EXPERIMENTAL ELECTRON SCATTERING FROM ATOMIC
AND MOLECULAR HYDROGEN, HELIUM, NEON
ARGON AND KRYPTON.

by

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SUMMARY

This thesis describes the measurements of absolute differential cross-sections for electrons scattered by atomic and molecular hydrogen, neon, argon and krypton, using a modulated beam apparatus. Both elastic and inelastic cross-sections are presented. The energy range for elastically scattered electrons lies between 50 eV. and 300 eV.. Excitation cross-sections for atomic hydrogen to the combined 2s and 2p states were measured at 50 eV., 100 eV. and 200 eV..

Absolute values were obtained by measuring ratios of cross-sections between the above named scattering centres and helium. Using the absolute helium cross-sections of Chamberlain et. al. it was then possible to predict other absolute cross-sections.

A mass-spectrometer was calibrated to measure the relative number densities of each scattering centre in the interaction region with the electron beam. Scattered electrons were energy analysed with a parallel plate electron spectrometer and detected by a channel electron multiplier.

The results are compared with other available experimental data and with existing theoretical treatments. The more important calculations and their regions of validity are discussed.
This thesis contains no material which has been accepted
for the award of any other degree or diploma in any University.
To the best of the author's knowledge and belief it contains
no material previously published or written by another person,
except when due reference is made in the text.

R. R. Böhm.
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CHAPTER 1

INTRODUCTION TO ELECTRON SCATTERING

1.1 INTRODUCTION

Interest in electron scattering from atoms and molecules has been stimulated in recent years by the need for accurate cross-sections in such fields as astrophysics, gaseous discharges, spectroscopy, physics of the atmosphere, atomic physics and solid state physics. Collision cross-sections are also necessary to understand high temperature plasmas in the quest of controlled thermo-nuclear reactions. (Massey and Burhop 1952 and 1969, Veldre 1966).

Hydrogen cross-sections are of particular interest due to the abundance of hydrogen in the Universe and because it is the simplest atom (and molecule) thus making it an ideal test for theoretical quantum mechanics. (Bethe 1930, Burke 1969, Gerjuoy 1971, Khare and Shoba 1972, Moisewitsch and Smith 1968, Trajmer et al. 1970, Vriens et al. 1968).

The difficulties associated in solving a three (or more) body problem in quantum mechanics have made it necessary to look for approximate solutions. Without a knowledge of absolute experimental cross-sections it is not possible to determine the range of validity of such approximations. According to the literature (Lassette
et. al. 1964, Moisewiçitsch and Smith 1968), even minor variations in the wave functions used produce quite considerable errors in their calculated differential cross-sections. Experimental results are therefore of fundamental importance.

This thesis describes an experiment designed to find absolute differential cross-sections of atomic hydrogen, using a chopped neutral beam apparatus as first described by Fite and Brackman (1958). The electron energy range involved is from 50 eV to 300 eV. Both elastic and inelastic events are considered. For the latter the resolution of the instrument was such as to allow only observations to the combined 2 $s$ and 2 $p$ excitation states.

This energy range was particularly chosen to complement results obtained in recent years which were preoccupied with resonance effects found at low energies, that is, near the threshold for ionization (Ehrhardt 1969, Takayanagi 1972, Williams and McGowan 1968), where a wealth of fine structure has been found in high resolution measurements (Burke 1969).

It was the aim of this project to fill the gap in the range of known cross-sections between low energies (i.e. threshold and less) and the higher energies where theoretical calculations were expected to be sufficiently reliable, e.g. the Born approximation.
1.2(a) HISTORICAL REVIEW

The widespread interest in electron scattering during the 1920's and 1930's, and again over the last decade, has mainly been limited to measurements of angular distributions or total cross-sections which have been normalized to the Born theory at high energies, (i.e. >500 eV) (Arnot 1931, MacMillan 1930, Mohr and Nichols 1932, Webb 1935 and Tai et al. 1970).

The earliest attempts to find absolute cross-sections came from Werner (1933) and Westin (1949). Werner measured absolute differential cross-sections of helium directly at two angles, 45° and 90°, in a static gas scattering apparatus. Incident electrons were collected by a Faraday cup situated on the axis of the beam, while the scattered electron signal was measured by a Faraday cup "ring", also centred on the beam axis. The number of scattering centres per unit volume was obtained from the pressure measured by a McLeod gauge. A check for double scattering was performed by finding the ratio of the scattered to incident electrons as a function of pressure. The results are given as 10% accurate and agree quite well with those recently obtained by Chamberlain et. al. (1970) and Vriens et. al. (1968).

Westin in a similar experiment used a magnetic electron spectrometer. The agreement with Chamberlain et. al. is reasonable at
higher energies. Stray magnetic fields may have contributed to inaccuracies at lower energies. Both Werner and Westin used a McLeod gauge for their pressure measurements, without correcting for the pumping effect of these gauges. These corrections are however small at the relatively high pressures used.

Hughes et al. (1932) normalized their angular distributions to the Born approximation (as calculated by Mott 1930) at 700 eV. Although the Born theory probably holds at that energy, there is some doubt on whether their energy dependence work is correct (Vriens et al. 1968).

1.2(b) **EQUATION BY MOTT**

The Born approximation is essentially an equation in which the scattering amplitude is expressed as the fourier transform of the potential set up by the atom (shown in a later section). In Mott's version, this equation is rewritten so that the scattering amplitude is proportional to the fourier transform of the charge distribution within the atom (called the "atomic form factor" here and may be interpreted as the contribution to the scattering amplitude by the electrical charge distribution about the atom).

Although they are equivalent, Mott's equation shows the relationship between the Born approximation and Coulomb scattering more clearly. The expressions for the scattering amplitude $f(\theta)$ are:
\[ f(\theta) = \frac{Ze^2}{2mv^2} \csc^2 \left( \frac{1}{2} \theta \right) \text{ (Coulomb scattering)}, \]

and \[ g(\theta) = \frac{e^2}{2mv^2} (Z - f(\theta)) \csc^2 \left( \frac{1}{2} \theta \right) \text{ (Born approx)}, \]

where \( f(\theta) \) is the atomic form factor,

\( Z \) is the atomic number of the atom, or the number of charges in the case of Coulomb scattering

\( e \) refers to an electron charge, and

\( \theta \) is the scattering angle.

It should be noted here that a term widely used instead of the atomic form factor (but which is proportional to it), is called the "generalized oscillator strength" (Moiseiwitsch and Smith 1968, Mott 1930, Vriens 1968).

1.2(c) **RECENT EXPERIMENTS**

More recently an attempt to find absolute cross-sections had been made by Vriens et. al. (1968). Basically their work consisted of measuring angular distributions for both elastically and inelastically scattered electrons from helium. These angular distributions were then converted to absolute differential cross-sections via the Born theory which was expressed in terms of the generalized oscillator strength \( f(K) \). (\( K \) is the momentum transfer, Bethe 1930).
From a knowledge of the shape of the differential cross-sections it was possible to determine relative values for the \( f(K) \) (Vriens 1967) over a wide range of \( K \). Since the absolute value of \( f(K = 0) \) is known (i.e. the optical oscillator strength), a calibration to absolute values of all the \( f(K) \) was possible by plotting \( f(K) \) versus \( K \) and extrapolating the curve to \( K = 0 \). The measurements were made in the energy range 100 eV to 400 eV for angles between \( 5^\circ \) and \( 30^\circ \) in the case of elastic scattering and \( 5^\circ \) to \( 20^\circ \) for inelastic scattering. The apparatus was the same as used by Chamberlain et. al., mentioned below.

The most rigorously obtained experimental cross-sections of helium are those of Chamberlain et. al. (1970). Their apparatus included a well defined electron beam which enabled them to take measurements at very small angles. The number density of the scattering centres was obtained by means of an oil manometer pressure gauge. Care was taken regarding any temperature gradients along the apparatus. The energy range involved was from 50 eV to 400 eV and all measurements (of both elastic and inelastic scattering) were obtained at a scattering angle of \( 5^\circ \). Determination of the cross-sections required the ratio of the scattered electron current to the incident electron current, as detected by Faraday cups which were designed to effectively trap all electrons that pass their entrance. A correction for the ion production along the
electron beam was also made. The energy resolution varied from 0.04 eV to 0.1 eV. It was achieved with the aid of an electron monochromator and an analyser, both of which were of the "hemi-
spherical electrostatic deflector" type, designed so as not to lose any electrons. Errors are given and vary from 5% at higher energies to 15% at 50 eV.

The foregoing reviews were all concerned with helium. Only recently were the first absolute differential cross-sections for the hydrogen molecule published (Trajmer et. al. 1970). Their energy range (from 7 eV to 81.6 eV) partly overlapped that of the present work and therefore enabled a comparison to be made. The method used by Trajmer et. al. relied on an integration of angular distributions, which were then normalized to known total cross-sections (Truhlar and Rice 1970). Since their experiment was limited to angles between 10° and 80°, it was necessary to extend the angular range (if an integration was to be achieved) by an extrapolation.

It is pointed out that the contribution to the total cross-section between 0° and 10° is relatively small so that any extrapolation would not contribute large errors to the integrated values. However, for just this reason, it is obvious that such data is not a very sensitive test of the shape of the angular
distributions at these angles.

In addition it should be noted that Trajmer et. al. have indicated that their measurements at $10^\circ$ may be subject to errors. Since angular distributions obtained with the present apparatus are generally less steep than those of Trajmer et.al. and agree with the results of Webb (1932, for $E = 100$ eV) and Williams (1969), it is suggested that the angular distributions of Trajmer et. al. are not reliable at small angles (a comparison is given in Chapter 5).

The only available absolute values for the differential cross-sections of rare gases other than helium are those for argon. They were measured by Berman (published by Kieffer 1966) and Kurepa and Vuskovic (1972).

The results of Berman only extend over a very small angular range ($\theta < 10^\circ$) for energies above 200 eV. No details are given of the method used. Kurepa and Vuskovic have published their results in abstract form for energies of 80, 90 and 100 eV. Their experimental procedure is stated to be the same as that used by Bromberg (1968), who found absolute differential cross-sections for helium at 500 eV. Neither publication gives an indication of the accuracy of the data presented.
1.3 OUTLINE OF PRESENT EXPERIMENT

The direct measurement of absolute cross-sections, without a normalization to some standard value, would require not only an accurate knowledge of the absolute detection efficiency of all detectors, but also the number density of the gas in the intersection region and the appropriate geometry factors at the intersection of the two beams. To obtain this information in the present apparatus was quite impractical.

Therefore, since Chamberlain et. al. had already produced reliable helium cross-sections to a high degree of accuracy, the method employed here was to find ratios of cross-sections between hydrogen (atomic and molecular) and helium. The only information required to obtain absolute values in this way was the relative number density of hydrogen and helium in the scattering region of the apparatus. (A mass spectrometer was calibrated for this purpose, details of which will be given in Chapter 4). Other parameters, such as the transmission efficiency of the electron spectrometer and the geometry factors were common to all measurements.

The apparatus was of the modulated beam type (Fite and Brackman 1958). Hydrogen atoms were produced by dissociation of molecular hydrogen gas in a heated tungsten oven (T = 2,600°C). A beam of partially dissociated hydrogen was formed and this
intersected the electron beam in the scattering chamber. The neutral beam was chopped at a rate of 100 times per second. The scattered electrons were energy analysed by means of an electrostatic (parallel plate) spectrometer and detected with a channel electron multiplier.

The scattered electron signal which arrived at the scalers during a beam "on" condition was added to the total, while the signal which arrived during the beam "off" condition was subtracted, thus eliminating the background scattering effect.

1.4 THEORETICAL REVIEW

This section gives a brief introduction to the theoretical aspects of electron scattering. Only a few of the theories available have been selected. Further information is given in Mott and Massey (1965), Massey and Burhop (1952 and 1969), Moiseiwitsch and Smith (1968) and Velde (1966).

For those calculations which enable a direct comparison with the present experimental results, a more detailed discussion is given in Chapter 5.

1.4(a) GENERAL SCATTERING FORMULAE

The usual method of treating the electron - atom (or molecule)
scattering problem in wave mechanics is to consider the wave function $\psi$ of a particle which is scattered by some potential $V$, to be composed of an incident plane wave $\exp(\mathbf{i}k \cdot \mathbf{r})$ plus a scattered wave $g$.

$$i.e. \quad \psi = \exp(\mathbf{i}k \cdot \mathbf{r}) + g(\mathbf{r})$$

where $k$ is the incident particle wave vector and $\mathbf{r}$ is the vector joining the scattering centre and the incident particle.

In particular at a large distance from the scatterer $g(\mathbf{r})$ will appear as a spherically divergent wave,

$$i.e. \quad g(\mathbf{r}) \rightarrow \frac{\exp(\mathbf{i}kr)}{r} f(\theta) \quad (\theta = \text{angle of scattering})$$

where $f(\theta)$ is the amplitude of the scattered wave.

The differential cross-section can be shown to be

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2$$

The Schrödinger equation for the problem is:

$$\frac{\hbar^2}{2m} \nabla^2 \psi + V\psi = E\psi$$

Substituting for $\psi$ and remembering that $(V^2 + k^2) \exp(\mathbf{i}k \cdot \mathbf{r}) = 0$, we get: $(V^2 + k^2)g = \frac{2m}{\hbar^2} V\psi$. Now in general $(V^2 + k^2)\phi = 0$ represents
the wave equation of a free particle. Therefore the term $\frac{2m}{\hbar^2} V\psi$
in the above equation will represent the strength of the waves
scattered by the potential at a point $\mathbf{r}'$. Hence if $G(\mathbf{r}, \mathbf{r}')$ is
the wave produced by a unit point source at $\mathbf{r}'$ so that:

$$(\nabla^2 + k^2) G = \delta(\mathbf{r} - \mathbf{r}')$$

then we may expect

$$g(\mathbf{r}) = \frac{2m}{\hbar^2} \int G(\mathbf{r}, \mathbf{r}') V(\mathbf{r}') \psi(\mathbf{r}') d^3r'$$

...1.1

where the integration is over the range of the potential (i.e. $\mathbf{r}'$). $G$ is called the Green's function and is given by:

$$G(\mathbf{r}, \mathbf{r}') = -\frac{1}{4\pi} \frac{\exp(ik|\mathbf{r} - \mathbf{r}'|)}{|\mathbf{r} - \mathbf{r}'|}$$

making the approximation that the potential has a finite value
over only a limited region, then for large $r$,

$$g(\mathbf{r}) = -\frac{m}{2\pi\hbar^2} \frac{\exp(ikr)}{r} \int \exp(-ik' \cdot \mathbf{r}) V(\mathbf{r}') \psi(\mathbf{r}') d^3r'$$

where $k'$ is in the direction of the scattered particle, hence

$$f(\theta) = -\frac{m}{2\pi\hbar^2} \int \exp(-ik' \cdot \mathbf{r}) V(\mathbf{r}') \psi(\mathbf{r}') d^3r'$$

...1.2

1.4(b) **FIRST BORN APPROXIMATION**

It has not been possible to perform the integration of
equation 1.2 as it stands. An approximation suggested by Born, which greatly simplifies the problem is to consider the scattering under conditions in which the potential energy between incident particle and scattering centre is small when compared to the kinetic energy of the particle. In this situation \( \psi \) is approximated by a plane wave. This enables the integration to be performed easily, i.e.

\[
f(\theta) \approx - \frac{m}{2\pi \hbar^2} \int \exp(-i\mathbf{k} \cdot \mathbf{r}') V(\mathbf{r}') \exp(i\mathbf{k} \cdot \mathbf{r}') d^3r'
\]

using \( \mathbf{q} = \mathbf{k} - \mathbf{k}' \) (equals momentum transfer)

therefore

\[
f(\theta) \approx - \frac{m}{2\pi \hbar^2} \int \exp(i\mathbf{q} \cdot \mathbf{r}') V(\mathbf{r}') d^3r'
\]

It may be noted that since \( \mathbf{q} \) is a function of \( \theta \) (i.e. \( \mathbf{q} = 2k\sin\theta \)), \( f(\theta) \) is proportional to the Fourier transform of \( V(\mathbf{r}') \). This implies that a long range potential will contribute mainly to scattering in the forward direction (i.e. \( \theta \) small).

1.4(c) BORN - OPPENHEIMER APPROXIMATION

An extension to the first Born approximation is to include exchange by using a symmetrized wave function. It is not clear whether this will lead to improved results, as it is expected that the inclusion of exchange is most important in an energy region
where the Born approximation is unlikely to be valid (e.g. 50 eV). A comparison with experiment will be given in Chapter 5.

1.4(d) **SECOND BORN APPROXIMATION**

A further development on the first Born approximation (called the second Born approximation) is to approximate the total wave function \( \psi \) by

\[
\psi = \exp(ik \cdot r) + \frac{2m}{\hbar^2} \int G(r,r')V(r')\exp(ik \cdot r')d^3r'
\]

instead of a plane wave. (See equation 1.1). In this way allowance is made for the distortion of the incident wave by the target atom.

Instead of considering electron scattering from a static potential, allowance can also be made for the target electron(s) to be excited to other states. Thus the atom is able to adjust to the influence of the incident electron. Such an approach is necessary if the Born theory is to be extended to inelastic scattering. The scattering amplitude thus obtained is given by Moiseiwitsch and Smith (1968) and explicitly contains the eigenfunctions of all the states of the atom.

The influence of the incident electron, as experienced by the target, corresponds to the atom being polarized. This (long range) polarization potential may, at sufficiently low energies, be an
important factor in small angle scattering. For example Holt et. al. (1972) have accounted for the forward scattering of $e^{-}$ -He for energies of 100 eV and above by using a simplified second Born approximation. Their calculations referred to the differential excitation cross-sections, $1s - 2s^1$, $1s - 2p^1$. They evaluated terms arising from the first three eigenstates exactly and then approximated for the other states.

However below 100 eV the validity of the second Born approximation decreases rapidly (Burke 1972). Considering the amount of work involved and the fact that other approximations (e.g. Glauber and even the first Born theory) give good agreement with experiment at these energies, this approximation is not often used.

1.4(e) **TRUNCATED EIGENFUNCTION EXPANSION (or close coupling approximation)**

In this approximation the total wave function is expanded in terms of a chosen set of functions, usually the eigenfunctions of the undisturbed atom. The resulting coupled integro-differential equations can then be solved numerically provided the infinite series of terms is truncated.

As an example, consider the hydrogen atom. Although including the $1s$ and $2s$ states only, will lead to an improvement over the
Born theory, a more useful expansion is the 1s - 2s - 2p close coupling approximation because two-thirds of the total polarizability of the atom is taken into account in this way (Burke and Smith 1962). Exchange is usually included by symmetrizing the wave functions involved.

Accurate theoretical results have been obtained by the close coupling approximation for electron scattering at low energies, particularly below the ionization threshold, where the number of open channels is limited and the partial wave expansion more suitable.

For example experimental results obtained by Schulz and Fox (1957) compare well with the calculations by Burke, et. al. (1966). The close coupling approximation has also been found applicable to describing resonance effects.

Extending the close coupling approximation to terms beyond the 2p state does not lead to improved calculations since the inclusion of continuum states contributes more to the cross-section than the inclusion of higher discrete states.

An approximate method is therefore usually fashioned to include the effects of the truncated terms. Taylor and Burke (1967) simply used ad. hoc. terms with adjustable parameters. Without these extra
terms the scattering potential obtained will not have the correct long range effect (Burke et. al. 1967, Fano 1970, Gailitis 1964, Hahn et. al. 1964, McKinley and Macek 1964, Percival and Richards 1970).

1.4(f) POLARIZED ORBITAL METHOD

A different way of taking into account the polarization of the atom is to consider the distortion of the electron charge distribution by an incident electron. This method (called the "polarized orbital method") lends itself particularly to low energies where the adiabatic approximation holds (i.e. the incident electron velocity is small enough for the scattering centre to adjust fully to the distortion at each position of the electron, Burke et. al. 1969, Lane and Henry 1968, Temkin and Lamkin 1961.

The form of the long range polarization potential has been shown to be given by \(-\frac{\alpha}{r^4}\) where \(\alpha\) is the polarizability of the atom. (Mott and Massey 1965).

1.4(g) THE GLAUDER APPROXIMATION

This theory has given promising results just in an energy region where the first Born theory may be considered suspect, that is, between 50 eV and 200 eV. Although appearing to be a small angle approximation, it produces useful results at surprisingly
large angles (see Chapter 5).

In this case the total wave function $\psi$ within the scattering region is approximated by a plane wave modulated by some function $\phi$ (Glauber 1959),

\[ \psi(\mathbf{r}) = \exp(ik \cdot \mathbf{r}) \phi(\mathbf{r}), \]

where $\phi(\mathbf{r})$ is assumed to vary slowly over a distance equivalent to the incident particle wavelength. In obtaining a form for $\phi(\mathbf{r})$ the approximation is made that only waves which are nearly parallel to the incident wave are considered. This gives a much simplified integration.

Essentially the Glauber theory is a diffraction approximation wherein it is assumed that the incident plane wave sweeps virtually undeviated through the region of interaction and emerges suffering only/impact parameter dependent change of phase and amplitude. (Burke 1972, Franco 1968, McDonald and Nuttal 1969, Tai et. al. 1970).

1.4(h) SUMMARY

In Chapter 5 the experimental results obtained from this work are compared with available theoretical calculations. Such comparisons make it possible to state the energy range in which
each approximation is valid. In view of the fact that no one theory is capable of producing accurate cross-sections over the entire energy range, a set of approximations have been chosen which combine to achieve this goal. For energy ranges where more than one approximation is applicable the simplest is presented.

The conclusions reached in Chapter 5 are that the first Born theory is useful for energies greater than 200 eV, while the Glauber approximation is a good representation for cross-sections between 50 eV and 200 eV. At lower energies still the close-coupling equations, although tedious, give good results, (references as in 1.4(e)).

1.5 OUTLINE OF THESIS

The remaining part of this thesis is divided into four sections. The first describes the electron gun and electron beam production (Chapter 2). The data handling technique and the vacuum technology are briefly discussed in Chapter 3. Chapter 4 deals with the mass-spectrometer calibration and gives the information required to find the ratios of number densities of the scattering centres at the intersection of the electron and neutral beam. Chapter 5 deals with the results from the electron scattering, which include angular distributions and their normalization. Molecular hydrogen elastic scattering is dealt with first, followed
by atomic hydrogen (elastic and inelastic) and the normalization of the rare gas cross-sections is presented last.
CHAPTER 2
ELECTRON OPTICS

2.1 INTRODUCTION

When attempting to measure angular distributions it is important that the initial direction of the electron beam is well defined. This is particularly so if scattering at small angles is to be attempted.

During the previous work with this apparatus (Williams 1969), angular distributions were limited to angles greater than 20°. The reason could have been space charge repulsion in the beam or poor focussing by the electron gun. It was therefore decided that an investigation would be carried out, as part of this project, to determine electron beam profiles for various focus conditions and distances from the electron gun.

2.2 THE ELECTRON GUN

A description of the construction of the electron gun was given by Teubner (1967). It consisted basically of a cathode-anode arrangement as described by Frost et. al. (1962). An einzel lens was situated in front of the anode so that the beam could be focussed (Simpson and Kujatt 1963).
The barium-oxide cathode was of the dispenser type (Harris and Bakish 1962), enabling the experimenter to reactivate its surface should it become necessary to open the system to air. It consisted of a tungsten matrix containing a barium compound which reduced to BaO on heating to 1150°C in a vacuum of 10⁻⁶ torr or better. (Haas, published by Hughes and Schultz 1967).

2.3 SPACE CHARGE REPULSION IN THE BEAM

A factor affecting the focusing of an electron beam is the mutual repulsion between electrons in the beam. Considering the cylindrical symmetry of an electron beam carrying a total current I, the electrons will move in the z direction with velocity

\[ v = \sqrt{-\frac{2q}{m}} \]

where \( V \) = electron energy,

\( m \) = mass of an electron, and

\( q \) = charge of an electron.

The radial repulsion force giving rise to the spreading of the beam is given by:

\[ \frac{d^2r}{dt^2} = -\frac{q}{m} E_r \]

where

\[ E_r = \frac{\phi}{2\pi\varepsilon_0 r} \]
and \( Q \) = total charge per unit length.

Neglecting axial space charge forces, Harris (published in Dakish 1962) shows that the above equations can be used to obtain an expression for \( \frac{dr}{dz} \), i.e. the amount of spreading which occurs in the beam with distance along \( z \) is:

\[
\frac{dr}{dz} = \pm K \sqrt{\frac{\ln r}{r_o}}
\]

where \( r_o \) = beam radius at \( \frac{dr}{dz} = 0 \) and \( K \) is a function of \( I V^{-3/2} \).

Using this information (plotted as a Universal beam spread curve in Dakish), it was seen that for the gun currents used here, space charge repulsion was not the main contribution to the beam spread. It was therefore necessary to observe the beam profiles and attempt to improve the focussing of the electron gun.

One method of doing this is to insert a Faraday cup into the electron beam and measure the electron current which it collects. To find the actual shape of the electron beam profiles, a cluster of small cups can be used to plot out the charge density across a section of the beam. The design of the Faraday cup must take these secondary emission phenomena into account. If the cup is deep and narrow, the probability of a secondary electron escaping from it is small.
2.4 SECONDARY ELECTRON EMISSION

Secondary electron emission will take place whenever electrons are incident on the surface of any material (Hughes and Schultz 1967). It is dependent on the primary electron energy, the angle of incidence of the electrons with the surface, the properties of the material being bombarded and the surface conditions of the material (that is, the history of the surface is important).

A characteristic property of secondary emission is that the emitted electron energy is usually in the range of 1 eV to 10 eV independent of the incident electron energy. However a few secondary electrons will have energies up to and including the primary electron energy.

Low energy secondary electrons are usually produced deep inside the material and have come to the surface by a diffusion process after which they escape through the surface barrier, while high energy secondaries have only undergone collisions near the surface (Spangenburg 1948).

2.5 DESIGN OF THE FARADAY CUP DETECTORS

The size of the electron beam was estimated to be less than 2 cm in diameter at the interaction region, (previous work by Williams 1969). Consequently a cluster of Faraday cups, each
about 3 cm deep and 3 mm in diameter, was built and inserted into the electron beam. The cluster contained nine cups in a matrix form of 3 x 3. The Faraday cups were made of copper tubes and fixed in position on a grounded metal plate, but insulated from it (with teflon) in such a way that no insulating material was in the direct path of the incident electrons. Consequently any charge built up would be minimized. A multiple switch was used to monitor each cup in turn on an ammeter. Results from this initial attempt indicated that either the beam was much wider than expected or that secondary emission was affecting the measurements.

Since the incident electrons struck the Faraday cups at grazing angles, large numbers of secondary electrons may have been produced (Haas, published by Hughes and Schultz 1967). These were then detected by neighbouring cups. It was therefore necessary to investigate this matter further.

Using a single Faraday cup and entirely surrounding it with a fine wire mesh (transparency = 90%) a study was made to find out more about the secondary emission process. The wire mesh was connected to a variable power supply with both negative and positive outputs. This unit was then placed in position, the electron beam focussed on it and the beam current measured as a function of the potential on the wire mesh. A typical result is seen in
Figure 2.1 The electron current (as measured by the faraday cup, arbitrary units) is shown as a function of the voltage on the wire mesh (grid) which completely surrounded the faraday cup. The electron energy was 50 eV.
Figure 2.1. It is clear that as the grid potential increased in the negative sense, the signal increased because the loss of secondary electrons from the cup was reduced. In fact the increase in the signal was so great that it is unlikely that secondary electrons from the Faraday cup alone contributed. For instance, secondary electrons produced at the negative grid would have been readily attracted to the Faraday cup. It is to be noted that the curve reaches a saturation value around -15V on the grid. This is just the energy region in which most secondaries are produced. The gradual fall off with more negative grid voltages, before cut off, was probably due to defocussing of the incident electron beam by the large negative potential obstructing its path.

For positive voltages on the wire mesh, a shallow minimum was observed. This may be explained by the fact that secondary electrons escaped from the Faraday cup when the wire mesh was at ground or some positive potential. On the other hand less secondary electrons reached the cup from the wire mesh as it became more positive. At higher positive voltages the curve increased slightly due to a field being set up by the grid which accelerated electrons within the scattering chamber in the direction of the Faraday cup.

The importance of secondary electrons was further illustrated by applying a varying potential to the Faraday cup and monitoring
Figure 2.2 The electron current is monitored on the grid for varying voltages on the Faraday cup.
the current on the grid. Results are plotted in Figure 2.2, from which it is immediately seen that the number of secondaries produced in the scattering chamber and collected by the grid exceed the number of incident electrons on the grid.

2.6 CONSTRUCTION OF THE FARADAY CUP SYSTEM

An improved system consisting of two Faraday cups was therefore designed in which secondary electrons were prevented from contributing to the signal. This was achieved by completely enclosing the cups within an electrically grounded cylinder, leaving open only entrance apertures to each cup. These entrance apertures were used as collimators so constructed that any electron passing them would land deep inside a Faraday cup (Figure 2.3). They were made from two parallel plates with holes drilled through them. A barrier to any secondary electrons was placed between the entrance of each cup and the collimator plates in the form of a suppressor plate. This plate was normally charged negative. The apertures of the suppressor plate were made large enough so as to be out of view from the incident electron beam and consequently did not contribute secondary electrons. To further reduce secondary emission, all plates were made of thin material, reduced to a knife edge at each aperture.
Figure 2.3 The faraday cup system used for the determination of electron beam profiles. Shaded regions refer to teflon insulators.
All Faraday cups were held in position by means of teflon (insulator) fittings, made in such a way that it was not possible for charge to accumulate on the insulation surface. Typical resistances for these insulators were of the order of $10^9$ ohms, measured with a Keithley electrometer. Electron currents were measured with a Hewlett-Packard microvolt-ammeter. Since the input impedance of the latter was less than or equal to $10^6$ ohms, leakage in the insulators was insignificant.

A condition which the collimators were to satisfy, was that each cup had to see the total cross-sectional area from where the electron beam originated. Provided the cups were kept at least 2 cm from the electron gun exit this condition was satisfied.

The secondary electron emission effect in this device was then investigated using the suppressor plate. By applying a negative voltage to this plate secondary electrons could be prevented from passing through its aperture. The percentage variation of the potential across the apertures is given approximately as $\frac{r}{d}$ where $r$ = radius of aperture and $d$ = distance between suppressor and nearest grounded plate. Making this factor as small as was practical, an integral spectrum was found for electrons detected by the cup, by varying the suppressor
voltage between zero and the incident electron energy. Results showed that the secondary electron production at the knife edges was negligible, so the suppressor was earthed. Those produced elsewhere (except inside the Faraday cup itself) were unable to contribute to the signal due to the construction of the cup system.

It was now possible to measure the beam profiles by merely deflecting the primary electron beam across a Faraday cup and plotting the results as a function of deflection voltage. This could be converted back into units of length by using the known distance between two Faraday cups as a calibrating standard. However the deflecting process introduced a considerable amount of distortion to the beam profiles, despite the use of a symmetric power supply which applied an equal but opposite potential about the mean electron energy to the two electrodes on either side of the beam, to the deflector about the outer einzel ring potential.

To eliminate this problem it was necessary to move the Faraday cup system across the electron beam. This was done by mounting the Faraday cup, off-axis, on a rod which passed into the vacuum system through a differentially pumped rotary seal. The cup could thus be moved along the beam axis, as well as across it, by rotating the rod. The length of arc through which
the Faraday cup needed to move was sufficiently small to be approximated by a straight line. Consequently, the calibration could be achieved as described before.

RESULTS AND CONCLUSIONS

A sample of the electron beam profiles obtained can be seen in Figure 2.4. The results indicate that although it was possible to optimize the focus condition to obtain an electron beam with very small diameter at some small distance from the electron gun, it was impossible to produce a well collimated beam which did not spread appreciably with distance. Since space charge repulsion was not appreciable it must be concluded that the einzel lens was responsible. It was therefore not possible to reduce the electron beam spread so as to measure angular distributions at angles smaller than 20°.

It should also be noted that the ability to focus the beam varied with the electron energy. At low energies, difficulties were experienced with the electron beam which caused data taking below 50 eV to be unreliable.
Figure 2.4 Profiles found for an electron beam of energy 100 eV at distances of 2 cm, 4 cm, 6 cm, 8 cm respectively from the gun. Beam width given in mms.
CHAPTER 3

THE ELECTRON SCATTERING SYSTEM

3.1 INTRODUCTION

A detailed account of the basic vacuum system and method of data recording for this type of apparatus has been given by Fite and Brackman (1958) and was also described by Teubner (1967) and Williams (1968). However, since several modifications and additions to the apparatus have been performed, a further description was found necessary.

The purpose of using a modulated beam apparatus is to be able to consider electron scattering from chemically unstable gases such as atomic hydrogen. It has other advantages too. For instance, the experimental study of electron scattering usually involves a component of background scattering which arises from stray electrons as well as from a presence of foreign gases (e.g. from outgassing of the chamber walls) in the scattering chamber. Details will be given in this chapter to show that it is possible to separate and thus eliminate this background component.

3.2 DESCRIPTION OF APPARATUS

The apparatus consisted of four stages: the oven chamber,
the chopping chamber, the scattering chamber, and the mass-spectrometer (Figure 3.1). All chambers were individually pumped and were connected by only small apertures in order to isolate each stage from its neighbour. The oven chamber contained the gas inlet system and the atomic hydrogen oven (details are given in Fite and Brackman 1958 and Teubner 1967). The latter consisted of a tungsten tube with a narrow slit cut into it by a spark erosion process. It was held in a vertical position with heavy, water cooled copper leads. By passing currents of the order of 200 to 300 amperes through the tungsten oven, temperatures between 2,000 °K to 3,000 °K, adequate for partially dissociating molecular hydrogen, were obtained.

The gas under study entered the tungsten tube through one end, while the other was closed. Thus the gas passed through the slit and spread according to a cosine distribution (Ramsey 1956). A narrow cone of it was selected to form the required beam, the rest was pumped away. Typically the background pressure in this chamber with gas diffusing into it, was $10^{-4}$ torr. The pressure in the hydrogen oven was usually a few torr.

The beam then passed into the chopping chamber, where it was chopped by a rotating mechanical shutter at the rate of 100 times each second. A pressure of about $10^{-5}$ torr was maintained
Figure 3.1 Schematic diagram of a modulated beam apparatus. The plane containing the electron spectrometer is perpendicular to the page.
in this chamber.

In the scattering chamber the gas beam was intercepted by an electron beam. Electrons scattered between angles \( \theta \) and \( \theta' \) were energy analysed by the electron spectrometer (described in Chapter 5) before being detected by an electron multiplier.

Ions produced at the intersection of the two beams were accelerated and focussed onto the mass-spectrometer entrance slit. After being mass-analysed the ions were detected by means of an electron multiplier (described in Chapter 4).

After passing through the scattering chamber the gas beam entered the mass-spectrometer system. A pump was added to this system to reduce the pressure fluctuations in the scattering chamber, caused by the chopping of the beam. From the geometry of the apparatus it was considered that the neutral beam would be sufficiently well collimated to pass through the scattering chamber into the fourth stage where it would be stopped by the mass-spectrometer entrance slit (which was of very small dimensions compared to the beam diameter). Hence there were two passages along which this gas could diffuse, either back to the scattering chamber or into the mass-spectrometer pump. Provided the pumping rate was sufficiently high, leakages back into the scattering chamber would be small. The consequent construction
of the connection, between pump and mass-spectrometer, had to be chosen accordingly.

The quantity of gas that flows through a short tube per second is given by (Green (1968))

\[ U = \frac{65}{D^3} \frac{1}{\sqrt{M}} \frac{1}{(L + \frac{4D}{3})} \text{ (litres/sec)} \]

where \( U \) is called the conductance of the tube,

\( D \) is the diameter of the tube,

\( L \) is the length of the tube, and

\( M \) is the mass number of the particles.

From a calculation of the above formulae it was possible to make the conductance of the gas back into the scattering chamber approximately one-tenth that of the conductance to the pump. (A correction was made for the valve introduced between the mass spectrometer and the pump). Thus the pressure increase which normally occurred in the scattering chamber when a gas beam was passed into the system (and consequently the pressure fluctuations when the beam is chopped) was expected to be greatly reduced.

When tried in practice however, it was found that the pressure fluctuations were reduced by only about 20% to 30%,
depending on the beam strength. Two possible factors may have been responsible. Firstly, more scattering of particles out of the beam occurred than was expected (the pressure in the beam was approximately $10^{-5}$ torr in the interaction region) and secondly, small leakages of gas occurred from the higher pressure chambers. These leakages were not collimated and could therefore not pass through the scattering chamber in the same way as the beam.

All stages were pumped with oil diffusion pumps operated with cold traps which were constantly maintained at liquid air temperature by an automated filler system (described in Appendix I). This was found necessary to eliminate the backstreaming of oil, which produced an insulating layer covering the chamber walls. As a result a charge accumulation occurred which interfered with the electron trajectories. The base pressure obtained in the scattering chamber with the use of liquid air traps was $2 \times 10^{-7}$ torr, the operating pressure (i.e. when a beam passed through it) was about $10^{-6}$ torr.

3.3 DATA HANDLING TECHNIQUE

A full description of the data handling electronics for this apparatus was given by Williams (1969). It is pointed out that the choice of a digital system was necessitated by the low
count rate obtained for large angle scattering.

Scattered electrons and ions produced in the interaction region of the two beams are detected by separate electron multipliers to produce pulses which are then amplified and passed through a discriminator unit set to reject all noise pulses. The digital signal thus obtained is fed into two scalers. One of these adds all pulses to previous entries during the "beam on" condition, while pulses arriving during the "beam off" condition are subtracted. Provided that the total integrated background signal is the same both when the beam is on or off, this scaler will record only scattering events from the neutral beam (called the beam scaler, or "add-subtract" scaler). The other scaler adds pulses reaching it during both the beam on and off conditions. It is conveniently called the background scaler.

The beam scaler was switched between the add and subtract mode by a reference signal which was generated when a light beam falling on a photo sensitive transistor was chopped with the same shutter as the neutral beam. The reference signal was brought into exact phase with the chopped beam by a variable delay unit.

An unfortunate property of the chopper was that its rate
of rotation was not constant but fluctuated slightly. To overcome this problem Williams (1969) limited the scaling time, during both on and off conditions of the beam, to a "window period" which was accurately determined by the interval of time required to count a preselected number of oscillations produced by a crystal oscillator. This window period was variable both in width as well as phase with respect to the reference period.

To record the data, facilities were available to store the information in a multi-channel digital recorder or to plot it on an X-Y plotter (via a digital to analog converter) modified so that both the beam and background signals were recorded simultaneously.

3.4 PRESSURE FLUCTUATIONS IN THE VACUUM SYSTEM

Since the background signal was proportional to the pressure in the scattering chamber at any given time, it was necessary to control any fluctuations in this pressure if the add-subtract scaler was to give meaningful results. The pressure fluctuations were of two types:

Random fluctuations resulted from irregular changes in the pumping speed of the diffusion pumps. Although they could not be completely removed these fluctuations were minimized by using
two diffusion pumps in series. This was done with both the scattering and chopping chamber pumps.

Coherent fluctuations of the background pressure were produced at the modulation frequency, by the introduction of the neutral beam during only half of each cycle. In particular the chopping of the neutral beam caused pressure fluctuations in both the chopping and scattering chambers which were out of phase with each other by 180 degrees and which had the property of being exponential (Green 1968) in character as shown in Figure 3.2(a), (b) and (c).

Now the contribution to the background signal at any instant of time will be directly proportional to the background pressure, in the scattering chamber, at that instant of time. The integrated contribution to the signal from the background during the beam on period, can therefore only be equal to the contribution during the beam off period, when the pressure changes in 3.2(b) are linear.

A necessary condition for the linearity of these pressure changes is that the characteristic time constant of the vacuum system is large compared to a half cycle of the chopping period. A linear variation is also needed in the chopping chamber to ensure that the same quantity of gas will pass from the (higher
Figure 3.2 (a) The reference signal which contains the information whether the gas beam is "on" or "off".
(b) The pressure fluctuations in the scattering chamber.
(c) "..." "chopping"
(d) Shows the "window time", i.e., the period when data is recorded.
pressure) chopping chamber into the scattering chamber during both of the half cycles of the chopping frequency.

The time constant involved is given by the ratio of the chamber volume to the speed of the pumping system. Since however the effective pumping speed is difficult to predict accurately, only an approximate value (equal to about one-tenth of a second) can be calculated.

To provide a more accurate value an alternate method had to be devised. Obtaining a direct measurement of the time taken to reduce the pressure by a factor of 1/e was impractical since the time constant was too small for any pressure gauge to respond quickly enough.

The procedure therefore used was to first pump the system down to the lowest pressure obtainable. Introducing a gas beam caused the pressure to rise in an exponential way (Green 1968) until it was interrupted by the shutter, causing the pressure to fall, also in an exponential manner. Hence in chopping the beam, pressure fluctuations of the type seen in Figure 3.2(b) and 3.2(c) were expected. These curves could be obtained in the following way.

Earlier in this chapter it was mentioned that the scalers
only accumulated data during a selected interval of time
within each half cycle of the reference signal. This window
time could be varied in size with respect to the chopping period.
Thus, while during normal operation it covered approximately
90% of each half cycle of the reference signal, for the purpose
of plotting out curve 3.2(b) it was made very small with respect
to the period of the reference signal (e.g. by slowing down the
chopper wheel). The window interval was then positioned in
the centre of the reference signal as indicated in Figure 3.2(d).
Provided that the contribution to the scattering signal by the
beam was eliminated, the add-subtract scalars would record the
difference between the on and off condition in the background
signal. Consequently a shutter was placed across the beam
entrance to the scattering chamber, however in such a way that
gas could still enter the chamber, to produce the pressure
fluctuations described previously. If the signal contribution
within the window time (Figure 3.2(d)) during the beam on
period equalled $Q_{ON}$ and during the beam off period equalled
$Q_{OFF}$, then the data recorded by the scalers was,

$$\Delta Q = Q_{ON} - Q_{OFF}$$

This difference in the contribution to the background signal
during the two half cycles of the chopping period could then be
used to predict the exponential functions involved and in particu-
lar to find the time constant of the system. The difference 
\( Q_{\text{ON}} - Q_{\text{OFF}} \) can be shown (Appendix II) to be given by:

\[
\Delta Q = K \left(1 - \frac{2e^{-t/T}}{1+e^{-T/\tau}}\right)
\]

where \( t \) = the time measured from the beginning of a chop-
ping period,

\( T \) = chopping period,

\( \tau \) = time constant of system

\( \tau \) was found to be equal to 150 milliseconds which is long com-
pared to a typical half cycle of the chopping period (i.e. 5 
milliseconds).

3.5 **ELIMINATION OF THE BACKGROUND SIGNAL**

A final test to show that the background contribution to 
the total signal was eliminated, could be demonstrated with the 
aid of a shutter blocking the entrance to the scattering chamber. 
As before the shutter was constructed and positioned in a manner 
which, although stopping the beam, allowed the gas to neverthe-
less enter the chamber. Consequently the usual background 
pressure fluctuations of a chopped beam experiment were simulated 
without having a beam contributing to the signal.
Allowing the add-subtract scalers to accumulate data over a period of 30 minutes, under the above conditions, produced a negligible total signal (i.e. after allowing for statistical effects). Repeating the procedure for a variety of source pressures (or beam strengths) gave the experimenter complete confidence in the apparatus.
CHAPTER 4
MASS SPECTROMETRY

4.1 INTRODUCTION

As outlined in Chapter 1, the object of this experiment was to find ratios between the differential cross-sections of hydrogen and helium. It was therefore necessary to know the relative number density of each species in the interaction region. The present chapter describes how a 120 degree magnet mass-spectrometer was calibrated to detect quantitatively the ion species mentioned above.

The mass-spectrometer was first calibrated to detect relative number densities of molecular hydrogen and helium. This established the relation between the detecting efficiency of the spectrometer and the mass of the ions. However it was also necessary to check this relationship with atomic hydrogen.

4.2 DESCRIPTION OF THE APPARATUS

Ions formed in the interaction region, at the intersection of the electron and neutral beam, were extracted by means of a parallel electrostatic field, produced by applying voltages +V and
Figure 4.1 The ion extraction and detection system.
The magnetic field applied to the mass-spectrometer was perpendicular to the plane of the paper.
-V respectively to two flat metallic surfaces which were symmetrically placed about the electron beam in a plane perpendicular to the neutral beam (Figure 4.1). In this way the electron beam passed through a region essentially at earth potential, thus ensuring that the electron energy was determined only by the potential on the cathode of the electron gun. Unfortunately however, the value of this extraction voltage was large enough to significantly change the direction of the electron path. Nevertheless the problem could be reduced by using a sufficiently high electron energy.

The value of the extraction voltage was chosen so that any further increase did not produce a change in the mass-spectrometer signal, that is, the extraction voltage was normally operated at saturation level. Under these circumstances V was equal to about 20 volts. The initial momentum thus imparted to the ions caused them to enter a linear accelerator (instead of a drift tube as in the previous arrangement) which consisted of a set of equally spaced annular rings. By placing a wire mesh across the first and last rings and using a resistor chain to provide equal voltage increments between the rings, a parallel electric accelerating field was produced. A schematic diagram of the mass-spectrometer is given in Figure 4.1.
Accelerating the ions, to their final energy (usually in excess of 100 eV) as quickly as possible reduced the amount of spread in the ion beam and consequently lessened the problem of ion loss from collisions with the surrounding cylinder walls. The next stage reached by the ions was an einzel lens. Its function was to focus the beam onto the entrance slit of the mass-spectrometer. Horizontal and vertical deflector electrodes were also included in the apparatus, ensuring that the beam could be properly centred on the entrance slit. (A necessity because the stray magnetic field from the mass-spectrometer magnet caused the beam to be deviated before it actually reached the entrance slit.)

The pumping system associated with the mass-spectrometer was placed between the einzel lens and the entrance to the mass-spectrometer. As a consequence a drift tube, made of wire mesh and raised to a potential equivalent to the ion energy, was inserted into this region. It produced a field free region for the ions to pass through, without being defocussed.

Finally the ions were selected according to their mass by the magnetic field and detected by an electron multiplier tube.
The exit slit of the mass-spectrometer was sufficiently large to allow effectively all ions of a particular species through at one particular setting of the magnetic field. This was done in order to overcome the undesirable non-linearity of the peak widths obtained when the magnetic field $B$ is uniformly stepped through peaks of different mass.

The equation describing the ion trajectories in a uniform magnetic field is:

$$B = \frac{(2Em)^{\frac{1}{2}}}{qr}$$

where $m = \text{mass of the ions}$

$E = \text{energy of the ions}$

$q = \text{charge of the ions}$

$r = \text{radius of curvature of the ion path}$.

Since $E$, $q$ and $r$ are constant in the present situation, the non-linear relationship between $B$ and $m$ can be easily seen.

The optimum size for the exit slit was found by trying slits of several different sizes. From a convolution consideration (Figure 4.2) the size which would transmit all of a given species at one setting, but not other species, was then chosen. With a narrow slit, the ion beam profile was effectively reproduced.
Figure 4.2 The ion beam profiles as detected by the mass-spectrometer consist of a convolution of the true profiles and the exit slit.
Wider slits eventually produced a profile with a flat region in the middle as desired.

4.3 THE CALIBRATION PROCEDURE

One method of finding the relative detecting efficiency of a mass-spectrometer for different ions is by means of a gas mixture of known composition. Introducing this mixture into the scattering chamber, enables a measurement to be made of the relative signal strength of each species. This information is then compared with the expected results after allowance has been made for the ionization cross-section of each species. (Values for the ionization cross-sections were obtained from Kieffer and Dunn, 1966).

Thus a 50% hydrogen and 50% helium mixture (by volume) was obtained in a gas cylinder pressurized to about 100 times atmospheric pressure. By means of a pressure reducing valve a sample of this mixture could be introduced into the scattering chamber. It was however important that the gas mixture remained unchanged in composition while passing through the valve.

The gas flow under high pressure conditions, when the mean free path of the particles is much smaller than the slit size
through which they pass, may be calculated (Starling and Woodall, 1957) by equating the work done by the particles in the cylinder on an area A (i.e. \( (p_1 - p_2)A \)), to the kinetic energy transfer to that area (i.e. \( \frac{1}{2}mN\bar{v}^2 \)). The area A may be considered as the area of the valve opening.

Where \( N \) = number of particles effusing,
\( V \) = volume effusing (at the cylinder pressure)
\( p_1 - p_2 \) = pressure difference across valve
\( \frac{1}{2}m\bar{v}^2 \) = average kinetic energy of each particle.

This leads to the equation:

\[
\frac{N}{V} = \frac{p_1 - p_2}{\frac{1}{2}m\bar{v}^2}
\]

Consequently no change in composition will occur since the particles of each species in the cylinder will be at the same temperature.

Before any measurement with the mass-spectrometer could be taken, it was necessary to ensure that the focus conditions for all ion species were identical. Thus helium and molecular hydrogen ions of equivalent energy were focussed on the entrance slit of the mass-spectrometer. The mass-spectrometer was dismantled for this purpose, only leaving the ion accelerating and focussing
stages intact. The ion detector was placed at the end of the drift tube in line with the initial direction of travel of the neutral beam. A slit in front of the ion detector simulated the entrance to the mass-spectrometer. The purity of the ion beams (produced separately for this purpose, i.e. either H\textsubscript{2} or He) relied on using high source pressures and flushing the chamber with the gas under study. It should be pointed out that an ion beam of approximately 90% purity would have been sufficient, as only differences in the profiles were being sought. By means of the horizontal deflector electrodes, each ion beam was in turn progressively deflected across the slit and the resultant profiles compared. As shown Figure 4.3, the profiles were found to be identical (even though some distortion may have been expected from the deflecting field, the method would nevertheless have shown significant differences in the profiles).

Defocussing the ion beams reduced the signal of each species in the same proportion. Consequently it was not necessary to have stringent control of the focus conditions, thus greatly simplifying the data taking. Results were also taken with the electron gun (which was rotated about the neutral beam here instead of the detector) in different angular positions to decide whether various structures inside the scattering chamber may have interfered with the extraction field. Only the Faraday cup,
Figure 4.3 Beam profiles of molecular hydrogen and helium ions at the entrance slit to the mass spectrometer.

Figure 4.4 H$_2$/He ratios in the mixed beam as a function of the source pressure.
monitoring the electron beam, was a problem. It was therefore moved well away from the interaction region.

It was now possible to perform a calibration test on the mass-spectrometer. First the vacuum system was pumped down to a pressure of approximately $2 \times 10^{-7}$ torr. The gas mixture was introduced directly into the scattering chamber via a needle valve. All pumps were then closed off from the system. The pressure was allowed to rise to a value between $10^{-5}$ and $10^{-4}$ torr before the needle valve was closed, ensuring that impurities in the chamber would be negligible. At the pressures used the mean free path of the particles was still sufficiently large for the present purpose. An ionization gauge was used to monitor the pressure to ensure that it remained constant while data was being accumulated on the background scalers (Chapter 3), which were convenient for this purpose.

The initial results thus obtained indicated that the relative efficiency of detecting hydrogen and helium ions, changed with the use of the detector. Both channel electron multipliers as well as multistage electron multipliers were used and similar performances found for both.
4.4 METHOD OF ION DETECTION

The detector first used with the mass-spectrometer was a Mullard channeltron. It was operated in the 2K to 2.5K volt region. During the process of calibration with the mixed gases (50% He, 50% H₂), it was found that its detecting efficiency decreased with continual hydrogen ion bombardment. Even when the operating voltage was increased to run the channeltron in saturation, this problem persisted. A possible solution was to allow the detector a "warm up" period. However the time involved was far too large to allow efficient data taking.

It was thought that the oxide surface of the channeltron was gradually reduced to a hydroxide layer. An electron multiplier (17 stage, Be Cu 0 surface) also behaved in a similar manner, however its sensitivity to hydrogen ions deteriorated even more drastically than the sensitivity of the channeltron. It was therefore decided that it would be desirable to allow the ions to impinge on a chemically inert surface, such as gold. The most straightforward method of achieving this, was to deposit a layer of gold on the first dynode of the electron multiplier by means of an evaporation process. A multiplier tube treated in this way showed no change in its sensitivity during data taking.

The ratio of signals thus obtained from the mass-
spectrometer with hydrogen and helium gas indicated that the gold coated ion detector was sensitive to the impact velocity of the ions. That is, the hydrogen-helium ratio, after correction for the ionization cross-sections, was equal to 1.4 instead of unity. Since the hydrogen and helium ions were accelerated to the same energy their velocities differed by a factor of $\sqrt{2}$. A further investigation of this result was therefore undertaken.

When ions of sufficient energy are incident on the surface of a dynode in the electron multiplier tube (Haas 1967), they will cause secondary electrons to be emitted. It is claimed (Bethe 1930, Bohr 1948 and Oliphant 1930) that these secondary electrons are produced by the ionization of the target atoms, but only electrons formed within $10^{-8}$ cm of the surface are expected to escape. Since this distance is small compared to the typical penetration of the incident ions (between $10^{-7}$ and $10^{-6}$ cm), the ionization producing secondary electrons occurs at the full impact velocity.

An experimental check to give the details of how the secondary electron emission depends on the velocity in the energy range between 1 KeV and 3 KeV was therefore made. Both hydrogen and helium ions were studied by providing a constant source of each and measuring the increase in signal produced by an increase.
in the ion energy. To ensure a uniform amplification by the electron multiplier tube, a constant floating voltage was supplied between the 1st and 17th dynode, while a separate power unit supplied the required voltage difference between the mass spectrometer output and (gold coated) first dynode. Results are shown in Figure 4.5. It can be seen that both the helium and hydrogen signals increased linearly with velocity in this range.

Studies to determine the secondary electron emission from various target materials have been made both theoretically (Bethe and Bohr, as above) and experimentally (Ploch 1951, Oliphant 1930). For instance Bethe shows that the detection efficiency depends explicitly on the velocity of the ions. An experimental investigation by Ploch (shown in Figure 4.6), in an energy region between 1 KeV and 6 KeV confirms that the secondary electron emission is dependent on the ion velocity only. In particular, within the energy range indicated above, a linear relation is obtained.

4.5 MOLECULAR BEAM TECHNIQUE

The next step was to introduce the gas mixture into the system as a beam. The source pressure of such gas beams are usually sufficiently low for molecular flow to occur. However
Figure 4.5 The ion signal detected by the gold-plated detector, as a function of the ion velocity. (Units for both are arbitrary.)

Figure 4.6 Ploch's results, replotted as a function of velocity.
in the present experiment higher pressures were also used. The
calibration was therefore performed over a wide pressure range
including very low source pressures. The criterion for molecular
flow is that the mean free path of the particles within the
source is much larger than the width of the slit from which they
emerge (Ramsey 1956).

According to Ramsey, the number of particles $dQ$ being
emitted per second from an aperture of area $A$ into a solid angle
$\Delta \omega$, under conditions of molecular flow, is given by:

$$
\frac{d\omega}{dQ} = \frac{A n \bar{v} \cos \theta}{4\pi}
$$

where $n =$ number of particles per unit volume inside the
source

$\bar{v} =$ mean velocity of particles in the source.

Thus if a 50% - 50% mixture of hydrogen and helium is fed into
the source, more hydrogen molecules will leave per second
because of the velocity dependence in the above equation, until
an equilibrium condition is reached in which equal numbers of
each will pass through the slit per second (since equal numbers
enter the source from the gas cylinder, as shown previously).
Therefore equal numbers of hydrogen and helium particles will
cross the electron beam per second. But since the hydrogen
molecules have a higher velocity (by a factor of $\sqrt{2}$) they will spend less time in the interaction region, consequently the number density ratio of hydrogen to helium (for the mixed beam) is expected to be $1: \sqrt{2}$.

Similarly, equal source pressures of different gases (not mixed) will result in identical number densities in the interaction region.

In practice the accuracy of the above arguments will depend on whether the source pressures are low enough for molecular flow to occur. It was therefore desirable to work at pressures as low as the apparatus allowed. In the present case a source pressure of 0.1 torr. Under these conditions the mean free path in the source was approximately twenty times as large as the slit width.

To test the foregoing arguments, a mixed hydrogen-helium beam (the mixture in the ratio 1:1) was produced over a range of source pressures and the ratios measured. Figure 4.4 shows a sample of the results obtained. The ratio of $H_2$/He changes with pressure above a few torr, showing that hydrogen is scattered out of the beam more strongly than helium. (Indicating that Ramsey's equation breaks down at lower pressures for hydrogen than for helium, the mean free path of hydrogen being less than that of helium at a given pressure). Ratios at lower pressures were as predicted above.
A further check using separate hydrogen and helium beams followed. It showed that equal source pressures will indeed produce equal number densities in the beam. Source pressures were measured with a diaphragm pressure gauge (Baratron pressure meter, type 77) to an accuracy of 0.1%. The values of the above ratios were obtained by dividing the mass-spectrometer signal output for each ion species by the corresponding ionization cross-section. The numbers thus obtained were in turn corrected to allow for the sensitivity of the detector to the impact velocity of the ions.

The measurements were repeated under different conditions. Particular attention was paid to the varying extraction voltage, energy and focus conditions of the ion beam. The extraction voltage was varied between 20 volts and 200 volts without affecting the ratios.

To further underline the validity of the above it should be noted that if a pump was opened to the system during the static gas calibration then the hydrogen-helium ratios were gradually reduced in value until similar results were obtained to the beam experiments. The faster diffusion property of hydrogen therefore again reduced its number density in the chamber.

The consistency in the above results enabled an extension of
the original project (i.e. hydrogen cross-sections only) to
other gases for which the mass-spectrometer was not suitable (e.g.
the rare gases Ne, Ar and Kr).

4.6 ION DETECTION WITH A FARADAY CUP

Considering the complexity of the detecting process for these
ions and the consequent uncertainty that the explanations for the
various effects were correct, a further (but simple) check was
desirable. By maximizing the count rate as much as the apparatus
would allow, an analogue detection by means of a Faraday cup was
found to be possible. Such a detection system would be independent
of the chemistry of the detector and the velocity of the ions.
The cup was filled with a honeycomb structure and coated with
colloidal graphite to reduce the secondary electron emission.
Since the cup was operated at a voltage equivalent to the ion
energy, the ion detector (a Keithley electrometer, model 610B)
was operated with a floating earth.

A measure of the quantity of ions collected by the Faraday
cup was therefore recorded on the electrometer. The gas mixture
was again introduced as described in the static gas calibration
test. Electrical currents measured were of the order of $10^{-11}$
amps. The results thus obtained confirmed the previous work.
As will be described in the next section, precautions during the above procedure had to be taken due to the adsorption of hydrogen on the walls.

4.7 ADSORPTION AND OUTGASSING FROM WALLS

During the static gas calibration procedure, the most consistent results were obtained when operating at the highest pressure practical under the circumstances (the upper limit was due to mean free path considerations within the mass-spectrometer). The reason for this was the large amount of adsorption of hydrogen on the walls of the chamber.

From the practical point of view, it was found that after having partially degassed the equipment (only partial degassing was possible as the system was not bakeable), it was necessary to flush it briefly with the gas mixture and then perform the experiment as quickly as possible. If readings were delayed for several minutes, the slow process of hydrogen dissolving within the metal (see later) became quite significant. Evidence of this phenomenon was found during scattering experiments when the background scalers would always show an unusually low hydrogen content at the beginning of each experiment after the system had been pumped for some time. Similarly at the end of an experiment a much greater hydrogen signal, as compared to helium, would
persist for long periods of time.

A better illustration of this phenomenon could be observed by passing the gas mixture into the system in the form of a beam (i.e. through the tungsten oven) with a shutter in the scattering chamber which prevented the beam from passing through the interaction region. The resultant ratio of the $\text{H}_2$/He content was measured on the background scalers as a function of the source pressure (i.e. quantity of gas entering the system). As this quantity was increased in stages over several minutes, so the $\text{H}_2$/He ratio increased. (Shown in Figure 4.7).

After the gas flow had continued for approximately 30 minutes, the above procedure was reversed (i.e. the gas flow was steadily being decreased in steps) resulting in an increased value for the $\text{H}_2$/He ratio. Thus as the gas quantity entering became less so the hydrogen outgassing from the walls became more significant.

In general the $\text{H}_2$/He ratio was always large in the background after hydrogen had been admitted for some time, particularly if the number density in the sample measured was small.
Figure 4.7 $\text{H}_2/\text{He}$ ratios in the background measured as the source pressure of the mixed beam is increased slowly and then decreased again.

Figure 4.8 Trajectories are shown of energetic ions produced by dissociative ionization.
4.8 THE MASS-SPECTROMETER CALIBRATION WITH ATOMIC HYDROGEN

The next step in the calibration process was to confirm the mass-dependence of the detecting system with atomic hydrogen. Particular attention was paid to the relation between the detection efficiency and the velocity of the ions. Confidence in the method would be attained if this effect was found self consistent for all ions used.

Although the total ionization cross-sections for atomic hydrogen are known to the same accuracy as those for molecular hydrogen and helium the previous method was not as suitable here due to the inability of being able to obtain a pure beam of atomic hydrogen. Fite and Brackman obtained a 96% dissociation percentage, at source pressures somewhat lower than were practical with the present apparatus.

One method of calibration which seemed worth pursuing was to measure the dissociative cross-section of molecular hydrogen into an atom and an atomic ion, thus:

\[ \text{H}_2 + e^- \rightarrow \text{H} + \text{H}^+ + 2e^- \]

Results would then be compared with those of Rapp et. al. (1965), who measured this cross-section as a function of energy. Consequently the detection efficiency could be found.
4.9 DISSOCIATIVE IONIZATION OF MOLECULAR HYDROGEN

As explained by Rapp et. al. (1965) and Stevenson (1947), when molecular hydrogen is bombarded with electrons of energies greater than 16 eV, the molecular ions thus formed may dissociate into a proton and a free atom provided the molecular hydrogen ion \( \text{H}_2^+ \) is formed above the dissociative limit of the \( 2\Sigma_g^+ \) state. If the electron energy is greater than 27 eV, the \( \text{H}_2^+ \) ion may be excited to the repulsive antisymmetric \( 2\Sigma_u^+ \) state to again produce a proton and a hydrogen atom.

With higher electron energies other excited states become possible with the same end products. However the atomic hydrogen ions (i.e. protons) obtained from a repulsive state of the molecular \( \text{H}_2^+ \) ions will be produced with a kinetic energy of up to 15 eV. Since the direction of these ions is random some difficulty is experienced when trying to collect them through a slit.

The system used here was designed for the detection of non-energetic ions which would conveniently pass through a slit to form a beam before being mass analyzed. Some modifications in the extraction system were therefore necessary. Normally, with ions of thermal energy variations, an extraction of some 20 volts were applied across the interaction region. This potential difference was found to produce a sufficiently high extraction field to
obtain a saturated beam signal. Therefore by increasing the value of this extraction field it appeared feasible to be able to fully extract even these energetic ions. Figure 4.8 illustrates the situation. An expression for the expected ion trajectories is given in Appendix III.

The aperture through which the ions had to pass was 2 cm in diameter, and the region in which the ions were produced had an area of projection along the axis of the neutral beam of approximately 1 cm x \( \frac{1}{4} \) cm. An estimate of the expected spread of such ions with an initial kinetic energy of 10 eV and extraction voltage of 200v was calculated and is shown in Appendix III. It can be seen that although an ion formed in the centre of the atomic beam would pass through the extraction aperture, to get a large percentage of all such ions into the mass-spectrometer, a larger field would be required. Potential difference\(^5\) across the extraction plates of up to 300 volts were applied (equivalent to a field of 150 v/cm). Higher voltages deflected the electron beam too drastically and were therefore not suitable. (The apparatus used here only allowed a maximum electron energy of 300 eV).

Using this maximum electron energy and an extraction voltage which could be varied between zero volts and 300 volts, the ratio of the peak heights of \( \text{H}^+ \) and \( \text{H}_2^+ \) ion were measured as a function
of the extraction voltage. Since the ion extraction field caused the electron beam to miss the Faraday cup it became necessary to check the gun current stability from time to time between data taking. As the extraction field was increased so the ion focus conditions were adjusted accordingly.

The results obtained were expected to show an increasing ratio of $\text{H}^+/\text{H}_2^+$ with increase in the extraction field, until a saturation level in agreement with the data published by Rapp et al. (1965), was reached. The ratios obtained with this method were however much smaller than the results in the literature. Figure 4.9 represents the results graphically.

One way of improving the above method was to allow for a greater tolerance in the transverse ion drift (i.e. perpendicular to the motion of the ion beam), by restricting the region in which the ions were produced. For instance, reducing the diameter of the atomic beam size would have such an effect. The limiting aperture of the atomic beam size (i.e. before the beam enters the scattering chamber) was therefore reduced, as indicated in Figure 4.10, to about one half the previous area. The shape of the neutral beam was first changed to a rectangular cross-section. Because the electron beam had a somewhat smaller diameter, a reduced interaction region resulted. However ratios thus obtained did not significantly differ from the previous ones, possibly
Figure 4.9 The quantity of H⁺ ions detected (from the dissociation of H₂) with increasing extraction voltage.

Figure 4.10 The reduced cross-sectional beam size.
indicating that the neutral beam was less well defined than was originally thought. Consequently in travelling from the aperture of the scattering chamber to the place where intersected by the electron beam a considerable amount of divergence could have occurred. Unfortunately this distance could not be made smaller than 1 cm, due to the construction of the electron gun.

Although some effort was made to resolve this problem it was not possible to obtain a completely satisfactory explanation, but it is probable that a saturation condition could not be reached with an extraction of only 300 volts. In view of these difficulties, an alternative method was therefore attempted.

4.10 ALTERNATIVE CALIBRATION METHOD FOR ATOMIC HYDROGEN

From the work of Fite and Brackman (1958) it has been shown that in the dissociation of hydrogen molecules by a heated tungsten surface, a neutral beam with an atomic hydrogen content of up to 96% could be achieved. Using the most ideal conditions for such a process (i.e. high temperatures and low source pressures) it was feasible to obtain dissociation fractions almost as large with the present apparatus. By making a correction for the undissociated hydrogen remaining in the beam (which could be estimated from the H₂/He ratio measurements) the number density
of hydrogen atoms could be predicted with the aid of the hydrogen-helium mixture used previously.

Source pressures used for this purpose were around $\frac{1}{2}$ torr and the tungsten oven temperature in the vicinity of $3,000^\circ$K (measured with an optical pyrometer and corrected to black body radiation). The mixed beam was introduced while the oven was gradually raised in temperature and the increase in the $H^+$ signal noticed.

Since the relative detecting efficiency of molecular hydrogen and helium had already been measured, an estimate of the amount of molecular hydrogen left undissociated could be made. And since each molecule gives rise to two atoms, an estimate of the total number of atoms produced could also be made. Realizing that the hydrogen atoms (from gas kinetics) have a higher mean velocity than the hydrogen molecules (i.e. inversely as the square root of the mass) the time spent in the interaction region by the hydrogen atoms will be reduced by a factor of $\sqrt{2}$. Therefore if $N$ molecules were dissociated and therefore $2N$ atoms produced, the number density of hydrogen atoms will be given by $\sqrt{2N}$.

By raising the temperature until the percentage of undissociated hydrogen fell to about 10%, the hydrogen atom signal confirmed that the ion detection efficiency was indeed dependent
on the ion velocity.

An attempt was also made to measure the variation in the beam signal as the oven temperature was gradually raised while keeping the oven pressure constant. If the square root dependence of the number density on the oven temperature could be demonstrated, a further method was available of predicting relative number densities (Teubner 1967). That is, it would have been possible to calculate the (hypothetical) number density of hydrogen molecules in a hot oven had there been no dissociation. Therefore by measuring the actual quantity of both molecular and atomic hydrogen with the mass-spectrometer and converting the atomic hydrogen number densities into expected molecular hydrogen number densities (i.e. as if there were no dissociation), a further check was possible. However difficulty was experienced due to the expansion of the tungsten oven as it was heated causing it to move within the fittings which held it in place. This caused gas to leak into the oven chamber in an irregular manner, making meaningful data taking difficult.

4.11 ABSORPTION OF ATOMIC HYDROGEN INTO THE METALLIC WALLS

During the normal process of data taking, readings of the background signal were also noted, since this was necessary to
calculate statistical uncertainties. As a result it was observed that there was a considerable quantity of atomic hydrogen in the background. Since no immediate explanation was available, an effort was made to trace its origin.

It is known (Pirani and Yarwood, 1961), that gases adsorbed on the surface of metals, may diffuse into the interior and form a solution. The solubility increases with the temperature of the metal and also the pressure of the gas. Moreover a dissolved diatomic gas exists in the atomic rather than the molecular state, the dissociation occuring at the surface. When re-emitted from the metal, there may consequently be a probability that a portion of the gas remains in the atomic form. The detailed properties of the above depends on the species of metal, for instance some metals have an enormous solubility due to the formation of pseudo hydrides. (e.g. Titanium, zirconium).

An attempt was consequently made to decide whether this was indeed the source of the atomic hydrogen observed. Initial evidence came from noting the change in the atomic hydrogen content during the time an experiment was performed. That is, while hydrogen gas was being admitted into the system, the apparent content of atomic hydrogen rose steadily. For the purpose of illustration, a mixed hydrogen-helium gas beam was admitted into
the system and the respective ratios of H/He and H/H₂ in the background gas, measured. Since helium has not been observed to form a solution in metals (Pirani and Yarwood, 1961) such a ratio measurement would give a good indication of the atomic hydrogen build up in the chamber. The quantity of H₂ observed will, on the other hand, be related to the H content since an increase in H must also produce some change in the quantity of H₂. Figures 4.11(a) and 4.11(b) show the results obtained. It may be noted that the H/H₂ ratio rises less steeply than the H/Hₑ.

The above ratios in the background, immediately after admitting the mixed gas beam, showed that there was an initial deficiency of hydrogen, presumably because of adsorption on the walls. The above evidence does not however, preclude the production of atomic hydrogen from some other source which increases with time. For instance a water vapour build up may have occurred. A feasible possibility is therefore that water molecules dissociated under electron impact.

\[ \text{i.e.} \quad H₂O + e^- \rightarrow OH^- + H^+ + e^- \]

The chamber was therefore flooded with a moist argon beam for a similar period as before while the atomic hydrogen content (there was always a residual amount in the background) was
Figure 4.11(a) Ratio of $H/\text{H}_2$ in the background after emitting the mixed gas beam into the system for a period of time.

Figure 4.11(b) Ratio of $H/\text{He}$ in the background under similar conditions to the above. (Note that the curves depended on the beam strength used.)
being monitored. Although an increase of H was observed it was considerably smaller than that previously observed.

To increase the water vapour content even further, moist air was then admitted into the system for an hour. The results showed that water vapour decomposition was not the complete explanation for this problem.

Considering that some atomic hydrogen ions were produced by dissociation, with some initial K.E., a brief calculation was made to find an upper limit produced in this way, which may have drifted into the mass-spectrometer system even though they were produced elsewhere in the scattering chamber. It was assumed that the ions were produced along the electron beam and some fraction of these would be detected no matter where they were produced. This fraction was estimated approximately from a solid angle consideration, since the initial velocity of the ions would have been random. It was clearly shown that only a very small fraction of the total atomic hydrogen content could be accounted for in this way.

There is a fundamental difference between adsorption on the surface of a material and the absorption of gas into the interior of a metal. This difference is the time constant involved for these two processes. According to Dushman (1962)
the solubility and diffusion of a gas in a metal are intimately related. It is shown that diffusion into a metal increases with the square root of the gas pressure and exponentially with the temperature. Times of diffusion also depend on other factors such as the history of the material, but are measured typically in hours. This can then be compared with the much faster process of surface adhesion.

To demonstrate this effect, hydrogen and helium were passed into the chamber for a considerable period of time. After turning off this source the relative atomic hydrogen and helium concentration could be measured in the background. Figure 4.12 illustrates the slow decay of the H signal. A preliminary conclusion was therefore reached that a quantity of hydrogen re-emerged from the metal in the atomic form.

Note: From a more recent investigation (Goonan 1973) it now seems likely that the large atomic hydrogen signal was produced by $H^+$ ions being released from the chamber walls (covered with hydrogen) under electron impact (Redhead et. al. 1968).
Figure 4.12 The quantity of H and He remaining in the background after the system had contained both hydrogen and helium for a period of several hours. Both ion signals are normalized to the same value at $T = 0$. 
CHAPTER 5

MEASUREMENTS OF DIFFERENTIAL CROSS-SECTIONS

SECTION 1. MOLECULAR HYDROGEN

5.1.1. INTRODUCTION

Using the gold coated electron multiplier tube as the ion detector in the mass-spectrometer system, it was possible to determine the relative number densities of hydrogen and helium in the interaction region. This information could then be used to find the ratios between the differential cross-sections of:

(a) molecular hydrogen and helium,
(b) atomic hydrogen and helium,
(c) the rare gases and helium.

Consequently, since absolute helium differential cross-sections are known, the unknown cross-sections can be found. This section will consider part (a) only. Parts (b) and (c) are discussed in Sections 2 and 3 respectively. The helium cross-sections used were those of Chamberlain et al. (1970) extended to larger angles with the aid of the angular distributions of Vriens et al. (1967).

In obtaining molecular hydrogen differential cross-sections, it was only necessary to measure ratios of $H_2$ and He cross-sections at one or two angles. Values at other angles could then be obtained
by means of the appropriate angular distribution.

Although a considerable amount of data was available on angular distributions for H₂, it was nevertheless necessary to produce new angular distributions in order to cover the present energy range (i.e. 50 eV to 300 eV) effectively. To check the reliability of the apparatus, several generally accepted angular distributions published in the literature, were remeasured and a comparison made.

5.1.2 ANGULAR DISTRIBUTIONS

Data taking for angular distributions with the present system has been described by Williams (1969). The apparatus consisted of an electron gun which was moved (instead of the detector) about the interaction region in increments of angle of 5 degrees. A parallel plate electron spectrometer energy analysed the scattered electrons. A staircase function generator stepped through the energy range of the scattered electrons. The value of the scattered electron signal at each step of the staircase function generator, was accumulated in a separate channel of a multi-channel analyser, used for the data recording.

Due to the low signal to noise ratio, a knowledge of the statistical accuracy was always necessary, as it was one of the major error contributions. If the scattered electron signal accumulated
in a particular channel \( n \) is given by \( N_n \) and the corresponding background signal by \( M_n \), then the standard deviation in the total electron signal is given by

\[
\sigma = \left[ \sum_n (N_n + 2M_n) \right]^{1/2}
\]

The summation is over the number of steps in the staircase function generator (or channel numbers) used. As pointed out before, the background scalar actually added all data arriving both during the beam on period (i.e. equal to \( N_n + M_n \) for channel \( n \)) and during the beam off period (equal to \( M_n \)). Consequently by taking the square root of the accumulated data in the background scaler, the statistical uncertainty in the cross-section measurements was obtained.

The problem of double scattering has been treated both by Williams and other authors at some length (e.g. Vriens et al. 1967, Chamberlain et al. 1970) and the reader is therefore referred to them. Suffice it to say that it was not a problem due to the low operating pressure used here.

Considering the rapid change of countrate with angle and the limited frequency response of the electron detector, it was necessary to obtain the angular distributions in small sections, each overlapping the other. The sections were then fitted
together. A compromise was usually made between the count rate desired and the effects of dead time of the detector.

To reduce the part played by stray magnetic fields in altering the electron trajectories, the scattering chamber was made of mild steel thus shielding the enclosed region from magnetic fields (Teubner 1967). This helped to reduce the earth’s field. To test its effectiveness against the mass-spectrometer magnet, angular distribution measurements were made while the mass-spectrometer electro magnet (while slightly magnetized) was moved to different positions with respect to the scattering chamber. Results from these tests showed that any such residual magnetism did not alter the angular distributions in a measurable way.

As stated in Chapter 2, the focus conditions of the electron beam did not allow the extension of angular distributions to angles of less than 20 degrees. Since the number of scattered electrons represented only a very tiny fraction (of the order of 1 in $10^{10}$) of the total electrons in the electron beam, it can readily be seen how a small portion of poorly focussed electrons would saturate the detectors at small scattering angles.
Having achieved the consistent reproduction of well established angular distributions, others at energies 50 eV, 75 eV, 150 eV and 300 eV, were measured. Results are shown in Figures 5.1 and 5.2.

Although angular distributions at some of these energies were available by Arnot (1931), Trajmer et al. (1970), Teubner (1967), the agreement between them was not satisfactory. The present measurement of 75 eV agreed most closely with the results of Arnot (Figure 5.2). In particular it may be seen that the angular distribution by Trajmer et al. is much too steep at angles of 30° or less.

Figures 5.1 and 5.2 also show a comparison between experiment and the Born approximation. It is evident that in the angular range indicated, the Born approximation fails at energies of 75 eV and 50 eV at small angles.

5.1.3 THE DETERMINATION OF ELASTIC MOLECULAR HYDROGEN CROSS-SECTIONS

The ratio measurements were performed in the following way. A molecular hydrogen beam was admitted into the chamber and a reading obtained on the mass-spectrometer (after allowing a "warm up" period for the detector) as explained in Chapter 4.
Figure 5.1 Angular distributions for elastically scattered electrons from molecular hydrogen compared with the Born approximation. The statistical error is < 5% for angles < 60°.
Figure 5.2 A comparison between measured angular distributions and the Born approximation. The statistical error is < 5% for angles < 60°.
An average of several readings was usually taken. The electron gun current had to be monitored both before and immediately after the mass-spectrometer measurements were taken to ensure a stable electron beam current (as explained in Chapter 4 it was not possible to monitor the electron current continuously as the ion extraction field deflected the beam past the Faraday cup).

The hydrogen beam was then turned off and a helium beam introduced. The helium peak height was found and consequently the relative number densities of hydrogen and helium, in the interaction region, calculated. By carefully noting the source pressure of each beam, the above number density ratio could be reproduced whenever required (as described in Chapter 4). As a consequence data taking was considerably simplified. Once the relative number densities of the two species involved were known, it was only necessary to measure the number of scattered electrons in each case.

If the number density ratio of two species is given by $N_1/N_2$ and the scattered electron signal ratio by $S_1/S_2$, then the ratio of the cross-sections is given by:

$$ R = \frac{S_1}{S_2} \times \frac{N_2}{N_1} $$
During electron scattering with different gases it was observed that the electron current, as detected by the Faraday cup, varied with a change of the gas species. Similar observations had been made by Williams (1968) who explained it in terms of the positive ion production along the beam path resulting in a reduction of the space charge repulsion. This effect was however not as pronounced with Argon. Given that the ionization cross-sections of molecular hydrogen and argon are approximately equal, a similar number of positive ions should have been produced in each case. Since this was not so it was thought that the chemically active hydrogen influenced the function of the electron gun cathode. The degree to which the electron current was affected depended on the quantity of hydrogen involved. Provided the chamber pressure was kept to less than $10^{-6}$ torr, this effect was not important.

The electron detection efficiency by the channel electron multiplier, was also compared with different background gases. During scattering from a helium beam, hydrogen was admitted through a valve in the side of the scattering chamber. Provided the overall pressure in the system was not raised so much that dead time corrections became large, no significant change in count rate was observed.

The limited range of count rate acceptable to the detecting
system made it desirable to keep the signal strength at the output of the electron and mass-spectrometers approximately equal. Otherwise a change in the electron current would have been necessary. Such a change was not trivial with the present electron gun and amounted to a considerable time loss. Consequently the various factors determining the count rate, such as the electron gun current, the angle of scattering and the size of the entrance slit to the mass-spectrometer were all chosen accordingly, for more efficient data taking.

In an effort to reduce any errors due to uncertainties in the angular position (particularly important for inelastic cross-section ratios, because of the rapid change in count rate with angle), ratios were always taken at any one angle at a time. Normalizations between different angles were compared with the aid of angular distributions. The normalization of each angular distribution was usually performed at two different angles.

5.1.4 THE ELECTRON SPECTROMETER

The electron spectrometer was described in detail by Harrower (1955). Electrons were deflected by a uniform electrostatic field produced by two parallel plates as shown in Figure 5.3. The energy resolution for the device is given by the approximate formulae,
DEFLECTOR PLATE
(-ve potential)

INCIDENT ELECTRONS

Dimensions
\[ x_0 = 2.00'' \]
\[ d = 0.75'' \]
\[ \Delta x_0 = 0.01'' \]
\[ \alpha = 0.08^\circ \]

RESISTOR CHAIN

ANNULAR GUARD RINGS

\(-ve potential\)

EINZEL LENS

Figure 5.3 The electron spectrometer.
\[ \frac{\Delta E}{E} = \frac{2\Delta \chi}{\chi} \]

where \( \Delta \chi \) = the width of both entrance and exit slits

and \( \chi \) = the distance between the slits.

The value for \( \Delta E \) was equal to 1% of the electron energy involved. Hence a primary monochromatic electron beam of 100 eV resulted in a peak one volt wide, measured at FWHM. In addition the electron beam had a thermal energy spread of approximately 0.3 eV. The angular resolution of the spectrometer was approximately 5 degrees. When taking measurements, a staircase function generator stepped the voltage on one of the electron spectrometer plates through a range of voltages to produce the particular peak of interest. The step sizes were variable between .01 and .15 volts. An integration over each peak was then performed.

5.1.5 THE DETERMINATION OF DIFFERENTIAL CROSS-SECTIONS AS A FUNCTION OF ENERGY

The aim of this project was to obtain absolute cross-sections in the energy range 50 eV to 300 eV. Unfortunately however, no absolute helium cross-sections were available below 100 eV at angles greater than or equal to 20°. For this reason
it was decided to try to extend the energy range of the helium
differential cross-sections at 30°, from 100 eV to 50 eV. To
achieve this it was necessary to calibrate the electron detection
system.

Basically the electron detection system consisted of a
spectrometer, to energy analyse the scattered electrons and a
channel electron multiplier to detect them. To reduce the loss
of electrons, as they pass from the analyser to the detector, an
einzel lens was inserted between these devices. The negative
voltage on one of the rings of this lens also served the purpose
of preventing stray secondary electrons from saturating the
detector. A positive potential applied to the entrance of the
electron multiplier further helped to direct the electrons
towards the detector.

There were therefore three factors contributing to a change
in the detecting efficiency of this system as the electron energy
was varied. These were the transparency of the spectrometer
(i.e. the signal output from the device for a given input varied
with energy), the detecting efficiency of the electron multi-
plier and the focussing properties of the einzel lens. Each of
these needed to be investigated separately.

The dependence of the detected signal on the impact energy
of the electrons was considered first. Keeping the potential difference across the electron multiplier constant, the electron impact energy was changed progressively from 50 eV to 800 eV. (Figure 5.4 illustrates how two power supplies were combined to enable this to be done).

The total number of scattered electrons passing through the spectrometer was kept constant by monitoring both the electron gun current and the neutral beam strength as well as keeping the electron energy and the scattering angle fixed. Therefore any change in the count rate for a given electron beam, was a function of the impact energy of the electrons only.

The results for a 50 eV and 100 eV beam are shown in Figure 5.5. With impact energies of 400 eV and higher the two curves displayed the same properties independent of the focus conditions of the einzel lens. But at smaller impact energies, the curves were quite different and changed with the focus conditions of the einzel lens. Consequently the entrance of the detector was always operated above 400 volts.

It was now necessary to consider the variation in the transparency of the electron spectrometer as a function of energy. From the equation giving the energy resolution, in Section 5.1.4, it is apparent that the peak widths, as obtained by uniformly
Figure 5.4 Arrangement of the power supplies for the electron detector (Mullard Channeltron). Power supply 1 determines the impact energy of the electrons (after adding the electron energy).
Figure 5.5 The variation in count rate of the electron detector with the impact energy of the incident electrons.
stepping the electron spectrometer through an energy region, will increase with the energy of the electrons being detected. Consequently a given electron current, produced by the electron gun, will produce a signal at the spectrometer output which depends on the electron energy. Since in the present situation data was obtained by integrating over each peak, the change in the peak area had to be measured as a function of energy for a fixed number of electrons scattered per second. By setting the angle of scattering to a fixed value of 30°, the scattered electron signal from helium, was measured over an energy range of 100 eV to 300 eV. These measurements were then compared with the known differential helium cross-sections thereby establishing the efficiency of transmission as a function of energy.

It was of course important to have an accurate knowledge of the electron beam current at each energy used. The Faraday cup which collected these electrons was therefore placed as close to the electron gun as possible. In this way few electrons in the incident beam were expected to escape detection. Since the degree of focus obtained varied with the electron beam energy and since the Faraday cup detection efficiency may have been energy dependent (e.g. the secondary emission phenomenon changes with energy) the incident electron production was however expected to be a source of error.
With the aid of the multiple Faraday cup (as explained in Chapter 2) it was possible to obtain reasonably similar beam profiles (i.e. electrons travelling parallel to each other in the interaction region) at different beam energies. The source pressure of the helium beam was monitored continuously to ensure it remained constant throughout the data taking process.

A staircase function generator stepped the energy analyser through the required peak in equal step sizes. For simplicity and speed of data taking, each peak was terminated when its individual values fell to less than 10% of the central maximum. The step sizes were kept constant over a particular energy range, but the process was repeated with a variety of step sizes.

Thus by dividing the scattered electron signal by the electron beam current at each energy, a calibration curve was plotted in the 100 eV to 300 eV energy range. Assuming that this curve could be represented by a polynomial function, values were plotted on log-log graph paper and the best visual straight line fit chosen. By extending the graph to lower energies the 50 eV and 75 eV helium cross-sections at 30° could be predicted. Figure 5.6 shows the change in transmission efficiency of the electron spectrometer with energy.

The helium cross-section, as a function of energy, at 30° thus obtained, is plotted in Figure 5.7 together with the
Figure 5.6 The energy dependence of the electron spectrometer.
Figure 5.7 Differential cross-section of helium at 30°, plotted as a function of energy.
calculations of LaBahn and Callaway (1969 and 1970). These 
were slightly scaled to fit the experimental data points of 
Vriens et al. exactly. Considering the excellent agreement 
obtained in this way they provided a useful check on the present 
work. The He cross-section adopted in this work at 50 eV was an 
average between this experiment and the scaled calculations by 
La Bahn and Callaway.

Absolute differential cross-sections of the hydrogen mole 
cule obtained from cross-section ratio measurements are given in 
Figure 5.8.

5.1.6 THEORETICAL REVIEW OF ELECTRON-MOLECULAR HYDROGEN 
SCATTERING AND DISCUSSION

A general introduction to the theory of electron scatter-
ing was presented in Chapter 1. The present chapter will deal 
with theoretical treatments which contain calculations of cross-
sections directly comparable with experimental results obtained 
here. Molecular hydrogen cross-sections are considered first; 
calculations on atomic hydrogen and the rare gases will be dis-
cussed in later sections.

The first attempt to calculate differential cross-sections 
for the hydrogen molecule, were made by Massey and Mohr (1932) 
who used the Born approximation for this purpose. The wave
Figure 5.8 Elastic differential cross-sections of the hydrogen molecule between 20° and 90° as measured with the modulated crossed beam apparatus. The error estimation is $\sim 10\%$ except for 50 e.V. where it is $\sim 15\%$. 
function describing the hydrogen molecule consisted of two parts, one for each atom within the molecule. As a consequence, the incident electron wave was coherently scattered at two similar obstacles which gave rise to a diffraction term in the expression for the scattering amplitude:

\[
\frac{\sin x}{1 + \frac{x}{\lambda}}
\]

where \(x = \frac{4\pi d}{\lambda} \sin \frac{1}{2} \theta\),
d being the equilibrium nuclear separation
\(\theta\) the scattering angle, and
\(\lambda\) the wavelength of the electron.

Massey and Mohr presented their calculated angular distributions at energies of 30 eV, 80 eV and 400 eV. They also presented ratios between cross-sections of molecular and atomic hydrogen with particular attention being given to the effect of the diffraction term. Figure 5.9 compares the 80 eV angular distribution of Massey and Mohr with the 75 eV measurements of the present experiment.

Measurements of the cross-sections for the hydrogen atom which are presented in the next section provided a check on the \(\text{H}_2/2\text{H}\) cross-section ratios by Massey and Mohr. The table below shows that these ratios did not at all agree with the
Figure 5.9 A comparison between experimental measurements and the calculations by Massey and Mohr. The angular distribution of Massey and Mohr has been normalized to the present experimental measurements at 60°.
experimental measurements. The calculated ratios seem to be better without the diffraction term.

<table>
<thead>
<tr>
<th>Electron Energy</th>
<th>Angle of Scattering</th>
<th>$\text{H}_2/2\text{H}$ Ratios</th>
</tr>
</thead>
<tbody>
<tr>
<td>75 eV</td>
<td>$30^\circ$</td>
<td>Expt.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>With diff.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.7</td>
</tr>
<tr>
<td>300 eV</td>
<td>$30^\circ$</td>
<td>0.7</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Massey &amp; Mohr Without diff.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1.0</td>
</tr>
<tr>
<td></td>
<td></td>
<td>.9</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1.0</td>
</tr>
</tbody>
</table>

More recently Truhlar and Rice (1970) have calculated differential cross-sections for the hydrogen molecule by including a polarization potential, to account for the breakdown of the Born approximation at small angles. The total scattering potential was $V = V_1 + V_2$, where $V_1$ was a first order potential due to the undisturbed hydrogen molecule, and $V_2$ was a second order potential due to the distortion of the electronic charge distribution by the influence of the incident electron.

The potential $V_1$ was calculated by considering the molecule as two spherically symmetric charge distributions centred at the two nuclei. The polarization potential was calculated with the aid of the adiabatic approximation. This assumed that the incident velocity of the electron was sufficiently small for the molecule to have time to fully adjust to the perturbing field (Mohr, 1970). The expression obtained was of the form $-ar^{-4}$,
where $\alpha$ is the dipole moment of the molecule. (The dipole moment of course depends on the direction of the internuclear axis relative to the field).

Although it may be expected that the adiabatic approximation produces useful results at low incident electron energies, it suffers from the defect that if the incident electron penetrates the charge distribution of the molecule, a significant increase in its velocity will be obtained due to the large attractive nuclear potential. Under these circumstances (Truhlar and Rice) the adiabatic approximation will break down.

To rectify the situation non-adiabatic terms were added to the polarization potential. The most significant of these was called the distortion potential. It arose from the inability of the induced dipole moment of the molecule to follow the motion of the electron at small distances of approach. For this reason, the dipole orientation relative to the direction of the incident electron was quite random, resulting in no net polarization at all (Kleinmann, Hahn and Spruch, 1968). The distortion potential is therefore of short range and opposite in sign (i.e. positive) to the polarization potential. Thus, although it had relatively small effect on the total potential at large distances, it conveniently cancelled the polarization potential
at small distances.

Truhlar and Rice also allowed for "some" distortion of the incident electron wave. They claim that this will improve the cross-sections at large angles. It was achieved by expanding the electron wave function in terms of partial waves of angular momentum. Since it may be argued that the $l = 0$ and $l = 1$ partial waves contributed most to the cross-section, the calculations were simplified by only considering distortion in these two terms.

(Note: from the discussion on partial waves in a later section, a correction to the $l = 0$ term is not important at $E > 50$ eV.) A limited distorted wave approximation was therefore produced. Truhlar and Rice also included exchange in their calculations. As pointed out in Chapter 1, the experimental results of Trajmer et al. (1972) were normalized with the aid of the above theory to give absolute cross-sections.

Using a similar procedure, Khare and Shobha (1972) also calculated differential cross-sections of the hydrogen molecule. The polarization potential included both adiabatic and non-adiabatic terms, but the incident electron was treated as a plane wave.

The foregoing calculations together with the present experimental measurements are presented in Figures 5.10 to 5.15. Each
Figure 5.10 The elastic differential cross-section of the hydrogen molecule for incident electrons of 50 eV. The calculations by Truhlar and Rice and Khare and Shobha take into consideration the polarization of the molecule.
Figure 5.11 The elastic differential cross-section of the hydrogen molecule for incident electrons of 75 eV. The calculations by Truhlar and Rice (at 81.6 eV.) take into consideration the polarization of the molecule.
Figure 5.12 Elastic differential cross sections of the hydrogen molecule for incident electrons of 100 e.V. The calculations by Truhlar and Rice and Khare and Shobha take into consideration the polarization of the molecule.
Figure 5.13 Elastic differential cross-sections of the hydrogen molecule for incident electrons of 150 e.V. The calculation by Truhlar and Rice represents the Born approx. without polarization.
Figure 5.14 Elastic differential cross-sections of the hydrogen molecule for incident electrons of 200 e.V. The calculations by Khare and Shobha take into consideration the polarization of the molecule.
Figure 5: Elastic differential cross-sections of the hydrogen molecule for incident electrons of 300 eV, compared with the calculations, which include a polarization potential, by Khare and Shobha and Truhlar and Rice.
data point represented in these graphs was taken from Figure 5.8 and error bars added to give an indication of the accuracy involved. The contributing factors to the total error were estimated to be 6% due to statistical uncertainties in the scattered signal, 5% due to the uncertainty in the number densities of each species in the interaction region, 3% due to variations in the electron gun current over long periods of time and 5% in the helium standards. Other errors (e.g. the source pressure) were expected to be small in comparison to the above. Taking a root mean square total produces an error of approximately 10%. In the case of the 50 eV cross-section a 10% error was allowed for the standard helium cross-section. The reason for this was the significant difference between present measurements on helium and the theoretical curve of La Bahn and Callaway whose energy dependence otherwise appear to agree with the results of Chamberlain et al. and Vriens et al.

The calculations by Truhlar and Rice, although agreeing with the present experimental results at large angles, are consistently too high at small angles suggesting that the polarization potential (even with non-adiabatic terms) overcompensates for the general defect of the Born approximation. The calculations by Khare and Shoba are similarly too steep at small angles. In addition they are generally too high at all angles (except at 300 eV).
SECTION 2. ATOMIC HYDROGEN

5.2.1 INTRODUCTION

The previous method of measuring ratios of cross-sections required a modification here because a pure atomic hydrogen beam was unattainable in practice. The contribution to the scattered signal by the molecular hydrogen component in the beam therefore had to be separated from the atomic hydrogen signal. This separation could be achieved with a knowledge of both the absolute molecular hydrogen and helium cross-sections and the relative number density of the H, H₂ and He particles in the interaction region.

5.2.2 EXPERIMENTAL METHOD

Hydrogen is again passed into the tungsten oven via a needle valve, to produce a neutral beam. As before, the oven pressure was continuously monitored with the Baratron pressure gauge, to ensure a uniform beam strength during the data taking process.

The heating of the hydrogen oven was achieved by passing an alternating current through it (Teubner 1967). Considerable care had to be taken during the heating process to prolong the life time of the tungsten tubes. Rapid expansions or contractions usually resulted in breakages. The life time of a tube
also depended on the temperature at which it was operated. Since the dissociation process increased with temperature a compromise had to be made with the degree of dissociation desired. Temperatures were usually between $2,300^\circ$ K and $2,600^\circ$ K (measured with an optical pyrometer) and the percentage of dissociation between 50% and 60%.

Measurements with the mass-spectrometer were taken as described in Chapter 4. In particular it was found that the number density of particles in a beam could always be reproduced by simply reproducing the source pressure of the beam (provided, of course, that the oven temperature remained constant). The ratio measurements could therefore be made more convenient by performing the mass-spectrometer work on each beam first and then reproducing a desired beam as required. Since oven pressures could be measured to 0.1% accuracy, no significant errors were introduced in this way.

A problem encountered with electron scattering from atomic hydrogen was the low signal to noise ratio. To improve this situation the base pressure in the scattering chamber was reduced to the limit the apparatus allowed, i.e. $2 \times 10^{-7}$ torr. Consequently typical conditions consisted of a source pressure for the beam of 3 torr and an operating pressure in the scattering chamber of $7 \times 10^{-7}$ torr.
5.2.3 **CALCULATION OF H/He CROSS-SECTION RATIOS**

Let the measured number densities of atomic, molecular hydrogen and helium be \( N_H \), \( N_{H_2} \) and \( N_{He} \) respectively. The signal obtained by the electron spectrometer at some scattering angle \( \theta \) was \( S_{H+H_2} \) for the hydrogen beam and \( S_{He} \) for the helium beam. Knowing the ratio of the elastic scattering cross-sections of \( H_2 \) and He, the \( H_2 \) contribution to the total hydrogen signal can be calculated thus:

\[
S_{H_2} = S_{He} \times \frac{N_{H_2}}{N_{He}} \times (R_{H_2/He})_{\theta}
\]

where \((R_{H_2/He})_{\theta}\) is the ratio of the elastic molecular hydrogen and helium cross-section at the angle \( \theta \). Consequently the ratio of the differential cross-section between H and He at the scattering angle \( \theta \) is given by:

\[
\frac{\partial \sigma_H}{\partial \sigma_{He}} = \left( \frac{S_{H+H_2} - S_{H_2}}{S_{He}} \right) \times \frac{N_{He}}{N_H}
\]

5.2.4 **ANGULAR DISTRIBUTIONS**

It was originally decided to generate angular distributions for atomic hydrogen by taking ratio measurements along the entire angular range. However due to the rather short life times of the tungsten tubes, this method was not practical. So instead,
ratio measurements were only taken at 20° and 40° and the angular range of the resulting cross-sections extended another 10° to 20° by measuring angular distributions of the atomic and molecular hydrogen mixture. These angular distributions were then compared to those of molecular hydrogen. It was found that at least over a limited range of angles these two angular distributions agreed. Consequently it could be concluded that the atomic hydrogen differential cross-sections were very similar in shape to the cross-sections of the molecule (at least over the range of angles presented here).

Comparisons of the angular shapes with angular distributions published by Tai et al. (1969) appear to agree very well.

5.2.5 ERROR ESTIMATION

In addition to errors discussed for the hydrogen molecule cross-sections, the main sources of error were obtained from

(a) the lower signal to noise ratio, making the statistical uncertainties larger, and

(b) an extra error from the determination in the number densities in the interaction region.

It was expected that these factors would add another 10% to the total error. Consequently the possible error was taken as 15%
Figure 5.16 The experimental atomic hydrogen cross-sections. The estimated possible error is 15% except at 50 eV, where it is ≈ 20%.
(root mean square addition). The 50 eV results are given as 20% accurate. The elastic H cross-sections are shown in figures 5.16 to 5.20.

5.2.6 THEORETICAL CROSS-SECTIONS FOR THE HYDROGEN ATOM.

THE CLOSE COUPLING APPROXIMATION

As already mentioned in Chapter 1, the truncated eigen-function expansion may be improved by making an approximate correction for the truncated terms.

Bransden and Coleman (1972) and Bransden et al. (1972) have made calculations, using such a method, for both elastic and inelastic differential cross-sections. Their procedure was to expand the total wave function \( \Psi \) in terms of eigenfunctions of the unperturbed target,

\[
\Psi (r, x) = \sum_n \phi_n (r) F_n (x)
\]

where \( r \) refers to the target electron \((s)\) and \( x \) to the incident electron coordinates.

The summation also includes the continuum states. Inserting this into the Schrödinger equation and rearranging, the set of coupled equations can be written in the form,

\[
(\mathcal{W}^2 + \mathcal{k}_n^2) F_n (x) = 2\sum_m V_{nm} (x) F_m (x)
\]
Figure 5.17 The differential atomic hydrogen cross-section at 50 eV compared to various theories and the expt. by Teubner et. al. The Born, Glauber and Schulz calculations merge at large angles.
Figure 5.18 The experimental 75 eV. differential H cross-section compared with the Born theory and the calculations by Schulz.
Figure 5.19 The differential atomic hydrogen cross-section at 100 eV compared with various calculations. The theories of Born, Glauber and Schulz merge at large angles.
Figure 5.20 The experimental differential $\dagger$ cross-section at 200 e.V. is compared with various calculations.
where $V_{nm}(x) = \int \phi_n^*(x) \, V(x, \xi) \, \phi_m(x) \, d\xi$.

This infinite set of coupled integro-differential equations is then terminated to a convenient number, say $N$. The set of equations referring to $n > N$ are modified in such a way that the $\phi_m$ in the equation for the potential are restricted to $m \leq N$ and at the same time the eigen-energies of the target of the states $n > N$ are substituted by some average value.

The authors proceed by setting

$$F_n(x) = \exp(ikp \cdot x) \, f_n(x)$$

Thus the $F_n(x)$, which describe the incident and scattered waves, are considered as a plane wave multiplied by a modulation factor, in a similar approach to that used by Glauber. However, here, instead of making a small angle approximation, the terms in $\nabla^2 f_n(x)$ are neglected. Since the scattering from light atoms is weak, $f_n(x)$ will vary only slowly (as argued by Glauber) consequently $\nabla^2 f_n(x)$ will be smaller than terms such as $V \, f_n(x)$.

In general it was therefore expected by Bransden et al. that this theory will provide more reliable results at larger angles.

The calculations by Bransden et al. are compared with the present experimental measurements in Figures 5.17, 5.19 and 5.20. It is seen that although the correct shapes are obtained, the
cross-sections are too large.

5.2.7 GLAUBER THEORY

The Glauber theory has been introduced in Chapter 1. It is an eikonal approximation which, in quantum mechanical potential scattering, give the solution to the wave equation in terms of path integral along the geometric rays perpendicular to the wave fronts; valid at short wavelengths (Goldstein, 1959).

In representing the total electron wave function by a plane wave modulated by some slowly varying function \( \phi \), allowance has been made for the distortion of the incident wave by the target atom. For elastic scattering the atom is considered to remain unperturbed.

The total and scattered waves are given by (Chapter 1):

\[
\psi(\mathbf{r}) = e^{i \mathbf{k} \cdot \mathbf{r}} + g(\mathbf{r})
\]

and

\[
g(\mathbf{r}) = \frac{-2m}{4\pi\hbar^2} \int \frac{\exp(i\mathbf{k}|\mathbf{r}-\mathbf{r}'|)}{|\mathbf{r}-\mathbf{r}'|} V(\mathbf{r}') \psi(\mathbf{r}') d\mathbf{r}'
\]

Substituting

\[
\psi(\mathbf{r}) = \exp(i\mathbf{k} \cdot \mathbf{r}) \phi(\mathbf{r}),
\]

Glauber obtains the equation

\[
\phi(\mathbf{r}) = 1 - \frac{2m}{4\pi\hbar^2} \int \frac{\exp[(i\mathbf{k}|\mathbf{r}-\mathbf{r}'| - i\mathbf{k} \cdot (\mathbf{r}-\mathbf{r}'))]}{|\mathbf{r}-\mathbf{r}'|} V(\mathbf{r}') \phi(\mathbf{r}') d\mathbf{r}'
\]
By assuming that $V(x)\phi(x)$ varies slowly within a particle wavelength (i.e. a weak potential and high energy particles), then for large differences between $k|x-x'|$ and $k.(x-x')$, the exponential term will oscillate rapidly resulting in a negligible contribution to the integral. Hence the integration may be performed along the incident direction of the particle. And $\phi$ is given (in rectangular coordinates) by:

$$\phi(x,y,z) = 1 - \frac{i}{\hbar v} \int V(x,y,z')\phi(x,y,z') \, dz'$$

where the direction of propagation is chosen to be along the $z$-axis. The solution is given by

$$\phi = \exp\left[-\frac{i}{\hbar v} \int_{-\infty}^{z} V(x,y,z') dz'\right] \quad \ldots(5.1)$$

and hence substituting in the scattering formulae presented in Chapter 1:

$$f(\theta) = \frac{2m}{4\pi \hbar^2} \int \exp(i\mathbf{r} \cdot (\mathbf{k} - \mathbf{k}')) V(r) \exp\left(-\frac{i}{\hbar v} \int_{-\infty}^{z} Vdz'\right) dzd^2b \quad \ldots(5.2)$$

where $d^2b$ is equivalent to $dx$ and $dy$, i.e. the plane of the impact parameters.

Glauber shows how this integral can be evaluated further if the small angle approximation is made that the $\exp[i(k-k').r] \approx \exp[i(k-k').\hat{b}]$, where $\mathbf{r} = \hat{b} + \mathbf{Kz}$ and $\hat{b}$ and $\mathbf{K}$ are perpendicular
and \( k \) is parallel to \( k \). Thus for large impact parameters \( b \) within a finite spherical scattering potential, \( r \) will be approximately equal to \( b \). The scattering amplitude is then given by:

\[
f(\theta) = \frac{k}{2\pi i} \int \exp[i(k-k').b] \left\{ \exp\left[ -\frac{i}{\hbar v} \int (b+kz')dz' \right] - 1 \right\} d^2b
\]

The resultant scattering intensities are plotted in Figures 5.17, 5.19 and 5.20. It is evident that the agreement with experiment extends to much larger angles than may have been expected. This is further discussed in a later sub-section.

5.2.8 OTHER CALCULATIONS

Another eikonal approximation, proposed by Chen et al., has been used to predict elastic atomic hydrogen cross-sections by Sinfailam and Chen (1972). In the first order approximation in their three body multiple scattering expansion, this theory predicts cross-sections more than an order of magnitude too large (for \( 50 \text{ eV} \leq E \leq 200 \text{ eV} \)). It has been seriously questioned by Byron and Joachain (1973). As a result, second order terms have also been included in this theory, producing quite reasonable cross-sections. (These are not plotted here, see Chen et al. 1973).

Schulz (private communication, 1973) calculated the differential \( H \) cross-sections using a variational method and included
for the effect of exchange. The results appear to be very good within the present range of angles.

The calculations by Khare and Shobha (also in a private communication, 1973) also agree quite well with the experimental values. Their work has not as yet been published.

It is particularly remarkable how well the Born approximation agrees with experiment. The agreement is very accurate provided the scattering angle \( \theta > \theta_o \), where \( \theta_o \) depends on the electron energy.

5.2.9 GENERAL DISCUSSION

Consider the scattering amplitude for elastic scattering as presented in Chapter 1.

\[
f(\theta) = \frac{-m}{2\pi\hbar^2} \int \exp(-ik\cdot\mathbf{r}) V(\mathbf{r}') \psi(\mathbf{r}') \, d^3\mathbf{r}'
\]

In order to simplify this integral, an approximation has to be made in either the representation of the wave function \( \psi \) or the potential \( V \), or both. For example, in the first Born approximation, \( \psi \) is represented by a plane wave and \( V \) by the static potential set up by the target atom in its ground state. More sophisticated treatments consider some kind of distortion occurring in either the target or the incident wave. The success of
one or other of these approximations will then indicate important features of the scattering process.

A distortion of the electron cloud (of the atom) may be treated by including a polarization term in the expression for the potential. Alternatively the excitations of the target electrons, during the scattering process, may be taken into consideration in the scattering formulae (e.g. 2nd Born approximation, Moiseiwitsch and Smith, 1968). However considering the poor agreement between experimental measurements and the calculations by Truhlar and Rice, which included a polarization potential, it is not clear whether polarization plays an important role for elastic scattering at energies greater than 50 eV. [Note: For inelastic scattering (Massey and Mohr, 1933) polarization is expected to be important at all energies since the atom is always "disturbed" during an inelastic event].

Allowance for the distortion of the incident electron wave is made in the Glauber approximation. For elastic scattering, the atom is treated as a static spherically symmetric potential. The success of this theory demonstrates the importance of the distortion to the incident wave for small angle scattering.

Of particular interest is the unexpected validity of the Glauber approximation at large angles. Similarly the Born
approximation, which has been considered as a small angle approximation (Mott and Massey 1965, and explained later) gives good agreement with experiment at large angles.

5.2.10 COMPARISON OF THE BORN AND GLAUBER THEORIES

It has been shown by Moore (1970) that the Glauber scattering amplitude for a spherically symmetric potential may be expanded to give a series with the first term equal to the first Born approximation plus higher order terms. Consequently it may be expected that in an energy region where the first Born approximation provides reasonable cross-sections, the Glauber approximation must also produce reasonable results.

An attempt is now made to show the similarity between the Born and Glauber theories more clearly. Consider the scattering amplitude for the Glauber approximation as expressed by equation 5.2. Making the small angle approximation (see Section 5.2.3)

\[ \exp[i(k-k') \cdot x] \approx \exp[i(k-k') \cdot b] \]

this equation can be written in the form

\[ f(\theta) = \frac{-2m}{4\pi \hbar^2} \int \exp[i(k-k') \cdot b - \frac{iF(b,z)}{\hbar v}] V \, dz \, d^2b \quad (5.3) \]

where

\[ F(b,z) = \int_{-\infty}^Z V(b,z') \, dz' \]
Now an assumption made in deriving the Glauber approximation is that \( \phi \) is close to unity and varies only slowly in a distance \( \lambda \) (the wavelength of the incident electron). Therefore \( \frac{F(b, z)}{h \nu} \) is also slowly varying and small compared to unity (see equation 5.1). This assumes that \( b \) is sufficiently large (an assumption made in deriving the Glauber approximation and discussed below) so that we are dealing with a region in which the potential is weak so that \( \frac{1}{h \nu} \int V dz' \) is much smaller than \((k-k') \cdot b\) for intermediate and large scattering angles (e.g. for \( \theta \geq 30^\circ \) this condition is satisfied in the present energy range). Consequently \( -\frac{iF}{h \nu} \) may be neglected in equation 5.3 and the Glauber approximation rewritten as,

\[
\begin{align*}
\frac{f(\theta)}{(\theta \text{ large})} & = -\frac{-2m}{4\pi^2} \int \exp[i(k-k') \cdot b] V dz' \, dz^2 b
\end{align*}
\]

But this expression can be shown to be the scattering amplitude of the Born approximation (Moore 1970) for a spherically symmetric potential.

For small angles where \((k-k') \cdot b \approx \frac{F}{h \nu}\), the exponential term in equation 5.3, will oscillate less rapidly (as compared with the exponential in the Born theory), therefore increasing the contribution to the scattering amplitude at these angles. Therefore the Glauber theory will predict a larger cross-section than the
Born theory, at small scattering angles and will become essentially identical to the Born theory at larger angles.

The justification for considering only "sufficiently large" values of $b$ in the above argument is that the potential near the nucleus in an atom can, to a very good approximation, be represented by a Coulomb potential. It is known (Gerjouy, Massey and Burhop, Williams, 1945) that for scattering from a Coulomb potential, both the Glauber and Born approximations give the correct scattering amplitude.

A comparison of the Coulomb potential and the hydrogen atom potential is given in Figure 5.21 and Appendix V.

5.2.11 LARGE ANGLE SCATTERING

(MOTT AND MASSEY 1965, MASSEY AND BURHOP, 1952)

Consider the Born approximation as expressed in the equation by Mott (Chapter 1)

$$f(\theta) = \frac{q^2}{2mv^2} (Z - F(\theta)) \csc^2 \left(\frac{1}{2} \theta\right)$$

where

$$F(\theta) = 4\pi \int_0^\infty p(r) \frac{\sin(2kr \sin^2 \theta)}{2ksin \frac{1}{2} \theta} rdr$$

and $k$ is the wave number,
Figure 5.21 A comparison of the H-atom and coulomb potentials.
\[ \rho(r) = \text{charge distribution of the electrons.} \]

For large scattering angles, \(\sin(2kr \sin \frac{1}{2} \theta)\) will oscillate rapidly over the smoothly varying charge distribution of the electrons, therefore reducing the integral to a small value.

To show this more convincingly, the expression for the atom form factor \(F(\theta)\) has been evaluated in Appendix IV and the range of angles given for which a contribution of \(\leq 10\%\) is obtained. The large angle scattering in the Born theory is therefore predominantly nuclear scattering. The same is also true for the Glauber theory, Gerjouy (1971). As a consequence (due to the special properties of the Coulomb potential) both the Glauber and Born approximations are expected to provide accurate cross-sections at large angles.

5.2.12 THE SCATTERING CROSS-SECTIONS AT INTERMEDIATE ANGLES

(I.E. \(30^\circ \leq \theta \leq 80^\circ\))

It has been shown that large angle scattering is adequately dealt with by the Born theory (a consequence of the unique property of the Coulomb potential, Williams 1945) provided, of course, that the general validity condition for the Born theory is satisfied (i.e. the scattering is weak). In the present energy range this would only apply to hydrogen and helium atoms. For the same reason the Glauber theory also produces the correct large
angle scattering intensities (Gerjouy 1971). The "Coulomb" scattering cross-section (i.e. scattering by a proton) are plotted in Figures 5.17 to 5.20.

It now remains to be shown why both the Born and Glauber approximation provide such accurate results for the intermediate range of angles, since both are expected to produce satisfactory results only at small angles. To clarify the situation, consider the scattering amplitude in terms of phase shifts of the incident wave which is conveniently divided into partial waves of angular momentum for this purpose (Mott and Massey, 1965, Schiff, 1955, Eisberg 1961). The scattering amplitude is given by,

$$ f(\theta) = \frac{1}{2ik} \sum_{\ell=0}^{\infty} (2\ell + 1) [e^{2in_\ell} - 1] P_{\ell} (\cos \theta) $$

...(5.4)

where $\eta_\ell$ is the phase shift of the $\ell^{th}$ partial wave

and $P_{\ell}$ is the $\ell^{th}$ Legendre polynomial.

The phase shifts can be calculated with the formulae,

$$ e^{2in_\ell} \sin 2\eta_\ell = -\frac{2mk}{\hbar^2} \int_0^\infty V(r)R_\ell (r) j_{\ell} (r)r^2 dr $$

...(5.5)

where $j_\ell$ are the radial wave functions for the partial waves without the presence of the potential

and $R_\ell$ the radial wave functions in the presence of the potential.
By setting \( R_\ell \) equal to \( j_\ell \) and replacing the L.H.S. by \( 2\eta_\ell \) the phase shifts as used in the Born approximation (Schiff) are obtained,
\[
i.e. \quad 2\eta_\ell = - \frac{2\hbar k}{\hbar^2} \int V(r) \, (j_\ell (r))^2 \, r^2 dr
\]
In particular it is possible to write the Born approximation in terms of partial wave phase shifts,
\[
f(\theta) = \frac{1}{2k} \sum \ell (2\ell+1) \, 2\eta_\ell \, P_\ell (\cos \theta)
\]
Thus the approximations made in the Born theory are that \( (e^{2i\eta_\ell} - 1) = 2i\eta_\ell \) and \( R_\ell = j_\ell \).

For an attractive potential the radial wave function \( R_\ell \) will contribute more to the integral (because the wave is "pulled in" towards the nucleus so that \( R_\ell \) will be larger than \( j_\ell \) in a region where \( V(r) \) is very large - Eisberg), therefore the Born phase shifts will in general be smaller than the correct values.

Considering the hydrogen atom, the correct phase shifts are sufficiently small (within the energy range considered here) for the above approximation of the Born theory to produce phase shifts correct to about 20%. Since the phase shifts decrease with increasing \( \ell \), the "Born phase shifts" become more accurate
at large $\ell$. Therefore it is expected (Mott and Massey) that at a sufficiently high energy where many partial waves contribute to the value of $f(\theta)$, the more accurate (i.e. smaller) phase shifts corresponding to large $\ell$, will dominate the cross-section. This will occur particularly at small scattering angles, where the $P_{\ell}(\cos \theta)$ are all of the order of unity, as seen from Figure 5.22. For intermediate scattering angles the $P_{\ell}(\cos \theta)$ values become smaller and alternate in sign, causing a considerable amount of cancelation among the higher $\ell$ contributions in the expression for $f(\theta)$ (equation 5.4). (Note: It is for this reason that the Born theory is expected to produce the best results at small angles).

However, although $(e^{2i\eta} - 1)^2$ is not a good approximation to $(2\eta)^2$ for angles as large as obtained for the $\ell = 0$ phase shift in atomic hydrogen at 50 eV, and $R_{\ell}$ is a similarly poor approximation for $j_{\ell}$, at this energy, these two inaccuracies have the effect of cancelling each other. For example taking

$$|e^{2i\eta_0} - 1|^2 = |2\eta_0(B)|^2$$

where $\eta_0 =$ correct $\ell = 0$ shift

$\eta_0(B) =$ "Born phase shift"

will only introduce an error of approximately 10% for 50 eV electron scattering and 2% at 100 eV.

The above argument becomes less accurate if the incorrect
Figure 5.22 Zonal harmonics, $P_l(\cos \theta)$, for $l = 0, 1, 2, 3$. 
$l = 1$ and $l = 2$ contributions are also added into the expression for the scattering intensity. Therefore the Born theory will be most accurate at angles where much cancellation occurs among the $l = 1, 2, 3 \ldots$ contributions to $|f(\theta)|^2$. For example, at 50 eV, the $l = 1, 2, 3 \ldots$ contribution to $|f(\theta)|^2$ between $60^\circ$ and $70^\circ$ will be negligibly small while at $\theta = 0^\circ$ the contribution will be greater than from the $l = 0$ partial wave.

At higher energies the above arguments will become even more applicable, so that the Born approximation (and hence the Glauber approximation which is identical with it at intermediate and large angles) will provide essentially the exact scattering intensities at these angles.

(Note: From the foregoing arguments a plane wave approximation seems to be quite sufficient to provide accurate scattering intensities at these energies and angles for hydrogen and helium atoms).

It is also interesting to observe the effect of exchange on the scattering amplitude, which as shown by Mott and Massey (1965), introduces another term in the expression of the total wave function for the collision process. This "scattered wave due to electron exchange", appears to improve the phase shifts in the partial waves, as obtained from equation 5.5, thereby improving
the small angle scattering intensities (e.g. Figures 5.17, 5.18).

The variation calculation by Schulz which also gives excellent agreement can probably be explained in the same way.

These arguments would indicate a great sensitivity of the elastic cross-sections at small angles to the introduction of extra scattered waves in the expression for the wave function. Thus, the real test for any theory to predict the correct scattering intensities (for small atoms or molecules) at energies between 50 eV and 300 eV occurs at small angles. Predictions at larger angles by Born type approximations are insensitive to the details of the scattering process and, as in the case of the Glauber theory, give good results without being applicable there.

5.2.13 INELASTIC DIFFERENTIAL CROSS-SECTIONS

The method of measuring ratios between cross-sections was particularly suited to inelastic scattering because it was now possible to distinguish between electrons scattered from atomic and molecular hydrogen. As a result ratios of cross-sections between atomic hydrogen and helium were obtained directly without the need to estimate the signal contribution from molecular hydrogen. This removal of a source of error compensated for the increase in statistical uncertainties due to the much reduced count rate.
Ratios were measured between the unknown inelastic cross-sections of atomic hydrogen and the known elastic helium cross-sections, used previously. Since inelastic helium cross-sections of absolute value were also available (Opal and Beaty, 1972) Chamberlain et al. 1970) a check could therefore be made on the method of ratio measurements to predict inelastic cross-sections. That is, ratios between the elastic and inelastic helium cross-sections were measured and a comparison made with the published cross-sections. The agreement was found to be very good.

The only inelastic cross-sections of atomic hydrogen and helium which could be measured with this apparatus were the combined excitation cross-sections of the n = 2 state. This limitation was determined by the resolution of the equipment.

5.2.14 THE ENERGY LOSS-SPECTRA OF HYDROGEN AND HELIUM

As the absolute resolution of the spectrometer depended on the incident electron energy (as explained previously), the peak widths increased with energy. Consequently it was expected that for some energy E, the resolution would be insufficient to detect even the combined 2S and 2p states, in the hydrogen atom.

Energy loss spectra for hydrogen (both H$_2$ and a mixture of H and H$_2$) and helium are shown in Figures 5.23 and 5.24. The H
Figure 5.23 The energy loss spectrum of molecular hydrogen and helium. The incident electron energy is 100 eV.
Figure 5.24 The energy loss spectrum of a partially dissociated hydrogen beam for incident electrons of 50 eV, 100 eV, and 200 eV.
peak for the $n = 2$ states was only just resolved from the molecular hydrogen ($b^3 \Sigma_u^+$) peak at an energy of 200 eV.

A characteristic of the molecular hydrogen spectra was the continuum due to the rotational and vibrational states of the molecule at the higher energy loss side of the peak. These states unfortunately overlapped with the $n = 2$ states of helium. Thus if ratio measurements between the inelastic events of $H$ and $H_e$ were to be measured, the hydrogen and helium beams had to be kept separate. Under these circumstances it was easier to take ratios with the elastic helium cross-sections, particularly considering the larger count rates obtained.

5.2.15 EXPERIMENTAL PROCEDURE

The determination of number densities in the interaction region was again performed with the mass-spectrometer.

To ensure that no contribution to the scattered signal from the molecular hydrogen $b^3 \Sigma_u^+$ state was added to the data, an energy loss spectrum from a pure molecular hydrogen beam was always taken before a ratio measurement was attempted and the channel number of the recorder in which the first significant entry had been made, carefully noted. Hence with identical settings on the data recorder and electron spectrometer (i.e. the staircase function
generator voltage) the atomic hydrogen peak could be terminated exactly where the first contribution to the molecular peak started. The truncated part of this peak could then be reconstructed from symmetry.

To overcome the vast difference in the count rates between the elastic and inelastic scattering cross-sections, measurements for the inelastic scattering events were taken at 20° while for the elastic an angle of 50° or 60° was usually chosen. Ratios could then be calculated with the aid of elastic angular distributions which were accurately known in this range of angles.

5.2.16 VARIATION IN THE DETECTION EFFICIENCY WITH ELECTRON ENERGY

The results of Section 5.1.5 showed that the electron multiplier efficiency decreased with increasing electron impact energy above about 200 volts. Thus a decrease in electron energy of 10 volts would have increased the count rate by some 5% at the impact energies used. Conversely, the decreased transparency of the electron spectrometer when analyzing electrons of reduced energy (by 10V) was 10%, 7% and 5% respectively for 50 eV, 100 eV and 200 eV electrons. These two effects therefore approximately cancelled each other and only a small correction was required.

The errors in these measurements were similar to those
previously discussed. Statistical uncertainties were however higher. It was estimated that the total error was between 15% and 20% except for the 50 eV measurements, which were, as before, a little higher.

5.2.17 RESULTS AND DISCUSSION

Having thus measured the absolute differential cross-sections (for 50 eV, 100 eV and 200 eV electrons) at one angle, an extension to other angles was achieved with the angular distributions measured by Williams (1968). The results are shown in Figure 5.25.

Both the Born and Glauber theories are again plotted for comparison with experiment (Figures 5.26, 5.27). The Born theory is seen to fail badly for all but the small angles. This is because for inelastic scattering the first Born theory only consists of electron-electron interactions. The interaction with the proton is eliminated due to an orthogonality property of the wave functions concerned (Moiseiwitsch and Smith 1968, Gerjuoy 1971). It is generally considered that the large angle inelastic scattering consists of two processes: firstly an inelastic interaction with the bound electron (which only causes small deflections) and secondly an elastic deflection by the nucleus (Gerjuoy 1971). This hypothesis is supported by the fact that both
Figure 5.25 The excitation cross-sections of atomic hydrogen to the combined 2s and 2p states. The points of normalization (at 20°) are indicated. The angular distributions are those of Williams.
Figure 5.26 The experimental excitation cross-section to the $n=2$ state of atomic hydrogen at 100 eV compared with theory.
Figure 5.27 Excitation cross-sections for the $n = 2$ state in atomic hydrogen at 50 e.V. and 200 e.V.
elastic and inelastic angular distributions are very similar at large angles.

The Glauber theory for inelastic scattering is obtained by (Gerjuoy 1971) a folding of the static potential scattering amplitude between the initial and final bound states.

Although the agreement with experiment is better than for the Born theory (the electron-nucleus interaction does not drop out of the equation in the Glauber approximation) it is by no means satisfactory for the 50 eV and 100 eV cross-sections.

A close coupling calculation by Scott (1969 in thesis by Williams) for 50 eV electrons is however in excellent agreement (both in absolute value as in shape) with experiment.

The calculations by Bransden et al. (1972) neither give the correct absolute values nor shapes for the differential cross-sections at 50 eV and 100 eV.

SECTION 3

5.3.1 EXTENSION OF THE ABSOLUTE CROSS-SECTION MEASUREMENTS TO NEON, ARGON AND KRYPTON

Although the mass-spectrometer was not suitable for measuring number densities of Neon, Argon and Krypton, the previous
method could nevertheless be extended to accommodate these atoms. The method relied on predicting number densities with the aid of the source pressure of each neutral beam. Indeed, provided that the source pressure is low enough so that the mean free path within the source is larger than the exit slit width, Ramsey's equation suggests the validity of such a prediction. To determine how closely Ramsey's equation was followed, the mass-spectrometer signal was monitored as a function of the source pressure, keeping all other parameters constant. It was found that between one half and five torr, the signal variation with the source pressure was for the present purpose sufficiently close to linear. Consequently source pressures were always kept below 5 torr and the ratio of the number densities in the interaction region between two species of gas, became the ratio of their source pressures.

5.3.2 RESULTS AND DISCUSSION

Results are shown in Figures 5.28, 5.29 and 5.30 together with other measurements (see Chapter 1) and in particular the theory by Furness and McCarthy (1973, and also by private communication. These authors requested these measurements due to the lack of reliable absolute cross-sections for the rare gases). Their method made use of an optical potential which consisted of terms representing the ground state potential (with an exchange
Figure 5.28 The differential cross section of neon at a scattering angle of 40°. The possible errors are indicated.
Figure 5.20 The differential cross-section of argon at scattering angle of 40°. The possible errors are indicated.
Differential cross-section at 40° (in units $a_0^2/s.r.$)

Figure 5.30: The differential cross-section of krypton scattering at 40°. Possible errors are indicated. There are no other absolute cross-sections for comparison.

Electron energy (eV)

0 100 200
term included), a polarization potential and a short range complex potential for the virtual excitations which may occur during the scattering process.
APPENDIX I

THE AUTOMATED LIQUID AIR FILLER SYSTEM

To keep the cold traps above the diffusion pumps at the temperature of liquid air, a filler system was constructed which pumped liquid air to each trap if it became empty. The electronics necessary, is described below.

Two temperature sensors were each positioned near the top and the bottom of the trap respectively. The best sensors available were 91 Germanium diodes. To cause the filler system to stop pumping liquid air when the top sensor became "cold" and to restart when both sensors were "warm", a memory unit in the form of an R.S. flip-flop was required. The electrical circuit is shown in Figure (a), the truth table in Figure (b). Suppose that to turn on the liquid air, A and B where high (corresponding to warm sensors), then

(1) \( R = 0, \ S = 1 \)

\[ \therefore \quad Q = 1 \quad \text{(i.e. high to turn switch on)} \]

later  

(2) \( B \rightarrow 0, \ \text{i.e.} \ A = 1, \ B = 0 \)

\[ \therefore \quad R = 0, \ S = 0 \]

\[ \therefore \quad Q = 1 \quad \text{(i.e. switch still on)} \]

then  

(3) \( A \rightarrow 0, \ \text{i.e.} \ A = 0, \ B = 0 \)
\[ R = 1, S = 0 \]
\[ Q = 0 \] (liquid air pumping is stopped).

if \( A \rightarrow 1 \) (i.e. one sensor warming)
\[ R = 0, S = 0 \]
\[ Q \text{ remains } = 0 \]

but when \( B \rightarrow 1 \) so that both sensors are warm
i.e. \( B = 1, A = 1 \)
then \( R = 0, S = 1 \)
\[ Q = 1 \text{ and liquid air will be pumped again.} \]
Figure (a)

R.S. FLIP-FLOP

TRUTH TABLE FOR
A NOR GATE.

TRUTH TABLE FOR
R.S. FLIP-FLOP.
APPENDIX II

According to Green, the equation governing a vacuum system
of volume $V$, being pumped with speed $S$ while a leak $L$ is present,
is given by:

$$\frac{dp}{dt} = \frac{L}{V} \frac{pS}{V} = \text{L in pressure x Vol/sec}$$

The time constant of the system is given by $V/S$. Hence re-
arranging the above

$$\frac{dp}{dt} = \frac{L}{S} \frac{S}{V} \frac{pS}{V} = \tau = \text{time constant}$$

$$\tau = \frac{L}{S} \frac{(p)}{/}\tau$$

hence

$$\frac{dp}{dt} = \frac{dt}{\frac{(L}{S} - p)} \tau$$

Integrating,

$$\ln (\frac{L}{S} - p) = \frac{t}{\tau} + K$$

$$\rightarrow -Ke^{-t/\tau} = \left(\frac{L}{S} - p\right)$$

at $t = 0, -K = \left(\frac{L}{S} - p_0\right)$ (where $p_0 = p(t)$ at $t=0$)

Hence when a gas beam enters the chamber,
\[ p(t) = \frac{L}{S} + \left( p_0 - \frac{L}{S} \right) e^{-t/\tau} \]  
\[ \ldots (1) \]

And when the gas beam is switched off,

\[ \frac{dp'}{dt'} = \frac{L'}{S} - \frac{p}{v} \]

and \[ p'(t' = 0) = p_1 \]

(performing the primed symbols refer to the "beam off" condition).

\[ \text{hence } p'(t') = \frac{L'}{S} + \left( p_1 - \frac{L'}{S} \right) e^{-t'/\tau} \]  
\[ \ldots (2) \]

Now the condition \( p(t) = p'(t') \) must be satisfied when \( t = T \) 
and \( t' = 0 \), where \( T \) is the half-period of the beam modulation.

\[ \therefore \frac{L}{S} + \left( p_0 - \frac{L}{S} \right) e^{-T/\tau} = \frac{L}{S} + \left( p_1 - \frac{L}{S} \right) e^{-T/\tau} \]

\[ \text{gives } p_1 = \frac{L}{S} + \left( p_0 - \frac{L}{S} \right) e^{-T/\tau} \]  
\[ \ldots (3) \]

\[ \text{Similarly } \]
\[ p_0 = \frac{L'}{S} + \left( p_1 - \frac{L'}{S} \right) e^{-T/\tau} \]  
\[ \ldots (4) \]

Obtaining the expressions (3) and (4) independent of \( p_0 \) and \( p_1 \).

\[ p_1 = \left( \frac{L}{S} + \frac{L'}{S} e^{-T/\tau} \right) / 1 + e^{-T/\tau} \]
and \[ p_0 = \left( \frac{L'}{S} + \frac{L}{S} e^{-T/\tau} \right) / 1 + e^{-T/\tau} \]

Now obtaining \( p(t) \) and \( p'(t') \)

\[
p'(t') = \frac{L'}{S} + \left( p_1 - \frac{L'}{S} \right) e^{-t'/\tau} = \frac{L'}{S} + \frac{L + L' e^{-T'/\tau}}{1 + e^{-T/\tau}} - \frac{L'}{S} e^{-t'/\tau}
\]

\[
p'(t') = \frac{L'}{S} + \left( \frac{L}{S} - \frac{L'}{S} \right) \frac{e^{-t'/\tau}}{1 + e^{-T/\tau}}
\]

Similarly,

\[
p(t) = \frac{L}{S} + \left( \frac{L}{S} - \frac{L'}{S} \right) \frac{e^{-t/\tau}}{1 + e^{-T/\tau}}
\]

Subtracting \( p'(t') \) from \( p(t) \) and putting \( t = t' \) (i.e. the window will be placed in the same position during both half-cycles to get \( \Delta Q \), the difference in signal between the "beam on" and "beam off" conditions.

\[ \therefore \Delta Q = p(t) - p'(t') \]

\[
= \left( \frac{L}{S} - \frac{L'}{S} \right) + \frac{e^{-t/\tau}}{1 + e^{-T/\tau}} \left[ \frac{L'}{S} - \frac{L}{S} - \frac{L}{S} + \frac{L'}{S} \right]
\]

\[ \therefore \Delta Q = K \left[ 1 - \frac{2 e^{-t/\tau}}{1 + e^{-T/\tau}} \right] \quad \text{(putting} \left( \frac{L}{S} - \frac{L'}{S} \right) = K) \]
By taking the two special cases, \( t = \frac{T}{2} \) and \( t = 0 \),

\[
\Delta Q \left( \frac{T}{2} \right) = K \left( 1 - \frac{2e^{-T/2\tau}}{1+e^{-T/\tau}} \right) \quad \ldots(5)
\]

and

\[
\Delta Q \ (t=0) = K \left( 1 - \frac{2}{1+e^{-T/\tau}} \right) \quad \ldots(6)
\]

Dividing (5) by (6),

\[
\frac{\Delta Q \left( \frac{T}{2} \right)}{Q(t=0)} = \frac{e^{-T/2\tau} - 1}{e^{-T/2\tau} + 1}
\]

This ratio was equal to -0.17 (\( \Delta Q(t=0) \) being negative).

Hence \( \tau \approx 150 \text{ milli-seconds} \).
APPENDIX III

Suppose the ions are launched with initial kinetic energy $T$ and velocity $v$, into a uniform electrostatic field $E$. The direction of the electrostatic field $E$ is parallel to the atomic beam path and $v$ makes an angle $\theta$ with it.

Hence we can write,

$$ F = m \frac{d^2x}{dt^2} \quad \text{(x measured along the field direction)}$$

$$ = -Eq \quad \text{(q = ionic charge)}$$

$$ = \frac{-Vq}{S_D} \quad \text{(S_D = distance between the extraction plates and V = voltage difference)}$$

$$ \therefore \frac{d^2x}{dt^2} = \frac{-Vq}{mS_D}$$

$$ \therefore \frac{dx}{dt} = \frac{-Vqt}{mS_D} - K$$

Putting $\frac{dx}{dt}$ = velocity component in the direction field

$$ \frac{dx}{dt} = \left(\frac{2T}{m}\right)^{1/2} \cos \theta, \text{ when } t = 0$$

On further integration,
\[ x = \frac{-Vq t^2}{2mS_D} + \left( \frac{2T}{m} \right)^{1/2} \cos \theta (t) + c \]

since \( x = 0 \) at \( t = 0 \) \( \therefore c = 0 \).

Therefore
\[ x = \frac{-Vq t^2}{2mS_D} + \left( \frac{2T}{m} \right)^{1/2} t \cos \theta \]

It is necessary to find the time taken for an ion produced half way between the extractor plates to travel a distance \( \frac{1}{2} S_D \).
Consequently the lateral spread of such ions may be obtained.

Thus
\[ \frac{Vq}{2mS_D} (t^2) - \left( \frac{2T}{m} \right)^{1/2} \cos \theta (t) + \frac{S_D}{2} = 0 \]

and hence an expression for \( t \) may be found.

If the distance moved by the ions perpendicular to the beam direction, is \( S_p \), then,
\[ S_p = v_p t \]
\[ = \frac{mS_D}{Vq} \left[ \frac{T}{m} \sin 2\theta \pm \left\{ \frac{4T^2}{m^2} \sin \theta \cos \theta \right\}^{1/2} \right] \]

For an extraction voltage of 200 volts and an ion energy of 10 eV, the spread of the ions will be less than 0.3 cm, for all initial angles \( \theta \).
APPENDIX IV

The atom form factor is given by,

$$F(0) = 4\pi \int_0^\infty \rho(r) \frac{\sin K r}{K} \, r \, dr$$

where

$$K = 2k \sin \frac{1}{2} \theta .$$

Putting \( \rho(r) = \frac{Z^3}{\pi a_0^3} e^{-2Kr} \frac{a_0}{a} \)

and letting \( a = \frac{Z}{a} \) for convenience

then

$$F(0) = \frac{4}{a^3 K \pi} \int_0^\infty r e^{-2r/a} \sin K r \, dr$$

Hence integrating by parts

$$F(0) = \frac{4}{a^3 K^2} \left[ -\frac{\cos K r}{K} r e^{-2r/a} \right]_0^\infty + \frac{4}{a^3 K} \int_0^\infty \frac{\cos K r}{K} e^{-2r/a} \, \frac{r}{a} \left[ -2e^{-2r/a} \right] \, dr$$

$$= \frac{4}{a^3 K^2} \left[ \frac{e^{-2r/a}}{(-\frac{2}{a} + K)} \left( -\frac{2}{a} \cos K r + K \sin K r \right) \right]_0^\infty$$
\[- \frac{8}{a^4K^2} \left[ \frac{\sin Kr}{K} \right] \left[ r e^{-2r/a} \right]_{r=0}^{\infty} \]

\[+ \frac{8}{a^4K^2} \int_{0}^{\infty} \frac{\sin Kr}{K} \left[ e^{-2r/a} - \frac{2r}{a} e^{-2r/a} \right] dr \]

Now

\[- \frac{8}{a^4K^2} \int_{0}^{\infty} \frac{\sin Kr}{K} \left[ e^{-2r/a} - \frac{2r}{a} e^{-2r/a} \right] dr \]

\[= \frac{-8}{a^4K^3} \left[ e^{-2r/a} \right]_{r=0}^{\infty} \left[ \frac{2}{a} \sin Kr + K\cos Kr \right] \]

\[- \frac{16}{a^5K^3} \int_{0}^{\infty} e^{-2r/a} \sin Kr \ dr \]

Bringing this last integral back to the R.H.S. and rearranging, then:

\[\frac{4}{a^3K} \int r e^{-2r/a} \sin Kr = \frac{a^2K^2}{(a^2K^2 + 4)} \left[ \frac{2}{a\left(\frac{4}{a^2} + k^2\right)} \right] \]

\[- \frac{8}{a^4K^3} \left[ \frac{-K}{\frac{4}{a^2} + k^2} \right] \]
\[ F = \frac{16}{(4 + a^2 k^2)^2} \]

The angle of scattering where \( F(\theta) \) becomes small compared to unity, (i.e. \( F(0) = \frac{1}{10} \)) can now be found for the case of the hydrogen atom.

Thus \( (4 + a^2 k^2)_0^2 > 160 \)

or \( a^2 k^2 \geq 9 \)

since \( K = 2k \sin \frac{1}{2} \theta \) and \( k = \frac{2\pi m v}{h} \)

then \( \sin \frac{1}{2} \theta \geq \frac{3 \times 10^8}{v} \)

where \( \theta = \) scattering angle

and \( v = \) velocity of incident electron.

Consequently calculating these angles \( \theta_c \)

<table>
<thead>
<tr>
<th>( \theta_c )</th>
<th>Velocity</th>
<th>Energy (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>95°</td>
<td>4.1 x 10^8 cm/sec</td>
<td>50 eV</td>
</tr>
<tr>
<td>75°</td>
<td>5 x 10^8 &quot;</td>
<td>75 &quot;</td>
</tr>
<tr>
<td>62°</td>
<td>5.8 x 10^8 &quot;</td>
<td>100 &quot;</td>
</tr>
<tr>
<td>50°</td>
<td>7.1 x 10^8 &quot;</td>
<td>150 &quot;</td>
</tr>
<tr>
<td>43°</td>
<td>8.2 x 10^8 &quot;</td>
<td>200 &quot;</td>
</tr>
<tr>
<td>35°</td>
<td>10 x 10^8 &quot;</td>
<td>300 &quot;</td>
</tr>
</tbody>
</table>

It should be noted that in the present energy range, it is
not possible to obtain a critical angle $\theta_c$ for other atoms, except for helium. Consequently, the Born and Glauber theories are only expected to give the large angle scattering correctly for the hydrogen and helium atom (N.B. within the present energy range).
APPENDIX V

The screened Coulomb potential of the hydrogen atom is given by (Mott and Massey 1965).

\[ V = - \frac{q^2}{a_0} \left( e^{-2r/a_0} - \frac{a_0}{r} \right) \]

where \( q \) = charge on an electron

and \( a_o \) = Bohr radius

The pure Coulomb potential is given by

\[ V_c = - \frac{q^2}{r} \]

Require \[ [V - V_c] = - \frac{q^2}{r} \left( e^{-2r/a_o} + \frac{r}{a_o} e^{-2r/a_o} - 1 \right) \]

Thus expanding the exponential and only keeping second order terms

\[ (V - V_c) = - \frac{q^2}{r} \left( 1 - \frac{2r}{a_o} + \frac{4r^2}{2a_o^2} \ldots + \frac{r}{a_o} - \frac{2r^2}{a_o^2} \ldots - 1 \right) \]

i.e.

\[ (V - V_c) = \frac{q^2}{a_o} \left( 1 - \frac{4r^2}{3a_o^2} \right) \]

Thus for small \( r \), the atomic potential may be approximated by a Coulomb potential.
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