rho})$$

where $g_i(\underline{x}, \underline{\rho})$ is the solution of (2) with the right hand side neglected, and boundary conditions

$$g_i(\underline{x}, \underline{\rho}) \underset{x \to \infty}{\sim} \exp(i\, \underline{k}_i \cdot \underline{\rho}) .$$

The distorting potential $U_i$ is defined by the equation

$$(H_i + U_i - E)\, \chi_i^+ = 0 ,$$

and is easily seen to be

$$U_i = -\frac{1}{x} + \frac{1}{\rho} + \frac{1}{a} \underline{\nabla}_r (\ln \psi_{1s}) \cdot \underline{\nabla}_r (\ln g_i) .$$

The exact transition amplitude is given by (4.1.7)

$$T_{if} = \langle \varphi_f | V_f - W_i | \chi_i^+ \rangle + \langle \Psi_f^- | W_i | \chi_i^+ \rangle .$$

Since $\varphi_f$ and $\chi_i^+$ both contain bound state functions, the surface terms arising in the application of Green's theorem to the first term vanish and this term is

$$\langle \varphi_f | V_f - V_i + U_i | \chi_i^+ \rangle = \langle \varphi_f | V_f - V_i + E - H_i | \chi_i^+ \rangle$$

$$= \langle \varphi_f | E - H_f | \chi_i^+ \rangle$$

$$= 0 .$$

The first order distorted wave approximation is obtained by replacing the exact wave function $\Psi_f^-$ by the distorted wave $\zeta_f^- = \psi_f(\underline{x})\, g_f(\underline{r}, \underline{\rho})$ which is a solution of the equation

$$(H_f + U_f - E)\, \zeta_f^- = 0 ,$$

where

$$U_f = -\frac{1}{r} + \frac{1}{\rho} - \frac{1}{b} \underline{\nabla}_x \ln \psi_f \cdot \underline{\nabla}_x g_f .$$

Finally, if terms of order $^1/M$ are neglected,

$$W_i = V_i - U_i = \underline{\nabla}_r \ln \psi_{1s} \cdot \underline{\nabla}_r \ln g_i = \frac{\underline{r}}{r} \cdot \underline{\nabla}_r \ln g_i ,$$

and

$$T_{if}^{DWB} = \left\langle \zeta_f^- \,\middle|\, \frac{\underline{r}}{r} \cdot \underline{\nabla}_r \ln g_i \,\middle|\, \chi_i^+ \right\rangle . \qquad (4.2.3)$$

No calculations have been reported using this equation. As pointed out by McCarroll and Salin, the approximation is the quantal equivalent of the continuum distorted wave approximation of Cheshire (1964) (see Chapter 6 § 2), and therefore has the same high energy behaviour as Drisko's second Born approximation.

## Chapter 5.

## IMPACT PARAMETER METHODS

### 1) Introduction.

Because the masses $M_1$, $M_2$ are much larger than the mass of the electron, the de Broglie wavelength associated with the relative motion of particles 1 and 2 is much smaller than the atomic unit of length. This motion may therefore be treated classically. Furthermore, Bates and Boyd (1962) showed that the motion is approximately rectilinear with constant relative velicity $\underline{v}$. These simplifications are used in the impact parameter methods.

The notation used in the present section is slightly different from that used previously. Let $\underline{r}_1, \underline{r}_2, \underline{r}$ denote the coordinates of the electron with respect to particles 1, 2 and 0, the centre of the internuclear line. Bates and McCarroll (1958) showed that the results obtained do not depend on the position of 0 on this line, but the present choice is made to simplify the analysis. Particle 1 moves along a straight line with constant velocity $\underline{v} = \frac{\partial \underline{R}}{\partial t}$, past the nucleus 2 which is regarded as fixed. Thus the distance of closest approach of the two heavy particles is equal to the impact parameter $\rho$. If the origin of time is chosen to be the instant of closest approach, then $\underline{R} = \underline{\rho} + \underline{v}\,t$, where, as before, $\underline{R}$ is the position vector of particle 1 with respect to particle 2.

The exact electronic wave function $\Psi(\underline{r}, t)$ which describes the motion of the electron in the field of the two nuclei satisfies the time dependent Schrödinger equation

$$\mathcal{H}_e \, \Psi(\underline{r},t) = i \frac{\partial}{\partial t} \Psi(\underline{r},t) \qquad (5.1.1)$$

where

$$\mathcal{H}_e = -\tfrac{1}{2} \nabla_r^2 + V_{13}(\underline{r}_1) + V_{23}(\underline{r}_2), \qquad (5.1.2)$$

If $\psi_n^{(1)}(\underline{r}_1)$, $\psi_m^{(2)}(\underline{r}_2)$ denote the eigenfunctions of the electron in the field of particle 1 or 2 repsectively, and $\epsilon_n^{(1)}$, $\epsilon_m^{(2)}$ the corresponding eigenenergies then

$$\left( -\frac{1}{2} \nabla_1^2 + V_{13}(\underline{r}_1) - \epsilon_n^{(1)} \right) \psi_n^{(1)}(\underline{r}_1) = 0$$

and $$\left( -\frac{1}{2} \nabla_2^2 + V_{23}(\underline{r}_2) - \epsilon_m^{(2)} \right) \psi_m^{(2)}(\underline{r}_2) = 0.$$

The exact wave function $\Psi(\underline{r},t)$ may be expanded in either of the following ways:-

$$\Psi(\underline{r},t) = \sum_n b_n(t) \, \Phi_n^{(1)}(\underline{r}_1,t) \qquad (5.1.3)$$

$$= \sum_m a_m(t) \, \Phi_m^{(2)}(\underline{r}_2,t) \qquad (5.1.4)$$

where

$$\Phi_n^{(1)}(\underline{r}_1,t) = \psi_n^{(1)}(\underline{r}_1) \exp\left( \tfrac{1}{2} i \underline{v}.\underline{r} - \tfrac{1}{8} i v^2 t - i \epsilon_n^{(1)} t \right), \qquad (5.1.5)$$

$$\Phi_m^{(2)}(\underline{r}_2,t) = \psi_m^{(2)}(\underline{r}_2) \exp\left( -\tfrac{1}{2} i \underline{v}.\underline{r} - \tfrac{1}{8} i v^2 t - i \epsilon_m^{(2)} t \right). \qquad (5.1.6)$$

The extra exponential terms allow for the translational motion of the electron and ensure that each term of the expansion (3) or (4) is a solution of (1) in the limit of infinite nuclear separation (if terms of order $^1/M$ are neglected.) In this connection, it should be noted that the time differentiation in (1) is to be carried out keeping $\underline{r}$ constant, not $\underline{r}_1$ or $\underline{r}_2$. Since

$$\underline{r}_1 = \underline{r} - \tfrac{1}{2}\underline{R} \quad = \underline{r} - \tfrac{1}{2}\underline{\rho} - \tfrac{1}{2}\underline{v}\,t,$$

and

$$\underline{r}_2 = \underline{r} + \tfrac{1}{2}\underline{R} \quad = \underline{r} + \tfrac{1}{2}\underline{\rho} + \tfrac{1}{2}\underline{v}\,t,$$

it follows that $\psi_n^{(1)}(\underline{r}_1), \psi_m^{(2)}(\underline{r}_2)$ are themselves functions of $t$.

It may be shown that

$$\left(\mathcal{H}_e - i\frac{\partial}{\partial t}\right)\Phi_n^{(1)}(\underline{r}_1,t) = V_{23}(\underline{r}_2)\,\Phi_n^{(1)}(\underline{r}_1,t) \tag{5.1.7}$$

and
$$\left(\mathcal{H}_e - i\frac{\partial}{\partial t}\right)\Phi_m^{(2)}(\underline{r}_2,t) = V_{13}(\underline{r}_1)\,\Phi_m^{(2)}(\underline{r}_2,t). \tag{5.1.8}$$

Substitution of (3) in (1) and use of (7) gives

$$i\,\dot{b}_f = \langle \Phi_f^{(1)} \mid V_{23} \mid \Psi \rangle, \tag{5.1.9}$$

and, similarly, (1), (4) and (8) give

$$i\,\dot{a}_n = \langle \Phi_n^{(2)} \mid V_{13} \mid \Psi \rangle, \tag{5.1.10}$$

where
$$\langle \Phi_f^{(1)} \mid V_{23} \mid \Psi \rangle = \int d\underline{r}\;\Phi_f^{(1)}(\underline{r}_1,t)^{*}\,V_{23}(\underline{r}_2)\,\Psi(\underline{r},t).$$

Since initially the electron is bound to nucleus 2, (9), (10) must be solved subject to the boundary conditions

$$|a_m(-\infty)| = \delta_{mi}\ , \qquad |b_n(-\infty)| = 0.$$

(but see later note, p. 67).

The probability of capture into state f occurring at impact parameter $\rho$ is

$$P = |b_f(\infty)|^2 \tag{5.1.11}$$

and the cross section for capture from state i to state f is obtained by integrating over all impact parameters,

$$Q_{if} = \int P \, d\rho \qquad \text{(in atomic units).}$$

This can usually be written

$$Q_{if} = 2\int_0^\infty P \rho \, d\rho \qquad \text{(in units of } \pi a_0^2 \text{).} \qquad (5.1.12)$$

Use of (4) in (9), (10) yields the equations

$$i \dot{b}_f = \sum_m a_m(t) \langle \Phi_f^{(1)} | V_{23} | \Phi_m^{(2)} \rangle, \qquad (5.1.13)$$

$$i \dot{a}_n = \sum_m b_m(t) \langle \Phi_n^{(2)} | V_{13} | \Phi_m^{(1)} \rangle. \qquad (5.1.14)$$

If $a_m(t)$ is known, (13) gives

$$i b_f(t) = \sum_m \int_{-\infty}^{t} \langle \Phi_f^{(1)} | V_{23} | \Phi_m^{(2)} \rangle \, a_m(t) \, dt. \qquad (5.1.15)$$

The impact parameter equivalent of the OBK approximation is obtained by setting $a_m(t) = \delta_{mi}$ in (15) and using the resulting expression for $b_f(\infty)$ in (12). A more refined approximation is obtained by solving (14) for $a_n(t)$, keeping only diagonal terms. This gives

$$a_n(t) = \delta_{ni} \exp\left\{ i\int_{-\infty}^{t} \langle \Phi_n^{(2)} | V_{13} | \Phi_n^{(2)} \rangle \, dt' \right\} \qquad (5.1.16)$$

Use of this expression in (15) yields a cross section $Q^{DI}$, which is the equivalent for capture of the distortion approximation for excitation (Bates, 1959). Cheshire (1964) has calculated values of $Q^{DI}$ for the process

$$H^+ + H(1s) \rightarrow H(1s) + H^+,$$

and results are given in table (6.2.1).

It should not be supposed that the impact parameter method favours the OBK approximation. One of the unsatisfactory aspects of this work is that any potential $W(R)$ which depends only on the internuclear coordinate may be added to $\mathcal{H}_e$ . The only difference this makes is to add a term $W(R)$ to the potentials occurring in (9), (10), (13), (14), (15), (16). The choice $W(R) = V_{12}(R)$, together with the substitution $a_m = \delta_{mi}$ in (15), leads to the impact parameter equivalent of the Jackson-Schiff approximation.

Bates (1958b) showed that the uncertainty about the correct choice of interaction potential arises because no allowance has been made for the fact that the unperturbed functions $\Phi_n^{(1)}$, $\Phi_n^{(2)}$ are not orthogonal except in the limit of infinite internuclear separation. The difficulty may be resolved by taking proper account of this lack of orthogonality. Instead of using either of the expansions (3), (4), $\Psi(\underline{r},t)$ is written

$$\Psi(\underline{r},t) = \sum_n a_n(t)\,\Phi_n^{(2)}(\underline{r}_2,t) + \sum_m b_m(t)\,\Phi_m^{(1)}(\underline{r}_1,t). \qquad (5.1.17)$$

Substitution in (1) now leads to the following exact equations:

$$i\dot{a}_n + i\sum_m \dot{b}_m \langle \Phi_n^{(2)} | \Phi_m^{(1)} \rangle$$
$$= \sum_m a_m \langle \Phi_n^{(2)} | V_{13} | \Phi_m^{(2)} \rangle + \sum_m b_m \langle \Phi_n^{(2)} | V_{23} | \Phi_m^{(1)} \rangle, \qquad (5.1.18)$$

and

$$i\dot{b}_n + i\sum_m \dot{a}_m \langle \Phi_n^{(1)} | \Phi_m^{(2)} \rangle$$
$$= \sum_m b_m \langle \Phi_n^{(1)} | V_{23} | \Phi_m^{(1)} \rangle + \sum_m a_m \langle \Phi_n^{(1)} | V_{13} | \Phi_m^{(2)} \rangle. \qquad (5.1.19)$$

## 2) The two state approximation.

This is obtained by neglecting all terms which involve a state other than the initial or final one. Then (18), (19) give

$$i(1-S^2)\dot{a}_i = a_i(H_{ii} - S_{if}K_{fi}) + b_f(K_{if} - S_{if}H_{ff})\exp\{-i(\epsilon_f^{(1)} - \epsilon_i^{(2)})t\}, \tag{5.2.1}$$

$$i(1-S^2)\dot{b}_f = b_f(H_{ff} - S_{fi}K_{if}) + a_i(K_{fi} - S_{fi}H_{ii})\exp\{-i(\epsilon_i^{(2)} - \epsilon_f^{(1)})t\}, \tag{5.2.2}$$

where

$$S_{if} = \int \psi_i^{(2)}(\underline{r}_2)^{*}\,\psi_f^{(1)}(\underline{r}_1)\,e^{i\underline{v}.\underline{r}}\,d\underline{r} = S_{fi}^{*}, \tag{5.2.3}$$

$$K_{if} = \int \psi_i^{(2)}(\underline{r}_2)^{*}\,V_{23}(\underline{r}_2)\,\psi_f^{(1)}(\underline{r}_1)\,e^{i\underline{v}.\underline{r}}\,d\underline{r}, \tag{5.2.4}$$

$$K_{fi} = \int \psi_i^{(2)}(\underline{r}_2)\,V_{13}(\underline{r}_1)\,\psi_f^{(1)}(\underline{r}_1)^{*}\,e^{-i\underline{v}.\underline{r}}\,d\underline{r},$$

$$H_{im} = \int \psi_i^{(2)}(\underline{r}_2)^{*}\,V_{13}(\underline{r}_1)\,\psi_m^{(2)}(\underline{r}_2)\,d\underline{r},$$

$$H_{fn} = \int \psi_f^{(1)}(\underline{r}_1)^{*}\,V_{23}(\underline{r}_2)\,\psi_n^{(1)}(\underline{r}_1)\,d\underline{r},$$

and $S = |S_{if}|$.

If $a_i$, $b_f$ are written in the forms

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

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

where

$$\alpha_i = \frac{H_{ii} - S_{if}K_{fi}}{1-S^2}, \quad \beta_f = \frac{H_{ff} - S_{fi}K_{if}}{1-S^2}, \tag{5.2.5}$$

then (1), (2) reduce to

$$i\dot{A}_i = B_f\left[\frac{K_{if} - S_{if}H_{ff}}{1-S^2}\right]\exp\left\{-i(\epsilon_f^{(1)} - \epsilon_i^{(2)})t + i\delta_{if}\right\} \tag{5.2.6}$$

and

$$i\dot{B}_f = A_i\left[\frac{K_{fi}-S_{fi}H_{ii}}{1-S^2}\right]\exp\left\{-i(\epsilon_i^{(2)}-\epsilon_f^{(1)})t - i\delta_{if}\right\}, \qquad (5.2.7)$$

where

$$\delta_{if} = \int_{-\infty}^{t}(\alpha_i - \beta_f)\,dt. \qquad (5.2.8)$$

The term $\delta_{if}$ arises because of the difference between the effects of the interaction of the colliding systems when in the initial or final state. Because of the exponential factor occurring in the integrands of (3), (4), $S_{fi}$, $K_{fi}$ may be expected to be small when the relative motion of the colliding particles is large. Then $1-S^2 \simeq 1$ , and

$$\delta_{if} = \int_{-\infty}^{t}(H_{ii} - H_{ff})\,dt.$$

Since the imaginary parts of $\alpha_i, \beta_j$ are antisymmetric with respect to $t$ ,

$$|a_i(\infty)| = |A_i(\infty)| \quad \text{and} \quad |b_f(\infty) = |B_f(\infty)|.$$

In order to obtain $B_f(\infty)$ and hence the cross section, (6), (7) must be solved subject to the boundary conditions

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

McCarroll (1961) showed that, for the symmetric resonance process

$$H^+ + H(1s) \rightarrow H(1s) + H^+, \qquad (5.2.9)$$

the equations simplify considerably and can be solved without further approximation. For in this case $H_{ii} = H_{ff}$, $S_{if} = S_{fi}$, $K_{if} = K_{fi}$ and $\delta_{if} = 0$, so (6), (7) become

$$i\dot{A}_i = B_f\left[\frac{K_{fi} - S_{fi}H_{ii}}{1-S^2}\right],$$

and

$$i\dot{B}_f = A_i\left[\frac{K_{fi} - S_{fi}H_{ii}}{1-S^2}\right].$$

These can be uncoupled and solved, giving

$$|b_f(\infty)| = |B_f(\infty)| = \left| \sin \int_{-\infty}^{\infty} \left( \frac{K_{fi} - S_{fi} H_{ii}}{1 - S^2} \right) dt \right| . \qquad (5.2.10)$$

Sil (1960) used a linear combination of the initial and final state wave functions as a trial function in a variational treatment and obtained a result equivalent to (10).

For any process other than (9), a further approximation must be made. The usual method is to ignore back-coupling from the final to the initial state i.e. it is assumed that $b_f(t) << a_i(t)$ throughout the encounter and the second term on the right hand side of (1) is neglected. The relevant solution of (6) is now

$$A_i(t) = 1 ,$$

and using this in (7) gives

$$|b_f(\infty)| = |B_f(\infty)| = \left| \int_{-\infty}^{\infty} M_{if} \, dt \right| , \qquad (5.2.11)$$

where

$$M_{if} = \left( \frac{K_{fi} - S_{fi} H_{ii}}{1 - S^2} \right) \exp\left( -i(\epsilon_i^{(1)} - \epsilon_f^{(1)})t - i\delta_{if} \right) \qquad (5.2.12)$$

and $\delta_{if}$ is defined by (8).

For symmetric resonance, the exact expression (10) may be written

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

so that, for this process, neglect of back-coupling involves the approximation

$$\sin\left( \int_{-\infty}^{\infty} M_{if} \, dt \right) \simeq \int_{-\infty}^{\infty} M_{if} \, dt . \qquad (5.2.13)$$

It is easy to see from (11), (12) that the unphysical dependence of of the cross section on the potential $V_{12}$ has now been removed. For if any function $W(R)$ of the internuclear distance is added to $\mathcal{H}_e$, then

$$K'_{fi} = \int \psi_f^{(1)}(\underline{r}_1)^* \, (V_{13} + W)\, \psi_i^{(2)}(\underline{r}_2)\, e^{-i\underline{v}\cdot\underline{r}} \, d\underline{r} = K_{fi} + W S_{fi} ,$$

$$H'_{ii} = \int \psi_i^{(2)}(\underline{r}_2)^* \, (V_{13} + W)\, \psi_i^{(2)}(\underline{r}_2)\, d\underline{r} = H_{ii} + W,$$

so that
$$K'_{fi} - S_{fi} H'_{ii} = K_{fi} - S_{fi} H_{ii} ,$$

and the inclusion of $W(R)$ does not affect the value of $M_{if}$. This result depends on the inclusion of the term $S_{fi}$ which allows for the nonorthogonality of the unperturbed functions.

However, Cheshire (1964) drew attention to the fact that the omission of the potential $V_{12}(R)$ alters the boundary condition on the exact wave function. Consider, for example, the collision of a charged ion with a neutral atom. If the whole interaction $V_{12} + V_{13}$ is included in $\mathcal{H}_e$, then in the limit of infinite nuclear separation the electron moves in the field of the isolated nucleus (2), and

$$\Psi(\underline{r}, t) \xrightarrow[t \to -\infty]{} \Phi_i^{(2)}(\underline{r}_2, t) .$$

If $V_{12}$ is omitted, the electron is influenced by the Coulomb field of the projectile even in this limit, and the correct boundary condition is

$$\Psi(\underline{r}, t) \xrightarrow[t \to -\infty]{} \Phi_i^{(2)}(\underline{r}, t) \exp\left\{ -\frac{i}{v} \ln (vR - \underline{v}\cdot\underline{R}) \right\} .$$

This result was first obtained by Wick (see footnote to paper by Jackson and Schiff, 1953). He pointed out that if the projectile and nucleus were considered to be classical particles moving in straight line paths, and $\Psi(\underline{r},t)$ is the exact electronic wave function satisfying the equation

$$(H_0 + V_{12} + V_{13} + V_{23})\,\Psi = i\,\frac{\partial \Psi}{\partial t},$$

then $\tilde{\Psi}(\underline{r},t) = \exp\left\{-\frac{i}{v}\ln(vR-\underline{v}.\underline{R})\right\}\Psi(\underline{r},t)$ satisfies

$$(H_0 + V_{13} + V_{23})\,\tilde{\Psi} = i\,\frac{\partial}{\partial t}\tilde{\Psi}.$$

Therefore the potential $V_{12}$ should not affect the probability of electron capture if the impact parameter method is used. In an exact quantum mechanical calculation, $V_{12}$ may be expected to give a contribution of order $1/M$ which can be neglected in comparison with contributions from other interactions. However, it does not follow that $V_{12}$ can be neglected when approximate methods are used. Returning to the point made by Cheshire, it is clear that the correct boundary conditions have been used in the work of Bates provided the choice $W(R) = V_{12}(R)$ is made. However, the OBK approximation obtained from (5.1.15) employs a wave function with incorrect boundary conditions. Cheshire (1965) obtained a modified OBK cross section $Q^{MBK}$ by writing

$$a_m(t) = \delta_{mi}\exp\left(-\frac{i}{v}\ln(vR-\underline{v}.\underline{R})\right)$$

in (15). Values of $Q^{MBK}$ for the symmetric process (9) are given in Table (6.2.1). Examination of (16) shows that

$$a_n(t) \xrightarrow[t\to-\infty]{} \delta_{ni}\exp\left(-\frac{i}{v}\ln(vR-\underline{v}.\underline{R})\right),$$

so the wave function used to obtain $Q^{DI}$ satisfies the correct boundary conditions.

The results obtained by McCarroll (1961) for reaction (9) are presented in Table (1), which is taken mainly from Bates and McCarroll (1962). Cross sections obtained using the two-state approximation are denoted by $Q_2$ and the superscript $b$ is added when back-coupling has been included. Comparison of $Q_2$ and $Q_2^b$ shows that this is unimportant at energies greater than 100 kev.

Allowance for the non-orthogonality of the initial and final unperturbed wave functions can also be made in a wave treatment (Bates 1958b), although most calculations have used the impact parameter formulation. The distorted wave method of Bassel and Gerjouy (1960) discussed in Chapter 4 § 2, is equivalent to the two-state approximation with both back-coupling and the term $S^2$ neglected. At energies above 200 kev this term becomes very small, and it can be seen from table (1) that $Q_2$ and $Q^{BG}$ are in close agreement, whereas at lower energies $Q^{BG} < Q_2$ . Also included in table (1), for comparison, are values of $Q^B$, $Q^{BK}$ calculated by McCarroll from (3.3.5), (3.1.9).

Since $Q^{BG} \sim Q^{BK}$ as v tends to infinity, the same is true of $Q_2$.

McElroy (1963) used the two-state approximation to calculate cross sections for the reactions

$$H^+ + H(1s) \rightarrow H(2s \text{ or } 2p) + H^+. \qquad (5.2.14$$

Two additional approximations were made to simplify the numerical work:-

(i) Back coupling was neglected.

(ii) The exact distortion term $\delta_{if}$ was replaced by one of the following expressions

a) $$\delta_{if} = \int_{-\infty}^{t} (H_{ii} - H_{ff})\, dt', \qquad (5.2.15)$$

b) $$\delta_{if} = 0. \qquad (5.2.16)$$

Results are given in table (2). $Q_2^{\delta}$, $Q_2^{0}$ denote cross sections obtained by using (15), (16) respectively in (12). It is clear that inclusion of the distortion term has a considerable effect on the values of the cross sections, and except at the lowest energy considered, (25 kev), $Q_2^{\delta} > Q_2^{0}$.

Lovell and McElroy (1965) investigated the error incurred by making the additional approximations (i), (ii) by considering the process

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

and solving the coupled equations (6), (7) numerically without further approximation. Their results are given in table (2), denoted by $Q_2^{b\delta}(2s)$, the superscripts indicating that both back coupling and distortion have been allowed for. Comparison with $Q_2^{\delta}(2s)$ of McElroy, indicates that at energies above 50 kev back coupling is unimportant, and that (15) is a good approximation to $\delta_{if}$ at these energies.

Table (2) also contains total cross sections, $Q_2^{\delta}(\Sigma)$, calculated by assuming that

$$Q_2^{\delta}(n) = Q_2^{\delta}(2)\, \frac{Q^{BK}(n)}{Q^{BK}(n)}, \qquad (5.2.17$$

and using the $n^{-3}$ rule. Then

$$Q_2^{\delta}(\Sigma) = Q_2^{\delta}(1s) + 1.62\ Q_2^{\delta}(2). \qquad (5.2.18)$$

## Table 5.2.1

Cross sections in units of $\pi a_0^2$ for $H^+ + H(1s) \rightarrow H(1s) + H^+$.

| Energy (kev) | $Q^{BK}$ | $Q^{B}$ | $Q_2$ | $Q_2{}^b$ | $Q^{BG}$ | $Q^{GS}$ |
|---|---|---|---|---|---|---|
| 0.1 | 1.27, 4 | - | - | 2.91, 1 | - | - |
| 1 | 1.22, 3 | - | - | 1.86, 1 | - | - |
| 5 | 2.01, 2 | - | 4.61, 1 | 1.13, 1 | - | - |
| 10 | - | - | - | - | 1.18, 1 | 1.71, 1 |
| 15 | 4.24, 1 | - | 9.25 | 6.37 | - | - |
| 20 | - | - | - | - | 4.23 | 6.14 |
| 25 | 1.68, 1 | 2.30 | 3.68 | 3.14 | - | - |
| 30 | - | - | - | - | 2.06 | 3.01 |
| 40 | - | - | - | - | 1.16 | 1.69 |
| 50 | 3.37 | 5.20,-1 | 8.04,-1 | 7.70,-1 | - | - |
| 60 | - | - | - | - | 4.54,-1 | 6.68,-1 |
| 70 | - | - | - | - | - | - |
| 75 | 1.04 | 1.77,-1 | 2.74,-1 | 2.69,-1 | - | - |
| 80 | - | - | - | - | 2.12,-1 | 3.12,-1 |
| 100 | 4.00,-1 | 7.35,-2 | 1.16,-1 | 1.15,-1 | 1.10,-1 | 1.63,-1 |
| 120 | - | - | - | - | 6.21,-2 | 9.13,-2 |
| 150 | 8.74,-2 | 1.81,-2 | 2.98,-2 | 2.98,-2 | - | - |
| 200 | 2.63,-2 | 6.00,-3 | 1.02,-2 | 1.02,-2 | 1.01,-2 | 1.47,-2 |
| 300 | 4.17,-3 | 1.08,-3 | 1.95,-3 | 1.95,-3 | - | - |
| 400 | 1.02,-3 | 2.92,-4 | 5.39,-4 | 5.39,-4 | - | - |
| 500 | 3.29,-4 | 1.01,-4 | 1.97,-4 | 1.97,-4 | 1.91,-4 | 2.65,-3 |
| 600 | 1.27,-4 | 4.09,-5 | - | - | - | - |
| 700 | 5.58,-5 | 1.88,-5 | - | - | - | - |
| 800 | 2.71,-5 | 9.46,-6 | - | - | - | - |
| 900 | 1.42,-5 | 5.12,-6 | - | - | - | - |
| 1000 | 7.95,-6 | 2.94,-6 | 5.82,-6 | 5.82,-6 | - | - |

### Table 5.2.2.

Cross sections $Q_2$ (nl), in units of $\pi a_0^2$, calculated by McElroy (1963), and by Lovell and McElroy (1965), for the process

$$H^+ + H\,(1s) \longrightarrow H\,(nl) + H^+.$$

| Energy (kev) | $Q_2^{0}(2s)$ | $Q_2^{\delta}$ (2s) | $Q_2^{b\delta}$ (2s) | $Q_2^{0}$ (2p) | $Q_2^{\delta}$ (2p) | $Q_2^{\delta}$ ($\Sigma$) |
|---|---|---|---|---|---|---|
| 1 | - | - | 1.34,-5 | - | - | - |
| 5 | - | - | 3.06,-2 | - | - | - |
| 12.5 | - | - | 2.32,-1 | - | - | - |
| 25 | 3.87,-1 | 3.58,-1 | 2.61,-1 | 2.97,-1 | 2.95,-1 | 4.20 |
| 50 | 1.06,-1 | 1.56,-1 | 1.55,-1 | 9.39,-2 | 1.11,-1 | 1.21 |
| 100 | 1.71,-2 | 2.81,-2 | 2.80,-2 | 1.11,-2 | 1.40,-2 | 1.83,-1 |
| 200 | 1.54,-3 | 2.33,-3 | 2.33,-3 | 5.68,-4 | 7.13,-4 | 1.51,-2 |
| 400 | 7.84,-5 | 1.04,-4 | 9.60,-5 | 1.53,-5 | 1.80,-5 | 7.37,-4 |
| 800 | 2.54,-6 | 2.99,-6 | - | 1.28,-7 | 1.42,-7 | 2.33,-5 |

### 3) Other coupled state calculations.

The approximations discussed so far fail to take account of states other than those directly involved in the transition. Bates and McCarroll (1962) pointed out that one could take account of the virtual sequences $i - m - f, i - n - f$ by keeping terms corresponding to the intermediate states m and n in expansion (5.1.17) for $\Psi(\underline{r},t)$. This approach was applied by Lovell and McElroy (1965) to the processes

$$H^+ + H(1s) \rightarrow H(1s \text{ or } 2s) + H^+,$$

the four states included being the 1s and 2s states of the target and projectile. Only three of the four states were kept in each calculation, and the resulting coupled equations were solved numerically, so that the effects of both back-coupling and distortion were allowed for. The results showed that the inclusion of an intermediate state had little effect on the cross section for the 1s - 1s transition, but that for the 1s - 2s transition the effect was considerable, especially at low energies.

If coupling to intermediate 2s states is important, one would expect coupling to 2p states to be also. Wilets and Gallaher (1966) have investigated the effect of keeping more states in expansion (5.1.17). Because they considered the scattering of protons by ground state hydrogen atoms they were able to use the symmetries of the system to halve the number of coupled equations which have to be solved. For this system, the Hamiltonian, $\mathcal{H}_e$, given by (5.1.2) is invariant under inversion through the centre of mass of the two protons ( $\underline{r}_1 \rightarrow -\underline{r}_2$, $\underline{r}_2 \rightarrow -\underline{r}_1$ ). The Schrödinger equation (5.1.1) therefore possesses solutions $\Psi^{\pi}$, which have definite parity,

$$\Psi(\underline{r},t) = \pi\,\Psi(-\underline{r},t), \qquad \text{where } \pi = \pm 1.$$

$\Psi^{\pi}$ is expanded in a set of parity-conserving states

$$\Psi^{\pi} = \sum_{k} a_k^{\pi}(t)\,\Phi_k^{\pi}(\underline{r},t), \tag{5.3.1}$$

where

$$\Phi_k^{\pi}(\underline{r},t) = 2^{-1/2}\left(\Phi_k^{(2)}(\underline{r}_2) + \pi(-1)^{\ell}\,\Phi_k^{(1)}(\underline{r}_1)\right), \tag{5.3.2}$$

and the functions $\Phi_k^{(j)}(\underline{r}_j)$, $j$ = 1, 2, defined by (5.1.5), (5.1.6) can be written

$$\Phi_k^{(j)}(\underline{r}_j) = \varphi_k^{(j)}(\underline{r}_j)\exp(-i\epsilon_k t),$$

with

$$\varphi_k^{(j)}(\underline{r}_j) = \psi_k^{(j)}(\underline{r}_j)\exp\left(\mp\tfrac{1}{2}i\underline{v}\cdot\underline{r} - \tfrac{1}{8}iv^2t\right),$$

the plus sign being taken for j = 1 and the minus sign for j = 2.

The following expansion is made in place of (5.1.17).

$$\Psi(\underline{r},t) = 2^{-1/2}\left(\Psi^{+}(\underline{r},t) + \Psi^{-}(\underline{r},t)\right)$$

$$= \frac{1}{2}\sum_{k}\left\{(a_k^{+} + a_k^{-})\,\Phi_k^{(2)}(\underline{r}_2) + (a_k^{+} - a_k^{-})(-1)^{\ell}\,\Phi_k^{(1)}(\underline{r}_1)\right\} \tag{5.3.3}$$

If the electron is initially bound to proton (2) in the ground state, the boundary conditions are

$$a_k^{+}(-\infty) = a_k^{-}(-\infty) = \delta_{1k}.$$

Coupled equations for the coefficients $a_k^{\pi}$ are obtained in the usual way by substituting (1) into (5.1.1). The equations are then solved twice, once for each parity. The probability of capture into

into state f occurring at some impact parameter $\rho$ is

$$\mathcal{P} = \left| \frac{a_f^+(\infty) - a_f^-(\infty)}{2} \right|^2 . \qquad (5.3.4)$$

Wilets and Gallaher evaluated cross sections for the reactions

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

Most of their calculations included the 1s, 2s, $2p_0$ and $2p_{\pm 1}$ states of both target and projectile (the eight state approximation) but a few results were obtained including also 3s, $3p_0$ and $3p_{\pm 1}$ states (the fourteen state approximation). Their results are given in tables (6.3.1), (6.3.2) (6.3.3) denoted by $Q_8^H(nl)$, $Q_{14}^H(nl)$. For the symmetric process, the eight state results are in very close agreement with $Q_2^b$ of McCarroll (1961), and the fourteen state results do not differ significantly. For capture into the 2s state, the addition of extra states does make an appreciable difference, especially at 9 kev. At energies above 30 kev, where comparison is possible, reasonable agreement with $Q_2^s$ of McElroy is obtained. For capture into 2p , it can be seen that adding in extra states has little effect at 9 kev but increases the cross section considerably at 25 kev, smoothing out the rather peculiar dip in the eight state calculations. This work indicates that the rate of convergence of the close-coupling method is rather slow.

## 4) Collisions involving alpha particles.

Cross sections have been calculated in the two-state approximation for

$$He^{++} + H(1s) \rightarrow He^{+}(1s) + H^{+} \qquad (5.4.1)$$

by McCarroll and McElroy (1962), and for

$$He^{++} + H(1s) \rightarrow He^{+}(2s \text{ or } 2p) + H^{+} \qquad (5.4.2)$$

by McElroy (1963). The same additional assumptions were made as for proton impact. Results are given in table (1), where $Q_2^{\delta}$, $Q_2^{o}$ have the same meanings as before. For process (1), it can be seen that $Q_2^{\delta}$ is much greater than $Q_2^{o}$ at all energies.

One would expect distortion to have a considerable effect on these processes because of the Coulomb repulsion in the final state. For this reason, Macomber and Webb (1967) performed calculations for process (1) using (5.2.11) with the exact expression for $\delta_{if}$. They found that $Q_2^{\delta}$ of McElroy considerably overestimates the true two-state cross section at all energies up to 800 kev, whereas $Q_2^{o}$ overestimates at energies below 100 kev and underestimates at higher energies. Although distortion is expected to be less important for proton impact than for alpha particle impact, nevertheless it is clear that McElroy's results for process (5.2.14) must be regarded as unreliable until calculations using the exact distortion term have been made.

Macomber and Webb also investigated the effect of backcoupling by solving (5.2.6), (5.2.7) numerically with no further approximation, and found that it is unimportant at energies above 100 kev.

Another calculation which takes exact account of distortion has been carried out by Basu, Bhattacharya and Chatterjee (1967). They used a four-state approximation to obtain cross sections for reactions (1), (2) in the energy range 1.6 to 32.4 kev, the coupled equations which arise being solved numerically. Their results are given in table (3), labelled $Q_4$ (nl), and it can be seen that the cross sections for the accidentally resonant processes decrease with decreasing energy as does the cross section Q (1s) for the non-resonant process. This is in accord with general predictions made by Bates and Lynn (1959) on the differences between the effects of symmetrical and accidental resonance. Estimates made by Basu et al of total cross sections agree well with the experimental results of Fite et al (1962) which are clearly non-resonant in form.

If the results found by Macomber and Webb for process (1) hold for (2) also, then McElroy's results overestimate the true two-state approximation result at all energies up to 800 kev. His results are given because they are the only ones for this reaction available for comparison with the impulse approximation.

Estimates by McElroy of total cross sectionf for the process

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

are given in table (2). They are based on the assumption that (5.2.17) and the $n^{-3}$ rule hold for alpha-particle impact also.

Then

$$Q_2^{\delta}(\Sigma) = Q_2^{\delta}(1) + Q_2^{\delta}(2) + 2.1\, Q_2^{\delta}(2)\, \frac{Q^{BK}(3)}{Q^{BK}(2)} .$$

(see ($\overline{3.3.11}$)).

McElroy states that at 25 kev, the third term contributes as much as 53 per cent of the first and second. This is not surprising since one might expect Q(3) to be greater than Q(1) at low energies for alpha-particle impact.

## Table 5.4.1.

Cross sections $Q_2(nl)$ in units of $\pi a_0^2$ for $He^{++} + H(1s) \rightarrow He^{+}(nl) + H^{+}$ calculated by McCarroll and McElroy (1962) and McElroy (1963).

| Energy (kev) | $Q_2(1s)$ | $Q_2^{\delta}(1s)$ | $Q_2(2s)$ | $Q_2^{\delta}(2s)$ | $Q_2(2p)$ | $Q_2^{\delta}(2p)$ |
|---|---|---|---|---|---|---|
| 25 | 1.21,-1 | 3.20,-1 | 2.05,+1 | 3.98 | 1.60,+1 | 1.41, 1 |
| 50 | 1.46,-1 | 6.43,-1 | 5.07 | 2.95 | 7.11 | 1.11, 1 |
| 75 | 1.49,-1 | 7.11,-1 | - | - | - | - |
| 100 | 1.43,-1 | 6.78,-1 | 8.76,-1 | 1.22 | 2.44 | 5.53 |
| 150 | 1.29,-1 | 5.36,-1 | - | - | - | - |
| 200 | 1.15,-1 | 4.11,-1 | 9.26,-2 | 3.23,-1 | 5.72,-1 | 1.66 |
| 250 | 9.83,-2 | 3.16,-1 | - | - | - | - |
| 400 | 6.19,-2 | 1.49,-1 | 6.36,-3 | 3.78,-2 | 9.29,-2 | 2.73,-1 |
| 800 | 1.67,-2 | 2.66,-2 | 2.30,-3 | 1.29,-2 | 1.03,-2 | 2.30,-2 |
| 1600 | 2.73,-3 | 3.36,=3 | - | - | - | - |

## Table 5.4.2.

Total electron capture cross sections in units of $\pi a_0^2$ for $He^{++} + H(1s) \longrightarrow He^{+} + H^{+}$ calculated by McElroy (1963)

| E(kev) | $Q_2$(total) | $Q_2^S$ (total) |
|---|---|---|
| 25 | 5.65,1 | 2.80, 1 |
| 50 | 2.58,1 | 3.01, 1 |
| 100 | 8.41 | 1.75, 1 |
| 200 | 1.76 | 5.32 |
| 400 | 2.84,-1 | 8.47,-1 |
| 800 | 4.13,-3 | 9.66,-2 |

## Table 5.4.3.

Cross sections $Q_4(nl)$, in units of $\pi a_0^2$, for

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

calculated by Basu et al (1967)

| Energy (kev) | $Q_4(1s)$ | $Q_4(2s)$ | $Q_4(2p)$ |
|---|---|---|---|
| 1.6 | 2.6,-7 | 3.63,-8 | 1.01,-7 |
| 3.6 | 6.4,-6 | 1.44,-7 | 3.35,-7 |
| 6.4 | 1.8,-4 | 2.56,-7 | 7.08,-7 |
| 10 | 4.8,-4 | 3.43,-7 | 1.05,-6 |
| 12 | 9.0,-4 | 4.05,-7 | 1.22,-6 |
| 14.4 | 1.43,-3 | 4.49,-7 | 1.38,-6 |
| 16 | 1.93,-3 | 4.58,-7 | 1.45,-6 |
| 19.6 | 4.26,-3 | 4.50,-7 | 1.58,-6 |
| 25.6 | 1.43,-2 | 4.11,-7 | 1.73,-6 |
| 32.4 | 3.22,-2 | 3.73,-7 | 1.82,-6 |

# Chapter 6

## SECOND ORDER METHODS

### 1) Introduction

The lack of convergence of close-coupling expansions suggested by the work of Lovell and McElroy and Wilets and Gallaher is probably due to the fact that approximations based on expansion (5.1.17) and the resulting coupled equations (5.1.18), (5.1.19) take account only of transitions between a limited number of bound states. For rearrangement collisions, transitions to other states, particularly those in the continuum, may have an important effect. The term "second order" is applied to methods which attempt to allow for such transitions.

Cheshire (1965) showed that second order differential equations for the coefficients in (5.1.3) and (5.1.4) can be obtained whose solutions do take account of coupling to all states not explicitly included in the calculation. The second order analogue of (5.1.10) is

$$\ddot{a}_n - i\sum_m \dot{a}_m \langle \Phi_n^{(2)} | V_{13} T_1 V_{13}^{-1} | \Phi_m^{(2)} \rangle + \sum_m a_m \langle \Phi_n^{(2)} | V_{13} V_{23} | \Phi_m^{(2)} \rangle = 0,$$

where $$T_1 = \frac{1}{2} \nabla_r^2 + V_{13} + i \frac{\partial}{\partial t} .$$

If only terms involving the initial state are kept, the following equation is obtained :

$$\ddot{a}_i - i \dot{a}_i \langle \Phi_i^{(2)} | V_{13} T_1 V_{13}^{-1} | \Phi_i^{(2)} \rangle + a_i \langle \Phi_i^{(2)} | V_{13} V_{23} | \Phi_i^{(2)} \rangle = 0.$$

Denote by $a_i^{(2)}(t)$ the solution of this equation with boundary condition

$$a_i^{(2)}(t) \underset{t \to -\infty}{\sim} \exp\left\{ -\frac{i}{v} \ln \left( vR - \underline{v}.\underline{R} \right) \right\}.$$

The second order distortion approximation to the cross section, $Q^{D2}$, is obtained by putting

$$a_n(t) = \delta_{ni}\, a_i^{(2)}(t)$$

in (5.1.15). Cheshire calculated values of $Q^{D2}$ for the process

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

and his results are given in table (6.2.1) At energies above 40 kev, they lie close to $Q^{GS}$ of Grant and Shapiro.

2) <u>The continuum distorted wave method</u>.

Another second order approximation which has been developed within the framework of the impact parameter method and applied to the process

$$H^+ + H(1s) \rightarrow H(1s) + H^+ \qquad (6.2.1)$$

is the continuum distorted wave method of Cheshire (1964).

It was shown in Chapter 4 that, in a wave treatment, the transition amplitude for capture into state f can be written

$$T_{if} = \langle \zeta_f^- \,|\, V_f - U_f \,|\, \Psi_i^+ \rangle,$$

where the distorted wave $\zeta_f^-$ satisfies the equation

$$\left( -\frac{1}{2\mu_f} \nabla_\rho^2 - \frac{1}{2a} \nabla_x^2 + V_{13} + U_f - E \right) \zeta_f^- = 0$$

(in the notation of Chapter 4.)

The equivalent result in an impact parameter formulation is that the probability for capture into state f occurring at an impact parameter $\rho$ is $|\, b_f(\infty) |^2$, where

$$b_f(t) = -i \int_{-\infty}^{t} \langle \zeta_f^- \,|\, V_f - U_f \,|\, \Psi_i^+ \rangle \, dt', \qquad (6.2.2)$$

provided that $b_f(-\infty) = 0$, and now $\zeta_f^-$, $\Psi_i^+$ are electronic wave functions. The distorted wave function $\zeta_f^-$ satisfies

$$\left(-\frac{1}{2}\nabla_r^2 + V_{13} + U_f - i\frac{\partial}{\partial t}\right)\zeta_f^- = 0.$$

Within the limits of the impact parameter method, (2) is exact.

The distorted waves used by Cheshire were chosen in the following way. Suppose $\Psi_i$, $\Psi_f$ are exact solutions of the equation

$$\left(-\frac{1}{2}\nabla_r^2 + V_{13} + V_{23} + V_{12} - i\frac{\partial}{\partial t}\right)\Psi(\underline{r},t) = 0.$$

Write $\Psi_i = \Phi_i^{(2)}\mathcal{L}_i$, $\Psi_f = \Phi_f^{(1)}\mathcal{L}_f$,

where $\Phi_f^{(1)}$, $\Phi_i^{(2)}$ are defined by (5.1.5), (5.1.6).

Then, for reaction (1), $\mathcal{L}_i, \mathcal{L}_f$ satisfy the equations

$$\left(-\frac{1}{2}\nabla_r^2 + V_{12} + V_{13} - i\frac{\partial}{\partial t} + \frac{i}{2}\underline{v}\cdot\underline{\nabla}_r\right)\mathcal{L}_i = -\frac{\underline{r}_1}{r_1}\cdot\underline{\nabla}_r\mathcal{L}_i, \qquad (6.2.3)$$

$$\left(-\frac{1}{2}\nabla_r^2 + V_{12} + V_{23} - i\frac{\partial}{\partial t} + \frac{i}{2}\underline{v}\cdot\underline{\nabla}_r\right)\mathcal{L}_f = -\frac{\underline{r}_2}{r_2}\cdot\underline{\nabla}_r\mathcal{L}_f, \qquad (6.2.4)$$

with boundary conditions

$$\mathcal{L}_i \xrightarrow[t\to-\infty]{} 1, \quad \mathcal{L}_f \xrightarrow[t\to+\infty]{} 1.$$

The distorted waves are taken to be

$$X_i = \Phi_i^{(2)}\mathcal{L}_i', \quad \zeta_f = \Phi_f^{(1)}\mathcal{L}_f', \qquad (6.2.5)$$

where $\mathcal{L}_i', \mathcal{L}_f'$ are solutions of the equations obtained by neglecting the terms on the right hand sides of (3) and (4). It can be shown that the distorting potentials are

$$U_i = V_i - A_i, \quad U_f = V_f - A_f$$

where

$$A_i X_i = \Phi_i^{(2)}\left(\frac{\underline{r}_2}{r_2}\cdot\underline{\nabla}_1\mathcal{L}_i'\right),$$

$$A_f \zeta_f = \Phi_f^{(1)}\left(\frac{\underline{r}_1}{r_1}\cdot\underline{\nabla}_2\mathcal{L}_f'\right).$$

## Table 6.2.1.

Cross sections in units of $\pi a_0^2$ for $H^+ + H(1s) \rightarrow H(1s) + H^+$

| Energy (kev) | $Q^{BK}$ | $Q^{MBK}$ | $Q_2^{b}$ | $Q^{CD}$ | $Q^{D1}$ | $Q^{D2}$ |
|---|---|---|---|---|---|---|
| 0.1 | 1.27, 4 | - | 2.91, 1 | 6.85, 5 | - | - |
| 1 | 1.22, 3 | - | 1.86, 1 | 6.70, 3 | - | - |
| 5 | 2.01, 2 | 5.02 | 1.13, 1 | 2.43, 2 | 4.38 | 4.08 |
| 15 | 4.24, 1 | - | 6.37 | 2.08, 1 | - | - |
| 25 | 1.68, 1 | 3.81 | 3.14 | 5.83 | 4.87 | 3.08 |
| 50 | 3.37 | 1.19 | 7.70,-1 | 7.89,-1 | 1.52 | 1.00 |
| 100 | 4.00,-1 | 1.83,-1 | 1.15,-1 | 7.33,-2 | 3.31,-1 | 1.55,-1 |
| 200 | 2.63,-2 | - | 1.02,-2 | 4.31,-3 | - | - |
| 400 | 1.02,-3 | 6.15,-4 | 5.39,-4 | 1.69,-4 | 7.86,-4 | 5.29,-4 |
| 500 | 3.29,-4 | - | 1.97,-4 | 5.55,-5 | - | - |
| 1000 | 7.95,-6 | 6.87,-6 | 5.82,-6 | 1.49,-6 | 8.77,-6 | 5.5,-6 |

Equation (2) now becomes

$$b_f(t) = -i\int_{-\infty}^{t} dt \, \langle \zeta_f^- | A_f | \Psi_i^+ \rangle , \qquad (6.2.6)$$

and the continuum distorted wave approximation is obtained by replacing $\Psi_i^+$ by $\chi_i$.

Cross sections calculated using (5) and (6) are labelled $Q^{CD}$ in table (1). It can be seen that the cross section falls off more rapidly with increasing energy than do those calculated using first order methods. Cheshire showed that

$$Q^{CD} \underset{v \to \infty}{\sim} \left( 0.2946 + \frac{5\pi v}{2^{12}} \right) Q^{BK} ,$$

which agrees exactly with the result obtained by Drisko using the second Born approximation.

## 3) Sturmian function expansions.

A variant of the close-coupling method, in which the total wave function is expanded in terms of Sturmian functions instead of hydrogenic functions, has recently been used by Gallaher and Wilets (1968) to describe proton-hydrogen scattering. The importance of the Sturmian functions is that they form a complete, discrete set which is not orthogonal to the hydrogen continuum. Therefore the method makes some allowance for virtual transitions to this.

It is essentially the same as that used previously by these authors (see Chapter 5 § 3) but the hydrogen wave function

$$| \mathbf{k} \rangle \equiv \psi_{\mathbf{k}}(\mathbf{r}) = R_{nl}(r) \, Y_{lm}(\theta, \varphi)$$

is replaced by the function

$$| \hat{\mathbf{k}} \rangle \equiv \hat{\psi}_{\mathbf{k}}(\mathbf{r}) = \frac{S_{nl}(r)}{r} \, Y_{lm}(\theta, \varphi).$$

The functions $S_k(r) \equiv S_{nl}(r)$ are Sturmian functions, similar to those first introduced into atomic scattering problems by Rotenburg (1962). Those used by Gallaher and Wilets are scaled hydrogenic functions

$$S_k(r) = r\,\alpha_k^{3/2}\,R_k(\alpha_k r)$$

where $\alpha_k = \dfrac{n}{l+1}$ .

With this definition, the functions $\hat{\psi}_{nl}$ with $l = n - 1$, coincide with the corresponding hydrogenic functions. In this section, the function obtained by the replacement, in a function g defined in Chapter 5 § 3,

of $\psi_k(\underline{r})$ by $\hat{\psi}_k(\underline{r})$ and

of $\epsilon_k$ by $\hat{\epsilon}_k = \langle \hat{k} | H | \hat{k} \rangle = \dfrac{1}{n(l+1)} - \dfrac{1}{2(l+1)^2}$,

will be denoted by $\hat{g}$.

The function $\Psi^{\pi}(\underline{r},t)$ may be written in either the hydrogenic or Sturmian representations.

$$\Psi^{\pi}(\underline{r},t) = \sum_k a_k^{\pi}(t)\,\Phi_k^{\pi}(\underline{r},t) = \sum_k b_k^{\pi}(t)\,\hat{\Phi}_k^{\pi}(\underline{r},t) \qquad (6.3.1)$$

where $\Phi_k^{\pi}(\underline{r},t)$ is defined by (5.3.2). Equation (1) gives

$$\sum_k a_k^{\pi}\left(\Phi_k^{(2)} + \pi(-1)^l\,\Phi_k^{(1)}\right) = \sum_k b_k^{\pi}\left(\hat{\Phi}_k^{(2)} + \pi(-1)^l\,\hat{\Phi}_k^{(1)}\right),$$

from which it can be shown that

$$a_k^{\pi} = \sum_{k'} b_{k'}^{\pi}\,\langle \Phi_k^{(j)} | \hat{\Phi}_{k'}^{(j)} \rangle$$

$$= \sum_{k'} b_{k'}^{\pi}\,\langle k | \hat{k}' \rangle \exp\{i(\epsilon_k - \hat{\epsilon}_{k'})t\}. \qquad (6.3.2)$$

The probability of capture into state f at impact parameter $\rho$ is given by (5.3.4) and (2) shows that the problem is solved if the coefficients $b_{k'}^{\pi}$ can be found. Coupled differential equations for them are obtained in the usual way and must be solved for each parity subject to the boundary conditions

$$b_{k'}^{+}(-\infty) = b_{k'}^{-}(-\infty) = \delta_{1k'},$$

since $\Psi(\underline{r},t)$ can be written

$$\Psi(\underline{r},t) = \frac{1}{2}\sum_{k}\left\{ (b_k^{+}+b_k^{-})\,\hat{\Phi}_k^{(2)} + (b_k^{+}-b_k^{-})(-1)^{l}\,\hat{\Phi}_k^{(1)} \right\},$$

and $\hat{\Phi}_{1s}^{(j)}$ coincides with $\Phi_{1s}^{(j)}$.

If only a finite number of terms is retained in (1), numerical solution is possible. However, a difficulty then arises when (2) is used to calculate $a_k^{\pi}$. This is because, although it is obvious from (1) that the complete expansion $\sum_k b_k^{\pi}\,\hat{\Phi}_k^{\pi}$ contains the whole of any hydrogenic state, the same is not true of any truncated expansion. For example, the table of overlap matrix elements given by Gallaher and Wilets shows that although $\hat{\psi}_{1s} = \psi_{1s}$, nevertheless

$$b_1\hat{\psi}_{1s} + b_2\hat{\psi}_{2s}$$
$$= (b_1 - 0.5\,b_2)\psi_{1s} + b_2(0.558\,\psi_{2s} + 0.224\,\psi_{3s} + 0.147\,\psi_{4s} + \cdots).$$

Thus, although parts of higher s hydrogenic states, including those in the continuum, are added by coupling in the 2s Sturmian state, some of $\psi_{1s}$ is actually removed. Thus, the actual amount of any hydrogenic state present in the Sturmian expansion of the wave function, depends on the overlap matrix elements as well as on the number of Sturmian states used. One possible method of avoiding this difficulty would be to use functions $\hat{\psi}'_k(\underline{r})$ in place of $\hat{\psi}_k(\underline{r})$ in expansion (1), defined by

$$\hat{\psi}'_k(\underline{r}) = \hat{\psi}_k(\underline{r}) + \sum_{k'<k} c_{k'}\psi_{k'}(\underline{r})$$

with coefficients chosen so that $\hat{\psi}'_k(\underline{r})$ is orthogonal to $\psi_l(\underline{r})$, $l < k$. However, this was not done by Gallaher and Wilets and this is a major defect of their method.

They calculated cross sections for the processes

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

for incident energies in the range 1 to 1000 kev. The majority of results were obtained using Sturmian states 1s, 2s, $2p_0$, $2p_{\pm 1}$ centred on both target and projectile; a few calculations were carried out including states 3s, $3p_0$, $3p_{\pm 1}$ and also 4s. Results are given in tables (1), (2), (3) and in fig (1). $Q_8^S(1s)$ agrees well with $Q_8^H(1s)$ at energies below 100 kev, but falls off slightly more quickly with increasing energy. Comparison with $Q_{14}^S(1s)$ shows satisfactory convergence. $Q_8^S(2s)$ lies well above $Q_8^H(2s)$ and, in fact, at energies above 70 kev exceeds $Q^{BK}(2s)$ obtained by Mapleton (1962). It must therefore be regarded as totally unrealistic. Comparison of $Q_8^S(2p)$, $Q_{14}^S(2p)$ and $Q_{16}^S(2p)$ shows that convergence is very slow and the cross sections are appreciably reduced when more states are coupled in. Even the addition of the two 4s states to the fourteen state expansion has this effect, and values of $Q_{16}^S(2p)$ lie close to those of $Q_8^H(2p)$. The latter are in reasonable agreement with the experimental results of Stebbings et al (1965) but the validity of these is in some doubt.

In view of the lack of convergence shown by the results and also the difficulty about obtaining the true cross section from the formulation used, cross sections based on the Sturmian expansion must be regarded with some caution.

## Table 6.3.1.

Cross sections in units of $\pi a_0^2$ for $H^+ + H(1s) \rightarrow H(1s) + H^+$

| Energy (kev) | $Q_2^b$ | $Q_8^H$ | $Q_{14}^H$ | $Q_8^S$ | $Q_{14}^S$ |
|---|---|---|---|---|---|
| 1 | 1.86, 1 | 1.558,1 | - | 1.97, 1 | - |
| 2 | - | 1.715,1 | - | 1.666,1 | - |
| 4 | - | 1.091,1 | - | 1.232,1 | - |
| 5 | 1.13, 1 | - | - | 1.138,1 | - |
| 6.25 | - | - | - | 1.038,1 | - |
| 7.5 | - | - | - | 9.75 | - |
| 9 | - | 9.40 | 9.40 | 8.94 | - |
| 15 | 6.37 | - | - | - | - |
| 16 | - | 6.09 | - | 5.57 | - |
| 25 | 3.14 | 3.33 | 3.33 | 3.214 | 3.235 |
| 30 | - | - | - | 2.382 | - |
| 40 | - | 1.37 | - | 1.363 | 1.270 |
| 50 | 7.70,-1 | - | - | - | - |
| 70 | - | 3.2,-1 | - | 3.10, -1 | 2.90, -1 |
| 75 | 2.69,-1 | - | - | - | - |
| 100 | 1.15,-1 | 1.1,-1 | - | 9.6, -2 | 9.46, -2 |
| 150 | 2.98,-2 | - | - | - | - |
| 200 | 1.02,-2 | - | - | 8.0, -3 | - |

## Table 6.3.2.

Cross sections in units of $\pi a_0^2$ for $H^+ + H(1s) \rightarrow H(2s) + H^+$

| Energy (kev) | $Q^{BK}$ | $Q_2^{\delta}$ | $Q_8^{H}$ | $Q_{14}^{H}$ | $Q_8^{S}$ |
|---|---|---|---|---|---|
| 1 | | - | 3.5,-2 | - | |
| 2 | | - | 8.8,-2 | - | |
| 4 | | - | 4.4,-2 | - | 2.4, -3 |
| 5 | | - | - | - | 8.2, -3 |
| 6.25 | | - | - | - | 1.38,-2 |
| 7.5 | | - | - | - | 4.15,-2 |
| 9 | | - | 1.93,-1 | 1.28,-1 | 8.26,-2 |
| 16 | | - | 3.33,-1 | - | 2.56,-1 |
| 25 | | 3.58,-1 | 4.10,-1 | 4.17,-1 | 5.70,-1 |
| 30 | | - | - | - | 6.60,-1 |
| 40 | | - | 2.94,-1 | - | 6.21,-1 |
| 50 | | 1.56,-1 | - | - | - |
| 70 | | - | 9.1, -2 | - | 2.27,-1 |
| 100 | | 2.81,-2 | 3.1, -2 | - | 8.21,-2 |
| 200 | | 2.33,-3 | - | - | 8.0, -3 |

## Table 6.3.3.

Cross sections in units of $\pi a_0^2$ for $H^+ + H(1s) \rightarrow H(2p) + H^+$

| Energy (kev) | $Q_8^H$ | $Q_{14}^H$ | $Q_8^S$ | $Q_{14}^S$ | $Q_{16}^S$ | $Q_8^S(\Sigma)$ |
|---|---|---|---|---|---|---|
| 1 | 9.0, -2 | - | 1.334,-1 | - | - | 1.981, 1 |
| 2 | 6.0, -2 | - | 2.38, -1 | - | - | 1.723, 1 |
| 4 | 1.77,-1 | - | 3.994,-1 | - | - | 1.275, 1 |
| 5 | - | - | 4.49, -1 | - | 2.31, -1 | 1.188, 1 |
| 6.25 | - | - | 5.14, -1 | - | - | 1.085, 1 |
| 7.5 | - | - | 5.50, -1 | - | - | 1.040, 1 |
| 9 | 2.68,-1 | 2.73,-1 | 4.914,-1 | - | 2.79, -1 | 9.61 |
| 16 | 1.86,-1 | - | 4.08, -1 | - | - | 6.56 |
| 25 | 8.6, -2 | 1.01,-1 | 3.004,-1 | 1.968,-1 | 2.065,-1 | 4.84 |
| 30 | - | - | 2.44, -1 | - | - | 4.17 |
| 40 | 5.6,-2 | - | 1.585,-1 | 1.120,-1 | - | 3.01 |
| 70 | 1.7,-2 | - | 3.85, -2 | 2.58,-2 | - | 8.96, -1 |
| 100 | 6 ,-3 | - | 9.8, -3 | 5.2, -3 | - | 2.92, -1 |
| 200 | - | - | 3 , -4 | - | - | 2.73, -2 |
| 400 | - | - | 4 , -4 | - | - | 1.80, -3 |
| 1000 | - | - | - | - | - | 3.0, -4 |

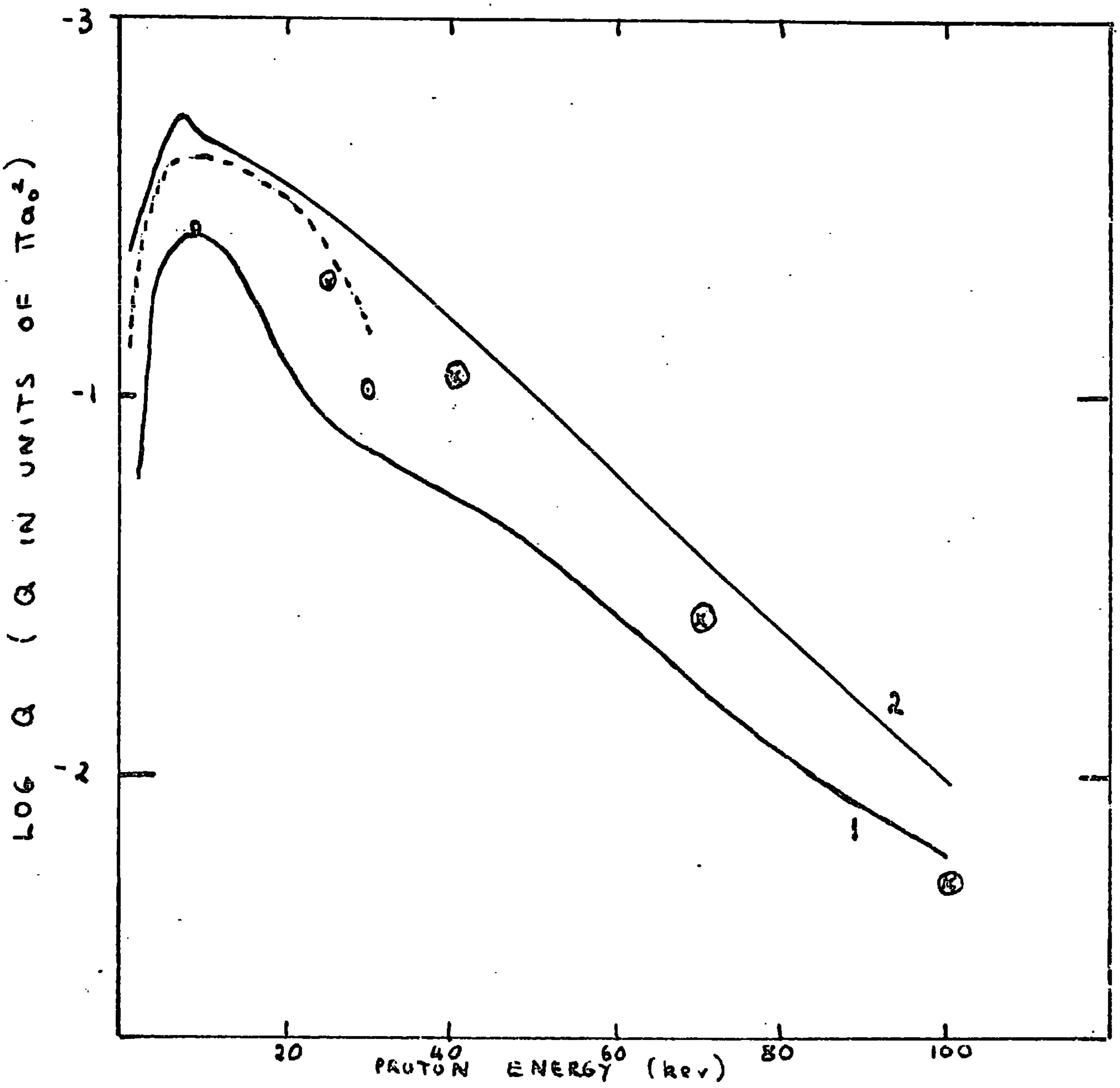


Fig 6.3.1. Cross sections for $H^+ + H(1s) \rightarrow H(2p) + H^+$

Curve 1; $Q_8^H$ , Wilets and Gallaher (1966)
Curve 2; $Q_8^S$ , Gallaher and Wilets (1968)

----- Experiment, Stebbings et al (1965)
⊙ ; $Q_{14}^H$ ; Ⓚ ; $Q_{14}^S$ .

## Chapter 7.

# THE IMPULSE APPROXIMATION

### 1) Introduction.

The name "impulse approximation" arises from the assumption made that at high energies the binding forces in the target atom are unimportant during the actual collision. Their function is to determine the initial momentum distribution of the collection of free particles with which the projectile reacts. The name masks the fact that it is also assumed that the reaction with each target particle can be considered separately, so that the total scattering amplitude can be expressed as the sum of two-body amplitudes.

The approximation was first proposed by Chew (1950) and the assumptions involved were investigated by Chew and Wick (1952) and Ashkin and Wick (1952). A formal derivation was given by Chew and Goldberger (1952) and the same approximation was obtained from a different viewpoint by Epstein (1952). The derivation given here is due to Coleman (1969) and brings out clearly the basic assumptions involved in the method.

### 2) Formulation of the approximation.

The wave function for the three particle system, corresponding to an initial state $\varphi_i$, is given by (2.3.7) in the form

$$\Psi_i^+ = \Omega^+ \varphi_i,$$

where $\Omega^+ = 1 + G^+ V_i,$

and $G^+$ is the three-body Green's function

$$G^+ = \lim_{\epsilon \to 0+} (E - H + i\epsilon)^{-1}.$$

The exact amplitude for a transition to state $\varphi_f$ is

$$T_{if} = \langle \varphi_f \mid V_f \mid \Omega^+ \varphi_i \rangle \tag{7.2.1}$$

This equation will now be rewritten in a form suitable for the application of the "impulse hypothesis".

Let $X_m$ be a member of the complete set of free particle wave functions satisfying the Schrödinger equation

$$(H_0 - E_m)\, X_m = 0.$$

An operator $\omega_i^+[m]$ is introduced, defined by the equation

$$\begin{aligned}\omega_i^+[m]\, X_m\rangle &= \left(1 + \frac{1}{E_m - H_0 - V_i + i\epsilon} V_i\right) X_m\rangle \\ &= \psi_i^+[m].\end{aligned} \tag{7.2.2}$$

Let

$$b_i^+[m] = \omega_i^+[m] - 1 .$$

The operators $\omega_i^+[m]$, $b_i^+[m]$ are only defined with reference to the plane wave basis $X_m\rangle$ and this is to be understood in what follows. With

$$A = E - H_0 + i\epsilon, \qquad B = E_m - H_0 - V_i + i\epsilon,$$

the operator identity (2.3.8) gives

$$\frac{1}{E - H + i\epsilon} = \frac{1}{E_m - H_0 - V_i + i\epsilon} + \frac{1}{E - H + i\epsilon}\,(E_m - E + V_{23})\,\frac{1}{E_m - H_0 - V_i + i\epsilon} .$$

Thus

$$G^+ V_i = b_i^+[m] + G^+(E_m - E + V_{23})\, b_i^+[m]$$

and

$$\mathcal{G}^+ V_i \varphi_i = \sum_m \mathcal{G}^+ V_i \chi_m \rangle \langle \chi_m | \varphi_i \rangle$$

$$= \sum_m \left( b_i^+[m] + \mathcal{G}^+ (E_m - E + V_{23})\, b_i^+[m] \right) \chi_m \rangle \langle \chi_m | \varphi_i \rangle. \tag{7.2.3}$$

Now

$$(E_m - E) \langle \chi_m | \varphi_i \rangle = \langle E_m \chi_m | \varphi_i \rangle - \langle \chi_m | E \varphi_i \rangle \tag{7.2.4}$$

and

$$E_m \chi_m = H_0 \chi_m , \qquad E \varphi_i = (H_0 + V_{23}) \varphi_i .$$

Therefore,

$$\begin{aligned} (E_m - E) \langle \chi_m | \varphi_i \rangle &= \langle \chi_m | H_0 | \varphi_i \rangle - \langle \chi_m | H_0 + V_{23} | \varphi_i \rangle \\ &= - \langle \chi_m | V_{23} | \varphi_i \rangle , \end{aligned}$$

so that (3) becomes

$$\mathcal{G}^+ V_i \varphi_i = ( b_i^+ + \mathcal{G}^+ [ V_{23} , b_i^+ ] ) \varphi_i ,$$

where [a, b] denotes the commutator of the operators a and b,

and
$$b_i^+ = \sum_m b_i^+[m] \chi_m \rangle \langle \chi_m .$$

If
$$\omega_i^+ = b_i^+ + 1$$

then
$$\Omega^+ = \omega_i^+ + \mathcal{G}^+ [ V_{23} , \omega_i^+ ] ,$$

and (1) can be written

$$T_{if} = \langle \varphi_f | V_f | ( \omega_i^+ + \mathcal{G}^+ [ V_{23} , \omega_i^+ ] ) \varphi_i \rangle , \tag{7.2.5}$$

which is the desired relation.

If the potential $V_{23}$ were constant throughout the collision then

a) the commutator would vanish identically, and

b) $V_{23}$ would not affect the transition probability.

Therefore, if it is assumed that the effect of the potential $V_{23}$ is negligible during the collision, it seems reasonable to neglect the commutator term in (5). The resulting matrix element will be denoted by $T_{if}^{IMP2}$ i.e.

$$T_{if}^{IMP2} = \langle \varphi_f \mid V_f \mid \omega_i^+ \varphi_i \rangle . \qquad (7.2.6)$$

This matrix element can also be obtained as an approximation to (4.1.21) which was derived using the distorted wave formalism of Dodd and Greider (1966). If $V_f$ is chosen to be zero, (4.1.21) and (6) differ only in the energies E, $E_m$ respectively occurring in the denominators, and it can be shown that

$$T_{if}^{I} = T_{if}^{IMP2} + \sum_m \langle \varphi_f | V_f | \frac{1}{E - H_0 - V_i + i\epsilon} \left( \psi_i^+[m] - \chi_m \right) \rangle \langle \chi_m | V_{23} | \varphi_i \rangle .$$

McCarroll and Salin (1967) used $T_{if}^{IMP2}$ as an approximation to $T_{if}^{I}$ in a discussion of the high energy behaviour of the electron capture cross section, though the justification for doing so is not obvious.

It is clear that the use of (6) as an approximation to the exact transition amplitude (1) involves the replacement of the exact wave function $\Psi_i^+$ by

$$\Psi_i^{IMP2} = \omega_i^+ \varphi_i = \sum_m \psi_i^+[m] \langle \chi_m \mid \varphi_i \rangle \qquad (7.2.7)$$

This equation is only useful if it is possible to obtain an analytic expression for the function $\psi_i^+[m]$ by solving (2), which is equivalent to the equation

$$\left( H_0 + V_{12} + V_{13} - E_m \right) \psi_i^+[m] = 0 \qquad (7.2.8)$$

provided that

$$\lim_{\epsilon \to 0+} \epsilon \, \psi_i^+[m] = 0,$$

Since particles 1 and 2 are much heavier than the electron 3, to a good approximation $H_0$ separates exactly into two parts, one depending only on the argument of $V_{12}$ and the other on that of $V_{13}$. Equation (8) is then exactly soluble and $\psi_i^+[m]$ is the product of two single particle wave functions. This idea is also used in Chapter 9.

No numerical calculations have so far been carried out using $T_{if}^{IMP2}$.

Equation (6), which was obtained using only the "impulse hypothesis" that the effect of the binding forces could be neglected, does not give the transition amplitude as the sum of two-body scattering approximation. The usual form of the impulse approximation will now be derived. The further assumption must be made that multiple scattering terms can be neglected.

First the operator $\omega_i^+$ is exapnded in terms of true two-body operators $\omega_{ij}^+[m]$, defined by the equation

$$\omega_{ij}^+[m]\,\chi_m = \left(1 + \frac{1}{E_m + i\epsilon - H_0 - V_{ij}} V_{ij}\right)\chi_m = \psi_{ij}^+[m]. \qquad (7.2.9)$$

$\omega_{ij}^+[m]$ differs from $\omega_i^+[m]$ in that now only one potential occurs. It is again convenient to introduce operators

$$b_{ij}^+[m] = \omega_{ij}^+[m] - 1 .$$

If

$$\lim_{\epsilon \to 0+} \epsilon \, \psi_{ij}^+[m] = 0, \qquad (7.2.10)$$

it is clear that $\Psi^{+}_{ij}[m]$ satisfies the differential equation

$$(H_0 - V_{ij} - E_m)\,\Psi^{+}_{ij}[m] = 0. \qquad (7.2.11)$$

If $V_{ij}$ is a Coulomb potential, condition (10) is not satisfied and it is found that the normalization of the functions obtained by solving (9) and (11) differs. However, Mapleton (1961) pointed out that the correct function is the solution of (11).

Use of the operator identity (2.3.8) gives

$$\frac{1}{E_m - H_0 - V_i + i\epsilon} = \left(1 + \frac{1}{E_m - H_0 - V_i + i\epsilon}\,(V_i - V_{ij})\right)\frac{1}{E_m - H_0 - V_{ij} + i\epsilon}.$$

Thus,

$$\omega_i^{+}[m]\,\chi_m = \left(\omega_{13}^{+}[m] + \omega_{12}^{+}[m] - 1\right)\chi_m + \frac{1}{E_m - H_0 - V_i + i\epsilon}\left(V_{12}\,b_{13}^{+}[m] + V_{13}\,b_{12}^{+}[m]\right). \qquad (7.2.12)$$

The second and third terms correspond to multiple scattering in which the incident particle is scattered by the potentials $V_{12}$ and $V_{13}$ successively. If $V_{12} \equiv 0$, the terms are both zero. For electron capture collisions it has been shown (Chapter 5 § 2) that in an exact calculation the effect of the potential $V_{12}$ is negligible. It therefore seems reasonable to neglect the multiple scattering terms when considering such collisions, and also to make the further approximation $\omega_{12}^{+} \simeq 1$.

Then (7), (12) give

$$\Psi_i^{IMP} = \omega_{13}^{+}\,\varphi_i$$

and (6) becomes

$$T_{if}^{IMP} = \langle \varphi_f \,|\, V_f \,|\, \omega_{13}^{+}\,\varphi_i \rangle. \qquad (7.2.13)$$

All the impulse approximation calculations considered in this thesis are based on this expression.

Expressions (6) and (13) may be regarded as the "post" forms of the two impulse approximation matrix elements. The "prior" forms are obtained by starting with the alternative expression for the exact matrix element

$$T_{if} = \langle \Psi_f^- \mid V_i \mid \varphi_i \rangle,$$

where

$$\Psi_f^- = \Omega^- \varphi_f = (1 + G^- V_f)\, \varphi_f .$$

$\Omega^-$ is expanded in terms of the operator

$$\omega_f^- = \sum_m \omega_f^-[m]\, \chi_m \rangle \langle \chi_m$$

and

$$\omega_f^-[m]\, \chi_m = \left( 1 + \frac{1}{E_m - H_0 - V_f - i\epsilon} V_f \right) \chi_m .$$

Proceeding as before, the following equation is obtained

$$T_{if} = \langle \omega_f^- + G^-[V_{ij}, b_f^-]\, \varphi_f \mid V_i \mid \varphi_i \rangle, \qquad (7.2.14)$$

which is the "prior" form of (5). The two expressions are equal on the energy shell. If the term involving the commutator is dropped, one obtains

$$T_{if}^{IMP2} = \langle \omega_f^- \varphi_f \mid V_i \mid \varphi_i \rangle. \qquad (7.2.15)$$

Expressions (6) and (15) are only automatically equal if the initial and final systems are identical.

The "prior" form of (13) is obtained by expanding $\omega_f^-[m]$ in terms of the two-body operators $\omega_{ij}^-[m]$, where

$$\omega_{ij}^-[m]\, \chi_m = \left( 1 + \frac{1}{E_m - H_0 - V_{ij} - i\epsilon} V_{ij} \right) \chi_m .$$

The equation corresponding to (12) is

$$\omega_f^-[m]X_m = \left(\omega_{12}^-[m] + \omega_{23}^-[m] - 1\right)X_m$$

$$+ \frac{1}{E_m - H_0 - V_f - i\epsilon}\left(V_{12}\, b_{23}^-[m] + V_{23}\, b_{12}^-[m]\right)X_m .$$

Substituting in (15) gives

$$T_{if}^{IMP} = \langle \omega_{23}^- \varphi_f \,|\, V_i \,|\, \varphi_i \rangle$$

when multiple scattering terms are dropped and $\omega_{12}^-$ is replaced by 1.

Pradhan (1957) first applied the impulse approximation to electron capture and considered the process

$$H^+ + H(1s) \rightarrow H(1s) + H^+.$$

However, rather than evaluate (13), he used the simpler expression $\langle \varphi_f | V_{13} | \omega_{13}^+ \varphi_i \rangle$, which, as pointed out by Bassel and Gerjouy (1960), corresponds to a quite different physical process. The correct matrix element was used by McDowell (1961) and Cheshire (1963) although the former made an approximation to simplify the analysis. Cross sections for various processes have been calculated by Coleman and McDowell (1965), and by Coleman and the present author. The analysis is given in the next section.

### 3) Reduction of the matrix element.

Consider a collision in which a structureless particle $A^+$ of charge $Z_1$, mass $M_1$, collides with a hydrogen atom in either the 1s or 2s state, and captures the bound electron. i.e. a process of the form

$$A^+ + H(n'l') \rightarrow A(nl) + H^+.$$

Equation (7.2.13) can then be written

$$T_{if}^{IMP} = I_{12} + I_{23} ,$$

where

$$I_{ij} = \langle \varphi_f \,|\, V_{ij} \,|\, \omega_{13}^{+} \varphi_i \rangle , \qquad (7.3.1)$$

$$V_{12} = \frac{Z_1}{|\underline{r} - \underline{x}|} , \qquad V_{23} = -\frac{1}{r} .$$

The cross section is given by the equation

$$Q^{IMP}(nl) = \frac{1}{4\pi^2 a v^2} \left( \frac{\mu_f}{\mu_i} \right) \int_{\rho^2_{min}}^{\rho^2_{max}} |T_{if}^{IMP}|^2 \, d(\rho^2) . \qquad (7.3.2)$$

The impulse approximation wave function is

$$\Psi_i^{IMP} = \omega_{13}^{+} \varphi_i = \sum_m \langle \chi_m | \varphi_i \rangle \, \Psi_{13}^{+}[m] , \qquad (7.3.3)$$

where $\Psi_{13}^{+}[m]$ satisfies the equation

$$(H_0 + V_{13} - E_m) \, \Psi_{13}^{+}[m] = 0 . \qquad (7.3.4)$$

The free particle wave function $\chi_m$ is taken to be

$$\chi_m = (2\pi)^{-3} \exp\{ i(\underline{K}\cdot\underline{x} + \underline{k}\cdot\underline{\rho}) \} ; \qquad (7.3.5)$$

the energy $E_m$ is then given by

$$E_m = \frac{1}{2} \left( \frac{K^2}{a} + \frac{k^2}{\mu_f} \right) ,$$

and the summation over m in (3) stands for integrations over $\underline{k}$ and $\underline{K}$. Equation (4) may be written

$$\left( \frac{1}{2\mu_f} \nabla_\rho^2 + \frac{1}{2a} \nabla_x^2 + \frac{Z_1}{x} + \frac{k^2}{2\mu_f} + \frac{K^2}{2a} \right) \Psi_{13}^{+} = 0,$$

which is satisfied by

$$\Psi_{13}^{+} = (2\pi)^{-3} \exp\{ i(\underline{K}.\underline{x} + \underline{k}.\underline{\rho}) \} N(K) \, {}_1F_1\left[ \frac{i\alpha}{K}, 1, i(Kx - \underline{K}.\underline{x}) \right], \qquad (7.3.6)$$

with $\alpha = a Z_1$ and $N(K) = \exp\left( \frac{\pi\alpha}{2K} \right) \Gamma\left( 1 - \frac{i\alpha}{K} \right)$.

From (5) and (2.3.2), it follows that

$$\langle \chi_m | \Phi_i \rangle = \delta( \underline{k}_i + \underline{K} - a\underline{k} ) \, G_{n'l'} ( b\underline{k}_i - \underline{K} ), \qquad (7.3.7)$$

where $G_{n'l'}(\underline{t}) = \int \Psi_{n'l'}(\underline{r}) \exp( i\underline{t}.\underline{r} ) \, d\underline{r}$.

Using (6) and (7) in (3), it can be seen that

$$\begin{aligned} \omega_{13}^{+} \Phi_i &= (2\pi)^{-3} \int d\underline{k} \int d\underline{K} \; N(K) \exp\{ i(\underline{K}.\underline{x} + \underline{k}.\underline{\rho}) \} G_{n'l'} ( b\underline{k}_i - \underline{k} ) \\ &\qquad \delta( \underline{k}_i + \underline{K} - a\underline{k} ) \, {}_1F_1\left[ \frac{i\alpha}{K}, 1, i(Kx - \underline{K}.\underline{x}) \right] \\ &= (2\pi a)^{-3} \int d\underline{K} \; N(K) G_{n'l'} \left( \underline{k}_i (b - 1/a) - 1/a \, \underline{K} \right) \exp ( -i\underline{x}.\underline{k}_i \\ &\qquad \exp\left( \frac{i}{a} (\underline{k}_i + \underline{K}).\underline{r} \right) {}_1F_1\left[ \frac{i\alpha}{K}, 1, i(Kx - \underline{K}.\underline{x}) \right], \end{aligned} \qquad (7.3.8)$$

where the relation

$$\delta( \underline{k}_i + \underline{K} - a\underline{k} ) = \frac{1}{a^3} \, \delta\left( \frac{1}{a} (\underline{k}_i + \underline{K}) - \underline{k} \right)$$

has been used to obtain the final result.

If (2.3.10) and (8) are used in (1), and the order of integration is changed, then

$$I_{23} = -(2\pi a)^{-3}\int d\underline{K}\; N(K)\, G_{n'l'}\left(\underline{k}_i\left(b-{}^1\!/_a\right)-{}^1\!/_a\,\underline{K}\right) \qquad (7.3.9)$$

$$\times\int d\underline{x}\int d\underline{r}\; \psi^*_{nl}(\underline{x})\,\frac{1}{r}\,\exp\left\{i\left(\underline{p}.\underline{x}+\frac{1}{a}(\underline{K}-\underline{p}).\underline{r}\right)\right\}\,{}_1F_1\left[\frac{i\alpha}{K},1,i(Kx-\underline{K}.\underline{x})\right].$$

Now, $\quad \underline{k}_i\left(b-{}^1\!/_a\right)-{}^1\!/_a\,\underline{K} = \underline{q}-\underline{t},$

where $\quad \underline{t} = \frac{1}{a}(\underline{K}-\underline{p}).$

Since $\quad \int \frac{d\underline{r}}{r}\exp(-i\underline{t}.\underline{r}) = \frac{4\pi}{t^2},$

(9) becomes

$$I_{23} = -\frac{1}{2\pi^2a^3}\int d\underline{K}\;\frac{1}{t^2}\,N(K)\,G_{n'l'}(\underline{q}-\underline{t})\,\mathcal{J}(\underline{K},nl,\underline{p}), \qquad (7.3.10)$$

where

$$\mathcal{J}(\underline{K},nl,\underline{p}) = \int d\underline{x}\;\psi^*_{nl}(x)\exp(i\underline{p}.\underline{x})\,{}_1F_1\left[\frac{i\alpha}{K},1,i(Kx-\underline{K}.\underline{x})\right]. \qquad (7.3.11)$$

Similarly, using the result

$$\int\frac{d\underline{r}}{|\underline{r}-\underline{x}|}\exp(i\underline{t}.\underline{r}) = \frac{4\pi}{t^2}\exp(i\underline{t}.\underline{x}),$$

$I_{12}$ can be written as

$$I_{12} = \frac{Z_1}{2\pi^2a^3}\int d\underline{K}\;\frac{N(K)}{t^2}\,G_{n'l'}(\underline{q}-\underline{t})\,\mathcal{J}(\underline{K},nl,\underline{p}') \qquad (7.3.12)$$

where $\underline{p}' = \underline{p} + \underline{t}$. $\qquad$ (7.3.13)

If the quantity of interest is the total cross section for capture into a state with given values of n and l, then the wave functions can be referred to a reference frame OXYZ in which the Z-axis is taken to be in the direction of $\underset{\sim}{p}$, and the X - Z plane is the plane of $\underset{\sim}{p}$ and $\underset{\sim}{k}_i$. The evaluation of the cross section involves an integration over all values of the momentum transfer $\underset{\sim}{p}$. With this choice of axes, the total cross section for capture into a state with a given value of l is the sum of the results obtained using the wave functions of the various magnetic substates in turn in (11), but the separate results do not have a direct physical meaning. Of course, for capture into s states there is no difficulty because the wave functions are spherically symmetric.

If cross sections for capture into the separate magnetic substates are required, then the final state wave functions must be referred to a fixed system of axes, usually chosen with the polar axis in the direction of the incident beam. The method of evaluation of these cross sections from the results obtained using the other system of axes is described in the next section.

In order to carry out the $\underline{K}$ - integration in the frame OXYZ, spherical polar coordinates $(K, \nu, \gamma)$ are introduced.

The function $\mathcal{J}(\underset{\sim}{K}, nl, \underset{\sim}{p})$ must be evaluated separately for each final state considered since it depends on the final state wave function. The analysis is given in Appendix 1 and the results are summarised here. For capture into an s state, $\mathcal{J}(\underset{\sim}{K}, ns, \underset{\sim}{p})$ is a function of K and $\nu$ but is independent of the azimuthal angle $\gamma$.

For capture into p states

$$\mathcal{J}(\underline{K}, np_z, \underline{\rho}) = \sin\beta\ \mathcal{J}'(\underline{K}, np_x, \underline{\rho}) + \cos\beta\ \mathcal{J}'(\underline{K}, np_z, \underline{\rho}),$$

$$\mathcal{J}(\underline{K}, np_y, \underline{\rho}) = \cos\gamma\ \mathcal{H}(\underline{K}, np_x, \underline{\rho}),$$

$$\mathcal{J}(\underline{K}, np_x, \underline{\rho}) = -\sin\gamma\ \mathcal{H}(\underline{K}, np_x, \underline{\rho}), \qquad (7.3.14)$$

where

$$\mathcal{H}(\underline{K}, np_x, \underline{\rho}) = \cos\beta\ \mathcal{J}'(\underline{K}, np_x, \underline{\rho}) - \sin\beta\ \mathcal{J}'(\underline{K}, np_z, \underline{\rho}), \qquad (7.3.15)$$

and $\cos\beta = {}^{1}/_{\lambda}\,(p - K\cos\nu).$

The functions $\mathcal{J}'(\underline{K}, nl, \underline{\rho})$ depend on K and $\nu$ but are independent of $\gamma$. The exact form depends on the values of n and l, but may always be written

$$\mathcal{J}'(\underline{K}, nl, \underline{\rho}) = N_{nl}\left(\frac{c - id}{T}\right)^{-i\alpha/K}\left(\frac{A_0}{T} + \frac{A_1}{T^2} + \frac{A_2}{T^3} + \frac{A_3}{T^4}\right)$$

where

$$c = \beta^2 + \lambda^2 - K^2, \qquad d = 2\beta K,$$
$$\lambda = at, \qquad \beta = \alpha/n,$$
$$T = \beta^2 + \rho^2.$$

The constants $N_{nl}$ and the functions $A_i$ (i = 0, 1, 2, 3) are given in the appendix.

For convenience, define

$$\mathcal{H}(\underline{K}, ns \text{ or } np_z, \underline{\rho}) \equiv \mathcal{J}(\underline{K}, ns \text{ or } np_z, \underline{\rho}). \qquad (7.3.16)$$

The Fourier transform of the initial state is easily evaluated. The wave functions are

$$\psi_{1s}(\underline{r}) = \frac{b^{3/2}}{\pi^{1/2}} e^{-br}$$

and

$$\psi_{2s}(\underline{r}) = \frac{b^{3/2}}{4 . 2^{1/2} \pi^{1/2}} (2 - br) e^{-br/2} ,$$

so that

$$G_{1s}(\underline{q} - \underline{t}) = \frac{8 \pi^{1/2} b^{5/2}}{\left[ b^2 + (\underline{q} - \underline{t})^2 \right]^2} ,$$

$$G_{2s}(\underline{q} - \underline{t}) = 2^{3/2} \pi^{1/2} b^{5/2} \left\{ \frac{1}{\left( b^2/4 + (\underline{q} - \underline{t})^2 \right)^2} - \frac{b^2/2}{\left( b^2/4 + (\underline{q} - \underline{t})^2 \right)^3} \right\} .$$

It can be shown that

$$b^2 + (\underline{q} - \underline{t})^2 = A + B \cos \gamma \tag{7.3.17}$$

where

$$A = b^2 + v^2 + \frac{K^2}{a^2} - \frac{K}{p} \cos \nu \left( v^2 + b \Delta E + \frac{1}{a^2} (1 - ab) p^2 \right)$$

and

$$B = K^2 (\cos^2 \nu - 1) \left( \frac{(v^2 + b \Delta E)^2}{p^2} + \frac{(1 - ab)^2 p^2}{a^4} \right.$$

$$\left. + \frac{2b(1 - ab) \Delta E}{a^2} - \frac{2(1 + ab) v^2}{a^2} \right) .$$

Let

$$\left(b/_2\right)^2 + \left(\underline{q}-\underline{t}\right)^2 = A' + B\cos\gamma,$$

where $A'$ is obtained from A by replacing the first term by $(b/2)^2$.

Now consider expression (10) for $I_{23}$. The azimuthal integration with respect to $\gamma$ can be done analytically in all cases although it is rather lengthy.

For capture into an s or $p_z$ state, the integral is

$$\int G_{n'l'}\left(\underline{q}-\underline{t}\right)d\gamma\,;$$

for capture into a $p_x$ or $p_y$ state it is

$$\int G_{n'l'}(\underline{q}-\underline{t})\cos\gamma\,d\gamma, \qquad \int G_{n'l'}(\underline{q}-\underline{t})\sin\gamma\,d\gamma$$

respectively. In each case, the result may be written in the form

$$N_{n'l'}\;J(n'l'\,;\,nl)\,,$$

where $n'l'$, nl refer to the initial and final states respectively,

$$N_{1s} = 16\pi^{3/2}b^{5/2}, \qquad N_{2s} = (2\pi)^{3/2}b^{5/2},$$

$$J(1s;\, ns \text{ or } np_z) = A\,(A^2-B^2)^{-3/2},$$

$$J(1s;\, np_x) = -B\,(A^2-B^2)^{-3/2},$$

$$J(2s;\, ns \text{ or } np_z) = 2A'(A'^2-B^2)^{-3/2} - b^2/_2\,(2A'^2+B'^2)(A'^2-B^2)^{-5/2},$$

$$J(2s;\, np_x) = -2B(A'^2-B^2)^{-3/2} + b^2/_2\,(3A'B)(A'^2-B^2)^{-5/2},$$

$$J(1s;\, np_y) = J(2s;\, np_y) = 0.$$

Thus, (10) may be written

$$I_{23} = -\frac{N_{n'l'}}{2\pi^2 a^3}\int_0^\infty dK\, K^2 N(K)\int_{-1}^{+1} d(\cos\nu)\,\frac{1}{t^2}\,J(n'l';nl)\,\mathcal{H}(\underline{K},nl,\underline{p}),$$

where the functions $\mathcal{H}(\underline{k},nl,\underline{p})$ are defined by (15), (16). A similar expression may be obtained for $I_{12}$.

It can easily be shown that $I_{12}$ vanishes in the limit $^1/M \longrightarrow 0$; the proof given here is due to Pradhan (1957). From (13) and the definition of $\underline{t}$ it is clear that

$$\underline{p}' = \underline{p}\left(1-\frac{1}{a}\right) + \frac{1}{a}\underline{K}\,.$$

The first term vanishes as $(^1/M) \longrightarrow 0$, so (12) gives

$$\lim_{1/M\to 0} I_{12} = \frac{Z_1}{2\pi^2}\int d\underline{K}\; N(K)\; G_{n'l'}(\underline{q}-\underline{t})\,\frac{1}{t^2}\int d\underline{x}\;\psi^*_{nl}(\underline{x})\exp(i\,\underline{K}.\underline{x})\,{}_1F_1\left[\frac{i\alpha}{K},1,i(Kx-\underline{K}.\underline{x})\right]$$

However, since $\psi_{nl}(\underline{x})$ and $N(K)\exp(i\underline{K}.\underline{x})\,{}_1F_1\left[\frac{i\alpha}{K},1,i(Kx-\underline{K}.\underline{x})\right]$ are eigenfunctions of the same Hamiltonian corresponding to different eigenenergies, they are orthogonal, so that

$$\lim_{1/M\to 0} I_{12} = 0.$$

Consequently, it seems reasonable to neglect the contribution from $I_{12}$ when calculating electron capture cross sections. Coleman (1965) found by numerical calculations that this assumption is justified. The cross sections quoted in Chapter 8 were all obtained from the expression

$$Q^{IMP}(nl) = \frac{1}{4\pi^2 a v^2}\left(\frac{\mu_f}{\mu_i}\right)\int_{\rho^2_{min}}^{\rho^2_{max}} |I_{23}|^2 \, d(\rho^2).$$

## 4) Evaluation of cross sections for capture into definite magnetic substates.

In the usual notation, the exact transition matrix element is

$$T_{if} = \langle \varphi_f | V_f | \Psi_i^+ \rangle. \tag{7.4.1}$$

Since, in this thesis, only capture from states 1s, 2s of the target hydrogen atom is considered, the wave function $\Psi_i^+$ is independent of the system of axes chosen. In order to calculate cross sections for capture into definite magnetic sublevels of the final atom, the final state wave function must be referred to a fixed system of axes. Usually a reference frame $OX'Y'Z'$ is chosen with axis $OZ'$ in the direction $k_i$, and the $X' - Z'$ plane as the collision plane. In the previous section, matrix elements $I_{23}$ have been calculated using final bound state wave functions referred to a frame OXYZ, with Z-axis along $\underline{p}$ and the X - Z plane the plane of $\underline{p}$ and $\underline{k}_i$.

Now

$$\psi_{nlm}^{\underline{k}_i}(\underline{x}) = \sum_{m'} R^l_{m'm}(\alpha,\beta,\gamma)\, \psi^{f}_{nlm'}(\underline{x}) \tag{7.4.2}$$

where $\psi^{\underline{k}_i}_{nlm}(\underline{r}), \psi^{f}_{nlm}(\underline{r})$ denote wave functions in the frames $OX'Y'Z'$, OXYZ respectively. $R^{l}_{m'm}(\alpha,\beta,\gamma)$ are the elements of the rotation matrix and $\alpha,\beta,\gamma$ are the Euler angles of the rotation which takes OXYZ into $OX'Y'Z'$. In the present case, $\alpha = 0 = \gamma$, $\beta = \cos^{-1} \hat{\underline{p}}.\hat{\underline{k}}_i$. Only capture into s and p states has been considered. For $l = 1$, the elements of the rotation matrix are

$$R^{1}_{00} = \cos\beta \,, \qquad R^{1}_{0\pm1} = \pm\frac{1}{\sqrt{2}}\sin\beta\,\exp(\mp i\gamma)\,,$$

$$R^{1}_{10} = -R^{1}_{-10} = \frac{1}{\sqrt{2}}\sin\beta\,, \tag{7.4.3}$$

$$R^{1}_{\pm11} = \frac{1}{2}\left(1 \pm \cos\beta\right)\exp(-i\gamma) = \left[R^{1}_{\mp1,1}\right]^{*},$$

where the asterisk denotes complex conjugation. Using these in (2), substituting in (1) and writing $T_f$ in place of $T_{if}$ to simplify the notation one obtains

$$T^{\underline{k}_i}_{2p_0} = \frac{1}{\sqrt{2}}\sin\beta\, T^{f}_{2p_{-1}} + \cos\beta\, T^{f}_{2p_0} - \frac{1}{\sqrt{2}}\sin\beta\, T^{f}_{2p_1}\,,$$

$$T^{\underline{k}_i}_{2p_{-1}} = \frac{1}{2}\left(1+\cos\beta\right) T^{f}_{2p_{-1}} - \frac{1}{\sqrt{2}}\sin\beta\, T^{f}_{2p_0} + \frac{1}{2}\left(1-\cos\beta\right) T^{f}_{2p_{+1}}\,,$$

$$T^{\underline{k}_i}_{2p_{+1}} = \frac{1}{2}\left(1-\cos\beta\right) T^{f}_{2p_{-1}} + \frac{1}{\sqrt{2}}\sin\beta\, T^{f}_{2p_0} + \frac{1}{2}\left(1+\cos\beta\right) T^{f}_{2p_{+1}}\,.$$

Now

$$T_{2p_x} = \frac{1}{\sqrt{2}}\left(T_{2p_{-1}} - T_{2p_{+1}}\right),$$

$$T_{2p_y} = \frac{i}{\sqrt{2}}\left(T_{2p_{-1}} + T_{2p_{+1}}\right),$$

$$T_{2p_z} = T_{2p_0}\,.$$

Therefore

$$T_{2p_x}^{\underline{k}_i} = \cos\beta \, T_{2p_x}^{p} - \sin\beta \, T_{2p_z}^{p}, \qquad (7.4.4)$$

$$T_{2p_y}^{\underline{k}_i} = T_{2p_y}^{p} = 0$$

$$T_{2p_z}^{\underline{k}_i} = \sin\beta \, T_{2p_x}^{p} + \cos\beta \, T_{2p_z}^{p}. \qquad (7.4.5)$$

The following relations are also needed;

$$T_{2p_{\pm 1}} = \mp \frac{1}{\sqrt{2}} T_{2p_x}.$$

From this last result it can be seen that

$$Q\,(2p_1) = Q\,(2p_{-1}).$$

Using the equations $\underline{p} = a\underline{k}_f - \underline{k}_i$, and $\Delta E = \frac{\underline{k}_i^2}{\mu_i^2} - \frac{\underline{k}_f^2}{\mu_f^2}$, $\cos\beta$ can be written

$$\cos\beta = -\frac{1}{2pk_i}\left( p^2 + k_i^2 - a^2 \frac{\mu_f}{\mu_i} k_i^2 + a^2 \mu_f \, \Delta E \right).$$

If $M_1 = M_2$, this reduces to

$$\cos\beta = -\left( \frac{av^2 + a^2 \Delta E + p^2/\mu}{2pv} \right).$$

Cross sections for capture into definite magnetic substates $2p_x$, $2p_y$ can be calculated from (7.3.2) using matrix elements $T_{if}$ given by (4) and (5).

5) Numerical methods.

Coleman (1965) calculated cross sections for the following processes:

$$H^+ + H(1s) \longrightarrow H(1s, 2s \text{ or } 2p) + H^+ \qquad (7.5.1)$$

$$He^{++} + H(1s) \longrightarrow He^+(1s, 2s \text{ or } 2p) + H^+, \qquad (7.5.2)$$

His cross sections for capture into the 2p level of the projectile are in error due to an incorrect choice of the axis of quantization for the target atom. The present author has extended his work and has considered the processes

$$H^+ + H(1s) \longrightarrow H(2p) + H^+ \qquad (7.5.3)$$

$$H^+ + H(1s) \longrightarrow H(3s) + H^+ \qquad (7.5.4)$$

$$H^+ + H(1s) \longrightarrow H(3p) + H^+ \qquad (7.5.5)$$

$$H^+ + H(2s) \longrightarrow H(2p) + H^+ \qquad (7.5.6)$$

$$He^{++} + H(1s) \longrightarrow He^+(2p) + H^+ \qquad (7.5.7)$$

$$He^{++} + H(1s) \longrightarrow He^+(3s) + H^+ . \qquad (7.5.8)$$

The numerical methods used to calculate cross sections for processes (3) - (8) are very similar to those used by Coleman for processes (1) and (2). Three numerical integrations are involved, those with respect to $\nu$, K and p.

A Simpson integration procedure was used for the final p integration. Because the probability of a large transfer of momentum from the heavy incident particle to the target nucleus is very slight, $|I_{23}|^2$ falls off very rapidly with increasing p, and it was found to be unnecessary to consider values of p greater than 12. For some processes, an even smaller range was sufficient.

The energies to be used were carefully chosen to simplify the numerical work. For each process considered, the value of $p_{min}$ depends on the incident energy according to the equation

$$p_{min}^2 = \frac{1}{4v^2}\left(v^2 + \Delta E\right)^2,$$

where $\Delta E$ is the appropriate energy defect. For processes (3) - (8) it takes the values

a x (0.75, 8/9, 8/9, 0, 0, 5/9),

respectively.

For (3), the p values and steplengths used were as follows:-

p = 0.87 (0.015) 0.9 (0.05) 1.1 (0.1) 1.5 (0.25) 3.0 (0.5) 6.0 (1.0) 8.0.

The above equation was solved for $v^2$ using these values of p, and the cross section was calculated for a selection of the energies thus obtained. This ensured that $p_{min}$ for each energy coincided with one of the pivot points.

A similar procedure was followed for the other processes. The steplengths used were as follows:-

For (4) and (5),

p = 0.95 (0.025) 1.0 (0.05) 1.1 (0.1) 1.5 (0.25) 3.0 (0.5) 6.0 (1.0) 8.0 (2.0) 12.0.

For (6),

p = 0.2 (0.1) 1.2 (0.2) 2.0 (0.25) 3.0 (0.5) 6.0.

For (7),

p = 0.1 (0.1) 1.2 (0.2) 2.0(0.25) 3.0 (0.5) 6.0.

For (8),

p = 0.75 (0.025) 0.8 (0.05) 1.1 (0.1) 1.5 (0.25 ) 3.0 (0.5) 6.0.

Direct tests on the p integration were not in general possible because of the enormous amount of computer time involved. However, for (3), an indirect test showed that the cross sections were accurate to at least three figures at low energies and that the accuracy was much greater at high energies. It can probably be assumed that for all processes the results given are accurate to three figures.

The integration with respect to $\nu$ was performed using a 96 point Gaussian quadrature formula. Detailed tests showed that this procedure gave at least five figure accuracy in the integration in most cases.

N(K) includes the complex gamma function $\Gamma(1 - i\alpha/K)$. This was evaluated in the following way.

The real part of $\ln \Gamma(1 - i\alpha/K)$ was calculated exactly. The imaginary part of $\ln \Gamma(10 - i\alpha/K)$ was calculated from the first three terms of Stirling's asymptotic series (see Erdélyi vol 1. p 47) and the imaginary part of $\ln \Gamma(1 - i\alpha/K)$ was then obtained by repeated use of the identity $\Gamma(1+z) = z\Gamma(z)$. The routine gives $\Gamma(1 - i\alpha/K)$ correct to seven significant figures.

Simpson's method was used for the K integration. It was found that contributions from the ranges $0 \leq K \leq 0.05$ and $K \geq 100$ were negligible. The range $0.05 \leq K \leq 100$ was split into several parts and the steplengths were chosen to give four or five figure accuracy in each part. Near K = 0.05 a very small steplength was necessary because of the very rapid oscillations of the complex gamma function.

For processes (3), (4), (6), (7), (8), the basic steplengths used were as follows:-

K = 0.05 (0.001) 0.08 (0.0025) 0.14 ( 0.005) 0.20 (0.01) 0.4
(0.025) 1.5 (0.0625) 3.0 (0.125) 7.0 (0.25) 9.0
(0.5) 18.0 (1.0) 30.0 (2.5) 60.0 (5.0) 100.0.

For (5), slightly different values were used.

A detailed investigation showed that for each process it was necessary to decrease the steplength near K = p for each value of p. Tests were made for each case, but in general it was found that if h were the normal steplength, the required accuracy was obtained by using a steplength h/2 for a small range of K below K = p and h/4 for a small range above K = p.

The layout of the calculation was as follows. A value of p was chosen, then a value of K. The integration with respect to $\nu$ was carried out for a number of values of the incident energy and the results were stored in the computer as the first row of a matrix. A second value of K was then chosen, the $\nu$ integration carried out, and the results stored as the second row of the matrix. This procedure was continued until the inner integral had been evaluated for all the required values of K. Each row of the matrix then corresponded to a given value of K and each column to a given value of the energy E. By reading the appropriate column from the store, it was then possible to evaluate the K - integral and thus obtain a value for $T_{if}$. When $T_{if}$ had been evaluated for all the required energies, a new value of p was chosen and the entire procedure repeated. A separate programme was used for the p integration, the calculated values of $T_{if}$ being fed in as data.

## Chapter 8.

## RESULTS

### 1) Electron capture by protons in hydrogen.

Cross sections for processes (7.5.1), calculated by Coleman (1965), and (7.5.3), (7.5.4), (7.5.5), calculated by the present author, are presented in tables (1), (2) and (3), and graphically in figs (1) to (8), where they are compared with the results of other theories, and with experimental results where possible.

The derivation of the impulse approximation involves the assumption that for the duration of the collision the binding forces of the target are unimportant. One would expect this to be so when the speed of the projectile is greater than the orbital speed of the bound electron. For protons incident on hydrogen atoms in their ground state, this implies an incident energy greater than 25 kev. In general, it is found that at energies above 25 kev, $Q^{IMP}$ (nl) lies below the results of all other theories. The exception is $Q^{IMP}$ (2p) which is greater than $Q_8^{H}$ (2p) of Wilets and Gallaher (Chapter 5 § 3) for some energies below 50 kev.

For the resonant process, the calculation of Coleman differed from that of Cheshire (1963) only in the numerical methods used, and confirmed Cheshire's results. At 25 kev, the Born and impulse approximation results are in close agreement, but $Q^{IMP}$ (1s) falls off more rapidly as the energy increases.

Fig (3) shows that neither $Q^{IMP}$ (2s) nor $Q^{B}$ (2s) is in good agreement with the experimental results. Although $Q_8^{H}$ (2s) does agree well, it should be remembered that adding in more states altered the cross section somewhat at 9 kev.

It is clear from fig. (5) that $Q^{IMP}$ (2p) and $Q_8^{S}$ (2p) are in close agreement with the experimental results of Stebbings et al (1962) but the validity of these results is questionable (see Chapter 1 § 4). Again, the close coupling results show a definite lack of convergence. Figs. (6), (7) compare various theoretical results. The behaviour of $Q_2^{S}$ (2p) of McElroy (1963) at high energies is rather surprising. One would expect it to tend to $Q^{BK}$ but it is almost equal to $Q^{B}$ at 800 kev.

Values of $Q^{IMP}$ (3s) and $Q^{IMP}$ (3p) are listed in table (3) and are compared with the corresponding Born approximation results in fig. (8). The relative behaviour of the s and p cross sections in the two approximations is quite different. $Q^{IMP}$ (3p) is less than $Q^{IMP}$ (3s) at all energies whereas whereas $Q^{B}$ (3p) is greater than $Q^{B}$ (3s) in the energy range 5 kev to 80 kev. A similar result is observed for the 2s and 2p cross sections.

Cross sections for the process

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

calculated using the impulse approximation, are given in table (4). No other theoretical values for the process are known to the present author. The cross section behaves at low energies in a manner typical of symmetric resonance, increasing rapidly as the energy decreases.

The reaction is of interest particularly in the field of astrophysics.

The rate at which metastable hydrogen atoms in the 2s state decay spontaneously to the ground state is very slow, since the transition is optically forbidden. The double process in which hydrogen atoms in the 2p state are formed by the above process and then decay spontaneously to the ground state with the emission of Lyman-alpha radiation provides another mechanism by which the 2s level may be depopulated.

## Table 8.1.1

Impulse approximation cross sections, in units of $\pi a_0^2$, for the process $H^+ + H(1s) \longrightarrow H(1s) + H^+$.

| Energy (kev) | Q (1s) |
|---|---|
| 25.0 | 2.19 |
| 36.0 | 9.48,-1 |
| 49.0 | 4.22,-1 |
| 64.0 | 1.93,-1 |
| 81.0 | 9.07,-2 |
| 100 | 4.39,-2 |
| 156 | 8.01,-3 |
| 225 | 1.71,-3 |
| 306 | 4.24,-4 |
| 400 | 1.19,-4 |
| 506 | 3.79,-5 |
| 624 | 1.31,-5 |
| 899 | 2.08,-6 |
| 1224 | 4.04,-7 |
| 1598 | 9.52,-8 |

## Table 8.1.2.

Impulse approximation cross sections Q(nl), in units of $\pi a_0^2$, for capture into the n = 2 level of hydrogen.

| Energy (kev) | Q(2s) | Q(2p) | Q(2)=Q(2s)+Q(2p) |
|---|---|---|---|
| 0.41 | - | 2.16,-3 | - |
| 0.97 | 7.24,-2 | 1.29,-2 | 8.53,-2 |
| 1.89 | 1.87,-1 | 3.51,-2 | 2.22,-1 |
| 2.72 | - | 7.32,-2 | - |
| 4.44 | 4.26,-1 | 1.88,-1 | 6.14,-1 |
| 6.23 | 5.01,-1 | 2.95,-1 | 7.96,-1 |
| 10.7 | 4.95,-1 | 3.84,-1 | 8.79,-1 |
| 15.4 | 4.08,-1 | 3.30,-1 | 7.38,-1 |
| 22.8 | 2.77,-1 | 2.11,-1 | 4.88,-1 |
| 32.8 | - | 1.07,-1 | - |
| 56.2 | 4.75,-2 | 2.39,-2 | 7.14,-2 |
| 79.0 | 1.71,-2 | 7.01,-3 | 2.41,-2 |
| 103 | - | 2.39,-3 | - |
| 129 | 2.95,-3 | 8.89,-4 | 3.84,-3 |
| 156 | - | 3.55,-4 | - |
| 185 | 6.58,-4 | 1.59,-4 | 8.17,-4 |
| 216 | - | 6.87,-5 | - |
| 267 | - | 2.41,-5 | - |
| 284 | - | 1.62,-5 | - |
| 361 | 2.93,-5 | 4.50,-6 | 3.38,-5 |
| 468 | 8.07,-6 | 1.06,-6 | 9.13,-6 |
| 586 | 2.55,-6 | 2.81,-7 | 2.83,-6 |
| 861 | 3.75,-7 | 2.92,-8 | 4.04,-7 |
| 1186 | 7.72,-8 | - | - |
| 2459 | 1.07,-9 | - | - |

## Table 8.1.3.

Impulse approximation cross sections Q(nl), in units of $\pi a_0^2$, for capture into the n = 3 level of hydrogen

| Energy (kev) | Q(3s) | Q(3p) | Q(3s) + Q(3p) |
|---|---|---|---|
| 0.58 | 3.05,-3 | - | |
| 0.85 | 6.80,-3 | | |
| 1.39 | 1.59,-2 | 3.25,-3 | |
| 2.77 | 4.29,-2 | 9.24,-3 | |
| 4.09 | 6.59,-2 | - | |
| 7.09 | 9.84,-2 | - | |
| 11.1 | 1.09,-1 | 7.47,-2 | |
| 17.3 | 9.40,-2 | 7.28,-2 | |
| 28.5 | 5.61,-2 | 4.16,-2 | 9.77,-2 |
| 44.5 | 2.50,-2 | 1.58,-2 | 4.08,-2 |
| 69.4 | 7.84,-3 | 3.88,-3 | 1.17,-2 |
| 120 | 1.20,-3 | 4.25,-4 | 1.63,-3 |
| 178 | 2.50,-4 | 7.00,-5 | 3.20,-4 |
| 260 | 4.45,-5 | 9.74,-6 | 5.42,-5 |
| 354 | 9.94,-6 | 1.79,-6 | 1.17,-5 |
| 460 | 2.68,-6 | 4.03,-7 | 3.09,-6 |
| 518 | 1.43,-6 | - | - |
| 579 | 8.09,-7 | 1.05,-7 | 9.14,-7 |
| 644 | 4.70,-7 | - | - |
| 854 | 1.09,-7 | 1.07,-8 | 1.19,-7 |
| 1179 | 1.93,-8 | - | - |
| 2453 | 3.36,-10 | - | - |

### Table 8.1.4

Impulse approximation cross sections, in units of $\pi a_0^2$, for the process process $H^+ + H(2s) \rightarrow H(2p) + H^+$.

| Energy (kev) | Q (2s - 2p) |
|---|---|
| 4.00 | 2.13, 1 |
| 8.99 | 2.56 |
| 16.0 | 7.90,-1 |
| 25.0 | 2.93,-1 |
| 36.0 | 9.46,-2 |
| 48.9 | 2.88,-2 |
| 63.9 | 8.90,-3 |
| 80.9 | 2.87,-3 |
| 99.9 | 9.82,-4 |
| 144 | 1.40,-4 |
| 256 | 5.53,-6 |
| 400 | 4.14,-7 |
| 624 | 2.87,-8 |
| 899 | 3.22,-9 |

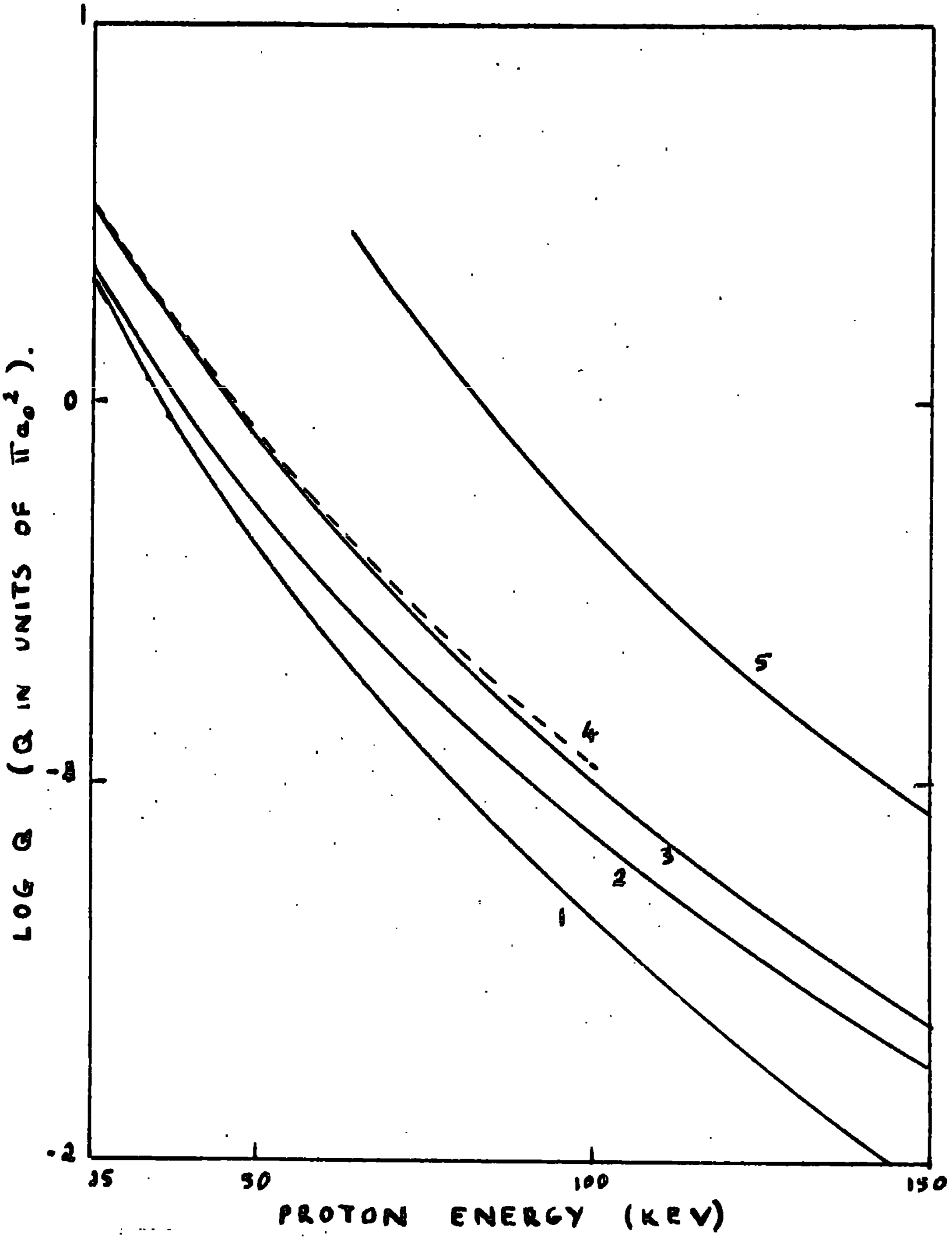


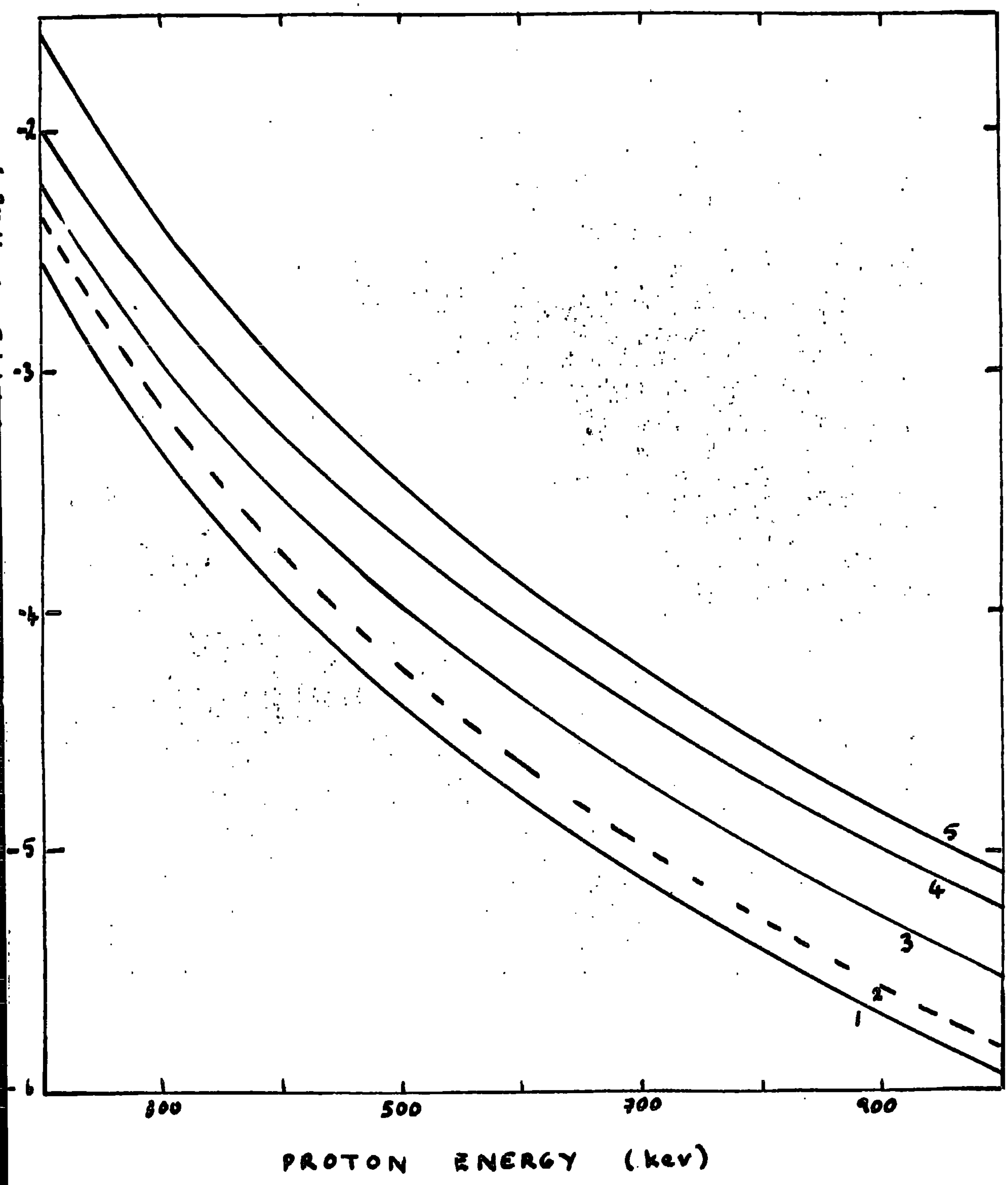
Fig. 8.1.1. Cross sections for $H^+ + H(1s) \rightarrow H(1s) + H^+$.

Curve 1; $Q^{IMP}$ Curve 2; $Q^{B}$

Curve 3; $Q_B^{S}$ Curve 4; $Q_B^{H}$

Curve 5; $Q^{BK}$.

Curves 3 and 4 are taken from Table (6.3.1);
Curves 2 and 5 are taken from Tables (3.3.3) and (3.3.2).



ig. 8.1.2. Cross sections for $H^+ + H(1s) \rightarrow H(1s) + H^+$

Curve 1 ; $Q^{IMP}$ Curve 2 ; $Q^{CD}$

Curve 3 ; $Q^{B}$ Curve 4; $Q_2^{b}$

Curve 5 ; $Q^{BK}$

Curves 3, 4, 5 are plotted from table (5.2.1)

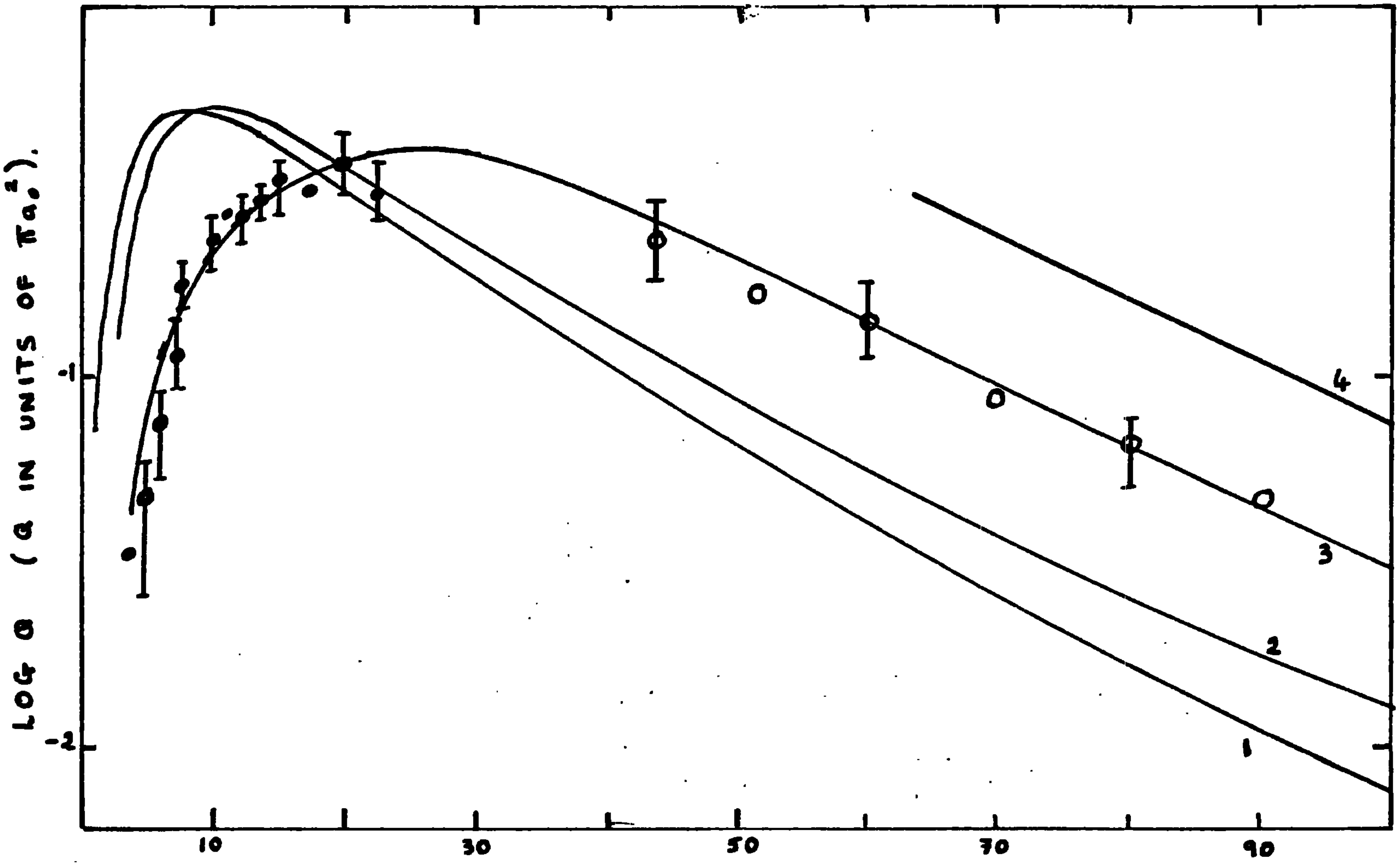


Fig 8.1.3. Cross sections for $H^+ + H(1s) \rightarrow H(2s) + H^+$.
Curve 1; $Q^{IMP}$, Coleman (1965); Curve 3; $Q_B^H$, Wilets and Gallaher (1966);
Curve 2; $Q^B$, Bates and Dalgarno (1953), Mapleton (1962); Curve 4; $Q^{BK}$, Mapleton (1962).
● experiment (Bayfield 1968).
○ experimental results of Ryding et al. (1966) normalised by Gaily (1968b).

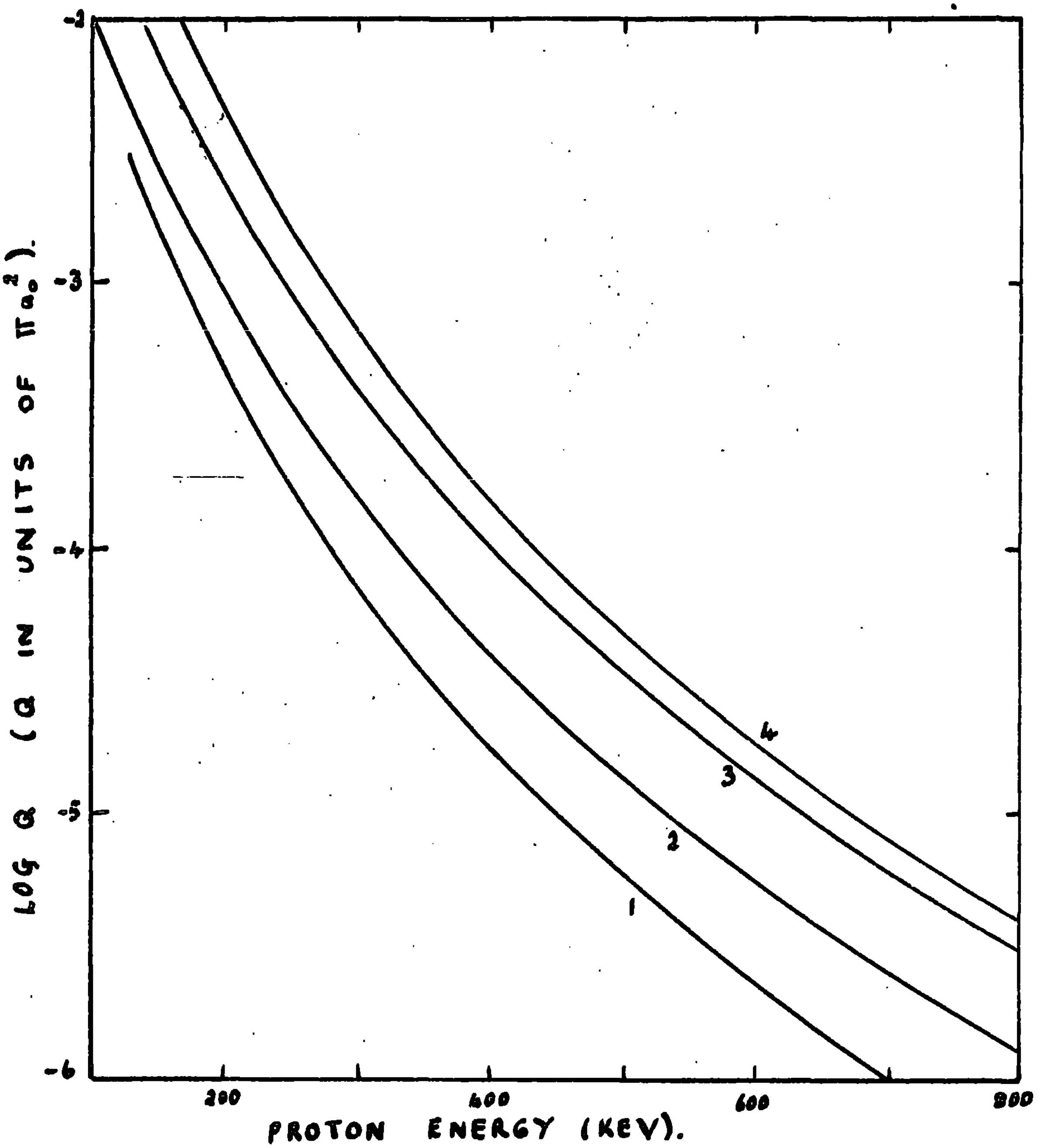


Fig. 8.1.4. Cross sections for $H^+ + H(1s) \rightarrow H(2s) + H^+$.

Curve 1; $Q^{IMP}$, Coleman (1965)

Curve 2; $Q^B$, Mapleton (1962)

Curve 3; $Q_2^S$, McElroy (1963)

Curve 4; $Q^{BK}$, Mapleton (1962).

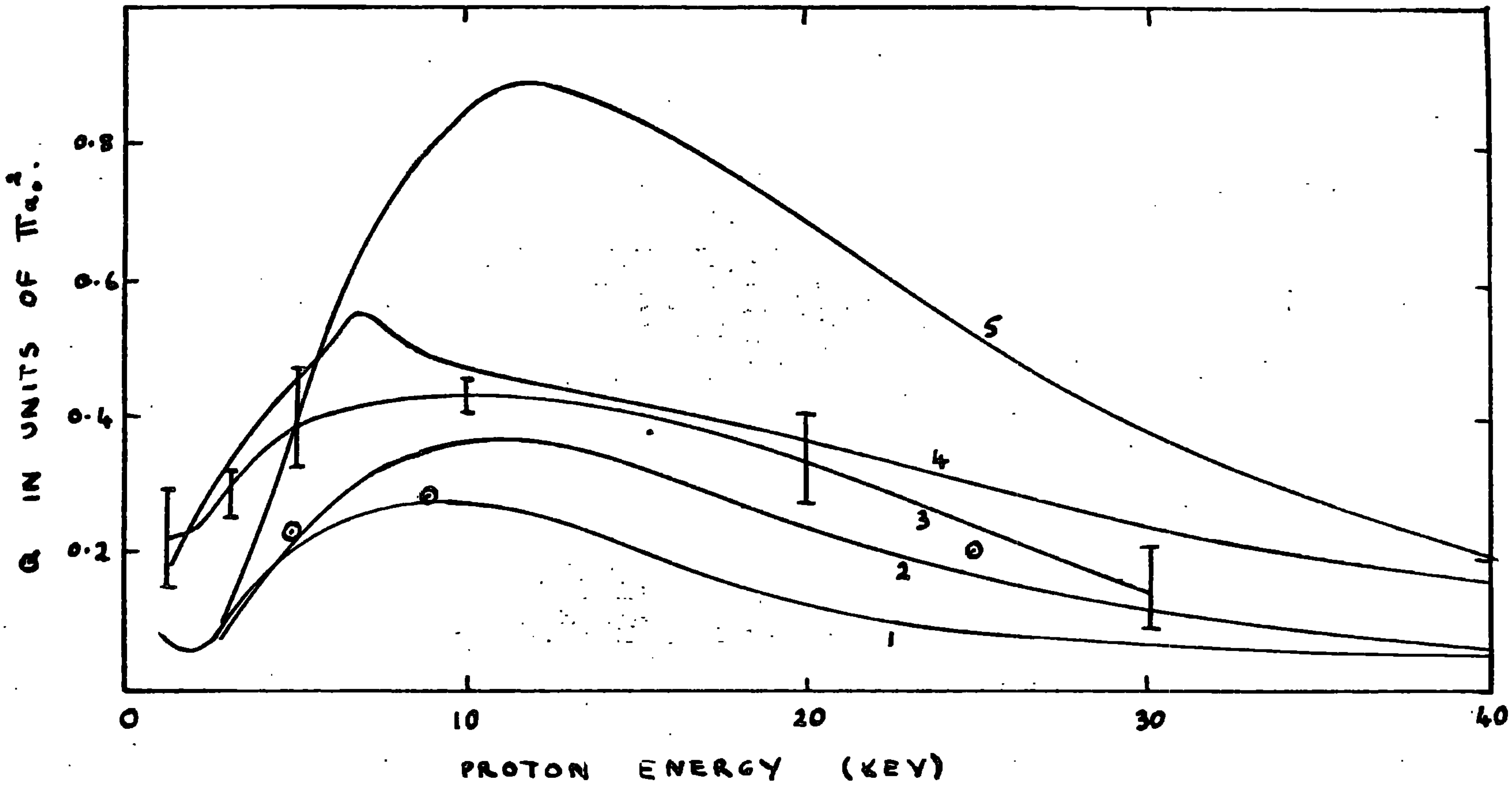


Fig. 8.1.5. Cross sections for $H^+ + H(1s) \rightarrow H(2p) + H^+$.

Curve 1; $Q_8^H$, Wilets and Gallaher (1966).
Curve 2; $Q^{IMP}$, present work.
Curve 3; Experiment, Stebbings et. al (1965).
Curve 4; $Q_8^S$, Gallaher and Wilets (1968).
Curve 5; $Q^B$, Bates and Dalgarno (1953)
⊙ $Q_{16}^S$, Gallaher and Wilets (1968).

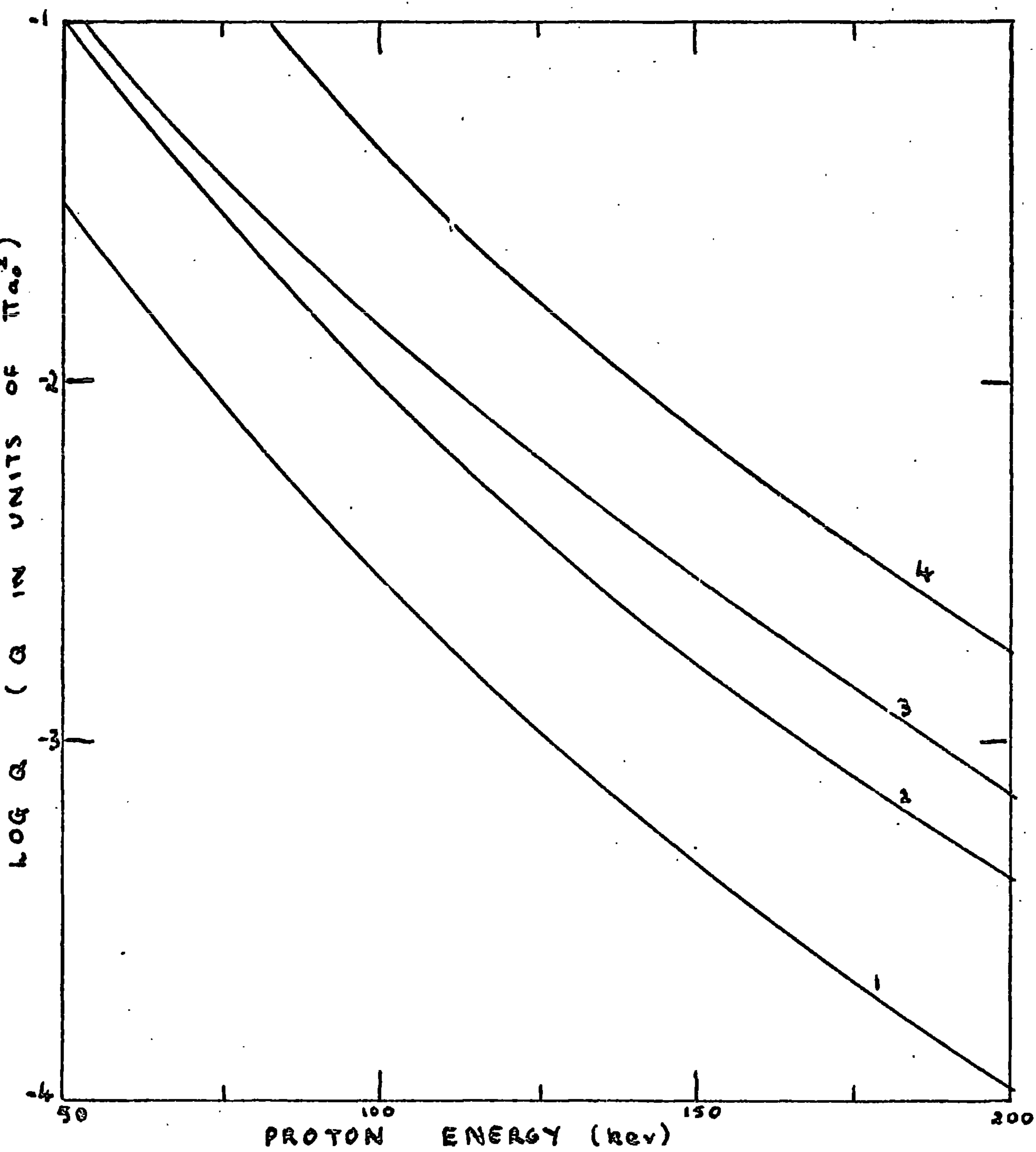


Fig 8.1.6.

Cross sections for $H^+ + H(1s) \rightarrow H(2p) + H^+$

Curve 1; $Q^{IMP}$, present work

Curve 2; $Q^{B}$, Mapleton (1962)

Curve 3; $Q_2^{S}$, McElroy (1963)

Curve 4; $Q^{BK}$, Mapleton (1962)

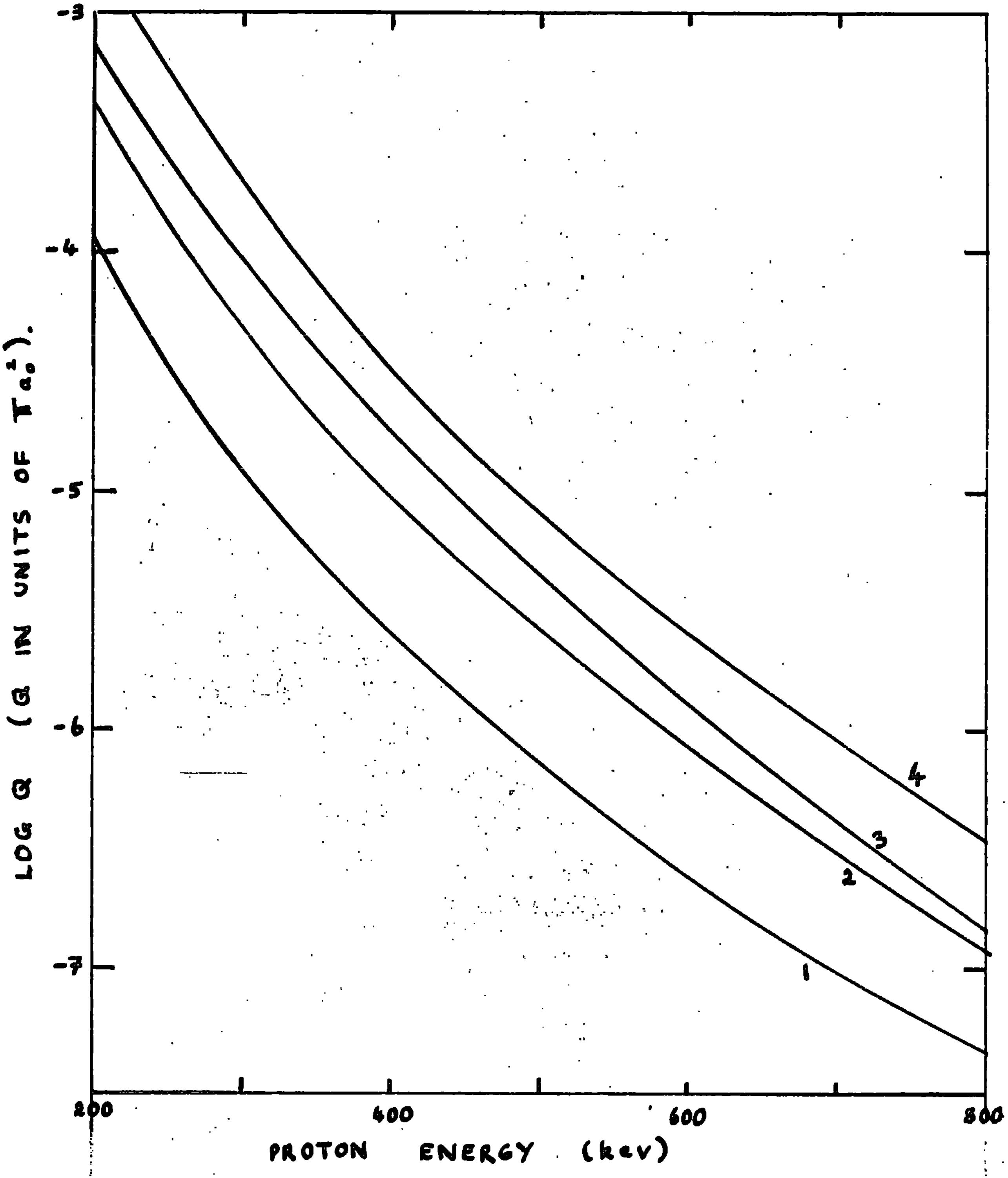


Fig 8.1.7. Cross sections for $H^+ + H(1s) \rightarrow H(2p) + H^+$.
Curve labels as in fig 8.1.6.

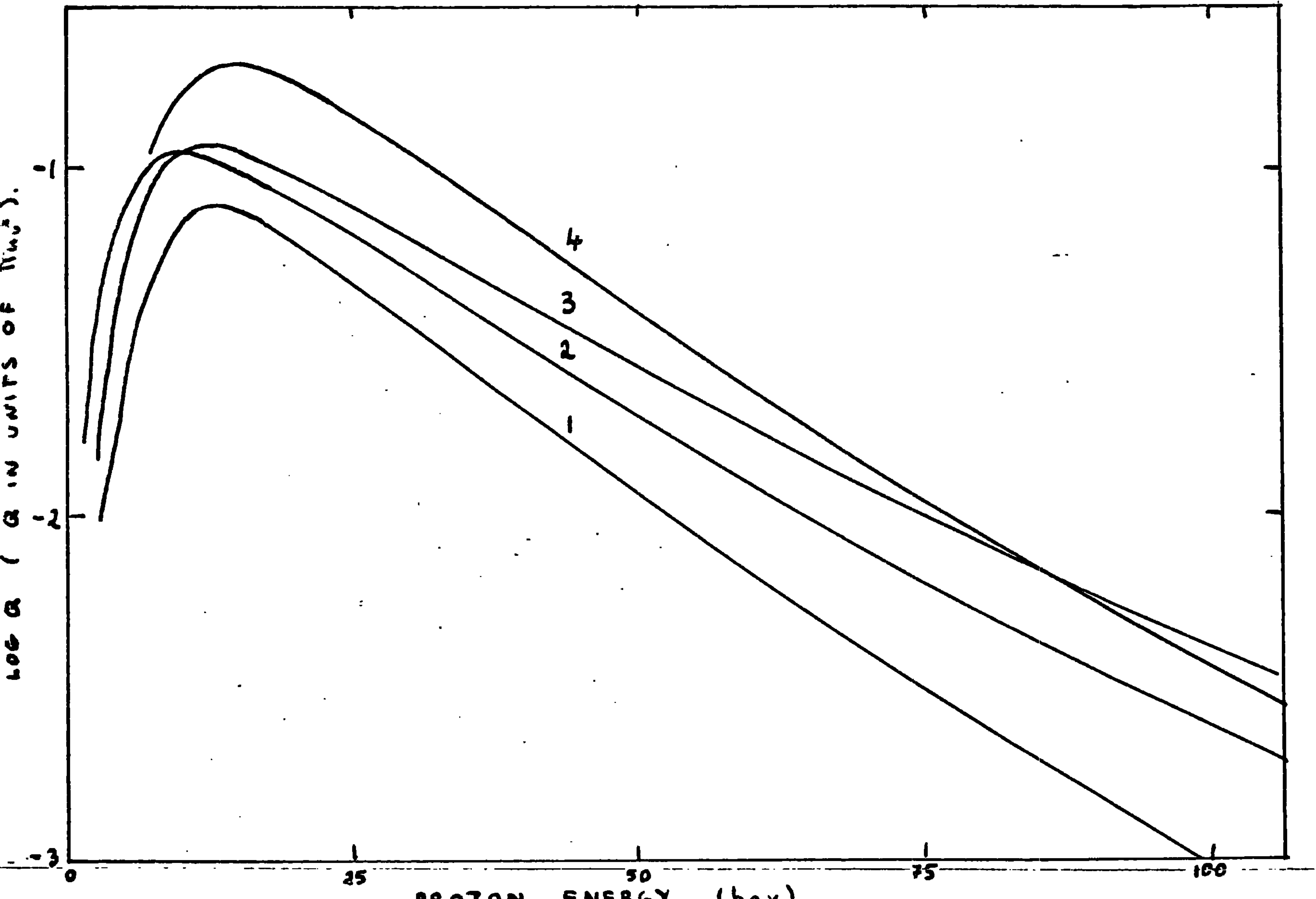


Fig 8.1.8. Cross sections for $H^+ + H(1s) \longrightarrow H(3s \text{ or } 3p) + H^+$.
Curve 1 ; $Q^{IMP}(3p)$ , Curve 2 ; $Q^{IMP}(3s)$ , present work.
Curve 3 ; $Q^{B}(3s)$ , Curve 4 ; $Q^{B}(3p)$, Bates and Dalgarno (1953).

2) Ratios and total cross sections.

It was shown in Chapter 3 § 3 that, for the Born approximation, an estimate of the cross section for capture into an excited state with quantum numbers n and l could be obtained from (3.3.9);

$$Q^{B}(nl) = \frac{Q^{B}(1s)}{Q^{BK}(1s)}\, Q^{BK}(nl)\,.$$

One of the reasons for performing the present calculations was to see whether it could be assumed that

$$Q^{IMP}(nl) = \frac{Q^{IMP}(1s)}{Q^{BK}(1s)}\, Q^{BK}(nl)\,. \tag{8.2.1}$$

If (1) holds, then so does the relation

$$Q^{IMP}(n) = \frac{Q^{IMP}(1s)}{Q^{BK}(1s)}\, Q^{BK}(n)\,, \tag{8.2.2}$$

where Q (n) denotes the total cross section for capture into a state with principal quantum number n. (2) implies that the ratio

$$R^{IMP}(n) = \frac{Q^{IMP}(n)}{Q^{IMP}(1s)}$$

tends to $n^{-3}$ as the energy of the projectile increases.

The ratios R(2s), R(2p), R(3s), R(3p) given by the OBK, Born and impulse approximations are compared in figs (1), (2). For capture into s states, the agreement between $R^{IMP}$ and $R^{BK}$ is excellent, even down to energies of 200 kev. For this reason, $R^B(2p)$ and $R^B(3p)$ are not shown in figs (1) and (2). $R^{IMP}$ is in reasonable agreement with the other two at energies above 700 kev. It is clear that use of (1), (2) slightly overestimates the true value of $Q^{IMP}$ (nl) in each case.

The evaluation of $Q^{IMP}$ (3d) would require an enormous amount of computer time and has not been undertaken. Using the OBK approximation, it is found that the contribution of $Q^{BK}$ (3d) to the cross section for capture into the n = 3 level is approximately 7% at 60 kev, 3% at 120 kev, 1.5% at 200 kev, and considerably less at higher energies. These figures indicate that capture into the 3d state is unimportant except at low energies. For this reason the ratio R (3) has been taken to be

$$R(3) = R(3s) + R(3p)$$

in the present discussion.

Fig (3) compares the ratios R (2), R (3) given by the OBK, Born and impulse approximations. In both cases they are in good agreement at energies above 500 kev but the approach to the limit $n^{-3}$ is very slow, and it is clear that the $n^{-3}$ rule applied to the 1s cross section considerably underestimates the cross sections for capture into the n = 2, 3 states. Therefore, it is probably more accurate to base estimates of total capture cross sections on the assumption that (2) holds for all n, rather than use this rule.

Then
$$Q^{IMP}(\Sigma) = Q^{IMP}(1s) + Q^{IMP}(2) + Q^{IMP}(3) + \frac{Q^{IMP}(1s)}{Q^{BK}(1s)} \sum_{n=4}^{\infty} Q^{BK}(n) \,. \qquad (8.2.3)$$

The sum of the OBK cross sections can be evaluated to any required degree of accuracy using the sum rule of May (1964) (see 3.1.11). Total cross sections, $Q^{1}(\Sigma)$, calculated from (3), are given in table (1).

Since (2) slightly overestimates the true impulse approximation cross section, particularly at low energies, a better estimate of $Q^{IMP}(n)$, for $n \geqslant 4$, might be

$$Q^{IMP}(n) = \frac{Q^{IMP}(3)}{Q^{BK}(3)} \; Q^{BK}(n). \qquad (8.2.4)$$

Total cross sections obtained using (4) are denoted by $Q^{2}(\Sigma)$ in table (1). As expected, $Q^{2}(\Sigma)$ is slightly less than $Q^{1}(\Sigma)$.

In figs (4), (5) several theoretical estimates of total cross sections are compared with experimental results. Values of $Q^{B}(\Sigma)$ were obtained by applying the $n^{-3}$ rule to the results of Mapleton. Values of $Q_{2}^{s}(\Sigma)$ were calculated by McElroy using (5.2.18). The experimental values of Stier and Barnett (1956) and Barnett and Reynolds (1958) are half the cross sections obtained from measurements on molecular hydrogen and lie above the results of Wittkower et al (1966) at energies above 50 kev. The well-known fact that predictions of the first Born approximation agree best with the experimental results is obvious from the figures. Values of $Q^{IMP}(\Sigma)$ lie below the experimental results and the difference increases with increasing energy.

## Table 8.2.1

Cross sections in units of $\pi a_0^2$ for $H^+ + H(1s) \rightarrow H + H^+$.

| Energy (kev) | $Q^1(\Sigma)$ | $Q^2(\Sigma)$ |
|---|---|---|
| 56 | 4.23,-1 | 4.03,-1 |
| 79 | 1.44,-1 | 1.39,-1 |
| 128.8 | 2.43,-2 | 2.37,-2 |
| 185.5 | 5.38,-3 | 5.31,-3 |
| 361.5 | 2.51,-4 | 2.50,-4 |
| 468 | 7.08,-5 | 7.05,-5 |
| 587 | 2.27,-5 | 2.26,-5 |

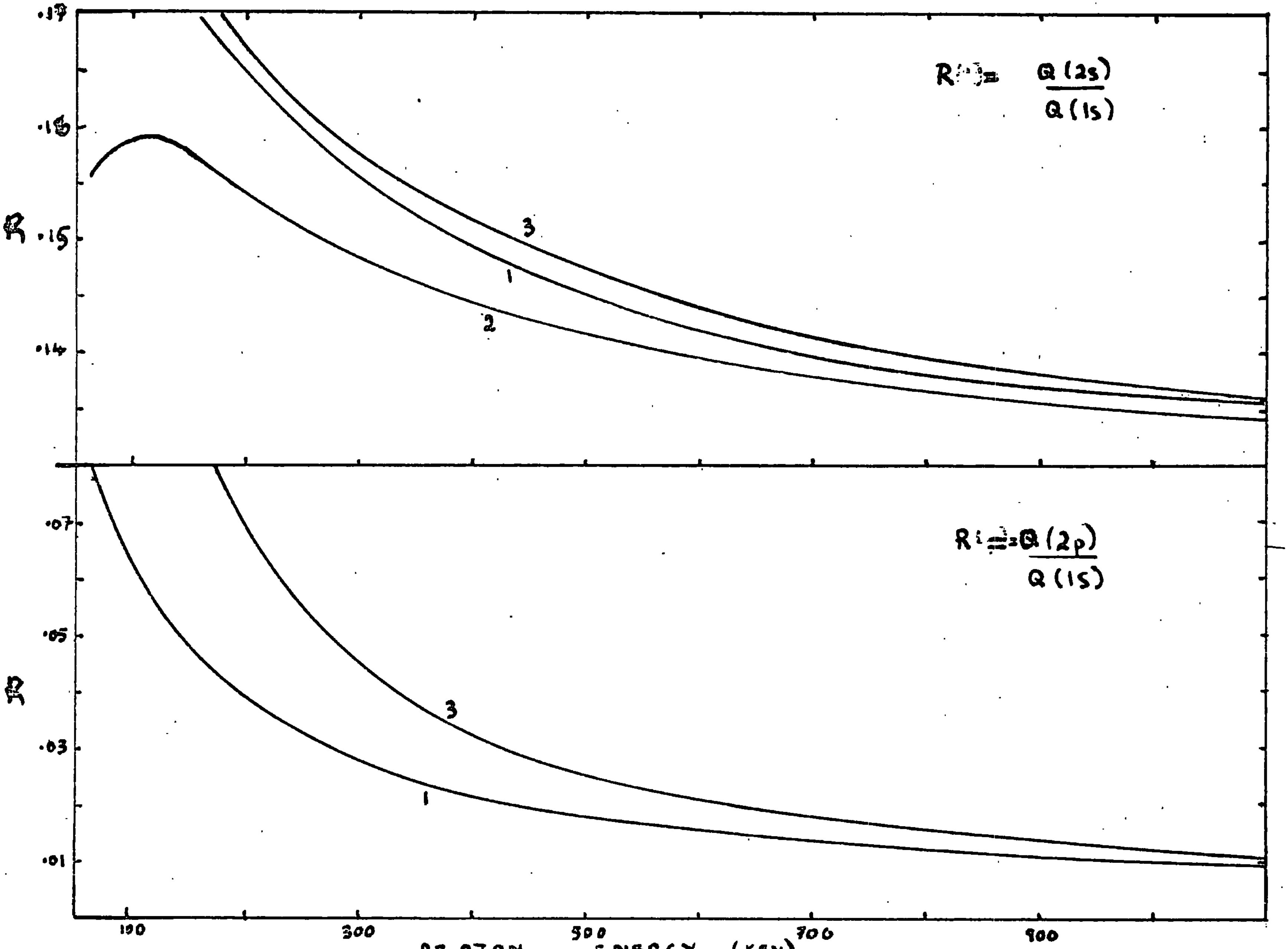


Fig 8.2.1. Cross section ratios for proton impact.
Curve 1; $R^{IMP}$ ; Curve 2; $R^{B}$; Curve 3; $R^{BK}$.

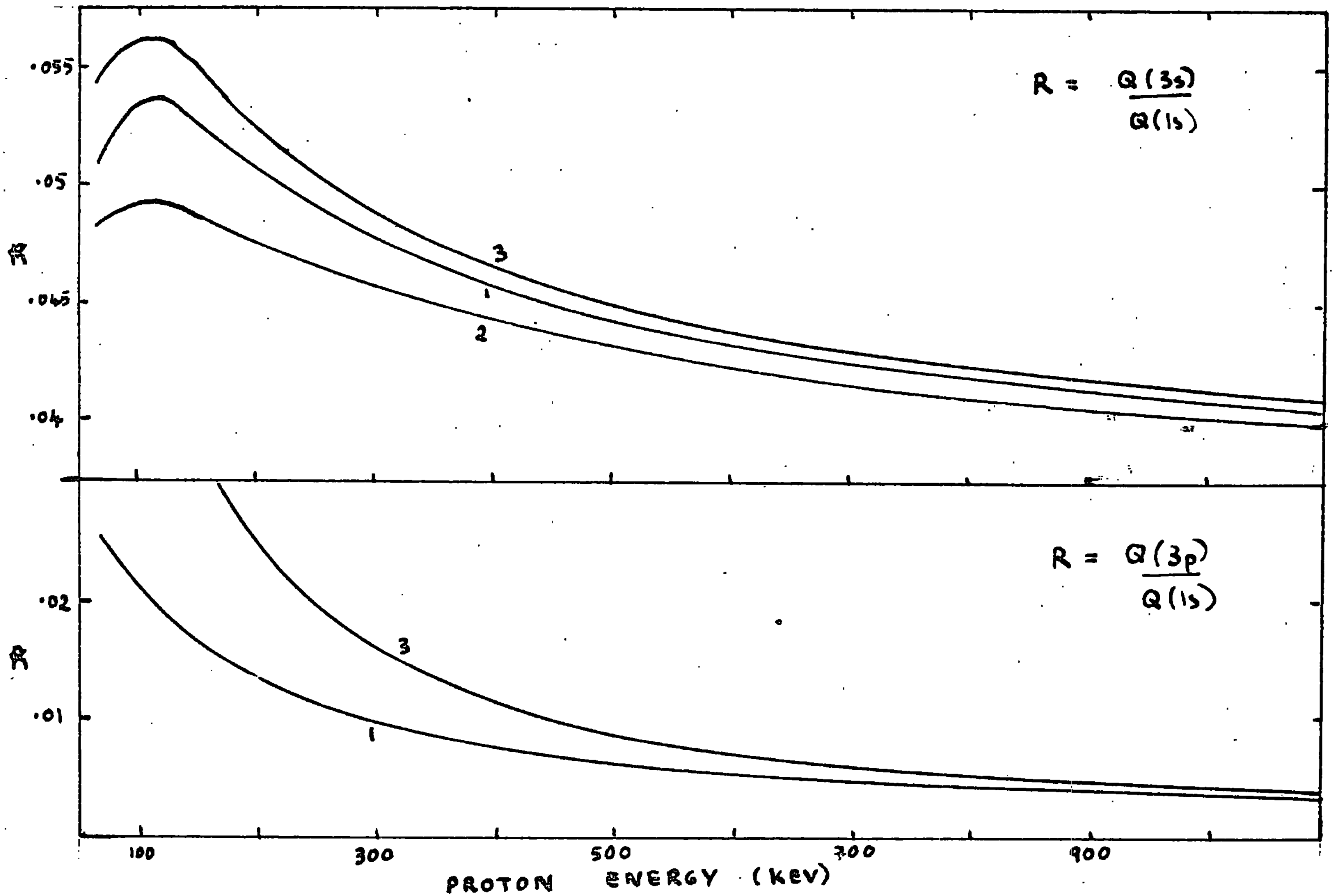


Fig 8.2.2. Cross section ratios for proton impact.
Curve labelling as in fig (8.2.1).

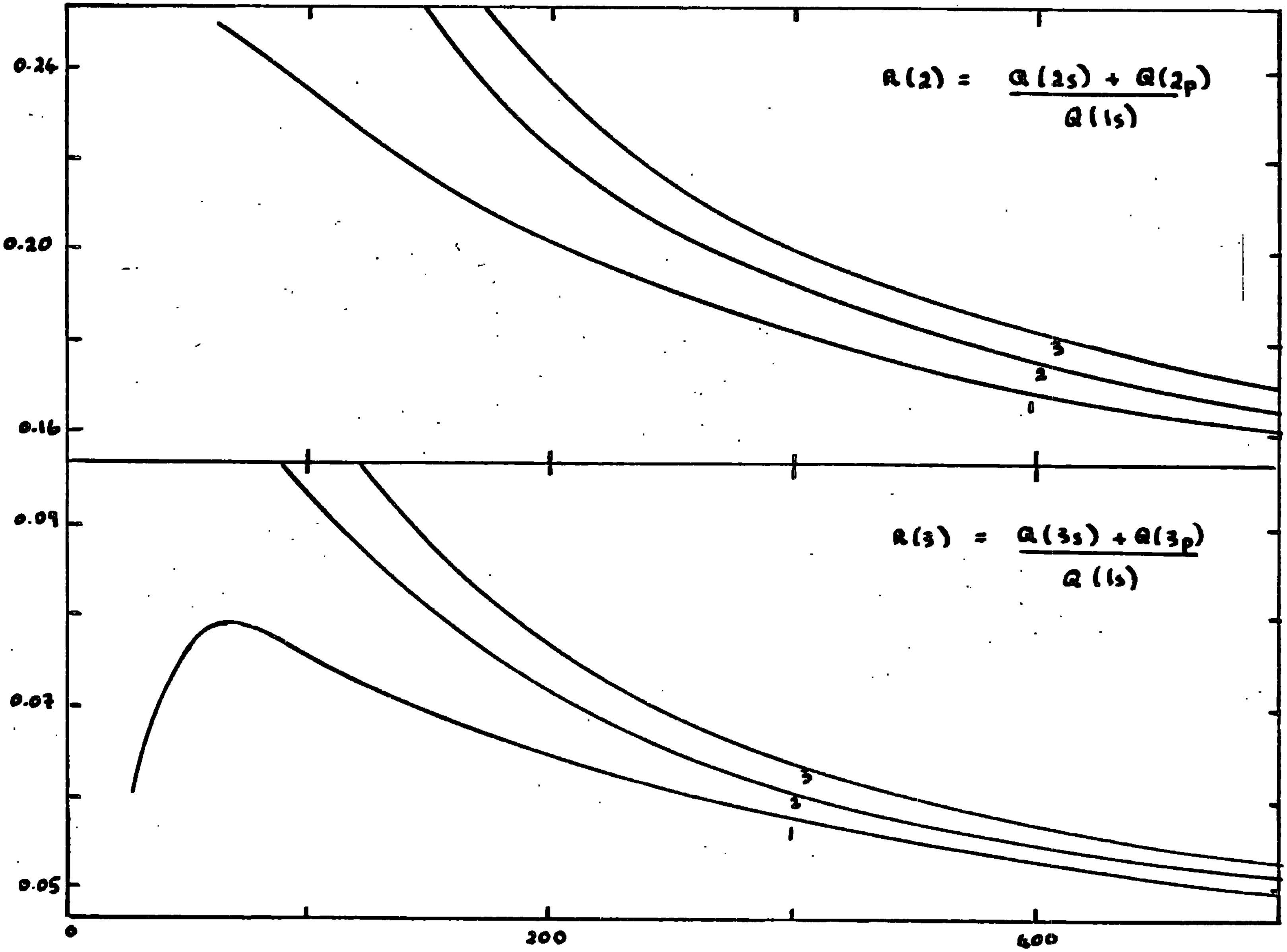


Fig 8.2.3. Cross section ratios for proton impact.

Curve labels as in Fig 8.2.1.

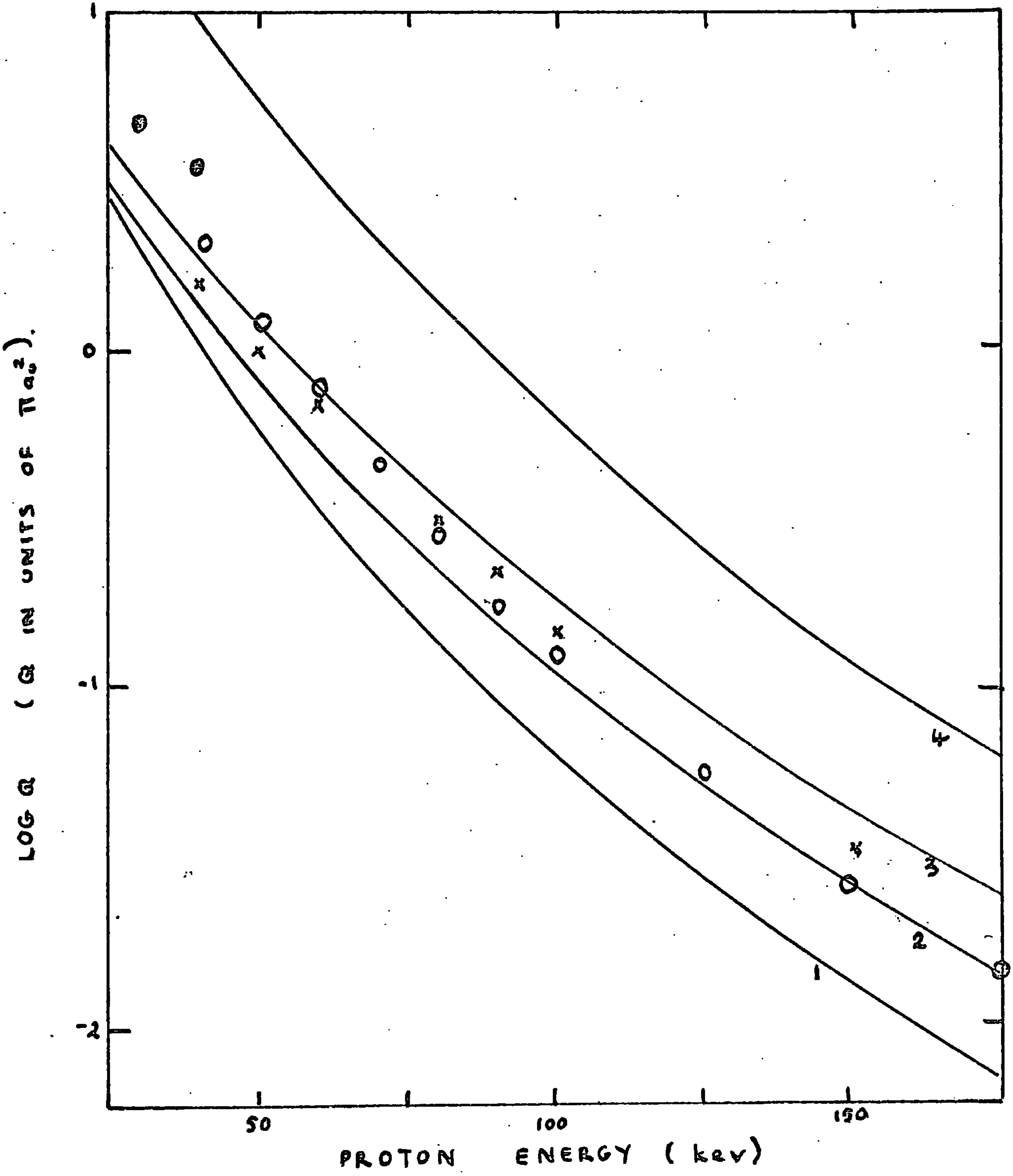


Fig 8.2.4. Cross sections for $H^+ + H(1s) \rightarrow H + H^+$

1.) $Q^{IMP}(\Sigma)$ ; 2) $Q^{B}(\Sigma)$ ; 3). $Q_2^{S}(\Sigma)$ ; 4) $Q^{BK}(\Sigma)$.

x Stier and Barnett (1956) ; ⊗ Fite et al. (1960);

o Wittkower et. al (1966)

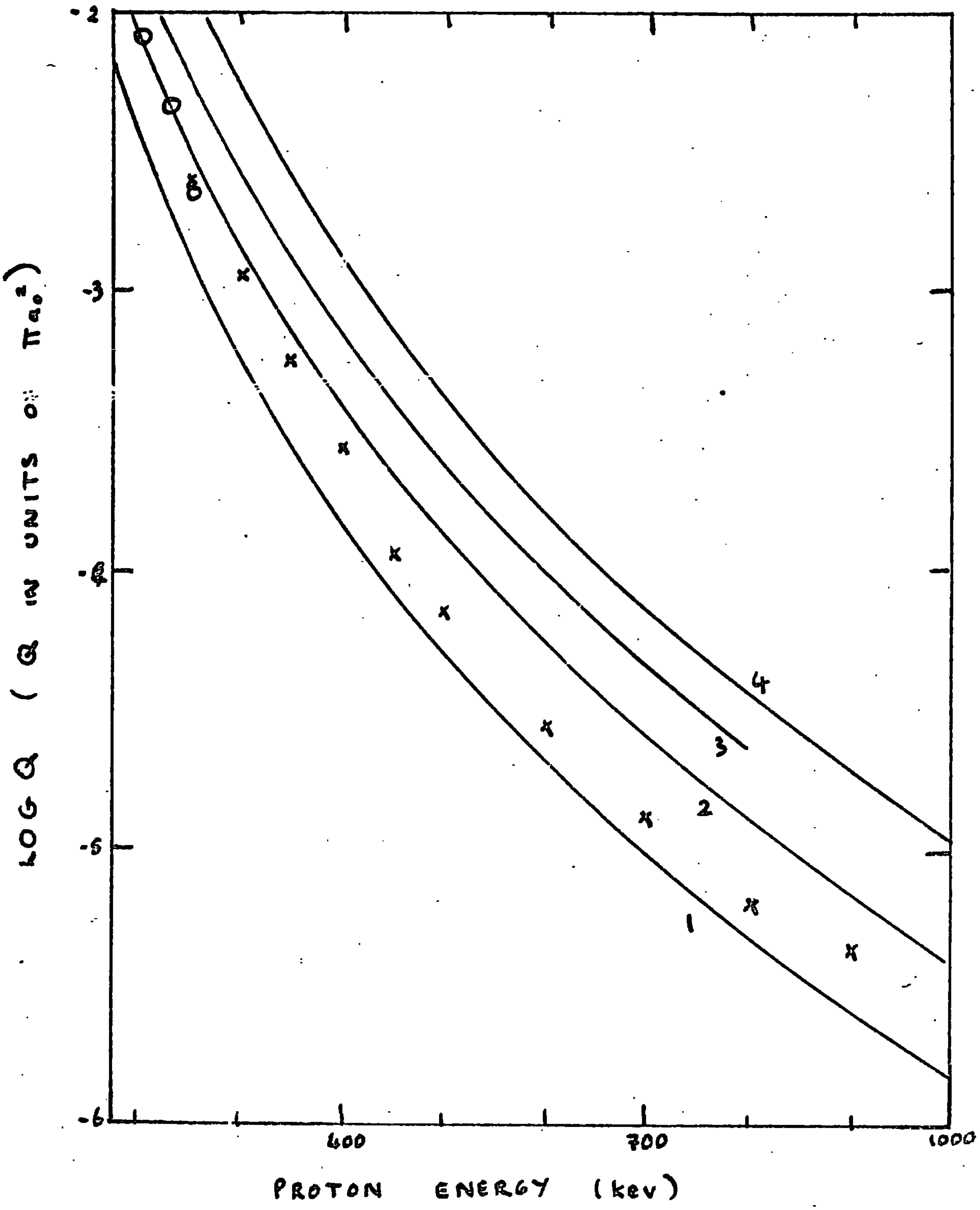


Fig 8.2.5. Cross sections for $H^+ + H(1s) \rightarrow H + H^+$

1) $Q^{IMP}(\Sigma)$; 2) $Q^{B}(\Sigma)$; 3) $Q_2^{S}(\Sigma)$; 4.) $Q^{BK}(\Sigma)$

x Barnett and Reynolds (1958)

o Wittkower et al (1966)

## 3) Electron capture by alpha particles in hydrogen.

Coleman (1965) considered the reactions

$$He^{++} + H\,(1s) \longrightarrow He^{+}\,(1s) + H^{+}, \qquad (8.3.1)$$

$$He^{++} + H\,(1s) \longrightarrow He^{+}\,(2s) + H^{+}, \qquad (8.3.2)$$

and the present author has extended his calculations to the processes

$$He^{++} + H\,(1s) \longrightarrow He^{+}\,(2p) + H^{+}, \qquad (8.3.3)$$

$$He^{++} + H\,(1s) \longrightarrow He^{+}\,(3s) + H^{+}. \qquad (8.3.4)$$

Results are given in tables (1), (2) and the cross sections are compared in figs (1) and (2).

Processes (2) and (3) are examples of accidental resonance. A defect of the present work is that the impulse approximation, in the form used, fails to take account of the effects of the Coulomb repulsion in the final state. For this reason, Q (2s) and Q (2p) behave at low energies in a manner typical of symmetric resonance, whereas, if proper allowance for distortion were made, the cross sections would tend to zero as the energy decreased. Below 50 kev, Q (3s) is larger than Q (1s). This is not surprising since at these low energies resonant effects are important and the energy defect for (4) is smaller than that for (1).

The two state approximation results of McElroy (1963), $Q_2^{\delta}$ (2p) are compared with $Q^{IMP}$ (2p) in fig (3). However, the exact distortion term (5.2.8) was not used by McElroy, and the effect of this on the values of the cross sections is not yet known. At high energies, where the effects of continuum intermediate states become important, the impulse approximation should be the more accurate.

Fig. (4) shows the relative behaviour of R (2) = Q (2) / Q (1s) given by the OBK, Born and impulse approximations. The OBK and Born ratios have already been discussed (Chapter 3 § 3). As expected, the difference between $R^{BK}$ (2) and $R^{IMP}$ (2) is considerable at low energies. At high energies there is a marked departure from the $n^{-3}$ rule which predicts the value 0.125 for R (2).

Assuming that

$$Q^{IMP}(n) = \frac{Q^{IMP}(2)}{Q^{BK}(2)} \; Q^{BK}(n) , \qquad n \geqslant 3,$$

an estimate of total cross sections for capture into all excited states of $He^+$ can be obtained:

$$Q^{IMP}(\Sigma) = Q^{IMP}(1s) + Q^{IMP}(2) + \frac{Q^{IMP}(2)}{Q^{BK}(2)} \sum_{n=3}^{\infty} Q^{BK}(n).$$

Values calculated from this relation are given in table (3). Experimental results are at present available only for energies below 36 kev (Fite et al 1962) and the impulse approximation cannot be expected to be reliable at such low energies where distortion due to the final state Coulomb repulsion is important.

# Table 8.3.1

Impulse approximation cross sections Q(nl), in units of $\pi a_0^2$, for the process $He^{++} + H(1s) \rightarrow He^{+}(nl) + H^{+}$.

| Energy (kev) | Q (1s) | Energy (kev) | Q (3s) |
|---|---|---|---|
| | | 1.29 | 5.10,-2 |
| | | 3.93 | 1.81,-1 |
| 6.00 | 1.27,-3 | 5.52 | 2.07,-1 |
| | | 8.46 | 2.08,-1 |
| | | 11.1 | 1.92,-1 |
| | | 15.6 | 1.67,-1 |
| 29.3 | 3.73,-2 | 25.9 | 1.32,-1 |
| 41.6 | 6.90,-2 | 44.0 | 1.02,-1 |
| 62.5 | 1.27,-1 | 69.4 | 8.13,-2 |
| 100 | 2.07,-1 | | |
| 123 | 2.30,-1 | 119 | 6.52,-2 |
| 152 | 2.38,-1 | | |
| 190 | 2.24,-1 | 197 | 4.72,-2 |
| 212 | 2.10,-1 | | |
| 267 | 1.70,-1 | 277 | 3.07,-2 |
| 337 | 1.25,-1 | | |
| 377 | 1.03,-1 | 364 | 1.85,-2 |
| 423 | 8.33,-2 | | |
| 474 | 6.58,-2 | | |
| 530 | 5.09,-2 | 559 | 6.07,-3 |
| 591 | 3.86,-2 | | |
| 732 | 2.10,-2 | 784 | 1.96,-3 |
| 899 | 1.09,-2 | 1110 | 5.00,-4 |
| 1436 | 1.95,-3 | 1486 | 1.39,-4 |
| 2156 | 3.53,-4 | 2386 | 1.46,-5 |

Table 8.3.2

Impulse approximation cross sections Q(nl), in units of $\pi a_0^2$, for the process $He^{++} + H(1s) \rightarrow He^{+}(nl) + H^{+}$.

| Energy (kev) | Q (2s) | Q (2p) | Q(2s) + Q(2p) |
|---|---|---|---|
| 4.0 | 1.51, 1 | 5.95, 1 | 7.46, 1 |
| 16.0 | 2.69 | 1.78, 1 | 2.05, 1 |
| 36.0 | 6.76,-1 | 9.22 | 9.90 |
| 64.0 | 2.33,-1 | 5.42 | 5.65 |
| 99.9 | 1.59,-1 | 3.12 | 3.28 |
| 144 | 1.43,-1 | 1.68 | 1.82 |
| 196 | 1.20,-1 | 8.60,-1 | 9.80,-1 |
| 256 | 8.91,-2 | 4.24,-1 | 5.13,-1 |
| 324 | 6.09,-2 | 2.06,-1 | 2.67,-1 |
| 400 | 3.93,-2 | 9.92,-2 | 1.39,-1 |
| 576 | - | 2.37,-2 | - |
| 624 | 1.16,-2 | - | - |
| 784 | - | 6.07,-3 | - |
| 899 | 3.25,-3 | - | - |
| 1023 | - | 1.67,-3 | - |
| 1224 | 9.46,-4 | - | - |
| 1599 | 2.94,-4 | 1.64,-4 | 4.58,-4 |
| 2023 | 9.80,-5 | - | - |
| 2498 | 3.57,-5 | 1.36,-5 | 1.13,-4 |
| 3597 | - | 1.65,-6 | - |

## Table 8.3.3.

Cross sections for $He^{++} + H\ (1s) \rightarrow He^{+} + H^{+}$.

| E(kev) | 99.9 | 144 | 196 | 256 | 400 | 576 | 784 | 1023 |
|---|---|---|---|---|---|---|---|---|
| Q | 8.9 | 5.4 | 3.1 | 1.6 | 4.4,-1 | 1.3,-1 | 4.2,-2 | 1.4,-2 |

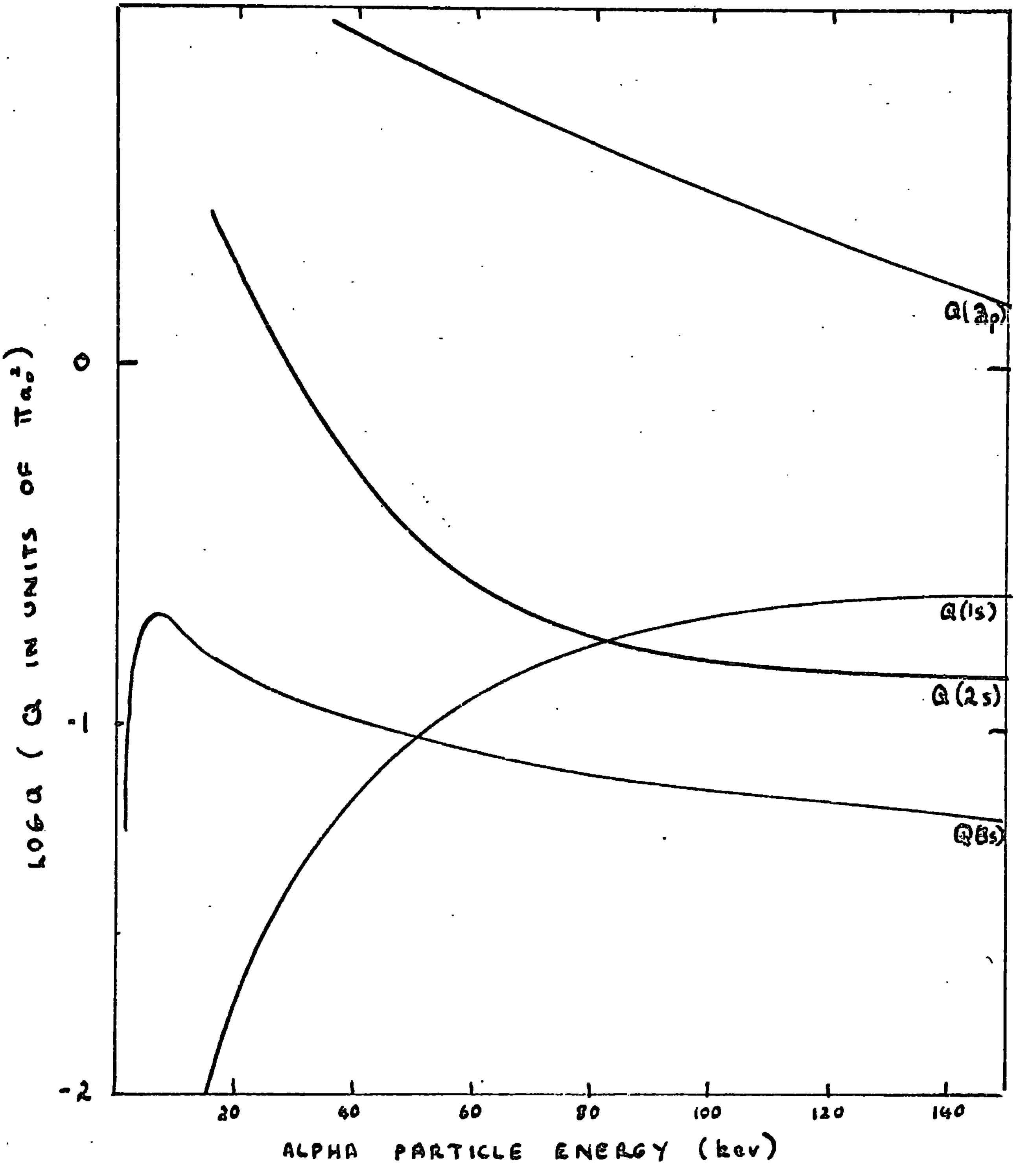


Fig 8.3.1, Impulse approximation cross sections $Q(nl)$ for $He^{++} + H(1s) \rightarrow He^{+}(nl) + H^{+}$

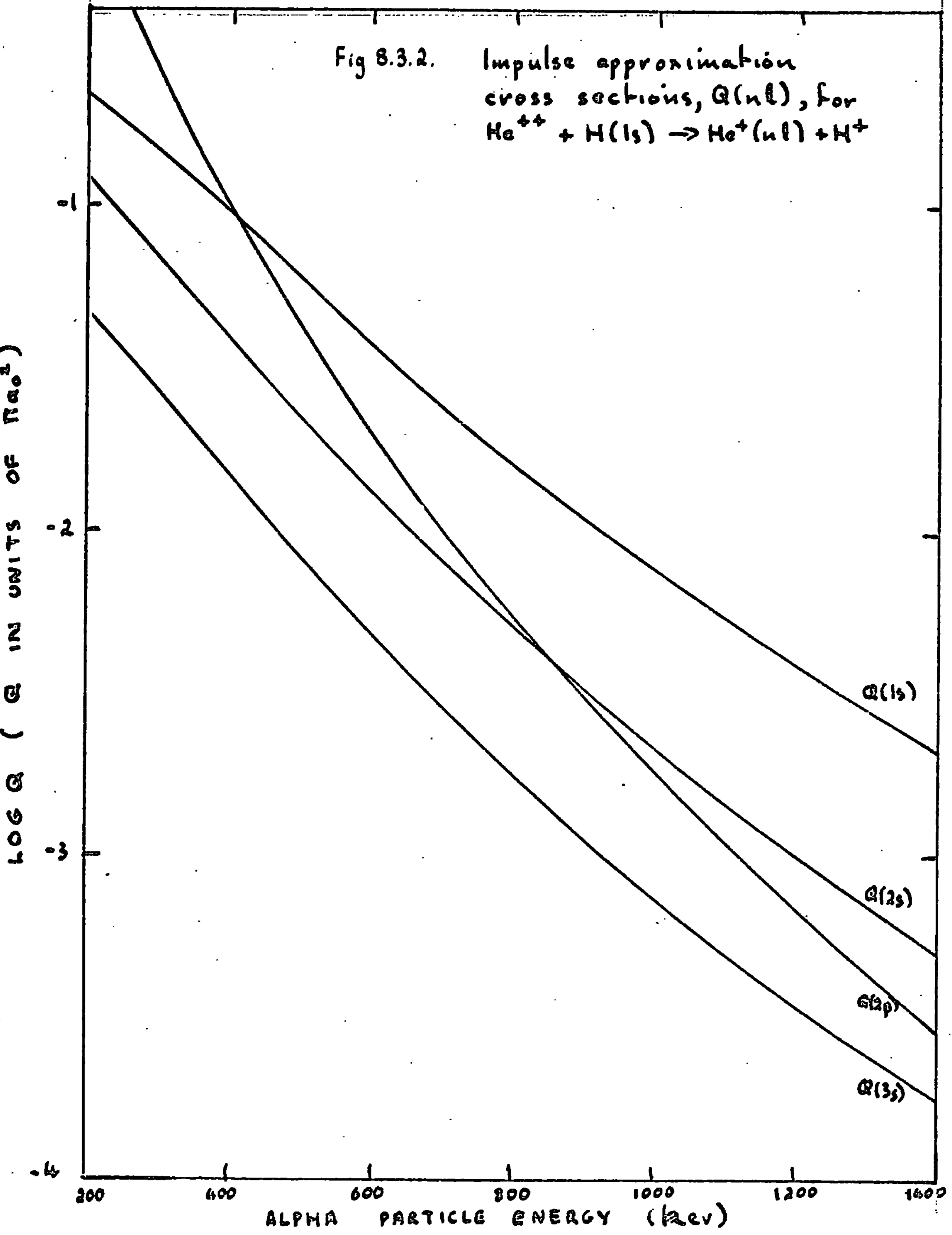


Fig 8.3.2. Impulse approximation cross sections, Q(nl), for $He^{++} + H(1s) \rightarrow He^{+}(nl) + H^{+}$

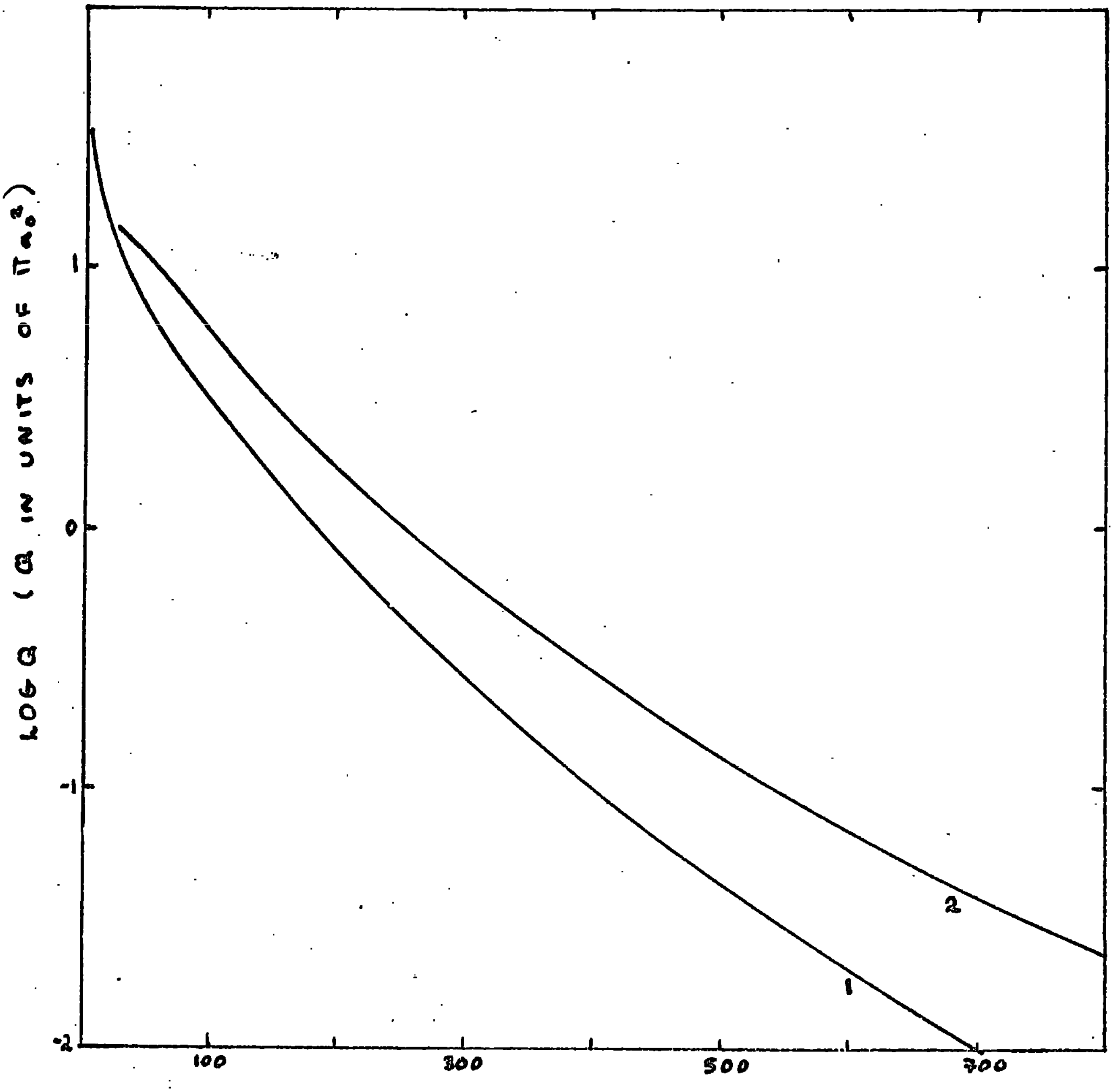


Fig 8.3.3. Cross sections for $He^{++} + H(1s) \rightarrow He^{+}(2p) + H^{+}$

Curve 1; $Q^{IMP}$, present work
Curve 2; $Q_2^{S}$, McElroy (1963)

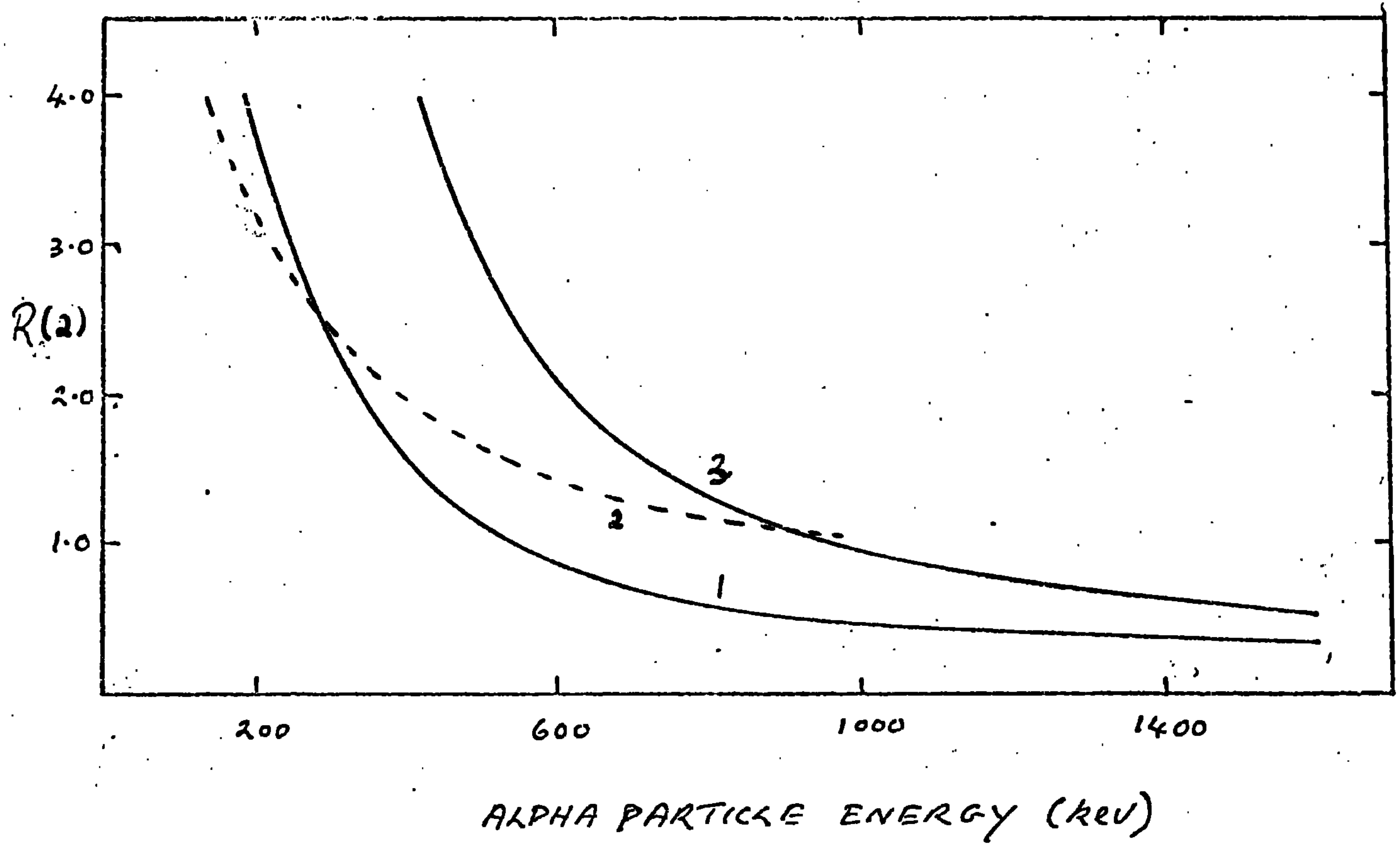


Fig 8.3.4. The ratio $R(2) = \frac{Q(2)}{Q(1s)}$ for alpha particle impact.

Curve 1; impulse approximation
Curve 2; Born approximation, Schiff (1954).
Curve 3; OBK approximation.

## 4) Polarization.

It is observed experimentally that when a gas is excited by a unidirectional beam of particles, the radiation subsequently emitted is polarized and has a non-uniform angular distribution. The degree of polarization is usually determined by viewing the radiating gas atoms in a direction at right angles to the incident beam. For example, suppose the incident beam is in the direction $Oz$. Consider light propagating in the $Ox$ direction. Let $I^{\parallel}$ and $I^{\perp}$ be the intensities of light with electric vector parallel and perpendicular to $Oz$ respectively. The polarization is defined to be

$$p = \frac{I^{\parallel} - I^{\perp}}{I^{\parallel} + I^{\perp}} \qquad (8.4.1)$$

For convenience, the discussion is now restricted to Lyman-alpha radiation emitted by hydrogen atoms excited by collisions with a charged beam of particles. The phenomena of polarization can be explained as follows.

If the hydrogen atoms are initially in their ground state, they are spherically symmetric. The anisotropy of the problem is introduced entirely through the motion of the incident particles. One therefore considers excitation of the states $2p_0$, $2p_{\pm 1}$ of the hydrogen atom, where 0, ± 1 refer to the values of the magnetic quantum number m defined with respect to axis of quantization in the direction of the incident beam. The excited states have cylindrical symmetry so it is not necessary to distinguish between the states $2p_{+1}$ and $2p_{-1}$ , and the angular distribution of the resulting radiation will also possess such symmetry.

From the conservation laws of angular momentum it follows that the transitions $2p_{\pm 1} \rightarrow 1s$ and $2p_0 \rightarrow 1s$ are accompanied by the emission of a photon in a direction parallel to and perpendicular to Oz, respectively. One would therefore expect

$$\frac{I^{\perp}}{I^{\parallel}} = \frac{Q\,(2p_{\pm 1})}{Q\,(2p_0)} = x \qquad (8.4.2)$$

and consequently, from (1),

$$P = \frac{1 - x}{1 + x} \,. \qquad (8.4.3)$$

In fact, the above explanation is very crude and no allowance has been made for the effects of the spins of

a) the atomic electron (fine structure)

b) the nucleus of the hydrogen atom (hyperfine structure)

c) the incident particle.

Penney (1932) showed that such effects are important. Percival and Seaton (1958) carried out a detailed calculation and obtained the formula

$$P = \frac{1 - x}{a + bx} \qquad (8.4.4)$$

where x is defined by (2) and a and b are constants which express the effects of the spins.

For the 2p - 1s transition in hydrogen

$$a = 2.375, \quad b = 3.749,$$

so it can be seen that allowance for these effects reduces the polarization to about one third of its uncorrected value.

P depends on the target gas and on the mass and velocity of the incident particles, and in general numerical values can only be obtained by detailed calculations of the cross sections $Q\,(2p_0)$, $Q\,(2p_{\pm 1})$. Fennema (1963) considered the problem of determining the polarization of Lyman-radiation from hydrogen atoms excited by a beam of electrons or other particles. He used the Born approximation to obtain analytic expressions for $Q\,(2p_0)$, $Q\,(2p_{\pm 1})$ and then attempted to represent the resulting expression for P analytically as a function of the mass and energy of the incoming particles by expanding these cross sections in terms of two parameters related to these quantities, and substituting in (4). The values of $P_0$ so obtained decrease from + 0.28 at 1 ev to - 0.24 at 850 kev. These values were used by Stebbings et al (1965) (See Chapter 1 § 4.)

The polarization of the Lyman - α radiation emitted by hydrogen atoms in the 2p state formed by the capture process

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

is also of interest in the analysis of experiments. The present author has used (3) and (4) to calculate values of the polarization $P_0$, P from the OBK cross sections given by van den Bos and de Heer (1967), and cross sections $Q_2^{\delta}$ calculated by McElroy (1963) using the two state approximation.

It should be noted that since $Q\ (2p_y) = 0,\ Q\ (2p_x)\ =\ 2\ Q\ (2p_{\pm 1})$. Results are given in table (1), denoted by $P^{BK}$, $P^{(2)}$ respectively.

It was shown in Chapter 7 § 4 that cross sections for capture into definite magnetic substates can be obtained using the impulse approximation and the results have been used to evaluate $P_o^{IMP}$, $P^{IMP}$, values of which are given in table (2).

Values of P given by the three theories are compared in fig (1). It can be seen that $P^{(2)}$ tends to $P^{BK}$ at high energies, and both take the value 0.339 at 800 kev. $P^{IMP}$ decreases much more rapidly with increasing energy.

## Table 8.4.1.

Polarization for process $H^+ + H(1s) \rightarrow H(2p) + H^+$

| Energy (kev) | OBK approximation van den Bos and de Heer (1967) |  | Two-state approximation McElroy (1963) |  |
|---|---|---|---|---|
|  | $P_\theta^{BK}$ | $P^{BK}$ | $P_\theta^{(2)}$ | $P^{(2)}$ |
| 0.5 | 0.707 | 0.339 | - | - |
| 1 | 0.698 | 0.336 | - | - |
| 5 | 0.661 | 0.326 | - | - |
| 10 | 0.644 | 0.321 | - | - |
| 25 | 0.638 | 0.319 | 0.669 | 0.257 |
| 50 | 0.652 | 0.323 | 0.737 | 0.288 |
| 100 | 0.671 | 0.328 | 0.786 | 0.312 |
| 150 | 0.682 | 0.332 | - | - |
| 200 | - | - | 0.816 | 0.326 |
| 250 | 0.693 | 0.335 | - | - |
| 400 | - | - | 0.832 | 0.334 |
| 500 | 0.703 | 0.338 | - | - |
| 800 | - | - | 0.841 | 0.339 |
| 1000 | 0.709 | 0.339 | - | - |
| 2500 | 0.711 | 0.340 | - | - |

# Table 8.4.2.

| Energy (kev) | Impulse approximation $P_e^{IMP}$ | $P^{IMP}$ |
|---|---|---|
| 0.97 | 0.726 | 0.283 |
| 1.89 | 0.794 | 0.316 |
| 2.68 | 0.858 | 0.347 |
| 4.44 | 0.889 | 0.363 |
| 6.23 | 0.886 | 0.361 |
| 10.7 | 0.871 | 0.353 |
| 15.4 | 0.860 | 0.348 |
| 22.8 | 0.850 | 0.343 |
| 32.8 | 0.840 | 0.338 |
| 56.3 | 0.817 | 0.327 |
| 79 | 0.796 | 0.317 |
| 103 | 0.771 | 0.305 |
| 156 | 0.733 | 0.282 |
| 217 | 0.683 | 0.264 |
| 285 | 0.656 | 0.251 |

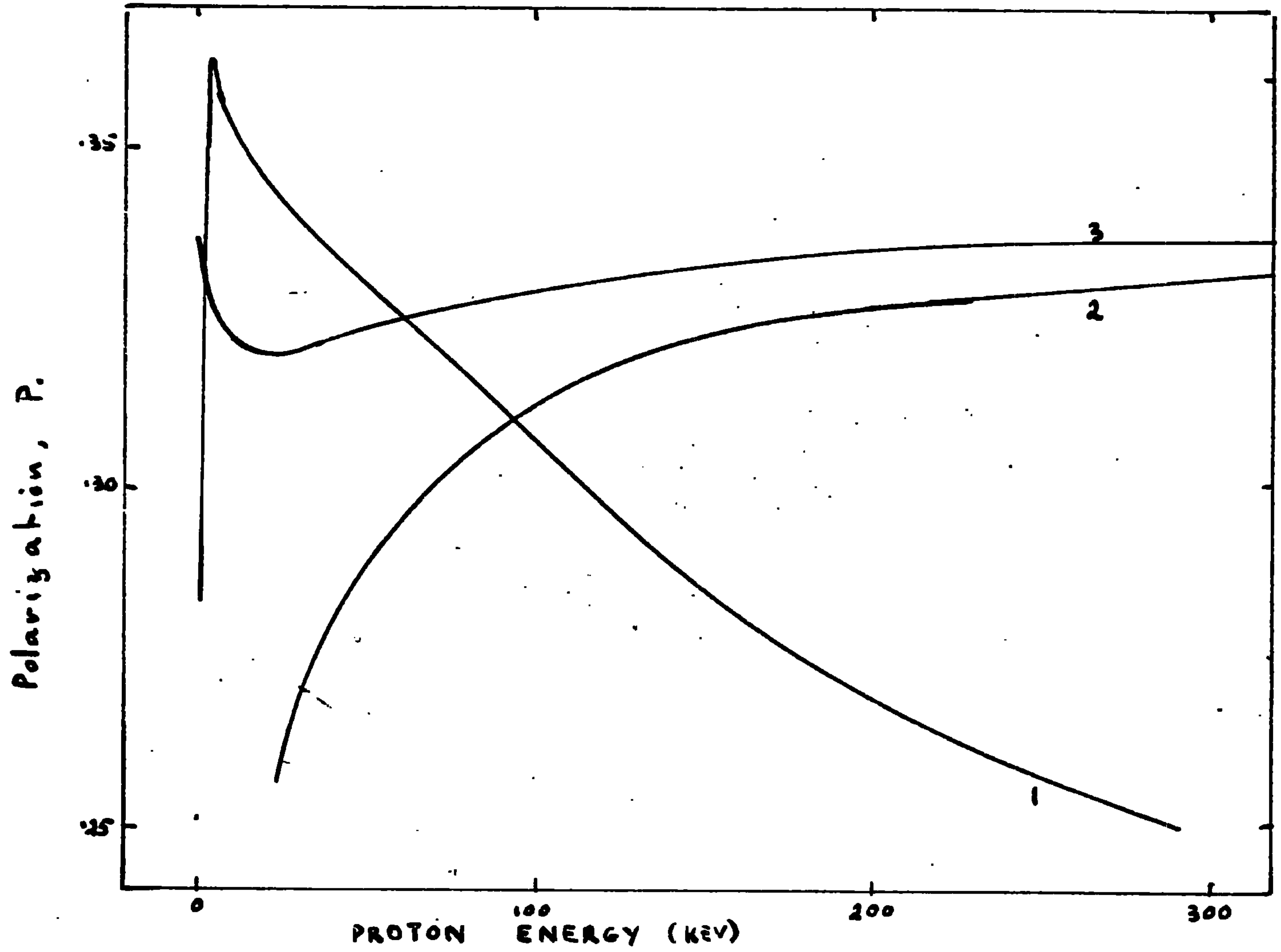


Fig. 8.4.1. Polarization for $H^+ + H(1s) \rightarrow H(2p) + H^+$

Curve 1; Impulse approximation, present work
Curve 2; 2 state approximation, McElroy (1963)
Curve 3; OBK approximation, van den Bos and de Heer (1967)

## 5) Angular distributions and transition probabilities.

It has frequently been stated that, for rearrangement collisions involving heavy particles, the majority of particles are scattered through very small angles, so that the differential cross section is very strongly peaked in the forward direction. It is of interest to consider the form of the angular distribution given by various approximations.

Bassel and Gerjouy (1960) plotted $|T_{if}|^2$ as a function of $p^2$ for the process

$$H^+ + H(1s) \rightarrow H(1s) + H^+, \qquad (8.5.1)$$

using both $T_{if}^{B}$ and $T_{if}^{BG}$. They found that $|T_{if}^{B}|^2$ is sharply peaked about $p^2 = p^2_{min}$ ($\theta = 0$) and decreases steeply to a deep minimum as the value of p is increased. This minimum is caused by cancellation of terms arising from the two potentials $V_{12}$, $V_{23}$. The dip is followed by a tail, which corresponds to scattering by the potential $V_{12}$ through larger angles (though still less than one degree), and which contributes significantly to the cross section. The angular distribution obtained using $T_{if}^{BG}$ is much more strongly peaked in the forward direction and the tail is effectively cancelled.

The angular distribution for process (1) obtained by Coleman (1965) using $T_{if}^{IMP} = I_{23}$ (see (7.3.1)) is shown in fig. (1). For each energy $|I_{23}|^2$ takes its maximum value at $p = p_{min}$ and decreases as p increases. Thus, as pointed out by Bransden and Cheshire (1963), although the actual cross sections for process (1) given by the Born and impulse approximations do not differ very much, there is a considerable difference in the angular distributions.

Curves similar to those shown in fig. (1) were obtained for all the processes investigated by the present author. Typical results are shown in figs. (2) and (3).

If the impact parameter method is used, the probability of electron capture into state f occurring at an impact parameter $\rho$ is given by (5.1.11) as

$$P = | b_f ( \infty ) |^2 .$$

When a structureless projectile 1 collides with a bound system (2 + 3) there are three possibilities:-

a) A direct collision may take place in which particle 1 is scattered leaving the bound system in either the ground or an excited state.

b) The target may be ionised.

c) A rearrangement collision may occur.

For a particle incident at impact parameter $\rho$ , the sum of the probabilities of these three events occurring must be unity and therefore any physically meaningful approximation will give a probability less than one for event (c). Schiff (1954) showed how results obtained using a wave formalism could be used to determine the capture probability at an impact parameter $\rho$, thus providing a test on the approximate wave method used.

The method depends on the fact that for rearrangement collisions the angular distribution of the scattered heavy particles is very strongly peaked in the forward direction, and consequently partial waves of very high angular momentum must contribute to the cross section.

In the following analysis, $c_\ell$ or $c(\rho)$ is written in place of $b_f(\infty)$. The first step is to expand $T_{if}$ in terms of Legendre polynomials,

$$T_{if} = \frac{\pi}{\sqrt{\mu_i \mu_f k_i k_f}} \sum_{\ell=0}^{\infty} (2\ell+1)\, c_\ell\, P_\ell(\cos\theta). \tag{8.5.2}$$

Use of this in (2.3.19) gives

$$\begin{aligned} Q(if) &= \frac{1}{2k_i^2} \int_{-1}^{+1} \left| \sum_{\ell=0}^{\infty} (2\ell+1)\, c_\ell\, P_\ell(\cos\theta) \right|^2 d(\cos\theta) \\ &= \frac{1}{k_i^2} \sum_{\ell=0}^{\infty} (2\ell+1)\, |c_\ell|^2 . \end{aligned}$$

Since a large number of $\ell$ values contribute to the cross section, the classical relation $\ell = \rho k_i$ can be used to transform the summation with respect to $\ell$ into an integration with respect to $\rho$, giving

$$Q(if) = 2\int_0^{\infty} |c(\rho)|^2 \rho\, d\rho .$$

Comparison with (5.1.12) shows that $|c(\rho)|^2$ is the probability of capture at impact parameter $\rho$.

Using the orthogonality of the Legendre polynomials, it follows from (2) that

$$c(\rho) = \frac{\sqrt{\mu_i \mu_f k_i k_f}}{2\pi} \int_{-1}^{+1} T_{if}\, P_\ell(\cos\theta)\, d(\cos\theta). \tag{8.5.3}$$

$T_{if}$ is appreciable only for small values of $\theta$, and for such $\theta$

$$P_\ell(\cos\theta) \simeq J_0(\ell\theta) = J_0(\rho k_i \theta).$$

But
$$1 - \cos\theta = \frac{p^2 - p_{min}^2}{2 a k_i k_f} ,$$

so for small $\theta$, $\quad \theta \simeq \sqrt{\frac{p^2 - p_{min}^2}{a k_i k_f}} .$

Also $a \simeq 1$, $k_i \simeq k_f$ and $\mu_i \simeq \mu_f$ .

If these approximations are made, and $p_{max}$ is replaced by infinity, (3) becomes
$$c(\rho) = \frac{1}{4\pi v} \int_{p_{min}^2}^{\infty} T_{if} \, J_0\left(\rho \sqrt{p^2 - p_{min}^2}\right) d(p^2). \qquad (8.5.4)$$

For the transition

$$H^+ + H(1s) \rightarrow H(1s) + H^+ ,$$

expression (4) can be evaluated in closed form for the OBK and Born approximations. Brinkman and Kramers (1930) obtained
$$\left| c^{BK}(\rho) \right|^2 = \frac{4\rho^4 \left( K_2(x) \right)^2}{v^2 \left( 1 + v^2/4 \right)^2} \qquad (8.5.5)$$

where
$$x = \rho \left( 1 + v^2/4 \right)^{1/2} ,$$

and Schiff (1954) showed that
$$\left| c^B(\rho) \right|^2 = \frac{4}{v^2} \left[ 6\lambda_5 K_0(x) + \frac{4\lambda_3 \rho K_1(x)}{\left(1 + v^2/4\right)^{1/2}} + \frac{(2\lambda_1 - 1)\rho^2 K_2(x)}{\left(1 + v^2/4\right)^2} \right]^2 \qquad (8.5.6)$$

where
$$\lambda_n = \int_0^1 \frac{x(1-x)\,dx}{\left[1 + v^2 x(1-x)\right]^{n/2}} .$$

$K_n(x)$ is the modified Bessel function of the second kind of order n.

Values of the transition probabilities calculated from (5), (6) led Bates and McCarroll (1962) to conclude that $Q^{BK}$ (1s) is too large at 25 kev and unreliable at energies well above 100 kev and that the validity of the Born approximation may be doubtful up to 100 kev.

Transition probabilities for processes (7.5.1) to (7.5.8) have been calculated by Coleman (1965) and by the present author, using (4) and calculated values of $T_{if}^{IMP}$. For the non-resonant reactions the transition probability is found to be less than unity for all energies and impact parameters, but in the case of accidental resonance it exceeds unity for energies less than 100 kev. For example, for (7.5.7) and an incident energy of 64 kev, it takes values 1.5, 1.1 at $\rho = 0, 1.0$ respectively. For the symmetric process unitarity is violated at energy 25 kev, $|c(\rho)|^2$ taking values 1.03, 1.02 at $\rho = 0, 0.1$, but at higher energies it is always less than unity.

If a graph of $\rho|c(\rho)|^2$ against $\rho$ is drawn, the area underneath is proportional to the cross section, so it can be seen which range of values of impact parameter is the most important. In figs (4), (5) values of $\rho|c(\rho)|^2$ for process (1) given by the OBK, Born, McCarroll and impulse approximations are compared. Clearly the OBK and impulse approximations favour slightly closer encounters than do the other two. Values of $\rho|c(\rho)|^2$ given by the impulse approximation for processes (7.5.4), (7.5.7) are plotted in figs (6) and (7).

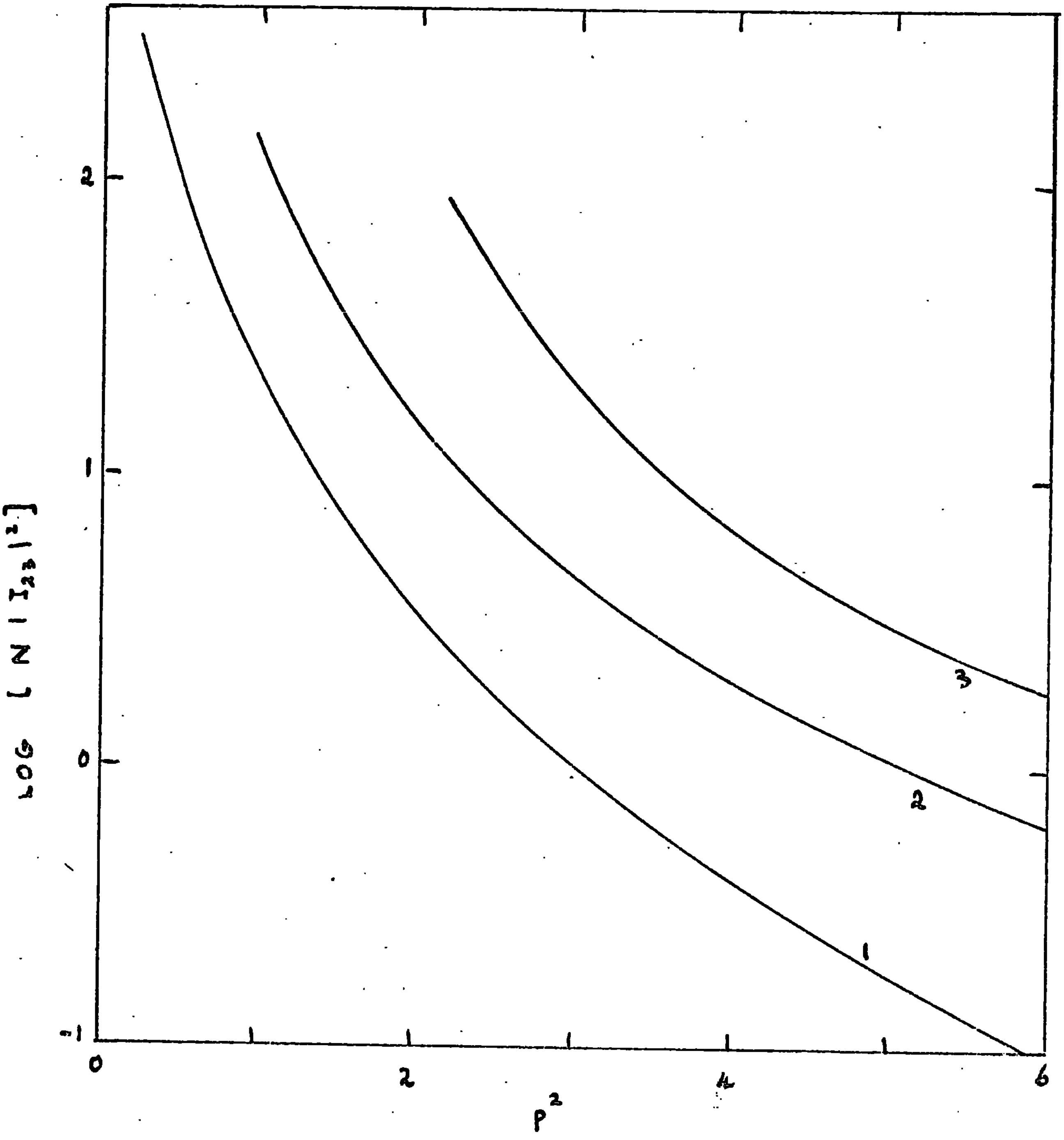


Fig 8.5.1. Impulse approximation angular distribution for $H^+ + H(1s) \rightarrow H(1s) + H^+$

(1) E = 25 kev , N = 1 ;
(2) E = 100 kev , N = 10;
(3) E = 225 kev , N = 100.

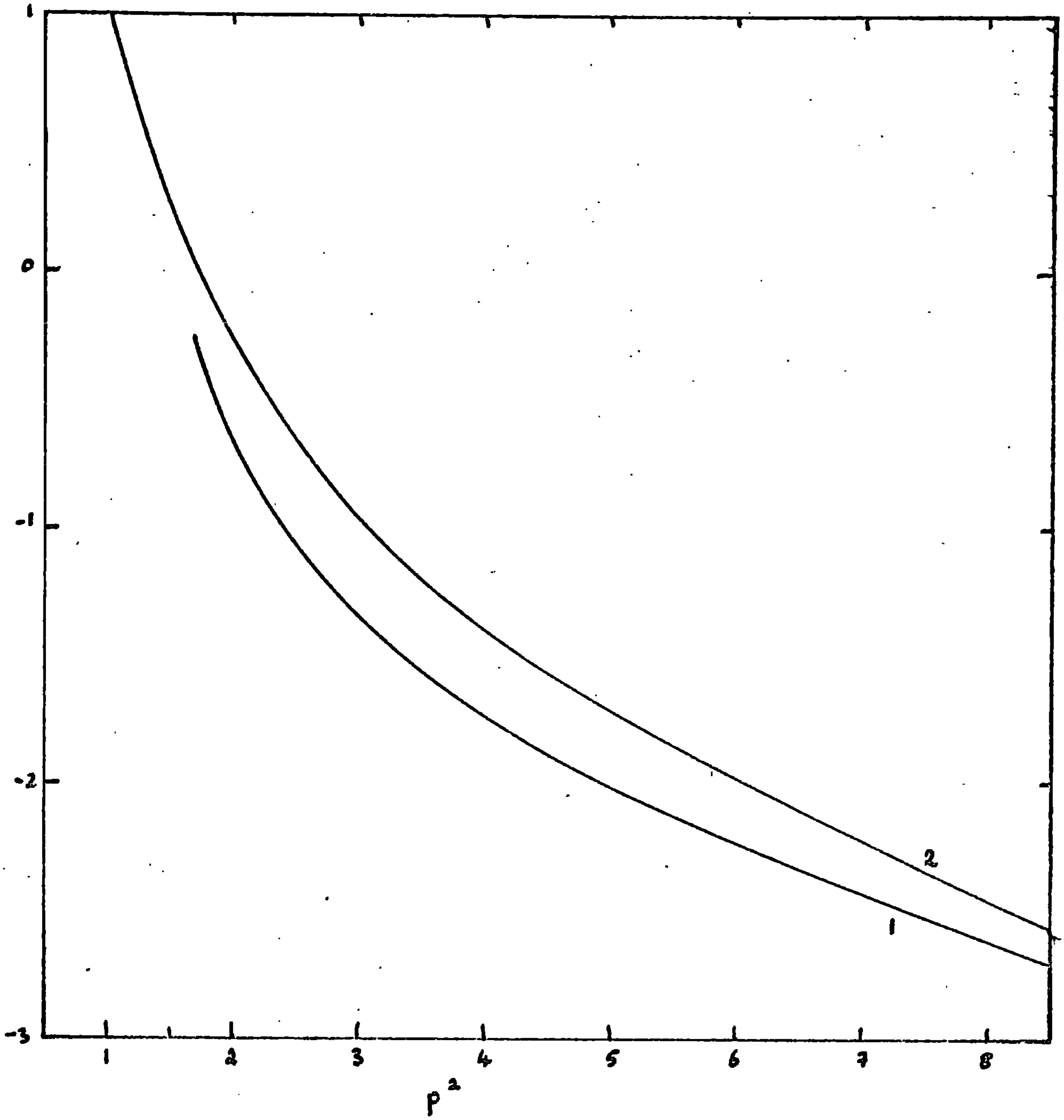


Fig 8.5.2. Impulse approximation angular distribution for
$H^+ + H(1s) \longrightarrow H(2p) + H^+$

Curve 1; E = 129 kev
Curve 2; E = 22.8 kev.

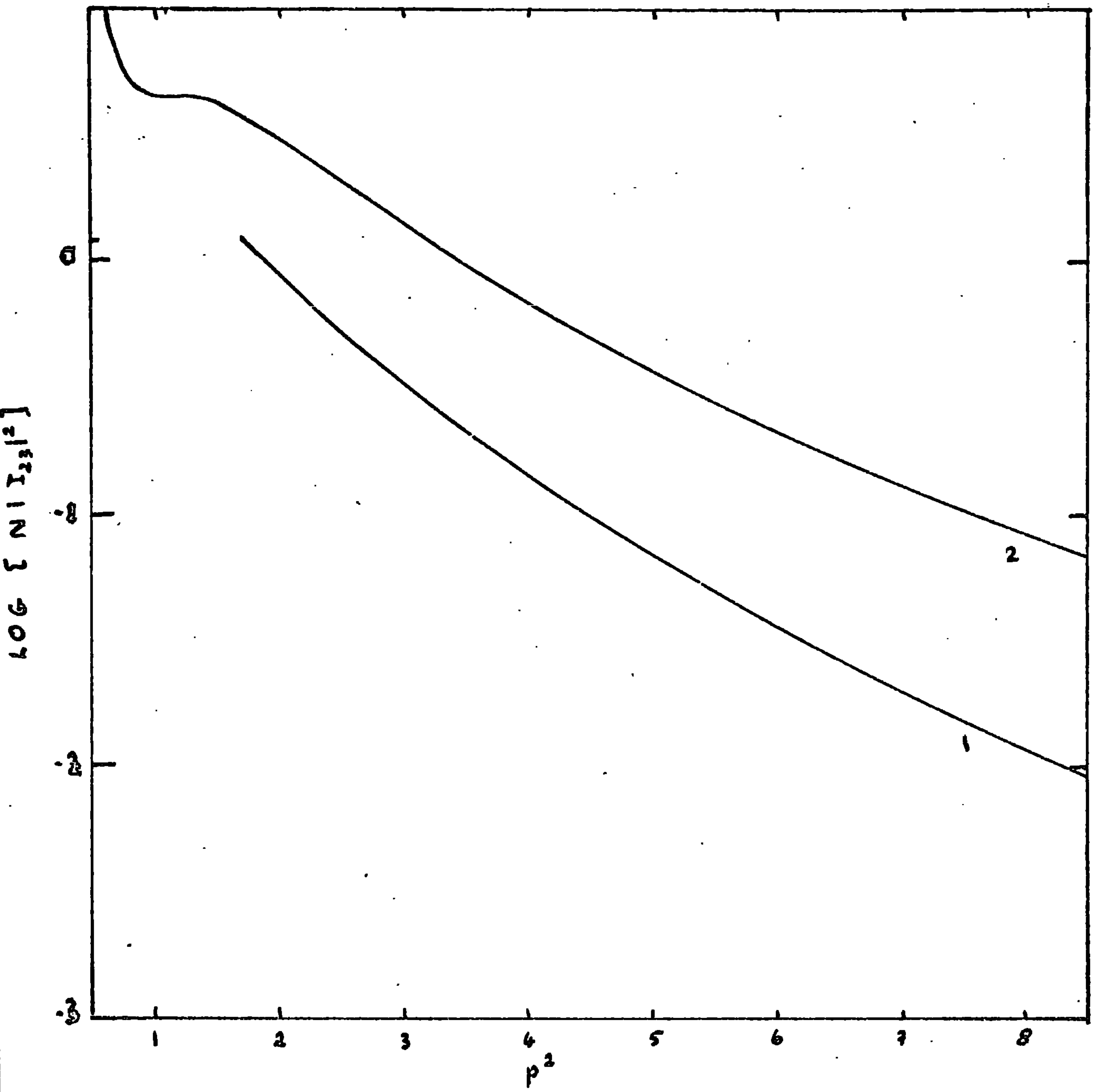


Fig 8.5.3. Impulse approximation angular distribution for $He^{++} + H(1s) \rightarrow He^{+}(3s) + H^{+}$

Curve 1; E = 559 kev, N=1

Curve 2; E = 25.9 kev, N=10

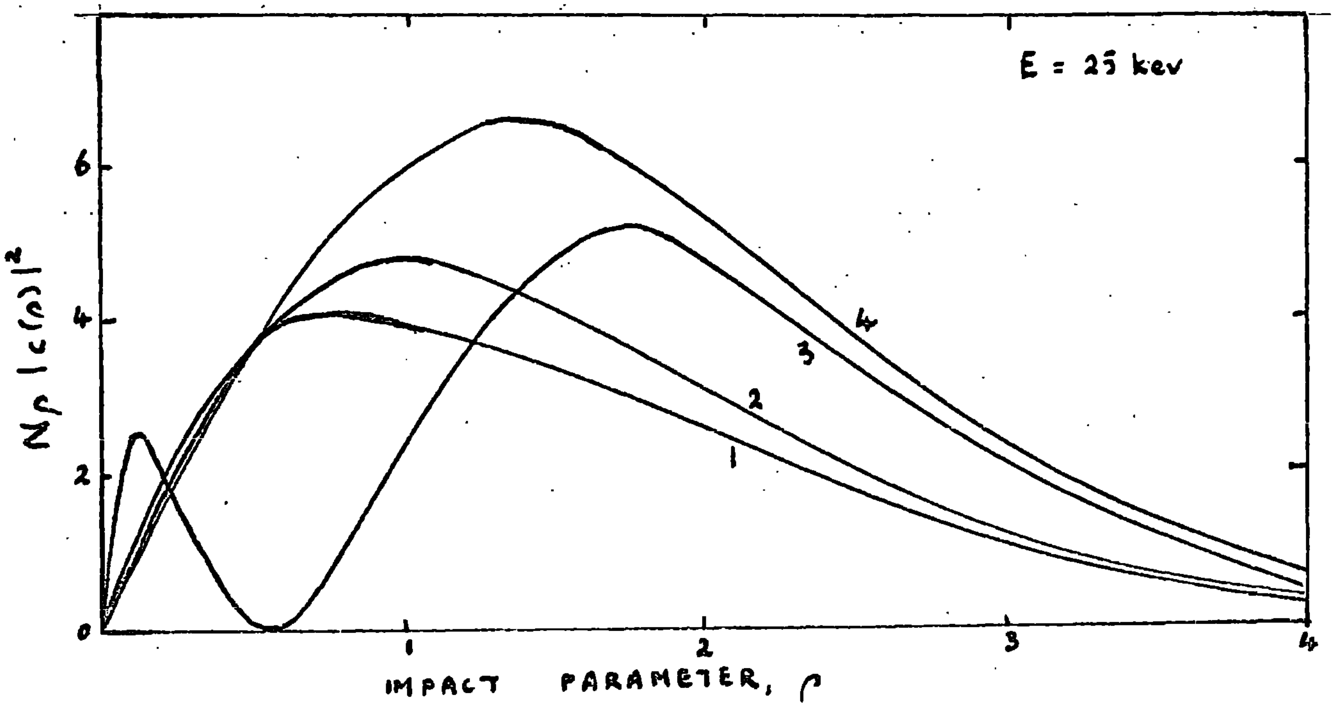


Fig 8.5.4. Graph of $N\rho\,|c(\rho)|^2$ against $\rho$ for
$H^+ + H(1s) \rightarrow H(1s) + H^+$.

Curve 1; OBK approximation, N = 1.

Curve 2; Impulse approximation, N = 10

Curve 3; Born approximation, N = 10
Schiff (1956)

Curve 4; McCarroll (1961), N = 10.

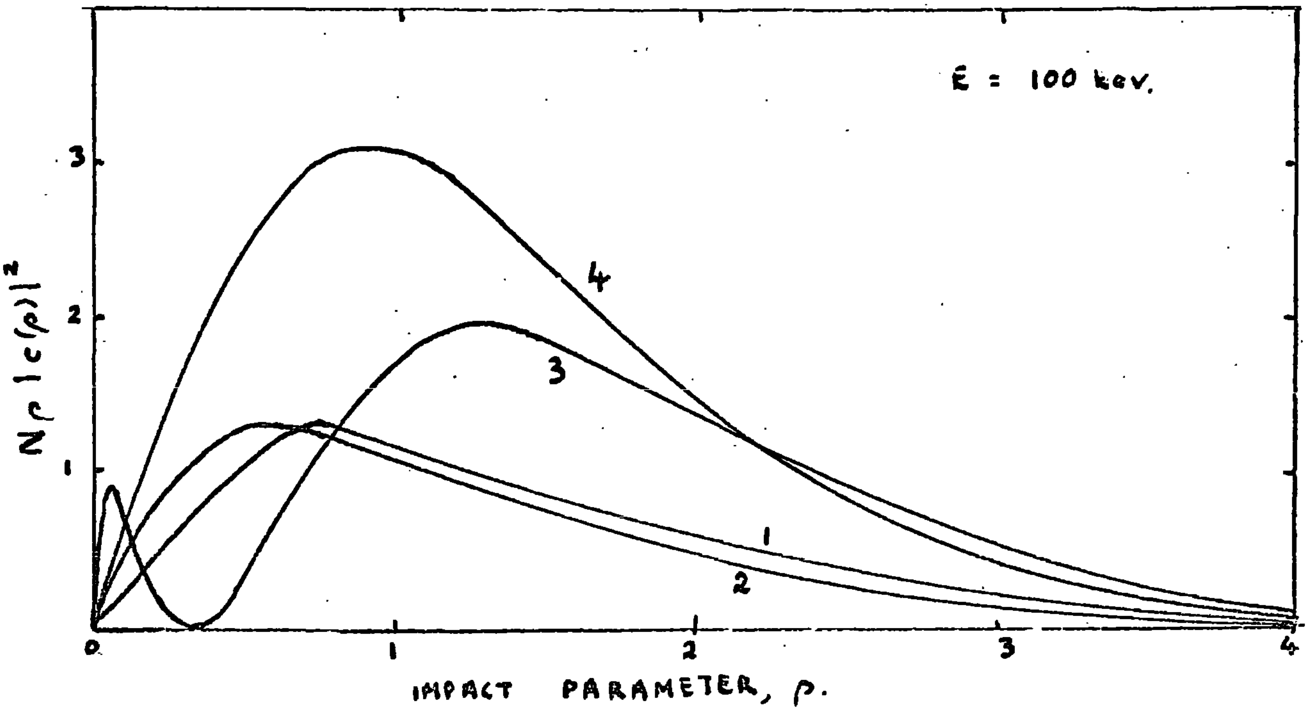


Fig 8.5.5. Graph of $\rho|c(\rho)|^2$ against $\rho$ for $H^+ + H(1s) \rightarrow H(1s) + H^+$

Curve 1; OBK approximation, N = 10

Curve 2; Impulse approximation, N = 100

Curve 3; Born approximation, N = 100 (Schiff, 1954)

Curve 4; McCarroll (1961), N = 100

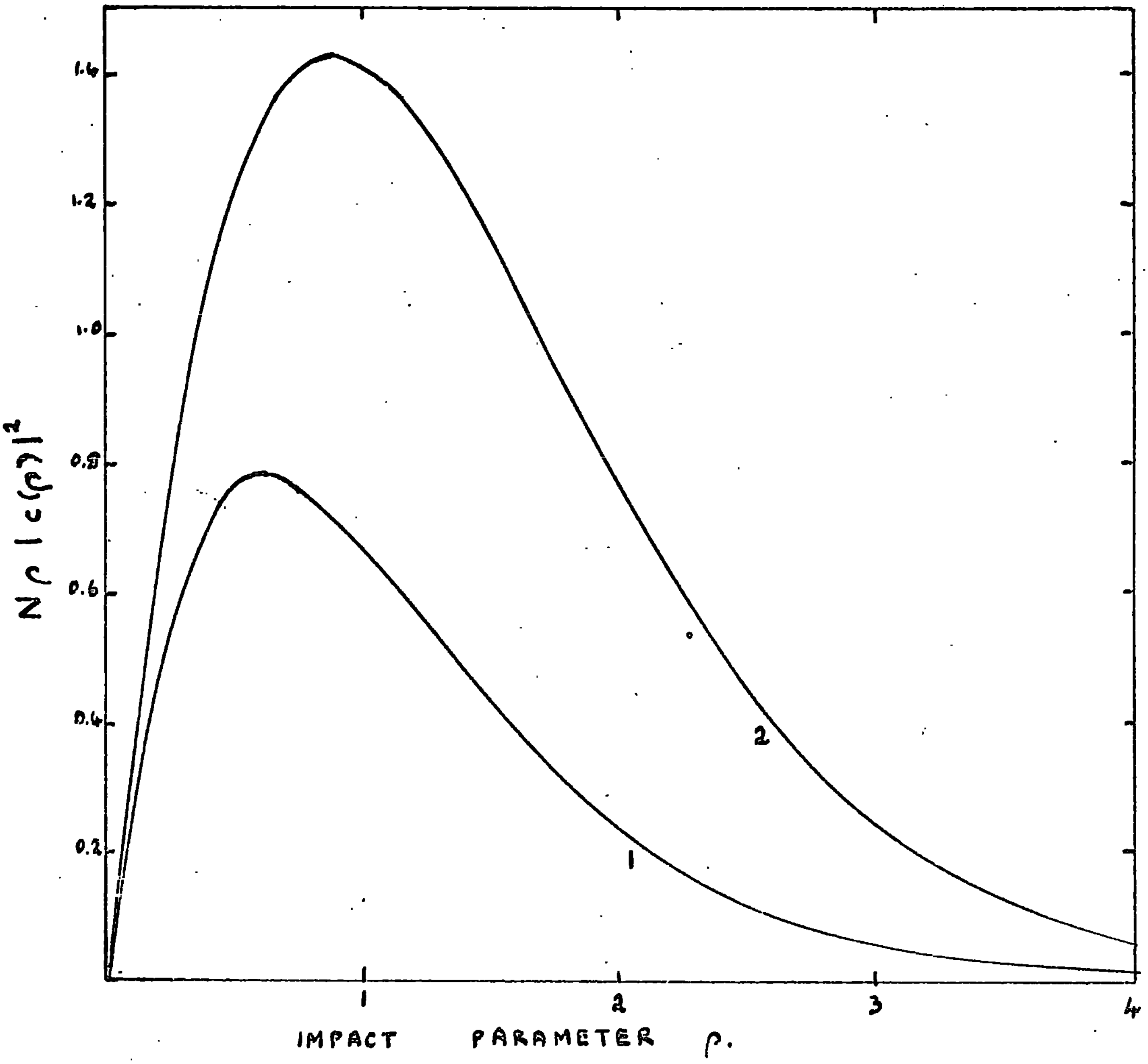


Fig 8.5.6. Graph of $N\rho\,|c(\rho)|^2$ against $\rho$ for $H^+ + H(1s) \rightarrow H(3s) + H^+$.

Curve 1; $E = 120$ kev, $N = 2 \times 10^3$

Curve 2; $E = 28.4$ kev, $N = 10^2$

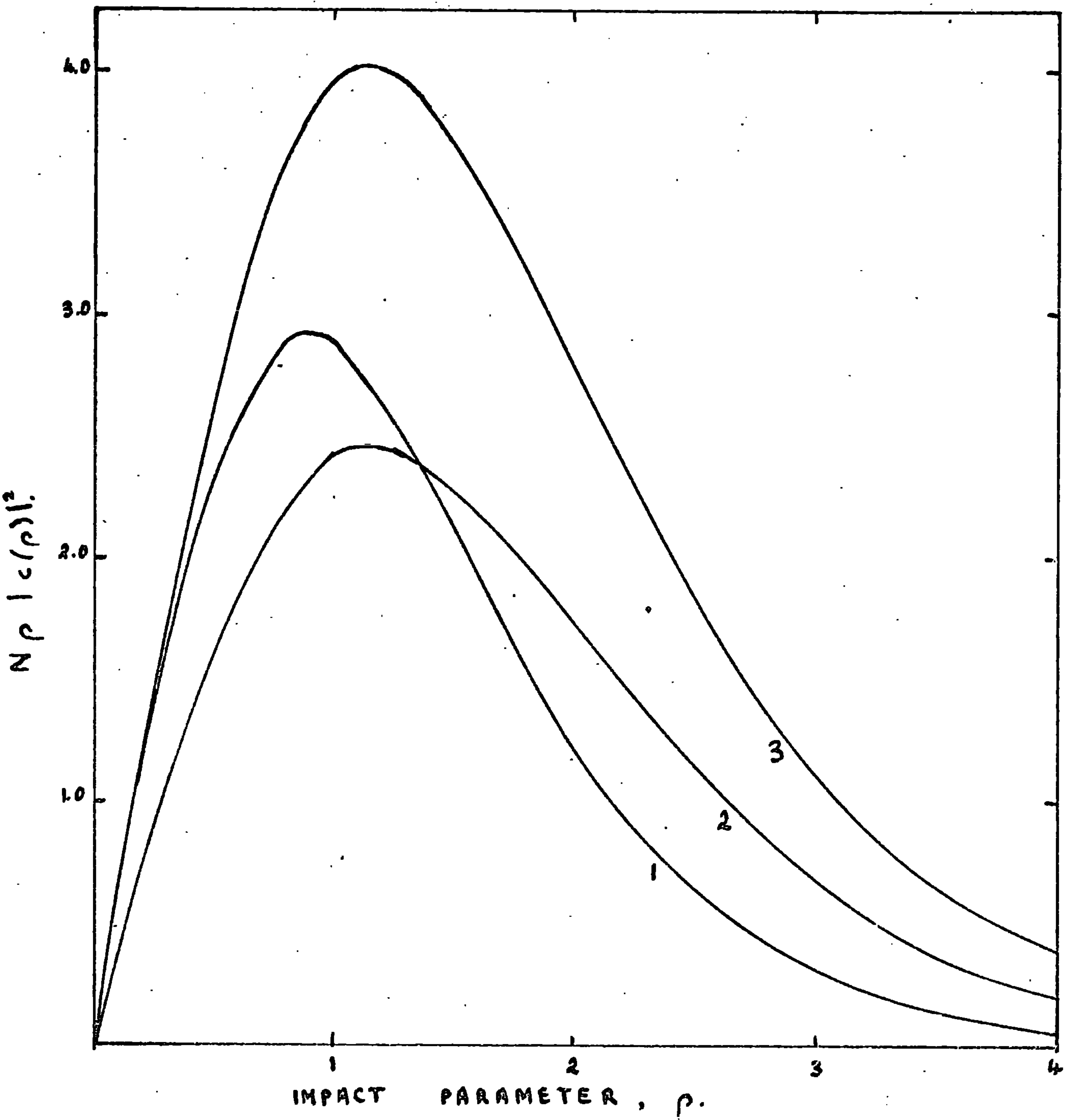


Fig 8.5.7. Graph of $N\rho|c(\rho)|^2$ against $\rho$ for
$He^{++} + H(1s) \rightarrow He^{+}(2p) + H^{+}$

Curve 1; E = 400 kev, N = $10^2$
Curve 2; E = 64 kev, N = 2
Curve 3; E = 16 kev, N = 1.

## 6) Conclusion.

For proton-hydrogen collisions the impulse hypothesis (that for the duration of the collision the effects of the binding forces are unimportant) cannot be expected to be valid at energies below 25 kev. Furthermore, the work of McCarroll and McElroy, discussed in Chapter 5 § 2, indicates that, for the processes

$$H^{+} + H(1s) \longrightarrow H(1s \text{ or } 2s) + H^{+},$$

back coupling is important at energies below 30 kev. The impulse approximation makes no allowance for back coupling, and consequently the computed transition probabilities exceed unity at low energies and small impact parameters. Values of $Q^{IMP}(nl)$ may therefore be too large at energies below 30 kev. For these reasons the disagreement of $Q^{IMP}(2s)$ with the experimental results of Bayfield is not unexpected. The lack of agreement between $Q^{IMP}(2s)$ and the results of Ryding et al (as renormalised by Gaily) is more disturbing. $Q^{IMP}(2p)$ appears to agree well with the values obtained by Stebbings et al but recent measurements have shown that these are not reliable.

Comparison with experimental values of total capture cross sections cannot be made until estimates of the cross sections for capture into all excited states of the projectile are available. It was shown in § 2 that the values of $Q^{IMP}(3s)$ and $Q^{IMP}(3p)$ calculated by the present author enable reliable estimates to be obtained. However, it is clear from figs (8.2.4), (8.2.5) that total cross sections predicted by the impulse approximation lie below the experimental values. The reason for the discrepancy is not known but Coleman has suggested that it may be due to an inconsistent treatment of the effects of the potential $V_{12}$. Since $V_{12}$ itself has been neglected completely in all the calculations, there is an unscreened Coulomb potential, and the boundary conditions on the wave functions should be altered. Thus the plane wave in $\varphi_f$ should be replaced by a Coulomb wave.

For collisions of alpha particles with hydrogen atoms, the impulse hypothesis should be valid at energies above 100 kev. At lower energies it was found that the transition probabilities exceed unity for the accidentally resonant processes. Values of the cross sections at low energies are in any case meaningless because the effect of the Coulomb repulsion between the collision products is neglected. No conclusions can be drawn about the accuracy of the results at high energies because experimental results are available only at energies below 36 kev.

## Chapter 9.

## THE HIGH ENERGY BEHAVIOUR OF ELECTRON CAPTURE CROSS SECTIONS

### 1. Review of previous work.

Several attempts have been made in recent years to determine the high energy form of the exact cross section for electron capture processes. However, even for the simplest reaction

$$H^+ + H(1s) \rightarrow H(1s) + H^+,$$

no rigorous derivation of the high energy limit has yet been given. The rest of this chapter is concerned with this reaction. If the asymptotic forms of the various approximations considered in this thesis are compared, a difference is immediately apparent between first and second order methods. This is not surprising in view of the fact that virtual transitions to excited or continuum states play an important part in the capture process at high energies since the capture cross section becomes small in comparison with that for either excitation or ionization. Second order methods attempt to take some account of these transitions whereas first order methods ignore them completely. The present situation is briefly as follows.

Suppose first that terms of order $^1/M$ are neglected. Then the first Born approximation gives

$$Q^B \underset{V \rightarrow \infty}{\sim} 0.661\, Q^{BK},$$

the distorted wave methods of Bassel and Gerjouy, and Grant and Shapiro, and the two state approximation of McCarroll, give

$$Q^{BG},\ Q^{GS},\ Q_2 \underset{v\to\infty}{\sim} Q^{BK},$$

the continuum distorted wave method of Cheshire, the distorted wave method of McCarroll and Salin, and the second Born approximation of Drisko give

$$Q^{CD},\ Q^{B2} \underset{v\to\infty}{\sim} \left(0.2946 + \frac{5\pi v}{2^{12}}\right) Q^{BK}, \qquad (9.1.1)$$

and the third Born approximation of Drisko gives

$$Q^{B3} \underset{v\to\infty}{\sim} \left(0.319 + \frac{5\pi v}{2^{12}}\right) Q^{BK},$$

where the Brinkman-Kramers cross section

$$Q^{BK} = \frac{2^8}{5v^2\left(1+v^2/4\right)^5} .$$

If terms of order 1/M are included, and the protons are regarded as distinguishable, back scattering eventually becomes the dominant process, and

$$Q^{B},\ Q^{BG} \underset{v\to\infty}{\sim} \frac{16}{3M^2}\, v^{-6} . \qquad (9.1.2)$$

Bransden and Cheshire (1963) considered the high energy form of the impulse approximation cross section and showed that, if the effect of the internuclear potential is neglected,

$$Q^{IMP} \underset{v\to\infty}{\sim} \left(0.2946 + \frac{5\pi v}{2^{11}}\right) Q^{BK} . \qquad (9.1.3)$$

This differs from the high energy form of $Q^{B2}$ only by a factor of 2 in the second term. It is interesting to note that a simpler version of the continuum distorted wave method, obtained by replacing $\Psi_i^+$ in (6.2.6) by $\Phi_i^{(2)} \exp\left\{-\frac{i}{v} \ln(vR - v^2 t)\right\}$ instead of by $\chi_i$, yields a cross section whose asymptotic form is given by (3), instead of by (1). The missing factor of 2 may arise because the wave function $\Phi_i^{(2)} \exp\left\{-\frac{i}{v} \ln(vR - v^2 t)\right\}$ and the impulse approximation wave function used by Bransden and Cheshire do not satisfy the correct boundary conditions.

Coleman (1965) showed that, although the matrix element $I_{12}$, involving the internuclear potential, vanishes in the limit $^1/M$ tends to zero, nevertheless, as in the Born approximation, it determines the asymptotic form of the cross section. Thus

$$Q^{IMP} \underset{v \to \infty}{\sim} \frac{16}{3M^2} v^{-6},$$

which is the same as (2). If $I_{12}$ is retained, it is inconsistent to replace $\omega_{12}^+$ by unity. However, Coleman was able to show that such a replacement does not affect the result. He also carried out detailed calculations which indicate that the $v^{-6}$ behaviour occurs only when $M_1 = M_2$, and the $v^{-11}$ behaviour is correct for all other cases.

2) <u>The high energy behaviour of a modified first Born approximation.</u>

Although second order methods appear to favour the second Born approximation result, the convergence of the Born series (and of the usual distorted wave Born series) is in some doubt, and in any case the work of Drisko suggests that third and higher order Born terms are important. In Chapter 4 § 1, the distorted wave formalism of Dodd and Greider was used to obtain a new integral equation (4.1.18) for the exact distorted wave transition operator. It was shown that the kernel of this equation could be made completely continuous. Thus the difficulties associated with the usual Born and distorted wave Born series do not occur with the series obtained by iteration of this equation, and it may be that the inhomogeneous term yields the correct high energy limit of the exact transition amplitude. This will certainly be true if the iterated series converges to its first term, but the convergence has not yet been considered.

With the choice $U_i = 0$, $V_x = V_{23}$, the inhomogeneous term is given by (4.1.21);

$$T_{if}^{I} = \langle \zeta_f^- \,|\, W_f + W_f \frac{1}{E - H_0 - V_i + i\epsilon} V_i \,|\, \varphi_i \rangle .$$

If $U_f = 0$ also, $T_{if}^{I}$ reduces to a modified first Born approximation matrix element

$$T_{if}^{MB} = \langle \varphi_f \,|\, V_f + V_f \frac{1}{E - H_0 - V_i + i\epsilon} V_i \,|\, \varphi_i \rangle .$$

The high energy behaviour of $T_{if}^{I}$ has been investigated by McCarroll and Salin (1967b), but they made an approximation which had the effect of replacing

$$\frac{1}{E - H_0 - V_i + i\epsilon} V_i \, \varphi_i \quad \text{by} \quad \sum_m \frac{1}{E_m - H + V_i + i\epsilon} \, \chi_m \rangle \langle \chi_m \,|\, V_i \,|\, \varphi_i \rangle ,$$

(Coleman, 1968) where the wave functions $\chi_m$ are solutions of the equation

$$(H_0 - \epsilon_m)\,\chi_m = 0.$$

They made three different choices for $U_f$, one being $U_f = 0$ in which case their matrix element reduces to $T_{if}^{IMP\,2}$ instead of to $T_{if}^{MB}$. In order to evaluate the integrals they obtained, they were forced to make rather crude peaking approximations similar to those described later in this chapter. The choices $U_f = 0$, $U_f = V_{12}$ led to cross sections with the same asymptotic form as $Q^{IMP}$ (see 9.1.3), while a different choice gave the same result as $Q^{CD}$ (see 9.1.1).

The work described in the rest of this chapter was undertaken in an attempt to determine the high energy behaviour of $T_{if}^{MB}$. The approximation introduced by McCarroll and Salin has not been made.

$T_{if}^{MB}$ may be written

$$T_{if}^{MB} = T_{if}^{B} + T_{if}^{M},$$

where
$$T_{if}^{M} = \langle \varphi_f | V_f \frac{1}{E - H_0 - V_{12} - V_{13} + i\epsilon} (V_{12} + V_{13}) | \varphi_i \rangle$$

$$= I(V_{23}, V_{12}) + I(V_{23}, V_{13}) + I(V_{12}, V_{13}) + I(V_{12}, V_{12}), \qquad (9.2.1)$$

where
$$I(U, V) = \langle \varphi_f | U \frac{1}{E - H_0 - V_{12} - V_{13} + i\epsilon} V | \varphi_i \rangle. \qquad (9.2.2)$$

To simplify the matrix element I(U,V), complete sets of solutions of the equation

$$\left( E_n - H_0 - V_{12} - V_{13} \right) \chi_n = 0 \qquad (9.2.3)$$

are introduced, so that (2) becomes

$$I(U,V) = \sum_n \frac{\langle \Phi_f | U | \chi_n \rangle \langle \chi_n | V | \Phi_i \rangle}{E - E_n + i\epsilon} , \qquad (9.2.4)$$

provided that the functions $\chi_n$ are orthonormal.

Equation (3) may be written

$$\left( -\frac{1}{2\mu} \nabla_\rho^2 - \frac{1}{2a} \nabla_x^2 + \frac{1}{\rho} - \frac{1}{x} - E_n \right) \chi_n = \left( \frac{1}{\rho} - \frac{1}{R} \right) \chi_n ,$$

where $a = \dfrac{M}{M+1}$, $\mu = \dfrac{M(M+1)}{2M+1}$, and M is the mass of a proton. If terms of order 1/M are neglected, the right hand side of this equation vanishes, and $\chi_n$ may be written as the product of two Coulomb functions. It takes either the form

$$\chi_n^b (\underline{x}, \rho) = \psi_{nlm}(\underline{x}) F_{\underline{K}}(\rho) ,$$

or

$$\chi_n^c (\underline{x}, \rho) = \chi_{\underline{k}}(\underline{x}) F_{\underline{K}}(\rho) ,$$

where $\psi_{nlm}(\underline{x})$ is a hydrogen bound state wave function, and $\chi_{\underline{k}}(\underline{x})$, $F_{\underline{K}}(\rho)$ are continuum hydrogen wave functions,

$$\chi_{\underline{k}}(\underline{x}) = (2\pi)^{-3/2} e^{\frac{1}{2}\nu\pi} \Gamma(1 - i\nu) \exp(i\underline{k}.\underline{x}) \, {}_1F_1[i\nu, 1, i(kx - \underline{k}.\underline{x})] ,$$

$$F_{\underline{K}}(\rho) = (2\pi)^{-3/2} e^{-\frac{1}{2}\Lambda\pi} \Gamma(1 + i\Lambda) \exp(i\underline{K}.\underline{\rho}) \, {}_1F_1[-i\Lambda, 1, i(K\rho - \underline{K}.\underline{\rho})] ,$$

where $\nu = a/k$, $\Lambda = \mu/K$.

The summation sign in (4) denotes a summation over all bound states and integrations over $\underline{k}$ and $\underline{K}$. It is convenient to consider contributions from intermediate bound states $\chi_n^b$, and from intermediate continuum states $\chi_n^c$ separately, so (4) is written

$$I(U,V) = I^b(U,V) + I^c(U,V)$$

where

$$I^b(U,V) = \sum_n \int d\underline{K} \; \frac{\langle \varphi_f | U | \chi_n^b \rangle \langle \chi_n^b | V | \varphi_i \rangle}{E - E_{n,\underline{K}} + i\epsilon}$$

and

$$I^c(U,V) = \int d\underline{k} \int d\underline{K} \; \frac{\langle \varphi_f | U | \chi_n^c \rangle \langle \chi_n^c | V | \varphi_i \rangle}{E - E_{\underline{k},\underline{K}} + i\epsilon}, \qquad (9.2.5)$$

with

$$E_{n,\underline{K}} = K^2/2\mu + \epsilon_n, \quad \epsilon_n < 0,$$

and

$$E_{\underline{k},\underline{K}} = K^2/2\mu + k^2/2a.$$

In the following work, terms of order $1/M$ compared with unity are neglected. Thus for example, $\nu$ is written $1/k$. Some of the notation used is now introduced.

Let

$$g_{nlm}(b,\underline{A}) = \int \frac{d\underline{x}}{x} \, e^{-bx} e^{i\underline{A}\cdot\underline{x}} \, \psi_{nlm}(\underline{x}), \qquad (9.2.6)$$

$$G_{nlm}(b,\underline{A}) = \int d\underline{x} \; e^{-bx} e^{i\underline{A}\cdot\underline{x}} \, \psi_{nlm}(\underline{x}). \qquad (9.2.7)$$

Integrals of this kind have been evaluated by Podolsky and Pauling (1929) and by Massey and Mohr (1931). The analysis is given in appendix (2

In the notation of chapter 3 § 1,

$$g_{nlm}(0,\underline{A}) = g_{nlm}(\underline{A}), \qquad G_{nlm}(0,\underline{A}) = G_{nlm}(\underline{A}).$$

Write

$$f_{\underline{K}}(\lambda,\alpha,\underline{Q}) = \int \frac{d\underline{\rho}}{\rho}\, e^{-\lambda\rho}\, e^{i\underline{Q}\cdot\underline{\rho}}\, {}_1F_1[\, i\alpha, 1, i(K\rho - \underline{K}\cdot\underline{\rho})], \qquad (9.2.8)$$

$$\mathcal{L}_{\underline{K}}(\lambda,\alpha,\underline{Q}) = \int d\underline{\rho}\, e^{-\lambda\rho}\, e^{i\underline{Q}\cdot\underline{\rho}}\, {}_1F_1[\, i\alpha, 1, i(K\rho - \underline{K}\cdot\underline{\rho})]. \qquad (9.2.9)$$

These integrals may be evaluated using a technique due to Nordsieck. The method is described in appendix (3) and the results are given here for reference.

$$f_{\underline{K}}(\lambda,\alpha,\underline{Q}) = \frac{4\pi}{\lambda^2+Q^2}\, f, \qquad (9.2.10)$$

where

$$f = \left[\frac{\lambda^2+Q^2}{\lambda^2+Q^2-2\underline{K}\cdot\underline{Q}-2i\lambda K}\right]^{i\alpha}, \qquad (9.2.11)$$

and

$$\mathcal{L}_{\underline{K}}(\lambda,\alpha,\underline{Q}) = \frac{8\pi}{(\lambda^2+Q^2)^2}\, F, \qquad (9.2.12)$$

where

$$F = \left[\frac{\lambda^2+Q^2}{\lambda^2+Q^2-2\underline{K}\cdot\underline{Q}-2i\lambda K}\right]^{i\alpha}\left(\lambda(1-i\alpha) + \frac{\alpha(K+i\lambda)(\lambda^2+Q^2)}{\lambda^2+Q^2-2\underline{K}\cdot\underline{Q}-2i\lambda K}\right). \qquad (9.2.1$$

## 3) The contribution from intermediate bound states.

### Evaluation of the matrix elements.

Write $N_1 = e^{-\frac{1}{2}\Lambda\pi}\,\Gamma(1+i\Lambda)$.

1.) $\langle \varphi_f | V_{23} | \chi_n^b \rangle$

If the potential $V_{23}(\underline{r})$ is written in terms of its Fourier transform, then

$$\langle \varphi_f | V_{23} | \chi_n^b \rangle = -\frac{1}{2\pi^2}\int d\underline{x}\int d\underline{\rho}\,\exp(-i\underline{k}_f.\underline{\rho})\,\psi_{1s}(\underline{x})\,\psi_{nlm}(\underline{x})\,F_{\underline{K}}(\underline{\rho})\int \frac{d\underline{t}}{t^2}\exp\left(-i\underline{t}.(\underline{\rho}+a\underline{x})\right).$$

Because the bound state wave function $\psi_{1s}(\underline{x})$ contains a decaying exponential factor, the integral with respect of $\underline{x}$ is uniformly convergent for all values of $\underline{t}$. However, the same is not true of the $\underline{\rho}$ integral, and to enable the order of the $\underline{x}$ and $\underline{\rho}$ and $\underline{t}$ integrations to be interchanged, a convergence factor $e^{-\lambda\rho}$ is introduced. The limit $\lambda \to 0$ is taken after all integrations have been performed.

Then

$$\langle \varphi_f | V_{23} | \chi_n^b \rangle = -\lim_{\lambda\to 0}\frac{N_1}{2^{5/2}\pi^4}\int \frac{d\underline{t}}{t^2}\,G_{nlm}(1,-\underline{t})\,\mathcal{L}_{\underline{K}}(\lambda,-\Lambda,\underline{t}_1,-\underline{t}) \qquad (9.3.1)$$

where $\underline{t}_1 = \underline{K} - \underline{k}_f$, and $G_{nlm}(b,\underline{B})$, $\mathcal{L}_{\underline{K}}(\lambda,\Lambda,\underline{Q})$ are defined by (9.2.7), (9.2.9) respectively.

a) <u>The intermediate ground state.</u>

The ground state hydrogen wave function is

$$\psi_{1s}(\underline{x}) = \pi^{-1/2} e^{-x} .$$

Now

$$G(1;-\underline{t}) = \frac{16\pi^{1/2}}{(4+t^2)^2} ,$$

and $\mathcal{L}_{\underline{K}}(\lambda,\alpha,\underline{Q})$ is given by (9.2.12)

Substituting these values in (1), the $\underline{t}$ - integral is

$$J = \int \frac{d\underline{t} \quad F_1}{t^2(4+t^2)^2(\lambda^2+(\underline{t}_1-\underline{t})^2)^2} , \qquad (9.3.2)$$

where $F_1$ is defined by (9.2.13) with $\underline{Q} = \underline{t}_1 - \underline{t}$, $\alpha = -\Lambda$. The $\underline{t}$ - integrand has two peaks, a very sharp one at $\underline{t} = \underline{t}_1$ and a less well-defined one at $\underline{t} = 0$. The Coulomb factor $F_1$ is a slowly varying function of $\underline{t}$ at both peaks and, provided $\underline{K} \neq \underline{k}_f$, the factor $(4 + t^2)^{-2}$ is slowly varying for values of $\underline{t}$ near $\underline{t}_1$. The contribution to J from this peak can be written

$$\frac{F_{11}}{(4+t_1^2)^2} \int \frac{d\underline{t}}{t^2(\lambda^2+(\underline{t}_1-\underline{t})^2)^2} = \frac{\pi^2 [F_{11}/\lambda]}{(4+t_1^2)^2(\lambda^2+t_1^2)} , \qquad (9.3.3)$$

where

$$F_{11}/\lambda = \left(\frac{\lambda}{\lambda-2iK}\right)^{-i\Lambda}\left(1+i\Lambda - \frac{\Lambda(K+i\lambda)}{\lambda-2iK}\right).$$

Thus, if the contribution from the other peak is neglected, and $\underline{K} \neq \underline{k}_f$,

$$\langle \varphi_f | V_{23} | \psi_{1s,\underline{K}} \rangle = -\lim_{\lambda\to 0} \frac{2^{9/2} N_1 (F_{11}/\lambda)}{\pi^{1/2}(4+t_1^2)^2(\lambda^2+t_1^2)} . \qquad (9.3.4)$$

In order to test the validity of the peaking approximation, the Coulomb factor F in (2) was replaced by its value at $\underline{t} = \underline{t}_1$, and the remaining integral was evaluated exactly. The analysis is very lengthy, and will not be given here, but the leading term, in the limit $\lambda \to 0$, is

$$\frac{\pi^2 \left( F_{11} / \lambda \right)}{\left(4 + t_1^2\right)^2 \left( \lambda^2 + t_1^2 \right)} ,$$

which agrees exactly with result (3). This fact provides some justification for the neglect of the peak at $\underline{t} = 0$. It also indicates that although $(4 + t^2)^{-2}$ is not a slowly-varying function of $\underline{t}$ near $\underline{t} = \underline{t}_1$ where $\underline{K} = \underline{k}_f$, nevertheless the procedure of replacing it by $(4 + t_1^2)^{-2}$ and carrying out the remaining integration leads to the correct answer in the limit $\lambda \to 0$. This is not surprising since in this limit the peak in the other factor is very much sharper. It will therefore be assumed that $\langle \varphi_f | V_{23} | \psi_{13} F_{\underline{K}} \rangle$ is correctly given by (4) for all values of $\underline{K}$.

An expression very similar to (4) may be obtained by a different method. Once the peaking approximation has been made, (1) may be written

$$\langle \varphi_f | V_{23} | \psi_{13} F_{\underline{K}} \rangle = - \lim_{\lambda \to 0} \frac{N_1}{2^{5/2} \pi^4} G_{13}(1, -\underline{t}_1) \int \frac{d\underline{t}}{t^2} \mathcal{L}_{\underline{K}} (\lambda, -\Lambda, \underline{t}_1 - \underline{t}).$$

If the order of the $\underline{\rho}$ and $\underline{t}$ integrations is reversed, which is legitimate provided $\lambda \neq 0$, then

$$\int \frac{d\underline{t}}{t^2} \exp(-i \underline{t} . \underline{\rho}) = \frac{2\pi^2}{\rho} ,$$

and

$$\langle \phi_f | V_{23} | \psi_{1s} F_{\underline{K}} \rangle = - \lim_{\lambda \to 0} \frac{N_1}{2^{3/2}\pi^2} \, G_{1s}(1, -\underline{t}_1) \, f_{\underline{K}}(\lambda, -\Lambda, \underline{t}_1)$$

$$= - \frac{2^{9/2} N_1 f_1}{\pi^{1/2} t_1^2 (4 + t_1^2)^2} , \qquad (9.3.5)$$

where $f_{\underline{K}}(\lambda, \alpha, \underline{Q})$ is defined by (9.2.8)

and

$$f_1 = \left( \frac{t_1^2}{t_1^2 - 2\underline{K} \cdot \underline{t}_1} \right)^{-i\Lambda} .$$

Equation (5) differs from (4) only in the appearance of the factor $f_1$ instead of $(F_{11}/\lambda)$. In the present work it is immaterial which result is used since the $\underline{K}$- integration involved in the evaluation of the expressions I (U, V) is performed by the use of a peaking approximation, and the values at the peak of both the factors $(F_{11}/\lambda)$ and $f_1$ tend to unity in the high energy limit. In the evaluation of the other matrix elements, the method which led to (5) will be adopted.

b) Other intermediate bound states.

The major contribution to the $\underline{t}$ - integral comes from the region $\underline{t} = \underline{t}_1$, due to the strong singularity in the term $[\lambda^2 + (\underline{t}_1 - \underline{t})^2]^{-2}$ which appears in $\mathcal{L}_{\underline{K}}(\lambda, -\Lambda, \underline{t}_1 - \underline{t})$. If the slowly-varying factors are removed from the integral,

$$\langle \phi_f | V_{23} | \chi_n^b \rangle = \frac{- 2^{1/2} N_1 f_1 G_{nlm}(1, -\underline{t}_1)}{\pi t_1^2} , \qquad (9.3.6)$$

where $G_{nlm}(b, \underline{A})$ is given by (A2.25).

2) $\underline{\langle \varphi_f | V_{12} | \chi_n^b \rangle}$.

In deriving the form of the intermediate bound state wave function, the potential $V_{12} = \frac{1}{R}$ was replaced by $1/\rho$. The same replacement is made here.

Then

$$\langle \varphi_f | V_{12} | \chi_n^b \rangle = \lim_{\lambda \to 0} \int d\underline{x}\, \psi_{1s}(\underline{x})\, \psi_{nlm}(\underline{x}) \int d\underline{\rho}\, \frac{e^{-\lambda\rho}}{\rho} \exp(-i\underline{k}_f \cdot \underline{\rho}) F_{\underline{K}}(\rho)$$

$$= \frac{N_1}{(2\pi)^{3/2}} \delta_{n1} \lim_{\lambda \to 0} f_{\underline{K}}(\lambda, -\Lambda, \underline{t}_1)$$

$$= \delta_{n1} \frac{2^{1/2}}{\pi^{1/2}} \frac{N_1 f_1}{t_1^2}, \qquad (9.3.7)$$

3) $\underline{\langle \chi_n^b | V_{13} | \varphi_i \rangle}$.

$\psi_{1s}(r)$ is written in terms of its Fourier transform and a convergence factor $e^{-\lambda\rho}$ is introduced.

Then

$$\langle \chi_n^b | V_{13} | \varphi_i \rangle = - \lim_{\lambda \to 0} \frac{N_1^*}{(2\pi)^{9/2}} \int d\underline{s}\, G_{1s}(\underline{s})\, g^*_{nlm}(\underline{s}+\underline{v})\, \mathcal{L}^*_{\underline{K}}(\lambda, -\Lambda, \underline{t}_2 + \underline{s}),$$

where $\underline{t}_2 = \underline{K} - a\underline{k}_i$.

At high energies it seems reasonable to neglect $\underline{s}$ in comparison with $\underline{v}$ in the argument of $g^*_{nlm}$, especially since $G_{1s}(\underline{s})$ is peaked about the value $\underline{s} = 0$. The remaining $\underline{s}$ - integration may then be carried out to give

$$\int G_{1s}(\underline{s}) \exp(-i\underline{s} \cdot \underline{\rho})\, d\underline{s} = \frac{(2\pi)^3}{\pi^{1/2}} e^{-\rho}.$$

Then

$$\langle \chi_n^b | V_{13} | \varphi_i \rangle = - \lim_{\lambda \to 0} \frac{N_1^*}{2^{3/2}\pi^2} \, g_{nlm}^*(\underline{v}) \, \mathcal{L}_{\underline{K}}^*(1+\lambda, -\Lambda, \underline{t}_2)$$

$$= - \frac{2^{3/2} N_1^*}{\pi} \, \frac{F_2^* \, g_{nlm}^*(\underline{v})}{(1+t_2^2)^2} \tag{9.3.8}$$

where

$$F_2 = \left[ \frac{1+t_2^2}{1+t_2^2 - 2\underline{K}.\underline{t}_2 - 2iK} \right]^{-i\Lambda} \left\{ 1 + i\Lambda - \frac{\Lambda(K+i)(1+t_2^2)}{1+t_2^2 - 2\underline{K}.\underline{t}_2 - 2iK} \right\}$$

and $g_{nlm}(\underline{v})$ is given by (A2.22).

For the intermediate ground state,

$$g_{1s}^*(\underline{v}) = \frac{4\pi^{1/2}}{1+v^2} ,$$

so that

$$\langle \psi_{1s} F_{\underline{k}} | V_{13} | \varphi_i \rangle = \frac{-2^{7/2} N_1^* F_2^*}{\pi^{1/2}(1+v^2)} \cdot \frac{1}{(1+t_2^2)^2} . \tag{9.3.9}$$

4) $\underline{\langle \chi_n^b | V_{12} | \varphi_i \rangle}$

If $V_{12}$ is replaced by $1/\rho$, $\psi_{1s}$ is written in terms of its Fourier transform, and a convergence factor $e^{-\lambda\rho}$ is introduced, then

$$\langle \chi_n^b | V_{12} | \varphi_i \rangle = \lim_{\lambda \to 0} \frac{N_1^*}{(2\pi)^{9/2}} \int d\underline{s} \; G_{1s}(\underline{s}) \, G_{nlm}^*(\underline{s}+\underline{v}) \, f_{\underline{K}}^*(\lambda, -\Lambda, \underline{t}_2 + \underline{s}) .$$

As in the evaluation of $\langle \chi_n^b | V_{13} | \varphi_i \rangle$, the argument $\underline{s} + \underline{v}$ of the Fourier transform is replaced by $\underline{v}$. The remaining $\underline{s}$ - integration can then be carried out exactly, with the result

$$\langle \chi_n^b | V_{12} | \varphi_i \rangle = \frac{N_1^*}{2^{3/2}\pi^2} \, G_{nlm}^*(\underline{v}) \, f_{\underline{K}}^*(1, -\Lambda, \underline{t}_2) ,$$

$$= \frac{2^{1/2} N_1^*}{\pi} \, \frac{f_2^*}{(1+t_2^2)} \, G_{nlm}^*(\underline{v}) , \tag{9.3.10}$$

where

$$f_2 = \left( \frac{1 + t_2^2}{1 + t_2^2 - 2\underline{K}.\underline{t}_2 - 2iK} \right)^{-i\Lambda} , \quad \underline{t}_2 = \underline{K} - a\underline{k}_i ,$$

and $\mathcal{G}_{nlm}(\underline{v})$ is given by (A2.28).

Since

$$\mathcal{G}_{1s}(\underline{v}) = \frac{8\pi^{1/2}}{(1+v^2)^2} ,$$

$$\langle \psi_{1s} F_{\underline{K}} | V_{12} | \varphi_i \rangle = \frac{2^{7/2} N_1^* f_2^*}{\pi^{1/2}(1+v^2)^2(1+t_2^2)} \qquad (9.3.11)$$

### The contribution to the transition amplitude from the intermediate ground state.

Define

$$I_{nlm}^{b}(U,V) = 2\mu \int d\underline{K} \frac{\langle \varphi_f | U | \chi_n^b \rangle \langle \chi_n^b | V | \varphi_i \rangle}{k_f^2 - K^2 + i\epsilon + \delta}$$

where $\delta = 2\mu(\epsilon_f - \epsilon_n)$.

a) From (5), (7) and (11), it can be seen that

$$I_{1s}^{b}(V_{23}, V_{12}) + I_{1s}^{b}(V_{12}, V_{12})$$

$$= \frac{32\mu}{\pi(1+v^2)^2} \int \frac{d\underline{K}\ C_1(\underline{K}) \left( 1 - \frac{16}{(4+t_1^2)^2} \right)}{(k_f^2 - K^2 + i\epsilon)(1+t_2^2)\, t_1^2} \qquad (9.3.12)$$

where

$$C_1(\underline{K}) = |N_1|^2 \left[ \frac{t_1^2}{t_1^2 - 2\underline{K}.\underline{t}_1} \right]^{-i\Lambda} \left[ \frac{1 + t_2^2}{1 + t_2^2 - 2\underline{K}.\underline{t}_2 + 2iK} \right]^{i\Lambda} . \qquad (9.3.13)$$

The major contribution to the integral in (12) comes from the range of $\underline{K}$ near $\underline{k}_f$ i.e. $\underline{t}_1 = 0$, $\underline{t}_2 = -\underline{q}$. When $\underline{K} = \underline{k}_f$, $\Lambda = \mu/k_f \approx \frac{1}{v_f}$ and tends to zero as $v_f$ tends to infinity. Since $|N_1|^2 \rightarrow 1$ as $\Lambda \rightarrow 0$, the value of $C_1(\underline{K})$ at the peak tends to 1 in the high energy limit. If the slowly varying factor $(1 + t_2{}^2)^{-1}$ is also replaced by its value at the peak, one obtains

$$I_{15}^{b}(V_{23}, V_{12}) + I_{15}^{b}(V_{12}, V_{12})$$

$$\simeq \frac{32\mu}{\pi(1+v^2)^2} \frac{C_1(k_f)}{(1+q^2)} \int \frac{d\underline{K}\ (8+t_1^2)}{(k_f^2 - K^2 + i\epsilon)(4+t_1^2)^2}$$

$$= \frac{32\mu}{\pi(1+v^2)^2} \frac{C_1(k_f)}{(1+q^2)} \left( I_1(4, \underline{k}_f) + 4\, I_2(4, \underline{k}_f) \right),$$

where $$I_n(\alpha^2, \underline{t}) = \int \frac{d\underline{K}}{(k_f^2 - K^2 + i\epsilon)(\alpha^2 + (\underline{K} - \underline{t})^2)^n}.$$

The evaluation of $I_1$ and $I_2$ is discussed in appendix (4). There it is shown that

$$I_1(4, \underline{k}_f) = -\pi^2/k_f \left( \tan^{-1} k_f + i/2 \ln(1+k_f^2) \right),$$

$$I_2(4, \underline{k}_f) = -\frac{\pi^2(1+ik_f)}{8(1+k_f^2)}.$$

Therefore

$$I_{15}^{b}(V_{23}, V_{12}) + I_{15}^{b}(V_{12}, V_{12})$$

$$\simeq \frac{-32\mu\pi}{(1+v^2)^2} \frac{C_1(k_f)}{(1+q^2)k_f} \left( \frac{k_f(1+ik_f)}{2(1+k_f^2)} + \tan^{-1} k_f + \frac{i}{2} \ln(1+k_f^2) \right)$$

$$\underset{v \rightarrow \infty}{\sim} -\frac{2^7 \pi i \ln v}{v^7 (1+\lambda)}, \qquad (9.3.14)$$

where $\lambda = 4M^2 \sin^2 \theta/2$, and $\theta$ is the angle of scattering.

b) Evaluation of $I_{15}^{b}(V_{23}, V_{13}) + I_{15}^{b}(V_{12}, V_{13})$.

From (5), (7) and (9) it follows that

$$I_{15}^{b}(V_{23}, V_{13}) + I_{15}^{b}(V_{12}, V_{13})$$

$$= -\frac{2^5\mu}{\pi(1+v^2)} \int \frac{d\underline{K}\; C_2(\underline{K}) \left(1 - \frac{16}{(4+t_1^2)^2}\right)}{(k_f^2 - K^2 + i\epsilon)(1+t_2^2)^2\; t_1^2}$$

where $C_2(\underline{K}) = |N_1|^2 \left(\frac{t_1^2}{t_1^2 - 2\underline{K}.\underline{t}_1}\right)^{-i\Lambda} \left(\frac{1 + t_2^2}{1 + t_2^2 - 2\underline{K}.\underline{t}_2 + 2iK}\right)^{i\Lambda}$

$$\times \left(1 - i\Lambda - \frac{\Lambda(K-i)(1+t_2^2)}{1 + t_2^2 - 2\underline{K}.\underline{t}_2 + 2iK}\right).$$

The integrand has strong peaks at $\underline{K} = a\underline{k}_i$ and at $\underline{K} = \underline{k}_f$. At the first of these a simple peaking approximation may be used, and the contribution from the second peak is evaluated in the way described in the previous section. At each peak, $C_2(\underline{K})$ tends to unity in the high energy limit, and it is replaced by this value.

Thus

$$I_{15}^{b}(V_{23}, V_{13}) + I_{15}^{b}(V_{12}, V_{13})$$

$$= -\frac{2^5\mu\pi}{(1+v^2)} \left[\frac{1}{q^2(k_f^2 - a^2k_i^2)}\left(1 - \frac{16}{(4+q^2)^2}\right) + \frac{1}{(1+q^2)^2 k_f}\left(-\tan^{-1}k_f - \frac{i}{2}\ln(1+k_f^2) - \frac{k_f(1+ik_f)}{2(1+k_f^2)}\right)\right]$$

$$\simeq \frac{-2^7\pi}{v^6(1+\lambda)}\left(1 - \frac{16}{(4+q^2)^2}\right) - \frac{2^9\pi}{v^8(1+\lambda)^2}\left(-\frac{\pi}{2} + \tan^{-1}\frac{1}{k_f} - \frac{i}{2}\ln(1+k_f^2) - \frac{k_f(1+ik_f)}{2(1+k_f^2)}\right).$$

At high energies, the leading term is the first. Thus

$$I_{15}^{b}(V_{23}, V_{13}) + I_{15}^{b}(V_{12}, V_{13}) \underset{v \to \infty}{\sim} -\frac{2^7\pi}{v^6(1+\lambda)}. \qquad (9.3.15)$$

The contribution from other bound states.

From (6), (7), (8) and (10), it can be seen that, if $n \neq 1$, then

$$I^{b}_{nlm}(V_{12}, V_{12}) = 0 = I^{b}_{nlm}(V_{12}, V_{13}).$$

$$I^{b}_{nlm}(V_{23}, V_{12}) = -\frac{4\mu}{\pi^2}\int \frac{d\underline{K}\; |N_1|^2 f_1 f_2^{*}\, G_{nlm}(1, -\underline{t}_1)\, G^{*}_{nlm}(\underline{v})}{(k_f^2 - K^2 + i\epsilon + \delta)\, t_1^2\, (1 + t_2^2)} ,$$

$$I^{b}_{nlm}(V_{23}, V_{13}) = \frac{8\mu}{\pi^2}\int \frac{d\underline{K}\; |N_1|^2 f_1 F_2^{*}\, G_{nlm}(1, -\underline{t}_1)\, g^{*}_{nlm}(\underline{v})}{(k_f^2 - K^2 + i\epsilon + \delta)\, t_1^2\, (1 + t_2^2)^2} .$$

For each intermediate state a peaking approximation is used to evaluate the integrals. The values taken at the peaks by the Coulomb factors $|N_1|^2 f_1 f_2^*$ and $|N_1|^2 f_1 F_2^*$ both tend to unity in the high energy limit. These factors are therefore omitted in the following analysis. Also $k_f^2 + \delta$ is replaced by $k_f^2$.

Then

$$I^{b}_{nlm}(V_{23}, V_{12}) = -\frac{4\mu}{\pi^2}\, G^{*}_{nlm}(\underline{v}) \int \frac{d\underline{K}\; G_{nlm}(1, -\underline{t}_1)}{(k_f^2 - K^2 + i\epsilon)\, t_1^2\, (1 + t_2^2)} ,$$

$$I^{b}_{nlm}(V_{23}, V_{13}) = \frac{8\mu}{\pi^2}\, g^{*}_{nlm}(\underline{v}) \int \frac{d\underline{K}\; G_{nlm}(1, -\underline{t}_1)}{(k_f^2 - K^2 + i\epsilon)\, t_1^2\, (1 + t_2^2)^2} .$$

It is shown in the appendix (A2.25) that $\mathcal{G}_{nlm}(1,-\underline{t}_1)$ can be written

$$\mathcal{G}_{nlm}(1,-\underline{t}_1) = H_l\, Y_l^m(\Theta,\Phi)\, T_l(t_1)\, \frac{t_1^{\,l}}{(\beta^2+t_1^2)^{l+2}},$$

where $\beta = \frac{n+1}{n}$, $\cos\Theta = -\frac{\underline{t}_1\cdot\underline{k}_i}{t_1 k_i}$ and $\Phi$ is the angle between the plane of $-\underline{t}_1$ and $\underline{k}_i$ and that of $\underline{k}_i$ and $\underline{k}_f$. The functions $H_l$, $T_l$ are defined in the appendix (A2.26),(A2.27).

The contribution from s - states with $n>1$.

a) $$I^b_{ns}(V_{23},V_{12}) = -\frac{4\mu}{\pi^2}\,\mathcal{G}^*_{n00}(\underline{v})\int\frac{d\underline{K}}{(k_f^2-K^2+i\epsilon)}\;\frac{\mathcal{G}_{n00}(1,-\underline{t}_1)}{t_1^2(1+t_2^2)}.$$

Although $\mathcal{G}_{n00}(1,0)=0$, it can be shown that

$$\lim_{t_1\to 0}\left[\frac{1}{t_1^2}\,\mathcal{G}_{n00}(1,-\underline{t}_1)\right] = \frac{2^5\,\pi^{1/2}\,n^{1/2}}{\Gamma(4)}\;\frac{n^4}{(n+1)^6}\left(\frac{n-1}{n+1}\right)^{n-3}, \qquad n>1.$$

Therefore, the region $\underline{K} = \underline{k}_f$, ($\underline{t}_1 = 0$), provides the major contribution to the integral. A peaking approximation is used, giving

$$I^b_{ns}(V_{23},V_{12}) = -\frac{32\mu}{\pi^2}\,\mathcal{G}^*_{n00}(\underline{v})\,\frac{\pi^{1/2}\,n^{1/2}\,T_0(0)}{n^4(1+q^2)}\;I_2(\beta^2,\underline{k}_f),$$

where $I_2(A,\underline{t})$ is given by (A4.1),

and $$T_0(0) = \frac{4n^4}{\Gamma(4)(n+1)^2}\left(\frac{n-1}{n+1}\right)^{n-3}.$$

Thus $$I^b_{ns}(V_{23},V_{12}) \underset{v\to\infty}{\sim} \frac{2^{10}\,\pi i n}{3(n+1)^4}\left(\frac{n-1}{n+1}\right)^{n-3}\frac{1}{(1+\lambda)}\cdot\frac{1}{v^7}.$$

b) $$I^{b}_{ns}(V_{23}, V_{13}) = \frac{8\mu}{\pi^2}\, g^{*}_{n00}(\underline{v}) \int \frac{d\underline{K}\;\; G_{n00}(1, -\underline{t}_1)}{(k_f^2 - K^2 + i\epsilon)\, t_1^2\, (1 + t_2^2)^2} \;.$$

The $\underline{K}$ - integrand has peaks at $\underline{K} = \underline{k}_f$, ($\underline{t}_1 = 0$), and at $\underline{K} = a\underline{k}_i$, ($\underline{t}_2 = 0$). Use of a peaking approximation gives

$$I^{b}_{ns}(V_{23}, V_{13})$$
$$= \frac{8\mu}{\pi^2}\, g^{*}_{n00}(\underline{v}) \left[ \frac{8\pi^{1/2} n^{1/2}\, T_0(0)}{(1+q^2)^2\, n^4}\, I_2(\beta^2, \underline{k}_f) + \frac{G_{n00}(1, -\underline{q})}{q^2}\, I_2(1, a\underline{k}_i) \right].$$

In the high energy limit, the leading term comes from the first peak.

$$I^{b}_{ns}(V_{23}, V_{13}) \underset{v \to \infty}{\sim} -\frac{2^{12}\pi i}{3}\, \frac{n}{(n+1)^4} \left(\frac{n-1}{n+1}\right)^{n-3} \frac{1}{(1+\lambda)^2} \cdot \frac{1}{v^7} \,.$$

### The contribution from p states.

a) $$I^{b}_{n1m}(V_{23}, V_{12}) = -\frac{4\mu}{\pi^2}\, G^{*}_{n1m}(\underline{v}) \int \frac{d\underline{K}\;\; H_1\, T_1(t_1)\, Y_{1m}(\Theta, \Phi)\, t_1}{(k_f^2 - K^2 + i\epsilon)\, t_1^2\, (1 + t_2^2)(\beta^2 + t_1^2)^3} \;.$$

The major contribution to the integral comes from the region near $\underline{K} = \underline{k}_f$, so a peaking approximation is used. If the slowly-varying factors are taken outside the integral sign, and the variable of integration is changed to $\underline{t}_1$, then

$$I^{b}_{n1m}(V_{23}, V_{12}) = \frac{4\mu}{\pi^2}\, G^{*}_{n1m}(\underline{v})\, \frac{H_1\, T_1(0)}{(1+q^2)} \int \frac{d\underline{t}_1\;\; Y_{1m}(\Theta, \Phi)}{t_1 (t_1^2 + 2\underline{k}\cdot\underline{t}_1 - i\epsilon)(\beta^2 + t_1^2)^3} \;,$$

where

$$T_1(0) = \frac{10n\,\Gamma(n+2)}{\Gamma(6)\,\Gamma(n-1)} \left(\frac{n-1}{n+1}\right)^{n-3} .$$

It proves convenient to carry out the $\underline{t}_1$ - integration in a frame Oxyz with z - axis in the direction $\underline{k}_f$ and the plane of $\underline{k}_i$ and $\underline{k}_f$ as the x - z plane. Let OXYZ denote the frame with Z - axis in the direction $\underline{k}_i$, the xz and XZ planes being the same. Spherical polar coordinates in the two frames are denoted by $(t_1, \theta, \varphi)$, $(t_1, \Theta', \Phi')$ respectively. Then, in terms of the angles $\Theta$, $\Phi$ defined on page 192,

$$\Theta' = \pi - \Theta, \qquad \Phi' = \pi + \Phi,$$

and

$$Y_{1m}(\Theta, \Phi) = -Y_{1m}(\Theta', \Phi') = -\sum_{m'=-1}^{1} Y_{1m'}(\theta, \varphi) R^{(1)}_{m'm}(\alpha, \beta, \gamma),$$

where the functions $R^{(1)}_{m'm}(\alpha, \beta, \gamma)$ are the elements of the rotation matrix and $\alpha, \beta, \gamma$ are the Euler angles of the rotation which takes Oxyz into OXYZ. (see for example, Messiah (1962) p.1068.)

In the present case,

$\alpha = \gamma = 0$, and $\beta$ is the scattering angle, $\theta_0$.

Now

$$\int \frac{d\underline{t}_1 \; Y_{1m}(\Theta, \Phi)}{t_1 (\beta^2 + t_1^2)^3 (t_1^2 + 2\underline{k}.\underline{t}_1 - i\epsilon)}$$

$$= -\sum_{m'=-1}^{1} R^{(1)}_{m'm}(0, \theta_0, 0) \int_0^\infty \frac{t_1 \, dt_1}{(\beta^2 + t_1^2)^3} \int_0^{2\pi} d\varphi \int_{-1}^{+1} \frac{Y_{1m'}(\theta, \varphi) \, dy}{(t_1^2 + 2k_f t_1 y - i\epsilon)},$$

where $y = \cos \theta$.

The $\varphi$ integration gives $2\pi\delta_{m'0}$, so

$$I^{b}_{n1m}(V_{23},V_{12}) = \frac{4.3^{1/2}\mu}{\pi^{3/2}}\, \mathcal{G}^{4}_{n1m}(\underline{y})\, \frac{H_1 T_1(0)}{(1+q^2)} \cdot R^{(1)}_{0m}(0,\theta_0,0)\, J,$$

where

$$R^{(1)}_{0m}(0,\theta_0,0) = \begin{cases} \pm \frac{1}{\sqrt{2}} \sin\theta_0 \,; & m = \pm 1, \\ \cos\theta_0 \,, & m = 0, \end{cases}$$

$$J = \int_k^\infty \frac{t\,dt}{(\beta^2+t^2)^3} \int_{-1}^{+1} \frac{y\,dy}{t^2+2kty-i\epsilon},$$

and suffices on $t_1$ and $k_f$ have been dropped. Since the lower limit of the t - integration is k, not 0, it seems legitimate to divide through by t and replace $\epsilon/t$ by $\epsilon$. Then, carrying out the y - integration, one obtains

$$\begin{aligned} J &= \frac{1}{2k}\int_k^\infty \frac{dt}{(\beta^2+t^2)^3}\left\{2 - \left(\frac{t}{2k} - i\epsilon\right)\ln\left(\frac{t+2k-i\epsilon}{t-2k-i\epsilon}\right)\right\} \\ &= J_1 - J_2 + J_3 \end{aligned}$$

where

$$J_1 = \frac{1}{k}\int_k^\infty \frac{dt}{(\beta^2+t^2)^3},$$

$$J_2 = \frac{1}{4k^2}\int_k^\infty \frac{t\,dt}{(\beta^2+t^2)^3} \ln\left(\frac{t+2k-i\epsilon}{t-2k-i\epsilon}\right),$$

and

$$J_3 = \frac{i\epsilon}{2k}\int_k^\infty \frac{dt}{(\beta^2+t^2)^3} \ln\left(\frac{t+2k-i\epsilon}{t-2k-i\epsilon}\right).$$

It can be shown that $J_3 \to 0$ as $\epsilon \to 0$,

$$\lim_{\epsilon \to 0} J_2 = O(k^{-6}) \quad \text{as } k \to \infty,$$

and $$J_1 = O(k^{-1}) \quad \text{as } k \to \infty.$$

Thus, the leading term in the high energy limit comes from $J_1$ and

$$I^{b}_{n1m}(V_{23}, V_{12}) = O(v^{-8}) \quad \text{as } v \to \infty.$$

b) $$I^{b}_{n1m}(V_{23}, V_{13}) = \frac{8\mu}{\pi^2} g^{*}_{n1m}(\underline{v}) \int \frac{d\underline{K}\; H_1 T_1(\underline{t}_1) Y_{1m}(\Theta, \Phi)\, t_1}{(k_f^2 - K^2 + i\epsilon) t_1^2 (1+t_2^2)^2 (\beta^2 + t_1^2)^3}.$$

The $\underline{K}$ - integrand has two peaks, at $\underline{t}_1 = 0$ and at $\underline{t}_2 = 0$. The leading term in the high energy limit comes from the first peak, and

$$I^{b}_{n1m}(V_{23}, V_{13}) = 0(v^{-8}) \text{ as } v \to \infty.$$

<u>The contribution from d - states.</u>

a) $$I^{b}_{n2m}(V_{23}, V_{12}) = -\frac{4\mu}{\pi^2} G^{*}_{n2m}(\underline{v}) \int \frac{d\underline{K}\; G_{n2m}(1, -\underline{t}_1)}{(k_f^2 - K^2 + i\epsilon) t_1^2 (1+t_2^2)}$$

$$= -\frac{4\mu}{\pi^2} G^{*}_{n2m}(\underline{v}) H_2 \int \frac{d\underline{K}\; Y_{2m}(\Theta, \Phi) T_2(\underline{t}_1)}{(k_f^2 - K^2 + i\epsilon)(1+t_2^2)(\beta^2 + t_1^2)^4}.$$

The $\underline{K}$ - integrand is strongly peaked at $\underline{K} = \underline{k}_f$, and the integral is evaluated in the usual way. The result is

$$I^{b}_{n2m}(V_{23}, V_{12}) = -\frac{4\mu}{\pi^2} H_2 G^{*}_{n2m}(\underline{v}) \frac{Y_{2m}(0,0)\, T_2(0)}{1+q^2} \; I_4(\beta^2, \underline{k}_f).$$

Now, $Y_{2m}(0,0) = \sqrt{\frac{5}{4\pi}}\,\delta_{m0}\,, \quad T_2(0) = \left(\frac{n-1}{n+1}\right)^{n-4} \frac{28n\,\Gamma(n+3)}{\Gamma(8)\,\Gamma(n-2)}\,,$

$$\mathcal{G}^{*}_{n20}(\underline{v}) \underset{v\to\infty}{\sim} -2^4\left[\frac{\Gamma(n+3)}{\Gamma(n-2)}\right]^{1/2} \frac{1}{n^4 v^6}\, P_2(\cos\theta),$$

and

$$I_4(\beta^2, \underline{k}_f) \underset{v\to\infty}{\sim} \frac{-i\pi^2}{3\mu v \beta^6}\,.$$

Thus,

$$I^{b}_{n2m}(V_{23}, V_{12}) \underset{v\to\infty}{\sim} \delta_{m0}\,\frac{2^{19}\,i\,\pi}{3\,\Gamma(7)}\,\frac{\Gamma(n+3)}{\Gamma(n-2)}\left(\frac{n-1}{n+1}\right)^{n-4} \frac{P_2(\cos\theta)}{n^2\,(n+1)^6}\,\frac{1}{v^9(1+\lambda)}\,.$$

b) $I^{b}_{n2m}(V_{23}, V_{13}) = \frac{8\mu}{\pi^2}\, g^{*}_{n2m}(\underline{v}) \int \frac{d\underline{K}\;\mathcal{G}_{n2m}(1, -\underline{t}_1)}{(k_f^2 - K^2 + i\epsilon)\, t_1^2\,(1+t_2^2)^2}\,.$

The integrand has two peaks, one at $\underline{K} = \underline{k}_f$ and the other at $\underline{K} = a\underline{k}_i$. In the high energy limit, the leading term comes from the first and is $O(v^{-9})$.

<u>The contribution from states with $l > 2$.</u>

For such states, $t_1^{-2}\,\mathcal{G}_{nlm}(1, \underline{t}_1) = 0$ when $\underline{t}_1 = 0$. The major contribution to the $\underline{K}$ - integrals now comes from the range of $\underline{K}$ near $a\underline{k}_i$ ($\underline{t}_2 = 0$). Making the usual peaking approximation

$$I^{b}_{nlm}(V_{23}, V_{12}) = -\frac{4\mu}{\pi^2 q^2}\,\mathcal{G}^{*}_{nlm}(\underline{v})\,\mathcal{G}_{nlm}(1, -\underline{q})\; I_1(1, a\underline{k}_i),$$

and

$$I^{b}_{nlm}(V_{23}, V_{13}) = \frac{8\mu}{\pi^2 q^2}\, g^{*}_{nlm}(\underline{v})\,\mathcal{G}_{nlm}(1, -\underline{q})\; I_2(1, a\underline{k}_i).$$

Then

$$I^{b}_{nlm}(V_{23},V_{12}) = O(v^{-(2l+11)}), \quad I^{b}_{nlm}(V_{23},V_{12}) = O(v^{-(2l+10)}).$$

4) The contribution from intermediate continuum states

$$\chi^{c}_{n} = \chi_{\underline{k}}(\underline{x})\, F_{\underline{k}}(\rho).$$

Evaluation of the matrix elements

Define $N_2 = e^{\frac{1}{2}(\nu-\Lambda)\pi}\,\Gamma(1-i\nu)\,\Gamma(1+i\Lambda).$

1) $\langle \varphi_f | V_{23} | \chi^{c}_{n} \rangle$

$V_{23}$ is written in terms of its Fourier transform and a convergence factor $e^{-\lambda\rho}$ is introduced.

Then

$$\langle \varphi_f | V_{23} | \chi^{c}_{n} \rangle = -\lim_{\lambda\to 0} \frac{N_2}{2^4\,\pi^{11/2}} \int \frac{d\underline{t}}{t^2}\, \mathcal{L}_{\underline{k}}(1,\nu,\underline{k}-a\underline{t})\,\mathcal{L}_{\underline{k}}(\lambda,-\Lambda,\underline{t}_1-\underline{t}). \qquad (9.4.1$$

Using (9.2.12) this may be written

$$\langle \varphi_f | V_{23} | \chi^{c}_{n} \rangle = -\lim_{\lambda\to 0} \frac{4N_2}{\pi^{9/2}} \int \frac{d\underline{t}}{t^2}\, \frac{F_1 F_3}{\left(1+(\underline{k}-a\underline{t})^2\right)^2 \left(\lambda^2+(\underline{t}_1-\underline{t})^2\right)^2} \qquad (9.4.2$$

where $F_1$, $F_3$ are given by (9.2.13) with $\underline{Q} = \underline{t}_1 - \underline{t}$, $\alpha = -\Lambda$, and $\underline{Q} = \underline{k} - a\underline{t}$, $\alpha = \nu$, $\lambda = 1$, respectively.

The main contribution to the $\underline{t}$ - integral comes from the region near $\underline{t} = \underline{t}_1$, due to the very sharp peak in the factor $\left(\lambda^2 + (\underline{t}_1 - \underline{t})^2\right)^{-2}$ at this point in the limit $\lambda \to 0$. Assuming that the other factors in (2) are slowly varying near this value of $\underline{t}$, the integration may be carried out to give

$$\langle \varphi_f | V_{23} | \chi_n^c \rangle = - \lim_{\lambda \to 0} \frac{4 N_2 \, F_{11} \, F_{31} / \lambda}{\pi^{3/2} \, t_1^2 \left( 1 + (\underline{k} - a\underline{t}_1)^2 \right)^2} \tag{9.4.3}$$

where $F_{11}$, $F_{31}$ are the values taken by $F_1$, $F_3$ when $\underline{t} = \underline{t}_1$. A difficulty arises in the passage to the limit $\lambda \to 0$. From (9.2.13), it can be seen that

$$F_{11}/\lambda = \left( \frac{\lambda}{\lambda - 2iK} \right)^{-i\Lambda} \left( 1 + i\Lambda - \frac{\Lambda(K + i\lambda)}{\lambda - 2iK} \right),$$

and $\lim_{\lambda \to 0} \left( F_{11}/\lambda \right)$ does not exist. In this work, the definition adopted by Mapleton (1967) has been used. He took

$$\lim_{\lambda \to 0} \left( \frac{\lambda}{\lambda - 2iK} \right)^{-i\Lambda} = 1, \tag{9.4.4}$$

so that

$$\lim_{\lambda \to 0} \left( F_{11}/\lambda \right) = 1 + \frac{i\Lambda}{2} = F_6 . \tag{9.4.5}$$

The reason for adopting the definition (4) is as follows.

The convergence factor, $e^{-\lambda\rho}$ was introduced into (1) so that the order of the $\underline{t}$ and $\rho$ integrations could be interchanged. However, suppose $\Lambda$ is equated to zero before the start of the calculation $\langle \varphi_f | V_{23} | \chi_n^c \rangle$. Then the intermediate state wave function $\chi_n^c$ is replaced by

$$\chi_n^0 = (2\pi)^{-3} N_1 \exp\left( i\underline{k}.\underline{x} + i\underline{K}.\rho \right) {}_1F_1\left[ i\nu, 1, i(kx - \underline{k}.\underline{x}) \right].$$

The matrix elements $\langle \varphi_f | V_{23} | \chi_n^0 \rangle$ can be evaluated exactly, with the result

$$\langle \varphi_f | V_{23} | \chi_n^0 \rangle = \frac{-4N_1 F_{31}}{\pi^{3/2} t_1^2 \left(1 + (\underline{k} - a\underline{t}_1)^2\right)^2} \tag{9.4.6}$$

Since $\lim_{\Lambda \to 0} N_2 = N_1$, comparison of (3) and (6) shows that

$$\lim_{\Lambda \to 0} \langle \varphi_f | V_{23} | \chi_n^c \rangle = \langle \varphi_f | V_{23} | \chi_n^0 \rangle \tag{9.4.7}$$

if $\lim_{\Lambda \to 0} \lim_{\Lambda \to 0} \left( F_{11}/\lambda \right) = 1.$

This condition is satisfied if

$$\lim_{\lambda \to 0} \left( F_{11}/\lambda \right) = 1 + \frac{i\Lambda}{2},$$

and this is the reason for the definition used. However it must be stressed that, since the integral $\langle \varphi_f | V_{23} | \chi_n^c \rangle$ is not uniformly convergent with respect to $\Lambda$, there is no reason for (7) to be satisfied, and the choice of limit made must be regarded as completely arbitrary.

The $\underline{t}$ - integrand in (2) has a second, less well-defined peak at $\underline{t} = +\frac{1}{a}\underline{k}$. This has been ignored in deriving (3) for reasons similar to those which led to the neglect of the peak at $\underline{t} = 0$ during the evaluatio of the 1s bound state term $\langle \varphi_f | V_{23} | \psi_{1s} F_{\underline{k}} \rangle$. When the peaks coincide, i.e. when $\underline{k} - a\underline{t}_1 = 0$, (2) can be written approximately as

$$\langle \varphi_f | V_{23} | \chi_n^c \rangle = -\lim_{\lambda \to 0} \frac{4N_2 F_{11} F_{31}}{\pi^{7/2}} \int \frac{d\underline{t}}{t^2 \left(1 + (\underline{k} - a\underline{t})^2\right)^2 \left(\lambda^2 + (\underline{k} - a\underline{t})^2\right)^2}.$$

The integral can be evaluated exactly, and the result, in the limit $\lambda \to 0$, is

$$\frac{\pi^2}{\lambda k^2} = \frac{\pi^2}{\lambda t_1^2} .$$

Thus, when $\underline{k} - a\underline{t}_1 = 0$,

$$\langle \varphi_f | V_{23} | \chi_n^c \rangle = - \lim_{\lambda \to 0} \frac{4 N_2}{\pi^{3/2}} \left( \frac{F_{31} \, F_{11}/\lambda}{t_1^2} \right) .$$

This is the same as the result given by (3) when $\underline{k} = a\underline{t}_1$. Later it will be shown that it is precisely those values of $\underline{k}$, $\underline{K}$ satisfying this equation which are the most important, so the value of $\langle \varphi_f | V_{23} | \chi_n^c \rangle$ given by (3) and (5) has been used in the following analysis.

i.e.
$$\langle \varphi_f | V_{23} | \chi_n^c \rangle = - \frac{4 N_2 \, F_{31} \, F_6}{\pi^{3/2} \, t_1^2 \left( 1 + (\underline{k} - a\underline{t}_1)^2 \right)^2} , \qquad (9.4.8)$$

Arguments similar to the one given above determined the choice of peaks used in the evaluation of the other matrix elements.

2) $\underline{\langle \varphi_f | V_{12} | \chi_n^c \rangle}$

This matrix element is zero because the functions $\psi_{1s}(\underline{x})$, $F_{\underline{k}}(\underline{x})$ are orthogonal.

3) $\underline{\langle \chi_n^c | V_{13} | \varphi_i \rangle}$

The initial bound state wave function is written in terms of its Fourier transform

$$\psi_{1s}(\underline{r}) = \frac{1}{\pi^{5/2}} \int d\underline{s} \; \frac{\exp\{ -i \underline{s} . (\underline{\rho} + a\underline{x}) \}}{(1 + s^2)^2} ,$$

and convergence factors $e^{-\lambda x}$, $e^{-\lambda \rho}$ are introduced. Then

$$\langle \chi_n^c | V_{13} | \varphi_i \rangle = -\lim_{\lambda \to 0} \frac{N_2^*}{8\pi^{11/2}} \int \frac{d\underline{s}}{(1+s^2)^2} f_{\underline{k}}^*(\lambda, \nu, \underline{k} + a\underline{s} + (1-a^2)\underline{k}_i) \times \mathcal{L}_{\underline{k}}^*(\lambda, -\Lambda, \underline{t}_2 + \underline{s}). \qquad (9.4.9)$$

Using (9.2.10), (9.2.12), this can be written

$$\langle \chi_n^c | V_{13} | \varphi_i \rangle = -\lim_{\lambda \to 0} \frac{4N_2^*}{\pi^{7/2}} \int \frac{d\underline{s}}{(1+s^2)^2} \frac{f_4^* \, F_4^*}{(\lambda^2 + (\underline{k} + (1-a^2)\underline{k}_i + a\underline{s})^2)(\lambda^2 + (\underline{t}_2 + \underline{s})^2)^2},$$

where $f_4$, $F_4$ are given by (9.2.11), (9.2.13) with $\underline{Q} = \underline{k} + (1 - a^2)\underline{k}_i + a\underline{s}$ $\alpha = \nu$, and $\underline{Q} = \underline{t}_2 + \underline{s}$, $\alpha = -\Lambda$, respectively. The major contribution to the integral comes from the region near $\underline{s} = -\underline{t}_2$ and the usual peaking approximation and use of (4) give

$$\langle \chi_n^c | V_{13} | \varphi_i \rangle = -\frac{4N_2^*}{\pi^{3/2}} \frac{f_{42}^* \, F_6^*}{(\underline{k}_i + \underline{k} - a\underline{K})^2 (1 + t_2^2)^2}, \qquad (9.4.10)$$

where $f_{42}$ is the value of $f_4$ when $\underline{s} = -\underline{t}_2$.

4) $\underline{\langle \chi_n^c | V_{12} | \varphi_i \rangle}$

$\psi_{13}(\underline{r})$ is written in terms of its Fourier transform, $V_{12}$ is replaced by $1/\rho$ and convergence factors $e^{-\lambda\rho}$, $e^{-\lambda x}$ are introduced. Then

$$\langle \chi_n^c | V_{12} | \varphi_i \rangle = \lim_{\lambda \to 0} \frac{N_2^*}{8\pi^{11/2}} \int \frac{d\underline{s}}{(1+s^2)^2} f_{\underline{k}}^*(\lambda, -\Lambda, \underline{t}_2 + \underline{s}) \mathcal{L}_{\underline{k}}^*(\lambda, \nu, \underline{k} + (1-a^2)\underline{k}_i + a\underline{s}).$$

The $\underline{s}$-integral is strongly peaked about the value

$$\underline{s} = -\frac{1}{a}(1-a^2)\underline{k}_i - \frac{1}{a}\underline{k}.$$

The integral is evaluated in the usual way, with the result

$$\langle \chi_n^c | V_{12} | \varphi_i \rangle = \frac{4N_2^*}{\pi^{3/2}} \frac{f_{52}^* \, F_7^*}{(\underline{k}_i + \underline{k} - a\underline{K})^2 (1 + (\underline{k} + (1-a^2)\underline{k}_i)^2)^2}, \qquad (9.4.11)$$

where $f_{52}$ is given by (9.2.11) with

$$\underline{Q} = a\underline{K} - \underline{k} - \underline{k}_1, \qquad \alpha = -\Lambda, \quad \lambda = 0,$$

and

$$F_7 = \lim_{\lambda \to 0} \left( \frac{\lambda}{\lambda - 2ik} \right)^{i\nu} \left( 1 - i\nu + \frac{\nu(k + i\lambda)}{\lambda - 2ik} \right)$$

$$= 1 - \frac{i\nu}{2} \qquad \text{(using (4)).}$$

## The contribution to the transition amplitude from the continuum intermediate states.

$I^c\,(U,V)$ was defined by (9.2.5). It proves convenient to introduce new coordinates $\underline{P}$, $\underline{Q}$ defined by

$$\underline{P} = \underline{K} - \underline{k}_f = \underline{t}_1, \quad \underline{Q} = \underline{k} - a\underline{K} + \underline{k}_i .$$

Write $E - E_{\underline{k},\underline{K}} + i\epsilon = \Delta/2a$ .

In terms of the new variables,

$$\Delta = \frac{a}{\mu}\left( k_f^2 - (\underline{P} + \underline{k}_f)^2 \right) - (\underline{Q} + a\underline{P} + p)^2 + 2a\epsilon_f + i\epsilon .$$

This may be written

$$-\Delta = (\underline{P} + \underline{Q})^2 - 2(1-a)\,\underline{P}.\underline{Q} - 2\underline{P}.\underline{q} + 2p.\underline{Q} + p^2 - 2a\epsilon_f - i\epsilon .$$

Let $C_1 = |N_2|^2 F_{31} f_{42}^* |F_6|^2,$

$C_2 = |N_2|^2 F_{31} f_{52}^* F_6 F_7^* .$

From (8), (10) and (11), it can be seen that

$$I^c(V_{23},V_{13}) = \frac{2^5}{\pi^3}\int \frac{d\underline{k}\,d\underline{K}\qquad C_1}{\Delta t_1^2(\underline{k}+\underline{k}_i-a\underline{K})^2(1+(\underline{k}-a\underline{t}_1)^2)^2(1+t_2^2)^2} \qquad (9.4.12)$$

and

$$I^c(V_{23},V_{12}) = -\frac{2^5}{\pi^3}\int \frac{d\underline{k}\,d\underline{K}\qquad C_2}{\Delta t_1^2(\underline{k}+\underline{k}_i-a\underline{K})^2(1+(\underline{k}-a\underline{t}_1)^2)^2(1+(\underline{k}+(1-a^2)\underline{k}_i)^2)^2} \qquad (9.4.13)$$

In terms of the new variables

$$I^c(V_{23},V_{13}) = \frac{2^5}{\pi^3}\int \frac{d\underline{p}\,d\underline{Q}\qquad C_1}{\Delta p^2 Q^2(1+(\underline{Q}+\underline{p})^2)^2(1+(\underline{p}-\underline{q})^2)^2}, \qquad (9.4.14)$$

$$I^c(V_{23},V_{12}) = -\frac{2^5}{\pi^3}\int \frac{d\underline{p}\,d\underline{Q}\qquad C_2}{\Delta p^2 Q^2(1+(\underline{Q}+\underline{p})^2)^2(1+(\underline{Q}+a\underline{p}-a\underline{q})^2)^2}. \qquad (9.4.15)$$

Consider (12). The main contribution to the integrations in the $\underline{k}$ and $\underline{K}$ spaces comes from values of $\underline{k}$, $\underline{K}$ satisfying

$$\underline{k} = a\underline{t}_1, \quad \underline{t}_2 = 0\,.$$

The expressions (8), (10) give the exact values of the matrix elements $\langle \varphi_f | V_{23} | \chi_n^c \rangle$, $\langle \chi_n^c | V_{13} | \varphi_i \rangle$ in the limit $\lambda \to 0$ for these values of $\underline{k}$ and $\underline{K}$. Similarly in (13) the expressions used for the matrix elements $\langle \varphi_f | V_{23} | \chi_n^c \rangle$, $\langle \chi_n^c | V_{13} | \varphi_i \rangle$ are exact (in limit $\lambda \to 0$ ) for the values of $\underline{k}$ and $\underline{K}$ which provide the major contribution to $I^c$ $(V_{23}, V_{12})$. It therefore seems reasonable to suppose that (12), (13) provide a good approximation to the true matrix elements $I^c$ (U, V). It can be shown that the values taken by the Coulomb factors $C_1$, $C_2$ at the peaks of the integrand both tend to 1 as $v \to \infty$.

Apart from the factor $C_1$, $I^c(V_{23}, V_{13})$ is identical with the second Born term $I(V_{23}, V_{13})$ given by Drisko. He showed that

$$I(V_{23}, V_{13}) \underset{v\to\infty}{\sim} \frac{-2^{11}\pi}{v^6(1+\lambda)^2(\lambda-3-16i/v)} . \qquad (9.4.16)$$

The evaluation of $I^c(V_{23}, V_{12})$.

The integrand in (15) has peaks at

$$\underline{Q} = -\underline{p},\ \underline{P} = \underline{q} + \frac{1}{a}\underline{p} .$$

At the peaks

$$-\Delta = \left(\underline{q} + \left(\frac{1}{a} - 1\right)\underline{p}\right)^2 + 2(1-a)\left(\underline{q} + \frac{1}{a}\underline{p}\right).\underline{p} - 2\left(\underline{q} + \frac{1}{a}\underline{p}\right).\underline{q} - p^2 - 2a\mathcal{E}_f - i\epsilon$$

$$= \left(1/a^2 - 3\right)p^2 - 2a\,\underline{p}.\underline{q} - 2a\mathcal{E}_f - i\epsilon,$$

where the relation $p^2 = q^2$ has been used. Thus

$$-\Delta \simeq \frac{1}{a^2}\left(1 - 2a\cos\theta\right)v^2 - i\epsilon,$$

and this can be zero. A contour integral method similar to that used by Drisko for the evaluation of $I^c(V_{23}, V_{13})$ is therefore used.

Let

$$\underline{P}' = \underline{Q} + a\underline{P} - a\underline{q},\quad \underline{Q}' = \underline{Q} + \underline{p} .$$

Then

$$-\Delta = \frac{1}{a^2}\left((1-a^2)Q'^2 - 2(1-a^2)\underline{P}'.\underline{Q}' + P'^2\right) + \frac{2}{a^2}(1-a^2)\underline{p}.\underline{P}'$$
$$+ 2\left(a\underline{q} + \frac{2a^2-1}{a^2}\underline{p}\right).\underline{Q}' + \frac{1}{a^2}(1-3a^2)p^2 - 2a\,\underline{p}.\underline{q} - 2a\mathcal{E}_f - i\epsilon,$$

and

$$I^{c}(V_{23},V_{12}) = -\frac{2^5}{\pi^3}\int \frac{d\underline{P}'\,d\underline{Q}'}{\Delta(1+P'^2)^2(1+Q'^2)^2(\underline{P}'-\underline{Q}'+\underline{p}+a\underline{q})^2(\underline{Q}'-\underline{p})^2} .$$

There are strong peaks at $\underline{P}' = 0$, $\underline{Q}' = 0$. $\Delta$ is therefore replaced by $\Delta_0$, where

$$-\Delta_0 = 2\,\underline{u}.\underline{P}' + 2\,\underline{w}.\underline{Q}' + A ,$$

with

$$\underline{u} = {}^{1}/_{a^2}(1-a^2)\,\underline{p} , \quad \underline{w} = a\underline{q} + {}^{1}/_{a^2}(2a^2-1)\,\underline{p} ,$$

and

$$A = {}^{1}/_{a^2}(1-3a^2)\,p^2 - 2a\,\underline{p}.\underline{q} - 2a\,\varepsilon_f ,$$

and $(\underline{P}' - \underline{Q}' + \underline{p} + a\underline{q})^2$, $(\underline{Q}' - \underline{p})^2$ are replaced by $(\underline{p} + a\underline{q})^2$, $p^2$ respectively. Then

$$I^{c}(V_{23},V_{12}) = \frac{-2^5}{\pi^3(\underline{p}+a\underline{q})^2p^2}\int \frac{d\underline{P}'\,d\underline{Q}'}{\Delta_0(1+P'^2)^2(1+Q'^2)^2} .$$

Cylindrical coordinate systems are introduced for both integrations, with axes in directions $\underline{u}$, $\underline{w}$.

Then $d\underline{P}' \rightarrow 2\pi P_r'\,dP_r'\,dP_z'$, $d\underline{Q}' \rightarrow 2\pi Q_r'\,dQ_r'\,dQ_z'$.

The integrals with respect to $P_r'$ and $Q_r'$ are easily evaluated, giving

$$I^{c}(V_{23},V_{12}) = \frac{2^5}{\pi(\underline{p}+a\underline{q})^2p^2}\int_{-\infty}^{\infty}\frac{dP_z}{(1+P_z^2)}\int_{-\infty}^{\infty}\frac{dQ_z}{(1+Q_z^2)(2uP_z+2wQ_z+A-i\epsilon} ,$$

where primes have been omitted.

The $Q_z$- integral may be evaluated using contour integration, taking as contour the real axis and an infinite semicircle in the lower half plane. The integrand has a pole at $Q_z = -i$, with residue $\dfrac{-1}{2i(1+P_z^2)(2uP_z-2i\omega+A)}$.

The same contour may then be used to evaluate the $P_z$ integral. The residue at the pole $P_z = -i$ is $\dfrac{1}{(2i)^2(-2iu-2i\omega+A)}$.

Finally,

$$I^c(V_{23},V_{12}) = \frac{2^5\pi}{(\underline{p}+a\underline{q})^2p^2\left(1/a^2(1-3a^2)p^2-2a\underline{p}.\underline{q}-2i(u+\omega)\right)}$$

$$= \frac{2^7\pi}{v^4(1+\lambda)\left(v^2(1-2\cos\theta)-2i(u+\omega)\right)}.$$

The imaginary part of the denominator is only important when $\cos\theta = \frac{1}{2}$, and then

$$|\underline{u}| = \frac{1}{a^2}(1-a^2)p = v, \qquad |\underline{\omega}| = v.$$

Thus

$$I^c(V_{23},V_{12}) = \frac{-2^7\pi}{v^6(1+\lambda)(1-\lambda/M^2+4i/v)}. \tag{9.4.17}$$

However, it was found that

$$I_{15}^b(V_{23},V_{13})+I_{15}^b(V_{12},V_{13}) \underset{v\to\infty}{\sim} -\frac{2^7\pi}{v^6(1+\lambda)},$$

and further analysis reveals that to obtain this result terms in $\lambda/M^2$ have been dropped. Therefore, for consistency, the term $\lambda/M^2$ is dropped in (17) also. The imaginary term is then insignificant, and

$$I^c(V_{23}, V_{12}) \underset{v \to \infty}{\sim} -\frac{2^7 \pi}{v^6(1+\lambda)} . \qquad (9.4.18)$$

## 5) Conclusion.

It was shown in § 2 of this chapter that the modified first Born approximation transition amplitude can be written

$$T_{if}^{MB} = T_{if}^{B} + T_{if}^{M}$$

where

$$T_{if}^{B} = T_{if}^{BK} + I^{JS}$$

and

$$T_{if}^{M} = I(V_{23}, V_{12}) + I(V_{23}, V_{13}) + I(V_{12}, V_{13}) + I(V_{12}, V_{12}).$$

Each separate term $I(U, V)$ can be split into two parts

$$I(U, V) = I^b(U, V) + I^c(U, V)$$

where $I^{b,c}(U, V)$ are defined by (9.2.5).

If terms of order $1/M$ are neglected

$$T_{if}^{B} \underset{v \to \infty}{\sim} \frac{-2^{11} \pi}{v^6(1+\lambda)^3} + \frac{2^8 \pi}{v^6(1+\lambda)} .$$

The asymptotic forms which have been derived for the various terms occurring in $T_{if}^{M}$ are given here for convenience.

1) <u>The bound state terms $I^{b}$ (U, V)</u>

The intermediate ground state terms

$$I_{1s}^{b}(V_{23},V_{13}) + I_{1s}^{b}(V_{12},V_{13}) \underset{v\to\infty}{\sim} -\frac{2^{7}\pi}{v^{6}(1+\lambda)}$$

$$I_{1s}^{b}(V_{23},V_{12}) + I_{1s}^{b}(V_{12},V_{12}) \underset{v\to\infty}{\sim} -\frac{2^{7}\pi i \ln v}{v^{7}(1+\lambda)} .$$

The contributions from s states with n > 1 are of order $v^{-7}$, while those from p and d states are of order $v^{-8}$, $v^{-9}$ respectively. For states with $\ell > 2$, $I_{nlm}^{b}(V_{23}, V_{13}) = 0(v^{-2\ell-11})$ and $I_{nlm}^{b}(V_{23}, V_{12}) = 0(v^{-2\ell-10})$.

2) <u>The continuum state terms $I^{c}$ (U, V)</u>

$$I^{c}(V_{23},V_{12}) \underset{v\to\infty}{\sim} -\frac{2^{7}\pi}{v^{6}(1+\lambda)}$$

$$I^{c}(V_{23},V_{13}) \underset{v\to\infty}{\sim} -\frac{2^{11}\pi}{v^{6}(1+\lambda)^{2}\left(\lambda-3-\frac{16i}{v}\right)} .$$

Thus, if terms whose asymptotic form decreases with energy more rapidly than $v^{-6}$ are ignored, the only contributions to the high energy form of $T_{if}^{M}$ come from the bound state terms $I_{1s}^{b}(V_{23}, V_{13}) + I_{1s}^{b}(V_{12}, V_{13})$ and the continuum state terms $I^{c}(V_{23}, V_{12})$, $I^{c}(V_{23}, V_{13})$. Clearly

$$I^{JS} + I_{1s}^{b}(V_{23}, V_{13}) + I_{1s}^{b}(V_{12},V_{13}) + I^{c}(V_{23}, V_{12}) = 0,$$

so, finally,

$$T_{if}^{MB} \underset{v\to\infty}{\sim} T_{if}^{BK} - \frac{2^{11}\pi}{v^{6}(1+\lambda)^{2}\left(\lambda-3-\frac{16i}{v}\right)} .$$

The asymptotic form of Drisko's second Born approximation is given by the same expression.

The work described in this chapter is unsatisfactory for several reasons. In particular, it was found necessary to use rather crude peaking approximations to evaluate the formidable integrals which arise, and although the validity of the methods used was carefully tested wherever possible, the results cannot be regarded as rigorous. Further difficulties arise over the contribution from the bound state terms. It has been assumed that the sum of an infinite number of terms, all with the same energy dependence, is finite, so that, for example, the contribution from all s states with n greater that 1 gives a term of order $v^{-7}$. This assumption may not be correct. The present author intends to look at this point in more detail but so far no alternative method for dealing with the terms has been found. Finally, to simplify the analysis, terms of order $^1/M$ have been dropped.

For these reasons, no definite conclusions can be drawn. However, the work indicates that the asymptotic form of $T_{if}^{MB}$ may well be the same as that of the second Born approximation.

## Appendix 1.

## Evaluation of the functions $\mathcal{J}(\underline{K}, nl, \underline{p})$.

### 1) Introduction.

Let the wave function $\psi_{nl}(\underline{x})$ of the final bound state be referred to a frame of reference OXYZ with Z-axis along $\underline{p}$ and such that the XZ plane is the plane of $\underline{p}$ and $\underline{k}_1$. It proves convenient to carry out the $\underline{x}$-integration involved in the definition of $\mathcal{J}(\underline{K}, nl, \underline{p})$ (see (7.3.11)) in a frame $Ox'y'z'$ with $z'$-axis in the direction of $\underline{\lambda} = \underline{p} - \underline{K}$, and with the plane of $\underline{\lambda}$ and $\underline{p}$ as the $x'z'$ plane. (Then $\underline{K}$ lies in the $x'z'$ plane.) Spherical polar coordinates in OXYZ and $Ox'y'z'$ are denoted by $(x, \Theta, \Phi)$, $(x, \theta, \varphi)$ respectively. In order to perform the integration, expressions for the wave functions $\psi_{nl}(\underline{x})$ referred to axes $Ox'y'z'$ must be found. In the present work it is only necessary to consider the cases $l = 0$, $l = 1$. Since the s state wave functions are spherically symmetric, they have the same form in both frames.

In the frame OXYZ,

$$\psi_{nlm}(\underline{x}) = R_{nl}(x)\, Y_{lm}(\Theta, \Phi),$$

where $R_{nl}(x)$ is the radial part of the wave function and

$$Y_{lm}(\Theta, \Phi) = (-1)^m \left[\frac{(2l+1)}{4\pi}\,\frac{(l-m)!}{(l+m)!}\right]^{1/2} P_l^m(\cos\Theta)\, e^{im\Phi}.$$

The spherical harmonics $Y_{lm}(\Theta, \Phi)$ transform, under rotation of the frame of reference, according to the equation

$$Y_{lm}(\Theta, \Phi) = \sum_{m'=-l}^{l} Y_{lm'}(\theta, \varphi)\, R^{l}_{m'm}(\alpha, \beta, \gamma), \qquad (A1.1.1)$$

where the functions $R^{l}_{m'm}(\alpha,\beta,\gamma)$ are the elements of the rotation matrix, and $\alpha,\beta,\gamma$ are the Euler angles of the rotation which takes $Ox'y'z'$ into $OXYZ$. (See, for example, Messiah (1962) p. 1068). In the present case, $\alpha = 0$, $\beta = \cos^{-1}(\underline{p}\cdot\underline{\lambda})$ and $\gamma$ is the angle which the plane of $\underline{p}$ and $\underline{\lambda}$ makes with that of $\underline{p}$ and $\underline{k}_i$. (i.e. $\gamma$ is just the azimuthal angle for the $\underline{K}$ integration.) The elements of the rotation matrix for $l = 1$ are given by (7.4.2).

Since

$$\psi_{np_z}(\underline{x}) = \psi_{np_0}(\underline{x}),$$

$$\psi_{np_y}(\underline{x}) = \frac{i}{\sqrt{2}}\left(\psi_{np_1}(\underline{x}) + \psi_{np_{-1}}(\underline{x})\right),$$

and

$$\psi_{np_x}(\underline{x}) = \frac{i}{\sqrt{2}}\left(\psi_{np_{-1}}(\underline{x}) - \psi_{np_1}(\underline{x})\right),$$

it can be seen from (A1.1.1) and (7.4.3) that

$$\psi_{np_z}(\underline{x}) = \cos\beta\,\psi'_{np_z}(\underline{x}) + \sin\beta\,\psi'_{np_x}(\underline{x}),$$

$$\psi_{np_y}(\underline{x}) = \sin\gamma\left(\sin\beta\,\psi'_{np_z}(\underline{x}) - \cos\beta\,\psi'_{np_x}(\underline{x})\right) + \cos\gamma\,\psi'_{np_y}(\underline{x}),$$

$$\psi_{np_x}(\underline{x}) = -\cos\gamma\left(\sin\beta\,\psi'_{np_z}(\underline{x}) - \cos\beta\,\psi'_{np_x}(\underline{x})\right) + \sin\gamma\,\psi'_{np_y}(\underline{x}),$$

where the primes are used to distinguish wave functions referred to the reference frame $Ox'y'z'$, the unprimed ones being referred to frame $OXYZ$. Substitution of these expressions in (7.3.11) gives

$$\mathcal{J}(np_z) = \cos\beta\,\mathcal{J}'(np_z) + \sin\beta\,\mathcal{J}'(np_x),$$

$$\mathcal{J}(np_y) = \sin\gamma\left(\sin\beta\,\mathcal{J}'(np_z) - \cos\beta\,\mathcal{J}'(np_x)\right) + \cos\gamma\,\mathcal{J}'(np_y),$$

$$\mathcal{J}(np_x) = -\cos\gamma\left(\sin\beta\,\mathcal{J}'(np_z) - \cos\beta\,\mathcal{J}'(np_x)\right) + \sin\gamma\,\mathcal{J}'(np_y),$$

where, for conciseness, $\mathcal{J}(\underline{K}, nl, \underline{p})$, $\mathcal{J}'(\underline{K}, nl, \underline{p})$ have been written as $\mathcal{J}(nl)$, $\mathcal{J}'(nl)$ and $\mathcal{J}'(\underline{K}, nl, \underline{p})$ is the result obtained by using in (7.3.11) the wave function $\psi'_{nl}(\underline{x})$ instead of $\psi_{nl}(\underline{x})$. That is,

$$\mathcal{J}'(\underline{K}, nl, \underline{p}) = \int d\underline{x} \left(\psi'_{nl}(\underline{x})\right)^{*} \exp(i\underline{p}\cdot\underline{x}) \, {}_1F_1\left[\frac{i\alpha}{K}, 1, i(Kx - \underline{K}\cdot\underline{x})\right].$$

In the present work, the functions $\mathcal{J}'(nl)$ are required for the following values of nl;

$2p_x$, $2p_y$, $2p_z$, $3s$, $3p_x$, $3p_y$, $3p_z$.

The value of $\mathcal{J}'(3s)$ is obtained by parametric differentiation of $\mathcal{J}'(1s)$ and the values for the 3p states are obtained from the corresponding expressions for the 2p states by the same technique. The basic integrals are given by Coleman (1965). It proves convenient to define

$$\mathcal{L}_m^{(n)}(\alpha, \beta) \equiv \left(\frac{\partial}{\partial\beta}\right)^n \mathcal{L}_m^{(0)}(\alpha, \beta) \qquad (A1.1.2)$$

where the functions $\mathcal{L}_m^{(0)}(\alpha, \beta)$ for m = 1, 3, 4, 5 are defined in the following pages.

2) <u>The evaluation of $\mathcal{J}'(\underline{K}, 3s, \underline{p})$</u>.

If finally, the bound system is in the 3s state, the wave function is

$$\psi_{3s}(\underline{x}) = \frac{\alpha^{3/2}}{81\sqrt{3\pi}} \left(27 - 18\alpha x + 2\alpha^2 x^2\right) e^{-\alpha x/3},$$

If

$$\mathcal{L}_1^{(0)}(\alpha, \beta) = \int e^{-\beta x} e^{i\underline{p}\cdot\underline{x}} \, {}_1F_1\left[\frac{i\alpha}{K}, 1, i(Kx - \underline{K}\cdot\underline{x})\right] d\underline{x},$$

then $\mathcal{J}'(\underline{K},3s,\underline{p})$ can be written

$$\mathcal{J}'(\underline{K},3s,\underline{p}) = \frac{\alpha^{3/2}}{88\sqrt{3\pi}}\left(27\,\mathcal{L}_1^{(0)}(\alpha,\alpha/3)+18\alpha\,\mathcal{L}_1^{(1)}(\alpha,\alpha/3)+2\alpha^2\,\mathcal{L}_1^{(2)}(\alpha,\alpha/3)\right) \qquad \text{(A1.2.1}$$

The value $\mathcal{L}_1^{(0)}(\alpha,\beta)$ is found by evaluating the integral

$$\mathcal{L}_1(\alpha,\beta) = \int \frac{e^{-\beta x}}{x}\, e^{i\underline{p}.\underline{x}}\; {}_1F_1\left[\frac{i\alpha}{K},1,i(Kx-\underline{K}.\underline{x})\right] d\underline{x},$$

and using the fact that

$$\mathcal{L}_1^{(0)}(\alpha,\beta) = -\frac{\partial}{\partial\beta}\mathcal{L}_1(\alpha,\beta). \qquad \text{(A1.2.2}$$

The analysis given here follows that of Massey and Mohr (1933) and McDowell (1961).

Let $n = -\frac{i\alpha}{K}$, $\cos\delta = \hat{\underline{K}}.\hat{\underline{x}}$, $v = x(1-\cos\delta)$, $\underline{\partial} = \underline{p}-\underline{K}$.

If Kummer's transformation,

$${}_1F_1\,(a,\ b;\ x) = e^x\,{}_1F_1\,(c-a,\ c;\ -x)$$

(see Erdélyi, 1953, Vol I p.253), is used

$$\mathcal{L}_1(\alpha,\beta) = \int \frac{1}{x}\exp\left(-(\beta-iK)x+i\underline{\partial}.\underline{x}\right){}_1F_1[1+n,1,-iKx]\,d\underline{x}.$$

But

$$\frac{\Gamma(\tfrac{1}{2}\nu+\tfrac{1}{2}\mu)\left(\frac{a}{2p}\right)^{\nu}}{2p^{\mu}\,\Gamma(\nu+1)}\;{}_1F_1\left[\tfrac{1}{2}\nu+\tfrac{1}{2}\mu;\nu+1;-\frac{a^2}{4p^2}\right]$$

$$= \int_0^\infty J_\nu(at)\exp(-p^2t^2)\,t^{\mu-1}\,dt.$$

(see Watson (1958) p.393).

With $\nu = 0$, $\mu = 2(n+1)$, $a = 2\sqrt{iKv}$, $p = 1$, this gives

$$ {}_1F_1[n+1, 1, -iKv] = \frac{1}{\Gamma(n+1)} \int_0^\infty J_0\left(\sqrt{4iKvy}\right) e^{-y} y^n \, dy , \qquad \text{(A1.2.3)} $$

where the change of variable $y = t^2$ has been made. Therefore,

$$ \mathcal{L}_1(\alpha,\beta) = \frac{1}{\Gamma(n+1)} \int \frac{d\underline{x}}{x} \exp\left(-(\beta - iK)x + i\,\underline{\lambda}.\underline{x}\right) \int_0^\infty J_0\left(\sqrt{4iKvy}\right) e^{-y} y^n \, dy . $$

Now, $\varphi$ is the angle which the plane of $\underline{\lambda}$ and $\underline{x}$ makes with the plane of $\underline{\lambda}$ and $\underline{K}$, and $\hat{\underline{\lambda}}.\hat{\underline{x}} = \cos\theta$. Therefore, if $\hat{\underline{K}}.\hat{\underline{\lambda}} = \cos\chi$, then

$$ v = x(1 - \cos\delta) = x(1 - \cos\chi\cos\theta - \sin\chi\sin\theta\cos\varphi). \qquad \text{(A1.2.4)} $$

Parabolic coordinates $(\xi, \eta, \varphi)$ are now introduced, where

$$ \xi = x(1 + \cos\theta), \qquad \eta = x(1 - \cos\theta). \qquad \text{(A1.2.5)} $$

In this coordinate system, the volume element $d\underline{x}$ is given by

$$ d\underline{x} = \tfrac{1}{4}(\xi + \eta)\, d\xi \, d\eta \, d\varphi . $$

Since $x = \frac{1}{2}(\xi + \eta)$, (4) becomes

$$ v = \xi \sin^2 \chi/2 + \eta \cos^2 \chi/2 - 2\sqrt{\xi\eta} \cos \chi/2 \sin \chi/2 \cos\varphi . $$

Therefore,

$$ \mathcal{L}_1(\alpha,\beta) = \frac{1}{2\Gamma(n+1)} \int_0^\infty dy \int_0^\infty d\xi \int_0^\infty d\eta \int_0^{2\pi} d\varphi \; y^n \exp\left(-\tfrac{1}{2}a_1\xi - \tfrac{1}{2}a_2\eta - y\right) J_0(z) , \qquad \text{(A1.2.6} $$

where

$$a_1 = \beta - iK - i\lambda, \quad a_2 = \beta - iK + i\lambda, \tag{A1.2.7}$$

$$Z^2 = z_1^2 + z_2^2 - 2z_1 z_2 \cos\varphi,$$

$$z_1 = \sqrt{4iKy\xi\sin^2 \chi/2} \quad \text{and} \quad z_2 = \sqrt{4iKy\eta\cos^2 \chi/2}.$$

From Graf's addition theorem (Watson (1958), p.359), it follows that

$$J_0(Z) = \sum_{m=-\infty}^{\infty} J_m(z_1)\, J_m(z_2)\, e^{im\varphi}. \tag{A1.2.8}$$

Since

$$\int_0^{2\pi} e^{im\varphi}\, d\varphi = 2\pi\, \delta_{m0},$$

(6) reduces to

$$\mathcal{L}_1(\alpha,\beta) = \frac{\pi}{\Gamma(1+n)} \int_0^\infty dy \int_0^\infty d\xi \int_0^\infty d\eta\, y^n J_0(z_1) J_0(z_2) \exp\left(-\tfrac{1}{2}a_1\xi - \tfrac{1}{2}a_2\eta - y\right).$$

If one puts $\xi = z^2$, the $\xi$ - integral becomes

$$2\int_0^\infty J_0\left(z\sqrt{4iKy\sin^2\chi/2}\right)\exp\left(-\tfrac{1}{2}a_1 z^2\right) z\, dz$$

$$= \frac{2}{a_1}\exp\left(-\frac{2iKy}{a_1}\sin^2\chi/2\right) \tag{A1.2.9}$$

(see Watson (1958) p.393).

The integration with respect to $\eta$ may be carried out in a similar way.

Thus

$$\mathcal{L}_1(\alpha,\beta) = \frac{4\pi}{\Gamma(1+n)a_1 a_2} \int_0^\infty y^n \exp\left(-\frac{2iKy}{a_1}\sin^2\chi/2 - \frac{2iKy}{a_2}\cos^2\chi/2 - y\right) dy. \quad \text{(A1.2.}$$

From (7) it is clear that

$$a_1 a_2 = c - id \qquad (A1.2.11)$$

where $$c = \beta^2 - K^2 + \lambda^2, \quad d = 2\beta K. \qquad (A1.2.12)$$

Also,

$$-\frac{2iKy}{a_1 a_2}\left( a_2 \sin^2 \chi/_2 + a_1 \cos^2 \chi/_2 \right) - y$$
$$= -\frac{2iKy}{c-id}\left( \beta - iK - i\lambda \cos\chi \right) - y = -\frac{Ty}{c-id}, \qquad (A1.2.13)$$

where $T = \beta^2 + p^2$. (A1.2.14)

If results (11) and (13) are used in (10) it becomes

$$\mathcal{L}_1(\alpha,\beta) = \frac{4\pi}{c-id}\int_0^\infty y^n \exp\left( \frac{-Ty}{c-id}\right) dy$$
$$= \frac{4\pi}{T}\left( \frac{c-id}{T}\right)^n . \qquad (A1.2.15)$$

Using (15) in (2), one obtains

$$\mathcal{L}_1^{(0)}(\alpha,\beta) = -\frac{8\pi}{T}\left( \frac{c-id}{T}\right)^n \left( \frac{n(\beta - iK)}{c-id} - \beta\frac{(n+1)}{T}\right).$$

Then, from (A1.1.2) it follows that

$$\mathcal{L}_1^{(1)}(\alpha,\beta) = -8\pi\left(\frac{c-id}{T}\right)^n \left( \frac{n}{(c-id)T} + \frac{2n(n-1)(\beta-iK)^2}{(c-id)^2 T} - \frac{4n(n+1)\beta(\beta-iK)}{T^2(c-id)} - \frac{(n+1)}{T^2} + \frac{2\beta^2(n+1)(n+2)}{T^2}\right), \qquad (A1.2.16)$$

and $$\mathcal{I}_1^{(2)}(\alpha,\beta) = -8\pi\left(\frac{c-id}{T}\right)^n\left(\frac{B_0}{T}+\frac{B_1}{T^2}+\frac{B_2}{T^3}+\frac{B_3}{T^4}\right), \tag{A1.2.17}$$

where $$B_0 = \frac{6n(n-1)(\beta-iK)}{(c-id)^2} + \frac{4n(n-1)(n-2)(\beta-iK)^3}{(c-id)^3},$$

$$B_1 = \frac{-6(n+1)(2\beta-iK)}{c-id} - \frac{12n(n-1)(n+1)\beta(\beta-iK)^2}{(c-id)^2},$$

$$B_2 = 6(n+1)(n+2)\beta + \frac{12n(n+1)(n+2)\beta^2(\beta-iK)}{c-id},$$

$$B_3 = -4(n+1)(n+2)(n+3)\beta^4.$$

If (16) and (17) are substituted in (1), the result is

$$\mathcal{J}'(\underline{K},3s,p) = N_{3s}\left(\frac{c-id}{T}\right)^n\left(\frac{A_0}{T}+\frac{A_1}{T^2}+\frac{A_2}{T^3}+\frac{A_3}{T^4}\right),$$

where

$$N_{3s} = -\frac{8\pi\alpha^{3/2}}{81\sqrt{3\pi}}, \quad \beta = \frac{\alpha}{3},$$

$$A_0 = 9n\frac{(2\alpha+3\beta-3iK)}{c-id} + \frac{12\alpha n(n-1)(\beta-iK)(3\beta-3iK+\alpha)}{(c-id)^2} + \frac{8n(n-1)(n-2)\alpha^2(\beta-iK)^3}{(c-id)^3},$$

$$A_1 = -9(n+1)(3\beta+2\alpha) - \frac{12n(n+1)\alpha(2\beta(\alpha+3\beta)-iK(\alpha+6\beta))}{c-id} + \frac{24n(n-1)(n+1)\alpha^2\beta(\beta-iK)^2}{(c-id)^2},$$

$$A_2 = 12(n+1)(n+2)\alpha\beta(\alpha+3\beta) + \frac{24n(n+1)(n+2)\alpha^2\beta^2(\beta-iK)}{c-id},$$

$$A_3 = -8(n+1)(n+2)(n+3)\alpha^2\beta^3.$$

3) i) The evaluation of $\mathcal{J}'(\underline{K}, 2p_z, \underline{p})$.

The $2p_z$ wave function is

$$\psi_{2p_z}(\underline{x}) = \frac{\alpha^{5/2}}{4\sqrt{2\pi}}\, x\cos\theta\, e^{-\alpha x/2} .$$

Therefore,

$$\mathcal{J}'(\underline{K}, 2p_z, \underline{p}) = \frac{\alpha^{5/2}}{4\sqrt{2\pi}}\, \mathcal{L}_3^{(0)}(\alpha, \alpha/2) \qquad (A1.3.1)$$

where

$$\mathcal{L}_3^{(0)}(\alpha,\beta) = \int x\cos\theta\, e^{-\beta x}\, e^{i\underline{p}.\underline{x}}\, {}_1F_1\left[\frac{i\alpha}{K}, 1, i(Kx-\underline{K}.\underline{x})\right] d\underline{x} \qquad (A1.3.2)$$

$$= \frac{1}{\Gamma(n+1)}\int d\underline{x}\; x\cos\theta \exp\left(-(\beta-iK)x+i\underline{p}.\underline{x}\right)\int_0^\infty dy\, y^n e^{-y} J_0\left(\sqrt{4iKvy}\right). \qquad (A1.3.3$$

The parabolic coordinates introduced in the previous section are again used. Since

$$x\cos\theta = \tfrac{1}{2}(\xi-\eta),$$

(3) becomes

$$\mathcal{L}_3^{(0)}(\alpha,\beta) = \frac{1}{8\Gamma(n+1)}\int_0^\infty dy\int_0^\infty d\xi\int_0^\infty d\eta\int_0^{2\pi} d\varphi\; y^n(\xi-\eta)(\xi+\eta)\exp\left(-\frac{a_1\xi}{2}-\frac{a_2}{2}\eta-y\right)J_0(Z),$$

where $a_1$, $a_2$, $z_1$, $z_2$, Z are defined by (A1.2.7). Using (A1.2.8), and carrying out the integration with respect to $\varphi$, it can be seen that

$$\mathcal{L}_3^{(0)}(\alpha,\beta) = \frac{-\pi}{2\Gamma(n+1)}\frac{\partial}{\partial\beta}\mathcal{L}_2(\alpha,\beta) \qquad (A1.3.4)$$

where

$$\mathcal{L}_2(\alpha,\beta) = \frac{8}{a_1 a_2}\int_0^\infty dy\, y^n \exp\left(-y - 2iKy\left(\frac{\sin^2 X/_2}{a_1} + \frac{\cos^2 X/_2}{a_2}\right)\right)$$

$$\times\left(\frac{1}{a_1} - \frac{1}{a_2} - 2iKy\left(\frac{\sin^2 X/_2}{a_1^2} - \frac{\cos^2 X/_2}{a_2^2}\right)\right). \quad \text{(A1.3.5}$$

From (A1.2.7), (A1.2.11), (A1.2.12), it follows that

$$\frac{\cos^2 X/_2}{a_2^2} - \frac{\sin^2 X/_2}{a_1^2} = \frac{\mu}{c-id} - \frac{2\lambda(\lambda\mu+K+i\beta)}{(c-id)^2},$$

where $\mu = \cos X$.

Substituting this result in (5), and using (A1.2.11), (A1.2.12) one obtains

$$\mathcal{L}_2(\alpha,\beta) = \frac{8}{c-id}\int_0^\infty dy\, y^n \exp\left(\frac{-Ty}{c-id}\right)\left[\frac{2i\lambda}{c-id} + 2iKy\left(\frac{\mu}{c-id} - \frac{2\lambda(\lambda\mu+K+i\beta)}{(c-id)^2}\right)\right]$$

$$= 16i\,\Gamma(1+n)\left(\frac{c-id}{T}\right)^n\left[\frac{\lambda}{T(c-id)} + \frac{K\mu(n+1)}{T^2} - \frac{2\lambda K(n+1)(\lambda\mu+K+i\beta)}{T^2(c-id)}\right]. \quad \text{(A1.3.6}$$

If (6) is substituted in (4), the result is

$$\mathcal{L}_3^{(0)}(\alpha,\beta) = 16i\pi\left(\frac{c-id}{T}\right)^n\left(\frac{A_0}{T} + \frac{A_1}{T^2} + \frac{A_2}{T^3}\right), \quad \text{(A1.3.7)}$$

where

$$A_0 = \frac{\lambda(\beta-iK)(1-n)}{(c-id)^2},$$

$$A_1 = \frac{(n+1)(\lambda\beta+i\lambda K-\mu Kn(\beta-iK))}{c-id} - \frac{2\lambda K(1-n^2)(\beta-iK)(\lambda\mu+K+i\beta)}{(c-id)^2},$$

$$A_2 = K\mu\beta(n+1)(n+2) - \frac{2\lambda\beta K(n+1)(n+2)(\lambda\mu+K+i\beta)}{c-id}.$$

Finally,

$$\mathcal{F}'(\underline{K}, 2p_z, \underline{p}) = N_{2p_z}\left(\frac{c-id}{T}\right)^{n}\left(\frac{A_0}{T} + \frac{A_1}{T^2} + \frac{A_2}{T^3}\right),$$

where $N_{2p_z} = 2i\,\alpha^{5/2}\sqrt{2\pi}$ , $\beta = \alpha/2$.

ii) Evaluation of $\mathcal{F}'(\underline{K}, 2p_x, \underline{p})$

Since $\psi_{2p_x}(\underline{x}) = \dfrac{\alpha^{5/2}}{4\sqrt{2\pi}}\, x \sin\theta \cos\varphi\, e^{-\alpha x/2}$,

$$\mathcal{F}'(\underline{K}, 2p_x, \underline{p}) = \frac{\alpha^{5/2}}{4\sqrt{2\pi}}\, \mathcal{I}_4^{(0)}(\alpha, \alpha/2) \tag{A1.3.8}$$

where
$$\mathcal{I}_4^{(0)}(\alpha,\beta) = \int d\underline{x}\;\; x\sin\theta\cos\varphi\, e^{-\beta x} e^{i\underline{p}.\underline{x}}\, {}_1F_1\left[i\alpha/K, 1, i(Kx - \underline{K}.\underline{x})\right] \tag{A1.3.9}$$

From (A1.2.5) it follows that

$$x \sin\theta = \sqrt{\xi\eta}\,,$$

and therefore, using (A1.2.3), (A1.2.8), (9) can be written

$$\mathcal{I}_4^{(0)}(\alpha,\beta) = -\frac{1}{\Gamma(1+n)}\frac{\partial}{\partial\beta}\mathcal{L}_3(\alpha,\beta) \tag{A1.3.10}$$

where

$$\mathcal{L}_3(\alpha,\beta) = \int_0^\infty dy\int_0^\infty d\xi\int_0^\infty d\eta\int_0^{2\pi} d\varphi\, \sqrt{\xi\eta}\; y^{n} \cos\varphi$$
$$\times \exp\left(-\tfrac{1}{2}(a_1\xi + a_2\eta) - y\right)\sum_{m=-\infty}^{\infty} J_m(z_1)J_m(z_2)e^{im\varphi}. \tag{A1.3.11}$$

However, $\displaystyle\int_0^{2\pi} e^{im\varphi}\cos\varphi\, d\varphi = \begin{matrix} 0\,, & m \neq \pm 1 \\ \pi\,, & m = \pm 1\,, \end{matrix}$

and $J_{-1}(z) = -J_1(z)$.

(11) therefore reduces to

$$\mathcal{L}_3(\alpha,\beta) = 2\pi\int_0^\infty dy\int_0^\infty d\xi\int_0^\infty d\eta\; y^{n}\sqrt{\xi\eta}\, \exp\left(-\tfrac{1}{2}(a_1\xi + a_2\eta) - y\right)J_1(z_1)J_1(z_2).$$

Consider the integral

$$I = \int_0^\infty \xi^{1/2} e^{-1/2\, a_1 \xi} J_1(u \xi^{1/2})\, d\xi .$$

Using the Bessel function recurrence relation

$$\nu/_{z}\, J_\nu(z) - \partial/_{\partial z}\, J_\nu(z) = J_{\nu+1}(z)$$

with $\nu = 0$, and the result (A1.2.9), yields

$$I = -\frac{\partial}{\partial u} \int_0^\infty \exp(-1/_2\, a_1 \xi)\, J_0(u \xi^{1/2})\, d\xi = \frac{2u}{a_1^2} \exp\left(-\frac{u^2}{2a_1}\right).$$

Thus $\int_0^\infty \exp(-\tfrac{1}{2} a_1 \xi)\, \xi^{1/2} J_1\left(\sqrt{4iKy\xi \sin^2 X/_2}\right) d\xi$

$$= \frac{4\sqrt{iKy}\,\sin X/_2}{a_1^2} \exp\left(-\frac{2iKy}{a_1} \sin^2 X/_2\right),$$

and therefore

$$\mathcal{L}_3(\alpha,\beta) = \frac{16 i \pi K \sin X}{(c-id)^2} \int_0^\infty dy\, y^{n+1} \exp\left(-\frac{T}{c-id}\, y\right)$$

$$= \frac{16 i \pi K \sqrt{1-\mu^2}}{T^2} \left(\frac{c-id}{T}\right)^n \Gamma(n+2).$$

Finally, substitution in (10) yields

$$\mathcal{L}_4^{(0)}(\alpha,\beta) = \frac{16 i \pi K \sqrt{1-\mu^2}}{T^2} (n+1) \left(\frac{c-id}{T}\right)^n \left(\beta\frac{(n+2)}{T} - \frac{n(\beta - iK)}{c-id}\right). \qquad \text{(A1.3.12)}$$

(8) may therefore be written

$$\mathcal{J}'(\underline{K}, 2p_x, \beta) = N_{2p_x} K(n+1)\sqrt{1-\mu^2} \left(\frac{c-id}{T}\right)^n \left(\frac{A_1}{T^2} + \frac{A_2}{T^3}\right),$$

where

$$N_{2p_x} = \frac{\alpha^{5/2}}{4\sqrt{2\pi}} 16 i \pi = 2 i \alpha^{5/2} \sqrt{2\pi} , \quad \beta = \alpha/2 ,$$

$$A_1 = \frac{-n(\beta - iK)}{c - id} ,$$

$$A_2 = \beta(n+2).$$

iii) <u>The evaluation of $\mathcal{J}'(\underline{K}, 2p_y, \underline{p})$</u>.

The $2p_y$ wave function is

$$\psi_{2p_y} = \frac{\alpha^{5/2}}{4\sqrt{2\pi}} \, x \sin\theta \sin\varphi \, e^{-\alpha x/2} ,$$

so that

$$\mathcal{J}'(\underline{K}, 2p_y, \underline{p}) = \frac{\alpha^{5/2}}{4\sqrt{2\pi}} \, \mathcal{I}_5^{(0)}(\alpha, \alpha/2) ,$$

where

$$\mathcal{I}_5^{(0)}(\alpha,\beta) = \int d\underline{x} \; x \sin\theta \sin\varphi \, e^{-\beta x} e^{i\underline{p}\cdot\underline{x}} \, {}_1F_1\left[\frac{i\alpha}{K}, 1, i(Kx - \underline{K}\cdot\underline{x})\right]. \qquad (A1.3.13)$$

The $\varphi$ integrals in this case take the form

$$\int_0^{2\pi} e^{im\varphi} \sin\varphi \, d\varphi = \begin{cases} 0 , & m \neq \pm 1, \\ i\pi, & m = -1, \\ -i\pi, & m = +1. \end{cases}$$

Therefore

$$\sum_{m=-\infty}^{\infty} \int_0^{2\pi} e^{im\varphi} \sin\varphi \, J_m(z_1) J_m(z_2) \, d\varphi$$
$$= \pi i \left( J_{-1}(z_1) J_{-1}(z_2) - J_1(z_1) J_1(z_2) \right).$$

This expression vanishes since $J_{-1}(z) = J_1(z)$ and consequently

$$\mathcal{J}'(\underline{K}, 2p_y, \underline{p}) = 0$$

3) i) <u>The evaluation of $\mathcal{J}'(\underline{K}, 3p_z, \underline{p})$.</u>

$$\psi_{3p_z}(\underline{x}) = \frac{2\alpha^{5/2}}{81\sqrt{2\pi}}\, x(6-\alpha x)\exp\left(-\tfrac{1}{3}\alpha x\right)\cos\theta,$$

so
$$\mathcal{J}'(\underline{K}, 3p_z, \underline{p}) = \frac{2\alpha^{5/2}}{81\sqrt{2\pi}}\left(6\mathcal{I}_3^{(0)}(\alpha, \alpha/3) + \alpha\,\mathcal{I}_3^{(1)}(\alpha, \alpha/3)\right)$$

where $\mathcal{I}_3^{(0)}(\alpha,\beta)$, $\mathcal{I}_3^{(1)}(\alpha,\beta)$ are defined by A1.3.2), (A1.1.2) respectively.

The value of $\mathcal{I}_3^{(0)}(\alpha,\beta)$ is given by (A1.3.7), and

$$\mathcal{I}_3^{(1)}(\alpha,\beta) = 16i\pi\left(\frac{c-id}{T}\right)^n\left(\frac{B_0}{T} + \frac{B_1}{T^2} + \frac{B_2}{T^3} + \frac{B_3}{T^4}\right)$$

where
$$B_0 = -\frac{\lambda(n-1)}{(c-id)^2} - \frac{2\lambda(n-1)(n-2)(\beta-iK)^2}{(c-id)^3},$$

$$B_1 = \frac{(n+1)(\lambda+\mu Kn)}{c-id} + \frac{4\lambda K(n^2-1)(n-2)(\beta-iK)^2(\lambda\mu+K+i\beta)}{(c-id)^3}$$
$$+\frac{2(n+1)(n-1)}{(c-id)^2}\Big((\beta-iK)\{\lambda(\beta+iK)-\mu Kn(\beta-iK)+\beta\lambda\}+\lambda K\{\lambda\mu+2i(\beta-iK)\}\Big).$$

$$B_2 = K\mu(n+1)(n+2) - \frac{8(n+1)(n+2)(n-1)}{(c-id)^2}\lambda K\beta(\beta-iK)(\lambda\mu+K+i\beta)$$
$$+\frac{2(n+1)(n+2)}{c-id}\Big\{-\lambda\beta(\beta+iK)+2\mu n\beta K(\beta-iK)-K\lambda(\lambda\mu+K+2i\beta)\Big\}.$$

$$B_3 = -2\beta^2K\mu(n+1)(n+2)(n+3) + \frac{4(n+1)(n+2)(n+3)\lambda K\beta^2(\lambda\mu+K+i\beta)}{c-id}.$$

Therefore

$$\mathcal{J}'(\underline{K}, 3p_z, \underline{p}) = N_{3p_z}\left(\frac{c-id}{T}\right)^n\left(\frac{A_0}{T} + \frac{A_1}{T^2} + \frac{A_2}{T^3} + \frac{A_3}{T^4}\right),$$

where $N_{3p_z} = \dfrac{16 i \pi . 2\alpha^{5/2}}{81\sqrt{2\pi}}$, $\beta = \dfrac{\alpha}{3}$,

$$A_0 = -\frac{\lambda(n-1)(6\beta+\alpha-6iK)}{(c-id)^2} - \frac{2\alpha\lambda(n-1)(n-2)(\beta-iK)^2}{(c-id)^3},$$

$$A_1 = \frac{(n+1)}{(c-id)}\Big(\lambda(\alpha+6\beta+6iK) - \mu K n(\alpha+6\beta-6iK)\Big)$$
$$+ \frac{2(n^2-1)}{(c-id)^2}\Big(\lambda^2\mu K(\alpha+6\beta-6iK) + \alpha\lambda(2\beta+3iK)(\beta-iK) + K(6i\lambda-\mu n\alpha)(\beta-iK)^2\Big)$$
$$+ \frac{4\alpha\lambda K}{(c-id)^3}(n^2-1)(n-2)(\beta-iK)^2(\lambda\mu+K+i\beta),$$

$$A_2 = (\alpha+6\beta)K\mu(n+1)(n+2) - \frac{8\alpha\beta\lambda K(n+1)(n+2)(\beta-iK)(\lambda\mu+K+i\beta)(n-1)}{(c-id)^2}$$
$$+ \frac{2(n+1)(n+2)}{i(c-id)}\Big(-\beta\lambda\big(\alpha\beta+3iK(\alpha+2\beta)\big) + 2\mu\alpha\beta n K(\beta-iK) - (\alpha+6\beta)\lambda K(\lambda\mu+K)\Big),$$

$$A_3 = -2\alpha\beta^2 K\mu(n+1)(n+2)(n+3) + 4\frac{(n+1)(n+2)(n+3)}{c-id}\lambda\alpha K\beta^2(\lambda\mu+K+i\beta).$$

ii) Evaluation of $\mathcal{J}'(\underline{K}, 3p_x, \underline{p})$.

$$\psi_{3p_x}(\underline{x}) = \frac{2\alpha^{5/2}}{81\sqrt{2\pi}}\, x(6-\alpha x)\exp\left(-\tfrac{1}{3}\alpha x\right)\sin\theta\cos\varphi,$$

giving

$$\mathcal{J}'(\underline{K}, 3p_x, \underline{p}) = \frac{2\alpha^{5/2}}{81\sqrt{2\pi}}\left(6\,\mathcal{I}_4^{(0)}(\alpha, \alpha/3) + \alpha\,\mathcal{I}_4^{(1)}(\alpha, \alpha/3)\right),$$

where $\mathcal{I}_4^{(0)}(\alpha,\beta)$, $\mathcal{I}_4^{(1)}(\alpha,\beta)$ are defined by (A1.3.9), (A1.1.2) and the value of $\mathcal{I}_4^{(0)}(\alpha,\beta)$ is given by (A1.3.12).

$$\mathcal{I}_4^{(1)}(\alpha,\beta) = 16i\pi\sqrt{1-\mu^2}\,K(n+1)\left(\frac{c-id}{T}\right)^n$$
$$\times\left(\frac{-n}{(c-id)T^2} - \frac{2n(n-1)(\beta-iK)^2}{(c-id)^2T^2} + \frac{4n(n+2)\beta(\beta-iK)}{(c-id)\,T^3} + \frac{n+2}{T^3} - \frac{2(n+3)(n+2)\beta^2}{T^4}\right.$$

Therefore

$$\mathcal{H}(3p_x) = N_{3p_x}\sqrt{1-\mu^2}\,K(n+1)\left(\frac{c-id}{T}\right)^n\left(\frac{A_1}{T^2} + \frac{A_2}{T^3} + \frac{A_3}{T^4}\right)$$

where

$$N_{3p_x} = \frac{2\alpha^{5/2}\,16i\pi}{81\sqrt{2\pi}}, \quad \beta = \frac{\alpha}{3},$$

$$A_1 = \frac{-n(\alpha+6\beta-6iK)}{c-id} - \frac{2\alpha n(n-1)(\beta-iK)^2}{(c-id)^2},$$

$$A_2 = (\alpha+6\beta)(n+2) + \frac{4n(n+2)\alpha\beta(\beta-iK)}{c-id},$$

$$A_3 = -2(n+3)(n+2)\alpha\beta^2.$$

### iii) Evaluation of $\mathcal{J}'(\underline{K}, 3p_y, \underline{p})$.

The $3p_y$ wave function is

$$\psi_{3p_y}(\underline{r}) = \frac{2\alpha^{5/2}}{81\sqrt{2\pi}}\, x(6-\alpha x)\exp\left(-\tfrac{1}{3}\alpha x\right)\sin\theta\,\sin\varphi,$$

so that

$$\mathcal{J}'(\underline{K},3p_y,\underline{p}) = \frac{2\alpha^{5/2}}{81\sqrt{2\pi}}\left( 6\, I_5^{(0)}(\alpha, \alpha/3) + \alpha I_5^{(1)}(\alpha, \alpha/3)\right),$$

and is zero for the same reason as $\mathcal{J}'(\underline{K}, 2p_y, \underline{p})$.

## Appendix 2.

### 1) Evaluation of the functions $g_{nlm}(b, \underline{A})$, $G_{nlm}(b, \underline{A})$.

First consider the evaluation of the following integral

$$I_{nl}^{(k)}(\alpha, K) = \int_0^\infty e^{-\alpha y}\, y^{l+\frac{1}{2}+k}\, L_{n-l-1}^{2l+1}(y)\, J_{l+\frac{1}{2}}(Ky)\, dy\,, \qquad n \geq l+1,$$

where $J_{l+\frac{1}{2}}(x)$ is the ordinary Bessel function of order $l + \frac{1}{2}$ and $L_p^{\,k}(z)$ is the Laguerre polynomial of degree p defined by the relation

$$\sum_{p=0}^{\infty} \frac{u^p}{(p+k)!} L_p^k(z) = \frac{\exp\left(-\frac{zu}{1-u}\right)}{(1-u)^{k+1}}\,, \quad |u|<1. \qquad (A2.1)$$

Therefore

$$\sum_{n-l-1=0}^{\infty} \frac{u^{n-l-1}}{(n+l)!} L_{n-l-1}^{2l+1}(z) = \frac{\exp\left(-\frac{zu}{1-u}\right)}{(1-u)^{l+2}}\,, \quad |u|<1.$$

Write

$$I = \sum_{n=l+1}^{\infty} \frac{u^{n-l-1}}{(n+l)!} I_{nl}^{(k)}(\alpha, K) \qquad (A2.2)$$

$$= \int_0^\infty \frac{y^{l+\frac{1}{2}+k}}{(1-u)^{2l+2}} \exp\left(-\left(\alpha + \frac{u}{1-u}\right) y\right) J_{l+\frac{1}{2}}(Ky)\, dy \qquad (A2.3)$$

Now (see e.g. Copson p.341, Ex 7)

$$\int_0^\infty e^{-at} J_\nu(bt)\, t^{\mu-1}\, dt = \frac{b^\nu \Gamma(\mu+\nu)}{2^\nu a^{\mu+\nu} \Gamma(\nu+1)}\, {}_2F_1\left(\frac{\mu+\nu}{2}, \frac{\mu+\nu+1}{2}; \nu+1; -\frac{b^2}{a^2}\right) \qquad (A2.4)$$

if $\mathrm{Re}\,(\mu+\nu) > 0$, $\mathrm{Re}\,(a \pm ib) > 0$.

Put $\mu = l + \frac{3}{2} + k$, $\nu = l + \frac{1}{2}$, $b = K$, $a = \alpha + \frac{u}{1-u}$.

Then

$$I = \frac{K^{l+1/2}\,\Gamma(2l+2+k)}{2^{l+1/2}\,\Gamma(l+3/2)\left(\alpha+\frac{u}{1-u}\right)^{2l+2+k}(1-u)^{2l+2}}\;{}_2F_1\left[l+1+k/2,\, l+\frac{3+k}{2};\, l+3/2;\, \frac{-K^2}{\left(\alpha+\frac{u}{1-u}\right)^2}\right]$$

i) $k = 0.$ $F(a,b;b;z) = (1-z)^{-a}.$ (A 2.5)

ii) $k = 1.$ $F(a,b;a;z) = (1-z)^{-b}.$ (A 2.6)

Therefore

$$F\left[l+1,\, l+3/2;\, l+3/2;\, \frac{-K^2}{(\alpha+\frac{u}{1-u})^2}\right] = \frac{(\alpha(1-u)+u)^{2l+2}}{\left((\alpha(1-u)+u)^2+K^2(1-u)^2\right)^{l+1}},$$

$$F\left[l+3/2,\, l+2;\, l+3/2;\, \frac{-K^2}{(\alpha+\frac{u}{1-u})^2}\right] = \frac{(\alpha(1-u)+u)^{2l+4}}{\left((\alpha(1-u)+u)^2+K^2(1-u)^2\right)^{l+2}}.$$

d) <u>Suppose k = 0</u>

$$I^{(0)}_{nl}(\alpha,K) = \int_0^\infty e^{-\alpha y}\, y^{l+1/2}\, L^{2l+1}_{n-l-1}(y)\, J_{l+1/2}(Ky)\, dy, \quad \text{(A2.7)}$$

$$I = \frac{K^{l+1/2}\,\Gamma(2l+2)}{2^{l+1/2}\,\Gamma(l+3/2)}\left(\frac{1}{(\alpha(1-u)+u)^2+K^2(1-u)^2}\right)^{l+1} \quad \text{(A2.8)}$$

$$(\alpha(1-u)+u)^2+K^2(1-u)^2 = \left(1-2x\epsilon u+(\epsilon u)^2\right)(\alpha^2+K^2)$$

Where $$\epsilon^2 = \frac{(1-\alpha)^2+K^2}{\alpha^2+K^2}; \quad \text{(A2.9)}$$

$$\epsilon x = \frac{\alpha^2+K^2-\alpha}{\alpha^2+K^2}, \quad \text{(A2.10)}$$

$$\frac{1}{\left(1-2x\epsilon u+(\epsilon u)^2\right)^{l+1}} = \sum_{k=0}^{\infty}(\epsilon u)^k\, C^{l+1}_k(x). \quad \text{(A2.11)}$$

From eq. (2), (8), (11), we have

$$\sum_{n=l+1}^{\infty} \frac{u^{n-l-1}}{(n+l)!} I_{nl}^{(0)}(\alpha,K) = \frac{2^{l+1/2}\,\Gamma(l+1)\,K^{l+1/2}}{\pi^{1/2}\,(\alpha^2+K^2)^{l+1}} \sum_{k=0}^{\infty} (\epsilon u)^k\, C_k^{l+1}(x)$$

where the identity

$$\frac{\Gamma(2l+2)}{\Gamma(l+3/2)} = \frac{2^{2l+1}\,\Gamma(l+1)}{\pi^{1/2}}$$

has been used.

Equating coefficients of $u^{n-l-1}$

$$I_{nl}^{(0)}(\alpha,K) = \frac{2^{l+1/2}\,\Gamma(n+l+1)\,\Gamma(l+1)\,K^{l+1/2}}{\pi^{1/2}\,(\alpha^2+K^2)^{l+1}}\, \epsilon^{n-l-1}\, C_{n-l-1}^{l+1}(x) \qquad (A2.12)$$

where $\epsilon$, $x$ are defined by (9), (10).

b) <u>Suppose k = 1</u>

$$I_{nl}^{(1)}(\alpha,K) = \int_0^{\infty} e^{-\alpha y}\, y^{l+3/2}\, L_{n-l-1}^{2l+1}(y)\, J_{l+1/2}(Ky)\, dy.$$

Then, it follows from (5), (6) that

$$I = \frac{2^{l+3/2}\,\Gamma(l+2)\,K^{l+1/2}\left(\alpha + u(1-2\alpha) - u^2(1-\alpha)\right)}{\pi^{1/2}\,(\alpha^2+K^2)^{l+2}} \sum_{k=0}^{\infty} (\epsilon u)^k\, C_k^{l+2}(x)$$

$$= \sum_{n=l+1}^{\infty} \frac{u^{n-l-1}}{(n+l)!}\, I_{nl}^{(1)}(\alpha,K).$$

Equating coefficients of $u^{n-l-1}$

$$I_{nl}^{(1)}(\alpha,K) = \frac{2^{l+3/2}}{\pi^{1/2}}\,\Gamma(n+l+1)\,\Gamma(l+2)\,\frac{K^{l+1/2}}{(\alpha^2+K^2)^{l+2}}$$

$$\times\left(\alpha\,\epsilon^{n-l-1} C_{n-l-1}^{l+2}(x) + (1-2\alpha)\,\epsilon^{n-l-2} C_{n-l-2}^{l+2}(x) - (1-\alpha)\,\epsilon^{n-l-3} C_{n-l-3}^{l+2}(x)\right) \qquad (A2.12)$$

where $C_{\mu}^{\nu}(x) = 0$ if $\mu < 0$, $C_0^{\nu}(x) = 1$.

Evaluation of $g_{nlm}(b, \underline{A})$.

$$g_{nlm}(b, \underline{A}) = \int \frac{d\underline{x}}{x}\, e^{-bx}\, e^{i\underline{A}\cdot\underline{x}}\, \psi_{nlm}(\underline{x}) \qquad (A2.14)$$

where
$$\psi_{nlm}(\underline{x}) = \frac{2}{n^2}\left(\frac{\Gamma(n-l)}{(\Gamma(n+l+1))^3}\right)^{1/2} e^{-x/n}\left(\frac{2x}{n}\right)^{l} L^{2l+1}_{n-l-1}\left(\frac{2x}{n}\right) Y^{m}_{l}(\theta,\varphi). \qquad (A2.15)$$

It is convenient to carry out the $\underline{x}$-integration in spherical polar coordinates $(x, \theta, \varphi)$ such that $\underline{k}_i$ points in the direction $\theta = 0$ and the plane of $\underline{k}_i$ and $\underline{k}_f$ is the plane $\varphi = 0$. Let $\underline{A} = (A, \Theta, \Phi)$ in this coordinate system. Now, (Messiah I p.497),

$$\exp(i\underline{A}.\underline{x}) = 4\pi \sum_{l'=0}^{\infty} \sum_{m'=-l'}^{l'} i^{l'} j_{l'}(Ax)\, Y^{m'*}_{l'}(\theta,\varphi)\, Y^{m}_{l}(\Theta,\Phi) \qquad (A2.16)$$

and
$$\int Y^{m*}_{l}(\theta,\varphi)\, Y^{m'}_{l'}(\theta,\varphi)\, d(\cos\theta)\, d\varphi = \delta_{mm'}\delta_{ll'} \qquad (A2.17)$$

If expressions (15), (16) are substituted in (14), the angular integrations give $\delta_{mm'}\delta_{ll'}$.

Let $y = \frac{2x}{n}$. Then $j_l(Ax) = \left(\frac{\pi}{2Ax}\right)^{1/2} J_{l+1/2}(\tfrac{1}{2}Any)$.

Then
$$g_{nlm}(b,\underline{A}) = 2\pi i^{l}\left(\frac{\pi}{An}\,\frac{\Gamma(n-l)}{(\Gamma(n+l+1))^3}\right)^{1/2} Y^{m}_{l}(\Theta,\Phi)\, I^{(0)}_{nl}\left(\tfrac{1}{2}(nb+1), \tfrac{1}{2}An\right) \qquad (A2.18)$$

where $I^{(0)}_{nl}(\alpha, K)$ is defined by (7). Use of (12) then gives

$$g_{nlm}(b,\underline{A}) = 2^{2l+3}\pi i^{l}\left(\frac{\Gamma(n-l)}{\Gamma(n+l+1)}\right)^{1/2} \frac{\Gamma(l+1)}{n^{l+2}}\, \frac{A^{l}\, Y^{m}_{l}(\Theta,\Phi)}{\left(\left(\frac{nb+1}{n}\right)^2 + A^2\right)^{l+1}}\, \epsilon^{n-l-1} C^{l+1}_{n-l-1}(x), \qquad (A2.19$$

where $$\epsilon^2 = \frac{(nb-1)^2 + A^2n^2}{(nb+1)^2 + A^2n^2}, \qquad (A2.20)$$

and $$x = \frac{1}{\epsilon}\left(\frac{n^2b^2-1 + A^2n^2}{(nb+1)^2 + A^2n^2}\right). \qquad (A2.21)$$

When b = 0, and $\underline{A} = \underline{v}$,

then $\Theta = \Phi = 0, \quad \epsilon = 1, \quad x = \frac{n^2v^2-1}{n^2v^2+1}$.

Therefore, $\lim_{v\to\infty} x = 1$.

Since $$C^{l+1}_{n-l-1}(1) = \frac{\Gamma(n+l+1)}{\Gamma(n-l)\Gamma(2l+2)},$$

it follows that
$$g_{nlm}(\underline{v}) \underset{v\to\infty}{\sim} 2^{2l+3}\pi i^l\left[\frac{\Gamma(n+l+1)}{\Gamma(n-l)}\right]^{1/2}\frac{\Gamma(l+1)}{\Gamma(2l+2)}\,\frac{Y_{lm}(0,0)}{n^{l+2}\,v^{l+2}} \qquad (A2.22)$$

<u>Evaluation of $G_{nlm}(b, \underline{A})$</u>

$$G_{nlm}(b,\underline{A}) = \int d\underline{x}\; e^{-bx}\, e^{i\underline{A}\cdot\underline{x}}\,\psi_{nlm}(\underline{x}). \qquad (A2.23)$$

The angular integration may be carried out as before, with the result
$$G_{nlm}(b,\underline{A}) = \pi i^l\left[\frac{n\pi\,\Gamma(n-l)}{A\,\{\Gamma(n+l+1)\}^3}\right]^{1/2} Y_{lm}(\Theta,\Phi)\, I^{(1)}_{nl}\left(\tfrac{1}{2}(nb+1), \tfrac{1}{2}An\right), \qquad (A2.24)$$

where $I^{(1)}_{nl}$ $(\alpha, K)$ is given by (13).

Thus $$G_{nlm}(b,\underline{A}) = H_l\, Y_{lm}(\Theta,\Phi)\, T_l(A)\,\frac{A^l}{\left(\left(\frac{nb+1}{n}\right)^2 + A^2\right)^{l+2}}, \qquad (A2.25)$$

where $$H_l = 2^{2l+4}\pi i^l\left[\frac{\Gamma(n-l)}{\Gamma(n+l+1)}\right]^{1/2}\frac{\Gamma(l+2)}{n^{l+3}}, \qquad (A2.26)$$

$$T_l(A) = (nb+1)\epsilon^{n-l-1}C^{l+2}_{n-l-1}(x) - 2nb\epsilon^{n-l-2}C^{l+2}_{n-l-2}(x) + (nb-1)\epsilon^{n-l-3}C^{l+2}_{n-l-3}(x), \qquad (A2.27)$$

and $\epsilon$, $x$ are given by (20), (21).

<u>Particular cases.</u>

1) $b = 0$

Then $\epsilon = 1$, $x = \dfrac{n^2 A^2 - 1}{n^2 A^2 + 1}$

Since

$$C_{n-l-1}^{l+2}(x) - C_{n-l-3}^{l+2}(x) = \frac{n}{l+1} C_{n-l-1}^{l+1}(x),$$

$$G_{nlm}(\underline{A}) \doteq 2^{2l+4} \pi i^l \left[\frac{\Gamma(n-l)}{\Gamma(n+l+1)}\right]^{1/2} \frac{\Gamma(l+1)}{n^{l+2}} \frac{Y_{lm}(\Theta, \Phi) A^l}{(1/n^2 + A^2)^{l+2}} C_{n-l-1}^{l+1}(x) \qquad (A2.28)$$

2) $b = 0$, $\underline{A} = \underline{v}$

From (28), it follows that

$$G_{nlm}(\underline{v}) \underset{v \to \infty}{\sim} 2^{2l+4} \pi i^l \left[\frac{\Gamma(n+l+1)}{\Gamma(n-l)}\right]^{1/2} \frac{\Gamma(l+1)}{\Gamma(2l+2)} \frac{Y_{lm}(0,0)}{n^{l+2}} \frac{1}{v^{l+4}} .$$

## Appendix 3.

## Evaluation of the functions $f_{\underline{K}}(\lambda,\alpha,\underline{Q})$, $\mathcal{L}_{\underline{K}}(\lambda,\alpha,\underline{Q})$.

These functions are evaluated by a technique due to Nordsieck.

By definition (9.2.8)

$$f_{\underline{K}}(\lambda,\alpha,\underline{Q}) = \int \frac{e^{-\lambda r}\, e^{i\underline{Q}.\underline{r}}}{r}\, {}_1F_1[\,i\alpha, 1, i(Kr-\underline{K}.\underline{r})]\, d\underline{r}\,. \qquad (A3.1)$$

The confluent hypergeometric function may be represented by the following integral;

$${}_1F_1[\,b, 1, z] = \frac{1}{2\pi i}\oint_{C_1}\left(\frac{t}{t-1}\right)^{b}\frac{e^{zt}}{t}\,dt\,, \qquad (A3.2)$$

where $C_1$ is any simple closed contour which encircles the points t = 0, t = 1 once in the positive direction, and the function $\left(\frac{t}{t-1}\right)^b$ is made single-valued by a cut in the t - plane along [0, 1]. If (2) is used in (1), then

$$f_{\underline{K}}(\lambda,\alpha,\underline{Q}) = \frac{1}{2\pi i}\oint_{C_1}\left(\frac{t}{t-1}\right)^{i\alpha}\frac{1}{t}\,R(t)\,dt\,, \qquad (A3.3)$$

where

$$R(t) = \int \frac{e^{-\lambda r}}{r}\, e^{i\underline{Q}.\underline{r}}\, e^{i(Kr-\underline{K}.\underline{r})t}\, d\underline{r}\,. \qquad (A3.4)$$

The change in the order of integration is valid provided that the space integral R(t) converges uniformly for all values of t on the contour $C_1$. If $\lambda$ is real and positive, then

$$|R(t)| \leq 4\pi\int_0^\infty r\, e^{-\lambda r}\, e^{-2Kr\,\min(\mathcal{I}m\, t)}\, dr,$$

Hence, by the Weierstrass M - test, expression (3) is valid provided that

$$-\lambda - 2K \min(\operatorname{Im} t) < 0 \tag{A3.5}$$

for all values of t on $C_1$. It will now be assumed that $C_1$ has been chosen so that (5) is satisfied. The integral in (4) may easily be evaluated, giving

$$R(t) = \frac{4\pi}{\lambda^2 + Q^2 - 2t(\underline{Q}.\underline{K} + i\lambda K)} .$$

Substituting this value in (3) gives

$$f_{\underline{K}}(\lambda, \alpha, \underline{Q}) = \frac{2}{i}\oint_{C_1} \frac{1}{t}\left(\frac{t}{t-1}\right)^{i\alpha} \frac{dt}{\left(\lambda^2 + Q^2 - 2t(\underline{Q}.\underline{K} + i\lambda K)\right)} . \tag{A3.6}$$

The t-integral is single-valued and behaves like $t^{-2}$ as t tends to infinity. Therefore the integral round a circle of radius R, centre origin, tends to zero as R tends to infinity and the integral round $C_1$ is equal to the sum of the residues at the poles lying outside $C_1$ multiplied by $2\pi i$. The integrand has a pole at

$$t_1 = \frac{\lambda^2 + Q^2}{2(\underline{Q}.\underline{K} + i\lambda K)} .$$

Since

$$-\lambda - 2K \operatorname{Im} t_1 = \frac{\lambda Q^2 \sin^2\theta}{Q^2\cos^2\theta + \lambda^2} > 0,$$

where $\underline{Q}.\underline{K} = QK\cos\theta$,

it follows that $t_1$ lies outside $C_1$.

Thus

$$f_{\underline{K}}(\lambda,\alpha,\underline{Q}) = \frac{4\pi}{(\lambda^2+Q^2)}\left(\frac{\lambda^2+Q^2}{\lambda^2+Q^2-2\underline{Q}.\underline{K}-2i\lambda K}\right)^{i\alpha}.$$

$\mathcal{L}_{\underline{K}}(\lambda,\alpha,\underline{Q})$ may easily be evaluated using this result.

Thus

$$\mathcal{L}_{\underline{K}}(\lambda,\alpha,\underline{Q}) = -\frac{\partial}{\partial\lambda} f_{\underline{K}}(\lambda,\alpha,\underline{Q})$$

$$= \frac{8\pi}{(\lambda^2+Q^2)^2}\left(\frac{\lambda^2+Q^2}{\lambda^2+Q^2-2\underline{Q}.\underline{K}-2i\lambda K}\right)^{i\alpha}\left(\lambda(1-i\alpha) + \frac{\alpha(K+i\lambda)(\lambda^2+Q^2)}{\lambda^2+Q^2-2\underline{K}.\underline{Q}-2i\lambda K}\right).$$

## Appendix 4.

### Evaluation of the integrals $I_n(\alpha^2, \underline{t})$.

Let $$I_n(\alpha^2,\underline{t}) = \int \frac{d\underline{K}}{(k_f^2-K^2+i\epsilon)(\alpha^2+(\underline{K}-\underline{t})^2)^n}.$$

Now $$\frac{1}{\alpha^2+(\underline{K}-\underline{t})^2} = \int_{\alpha^2}^{\infty} \frac{dA}{(A+(\underline{K}-\underline{t})^2)^2}$$

and $\left|\frac{1}{(A+(\underline{K}-\underline{t})^2)^2}\right| \leq \left|\frac{1}{A^2}\right|$ for all $\underline{K}$.

Since $\int_{\alpha^2}^{\infty} \frac{dA}{A^2}$ converges provided $\alpha^2 \neq 0$, it follows from the comparison test that $\int_{\alpha^2}^{\infty} \frac{dA}{(A+(\underline{K}-\underline{t})^2)^2}$ converges uniformly for all $\underline{K}$. Therefore

$$\int \frac{d\underline{K}}{(k_f^2-K^2+i\epsilon)(\alpha^2+(\underline{K}-\underline{t})^2)} = \int_{\alpha^2}^{\infty} dA \int \frac{d\underline{K}}{(k_f^2-K^2+i\epsilon)(A+(\underline{K}-\underline{t})^2)^2}$$

i.e. $$I_1(\alpha^2,\underline{t}) = \int_{\alpha^2}^{\infty} I_2(A,\underline{t})\, dA.$$

### Evaluation of $I_2(A, \underline{t})$.

$$I_2(A,\underline{t}) = 2\pi \int_0^{\infty} \frac{K^2 dK}{(k_f^2-K^2+i\epsilon)} \int_{-1}^{+1} \frac{dy}{(A+K^2+t^2-2Kty)^2}$$

$$= -\frac{\pi}{t} \int_{-\infty}^{\infty} \frac{K\, dK}{(K^2-k_f^2+i\epsilon)(A+(K-t)^2)} .$$

The integral may be evaluated by contour integration. The integrand has poles at

$$K = k_f, \quad K = t + i\sqrt{A},$$

with residues

$$\frac{1}{2\left(A+(k_f-t)^2\right)}, \qquad \frac{t+i\sqrt{A}}{2i\sqrt{A}\left((t+i\sqrt{A})^2-k_f^2\right)}.$$

Taking as contour an infinite semicircle in upper half plane

$$I_2(A,\underline{t}) = -\frac{\pi^2}{t}\left(\frac{i}{A+(k_f-t)^2} + \frac{t+i\sqrt{A}}{\sqrt{A}\left((t+i\sqrt{A})^2-k_f^2\right)}\right) \qquad (A4.1)$$

### Evaluation of $I_1(\alpha^2, \underline{t})$

$$I_1(\alpha^2,\underline{t}) = -\frac{\pi^2}{t}\left(J_1 + J_2\right)\Big|_{\alpha^2}^{\infty}$$

where

$$J_1 = i\int\frac{dA}{A+(k_f-t)^2} = i\ln\left(A+(k_f-t)^2\right),$$

$$J_2 = \int\frac{(t+i\sqrt{A})\,dA}{\sqrt{A}\left((t+i\sqrt{A})^2-k_f^2\right)}.$$

Put $t + i\sqrt{A} = y$.

$$J_2 = \frac{2}{i} \int \frac{y\,dy}{y^2 - k_f^2} = \frac{1}{i} \ln \left\{ (t + i\sqrt{A})^2 - k_f^2 \right\}.$$

$$I_1(\alpha^2, \underline{t}) = \frac{i\pi^2}{t} \left[ \ln\left\{ (t + i\sqrt{A})^2 - k_f^2 \right\} - \ln\left\{ A + (k_f - t)^2 \right\} \right] \Bigg|_{\alpha^2}^{\infty}$$

$$= \frac{i\pi^2}{t} \left[ \ln\left( \alpha^2 + (k_f - t)^2 \right) - \ln\left( (t + i\alpha)^2 - k_f^2 \right) \right].$$

Special cases.

1) $\underline{t} = \underline{k}_f$

$$I_2(A, \underline{k}_f) = -\pi^2 \left[ \frac{1}{\sqrt{A}\,(A + 4k_f^2)} + \frac{i}{2k_f} \left( \frac{1}{A} - \frac{1}{A + 4k_f^2} \right) \right].$$

a) $$I_2(4, \underline{k}_f) = \frac{-\pi^2 (1 + ik_f)}{8(1 + k_f^2)}.$$

b) $$I_2\left( \left( \frac{n+1}{n} \right)^2, \underline{k}_f \right) = \frac{-\pi^2 n^3}{(n+1)} \left( 1 + \frac{2ik_f n}{n+1} \right) \left( \frac{1}{(n+1)^2 + 4n^2 k_f^2} \right).$$

c) $$I_1(4, \underline{k}_f) = -\pi^2/k_f \left( \tan^{-1} k_f + \frac{i}{2} \ln(1 + k_f^2) \right).$$

2) $\underline{t} = a\underline{k}_i$

a) $$I_2(A, a\underline{k}_i) = -\frac{\pi^2}{\sqrt{A}} \left[ \frac{A + a^2 k_i^2 - k_f^2 + 2i k_f \sqrt{A}}{(A + k_f^2 + a^2 k_i^2)^2 - 4a^2 k_i^2 k_f^2} \right].$$

b) $$I_1(A, a\underline{k}_i) = -\frac{\pi^2}{ak_i} \left[ \tan^{-1} \frac{2ak_i\sqrt{A}}{A + k_f^2 - a^2 k_i^2} + \frac{i}{2} \ln\left\{ \frac{(A + k_f^2 - a^2 k_i^2)^2 + 4a^2 A k_i^2}{\left(A + (k_f - ak_i)^2\right)^2} \right\} \right].$$

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