TRIPLE DIFFERENTIAL CROSS SECTIONS FOR IONIZATION OF HELIUM

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Chapter 4: The ionization of helium by electron impact. Calculations using a correlated wavefunction for the helium ground state.

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ABSTRACT

The first chapter of this thesis is devoted to the development of the theory for the ionization of an atom or ion by electron impact. We have pursued the particular approach adopted by Schiff and derived an expression for the triple differential cross section corresponding to the ionization process. Chapter 2 described alternative treatments of the problem and the various approximate models that have been used for calculations. Included amongst these approximate models is the first Born approximation and it is upon this that the calculations of chapters 3 and 4 are based. These calculations of the triple differential cross section for the ionization of helium by electron impact are restricted to impact energies below 260eV to enable a comparison with the experimental measurements of Ehrhardt et al.

The calculations of Chapter 3 use a simple uncorrelated function to describe the target ground state and constitute a preliminary investigation of the TDC with particular regard to the relative importance of the direct, exchange and capture contributions. The results of these calculations indicate that the capture process makes negligible contribution to the TDC in the energy region considered and it is consequently ignored in the later calculations.

In Chapter 4 the calculations of Chapter 3 are repeated using an accurate 6 configuration C.I. target wave function. The results obtained are compared both with experiment and results of calculations based on other approximate models.

Finally in Chapter 5 we examine a number of points arising from the preceding chapters.

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The calculations described in the thesis were performed by the CDC 6600 computer of the University of London.

CHAPTER I

INTRODUCTION

As atomic and nuclear processes play increasingly important roles in modern technology it becomes essential that such processes be well understood. In particular the current interest in thermonuclear research, plasma physics and the recently developed field of astrophysics necessitates the accurate evaluation of ionization cross-sections of atoms or ions by electron impact. Such cross-sections have been the subject of much theoretical and experimental research in recent years and considerable progress has been made in the determination of accurate data.

With regard to experimental research the large quantity of data available is mainly concerned with the single or multiple ionization of atoms or ions initially in their ground states. Although knowledge of these particular processes is extremely valuable they constitute but a small proportion of the wide range of ionization processes. However, the determination of many of the cross-sections of interest, such as those involving ionization from an excited state, present the experimentalist with immense observational difficulties. In such cases the desired information can only be obtained from a theoretical treatment of the problem.

The aim of the theorist is to evolve, from a mathematical model which faithfully reproduces the characteristic features of the more readily observable processes, a model, within the same framework, capable of predicting the essential features of processes presently outside the scope of the experimentalist. Clearly in order to test the reliability, and so ascertain the predictive value, of a theoretical model, detailed and consistent experimental data is required.

The considerable volume of data available for the single and multiple ionization of atoms and ions in their ground states has been the subject of a review by Kieffer and Dunn (1966).

From the review the fact emerges that there are appreciable differences between some sets of results. The degree of disparity depends upon the species and in the case of helium, the subject of our investigation, produces a 20-30% uncertainty in the cross-sections obtained by averaging the different data. However, although results are not as well defined as one would wish, the salient features of the ionization processes are clearly shown. In view of this present experimental results may be considered to provide a reliable test of theoretical models.

Theoretical calculations of ionization cross-sections are extensive but by no means exhaustive. Here, as in the case of the experimental studies, there exists a degree of conflict since alternative treatments of a problem have produced significantly different results. This is perhaps more understandable because of the approximate nature of the calculations.

Much of the theoretical work has been reviewed by Rudge (1968) who attempted to analyse and assess the validity of the various theoretical models and the assumptions upon which they are founded. The review presents a comprehensive account of the basic approximate methods, both quantal and classical, that have been developed in the field of ionization theory and indicates the degree of success acheived through each approach.

Often there is an energy region where the predictions of several theoretical models are in close agreement, although the models may be appreciably different in structure. Outside this region the predicted cross-sections may rapidly diverge from one another. However, in such cases it is quite usual for the region of disagreement to lie largely outside the range of validity of all the theoretical models. Such behaviour presents one with the problem of distinguishing which model most accurately describes the mechanics of the ionization process. This is particularly true for the high energy region where the behaviour of the ionization cross-section may be equally well reproduced by any one of several models.

For the case of ionization of helium by electron impact there exists a variety of theoretical results (Massey and Mohr 1933, Erskine 1954, Sloan 1964, Inokuti and Kim 1969, Economides and McDowell 1969, Peach 1971) most of which are variations on the first Born formulation. Essentially such models differ by virtue of the treatment afforded to a particular aspect of the problem. For instance the work of Peach is largely concerned with an accurate description of the initial state and the inclusion of the exchange process, whilst the calculations of Economides and McDowell attach greater importance to an improved description of the final state. However in the high energy region, where these models are truly applicable, the predicted cross-sections appear fairly insensitive to the choice of model. The threshold of the region of validity of these approximate treatments is not clearly defined, so although the predictions of the various models may diverge at lower energies this provides no reliable indication of which model is to be preferred.

In spite of the wide variety of calculations made in Born approximation they have all suffered from a common failing. Even after taking due account of the uncertainty in the experimental data, all the calculations have consistently overestimated the cross-section at intermediate energies.

Following the publication of the detailed experimental measurements of the triple differential cross-section (T D C) made by Ehrhardt et al (1972) there has been renewed interest in the theoretical treatment of the problem. Because of the several angular integrations required for the evaluation of the total cross-section it was not previously possible to form a clear picture of how the different angular regions contribute to the cross-section. The TDC data now available provide a critical test of the theoretical models, clearly indicating the points on which they fail. From the characteristic behaviour of the TDC it would seem likely that the general agreement between calculations of the total cross-section based on different variants of the Born approximation is at least in part due to cancellation of errors as a result of the angular integrations.

In the present work the measurements of Ehrhardt et al are compared with calculations based on a first Born formulation in which proper account is taken of all processes contributing to the final state of ionization.

§1 The Scattering Amplitude

In this section we shall develop a formal description of the scattering of a single particle by its interaction with a second particle and then generalise the results to the many body problem. The approach that we shall use is basically that of Schiff (1968).

1.1 The S Matrix approach to Scattering Theory.

The relative motion of the two particles is described by a wave function $\psi(\underline{r},t)$ satisfying the time dependent Schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}\psi(\underline{r},t) = H\psi(\underline{r},t) = [H_0 + V(\underline{r},t)]\psi(\underline{r},t)$$

$$H_0 = -\frac{\hbar^2}{2\mu}\nabla^2$$

where μ denotes the reduced mass of the system and $V(\underline{r},t)$ the interaction potential between the particles.

The Schrodinger equation is characterised by two basic properties. Firstly it is linear in ψ which allows the superposition of solutions. Secondly since it is easily seen that each time derivative of ψ may be expressed in terms of ψ itself then clearly the values of ψ for all $\underline{r}$ at a particular time are sufficient to determine ψ for all $\underline{r}$ at all other times. These properties imply that the quantities $\psi(\underline{r},t_0)$ for a particular time t_0, form a basis set of the vector space to which the $\psi(\underline{r},t)$ belong. It follows that ψ must satisfy a homogeneous integral equation of the form

$$\psi(\underline{r}',t') = i\int G(\underline{r}',t';\underline{r},t)\psi(\underline{r},t)\,d\underline{r} \tag{1.2}$$

where G is the Green's function corresponding to the Hamiltonian H.

It is convenient to split the domain of G, with respect to time, into two distinct parts. For forward propagation in time $(i.e.\ t'>t)$ we define the retarded Green's function

$$\begin{aligned} G^+(\underline{r}',t';\underline{r},t) &= G(\underline{r}',t';\underline{r},t) \qquad & t'>t \\ &= 0 & t'<t \end{aligned} \tag{1.3}$$

and corresponding to backward propagation in time $(i.e.\ t'<t)$ we define the advanced Green's function

$$\begin{aligned} G^-(\underline{r}',t';\underline{r},t) &= -G(\underline{r}',t';\underline{r},t) \qquad & t'<t \\ &= 0 & t'>t \end{aligned} \tag{1.4}$$

Simple manipulations with these two propagators yield the following self evident results.

$$\begin{aligned} G^+(\underline{r}',t';\underline{r},t) &= i\int G^+(\underline{r}',t';\underline{r}_1,t_1)G^+(\underline{r}_1,t_1;\underline{r},t)\,d\underline{r}_1 \ , & t'>t_1>t \\ G^-(\underline{r}',t';\underline{r},t) &= -i\int G^-(\underline{r}',t';\underline{r}_1,t_1)G^-(\underline{r}_1,t_1;\underline{r},t)\,d\underline{r}_1 \ , & t'<t_1<t \\ \delta(\underline{r}-\underline{r}') &= \int G^+(\underline{r}',t;\underline{r}_1,t_1)G^-(\underline{r}_1,t_1;\underline{r},t)\,d\underline{r}_1 & t>t_1 \\ \delta(\underline{r}-\underline{r}') &= \int G^-(\underline{r}',t;\underline{r}_1,t_1)G^+(\underline{r}_1,t_1;\underline{r},t)\,d\underline{r}_1 & t<t_1 \end{aligned} \tag{1.5}$$

In the absence of any interaction between the two particles comprising the system the potential V is identically zero and the time dependent Schrodinger equation reduces to

$$i\hbar\frac{\partial}{\partial t}\psi_0(\underline{r},t) = H_0\psi_0(\underline{r},t) \tag{1.6}$$

$\psi_0(\underline{r},t)$ being the free particle wave function.

If we denote the associated Green's function by G_0 then it may be readily shown to have the form

$$G_0(\underline{r}',t';\underline{r},t) = -i\left[\frac{\mu}{2\pi i\hbar(t'-t)}\right]^{3/2} e^{\frac{i\mu|\underline{r}'-\underline{r}|^2}{2\hbar(t'-t)}} \tag{1.7}$$

The corresponding retarded and advanced Green's functions, G_0^+ and G_0^- respectively, are defined in accordance with (1.3) and (1.4). It is easily seen that these are interdependent since they satisfy the complex conjugate relation

$$G_0^+(\underline{r}',t';\underline{r},t) = G_0^{-*}(\underline{r},t;\underline{r}',t') \tag{1.8}$$

which we shall see may be extended to $G^{\pm}$ provided that the interaction potential V is real.

We shall now examine the interaction problem by means of an approach due to Feynman. Basically we would like to know how the wave function ψ develops between the times t and t' $(t'>t)$ when the interaction potential is present. In order to do this we shall firstly consider V to act only during a finite number of intervals between t and t', denoted by $(t_i, t_i+\Delta t_i, i=1,n)$ with $t_{i+1} > t_i$. Hence in the time interval (t_i, t_{i+1}) initially ψ develops under the influence of both the free particle propagator G_0^+ and the potential V for a time Δt_i and then for the remainder of the interval solely under the influence of the propagator G_0^+. As a consequence of this the function $\psi(\underline{r},t)$ representing the state of the system at the time t, will transform into the corresponding function $\psi(\underline{r}',t')$, for the time t', according to the relation

$$\psi(\underline{r}',t') = \int\ldots\int i\, G_0^+(\underline{r}',t';\underline{r}_n,t_n)\left[1 - \frac{i}{\hbar}V(\underline{r}_n,t_n)\Delta t_n\right]$$
$$i\, G^+(\underline{r}_n,t_n;\underline{r}_{n-1},t_{n-1}) \ldots\ldots\ldots\; iG_0^+(\underline{r}_2,t_2;\underline{r}_1,t_1)\left[1 - \frac{i}{\hbar}V(\underline{r}_1,t_1)\Delta t_1\right]$$
$$i\, G_0^+(\underline{r}_1,t_1;\underline{r},t)\,\psi(\underline{r},t)\,d\underline{r}_n \ldots\ldots\ldots d\underline{r}_1 d\underline{r} \qquad (1.9)$$

this being to first order in Δt_i -

If we now expand the brackets appearing in the integrand and use the result of (1.5) concerning successive applications of the free particle propagator we obtain

$$\psi(\underline{r}',t') = i\int G_0^+(\underline{r}',t';\underline{r},t)\,\psi(\underline{r},t)\,d\underline{r}$$
$$+ \frac{i}{\hbar}\sum_i \iint G_0^+(\underline{r}',t';\underline{r}_i,t_i)V(\underline{r}_i,t_i)\Delta t_i\, G_0^+(\underline{r}_i,t_i;\underline{r},t)$$
$$\psi(\underline{r},t)\,d\underline{r}_i d\underline{r}$$
$$+ \frac{i}{\hbar^2}\sum_{ij} \iiint G_0^+(\underline{r}',t';\underline{r}_i,t_i)V(\underline{r}_i,t_i)\Delta t_i\, G_0^+(\underline{r}_i,t_i;\underline{r}_j,t_j)$$
$$V(\underline{r}_j,t_j)\Delta t_j\, G_0^+(\underline{r}_j,t_j;\underline{r},t)\psi(\underline{r},t)\,d\underline{r}_i d\underline{r}_j d\underline{r}$$
$$+ \ldots\ldots\ldots\ldots \qquad (1.10)$$

At this stage we shall allow the intervals Δt_i to become infinitesimal in size, but infinite in number in such a way that V acts continuously. Then $\sum_i \Delta t_i \rightarrow \int_{t_i} dt_i$

This limiting process leads to the result

$$\psi(\underline{r}',t') = i\int G_0^+(\underline{r}',t';\underline{r},t)\,\psi(\underline{r},t)\,d\underline{r}$$
$$+ \frac{i}{\hbar}\int dt_i \iint G_0^+(\underline{r}',t';\underline{r}_i,t_i)V(\underline{r}_i,t_i)G_0^+(\underline{r}_i,t_i;\underline{r},t)\psi(\underline{r},t)\,d\underline{r}_i d\underline{r}$$
$$+ \frac{i}{\hbar^2}\int dt_i \int dt_j \iiint G_0^+(\underline{r}',t';\underline{r}_i,t_i)V(\underline{r}_i,t_i)\,G_0^+(\underline{r}_i,t_i;\underline{r}_j,t_j)$$
$$V(\underline{r}_j,t_j)\,G_0^+(\underline{r}_j,t_j;\underline{r},t)\,\psi(\underline{r},t)\,d\underline{r}_i d\underline{r}_j d\underline{r}$$
$$+ \ldots\ldots\ldots\ldots \qquad (1.11)$$

Clearly the terms succeeding the first in (1.11) may be arranged in the following way

$$\frac{1}{\hbar}\int dt_i\int G_0^+(\underline{r}',t';\underline{r}_i,t_i)V(\underline{r}_i,t_i)\Big[i\int G_0^+(\underline{r}_i,t_i;\underline{r},t)\psi(\underline{r},t)\,d\underline{r}$$

$$+\frac{i}{\hbar}\int dt_j\iint G_0^+(\underline{r}_i,t_i;\underline{r}_j,t_j)V(\underline{r}_j,t_j)G_0^+(\underline{r}_j,t_j;\underline{r},t)\psi(\underline{r},t)\,d\underline{r}_j\,d\underline{r}$$

$$+\;\dots\dots\dots\Big]\,d\underline{r}_i$$

from which it is clear that the series expansion of (1.11) is in fact repeated within itself. Hence provided that the series converges we may reduce the expression contained in equation (1.11) to the following form

$$\psi(\underline{r}',t') = i\int G_0^+(\underline{r}',t';\underline{r},t)\,\psi(\underline{r},t)\,d\underline{r}$$

$$+\frac{1}{\hbar}\int dt_i\int G_0^+(\underline{r}',t';\underline{r}_i,t_i)V(\underline{r}_i,t_i)\psi(\underline{r}_i,t_i)\,d\underline{r}_i \tag{1.12}$$

Similarly we can evolve a series expansion form of the propagator G^+, for comparison of equations (1.2) and (1.11) yields the result

$$G^+(\underline{r}',t';\underline{r},t) = G_0^+(\underline{r}',t';\underline{r},t)$$

$$+\frac{1}{\hbar}\iint G_0^+(\underline{r}',t';\underline{r}_i,t_i)V(\underline{r}_i,t_i)\,G_0^+(\underline{r}_i,t_i;\underline{r},t)\,dt_i\,d\underline{r}_i$$

$$+\frac{1}{\hbar^2}\iiiint G_0^+(\underline{r}',t';\underline{r}_i,t_i)V(\underline{r}_i,t_i)G_0^+(\underline{r}_i,t_i;\underline{r}_j,t_j)$$

$$V(\underline{r}_j,t_j)\,G_0^+(\underline{r}_j,t_j;\underline{r},t)\,dt_i\,d\underline{r}_i\,dt_j\,d\underline{r}_j$$

$$+\;\dots\dots\dots\dots \tag{1.13}$$

As before, provided that this series converges, it may be summed to give the equation

$$G^+(\underline{r}',t';\underline{r},t) = G_0^+(\underline{r}',t';\underline{r},t) + \tfrac{1}{\hbar}\iint G_0^+(\underline{r}',t';\underline{r}_i,t_i)V(\underline{r}_i,t_i)G^+(\underline{r}_i,t_i;\underline{r},t)\,dt_i\,d\underline{r}_i \tag{1.14}$$

Alternatively our approach to the interaction problem could have been developed equally well from the point of view of backward propagation in time by using the advanced Green's functions G_0^- and G^-. This leads to results exactly analogous to those already obtained. Using the equation (1.11) and its counterpart in the alternative formulation, together with (1.8), it is possible to show that

$$G^+(\underline{r}',t';\underline{r},t) = G^{-*}(\underline{r},t;\underline{r}',t') \tag{1.15}$$

provided that V is real.

At this stage we have a formalism which enables us to describe how the collision process develops. With this it is possible to express the probability of a particular final state evolving from the interaction, as is shown by the following.

We assume that there exists a time $-T_1$ in the distant past such that for all $t<-T_1$ there is no interaction between the two particles. For such a time t the system is represented by a solution of the wave equation (1.6). In a similar fashion it is assumed that there exists a time T_2 in the distant future such that for all $t>T_2$ there once again is no interaction between the particles. It therefore follows that the wave function representing the system at such a time may be represented by a linear combination of the solutions $\phi_i(\underline{r},t)$ of (1.6) provided that no rearrangement has occurred during the collision. If the system may be considered to originate in a state $\phi_\alpha(\underline{r},t)$ in the distant past $(t<-T_1)$ then this will develop into some state ψ_α^+ under the influence of the interaction potential. Since ψ_α^+ is a solution of the full time dependent Schrodinger equation then we may express it in the integral form of equation (1.2). Hence we have

$$\psi_\alpha^+(\underline{r}',t') = i\int G^+(\underline{r}',t';\underline{r},t)\phi_\alpha(\underline{r},t)d\underline{r} \qquad t<-T_1 \tag{1.16}$$

In the region $t'>T_2$ the interaction potential is no longer effective and the quantity

$$\langle\beta|S|\alpha\rangle \equiv (\phi_\beta,\psi_\alpha^+) \tag{1.17}$$

is the amplitude of the free-particle state β that is contained, after the scattering has occurred, in the state that has developed from the free-particle state α describing the system prior to the interaction. The transition amplitude of (1.17) defines an element of the scattering matrix (S matrix). If in (1.17) the wave function ψ_α^+ is replaced by the integral form of (1.16) we obtain

$$\langle\beta|S|\alpha\rangle = i\iint\phi_\beta^*(\underline{r}',t')G^+(\underline{r}',t';\underline{r},t)\phi_\alpha(\underline{r},t)\,d\underline{r}'d\underline{r} \qquad t<-T_1\ ,\ t'>T_2 \tag{1.18}$$

Now substituting for G^+ from equation (1.14) we have

$$\langle\beta|S|\alpha\rangle = i\iint\phi_\beta^*(\underline{r}',t')G_0^+(\underline{r}',t';\underline{r},t)\,\phi_\alpha(\underline{r},t)\,d\underline{r}'d\underline{r}$$
$$+\frac{i}{\hbar}\iint\phi_\beta^*(\underline{r}',t')\iint G_0^+(\underline{r}',t';\underline{r}_i,t_i)V(\underline{r}_i,t_i)G^+(\underline{r}_i,t_i;\underline{r},t)$$
$$\phi_\alpha(\underline{r},t)\,dt_i\,d\underline{r}_i\,d\underline{r}'d\underline{r}$$

But from equation (1.15) it is clear that

$$\int\phi_\beta^*(\underline{r}',t')\,G_0^+(\underline{r}',t';\underline{r}_i,t_i)d\underline{r}'$$
$$=\int G_0^{-*}(\underline{r}_i,t_i;\underline{r}',t')\,\phi_\beta^*(\underline{r}',t')d\underline{r}'$$

Hence the S matrix element has the form

$$<\beta|S|\alpha> = i\iint \phi^{*}_{\beta}(\underline{r}',t')\,G^{+}_{0}(\underline{r}',t';\underline{r},t)\,\phi_{\alpha}(\underline{r},t)\,d\underline{r}'d\underline{r}$$

$$+\ \frac{i}{\hbar}\iiiint G^{-*}_{0}(\underline{r}_i,t_i;\underline{r}',t')\,\phi^{*}_{\beta}(\underline{r}',t')\,V(\underline{r}_i,t_i)\,G^{+}(\underline{r}_i,t_i;\underline{r},t)$$

$$\phi_{\alpha}(\underline{r},t)\,dt_i\,d\underline{r}_i\,d\underline{r}'d\underline{r}$$

(1.19)

By applying the result of (1.16) and its analogue and discarding the index i the equation (1.19) may be reduced to the form

$$<\beta|S|\alpha> = <\beta|\alpha> - \frac{i}{\hbar}\iint \phi^{*}_{\beta}(\underline{r},t)\,V(\underline{r},t)\,\Psi^{+}_{\alpha}(\underline{r},t)\,dt\,d\underline{r}$$

(1.20)

Clearly, provided that the wave functions corresponding to the states α and β are orthogonal, the probability of a transition to the final state β is given by

$$P_{\alpha\beta} = |<\beta|S|\alpha>|^{2}$$

(1.21)

In the more general case of scattering by a composite target rearrangement of the original system may occur as a result of the collision. Such a situation can give rise to the problem of non-orthogonal wave functions. To allow for non-orthogonality we replace the expression in (1.21) by the following

$$\begin{aligned} P_{\alpha\beta} &= |<\beta|S|\alpha> - <\beta|\alpha>|^{2} \\ &= |<\beta|S-1|\alpha>|^{2} \end{aligned}$$

(1.22)

Obviously the equations (1.21) and (1.22) are identical if the states α and β are orthogonal.

The expression in (1.22) represents the probability of a transition over the entire period of duration of the collision whereas the experimentally observed quantity is the transition probability per unit time. Let us represent this quantity by $W_{\alpha\beta}$ and consider a time t' during the interaction. Then we have

$$W_{\alpha\beta\,(t')} = \frac{\partial}{\partial t'} \left| \langle \beta | S-1 | \alpha \rangle \right|^2 \tag{1.23}$$

Substituting from equation (1.20) we obtain

$$W_{\alpha\beta\,(t')} = \frac{\partial}{\partial t'} \left| -\frac{i}{\hbar} \iint \phi_\beta(\underline{r},t)\, V(\underline{r},t)\, \psi_\alpha^+(\underline{r},t)\, dt\, d\underline{r} \right|^2 \tag{1.24}$$

If the interaction potential may be considered independent of time then we have a stationary situation for which we may write

$$\begin{aligned} \phi_\beta(\underline{r},t) &= u_\beta(\underline{r})\, e^{-i\omega_\beta t} \\ \psi_\alpha^+(\underline{r},t) &= \chi_\alpha^+(\underline{r})\, e^{-i\omega_\alpha t} \\ V(\underline{r},t) &= V(\underline{r})\, g(t) \end{aligned} \tag{1.25}$$

where $\omega_i = \frac{E_i}{\hbar}$, E_i being the energy corresponding to the state denoted by i , and the function $g(t)$ is defined by

$$\begin{aligned} g(t) &= 1 \qquad -T_1 < t < T_2 \\ &= 0 \qquad \text{otherwise} \end{aligned} \tag{1.26}$$

We can now use the results of (1.25) to separate the time and space dependence of the expression in (1.24). This gives

$$W_{\alpha\beta\,(t')} = \left| \langle u_\beta | V(\underline{r}) | \chi_\alpha^+ \rangle \right|^2 \frac{\partial}{\partial t'} \left| -\frac{i}{\hbar} \int_{-\infty}^{t'} g(t)\, e^{i\omega_{\beta\alpha} t}\, dt \right|^2$$

$$\text{where} \quad \omega_{\beta\alpha} = \omega_\beta - \omega_\alpha \tag{1.27}$$

Hence making the identification

$$T_{\alpha\beta} = \langle u_\beta | V(r) | \chi_\alpha^+ \rangle \tag{1.28}$$

and carrying out the differentiation we obtain

$$\underset{(t')}{W_{\alpha\beta}} = |T_{\alpha\beta}|^2 \frac{1}{\hbar^2} \Big\{ g(t') e^{i\omega_{\beta\alpha}t'} \int_{-\infty}^{t'} g(t) e^{-i\omega_{\beta\alpha}t}\, dt$$

$$+ g(t') e^{-i\omega_{\beta\alpha}t'} \int_{-\infty}^{t'} g(t) e^{i\omega_{\beta\alpha}t}\, dt \Big\} \tag{1.29}$$

Since t' lies within the period of interaction we must have $g(t')=1$. Applying this result to (1.29) and combining the two terms within the brackets leads to the equation

$$\underset{(t')}{W_{\alpha\beta}} = |T_{\alpha\beta}|^2 \frac{1}{\hbar^2} \Big\{ 2 \int_{-\infty}^{t'} g(t) \cos[\omega_{\beta\alpha}(t-t')]\, dt \Big\} \tag{1.30}$$

Since we are considering a situation in which energy is conserved we are concerned with the limiting case $\omega_{\beta\alpha} \to 0$. Hence for present purposes we may regard $\omega_{\beta\alpha}$ as a very small quantity (in accordance with the Uncertainty Principle). Consequently, since the integrand appearing in (1.30) peaks at $t=t'$, the region $t<-T_1$ may be considered to make negligible contribution to the integral. This now allows us to replace $g(t)$ by unity over the entire range of integration, so leading to the result

$$\underset{(t')}{W_{\alpha\beta}} = |T_{\alpha\beta}|^2 \frac{1}{\hbar^2} \Big\{ 2 \int_{-\infty}^{t'} \cos[\omega_{\beta\alpha}(t-t')]\, dt \Big\} \tag{1.31}$$

The change of variable $\tau = t-t'$ transforms equation (1.31) to the form

$$\underset{(t')}{W_{\alpha\beta}} = |T_{\alpha\beta}|^2 \frac{1}{\hbar^2} \Big\{ 2 \int_{-\infty}^{0} \cos\omega_{\beta\alpha}\tau\, d\tau \Big\}$$

$$= |T_{\alpha\beta}|^2 \frac{1}{\hbar^2} \int_{-\infty}^{\infty} \cos\omega_{\beta\alpha}\tau\, d\tau \tag{1.32}$$

Now from the theory of distributions comes the result

$$\int_{-\infty}^{\infty} \cos \omega_{\beta\alpha} \tau \, d\tau = 2\pi \delta(\omega_{\beta\alpha}) \tag{1.33}$$

which when applied to equation (1.32) leads to the following expression for $W_{\alpha\beta}(t')$

$$\begin{aligned} W_{\alpha\beta}(t') &= |T_{\alpha\beta}|^2 \frac{2\pi}{\hbar^2} \delta(\omega_{\beta\alpha}) \\ &= \frac{2\pi}{\hbar} \delta(E_\beta - E_\alpha) |T_{\alpha\beta}|^2 \end{aligned} \tag{1.34}$$

It should be noted that this result is independent of time. The matrix T having elements $T_{\alpha\beta}$ is known as the transition matrix.

1.2 The relation between the scattering amplitude and T matrix

We shall assume that the results of the last section may be generalized to scattering by a composite target.

First of all we shall derive an explicit expression for the Green's function corresponding to the stationary scattering problem. The potential V appearing in the equation (1.1) is now independent of time and consequently it is possible to express the wave function $\psi(\underline{r},t)$ as an expansion in energy eigenfunctions

$$\psi(\underline{r},t) = S_\alpha A_\alpha(t) \chi_\alpha(\underline{r})$$

with $$A_\alpha(t) = \int \chi_\alpha^*(\underline{r}) \psi(\underline{r},t) \, d\underline{r} \tag{1.35}$$

where the functions $\chi_\alpha(\underline{r})$ are solutions of the time independent Schrodinger equation

$$(H_0 + V(\underline{r})) \chi_\alpha(\underline{r}) = E_\alpha \chi_\alpha(\underline{r}) \tag{1.36}$$

The symbol S_α denotes summation over discrete states and integration over the continuum.

If the form (1.35) is now substituted into the equation (1.1) we obtain

$$i\hbar \mathop{S}_{\alpha} \chi_{\alpha}(\underline{r}) \frac{d}{dt} A_{\alpha}(t) = \mathop{S}_{\alpha} A_{\alpha}(t) E_{\alpha} \chi_{\alpha}(\underline{r})$$

However since the functions $\chi_{\alpha}(\underline{r})$ form an orthogonal set then there can be no linear dependence between them. As a consequenc of this we must have

$$i\hbar \frac{d}{dt} A_{\alpha}(t) = E_{\alpha} A_{\alpha}(t) \tag{1.37}$$

Clearly this equation may be integrated to give the following form for the coefficients $A_{\alpha}(t)$

$$A_{\alpha}(t) = A_{\alpha}(t_0) e^{-i\omega_{\alpha}(t-t_0)} \tag{1.38}$$

where $\omega_{\alpha} = \frac{E_{\alpha}}{\hbar}$

The $A_{\alpha}(t)$ appearing in the expansion (1.35) can be replaced by these explicit forms, so giving

$$\psi(\underline{r},t) = \mathop{S}_{\alpha} A_{\alpha}(t_0) e^{-i\omega_{\alpha}(t-t_0)} \chi_{\alpha}(\underline{r}) \tag{1.39}$$

But we know that

$$A_{\alpha}(t_0) = \int \chi^*_{\alpha}(\underline{r}') \psi(\underline{r}',t_0) d\underline{r}'$$

Hence substituting in equation (1.39) we obtain

$$\psi(\underline{r},t) = \mathop{S}_{\alpha} \int \chi^*_{\alpha}(\underline{r}') \psi(\underline{r}',t_0) e^{-i\omega_{\alpha}(t-t_0)} \chi_{\alpha}(\underline{r}) d\underline{r}'$$

$$= \int \Big[\mathop{S}_{\alpha} \chi^*_{\alpha}(\underline{r}') \chi_{\alpha}(\underline{r}) e^{-i\omega_{\alpha}(t-t_0)} \Big] \psi(\underline{r}',t_0) d\underline{r}' \tag{1.40}$$

If we compare the equations (1.40) and (1.2) we see that it is now possible to write down an explicit expression for the Green's function G. i.e.

$$G(r',t';r,t) = -i\sum_\alpha \chi_\alpha(r')\chi^*_\alpha(r)\,e^{-i\omega_\alpha(t'-t)} \tag{1.41}$$

To obtain the explicit form of the retarded Green's function G^+ we make use of the Heaviside function $\theta(\tau)$ defined by

$$\begin{aligned}\theta(\tau) &= 1 \qquad \tau>0\\ &= 0 \qquad \tau<0\end{aligned} \tag{1.42}$$

Then in accordance with the definition of G^+ given in equation (1.3) we may write

$$\begin{aligned}G^+(r',t';r,t) &= \theta(t'-t)\,G(r',t';r,t)\\ &= \theta(t'-t)\left\{-i\sum_\alpha \chi_\alpha(r')\chi^*_\alpha(r)\,e^{-i\omega_\alpha(t'-t)}\right\}\end{aligned} \tag{1.43}$$

The theory of distributions shows that it is possible to express $\theta(\tau)$ in the following integral form

$$\theta(\tau) = -\frac{1}{2\pi i}\int_{-\infty}^{\infty} e^{-i\omega\tau}\frac{d\omega}{\omega+i\epsilon} \tag{1.44}$$

in which the limit $\epsilon \to 0^+$ is implied.

If we now combine the equations (1.43) and (1.44) we obtain

$$G^+(r',t';r,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\sum_\alpha (\omega+i\epsilon)^{-1}\chi_\alpha(r')\chi^*_\alpha(r)\,e^{-i(\omega+\omega_\alpha)(t'-t)}\,d\omega \tag{1.45}$$

By changing the variable of integration from ω to $\omega+\omega_\alpha$ the expression of (1.45) is transformed to the following form

$$G^+(\underline{r}',t';\underline{r},t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathop{S}_{\alpha} (\omega-\omega_\alpha+i\epsilon)^{-1}\chi_\alpha(\underline{r}')\chi^*_\alpha(\underline{r})\, e^{-i\omega(t'-t)}\, d\omega \tag{1.46}$$

Clearly the corresponding expression for the free particle propagator is derived in a similar way. By analogy we have

$$G_0^+(\underline{r}',t';\underline{r},t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathop{S}_{\alpha} (\omega-\omega_\alpha+i\epsilon)^{-1} u_\alpha(\underline{r}') u^*_\alpha(\underline{r})\, e^{-i\omega(t'-t)}\, d\omega \tag{1.47}$$

where the wave functions $u_\alpha(\underline{r})$ are solutions of the time independent Schrödinger equation

$$(H_0 - E_\alpha)\, u_\alpha(\underline{r}) = 0 \tag{1.48}$$

We shall now combine these results with those already obtained for the general scattering process. In this context it is convenient to choose equation (1.12) as our starting point

$$\psi^+(\underline{r}',t') = i\int G_0^+(\underline{r}',t';\underline{r},t)\,\psi(\underline{r},t)\, d\underline{r} + \frac{1}{\hbar}\int dt_i \int G_0^+(\underline{r}',t';\underline{r}_i,t_i)\, V(\underline{r}_i,t_i)\, \psi^+(\underline{r}_i,t_i)\, d\underline{r}_i$$

Taking t as a time in the distant past at which no interaction is present we may write

$$\psi(\underline{r},t) = u_{\alpha_0}(\underline{r})\, e^{-i\omega_{\alpha_0} t}$$

$$\psi^+(\underline{r}',t') = \chi^+_{\alpha_0}(\underline{r}')\, e^{-i\omega_{\alpha_0} t'} \quad \text{where } \omega_{\alpha_0} = \frac{E_{\alpha_0}}{\hbar} \tag{1.49}$$

If we now consider the time of interaction to approach infinity then the function $g(t)$ expressing the time dependence of the potential $V(\underline{r},t)$ (equation (1.25)) may be assumed identically equal to unity. Thus applying the results of (1.47) and (1.49) to equation (1.12) we obtain

$$\begin{aligned}\chi^{+}_{\alpha_0}(\underline{r}')e^{-i\omega_{\alpha_0}t'} &= u_{\alpha_0}(\underline{r}')e^{-i\omega_{\alpha_0}t'} \\ &+ \frac{1}{\hbar}\int dt_i \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathop{\mathrm{S}}_{\alpha} (\omega-\omega_{\alpha}+i\epsilon)^{-1}\int u_{\alpha}(\underline{r}')u^{*}_{\alpha}(\underline{r}_i)e^{-i\omega(t'-t_i)} \\ &\qquad V(\underline{r}_i)\chi^{+}_{\alpha_0}(\underline{r}_i)e^{-i\omega_{\alpha_0}t_i}\,d\underline{r}_i\,d\omega\end{aligned} \tag{1.50}$$

Let us now consider the integration over the variable t_i. This has the form

$$\begin{aligned}&\int_{t}^{t'} dt_i\, e^{-i\omega(t'-t_i)}e^{-i\omega_{\alpha_0}t_i} \\ &= e^{-i\omega t'}\int_{t}^{t'} dt_i\, e^{it_i(\omega-\omega_{\alpha_0})}\end{aligned}$$

We shall make the identification

$$F(t,t',\omega) = \int_{t}^{t'} dt_i\, e^{it_i(\omega-\omega_{\alpha_0})} \tag{1.51}$$

By making the further identification

$$G^{+}_{0\omega}(\underline{r}',\underline{r}_i) = \mathop{\mathrm{S}}_{\alpha}(\omega-\omega_{\alpha}+i\epsilon)^{-1}u_{\alpha}(\underline{r}')u^{*}_{\alpha}(\underline{r}_i) \tag{1.52}$$

we are able to simplify equation (1.50) to the following

$$\begin{aligned}\chi^{+}_{\alpha_0}(\underline{r}')e^{-i\omega_{\alpha_0}t'} &= u_{\alpha_0}(\underline{r}')e^{-i\omega_{\alpha_0}t'} \\ &+ \frac{1}{2\pi\hbar}e^{-i\omega_{\alpha_0}t'}\iint_{-\infty}^{\infty} e^{-it'(\omega-\omega_{\alpha_0})}F(t,t',\omega) \\ &\qquad G^{+}_{0\omega}(\underline{r}',\underline{r}_i)V(\underline{r}_i)\chi^{+}_{\alpha_0}(\underline{r}_i)\,d\underline{r}_i\,d\omega\end{aligned}$$

Cancellation of the exponential factor $e^{-i\omega_{\alpha_0}t'}$ results in the form

$$\chi^+_{\alpha_0}(\underline{r}') = u_{\alpha_0}(\underline{r}') + \frac{1}{2\pi\hbar}\iint_{-\infty}^{\infty} e^{-it'(\omega-\omega_{\alpha_0})}F(t,t';\omega)\,G^+_{0\omega}(\underline{r}';\underline{r}_i)$$

$$V(\underline{r}_i)\chi^+_{\alpha_0}(\underline{r}_i)\,d\underline{r}_i\,d\omega \tag{1.53}$$

Now since we are interested in the state of the system after the scattering has occurred and the interaction is no longer present we shall take t' to be a time in the distant future. Hence we wish to examine the limiting form of equation (1.53) as $t \to -\infty$ and $t' \to +\infty$ simultaneously. In this limit we have

$$\chi^+_{\alpha_0}(\underline{r}') = u_{\alpha_0}(\underline{r}') + \frac{1}{2\pi\hbar}\iint_{-\infty}^{\infty} \underset{\substack{t\to-\infty \\ t'\to+\infty}}{\mathrm{Lmt}}\left\{e^{-it'(\omega-\omega_{\alpha_0})}F(t,t';\omega)\right\}$$

$$G^+_{0\omega}(\underline{r}';\underline{r}_i)V(\underline{r}_i)\chi^+_{\alpha_0}(\underline{r}_i)\,d\underline{r}_i\,d\omega$$

$$= u_{\alpha_0}(\underline{r}') + \frac{1}{2\pi\hbar}\iint_{-\infty}^{\infty} \underset{\substack{t\to-\infty \\ t'\to+\infty}}{\mathrm{Lmt}}\left\{e^{-it'(\omega-\omega_{\alpha_0})}\right\}\underset{\substack{t\to-\infty \\ t'\to+\infty}}{\mathrm{Lmt}}\left\{F(t,t';\omega)\right\}$$

$$G^+_{0\omega}(\underline{r}';\underline{r}_i)V(\underline{r}_i)\chi^+_{\alpha_0}(\underline{r}_i)\,d\underline{r}_i\,d\omega \tag{1.54}$$

But from the theory of distributions we have the result

$$\underset{\substack{t\to-\infty \\ t'\to+\infty}}{\mathrm{Lmt}} F(t,t';\omega) = 2\pi\delta(\omega-\omega_{\alpha_0}) \tag{1.55}$$

Hence applying this result to (1.54) and simplifying, we obtain

$$\chi^+_{\alpha_0}(\underline{r}') = u_{\alpha_0}(\underline{r}') + \frac{1}{\hbar}\int G^+_{0\omega_{\alpha_0}}(\underline{r}';\underline{r}_i)V(\underline{r}_i)\chi^+_{\alpha_0}(\underline{r}_i)\,d\underline{r}_i \tag{1.56}$$

which is an integral equation for the spatial wave function $\chi_{\alpha_0}(\underline{r})$

We shall now consider scattering by a composite target. Let us assume the target to be an n electron atom and denote the corresponding position vectors by $\underline{R} = (\underline{r}_1, \underline{r}_2, \ldots\ldots \underline{r}_n)$, these being measured relative to the nucleus. The position vector of the incident electron is denoted by $\underline{r}$. Then generalization of (1.56) leads to the form

$$\chi^{+}_{\alpha_0}(\underline{r}', \underline{R}') = u_{\alpha_0}(\underline{r}', \underline{R}') + \frac{1}{\hbar}\int G^{+}_{0\omega_{\alpha_0}}(\underline{r}', \underline{R}'; \underline{r}, \underline{R})\, V(\underline{r}, \underline{R})\, \chi^{+}_{\alpha_0}(\underline{r}, \underline{R})\, d\underline{r}\, d\underline{R}$$

where

$$H = H_0 + V(\underline{r}, \underline{R}) = H_0 + \sum_{i=1}^{n} \frac{e^2}{|\underline{r} - \underline{r}_i|} - \frac{Z_n e^2}{|\underline{r}|}$$

with $Z_n = n$ for a neutral target. (1.57)

and the wavefunctions $\chi^{+}_{\alpha_0}(\underline{r}, \underline{R})$, $u_{\alpha_0}(\underline{r}, \underline{R})$ satisfy the time independent Schrödinger equations (1.58a) and (1.59a) respectively

$$(H - E_{\alpha_0})\, \chi^{+}_{\alpha_0}(\underline{r}, \underline{R}) = 0 \qquad (1.58a)$$

$$(H_0 - E_{\alpha_0})\, u_{\alpha_0}(\underline{r}, \underline{R}) = 0 \qquad (1.59a)$$

By analogy with (1.52) the retarded Green's function $G^{+}_{0\omega_{\alpha_0}}(\underline{r}', \underline{R}'; \underline{r}, \underline{R})$ appearing in (1.57) may be expressed as follows

$$G^{+}_{0\omega_{\alpha_0}}(\underline{r}', \underline{R}'; \underline{r}, \underline{R}) = \mathop{\mathrm{S}}_{\alpha} (\omega_{\alpha_0} - \omega_{\alpha} + i\epsilon)^{-1} u_{\alpha}(\underline{r}', \underline{R}')\, u^{*}_{\alpha}(\underline{r}, \underline{R}) . \qquad (1.58)$$

The unperturbed hamiltonian H_0, corresponding to the system prior to interaction, is composed of two parts

$$H_0 = H_T + H_E \qquad (1.59)$$

Where H_T corresponds to the target system and H_E to the incident electron. Hence the wavefunctions $u_{\alpha}(\underline{r}, \underline{R})$ are separable and may be expressed as products of two functions.

Let m characterize the state of the target system described by the wavefunction $\phi_m(\underline{R})$. If $\mathcal{E}_m$ is the energy associated with this state then $\phi_m(\underline{R})$ satisfies the Schrödinger equation

$$(H_T - \mathcal{E}_m)\phi_m(\underline{R}) = 0 \tag{1.60}$$

The energy eigenfunctions of the free particle hamiltonian will be represented by the functions $v_{k_\alpha}(\underline{r})$ where

$$(H_E - \varepsilon_\alpha) v_{k_\alpha}(\underline{r}) = 0 \tag{1.61}$$

ε_α being the energy of the free particle state having momentum $k_\alpha \hbar$.

Hence applying these results to equation (1.58) enables us to express $G^+_{0\omega_{\alpha_0}}(\underline{r}', \underline{R}'; \underline{r}, \underline{R})$ in the form

$$G^+_{0\omega_{\alpha_0}}(\underline{r}', \underline{R}'; \underline{r}, \underline{R}) = \mathop{S}_m \int (\omega_{\alpha_0} - \omega_\alpha + i\epsilon)^{-1} v_{k_\alpha}(\underline{r}') \phi_m(\underline{R}') v^*_{k_\alpha}(\underline{r}) \phi^*_m(\underline{R})\, d\underline{k}_\alpha$$

where $$\hbar\omega_\alpha = E_\alpha = \mathcal{E}_m + \varepsilon_\alpha \tag{1.62}$$

If we now write

$$E_{\alpha_0} = \mathcal{E}_m + \varepsilon_{m\alpha_0}$$

where $$\varepsilon_{m\alpha_0} = \frac{1}{2\mu} k^2_{m\alpha_0} \hbar^2 \tag{1.63}$$

and make the change $\epsilon \rightarrow \frac{2\mu}{\hbar}\epsilon$ then equation (1.62) may be transformed to

$$G^+_{0\omega_{\alpha_0}}(\underline{r}', \underline{R}'; \underline{r}, \underline{R}) = \frac{2\mu}{\hbar} \mathop{S}_m \int (k^2_{m\alpha_0} - k^2_\alpha + i\epsilon)^{-1} v_{k_\alpha}(\underline{r}') \phi_m(\underline{R}') \\ v^*_{k_\alpha}(\underline{r}) \phi^*_m(\underline{R})\, d\underline{k}_\alpha \tag{1.64}$$

But we know the explicit form of the function $v_{k_\alpha}(\underline{r})$ to be

$$v_{k_\alpha}(\underline{r}) = \frac{1}{(2\pi)^{3/2}} e^{i\underline{k}_\alpha \cdot \underline{r}} \tag{1.65}$$

Hence if we now substitute this form of $v_{k_\alpha}(\underline{r})$ in equation (1.64) then we obtain

$$G^{+}_{0\omega_{\alpha_0}}(\underline{r}',\underline{R}';\underline{r},\underline{R}) = \frac{\mu}{4\pi^3\hbar} \mathop{S}_m \int (k_{m\alpha_0}^2 - k_\alpha^2 + i\epsilon)^{-1} e^{i\underline{k}_\alpha\cdot(\underline{r}'-\underline{r})} \phi_m(\underline{R}')\phi_m^*(\underline{R})\, d\underline{k}_\alpha \qquad (1.66)$$

The integration over momentum space appearing in equation (1.66) is readily evaluated to give the result

$$G^{+}_{0\omega_{\alpha_0}}(\underline{r}',\underline{R}';\underline{r},\underline{R}) = -\frac{\mu}{2\pi\hbar} \mathop{S}_m |\underline{r}'-\underline{r}|^{-1} e^{ik_{m\alpha_0}|\underline{r}'-\underline{r}|} \phi_m(\underline{R}')\phi_m^*(\underline{R}) \qquad (1.67)$$

We shall now return to equation (1.57). In order to ascertain the effect of the scattering process we need to examine the state of the system when there is large separation between the target and scattered electron. Thus our interest is directed toward the asymptotic region $r'\to\infty$. Clearly the form of the wavefunction $\chi^{+}_{\alpha_0}(\underline{r}',\underline{R}')$ in the region of interest is largely dependent upon the asymptotic behaviour of $G_{0\omega_{\alpha_0}}$. Therefore let us consider the form of $G_{0\omega_{\alpha_0}}$ as $r'\to\infty$. Now since

$$|\underline{r}'-\underline{r}| = r' - r\cos\theta' + O\left(\frac{r^2}{r'}\right)$$

where θ' is the angle between $\underline{r}'$ and $\underline{r}$

and
$$|\underline{r}'-\underline{r}|^{-1} = \frac{1}{r'} + O\left(\frac{r}{r'^2}\right)$$

then

$$G^{+}_{0\omega_{\alpha_0}}(\underline{r}',\underline{R}';\underline{r},\underline{R}) \xrightarrow[r'\to\infty]{} -\frac{\mu}{2\pi\hbar} \mathop{S}_m \frac{e^{ik_{m\alpha_0}(r'-r\cos\theta')}}{r'} \phi_m(\underline{R}')\phi_m^*(\underline{R}) \qquad (1.68)$$

This result enables us to determine the asymptotic form of equation (1.57). Clearly for $r'\to\infty$ we have

$$\chi^{+}_{\alpha_0}(\underline{r}',\underline{R}') \underset{r'\to\infty}{\rightarrow} u_{\alpha_0}(\underline{r}',\underline{R}') - \frac{\mu}{2\pi\hbar^2} \mathop{S}_{m} \frac{e^{ik_{m\alpha_0}r'}}{r'} \phi_m(\underline{R}')$$

$$\int e^{-ik_{m\alpha_0} r\cos\theta'} \phi^{*}_{m}(\underline{R}) V(\underline{r},\underline{R}) \chi^{+}_{\alpha_0}(\underline{r},\underline{R})\, d\underline{r}\, d\underline{R} \qquad (1.69)$$

We now introduce a vector $\underline{k}_{m\alpha_0}$ having magnitude equal to $k_{m\alpha_0}$ and direction parallel to that of $\underline{r}$. This enables us to replace $k_{m\alpha_0} r\cos\theta'$ by $\underline{k}_{m\alpha_0}\cdot\underline{r}$. Hence equation (1.69) becomes

$$\chi^{+}_{\alpha_0}(\underline{r}',\underline{R}') \underset{r'\to\infty}{\longrightarrow} u_{\alpha_0}(\underline{r}',\underline{R}') - \frac{\mu}{2\pi\hbar^2} \mathop{S}_{m} \frac{e^{ik_{m\alpha_0}r'}}{r'} \phi_m(\underline{R}')$$

$$\int e^{-i\underline{k}_{m\alpha_0}\cdot\underline{r}} \phi^{*}_{m}(\underline{R}) V(\underline{r},\underline{R}) \chi_{\alpha_0}(\underline{r},\underline{R})\, d\underline{r}\, d\underline{R}$$

$$(1.70)$$

From a purely physical approach it would be expected that the wavefunction describing the system would have the asymptotic form

$$\chi^{+}_{\alpha_0}(\underline{r}',\underline{R}') \underset{r'\to\infty}{\longrightarrow} u_{\alpha_0}(\underline{r}',\underline{R}') + \frac{1}{(2\pi)^{3/2}} \mathop{S}_{m} \frac{e^{ik_{m\alpha_0}r'}}{r'} f(m,\underline{k}_{m\alpha_0}) \phi_m(\underline{R}')$$

$$(1.71)$$

The first term corresponds to the majority of the incident electron beam experiencing no interaction with the target system, whilst the second term describes the small scattered part of the beam appearing to radiate from the target system, excited to some state m by the collision. The scattering amplitude $f(m,\underline{k}_{m,\alpha_0})$ playing the role of an angular dependent weight factor, is defined by the form of the wavefunction appearing in (1.71). By comparing (1.70) and (1.71) we are able to obtain an explicit expression for the scattering amplitude

$$f(m,\underline{k}_{m\alpha_0}) = -\frac{(2\pi)^{1/2}\mu}{\hbar^2} \int e^{-i\underline{k}_{m\alpha_0}\cdot\underline{r}} \phi_m(\underline{R}) V(\underline{r},\underline{R}) \chi^{+}_{\alpha_0}(\underline{r},\underline{R})\, d\underline{r}\, d\underline{R}$$

$$(1.72)$$

Equation (1.72) can be written in the more compact form

$$f(m,\underline{k}_{m\alpha_0}) = -\frac{(2\pi)^2\mu}{\hbar^2}\langle u_{m\alpha_0}|V(\underline{r},\underline{R})|\chi^+_{\alpha_0}\rangle \tag{1.73}$$

where $u_{m\alpha_0}(\underline{r},\underline{R}) = \frac{1}{(2\pi)^{3/2}} e^{i\underline{k}_{m\alpha_0}\cdot\underline{r}}\,\phi_m(\underline{R})$

Hence generalizing the definition of the T matrix, given in equation (1.28), we may write

$$f(m,\underline{k}_{m\alpha_0}) = -\frac{(2\pi)^2\mu}{\hbar^2}\,T_{\alpha_0,m\alpha_0} \tag{1.74}$$

1.3 Rearrangement Collisions

So far we have only considered the scattering situation in which the scattered particle and target system retain their prior-interaction identities. However, for the case of the scattering of an electron by an atom or ion there exists the possibility of an exchange between the incident electron and an electron belonging to the target. This is known as a rearrangement collision. Since the rearrangement collision is experimentally indistinguishable from direct scattering we must take full account of such collisions. The interaction potential will now depend on whether we are observing the situation before or after the rearrangement has occurred and so is no longer unique. It therefore follows that the T matrix element corresponding to a rearrangement collision cannot be obtained by direct analogy with (1.28), since this involves a potential. Hence we must seek a form of the T matrix element that does not explicitly involve the potential. In order to obtain an alternative formulation we shall revert to the simpler problem of scattering by a single potential.

From equation (1.17) we have

$$\langle\beta|S-1|\alpha\rangle = \int \phi^*_\beta(\underline{r},t')\left(\psi^+_\alpha(\underline{r},t') - \phi_\alpha(\underline{r},t')\right)d\underline{r}$$

whilst equation (1.20) gives the following expression for the same quantity

$$\langle\beta|S-1|\alpha\rangle = -\frac{i}{\hbar}\iint \phi^{*}_{\beta}(\underline{r},t)V(\underline{r},t)\psi^{+}_{\alpha}(\underline{r},t)\,dt\,d\underline{r}$$

For the stationary situation we may use the results (1.25) to obtain

$$\langle\beta|S-1|\alpha\rangle = (u_{\beta},(\chi^{+}_{\alpha}-u_{\alpha}))e^{i/\hbar(E_{\beta}-E_{\alpha})t'} \tag{1.75}$$

and

$$\langle\beta|S-1|\alpha\rangle = -\frac{i}{\hbar}\langle\beta|T|\alpha\rangle\int_{\infty}^{t'} g(t)e^{i/\hbar(E_{\beta}-E_{\alpha})t}dt \tag{1.76}$$

respectively

To enable us to evaluate the integral in (1.76) we shall replace E_{α} by $E_{\alpha}+i\epsilon$ where the limit $\epsilon \rightarrow 0^{+}$ is implied. Since this will result in zero contribution from the lower limit of the integration we may set $g(t)=1$ in the integrand. Hence the integrand over time becomes

$$\int_{-\infty}^{t'} e^{i/\hbar(E_{\beta}-E_{\alpha}-i\epsilon)t}dt = \frac{\hbar}{i(E_{\beta}-E_{\alpha}-i\epsilon)}e^{i/\hbar(E_{\beta}-E_{\alpha}-i\epsilon)t'} \tag{1.77}$$

Combining equations (1.75) and (1.76) and applying the result (1.77) we obtain:

$$(u_{\beta},(\chi^{+}_{\alpha}-u_{\alpha})) = \frac{-1}{(E_{\beta}-E_{\alpha}-i\epsilon)}\langle\beta|T|\alpha\rangle \tag{1.78}$$

Since energy is conserved $E_{\beta}=E_{\alpha}$ and (1.78) becomes

$$\langle\beta|T|\alpha\rangle = i\epsilon(u_{\beta},(\chi^{+}_{\alpha}-u_{\alpha})) \tag{1.79}$$

Now this expression for the T matrix element does not involve the potential and consequently we shall assume that the analogous result holds true for rearrangement collisions.

At this stage in the discussion it is useful to introduce the Lippmann-Schwinger equations. The Lippmann-Schwinger approach provides a symbolic way of expressing the integral equation for the wavefunction. Let us consider the Schrödinger time independent equation

$$(H_0 + V - E_\alpha)\chi_\alpha(\underline{r}) = 0 \tag{1.80}$$

Here the H_0 is a differential operator and subsequent rearrangement of (1.80) produces the inhomogeneous differential equation

$$(E_\alpha - H_0)\chi_\alpha(\underline{r}) = V(\underline{r})\chi_\alpha(\underline{r}) \tag{1.81}$$

The general solution of (1.81) will be composed of the solution of the homogeneous differential equation

$$(E_\alpha - H_0)u_\alpha(\underline{r}) = 0$$

together with a particular integral of (1.81). If $\mathcal{L}$ is the inverse integral operator corresponding to $(E_\alpha - H_0)$ we obtain the integral equation

$$\chi_\alpha(\underline{r}) = u_\alpha(\underline{r}) + \mathcal{L}V(\underline{r})\chi_\alpha(\underline{r}) \tag{1.82}$$

Symbolically we might write $\mathcal{L} = (E_\alpha - H_0)^{-1}$. However to avoid the singularity occurring at $E = E_\alpha$ we make the change $E_\alpha \to E_\alpha \pm i\epsilon$ where, as before, the limit $\epsilon \to 0^+$ is implied. It can be shown that the plus and minus signs correspond to outgoing and ingoing waves respectively. Hence we have

$$\chi_\alpha^+(\underline{r}) = u_\alpha(\underline{r}) + (E_\alpha - H_0 + i\epsilon)^{-1}V(\underline{r})\chi_\alpha^+(\underline{r}) \tag{1.83}$$

$$\chi_\alpha^-(\underline{r}) = u_\alpha(\underline{r}) + (E_\alpha - H_0 - i\epsilon)^{-1}V(\underline{r})\chi_\alpha^-(\underline{r}) \tag{1.84}$$

We shall now show how these results may be applied to rearrangement collisions.

Let us suppose that the collision of two systems a and b results in a rearrangement for which the component systems are c, d. In this event the full hamiltonian H can be written in either of two ways

$$H = H_{ab} + H'_{ab} = H_{cd} + H'_{cd}$$

where H_{ab} describes the internal and kinetic energies of a and b and H'_{ab} their interaction. H_{cd} and H'_{cd} are similarly defined. If χ^+_{ab} and χ^-_{cd} are the outgoing and ingoing waves corresponding to this scattering process then, in accordance with equations (1.83) and (1.84), they satisfy Lippmann-Schwinger equations of the form

$$\chi^+_{ab} = u_{ab} + (E - H_{ab} + i\epsilon)^{-1} H'_{ab} \chi^+_{ab} \tag{1.85}$$

and

$$\chi^-_{cd} = u_{cd} + (E - H_{cd} - i\epsilon)^{-1} H'_{cd} \chi^-_{cd} \tag{1.86}$$

where E is the total energy.

We now introduce operators $\mathcal{L}_{cd}$ and $\mathcal{L}_{ab}$ defined by

$$\mathcal{L}_{cd} = (E - H_{cd} + i\epsilon)$$

and

$$\mathcal{L}_{ab} = (E - H_{ab} + i\epsilon)$$

By using the second of these we can write (1.85) in the form

$$\chi^+_{ab} - u_{ab} = \mathcal{L}^{-1}_{ab} H'_{ab} \chi^+_{ab} \tag{1.87}$$

From equation (1.79) the T matrix element corresponding to the rearrangement collision is given by

$$\langle cd | T | ab \rangle = i\epsilon (u_{cd}, (\chi^+_{ab} - u_{ab}))$$

Now

$$i\epsilon (u_{cd}, (\chi^+_{ab} - u_{ab})) = i\epsilon (u_{cd}, \mathcal{L}^{-1}_{cd} \mathcal{L}_{cd} (\chi^+_{ab} - u_{ab}))$$
$$= i\epsilon (\mathcal{L}^{-1*}_{cd} u_{cd}, \mathcal{L}_{cd} (\chi^+_{ab} - u_{ab}))$$

But

$$\mathcal{L}^{-1*}_{cd} u_{cd} = (E - H_{cd} - i\epsilon)^{-1} u_{cd}$$
$$= i/\epsilon$$

Hence we obtain

$$\langle cd | T | ab \rangle = (u_{cd}, \mathcal{L}_{cd} (\chi^+_{ab} - u_{ab})) \tag{1.88}$$

Let us now consider the quantity $\mathcal{L}_{cd} (\chi^+_{ab} - u_{ab})$. From the definition of the operator $\mathcal{L}_{cd}$ we have

$$\mathcal{L}_{cd} = E - H_{cd} + i\epsilon = E - H + H'_{cd} + i\epsilon$$

However since $H=H_{ab}+H'_{ab}$, an alternative expression for $\mathcal{L}_{cd}$ is

$$\mathcal{L}_{cd} = E+i\epsilon-H_{ab}-H'_{ab}+H'_{cd}$$

This leads to the result

$$\mathcal{L}_{cd}(X^+_{ab}-u_{ab})=(E+i\epsilon-H_{ab}-H'_{ab}+H'_{cd})(X^+_{ab}-u_{ab})$$

$$=\mathcal{L}_{ab}(X^+_{ab}-u_{ab})-(H'_{ab}-H'_{cd})(X^+_{ab}-u_{ab})$$

Applying the result (1.87) we obtain

$$\mathcal{L}_{cd}(X^+_{ab}-u_{ab})=\mathcal{L}_{ab}\mathcal{L}^{-1}_{ab}H'_{ab}X^+_{ab}-(H'_{ab}-H'_{cd})(X^+_{ab}-u_{ab})$$

$$=H'_{ab}X^+_{ab}-(H'_{ab}-H'_{cd})(X^+_{ab}-u_{ab})$$

$$=H'_{cd}X^+_{ab}+(H'_{ab}-H'_{cd})u_{ab} \tag{1.89}$$

If we now substitute this result in equation (1.88) the T matrix element will take the following form

$$\langle cd|T|ab\rangle=(u_{cd}, H'_{cd}X^+_{ab}+(H'_{ab}-H'_{cd})u_{ab})$$

$$=(u_{cd},H'_{cd}X^+_{ab})+(u_{cd},(H'_{ab}-H'_{cd})u_{ab}) \tag{1.90}$$

Since $H_{ab}+H'_{ab}=H_{cd}+H'_{cd}$ the second term in (1.90) may be rewritten as

$$(u_{cd}, (H_{cd}-H_{ab})u_{ab})$$

$$=(u_{cd}, H_{cd}u_{ab})-E(u_{cd}, u_{ab})$$

$$=E(u_{cd},u_{ab})-E(u_{cd},u_{ab})$$

$$=0$$

Hence equation (1.90) becomes

$$\langle cd|T|ab\rangle=(u_{cd},H'_{cd}X^+_{ab}) \tag{1.91}$$

However we could equally well start from the formulation of the T matrix element in terms of the ingoing wave

$$\langle cd|T|ab\rangle = i\epsilon(\chi^{-}_{cd}-u_{cd}, u_{ab})$$

In this case if we manipulate the original form in a way similar to that previously described then we obtain

$$\langle cd|T|ab\rangle = (\chi^{-}_{cd}, H'_{ab}u_{ab}) \qquad (1.92)$$

The equations (1.91) and (1.92) are referred to as the post and prior forms of the T matrix element respectively.

It should be noted that throughout the analysis leading to equations (1.91) and (1.92) it is assumed that the operators H_{ab}, H'_{ab}, H_{cd} and H'_{cd} are all hermitian.

1.4 The Ionization of Helium by Electron Impact

Having developed a formulation capable of dealing with all eventualities arising from the collision of two systems we are now in a position to consider the single ionization of helium by electron impact. By virtue of the indistinguishability of the electrons involved there are three distinct processes that contribute to each observed final state. In addition to direct scattering, for which the incident electron emerges as the more energetic of the two ionization electrons present in the final state, there are two types of rearrangement collision that may occur. Firstly there is the possibility of exchange for which the roles of the two ionization electrons are interchanged and secondly capture for which the two atomic electrons are excited to the continuum and the incident electron de-excited to a bound state of the residue ion.

In the discussion that follows we shall refer to the more energetic ionization electron as the 'fast' electron and the other as the 'slow', denoting the respective momenta by $\underline{k}_f$ and $\underline{k}_s$.

Associated with the three processes described we have the direct, exchange and capture amplitudes which, in accordance with the work of Rudge (1968), we denote by $f(\underline{k}_f,\underline{k}_s)$, $g(\underline{k}_f,\underline{k}_s)$ and $\omega(\underline{k}_f,\underline{k}_s)$ respectively. Each amplitude is related to a T matrix element, corresponding to the particular transition with which the amplitude is associated, through an equation of the form (1.74).

Our present intention is to show how the amplitudes combine to give the probability for each final state of ionization. In order to do this we need to determine the relation between the amplitudes and the asymptotic form of the wavefunction representing the system.

If we denote the spatial co-ordinates of the two atomic electrons by $\underline{r}_2$ and $\underline{r}_3$ and those of the incident electron by $\underline{r}_1$ then the full hamiltonian corresponding to the electron-helium interaction has the form

$$H(1,2,3) = H_e(1) + H_T(2,3) + V(1;2,3)$$

where $H_e(1)$ is the free-electron hamiltonian, $H_T(2,3)$ the hamiltonian for the target system and $V(1;2,3)$ the interaction potential, is given by

$$V(1;2,3) = -\frac{2e^2}{r_1} + \frac{e^2}{r_{12}} + \frac{e^2}{r_{13}}$$

Now since the initial symmetry of the system must be retained then $\chi^+(\underline{r}_2,\underline{r}_3;\underline{r}_1)$, the solution of the full Schrödinger equation that develops from the wavefunction describing the initial state of the system, must be symmetric with respect to interchange of $\underline{r}_2$ and $\underline{r}_3$. Let $\{\underline{x}_i, i=1,3\}$ represent both the spatial and spin co-ordinates of the electrons. Hence if we take full account of spin the anti-symmetrized wavefunction representing the system is

$$\chi^+(\underline{x}_2,\underline{x}_3;\underline{x}_1) = \sum_{\text{cyclic permutations of indexes}} \upsilon(S_A, M_{S_A}|\sigma_2,\sigma_3)\,\delta(\mu_1|\sigma_1)\,\chi^+(\underline{r}_2,\underline{r}_3;\underline{r}_1) \tag{1.93}$$

where $\upsilon(S_A, M_{S_A}|\sigma_2, \sigma_3)$ is the spin function representing a state of the target that has total spin S_A and z-component M_{S_A}, $\delta(\mu_1|\sigma_1)$ is the spin function of an electron having spin μ_1, and $\{\sigma_i, i=1,3\}$ denote the spin co-ordinates of the electrons.

Our interest is confined to those collisions that result in ionization and so we shall retain only such states in the asymptotic form of χ^+. Hence we obtain

$$\chi^+(\underline{x}_2, \underline{x}_3; \underline{x}_1) \sim \ldots\ldots \sum_{\mu_1'\mu_2'\mu_3'} \delta(\mu_1'|\sigma_1)\delta(\mu_2'|\sigma_2)\delta(\mu_3'|\sigma_3)$$

$$\sum_{E(m,k_f,k_s)=E} f_{k_f k_s}(S_A, M_{S_A}, \mu_1|\mu_1'\mu_2'\mu_3'; \hat{r}_1, \hat{r}_2)\frac{1}{(2\pi)^{3/2}}\frac{e^{ik_f r_1}}{r_1}\phi_{mk_s}(\underline{r}_2, \underline{r}_3)\ldots \tag{1.94}$$

In the asymptotic form of (1.94) the wavefunction $\phi_{mk_s}(\underline{r}_2, \underline{r}_3)$ describes the excited state of the target system which is composed of the residual ion, in some state m, together with the less energetic ionization electron. The quantities E and $E(m, k_f, k_s)$ are the total energies of the initial and final states of the system respectively. Finally, the quantity $f_{k_f k_s}$ is the combination of amplitudes obtained after projecting the associated spin functions onto the function $\delta(\mu_1'|\sigma_1)\delta(\mu_2'|\sigma_2)\delta(\mu_3'|\sigma_3)$.

Since the present work is concerned with the ionization of a helium atom initially in its ground state we have $S_A = M_{S_A} = 0$ and the corresponding form of $f_{k_f k_s}$ is

$$\begin{aligned} f_{k_f k_s}&(0, 0, \mu_1|\mu_1'\mu_2'\mu_3'; \hat{r}_1, \hat{r}_2) \\ &= C(\tfrac{1}{2}, \tfrac{1}{2}, 0; \mu_2', \mu_3', 0)\,\delta_{\mu_1\mu_1'}\, f(\underline{k}_f, \underline{k}_s) \\ &+ C(\tfrac{1}{2}, \tfrac{1}{2}, 0; \mu_3', \mu_1', 0)\,\delta_{\mu_1\mu_2'}\, g(\underline{k}_f, \underline{k}_s) \\ &+ C(\tfrac{1}{2}, \tfrac{1}{2}, 0; \mu_1', \mu_2', 0)\,\delta_{\mu_1\mu_3'}\, \omega(\underline{k}_f, \underline{k}_s) \end{aligned} \tag{1.95}$$

where the C's are Clebsch-Gordon coefficients.

We must now examine the different combinations of spins that may occur. Let the initial spins be $\mu_1 = +\frac{1}{2}$, $\mu_2 = +\frac{1}{2}$ and $\mu_3 = -\frac{1}{2}$. In this case the spin function for the ground state of the helium atom is given by

$$v(0,0\,|\,\sigma_2,\sigma_3) = \frac{1}{\sqrt{2}}\left\{\delta(\tfrac{1}{2}|\sigma_2)\delta(-\tfrac{1}{2}|\sigma_3) - \delta(-\tfrac{1}{2}|\sigma_2)\delta(\tfrac{1}{2}|\sigma_3)\right\} \qquad (1.96)$$

If we consider the final state we see that μ_1', μ_2' and μ_3' may form any of the following combinations

	μ_1'	μ_2'	μ_3'
a)	$+\frac{1}{2}$	$+\frac{1}{2}$	$-\frac{1}{2}$
b)	$+\frac{1}{2}$	$-\frac{1}{2}$	$+\frac{1}{2}$
c)	$-\frac{1}{2}$	$+\frac{1}{2}$	$+\frac{1}{2}$

which give rise to the contributions

a) $$f_{k_f k_s}(0,0,\tfrac{1}{2}\,|\,\tfrac{1}{2},\tfrac{1}{2},-\tfrac{1}{2}) = C(\tfrac{1}{2},\tfrac{1}{2},0;\tfrac{1}{2},-\tfrac{1}{2},0)\delta_{\frac{1}{2}\frac{1}{2}}f(\underline{k}_f,\underline{k}_s) + C(\tfrac{1}{2},\tfrac{1}{2},0;-\tfrac{1}{2},\tfrac{1}{2},0)\delta_{\frac{1}{2}\frac{1}{2}}g(\underline{k}_f,\underline{k}_s) + C(\tfrac{1}{2},\tfrac{1}{2},0;+\tfrac{1}{2},\tfrac{1}{2},0)\delta_{\frac{1}{2}-\frac{1}{2}}\omega(\underline{k}_f,\underline{k}_s)$$

b) $$f_{k_f k_s}(0,0,\tfrac{1}{2}\,|\,\tfrac{1}{2},-\tfrac{1}{2},\tfrac{1}{2}) = C(\tfrac{1}{2},\tfrac{1}{2},0;-\tfrac{1}{2},\tfrac{1}{2},0)\delta_{\frac{1}{2}\frac{1}{2}}f(\underline{k}_f,\underline{k}_s) + C(\tfrac{1}{2},\tfrac{1}{2},0;\tfrac{1}{2},\tfrac{1}{2},0)\delta_{\frac{1}{2}-\frac{1}{2}}g(\underline{k}_f,\underline{k}_s) + C(\tfrac{1}{2},\tfrac{1}{2},0;\tfrac{1}{2},-\tfrac{1}{2},0)\delta_{\frac{1}{2}\frac{1}{2}}\omega(\underline{k}_f,\underline{k}_s)$$

c) $$f_{k_f k_s}(0,0,\tfrac{1}{2}\,|\,-\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2}) = C(\tfrac{1}{2},\tfrac{1}{2},0;\tfrac{1}{2},\tfrac{1}{2},0)\delta_{\frac{1}{2}-\frac{1}{2}}f(\underline{k}_f,\underline{k}_s) + C(\tfrac{1}{2},\tfrac{1}{2},0;\tfrac{1}{2},-\tfrac{1}{2},0)\delta_{\frac{1}{2}\frac{1}{2}}g(\underline{k}_f,\underline{k}_s) + C(\tfrac{1}{2},\tfrac{1}{2},0;-\tfrac{1}{2},\tfrac{1}{2},0)\delta_{\frac{1}{2}\frac{1}{2}}\omega(\underline{k}_f,\underline{k}_s)$$

Now the only non-zero Clebsch-Gordon coefficients are $C(\frac{1}{2},\frac{1}{2},0;\frac{1}{2},-\frac{1}{2},0)$ and $C(\frac{1}{2},\frac{1}{2},0;-\frac{1}{2},\frac{1}{2},0)$ and these are given by

$$C(\tfrac{1}{2},\tfrac{1}{2},0;\tfrac{1}{2},-\tfrac{1}{2},0) = \frac{1}{\sqrt{2}}\int\left\{\delta(\tfrac{1}{2}|\sigma_2)\delta(-\tfrac{1}{2}|\sigma_3) - \delta(-\tfrac{1}{2}|\sigma_2)\delta(\tfrac{1}{2}|\sigma_3)\right\}^* \delta(\tfrac{1}{2}|\sigma_2)\delta(-\tfrac{1}{2}|\sigma_3)\,d\sigma_2 d\sigma_3$$

$$= \frac{1}{\sqrt{2}}$$

and

$$C(\tfrac{1}{2},\tfrac{1}{2},0;-\tfrac{1}{2},\tfrac{1}{2},0) = \frac{1}{\sqrt{2}}\int\{\delta(\tfrac{1}{2}|\sigma_2)\delta(-\tfrac{1}{2}|\sigma_3)-\delta(-\tfrac{1}{2}|\sigma_2)\delta(\tfrac{1}{2}|\sigma_3)\}^{*}$$

$$\delta(-\tfrac{1}{2}|\sigma_2)\delta(\tfrac{1}{2}|\sigma_3)d\sigma_2 d\sigma_3$$

$$= -\frac{1}{\sqrt{2}}$$

Hence, applying these results, we obtain

$$f_{k_f k_s}(0,0,\tfrac{1}{2}|\tfrac{1}{2},\tfrac{1}{2},-\tfrac{1}{2}) = \frac{1}{\sqrt{2}}f(\underline{k}_f,\underline{k}_s) - \frac{1}{\sqrt{2}}g(\underline{k}_f,\underline{k}_s)$$

$$f_{k_f k_s}(0,0,\tfrac{1}{2}|\tfrac{1}{2},-\tfrac{1}{2},\tfrac{1}{2}) = -\frac{1}{\sqrt{2}}f(\underline{k}_f,\underline{k}_s) + \frac{1}{\sqrt{2}}\omega(\underline{k}_f,\underline{k}_s)$$

$$f_{k_f k_s}(0,0,\tfrac{1}{2}|-\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2}) = \frac{1}{\sqrt{2}}g(\underline{k}_f,\underline{k}_s) - \frac{1}{\sqrt{2}}\omega(\underline{k}_f,\underline{k}_6)$$

(1.97)

Now the probability for any particular transition is proportional to the square of the associated amplitude, as indicated by equations (1.34) and (1.74). Consequently our interest is directed toward the quantity

$$\sum_{\mu_1,\mu_1'\mu_2'\mu_3'} \left| f_{k_f k_s}(0,0,\mu_1|\mu_1'\mu_2'\mu_3')\right|^2 \qquad (1.98)$$

Since μ_1 has two possible values, each giving an equal contribution to the sum of (1.98) then, using the expressions of (1.97), we have

$$\sum_{\mu_1,\mu_1'\mu_2'\mu_3'} \left| f_{k_f k_s}(0,0,\mu_1|\mu_1'\mu_2'\mu_3')\right|^2$$

$$= 2\left\{ \left|\frac{1}{\sqrt{2}}f(\underline{k}_f,\underline{k}_s)-\frac{1}{\sqrt{2}}g(\underline{k}_f,\underline{k}_s)\right|^2 + \left|-\frac{1}{\sqrt{2}}f(\underline{k}_f,\underline{k}_s)+\frac{1}{\sqrt{2}}\omega(\underline{k}_f,\underline{k}_s)\right|^2 \right.$$

$$\left. + \left|\frac{1}{\sqrt{2}}g(\underline{k}_f,\underline{k}_s)-\frac{1}{\sqrt{2}}\omega(\underline{k}_f,\underline{k}_6)\right|^2 \right\}$$

$$= 2\left\{ |f(\underline{k}_f,\underline{k}_s)|^2 + |g(\underline{k}_f,\underline{k}_s)|^2 + |\omega(\underline{k}_f,\underline{k}_s)|^2 - \mathcal{R}e.\left[f(\underline{k}_f,\underline{k}_s)g^*(\underline{k}_f,\underline{k}_s)\right] - \mathcal{R}e.\left[\omega^*(\underline{k}_f,\underline{k}_s)\left(f(\underline{k}_f,\underline{k}_s)+g(\underline{k}_f,\underline{k}_s)\right)\right]\right\}$$

If we now average over the spin states of the target and incident electron, representing the averaged sum by $q(\underline{k}_f,\underline{k}_s)$, we obtain

$$q(\underline{k}_f,\underline{k}_s) = [2(2S_A+1)]^{-1}{\sum}' \left| F_{\underline{k}_f\underline{k}_s}(0,0,\mu_1|\mu_1'\mu_2'\mu_3')\right|^2$$
$$= |f(\underline{k}_f,\underline{k}_s)|^2 + |g(\underline{k}_f,\underline{k}_s)|^2 + |\omega(\underline{k}_f,\underline{k}_s)|^2$$
$$- \mathcal{R}e.\left[f(\underline{k}_f,\underline{k}_s)g^*(\underline{k}_f,\underline{k}_s)\right]$$
$$- \mathcal{R}e.\left[\omega^*(\underline{k}_f,\underline{k}_s)\left(f(\underline{k}_f,\underline{k}_s)+g(\underline{k}_f,\underline{k}_s)\right)\right] \tag{1.99}$$

Let $W_{m\underline{k}_f\underline{k}_s}$ represent the transition probability per unit time, taking full account of all rearrangements that may contribute to the final state of ionization. Then from the analogues of equations (1.34) and (1.74) it follows that this is given by

$$W_{m\underline{k}_f\underline{k}_s} = \frac{\hbar^3}{(2\pi)^3\mu^2}\,\delta(E(m,\underline{k}_f,\underline{k}_s)-E)\,q(\underline{k}_f,\underline{k}_s) \tag{1.100}$$

It is convenient at this stage to adopt the system of atomic units $(a.u.)$ for our measurements. This merely requires that we set $\mu = 1,\ \hbar = 1$ in all previous expressions, where appropriate.

Now as a consequence of the Uncertainty Principle there will be a group of states, centred around $E(m,k_f,k_s) = E$, into which the system may make transitions, all of which will be observed as the same excitation process. The probability of transitions, per unit time, to a group of such states is

$$W_{m\underline{k}_f\underline{k}_s} = \int_{E-\Delta E}^{E+\Delta E} W_{m\underline{k}_f\underline{k}_s}\,\rho(E(m,k_f,k_s))\,dE(m,k_f,k_s)\,d\Omega_f \qquad (1.101)$$

where $\rho(E(m,k_f,k_s))$ the density of states per unit solid angle, may be replaced by $\rho(k_f)$ the density of states per unit solid angle for the 'fast' outgoing electron.

Then substituting from (1.100) we obtain

$$W_{m\underline{k}_f\underline{k}_s} = \frac{1}{(2\pi)^3}\,\rho(k_f)\,q(\underline{k}_f,\underline{k}_s)\,d\Omega_f$$

When deriving an expression for the density of states, $\rho(k_f)$, it is convenient to initially consider the ionization process to be restricted to a finite volume of space. In this event we may use box normalization, the normalization factor associated with a free electron wavefunction being $L^{-3/2}$, where L is the edge length of the confining cube. Later we shall take the limit in which the cube encompasses all space. For the present situation it is easily shown that $\rho(k_f) = k_f\left(\frac{L}{2\pi}\right)^3$ and so we arrive at the following expression for the probability of transitions per unit time

$$W_{m\underline{k}_f\underline{k}_s} = \frac{L^3}{(2\pi)^6}\,k_f\,q(\underline{k}_f,\underline{k}_s)\,d\Omega_f \qquad (1.102)$$

The target system experiences a transition to an ionized state, which may be regarded as an excitation to a continuum state. However unlike the ordinary case of excitation for which each electron occupies a discrete state, we now have an electron flux, of magnitude k_s into a group of continuum states. The experimentally observed quantity would be the electron flux, per unit solid angle, into the continuum states, resulting from an incident beam of unit flux. Since the flux of the incident beam is $k_0 L^{-3}$ per unit area and time then the probability per unit time, dP, corresponding to the scattering of the 'slow' electron into an element of solid angle, $d\Omega_s$, is given by

$$dP = W_{m\underline{k}_f\underline{k}_s} L^3 \frac{k_s}{k_0}\, d\Omega_s$$

where k_0 is the magnitude of the momentum of an incident electron.

Thus applying the result of (1.102) we obtain

$$dP = \left(\frac{L}{2\pi}\right)^6 \frac{k_f k_s}{k_0}\, q(\underline{k}_f, \underline{k}_s)\, d\Omega_f\, d\Omega_s \tag{1.103}$$

Let P be the total probability, per unit time, of observing a final state in which the electron momenta have magnitudes k_f and k_s. Then clearly

$$P = \int dP = \iint \frac{L^6}{(2\pi)^6} \frac{k_f k_s}{k_0}\, q(\underline{k}_f, \underline{k}_s)\, d\Omega_f\, d\Omega_s \tag{1.104}$$

by use of equation (1.103).

If we introduce the quantity $I(\hat{\underline{k}}_f, \hat{\underline{k}}_s)$ to represent the probability, per unit time, that the particular state of ionization characterized by the two momentum vectors $\underline{k}_f$ and $\underline{k}_s$ will result from the impact by an incident beam of unit flux, then

$$P = \iint I(\hat{\underline{k}}_f, \hat{\underline{k}}_s)\, d\Omega_f\, d\Omega_s \tag{1.105}$$

Comparison of equations (1.104) and (1.105) leads to the result

$$I(\hat{\underline{k}}_f, \hat{\underline{k}}_s) = \frac{L^6}{(2\pi)^6} \frac{k_f k_s}{k_0}\, q(\underline{k}_f, \underline{k}_s) \tag{1.106}$$

Since the quantity $q(\underline{k}_f, \underline{k}_s)$ is a combination of products of pairs of the amplitudes and each amplitude involves two free electron wavefunctions, with associated normalization factors $L^{-3/2}$, it is clear that a factor L^{-6} arises from $q(\underline{k}_f, \underline{k}_s)$. Consequently the expression of (1.106) is independent of the choice of normalization. In the limit of infinite interaction space, adopting the usual normalization proceedure, $L^{-3/2}$ is replaced by $(2\pi)^{-3/2}$ and (1.106) becomes

$$\mathcal{I}(\hat{\underline{k}}_f,\hat{\underline{k}}_s) = \frac{k_f k_s}{k_0} q(\underline{k}_f,\underline{k}_s) \qquad (1.107)$$

Because, for fixed incident energy, $\mathcal{I}(\hat{\underline{k}}_f,\hat{\underline{k}}_s)$ depends upon the angular co-ordinates of both outgoing electrons and the energy of either, it is known as the triple differential cross-section. It is sometimes convenient to indicate this by writing it in the form

$$\mathcal{I}(\hat{\underline{k}}_f,\hat{\underline{k}}_s) = \frac{d^3\sigma}{d\hat{\underline{k}}_f d\hat{\underline{k}}_s d\epsilon_s} \qquad (1.108)$$

where the symbol σ denotes the total cross-section and $\epsilon_s=\frac{1}{2}k_s^2$, the energy of the 'slow' ionization electron.

* we recall that the wavefunction satisfying the full Schrodinger equation has developed from an initial state containing a free electron wavefunction.

CHAPTER 2

In developing the formulation contained in Chapter 1 it was assumed that it is possible to distinguish times in the remote past and future for which the interaction is absent. This is equivalent to considering the interaction potential to be of limited range. However, in electron-atom collisions the incident electron interacts with the target atom via coulomb potentials, which are well known for their long range effects. In the initial state the incoming electron will see an electrically neutral target and only as it nears the target will it be able to distinguish between the individual potentials of the constituent particles. Hence although we are dealing with Coulomb potentials it is sensible to refer to a prior interaction state in the distant past. However, after ionization has occurred, although the slower outgoing electron will tend to screen the 'fast' electron from the charge of the residual ion, it is unlikely that the ion and 'slow' electron will appear sufficiently localized to be considered electrically neutral. Clearly the asymptotic form of the wave function representing the interacting systems is dependent upon the character of the interactio potential existing in the final state. Should this potential behave like a screened Coulomb potential then it is not possible to represent the 'fast' electron by a plane wave, irrespective of how energetic it may be. Hence it would not be possible to distinguish a time in the distant future at which the interaction was absent. For such a situation the approach to the ionization problem previously used is no longer applicable.

If the interaction potential in the ionized state is of a short range nature then a plane wave representation for the 'fast' outgoing electron in the asymptotic form of the full wave function is adequate and the approach presented in Chapter 1 remains valid.

To allow for the presence of a long range interaction potential in the ionized state it is necessary to seek an alternativ approach to the ionization problem. In 2.1 we shall outline an approach due to Rudge (1968).

2.1 Solution in hyperspherical co-ordinates.

In this section it is our intention to rewrite the usual time independent Schrodinger equation in terms of hyperspherical co-ordinates and then transform this to give the corresponding integral form for the wave function from which, by due consideration of the asymptotic form, we may extract an expression for the scattering amplitude.

One advantage resulting from the use of hyperspherical co-ordinates is that it is possible to investigate the asymptotic form of the wave function when both outgoing electrons are far removed from the residual ion by considering the asymptotic dependence upon a single variable in the hyperspherical co-ordinate system.

We shall develop this alternative treatment through consideration of the particular case of the ionization of atomic hydrogen b electron impact. The results so obtained may be easily generalized to the ionization of more complex atoms.

The wave function $\Psi(\underline{r}_1,\underline{r}_2)$ representing the interacting systems satisfies the time independent Schrodinger equation

$$\mathcal{H}\,\Psi(\underline{r}_1,\underline{r}_2) = \frac{1}{2}\chi^2\,\Psi(\underline{r}_1,\underline{r}_2) \tag{2.1}$$

where $\frac{1}{2}\chi^2 = E$, the total energy of the interacting systems and

$$\mathcal{H} = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - \frac{1}{r_1} - \frac{1}{r_2} + \frac{1}{r_{12}}$$

We shall now introduce the system of hyperspherical co-ordinate $(\theta_1,\phi_1,\theta_2,\phi_2,\alpha,\rho)$ where $(\theta_i,\phi_i,\ i=1,2)$ are the usual angular co-ordinates of the two electrons, as measured in the spherical polar co-ordinate system, and the quantities α, ρ are defined by

$$\left.\begin{aligned} r_1 &= \rho\cos\alpha \\ r_2 &= \rho\sin\alpha \end{aligned}\right\} \quad 0 \leqslant \alpha \leqslant \frac{\pi}{2} \tag{2.2}$$

Defining an additional quantity

$$\zeta(\hat{r}_1, \hat{r}_2, \alpha) = (\sin\alpha)^{-1} + (\cos\alpha)^{-1} - (1 - \cos\theta_{12}\sin 2\alpha)^{-1/2} \tag{2.3}$$

enables us to transform equation (2.1) to the hyperspherical form

$$\mathcal{L}\Phi = (\rho^{-2})\Lambda\Phi \tag{2.4}$$

having made the substitution $\Psi(r_1, r_2) = \Phi(r_1, r_2)\rho^{-5/2}$

In equation (2.4) $\mathcal{L}$ and Λ denote differential operators having the following forms

$$\begin{aligned} \mathcal{L} &= \frac{\partial^2}{\partial\rho^2} + x^2 + \frac{2\zeta}{\rho} - \frac{15}{4\rho^2} \\ \Lambda &= (\sin^2\alpha\cos^2\alpha)^{-1}\Big\{\cos^2\alpha\, L_2^2 + \sin^2\alpha\, L_1^2 \\ &\qquad - \frac{\partial}{\partial\alpha}\Big(\sin^2\alpha\cos^2\alpha\frac{\partial}{\partial\alpha}\Big)\Big\} \end{aligned} \tag{2.5}$$

with $L_i^2 = -(\sin\theta_i)^{-1}\dfrac{\partial}{\partial\theta_i}\Big(\sin\theta_i\dfrac{\partial}{\partial\theta_i}\Big) - (\sin^2\theta_i)^{-1}\dfrac{\partial^2}{\partial\phi_i^2}$

The homogeneous differential equation associated with (2.4) is $\mathcal{L}\Phi = 0$ which is of a standard form having linearly independent solutions $F(\zeta, x, \rho)$ and $H(\zeta, x, \rho)$, denoting the radial Coulomb functions with asymptotic forms

$$\left.\begin{aligned} F(\zeta, x, \rho) &\sim x^{-5/2}\sin[f(\rho)] \\ H(\zeta, x, \rho) &\sim x^{-5/2}\exp[if(\rho)] \end{aligned}\right\} \rho \to \infty \tag{2.6}$$

where $f(\rho) = \chi\rho + (\zeta/\chi)\ln(2\chi\rho) - \frac{3}{4}\pi + \arg\Gamma(\frac{5}{2} - i\zeta/\chi)$

By using a suitable combination of these functions, such that the correct boundary conditions are satisfied, we are able to construct the Green's function for the problem. Proceeding in this way it is readily shown that the wave function $\Phi(\mathbf{r}_1, \mathbf{r}_2)$ satisfies the integral equation

$$\Phi(\zeta,\chi,\rho) = -\chi^4\Big[H(\zeta,\chi,\rho)\int_0^\rho \rho^{-2}F(\zeta,\chi,\rho)\Lambda\Phi\,d\rho + F(\zeta,\chi,\rho)\int_\rho^\infty \rho^{-2}H(\zeta,\chi,\rho)\Lambda\Phi\,d\rho\Big] \qquad (2.7)$$

Now in the final state of ionization we are concerned with the asymptotic behaviour of the wave function as r_1, r_2 and $r_{12} \to \infty$ simultaneously. This threefold limiting process may be achieved by considering the behaviour of the form of the wave function contained in (2.7) as $\rho \to \infty$ (provided that we exclude the points $\alpha = 0, \alpha = \pi/2$ and $(\alpha = \frac{\pi}{4}, \theta_{12} = 0)$).

If we retain only the leading term in this asymptotic form then we obtain

$$\Phi(\zeta,\chi,\rho) \sim -\chi^{3/2} e^{i[\chi\rho + (\zeta/\chi)\ln(2\chi\rho) - \frac{3}{4}\pi + \arg\Gamma(\frac{5}{2} - i\zeta/\chi)]} \int_0^\infty \rho^{-2}F(\zeta,\chi,\rho)\Lambda\Phi\,d\rho \qquad \rho \to \infty \qquad (2.8)$$

It is useful to make a comparison between the expression in (2.8) and the asymptotic form of the wave function corresponding to the scattering of an electron by an attractive Coulomb field (c.f. Landau and Lifshitz 1965). The factor $e^{i[\chi\rho + (\zeta/\chi)\ln(2\chi\rho)]}$ appearing in (2.8) is clearly the analogue of one such exponential factor occurring in the asymptotic coulomb function. An extension of this comparison of terms leads us to make the following identification for the scattering amplitude:

$$f(\hat{\mathbf{r}}_1,\hat{\mathbf{r}}_2,\alpha) = -\exp[i\arg\Gamma(\tfrac{5}{2}-i\tfrac{\zeta}{\chi})] \int_0^\infty \rho^{-2}F(\zeta,\chi,\rho)\Lambda\Phi\, d\rho \tag{2.9}$$

Hence we obtain the asymptotic form

$$\Phi(\zeta,\chi,\rho) \sim -i^{1/2}(\chi)^{3/2} f(\hat{\mathbf{r}}_1,\hat{\mathbf{r}}_2,\alpha)\, e^{i[\chi\rho+(\zeta/\chi)\ln(2\chi\rho)]}$$

from which follows

$$\Psi(\mathbf{r}_1,\mathbf{r}_2) \sim -i^{1/2}\left(\frac{\chi^3}{\rho^5}\right)^{1/2} f(\hat{\mathbf{r}}_1,\hat{\mathbf{r}}_2,\alpha)\, e^{i[\chi\rho+(\zeta/\chi)\ln(2\chi\rho)]} \qquad (r_1,r_2)\rightarrow\infty \tag{2.10}$$

However since this form of the scattering amplitude is of limited use we shall now show how it may be used to derive the more familiar integral form of the amplitude.

Let us consider the integral expression

$$\mathcal{I} = \int \Psi(\mathbf{r}_1,\mathbf{r}_2)(\mathcal{H}-E)\Phi(\mathbf{r}_1,\mathbf{r}_2)\, d\mathbf{r}_1 d\mathbf{r}_2 \tag{2.11}$$

where $\Psi(\mathbf{r}_1,\mathbf{r}_2)$ is the exact solution of the Schrödinger equation having the asymptotic form previously described, and $\Phi(\mathbf{r}_1,\mathbf{r}_2)$ is some wave function whose asymptotic form describes two continuum electrons moving in Coulomb like fields. We make the following choice for $\Phi(\mathbf{r}_1,\mathbf{r}_2)$

$$\Phi(\mathbf{r}_1,\mathbf{r}_2) \sim \phi_1(z_1,-\mathbf{k}_1|\mathbf{r}_1)\phi_2(z_2,-\mathbf{k}_2|\mathbf{r}_2) \qquad \rho\rightarrow\infty \tag{2.12}$$

where each ϕ_i is a solution of a differential equation of the form

$$[\nabla^2 + k_i^2 + \left(\frac{2z_i}{r}\right) + V_i(r)]\phi_i(z_i, -\underline{k}_i|\underline{r}) = 0$$

(2.13)

In the equations (2.12) and (2.13) $\underline{k}_i\,,\ i=1,2$ denote the momenta of the two continuum electrons in the final state of ionization, $k_i = |\underline{k}_i|,\ i=1,2\ ,\ V_i(r)$ represents some short range potential and the Z_i are effective charges which will be determined at a later stage.

The functions $\phi_i(z_i, -\underline{k}_i|\underline{r})$ have the asymptotic forms

$$\phi_i(z_i,-\underline{k}_i|\underline{r}) \underset{r\to\infty}{\sim} \left(\frac{2\pi}{ik_i r}\right)\Big\{\alpha(\hat{\underline{k}}_i,\hat{\underline{r}})e^{i[k_i r + (\frac{Z_i}{k_i})\ln(2k_i r)]} - \delta(\hat{\underline{k}}_i - \hat{\underline{r}})e^{-i[k_i r + (\frac{Z_i}{k_i})\ln(2k_i r)]}\Big\} \qquad (2.14)$$

where

$$\alpha(\hat{\underline{k}}_i,\hat{\underline{r}}) = \delta(\hat{\underline{k}}_i + \hat{\underline{r}}) + \left(\frac{ik_i}{2\pi}\right)f_{el.}(-\hat{\underline{k}}_i,\hat{\underline{r}})$$

$f_{el.}$ denoting the elastic scattering amplitude.

By applying a multi-dimensional form of the divergence theorem the integral $\mathcal{I}$ appearing in equation (2.11) may be reduced to a surface integral

$$\mathcal{I} = -\frac{1}{2}\mathop{\mathrm{Lmt.}}_{\rho\to\infty}\rho^5\int\left(\Psi\frac{\partial\Phi}{\partial\rho} - \Phi\frac{\partial\Psi}{\partial\rho}\right)\sin^2\alpha\cos^2\alpha\, d\alpha\, d\hat{\underline{r}}_1\, d\hat{\underline{r}}_2 \qquad (2.15)$$

This modified form of $\mathcal{I}$ may be evaluated by the application of two theorems concerning stationary phase (Jeffreys and Jeffreys 1956). These state that

$$\int_a^b f(x)e^{iRg(x)}dx \underset{R\to\infty}{\sim} f(x_0)\left[\frac{2\pi}{R|g''(x_0)|}\right]^{\frac{1}{2}} e^{i[g(x_0)R + \frac{1}{4}\pi\,\mathrm{sgn}(g''(x_0))]} \qquad (2.16)$$

provided that $g'(x_0) = 0,\ a \leqslant x_0 \leqslant b$. In the event of such a point not existing or if $f(x_0) = 0$, then

$$\int_a^b f(x)\,e^{iRg(x)}dx \sim \left\{\frac{f(x)\,e^{iRg(x)}}{iRg'(x)}\right\}\Bigg|_{x=a}^{x=b}$$

as $R\to\infty$

(2.17)

If we define

$$\left.\begin{aligned} k_1 &= X\cos\beta \\ k_2 &= X\sin\beta \end{aligned}\right\} \quad 0\leqslant\beta\leqslant\tfrac{1}{2}\pi$$

(2.18)

and substitute the asymptotic forms of the wave functions and their derivatives into the integral expression for $\mathcal{I}$, application of the stationary phase theorems (2.17) and (2.18) enables us to simplify to the following expression for $\mathcal{I}$

$$\mathcal{I} = -(2\pi)^{5/2} f(\hat{\underline{k}}_1,\hat{\underline{k}}_2)(\sin\beta)^{-2iZ_2/k_2}(\cos\beta)^{-2iZ_1/k_1}$$

$$\times \lim_{\rho\to\infty} e^{i[\zeta(\hat{\underline{k}}_1,\hat{\underline{k}}_2,\beta)/X - Z_1/k_1 - Z_2/k_2]\ln(2X\rho)}$$

(2.19)

the only contribution to the integral arising from the point of stationary phase corresponding to $\alpha=\beta$.

Now it is clear that the expression in (2.19) will contain a divergent phase factor unless the charge parameters satisfy the relation

$$\frac{Z_1}{k_1}+\frac{Z_2}{k_2} = \zeta(\hat{\underline{k}}_1,\hat{\underline{k}}_2,\beta)/X$$

which may be rewritten as

$$\frac{Z_1}{k_1}+\frac{Z_2}{k_2} = \frac{1}{k_1}+\frac{1}{k_2}-\frac{1}{|\underline{k}_1-\underline{k}_2|} \qquad (2.20)$$

Provided that the relation (2.20) is satisfied $\mathcal{I}$ is properly defined and given by

$$\mathcal{I} = -(2\pi)^{5/2} f(\hat{\underline{k}}_1,\hat{\underline{k}}_2)(\sin\beta)^{-2iZ_2/k_2}(\cos\beta)^{-2iZ_1/k_1}$$

(2.21)

A subsequent rearrangement of (2.21), after making the appropriate substitutions from (2.18), leads to the following expression for the scattering amplitude

$$f(\hat{\underline{k}}_1,\hat{\underline{k}}_2) = -(2\pi)^{-5/2}(\exp[i\Delta(\underline{k}_1,\underline{k}_2)])I \tag{2.22}$$

where $$\Delta(\underline{k}_1,\underline{k}_2) = 2\left[\frac{Z_1}{k_1}\ln\left(\frac{k_1}{X}\right)+\frac{Z_2}{k_2}\ln\left(\frac{k_2}{X}\right)\right]$$

Hence
$$f(\hat{\underline{k}}_1,\hat{\underline{k}}_2) = -(2\pi)^{-5/2}e^{i\Delta(\underline{k}_1,\underline{k}_2)}\int 2\Psi_S(\mathcal{H}-E)\Phi\, d\underline{r}_1 d\underline{r}_2$$

which may readily be generalized to the case of a target having an outer shell of n equivalent electrons

$$f(\hat{\underline{k}}_1,\hat{\underline{k}}_2) = -(2\pi)^{-5/2}e^{i\Delta(\underline{k}_1,\underline{k}_2)}\int 2\Psi_S(\underline{r}_1,\dots,\underline{r}_n)(\mathcal{H}-E)\Phi(\underline{r}_1,\dots,\underline{r}_n)\, d\underline{r}_1\dots\dots d\underline{r}_n \tag{2.23}$$

It should be noted that the definition of the scattering amplitude used in this section differs from that appearing in Chapter 1 in one fundamental respect. The final state wave function Φ in (2.23), unlike its counterpart in Chapter 1, has not been antisymmetrized and hence the term scattering amplitude as used in this and the previous Chapter describes two different quantities. For the case of helium the effect of this difference in the definition is to introduce an additional factor of two in the usual expression for the triple differential cross-section given by (1.107). This may be directly attributed to the fact that there are two equivalent electrons comprising the helium ground state.

Apart from this difference in definition, which may be easily remedied by simply replacing Φ by its anti-symmetric form in (2.23), we observe that the two forms of the amplitude are basically similar. However the wave function Φ in (2.23) now describes a final state in which the outgoing electrons continue to move under the influence of Coulomb like potentials, whereas before it was assumed that such interactions were absent. In addition we now have a momenta dependent phase factor associated with the amplitude, the significance of which we shall discuss later.

One interesting point that emerges from this alternative treatment is the fact that the final state wave function is not uniquely defined. Hence this approach does not actually resolve the problem regarding the exact nature of the final state wave function. Instead it provides a general form for this function characterized by effective charges Z_1 and Z_2 which are arbitrary, subject to the restriction imposed by (2.20). The relation (2.20) implies that the charges Z_1 and Z_2 are angle dependent quantities which asymptotically take full account of the Coulomb potentials. From purely physical considerations this situation would seem perfectly reasonable. By reason of the latitude present in the choice of final state wave function the approach outlined here is best regarded as essentially a trial function method. Although we are required to satisfy the relation (2.20) we have no prescription for the 'best' choice of effective charges.

Rudge and Schwartz (1966) have made calculations of the total ionization cross section of $H(1s)$ based on the theoretical model described. The final state wave function was represented by a product of two coulomb functions corresponding to the choice of effective charges:

$$\left.\begin{aligned} Z_1 &= 1 - \frac{k_1}{|\underline{k}_1 - \underline{k}_2|} \\ Z_2 &= 1 \end{aligned}\right\} \quad k_1 > k_2 \tag{2.24}$$

The results obtained did not represent a significant improvement over previous calculations and in fact in the intermediate and high energy regions were at even greater variance with experiment. It was argued that the choice of charges appearing in (2.24) might be partly responsible for the apparent failure of the calculations.

From physical considerations it would seem that the roles of the two outgoing electrons can be interchanged by merely interchanging the corresponding momentum vectors and consequently, since the effective charge seen by each electron is a function of the momenta alone, we might reasonably expect Z_1 and Z_2 to satisfy the relation

$$Z_1(\underline{k}_1, \underline{k}_2) = Z_2(\underline{k}_2, \underline{k}_1)$$

Such a symmetry relation is achieved by assigning the following values to Z_1 and Z_2

$$Z_1(\underline{k}_1, \underline{k}_2) = 1 - \frac{1}{2}\frac{k_1}{|\underline{k}_1 - \underline{k}_2|}$$

$$Z_2(\underline{k}_1, \underline{k}_2) = 1 - \frac{1}{2}\frac{k_2}{|\underline{k}_1 - \underline{k}_2|} \tag{2.25}$$

One consequence of such a choice would be that even at high energies the 'fast' outgoing electron would be moving in a Coulomb field since the corresponding effective charge will always be greater than zero. This remains so even when the 'slow' electron has zero energy and one might reasonably expect it to screen the 'fast' electron completely. Hence, in view of this discrepancy, the suitability of the choice of values in (2.25), although supported to some extent by physical considerations, must remain open to question. We shall see a further consequence of this particular choice at a later stage in this discussion.

Clearly it is possible to define the other two interaction amplitudes associated with the ionization of helium by simple analogy. Hence we obtain the following definitions for $f(\underline{k}_1, \underline{k}_2)$, $g(\underline{k}_1, \underline{k}_2)$ and $\omega(\underline{k}_1, \underline{k}_2)$ the direct, exchange and capture amplitudes respectively

$$f(\underline{k}_1,\underline{k}_2) = -(2\pi)^{-5/2} e^{i\Delta(\underline{k}_1,\underline{k}_2)} \int \Psi(\underline{r}_2,\underline{r}_3;\underline{r}_1)(\mathcal{H}-E) \Phi(\underline{r}_3,\underline{r}_1,\underline{r}_2)\, d\underline{r}_1 d\underline{r}_2 d\underline{r}_3$$

$$g(\underline{k}_1,\underline{k}_2) = -(2\pi)^{-5/2} e^{i\Delta(\underline{k}_1,\underline{k}_2)} \int \Psi(\underline{r}_2,\underline{r}_3;\underline{r}_1)(\mathcal{H}-E) \Phi(\underline{r}_3,\underline{r}_2,\underline{r}_1)\, d\underline{r}_1 d\underline{r}_2 d\underline{r}_3$$

$$\omega(\underline{k}_1,\underline{k}_2) = -(2\pi)^{-5/2} e^{i\Delta(\underline{k}_1,\underline{k}_2)} \int \Psi(\underline{r}_2,\underline{r}_3;\underline{r}_1)(\mathcal{H}-E) \Phi(\underline{r}_1,\underline{r}_2,\underline{r}_3)\, d\underline{r}_1 d\underline{r}_2 d\underline{r}_3 \tag{2.26}$$

where the wave function Ψ is the solution of the full time independent Schrödinger equation describing the collision process and Φ, the complex conjugate of the final state wave function, is formed from the product of two functions $\phi_i(z_i(\underline{k}_1,\underline{k}_2), -\underline{k}_i \,|\, \underline{r}_j)$, previously defined, and the complex conjugate of the function describing the ground state of the residual ion. The indexes 1, 2 and 3 appearing in the definitions (2.26) refer to the incident and atomic electrons respectively.

Since we expect the roles of the two outgoing electrons to be interchanged as a consequence of interchanging the corresponding momentum vectors then both $g(\underline{k}_1,\underline{k}_2)$ and $f(\underline{k}_2,\underline{k}_1)$ must relate to the same physical process and must therefore be proportional to each other. (This of course assumes that the form of the wave function chosen to describe each outgoing electron is appropriate for the entire momentum range.)

Peterkop (1961) independently developed a treatment of the ionization problem using an approach closely resembling that of Rudge et al and was the first to show that suitable definition of normalization and phase factors leads to the relation

$$g(\underline{k}_1,\underline{k}_2) = f(\underline{k}_2,\underline{k}_1) \tag{2.27}$$

A demonstration of the derivation of this relation is easily achieved by means of a simple manipulation of the expression representing the exchange amplitude in (2.26). Now from (2.26) we have

$$g(\underline{k}_1,\underline{k}_2) = -(2\pi)^{-5/2} e^{i\Delta(\underline{k}_1,\underline{k}_2)} \int \Psi(\underline{r}_2,\underline{r}_3;\underline{r}_1)(\mathcal{H}-E)$$

$$\psi^*(\underline{r}_3)\phi_1(z_1(\underline{k}_1,\underline{k}_2),-\underline{k}_1|\underline{r}_2)\phi_2(z_2(\underline{k}_1,\underline{k}_2),-\underline{k}_2|\underline{r}_1)d\underline{r}_1 d\underline{r}_2 d\underline{r}_3$$

But we have shown previously that the choice of effective charges Z_1 and Z_2 is arbitrary provided that the constraint imposed by (2.20) is satisfied. Hence if we replace $Z_2(\underline{k}_1,\underline{k}_2)$ by $Z_1(\underline{k}_2,\underline{k}_1)$ and $Z_1(\underline{k}_1,\underline{k}_2)$ by $Z_2(\underline{k}_2,\underline{k}_1)$ the relation (2.20) will still be satisfied and the phase $\Delta(\underline{k}_1,\underline{k}_2)$ is then replaced by $\Delta(\underline{k}_2,\underline{k}_1)$. Thus we obtain the relation (2.27). In subsequent discussion we shall refer to the form of the exchange amplitude resulting from the use of (2.27) as the "Peterkop form".

It should be noted that the choice of effective charges given by (2.25) leaves the phase factor unaltered under the transformation: $\underline{k}_1 \to \underline{k}_2,\ \underline{k}_2 \to \underline{k}_1$ associated with (2.27), since $\Delta(\underline{k}_1,\underline{k}_2) = \Delta(\underline{k}_2,\underline{k}_1)$ in this case.

The three amplitudes defined by (2.26) may be combined to give the triple differential cross section

$$\frac{d^3\sigma}{d\epsilon_1 d\hat{\underline{k}}_1 d\hat{\underline{k}}_2} = \frac{2k_1k_2}{k_0} q(\underline{k}_1,\underline{k}_2) \tag{2.28}$$

where $q(\underline{k}_1,\underline{k}_2)$ has form identical to that defined by equation (1.99), $\epsilon_1 = \frac{1}{2}k_1^2$ and $\underline{k}_0$ denotes the momentum of the incident electron. The presence of the factor 2 in (2.28) which does not appear in (1.107), has already been explained.

If we consider the form of $g(\underline{k}_1,\underline{k}_2)$ given by (1.99) it is clear that the phase factor associated with each amplitude only assumes any importance if we use the 'Peterkop form' of the exchange amplitude. In this case we obtain a phase difference of $\Delta(\underline{k}_1,\underline{k}_2)-\Delta(\underline{k}_2,\underline{k}_1)$ between the exchange amplitude and either of the other two amplitudes, which will obviously affect the way in which these amplitudes interfere. However, it is observed that the choice of effective charges given by (2.25) eliminates any phase difference and so leads to a simplification of the interference problem.

Other approximate models using the 'Peterkop form' of the exchange amplitude have also included a phase difference between the amplitudes although the prescription for the form of this quantity has varied somewhat, largely depending upon the particular approach to the problem used.

Yet another approach to the ionization problem is provided by Geltman (1969) who, like Rudge, also maintains that both outgoing electrons in the final state should be considered to move in Coulomb like fields. Hence the asymptotic form of the wave function corresponding to the ionization process should contain appropriate Coulomb-type wave representations of these electrons. Using the ionization of hydrogen as a simple example he demonstrates how the theory can be developed to achieve such a situation. Basically the approach consists of modifying the usual form of the integral equation derived from the Schrödinger equation such that the corresponding homogeneous equation describes two non-interacting electrons moving in pure Coulomb fields. The result of this alternative resolution for the integral equation is that, although the desired asymptotic form of the scattered part of the wave is obtained, the unperturbed part of the incident beam is now represented by a Coulomb function since it is contained in that part of the solution arising from the homogeneous equation. Clearly this does not seem to be in total accord with the physical situation.

Geltman has used this form of the wave function to derive the relation (2.27) but, in doing so, finds it necessary to eliminate the logarithmic phase factors appearing in the asymptotic forms of the Coulomb functions representing the outgoing electrons. This is achieved by assuming exponential damping of the Coulomb potentials. Such a device becomes necessary because the choice of effective charges takes no account of a possible energy dependence.

2.2. Approximate Methods

Although the various approaches examined in the previous discussion differ from each other in several aspects each associated form for the amplitudes is exact, within its terms of reference, in the sense that each has been derived without recourse to approximate forms of the wave functions. While it is true that the choice of representation of the final state of ionization is a source of contention, it should be recognised that this arises from a difference in the mathematical interpretation of the physical situation rather than a divergence of opinion upon the validity of different approximate methods.

All expressions so far obtained for the amplitudes involve the exact solution of the Schrödinger equation corresponding to the ionization process. In practice it is not possible to obtain the exact wave function describing any interaction process involving more than two distinct entities and one is forced to seek an approximate solution to the problem. In the following we shall describe a number of different approximate forms that have been used to replace the exact wave function.

Some approximations are readily suggested by particular ways in which we are able to express the exact wave function. The various orders of the Born approximation fall into such a class. These particular approximations are based on the theoretical approach to the ionization problem presented in Chapter 1, although one can easily derive their analogues using the alternative approaches contained in this chapter.

A suitable generalization of equation (1.56) yields the following integral form for the wave function $\chi^+_{\alpha_0}(\underline{r}',\underline{R}')$ describing the collision process

$$\chi^+_{\alpha_0}(\underline{r}',\underline{R}') = u_{\alpha_0}(\underline{r}',\underline{R}') + \int G^+_{0\omega_{\alpha_0}}(\underline{r}',\underline{R}';\underline{r},\underline{R}) \, V(\underline{r},\underline{R})\chi^+_{\alpha_0}(\underline{r},\underline{R})d\underline{r}\,d\underline{R} \qquad (2.29)$$

Where $u_{\alpha_0}(\underline{r}',\underline{R}')$ describes the unperturbed state, $G^+_{0\omega_{\alpha_0}}(\underline{r}',\underline{R}';\underline{r},\underline{R})$ denotes the corresponding retarded Green's function and V the interaction potential. In (2.29) $\underline{r}'$ denotes the spatial co-ordinates of the incident electron and $\underline{R}'=(\underline{r}_1',\ldots\ldots,\underline{r}_n')$ those of the n atomic electrons belonging to the target system.

Equation (2.29) may be written symbolically as

$$\chi^+_{\alpha_0} = u_{\alpha_0} + G^+_0 V \chi^+_{\alpha_0} \qquad (2.30)$$

where G^+_0 represents an integral operator.

Clearly the wave function $\chi^+_{\alpha_0}$ appearing on the right hand side of (2.30) may be replaced by the form given by (2.30), so leading to the result

$$\chi^+_{\alpha_0} = u_{\alpha_0} + G^+_0 V u_{\alpha_0} + G^+_0 V G^+_0 V \chi^+_{\alpha_0} \qquad (2.31)$$

This process may be continued indefinitely to generate the infinite Born or Neumann series

$$\chi^{+}_{\alpha_0} = \sum_{n=0}^{\infty} (G_0^{+}V)^n u_{\alpha_0} \tag{2.32}$$

We can obtain a whole class of approximations for the wave function $\chi^{+}_{\alpha_0}$ from (2.32) by merely terminating the series expansion after different numbers of terms. These give the Born approximations, the most commonly used being the first Born approximation obtained by terminating the series after the first two terms. In this case equation (2.29) is replaced by the approximate form

$$\chi^{+}_{\alpha_0}(\underline{r}',\underline{R}') = u_{\alpha_0}(\underline{r}',\underline{R}') + \int G^{+}_{0\omega_{\alpha_0}}(\underline{r}',\underline{R}';\underline{r},\underline{R}) \, V(\underline{r},\underline{R}) u_{\alpha_0}(\underline{r},\underline{R}) d\underline{r} d\underline{R} \tag{2.33}$$

Consequently wherever the function $\chi^{+}_{\alpha_0}$ appears in the expressions for the direct, exchange and capture amplitudes it is now replaced by the unperturbed function u_{α_0}.

The first Born approximation is valid for collisional processes involving high energy incident electrons since it can be shown to represent the dominant contribution to the process provided that Z, the charge carried by the nucleus of the target system, is not too large (see Schiff 1968)

Calculations of electron impact excitation (Woollings 1972) and double ionization (Tweed 1973) cross sections for various atoms have been made based on the second Born approximation but generally the repeated integrals involved render calculation so unwieldy as to be impractical without further approximation and a consequent loss in accuracy.

2.3. Approximate forms of the exchange amplitude

Even within the framework of the first Born approximation there exists considerable latitude in the choice of wave functions since it is not possible to construct exact functions describing electron-electron correlations. Of the approximate models that take account of exchange several use a modified form of the corresponding amplitude based upon the relation (2.27). Such modified forms are generally referred to as Born-exchange approximations. The phase factors associated with each of the amplitudes in the Rudge formulation are omitted but a phase difference between direct and exchange amplitudes is introduced by modifying (2.27) to the following form

$$g(\underline{k}_1,\underline{k}_2) = e^{i\tau(\underline{k}_1,\underline{k}_2)} f(\underline{k}_2,\underline{k}_1) \tag{2.34}$$

Whereas in the theoretical model developed by Rudge the presence of the phase factor $e^{i\tau(\underline{k}_1,\underline{k}_2)}$ was a natural consequence of the particular formulation of the problem used, in (2.34) it has become a form of parameter which may be adjusted to compensate for inaccuracies resulting from the approximate form of the exchange amplitude used. As an example of the use of the relation (2.34) we shall consider the calculations of Peach (1966) for the collisional ionization of a variety of atoms with outer s electrons. These calculations are based on the first Born approximation, the more energetic outgoing electron being represented by a plane wave and the other by a Coulomb function. Because each wave function is appropriate to a particular energy region we have the situation in which application of (2.34) leads to a totally inadequate description of the 'slow' electron for the exchange process. Clearly both phase and magnitude of the exchange amplitude are likely to be affected by the use of such an approximation. However, since exchange effects are most significant when the outgoing electrons have nearly equal energies, and in such cases plane wave descriptions for the two electrons may be adequate provided the energies are sufficiently large, then the Born-exchange approximation may provide a fairly good description of the exchange contrbution in the total cross section results.

The form of the phase difference $\tau(\underline{k}_1, \underline{k}_2)$ appearing in calculations based on the Born-exchange approximation has varied according to the particular criterion applied. Here we shall give two choices based on totally different criteria. The first of these, suggested by Peterkop [1962 (a)], is based on purely practical considerations. Since for intermediate and high energies first Born calculations tend to overestimate the total cross section it is advantageous to maximize the interference between the direct and exchange amplitudes since it is through the interference term that exchange makes its most significant contribution. This may be achieved by the choice

$$\tau(\underline{k}_1, \underline{k}_2) = \arg f(\underline{k}_1, \underline{k}_2) - \arg f(\underline{k}_2, \underline{k}_1) \tag{2.35}$$

The second choice which has been frequently used [Peterkop (1962a), Geltman, Rudge, and Seaton (1963) and Sloan (1965)] is given by

$$\tau(\underline{k}_1, \underline{k}_2) = \arg\Gamma(1 - iZ/k_1) - \arg\Gamma(1 - iZ/k_2) \tag{2.36}$$

where Z is the net charge on the new ion produced.
The origin of this choice of phase difference clearly stems from a Coulomb-type wave representation of the outgoing electrons.

Other approximate models have avoided the inaccuracy inherent in the use of the relation (2.27) by basing exchange calculations on the explicit form of the amplitude derived earlier. One such model is the Born-Oppenheimer approximation which has been used to calculate the ionization cross section of a variety of ions [Burke and Taylor (1965), $H(1s)$, $H(2s)$, $He^{+}(1s)$, $He^{+}(2s)$; Trefftz (1963), O^{+5}; Malik and Trefftz (1961), O^{+4}; Geltman (1960), H^{-}]. This approximation fails to reproduce the correct behaviour for the cross section, being in considerable error in the low and intermediate energy regions for the ionization of neutral species in an initial atomic 's' state as a result of spuriously large contributions to the cross section arising from 's' states of the scattered electron. Considerable improvement is obtained when the method is used to calculate ionization cross sections for positive ions (Burke and Taylor (1965)).

For the ionization of $H(1s)$ the approximation consists of adopting the following forms of the scattering amplitudes:

$$f(\underline{k}_1,\underline{k}_2) = -(2\pi)^{-5/2}\int \Psi(\underline{r}_1,\underline{r}_2)(H-E)\Phi(\underline{r}_1,\underline{r}_2)\,d\underline{r}_1\,d\underline{r}_2$$

$$g(\underline{k}_1,\underline{k}_2) = -(2\pi)^{-5/2}\int \Psi(\underline{r}_1,\underline{r}_2)(H-E)\Phi(\underline{r}_2,\underline{r}_1)\,d\underline{r}_1\,d\underline{r}_2 \qquad (2.37)$$

the capture process being excluded. In accordance with the first Born approximation the initial state wave function Ψ is given by the product of a free electron wave function and a hydrogenic $1s$ orbital while the final state wave function uses a plane wave description of the 'fast' outgoing electron and a Coulomb function ($Z = 1$) for the other.

Rudge and others have attributed the failure of the Born-Oppenheimer approximation to the lack of orthogonality between the functions $\Psi(\underline{r}_1,\underline{r}_2)$ and $\Phi(\underline{r}_2,\underline{r}_1)$ appearing in the exchange amplitude given by (2.37). They argue that the addition of a constant to the hamiltonian H would result in a change in the cross section as calculated from the amplitudes of (2.37), which contradicts the physical interpretation of such a change in the hamiltonion. However, as has been indicated by Schulz (1973), this situation does not arise.

Let us consider the Lippmann-Schwinger formulation for rearrangement collisions (§ 1.3). If two colliding systems a and b suffer a rearrangement resulting in component systems c and d then the corresponding ingoing and outgoing waves, χ^+_{ab} and χ^-_{cd} respectively, satisfy the equations (1.85) and (1.86), i.e.

$$\chi^+_{ab} = u_{ab} + (E - H_{ab} + i\epsilon)^{-1} H'_{ab} \chi^+_{ab} \qquad (2.38)$$

$$\chi^-_{cd} = u_{cd} + (E - H_{cd} - i\epsilon)^{-1} H'_{cd} \chi^-_{cd} \qquad (2.39)$$

where u_{ab} and u_{cd} satisfy the homogeneous equations

$$(H_{ab} - E) u_{ab} = 0 \quad , \quad (H_{cd} - E) u_{cd} = 0$$

We shall now examine the effect produced by introducing an additional constant, V_0, into the total hamiltonian H. For this purpose we need consider only the integral equation (2.38) together with the corresponding homogeneous equation. The quantity V_0 may be interpreted as an additional background potential and associated with this we must introduce an energy shift of E_0 in all states, where in our system of units (a.u.)

$$E_0 = V_0 \qquad (2.40)$$

Now formerly the Schrodinger equation corresponding to the collision process was given by the following

$$H\Psi = E\Psi \quad \text{or alternatively} \quad (H-E)\Psi = 0$$

However the additional background potential, V_0 , produces the energy shift $E \rightarrow E + E_0$ and so Ψ must satisfy the equation

$$(H + V_0)\Psi = (E + E_0)\Psi$$

which with the help of (2.40) reduces to the original form

$$(H - E)\Psi = 0$$

Hence the wave function Ψ describing the interaction of the systems is unaffected. Now since the potential V_0 is present in the unperturbed states existing before and after the interaction it cannot be considered to constitute part of the interaction potential (i.e. H'_{ab} and H'_{cd} remain unchanged). In the intial unperturbed state the same energy shift, E_0 , must be observed, so leading to the following equation for u_{ab}

$$(H_{ab} + V_0)u_{ab} = (E + E_0)u_{ab}$$

which reduces to

$$(H_{ab} - E)u_{ab} = 0$$

Consequently the wave function u_{ab} retains its original form. Clearly equation (2.38) is invariant with respect to this particular change in the hamiltonian. Similar manipulation of (2.39) and the corresponding homogeneous equation shows this to be true for these as well.

In essence the addition of a constant to the total hamiltonian produces a trivial shift in the energy levels that has no effect on the Born-Oppenheimer calculations for the exchange amplitude.

Consequently, as $\Psi(r_1, r_2)$ and $\Phi(r_2, r_1)$ are not eigen functions of the same hamiltonian, there is no necessity for them to be mutually orthogonal. However this does not imply that the wave functions should not be subject to some orthogonality condition since when approximate wave functions are used orthogonality conditions do at least introduce a measure of consistency into the model.

Another form of the exchange amplitude is provided by the Born-Ochkur approximation. Ochkur (1965) argued that the Born-Oppenheimer approximation was appropriate to high energy collisions and from this derived an alternative approximate form for the exchange amplitude, based on a series expansion, which he claimed to be valid for the entire energy range. Essentially the method used assumes that the wave function $\phi_{\underline{k}}(\underline{r})$ representing the 'slow' outgoing electron (and chosen to be a Coulomb wave in the Oppenheimer formulation) can be factorized into the form

$$\phi_{\underline{k}}(\underline{r}) = e^{i\underline{k}\cdot\underline{r}}\chi(\underline{k},\underline{r}) \tag{2.41}$$

where the function $\chi(\underline{k},\underline{r})$ varies slowly in comparison with $e^{i\underline{K}\cdot\underline{r}}$. $(\underline{K}=\underline{k}_0-\underline{k})$

This is equivalent to requiring that

$$|\underline{\nabla}\chi(\underline{k},\underline{r})| \ll |\underline{\nabla}e^{i\underline{K}\cdot\underline{r}}|$$

$$\text{i.e.} \quad |\underline{\nabla}\chi(\underline{k},\underline{r})| \ll K \tag{2.42}$$

Use of the form (2.41) leads to an integral of a similar nature to the usual Bethe integral appearing in first Born expressions for the direct amplitude. Repeated integration by parts with respect to two variables results in a series expansion in inverse powers of K. Provided that condition (2.42) is satisfied the dominant contribution arises from the first term of the series, all others containing derivatives of $\chi(\underline{k},\underline{r})$. By using an order of magnitude arguement, Ochkur shows that the contribution to the amplitude arising from the $1/r$ term in the interaction potential may be omitted. Hence he obtains the relation

$$g(\underline{k}_1,\underline{k}_2)=\frac{|\underline{k}_0-\underline{k}_1|^2}{|\underline{k}_0-\underline{k}_2|^2}f(\underline{k}_1,\underline{k}_2) \tag{2.43}$$

Ochkur provides no convincing explanation as to why this form should remain valid for collisional ionization at lower energies although in a number of cases this approximation, or modified forms of it, has shown considerable improvement over Born-exchange calculations. A particular example is given by the calculations of Peach (1966) for the ionization cross sections of He, Li, Be, Na and Mg from their ground states.

All approximate expressions for the exchange amplitude so far examined have been based on the first Born approximation for which Ψ the exact solution of the Schrödinger equation, is approximated with the wave function representing the initial unperturbed state of the systems. Burke and Taylor (1965) have attempted to remedy the situation by using an improved approximate form for the exact wave function. For the ionization of hydrogen this wave function takes the form

$$\Psi(\underline{r}_1,\underline{r}_2)=[1+(-1)^S P_{12}]\sum_{\gamma}\psi(\gamma|\underline{r}_2)F_{\gamma}(\underline{r}_1) \tag{2.44}$$

where the $\psi(\gamma|\underline{r})$ are hydrogenic orbitals and the summation is over the configurations (γ : $1s, 2s, 2p$). In equation (2.44) P_{12} is a permutation operator and S the total spin of the system.

The functions $F_{\gamma}(\underline{r})$ are obtained from the Hartree-Fock equations

$$\int\psi^*(\gamma|\underline{r}_2)(H-E)\Psi(\underline{r}_1,\underline{r}_2)\,d\underline{r}_2=0 \tag{2.45}$$

This model, which retains the Oppenheimer representation of the final state, has been referred to as the Distorted-Wave Born-Oppenheimer Method.

In spite of the greater sophistication of this model results obtained show no significant improvement over Born and Born-exchange calculations for ionization from the ground state. This would seem to indicate that better final state wave functions are required. However this method has been used with rather more success for the ionization of hydrogen from the 2s state.

2.4 SUMMARY

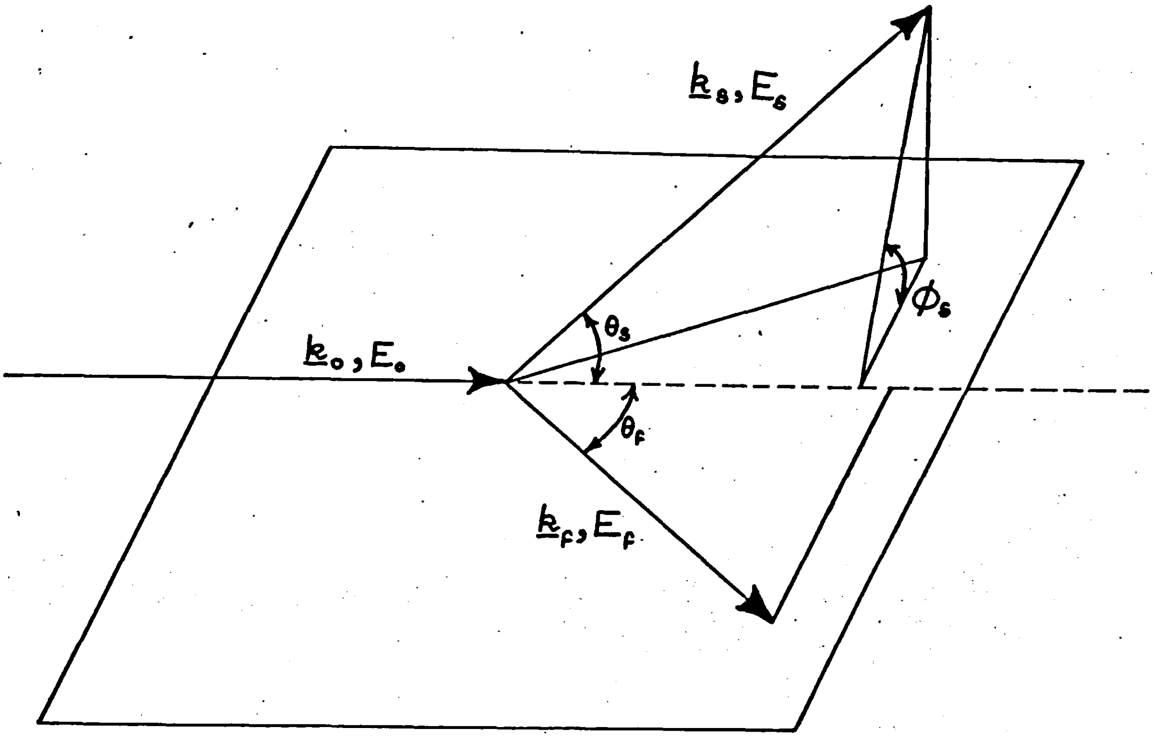
Before concluding this discussion on the use of approximate forms of the amplitudes we shall present a summary of the calculations that have been performed for the triple differential cross section corresponding to the ionization of helium. The three main contributors are Jacobs (1974), Geltman (1974) and Schulz (1973).

The approach used by Jacobs is based on the Born approximation the effects of exchange and capture being consistently excluded. In his treatment of the problem he is concerned with the development of a theoretical framework suitable for the calculation of triple differential cross sections corresponding to ionization in which target atom and residual ion occupy general states. The direct amplitude is expressed in terms of the Bethe generalized oscillator strength. This approach leads to a Legendre polynomial expansion for the amplitude which expresses the angular correlation between the two outgoing electrons in terms of the angle between the ejected electron momentum vector and the momentum transfer vector. The expansion obtained closely resembles the form of the amplitude given in chapters 3 and 4. In the subsequent calculations the main emphasis is on the accuracy of the helium ground state function, for which a 56-term Hylleraas expansion is used. The outgoing electrons are represented by $1s-2s-2p$ close coupling continuum functions.

We have already made mention of the Coulomb-projected Born approximation of Geltman et al. Basically this is designed to take specific account of the interaction between the "fast" outgoing electron and the target nucleus in the final state by using a Coulomb wave representation for this electron. Although this approximation requires the omission of a term from the interaction potential the effect is implicit in the wave functions and is not lost through orthogonality requirements as is the case with the ordinary Born approximation (c.f. Chapters 3 and 4). In the calculations of Geltman the "slow" outgoing electron is represented by a Coulomb function corresponding to an effective charge $27/16$ and the "fast" electron by a Coulomb function with effective charge 2. The ground state of the helium atom is represented by the simple one-parameter wave function defined in equation (3.5).

The model used by Schulz, although developed from different considerations, is of a similar nature to that of Geltman. In this model the two outgoing electrons are once again represented by Coulomb waves. However the two models differ in the choice of effective charges. Schulz has tried various combinations of effective charges, largely chosen in accordance with equation (2.20). In addition, from an analysis of the terms comprising the direct amplitude, Schulz is able to determine the dominant contributions to the binary and recoil peaks characterizing the differential cross section. He has used this information to produce a criterion on which to base the choice of effective charges. By this the charges are adjusted to achieve the largest value of the ratio between the sizes of the peaks. The calculations based on this model use a two-parameter Hartree-Fock wave function to represent the helium ground state.

FRAME OF REFERENCE FOR MEASUREMENT OF THE SCATTERING ANGLES



NOTATION:

$E_0, \underline{k}_0$	ENERGY AND MOMENTUM OF INCIDENT ELECTRON
$E_f, \underline{k}_f$	ENERGY AND MOMENTUM OF 'FAST' OUTGOING ELECTRON
$E_s, \underline{k}_s$	ENERGY AND MOMENTUM OF 'SLOW' OUTGOING ELECTRON

NOTE:

THE CALCULATIONS DESCRIBED IN THE FOLLOWING CHAPTERS ARE RESTRICTED TO THOSE CASES FOR WHICH THE TRAJECTORIES OF THE INCIDENT AND OUTGOING ELECTRONS ARE COPLANAR.

CHAPTER 3

The ionization of Helium by electron impact (using a simple one parameter wave function to represent the target system).

A variety of mathematical models used to calculate impact ionization cross sections for helium have been reviewed in the previous chapters. Although a number of these have taken account of the exchange process, to date all models have excluded the effects of capture. In this chapter it is our intention to assess the relative importance of the capture process in comparison with the direct and exchange scattering processes. In order to achieve this objective we have made calculations of $f(\underline{k}_f,\underline{k}_s)$, $g(\underline{k}_f,\underline{k}_s)$ and $\omega(\underline{k}_f,\underline{k}_s)$ the direct, exchange and capture amplitudes respectively as defined by Rudge (eq. 2.26), based on the first Born approximation (eq. 2.33).

These preliminary calculations are of an exploratory nature and hence the emphasis is largely on ease of computation, using adequate descriptions of the electron states involved, rather than high precision. With regard to the use of approximate wave functions it is recognised that while it is relatively simple to approximate a bound function to any desired degree of accuracy the same is not true for continuum state wave functions. Consequently the choice of representation for continuum states is a crucial factor in any calculations in which such states are involved. For this reason although we have used basic approximate bound state functions in these preliminary calculations considerable care has been taken to ensure a correct description of the continuum states involved.

3.1 The wave functions

The direct, exchange and capture amplitudes, denoted by $f(\underline{k}_f,\underline{k}_s)$, $g(\underline{k}_f,\underline{k}_s)$ and $\omega(\underline{k}_f,\underline{k}_s)$ respectively, are given by

$$f(\underline{k}_f,\underline{k}_s) = C\langle \Psi_{\underline{k}_f,\underline{k}_s}(1;2,3)|V(1,2,3)|\Psi_{\underline{k}_0}(1;2,3)\rangle$$

$$g(\underline{k}_f,\underline{k}_s) = C\langle \Psi_{\underline{k}_f,\underline{k}_s}(2;1,3)|V(1,2,3)|\Psi_{\underline{k}_0}(1;2,3)\rangle$$

$$\omega(\underline{k}_f,\underline{k}_s) = C\langle \Psi_{\underline{k}_f,\underline{k}_s}(2;3,1)|V(1,2,3)|\Psi_{\underline{k}_0}(1;2,3)\rangle \tag{3.1}$$

where $C = -(2\pi)^2 e^{i\Delta(\underline{k}_f,\underline{k}_s)}$, the quantity $\Delta(\underline{k}_f,\underline{k}_s)$ being a momenta dependent phase discussed in detail in chapter 2.

The indexes 1, 2 and 3 refer to the incident and atomic electrons respectively.

In accordance with the first Born approximation the wave functions $\Psi_{\underline{k}_0}(i;j,k)$ and $\Psi_{\underline{k}_f,\underline{k}_s}(i;j,k)$ describe the unperturbed states of the consistuent systems before and after ionization.

As before $\underline{k}_0$ denotes the momentum of the incident electron and $\underline{k}_f$ and $\underline{k}_s$ the momenta of the "fast" and "slow" outgoing electrons respectively.

The function $V(1,2,3)$ appearing in the expressions for the amplitudes given by equations (3.1) represents the interaction potential. There are two alternative forms for this potential depending on whether we use the interaction appropriate to the initial or final state of the systems. Corresponding to these two forms of the potential we have the prior and post formulations of the amplitudes respectively. (eqs. 1.91, 1.92). If the total hamiltonian corresponding to the collisional process is denoted by H and H_i and H_f are the respective hamiltonians associated with the intial and final unperturbed states then the forms of $V(1,2,3)$ appropriate to the prior and post formulations respectively are given by

$$V(1,2,3) = H - H_i \tag{3.2}$$

$$V(1,2,3) = H - H_f \tag{3.3}$$

Let us now direct our attention to the specific forms of the wave functions to be used in the expressions (3.1). The function $\Psi_{\underline{k}_0}$ describing the initial unperturbed state is clearly separable into the form

$$\Psi_{\underline{k}_0}(1;2,3) = \frac{1}{(2\pi)^{3/2}} e^{i\underline{k}_0\cdot\underline{r}_1}\,\Psi_0(\underline{r}_2,\underline{r}_3) \tag{3.4}$$

where the wave function Ψ_0 represents the target ground state and is, for the purposes of these calculations, approximated with the simple ansatz

$$\Psi_0(\underline{r}_2,\underline{r}_3) = \frac{\alpha^3}{\pi}\exp[-\alpha(r_2+r_3)] \qquad \alpha = \frac{27}{16} \tag{3.5}$$

The value of the parameter, α, is determined by means of the Rayleigh-Ritz variational principle.

For the final unperturbed state the corresponding wave function $\Psi_{\underline{k}_f,\underline{k}_s}$ must also be separable, i.e.

$$\Psi_{\underline{k}_f,\underline{k}_s}(i;j,k) = \frac{1}{(2\pi)^{3/2}} e^{i\underline{k}_f\cdot\underline{r}_i}\,\Psi_{\underline{k}_s}(\underline{r}_j,\underline{r}_k) \tag{3.6}$$

where $\Psi_{\underline{k}_s}$ describes the excited state of the target formed from the "slow" electron and residual ion. This excited state is approximated with the exchange-adiabatic model of Economides and

McDowell (1969). Their approach to the problem, which is a variant of the polarized orbital treatment of Sloan (1964), is outlined in the following section.

1 The Method of Polarized Orbitals.

Clearly the presence of the "Slow" continuum electron produces polarization of the residual ion with a consequent perturbation of the $1s$ state occupied by the remaining bound electron. The total antisymmetrized wave function for the electron-ion system is assumed to have the form

$$\begin{aligned}\Psi_{\underline{k}}^{A}(\underline{r}_1,\underline{r}_2) &= (1+P_{12})\Psi_{\underline{k}}(\underline{r}_1,\underline{r}_2)\\ &= (1+P_{12})\psi_{\underline{k}}(\underline{r}_1)[\psi_{1s}(Z,\underline{r}_2)+\psi^{pol}(\underline{r}_1,\underline{r}_2)]\end{aligned} \tag{3.7}$$

where P_{12} is the usual permutation operator and Z is the charge carried by the nucleus of the residual ion.

In the form (3.7) the function $\psi^{pol}(\underline{r}_1,\underline{r}_2)$ is an approximation to the first order perturbation of the ground state function $\psi_{1s}(Z,\underline{r}_2)$ produced by a stationary electron at $\underline{r}_1$. Following the method of Sloan we obtain the corresponding form of ψ^{pol},

$$\psi^{pol}(\underline{r}_1,\underline{r}_2) = -\frac{1}{(\pi Z)^{1/2}}\frac{\epsilon(\underline{r}_1,\underline{r}_2)}{r_1^2}e^{-Zr_2}\left(\frac{1}{2}Zr_2^2+r_2\right)\cos\theta_{12} \tag{3.8}$$

where

$$\epsilon(r_1,r_2) = \begin{cases}1 & r_1 > r_2\\ 0 & r_1 < r_2\end{cases}$$

and θ_{12} is the angle between the radial vectors $\underline{r}_1$ and $\underline{r}_2$.

When the continuum electron is far removed from the residual ion the function $\psi^{pol}(\underline{r}_1,\underline{r}_2)$ represents the dipole contribution to the first order perturbation of $\psi_{1s}(Z,\underline{r}_2)$.

In accordance with the variational principle applied by Sloan we take $\Psi_{\underline{k}}^{A}$ to be a solution of the equation:

$$\int \psi_{1s}^{*}(z,\underline{r}_2)(H-E)\Psi_{\underline{k}}^{A}(\underline{r}_1,\underline{r}_2)\,d\underline{r}_2=0 \tag{3.9}$$

where
$$H = -\frac{1}{2}(\nabla_1^2+\nabla_2^2)-\frac{z}{r_1}-\frac{z}{r_2}+\frac{1}{r_{12}}$$
and
$$E=\frac{1}{2}(k^2-z^2)$$

The function $\psi_{\underline{k}}(\underline{r})$ describing the continuum electron may be represented by a partial wave expansion (Faxén and Holtzmark 1929)

$$\psi_{\underline{k}}(\underline{r})=\frac{1}{(2\pi)^{3/2}k^{1/2}}\sum_{l=0}^{\infty}(2l+1)\,i^{l}e^{i(\sigma_l+\eta_l)}\frac{u_l(k,r)}{r}P_l(\hat{\underline{k}}\cdot\hat{\underline{r}}) \tag{3.10}$$

In the expansion (3.10) the function P_l is the Legendre polynomial of order l and $u_l(k,r)$ is a radial function, regular at the origin, with the asymptotic form

$$\underset{r\to\infty}{u_l(k,r)} \sim \frac{1}{k^{1/2}}\sin\left[kr+\frac{(z-1)}{k}\ln(2kr)-\frac{1}{2}l\pi+\sigma_l+\eta_l\right] \tag{3.11}$$

where $\sigma_l = \arg\Gamma(l+1-\frac{i(z-1)}{k})$, the usual Coulomb phase, while η_l denotes that part of the phase arising from non-Coulomb potentials.

Subsequent substitution for $\Psi_{\underline{k}}^{A}$ in (3.9) from equation (3.7), together with the use of the forms (3.8) and (3.10) indicates that the radial function $u_l(k,r)$ must satisfy the integro-differential equation

$$\left[\frac{d^2}{dr^2}+k^2+\frac{2(z-1)}{r}-\frac{l(l+1)}{r^2}+2e^{-2zr}\left(z+\frac{1}{r}\right)\right]u_l(k,r)$$

$$= -\frac{\beta(zr)}{(zr)^4}u_l(k,r)-4z^3(k^2+z^2)\delta_{l0}e^{-zr}r^{l+1}I(l+1,\infty)$$

$$+\frac{8z^3}{(2l+1)}e^{-zr}\left[r^{-l}I(l+1,r)+r^{l+1}J(-l,r)\right]$$

$$-\frac{4z}{(2l+1)}\delta_{l1}e^{-zr}\left[\frac{1}{2}r^3z(z^2+k^2)+r^2(k^2-z^2)\right]J(-l,r)$$

$$-\frac{4z}{(2l+1)}e^{-zr}(zr^3+2r^2)\left[\frac{(l+1)}{(2l+3)}r^{l+1}J(-l-3,r)+\frac{l}{(2l-1)}r^{l-1}J(-l-1,r)\right]$$

$$+\frac{4}{3}z\delta_{l1}e^{-2zr}\left[(-\frac{1}{2}z^2r^2+\frac{1}{2}zr+3)u_l(k,r)-(\frac{1}{2}zr^2+r)\frac{d}{dr}u_l(k,r)\right]$$

(3.12)

where

$$\beta(x)=\frac{9}{2}-\frac{2}{3}e^{-2x}(x^5+\frac{9}{2}x^4+9x^3+\frac{27}{2}x^2+\frac{27}{2}x+\frac{27}{4})$$

$$I(m,r)=\int_0^r e^{-zx}u_l(k,x)x^m dx \qquad (3.13)$$

$$J(m,r)=\int_r^\infty e^{-zx}u_l(k,x)x^m dx \qquad (3.14)$$

The quantity $\frac{\beta(zr)}{(zr)^4}$ is defined to be the direct polarization potential, having the asymptotic behaviour

$$\frac{\beta(zr)}{(zr)^4}\underset{r\to\infty}{\sim}\frac{\alpha}{r^4}$$

where $\alpha=\frac{9}{2z^4}$ is the dipole polarizability.

The exchange-adiabatic approximation of Economides and McDowell is obtained by neglecting the perturbation of the ground state in the exchange terms. Hence the terms contained in the last three square brackets of equation (3.12) are omitted. In addition all subsequent calculations are made using the unperturbed $1s$ state wave function to describe the ground state of the residual ion.

Due allowance for the neglect of specific terms in the modified form of equation (3.12) can be made by the introduction of the switching constants A_1, A_2, A_3 at the appropriate places in this equation

$$\left[\frac{d^2}{dr^2}+k^2+\frac{2(z-1)}{r}+2A_1(z+\frac{1}{r})e^{-2zr}-\frac{l(l+1)}{r^2}+A_2\frac{\beta(zr)}{(zr)^4}\right]u_l(k,r)$$

$$= \frac{8z^3}{(2l+1)} A_3 e^{-zr}\left[r^{-l} I(l+1,r) + r^{l+1}\left(I(-l,\infty) - I(-l,r) - \frac{1}{2}\delta_{l0}(z^2+k^2) I(l+1,\infty)\right)\right] \tag{3.15}$$

3.1.2 The normalization of the continuum wave functions.

To ensure the asymptotic behaviour prescribed by equation (3.11) it is necessary that the radial function $u_l(k,r)$ should be correctly normalized. This is achieved by use of the Strömgren method (cf. Bates and Seaton, 1949). The appropriate form of equation (3.15) for the asymptotic region will be

$$\frac{d^2}{dr^2} u_l(k,r) + \lambda(k,r) u_l(k,r) = 0 \tag{3.16}$$

which is satisfied by a function of the form

$$u_l(k,r) = C \zeta^{-\frac{1}{2}} \sin\{\phi(r) + \delta\} \tag{3.17}$$

where C is a constant and ζ, which represents $\frac{d\phi}{dr}$ is given by

$$\zeta^2 = \lambda(k,r) + \zeta^{\frac{1}{2}} \frac{d^2}{dr^2}(\zeta^{-\frac{1}{2}}) \tag{3.18}$$

The rapid convergence exhibited by the successive approximations to ζ arising from the solution of (3.18) by iteration renders the technique most suitable for this case. As $r \to \infty$, $\lambda(k,r)$ tends to k^2 and so the asymptotic amplitude of (3.17) is simply $Ck^{-\frac{1}{2}}$ The constant C may be evaluated in the following way: we select two values of r, denoted by r_1 and r_2, corresponding to points in the asymptotic region. Associated with these we define the quantities

$$\alpha = \frac{1}{2}\int_{r_1}^{r_2} \zeta \, dr \qquad a_1 = \zeta_1^{\frac{1}{2}} u_l(k,r_1) \qquad a_2 = \zeta_2^{\frac{1}{2}} u_l(k,r_2)$$

By suitable manipulation of these, in conjunction with equation (3.17), we obtain the following expression for C

$$C = \frac{1}{2}\left[(a_1+a_2)^2 \sec^2\alpha + (a_1-a_2)^2 \operatorname{cosec}^2\alpha\right]^{\frac{1}{2}} \tag{3.19}$$

which may easily be evaluated.

The method of solution of the equation (3.15), together with the numerical techniques involved is described in Appendix A. For the purposes of the calculations contained in this chapter the switching constants, A_i, $i=1,3$ are all set to unity.

3.2 Reduction of the amplitudes

As a further simplification to these preliminary calculations it was decided that the Peterkop form of the exchange amplitude given by equation (2.27) should be adopted. Hence we require only the explicit forms of the direct and capture amplitudes.

3.2.1 The direct amplitude

The direct scattering amplitude has the form

$$f(\underline{k}_f,\underline{k}_s) = \frac{-1}{(2\pi)} e^{i\Delta(\underline{k}_f,\underline{k}_s)} \iiint e^{i\underline{K}\cdot\underline{r}_1} \Psi^{*}_{\underline{k}_s}(\underline{r}_2,\underline{r}_3) V(\underline{r}_1;\underline{r}_2,\underline{r}_3) \Psi_0(\underline{r}_2,\underline{r}_3)\, d\underline{r}_1 d\underline{r}_2 d\underline{r}_3 \qquad (3.20)$$

where $$\Psi_{\underline{k}_s}(\underline{r}_2,\underline{r}_3) = \psi_{\underline{k}_s}(\underline{r}_2)\psi_{1s}(Z,\underline{r}_3) \qquad (3.21)$$

with $$\psi_{1s}(Z,\underline{r}_3) = \frac{Z^{3/2}}{\pi^{1/2}} e^{-Zr_3} \qquad (3.22)$$

also $$\underline{K} = \underline{k}_0 - \underline{k}_f$$

and $$V(\underline{r}_1;\underline{r}_2,\underline{r}_3) = -\frac{Z}{r_1} + \frac{1}{r_{12}} + \frac{1}{r_{13}} \qquad (3.23)$$

All other quantities are as previously defined.

Since Ψ_0 and $\Psi_{\underline{k}_s}$ are both taken to represent eigenstates of the target system then they are subject to the orthogonality condition

$$\langle \Psi_0(\underline{r}_j,\underline{r}_k) | \Psi_{\underline{k}_s}(\underline{r}_j,\underline{r}_k) \rangle = 0 \qquad (3.24)$$

This may be achieved by either

(a) requiring the s-wave of the polarized orbital expansion to be orthogonal to $e^{-\alpha r}$, or

(b) replacing ${}^2\bar{\Psi}_{\underline{k}_s}(\underline{r}_j,\underline{r}_k)$ by ${}^2\bar{\Psi}_{\underline{k}_s}(\underline{r}_j,\underline{r}_k) - \langle {}^2\bar{\Psi}_0 | {}^2\bar{\Psi}_{\underline{k}_s} \rangle {}^2\bar{\Psi}_0(\underline{r}_j,\underline{r}_k)$

In the first case the orthogonalized function has the form

$${}^2\bar{\Psi}^{(a)}_{\underline{k}_s}(\underline{r}_j,\underline{r}_k) = {}^2\bar{\Psi}_{\underline{k}_s}(\underline{r}_j,\underline{r}_k) + A^{(a)}\exp(-\alpha r_j - Z r_k)$$

and in the second case

$${}^2\bar{\Psi}^{(b)}_{\underline{k}_s}(\underline{r}_j,\underline{r}_k) = {}^2\bar{\Psi}_{\underline{k}_s}(\underline{r}_j,\underline{r}_k) + A^{(b)}\exp(-\alpha r_j - \alpha r_k)$$

where $A^{(a)}$, $A^{(b)}$ are constants.

Let us introduce the quantity $A(t)$ defined in the following way

$$A(Z) = A^{(a)}$$

$$A(\alpha) = A^{(b)}$$

$A(t) \equiv 0$ in the absence of any orthogonality condition.

This enables us to write the orthogonalized wave function in the general form

$$\left[{}^2\bar{\Psi}_{\underline{k}_s}(\underline{r}_j,\underline{r}_k)\right]_{\text{orthog.}} = {}^2\bar{\Psi}_{\underline{k}_s}(\underline{r}_j,\underline{r}_k) + A(t)\exp(-\alpha r_j - t r_k) \tag{3.25}$$

Substituting this form of the wave function into (3.20) and using the explicit form of the interaction potential given by (3.23) we obtain

$$f(\underline{k}_f,\underline{k}_s) = \frac{-1}{(2\pi)} e^{i\Delta(\underline{k}_f,\underline{k}_s)}\left\{F_1 + bF_2\right\} \tag{3.26}$$

where

$$F_1 = \iiint e^{i\underline{K}\cdot\underline{r}_1}\left[{}^2\bar{\Psi}^*_{\underline{k}_s}(\underline{r}_2,\underline{r}_3) + A^*(t)e^{-\alpha r_2 - t r_3}\right]\left(\frac{1}{r_{12}} + \frac{1}{r_{13}}\right) {}^2\bar{\Psi}_0(\underline{r}_2,\underline{r}_3)\, d\underline{r}_1\, d\underline{r}_2\, d\underline{r}_3 \tag{3.27}$$

and

$$F_2 = \iiint e^{i\underline{K}\cdot\underline{r}_1}\, {}^2\bar{\Psi}^*_{\underline{k}_s}(\underline{r}_2,\underline{r}_3)\left(\frac{-Z}{r_1}\right) {}^2\bar{\Psi}_0(\underline{r}_2,\underline{r}_3)\, d\underline{r}_1\, d\underline{r}_2\, d\underline{r}_3 \tag{3.28}$$

the associated constant b having the form $b = \delta_{A(t),0}$
The integration over the variable $\underline{r}_1$, occuring in (3.27), may be evaluated immediately since it involves only the familiar Bethe integral. The resulting expression for F_1 is

$$F_1 = \frac{4\pi}{K^2} \sum_{j=2,3} \iint e^{i\underline{k}\cdot\underline{r}_j} \left[{}^{2}\overline{\Psi}_{\underline{k}_s}^{*}(\underline{r}_2,\underline{r}_3) + A(t) e^{-\alpha r_2 - t r_3} \right] {}^{2}\overline{\Psi}_0(\underline{r}_2,\underline{r}_3)\, d\underline{r}_2\, d\underline{r}_3$$

Let us firstly consider that part of the integral involving the second term appearing within the brackets. Denoting this by F_{1A} we have

$$F_{1A} = \frac{4\pi}{K^2} A^{*}(t) \sum_{j=2,3} \iint e^{i\underline{k}\cdot\underline{r}_j} e^{-\alpha r_2 - t r_3}\, {}^{2}\overline{\Psi}_0(\underline{r}_2,\underline{r}_3)\, d\underline{r}_2\, d\underline{r}_3 \tag{3.29}$$

Since the wave function ${}^{2}\overline{\Psi}_0(\underline{r}_2,\underline{r}_3)$ is symmetric with respect to interchange of the vectors $\underline{r}_2$ and $\underline{r}_3$ then (3.29) may be rewritten as

$$F_{1A} = \frac{4\pi}{K^2} A^{*}(t) \left\{ I_0(t,\alpha) + I_0(\alpha,t) \right\} \tag{3.30}$$

where the integral $I_0(\gamma,\beta)$ is defined by

$$I_0(\gamma,\beta) = \iint e^{i\underline{k}\cdot\underline{r}_2} e^{-\gamma r_2 - \beta r_3}\, {}^{2}\overline{\Psi}_0(\underline{r}_2,\underline{r}_3)\, d\underline{r}_2\, d\underline{r}_3 \tag{3.31}$$

If we now substitute for ${}^{2}\overline{\Psi}_0$ from equation (3.5) we obtain the following explicit expression for I_0

$$I_0(\gamma,\beta) = \frac{\alpha^3}{\pi} \iint e^{i\underline{k}\cdot\underline{r}_2} e^{-(\gamma+\alpha) r_2} e^{-(\beta+\alpha) r_3}\, d\underline{r}_2\, d\underline{r}_3 \tag{3.32}$$

To facilitate the evaluation of the $\underline{r}_2$ integration we make use of the series expansion of $e^{i\underline{k}\cdot\underline{r}}$ in Legendre polynomials, ie.

$$e^{i\underline{k}\cdot\underline{r}} = \sum_{l=0}^{\infty} i^{l}(2l+1)\, j_l(kr)\, P_l(\hat{\underline{k}}\cdot\hat{\underline{r}}) \tag{3.33}$$

where $j_l(kr)$ is a spherical Bessel function of order l.
Substituting the form (3.33) into (3.32) and using the orthogonality properties of Legendre polynomials we obtain

$$\begin{aligned} I_0(\gamma,\beta) &= 16\alpha^3\pi\left(\int_0^\infty j_0(kr)r^2e^{-(\gamma+\alpha)r}dr\right)\left(\int_0^\infty e^{-(\beta+\alpha)r}r^2dr\right) \\ &= 16\alpha^3\pi\left(\frac{2\alpha_1}{(\alpha_1^2+k^2)^2}\right)\left(\frac{2}{\alpha_2^3}\right) \\ &= \frac{64\pi\alpha^3\alpha_1}{(\alpha_1^2+k^2)^2\alpha_2^3} \end{aligned} \tag{3.34}$$

where $\alpha_1=\gamma+\alpha$ and $\alpha_2=\beta+\alpha$.
Hence equation (3.30) may be reduced to the form

$$F_{1A}=\frac{256\pi^2\alpha^3}{K^2}A^*(t)\left\{\frac{(t+\alpha)}{([t+\alpha]^2+K^2)^2\cdot 8\alpha^3}+\frac{2\alpha}{(4\alpha^2+K^2)^2(t+\alpha)^3}\right\} \tag{3.35}$$

We shall now consider the remaining integral appearing in the expression for F_1,

$$F_{1B}=\frac{4\pi}{K^2}\sum_{j=2,3}\iint e^{i\underline{K}\cdot\underline{r}_j}\,{}^{2}\Psi^{S*}_{\underline{k}_s}(\underline{r}_2,\underline{r}_3)\,{}^{2}\Psi^{S}_{0}(\underline{r}_2,\underline{r}_3)\,d\underline{r}_2\,d\underline{r}_3$$

This expression may also be written in a symmetric form

$$F_{1B}=\frac{4\pi}{K^2}\left\{I_1(\underline{K},\underline{0})+I_1(\underline{0},\underline{K})\right\} \tag{3.36}$$

by defining the integral $I_1(\underline{K}_a,\underline{K}_b)$ in the following way

$$I_1(\underline{K}_a,\underline{K}_b)=\iint e^{i\underline{K}_a\cdot\underline{r}_2}e^{i\underline{K}_b\cdot\underline{r}_3}\,{}^{2}\Psi^{S*}_{\underline{k}_s}(\underline{r}_2,\underline{r}_3)\,{}^{2}\Psi^{S}_{0}(\underline{r}_2,\underline{r}_3)\,d\underline{r}_2\,d\underline{r}_3 \tag{3.37}$$

Subsequent substitution of the appropriate forms of the wave functions form (3.5), (3.21) gives the following expression for I_1

$$I_1(\underline{K}_a,\underline{K}_b)=\frac{Z^{3/2}}{\pi^{1/2}}\cdot\frac{\alpha^3}{\pi}\iint e^{i\underline{K}_a\cdot\underline{r}_2}e^{i\underline{K}_b\cdot\underline{r}_3}\,{}^{2}\psi^{S*}_{\underline{k}_s}(\underline{r}_2)\,e^{-Zr_3}e^{-\alpha(r_2+r_3)}\,d\underline{r}_2\,d\underline{r}_3$$

$$= \frac{Z^{3/2}\alpha^3}{\pi^{3/2}} \left(\int e^{i\underline{k}_a\cdot\underline{r}_2}\psi^*_{\underline{k}_s}(\underline{r}_2)e^{-\alpha r_2}d\underline{r}_2\right)\left(\int e^{i\underline{k}_b\cdot\underline{r}_3}e^{-(Z+\alpha)r_3}d\underline{r}_3\right) \qquad (3.38)$$

We shall firstly direct our attention to the integration over the variable $\underline{r}_2$ in equation (3.38). By using the partial wave expansion representation of $\psi^*_{\underline{k}_s}$, given by equation (3.10), in conjunction with the expansion of P_l in Spherical Harmonics

$$P_l(\hat{\underline{x}}_1\cdot\hat{\underline{x}}_2) = \sum_{m=-l}^{l}\frac{4\pi}{(2l+1)}Y_{lm}(\hat{\underline{x}}_1)Y^*_{lm}(\hat{\underline{x}}_2) \qquad (3.39)$$

and (3.33) we can perform the angular part of the integration and so obtain

$$\int e^{i\underline{k}_a\cdot\underline{r}_2}\psi^*_{\underline{k}_s}(\underline{r}_2)e^{-\alpha r_2}d\underline{r}_2$$

$$= \frac{4\pi}{(2\pi)^{3/2}k_s^{1/2}}\sum_{l=0}^{\infty}(2l+1)e^{-i(\sigma_l+\eta_l)}P_l(\hat{\underline{k}}_a\cdot\hat{\underline{k}}_s)\int_0^\infty j_l(k_a r)u_l(k_s,r)re^{-\alpha r}dr \qquad (3.40)$$

The corresponding integration over the variable $\underline{r}_3$ gives us the result

$$\int e^{i\underline{k}_b\cdot\underline{r}_3}e^{-(Z+\alpha)r_3}d\underline{r}_3 = 4\pi.\frac{2(Z+\alpha)}{([Z+\alpha]^2+k_b^2)^2} \qquad (3.41)$$

Using the results (3.40) and (3.41) in the equation (3.38) yields the following form for I_1

$$I_1(\underline{k}_a,\underline{k}_b) = \frac{8\sqrt{2}(Z+\alpha)Z^{3/2}\alpha^3}{\pi k_s^{1/2}([Z+\alpha]^2+k_b^2)^2}\sum_{l=0}^{\infty}(2l+1)e^{-i(\sigma_l+\eta_l)}P_l(\hat{\underline{k}}_a\cdot\hat{\underline{k}}_s)$$

$$\int_0^\infty j_l(k_a r)u_l(k_s,r)re^{-\alpha r}dr \qquad (3.42)$$

Hence

$$I_1(\underline{k},0) = \frac{8\sqrt{2}\,Z^{3/2}\alpha^3}{\pi k_s^{1/2}(Z+\alpha)^3}\sum_{l=0}^{\infty}(2l+1)e^{-i(\sigma_l+\eta_l)}P_l(\hat{\underline{k}}\cdot\hat{\underline{k}}_s)$$

$$\int_0^\infty j_l(Kr)\,u_l(k_s,r)\,r\,e^{-\alpha r}\,dr$$

and

$$I_1(\underline{0},\underline{K}) = \frac{8\sqrt{2}(z+\alpha)z^{3/2}\alpha^3}{\pi k_s^{1/2}([z+\alpha]^2+K^2)^2}\,e^{-i(\sigma_0+\eta_0)}\int_0^\infty u_0(k_s,r)\,r\,e^{-\alpha r}\,dr$$

Consequently the term F_{1B} is given by the expression

$$F_{1B} = \frac{32\sqrt{2}z^{3/2}\alpha^3}{K^2 k_s^{1/2}}\left\{\frac{1}{(z+\alpha)^3}\sum_{l=0}^{\infty}(2l+1)e^{-i(\sigma_l+\eta_l)}P_l(\hat{\underline{K}}\cdot\hat{\underline{k}}_s)\right.$$

$$\left.\int_0^\infty j_l(Kr)\,u_l(k_s,r)\,r\,e^{-\alpha r}\,dr + \frac{(z+\alpha)}{([z+\alpha]^2+K^2)^2}\cdot e^{-i(\sigma_0+\eta_0)}\int_0^\infty u_0(k_s,r)\,r\,e^{-\alpha r}\,dr\right\} \tag{3.43}$$

Let us now consider the quantity F_2 as defined by (3.28). Since

$$A(\alpha) = A^{(b)} = -\frac{\pi}{\alpha^3}\langle {}^2\Psi_0 | {}^2\Psi_{\underline{k}_s}\rangle$$

then clearly F_2 can be rewritten in the form

$$F_2 = -\frac{\alpha^3}{\pi}A^*(\alpha)\int e^{i\underline{K}\cdot\underline{r}_1}\,\frac{-z}{r_1}\,d\underline{r}_1$$

which involves the usual Bethe integral.

Hence, following the evaluation of this integral, we obtain

$$F_2 = \frac{4z\alpha^3 A^*(\alpha)}{K^2} \tag{3.44}$$

It now only remains to find an explicit expression for the overlap integral denoted by $A(t)$

$$A(t) = -\iint e^{-\alpha r_2 - t r_3}\,\frac{z^{3/2}}{\pi^{1/2}}\,e^{-z r_3}\,\psi_{\underline{k}_s}(\underline{r}_2)\,d\underline{r}_2\,d\underline{r}_3$$

$$= -\frac{z^{3/2}}{\pi^{1/2}}\left(\int e^{-\alpha r_2}\psi_{\underline{k}_s}(\underline{r}_2)\,d\underline{r}_2\right)\left(\int e^{-(t+z)r_3}\,d\underline{r}_3\right) \tag{3.45}$$

But

$$\int e^{-(t+z)r}\,d\underline{r} = \frac{8\pi}{(t+z)^3}$$

and $$\int e^{-\alpha r}\psi^{S}_{\underline{k}_s}(\underline{r})\,d\underline{r} = \frac{4\pi}{k_s^{1/2}(2\pi)^{3/2}}\,e^{i(\sigma_0+\eta_0)}\int_0^\infty e^{-\alpha r}u_0(k_s,r)\,r\,dr$$

Combining the results of the two integrals above we arrive at the expression for $A(t)$ required

$$A(t) = -\frac{8\sqrt{2}\,Z^{3/2}}{k_s^{1/2}(t+Z)^3}\,e^{i(\sigma_0+\eta_0)}\int_0^\infty e^{-\alpha r}u_0(k_s,r)\,r\,dr \tag{3.46}$$

3.2.2 The capture amplitude

The capture amplitude is defined by equation (3.1). Substituting the appropriate forms of the wave functions from equations (3.4), (3.6) and (3.25) we obtain

$$\omega(\underline{k}_f,\underline{k}_s) = -\frac{1}{2\pi}e^{i\Delta(\underline{k}_f,\underline{k}_s)}\iiint e^{i\underline{k}_0\cdot\underline{r}_1}\,\Psi^{S}_{0}(\underline{r}_2,\underline{r}_3)\,V(1,2,3)\,e^{-i\underline{k}_f\cdot\underline{r}_2}$$
$$\left[\Psi^{S*}_{\underline{k}_s}(\underline{r}_3,\underline{r}_1) + A^*(t)\,e^{-\alpha r_3 - t r_1}\right]d\underline{r}_1\,d\underline{r}_2\,d\underline{r}_3 \tag{3.47}$$

The post form of the amplitude is obtained if the interaction potential is taken to be

$$V(1,2,3) = V(2;1,3) = \frac{1}{r_{12}} + \frac{1}{r_{32}} - \frac{Z}{r_2}$$

while the prior form corresponds to the choice

$$V(1,2,3) = V(1;2,3)$$

If $\omega^-(\underline{k}_f,\underline{k}_s)$ and $\omega^+(\underline{k}_f,\underline{k}_s)$ denote the prior and post formulations of the amplitude respectively, then these are given by

$$\omega^-(\underline{k}_f,\underline{k}_s) = -\frac{1}{2\pi}e^{i\Delta(\underline{k}_f,\underline{k}_s)}\iiint e^{i\underline{k}_0\cdot\underline{r}_1}\,\Psi^{S}_{0}(\underline{r}_2,\underline{r}_3)\,V(1;2,3)\,e^{i\underline{k}_f\cdot\underline{r}_2}$$
$$\left[\psi^{S*}_{\underline{k}_s}(\underline{r}_3)\frac{Z^{3/2}}{\pi^{1/2}}e^{-Zr_1} + A^*(t)\,e^{-\alpha r_3 - t r_1}\right]d\underline{r}_1\,d\underline{r}_2\,d\underline{r}_3 \tag{3.48}$$

and

$$\omega^+(\underline{k}_f,\underline{k}_s)=-\frac{1}{2\pi}e^{i\Delta(\underline{k}_f,\underline{k}_s)}\iiint e^{i\underline{k}_0\cdot\underline{r}_1}\Psi_0(\underline{r}_2,\underline{r}_3)V(2;1,3)e^{i\underline{k}_f\cdot\underline{r}_2}$$
$$\left[\psi^*_{\underline{k}_s}(\underline{r}_3).\frac{z^{3/2}}{\pi^{1/2}}e^{-zr_1}+A^*(t)e^{-\alpha r_3-tr_1}\right]d\underline{r}_1d\underline{r}_2d\underline{r}_3 \tag{3.49}$$

Interchanging the indexes 1 and 2 in (3.49) we obtain

$$\omega^+(\underline{k}_f,\underline{k}_s)=-\frac{1}{2\pi}e^{i\Delta(\underline{k}_f,\underline{k}_s)}\iiint e^{i\underline{k}_0\cdot\underline{r}_2}\Psi_0(\underline{r}_1,\underline{r}_3)V(1;2,3)e^{i\underline{k}_f\cdot\underline{r}_1}$$
$$\left[\psi^*_{\underline{k}_s}(\underline{r}_3).\frac{z^{3/2}}{\pi^{1/2}}e^{-zr_2}+A^*(t)e^{-\alpha r_3-tr_2}\right]d\underline{r}_1d\underline{r}_2d\underline{r}_3 \tag{3.50}$$

where we have made the appropriate substitutions from (3.21) and (3.22). If we now replace Ψ_0 by the explicit form (3.5) and introduce the quantities $W_1(\underline{k}_a,\underline{k}_b,\beta,\gamma)$, $W_2(\underline{k}_a,\underline{k}_b,\beta,\gamma)$ defined by

$$W_1(\underline{k}_a,\underline{k}_b,\beta,\gamma)=\frac{\alpha^3z^{3/2}}{\pi^{3/2}}\iiint e^{i\underline{k}_a\cdot\underline{r}_1}e^{-\beta r_1}e^{i\underline{k}_b\cdot\underline{r}_2}e^{-\gamma r_2}V(1;2,3)$$
$$e^{-\alpha r_3}\psi^*_{\underline{k}_s}(\underline{r}_3)d\underline{r}_1d\underline{r}_2d\underline{r}_3 \tag{3.51}$$

$$W_2(\underline{k}_a,\underline{k}_b,\beta,\gamma)=\frac{\alpha^3}{\pi}\iiint e^{i\underline{k}_a\cdot\underline{r}_1}e^{-\beta r_1}e^{i\underline{k}_b\cdot\underline{r}_2}e^{-\gamma r_2}V(1;2,3)$$
$$e^{-2\alpha r_3}d\underline{r}_1d\underline{r}_2d\underline{r}_3 \tag{3.52}$$

then clearly both ω^- and ω^+ have the same basic structure, the corresponding expressions being

$$\omega^-(\underline{k}_f,\underline{k}_s)=-\frac{1}{2\pi}e^{i\Delta(\underline{k}_f,\underline{k}_s)}\left\{W_1(\underline{k}_0,-\underline{k}_f,z,\alpha)+A^*(t)W_2(\underline{k}_0,-\underline{k}_f,t,\alpha)\right\} \tag{3.53}$$

$$\omega^+(\underline{k}_f,\underline{k}_s)=-\frac{1}{2\pi}e^{i\Delta(\underline{k}_f,\underline{k}_s)}\left\{W_1(-\underline{k}_f,\underline{k}_0,\alpha,z)+A^*(t)W_2(-\underline{k}_f,\underline{k}_0,\alpha,t)\right\} \tag{3.54}$$

Substituting the explicit form of the potential $V(1;2,3)$ into (3.51) we obtain the following expression for W_1

$$W_1(\underline{k}_a,\underline{k}_b,\beta,\gamma)=\frac{\alpha^3z^{3/2}}{\pi^{3/2}}\left(W_{1A}+W_{1B}\right) \tag{3.55}$$

where
$$W_{1A} = \iiint e^{i\underline{k}_a\cdot\underline{r}_1} e^{-\beta r_1} e^{i\underline{k}_b\cdot\underline{r}_2} e^{-\gamma r_2}\left(\frac{1}{r_{12}}+\frac{1}{r_{13}}\right) e^{-\alpha r_3}\psi^*_{\underline{k}_s}(\underline{r}_3)\, d\underline{r}_1 d\underline{r}_2 d\underline{r}_3 \tag{3.56}$$

and
$$W_{1B} = \iiint e^{i\underline{k}_a\cdot\underline{r}_1} e^{-\beta r_1} e^{i\underline{k}_b\cdot\underline{r}_2} e^{-\gamma r_2}\left(-\frac{z}{r_1}\right) e^{-\alpha r_3}\psi^*_{\underline{k}_s}(\underline{r}_3)\, d\underline{r}_1 d\underline{r}_2 d\underline{r}_3 \tag{3.57}$$

We shall now examine the integration over the variable $\underline{r}_1$ involved in (3.56)

$$W_{1A} = \iint e^{i\underline{k}_b\cdot\underline{r}_2} e^{-\gamma r_2} e^{-\alpha r_3}\psi^*_{\underline{k}_s}(\underline{r}_3)\left(\int e^{i\underline{k}_a\cdot\underline{r}_1} e^{-\beta r_1}\left[\frac{1}{r_{12}}+\frac{1}{r_{13}}\right] d\underline{r}_1\right) d\underline{r}_2 d\underline{r}_3$$

In order to evaluate the $\underline{r}_1$ integration we need to make use of the series expansion

$$\frac{1}{r_{ij}} = \sum_{l=0}^{\infty} \frac{r_<^l}{r_>^{l+1}} P_l(\hat{\underline{r}}_i\cdot\hat{\underline{r}}_j) \tag{3.58}$$

where $r_>$ and $r_<$ denote the greater and lesser of r_i and r_j respectively.

If we introduce the function $v_l(r_i,k,\beta)$ defined by

$$v_l(r_i,k,\beta) = \int_0^{\infty} j_l(kr) e^{-\beta r} \gamma_l(r; r_i)\, r^2 dr \tag{3.59}$$

where $\gamma_l(r; r_i) = \frac{r_<^l}{r_>^{l+1}}$,

then the evaluation of the $\underline{r}_1$ integration associated with W_{1A}, subsequent to the substitution of the expansion (3.58) together with the use of (3.39), yields the result

$$W_{1A} = 4\pi\sum_{l=0}^{\infty} i^l \iint e^{i\underline{k}_b\cdot\underline{r}_2} e^{-\gamma r_2} e^{-\alpha r_3}\psi^*_{\underline{k}_s}(\underline{r}_3)\left[P_l(\hat{\underline{r}}_2\cdot\hat{\underline{k}}_a) v_l(r_2,k_a,\beta) + P_l(\hat{\underline{r}}_3\cdot\hat{\underline{k}}_a) v_l(r_3,k_a,\beta)\right] d\underline{r}_2 d\underline{r}_3 \tag{3.60}$$

The first term contained in the brackets appearing in (3.60) gives the following contribution to the integral

$$\iint 4\pi\sum_{l=0}^{\infty} i^l P_l(\hat{\underline{r}}_2\cdot\hat{\underline{k}}_a)\, v_l(r_2,k_a,\beta)\, e^{i\underline{k}_b\cdot\underline{r}_2} e^{-\gamma r_2} e^{-\alpha r_3}\, \psi^*_{\underline{k}_s}(\underline{r}_3)\, d\underline{r}_2\, d\underline{r}_3$$

Appropriate use of the expansion (3.33) enables us to perform the angular part of the $\underline{r}_2$ integration and so obtain

$$16\pi^2\sum_{l=0}^{\infty}(-1)^l P_l(\hat{\underline{k}}_a\cdot\hat{\underline{k}}_b)\left(\int_0^{\infty} v_l(r,k_a,\beta)\, j_l(k_b r)\, e^{-\gamma r} r^2 dr\right)\int e^{-\alpha r_3}\psi^*_{\underline{k}_s}(\underline{r}_3)\, d\underline{r}_3 \tag{3.61}$$

But
$$\int e^{-\alpha r}\psi^*_{\underline{k}_s}(\underline{r})\, d\underline{r} = \frac{4\pi}{k_s^{1/2}(2\pi)^{3/2}}\, e^{-i(\sigma_0+\eta_0)}\int e^{-\alpha r} u_0(k_s,r)\, r\, dr$$

Hence (3.61) takes the form

$$\frac{16\sqrt{2}\,\pi^{3/2}}{k_s^{1/2}}\, e^{-i(\sigma_0+\eta_0)}\int_0^{\infty} e^{-\alpha r} u_0(k_s,r)\, r\, dr \sum_{l=0}^{\infty}(-1)^l P_l(\hat{\underline{k}}_a\cdot\hat{\underline{k}}_b)$$
$$\int_0^{\infty} v_l(r,k_a,\beta)\, j_l(k_b r)\, e^{-\gamma r} r^2 dr \tag{3.62}$$

Let us now consider the contribution arising from the remaining term within the brackets of (3.60)

$$\iint 4\pi\sum_{l=0}^{\infty} i^l P_l(\hat{\underline{r}}_3\cdot\hat{\underline{k}}_a)\, v_l(r_3,k_a,\beta)\, e^{i\underline{k}_b\cdot\underline{r}_2} e^{-\gamma r_2} e^{-\alpha r_3}\, \psi^*_{\underline{k}_s}(\underline{r}_3)\, d\underline{r}_2\, d\underline{r}_3$$

Replacing $\psi_{\underline{k}_s}$ by the partial wave expansion (3.10) allows us to evaluate the $\hat{\underline{r}}_3$ integration which results in the expression

$$\frac{16\pi^2}{k_s^{1/2}(2\pi)^{3/2}}\sum_{l=0}^{\infty} e^{-i(\sigma_l+\eta_l)} P_l(\hat{\underline{k}}_a\cdot\hat{\underline{k}}_s)\left(\int_0^{\infty} v_l(r,k_a,\beta)\, e^{-\alpha r} u_l(k_s,r)\, r\, dr\right)$$
$$\int e^{i\underline{k}_b\cdot\underline{r}_2} e^{-\gamma r_2}\, d\underline{r}_2 \tag{3.63}$$

But
$$\int e^{i\underline{k}_b\cdot\underline{r}} e^{-\gamma r}\, d\underline{r} = 4\pi\int_0 j_0(k_b r)\, e^{-\gamma r} r^2 dr$$
$$= \frac{8\pi\gamma}{(\gamma^2+k_b^2)^2}$$

Hence (3.63) may be reduced to the form

$$\frac{32\sqrt{2}\,\pi^{3/2}\gamma}{k_s^{1/2}(\gamma^2+k_b^2)^2}\sum_{l=0}^{\infty} e^{-i(\sigma_l+\eta_l)} P_l(\hat{\underline{k}}_a\cdot\hat{\underline{k}}_s)\int_0^{\infty} v_l(r,k_a,\beta)\, e^{-\alpha r} u_l(k_s,r)\, r\, dr \tag{3.64}$$

Combining the results (3.62) and (3.64) we obtain

$$W_{1A} = \frac{16\sqrt{2}\pi^{3/2}}{k_s^{1/2}} \sum_{l=0}^{\infty} \Big[\Big(e^{-i(\sigma_0+\eta_0)} \int_0^\infty e^{-\alpha r} u_0(k_s,r)\, r\, dr \Big) (-1)^l P_l(\hat{\underline{k}}_a \cdot \hat{\underline{k}}_b)$$

$$\int_0^\infty v_l(r;k_a,\beta)\, j_l(k_b r)\, e^{-\gamma r} r^2 dr$$

$$+ \frac{2\gamma}{(\gamma^2+k_b^2)^2}\, e^{-i(\sigma_l+\eta_l)} P_l(\hat{\underline{k}}_a \cdot \hat{\underline{k}}_s) \int_0^\infty v_l(r;k_a,\beta)\, u_l(k_s,r)\, e^{-\alpha r} r\, dr \Big] \tag{3.65}$$

Let us now examine the term W_{1B} as given by (3.57). In this case the integration over the three configuration spaces is separable

$$W_{1B} = \int -\frac{z}{r_1} e^{i\underline{k}_a\cdot\underline{r}_1} e^{-\beta r_1} d\underline{r}_1 \int e^{i\underline{k}_b\cdot\underline{r}_2} e^{-\gamma r_2} d\underline{r}_2 \int e^{-\alpha r_3} \psi^*_{\underline{k}_s}(\underline{r}_3)\, d\underline{r}_3$$

From the $\underline{r}_1$, integration we obtain

$$\int -\frac{z}{r} e^{i\underline{k}_a\cdot\underline{r}} e^{-\beta r} d\underline{r} = -4\pi z \int j_0(k_a r)\, e^{-\beta r} r\, dr$$

$$= -\frac{4\pi z}{(\beta^2+k_a^2)}$$

where $e^{i\underline{k}_a\cdot\underline{r}}$ has been replaced by the series expansion (3.33)

Also

$$\int e^{i\underline{k}_b\cdot\underline{r}} e^{-\gamma r} d\underline{r} = 4\pi \int j_0(k_b r)\, e^{-\gamma r} r^2 dr$$

$$= 4\pi . \frac{2\gamma}{(\gamma^2+k_b^2)^2}$$

and

$$\int e^{-\alpha r} \psi^*_{\underline{k}_s}(\underline{r})\, d\underline{r} = \frac{\sqrt{2}}{k_s^{1/2}\pi^{1/2}}\, e^{-i(\sigma_0+\eta_0)} \int_0^\infty e^{-\alpha r} u_0(k_s,r)\, r\, dr$$

Hence W_{1B} is given by the expression

$$W_{1B} = \frac{-32\sqrt{2}\pi^{3/2} z\gamma}{k_s^{1/2}(\beta^2+k_a^2)(\gamma^2+k_b^2)^2}\, e^{-i(\sigma_0+\eta_0)} \int_0^\infty e^{-\alpha r} u_0(k_s,r)\, r\, dr \tag{3.66}$$

When evaluating the term W_2 defined by (3.52) it is convenient to separate it into two parts as was done with W_1, i.e.

$$W_2 = \frac{\alpha^3}{\pi}\left[W_{2A} + W_{2B}\right] \tag{3.67}$$

where

$$W_{2A} = \iiint e^{i\underline{k}_a\cdot\underline{r}_1} e^{-\beta r_1} e^{i\underline{k}_b\cdot\underline{r}_2} e^{-\gamma r_2}\left[\frac{1}{r_{12}} + \frac{1}{r_{13}}\right] e^{-2\alpha r_3}\, d\underline{r}_1\, d\underline{r}_2\, d\underline{r}_3 \tag{3.68}$$

and

$$W_{2B} = \iiint e^{i\underline{k}_a\cdot\underline{r}_1} e^{-\beta r_1} e^{i\underline{k}_b\cdot\underline{r}_2} e^{-\gamma r_2}\left(\frac{-Z}{r_1}\right) e^{-2\alpha r_3}\, d\underline{r}_1\, d\underline{r}_2\, d\underline{r}_3 \tag{3.69}$$

If we firstly consider W_{2A} and evaluate the $\underline{r}_1$ integration as we did for W_{1A} (cf. eq. 3.60) then we obtain

$$W_{2A} = 4\pi \sum_{l=0}^{\infty} i^l \iint e^{i\underline{k}_b\cdot\underline{r}_2} e^{-\gamma r_2} e^{-2\alpha r_3}\left[P_l(\hat{\underline{r}}_2\cdot\hat{\underline{k}}_a)\, v_l(r_2, k_a, \beta) + P_l(\hat{\underline{r}}_3\cdot\hat{\underline{k}}_a)\, v_l(r_3, k_a, \beta)\right] d\underline{r}_2\, d\underline{r}_3 \tag{3.70}$$

In equation (3.70) the first term within the brackets gives rise to the integral

$$\iint 4\pi \sum_{l=0}^{\infty} i^l P_l(\hat{\underline{r}}_2\cdot\hat{\underline{k}}_a)\, v_l(r_2, k_a, \beta)\, e^{i\underline{k}_b\cdot\underline{r}_2} e^{-\gamma r_2} e^{-2\alpha r_3}\, d\underline{r}_2\, d\underline{r}_3$$

which, after evaluation of the $\hat{\underline{r}}_2$ integration, may be reduced to the expression

$$16\pi^2 \sum_{l=0}^{\infty} (-1)^l P_l(\hat{\underline{k}}_a\cdot\hat{\underline{k}}_b)\left(\int_0^{\infty} v_l(r, k_a, \beta)\, j_l(k_b r)\, e^{-\gamma r} r^2\, dr\right)\int e^{-2\alpha r_3}\, d\underline{r}_3 \tag{3.71}$$

But

$$\int e^{-2\alpha r_3}\, d\underline{r}_3 = \frac{4\pi}{4\alpha^3} = \frac{\pi}{\alpha^3}$$

Thus (3.71) becomes

$$\frac{16\pi^3}{\alpha^3} \sum_{l=0}^{\infty} (-1)^l P_l(\hat{\underline{k}}_a\cdot\hat{\underline{k}}_b)\int_0^{\infty} v_l(r, k_a, \beta)\, j_l(k_b r)\, e^{-\gamma r} r^2\, dr \tag{3.72}$$

The second term arising from (3.70) has the form

$$\iint 4\pi \sum_{l=0}^{\infty} i^{l} P_l(\hat{\underline{r}}_3 \cdot \hat{\underline{k}}_a) v_l(r_3, k_a, \beta) e^{i\underline{k}_b \cdot \underline{r}_2} e^{-\gamma r_2} e^{-2\alpha r_3} d\underline{r}_2 d\underline{r}_3$$

Performing the integration over $\hat{\underline{r}}_3$ we obtain

$$16\pi^2 \int_0^{\infty} v_0(r, k_a, \beta) e^{-2\alpha r} r^2 dr \int e^{i\underline{k}_b \cdot \underline{r}_2} e^{-\gamma r_2} d\underline{r}_2 \qquad (3.73)$$

Now from (3.59) we have

$$v_0(r_i, k, \beta) = \int_0^{\infty} j_0(kr) e^{-\beta r} \frac{1}{r_>} r^2 dr$$

$$= \frac{1}{r_i} \int_0^{r_i} j_0(kr) e^{-\beta r} r^2 dr + \int_{r_i}^{\infty} j_0(kr) e^{-\beta r} r\, dr$$

which may be evaluated to give

$$v_0(r, k, \beta) = \frac{1}{k(\beta^2+k^2)^2} \cdot \frac{1}{r} \left[2\beta k - (2\beta k \cos kr + (\beta^2 - k^2) \sin kr) e^{-\beta r} \right]$$

Hence

$$\int_0^{\infty} v_0(r, k_a, \beta) e^{-2\alpha r} r^2 dr$$

$$= \frac{1}{k_a(\beta^2+k_a^2)^2} \int_0^{\infty} \{ 2\beta k_a e^{-2\alpha r} r - 2\beta k_a \cos k_a r . e^{-(2\alpha+\beta) r} r$$

$$- (\beta^2 - k_a^2) \sin k_a r . e^{-(2\alpha+\beta) r} r \} dr$$

$$= \frac{1}{k_a(\beta^2+k_a^2)^2} \left\{ \frac{2\beta k_a}{(2\alpha)^2} - 2\beta k_a \frac{[(2\alpha+\beta)^2 - k_a^2]}{[(2\alpha+\beta)^2 + k_a^2]^2} \right.$$

$$\left. - (\beta^2 - k_a^2) . \frac{2(2\alpha+\beta) k_a}{[(2\alpha+\beta)^2 + k_a^2]^2} \right\}$$

$$= \frac{2}{(\beta^2+k_a^2)^2} \left\{ \frac{\beta}{4\alpha^2} - \frac{[\beta(2\alpha+\beta) - k_a^2](2\alpha + 2\beta)}{[(2\alpha+\beta)^2 + k_a^2]^2} \right\} \qquad (3.74)$$

Finally the $\underline{r}_2$ integration in (3.73) yields the result

$$\int e^{i\underline{k}_b \cdot \underline{r}} e^{-\gamma r} d\underline{r} = 8\pi\gamma / (\gamma^2 + k_b^2)^2$$

Using this and the result (3.74) we can reduce (3.73) to the form

$$\frac{256\pi^3\gamma}{(\beta^2+k_a^2)^2(\gamma^2+k_b^2)^2}\left\{\frac{\beta}{4\alpha^2}-\frac{[\beta(2\alpha+\beta)-k_a^2]\,(2\alpha+2\beta)}{[(2\alpha+\beta)^2+k_a^2]^2}\right\} \tag{3.75}$$

Combining equations (3.72) and (3.75) yields the following expression for W_{2A}

$$W_{2A}=16\pi^3\Bigg(\frac{1}{\alpha^3}\sum_{l=0}^{\infty}(-1)^l P_l(\hat{\mathbf{k}}_a\cdot\hat{\mathbf{k}}_b)\int_0^{\infty}v_l(r,k_a,\beta)\,j_l(k_b r)\,e^{-\gamma r}r^2\,dr$$

$$+\frac{16\gamma}{(\beta^2+k_a^2)^2(\gamma^2+k_b^2)^2}\left\{\frac{\beta}{4\alpha^2}-\frac{[\beta(2\alpha+\beta)-k_a^2](2\alpha+2\beta)}{[(2\alpha+\beta)^2+k_a^2]^2}\right\}\Bigg) \tag{3.76}$$

The term W_{2B} defined by (3.69) is separable with respect to the integrations involved and may be rewritten in the form

$$W_{2B}=\int\left(-\frac{Z}{r_1}\right)e^{i\mathbf{k}_a\cdot\mathbf{r}_1}e^{-\beta r_1}d\mathbf{r}_1\int e^{i\mathbf{k}_b\cdot\mathbf{r}_2}e^{-\gamma r_2}d\mathbf{r}_2\int e^{-2\alpha r_3}d\mathbf{r}_3$$

$$=\left(-\frac{4\pi Z}{(\beta^2+k_a^2)}\right)\left(\frac{8\pi\gamma}{(\gamma^2+k_b^2)^2}\right)\left(\frac{\pi}{\alpha^3}\right)$$

$$=\frac{-32\pi^3 Z\gamma}{\alpha^3(\beta^2+k_a^2)(\gamma^2+k_b^2)^2} \tag{3.77}$$

where we have used the results for the integrals as previously found.

Integrals appearing in the previous analysis that cannot be reduced to closed analytic forms are integrated numerically using Simpson's Rule over 1500 points. For this purpose the range of integration is divided into three parts corresponding to steplengths of 0.005, 0.01 and 0.02, the first of these containing the first 100 function values, the second the next 200 and the third the remaining 1200. The integration routines used in the calculation of the direct and exchange amplitudes are easily checked by running the program for the plane-plane approximation as described in Appendix B (retaining only terms corresponding to the simple ground state wave function in the alternative analysis). This proceedure provided an adequate check on the calculations for both the direct and exchange amplitudes since they share the same coding.

The capture amplitude presents more of a problem since even for the plane-plane approximation some of the associated integrals cannot be easily reduced to analytic forms. In particular we require some check on the method used to generate the integrals:

$$\int_0^\infty v_l(r,k',\beta)\, u_l(k,r)\, e^{-\alpha r}\, r\, dr$$

appearing in the expression for W_{1A} given by equation (3.65). If we make the Bessel function replacement corresponding to the plane-plane approximation the integral becomes

$$\int_0^\infty e^{-\alpha r} r^2 j_l(kr)\, v_l(r,k',\beta)\, dr$$

Because of the form of the function v_l, defined by (3.59), this integral has particular symmetry properties and may also be expressed in the form

$$\int_0^\infty e^{-\beta r} r^2 j_l(k'r)\, v_l(r,k,\alpha)\, dr$$

Subsequent evaluation of this integral using both forms presented here produced results that agreed to at least four significant figures. This clearly indicated the reliability of the numerical integration technique used.

3.3 Results

We have calculated the triple differential cross section for the ionization of helium by electron impact using the expressions for the amplitudes given in this chapter. Results are presented for the energy regions investigated by Erhardt et al (1972). During the course of our calculations we have examined the effects of orthogonality upon the amplitudes. In particular we are interested in the extent to which the different methods of achieving orthogonality affect the results. For this purpose we have calculated the amplitudes using both forms of the orthogonalized final state wave function. Tables 1 to 3 compare the results obtained from the two choices of orthogonality for selected energies and angles.

We have also evaluated $\omega(\underline{k}_f,\underline{k}_s)$ in both the past and prior formulations. If the wave functions Ψ_0 and $\Psi^{(a,b)}_{\underline{k}_s}$ are exact these two expressions are of course, identical, but otherwise the post-prior discrepancy gives a crude measure of the unreliability of the wave functions. The tables 4 - 6 show a comparison between values of the capture amplitude calculated from the post and prior forms for a number of cases.

If we denote the capture probability by $P_{cap}(\underline{k}_f,\underline{k}_s)$ then we have the following definition:

$$P_{cap}(\underline{k}_f,\underline{k}_s) = \frac{2k_f k_s}{k_0}\left|\omega(\underline{k}_f,\underline{k}_s)\right|^2$$

The figures 1 -3 show the variation of P_{cap} with angle, using both post and prior approximations, for representative sets of collision parameters. An inspection of these probability distributions clearly indicates basic differences between the two approximations. Although the Kidney shape is common to both, and may therefore be considered a characteristic of the capture probability distribution, the positions of the maxima in either one are completely reversed in the other. However the minima of the two distributions roughly coincide. Another difference that is apparent is that while the curve corresponding to the prior approximation is symmetrical about the direction of the incident electron that for the post approximation is symmetrical about the direction of the "fast" outgoing electron.

Tables 7 - 9 show the relative magnitudes of the direct, exchange and capture amplitudes for three sets of collision parameters. Finally figures 4 – 9 show the variation of the triple differential cross section with angle. We have only included those cases for which there is experimental data available for comparison. The triple differential cross section is characterized by a forward and backward peak, referred to as the binary and recoil peaks respectively. Since the measurements of Ehrhardt et al are not absolute it has been necessary to normalize the results of our calculations to these measurements. This is achieved by requiring that the maximum of the forward peak, as measured experimentally, should be in agreement with the calculated value. We observe that the curves corresponding to the calculations tend to underestimate the magnitude of the recoil peak. A more detailed discussion of the differences between the experimental and calculated curves, and the reasons for them, is contained in Chapter 4.

3.4 Conclusions

We have evaluated the direct, exchange and capture amplitudes, corresponding to the ionization of Helium by electron impact, using the first Born approximation. Particular consideration has been given to the effects of orthogonality and to differences arising from the use of the post and prior forms of the capture amplitude. Also preliminary calculations for the triple differential cross section have been made corresponding to an incident energy of 256.5eV.

The results obtained lead us to the following conclusions:

Firstly, that, at least in the energy range considered, the choice of orthogonality condition is unimportant (provided that equation 3.24 is satisfied).

Secondly, although both post and prior forms of the capture amplitude produce results of the same order of magnitude, there is considerable discrepancy between the two. This would seem to indicate that the correlation in the He ground state, which has been neglected in these calculations, is an important consideration in the evaluation of the capture amplitude.

Thirdly, it is clear that the capture process is only significant at these relatively high energies where the triple differential cross section is small, but it may dominate the exchange contribution in these regions.

Finally, the calculations of the triple differential cross section, although reproducing the salient features of the experimental measurements, differ from the experimental measurements in several respects. In particular there exists a serious discrepancy in the relative magnitudes of the binary and recoil peaks.

CASE: $E_0 = 256.5eV$ $E_f = 226eV$ $\theta_f = 4°$

	ORTHOGONALITY CONDITION (a)		ORTHOGONALITY CONDITION (b)		NO ORTHOGONALITY CONDITION	
ANGLE θ_s	$\mathcal{R}.f(\underline{k}_f,\underline{k}_s)$	$\mathcal{I}.f(\underline{k}_f,\underline{k}_s)$	$\mathcal{R}.f(\underline{k}_f,\underline{k}_s)$	$\mathcal{I}.f(\underline{k}_f,\underline{k}_s)$	$\mathcal{R}.f(\underline{k}_f,\underline{k}_s)$	$\mathcal{I}.f(\underline{k}_f,\underline{k}_s)$
30°	0.339(-2)	0.404(-3)	0.339(-2)	0.399(-3)	0.330(-2)	0.472(-3)
60°	-0.224(-2)	-0.454(-2)	-0.223(-2)	-0.454(-2)	-0.233(-2)	-0.447(-2)
90°	-0.656(-2)	-0.710(-2)	-0.655(-2)	-0.711(-2)	-0.665(-2)	-0.703(-2)
120°	-0.877(-2)	-0.805(-2)	-0.877(-2)	-0.805(-2)	-0.887(-2)	-0.797(-2)
150°	-0.871(-2)	-0.802(-2)	-0.870(-2)	-0.803(-2)	-0.881(-2)	-0.795(-2)
180°	-0.637(-2)	-0.701(-2)	-0.636(-2)	-0.702(-2)	-0.647(-2)	-0.694(-2)
210°	-0.195(-2)	-0.433(-2)	-0.194(-2)	-0.434(-2)	-0.205(-2)	-0.426(-2)
240°	0.370(-2)	0.745(-3)	0.371(-2)	0.739(-3)	0.361(-2)	0.812(-3)
270°	0.888(-2)	0.752(-2)	0.889(-2)	0.752(-2)	0.880(-2)	0.759(-2)
300°	0.118(-1)	0.127(-1)	0.118(-1)	0.127(-1)	0.118(-1)	0.128(-1)
330°	0.117(-1)	0.125(-1)	0.117(-1)	0.125(-1)	0.117(-1)	0.126(-1)
360°	0.865(-2)	0.715(-2)	0.865(-2)	0.715(-2)	0.856(-2)	0.722(-2)

CASE: $E_0 = 256.5eV$ $E_f = 229eV$ $\theta_f = 6°$

30°	0.213(-2)	-0.178(-2)	0.214(-2)	-0.179(-2)	0.199(-2)	-0.173(-2)
60°	-0.126(-2)	-0.715(-2)	-0.125(-2)	-0.716(-2)	-0.140(-2)	-0.710(-2)
90°	-0.398(-2)	-0.988(-2)	-0.396(-2)	-0.988(-2)	-0.411(-2)	-0.983(-2)
120°	-0.503(-2)	-0.107(-1)	-0.502(-2)	-0.107(-1)	-0.517(-2)	-0.107(-1)
150°	-0.415(-2)	-0.100(-1)	-0.414(-2)	-0.100(-1)	-0.429(-2)	-0.998(-2)
180°	-0.157(-2)	-0.751(-2)	-0.155(-2)	-0.752(-2)	-0.170(-2)	-0.746(-2)
210°	0.183(-2)	-0.240(-2)	0.184(-2)	-0.241(-2)	0.168(-2)	-0.235(-2)
240°	0.447(-2)	0.519(-2)	0.448(-2)	0.518(-2)	0.432(-2)	0.525(-2)
270°	0.532(-2)	0.128(-1)	0.533(-2)	0.128(-1)	0.517(-2)	0.129(-1)
300°	0.524(-2)	0.163(-1)	0.525(-2)	0.163(-1)	0.509(-2)	0.164(-1)
330°	0.532(-2)	0.134(-1)	0.534(-2)	0.134(-1)	0.518(-2)	0.134(-1)
360°	0.462(-2)	0.596(-2)	0.463(-2)	0.596(-2)	-	-

TABLE 3.1

VARIATION OF THE DIRECT SCATTERING AMPLITUDE WITH ANGLE θ_s FOR THE VARIOUS CHOICES OF ORTHOGONALITY EXAMINED.

CASE: E_0 =256.5eV E_f =226eV θ_f=4°

	ORTHOGONALITY CONDITION (a)		ORTHOGONALITY CONDITION (b)		NO ORTHOGONALITY CONDITION	
θ_s ANGLE	$R.g(k_f,k_s)$	$I.g(k_f,k_s)$	$R.g(k_f,k_s)$	$I.g(k_f,k_s)$	$R.g(k_f,k_s)$	$I.g(k_f,k_s)$
30°	0.114(-3)	0.358(-4)	0.114(-3)	0.357(-4)	0.117(-3)	0.389(-4)
60°	0.628(-4)	0.203(-4)	0.628(-4)	0.202(-4)	0.656(-4)	0.231(-4)
90°	0.362(-4)	0.176(-5)	0.361(-4)	0.172(-5)	0.386(-4)	0.422(-5)
120°	0.261(-4)	-0.123(-4)	0.260(-4)	-0.124(-4)	0.283(-4)	-0.102(-4)
150°	0.260(-4)	-0.193(-4)	0.259(-4)	-0.193(-4)	0.280(-4)	-0.173(-4)
180°	0.344(-4)	-0.218(-4)	0.344(-4)	-0.219(-4)	0.364(-4)	-0.199(-4)
210°	0.530(-4)	-0.217(-4)	0.529(-4)	-0.218(-4)	0.550(-4)	-0.197(-4)
240°	0.844(-4)	-0.161(-4)	0.844(-4)	-0.161(-4)	0.866(-4)	-0.139(-4)
270°	0.129(-3)	0.843(-7)	0.129(-3)	0.387(-7)	0.131(-3)	0.253(-5)
300°	0.176(-3)	0.233(-4)	0.176(-3)	0.232(-4)	0.179(-3)	0.261(-4)
330°	0.201(-3)	0.399(-4)	0.201(-3)	0.398(-4)	0.204(-3)	0.431(-4)
360°	0.175(-3)	0.433(-4)	0.175(-3)	0.432(-4)	0.178(-3)	0.466(-4)

CASE: E_0 = 256.5eV E_f =229eV θ_f=6°

30°	0.106(-3)	0.299(-4)	0.106(-3)	0.298(-4)	0.108(-3)	0.329(-4)
60°	0.636(-4)	0.180(-4)	0.635(-4)	0.180(-4)	0.661(-4)	0.208(-4)
90°	0.416(-4)	0.406(-5)	0.415(-4)	0.401(-5)	0.439(-4)	0.652(-5)
120°	0.347(-4)	-0.775(-5)	0.346(-4)	-0.778(-5)	0.368(-4)	-0.551(-5)
150°	0.385(-4)	-0.150(-4)	0.384(-4)	-0.151(-4)	0.405(-4)	-0.129(-4)
180°	0.525(-4)	-0.182(-4)	0.524(-4)	-0.182(-4)	0.545(-4)	-0.161(-4)
210°	0.785(-4)	-0.175(-4)	0.785(-4)	-0.176(-4)	0.805(-4)	-0.155(-4)
240°	0.118(-3)	-0.112(-4)	0.118(-3)	-0.112(-4)	0.120(-3)	-0.896(-5)
270°	0.164(-3)	0.285(-5)	0.164(-3)	0.280(-5)	0.166(-3)	0.530(-5)
300°	0.199(-3)	0.207(-4)	0.199(-3)	0.206(-4)	0.201(-3)	0.234(-4)
330°	0.200(-3)	0.333(-4)	0.200(-3)	0.333(-4)	0.202(-3)	0.363(-4)
360°	0.160(-3)	0.360(-4)	0.160(-3)	0.359(-4)	-	-

TABLE 3.2

VARIATION OF THE EXCHANGE AMPLITUDE (PETERKOP FORM) WITH ANGLE θ_s FOR THE VARIOUS CHOICES OF ORTHOGONALITY EXAMINED.

CASE: $E_o = 256.5\,eV$ $E_f = 226\,eV$ $\theta_f = 4°$

	ORTHOGONALITY CONDITION (a)		ORTHOGONALITY CONDITION (b)		NO ORTHOGONALITY CONDITION	
ANGLE θ_s	$R.\omega(k_f,k_s)$	$I.\omega(k_f,k_s)$	$R.\omega(\underline{k}_f,\underline{k}_s)$	$I.\omega(\underline{k}_f,\underline{k}_s)$	$R.\omega(\underline{k}_f,\underline{k}_s)$	$I.\omega(\underline{k}_f,\underline{k}_s)$
30°	0.211(-4)	0.192(-5)	0.210(-4)	0.198(-5)	0.195(-4)	0.313(-5)
60°	0.172(-4)	-0.394(-5)	0.171(-4)	-0.388(-5)	0.156(-4)	-0.273(-5)
90°	0.120(-4)	-0.949(-5)	0.119(-4)	-0.943(-5)	0.104(-4)	-0.828(-5)
120°	0.729(-5)	-0.130(-4)	0.720(-5)	-0.130(-4)	0.562(-5)	-0.118(-4)
150°	0.417(-5)	-0.147(-4)	0.408(-5)	-0.146(-4)	0.250(-5)	-0.135(-4)
180°	0.310(-5)	-0.151(-4)	0.301(-5)	-0.151(-4)	0.144(-5)	-0.139(-4)
210°	0.417(-5)	-0.147(-4)	0.408(-5)	-0.146(-4)	0.250(-5)	-0.135(-4)
240°	0.729(-5)	-0.130(-4)	0.720(-5)	-0.130(-4)	0.562(-5)	-0.118(-4)
270°	0.120(-4)	-0.949(-5)	0.119(-4)	-0.943(-5)	0.104(-4)	-0.828(-5)
300°	0.172(-4)	-0.394(-5)	0.171(-4)	-0.388(-5)	0.156(-4)	-0.273(-5)
330°	0.211(-4)	0.192(-5)	0.210(-4)	0.198(-5)	0.195(-4)	0.313(-5)
360°	0.225(-4)	0.456(-5)	0.224(-4)	0.462(-5)	0.209(-4)	0.577(-5)

CASE: $E_o = 256.5\,eV$ $E_f = 229\,eV$ $\theta_f = 6°$

30°	0.202(-4)	0.784(-5)	0.200(-4)	0.789(-5)	0.176(-4)	0.878(-5)
60°	0.190(-4)	0.992(-6)	0.188(-4)	0.104(-5)	0.164(-4)	0.193(-5)
90°	0.163(-4)	-0.654(-5)	0.162(-4)	-0.649(-5)	0.138(-4)	-0.561(-5)
120°	0.131(-4)	-0.123(-4)	0.129(-4)	-0.122(-4)	0.105(-4)	-0.114(-4)
150°	0.105(-4)	-0.155(-4)	0.103(-4)	-0.155(-4)	0.793(-5)	-0.146(-4)
180°	0.953(-5)	-0.166(-4)	0.939(-5)	-0.165(-4)	0.698(-5)	-0.156(-4)
210°	0.105(-4)	-0.155(-4)	0.103(-4)	-0.155(-4)	0.793(-5)	-0.146(-4)
240°	0.131(-4)	-0.123(-4)	0.129(-4)	-0.122(-4)	0.105(-4)	-0.114(-4)
270°	0.163(-4)	-0.654(-5)	0.162(-4)	-0.649(-5)	0.138(-4)	-0.561(-5)
300°	0.190(-4)	0.992(-6)	0.188(-4)	0.104(-5)	0.164(-4)	0.193(-5)
330°	0.202(-4)	0.784(-5)	0.200(-4)	0.789(-5)	0.176(-4)	0.878(-5)
360°	0.204(-4)	0.107(-4)	0.203(-4)	0.107(-4)	-	-

TABLE 3.3

VARIATION OF THE CAPTURE AMPLITUDE (PRIOR FORM) WITH ANGLE θ_s FOR THE VARIOUS CHOICES OF ORTHOGONALITY EXAMINED.

CASE: $E_0 = 256.5\,eV$ $E_f = 229\,eV$ $\theta_f = 6°$

	PRIOR APPROXIMATION		POST APPROXIMATION	
ANGLE θ_S	$\mathcal{R}.\omega(\underline{k}_f,\underline{k}_s)$	$\mathcal{I}.\omega(\underline{k}_f,\underline{k}_s)$	$\mathcal{R}.\omega(\underline{k}_f,\underline{k}_s)$	$\mathcal{I}.\omega(\underline{k}_f,\underline{k}_s)$
15°	0.204(-4)	0.993(-5)	0.952(-5)	-0.184(-4)
30°	0.202(-4)	0.784(-5)	0.101(-4)	-0.178(-4)
45°	0.197(-4)	0.472(-5)	0.113(-4)	-0.166(-4)
60°	0.190(-4)	0.992(-6)	0.129(-4)	-0.147(-4)
75°	0.178(-4)	-0.289(-5)	0.147(-4)	-0.121(-4)
90°	0.163(-4)	-0.654(-5)	0.167(-4)	-0.874(-5)
105°	0.147(-4)	-0.972(-5)	0.185(-4)	-0.470(-5)
120°	0.131(-4)	-0.123(-4)	0.200(-4)	-0.195(-6)
135°	0.116(-4)	-0.142(-4)	0.211(-4)	0.437(-5)
150°	0.105(-4)	-0.155(-4)	0.217(-4)	0.847(-5)
165°	0.977(-5)	-0.163(-4)	0.219(-4)	0.115(-4)
180°	0.953(-5)	-0.166(-4)	0.220(-4)	0.131(-4)
195°	0.977(-5)	-0.163(-4)	0.220(-4)	0.129(-4)
210°	0.105(-4)	-0.155(-4)	0.219(-4)	0.110(-4)
225°	0.116(-4)	-0.142(-4)	0.216(-4)	0.771(-5)
240°	0.131(-4)	-0.123(-4)	0.209(-4)	0.347(-5)
255°	0.147(-4)	-0.971(-5)	0.197(-4)	-0.112(-5)
270°	0.163(-4)	-0.654(-5)	0.182(-4)	-0.555(-5)
285°	0.178(-4)	-0.288(-5)	0.163(-4)	-0.948(-5)
300°	0.190(-4)	0.992(-6)	0.143(-4)	-0.127(-4)
315°	0.197(-4)	0.472(-5)	0.125(-4)	-0.152(-4)
330°	0.202(-4)	0.784(-5)	0.110(-4)	-0.169(-4)
345°	0.204(-4)	0.993(-5)	0.998(-5)	-0.180(-4)
360°	0.204(-4)	0.107(-4)	0.947(-5)	-0.185(-4)

TABLE 3.4

A COMPARISON OF THE VALUES OF THE CAPTURE AMPLITUDE CALCULATED FROM THE PRIOR AND POST FORMULATIONS. ORTHOGONALITY CONDITION (b) IS IMPOSED.

It should be noted that tabulated values differ from the corresponding amplitudes by a multiplicative constant. (The entries in the tables should be multiplied by a factor $16\sqrt{2}\,\alpha^3 Z^{3/2}/\pi$ to obtain the actual values of the amplitudes.)

CASE: E_o = 256.5eV E_f = 226eV θ_f=4°

	PRIOR APPROXIMATION		POST APPROXIMATION	
ANGLE θ_s	$\mathcal{R}.\omega(\underline{k}_f,\underline{k}_s)$	$\mathcal{I}.\omega(\underline{k}_f,\underline{k}_s)$	$\mathcal{R}.\omega(\underline{k}_f,\underline{k}_s)$	$\mathcal{I}.\omega(\underline{k}_f,\underline{k}_s)$
15°	0.221(-4)	0.392(-5)	0.223(-5)	-0.163(-4)
30°	0.210(-4)	0.198(-5)	0.298(-5)	-0.160(-4)
45°	0.193(-4)	-0.787(-6)	0.432(-5)	-0.154(-4)
60°	0.171(-4)	-0.388(-5)	0.625(-5)	-0.144(-4)
75°	0.146(-4)	-0.686(-5)	0.869(-5)	-0.129(-4)
90°	0.119(-4)	-0.948(-5)	0.115(-4)	-0.108(-4)
105°	0.942(-5)	-0.115(-4)	0.146(-4)	-0.800(-5)
120°	0.720(-5)	-0.130(-4)	0.177(-4)	-0.459(-5)
135°	0.539(-5)	-0.140(-4)	0.204(-4)	-0.856(-6)
150°	0.408(-5)	-0.146(-4)	0.225(-4)	0.269(-5)
165°	0.328(-5)	-0.150(-4)	0.240(-4)	0.541(-5)
180°	0.301(-5)	-0.151(-4)	0.246(-4)	0.673(-5)
195°	0.328(-5)	-0.150(-4)	0.244(-4)	0.632(-5)
210°	0.408(-5)	-0.146(-4)	0.234(-4)	0.429(-5)
225°	0.539(-5)	-0.140(-4)	0.216(-4)	0.110(-5)
240°	0.720(-5)	-0.130(-4)	0.192(-4)	-0.261(-5)
255°	0.942(-5)	-0.115(-4)	0.163(-4)	-0.624(-5)
270°	0.119(-4)	-0.943(-5)	0.132(-4)	-0.940(-5)
285°	0.146(-4)	-0.686(-5)	0.102(-4)	-0.119(-4)
300°	0.171(-4)	-0.388(-5)	0.749(-5)	-0.137(-4)
315°	0.193(-4)	-0.786(-6)	0.528(-5)	-0.149(-4)
330°	0.210(-4)	0.198(-5)	0.362(-5)	-0.157(-4)
345°	0.221(-4)	0.392(-5)	0.256(-5)	-0.162(-4)
360°	0.224(-4)	0.462(-5)	0.209(-5)	-0.163(-4)

TABLE 3.5

A COMPARISON OF THE VALUES OF THE CAPTURE AMPLITUDE CALCULATED FROM THE PRIOR AND POST FORMULATIONS. ORTHOGONALITY CONDITION (b) IS IMPOSED.

CASE: E_0 = 256.5 eV E_f = 197 eV $\theta_f = 4°$

	PRIOR APPROXIMATION		POST APPROXIMATION	
ANGLE θ_s	$\mathcal{R}.\omega(\underline{k}_f, \underline{k}_s)$	$\mathcal{I}.\omega(\underline{k}_f, \underline{k}_s)$	$\mathcal{R}.\omega(\underline{k}_f, \underline{k}_s)$	$\mathcal{I}.\omega(\underline{k}_f, \underline{k}_s)$
15°	0.287(-4)	0.599(-6)	-0.192(-5)	-0.725(-5)
30°	0.250(-4)	-0.151(-5)	-0.150(-5)	-0.738(-5)
45°	0.200(-4)	-0.392(-5)	-0.686(-6)	-0.756(-5)
60°	0.149(-4)	-0.584(-5)	0.626(-6)	-0.777(-5)
75°	0.104(-4)	-0.704(-5)	0.257(-5)	-0.796(-5)
90°	0.676(-5)	-0.762(-5)	0.533(-5)	-0.795(-5)
105°	0.397(-5)	-0.778(-5)	0.909(-5)	-0.753(-5)
120°	0.193(-5)	-0.771(-5)	0.139(-4)	-0.642(-5)
135°	0.516(-6)	-0.756(-5)	0.197(-4)	-0.438(-5)
150°	-0.405(-6)	-0.741(-5)	0.258(-4)	-0.149(-5)
165°	-0.920(-6)	-0.730(-5)	0.309(-4)	0.148(-5)
180°	-0.108(-5)	-0.725(-5)	0.335(-4)	0.316(-5)
195°	-0.920(-6)	-0.730(-5)	0.327(-4)	0.262(-5)
210°	-0.405(-6)	-0.741(-5)	0.287(-4)	0.169(-6)
225°	0.616(-6)	-0.756(-5)	0.230(-4)	-0.291(-5)
240°	0.193(-5)	-0.771(-5)	0.169(-4)	-0.546(-5)
255°	0.397(-5)	-0.778(-5)	0.115(-4)	-0.704(-5)
270°	0.676(-5)	-0.762(-5)	0.720(-5)	-0.779(-5)
285°	0.104(-4)	-0.704(-5)	0.392(-5)	-0.799(-5)
300°	0.149(-4)	-0.584(-5)	0.157(-5)	-0.788(-5)
315°	0.200(-4)	-0.392(-5)	-0.550(-7)	-0.767(-5)
330°	0.250(-4)	-0.151(-5)	-0.112(-5)	-0.747(-5)
345°	0.287(-4)	0.599(-6)	-0.174(-5)	-0.731(-5)
360°	0.301(-4)	0.145(-5)	-0.200(-5)	-0.722(-5)

TABLE 3.6

A COMPARISON OF THE VALUES OF THE CAPTURE AMPLITUDE CALCULATED FROM THE PRIOR AND POST FORMULATIONS. ORTHOGONALITY CONDITION (b) IS IMPOSED.

CASE: $E_0 = 256.5\,eV$ $E_f = 229\,eV$ $\theta_f = 4°$

	$f(\underline{k}_f, \underline{k}_s)$		$g(\underline{k}_f, \underline{k}_s)$		$\omega(\underline{k}_f, \underline{k}_s)$	
θ_s ANGLE	$\mathcal{R}.f(\underline{k}_f, \underline{k}_s)$	$\mathcal{I}.f(\underline{k}_f, \underline{k}_s)$	$\mathcal{R}.g(\underline{k}_f, \underline{k}_s)$	$\mathcal{I}.g(\underline{k}_f, \underline{k}_s)$	$\mathcal{R}.\omega(\underline{k}_f, \underline{k}_s)$	$\mathcal{I}.\omega(\underline{k}_f, \underline{k}_s)$
15°	0.511(-2)	0.668(-2)	0.164(-3)	0.381(-4)	0.178(-4)	0.109(-4)
30°	0.344(-2)	0.142(-2)	0.139(-3)	0.341(-4)	0.176(-4)	0.878(-5)
45°	0.137(-2)	-0.338(-2)	0.115(-3)	0.285(-4)	0.172(-4)	0.566(-5)
60°	-0.883(-3)	-0.741(-2)	0.941(-4)	0.215(-4)	0.164(-4)	0.193(-5)
75°	-0.306(-2)	-0.106(-1)	0.783(-4)	0.139(-4)	0.152(-4)	-0.195(-5)
90°	-0.495(-2)	-0.128(-1)	0.671(-4)	0.618(-5)	0.138(-4)	-0.561(-5)
105°	-0.635(-2)	-0.143(-1)	0.597(-4)	-0.779(-6)	0.121(-4)	-0.879(-5)
120°	-0.717(-2)	-0.151(-1)	0.556(-4)	-0.655(-5)	0.105(-4)	-0.114(-4)
135°	-0.732(-2)	-0.153(-1)	0.543(-4)	-0.109(-4)	0.906(-5)	-0.133(-4)
150°	-0.682(-2)	-0.148(-1)	0.555(-4)	-0.140(-4)	0.793(-5)	-0.146(-4)
165°	-0.568(-2)	-0.137(-1)	0.592(-4)	-0.159(-4)	0.722(-5)	-0.154(-4)
180°	-0.401(-2)	-0.118(-1)	0.654(-4)	-0.169(-4)	0.698(-5)	-0.156(-4)
195°	-0.194(-2)	-0.902(-2)	0.742(-4)	-0.169(-4)	0.722(-5)	-0.154(-4)
210°	0.306(-3)	-0.540(-2)	0.858(-4)	-0.157(-4)	0.793(-5)	-0.146(-4)
225°	0.249(-2)	-0.944(-3)	0.100(-3)	-0.132(-4)	0.906(-5)	-0.133(-4)
240°	0.438(-2)	0.414(-2)	0.118(-3)	-0.890(-5)	0.105(-4)	-0.114(-4)
255°	0.578(-2)	0.947(-2)	0.137(-3)	-0.265(-5)	0.121(-4)	-0.879(-5)
270°	0.665(-2)	0.145(-1)	0.157(-3)	0.535(-5)	0.138(-4)	-0.561(-5)
285°	0.707(-2)	0.185(-1)	0.177(-3)	0.144(-4)	0.152(-4)	-0.195(-5)
300°	0.721(-2)	0.209(-1)	0.194(-3)	0.233(-4)	0.164(-4)	0.193(-5)
315°	0.723(-2)	0.214(-1)	0.206(-3)	0.310(-4)	0.172(-4)	0.566(-5)
330°	0.716(-2)	0.199(-1)	0.209(-3)	0.365(-4)	0.176(-4)	0.878(-5)
345°	0.690(-2)	0.165(-1)	0.202(-3)	0.395(-4)	0.178(-4)	0.109(-4)
360°	0.626(-2)	0.119(-1)	0.186(-3)	0.399(-4)	0.178(-4)	0.116(-4)

TABLE 3.7

VARIATION OF THE DIRECT, EXCHANGE AND CAPTURE (PRIOR FORM) AMPLITUDES WITH SCATTERING ANGLE θ_s. THE NON-ORTHOGONALIZED FINAL STATE WAVE FUNCTION IS USED.

CASE: $E_0 = 256.5\,eV$ $E_f = 229\,eV$ $\theta_f = 8^\circ$

	$f(k_f, k_s)$		$g(k_f, k_s)$		$\omega(k_f, k_s)$	
ANGLE θ_s	$\mathcal{R}.f(k_f,k_s)$	$\mathcal{I}.f(k_f,k_s)$	$\mathcal{R}.g(k_f,k_s)$	$\mathcal{I}.g(k_f,k_s)$	$\mathcal{R}\omega(k_f,k_s)$	$\mathcal{I}.\omega(k_f,k_s)$
15°	0.258(-2)	0.103(-3)	0.106(-3)	0.354(-4)	0.178(-4)	0.109(-4)
30°	0.136(-2)	-0.248(-2)	0.793(-4)	0.314(-4)	0.176(-4)	0.878(-5)
45°	0.170(-4)	-0.447(-2)	0.577(-4)	0.261(-4)	0.172(-4)	0.566(-5)
60°	-0.127(-2)	-0.588(-2)	0.418(-4)	0.200(-4)	0.164(-4)	0.193(-5)
75°	-0.236(-2)	-0.680(-2)	0.310(-4)	0.134(-4)	0.152(-4)	-0.195(-5)
90°	-0.315(-2)	-0.734(-2)	0.243(-4)	0.690(-5)	0.138(-4)	-0.561(-5)
105°	-0.360(-2)	-0.761(-2)	0.210(-4)	0.855(-6)	0.121(-4)	-0.879(-5)
120°	-0.369(-2)	-0.766(-2)	0.202(-4)	-0.434(-5)	0.105(-4)	-0.114(-4)
135°	-0.341(-2)	-0.750(-2)	0.218(-4)	-0.852(-5)	0.906(-5)	-0.133(-4)
150°	-0.277(-2)	-0.710(-2)	0.257(-4)	-0.117(-4)	0.793(-5)	-0.146(-4)
165°	-0.182(-2)	-0.637(-2)	0.321(-4)	-0.138(-4)	0.722(-5)	-0.154(-4)
180°	-0.613(-3)	-0.521(-2)	0.414(-4)	-0.152(-4)	0.698(-5)	-0.156(-4)
195°	0.728(-3)	-0.350(-2)	0.540(-4)	-0.156(-4)	0.722(-5)	-0.154(-4)
210°	0.203(-2)	-0.120(-2)	0.704(-4)	-0.149(-4)	0.793(-5)	-0.146(-4)
225°	0.310(-2)	0.167(-2)	0.907(-4)	-0.128(-4)	0.906(-5)	-0.133(-4)
240°	0.378(-2)	0.489(-2)	0.114(-3)	-0.881(-5)	0.105(-4)	-0.114(-4)
255°	0.401(-2)	0.808(-2)	0.140(-3)	-0.271(-5)	0.121(-4)	-0.879(-5)
270°	0.392(-2)	0.108(-1)	0.165(-3)	0.530(-5)	0.138(-4)	-0.561(-5)
285°	0.347(-2)	0.124(-1)	0.186(-3)	0.144(-4)	0.152(-4)	-0.195(-5)
300°	0.369(-2)	0.128(-1)	0.197(-3)	0.234(-4)	0.164(-4)	0.193(-5)
315°	0.383(-2)	0.117(-1)	0.198(-3)	0.308(-4)	0.172(-4)	0.566(-5)
330°	0.400(-2)	0.945(-2)	0.186(-3)	0.358(-4)	0.176(-4)	0.878(-5)
345°	0.394(-2)	0.644(-2)	0.164(-3)	0.381(-4)	0.178(-4)	0.109(-4)
360°	0.348(-2)	0.317(-2)	0.136(-3)	0.378(-4)	0.178(-4)	0.116(-4)

TABLE 3.8

VARIATION OF THE DIRECT, EXCHANGE AND CAPTURE (PRIOR FORM) AMPLITUDES WITH SCATTERING ANGLE θ_s. THE NON-ORTHOGONALIZED FINAL STATE WAVE FUNCTION IS USED.

CASE: E_0 =256.5eV E_f =197eV θ_f=4°

	$f(\underline{k}_f, \underline{k}_s)$		$g(\underline{k}_f, \underline{k}_s)$		$\omega(\underline{k}_f, \underline{k}_s)$	
ANGLE θ_s	$\mathcal{R}.f(\underline{k}_f, \underline{k}_s)$	$\mathcal{I}.f(\underline{k}_f, \underline{k}_s)$	$\mathcal{R}.g(\underline{k}_f, \underline{k}_s)$	$\mathcal{I}.g(\underline{k}_f, \underline{k}_s)$	$\mathcal{R}.\omega(\underline{k}_f, \underline{k}_s)$	$\mathcal{I}.\omega(\underline{k}_f, \underline{k}_s)$
15°	0.268(-2)	0.438(-3)	0.429(-4)	0.364(-4)	0.287(-4)	0.599(-6)
30°	0.166(-2)	0.198(-4)	0.152(-4)	0.269(-4)	0.250(-4)	-0.151(-5)
45°	0.721(-3)	-0.265(-3)	0.336(-5)	0.185(-4)	0.200(-4)	-0.392(-5)
60°	-0.586(-4)	-0.416(-3)	-0.161(-5)	0.117(-4)	0.149(-4)	-0.584(-5)
75°	-0.657(-3)	-0.466(-3)	-0.769(-5)	0.457(-5)	0.104(-4)	-0.704(-5)
90°	-0.109(-2)	-0.458(-3)	-0.145(-4)	-0.279(-5)	0.676(-5)	-0.762(-5)
105°	-0.140(-2)	-0.424(-3)	-0.196(-4)	-0.760(-5)	0.397(-5)	-0.778(-5)
120°	-0.159(-2)	-0.388(-3)	-0.220(-4)	-0.879(-5)	0.193(-5)	-0.771(-5)
135°	-0.171(-2)	-0.360(-3)	-0.222(-4)	-0.745(-5)	0.516(-6)	-0.756(-5)
150°	-0.176(-2)	-0.346(-3)	-0.210(-4)	-0.524(-5)	-0.405(-6)	-0.741(-5)
165°	-0.174(-2)	-0.350(-3)	-0.196(-4)	-0.338(-5)	-0.920(-6)	-0.730(-5)
180°	-0.167(-2)	-0.371(-3)	-0.189(-4)	-0.262(-5)	-0.108(-5)	-0.725(-5)
195°	-0.152(-2)	-0.404(-3)	-0.193(-4)	-0.332(-5)	-0.920(-6)	-0.730(-5)
210°	-0.127(-2)	-0.441(-3)	-0.204(-4)	-0.562(-5)	-0.405(-6)	-0.741(-5)
225°	-0.913(-3)	-0.466(-3)	-0.213(-4)	-0.927(-5)	0.516(-6)	-0.756(-5)
240°	-0.406(-3)	-0.453(-3)	-0.199(-4)	-0.132(-4)	0.193(-5)	-0.771(-5)
255°	0.275(-3)	-0.362(-3)	-0.144(-4)	-0.150(-4)	0.397(-5)	-0.778(-5)
270°	0.113(-2)	-0.153(-3)	-0.366(-5)	-0.113(-4)	0.676(-5)	-0.762(-5)
285°	0.213(-2)	0.197(-3)	0.110(-4)	-0.132(-6)	0.104(-4)	-0.704(-5)
300°	0.313(-2)	0.654(-3)	0.283(-4)	0.161(-4)	0.149(-4)	-0.584(-5)
315°	0.394(-2)	0.109(-2)	0.510(-4)	0.314(-4)	0.200(-4)	-0.392(-5)
330°	0.435(-2)	0.133(-2)	0.775(-4)	0.418(-4)	0.250(-4)	-0.151(-5)
345°	0.423(-2)	0.126(-2)	0.918(-4)	0.460(-4)	0.287(-4)	0.599(-6)
360°	0.361(-2)	0.905(-3)	0.771(-4)	0.438(-4)	0.301(-4)	0.145(-5)

TABLE 3.9

VARIATION OF THE DIRECT, EXCHANGE AND CAPTURE (PRIOR FORM) AMPLITUDES WITH SCATTERING ANGLE θ_s . ORTHOGONALITY CONDITION (b) IS IMPOSED.

CASE: E_0 = 256.5eV E_f = 229eV $\theta_f=6°$

ANGLE θ_8	EQUAL PHASES	COULOMB PHASES	MAXIMUM INTERFERENCE	RUDGE PHASE	BORN OCHKUR
15°	0.1491	0.1490	0.1490	0.1510	0.1515
30°	0.7084(-1)	0.7137(-1)	0.6959(-1)	0.7394(-1)	0.7118(-1)
45°	0.2219	0.2227	0.2250	0.2249	0.2176
60°	0.4988	0.4996	0.5013	0.5013	0.4894
75°	0.8050	0.8057	0.8072	0.8072	0.7916
90°	0.1069(+1)	0.1070(+1)	0.1072(+1)	0.1072(+1)	0.1053(+1)
105°	0.1247(+1)	0.1248(+1)	0.1250(+1)	0.1250(+1)	0.1231(+1)
120°	0.1316(+1)	0.1317(+1)	0.1319(+1)	0.1319(+1)	0.1300(+1)
135°	0.1268(+1)	0.1269(+1)	0.1271(+1)	0.1271(+1)	0.1253(+1)
150°	0.1107(+1)	0.1108(+1)	0.1112(+1)	0.1111(+1)	0.1095(+1)
165°	0.8557	0.8566	0.8516	0.8591	0.8467
180°	0.5525	0.5534	0.5490	0.5558	0.5472
195°	0.2643	0.2650	0.2620	0.2671	0.2624
210°	0.8360(-1)	0.8395(-1)	0.8305(-1)	0.8543(-1)	0.8436(-1)
225°	0.1149	0.1147	0.1145	0.1148	0.1164
240°	0.4367	0.4355	0.4336	0.4336	0.4359
255°	0.1044(+1)	0.1042(+1)	0.1037(+1)	0.1037(+1)	0.1038(+1)
270°	0.1802(+1)	0.1798(+1)	0.1789(+1)	0.1790(+1)	0.1787(+1)
285°	0.2458(+1)	0.2452(+1)	0.2440(+1)	0.2441(+1)	0.2434(+1)
300°	0.2747(+1)	0.2741(+1)	0.2728(+1)	0.2728(+1)	0.2719(+1)
315°	0.2542(+1)	0.2537(+1)	0.2525(+1)	0.2525(+1)	0.2516(+1)
330°	0.1934(+1)	0.1930(+1)	0.1921(+1)	0.1921(+1)	0.1916(+1)
345°	0.1174(+1)	0.1171(+1)	0.1166(+1)	0.1167(+1)	0.1166(+1)
360°	0.5252	0.5239	0.5226	0.5238	0.5249

TABLE 3.10

VALUES OF THE TDCS WITH THE INCLUSION OF EXCHANGE AND CAPTURE (PRIOR FORM), CALCULATED FOR VARIOUS FORMS OF THE EXCHANGE AMPLITUDE. THE FIRST FOUR APPROXIMATIONS CORRESPOND TO THE DIFFERENT CHOICES OF THE PHASE FACTOR ASSOCIATED WITH THE EXCHANGE AMPLITUDE, AS DESCRIBED IN CHAPTER 2. THE APPROXIMATION DENOTED BY RUDGE PHASE CORRESPONDS TO THE CHOICE OF EFFECTIVE CHARGES $z_1 = 1-(k_1/|\underline{k}_1-\underline{k}_2|)$, $z_2 = 1$.

E_0= 200eV E_f = 164.5eV θ_b= 30°

ANGLE θ_f	EQUAL PHASES	COULOMB PHASES	MAXIMUM INTERFERENCE	RUDGE PHASE	BORN OCHKUR
15°	0.2308(-1)	0.2304(-1)	0.2324(-1)	0.2324(-1)	0.2062(-1)
30°	0.2887(-2)	0.2860(-2)	0.2749(-2)	0.3103(-2)	0.2127(-2)
45°	0.2556(-3)	0.2473(-3)	0.2182(-3)	0.3272(-3)	0.1900(-3)
60°	0.4945(-4)	0.4965(-4)	0.4932(-4)	0.4367(-4)	0.4129(-4)
75°	0.2486(-4)	0.2507(-4)	0.2409(-4)	0.2010(-4)	0.2026(-4)
90°	0.1674(-4)	0.1577(-4)	0.8581(-5)	0.2122(-4)	0.1398(-4)
105°	0.1219(-4)	0.1155(-4)	0.9136(-5)	0.1576(-4)	0.1115(-4)
120°	0.9581(-5)	0.9905(-5)	0.9687(-5)	0.8981(-5)	0.9891(-5)
135°	0.1083(-4)	0.1108(-4)	0.1096(-4)	0.1067(-4)	0.1011(-4)
150°	0.2543(-4)	0.2384(-4)	0.1237(-4)	0.3219(-4)	0.1237(-4)
165°	0.6518(-4)	0.6088(-4)	0.9136(-4)	0.8272(-4)	0.1731(-4)
180°	0.6335(-4)	0.5865(-4)	0.2963(-4)	0.8373(-4)	0.2493(-4)
195°	0.3462(-4)	0.3316(-4)	0.2781(-4)	0.4206(-4)	0.2775(-4)
210°	0.5295(-4)	0.5412(-4)	0.4502(-4)	0.4816(-4)	0.4017(-4)
225°	0.5601(-4)	0.5688(-4)	0.4930(-4)	0.5226(-4)	0.4065(-4)
240°	0.4099(-4)	0.4073(-4)	0.4070(-4)	0.4451(-4)	0.3382(-4)
255°	0.3241(-4)	0.3143(-4)	0.2936(-4)	0.3872(-4)	0.2302(-4)
270°	0.3862(-4)	0.3733(-4)	0.4206(-4)	0.4216(-4)	0.1745(-4)
285°	0.3020(-4)	0.2934(-4)	0.2250(-4)	0.3384(-4)	0.4120(-4)
300°	0.1027(-3)	0.1050(-3)	0.1025(-4)	0.1107(-3)	0.2004(-3)
315°	0.1569(-2)	0.1577(-2)	0.1557(-2)	0.1565(-2)	0.1391(-2)
330°	0.2248(-1)	0.2247(-1)	0.2247(-1)	0.2279(-1)	0.1751(-1)
345°	0.2996	0.3003	0.2990	0.3017	0.2823
360°	0.2600(+1)	0.2602(+1)	0.2599(+1)	0.2606(+1)	0.2599(+1)

TABLE 3.11

VALUES OF THE TDC, WITH THE INCLUSION OF EXCHANGE AND CAPTURE (PRIOR FORM), CALCULATED FOR VARIOUS FORMS OF THE EXCHANGE AMPLITUDE.

THE CAPTURE PROBABILITY

(USING ORTHOGONALIZED FINAL STATE WAVE FUNCTION (b))

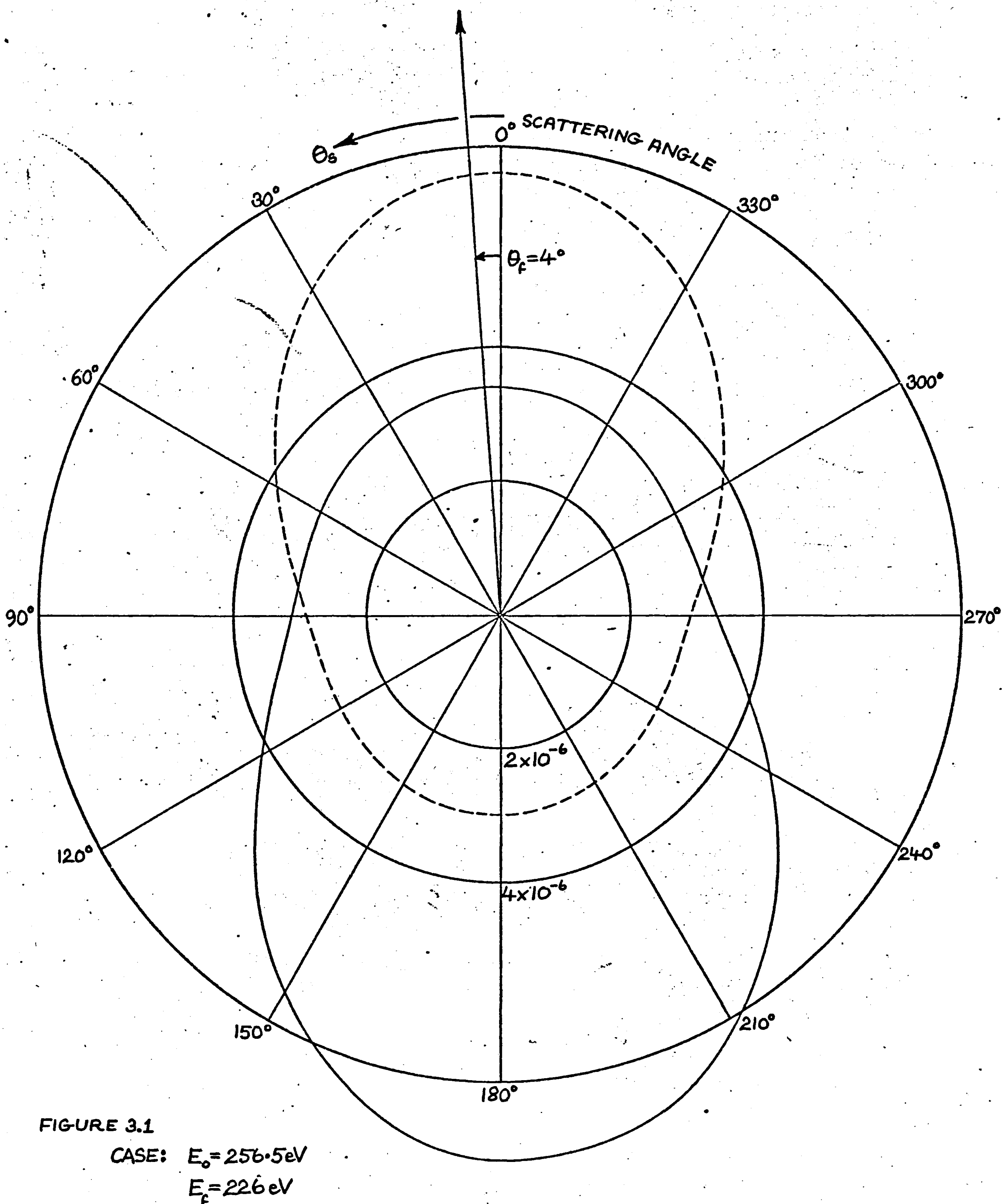


FIGURE 3.1

CASE: $E_o = 256 \cdot 5$ eV
$E_f = 226$ eV
$\theta_f = 4°$

THE FULL LINE CORRESPONDS TO THE POST APPROXIMATION AND THE BROKEN LINE TO THE PRIOR APPROXIMATION.

THE CAPTURE PROBABILITY *

(USING NON-ORTHOGONALIZED FINAL STATE WAVE FUNCTION)

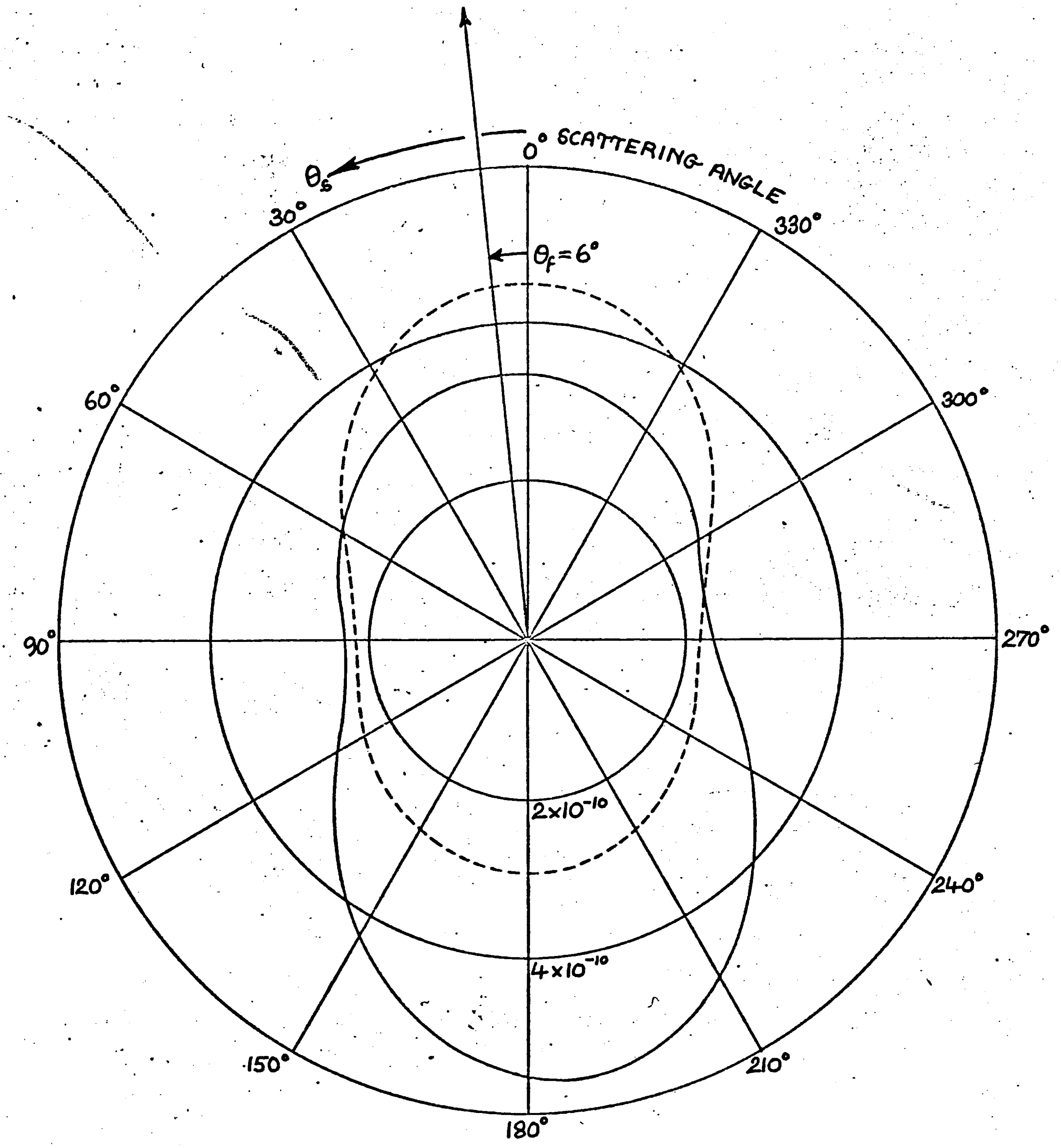


FIGURE 3.2

CASE: $E_0 = 256{\cdot}5\,eV$
$E_f = 229\,eV$
$\theta_f = 6°$

THE FULL LINE CORRESPONDS TO THE POST APPROXIMATION AND THE BROKEN LINE TO THE PRIOR APPROXIMATION.

* (IT SHOULD BE NOTED THAT THESE VALUES DIFFER FROM THE ACTUAL VALUES OF THE PROBABILITY BY A FACTOR $\frac{2k_f k_s}{k_0}\left(\frac{512\alpha^6 Z^3}{\pi^2}\right)$)

THE CAPTURE PROBABILITY*

(CALCULATED FROM THE PRIOR APPROXIMATION)
NON-ORTHOGONALIZED FINAL STATE WAVE FUNCTION.

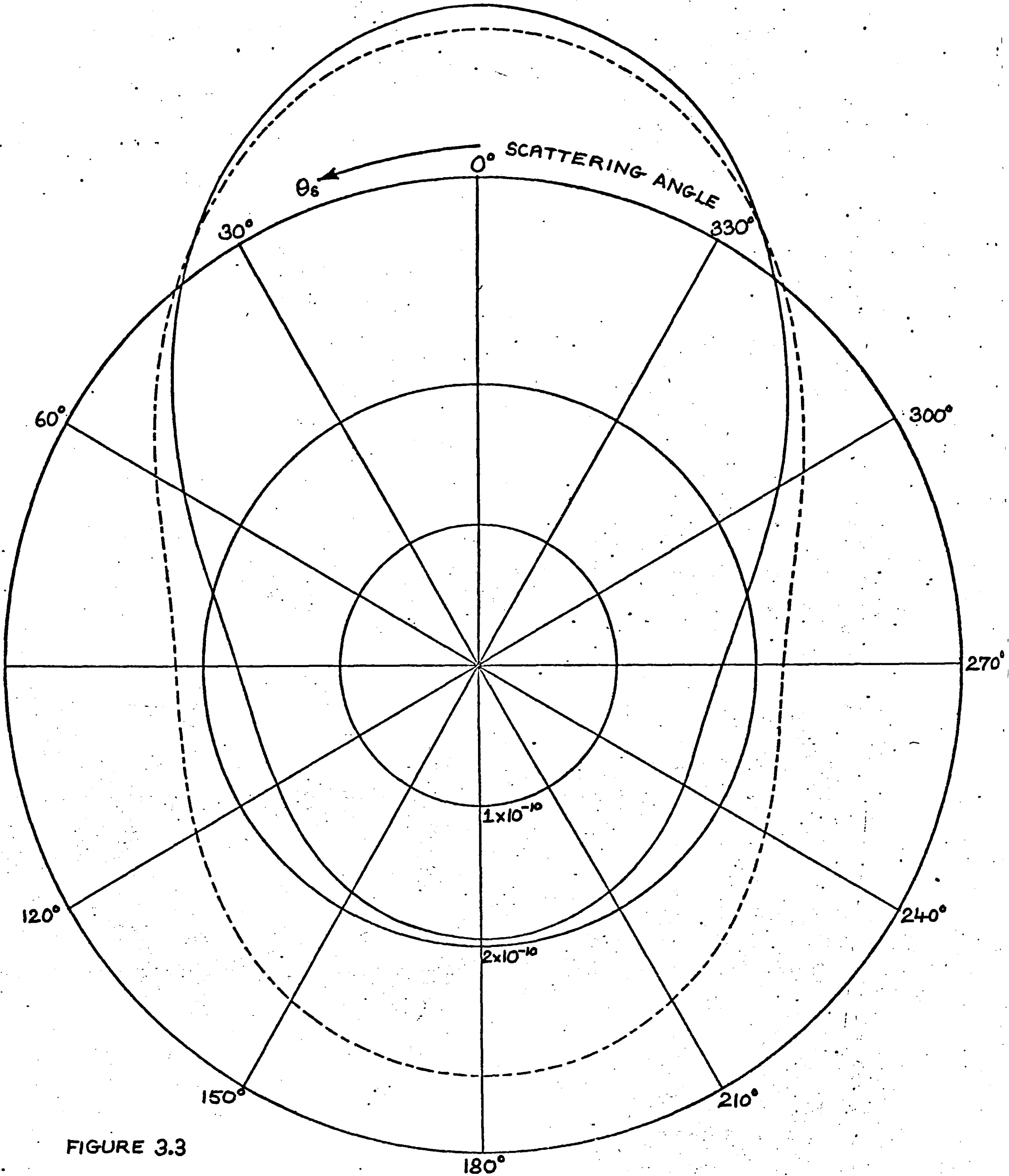


FIGURE 3.3

THE ENERGY DEPENDENCE OF THE CAPTURE PROBABILITY

CASES: $E_o = 256.5eV$
$E_f = 229eV$ (BROKEN LINE) $E_f = 226eV$ (FULL LINE)

IT SHOULD BE NOTED THAT THE PRIOR FORM OF THE CAPTURE PROBABILITY DOES NOT DEPEND ON θ_f.

THE TRIPLE DIFFERENTIAL CROSS SECTION

CASE: $E_o = 256.5\text{eV}$ $E_f = 226\text{eV}$ $\theta_f = 4°$

EXCHANGE INCLUDED

ORTHOGONALIZED FINAL STATE WAVE FUNCTION (a)

ANGLE	TDC
15°	0.639
30°	0.141
45°	0.748(-1)
60°	0.326
75°	0.740
90°	0.118(+1)
105°	0.155(+1)
120°	0.179(+1)
135°	0.186(+1)
150°	0.177(+1)
165°	0.151(+1)
180°	0.113(+1)
195°	0.687
210°	0.284
225°	0.625(-1)
240°	0.176
255°	0.729
270°	0.169(+1)
285°	0.284(+1)
300°	0.377(+1)
315°	0.410(+1)
330°	0.368(+1)
345°	0.270(+1)
360°	0.156(+1)

THE TRIPLE DIFFERENTIAL CROSS SECTION
(WITH THE INCLUSION OF EXCHANGE (PETERKOP FORM))

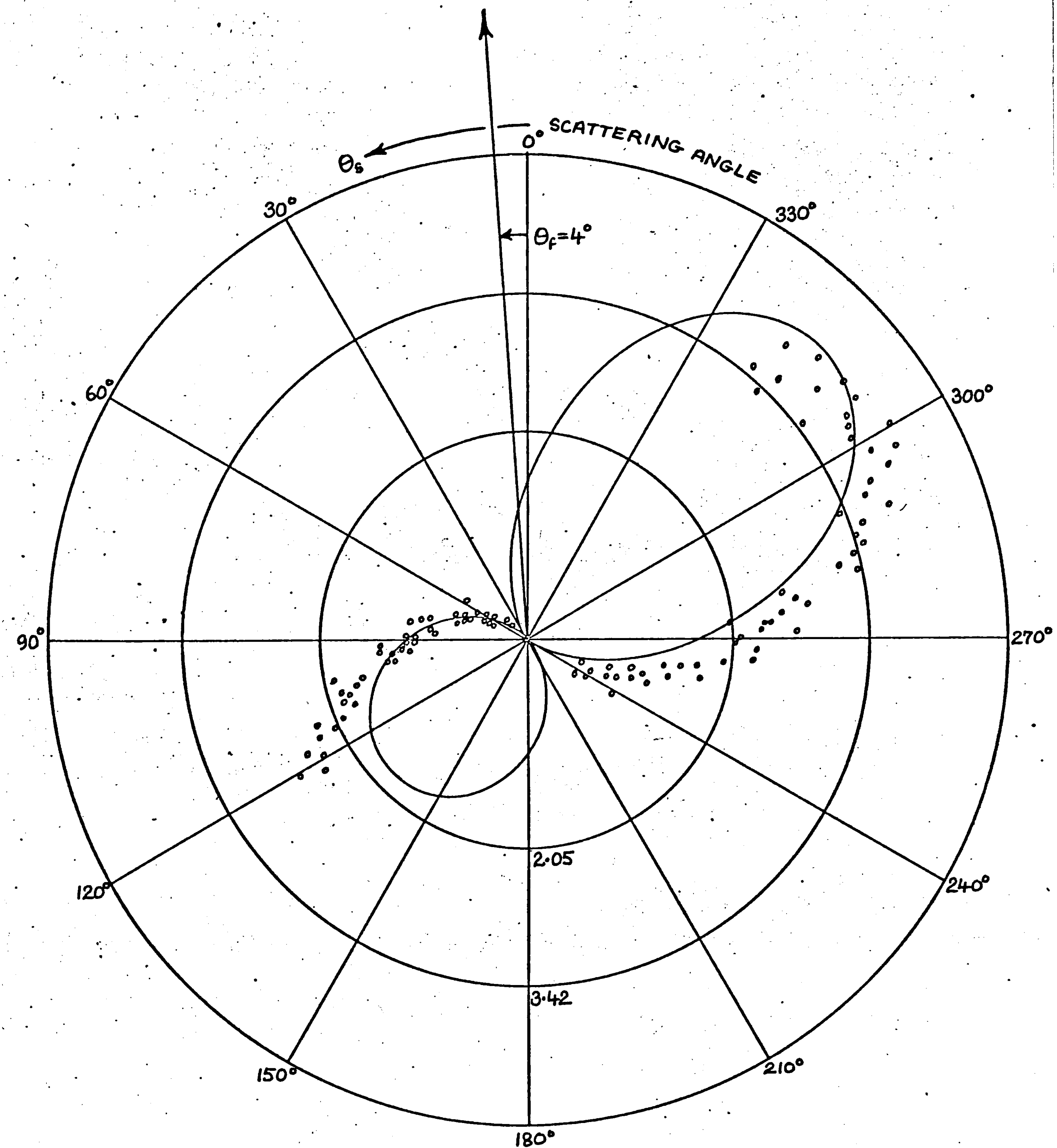


FIGURE 3.4

CASE: $E_0 = 256{\cdot}5\,\text{eV}$.
$E_f = 226\,\text{eV}$
$\theta_f = 4°$

. THE TRIPLE DIFFERENTIAL CROSS SECTION

CASE: E_0 = 256.5 eV E_f = 226 eV θ_f = 6°

EXCHANGE AND CAPTURE (PRIOR) INCLUDED

NON-ORTHOGONALIZED FINAL STATE WAVE FUNCTION

ANGLE θ_s	TDC
15°	0.142
30°	0.456(-1)
45°	0.144
60°	0.341
75°	0.560
90°	0.749
105°	0.879
120°	0.937
135°	0.919
150°	0.827
165°	0.667
180°	0.459
195°	0.242
210°	0.794(-1)
225°	0.600(-1)
240°	0.275
255°	0.769
270°	0.147(+1)
285°	0.215(+1)
300°	0.252(+1)
315°	0.240(+1)
330°	0.185(+1)
345°	0.113(+1)
360°	0.506

THE TRIPLE DIFFERENTIAL CROSS SECTION
(WITH THE INCLUSION OF EXCHANGE (PETERKOP FORM)
AND CAPTURE (PRIOR FORM))

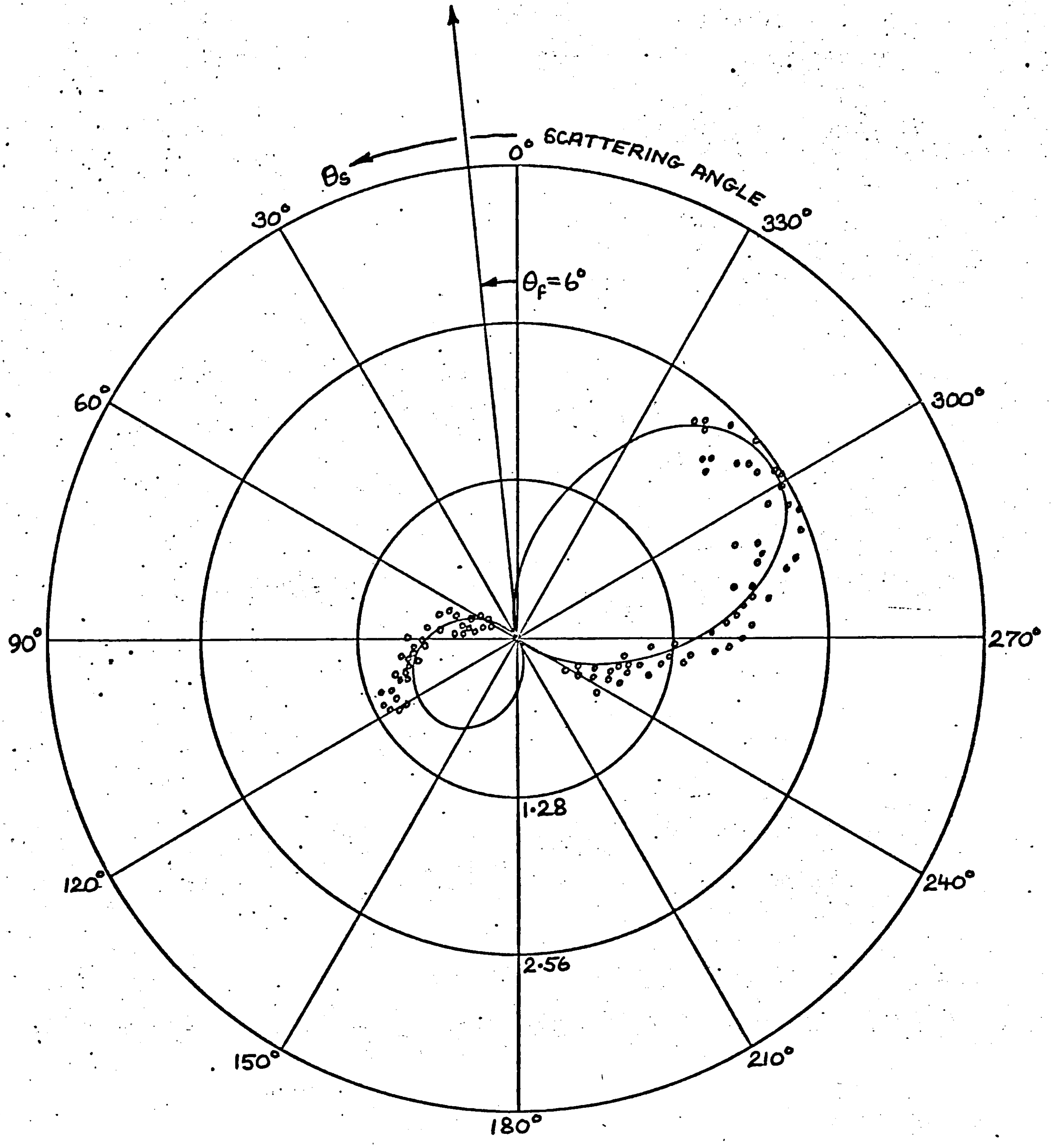


FIGURE 3.5

CASE: $E_0 = 256{\cdot}5\,eV$
$E_f = 226\ eV$
$\theta_f = 6°$

THE TRIPLE DIFFERENTIAL CROSS SECTION

CASE: E_o = 256.5eV E_f = 230.5eV θ_f=4°

EXCHANGE INCLUDED

ORTHOGONALIZED FINAL STATE WAVE FUNCTION (b)

ANGLE θ_s	TDC
15°	0.669
30°	0.132
45°	0.174
60°	0.675
75°	0.143(+1)
90°	0.222(+1)
105°	0.287(+1)
120°	0.325(+1)
135°	0.330(+1)
150°	0.300(+1)
165°	0.241(+1)
180°	0.164(+1)
195°	0.851
210°	0.265
225°	0.913(-1)
240°	0.478
255°	0.143(+1)
270°	0.275(+1)
285°	0.406(+1)
300°	0.493(+1)
315°	0.504(+1)
330°	0.434(+1)
345°	0.310(+1)
360°	0.174(+1)

THE TRIPLE DIFFERENTIAL CROSS SECTION

WITH THE INCLUSION OF EXCHANGE (PETERKOP FORM)

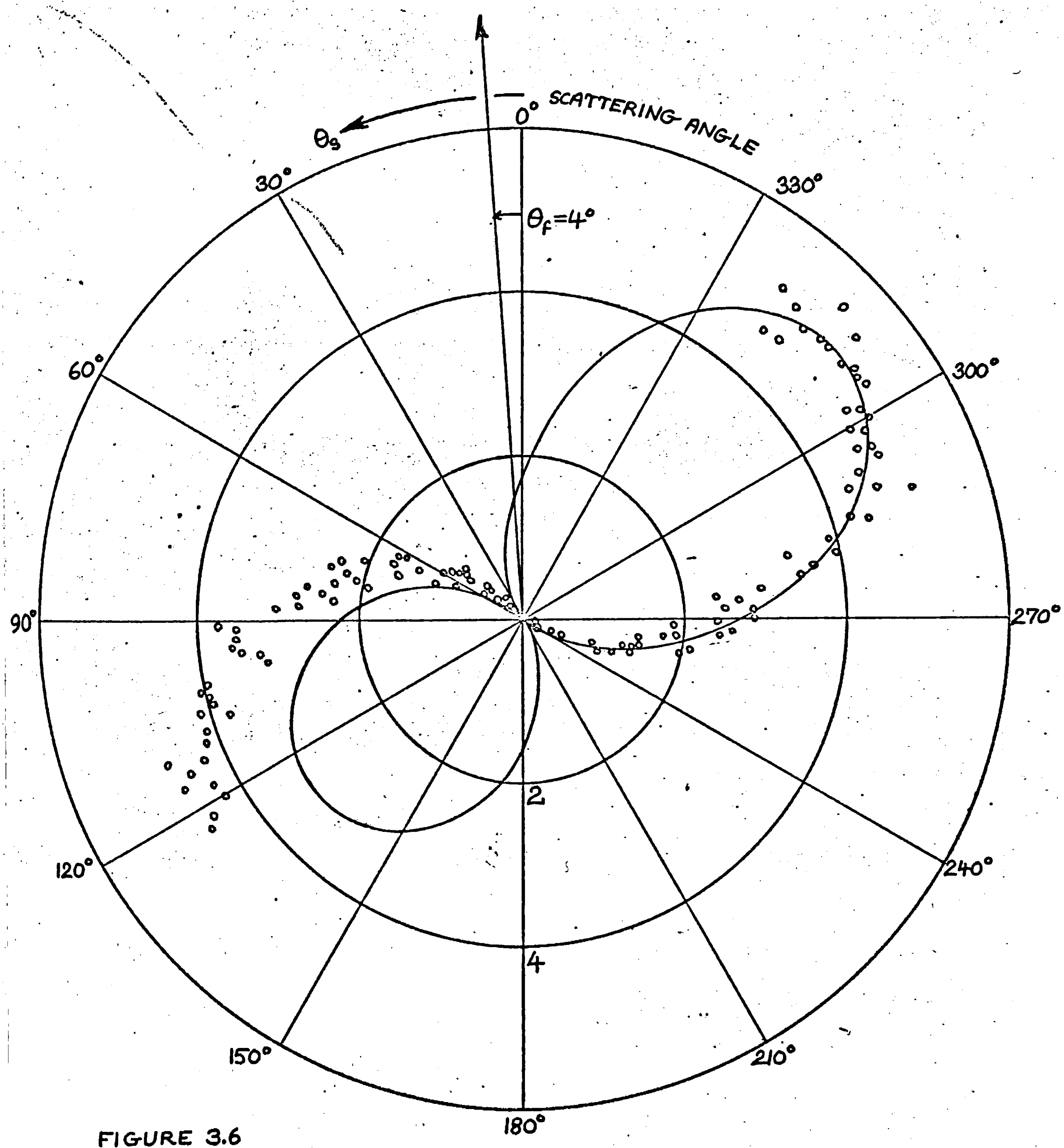


FIGURE 3.6

CASE : $E_0 = 256{\cdot}5\,eV$
$E_f = 230{\cdot}5\,eV$
$\theta_f = 4°$

THE TRIPLE DIFFERENTIAL CROSS SECTION

CASE: E_o = 256.5eV E_f = 229eV θ_f=6

EXCHANGE INCLUDED

ORTHOGONALIZED FINAL STATE WAVE FUNCTION (b)

ANGLE θ_s	TDC
15°	0.151
30°	0.718(-1)
45°	0.222
60°	0.499
75°	0.805
90°	0.107(+1)
105°	0.125(+1)
120°	0.132(+1)
135°	0.127(+1)
150°	0.111(+1)
165°	0.857
180°	0.554
195°	0.266
210°	0.847(-1)
225°	0.116
240°	0.437
255°	0.104(+1)
270°	0.180(+1)
285°	0.246(+1)
300°	0.275(+1)
315°	0.254(+1)
330°	0.194(+1)
345°	0.118(+1)
360°	0.527

THE TRIPLE DIFFERENTIAL CROSS SECTION

WITH THE INCLUSION OF EXCHANGE (PETERKOP FORM)

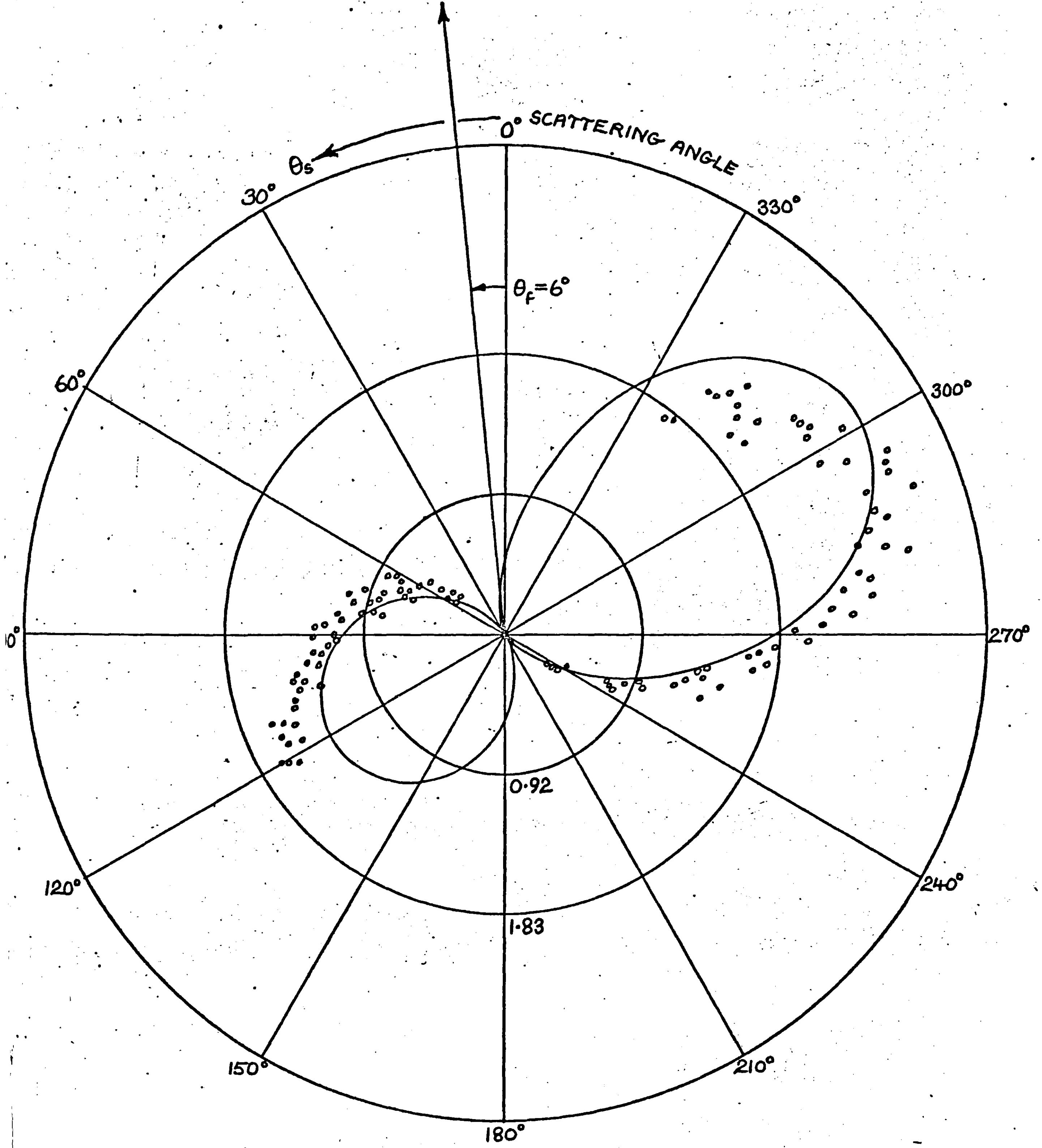


FIGURE 3.7

CASE: $E_0 = 256\cdot5$ eV

$E_f = 229$ eV

$\theta_f = 6°$

THE TRIPLE DIFFERENTIAL CROSS SECTION

WITH THE INCLUSION OF EXCHANGE (PETERKOP FORM)

CASE: $E_0 = 256{\cdot}5\,eV$
$E_f = 229\,eV$
$\theta_f = 6°$

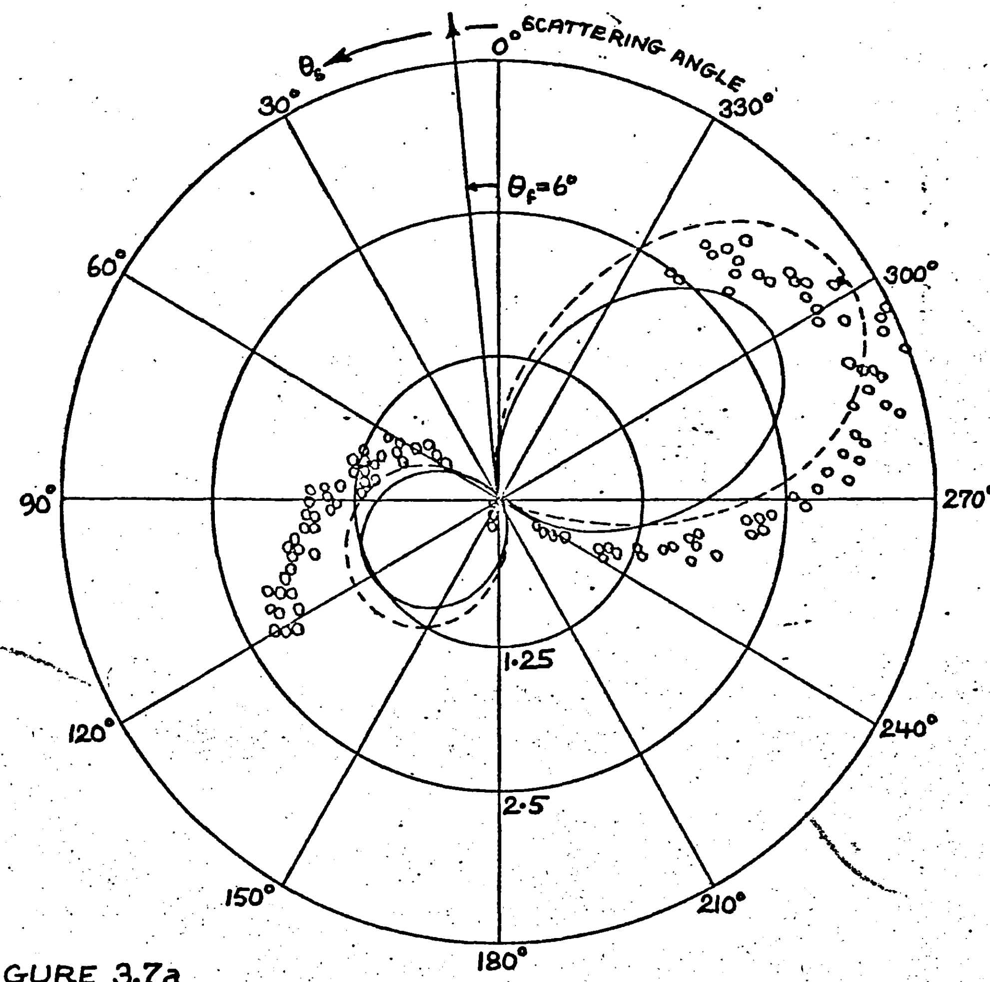


FIGURE 3.7a

THE FULL CURVE CORRESPONDS TO OUR EXCHANGE ADIABATIC CALCULATIONS AND THE BROKEN LINE TO BORN-COULOMB CALCULATIONS USING A H-F WAVE FUNCTION TO REPRESENT THE TARGET SYSTEM (SCHULZ).

THE EXPERIMENTAL DATA IS NORMALIZED WITH RESPECT TO THE BORN-COULOMB CALCULATIONS.

THE TRIPLE DIFFERENTIAL CROSS SECTION

CASE: $E_o = 256.5eV$ $E_f = 229eV$ $\theta_f = 4°$

EXCHANGE AND CAPTURE (PRIOR) INCLUDED

NON-ORTHOGONALIZED FINAL STATE WAVE FUNCTION

ANGLE θ_s	TDC
15°	0.654
30°	0.125
45°	0.124
60°	0.526
75°	0.114(+1)
90°	0.179(+1)
105°	0.232(+1)
120°	0.264(+1)
135°	0.271(+1)
150°	0.250(+1)
165°	0.206(+1)
180°	0.145(+1)
195°	0.800
210°	0.273
225°	0.642(-1)
240°	0.338
255°	0.115
270°	0.237(+1)
285°	0.367(+1)
300°	0.459(+1)
315°	0.479(+1)
330°	0.418(+1)
345°	0.300(+1)
360°	0.169(+1)

THE TRIPLE DIFFERENTIAL CROSS SECTION (WITH THE INCLUSION OF EXCHANGE (PETERKOP FORM) AND CAPTURE (PRIOR FORM))

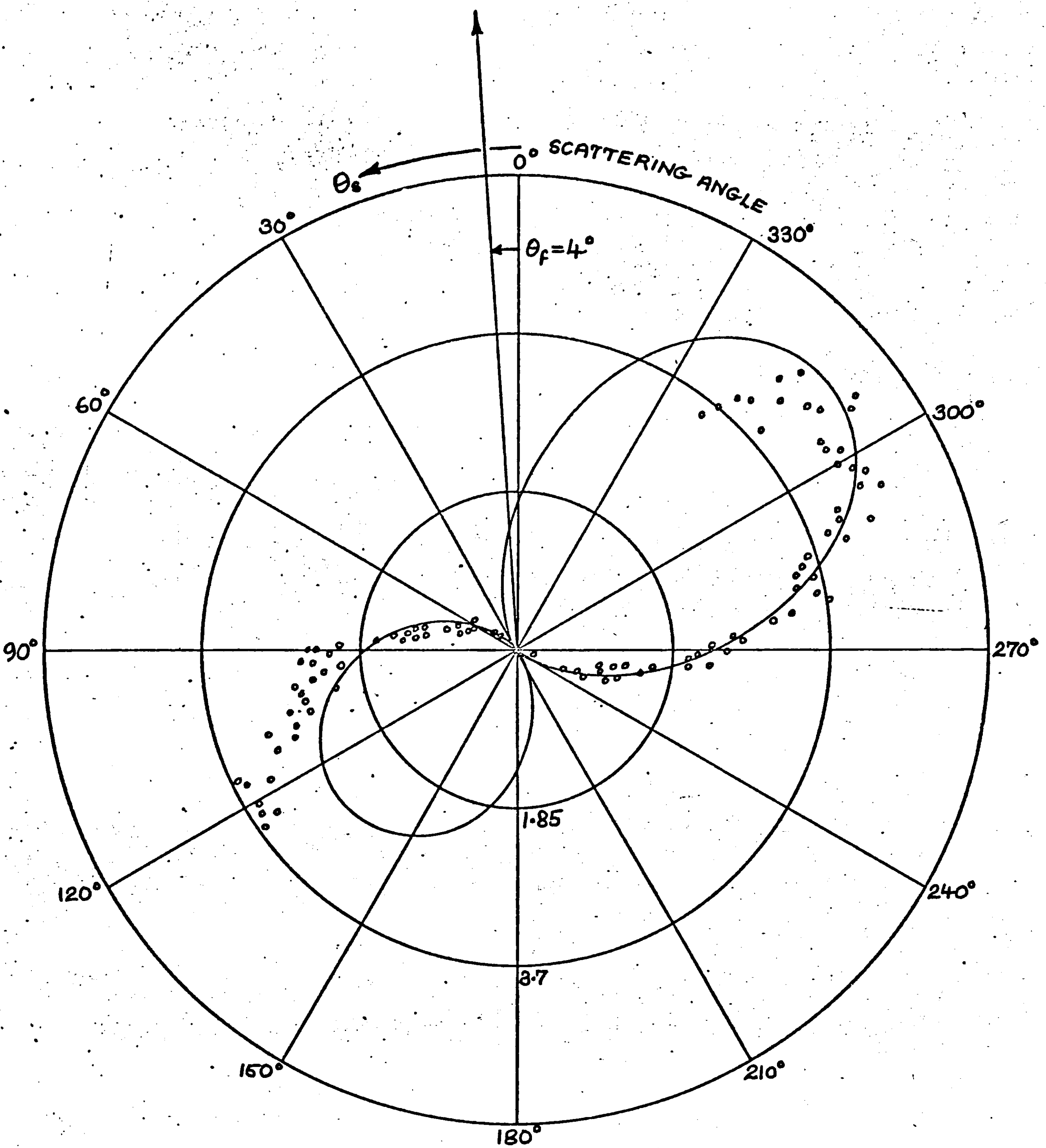


FIGURE 3.8

CASE: $E_0 = 256{\cdot}5\,eV$
$E_f = 229\,eV$
$\theta_f = 4°$

THE TRIPLE DIFFERENTIAL CROSS SECTION

CASE: $E_0 = 256.5eV$ $E_f = 197eV$ $\theta_f = 4^\circ$

EXCHANGE AND CAPTURE (PRIOR) INCLUDED

ORTHOGONALIZED FINAL STATE WAVE FUNCTION (b)

ANGLE θ_s	TDC
15°	0.195
30°	0.734(-1)
45°	0.157(-1)
60°	0.489(-2)
75°	0.177(-1)
90°	0.379(-1)
105°	0.572(-1)
120°	0.722(-1)
135°	0.820(-1)
150°	0.863(-1)
165°	0.851(-1)
180°	0.783(-1)
195°	0.660(-1)
210°	0.485(-1)
225°	0.279(-1)
240°	0.961(-2)
255°	0.548(-2)
270°	0.354(-1)
285°	0.123
300°	0.274
315°	0.447
330°	0.550
345°	0.513
360°	0.365

THE TRIPLE DIFFERENTIAL CROSS SECTION
(WITH THE INCLUSION OF EXCHANGE (PETERKOP FORM)
AND CAPTURE (PRIOR FORM))

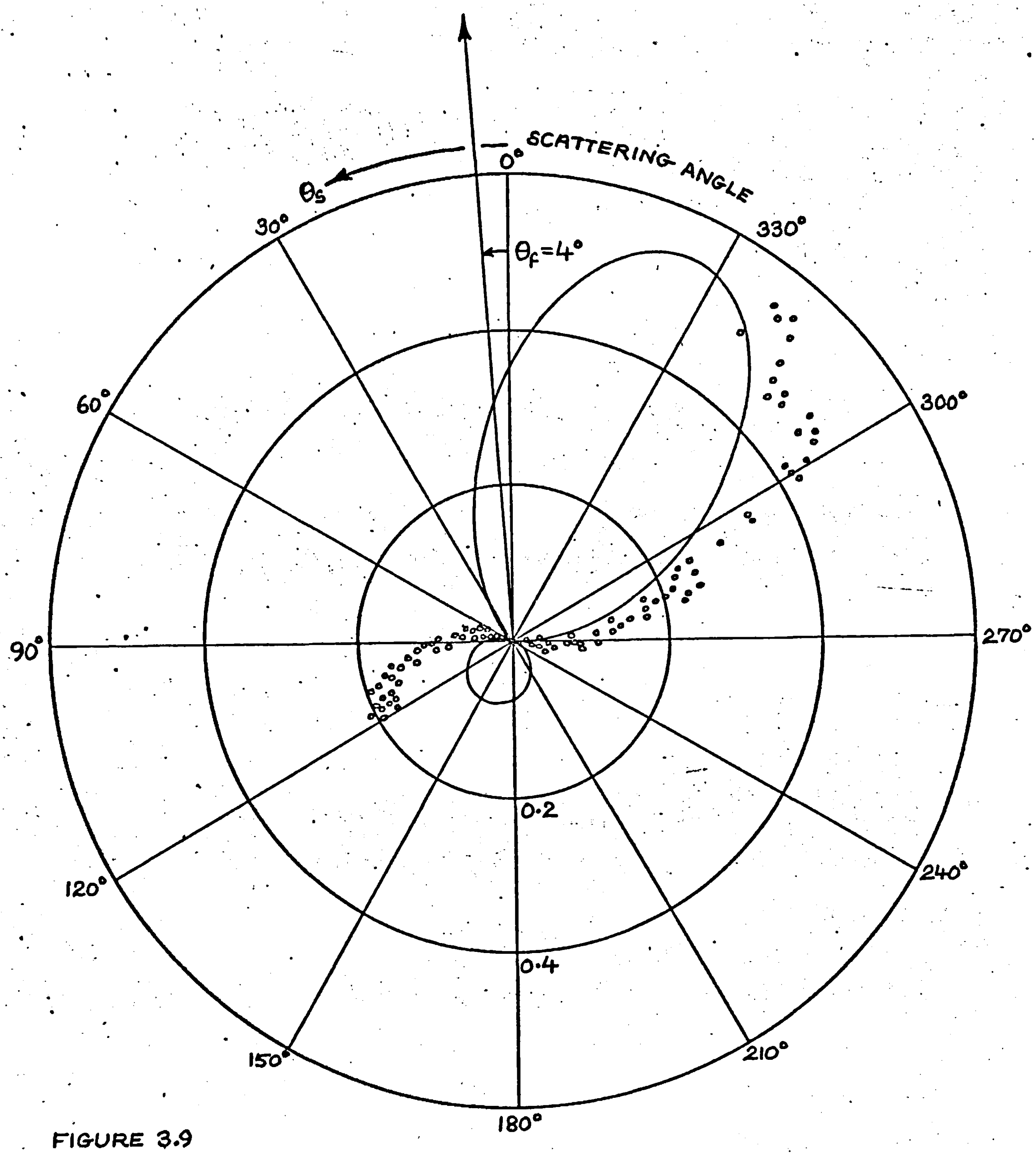


FIGURE 3.9

CASE: $E_0 = 256{\cdot}5\,\text{eV}$
$E_f = 197\,\text{eV}$
$\theta_f = 4°$

CHAPTER 4 .

As a consequence of the investigation described in the previous chapter we conclude that the capture process makes no significant contribution to the triple differential cross section in the energy region considered. Hence we can confidently neglect the effects of capture in subsequent calculations within the same energy region. In this chapter we attempt to evaluate the triple differential cross section for electron-helium ionizing collisions within the first Born approximation, to high accuracy, and hence to identify more clearly the angular regions in which the predictions of the first Born approximation are reliable. Unfortunately the experimental measurements are restricted to impact energies below 260 eV, and it is already clear from Bethe-Born plots of the total cross section (Inokuti 1972, Economides and McDowell 1969) that the first Born approximation gives an unsatisfactory result for the total cross section at such low energies.

Any attempt to assess the reliability of first Born predictions of the triple differential cross section for electron impact on complex atoms requires the use of accurate wave functions for the target, and for the slower of the outgoing electrons. Otherwise little siginificance can be attached to the degree of agreement with the experimental data.

For the purposes of these calculations we have retained the adiabatic-exchange description of the residual ion and "slow" outgoing electron (§ 3.1) while introducing an improved description of the target ground state. The simple one parameter wave function given by equation (3.5) is now replaced by a six configuration C.I. target wave function (Green et al 1953, 1954)

$$\Psi_0(\underline{r}_2,\underline{r}_3) = \sum_{i=1}^{6} a_i \chi_i(\underline{r}_2,\underline{r}_3) \tag{4.1}$$

The nature of the two-electron configuration wave functions $\chi_i(\underline{r}_2,\underline{r}_3)$ and the method by which the weights a_i are determined are described in the following section.

4.1. The correlated target wave function

Excellent wave functions describing the ground states of two-electron ions have been available for some time. The wave functions of Hylleraas provide one such example. However because of the way in which the electron-electron correlation is included in these, (i.e. through a dependence on the inter-electron radius vector $\underline{r}_{23}$) subsequent calculations involving such wave functions often prove difficult, frequently necessitating some type of approximation and so forfeiting the initial accuracy. A useful approach to the problem of achieving high accuracy while retaining simplicity of form is provided by Green et al (1953, 1954). In this work the wave function is represented by a series expansion in normalized Legendre Polynomials based on a accurate Hylleraas function

$$\Psi_0(\underline{r}_2,\underline{r}_3) = \sum_{i} b_i \Phi_i^N(r_2,r_3) P_i^N(\hat{\underline{r}}_2\cdot\hat{\underline{r}}_3) \tag{4.2}$$

The normalized function $\Phi_i^N(r_2,r_3)$ is determined by projecting $\Psi_0(\underline{r}_2,\underline{r}_3)$ onto $P_i^N(\hat{\underline{r}}_2\cdot\hat{\underline{r}}_3)$ in the usual way. Once the functions Φ_i^N have been obtained then each of these is expanded in combinations of hydrogenic orbitals (corresponding to a series of two-electron configurations). Since the orbital angular momenta of the two atomic electrons combine through Russell-Saunders Coupling and the total orbital angular momentum of the ground state is zero then it is clear that the configuration expansion can only include suitably symmetrized combinations of states having equal but anti-parallel momentum l . Moreoever the Spherical Harmonics Y_{lm} associated with the electron states must combine to give the Legendre Polynomial P_l^N corresponding to the function Φ_l^N since the former of these contains the entire angular dependence. Hence the expansion corresponding to Φ_0^N can contain only s-s configurations, that corresponding to Φ_1^N only p-p configurations and so on. In their initial calculations for the helium ground state Green et al used hydrogenic orbitals corresponding to an effective charge $Z = 2$. However the resulting configuration expansions exhibited slow convergence, it being necessary to include continuum states in order to ensure a good description. Subsequently the charge $Z = Z_l$ was treated as a variable parameter to be determined independently for each Φ_l^N expansion. In this case the coefficients $C_{n_1 l_1, n_2 l_2}$ of the various configurations were functions of Z_l . The method now consisted of terminating each configuration expansion after the desired number of terms and choosing Z_l so as to maximize the sum $\sum |C_{n_1 l_1, n_2 l_2}|^2$ and thus provide the best description possible from the limited (truncated) set of configurations.

For the present calculations we have adopted the form of the wave function suggested by Green et al but have determined the effective charges and configuration coefficients by a different technique. The wave function $\bar{\Phi}_0$ is represented by a linear combination of the two-electron configurations $(1s)^2$,(1s2s),$(2s)^2$, $(2p)^2$,(2p3p),$(3p)^2$ i.e.

$$\bar{\Phi}_0(\underline{r}_2,\underline{r}_3) = \frac{1}{4\pi} \sum_{\text{'s' states}} C_{n_1 l_1, n_2 l_2} (1 + \delta_{n_1 l_1, n_2 l_2})^{1/2} R_{n_1 l_1}(Z_0, r_2) R_{n_2 l_2}(Z_0, r_3) P_0^N(\hat{\underline{r}}_2 \cdot \hat{\underline{r}}_3)$$

$$+\frac{1}{4\pi}\sum_{\text{'p' states}} d_{n_1l_1,n_2l_2}(1+\delta_{n_1l_1,n_2l_2})^{1/2} R_{n_1l_1}(z_1, r_2) R_{n_2l_2}(z_1, r_3) P_1^N(\hat{r}_2 \cdot \hat{r}_3) \tag{4.3}$$

where the $R_{nl}(z_l, r)$ are suitably normalized radial functions. All correlation effects between the two atomic electrons are taken to be contained in the second summation appearing in (4.3). The quantities $c_{n_1l_1,n_2l_2}$, $d_{n_1l_1,n_2l_2}$, z_0 and z_1 now assume the roles of parameters which are determined in accordance with the Rayleigh-Ritz Variational Principle. This method consists of using the wave function given by (4.3) to obtain an explicit expression for the quantity $\frac{\langle {}^2\Psi_0 | H | {}^2\Psi_0 \rangle}{\langle \Psi_0 | {}^2\Psi_0 \rangle}$, where H is the hamiltonian for the two-electron system, and then minimizing the expression with respect to each of the parameters. For an exact wave function the quantity considered yields the energy of the atomic system which may be shown to provide a lower limit for the minimization procedure. The minimization is performed numerically (Powell 1964), using the results of Green et al to provide starting values for the parameters, and the values of the parameters corresponding to the stationary point are considered to be those most appropriate for the form of the wave function given by (4.3).

For the method described the criterion that we have sought to satisfy is that of an accurate ground state energy for the atomic system. However since the different regions of configuration space do not contribute equally to the energy this does not automatically ensure a good wave function. In order to obtain some measure of reliability of the wave function we have used it to calculate the atomic form factor $F(k)$ and the incoherent-scattering function $S_{inc.}(k)$ for helium over a range of values of k the momentum transfer. For a neutral atom of atomic number Z we have the definitions

$$F(k) = \sum_{j=1}^{Z} \langle {}^{2}\bar{\Psi}_0 | e^{i\underline{k}\cdot\underline{r}_j} | {}^{2}\bar{\Psi}_0 \rangle \tag{4.4}$$

$$S_{inc.}(k) = Z^{-1}\Big[\sum_{j,k=1}^{Z} \langle {}^{2}\bar{\Psi}_0 | e^{i\underline{k}\cdot(\underline{r}_j-\underline{r}_k)} | {}^{2}\bar{\Psi}_0 \rangle - |F(k)|^2\Big] \tag{4.5}$$

The quantities defined by (4.4) and (4.5) have been tabulated for a variety of wave functions ${}^{2}\bar{\Psi}_0$ over a wide range of momentum transfer (Kim and Inokuti 1968) and results obtained from the form of the wave function given in (4.3) are compared with a sample of these in the table 4.1. Clearly the wave function obtained from the minimization procedure compares favourably with the standard Hylleraas and Hartree-Fock forms in most respects.

4.2. Reduction of the amplitudes

Since it is our intention to retain the Peterkop form of the exchange amplitude in these calculations (eq. 2.27) it is only necessary to derive an explicit expression for the direct scattering amplitude. From equation (3.20) we have

$$f(\underline{k}_f,\underline{k}_s) = -\frac{1}{2\pi} e^{i\Delta(\underline{k}_f,\underline{k}_s)} \iiint e^{i\underline{k}\cdot\underline{r}_1}\, {}^{2}\bar{\Psi}^{*}_{\underline{k}_s}(\underline{r}_2,\underline{r}_3)\, V(\underline{r}_1;\underline{r}_2,\underline{r}_3)\, {}^{2}\bar{\Psi}_0(\underline{r}_2,\underline{r}_3)\, d\underline{r}_1 d\underline{r}_2 d\underline{r}_3 \tag{4.6}$$

where ${}^{2}\bar{\Psi}_0(\underline{r}_2,\underline{r}_3)$ is given by equation (4.3) and all other quantities are as previously defined in chapter 3.

If we now replace the function ${}^{2}\bar{\Psi}_{\underline{k}_s}(\underline{r}_2,\underline{r}_3)$ by the orthogonalized form specified by the choice (*b*) in the previous chapter we obtain

$$f(\underline{k}_f,\underline{k}_s) = -\frac{1}{2\pi} e^{i\Delta(\underline{k}_f,\underline{k}_s)} \iiint e^{i\underline{k}\cdot\underline{r}_1} \big[{}^{2}\bar{\Psi}^{*}_{\underline{k}_s}(\underline{r}_2,\underline{r}_3) + I^{*}_{0v}\, {}^{2}\bar{\Psi}_0(\underline{r}_2,\underline{r}_3)\big] \left(\frac{1}{r_{12}}+\frac{1}{r_{13}}-\frac{Z}{r_1}\right) {}^{2}\bar{\Psi}_0(\underline{r}_2,\underline{r}_3)\, d\underline{r}_1 d\underline{r}_2 d\underline{r}_3 \tag{4.7}$$

where we have replaced $V(1;2,3)$ by the explicit expression given in (3.23) and I_{ov} is an overlap integral defined by

$$I_{ov} = -\left\langle {}^2\bar{\Psi}^S_0(\underline{r}_2,\underline{r}_3) \middle| {}^2\bar{\Psi}^S_{\underline{k}_6}(\underline{r}_2,\underline{r}_3) \right\rangle \tag{4.8}$$

As a consequence of the particular orthogonality condition imposed on the wave functions it is apparent that the Z/r_1 term in the interaction potential makes no contribution to the amplitude. Hence (4.7) reduces to

$$f(\underline{k}_f,\underline{k}_s) = -\frac{1}{2\pi} e^{i\Delta(\underline{k}_f,\underline{k}_s)} \iiint e^{i\underline{K}\cdot\underline{r}_1} \left[{}^2\bar{\Psi}^{S*}_{\underline{k}_s}(\underline{r}_2,\underline{r}_3) + I^*_{ov}\, {}^2\bar{\Psi}^S_0(\underline{r}_2,\underline{r}_3) \right]$$

$$\left(\frac{1}{r_{12}} + \frac{1}{r_{13}} \right) {}^2\bar{\Psi}^S_0(\underline{r}_2,\underline{r}_3)\, d\underline{r}_1 d\underline{r}_2 d\underline{r}_3$$

Now the integration over the variable $\underline{r}_1$ involves the familiar Bethe integrals which may be evaluated to yield the result

$$f(\underline{k}_f,\underline{k}_s) = -\frac{1}{2\pi} e^{i\Delta(\underline{k}_f,\underline{k}_s)} \left\{ \frac{4\pi}{K^2} F_1 + \frac{4\pi}{K^2} I^*_{ov} F_2 \right\}$$

$$= -\frac{2}{K^2} e^{i\Delta(\underline{k}_f,\underline{k}_s)} \left\{ F_1 + I^*_{ov} F_2 \right\} \tag{4.9}$$

where

$$F_1 = \iint \sum_{j=2,3} e^{i\underline{K}\cdot\underline{r}_j}\, {}^2\bar{\Psi}^{S*}_{\underline{k}_s}(\underline{r}_2,\underline{r}_3)\, {}^2\bar{\Psi}^S_0(\underline{r}_2,\underline{r}_3)\, d\underline{r}_2 d\underline{r}_3 \tag{4.10}$$

and

$$F_2 = \iint \sum_{j=2,3} e^{i\underline{K}\cdot\underline{r}_j}\, {}^2\bar{\Psi}^S_0(\underline{r}_2,\underline{r}_3)\, {}^2\bar{\Psi}^S_0(\underline{r}_2,\underline{r}_3)\, d\underline{r}_2 d\underline{r}_3 \tag{4.11}$$

which is seen to be the form factor for the case of helium.

Let us firstly examine the quantity F_1 defined by (4.10). This may be expressed in the form

$$F_1 = F_{1A} + F_{1B}$$

where

$$F_{1A} = \iint e^{i\underline{k}\cdot\underline{r}_2}\,{}^{2}\bar{\Psi}^{*}_{\underline{k}_s}(\underline{r}_2,\underline{r}_3)\,{}^{2}\bar{\Psi}_{0}(\underline{r}_2,\underline{r}_3)\,d\underline{r}_2\,d\underline{r}_3 \tag{4.12}$$

and

$$F_{1B} = \iint e^{i\underline{k}\cdot\underline{r}_3}\,{}^{2}\bar{\Psi}^{*}_{\underline{k}_s}(\underline{r}_2,\underline{r}_3)\,{}^{2}\bar{\Psi}_{0}(\underline{r}_2,\underline{r}_3)\,d\underline{r}_2\,d\underline{r}_3 \tag{4.13}$$

If we now substitute for ${}^{2}\bar{\Psi}_{\underline{k}_s}$ from equations (3.21) and (3.22) and for ${}^{2}\bar{\Psi}_{0}$ from equation (4.3) then F_{1A} takes the form

$$\begin{aligned} F_{1A} = {} & \frac{1}{4\pi}\sum_{\text{'s' states}} c_{n_1l_1,n_2l_2}(1+\delta_{n_1l_1,n_2l_2})^{1/2}\iint e^{i\underline{k}\cdot\underline{r}_2}\,{}^{2}\psi^{*}_{\underline{k}_s}(\underline{r}_2)\frac{Z^{3/2}}{\pi^{1/2}}e^{-Zr_3} \\ & \qquad R_{n_1l_1}(Z_0,r_2)R_{n_2l_2}(Z_0,r_3)P^{N}_{0}(\hat{\underline{r}}_2\cdot\hat{\underline{r}}_3)\,d\underline{r}_2\,d\underline{r}_3 \\ & + \frac{1}{4\pi}\sum_{\text{'p' states}} d_{n_1l_1,n_2l_2}(1+\delta_{n_1l_1,n_2l_2})^{1/2}\iint e^{i\underline{k}\cdot\underline{r}_2}\,{}^{2}\psi^{*}_{\underline{k}_s}(\underline{r}_2)\frac{Z^{3/2}}{\pi^{1/2}}e^{-Zr_3} \\ & \qquad R_{n_1l_1}(Z_1,r_2)R_{n_2l_2}(Z_1,r_3)P^{N}_{1}(\hat{\underline{r}}_2\cdot\hat{\underline{r}}_3)\,d\underline{r}_2\,d\underline{r}_3 \end{aligned} \tag{4.14}$$

where $P^{N}_{l}(\hat{\underline{r}}_2\cdot\hat{\underline{r}}_3) = \left[\frac{(2l+1)}{2}\right]^{1/2}P_{l}(\hat{\underline{r}}_2\cdot\hat{\underline{r}}_3)$

In order to perform the angular part of the $\underline{r}_3$ integration it is necessary to write the $P_l(\hat{\underline{r}}_2\cdot\hat{\underline{r}}_3)$ in separable form. This is achieved by means of the following expansion in Spherical Harmonics

$$P_l(\hat{\underline{r}}_2\cdot\hat{\underline{r}}_3) = \frac{4\pi}{(2l+1)}\sum_{\mu=-l}^{l} Y_{l\mu}(\hat{\underline{r}}_2)Y^{*}_{l\mu}(\hat{\underline{r}}_3) \tag{4.15}$$

It now becomes obvious that due to the orthogonality of the Spherical Harmonics the second summation in (4.14) makes no contribution to F_{1A}. After performing the $\hat{\underline{r}}_3$ integration in the remaining terms we obtain

$$\begin{aligned} F_{1A} = {} & \frac{Z^{3/2}}{(2\pi)^{1/2}}\sum_{\text{'s' states}} c_{n_1l_1,n_2l_2}(1+\delta_{n_1l_1,n_2l_2})^{1/2}\left(\int_0^{\infty} e^{-Zr_3}R_{n_2l_2}(Z_0,r_3)\,r_3^2\,dr_3\right) \\ & \qquad \left(\int e^{i\underline{k}\cdot\underline{r}_2}\,{}^{2}\psi^{*}_{\underline{k}_s}(\underline{r}_2)R_{n_1l_1}(Z_0,r_2)\,d\underline{r}_2\right) \end{aligned} \tag{4.16}$$

For the particular set of configurations used to describe the target ground state the radial functions R_{nl} are all of the general form

$$R_{nl}(z_l,r) = (a_{nl}r^2 + b_{nl}r + c_{nl})e^{-\alpha_{nl}r} \tag{4.17}$$

and hence

$$\int_0^\infty e^{-zr}R_{nl}(z_l,r)r^2dr = \int_0^\infty e^{-(z+\alpha_{nl})r}(a_{nl}r^4 + b_{nl}r^3 + c_{nl}r^2)dr$$

$$= \frac{1}{(z+\alpha_{nl})^3}\left\{\frac{4!a_{nl}}{(z+\alpha_{nl})^2} + \frac{3!b_{nl}}{(z+\alpha_{nl})} + 2!c_{nl}\right\}$$

$$= \frac{2}{(z+\alpha_{nl})^3}\left\{\frac{12a_{nl}}{(z+\alpha_{nl})^2} + \frac{3b_{nl}}{(z+\alpha_{nl})} + c_{nl}\right\} \tag{4.18}$$

Let us now consider the $\underline{r}_2$ integration appearing in (4.16). To enable us to perform the angular integration it is necessary that both the "slow" electron wave function and the oscillatory exponential be replaced by the respective series expansions (3.10) and (3.33). The Legendre polynomials associated with each of these expansions are expressed in Spherical Harmonics by use of (4.15). From the subsequent angular integration we obtain

$$\int e^{i\underline{k}\cdot\underline{r}}\psi^*_{\underline{k}_s}(\underline{r})R_{n_1l_1}(z_0,r)d\underline{r} = 4\pi\sum_{l=0}^{\infty}(2l+1)P_l(\hat{\underline{k}}\cdot\hat{\underline{k}}_s)e^{-i(\sigma_l+\eta_l)}$$

$$\frac{1}{(2\pi)^{3/2}k_s^{1/2}}\int_0^\infty j_l(kr)u_l(k_s,r)rR_{n_1l_1}(z_0,r)dr \tag{4.19}$$

Combining the results (4.18) and (4.19) we obtain

$$F_{1A} = \frac{2z^{3/2}}{\pi k_s^{1/2}}\sum_{l=0}^{\infty}(2l+1)P_l(\hat{\underline{k}}\cdot\hat{\underline{k}}_s)e^{-i(\sigma_l+\eta_l)}\int_0^\infty j_l(kr)u_l(k_s,r)r\Big($$

$$\sum_{\text{'s' states}} C_{n_1l_1,n_2l_2}(1+\delta_{n_1l_1,n_2l_2})^{1/2}\cdot\frac{1}{(Z+\alpha_{n_2l_2})^3}\left[\frac{12a_{n_2l_2}}{(Z+\alpha_{n_2l_2})^2}+\frac{3b_{n_2l_2}}{(Z+\alpha_{n_2l_2})}+C_{n_2l_2}\right]$$

$$R_{n_1l_1}(Z_0,r)\Big)dr \tag{4.20}$$

The remaining terms in the expression for F_1 arise from the integral F_{1B} defined by (4.13). Substituting for $\Psi_{\underline{k}_s}$ and Ψ_0 as before we obtain

$$F_{1B} = \frac{1}{4\pi}\sum_{\text{'s' states}} c_{n_1l_1,n_2l_2}(1+\delta_{n_1l_1,n_2l_2})^{1/2}\iint e^{i\underline{k}\cdot\underline{r}_3}\psi^*_{\underline{k}_s}(\underline{r}_2)\frac{Z^{3/2}}{\pi^{1/2}}e^{-Zr_3}$$

$$R_{n_1l_1}(Z_0,r_2)R_{n_2l_2}(Z_0,r_3)P_0^N(\hat{\underline{r}}_2\cdot\hat{\underline{r}}_3)\,d\underline{r}_2\,d\underline{r}_3$$

$$+\frac{1}{4\pi}\sum_{\text{'p' states}} d_{n_1l_1,n_2l_2}(1+\delta_{n_1l_1,n_2l_2})^{1/2}\iint e^{i\underline{k}\cdot\underline{r}_3}\psi^*_{\underline{k}_s}(\underline{r}_2)\frac{Z^{3/2}}{\pi^{1/2}}e^{-Zr_3}$$

$$R_{n_1l_1}(Z_1,r_2)R_{n_2l_2}(Z_1,r_3)P_1^N(\hat{\underline{r}}_2\cdot\hat{\underline{r}}_3)\,d\underline{r}_2\,d\underline{r}_3 \tag{4.21}$$

It is convenient to split F_{1B} into two parts F_{1B}^{s} and F_{1B}^{p} corresponding to the contributions arising from the 's' and 'p' configurations of the target wave function respectively. With the aid of the appropriate substitutions from (3.33) and (4.15) the angular part of the $\underline{r}_3$ integration associated with F_{1B}^{s} may be evaluated to give

$$F_{1B}^{s} = \frac{Z^{3/2}}{(2\pi)^{1/2}}\sum_{\text{'s' states}} c_{n_1l_1,n_2l_2}(1+\delta_{n_1l_1,n_2l_2})^{1/2}\left(\int_0^\infty j_0(kr_3)e^{-Zr_3}R_{n_2l_2}(Z_0,r_3)r_3^2\,dr_3\right)$$

$$\left(\int\psi^*_{\underline{k}_s}(\underline{r}_2)R_{n_1l_1}(Z_0,r_2)\,d\underline{r}_2\right) \tag{4.22}$$

Using the form of the radial function prescribed by (4.17) we have

$$\int_0^\infty j_0(kr)e^{-zr}R_{nl}(z_l,r)r^2dr = \frac{1}{k}\int_0^\infty \sin kr.(a_{nl}r^3+b_{nl}r^2+c_{nl}r)e^{-(z+\alpha_{nl})r}dr$$

But

$$\int_0^\infty r^n \sin kr\, e^{-\beta r}dr = \mathcal{I}m.\left\{\frac{n!(\beta+ik)^{n+1}}{(\beta^2+k^2)^{n+1}}\right\}$$

Hence

$$\int_0^\infty j_0(kr)e^{-zr}R_{nl}(z_l,r)r^2dr$$

$$= \frac{1}{(\beta^2+k^2)^2}\left\{6a_{nl}\cdot\frac{4\beta(\beta^2-k^2)}{(\beta^2+k^2)^2}+2b_{nl}\frac{(3\beta^2-k^2)}{(\beta^2+k^2)}+2c_{nl}\beta\right\}$$

$$= \frac{2}{(\beta^2+k^2)^2}\left\{12a_{nl}\frac{\beta(\beta^2-k^2)}{(\beta^2+k^2)^2}+b_{nl}\frac{(3\beta^2-k^2)}{(\beta^2+k^2)}+c_{nl}\beta\right\}$$

where $\beta = z+\alpha_{nl}$ (4.23)

The angular integration associated with the remaining integral in (4.22) may be readily evaluated after substitution from (3.10)

$$\int \psi^*_{\underline{k}_s}(\underline{r})R_{n_1l_1}(z_0,r)d\underline{r} = \frac{4\pi}{(2\pi)^{3/2}k_s^{1/2}}e^{-i(\sigma_0+\eta_0)}\int_0^\infty u_0(k_s,r)rR_{n_1l_1}(z_0,r)dr \tag{4.24}$$

Combining results (4.23) and (4.24) yields the following expression for F_{1B}^s

$$F_{1B}^s = \frac{2z^{3/2}}{\pi k_s^{1/2}}e^{-i(\sigma_0+\eta_0)}\int_0^\infty u_0(k_s,r)r\sum_{\text{'s' states}}c_{n_1l_1,n_2l_2}(1+\delta_{n_1l_1,n_2l_2})^{1/2}R_{n_1l_1}(z_0,r)$$

$$\frac{1}{(\beta^2_{n_2l_2}+k^2)^2}\left\{12a_{n_2l_2}\beta_{n_2l_2}\frac{(\beta^2_{n_2l_2}-k^2)}{(\beta^2_{n_2l_2}+k^2)^2}+b_{n_2l_2}\frac{(3\beta^2_{n_2l_2}-k^2)}{(\beta^2_{n_2l_2}+k^2)}+c_{n_2l_2}\beta_{n_2l_2}\right\}dr$$

where $\beta_{n_2l_2} = z+\alpha_{n_2l_2}$ (4.25)

The 'p' contribution to the quantity F_{1B} is defined by

$$F_{1B}^{p} = \frac{1}{4\pi}\sum_{\text{'p' states}} d_{n_1l_1,n_2l_2}(1+\delta_{n_1l_1,n_2l_2})^{1/2}\iint e^{i\underline{k}\cdot\underline{r}_3}\psi^{*}_{\underline{k}_s}(\underline{r}_2)\frac{Z^{3/2}}{\pi^{1/2}}e^{-Zr_3}$$

$$R_{n_1l_1}(Z_1,r_2)R_{n_2l_2}(Z_1,r_3)P_1(\hat{\underline{r}}_2\cdot\hat{\underline{r}}_3)\,d\underline{r}_2\,d\underline{r}_3$$

If we substitute from (3.33) and (4.15) the $\hat{\underline{r}}_3$ integration may be evaluated so yielding the following result

$$F_{1B}^{p} = \frac{\sqrt{3}\,Z^{3/2}\,i}{(2\pi)^{1/2}}\sum_{\text{'p' states}} d_{n_1l_1,n_2l_2}(1+\delta_{n_1l_1,n_2l_2})^{1/2}\int_0^{\infty} j_1(kr_3)e^{-Zr_3}R_{n_2l_2}(Z_1,r_3)\,r_3^2\,dr_3$$

$$\int \psi^{*}_{\underline{k}_s}(\underline{r}_2)R_{n_1l_1}(Z_1,r_2)P_1(\hat{\underline{k}}\cdot\hat{\underline{r}}_2)\,d\underline{r}_2 \qquad (4.26)$$

Replacing $\psi_{\underline{k}_s}$ by the series expansion (3.10) and performing the $\hat{\underline{r}}_2$ integration produces the expression

$$F_{1B}^{p} = \frac{\sqrt{3}\,Z^{3/2}}{\pi k_s^{1/2}}e^{-i(\sigma_1+\eta_1)}P_1(\hat{\underline{k}}_s\cdot\hat{\underline{k}})\sum_{\text{'p' states}} d_{n_1l_1,n_2l_2}(1+\delta_{n_1l_1,n_2l_2})^{1/2}$$

$$\int_0^{\infty} j_1(kr)e^{-Zr}R_{n_2l_2}(Z_1,r)\,r^2\,dr\int_0^{\infty} u_1(k_s,r)\,r\,R_{n_1l_1}(Z_1,r)\,dr \qquad (4.27)$$

But

$$j_1(x) = -\frac{d}{dx}j_0(x)$$

Hence

$$\int_0^{\infty} j_1(kr)e^{-Zr}R_{nl}(Z_1,r)\,r^2\,dr = -\frac{\partial}{\partial k}\int_0^{\infty} j_0(kr)e^{-Zr}R_{nl}(Z_1,r)\,r\,dr$$

Substituting for R_{nl} from (4.7) we have

$$\int_0^{\infty} j_1(kr)e^{-Zr}R_{nl}(Z_1,r)\,r^2\,dr$$

$$= -\frac{\partial}{\partial k}\int_0^{\infty} j_0(kr)e^{-\beta r}(a_{nl}r^3+b_{nl}r^2+c_{nl}r)\,dr \qquad (4.28)$$

where $\beta = z + \alpha_{nl}$.

Evaluation of the integral on the right hand side of equation (4.28) leads to the result

$$\int_0^\infty j_1(Kr) e^{-zr} R_{nl}(z_1, r) r^2 dr$$

$$= -\frac{\partial}{\partial K}\left\{ \frac{2a_{nl}(3\beta^2 - K^2)}{(\beta^2 + K^2)^3} + \frac{2b_{nl}\beta}{(\beta^2 + K^2)^2} + \frac{c_{nl}}{(\beta^2 + K^2)} \right\}$$

$$= \frac{2K}{(\beta^2 + K^2)^2}\left\{ \frac{4a_{nl}(5\beta^2 - K^2)}{(\beta^2 + K^2)^2} + \frac{4b_{nl}\beta}{(\beta^2 + K^2)} + c_{nl} \right\} \tag{4.29}$$

Applying the result (4.29) to the expression in (4.27) we obtain

$$F_{1B}^{P} = \frac{2\sqrt{3}}{\pi k_s^{1/2}} z^{3/2} e^{-i(\sigma_1 + \eta_1)} P_1(\hat{\underline{k}}_s \cdot \hat{\underline{K}}) \int_0^\infty u_1(k_s, r) r \left(\sum_{\text{'p' states}} d_{n_1 l_1, n_2 l_2} (1 + \delta_{n_1 l_1, n_2 l_2})^{1/2} \right.$$

$$\left. \frac{K}{(\beta_{n_2 l_2}^2 + K^2)^2}\left\{ \frac{4a_{n_2 l_2}(5\beta_{n_2 l_2}^2 - K^2)}{(\beta_{n_2 l_1}^2 + K^2)^2} + \frac{4b_{n_2 l_2}\beta_{n_2 l_2}}{(\beta_{n_2 l_2}^2 + K^2)} + c_{n_2 l_2} \right\} R_{n_1 l_1}(z_1, r) \right) dr \tag{4.30}$$

Let us now examine the quantity F_2 defined by equation (4.11). Since this is symmetric with respect to the radius vectors $\underline{r}_2$ and $\underline{r}_3$ we can write

$$F_2 = 2 \iint e^{i\underline{K}\cdot\underline{r}_2}\, {}^2\Psi_0(\underline{r}_2, \underline{r}_3)\, {}^2\Psi_0(\underline{r}_2, \underline{r}_3)\, d\underline{r}_2\, d\underline{r}_3 \tag{4.31}$$

It is convenient to express the ground state wave function in the form

$${}^2\Psi_0(\underline{r}_2, \underline{r}_3) = \frac{1}{4\pi}\left\{ \Phi_0^s(r_2, r_3) P_0^N(\hat{\underline{r}}_2 \cdot \hat{\underline{r}}_3) + \Phi_0^P(r_2, r_3) P_1^N(\hat{\underline{r}}_2 \cdot \hat{\underline{r}}_3) \right\} \tag{4.32}$$

Then, substituting this form into (4.31), we obtain

$$F_2 = \frac{2}{16\pi^2}\Big\{ \iint e^{i\underline{k}\cdot\underline{r}_2}\,\Phi_0^s(r_2,r_3)\,\Phi_0^s(r_2,r_3)\,P_0^N(\hat{\underline{r}}_2\cdot\hat{\underline{r}}_3)\,P_0^N(\hat{\underline{r}}_2\cdot\hat{\underline{r}}_3)\,d\underline{r}_2\,d\underline{r}_3$$

$$+\,2\iint e^{i\underline{k}\cdot\underline{r}_2}\,\Phi_0^s(r_2,r_3)\,\Phi_0^p(r_2,r_3)\,P_0^N(\hat{\underline{r}}_2\cdot\hat{\underline{r}}_3)\,P_1^N(\hat{\underline{r}}_2\cdot\hat{\underline{r}}_3)\,d\underline{r}_2\,d\underline{r}_3$$

$$+\iint e^{i\underline{k}\cdot\underline{r}_2}\,\Phi_0^p(r_2,r_3)\,\Phi_0^p(r_2,r_3)\,P_1^N(\hat{\underline{r}}_2\cdot\hat{\underline{r}}_3)\,P_1^N(\hat{\underline{r}}_2\cdot\hat{\underline{r}}_3)\,d\underline{r}_2\,d\underline{r}_3\Big\} \qquad (4.33)$$

If we perform the $\hat{\underline{r}}_3$ integration appearing in the second term of (4.33) we obtain zero contribution by reason of the orthogonality of the Spherical Harmonics. Evaluation of the angular integrations associated with the remaining terms yields

$$F_2 = \iint j_0(kr_2)\,\Phi_0^s(r_2,r_3)\,\Phi_0^s(r_2,r_3)\,r_2^2 r_3^2\,dr_2\,dr_3$$

$$+\iint j_0(kr_2)\,\Phi_0^p(r_2,r_3)\,\Phi_0^p(r_2,r_3)\,r_2^2 r_3^2\,dr_2\,dr_3$$

which we shall write in the form

$$F_2 = F_2^s + F_2^p$$

where

$$F_2^s = \int_0^\infty\!\!\int_0^\infty j_0(kr_2)\,\Phi_0^s(r_2,r_3)\,\Phi_0^s(r_2,r_3)\,r_2^2 r_3^2\,dr_2\,dr_3 \qquad (4.34)$$

and

$$F_2^p = \int_0^\infty\!\!\int_0^\infty j_0(kr_2)\,\Phi_0^p(r_2,r_3)\,\Phi_0^p(r_2,r_3)\,r_2^2 r_3^2\,dr_2\,dr_3 \qquad (4.35)$$

Now

$$\Phi_0^s(r_2,r_3) = \sum_{\text{'s' states}} c_{n_1l_1;n_2l_2}\,(1+\delta_{n_1l_1,n_2l_2})^{\frac{1}{2}}\,R_{n_1l_1}(z_0,r_2)\,R_{n_2l_2}(z_0,r_3)$$

Hence, following the substitution of this into (4.34), we obtain

$$F_2^s = \sum_{n_1 n_2}\sum_{m_1 m_2} c_{n_1s,n_2s}\,c_{m_1s,m_2s}\,(1+\delta_{n_1n_2})^{\frac{1}{2}}(1+\delta_{m_1m_2})^{\frac{1}{2}}$$

$$\left(\int_0^\infty j_0(kr)\,r^2 R_{n_1s}(z_0,r)\,R_{m_1s}(z_0,r)\,dr\right)\left(\int_0^\infty R_{n_2s}(z_0,r)\,R_{m_2s}(z_0,r)\,r^2\,dr\right)$$

But from the orthogonality of the radial functions we have

$$\int_0^\infty R_{n_2s}(z_0,r)\,R_{m_2s}(z_0,r)\,r^2\,dr = \delta_{n_2m_2}$$

Thus

$$F_2^s=\sum_{n_1 n_2 m_1} c_{n_1 s, n_2 s}\, c_{m_1 s, n_2 s}(1+\delta_{n_1 n_2})^{1/2}(1+\delta_{m_1 n_2})^{1/2}$$

$$\int_0^\infty j_0(kr)\, r^2 R_{n_1 s}(z_0,r) R_{m_1 s}(z_0,r)\, dr$$

$$=\sum_{n_1 m_1}\Big(\sum_{n_2} c_{n_1 s, n_2 s}\, c_{m_1 s, n_2 s}(1+\delta_{n_1 n_2})^{1/2}(1+\delta_{m_1 n_2})^{1/2}\Big)$$

$$\int_0^\infty j_0(kr)\, r^2 R_{n_1 s}(z_0,r) R_{m_1 s}(z_0,r)\, dr \qquad (4.36)$$

Denoting the integral appearing in (4.36) by $I^s_{n_1 m_1}$ and substituting the explicit forms of the radial functions from (4.17) we obtain

$$I^s_{n_1 m_1} = \frac{1}{k}\sum_{n=1}^{5} H_n \int_0^\infty r^n \sin kr\, e^{-\alpha r}\, dr \qquad (4.37)$$

where

$$\begin{aligned}
H_1 &= c_{n_1 s} c_{m_1 s}\\
H_2 &= b_{n_1 s} c_{m_1 s} + b_{m_1 s} c_{n_1 s}\\
H_3 &= a_{n_1 s} c_{m_1 s} + a_{m_1 s} c_{n_1 s} + b_{n_1 s} b_{m_1 s}\\
H_4 &= a_{n_1 s} b_{m_1 s} + a_{m_1 s} b_{n_1 s}\\
H_5 &= a_{n_1 s} a_{m_1 s}\\
\alpha &= \alpha_{n_1 s} + \alpha_{m_1 s}
\end{aligned}$$

Evaluation of (4.37) yields the result

$$I^s_{n_1 m_1} = \frac{1}{k}\sum_{n=1}^{5} H_n\, \mathcal{I}m.\left\{\frac{n!\,(\alpha+ik)^{n+1}}{(\alpha^2+k^2)^{n+1}}\right\}$$

Hence

$$I^s_{n_1 m_1} = \sum_{n=1}^{5} H_n \frac{n!}{(\alpha^2+k^2)^{n+1}} \sum_{m=0}^{[\frac{n}{2}]} (-1)^m C^{n+1}_{2m+1}\, \alpha^{n-2m} k^{2m} \qquad (4.38)$$

Thus

$$F_2^s=\sum_{n_1 m_1}\Big(\sum_{n_2} c_{n_1 s, n_2 s}\, c_{m_1 s, n_2 s}(1+\delta_{n_1 n_2})^{1/2}(1+\delta_{m_1 n_2})^{1/2}\Big) I^s_{n_1 m_1} \qquad (4.39)$$

where the quantity $\mathcal{I}^{S}_{n_1 m_1}$ is as defined by equation (4.38). Since the term F_2^P, defined by (4.35), is of a form similar to that of F_2^S then by analogy

$$F_2^P = \sum_{n_1 m_1}\Big(\sum_{n_2} d_{n_1 p, n_2 p}\, d_{m_1 p, n_2 p}(1+\delta_{n_1 n_2})^{1/2}(1+\delta_{m_1 n_2})^{1/2}\Big)\mathcal{I}^{P}_{n_1 m_1} \tag{4.40}$$

The integral $\mathcal{I}^{P}_{n_1 m_1}$ appearing in (4.40) is the exact counterpart of $\mathcal{I}^{S}_{n_1 m_1}$ and is obtained from (4.38) by merely redefining the quantities $H_n\ (n=1,5)$ and α in terms of the corresponding 'p' state parameters.

It only remains now to derive an explicit expression for the overlap integral $\mathcal{I}_{ov}$ defined by (4.8). Appropriate substitutions from (3.21), (3.22) and (4.32) lead to the form

$$\mathcal{I}_{ov} = \frac{-Z^{3/2}}{4\pi^{3/2}}\iint \Phi_0^S(\underline{r}_2, \underline{r}_3)\, P_0^N(\hat{\underline{r}}_2\cdot\hat{\underline{r}}_3)\, \psi_{\underline{k}_s}(\underline{r}_2)\, e^{-Zr_3}\, d\underline{r}_2\, d\underline{r}_3$$

$$-\frac{Z^{3/2}}{4\pi^{3/2}}\iint \Phi_0^P(\underline{r}_2, \underline{r}_3)\, P_1^N(\hat{\underline{r}}_2\cdot\hat{\underline{r}}_3)\, \psi_{\underline{k}_s}(\underline{r}_2)\, e^{-Zr_3}\, d\underline{r}_2\, d\underline{r}_3$$

Let us consider the second term in this expression. By using the expansion in Spherical Harmonics given by (4.15) we are able to write the Legendre polynomial in separable form, which enables us to perform the associated $\hat{\underline{r}}_3$ integration. Clearly we obtain zero contribution. If we evaluate the angular integrations appearing in the remaining term we obtain

$$\mathcal{I}_{ov} = \frac{-Z^{3/2}}{\pi k_s^{1/2}}\, e^{i(\sigma_0+\eta_0)}\int_0^\infty\!\!\int_0^\infty \Phi_0^S(r_2, r_3)\, u_0(k_s, r_2)\, r_2\, e^{-Zr_3}\, r_3^2\, dr_2\, dr_3 \tag{4.41}$$

where we have replaced the wave function $\psi_{\underline{k}_6}$ by the partial wave expansion (3.10).

After substituting for Φ_0^S we have

$$\mathcal{I}_{ov} = \frac{-Z^{3/2}}{\pi k_s^{1/2}}\, e^{i(\sigma_0+\eta_0)}\sum_{n_1 n_2} C_{n_1 s, n_2 s}(1+\delta_{n_1 n_2})^{1/2}\Big(\int_0^\infty R_{n_1 s}(Z_0, r)\, u_0(k_s, r)\, r\, dr\Big)$$

$$\left(\int_0^\infty R_{n_2s}(z_0,r)\,r^2e^{-zr}dr\right)$$

But

$$\int_0^\infty R_{n_2s}(z_0,r)\,r^2e^{-zr}dr=\frac{2}{(z+\alpha_{n_2s})^3}\left\{\frac{12a_{n_2s}}{(z+\alpha_{n_2s})^2}+\frac{3b_{n_2s}}{(z+\alpha_{n_2s})}+c_{n_2s}\right\}$$

where we have used the form of the radial function given by (4.17). Hence

$$I_{ov}=\frac{-z^{3/2}}{\pi k_s^{1/2}}e^{i(\sigma_0+\eta_0)}\int_0^\infty u_0(k_s,r)\,r\left\{\sum_{n_1n_2}c_{n_1s,n_2s}(1+\delta_{n_1n_2})^{1/2}R_{n_1s}(z_0,r)\right.$$

$$\left.\frac{2}{(z+\alpha_{n_2s})^3}\left[\frac{12a_{n_2s}}{(z+\alpha_{n_2s})^2}+\frac{3b_{n_2s}}{(z+\alpha_{n_2s})}+c_{n_2s}\right]\right\}dr \qquad (4.42)$$

The partial wave calculations reported in this section were checked in two ways. Firstly, by a appropriate choice of parameters it was possible to recreate the model used in chapter 3 and so repeat some of the calculations reported there. The second check was achieved by specializing to a plane wave description of the slow outgoing electron, in which case the analysis can be evaluated in closed form (cf. Appendix B).

We found that contributions from $\ell>6$ were unimportant at the energy considered, the dominant contribution arising from $s\rightarrow p$ transitions. However in some angular regions there was an appreciable quadrapole transition probability ($s\rightarrow d$).

4.3 Results

In the figures 1 - 6 we compare our calculations of the triple differential cross section, for a number of representative cases, with the experimental measurements of Ehrhardt et al at the incident energy E_0 = 256.5e.V. We shall use E_f and θ_f to denote the energy and the angle of scattering, respectively, of the "fast" outgoing electron. The following table shows the sets of collision parameters for which calculations have been made.

FIGURE	E_0 (eV)	E_f(eV)	θ_f
1	256.5	226.0	4°
2	256.5	226.0	6°
3	256.5	226.0	8°
4	256.5	230.5	4°
5	256.5	229.0	6°
6	256.5	182.0	8°

Since the experimental measurements are not absolute it is necessary to normalize them against the calculated curves in some way. In this study the normalization is achieved by requiring that the maximum of the forward peak of the TDC, as measured experimentally, should be in agreement with the calculated value. The justification for this course of action is contained in the general discussion that follows.

A preliminary inspection of the results indicates that the use of the correlated wave function for the description of the target ground state effects localized variation in the magnitude of the TDC. In addition we observe that there is a significant decrease of the ratio of the two maxima characterizing the TDC. Hence we have the rather surprising result that the simpler model procides a better qualitative description of the TDC as measured experimentally. However such a situation should be regarded as being merely fortuitous since there can be little doubt that the later model provides a better description of the electron states and interactions associated with the ionization process. Indeed such a view is supported by the other features of the improved model, namely the constancy of normalization as is described at a later point in this discussion.

This somewhat misleading situation regarding the qualitative agreement betweem experimental and theoretical results raises the important point as to which features of the experimental results are most important when making a comparison with theoretical predictions. Our own investigations clearly indicate that the degree of qualitative agreement between calculations and experimental measurements is not a sufficiently good basis on which to judge a theoretical model.

Now it is noticeable that all the variants of the first Born approximation, together with all other approximations in common use, predict a maximum of the TDC in the forward direction. It would therefore seem logical to give first priority to obtaining the best possible description of this forward peak with regard to general shape and angular position. On this basis we have the justification for choosing to normalize the experimental measurements against the calculations at the maximum of the binary peak. In order to introduce some measure of consistency into the comparisons between theoretical and experimental results we need to relate the different sets of measurements together where possible. This is done through the normalization factor. Where appropriate one should make a comparison over a series of different cases using the same normalization factor. If the general agreement between the theoretical and experimental measurements of the binary peak persists then a more detailed comparison is justified. The next point to consider would be the general character of the "recoil" peak including the ratio of its maximum to that of the "binary" peak.

For the cases shown in figures 1 - 3 a constant normalization factor has been used. The results obtained indicate that the normalization is preserved by the form of the Born approximation used for the calculations. Another point of agreement apparent from these and the remaining cases is the general success of the calculations in reproducing the shape of the forward peak, albeit this peak may not be correctly positioned.

The TDC is characterized by a forward and backward peak separated by pronounced minima. These two peaks are referred to as 'binary' and 'recoil' peaks respectively. Firstly the calculations consistently underestimate the magnitude of the 'recoil peak as measured by Ehrhardt. Secondly the theoretical model tends to produce a 'binary' and 'recoil' peak with a common axis of symmetry, whereas the experimental results show a definite shift of one axis away from the other. The effect of this is for the angular position of the 'binary' peak, as predicted by our calculations, to lie too close to the polar axis defined by the direction of the incoming electron. This angular shift increases as the energy of the "slow" outgoing electron increases but the indications are that it is not strongly related to the angle of scattering of the "fast" outgoing electron. These conclusions are reinforced by the results of the calculations performed by Schulz (1973) and Jacobs (1974), some of which are included here.

With regard to the point concerning the symmetry of results Fano et al (1973), attributing the TDC exclusively to dipole-type ionization for large incident energies, predict that the "slow" electron distribution will exhibit axial symmetry about the momentum exchange vector $\underline{k}_0-\underline{k}_f$, which accurately describes the Born calculations presented here. At lower incident energies the repulsion between the outgoing electrons is expected to displace the peaks, with the consequent loss of symmetry. The neglect of the electron-electron interaction in the final state seems a likely reason for the discrepancy between calculation and experiment as regards the angular positions of the peaks.

Schulz (1973) has made extensive calculations using Coulomb waves to represent the outgoing electrons and varying the effective charges. By careful choice of effective charges Schulz has been able to obtain an improvement in both the angular positions of the peaks and their relative magnitudes. However the choice of charges is largely associated with curve fitting techniques rather than physical considerations and still fails to provide a completely satisfactory description of the 'recoil' peak. We have included a selection of the results for comparison. Also, Salin (1973) has used the impact parameter method to describe the ionization process. These calculations take particular account of the Coulomb interaction between the two outgoing electrons. The results obtained are qualitatively similar to those of Schulz.

The origin of the 'recoil' peak has been discussed in the recent publication by Schulz. Vriens (1969) attributed it to ionizing collisions in which an initially bound electron, leaving the ion in a forward direction, is reflected by the potential of the ion and consequently suffers a reversal of direction. It has been suggested by Schulz that another type of collision contributing to the 'recoil' peak is that involving the scattering of the incident electron by the nucleus or the electron that remains bound. In this case the mutual interaction of all the atomic particles could result in a nearly uniform distribution for the ejected electron. The contribution from the first type of collision decreases with the energy E_S, whilst that of the second increases with momentum transfer.

Since calculations based on the first Born approximation exclude the interaction between the incident electron and the nucleus, then the explanations suggested by Vriens and Schulz would at least seem compatible with the failure of these calculations to reproduce a 'recoil' peak of sufficient magnitude. Confirmation of this conclusio seems to be provided by the TDC calculations of Geltman (1974). He has used the Coulomb-projected Born approximation of Geltman and Hidalgo, which takes account of the electron-nucleus interaction, to calculate the TDC of helium for a wide range of collision parameters. In some respects the results obtained show a considerable improvement over calculations based on variants of the first Born approximation. The Coulomb-projected Born approximation produces improved predictions for the relative magnitudes of the 'binary' and 'recoil' peaks but fails to locate these correctly. In contrast to those calculations previously described the angular shift in the position of the binary encounter peak is now away from the polar axis. We include a selectio of Geltman's results to show the features described. In addition to the improved peak ratio the CPB approximation appears to have a wider application than one might expect, producing reasonable qualitative agreement at quite low incident energies. However the only guide that we have to quantitative agreement is the degree to which normalization is conserved and this is not indicated in the results.

It should be noted that these calculations are based on a simple description of the helium target, the wave function being identical to that used in our preliminary calculations of the TDC, and from our own experience it cannot be assumed that an improved description of the helium ground state will result in improved agreement with experiment.

The CPB approximation has been used for a variety of calculations and is generally comparable to the better theoretical models in common use. However there is one case in which it has been shown to be decidedly inferior. When used to calculate the 90° polarization of Lyman α radiation emitted by the 2p state of H excited by electron impact (incident energies in the range 40 - 200 eV) the CPB approximation produced results quite different from those determined from experimental measurements. In fact Morgan and Stauffer (1975) have found that the predictions of the CPB approximation have the opposite sign to that indicated both by experiment and other theoretical models. However this contrasts with the CPB calculations of the differential cross section for the excitation of all the n =2 levels in H, where there is satisfactory agreement with experiment. This indicates that there may be certain inherent weaknesses associated with the CPB approximation.

Let us now examine the double differential cross section obtained from the TDC by integrating over the angular co-ordinates of the "slow" outgoing electron

$$\frac{d^2\sigma}{d\hat{\underline{k}}_f d\varepsilon} = \int \frac{d^3\sigma}{d\hat{\underline{k}}_f d\hat{\underline{k}}_s d\varepsilon} d\hat{\underline{k}}_s \tag{4.43}$$

where $$d\hat{\underline{k}}_s = \sin\theta_s d\theta_s d\phi_s$$

Because all of the calculations have been confined to in-plane scattering ($\phi_s = 0°, 180°$) we cannot determine exactly the effect of the integration over the angular co-ordinates. However we can make a reasonable speculation. In the region about $\phi_s = 0°$ the θ_s integration has the form

$$\int \frac{d^3\sigma}{d\hat{\underline{k}}_f d\hat{\underline{k}}_s d\varepsilon} \sin\theta_s d\theta_s \tag{4.44}$$

Since the 'binary' and 'recoil' peaks of the TDC are almost diametrically opposite then the presence of the $\sin\theta_s$ factor in the integrand of (4.44) will result in some cancellation between the peaks. Hence it seems likely that any model underestimating the magnitude of the recoil peak will tend to overestimate the total cross section, as is the situation regarding Born calculations of the total cross section.

Finally we have made calculations to investigate how the various partial waves, appearing in the exchange adiabatic representation of the "slow" outgoing electron, contribute to the TDC. For the purposes of these calculations we have retained only the "s " state configurations of the C.I. wavefunction describing the target ground state.

We found that for the regions in which the TDC is most significant the largest contribution arises from the dipole transition (Δl =1). However in other angular regions, where the TDC is less significant, the quadrapole, and some higher order, contributions assume considerable importance. One such region is $0<\theta_s<90°$. The figures 7 and 8 show the dependence of the TDC upon the partial wave contributions in this angular region. The following table shows the values of the collision parameters in each case.

FIGURE	E_0(eV)	E_f(eV)	θ_f
7	256.5	230.5	4°
8	256.5	230.5	7°

4.4 Conclusions

We have calculated triple differential cross sections for the electron impact ionization of helium in first Born approximation at an incident energy of 256.5eV. Particular consideration has been given to the use of accurate wave functions to describe the target ground state and the 'slow' outgoing electron. The results show the first Born approximation to fail on two points; namely the prediction of the correct angular positions of the 'binary' and 'recoil' peaks and the magnitude of the 'recoil' peak. The various explanations for the behaviour of the TDC are presented, from which it is clear that the discrepancies between the calculations and experimental results arise through faults inherent in the first Born approximation. In this connection we have indicated why Born calculations overestimate the total cross sections in the energy region considered. Further we have shown that there are angular regions where the ionization process may be significantly different from a dipole transition.

PARAMETERS FOR THE TARGET WAVE FUNCTION

H$^-$

$C_{1s,1s}$	$C_{1s,2s}$	$C_{2s,2s}$	$d_{2p,2p}$
0.704981	-0.701157	-0.128315(-1)	-0.101926
$d_{2p,3p}$	$d_{3p,3p}$	Z_0	Z_1
0.234939(-1)	-165903(-1)	0.993914	0.215075(+1)

CORRESPONDING GROUND STATE ENERGY = -0.520823 au

He

$C_{1s,1s}$	$C_{1s,2s}$	$C_{2s,2s}$	$d_{2p,2p}$
0.991334	-0.112748	-0.222737(-1)	-0.624144(-1)
$d_{2p,3p}$	$d_{3p,3p}$	Z_0	Z_1
0.489151(-2)	-0.113886(-1)	0.175478(+1)	0.518423(+1)

CORRESPONDING GROUND STATE ENERGY = -0.287660 (+1) au

Li$^+$

$C_{1s,1s}$	$C_{1s,2s}$	$C_{2s,2s}$	$d_{2p,2p}$
0.997407	-0.572918(-1)	-0.125330(-1)	-0.410064(-1)
$d_{2p,3p}$	$d_{3p,3p}$	Z_0	Z_1
0.220681(-2)	-0.726350(-2)	0.273824(1)	0.812231(1)

CORRESPONDING GROUND STATE ENERGY = -0.725106(+1) au

MOMENTUM TRANSFER (Ka_0)	ATOMIC FORM FACTOR F(K)			
	C.I WAVE FUNCTION	3 TERM HF*	3 TERM HY†	6 TERM HY
0.166243	0.198890(+1)	0.19892(+1)	0.19890(+1)	0.198905(+1)
0.332485	0.195645(+1)	0.19571(+1)	0.19567(+1)	0.195481(+1)
0.498728	0.190489(+1)	0.19057(+1)	0.19046(+1)	0.190496(+1)
0.664971	0.183735(+1)	0.18372(+1)	0.18354(+1)	0.183613(+1)
0.831214	0.175726(+1)	0.17551(+1)	0.17524(+1)	0.175352(+1)
0.997456	0.166794(+1)	0.16626(+1)	0.16589(+1)	0.166065(+1)
0.132994(+1)	0.147339(+1)	0.14604(+1)	0.14546(+1)	0.145785(+1)
0.199491(+1)	0.108303(+1)	0.10602(+1)	0.10519(+1)	0.105819(+1)
0.265988(+1)	0.757991	0.7383	0.7303	0.73804
0.332485(+1)	0.519465	0.5089	0.5025	0.50995
0.398983(+1)	0.355121	0.3529	0.3482	0.35449
0.465480(+1)	0.244878	0.2481	0.2447	0.24965

*HF: HARTREE-FOCK WAVE FUNCTION †HY: HYLLERAAS WAVE FUNCTION

MOMENTUM TRANSFER (Ka_0)	INCOHERENT SCATTERING FUNCTION (VALUES LISTED ARE ZSinc(K) WITH Z = 2)			
	C.I WAVE FUNCTION	3 TERM HF	3 TERM HY	6 TERM HY
0.166243	0.208770(-1)	0.2163(-1)	0.2043(-1)	0.20691(-1)
0.332485	0.813874(-1)	0.8480(-1)	0.7995(-1)	0.80913(-1)
0.498728	0.175468	0.1843	0.1735	0.17546
0.664971	0.294990	0.3123	0.2938	0.29674
0.831214	0.431430	0.4598	0.4322	0.43599
0.997456	0.576992	0.6178	0.5802	0.58457
0.132994(+1)	0.870468	0.9336	0.8765	0.88094
0.199491(+1)	0.136271(+1)	0.14380(+1)	0.13593(+1)	0.136108(+1)
0.265988(+1)	0.167239(+1)	0.17274(+1)	0.16558(+1)	0.165524(+1)
0.332485(+1)	0.183911(+1)	0.18705(+1)	0.18186(+1)	0.181719(+1)
0.398983(+1)	0.192214(+1)	0.19377(+1)	0.19043(+1)	0.190286(+1)
0.465480(+1)	0.196211(+1)	0.19692(+1)	0.19487(+1)	0.194762(+1)

TABLE 4.1
VALUES OF THE ATOMIC FORM FACTOR AND INCOHERENT SCATTERING FUNCTION FOR HELIUM CALCULATED FROM STANDARD WAVE FUNCTIONS.

CASE: $E_0 = 256.5\,eV$ $E_f = 226\,eV$ $\theta_f = 4°$

ANGLE θ_s	$f(\underline{k}_f,\underline{k}_s)$		$g(\underline{k}_f,\underline{k}_s)$	
	$\mathcal{R}.f(\underline{k}_f,\underline{k}_s)$	$\mathcal{I}.f(\underline{k}_f,\underline{k}_s)$	$\mathcal{R}.g(\underline{k}_f,\underline{k}_s)$	$\mathcal{I}.g(\underline{k}_f,\underline{k}_s)$
18°	0.521	0.224	0.166(-1)	0.475(-2)
36°	0.172	-0.123	0.104(-1)	0.417(-2)
54°	-0.154	-0.364	0.627(-2)	0.320(-2)
72°	-0.429	-0.523	0.417(-2)	0.176(-2)
90°	-0.635	-0.621	0.322(-2)	0.179(-3)
108°	-0.771	-0.675	0.265(-2)	-0.104(-2)
126°	-0.838	-0.698	0.234(-2)	-0.179(-2)
144°	-0.835	-0.697	0.231(-2)	-0.220(-2)
162°	-0.761	-0.672	0.262(-2)	-0.242(-2)
180°	-0.620	-0.614	0.329(-2)	-0.254(-2)
198°	-0.406	-0.511	0.441(-2)	-0.260(-2)
216°	-0.126	-0.346	0.617(-2)	-0.255(-2)
234°	0.204	-0.957(-1)	0.886(-2)	-0.225(-2)
252°	0.552	0.261	0.128(-1)	-0.148(-2)
270°	0.851	0.723	0.184(-1)	-0.140(-4)
288°	0.102(+1)	0.121(+1)	0.251(-1)	0.202(-2)
306°	0.108(+1)	0.153(+1)	0.315(-1)	0.381(-2)
324°	0.107(+1)	0.152(+1)	0.342(-1)	0.480(-2)
342°	0.101(+1)	0.117(+1)	0.311(-1)	0.518(-2)
360°	0.828	0.678	0.242(-1)	0.507(-2)

TABLE 4.2
VARIATION OF THE DIRECT AND EXCHANGE (PETERKOP FORM) AMPLITUDES WITH SCATTERING ANGLE θ_s.

It should be noted that the tabulated values differ from the corresponding amplitudes by a multiplicative constant. (The entries in these tables should be multiplied by a factor $Z^{3/2}/\pi$ to obtain the actual values of the amplitudes.)

CASE: E_0 = 256.5eV E_f = 229eV θ_f= 6°

	$f(\underline{k}_f,\underline{k}_s)$		$g(\underline{k}_f,\underline{k}_s)$	
ANGLE θ_s	$\mathcal{R}.f(\underline{k}_f,\underline{k}_s)$	$\mathcal{I}.f(\underline{k}_f,\underline{k}_s)$	$\mathcal{R}.g(\underline{k}_f,\underline{k}_s)$	$\mathcal{I}.g(\underline{k}_f,\underline{k}_s)$
18°	0.374	-0.218(-1)	0.149(-1)	0.425(-2)
36°	0.117	-0.407	0.968(-2)	0.368(-2)
54°	-0.126	-0.656	0.636(-2)	0.284(-2)
72°	-0.319	-0.809	0.457(-2)	0.172(-2)
90°	-0.451	-0.895	0.372(-2)	0.509(-3)
108°	-0.528	-0.940	0.336(-2)	-0.527(-3)
126°	-0.544	-0.950	0.332(-2)	-0.128(-2)
144°	-0.496	-0.922	0.361(-2)	-0.177(-2)
162°	-0.391	-0.857	0.429(-2)	-0.208(-2)
180°	-0.229	-0.741	0.547(-2)	-0.224(-2)
198°	-0.680(-2)	-0.543	0.733(-2)	-0.228(-2)
216°	0.250	-0.231	0.102(-1)	-0.214(-2)
234°	0.487	0.242	0.146(-1)	-0.173(-2)
252°	0.586	0.875	0.210(-1)	-0.905(-3)
270°	0.433	0.153(+1)	0.294(-1)	0.398(-3)
288°	0.151	0.198(+1)	0.377(-1)	0.199(-2)
306°	0.692(-1)	0.208(+1)	0.417(-1)	0.339(-2)
324°	0.291	0.179(+1)	0.386(-1)	0.426(-2)
342°	0.543	0.121(+1)	0.308(-1)	0.460(-2)
360°	0.563	0.537	0.221(-1)	0.456(-2)

TABLE 4.3
VARIATION OF THE DIRECT AND EXCHANGE (PETERKOP FORM) AMPLITUDES WITH SCATTERING ANGLE θ_S.

CASE: $E_0 = 256.5\text{eV}$ $E_f = 230.5\text{eV}$ $\theta_f = 10°$

	$f(\underline{k}_f, \underline{k}_s)$		$g(\underline{k}_f, \underline{k}_s)$	
ANGLE θ_s	$\mathcal{R}.f(\underline{k}_f, \underline{k}_s)$	$\mathcal{I}.f(\underline{k}_f, \underline{k}_s)$	$\mathcal{R}.g(\underline{k}_f, \underline{k}_s)$	$\mathcal{I}.g(\underline{k}_f, \underline{k}_s)$
15°	0.401	0.567(-2)	0.734(-2)	0.350(-2)
30°	0.361	-0.277	0.488(-2)	0.314(-2)
45°	0.284	-0.484	0.316(-2)	0.266(-2)
60°	0.203	-0.624	0.208(-2)	0.206(-2)
75°	0.132	-0.710	0.148(-2)	0.139(-2)
90°	0.826(-1)	-0.762	0.122(-2)	0.708(-3)
105°	0.590(-1)	-0.789	0.117(-2)	0.713(-4)
120°	0.598(-1)	-0.788	0.128(-2)	-0.472(-3)
135°	0.852(-1)	-0.759	0.155(-2)	-0.906(-3)
150°	0.136	-0.705	0.202(-2)	-0.124(-2)
165°	0.208	-0.616	0.273(-2)	-0.147(-2)
180°	0.290	-0.472	0.375(-2)	-0.161(-2)
195°	0.365	-0.260	0.518(-2)	-0.165(-2)
210°	0.402	0.283(-1)	0.713(-2)	-0.158(-2)
225°	0.345	0.389	0.977(-2)	-0.134(-2)
240°	0.145	0.767	0.132(-1)	-0.909(-3)
255°	-0.192	0.106(+1)	0.174(-1)	-0.243(-3)
270°	-0.563	0.119(+1)	0.218(-1)	0.636(-3)
285°	-0.805	0.122(+1)	0.249(-1)	0.162(-2)
300°	-0.795	0.122(+1)	0.255(-1)	0.254(-2)
315°	-0.539	0.199(+1)	0.233(-1)	0.324(-2)
330°	-0.165	0.104(+1)	0.192(-1)	0.365(-2)
345°	0.164	0.742	0.147(-1)	0.380(-2)
360°	0.354	0.362	0.106(-1)	0.373(-2)

TABLE 4.4
VARIATION OF THE DIRECT AND EXCHANGE (PETERKOP FORM) AMPLITUDES WITH SCATTERING ANGLE θ_s

CASE: $E_0 = 256.5\text{eV}$ $E_f = 229\text{eV}$ $\theta_f = 4°$

	SUMMED PARTIAL WAVE CONTRIBUTIONS TO THE TDC				
ANGLE θ_S	$\sum_{l=0}$	$\sum_{l=0}^{1}$	$\sum_{l=0}^{2}$	$\sum_{l=0}^{5}$	$\sum_{l=0}^{6}$
15°	0.948(-2)	0.605	0.497	0.517	0.513
30°	0.934(-2)	0.126	0.996(-1)	0.113	0.113
45°	0.946(-2)	0.218(-1)	0.193	0.166	0.166
60°	0.984(-2)	0.319	0.550	0.484	0.485
75°	0.104(-1)	0.936	0.966	0.905	0.908
90°	0.111(-1)	0.171(+1)	0.133(+1)	0.132(+1)	0.132 (+1)
105°	0.116(-1)	0.242(+1)	0.159(+1)	0.164(+1)	0.164(+1)
120°	0.120(-1)	0.289(+1)	0.175(+1)	0.182(+1)	0.183(+1)
135°	0.121(-1)	0.299(+1)	0.178(+1)	0.185(+1)	0.187(+1)
150°	0.118(-1)	0.269(+1)	0.168(+1)	0.174(+1)	0.175(+1)
165°	0.113(-1)	0.207(+1)	0.147(+1)	0.149(+1)	0.148(+1)
180°	0.107(-1)	0.130(+1)	0.115(+1)	0.111(+1)	0.111(+1)
195°	0.101(-1)	0.581	0.750	0.679	0.682
210°	0.961(-2)	0.116	0.344	0.296	0.295
225°	0.936(-2)	0.255(-1)	0.955(-1)	0.928(-1)	0.932(-1)
240°	0.939(-2)	0.336	0.236	0.257	0.256
255°	0.964(-2)	0.966	0.942	0.955	0.952
270°	0.100(-1)	0.175(+1)	0.216(+1)	0.219(+1)	0.219(+1)
285°	0.104(-1)	0.247(+1)	0.355(+1)	0.369(+1)	0.369(+1)
300°	0.106(-1)	0.295(+1)	0.458(+1)	0.490(+1)	0.489(+1)
315°	0.107(-1)	0.304(+1)	0.480(+1)	0.517(+1)	0.515(+1)
330°	0.105(-1)	0.274(+1)	0.412(+1)	0.434(+1)	0.434(+1)
345°	0.102(-1)	0.211(+1)	0.283(+1)	0.289(+1)	0.290(+1)
360°	0.981(-2)	0.133(+1)	0.147(+1)	0.148(+1)	0.148(+1)

TABLE 4.5
VALUES OF THE TDC (WITH EXCHANGE AND CAPTURE EXCLUDED) SHOWING THE RELATIVE IMPORTANCE OF THE VARIOUS TERMS IN THE INFINITE SERIES EXPANSION ASSOCIATED WITH THE DIRECT AMPLITUDE.

CASE: $E_o = 256.5\,eV$ $E_f = 230.5\,eV$ $\theta_f = 4°$

ANGLE θ_s	SUMMED PARTIAL-WAVE CONTRIBUTIONS TO TDC				
	$\sum_{l=0}$	$\sum_{l=0}^{1}$	$\sum_{l=0}^{2}$	$\sum_{l=0}^{5}$	$\sum_{l=0}^{6}$
15°	0.119(-1)	0.676	0.559	0.637	0.634
30°	0.119(-1)	0.115	0.142	0.167	0.167
45°	0.119(-1)	0.503(-1)	0.307	0.277	0.276
60°	0.119(-1)	0.501	0.780	0.725	0.727
75°	0.119(-1)	0.135(+1)	0.134(+1)	0.130(+1)	0.130(+1)
90°	0.119(-1)	0.236(+1)	0.186(+1)	0.184(+1)	0.183(+1)
105°	0.119(-1)	0.327(+1)	0.227(+1)	0.224(+1)	0.224(+1)
120°	0.119(-1)	0.384(+1)	0.252(+1)	0.246(+1)	0.247(+1)
135°	0.119(-1)	0.391(+1)	0.255(+1)	0.248(+1)	0.250(+1)
150°	0.119(-1)	0.346(+1)	0.235(+1)	0.232(+1)	0.232(+1)
165°	0.119(-1)	0.261(+1)	0.197(+1)	0.196(+1)	0.195(+1)
180°	0.119(-1)	0.160(+1)	0.148(+1)	0.144(+1)	0.144(+1)
195°	0.119(-1)	0.687	0.921	0.866	0.869
210°	0.199(-1)	0.119	0.409	0.369	0.368
225°	0.199(-1)	0.478(-1)	0.139	0.149	0.149
240°	0.119(-1)	0.492	0.385	0.452	0.450
255°	0.119(-1)	0.133(+1)	0.134(+1)	0.143(+1)	0.143(+1)
270°	0.119(-1)	0.234(+1)	0.290(+1)	0.297(+1)	0.298(+1)
285°	0.119(-1)	0.325(+1)	0.461(+1)	0.466(+1)	0.466(+1)
300°	0.119(-1)	0.381(+1)	0.580(+1)	0.586(+1)	0.584(+1)
315°	0.119(-1)	0.388(+1)	0.595(+1)	0.601(+1)	0.599(+1)
330°	0.119(-1)	0.343(+1)	0.499(+1)	0.504(+1)	0.504(+1)
345°	0.119(-1)	0.259(+1)	0.335(+1)	0.341(+1)	0.342(+1)
360°	0.119(-1)	0.158(+1)	0.169(+1)	0.179(+1)	0.178(+1)

TABLE 4.6

VALUES OF THE TDC (WITH EXCHANGE AND CAPTURE EXCLUDED) SHOWING THE RELATIVE IMPORTANCE OF THE VARIOUS TERMS IN THE PARTIAL WAVE EXPANSION. THE 'p' STATES HAVE BEEN OMITTED FROM THE TARGET WAVE FUNCTION FOR THESE CALCULATIONS.

CASE: $E_o = 256.5\,eV$ $E_f = 230.5\,eV$ $\theta_f = 7°$

	SUMMED PARTIAL WAVE CONTRIBUTIONS TO THE TDC				
ANGLE θ_S	$\sum_{l=0}$	$\sum_{l=0}^{1}$	$\sum_{l=0}^{2}$	$\sum_{l=0}^{5}$	$\sum_{l=0}^{6}$
15°	0.163(-1)	0.887(-1)	0.119	0.152	0.152
30°	0.163(-1)	0.212(-1)	0.194	0.170	0.169
45°	0.163(-1)	0.180	0.378	0.322	0.324
60°	0.163(-1)	0.522	0.561	0.517	0.522
75°	0.163(-1)	0.958	0.718	0.706	0.700
90°	0.163(-1)	0.137(+1)	0.852	0.842	0.836
105°	0.163(-1)	0.165(+1)	0.948	0.908	0.922
120°	0.163(-1)	0.172(+1)	0.973	0.920	0.944
135°	0.163(-1)	0.156(+1)	0.918	0.890	0.895
150°	0.163(-1)	0.122(+1)	0.803	0.798	0.788
165°	0.163(-1)	0.785	0.660	0.636	0.636
180°	0.163(-1)	0.373	0.493	0.439	0.445
195°	0.163(-1)	0.929(-1)	0.303	0.255	0.254
210°	0.163(-1)	0.202(-1)	0.144	0.140	0.139
225°	0.163(-1)	0.174	0.155	0.210	0.209
240°	0.163(-1)	0.512	0.489	0.586	0.581
255°	0.163(-1)	0.943	0.118(+1)	0.126(+1)	0.127(+1)
270°	0.163(-1)	0.135(+1)	0.204(+1)	0.208(+1)	0.209(+1)
285°	0.163(-1)	0.163(+1)	0.273(+1)	0.278(+1)	0.276(+1)
300°	0.163(-1)	0.170(+1)	0.291(+1)	0.299(+1)	0.295(+1)
315°	0.163(-1)	0.154(+1)	0.251(+1)	0.255(+1)	0.254(+1)
330°	0.163(-1)	0.120(+1)	0.171(+1)	0.176(+1)	0.177(+1)
345°	0.163(-1)	0.772	0.877	0.970	0.971
360°	0.163(-1)	0.364	0.315	0.401	0.396

TABLE 4.7

VALUES OF THE TDC (WITH EXCHANGE AND CAPTURE EXCLUDED) SHOWING THE RELATIVE IMPORTANCE OF THE VARIOUS TERMS IN THE PARTIAL WAVE EXPANSION. THE 'p' STATES HAVE BEEN OMITTED FROM THE TARGET WAVE FUNCTION FOR THESE CALCULATIONS.

THE TRIPLE DIFFERENTIAL CROSS SECTION

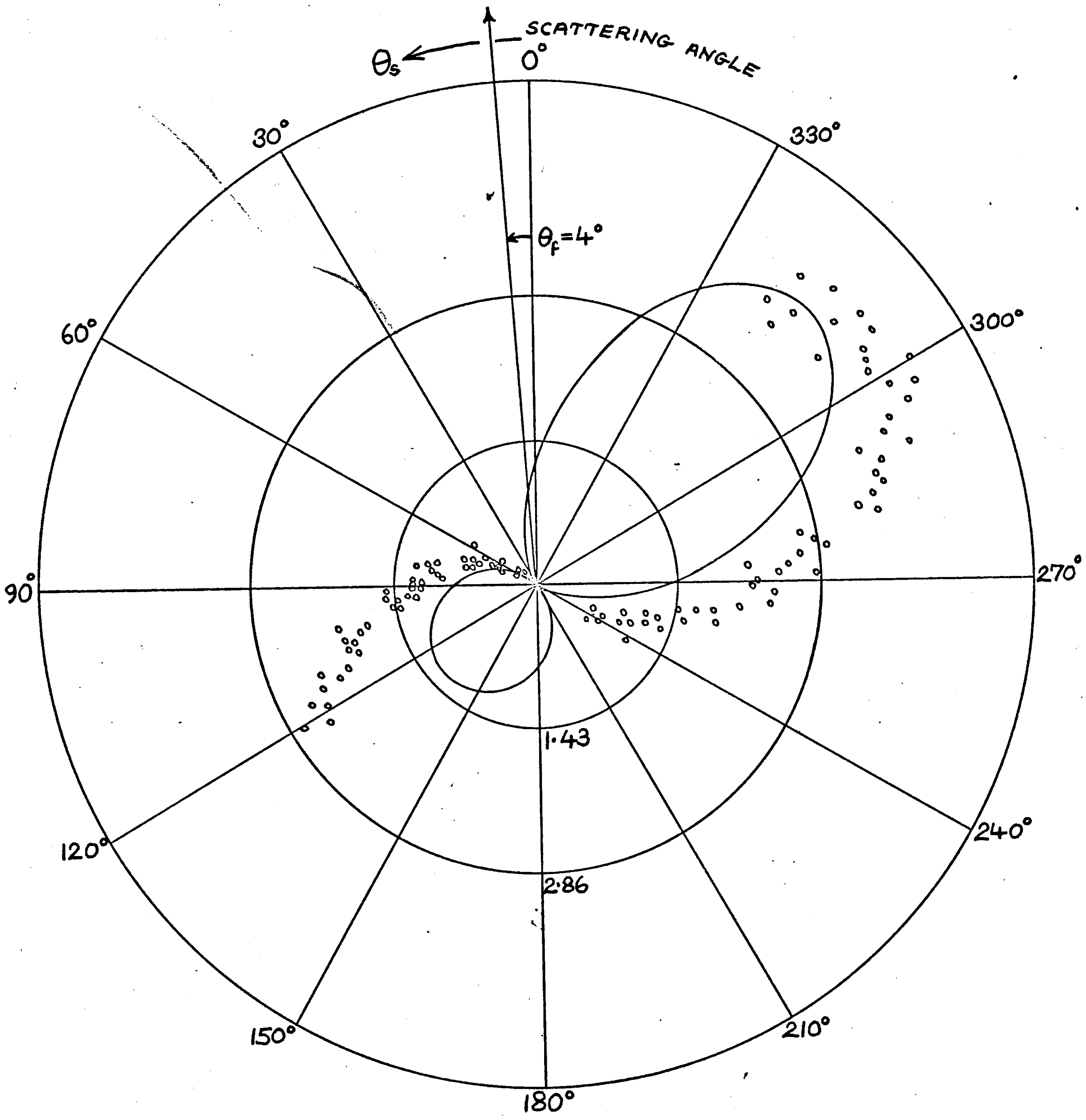


FIGURE 4.1

CASE: $E_0 = 256{\cdot}5\,eV$
$E_f = 226\,eV$
$\theta_f = 4°$

THE TRIPLE DIFFERENTIAL CROSS SECTION

CASE: $E_0 = 256.5 eV$ $E_f = 226 eV$ $\theta_f = 4°$

ANGLE θ_s	TDC
18°	0.332
36°	0.460(-1)
54°	0.169
72°	0.490
90°	0.843
108°	0.112(+1)
126°	0.127(+1)
144°	0.126(+1)
162°	0.110(+1)
180°	0.811
198°	0.455
216°	0.145
234°	0.520(-1)
252°	0.390
270°	0.131(+1)
288°	0.265(+1)
306°	0.370(+1)
324°	0.364(+1)
342°	0.251(+1)
360°	0.120(+1)

THE TRIPLE DIFFERENTIAL CROSS SECTION

CASE: $E_o = 256.5\,eV$ $E_f = 226\,eV$ $\theta_f = 6°$

ANGLE θ_s	TDC
15°	0.976(-1)
30°	0.479(-1)
45°	0.130
60°	0.271
75°	0.418
90°	0.540
105°	0.623
120°	0.663
135°	0.651
150°	0.590
165°	0.488
180°	0.352
195°	0.202
210°	0.804(-1)
225°	0.477(-1)
240°	0.193
255°	0.616
270°	0.134(+1)
285°	0.220(+1)
300°	0.276(+1)
315°	0.258(+1)
330°	0.181(+1)
345°	0.971
360°	0.381

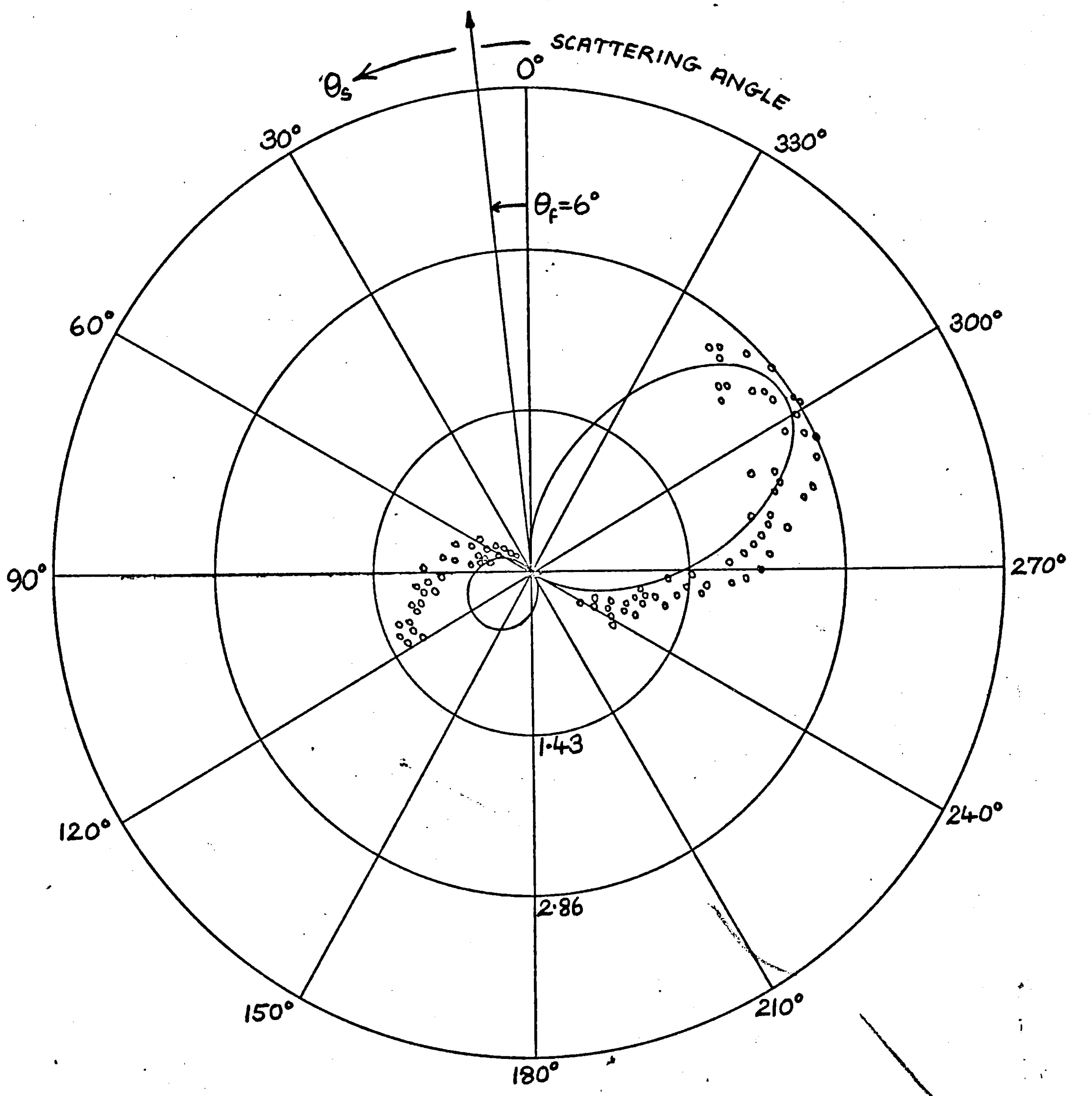


FIGURE 4.2

CASE: $E_0 = 256{\cdot}5\,eV$
$E_f = 226\,eV$
$\theta_f = 6°$

THE TRIPLE DIFFERENTIAL CROSS SECTION

CASE: $E_o = 256.5eV$ $E_f = 226eV$ $\theta_f = 8°$

ANGLE θ_s	TDC
15°	0.491(-1)
30°	0.609(-1)
45°	0.124
60°	0.203
75°	0.273
90°	0.323
105°	0.356
120°	0.367
135°	0.350
150°	0.312
165°	0.258
180°	0.184
195°	0.106
210°	0.507(-1)
225°	0.595(-1)
240°	0.210
255°	0.583
270°	0.119(+1)
285°	0.188(+1)
300°	0.216(+1)
315°	0.174(+1)
330°	0.103(+1)
345°	0.473
360°	0.158

THE TRIPLE DIFFERENTIAL CROSS SECTION

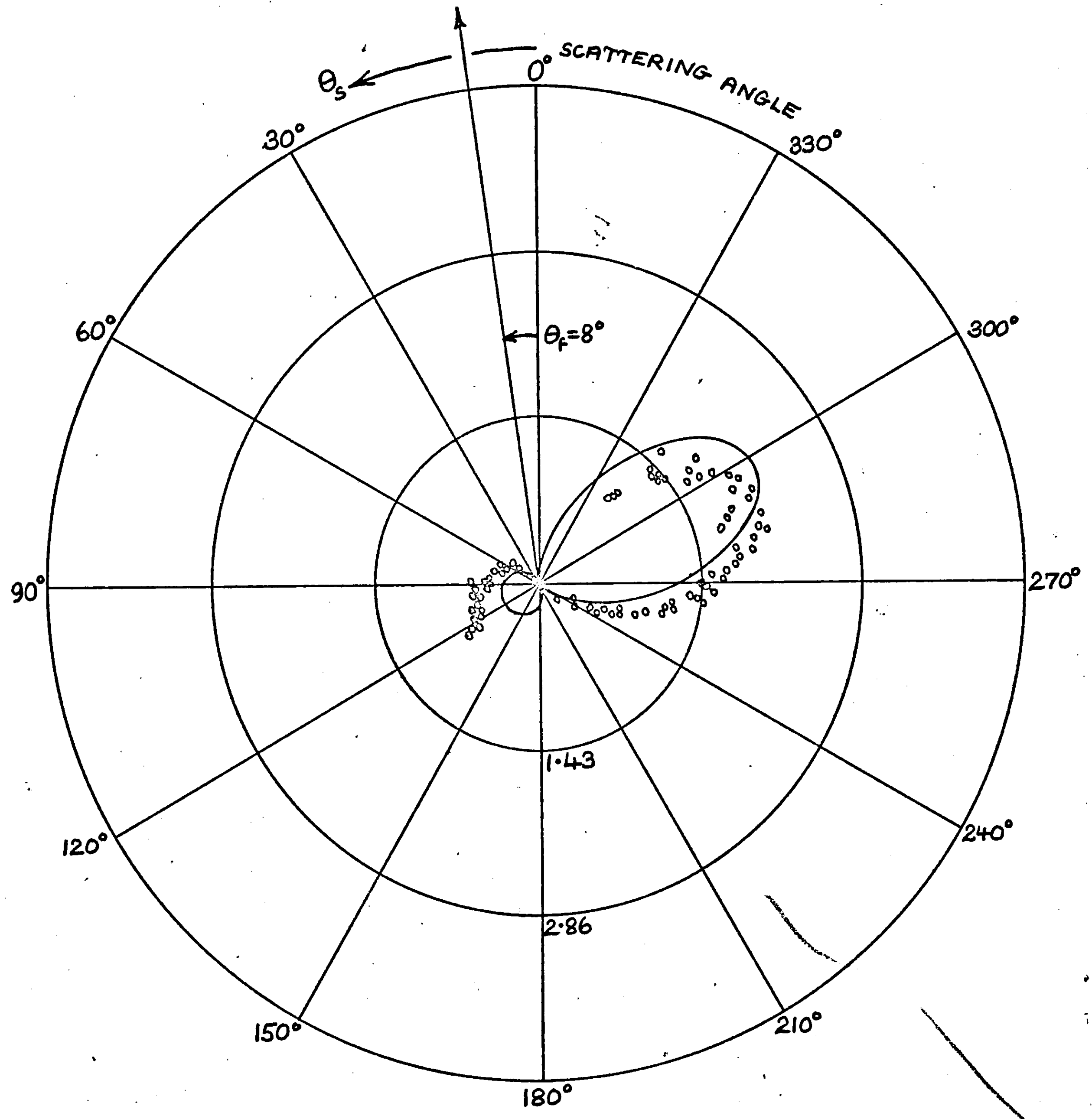


FIGURE 4.3

CASE: $E_0 = 256{\cdot}5$eV

$E_f = 226$

$\theta_f = 8°$

THE TRIPLE DIFFERENTIAL CROSS SECTION

CASE: $E_0 = 256.5\,eV$ $E_f = 230.5\,eV$ $\theta_f = 4^\circ$

ANGLE θ_s	TDC
15°	0.600
30°	0.158
45°	0.267
60°	0.698
75°	0.124(+1)
90°	0.174(+1)
105°	0.212(+1)
120°	0.233(+1)
135°	0.236(+1)
150°	0.219(+1)
165°	0.185(+1)
180°	0.137(+1)
195°	0.829
210°	0.355
225°	0.143
240°	0.427
255°	0.137(+1)
270°	0.290(+1)
285°	0.451(+1)
300°	0.566(+1)
315°	0.581(+1)
330°	0.487(+1)
345°	0.329(+1)
360°	0.180(+1)

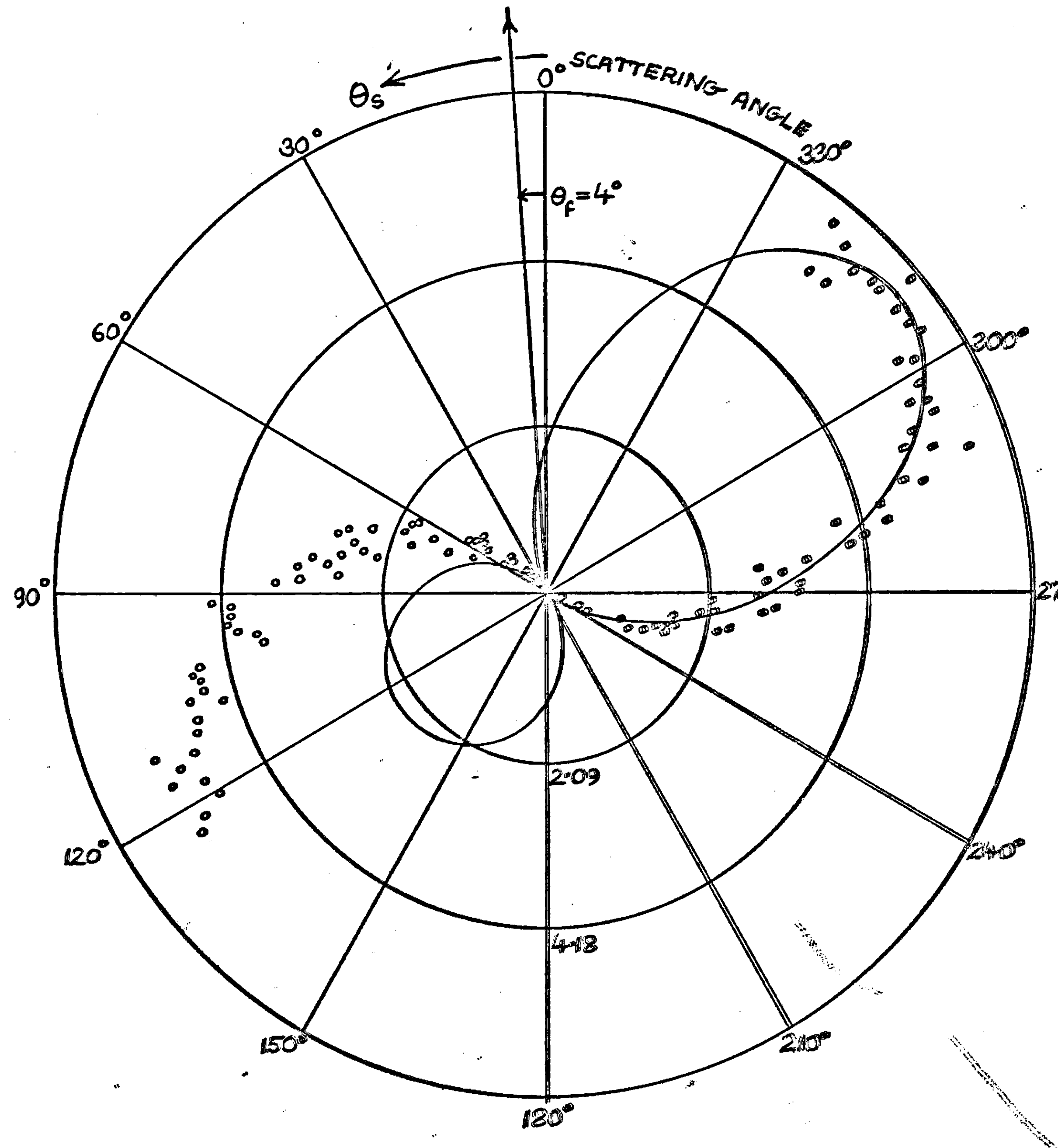


FIGURE 4.4

CASE: $E_0 = 256{\cdot}5\,\mathrm{eV}$
$E_f = 230{\cdot}5\,\mathrm{eV}$
$\theta_f = 4°$

THE TRIPLE DIFFERENTIAL CROSS SECTION
(ADDITIONAL GRAPH)

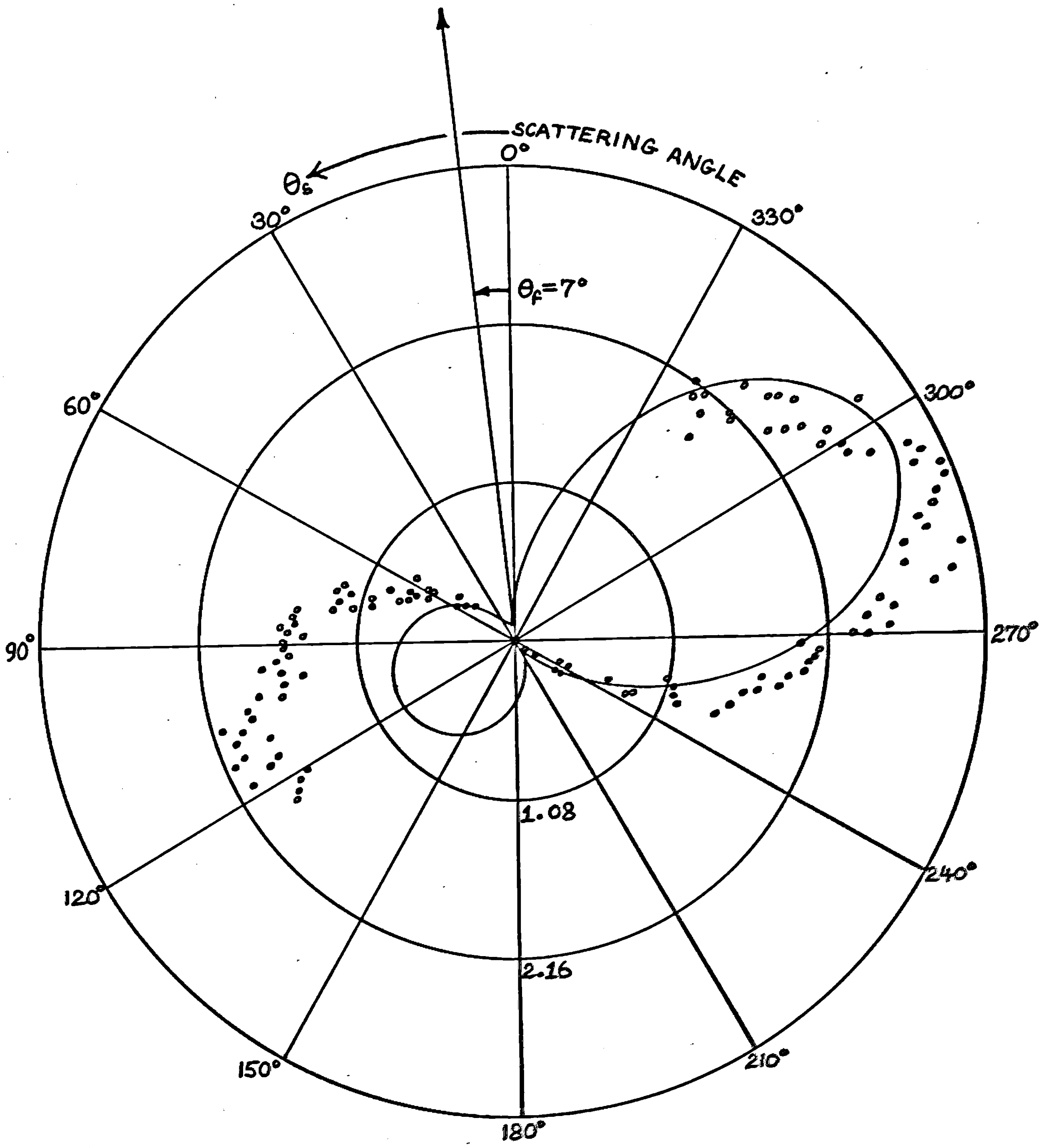


FIGURE 4.4A

CASE: $E_0 = 256{\cdot}5eV$
$E_f = 230{\cdot}5eV$
$\theta_f = 7°$

NORMALIZATION AS IN CASE $\theta_f = 4°$

THE TRIPLE DIFFERENTIAL CROSS SECTION

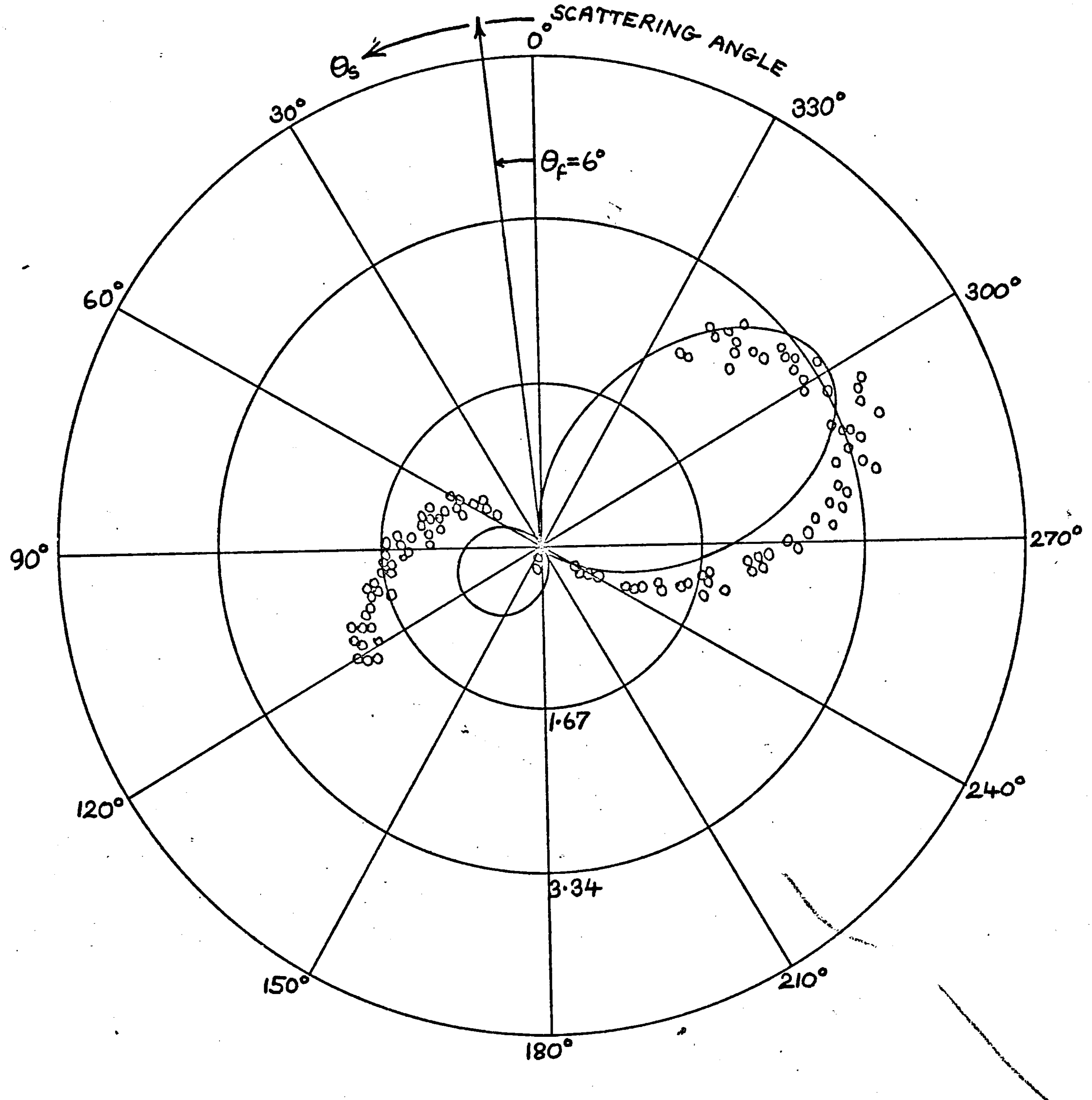


FIGURE 4.5

CASE: $E_0 = 256{\cdot}5\,eV$
$E_f = 229\,eV$
$\theta_f = 6°$

THE TRIPLE DIFFERENTIAL CROSS SECTION

CASE: E_o = 256.5eV E_f = 229eV θ_f = 4°

ANGLE θ_s	TDC
15°	0.148(+1)
30°	0.513
45°	0.113
60°	0.166
75°	0.485
90°	0.908
105°	0.132(+1)
120°	0.164(+1)
135°	0.183(+1)
150°	0.187(+1)
165°	0.175(+1)
180°	0.148(+1)
195°	0.111(+1)
210°	0.682
225°	0.295
240°	0.930(-1)
255°	0.256
270°	0.952
285°	0.219(+1)
300°	0.369(+1)
315°	0.489(+1)
330°	0.515(+1)
345°	0.434(+1)
360°	0.290(+1)

THE TRIPLE DIFFERENTIAL CROSS SECTION
(ADDITIONAL GRAPH)

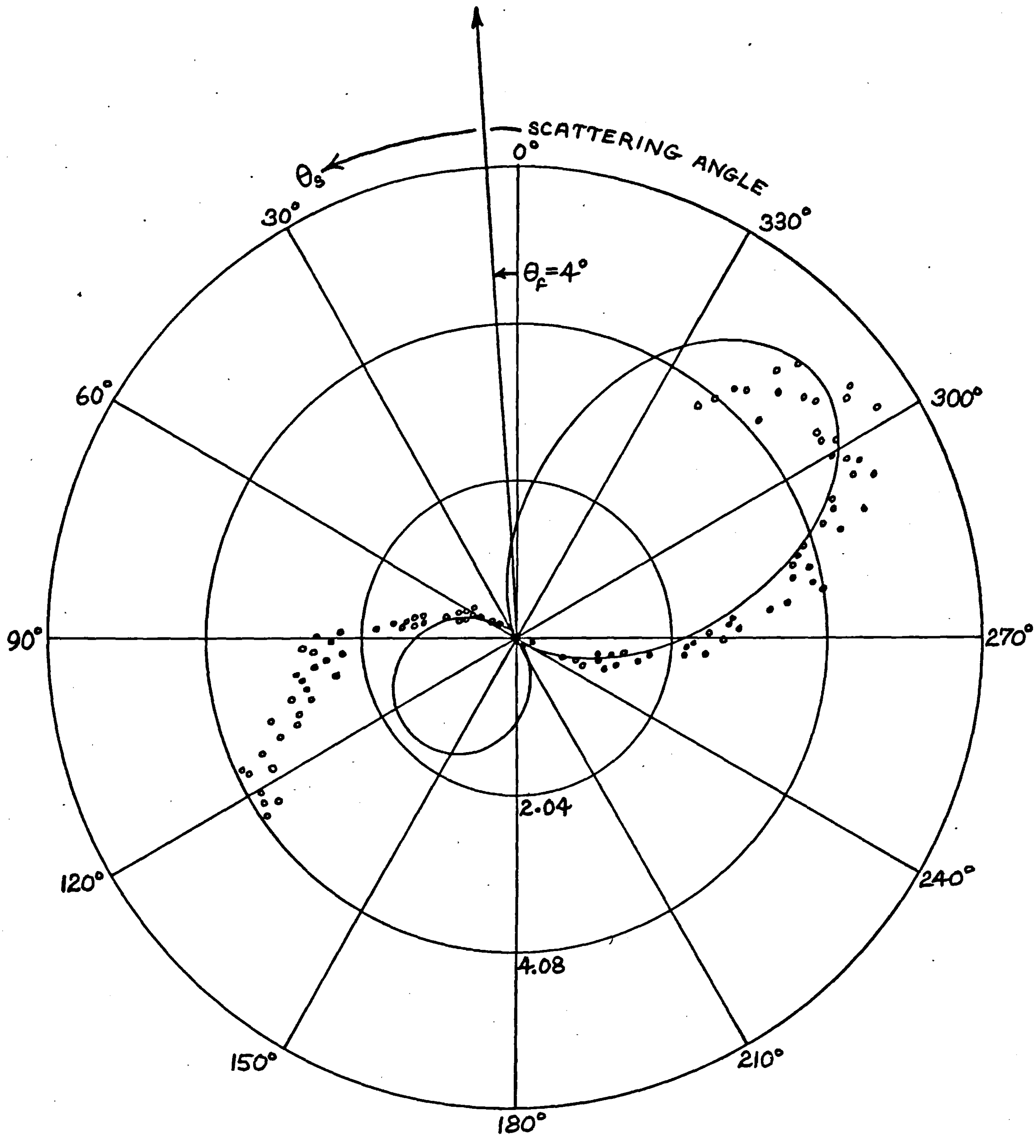


FIGURE 4.5A

CASE: $E_0 = 256.5\,eV$
$E_f = 229\,eV$
$\theta_f = 4°$

NORMALIZATION AS IN CASE $\theta_f = 6°$

THE TRIPLE DIFFERENTIAL CROSS SECTION

CASE: $E_o = 256.5$ eV $E_f = 182$ eV $\theta_f = 8°$

ANGLE θ_s	TDC
15°	0.229(-1)
30°	0.549(-2)
45°	0.135(-2)
60°	0.265(-2)
75°	0.521(-2)
90°	0.748(-2)
105°	0.917(-2)
120°	0.102(-1)
135°	0.106(-1)
150°	0.107(-1)
165°	0.104(-1)
180°	0.954(-2)
195°	0.805(-2)
210°	0.594(-2)
225°	0.340(-2)
240°	0.142(-2)
255°	0.329(-2)
270°	0.157(-1)
285°	0.481(-1)
300°	0.103
315°	0.156
330°	0.164
345°	0.121
360°	0.626(-1)

THE TRIPLE DIFFERENTIAL CROSS SECTION

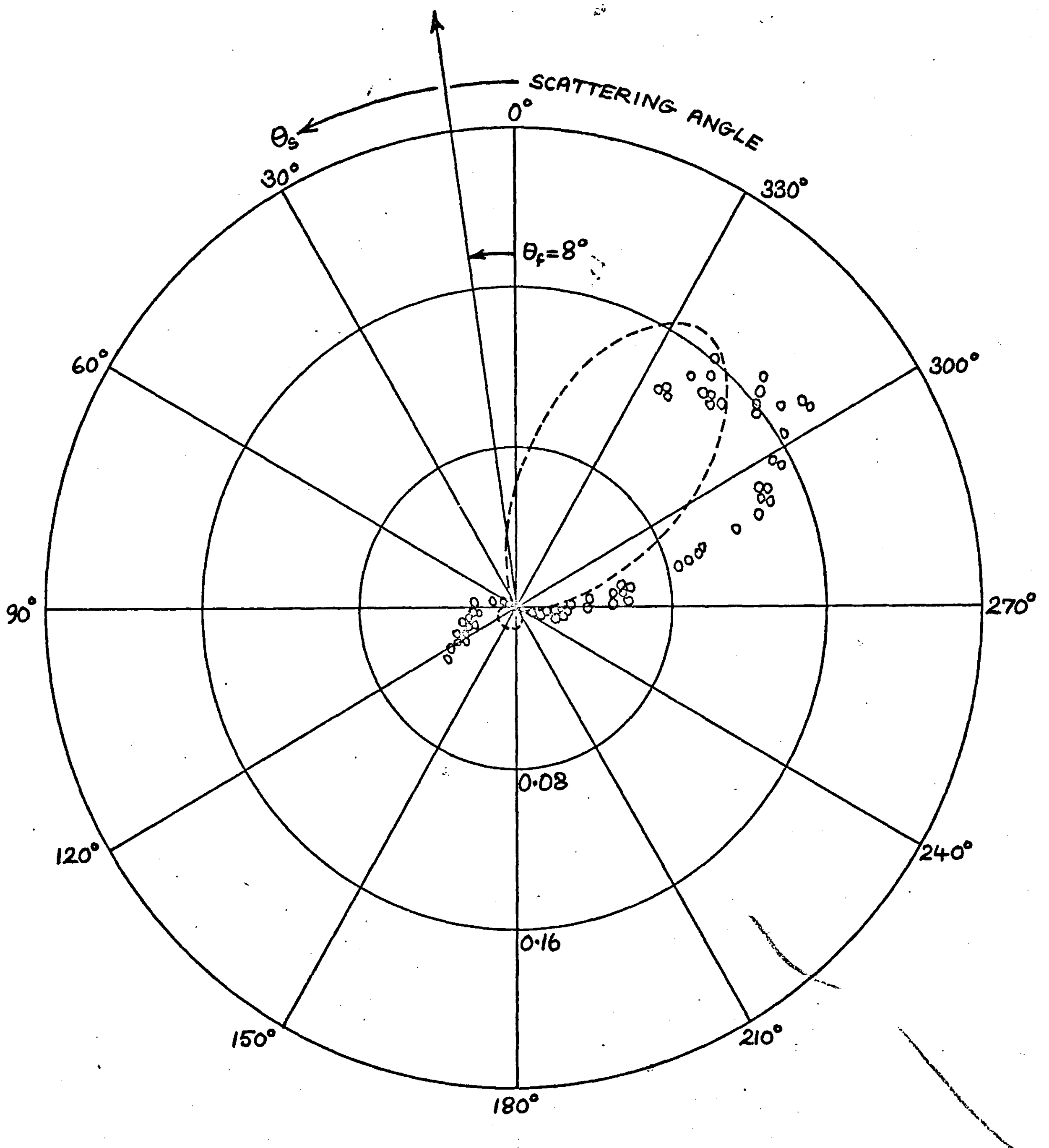
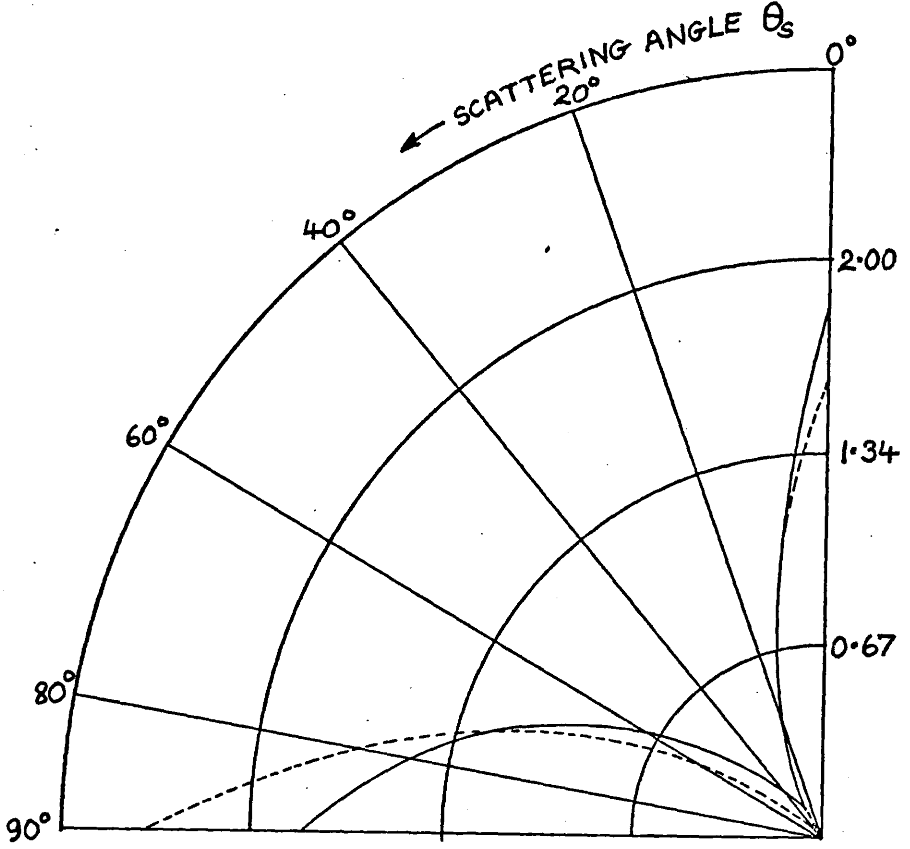


FIGURE 4.6

CASE: $E_0 = 256{\cdot}5$ eV
$E_f = 182$ eV
$\theta_f = 8°$

THE TRIPLE DIFFERENTIAL CROSS SECTION



CASE: $E_0 = 256{\cdot}5\,\text{eV}$
$E_f = 230{\cdot}5\,\text{eV}$
$\theta_f = 4°$

FIGURE 4.7
THE SUMMED PARTIAL WAVE CONTRIBUTIONS TO THE TRIPLE DIFFERENTIAL CROSS SECTION.

THE BROKEN CURVE CORRESPONDS TO THE TDC WITH THE INCLUSION OF THE TERMS L=0,1 AND THE FULL CURVE TO THE TDC WITH THE INCLUSION OF THE TERMS L=0,6.

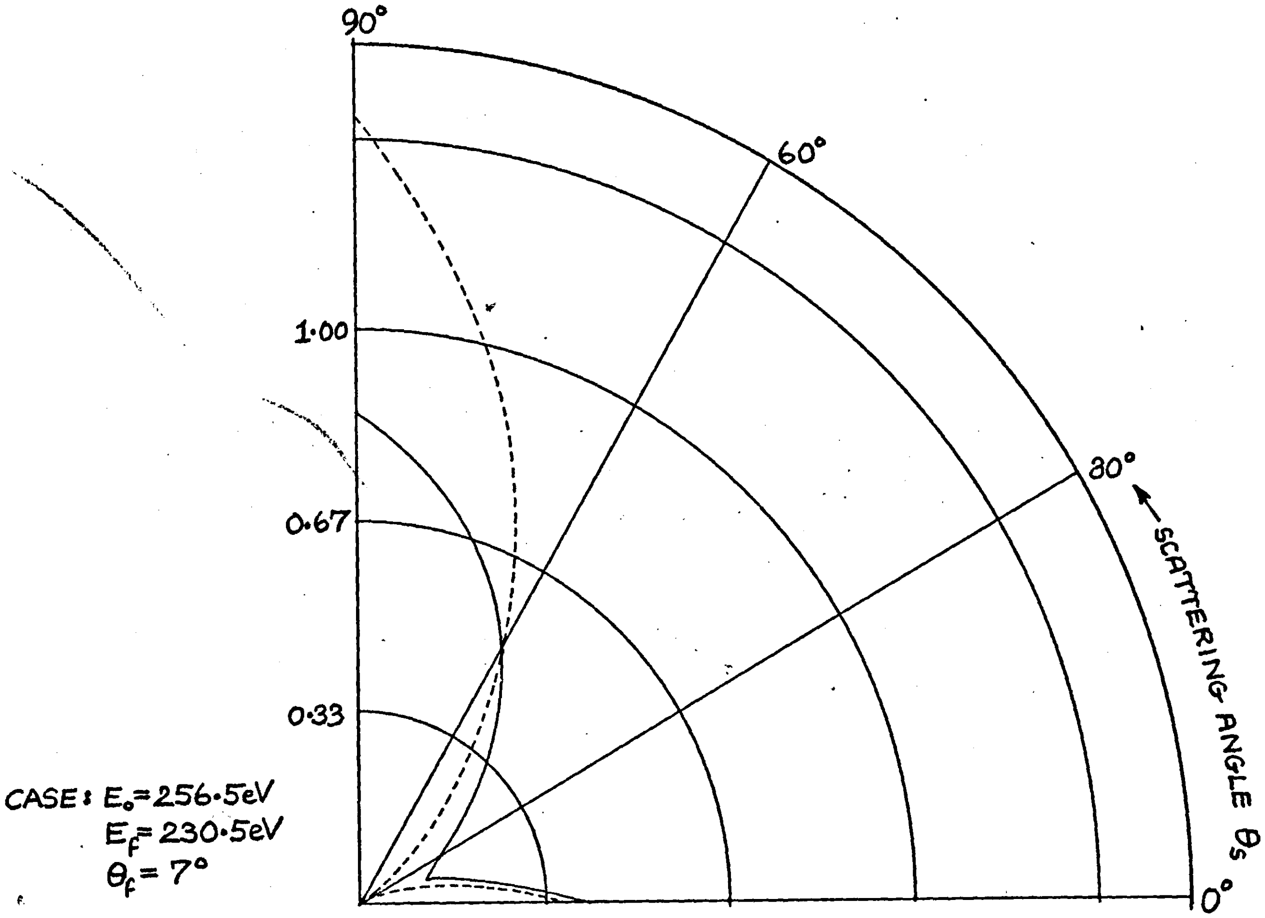
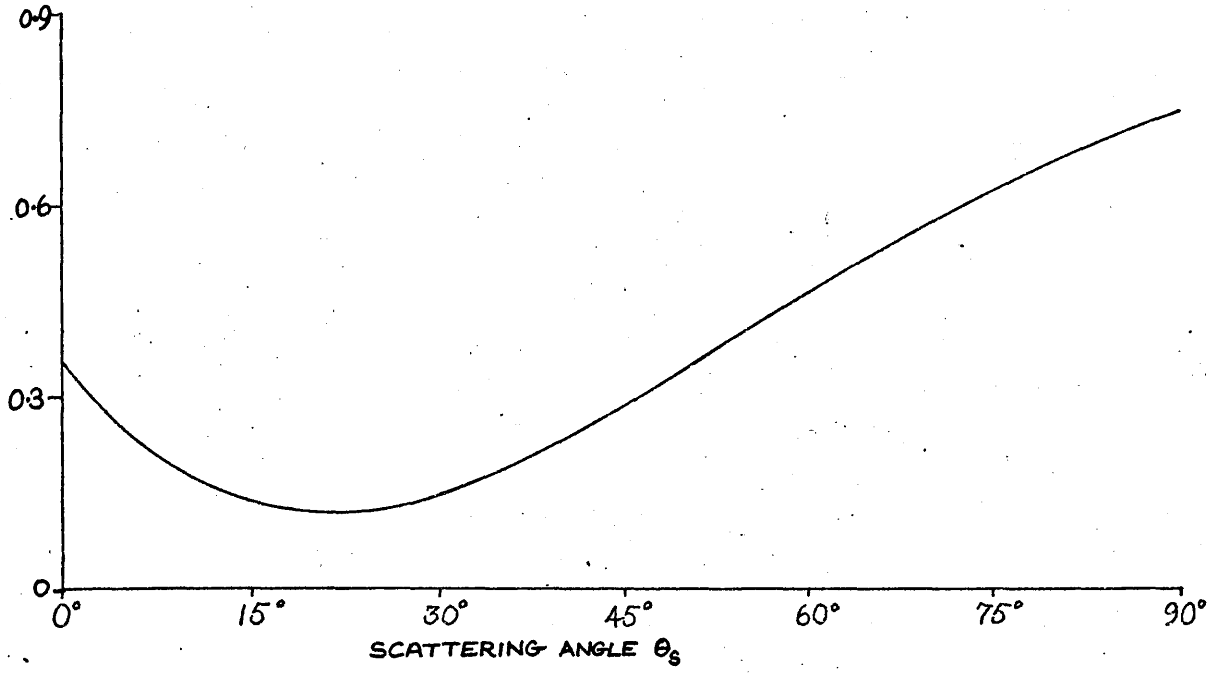


FIGURE 4.8

THE SUMMED PARTIAL WAVE CONTRIBUTIONS TO THE TRIPLE DIFFERENTIAL CROSS SECTION.

THE BROKEN CURVE CORRESPONDS TO THE TDC WITH THE INCLUSION OF THE TERMS $L=0,1$ AND THE FULL CURVE TO THE TDC WITH THE INCLUSION OF THE TERMS $L=0,6$.



DETAIL OF THE TRIPLE DIFFERENTIAL CROSS SECTION IN THE REGION OF A MINIMUM.

CASE: $E_0 = 256{\cdot}5\,\text{eV}$
$E_f = 230{\cdot}5\,\text{eV}$
$\theta_f = 7°$

THESE CALCULATIONS ARE BASED ON THE CORRELATED TARGET WAVE FUNCTION WITH THE 'P' TERMS EXCLUDED. THE PARTIAL WAVE CONTRIBUTIONS L=0,6 ARE INCLUDED.

FIGURE 4.9

THE TRIPLE DIFFERENTIAL CROSS SECTION

(RESULTS OBTAINED BY JACOBS)

CASE: $E_0 = 256.5\,eV$
$E_\delta = 3.0\,eV$
$\theta_f = 4°$

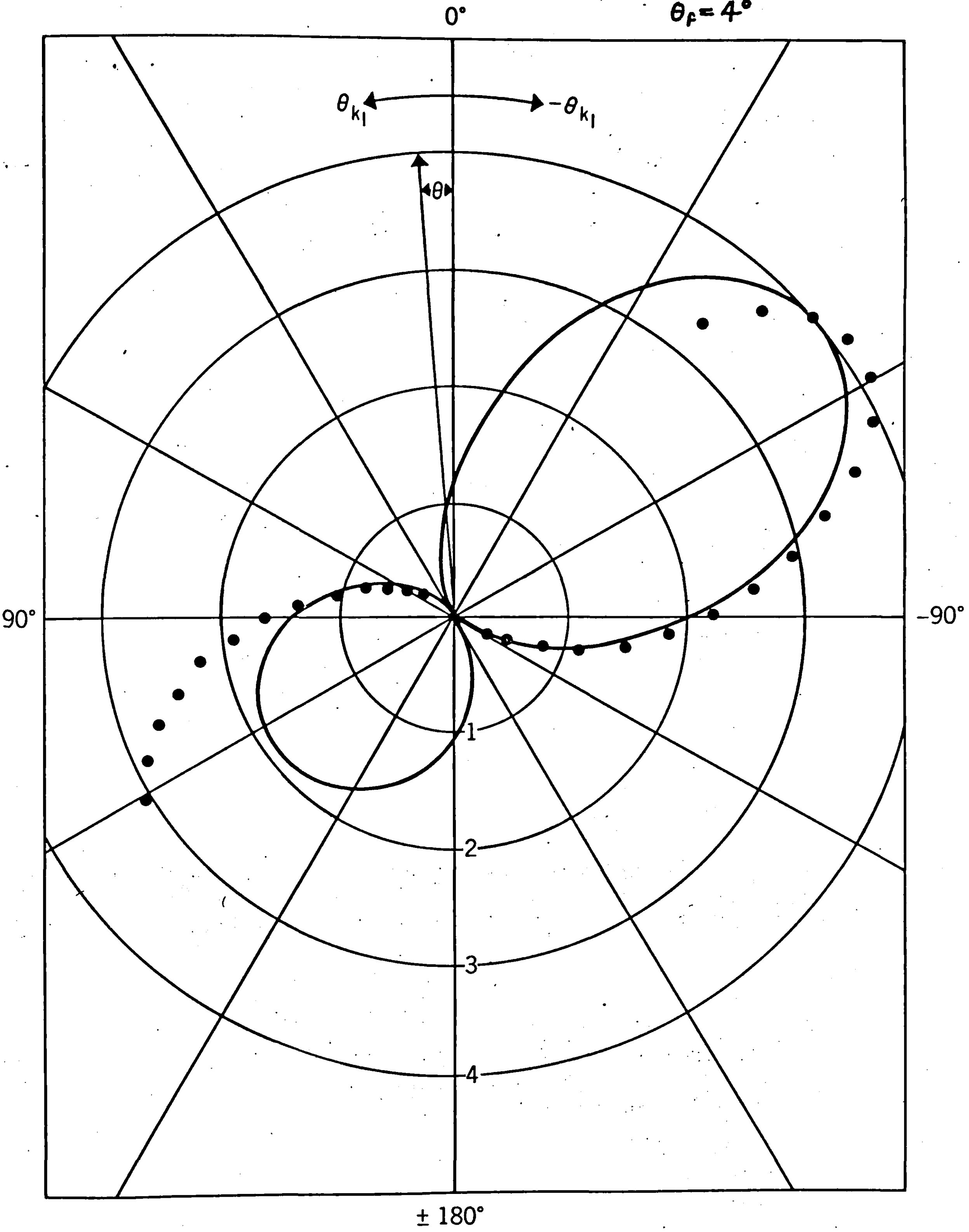


FIGURE 3.

——— CALCULATED CURVE

● ● ● ● ● ● ● EHRHARDT ET AL. (1972)

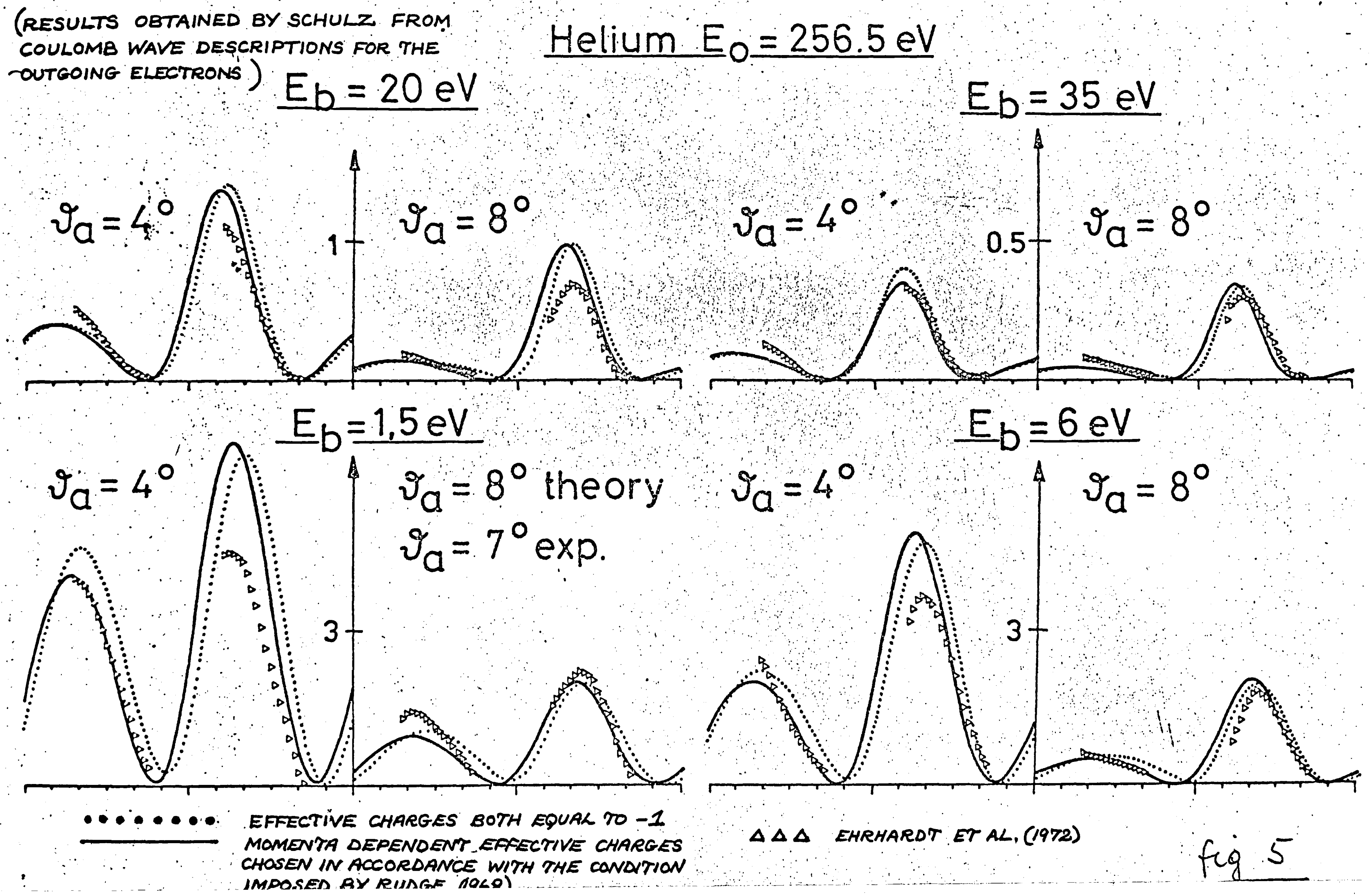

(RESULTS OBTAINED BY SCHULZ FROM COULOMB WAVE DESCRIPTIONS FOR THE OUTGOING ELECTRONS)
Helium $E_0 = 256.5$ eV
$E_b = 20$ eV
$\vartheta_a = 4°$
1
$\vartheta_a = 8°$
$E_b = 35$ eV
$\vartheta_a = 4°$
0.5
$\vartheta_a = 8°$
$E_b = 1{,}5$ eV
$\vartheta_a = 4°$
3
$\vartheta_a = 8°$ theory
$\vartheta_a = 7°$ exp.
$E_b = 6$ eV
$\vartheta_a = 4°$
3
$\vartheta_a = 8°$
•••••••• EFFECTIVE CHARGES BOTH EQUAL TO −1
MOMENTA DEPENDENT EFFECTIVE CHARGES CHOSEN IN ACCORDANCE WITH THE CONDITION IMPOSED BY RUDGE (1969)
△△△ EHRHARDT ET AL. (1972)

fig 5

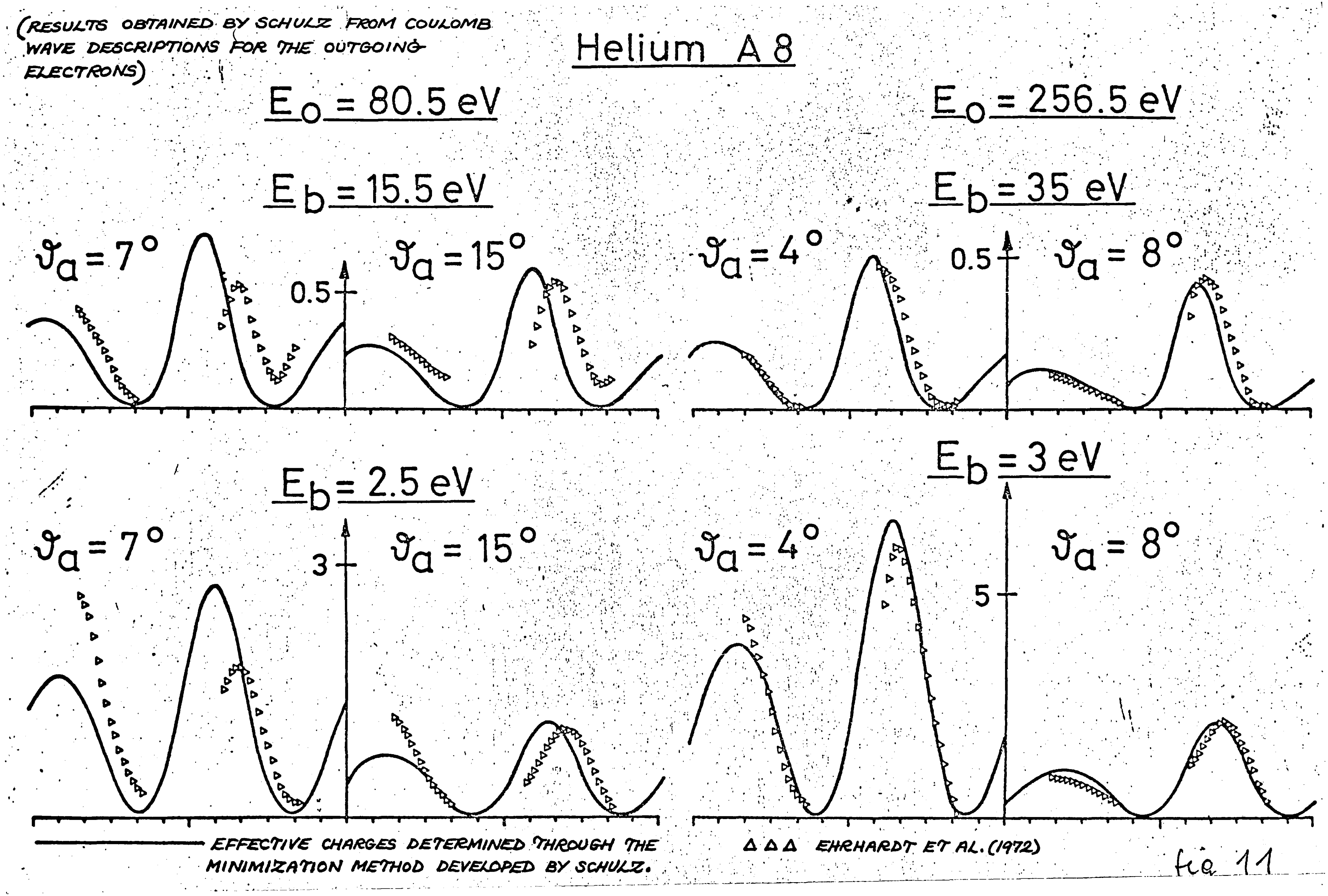
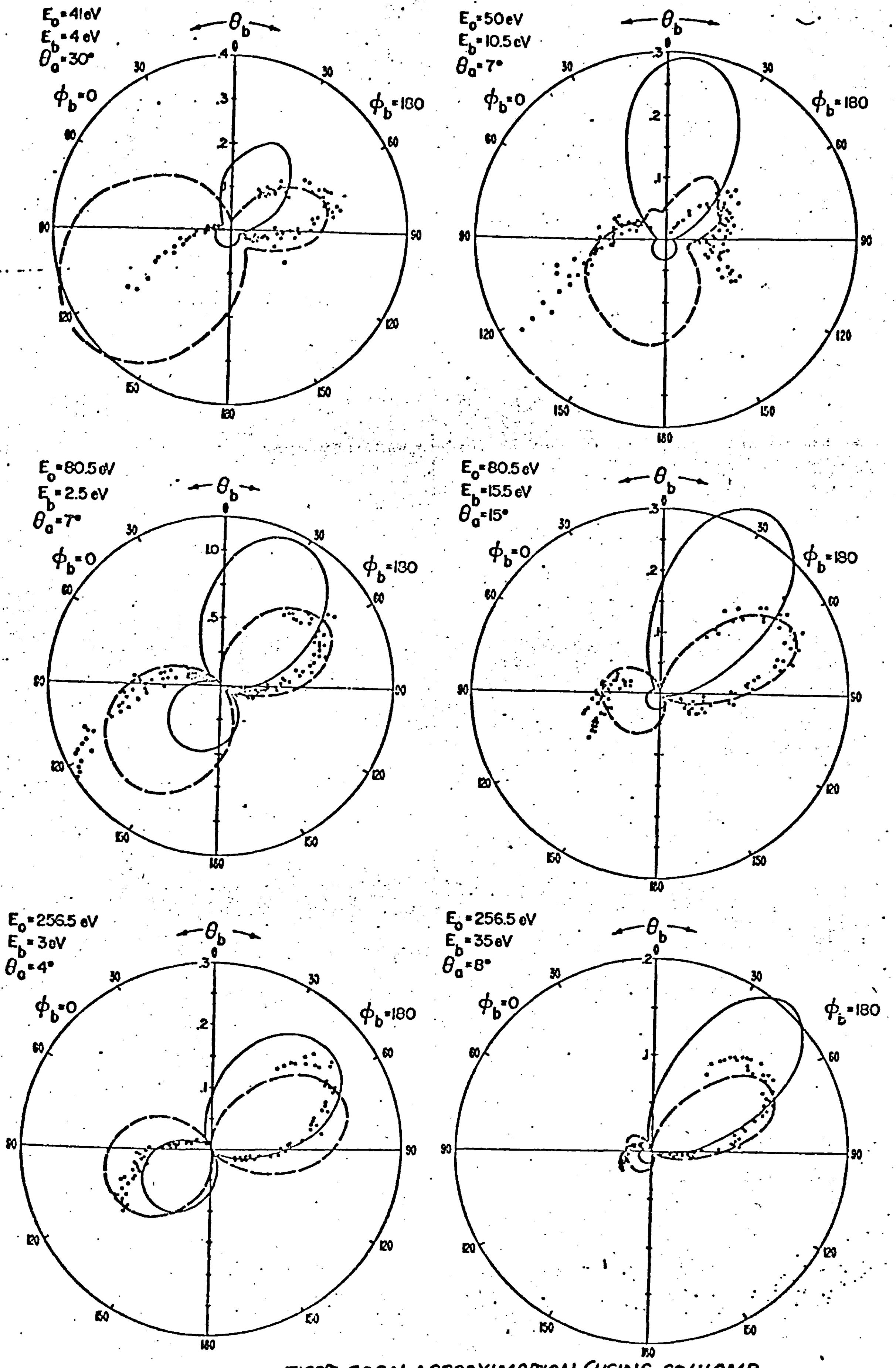

(RESULTS OBTAINED BY SCHULZ FROM COULOMB WAVE DESCRIPTIONS FOR THE OUTGOING ELECTRONS)
Helium A 8
$E_o = 80.5$ eV
$E_b = 15.5$ eV
$\vartheta_a = 7°$
0.5
$\vartheta_a = 15°$
$E_o = 256.5$ eV
$E_b = 35$ eV
$\vartheta_a = 4°$
0.5
$\vartheta_a = 8°$
$E_b = 2.5$ eV
$\vartheta_a = 7°$
3
$\vartheta_a = 15°$
$E_b = 3$ eV
$\vartheta_a = 4°$
5
$\vartheta_a = 8°$
EFFECTIVE CHARGES DETERMINED THROUGH THE MINIMIZATION METHOD DEVELOPED BY SCHULZ.
∆ ∆ ∆ EHRHARDT ET AL. (1972)

fig 11

TDC RESULTS OBTAINED BY GELTMAN



———— FIRST BORN APPROXIMATION (USING COULOMB WAVE DESCRIPTION OF SLOW OUTGOING ELECTRON) 0-74-816

Figure 4 — — — — COULOMB-PROJECTED BORN EXCHANGE CALCULATIONS

● ● ● ● ● EHRHARDT ET AL. (1972)

CHAPTER 5

Introduction

In this chapter we shall examine a number of points arising from the main section of the work, contained in chapters 3 and 4. Of these points the one which is of particular interest is the question of the validity of the exchange approximation used in the calculations. This approximation, derived from equation (2.27), was discussed in chapter 2 where due consideration was given to the inadequacies implicit in this form. Although (2.27) is clearly true for exact wave functions, when used with approximate wave functions it often results in an inadequate description of the physics of the exchange process. This is particularly true when the approximate wave functions are only appropriate to specific energy regions, as in the case of first Born calculations. In such a situation there appears to be little reason for preferring the "Peterkop approximation", derived from (2.27), to the very much simpler plane-plane approximation for the exchange amplitude. The main reason for using the "Peterkop approximation" in our calculations was that it allowed direct avaluation of the exchange amplitude whereas the corresponding expression given by the equations (3.1) presents formidable computational difficulties. However the results of the calculations of the exchange amplitude based on the "Peterkop approximation" and presented in chapters 3 and 4 indicate that the corresponding contribution to the triple differential cross section is consistently small. Indeed, in the energy region considered, it appears as no more than a first order correction throughout the angular range of the "slow" outgoing electron, even being dominated by the contribution from the capture amplitude in some angular regions. In view of the rather unexpected characteristics present in the behaviour of the exchange amplitude one is led to question the validity of the approximation upon which it is based. For this reason we have attempted to derive a more reliable approximate form of the exchange amplitude. It is not intended that this should lead to an accurate evaluation of the exchange contribution, but rather that it should provide an estimate of the correct order of magnitude.

Before seeking a method of approximation it is useful to first examine the sensitivity of the amplitude with respect to variation of the different approximate functions involved. It is not in fact necessary to conduct a specific investigation on this point since adequate data already exists. For instance comparison of triple differential cross section results obtained from the plane-plane approximation and Born-Coulomb calculations, or those contained in chapters 3 and 4, show that these may differ by an order of magnitude, from which it is clear that the TDC is highly sensitive to the manner of representation of the "slow" outgoing electron. We may therefore conclude that any approximation involving this continuum function is likely to have significant effect upon the amplitude. In addition since the "slow" electron continuum function carries all information relating to the scattering by the local potentials it would be unwise to apply any approximation involving some modification of this wave-function.

In contrast to this, comparison of the TDC results presented in chapters 3 and 4 indicates that variation of the target ground state function produces much less drastic changes in the TDC. Although these changes are non-negligible the characteristic behaviour is unaltered and magnitudes remain comparable. This of course assumes that the form of the function resulting from any variation remains appropriate to the system that it is intended to describe. As a result of the points raised in this discussion the method of approximation chosen involves modification of the target ground state function rather than the continuum function. A detailed description of the method is given in the following section.

5.1. An approximate form of the exchange amplitude

An explicit expression for the exchange amplitude is provided by the equations (3.1), being

$$g(\underline{k}_f,\underline{k}_s) = C\left\langle \bar{\Psi}_{\underline{k}_f,\underline{k}_s}(2;1,3)\middle| V(1,2,3) \middle| \bar{\Psi}_{\underline{k}_0}(1;2,3)\right\rangle \tag{5.1}$$

where $C = -(2\pi)^2 e^{i\Delta(\underline{k}_f,\underline{k}_s)}$

The final state wave function $\bar{\Psi}_{\underline{k}_f,\underline{k}_s}$ is given by

$$\bar{\Psi}_{\underline{k}_f,\underline{k}_s}(i;j,k) = \frac{1}{(2\pi)^{3/2}} e^{i\underline{k}_f\cdot\underline{r}_i}\bar{\Psi}_{\underline{k}_s}(\underline{r}_j,\underline{r}_k) \tag{5.2}$$

where

$$\bar{\Psi}_{\underline{k}_s}(\underline{r}_j,\underline{r}_k) = \psi_{\underline{k}_s}(\underline{r}_j)\psi_{1s}(Z=2,\underline{r}_k) \tag{5.3}$$

these wave functions being as previously defined.

The wave function $\bar{\Psi}_{\underline{k}_0}(1;2,3)$ describes the intial state of the system, and has the form

$$\bar{\Psi}_{\underline{k}_0}(1;2,3) = \frac{1}{(2\pi)^{3/2}} e^{i\underline{k}_0\cdot\underline{r}_1}\bar{\Psi}_0(\underline{r}_2,\underline{r}_3) \tag{5.4}$$

where $\bar{\Psi}_0(\underline{r}_2,\underline{r}_3)$ represents the ground state of the target system. In order to simplify the following analysis we have chosen to use the simple ansatz

$$\bar{\Psi}_0(\underline{r}_2,\underline{r}_3) = \frac{\alpha^3}{\pi} e^{-\alpha(r_2+r_3)} \quad , \quad \alpha = 27/16 \tag{5.5}$$

If we use the prior formulation of the exchange amplitude then the interaction potential appearing in (5.1) will have the form

$$V(1,2,3) = -\frac{Z}{r_1} + \frac{1}{r_{13}} + \frac{1}{r_{12}} \tag{5.6}$$

where z = 2 for helium.

When one attempts to evaluate the form of the amplitude given by (5.1) it is found that all but one of the terms contained therein reduce to single integrations over a radial variable which are easily evaluated by standard numerical techniques. It is the presence of this particular term that necessitates the use of some method of approximation. For the present we shall direct our attention toward this term, performing the more straightforward integrations associated with the remaining terms at a later stage. The term in question is

$$C\left\langle {}^{2}\Psi_{\underline{k}_f,\underline{k}_s}(2;1,3)\right|\frac{1}{r_{12}}\left|{}^{2}\Psi_{\underline{k}_0}(1;2,3)\right\rangle$$

Denoting this by I_{EX} we have the following

$$I_{EX} = -\frac{1}{2\pi}e^{i\Delta(\underline{k}_f,\underline{k}_s)}\iiint e^{-i\underline{k}_f\cdot\underline{r}_2}\,{}^{2}\psi^{*}_{\underline{k}_s}(\underline{r}_1)\,{}^{2}\psi^{*}_{1s}(\underline{r}_3)$$

$$\left[\frac{1}{r_{12}}\right]e^{i\underline{k}_0\cdot\underline{r}_1}\,{}^{2}\Psi_0(\underline{r}_2,\underline{r}_3)\,d\underline{r}_1\,d\underline{r}_2\,d\underline{r}_3 \qquad (5.7)$$

Substituting for ${}^{2}\Psi_0$ from (5.5) we obtain

$$I_{EX} = -\frac{1}{2\pi}e^{i\Delta(\underline{k}_f,\underline{k}_s)}\frac{\alpha^3}{\pi}\int {}^{2}\psi^{*}_{1s}(\underline{r}_3)\,e^{-\alpha r_3}\,d\underline{r}_3$$

$$\iint e^{-i\underline{k}_f\cdot\underline{r}_2}\,{}^{2}\psi^{*}_{\underline{k}_s}(\underline{r}_1)\frac{1}{r_{12}}e^{i\underline{k}_0\cdot\underline{r}_1}e^{-\alpha r_2}\,d\underline{r}_1\,d\underline{r}_2 \qquad (5.8)$$

Let us now examine the integration over the variable $\underline{r}_3$

$$\int {}^{2}\psi^{*}_{1s}(\underline{r}_3)\,e^{-\alpha r_3}\,d\underline{r}_3 = \frac{Z^{3/2}}{\pi^{1/2}}\int e^{-(Z+\alpha)r_3}\,d\underline{r}_3$$

$$= \frac{8\pi^{1/2}Z^{3/2}}{(Z+\alpha)^3}$$

Hence

$$I_{EX} = \frac{-4\alpha^3 Z^{3/2}}{\pi^{3/2}(Z+\alpha)^3}\,e^{i\Delta(\underline{k}_f,\underline{k}_s)}\,J_{EX} \qquad (5.9)$$

where
$$J_{EX} = \iint e^{-i\underline{k}_f\cdot\underline{r}_2}\psi^*_{\underline{k}_s}(\underline{r}_1)\frac{1}{r_{12}}e^{i\underline{k}_0\cdot\underline{r}_1}e^{-\alpha r_2}d\underline{r}_1 d\underline{r}_2 \tag{5.10}$$

We can transform the integral of (5.10) by changing the co-ordinate spaces in which we make our measurements.

i.e.
$$(\underline{r}_1, \underline{r}_2) \rightarrow (\underline{r}_1, \underline{r}_{12})$$

where
$$\underline{r}_{12} = \underline{r}_1 - \underline{r}_2$$

Then
$$\underline{r}_2 = \underline{r}_1 - \underline{r}_{12}$$

and
$$r_2 = |\underline{r}_1 - \underline{r}_{12}|$$

In this event we obtain
$$J_{EX} = \iint e^{-i\underline{k}_f\cdot\underline{r}_1}e^{i\underline{k}_f\cdot\underline{r}_{12}}\psi^*_{\underline{k}_s}(\underline{r}_1)\frac{1}{r_{12}}e^{i\underline{k}_0\cdot\underline{r}_1}e^{-\alpha|\underline{r}_1-\underline{r}_{12}|}\,d\underline{r}_1 d\underline{r}_{12} \tag{5.11}$$

Let us firstly consider the integration over the variable $\underline{r}_{12}$ appearing in equation (5.11). This takes the form
$$\int \frac{1}{r_{12}} e^{i\underline{k}_f\cdot\underline{r}_{12}} e^{-\alpha(r_1^2+r_{12}^2-2\underline{r}_1\cdot\underline{r}_{12})^{1/2}} d\underline{r}_{12} \quad , \tag{5.12}$$

which we shall denote by K_{EX}. In order to evaluate the integral (5.12) we shall seek an expansion of $e^{-\alpha(r_1^2+r_{12}^2-2\underline{r}_1\cdot\underline{r}_{12})^{1/2}}$ in terms of Legendré Polynomials. Although it may be shown that this can be done exactly it is necessary to introduce some type of approximation in order to reduce the complexity of the problem. The approximation used is achieved by replacing the quantity
$$|\underline{r}_1 - \underline{r}_{12}| = (r_>^2 + r_<^2 - 2r_>r_<\mu)^{1/2}$$

with
$$(r_> - \mu A r_<)$$

where $r_>$ and $r_<$ have the usual meanings, μ is the cosine of the angle between the two position vectors ($= \hat{\underline{r}}_1\cdot\hat{\underline{r}}_{12}$) and A is a parameter the value of which should be chosen so as to minimize the error arising from the approximation.

We shall now consider a series expansion of the function

$$e^{-\alpha(r_> - \mu A r_<)}$$

$$= e^{-\alpha r_>} e^{\beta\mu r_<} \qquad \text{where } \beta = A\alpha$$

Let

$$e^{\beta\mu r_<} = \sum G_l(\beta, r_<) P_l(\mu)$$

The radial functions $G_l(\beta, r_<)$ may be determined by applying the orthogonality properties of the Legendre Polynomials. i.e.

$$\int_{-1}^{+1} P_m(\mu) e^{\beta\mu r_<} d\mu = \sum_l G_l(\beta, r_<) \int_{-1}^{+1} P_m(\mu) P_l(\mu)\, d\mu$$

$$= \sum_l G_l(\beta, r_<) . \frac{2}{2m+1} \delta_{lm}$$

Hence

$$G_m(\beta, r_<) = \frac{(2m+1)}{2} \int_{-1}^{+1} P_m(\mu) e^{\beta\mu r_<} d\mu = \frac{(2m+1)}{2} \bar{G}_m \tag{5.13}$$

To obtain explicit expressions for the $G_l(\beta, r_<)$ we are required to evaluate integrals of the type contained in (5.13). These may all be constructed from the set of integrals of the form

$$H_n(r_<, \beta) = \int_{-1}^{1} \mu^n e^{\beta\mu r_<} d\mu \qquad n \geqslant 0 \tag{5.14}$$

It is easily seen that the integrals $H_n(r_<, \beta)$ may be generated by means of the relation

$$H_n(r_<, \beta) = \frac{\partial^n}{\partial x^n} \left[\int_{-1}^{+1} e^{x\mu} d\mu \right] \tag{5.15}$$

where $x = \beta r_<$.

Substituting the appropriate exponential function into the integrand of (5.12) we obtain

$$\int \frac{1}{r_{12}} e^{i\underline{k}_f\cdot\underline{r}_{12}} e^{-\alpha r_>} \sum_l G_l(\beta, r_<) P_l(\mu)\, d\underline{r}_{12} \tag{5.16}$$

But

$$e^{i\underline{k}_f\cdot\underline{r}_{12}} = 4\pi \sum_{\lambda m} i^\lambda j_\lambda(k_f r_{12}) Y_{\lambda m}(\hat{\underline{k}}_f) Y^*_{\lambda m}(\hat{\underline{r}}_{12})$$

and

$$P_l(\mu) = \frac{4\pi}{(2l+1)} \sum_n Y_{ln}(\hat{\underline{r}}_{12}) Y^*_{ln}(\hat{\underline{r}}_1)$$

Hence by appropriate use of these two expansions in Spherical Harmonics we are able to evaluate the angular part of the integration appearing in (5.16). The resulting expression has the form

$$4\pi \sum_l i^l P_l(\hat{\underline{k}}_f\cdot\hat{\underline{r}}_1) \int_0^\infty j_l(k_f r_{12}) e^{-\alpha r_>} G_l(\beta, r_<)\, r_{12}\, dr_{12} \tag{5.17}$$

We shall now make the identification

$$\mathcal{M}_l(r_1) = \int_0^\infty j_l(k_f r) e^{-\alpha r_>} \bar{G}_l(\beta, r_<)\, r\, dr$$

which enables us to write (5.17) in the more compact form

$$4\pi \sum_l i^l P_l(\hat{\underline{k}}_f\cdot\hat{\underline{r}}_1) \mathcal{M}_l(r_1) \frac{(2l+1)}{2}$$

Using this result we are now able to return to the expression for J_{EX}, given by (5.11), and consider the remaining integration contained there

$$J_{EX} = \int e^{i(\underline{k}_0 - \underline{k}_f)\cdot\underline{r}_1} \psi^*_{\underline{k}_s}(\underline{r}_1) 4\pi \sum_l i^l P_l(\hat{\underline{k}}_f\cdot\hat{\underline{r}}_1) \mathcal{M}_l(r_1)\, d\underline{r}_1 \frac{(2l+1)}{2} \tag{5.18}$$

Since our interest is confined to ionizing collisions involving small momentum transfer (i.e. $\underline{k}_0 - \underline{k}_f$ small) then we shall take only a two term expansion for the exponential function

i.e. $$e^{i\underline{K}\cdot\underline{r}_1} \simeq j_0(Kr_1) + 3i j_1(Kr_1) P_1(\hat{\underline{K}}\cdot\hat{\underline{r}}_1)$$

where $$\underline{K} = \underline{k}_0 - \underline{k}_f$$

If we now substitute this truncated expansion into (5.18) we obtain

$$J_{EX} = K_1 + K_2 \tag{5.19}$$

where

$$K_1 = \int j_0(kr_1)\psi^*_{\underline{k}_s}(\underline{r}_1)4\pi\sum_l i^l P_l(\hat{\underline{k}}_f\cdot\hat{\underline{r}}_1)\mathcal{M}_l(r_1)\,d\underline{r}_1\left(\frac{2l+1}{2}\right) \tag{5.20}$$

and

$$K_2 = \frac{3i}{2}\int j_1(kr_1)P_1(\hat{\underline{k}}\cdot\hat{\underline{r}}_1)\psi^*_{\underline{k}_s}(\underline{r}_1)4\pi\sum_l i^l P_l(\hat{\underline{k}}_f\cdot\hat{\underline{r}}_1)\mathcal{M}_l(r_1)\,d\underline{r}_1\frac{(2l+1)}{2} \tag{5.21}$$

Let us consider the integral K_1, given by (5.20). If we replace the continuum function $\psi^*_{\underline{k}_s}(\underline{r}_1)$ by its series expansion

$$\psi^*_{\underline{k}_s}(\underline{r}_1) = \frac{1}{(2\pi)^{3/2}k_s^{1/2}}\sum_{\lambda\mu}4\pi(-i)^\lambda e^{-i\delta_\lambda}\frac{u_\lambda(k_s,r_1)}{r_1}Y_{\lambda\mu}(\hat{\underline{r}}_1)Y^*_{\lambda\mu}(\hat{\underline{k}}_s)$$

(where $\delta_l = \sigma_l + \eta_l$ the total phase shift associated with the l^{th} partial wave)

and use the spherical harmonic expansion appropriate to the Legendre polynomial of order l, then we are able to perform the angular part of the $\underline{r}_1$ integration. From this we obtain

$$K_1 = \left(\frac{2\pi}{k_s}\right)^{1/2} 2\sum_l e^{-i\delta_l}P_l(\hat{\underline{k}}_f\cdot\hat{\underline{k}}_s)\int_0^\infty r_1 j_0(kr_1)u_l(k_s,r_1)\mathcal{M}_l(r_1)\,dr_1(2l+1) \tag{5.22}$$

By making the same replacements in the expression for K_2, given by equation (5.21), and evaluating the $\hat{\underline{r}}_1$ integration we are led to the result

$$K_2 = \frac{(4\pi)^3}{(2\pi)^{3/2}k_s^{1/2}}\,i\sum_{\lambda\mu}(-i)^\lambda e^{-i\delta_\lambda}Y^*_{\lambda\mu}(\hat{\underline{k}}_s)\sum_{lm}i^l\,Y^*_{lm}(\hat{\underline{k}}_f)$$

$$\frac{4\pi}{2}\sum_{n=-1}^{+1}Y^*_{1n}(\hat{\underline{k}})\left\langle\begin{matrix}\lambda & l & 1\\ \mu & m & n\end{matrix}\right\rangle\int_0^\infty j_1(kr)\,r\,u_\lambda(k_s,r)\mathcal{M}_l(r)\,dr \tag{5.23}$$

where the indices λ, l, μ, m, n are subject to the following restraints

(i) $\mu+m+n=0$

(ii) $\lambda+l+1 =$ an even integer

(iii) the triangle inequality

In view of the fact that we are almost entirely concerned with collisions involving small momentum transfer it is reasonable to use the approximation consequent from considering $\hat{\underline{k}}$ and $\hat{\underline{k}}_f$ to be orthogonal unit vectors. For the sake of convenience we shall take $\hat{\underline{k}}_f$ as the polar axis for our co-ordinate system.

Let us now consider the summation over the indices μ and m appearing in (5.23)

$$\sum_{\mu}\sum_{m}\sum_{n=-1}^{+1}(-1)^{\lambda}(i)^{\lambda+l+1}Y^{*}_{\lambda\mu}(\hat{\underline{k}}_s)Y_{1n}(\hat{\underline{k}})Y^{*}_{lm}(\hat{\underline{k}}_f)\left\langle\begin{matrix}\lambda & l & 1\\ \mu & m & n\end{matrix}\right\rangle$$

If for the present we exclude the cases $l=0$ or $\lambda=0$, then since $Y^{*}_{lm}(\hat{\underline{k}}_f)\propto P_l^m(\hat{\underline{k}}_f\cdot\hat{\underline{k}}_f)$, it follows that for non-zero $Y^{*}_{lm}(\hat{\underline{k}}_f)$ we require $m=0$. Consequently condition (i) reduces to the equality

$$\mu+n=0$$

Hence the summation becomes

$$\sum_{n=-1}^{+1}(-1)^{\lambda}(i)^{\lambda+l+1}Y^{*}_{\lambda,-n}(\hat{\underline{k}}_s)Y^{*}_{1,n}(\hat{\underline{k}})Y^{*}_{l,0}(\hat{\underline{k}}_f)\left\langle\begin{matrix}\lambda & l & 1\\ -n & 0 & n\end{matrix}\right\rangle$$

$$= (-1)^{\lambda}\,(i)^{\lambda+l+1}Y^{*}_{l0}(\hat{\underline{k}}_f)\Big\{Y^{*}_{\lambda,1}(\hat{\underline{k}}_s)Y^{*}_{1,-1}(\hat{\underline{k}})\left\langle\begin{matrix}\lambda & l & 1\\ 1 & 0 & -1\end{matrix}\right\rangle$$

$$+\,Y^{*}_{\lambda,0}(\hat{\underline{k}}_s)Y^{*}_{1,0}(\hat{\underline{k}})\left\langle\begin{matrix}\lambda & l & 1\\ 0 & 0 & 0\end{matrix}\right\rangle$$

$$+\,Y^{*}_{\lambda,-1}(\hat{\underline{k}}_s)Y^{*}_{1,1}(\hat{\underline{k}})\left\langle\begin{matrix}\lambda & l & 1\\ -1 & 0 & 1\end{matrix}\right\rangle\Big\}$$

But

$$Y^{*}_{1,0}(\hat{\underline{k}})\propto P_1^0(\hat{\underline{k}}\cdot\hat{\underline{k}}_f)=\cos\tfrac{\pi}{2}=0$$

and also

$$\left\langle\begin{matrix}\lambda & l & 1\\ -1 & 0 & 1\end{matrix}\right\rangle=(-1)^{\lambda+l+1}\left\langle\begin{matrix}\lambda & l & 1\\ 1 & 0 & -1\end{matrix}\right\rangle$$

$$=\left\langle\begin{matrix}\lambda & l & 1\\ 1 & 0 & -1\end{matrix}\right\rangle$$

since condition (ii) requires that the sum $\lambda+l+1$ be equal to an even integer. Using these results the summation reduces to the form

$$(-1)^{\lambda}(i)^{\lambda+l+1}Y^{*}_{l,0}(\hat{\underline{k}}_f)\left\langle\begin{matrix}\lambda & l & 1\\ 1 & 0 & -1\end{matrix}\right\rangle\Big\{Y^{*}_{\lambda,1}(\hat{\underline{k}}_s)Y^{*}_{1,-1}(\hat{\underline{k}}) + Y^{*}_{\lambda,-1}(\hat{\underline{k}}_s)Y^{*}_{1,1}(\hat{\underline{k}})\Big\} \qquad (5.24)$$

Now $Y_{l,-m}(\hat{\underline{k}}) = (-1)^m Y^{*}_{l,m}(\hat{\underline{k}})$

Hence (5.24) may be rewritten as

$$(-1)^{\lambda+1}(i)^{\lambda+l+1}Y^{*}_{l,0}(\hat{\underline{k}}_f)\left\langle\begin{matrix}\lambda & l & 1\\ 1 & 0 & -1\end{matrix}\right\rangle\Big\{Y^{*}_{\lambda,1}(\hat{\underline{k}}_s)Y_{1,1}(\hat{\underline{k}}) + Y_{\lambda,1}(\hat{\underline{k}}_s)Y^{*}_{1,1}(\hat{\underline{k}})\Big\}$$

$$= (-1)^{\lambda+1}(i)^{\lambda+l+1}Y^{*}_{l,0}(\hat{\underline{k}}_f)\left\langle\begin{matrix}\lambda & l & 1\\ 1 & 0 & -1\end{matrix}\right\rangle 2\mathrm{Re}\Big\{Y^{*}_{\lambda,1}(\hat{\underline{k}}_s)Y_{1,1}(\hat{\underline{k}})\Big\} \qquad (5.25)$$

If we now write the spherical harmonics in terms of associated Legendré functions we obtain

$$(-1)^{\lambda+1}(i)^{\lambda+l+1}Y^{*}_{l,0}(\hat{\underline{k}}_f)\left\langle\begin{matrix}\lambda & l & 1\\ 1 & 0 & -1\end{matrix}\right\rangle 2\left[\frac{(2\lambda+1).3.(\lambda-1)!}{4\pi.4\pi.(\lambda+1)!2}\right]^{\frac{1}{2}} P^{1}_{\lambda}(\hat{\underline{k}}_s.\hat{\underline{k}}_f)P^{1}_{1}(\hat{\underline{k}}.\hat{\underline{k}}_f) \qquad (5.26)$$

But $P^{1}_{1}(0) = 1$

and

$$\left\langle\begin{matrix}\lambda & l & 1\\ 1 & 0 & -1\end{matrix}\right\rangle = \left[\frac{(2\lambda+1)(2l+1)3}{4\pi}\right]^{\frac{1}{2}}\begin{pmatrix}\lambda & l & 1\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}\lambda & l & 1\\ 1 & 0 & -1\end{pmatrix}$$

Substituting these results into (5.26) leads to the following expression

$$(-1)^{\lambda+1}(i)^{\lambda+l+1}\frac{2(2\lambda+1).3}{4\pi}\left[\frac{(\lambda-1)!(2l+1)}{(\lambda+1)!\,8\pi}\right]^{1/2}\begin{pmatrix}\lambda & l & 1\\ 0 & 0 & 0\end{pmatrix}$$

$$\begin{pmatrix}\lambda & l & 1\\ 1 & 0 & -1\end{pmatrix}Y^{*}_{l,0}(\hat{\underline{k}}_f)P'_{\lambda}(\hat{\underline{k}}_s\cdot\hat{\underline{k}}_f)$$

which we shall denote by the quantity $A_{\lambda l}$

Now

$$Y^{*}_{l,0}(\hat{\underline{k}}_f) = \left[\frac{2l+1}{4\pi}\right]^{1/2}P_l(\hat{\underline{k}}_f\cdot\hat{\underline{k}}_f) = \left[\frac{2l+1}{4\pi}\right]^{1/2}$$

Hence we obtain

$$A_{\lambda l} = (-1)^{\lambda+1}(i)^{\lambda+l+1}\frac{6(2\lambda+1)(2l+1)}{16\pi^2}\left[\frac{1}{2\lambda(\lambda+1)}\right]^{1/2}$$

$$\begin{pmatrix}\lambda & l & 1\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}\lambda & l & 1\\ 1 & 0 & -1\end{pmatrix}P'_{\lambda}(\hat{\underline{k}}_s\cdot\hat{\underline{k}}_f)$$

(5.26)

In order to proceed further we require to evaluate the Wigner 3-J symbols appearing in (5.26). From the conditions (ii) and (iii) ($|\lambda-1|\leqslant l\leqslant |l+1|$) it follows that for each value of $\lambda>0$ we have the two corresponding values of $l:\lambda-1,\lambda+1$. We are therefore concerned with the evaluation of the quantities

$$\begin{pmatrix}\lambda & l & 1\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}\lambda & l & 1\\ 1 & 0 & -1\end{pmatrix}_{l=\lambda-1,\lambda+1}$$

It is easily shown that

$$\begin{pmatrix}\lambda & \lambda-1 & 1\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}\lambda & \lambda-1 & 1\\ 1 & 0 & -1\end{pmatrix} = \frac{(-1)^{2\lambda-3}}{(2\lambda+1)(2\lambda-1)}\left[\frac{\lambda(\lambda+1)}{2}\right]^{\frac{1}{2}}$$

and

$$\begin{pmatrix}\lambda & \lambda+1 & 1\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}\lambda & \lambda+1 & 1\\ 1 & 0 & -1\end{pmatrix} = \frac{(-1)^{2\lambda-2}}{(2\lambda+1)(2\lambda+3)}\left[\frac{(\lambda+1)\lambda}{2}\right]^{1/2}$$

Using these results in conjunction with equation (5.26) we obtain

$$A_{\lambda,\lambda-1} = \frac{3}{16\pi^2}P'_{\lambda}(\hat{\underline{k}}_s\cdot\hat{\underline{k}}_f)$$

$$A_{\lambda,\lambda+1} = \frac{3}{16\pi^2}P'_{\lambda}(\hat{\underline{k}}_s\cdot\hat{\underline{k}}_f)$$

(5.27)

Hence the integral K_2 now takes the form

$$K_2 = \frac{(4\pi)^4}{2(2\pi)^{3/2}k_s^{1/2}} \sum_{\lambda \geqslant 1} e^{-i\delta_\lambda} \cdot \frac{3}{16\pi^2} P'_\lambda(\hat{\underline{k}}_s \cdot \hat{\underline{k}}_f)$$

$$\int_0^\infty j_1(kr)\, r\, u_\lambda(k_s, r)\left[\mathcal{M}_{\lambda-1}(r) + \mathcal{M}_{\lambda+1}(r)\right] dr$$

$$+ \quad \left[\text{term corresponding to } \lambda = 0\right]$$

Let us consider the contribution to the summation arising from the value $\lambda = 0$. For this case we must have $l = 1$. In addition $\mu = 0$, which implies $n = 0$ (since $\mu = -n$). Consequently the only combination of spherical harmonics possible is

$$Y^*_{0,0}(\hat{\underline{k}}_s)\, Y^*_{1,0}(\hat{\underline{k}})\, Y^*_{1,0}(\hat{\underline{k}}_f)$$

But

$$Y^*_{1,0}(\hat{\underline{k}}) \propto P_1(\hat{\underline{k}} \cdot \hat{\underline{k}}_f) = 0$$

Thus we obtain zero contribution corresponding to $\lambda = 0$, so giving the following form for K_2

$$K_2 = \frac{12\sqrt{2}\,\pi^{1/2}}{2k_s^{1/2}} \sum_{\lambda \geqslant 1} e^{-i\delta_\lambda} P'_\lambda(\hat{\underline{k}}_s \cdot \hat{\underline{k}}_f) \int_0^\infty j_1(kr)\, r\, u_\lambda(k_s, r)\left[\mathcal{M}_{\lambda-1}(r) + \mathcal{M}_{\lambda+1}(r)\right] dr \tag{5.28}$$

The quantities K_1 and K_2 may be evaluated by numerical integration according to Simpson's Rule, over a 1500 point partition of the range of the radial variable. The corresponding values of the functions $\mathcal{M}_l(r)$ required are generated by a numerical technique described elsewhere (see Appendix C).

We must now examine the remaining terms involved in the expression for the exchange amplitude. If we take due account of orthogonality by replacing the final state function $\overline{\Psi}_{\underline{k}_f, \underline{k}_s}$ by $\overline{\Psi}^{(b)}_{\underline{k}_f, \underline{k}_s} = (2\pi)^{-3/2} e^{i\underline{k}_f \cdot \underline{r}_2}\, \overline{\Psi}^{(b)}_{\underline{k}_s}$ in equation (5.1), then we need consider the terms

$$-\frac{1}{2\pi}e^{i\Delta(\underline{k}_f,\underline{k}_s)}\Big[\iiint e^{-i\underline{k}_f\cdot\underline{r}_2}\bar{\Psi}^{*}_{\underline{k}_s}(\underline{r}_1,\underline{r}_3)\left(-\frac{Z}{r_1}+\frac{1}{r_{13}}\right)e^{i\underline{k}_0\cdot\underline{r}_1}\bar{\Psi}_0(\underline{r}_2,\underline{r}_3)\,d\underline{r}_1d\underline{r}_2d\underline{r}_3$$

$$+A^{(b)*}\iiint e^{-i\underline{k}_f\cdot\underline{r}_2}e^{-\alpha(r_1+r_3)}\left(-\frac{Z}{r_1}+\frac{1}{r_{13}}+\frac{1}{r_{12}}\right)e^{i\underline{k}_0\cdot\underline{r}_1}\bar{\Psi}_0(\underline{r}_2,\underline{r}_3)\,d\underline{r}_1d\underline{r}_2d\underline{r}_3\Big] \quad (5.29)$$

Denoting the first integral of (5.29) by L_1, and performing the integration over the variable $\underline{r}_2$ we obtain

$$L_1=\frac{8\alpha^4}{(\alpha^2+k_f^2)^2}\iint\bar{\Psi}^{*}_{\underline{k}_s}(\underline{r}_1,\underline{r}_3)\left(-\frac{Z}{r_1}+\frac{1}{r_{13}}\right)e^{i\underline{k}_0\cdot\underline{r}_1}e^{-\alpha r_3}d\underline{r}_1d\underline{r}_3$$

But

$$\bar{\Psi}_{\underline{k}_s}(\underline{r}_1,\underline{r}_3)=\psi_{\underline{k}_s}(\underline{r}_1)\psi_{1s}(Z,\underline{r}_3)$$

where

$$\psi_{1s}(\underline{r}_3)=\frac{Z^{3/2}}{\pi^{1/2}}e^{-Zr_3}$$

Hence

$$L_1=\frac{8\alpha^4Z^{3/2}}{\pi^{1/2}(\alpha^2+k_f^2)^2}\iint\psi_{\underline{k}_s}(\underline{r}_1)e^{i\underline{k}_0\cdot\underline{r}_1}\left(-\frac{Z}{r_1}+\frac{1}{r_{13}}\right)e^{-(\alpha+Z)r_3}d\underline{r}_1d\underline{r}_3 \quad (5.30)$$

When performing the $\underline{r}_3$ integration there are two terms that we must consider. Firstly

$$\int e^{-(\alpha+Z)r_3}d\underline{r}_3=\frac{8\pi}{(\alpha+Z)^3}$$

and secondly

$$\int\frac{1}{r_{13}}e^{-(\alpha+Z)r_3}d\underline{r}_3=4\pi\int_0^\infty\frac{1}{r_>}e^{-(\alpha+Z)r_3}r_3^2dr_3$$

$$=4\pi\left\{\frac{2}{r_1\beta^3}-\frac{e^{-\beta r_1}}{\beta^2}\left[1+\frac{2}{r_1\beta}\right]\right\}$$

where

$$\beta=\alpha+Z$$

Applying these results to equation (5.30) we obtain

$$L_1 = \frac{32\pi^{1/2}\alpha^4 Z^{3/2}}{(\alpha^2+k_f^2)^2\beta^3}\int \psi^{S}_{\underline{k}_s}(\underline{r})\, e^{i\underline{k}_0\cdot\underline{r}}\left[\frac{2(1-Z)}{r} - e^{-\beta r}\left(\beta+\frac{2}{r}\right)\right]d\underline{r} \tag{5.31}$$

If we now replace $\psi^{S}_{\underline{k}_s}(\underline{r})$ by the corresponding expansion in spherical harmonics, and at the same time make a similar substitution for the exponential function, then we are able to evaluate the angular part of the integration in (5.31)

i.e.

$$L_1 = \frac{32\sqrt{2}\,\alpha^4 Z^{3/2}}{(\alpha^2+k_f^2)^2\beta^3 k_s^{1/2}}\sum (2l+1)\, e^{-i[\sigma_l+\eta_l]}\, P_l(\hat{\underline{k}}_s\cdot\hat{\underline{k}}_0)$$

$$\int_0^\infty r\, u_l(k_s,r)\, j_l(k_0 r)\left[\frac{2(1-Z)}{r} - e^{-\beta r}\left(\beta+\frac{2}{r}\right)\right]dr \tag{5.32}$$

The remaining radial integration appearing in (5.32) may be carried out numerically. Let us consider the second integral contained in (5.29)

$$\iiint e^{-i\underline{k}_f\cdot\underline{r}_2}\, e^{-\alpha(r_1+r_3)}\left(-\frac{Z}{r_1}+\frac{1}{r_{13}}+\frac{1}{r_{12}}\right)e^{i\underline{k}_0\cdot\underline{r}_1}\,\Psi^{S}_{0}(\underline{r}_2,\underline{r}_3)\, d\underline{r}_1 d\underline{r}_2 d\underline{r}_3$$

It is convenient to split this integral, which we shall denote by L_2, into two parts

$$L_2 = L_{2A} + L_{2B} \tag{5.33}$$

where

$$L_{2A} = \iiint e^{-i\underline{k}_f\cdot\underline{r}_2}\, e^{-\alpha(r_1+r_3)}\left(-\frac{Z}{r_1}+\frac{1}{r_{13}}\right)e^{i\underline{k}_0\cdot\underline{r}_1}\,\Psi^{S}_{0}(\underline{r}_2,\underline{r}_3)\, d\underline{r}_1 d\underline{r}_2 d\underline{r}_3 \tag{5.34}$$

and

$$L_{2B} = \iiint e^{-i\underline{k}_f\cdot\underline{r}_2}\, e^{-\alpha(r_1+r_3)}\left(\frac{1}{r_{12}}\right)e^{i\underline{k}_0\cdot\underline{r}_1}\,\Psi^{S}_{0}(\underline{r}_2,\underline{r}_3)\, d\underline{r}_1 d\underline{r}_2 d\underline{r}_3 \tag{5.35}$$

The integration over the variable $\underline{r}_2$ involved in the expression for L_{2A} is identical to that associated with L_1. Hence we are able to reduce L_{2A} to the form

$$L_{2A} = \frac{8\alpha^4}{(\alpha^2+k_f^2)^2}\iint e^{-\alpha(r_1+r_3)}\left(\frac{-z}{r_1}+\frac{1}{r_{13}}\right)e^{i\underline{k}_0\cdot\underline{r}_1}e^{-\alpha r_3}d\underline{r}_1\,d\underline{r}_3 \tag{5.36}$$

If we now examine the $\underline{r}_3$ integration we observe that there are two types of integral that need to be considered. Firstly

$$\int e^{-2\alpha r_3}d\underline{r}_3 = \frac{\pi}{\alpha^3}$$

and secondly

$$\int e^{-2\alpha r_3}\frac{1}{r_{13}}\,d\underline{r}_3 = 4\pi\left\{\frac{2}{r_1\gamma^3} - \frac{e^{-\gamma r_1}}{\gamma^3}\left[\gamma+\frac{2}{r_1}\right]\right\}$$

where

$$\gamma = 2\alpha$$

i.e.

$$\int e^{-2\alpha r_3}\frac{1}{r_{13}}\,d\underline{r}_3 = \frac{\pi}{\alpha^3}\left\{\frac{1}{r_1} - e^{-2\alpha r_1}\left[\alpha+\frac{1}{r_1}\right]\right\}$$

Combining these results with (5.36) we obtain

$$L_{2A} = \frac{8\alpha\pi}{(\alpha^2+k_f^2)^2}\int e^{-\alpha r_1}e^{i\underline{k}_0\cdot\underline{r}_1}\left(\frac{(1-z)}{r_1} - e^{-2\alpha r_1}\left[\alpha+\frac{1}{r_1}\right]\right)d\underline{r}_1$$

The angular integration appearing in this expression may be evaluated directly, yielding the result

$$L_{2A} = \frac{32\alpha\pi^2}{(\alpha^2+k_f^2)^2}\int r^2 j_0(k_0 r)\left(\frac{(1-z)e^{-\alpha r}}{r} - e^{-3\alpha r}\left[\alpha+\frac{1}{r}\right]\right)dr$$

which when integrated reduces to the form

$$L_{2A} = \frac{32\alpha\pi^2}{(\alpha^2+k_f^2)^2}\left\{\frac{(1-z)}{(\alpha^2+k_0^2)} - \frac{6\alpha^2}{(9\alpha^2+k_0^2)^2} - \frac{1}{(9\alpha^2+k_0^2)}\right\}$$

$$= \frac{32\alpha\pi^2}{(\alpha^2+k_f^2)^2}\left[\frac{(1-z)}{(\alpha^2+k_0^2)} - \frac{(15\alpha^2+k_0^2)}{(9\alpha^2+k_0^2)^2}\right] \tag{5.37}$$

It now remains to evaluate the expression for L_{2B} given by equation (5.35). The integration over $\underline{r}_3$ may be performed to produce the following result

$$L_{2B} = \iint e^{-i\underline{k}_f\cdot\underline{r}_2} e^{-\alpha r_1} \left(\frac{1}{r_{12}}\right) e^{i\underline{k}_0\cdot\underline{r}_1} e^{-\alpha r_2} d\underline{r}_1 d\underline{r}_2$$

Let us consider the $\underline{r}_2$ integration involved in the previous expression. This takes the form

$$\int e^{-i\underline{k}_f\cdot\underline{r}_2} \frac{1}{r_{12}} e^{-\alpha r_2} d\underline{r}_2$$

By expressing the oscillatory exponential term and the inverse of the inter-electron separation as expansions in spherical harmonics we are able to evaluate the angular part of the integration. Hence we obtain

$$4\pi \sum_l P_l(\hat{\underline{k}}_f\cdot\hat{\underline{r}}_1)(-i)^l \int_0^\infty e^{-\alpha r_2} r_2^2 \gamma_l(r_2, r_1) j_l(k_f r_2) dr_2 \qquad (5.38)$$

where $\gamma_l(r_2, r_1) = \frac{r_<^l}{r_>^{l+1}}$; $r_>$, $r_<$ being the greater and lesser of r_2 and r_1 , respectively.

This may be written in terms of the function v_l defined by equation (3.59)

$$4\pi \sum_l (-i)^l P_l(\hat{\underline{k}}_f\cdot\hat{\underline{r}}_1) v_l(r_1, k_f, \alpha) \qquad (5.39)$$

The expression for L_{2B} may now be reduced to the form

$$L_{2B} = 4\pi \int e^{i\underline{k}_0\cdot\underline{r}_1} e^{-\alpha r_1} \sum_l (-i)^l P_l(\hat{\underline{k}}_f\cdot\hat{\underline{r}}_1) v_l(r_1, k_f, \alpha) d\underline{r}$$

If we once again replace the exponential term by the corresponding expansion in spherical harmonics this enables us to perform the angular integration with the result

$$L_{2B} = 16\pi^2 \sum_l P_l(\hat{\underline{k}}_0\cdot\hat{\underline{k}}_f) \int_0^\infty r^2 e^{-\alpha r} j_l(k_0 r) v_l(r, k_f, \alpha) dr \qquad (5.40)$$

The integrals involved in (5.40) are evaluated by means of standard numerical integration techniques.

Before presenting results of calculations based on the analysis described in this section we shall pause in order to mention a point concerning the convergence of the numerical integrations performed. With one exception it has been found that all the integrals computed have converged well within the range of integration used. This is of course to be expected, being a consequence of the presence of the negative exponential function appearing in most of the integrands. The exception is provided by the integrals contained in (5.32). We observe that one of the terms constituting the integrand of each integral does not involve an exponential factor, and it is this term that shows some reluctance to converge. In fact it was found necessary to make an appreciable extension of the range of integratio in this case, replacing the numerical function u_l by its limiting analytic form in the asymptotic region.

5.1.1 Results

We have made calculations of the exchange amplitude based on the approximation described in this section. These calculations were restricted to two cases which were considered representative for the energy regions associated with our investigations. In tables 1 and 2 we show a comparison between these values of the exchange amplitude and the corresponding values calculated from the Peterkop form of the amplitude. It is clear from this comparison that there is considerable discrepancy between the two sets of results. The results indicate that the Peterkop approximation may, in general, underestimate the magnitude of the exchange amplitude. If we introduce the probability associated with the exchange process, defined by

$$P_{EXCH} = \frac{2k_f k_s}{k_0} \left| g(\underline{k}_f, \underline{k}_s) \right|^2 .$$

then we can use the corresponding probability distributions to demonstrate the essential differences between the predictions of the two approximations examined. Figures 1 to 3 show the probability distributions for the cases considered. It is apparent that the differences between the predictions of the two forms of the amplitude are not merely quantitative but are qualitative as well. Although it is possible that the approximations used in the evaluation of the exchange amplitude defined by (5.1) may partially account for the quantitative differences between the two sets of results, it is unlikely that these would significantly modify the characteristic behaviour of the amplitude. For the approximate form of the amplitude described in this section P_{EXCH} is characterized by a three lobed distribution with approximate symmetry about the direction of the "fast" outgoing electron. The distribution corresponding to the Peterkop approximation shows a much simpler structure which is almost entirely at variance with that previously described. However the angular position of the maximum of this distribution does roughly coincide with that of one of the three maxima of the other distribution.

5.1.2 Conclusions

The calculations of the exchange amplitude described here indicate that the Peterkop approximation fails to provide an accurate description of the exchange process for first Born calculations. This failure is two-fold. Firstly the approximation tends to underestimate the magnitude of the amplitude. Secondly the behaviour of the amplitude as predicted by the Peterkop approximation bears little resemblance to that predicted by the alternative approximation based on the exact form of the amplitude.

CASE: $E_0 = 256.5\,eV$ $E_f = 230.5\,eV$ $\theta_f = 4°$

	PETERKOP FORM OF THE EXCHANGE AMPLITUDE		THE FORM OF THE AMPLITUDE DESCRIBED IN THIS SECTION*	
ANGLE θ_s	$\mathcal{R}.g(\underline{k}_f, \underline{k}_s)$	$\mathcal{I}.g(\underline{k}_f, \underline{k}_s)$	$\mathcal{R}.g(\underline{k}_f, \underline{k}_s)$	$\mathcal{I}.g(\underline{k}_f, \underline{k}_s)$
15°	0.181(-1)	0.324(-2)	-0.165(-1)	0.282(-1)
30°	0.160(-1)	0.292(-2)	-0.156(-1)	0.344(-1)
45°	0.139(-1)	0.244(-2)	-0.131(-1)	0.356(-1)
60°	0.120(-1)	0.185(-2)	-0.101(-1)	0.324(-1)
75°	0.105(-1)	0.119(-2)	-0.705(-2)	0.275(-1)
90°	0.936(-2)	0.526(-3)	-0.432(-2)	0.220(-1)
105°	0.859(-2)	-0.929(-4)	-0.250(-2)	0.148(-1)
120°	0.815(-2)	-0.625(-3)	-0.164(-2)	0.571(-2)
135°	0.801(-2)	-0.105(-2)	-0.832(-3)	-0.290(-2)
150°	0.815(-2)	-0.136(-2)	0.632(-3)	-0.870(-2)
165°	0.855(-2)	-0.155(-2)	0.191(-2)	-0.122(-1)
180°	0.922(-2)	-0.164(-2)	0.139(-2)	-0.163(-1)
195°	0.101(-1)	-0.162(-2)	0.179(-2)	-0.141(-1)
210°	0.113(-1)	-0.148(-2)	0.130(-2)	-0.109(-1)
225°	0.128(-1)	-0.121(-2)	-0.128(-3)	-0.678(-2)
240°	0.144(-1)	-0.787(-3)	-0.124(-2)	0.628(-3)
255°	0.162(-1)	-0.216(-3)	-0.202(-2)	0.986(-2)
270°	-	-	-0.324(-2)	0.178(-1)
285°	0.197(-1)	0.123(-2)	-0.535(-2)	0.296(-1)
300°	0.211(-1)	0.197(-2)	-0.813(-2)	0.296(-1)
315°	0.219(-1)	0.260(-2)	-0.113(-1)	0.344(-1)
330°	0.220(-1)	0.307(-2)	-0.144(-1)	0.351(-1)
345°	0.213(-1)	0.333(-2)	-0.166(-1)	0.307(-1)
360°	-	-	-	-

TABLE 5.1

VARIATION OF THE EXCHANGE AMPLITUDE WITH SCATTERING ANGLE θ_s

IT SHOULD BE NOTED THAT THE TABULATED VALUES IN THE TABLES 5.1 AND 5.2 DIFFER FROM THE ACTUAL VALUES OF THE AMPLITUDE BY A MULTIPLICATIVE CONSTANT $\frac{Z^{3/2}}{\pi}$

* THESE CALCULATIONS CORRESPOND TO THE VALUE A = 1 (SEE EQ. 5.12 ONWARDS)

CASE: $E_0 = 256.5eV$ $E_f = 230.5eV$ $\theta_f = 7^\circ$

	PETERKOP FORM OF THE EXCHANGE AMPLITUDE		THE FORM OF THE AMPLITUDE DESCRIBED IN THIS SECTION*	
ANGLE θ_s	$\mathcal{R}.g(\underline{k}_f, \underline{k}_s)$	$\mathcal{I}.g(\underline{k}_f, \underline{k}_s)$	$\mathcal{R}.g(\underline{k}_f, \underline{k}_s)$	$\mathcal{I}.g(\underline{k}_f, \underline{k}_s)$
15°	0.147(-1)	0.380(-2)	-0.134(-1)	0.159(-1)
30°	0.109(-1)	0.344(-2)	-0.131(-1)	0.211(-1)
45°	0.813(-2)	0.292(-2)	-0.116(-1)	0.226(-1)
60°	0.627(-2)	0.225(-2)	-0.986(-2)	0.209(-1)
75°	0.514(-2)	0.147(-2)	-0.803(-2)	0.182(-1)
90°	0.451(-2)	0.679(-3)	-0.618(-2)	0.152(-1)
105°	0.423(-2)	-0.493(-4)	-0.477(-2)	0.109(-1)
120°	0.421(-2)	-0.655(-3)	-0.411(-2)	0.520(-2)
135°	0.443(-2)	-0.112(-2)	-0.366(-2)	-0.466(-3)
150°	0.492(-2)	-0.146(-2)	-0.271(-2)	-0.450(-2)
165°	0.571(-2)	-0.169(-2)	-0.164(-2)	-0.698(-2)
180°	0.689(-2)	-0.181(-2)	-0.166(-2)	-0.946(-2)
195°	0.857(-2)	-0.182(-2)	-0.178(-2)	-0.921(-2)
210°	0.109(-1)	-0.171(-2)	-0.196(-2)	-0.705(-2)
225°	0.141(-1)	-0.145(-2)	-0.285(-2)	-0.493(-2)
240°	0.184(-1)	-0.979(-3)	-0.364(-2)	-0.625(-3)
255°	0.237(-1)	-0.280(-3)	-0.420(-2)	0.528(-2)
270°	0.295(-1)	0.630(-3)	-0.493(-2)	0.103(-1)
285°	0.345(-1)	0.165(-2)	-0.607(-2)	0.140(-1)
300°	0.367(-1)	0.261(-2)	-0.761(-2)	0.177(-1)
315°	0.354(-1)	0.335(-2)	-0.954(-2)	0.212(-1)
330°	0.310(-1)	0.382(-2)	-0.117(-1)	0.219(-1)
345°	0.252(-1)	0.402(-2)	-0.135(-1)	0.187(-1)
360°	0.195(-1)	0.400(-2)	-	-

TABLE 5.2

VARIATION OF THE EXCHANGE AMPLITUDE WITH SCATTERING ANGLE θ_s

* THESE CALCULATIONS CORRESPOND TO THE VALUE A = 1 (SEE EQ. 5.12 ONWARDS)

Peterkop exchange

THE EXCHANGE PROBABILITY
(CALCULATED FROM THE PETERKOP FORM OF THE EXCHANGE AMPLITUDE)

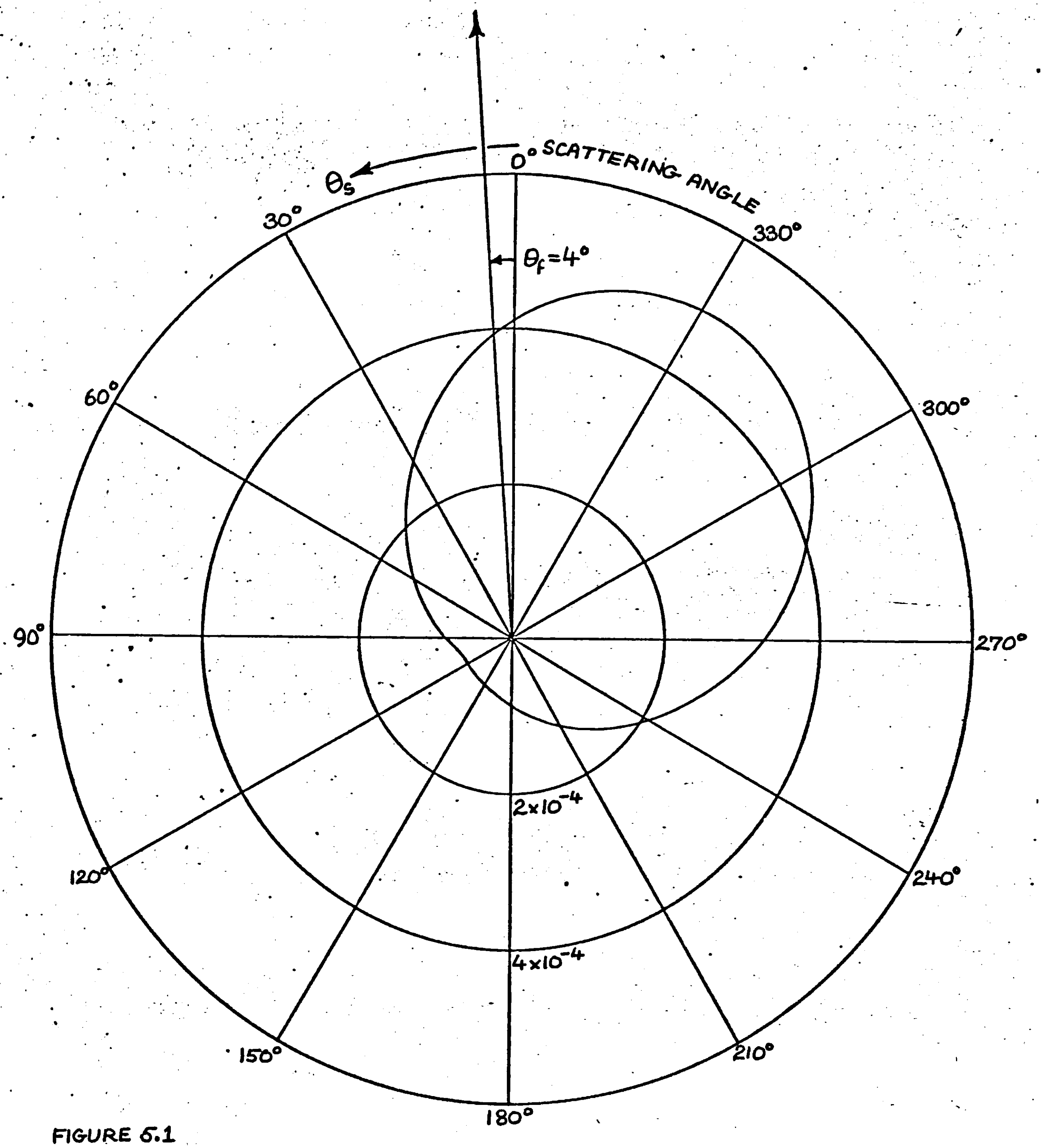


FIGURE 6.1

CASE: $E_o = 256{\cdot}5\,eV$
$E_f = 230{\cdot}5\,eV$
$\theta_f = 4°$

THE VALUES SHOWN HERE DIFFER FROM THE ACTUAL VALUES OF THE EXCHANGE PROBABILITY BY A MULTIPLICATIVE CONSTANT (THEY REQUIRE MULTIPLICATION BY $\frac{2k_f k_s}{k_o}\frac{Z^8}{\pi^2}$)

4°

THE EXCHANGE PROBABILITY

(CALCULATED FROM THE APPROPRIATE EXPRESSION BASED ON THE APPROXIMATE FORM OF THE EXCHANGE AMPLITUDE DESCRIBED IN §5.1)

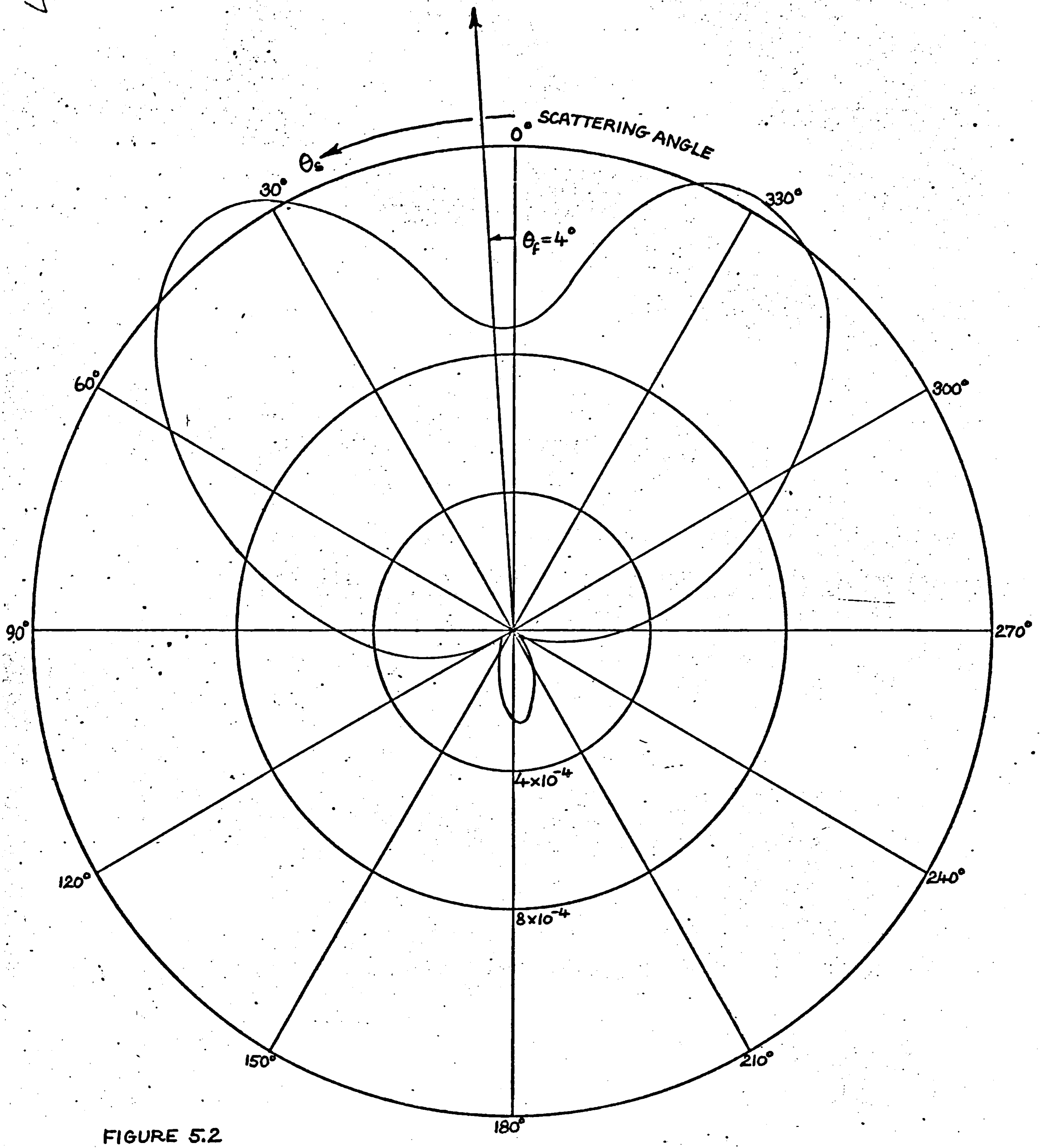


FIGURE 5.2

CASE: $E_0 = 256{\cdot}5\,\text{eV}$

$E_f = 230{\cdot}5\,\text{eV}$

$\theta_f = 4°$

THE VALUES SHOWN HERE DIFFER FROM THE ACTUAL VALUES OF THE EXCHANGE PROBABILITY BY A MULTIPLICATIVE CONSTANT (THEY REQUIRE MULTIPLICATION BY $\frac{2k_f k_s}{k_0} . \frac{Z^3}{\pi^2}$).

THE EXCHANGE PROBABILITY

(CALCULATED FROM THE APPROXIMATE FORM OF THE EXCHANGE AMPLITUDE DESCRIBED IN §5.1)

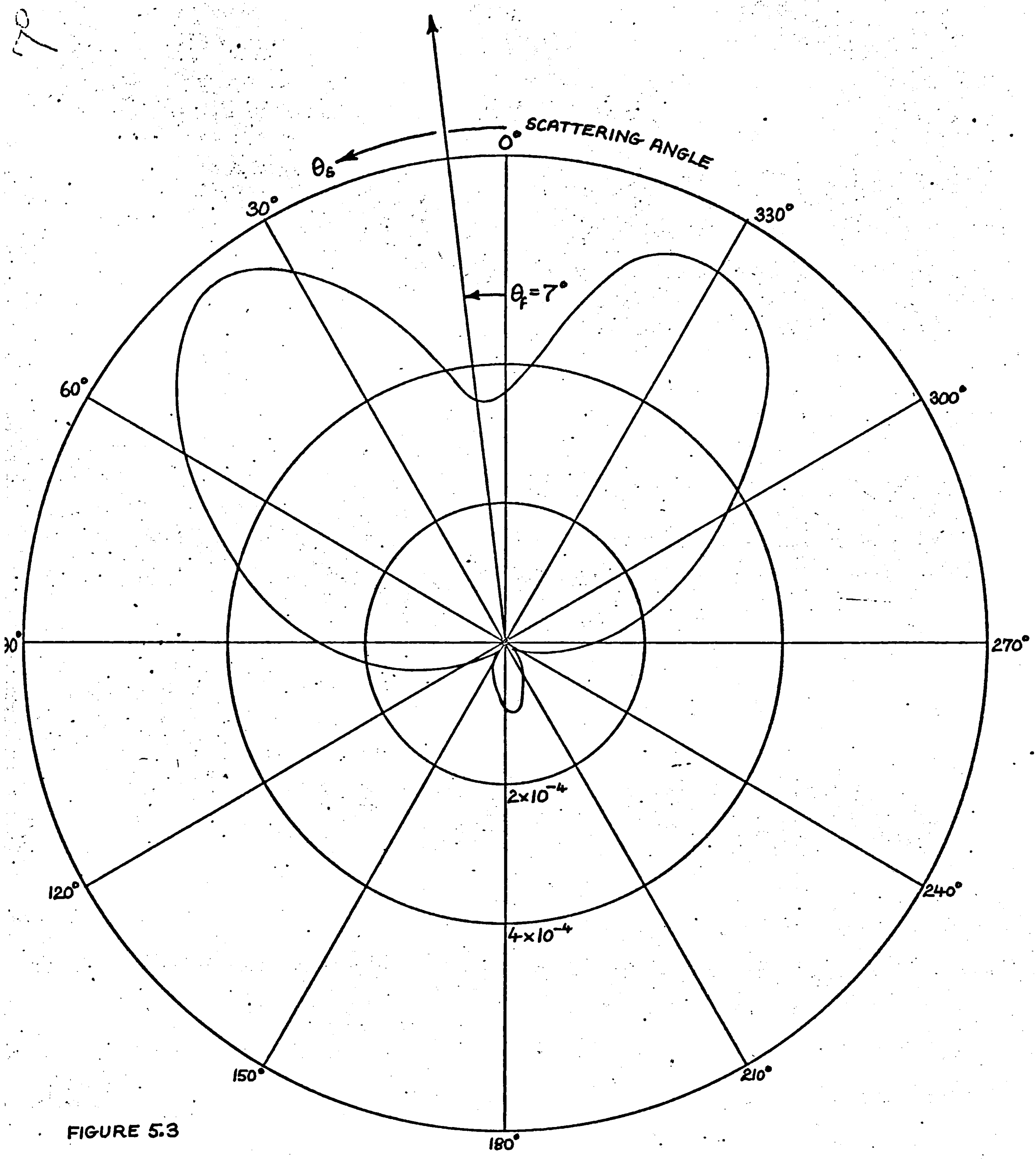


FIGURE 5.3

CASE: $E_0 = 256{\cdot}5\,\text{eV}$
$E_f = 230{\cdot}5\,\text{eV}$
$\theta_f = 7°$

THE VALUES SHOWN HERE DIFFER FROM THE ACTUAL VALUES OF THE EXCHANGE PROBABILITY BY A MULTIPLICATIVE CONSTANT (THEY REQUIRE MULTIPLICATION BY $\frac{2k_f k_s}{k_0} . \frac{Z^3}{\pi^2}$).

5.2. A rational approximation to the triple differential cross-section

Clearly even if both capture and exchange are excluded in our mathematical models describing the ionization process the expression for the triple differential cross section is still sufficiently complex to make the further integrations required for the other differential cross sections and ultimately the total cross section, extremely lengthy and involved. It was with this in mind that we attempted to construct a rational function capable of reproducing the triple differential cross section as calculated from the expressions contained in the previous chapters.

As with all curve fitting the success of the method is not measured merely by how faithfully the approximate function reproduces the original data but more importantly by the number of parameters required in the approximate form to reproduce the data to the desired degree of accuracy. It is for this reason that we have used a rational function, which is capable of exhibiting widely varying behaviour with the inclusion of a few terms only, rather than a polynomial.

The method that we have applied is the usual least squares fit by which the parameters of the approximate function are chosen to minimize the sum of the squares of the differences between the original and regenerated data. The minimization procedure is performed by means of the program VOA4A (Powell 1964). However before the minimization can proceed we need starting values for the parameters, and, if the procedure is to function efficiently, values that are not too far removed from the optimum. We shall now describe the method used to estimate these starting values.

So far we have made no suggestion as to a suitable variable on which to base the expansion corresponding to the approximate function. However since the techniques outlined in the following are of a general nature we shall leave the choice of variable until a later stage in the discussion. For the present let us simply represent this variable by x. From our knowledge of the functional form of the triple differential cross section, provided by the analysis of Chapters 3 and 4, we may ascribe to it the following form

$$\frac{d^3\sigma}{d\hat{\underline{k}}_f\, d\hat{\underline{k}}_s\, dE} = \frac{1}{K^4} F(x) \tag{5.41}$$

where K denotes the magnitude of the momentum transfer and all other quantities have their usual meaning. In (5.41) $F(x)$ represents the rational function that we wish to construct. As we have seen from the results of earlier analysis, the triple differential cross section is characterized by an appreciable maximum in the forward direction. The removal of the K^{-4} factor from the TDC obviously modifes this behaviour. However a well defined maximum is found to still exist in the same region as the original maximum. Since this is perhaps the most significant feature of the curve which we wish to reproduce we shall use this maximum as a starting point. Now the simplest rational approximation to the curve in the region of the maximum is provided by the Breit-Wigner resonance form

$$F(x) = \frac{\frac{1}{4}\Gamma^2 F_0}{\frac{1}{4}\Gamma^2 + (x-x_0)^2} \tag{5.42}$$

where $\Gamma/2$ denotes the half width of the maximum, F_0 the maximum value of the curve and x_0 the value of x at which this occurs. We can elaborate upon this form by including additional terms in numerator and denominator for which the associated parameters are initially set to zero when starting the minimization proceedure. By this method we construct our rational function. Hence the necessary starting values for the parameters are obtained in terms of the quantities Γ, F_0 and x_0. We now require a simple automatic way of extracting these quantities from the TDC data. In order to do this we first fit a simple polynomial to the modified triple-differential cross section curve (the curve approximated by $F(x)$ in (5.42)) in the region of the maximum. For this purpose we have chosen to use the cubic

$$f(x) = a_0x^3 + a_1x^2 + a_2x + a_3 \tag{5.43}$$

the parameters $\{a_i,\ i = 0,3\}$ being determined by fitting the function to four data points in the region of the maximum, these points being equally distributed on each side of the maximum.

We are now able to locate the maximum by examining the turning points of the function $f(x)$. These correspond to the solutions of the equation

$$\frac{df}{dx} = 3a_0x^2 + 2a_1x + a_2 = 0$$

i.e. $$x = \frac{-a_1 \pm (a_1^2 - 3a_0a_2)^{1/2}}{3a_0} \tag{5.44}$$

By evaluating the second derivative for each case we are able to determine which solution corresponds to the maximum.

i.e. $$\frac{d^2f}{dx^2} = 6a_0x + 2a_1 < 0\ , \quad \text{for the maximum} \tag{5.45}$$

We shall denote the appropriate value of x by x_0. Then substituting in (5.43) we obtain the maximum value of the curve, denoted by F_0 in equation (5.42)

$$F_0 = f(x_0) = a_0x_0^3 + a_1x_0^2 + a_2x_0 + a_3 \tag{5.46}$$

Finally we need to estimate the half-width of the curve at the maximum. This is defined to be the half-width of the curve at half its maximum value. Hence the half width is given by half the difference between the two real solutions of the equation

$$a_0x^3 + a_1x^2 + a_2x + a_3 = \tfrac{1}{2}F_0$$

i.e. $$a_0x^3 + a_1x^2 + a_2x + A_3 = 0 \tag{5.47}$$

with $A_3 = a_3 - \frac{1}{2}F_0$

Provided that we have reasonable estimates for the roots of this equation we can rapidly improve them by means of the following iterative method. If α is an approximation to a root α_0 then we may write $\alpha_0 = \alpha + \epsilon$, where ϵ is a small correction. Then substituting into the equation (5.47) and ignoring terms of order ϵ^2 (and higher powers) we obtain

$$a_0(\alpha^3 + 3\alpha^2\epsilon) + a_1(\alpha^2 + 2\alpha\epsilon) + a_2\alpha + a_2\epsilon + A_3 = 0$$

Hence $$\epsilon = -\frac{(a_0\alpha^3 + a_1\alpha^2 + a_2\alpha + A_3)}{(3a_0\alpha^2 + 2a_1\alpha + a_2)} \tag{5.48}$$

Using the quantity $\alpha + \epsilon$ as a new improved estimate we continue the proceedure until successive estimates converge within some specified limits. Initial estimates for the roots can be obtained quite simply. Let $\{x = z_i\ ,\ i = 1,4\}$ correspond to the four data points used to fit the cubic. We wish to estimate the points of intersection of the cubic with the line $y = \frac{1}{2}F_0$. If we assume that the slope of the curve is almost linear in these regions then we can obtain a reasonable first approximation for the points of intersection $\{(\omega_i, \frac{1}{2}F_0), i = 1,2\}$ by linear extrapolation

i.e. $$\frac{f(z_1) - f(\omega_1)}{z_1 - \omega_1} \simeq f'(z_1)$$

where $f'(z_1) = \dfrac{df(z_1)}{dx}$

But

$$f(\omega_1) = \tfrac{1}{2}F_0$$

Then $$\omega_1 \simeq z_1 - \frac{(f(z_1) - \frac{1}{2}F_0)}{f'(z_1)}$$

and similarly

$$\omega_2 \simeq z_4 - \frac{(f(z_4) - \frac{1}{2}F_0)}{f'(z_4)} \tag{5.49}$$

From these we obtain a first estimate for the halfwidth

$$\frac{1}{2}\Gamma = \frac{\omega_2 - \omega_1}{2} \tag{5.50}$$

With this information we are able to provide the starting values required for the curve fitting proceedure based on the form (5.42). As a test of the consistency of the method used we can derive a simple relation between the quantities extracted from the TDC data. Consider the Breit-Wigner form (5.42). This has half its maximum value when

$$\frac{1}{2}F_0 = \frac{\frac{1}{4}\Gamma^2 F_0}{\frac{1}{4}\Gamma^2 + (x - x_0)^2} \tag{5.51}$$

so

$$(x - x_0)^2 = 1/4\,\Gamma^2$$

Since $x = \omega_1$ or ω_2 when the function $F(x)$ takes half its maximum value, then we obtain

$$\Gamma = \omega_2 - \omega_1$$

and $$2x_0 = \omega_1 + \omega_2 \tag{5.52}$$

The second of these relations provides a useful check on our approach, as previously mentioned.

With regard to the form of the variable x several choices have been tried, with varying degrees of success. We shall give an account of two of these. Initially it was hoped to extract the total angular dependence of the TDC by constructing a composite variable containing the dependence on both outgoing electron scattering angles. If we examine the form of the TDC obtained from the plane-plane approximation (Appendix B) we find that in addition to the momentum transfer there is another angle dependent quantity, namely $K' = |\underline{K} - \underline{k}_s|$, the magnitude of the recoil momentum imparted to the residual ion. Here we have a quantity depending upon the scattering angles of both outgoing electrons, so seeming to provide the type of composite variable required for our calculations. However subsequent calculations based on a function of the form given by (5.42), with K' replacing the variable x, produced unsatisfactory results. The postulated curve could only be made to fit the data by the addition of an unacceptably large number of terms to the numerator and denominator of (5.42). Since minor modifications achieved no appreciable improvement it was clear that K' was an unsuitable choice of variable and it was consequently discarded.

Since our attempts to construct a composite variable containing the dependence on both scattering angles were unproductive it was subsequently decided to treat each dependence separately. Our investigation then centred on the form of a suitable variable for the θ_f dependence. An appropriate choice was found to be that given by $x = \sin\theta_f$. In the following we describe results obtained from this choice of variable.

The function $F(x)$ defined by equation (5.42) is taken to have the parametric form

$$F(x) = \frac{C_0 + C_1 x + C_2 x^2}{C_3 + C_4 x + C_5 x^2 + C_6 x^3 + C_7 x^4} \qquad (5.53)$$

where $C_0 = \frac{1}{4}\Gamma^2 F_0$ and $C_i\ ,\ i = 1, 7$ are parameters to be determined by the minimization proceedure.

Let F_D denote values of the function F extracted from the triple differential cross section data and F_R the corresponding values obtained from the rational form (5.53). The quantity that we have chosen to minimize is given by

$$S = \sum_{i=1}^{N_D} \left[\frac{F_D - F_R}{F_D \times 10^{-2}} \right]_i^2 \tag{5.54}$$

where N_D denotes the number of data points used.
If N_p indicates the number of parameters included in the rational form of F then a measure of the accuracy of the fitted curve is provided by the quantity

$$\chi = \left[\frac{S}{N_D - N_P} \right]^{1/2}$$

We now present results for two cases. Both correspond to the energies $E_0 = 200\,eV$, $E_f = 164.5\,eV$, the first case having the scattering angle of the slow electron fixed at 30°, the second at 45°. In each case we show the minimum value of χ obtained and the corresponding values of the parameters.

Case 1

$\theta_s = 30°$

$\chi = 0.85$

$x_0 = 0.016$ $x_1 = -0.223$ $x_2 = 0.932$ $x_3 = 0.373$

$x_4 = 0.384$ $x_5 = 0.279\text{x}10$ $x_6 = 0.719\text{x}10$ $x_7 = 0.189\text{x}10$

Case 2

$\theta_s = 45°$

$\chi = 0.35$

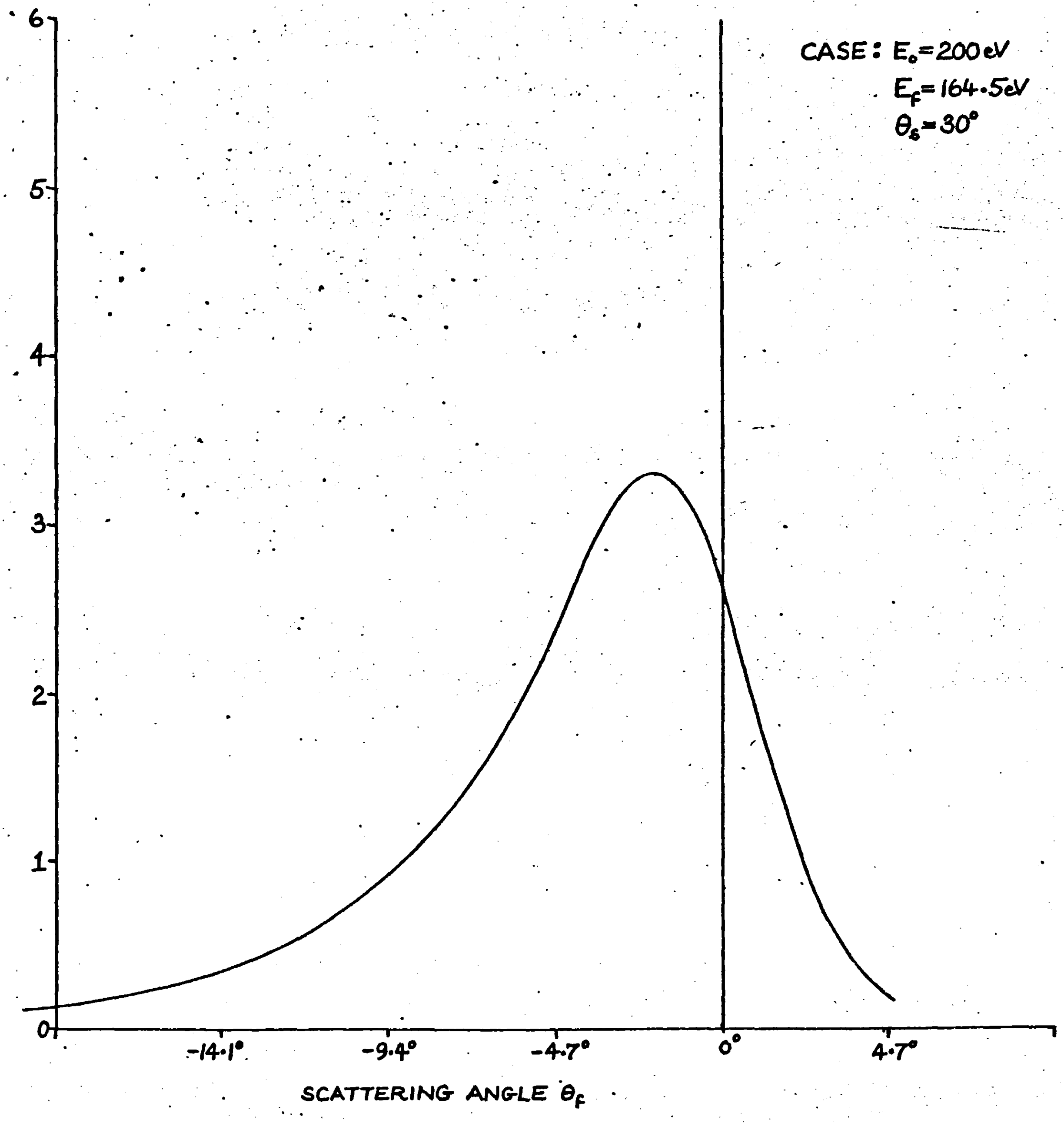
$x_0 = 0.021$ $x_1 = -0.472$ $x_2 = 0.295\text{x}10$ $x_3 = 0.856$

$x_4 = 0.278\text{x}10$ $x_5 = 0.112\text{x}10$ $x_6 = 0.252\text{x}10$ $x_7 = 0.433\text{x}10$

An inspection of the quantity χ for each case indicates that the fitted curve will reproduce the original data to within an error of 1% or less. Clearly then the type of rational function constructed

FIGURE 5.4 VARIATION OF THE TRIPLE DIFFERENTIAL CROSS SECTION WITH SCATTERING ANGLE θ_f.

(THE VALUES SHOWN HERE ARE CALCULATED FROM THE MODEL DESCRIBED IN CHAPTER 3, USING AN ORTHOGONALIZED FINAL STATE WAVE FUNCTION. EXCHANGE AND CAPTURE ARE EXCLUDED. THE θ_f DEPENDENCE OF THE TDC, ILLUSTRATED BELOW, IS THE SUBJECT OF THE CURVE FITTING PROCEEDURE OF §5.2)



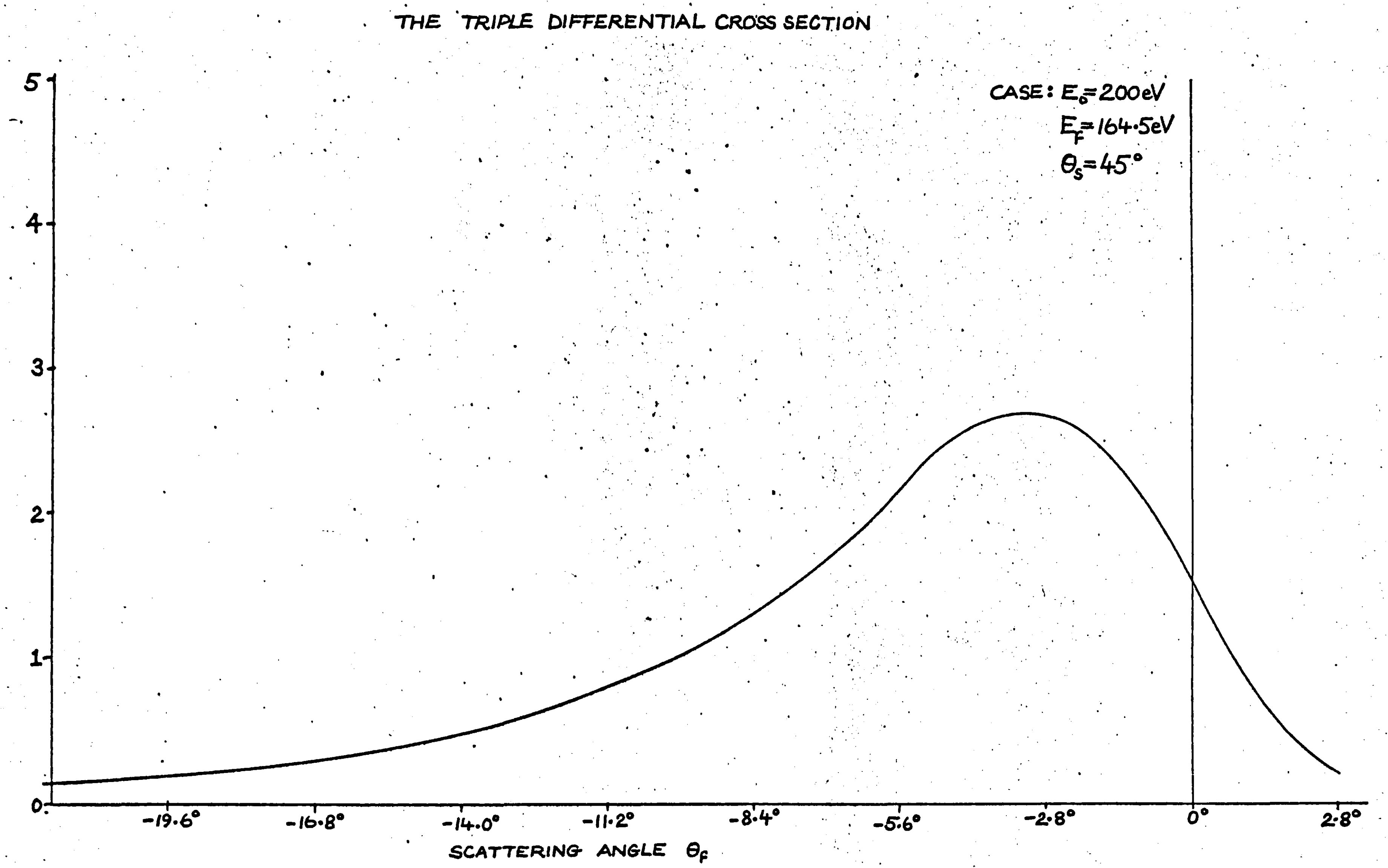


FIGURE 5.5

VARIATION OF THE TRIPLE DIFFERENTIAL CROSS SECTION WITH SCATTERING ANGLE θ_F

(THE VALUES SHOWN HERE ARE CALCULATED FROM THE MODEL DESCRIBED IN CHAPTER 3, USING AN ORTHOGONALIZED FINAL STATE WAVE FUNCTION. EXCHANGE AND CAPTURE ARE EXCLUDED. THE θ_F DEPENDENCE OF THE TDC, ILLUSTRATED ABOVE, IS THE SUBJECT OF THE CURVE FITTING PROCEEDURE OF §5.2) will provide a good representation of the differential cross section. However, since it is not clear how the parameters depend on the angle θ_s , this approach is at present of limited use.

5.3. An analysis of the shape of the double differential cross-section

In this section we shall examine the shape of the double differential cross section (dependent on energy and slow electron scattering angle) as predicted by the mathematical model of chapter 4. If we neglect the effects of capture and exchange the only contribution to the triple differential cross section arises from the direct amplitude which is, to within an arbitrary phase factor, given by

$$f(\underline{k}_f,\underline{k}_s) = -\frac{2}{K^2}\sum_{m=2}^{3}\int \Psi_0(\underline{r}_2,\underline{r}_3)\, e^{i\underline{K}\cdot\underline{r}_m}\, \Psi_{\underline{k}_s}^{N*}(\underline{r}_2,\underline{r}_3)\, d\underline{r}_2\, d\underline{r}_3 \tag{5.55}$$

where $\Psi_0(\underline{r}_2,\underline{r}_3)$ represents the target ground state and $\Psi_{\underline{k}_s}^{N}$ is a suitably normalized wave function representing the final state of excitation. The quantity $\underline{K}$ is the momentum transfer, defined in the usual way.

We shall now expand the exponential factor appearing in the integrand of (5.55) in powers of the quantity $i\underline{K}\cdot\underline{r}_m$

i.e. $$e^{i\underline{K}\cdot\underline{r}_m} = 1 + \frac{(i\underline{K}\cdot\underline{r}_m)}{1!} + \frac{(i\underline{K}\cdot\underline{r}_m)^2}{2!} + \ldots\ldots \tag{5.56}$$

By replacing the exponential in (5.55) by its expansion we are able to determine how the various terms in (5.56) contribute to the amplitude and hence the triple differential cross section. For this purpose we have chosen to retain only the first three terms of the expansion. Since we have imposed the orthogonality condition

$$\langle \Psi_0 | \Psi_{\underline{k}_s}^{N} \rangle = 0$$

then clearly the first term of the series expansion makes zero contribution to the amplitude. The contribution arising from the second term in the expansion has the form

$$-\frac{2}{K^2}\sum_{m=2}^{3}\int {}^2\bar{\Psi}_0(\underline{r}_2,\underline{r}_3)\, iKr_m\cos\theta_m\, {}^2\bar{\Psi}^{N*}_{\underline{k}_s}(\underline{r}_2,\underline{r}_3)\, d\underline{r}_2\, d\underline{r}_3 \qquad (5.57)$$

where we have chosen the polar axis to be along the direction of the momentum transfer $\underline{K}$.

Substituting the explicit forms of the wave functions ${}^2\bar{\Psi}_0$ and ${}^2\bar{\Psi}^N_{\underline{k}_s}$ from (3.21), (4.6) and associated equations we may, by means of the methods demonstrated in earlier chapters, evaluate the expression in (5.57) and so obtain

$$f_1(\underline{k}_f,\underline{k}_s) = -\frac{P_1(\hat{\underline{K}}\cdot\hat{\underline{k}}_s)\,J(k_s)}{K} \qquad (5.58)$$

the $f_1(\underline{k}_f,\underline{k}_s)$ indicating that this is the first order contribution to the amplitude. The function $J(k_s)$ is given by

$$J(k_s) = \frac{2z^{3/2}e^{-i\delta_1}}{k_s^{1/2}\pi}\Big\{\sum_{i,j=1,2} c_{ij}\,(1+\delta_{ij})^{1/2}\int_0^\infty {}^2\psi_{is}(r)\,r^2u_1(k_s,r)\,dr$$

$$\times\int_0^\infty {}^2\psi_{js}(r)\,e^{-zr}r^2\,dr + \frac{1}{\sqrt{3}}\sum_{k,l=2,3} d_{kl}\,(1+\delta_{kl})^{1/2}\int_0^\infty {}^2\psi_{kp}(r)\,r\,u_1(k_s,r)\,dr$$

$$\times\int_0^\infty {}^2\psi_{lp}(r)\,e^{-zr}r^3\,dr\Big\} \qquad (5.59)$$

the functions ${}^2\psi_{is}$ and ${}^2\psi_{kp}$ being respectively 's' and 'p' state one-electron radial functions appearing in the C.I. wave function representing the target ground state. The quantities c_{ij} and d_{kl} are the associated weights. All other quantities are as previously defined.

In order to find the required double differential cross section it is necessary to evaluate an integral of the form

$$\int |f(\underline{k}_f,\underline{k}_s)|^2 d\hat{\underline{k}}_f$$

The first order contribution to this integral, arising from the expansion of the amplitude $f(\underline{k}_f,\underline{k}_s)$ in "partial amplitudes" will be

$$\int |f_1(\underline{k}_f,\underline{k}_s)|^2 d\hat{\underline{k}}_f$$

$$= |J(k_s)|^2 \int \left(\frac{P_1(\hat{\underline{K}}\cdot\hat{\underline{k}}_s)}{K}\right)^2 d\hat{\underline{k}}_f \qquad (5.60)$$

Let us therefore examine the integral

$$\int \frac{\cos^2\theta_{\underline{K}\underline{k}_s}}{K^2} d\hat{\underline{k}}_f$$

where $\theta_{\underline{K}\underline{k}_s}$ denotes the angle between the vectors $\underline{K}$ and $\underline{k}_s$. Considerable simplification is achieved by means of the relation

$$\cos\theta_{\underline{K}\underline{k}_s} = \cos\theta_{\underline{K}}\cos\theta_{\underline{k}_s} + \sin\theta_{\underline{K}}\sin\theta_{\underline{k}_s}\cos(\phi_{\underline{K}} - \phi_{\underline{k}_s}) \qquad (5.61)$$

Since we are concerned with a situation in which the direction $\hat{\underline{k}}_s$ of the "slow" electron is fixed then we may use the vectors $\underline{k}_o$ and $\underline{k}_s$ to define the plane $\phi = 0$. Hence $\phi_{\underline{k}_s} = 0$, and equation (5.61) becomes

$$\cos\theta_{\underline{K}\underline{k}_s} = \cos\theta_{\underline{K}}\cos\theta_{\underline{k}_s} + \sin\theta_{\underline{K}}\sin\theta_{\underline{k}_s}\cos\phi_{\underline{K}} \qquad (5.62)$$

where we are using a frame of reference in which the polar axis is along the line of action of the vector $\underline{k}_o$. Clearly since the vectors $\underline{K}$ and $\underline{k}_f$ lie in the same azimuthal plane then we can replace $\phi_{\underline{K}}$ by $\phi_{\underline{k}_f}$ in equation (5.62). Thus

$$\cos\theta_{\underline{K}\underline{k}_s} = \cos\theta_{\underline{K}}\cos\theta_{\underline{k}_s} + \sin\theta_{\underline{K}}\sin\theta_{\underline{k}_s}\cos\phi_{\underline{k}_f}$$

and

$$\cos^2\theta_{\underline{K}\underline{k}_s} = \cos^2\theta_{\underline{K}}\cos^2\theta_{\underline{k}_s} + \sin^2\theta_{\underline{K}}\sin^2\theta_{\underline{k}_s}\cos^2\phi_{\underline{k}_f}$$
$$+ 2\cos\theta_{\underline{K}}\sin\theta_{\underline{K}}\cos\theta_{\underline{k}_s}\sin\theta_{\underline{k}_s}\cos\phi_{\underline{k}_f}$$

Using the results

$$\int_0^{2\pi}\cos^2\phi\, d\phi = \pi$$

and

$$\int_0^{2\pi}\cos\phi\, d\phi = 0$$

we may perform the integration over the azimuthal angle $\phi_{\underline{k}_f}$ appearing in (5.60) and so obtain

$$\int\frac{\cos^2\theta_{\underline{K}\underline{k}_s}}{K^2}\,d\hat{\underline{k}}_f = \pi\int_0^{\pi}\frac{1}{K^2}\left(2\cos^2\theta_{\underline{K}}\cos^2\theta_{\underline{k}_s} + \sin^2\theta_{\underline{K}}\sin^2\theta_{\underline{k}_s}\right)\sin\theta_{\underline{k}_f}\,d\theta_{\underline{k}_f}$$

(5.63)

This equation may be written as the sum of two terms

$$2\pi\cos^2\theta_{\underline{k}_s}\int_0^{\pi}\frac{\cos^2\theta_{\underline{K}}}{K^2}\sin\theta_{\underline{k}_f}\,d\theta_{\underline{k}_f}$$
$$+ \pi\sin^2\theta_{\underline{k}_s}\int_0^{\pi}\frac{\sin^2\theta_{\underline{K}}}{K^2}\sin\theta_{\underline{k}_f}\,d\theta_{\underline{k}_f}$$

By applying the Sine Rule to the triangle having sides corresponding to the vectors $\underline{k}_0$, $\underline{k}_f$ and $\underline{K}$ we obtain the relation

$$\sin^2\theta_{\underline{K}} = \frac{k_f^2}{K^2}\sin^2\theta_f \qquad (5.64)$$

In addition we have

$$\cos^2\theta_{\underline{K}} = \frac{(\underline{k}_0\cdot\underline{K})^2}{k_0^2K^2} = \frac{(k_0^2 - k_0k_f\cos\theta_f)}{k_0^2K^2} \qquad (5.65)$$

If we now substitute from equations (5.64) and (5.65) the expression in which we are interested becomes

$$\int \frac{\cos^2\theta_{\underline{k}\underline{k}_s}}{K^2}\, d\hat{\underline{k}}_f$$

$$= 2\pi\cos^2\theta_{\underline{k}_s}\int_0^{\pi}\left[\frac{\sin\theta_{\underline{k}_f}}{K^2} - \frac{k_f^2}{K^4}\sin^2\theta_f \sin\theta_{\underline{k}_f}\right] d\theta_{\underline{k}_f}$$

$$+ \pi\sin^2\theta_{\underline{k}_s}\int_0^{\pi} \frac{k_f^2}{K^4}\sin^2\theta_{\underline{k}_f}\sin\theta_{\underline{k}_f}\, d\theta_{\underline{k}_f} \tag{5.66}$$

Introducing the change of variable $\theta_{\underline{k}_f} \to \mu = \cos\theta_{\underline{k}_f}$ the integrals appearing in equation (5.66) may be transformed as shown

$$\int_0^{\pi}\left[\frac{\sin\theta_{\underline{k}_f}}{K^2} - \frac{k_f^2\sin^2\theta_{\underline{k}_f}\sin\theta_{\underline{k}_f}}{K^4}\right] d\theta_{\underline{k}_f}$$

$$= \int_{-1}^{+1}\left[\frac{1}{(k_0^2+k_f^2-2k_0k_f\mu)} - \frac{k_f^2}{(k_0^2+k_f^2-2k_0k_f\mu)^2} + \frac{k_f^2\mu^2}{(k_0^2+k_f^2-2k_0k_f\mu)^2}\right] d\mu \tag{5.67}$$

$$\int_0^{\pi} \frac{k_f^2}{K^4}\sin^2\theta_{\underline{k}_f}\sin\theta_{\underline{k}_f}\, d\theta_{\underline{k}_f}$$

$$= \int_{-1}^{+1}\left[\frac{k_f^2}{(k_0^2+k_f^2-2k_0k_f\mu)^2} - \frac{k_f^2\mu^2}{(k_0^2+k_f^2-2k_0k_f\mu)^2}\right] d\mu \tag{5.68}$$

There are three different types of integral that we need to evaluate. By making the identifications $A = k_0^2 + k_f^2$ and $B = -2k_0k_f$ these may be reduced to the forms

$$\int_{-1}^{+1}\frac{d\mu}{(A+B\mu)} \qquad \text{(i)}$$

$$\int_{-1}^{+1}\frac{d\mu}{(A+B\mu)^2} \qquad \text{(ii)}$$

$$\int_{-1}^{+1}\frac{\mu^2 d\mu}{(A+B\mu)^2} \qquad \text{(iii)}$$

These integrals are readily evaluated, yielding the following results

$$\int_{-1}^{+1} \frac{d\mu}{(A+B\mu)} = \frac{1}{B} \log_e \left[\frac{A+B}{A-B}\right] \qquad \text{(i)}$$

$$\int_{-1}^{+1} \frac{d\mu}{(A+B\mu)^2} = \frac{2}{(A^2-B^2)} \qquad \text{(ii)}$$

$$\int_{-1}^{+1} \frac{\mu^2 d\mu}{(A+B\mu)^2} = \frac{1}{B^2}\left\{2 + \frac{2A}{B} \log_e \left[\frac{A-B}{A+B}\right] + \frac{2A^2}{(A^2-B^2)}\right\} \qquad \text{(iii)}$$

By appropriate substitution of these results the integral of (5.67) may be simplified to the following

$$\frac{1}{B} \log_e \left[\frac{A-B}{A+B}\right] \left\{\frac{2k_f^2 A}{B^2} - 1\right\} + \frac{4k_f^2}{B^2}$$

Replacing A and B by the appropriate momenta dependent expressions we obtain

$$\frac{1}{2k_0^3 k_f}(k_0^2-k_f^2) \log_e \left[\frac{k_0+k_f}{k_0-k_f}\right] + \frac{1}{k_0^2}$$

In a similar way the integral in equation (5.68) may be shown to equal

$$-\frac{2k_f^2}{B^2}\left\{\frac{A}{B} \log_e \left[\frac{A-B}{A+B}\right] + 2\right\}$$

$$= \frac{(k_0^2+k_f^2)}{2k_0^3 k_f} \log_e \left[\frac{k_0+k_f}{k_0-k_f}\right] - \frac{1}{k_0^2}$$

Hence we arrive at the result

$$\int \frac{\cos^2\theta_{kk_s}}{K^2} d\hat{k}_f = 2\pi \cos^2\theta_{\underline{k}_s} \left\{\frac{(k_0^2-k_f^2)}{2k_0^3 k_f} \log_e \left[\frac{k_0+k_f}{k_0-k_f}\right] + \frac{1}{k_0^2}\right\}$$

$$+ \pi \sin^2\theta_{\underline{k}_s} \left\{\frac{(k_0^2+k_f^2)}{2k_0^3 k_f} \log_e \left[\frac{k_0+k_f}{k_0-k_f}\right] - \frac{1}{k_0^2}\right\}$$

(5.69)

In order to determine the shape of the curve corresponding to the function we shall make a further examination of the energy dependent coefficients of the two terms in equation (5.69). Clearly the coefficient of the first term is always positive. Let us therefore turn our attention to the coefficient of the second term. To facilitate our investigation we shall make the replacement $k_f = \alpha k_o$ where $0 < \alpha < 1$. The coefficient of interest may now be rewritten in the form

$$\frac{1}{k_o^2}\left[\frac{(1+\alpha^2)}{2\alpha}\log_e\left[\frac{1+\alpha}{1-\alpha}\right] - 1\right]$$

Using the appropriate series expansion for the logarithmic term we obtain

$$\frac{1}{k_o^2}\left[(1+\alpha^2)\left\{1+\frac{\alpha^2}{3}+\frac{\alpha^4}{5}+\ldots\ldots\right\} - 1\right] > 0$$

Hence this coefficient is also always positive for all cases. Taking the two coefficients in the order in which they occur in equation (5.69) we shall denote them by $C_1(k_o,k_f)$ and $C_2(k_o,k_f)$ respectively If we now eliminate the $\sin^2\theta_{\underline{k}_s}$ dependence equation (5.69) may be rewritten as

$$\int \frac{\cos^2\theta_{\underline{k}\underline{k}_s}}{K^2} d\hat{\underline{k}}_f = \pi\left\{C_3(k_o,k_f)\cos^2\theta_{\underline{k}_s} + C_2(k_o,k_f)\right\} \qquad (5.70)$$

where $C_3(k_o,k_f) = 2C_1(k_o,k_f) - C_2(k_o,k_f)$

To conclude our analysis of the functional form of (5.70) it is necessary to examine the behaviour of the coefficient $C_3(k_o,k_f)$.

Now

$$C_3(k_o,k_f) = \frac{(k_o^2-3k_f^2)}{2k_o^3k_f}\log_e\left[\frac{k_o+k_f}{k_o-k_f}\right] + \frac{3}{k_o^2}$$

$$= \frac{1}{k_o^2}\left\{\frac{(1-3\alpha^2)}{2\alpha}\log_e\left[\frac{1+\alpha}{1-\alpha}\right] + 3\right\} \qquad (5.71)$$

Or, replacing the logarithmic term by its series expansion,

$$C_3(k_0,k_f) = \frac{1}{k_0^2}\left\{4 - \alpha^2 \sum_{n=0}^{\infty} \alpha^{2n} \frac{(7n+8)}{(2n+1)(2n+3)}\right\} \tag{5.72}$$

It is immediately clear that the sign of this quantity depends upon the magnitude of α. For high energy ionizing collisions involving small energy loss of the incident electron α will be close to unity and $C_3(k_0,k_f)$ will consequently be negative. For small values of α, $C_3(k_0,k_f)$ will be positive.

The curve corresponding to the function in (5.70) will be symmetrical about $\theta = \pi/2$, the direction of curvature depending on the sign of $C_3(k_0,k_f)$. If $C_3(k_0,k_f)$ is negative then the curve will be convex and if it is positive the curve will be concave.

For the ionization of helium there are two sets of experimental measurements of the double differential cross section available (C.B. Opal et al 1971, Ehrhardt et al 1972). Unfortunately these data differ significantly in the region of smallest energy transfer to the ejected electron, which is the region of greatest interest. Although we can place no reliance on the data available for this region it is interesting to note that there is general qualitative agreement between the measurements of Opal et al at primary energies greater than 200 eV and the behaviour predicted by (5.70). However even here the experimental curves show signs of additional structure. As we allow a greater energy transfer to the ejected electron the two sets of experimental measurements approach general qualitative agreement, both indicating a highly structured form quite different to that predicted by (5.70). We must therefore conclude that even at high energies the higher order terms in the expansion (5.56) make a significant contribution to the cross section. Hence the ionization process is not a pure dipole transition.

APPENDIX A

In this appendix we present a description of the numerical techniques used in the generation of the radial functions $u_l(k,r)$ satisfying the equation (3.15). For this purpose we first rewrite equation (3.15) in the form

$$\frac{d^2}{dr^2}u_l(k,r) = f_l(k,r)u_l(k,r) + g_l(r)\int_0^r e^{-zx}u_l(k,x)\left\{r^{-l}x^{l+1} - r^{l+1}x^{-l}\right\}dx + r^{l+1}a\,g_l(r) \tag{A1}$$

where

$$f_l(k,r) = \frac{l(l+1)}{r^2} - k^2 - 2\frac{(z-1)}{r} - 2A_1\left(z+\frac{1}{r}\right)e^{-2zr} - A_2\frac{\beta(zr)}{(zr)^4} \tag{A2}$$

$$g_l(r) = \frac{8z^3A_3}{(2l+1)}e^{-zr} \tag{A3}$$

$$a = \int_0^\infty e^{-zx}u_l(k,x)x^{-l}\left\{1 - \frac{1}{2}\delta_{l0}x(z^2+k^2)\right\}dx \tag{A4}$$

Adopting the approach of Percival and Marriott [Marriott 1958] we consider the inhomogeneous integro-differential equation

$$\frac{d^2}{dr^2}Y_l(k,r) = f_l(k,r)Y_l(k,r) + g_l(r)\int_0^r e^{-zx}Y_l(k,x)\left\{r^{-l}x^{l+1} - r^{l+1}x^{-l}\right\}dx + r^{l+1}g_l(r) \tag{A5}$$

and the associated homogeneous equation

$$\frac{d^2}{dr^2}X_l(k,r) = f_l(k,r)X_l(k,r) + g_l(r)\int_0^r e^{-zx}X_l(k,x)\left\{r^{-l}x^{l+1} - r^{l+1}x^{-l}\right\}dx \tag{A6}$$

The solutions of these two equations are denoted by $Y_l(k,r)$ and $X_l(k,r)$ respectively. The general solution of the inhomogeneous equation (A1) may be expressed as a suitable combination of these functions and is given by

$$u_l(k,r) = X_l(k,r) + aY_l(k,r) \tag{A7}$$

Subsequent to the generation of the functions $X_l(k,r)$ and $Y_l(k,r)$ we are able to evaluate the quantity 'a' in terms of these since substitution of the form (A7) into (A4) yields the result

$$a = \frac{\int_0^\infty e^{-zx} X_l(k,x) x^{-l}\{1 - \tfrac{1}{2}\delta_{l0} x(z^2+k^2)\} dx}{1 - \int_0^\infty e^{-zx} Y_l(k,x) x^{-l}\{1 - \tfrac{1}{2}\delta_{l0} x(z^2+k^2)\} dx} \tag{A8}$$

We now turn our attention to the actual construction of the functions $X_l(k,r)$ and $Y_l(k,r)$. The function $u_l(k,r)$, of which these are component parts, is subject to the boundary conditions

$$u_l(k,0) = 0 \tag{A9}$$

and

$$\underset{r\to\infty}{u_l(k,r)} \sim \frac{1}{k^{1/2}} \sin\left[kr + \frac{(z-1)}{k}\ln(2kr) - \frac{1}{2}l\pi + \sigma_l + \eta_l\right] \tag{A10}$$

The first of these is most easily achieved by requiring that

$$X_l(k,0) = Y_l(k,0) = 0 \tag{A11}$$

Hence the series expansions corresponding to these functions are assumed to take the forms

$$X_l(k,r) = \sum_{n=0}^{\infty} a_n^l r^{n+\sigma} \tag{A12}$$

$$Y_l(k,r) = \sum_{n=0}^{\infty} b_n^l r^{n+\rho} \qquad \text{with } \sigma, \rho > 0 \tag{A13}$$

The coefficients a_0^l, b_0^l are arbitrary (but non zero) and all others are expressible in terms of them through recurrence relations. In the region of the origin the function $f_l(k,r)$ may be represented by the series expansion

$$f_l(k,r) = \frac{l(l+1)}{r^2} + \frac{Z_0}{r} + Z_1 + Z_2 r + Z_3 r^2 + O(r^3) \tag{A14}$$

where

$$Z_0 = -2(z-1+A_1) \qquad Z_1 = (2A_1 z - k^2)$$

$$Z_2 = -\frac{8A_2 z}{15}$$

$$Z_3 = -\frac{2}{3} z^2 (2A_1 z - A_2)$$

while the corresponding expression for $g_l(r)$ is

$$g_l(r) = \frac{2A_3'}{(2l+1)} \left[1 - zr + \tfrac{1}{2} z^2 r^2 + O(r^3)\right] \tag{A15}$$

with

$$A_3' = 4z^3 A_3$$

Appropriate substitution of the forms (A12),(A14) and (A15) in equation (A6) yields

$$\sum_{n=0}^{\infty} a_n^l (n+\sigma)(n+\sigma-1) r^{n+\sigma-2} = \left\{ \frac{l(l+1)}{r^2} + \frac{Z_0}{r} + Z_1 + Z_2 r + Z_3 r^2 + O(r^3) \right\}$$

$$\sum_{n=0}^{\infty} a_n^l r^{n+\sigma} - 2A_3' \sum_{n=0}^{\infty} a_n^l \left[\frac{r^{n+\sigma+2}}{(n+\sigma+l+2)(n+\sigma+1-l)} + O(r^{n+\sigma+3}) \right] \tag{A16}$$

from which we may obtain the recurrence relations linking the coefficients a_n^l. The equations satisfied (for) by the coefficients $\{a_n^l, n=0,4\}$ are

$$[\sigma(\sigma-1) - l(l+1)] a_0^l = 0 \tag{A17}$$

$$a_1^l [\sigma(\sigma+1) - l(l+1)] = Z_0 a_0^l \tag{A18}$$

$$a_2^{l}[(\sigma+1)(\sigma+2)-l(l+1)]=z_0a_1^{l}+z_1a_0^{l} \qquad \text{(A19)}$$

$$a_3^{l}[(\sigma+2)(\sigma+3)-l(l+1)]=a_2^{l}z_0+a_1^{l}z_1+a_0^{l}z_2 \qquad \text{(A20)}$$

$$a_4^{l}[(\sigma+3)(\sigma+4)-l(l+1)]=a_3^{l}z_0+a_2^{l}z_1+a_1^{l}z_2 + a_0^{l}\left[z_3-\frac{2A_3'}{(\sigma+l+2)(\sigma-l+1)}\right] \qquad \text{(A21)}$$

Equations (A18) - (A21) provide the means for expressing the coefficients succeeding a_0^{l} in terms of this quantity, while (A17) implies that

$$\sigma(\sigma-1)-l(l+1)=0 \qquad \text{(A22)}$$

since a_0^{l} is non zero.

Equation (A22) has roots $\sigma=l+1, \sigma=-l$, only the former of which satisfies the requirement $\sigma>0$. Substituting the value $\sigma=l+1$ into equations (A18) - (A21) allows the relevant coefficients to be determined, so enabling us to rewrite (A12) in the form

$$X_l(k,r)=r^{l+1}[a_0^{l}+a_1^{l}r+a_2^{l}r^2+a_3^{l}r^3+a_4^{l}r^4+O(r^5)] \qquad \text{(A23)}$$

Similarly we can obtain

$$Y_l(k,r)=r^{l+1}[b_0^{l}+b_1^{l}r+b_2^{l}r^2+b_3^{l}r^3+b_4^{l}r^4+O(r^5)] \qquad \text{(A24)}$$

We now make the following identifications

$$E_l(k,r)=\int_0^r e^{-zx}x^{l+1}X_l(k,x)\,dx \qquad \text{(A25)}$$

$$F_l(k,r)=\int_0^r e^{-zx}x^{-l}X_l(k,x)\,dx \qquad \text{(A26)}$$

$$G_l(k,r)=\int_0^r e^{-zx}x^{l+1}Y_l(k,x)\,dx \qquad \text{(A27)}$$

$$H_l(k,r)=\int_0^r e^{-zx}x^{-l}Y_l(k,x)\,dx \qquad \text{(A28)}$$

Using the quantities defined by these equations the differential equations satisfied by the functions X_l and Y_l may be written as

$$\frac{d^2}{dr^2} X_l(k,r) = f_l(k,r) X_l(k,r) + C_l(k,r) \tag{A29}$$

$$\frac{d^2}{dr^2} Y_l(k,r) = f_l(k,r) Y_l(k,r) + D_l(k,r) \tag{A30}$$

where

$$C_l(k,r) = g_l(r)\left[r^{-l} E_l(k,r) - r^{l+1} F_l(k,r)\right] \tag{A31}$$

and

$$D_l(k,r) = g_l(r)\left[r^{-l} G_l(k,r) - r^{l+1}\left\{H_l(k,r) - 1\right\}\right] \tag{A32}$$

In order to initiate the numerical technique used to construct the solutions of the equations (A29) and (A30) we require explicit expressions for the functions E_l, F_l, G_l and H_l in the region of the origin. These are obtained from equations (A25) - (A28), used in conjunction with (A23) and (A24). They are

$$E_l(k,r) = r^{2l+3}\left[\frac{a_0^l}{(2l+3)} + \frac{(a_1^l - z a_0^l) r}{(2l+4)} + \frac{(a_2^l - z a_1^l + \frac{1}{2} z^2 a_0^l) r^2}{(2l+5)} + O(r^3)\right] \tag{A33}$$

$$F_l(k,r) = r^2\left[\frac{a_0^l}{2} + \frac{(a_1^l - z a_0^l) r}{3} + \frac{(a_2^l - z a_1^l + \frac{1}{2} z^2 a_0^l) r^2}{4} + \frac{(a_3^l - z a_2^l + \frac{1}{2} z^2 a_1^l - \frac{1}{6} z^3 a_0^l) r^3}{5} + O(r^4)\right] \tag{A34}$$

$$G_l(k,r) = r^{2l+3}\left[\frac{b_0^l}{(2l+3)} + \frac{(b_1^l - z b_0^l) r}{(2l+4)} + \frac{(b_2^l - z b_1^l + \frac{1}{2} z^2 b_0^l) r^2}{(2l+5)} + O(r^3)\right] \tag{A35}$$

$$H_l(k,r) = r^2\left[\frac{b_0^l}{2} + \frac{(b_1^l - z b_0^l) r}{3} + \frac{(b_2^l - z b_1^l + \frac{1}{2} z^2 b_0^l) r^2}{4} + \frac{(b_3^l - z b_2^l + \frac{1}{2} z^2 b_1^l - \frac{1}{6} z^3 b_0^l) r^3}{5} + O(r^4)\right] \tag{A36}$$

Combining these expressions in accordance with equations (A31) and (A32) we obtain

$$C_l(k,r) = -2A_3' e^{-zr} r^{l+3} \left[\frac{a_0^l}{2(2l+3)} + \frac{(a_1^l - z a_0^l) r}{3(2l+4)} \right.$$

$$\left. + \frac{(a_2^l - z a_1^l + \frac{1}{2} z^2 a_0^l) r^2}{4(2l+5)} + O(r^3) \right] \tag{A37}$$

and

$$D_l(k,r) = -2A_3' e^{-zr} r^{l+1} \left[\frac{-1}{(2l+1)} + \frac{b_0^l}{2(2l+3)} r^2 + \frac{(b_1^l - z b_0^l) r^3}{3(2l+4)} \right.$$

$$\left. + \frac{(b_2^l - z b_1^l + \frac{1}{2} z^2 b_0^l) r^4}{4(2l+5)} + O(r^5) \right] \tag{A38}$$

The solutions of the integro-differential equations (A29) and (A30) are constructed by outward integration of the equations, performed by means of Numerov's method. For this purpose we introduce the quantities.

$$\alpha_j = 1 - \tfrac{1}{12} h^2 f_j \tag{A39}$$

$$\beta_j = 2 + \tfrac{5}{6} h^2 f_j \tag{A40}$$

where h is the integration step-length and $f_j = f(r_j)$. Use of the Numerov formula enables us to replace equations (A29) and (A30) by the recurrence relations

$$X_{j+1} = \frac{1}{\alpha_{j+1}} \left[\beta_j X_j - \alpha_{j-1} X_{j-1} + \frac{1}{12} h^2 (C_{j+1} + 10 C_j + C_{j-1}) \right] \tag{A41}$$

$$Y_{j+1} = \frac{1}{\alpha_{j+1}} \left[\beta_j Y_j - \alpha_{j-1} Y_{j-1} + \frac{1}{12} h^2 (D_{j+1} + 10 D_j + D_{j-1}) \right] \tag{A42}$$

The exchange integrals needed for the evaluation of the functions $C_l(k,r)$ and $D_l(k,r)$ may be evaluated in two different ways. In the work of Economides (1969) the evaluation is accomplished through the use of a seven-point Newton-Cotes formula (Abramowitz and Stegun, 1965). Applying this to the integral $E_l(k,r)$ (equation (A25)) we obtain

$$E_{j+1} = E_{j-6} + 0{\cdot}3h\left[11P_{j-4} - 14P_{j-3} + 26P_{j-2} - 14P_{j-1} + 11P_j\right] \tag{A43}$$

where

$$P_j = e^{-Zr_j} r_j^{l+1} X_j \tag{A44}$$

Similar expressions may be obtained for the remaining exchange integrals.

The second method of evaluation avoids the dissociation of the functions C_l and D_l into their component parts by calculating them directly. This is possible because the functions $g_l^{-1}C_l$ and $g_l^{-1}D_l$ satisfy differential equations of similar nature to (A29) and (A30). The appropriate equation for $K_l = g_l^{-1}C_l$ is

$$\frac{d^2K_l}{dr^2} = \frac{l(l+1)}{r^2}K_l - (2l+1)e^{-Zr}X_l \tag{A45}$$

These equations can be solved using the techniques already described.

The original program followed the method used by Economides. An alternative version of the program (for generating the radial functions) that used the second method described was produced by L. A. Morgan (1973). Although results produced by the two methods were in good agreement the Morgan version was adopted in place of the original because of its greater sophistication.

The formulae presented in this section generate successive function values from those preceding. To initiate the integration routine we require six starting values which are easily calculated from the series expansions about the origin (A23, A24 and A33 - A36).

APPENDIX B.

In this appendix we are concerned with the forms taken by the amplitudes when both outgoing electrons are represented by plane waves. This approximation leads to considerable simplification in the analysis and it is now possible to reduce all the integrals to simple closed forms, avoiding the infinite series expansions present in the original analysis. However in addition to obtaining these simple closed forms we are also interested in calculating the expressions that are directly analogous to those of Chapter 4.

This plane-plane approximation is achieved by replacing the function $\psi_{\underline{k}_s}(\underline{r})$ by the exponential form $(2\pi)^{-3/2} e^{i\underline{k}_s\cdot\underline{r}}$. Clearly the only terms in the amplitudes that need to be considered are those involving the function $\psi_{\underline{k}_s}(\underline{r})$. Referring to equation (4.9) we see that the relevant quantities are F_1 and I_{ov}. The quantity F_1 can be divided into two components F_{1A} and F_{1B} defined by equations (4.12) and (4.13) respectively. We shall firstly examine the modified form of F_{1A}. Although the expression for F_{1A} given by equation (4.16) involves a double integral the replacement associated with the present approximation will only affect the second of these integrals. This integral has the form

$$\int e^{i\underline{K}\cdot\underline{r}} \psi^*_{\underline{k}_s}(\underline{r}) R_{n_1 l_1}(z_0, r) d\underline{r} \tag{B1}$$

where the $R_{n_1 l_1}$ are hydrogenic radial functions corresponding to an effective charge Z_0 and have the general form

$$R_{nl}(z_l, r) = (a_{nl} r^2 + b_{nl} r + c_{nl}) e^{-\alpha_{nl} r} \tag{B2}$$

Using the plane wave representation for the slow electron the integral (B1) becomes

$$\frac{1}{(2\pi)^{3/2}}\int e^{i(\underline{k}-\underline{k}_s)\cdot\underline{r}}R_{n_1l_1}(z_0,r)\,d\underline{r}$$

If we introduce the momentum variable K' defined by $K'=|\underline{K}'|=|\underline{K}-\underline{k}_s|$, which is referred to as the recoil momentum, and perform the angular part of the integration then we obtain the radial integral

$$\frac{4\pi}{(2\pi)^{3/2}}\int_0^\infty j_0(rK')r^2R_{n_1l_1}(z_0,r)\,dr \tag{B3}$$

But from equation (4.23) we have the general result

$$\int_0^\infty j_0(Kr)e^{-zr}R_{nl}(z_l,r)r^2dr$$

$$=\frac{2}{(\beta^2+K^2)^2}\left\{12a_{nl}\frac{\beta(\beta^2-K^2)}{(\beta^2+K^2)^2}+b_{nl}\frac{(3\beta^2-K^2)}{(\beta^2+K^2)}+c_{nl}\beta\right\} \tag{B4}$$

where

$$\beta=z+\alpha_{nl}$$

Hence by an appropriate choice of parameters we can use the result (B4) to reduce (B3) to the form

$$\left(\frac{2}{\pi}\right)^{1/2}\frac{2}{(\beta^2+K'^2)^2}\left\{12a_{n_1l_1}\frac{\beta(\beta^2-K'^2)}{(\beta^2+K'^2)^2}+b_{n_1l_1}\frac{(3\beta^2-K'^2)}{(\beta^2+K'^2)}+c_{n_1l_1}\beta\right\} \tag{B5}$$

with $\beta=\alpha_{n_1l_1}$

The remaining integral appearing in (4.16) has the form

$$\int_0^\infty e^{-zr}R_{n_2l_2}(z_0,r)r^2dr$$

which is readily evaluated (equation (4.18)), yielding the result

$$\frac{2}{(z+\alpha_{n_2l_2})^3}\left\{\frac{12a_{n_2l_2}}{(z+\alpha_{n_2l_2})^2}+\frac{3b_{n_2l_2}}{(z+\alpha_{n_2l_2})}+c_{n_2l_2}\right\} \tag{B6}$$

If we now make the identifications

$$I^{(1)}_{n_1l_1}(K')=\frac{2}{(\beta^2+K'^2)^2}\left\{12a_{n_1l_1}\frac{\beta(\beta^2-K'^2)}{(\beta^2+K'^2)^2}\right.$$

$$+ b_{n_1l_1}\frac{(3\beta^2-K'^2)}{(\beta^2+K'^2)} + c_{n_1l_1}\beta \Bigg\}$$

and

$$I^{(2)}_{n_2l_2}(z) = \frac{2}{(z+\alpha_{n_2l_2})^3}\left\{\frac{12a_{n_2l_2}}{(z+\alpha_{n_2l_2})^2} + \frac{3b_{n_2l_2}}{(z+\alpha_{n_2l_2})} + c_{n_2l_2}\right\}$$

then the modified expression for F_{1A} has the form

$$F_{1A} = \frac{Z^{3/2}}{\pi}\sum_{\text{'s' states}} C_{n_1l_1,n_2l_2}(1+\delta_{n_1l_1,n_2l_2})^{1/2} I^{(1)}_{n_1l_1}(K')\, I^{(2)}_{n_2l_2}(z) \qquad \text{(B7)}$$

We shall now turn our attention to the quantity F_{1B}. This is composed of a "s" and a "p" contribution denoted by F^{s}_{1B} and F^{p}_{1B} respectively. The contribution F^{s}_{1B} is defined by equation (4.25) and may be expressed in the form

$$F^{s}_{1B} = \frac{Z^{3/2}}{\pi k_s^{1/2}}\sum_{\text{'s' states}} C_{n_1l_1,n_2l_2}(1+\delta_{n_1l_1,n_2l_2})^{1/2} I^{(1)}_{n_2l_2}(K,\beta=z+\alpha_{n_2l_2}) \int_0^\infty u_0(k_s,r)\, r R_{n_1l_1}(z_0,r)\,dr$$

By making the replacement $u_0(k_s,r) \rightarrow k_s^{1/2} r\, j_0(k_s r)$ we are able to transform this expression to the form appropriate to the plane-plane approximation

i.e.

$$F^{s}_{1B} = \frac{Z^{3/2}}{\pi}\sum_{\text{'s' states}} C_{n_1l_1,n_2l_2}(1+\delta_{n_1l_1,n_2l_2})^{1/2} I^{(1)}_{n_2l_2}(K,\beta=z+\alpha_{n_2l_2}) \int_0^\infty j_0(k_s r)\, r^2 R_{n_1l_1}(z_0,r)\,dr \qquad \text{(B8)}$$

But

$$\int_0^\infty j_0(k_s r)\, r^2 R_{n_1l_1}(z_0,r)\,dr = I^{(1)}_{n_1l_1}(k_s,\beta=\alpha_{n_1l_1})$$

Hence we obtain the result

$$F^{s}_{1B} = \frac{Z^{3/2}}{\pi}\sum_{\text{'s' states}} C_{n_1l_1,n_2l_2}(1+\delta_{n_1l_1,n_2l_2})^{1/2} I^{(1)}_{n_2l_2}(K,\beta=z+\alpha_{n_2l_2})\, I^{(1)}_{n_1l_1}(k_s,\beta=\alpha_{n_1l_1}) \qquad \text{(B9)}$$

The appropriate form of F^{p}_{1B} can be obtained from equation (4.30) by making the Spherical Bessel function replacement. In this case we have

$$F_{1B}^{P} = \sqrt{3}\,\frac{Z^{3/2}}{\pi} P_1(\hat{k}_s\cdot\hat{k}) \sum_{\text{'p' states}} d_{n_1l_1,n_2l_2}(1+\delta_{n_1l_1,n_2l_2})^{1/2}$$

$$I^{(3)}_{n_2l_2}(K,\beta=z+\alpha_{n_2l_2}) \int_0^\infty j_1(k_s r)\, r^2 R_{n_1l_1}(z_1,r)\,dr \qquad \text{(B10)}$$

where

$$I^{(3)}_{nl}(K) = \frac{2K}{(\beta^2+K^2)^2}\left\{\frac{4a_{nl}(5\beta^2-K^2)}{(\beta^2+K^2)^2}+\frac{4b_{nl}\beta}{(\beta^2+K^2)}+c_{nl}\right\} \qquad \text{(B11)}$$

Now from equation (4.29) we have the general result

$$\int_0^\infty j_1(Kr)e^{-zr}R_{nl}(z_1,r)\,r^2dr = I^{(3)}_{nl}(K)$$, as defined by equation (B11)

Hence it follows that

$$\int_0^\infty j_1(k_s r)\,r^2R_{n_1l_1}(z_1,r)\,dr = I^{(3)}_{n_1l_1}(k_s,\beta=\alpha_{n_1l_1})$$

which allows the expression for F_{1B}^{P} to be rewritten in the simple closed form

$$F_{1B}^{P} = \sqrt{3}\,\frac{Z^{3/2}}{\pi} P_1(\hat{k}_s\cdot\hat{k}) \sum_{\text{'p' states}} d_{n_1l_1,n_2l_2}(1+\delta_{n_1l_1,n_2l_2})^{1/2}$$

$$I^{(3)}_{n_2l_2}(K,\beta=z+\alpha_{n_2l_2})\, I^{(3)}_{n_1l_1}(k_s,\beta=\alpha_{n_1l_1}) \qquad \text{(B12)}$$

It now only remains to determine the expression for I_{ov} corresponding to the plane-plane approximation. If we make the appropriate replacement in equation (4.42) we obtain the result

$$I_{ov} = -\frac{Z^{3/2}}{\pi} \sum_{\text{'s' states}} C_{n_1l_1,n_2l_2}(1+\delta_{n_1l_1,n_2l_2})^{1/2} I^{(2)}_{n_2l_2}(z)$$

$$\int_0^\infty j_0(k_s r)\,r^2R_{n_1l_1}(z_0,r)\,dr$$

which may be written in the more convenient form

$$I_{ov} = -\frac{Z^{3/2}}{\pi}\sum_{\text{'s' states}} C_{n_1l_1,n_2l_2}\left(1+\delta_{n_1l_1,n_2l_2}\right)^{1/2} I^{(2)}_{n_2l_2}(Z)\, I^{(1)}_{n_1l_1}(k_s,\beta=\alpha_{n_1l_1}) \tag{B13}$$

In the analysis corresponding to the plane-plane approximation we have avoided the infinite series expansion associated with the quantity F_{1A} (cf. equation (4.20)). However it is also necessary to consider the form of this expansion resulting from the use of the present approximation. This will be

$$F_{1A} = \frac{Z^{3/2}}{\pi}\sum_{l=0}^{\infty}(2l+1)P_l(\hat{\underline{k}}\cdot\hat{\underline{k}}_s)\sum_{\text{'s' states}} C_{n_1l_1,n_2l_2}\left(1+\delta_{n_1l_1,n_2l_2}\right)^{1/2} I^{(2)}_{n_2l_2}(Z)\int_0^{\infty} j_l(kr)\, j_l(k_sr)\, r^2 R_{n_1l_1}(Z_0,r)\,dr \tag{B14}$$

In order to evaluate this expression we require a simple analytic form for the integral

$$\int_0^{\infty} j_l(kr)\, j_l(k_sr)\, r^2 R_{nl}(Z_0,r)\,dr$$

$$= \int_0^{\infty} j_l(kr)\, j_l(k_sr)\, r^2\left(a_{nl}r^2+b_{nl}r+c_{nl}\right)e^{-\alpha_{nl}r}\,dr$$

This integral may be split up into three components of the following forms

$$\int_0^{\infty} j_l(kr)\, j_l(k_sr)\, r^2 e^{-\alpha r}\,dr \qquad \text{(i)}$$

$$\int_0^{\infty} j_l(kr)\, j_l(k_sr)\, r^3 e^{-\alpha r}\,dr \qquad \text{(ii)}$$

$$\int_0^{\infty} j_l(kr)\, j_l(k_sr)\, r^4 e^{-\alpha r}\,dr \qquad \text{(iii)}$$

We are enabled to evaluate these integrals through a result given by Watson (Treatise on Bessel Functions). The appropriate form of this result is

$$\int_0^\infty J_{l+\frac{1}{2}}(k_s r) J_{l+\frac{1}{2}}(Kr) e^{-\alpha r} dr = \frac{1}{\pi (k_s K)^{\frac{1}{2}}} Q_l\left(\frac{\alpha^2+k_s^2+K^2}{2k_s K}\right) \tag{B15}$$

where Q_l is the Legendre function of the second kind and order l.

By use of the relation $j_l(\beta r) = \left(\frac{\pi}{2\beta r}\right)^{\frac{1}{2}} J_{l+\frac{1}{2}}(\beta r)$ we are able to rewrite the integral in (B15) as one involving Spherical Bessel functions of equal orders

i.e.

$$\int_0^\infty r\, j_l(k_s r) j_l(Kr) e^{-\alpha r} dr = \frac{1}{2k_s K} Q_l\left(\frac{\alpha^2+k_s^2+K^2}{2k_s K}\right) \tag{B16}$$

The first of the three integrals required may be obtained from the integral appearing in (B16) by differentiation with respect to α. Since $\frac{d}{d\alpha} = \frac{d\omega}{d\alpha} \cdot \frac{d}{d\omega}$, the result may be expressed in the form

$$\int_0^\infty j_l(Kr) j_l(k_s r) r^2 e^{-\alpha r} dr = \frac{-\alpha}{2(k_s K)^2} \frac{d}{d\omega} Q_l(\omega) \tag{B17}$$

where $\omega = \frac{\alpha^2+k_s^2+K^2}{2k_s K}$

The remaining integrals may be obtained by further differentiation with respect to α. Corresponding results for integrals (ii) and (iii) are

$$\int_0^\infty j_l(Kr) j_l(k_s r) r^3 e^{-\alpha r} dr = \frac{1}{2(k_s K)^2} \left\{ \frac{dQ_l}{d\omega} + \frac{\alpha^2}{k_s K} \frac{d^2 Q_l}{d\omega^2} \right\} \tag{B18}$$

$$\int_0^\infty j_l(kr)\, j_l(k_s r)\, r^4 e^{-\alpha r} dr = \frac{-\alpha}{2(k_s k)^3}\left\{ 3\frac{d^2 Q_l}{d\omega^2} + \frac{\alpha^2}{k_s k}\frac{d^3 Q_l}{d\omega^3} \right\} \tag{B19}$$

The evaluation of these integrals involves the generation of the Legendre functions Q_l and their derivatives. This is readily achieved by means of the recurrence relations linking these functions. The two basic recurrence relations are

$$(l+1)Q_{l+1}(\omega) = (2l+1)\omega Q_l(\omega) - lQ_{l-1}(\omega) \tag{B20}$$

and

$$(\omega^2-1)\frac{dQ_l}{d\omega} = l[\omega Q_l(\omega) - Q_{l-1}(\omega)] \tag{B21}$$

These can be supplemented by the recurrence relations satisfied by the higher derivatives, obtained from differentiation of (B21)

$$(\omega^2-1)\frac{d^2 Q_l}{d\omega^2} = (l-2)\omega\frac{dQ_l}{d\omega} + l\left[Q_l - \frac{dQ_{l-1}}{d\omega}\right] \tag{B22}$$

$$(\omega^2-1)\frac{d^3 Q_l}{d\omega^3} = (l-4)\omega\frac{d^2 Q_l}{d\omega^2} + (2l-2)\frac{dQ_l}{d\omega} - l\frac{d^2 Q_{l-1}}{d\omega^2} \tag{B23}$$

By using the relations B20 - B23 in conjunction with the explicit forms of the first three functions Q_l and the first derivative of the zero order function we are able to generate all the functions necessary to our calculations. The relevant explicit forms are given by

$$Q_0(\omega) = \frac{1}{2}\ln\left(\frac{\omega+1}{\omega-1}\right)$$

$$Q_1(\omega) = \frac{1}{2}\omega\ln\left(\frac{\omega+1}{\omega-1}\right)$$

$$Q_2(\omega) = \frac{1}{2}(3\omega^2-1)\frac{1}{2}\ln\left(\frac{\omega+1}{\omega-1}\right)$$

$$\frac{dQ_0(\omega)}{d\omega} = \frac{-1}{(\omega^2-1)}$$

Our purpose in performing the analysis for the plane-plane approximation is two fold. Firstly it may be used to provide a simple check on the coding of the program TRIPLE 3. This is achieved by replacing the radial function u_l/r by the Spherical Bessel function appropriate to the plane-plane approximation. Calculations are then made with this modified version of the program. Identical calculations are made using the simplified analysis provided by this appendix and a comparison of the two sets of results indicates the correctness of the coding. The second purpose of the simplified analysis arose from the check described. It was found that in some cases it was necessary to include a correction for the higher order terms neglected through the use of the truncated form of the series expansion $(l=0,6)$ contained in (4.20). This convergence problem was restricted to the calculations of the exchange amplitude. The correction that was made corresponds to using the Spherical Bessel function replacement in the higher order terms. It is obtained by calculating F_{1A} from (B7) and subtracting the sum of the first seven terms of the series expansion in (B14), evaluated by the use of the results B20 - B23.

APPENDIX C

(Numerical techniques associated with the evaluation of the form of the exchange amplitude given in chapter 5.)

In order to evaluate the integrals appearing in (5.28) we must devise a numerical method suitable for generating the functions

$$\mathcal{M}_l(r_1) = \int_0^\infty j_l(k_f r)\, e^{-\alpha r_>}\, G_l(\beta, r_<)\, r\, dr \tag{C1}$$

The functions $G_l(\beta, r_<)$, defined by (5.13), may be readily obtained in closed analytic form as indicated by (5.15).

The integral (C1) splits up into two parts, each defined on a different part of the range of r

$$\mathcal{M}_l(r_1) = e^{-\alpha r_1}\int_0^{r_1} r\, j_l(k_f r)\, G_l(\beta, r)\, dr$$

$$+\; G_l(\beta, r_1)\int_{r_1}^{\infty} r\, j_l(k_f r)\, e^{-\alpha r}\, dr \tag{C2}$$

For the purpose of numerical integration involving the $\mathcal{M}_l$ we are interested in evaluating these functions at selected points over the range of r_1. We shall consider some partition of the range of r_1 given by the values $\{r_1, r_2, \ldots\ldots r_N\}$. Let functions $F_{l1}(r_1)$ and $F_{l2}(r_1)$ denote the first and second terms in (C2) respectively. Then

$$\mathcal{M}_l(r_{i+1}) = F_{l1}(r_{i+1}) + F_{l2}(r_{i+1}) \tag{C3}$$

Now

$$F_{l1}(r_{i+1}) = e^{-\alpha r_{i+1}}\int_0^{r_{i+1}} r\, j_l(k_f r)\, G_l(\beta, r)\, dr$$

$$= e^{-\alpha(r_{i+1}-r_i)}\left\{e^{-\alpha r_i}\int_0^{r_{i+1}} r j_l(k_f r) G_l(\beta, r)\, dr\right\} \tag{C4}$$

But

$r_{i+1} = r_i + h$ where h is the step length in the region of integration.

Hence

$$F_{l1}(r_{i+1}) = e^{-\alpha h}\left\{e^{-\alpha r_i}\left(\int_0^{r_i} + \int_{r_i}^{r_{i+1}}\right) r j_l(k_f r) G_l(\beta, r)\, dr\right\}$$

$$= e^{-\alpha h}\left\{F_{l1}(r_i) + e^{-\alpha r_i}\int_{r_i}^{r_{i+1}} r j_l(k_f r) G_l(\beta, r)\, dr\right\} \tag{C5}$$

The integral contained in the previous expression may be evaluated by means of Simpson's Rule. It is found that a three point integration is adequate. Hence defining $r_a = r_i$, $r_b = r_i + h/2$ and $r_c = r_{i+1}$, we have

$$\int_{r_i}^{r_{i+1}} r j_l(k_f r) G_l(\beta, r)\, dr = \frac{h}{6}\left\{[r j_l(k_f r) G_l(\beta, r)]_{r=r_a}\right.$$

$$\left. + 4[r j_l(k_f r) G_l(\beta, r)]_{r=r_b} + [r j_l(k_f r) G_l(\beta, r)]_{r=r_c}\right\} \tag{C6}$$

Let us now turn our attention to the function F_{l2} appearing in equation (C3). In this case we may write

$$F_{l2}(r_{i+1}) = G_l(\beta, r_{i+1})\int_{r_{i+1}}^{\infty} r j_l(k_f r) e^{-\alpha r}\, dr \tag{C7}$$

Denoting the integral by $I(r_{i+1})$, we have

$$F_{l2}(r_{i+1}) = G_l(\beta, r_{i+1}) I(r_{i+1}) \tag{C8}$$

In contrast with the functions F_{l1} , which involved an outward integration, the generation of the function values for the F_{l2} requires inward integration. The approach used is outlined in the following

Now

$$
\begin{aligned}
F_{l2}(r_i) &= G_l(\beta, r_i)\int_{r_i}^{\infty} r\, j_l(k_f r)\, e^{-\alpha r}\, dr \\
&= G_l(\beta, r_i)\left\{ \int_{r_{i+1}}^{\infty} r\, j_l(k_f r)\, e^{-\alpha r}\, dr + \int_{r_i}^{r_{i+1}} r\, j_l(k_f r)\, e^{-\alpha r}\, dr \right\} \\
&= G_l(\beta, r_i)\left\{ I(r_{i+1}) + \int_{r_i}^{r_{i+1}} r\, j_l(k_f r)\, e^{-\alpha r}\, dr \right\}
\end{aligned}
\qquad \text{(C9)}
$$

As before it is found that a three point Simpson integration is adequate for the evaluation of the second term appearing within the brackets of (C9).

The fundamental difference between the methods used to generate the two sets of functions occurs in the evaluation of starting values for the two proceedures. To initiate the generation of the functions F_{l1} we need to calculate various function values at the lower limit of the range of r , which can be done directly, whereas in the case of the functions F_{l2} we must calculate the function values at the upper limit of the range of r. Since this upper limit is necessarily of finite size then clearly evaluating starting values at this point is rather more difficult than the previous case.

Let R_{max} correspond to the upper limit for the range of r; then to initiate the generation of the functions F_{l2} we need to evaluate $\mathcal{I}(R_{max})$

i.e.

$$\int_{R_{max}}^{\infty} r j_l(k_f r) e^{-\alpha r} dr \qquad \text{(C10)}$$

Now in this region of integration we may assume that the functions constituting the integrand of (C10) exhibit their asymptotic behaviours. Hence replacing the spherical Bessel function with its asymptotic form we obtain

$$\mathcal{I}(R_{max}) = \frac{1}{k_f}\int_{R_{max}}^{\infty} \sin(k_f r - \tfrac{1}{2}l\pi) e^{-\alpha r} dr$$

$$= \frac{1}{k_f}\cos\left(\frac{l\pi}{2}\right)\int_{R_{max}}^{\infty} \sin k_f r . e^{-\alpha r} dr + \frac{1}{k_f}\sin\left(\frac{l\pi}{2}\right)\int_{R_{max}}^{\infty} \cos k_f r . e^{-\alpha r} dr \qquad \text{(C11)}$$

If we introduce the quantities $S(R_{max})$ and $C(R_{max})$ defined by

$$S(R_{max}) = \frac{1}{k_f}\int_{R_{max}}^{\infty} \sin k_f r . e^{-\alpha r} dr = \frac{e^{-\alpha R_{max}}}{k_f(\alpha^2 + k_f^2)}\left[k_f \cos(k_f R_{max}) + \alpha \sin(k_f R_{max})\right]$$

$$C(R_{max}) = \frac{1}{k_f}\int_{R_{max}}^{\infty} \cos k_f r . e^{-\alpha r} dr = \frac{e^{-\alpha R_{max}}}{k_f(\alpha^2 + k_f^2)}\left[\alpha \cos(k_f R_{max}) - k_f \sin(k_f R_{max})\right] \qquad \text{(C12)}$$

then we may write

$$\mathcal{I}(R_{max}) = S(R_{max})\cos\left(\frac{l\pi}{2}\right) - C(R_{max})\sin\left(\frac{l\pi}{2}\right) \qquad \text{(C13)}$$

Using the formula (C13) to provide a starting value we are now able to generate the function values for the F_{l2} by use of the numerical technique previously described. These function values are combined with those corresponding to the F_{l1} , generated separately as previously described, in accordance with equation (C3).

The numerical techniques described here were tested by using a simple replacement for the function G_l , chosen to enable evaluation of the function $\mathcal{M}_l$ in closed analytic form. Since we are concerned with only a small range of values of l then it is sufficient to show that the techniques are reliable for the case $l=0$ (this not being special in any particular sense.) This case was tested by replacing G_0 by a simple exponential. The $\mathcal{M}_0$ function values generated by the numerical techniques were identical (to at least 6 figures) to those evaluated from the analytic form over the entire range of r.

Before concluding this section it is of interest to examine an alternative approach to the numerical construction of the F_{l2} functions. The inward integration involved in the method previously described may be replaced by the usual outward integration by rewriting the form of $\mathcal{I}(r_{i+1})$ in the following way

$$\mathcal{I}(r_{i+1}) = \int_{r_{i+1}}^{\infty} r j_l(k_f r) e^{-\alpha r} dr$$

$$= \int_0^{\infty} r j_l(k_f r) e^{-\alpha r} dr - \int_0^{r_{i+1}} r j_l(k_f r) e^{-\alpha r} dr \qquad \text{(C14)}$$

However subsequent application of this method showed it to be unstable, the resulting function values rapidly diverging from the true values in the asymptotic region. This alternative method involved the evaluation of the integrals $\int_0^{\infty} r j_l(k_f r) e^{-\alpha r} dr$, which were found to be expressable in closed analytic form. We shall now give a short account of the method used to generate these analytic forms.

Now $$j_l(k_f r) = \left(\frac{\pi}{2k_f r}\right)^{1/2} J_{l+1/2}(k_f r)$$

where $J_{l+\frac{1}{2}}(k_f r)$ denotes the ordinary Bessel function of order $l+\frac{1}{2}$

Hence

$$\int_0^\infty r\, j_l(k_f r) e^{-\alpha r} dr = \left(\frac{\pi}{2k_f}\right)^{\frac{1}{2}} \int_0^\infty r^{\frac{1}{2}} J_{l+\frac{1}{2}}(r k_f) e^{-\alpha r} dr$$

$$= \left(\frac{\pi}{2k_f}\right)^{\frac{1}{2}} \int_0^\infty r^{\mu-1} J_\nu(k_f r) e^{-\alpha r} dr$$

$$(\text{where } \mu = 3/2 \text{ and } \nu = l+1/2)$$

$$= \left(\frac{\pi}{2k_f}\right)^{\frac{1}{2}} \frac{\left(\frac{1}{2}\frac{k_f}{\alpha}\right)^{l+1/2} \Gamma(l+2)}{\alpha^{3/2}\, \Gamma(l+3/2)} \, {}_2F_1\left(\frac{l+2}{2}, \frac{l+3}{2}, l+3/2, -\frac{k_f^2}{\alpha^2}\right) \quad \text{(C15)}$$

In the previous expression ${}_2F_1$ denotes a hypergeometric function and Γ , the gamma function.

We wish to investigate the functional form of (C15) for integer values of l . If we exclude the simple case corresponding to $l=0$ then the cases to be considered fall into two classes. The first class corresponds to even values of l and the second to odd values.

(a) even values of l

Let $l = 2n$ (n an integer >0), and $z = \frac{k_f^2}{\alpha^2}$

Now

$$ {}_2F_1\left(\frac{l+2}{2}, \frac{l+3}{2}, l+3/2, -z\right) = {}_2F_1(n+1, n+3/2, 2n+3/2, -z) \quad \text{(C16)}$$

But

$$\frac{(1)_n (3/2)_n}{(n+3/2)_n} \, {}_2F_1(n+1, n+3/2, 2n+3/2, -z) = (-1)^n \frac{d^n}{dz^n} \, {}_2F_1(1, 3/2, n+3/2, -z)$$

(C17)

where we have the following definition

$$(x)_n = \frac{\Gamma(x+n)}{\Gamma(x)}$$

Also

$${}_2F_1(1,3/2,n+3/2,-z) = \frac{(5/2)_{n-1}(1+z)^{n-1}(-1)^{n-1}}{(3/2)_{n-1}(1)_{n-1}} \frac{d^{n-1}}{dz^{n-1}}\,{}_2F_1(1,3/2,5/2,-z) \qquad \text{(C18)}$$

If we now consider the series expansion of ${}_2F_1(1,3/2,5/2,-z)$ we find that it may be summed to give the result

$${}_2F_1(1,3/2,5/2,-z) = 3(z^{-1} - z^{-3/2}\tan^{-1} z^{1/2}) \qquad \text{(C19)}$$

Combining equations (C16 - C19) enables us to rewrite equation (C15) in the form

$$\int_0^\infty r j_{2n}(k_f r) e^{-\alpha r} dr = -\pi\left(\frac{k_f}{2}\right)^{2n} \frac{(2n)!}{[\alpha^{2n+2}(\Gamma(n+1/2))^2 n!(n-1)!]} \frac{d^n}{dz^n}\left\{(1+z)^{n-1}\frac{d^{n-1}}{dz^{n-1}}[z^{-1}-z^{-3/2}\tan^{-1}z^{1/2}]\right\} \qquad \text{(C20)}$$

(b) odd values of l

$$l = 2n+1$$

For these cases we need to consider the functions

$${}_2F_1(n+3/2,n+2,2n+5/2,-z)$$

But we have the result

$${}_2F_1(n+3/2,n+2,2n+5/2,-z) = \frac{(-1)^{n+1}(n+3/2)_{n+1}}{(1/2)_{n+1}(1)_{n+1}} \frac{d^{n+1}}{dz^{n+1}}\,{}_2F_1(1/2,1,n+3/2,-z) \qquad \text{(C21)}$$

Also

$$\frac{(1)_n(1/2)_n}{(3/2)_n}(1+z)^{-n}{}_2F_1(1/2,1,3/2+n,-z)=(-1)^n\frac{d^n}{dz^n}{}_2F_1(1/2,1,3/2,-z)$$

$$=(-1)^n\frac{d^n}{dz^n}[z^{-1/2}\tan^{-1}z^{1/2}]$$

(C22)

Using the results (C21) and (C22) we obtain

$$\int_0^\infty r j_{2n+1}(k_f r)e^{-\alpha r}dr=-\pi\left(\frac{k_f}{2}\right)^{2n+1}\cdot\frac{4}{\alpha^{2n+3}}\cdot\frac{(2n)!}{(\Gamma(n+1/2))^2(n!)^2}$$

$$\frac{d^{n+1}}{dz^{n+1}}\left\{(1+z)^n\frac{d^n}{dz^n}[z^{-1/2}\tan^{-1}z^{1/2}]\right\}$$

(C23)

where $z=\frac{k_f^2}{\alpha^2}$

The results contained in equations (C20) and (C23) were checked by numerical integration. The agreement between the numerical evaluation of the integrals and the corresponding results obtained from the analytic forms clearly showed these forms to be correct.

THE PROGRAMS

This section provides a brief description of the programs used for the calculation of the triple differential cross section based on the exchange adiabatic approximation of Economides and McDowell. The coding was written in FORTRAN IV and the programs were developed for use on the CDC series of London University. Consequently there are small sections of coding that are peculiar to the system used, but these can be easily modified.

For convenience the computation was split into two parts. The first part is concerned with the generation and storage of the angular independent quantities appearing in the calculations. The second part performs the majority of the calculations with the aid of the information previously stored. The corresponding programs are WRITEUP and TRIPLE 3 respectively.

WRITEUP

The main purpose of this program is to generate and store (on disc or tape) the numerical wave functions required in the calculatio
These wave functions fall into two classes. Firstly there are the exchange adiabatic or polarized orbital radial functions that appear in the partial wave expansion (3.10). The numerical techniques involved in the solution of the integro-differential equations satisfied by these functions have been described elsewhere. These functions are constructed by means of the sub-program POLORB (L. A. Morgan 1973).

Secondly there are the one electron radial functions used in the Configuration Interaction description of the target ground state given by equation (4.3). Since these functions have simple analytic forms expressible in terms of standard functions then they are easily generated without the need for a special subroutine. In addition the program also generates and stores the various combinations of these wave functions given by the "s" state summation appearing in the equation (4.20).

The various functions described here are evaluated at 1500 points (although this may be varied), the interval between successive points depending on the region. If i denotes the i^{th} point and h the step length then all our calculations are based on the partition $\{h = 0.005,\ i = 1,100;\ h = 0.01,\ i = 101,300;\ h = 0.02,\ i = 301,1500\}$. The information generated requires three cycles of permanent disc storage.

TRIPLE 3

For any particular set of values of the energy parameters this program may be used to calculate the triple differential cross section for a series of fixed values of θ_f and a range of values of θ_s covering the entire angular region. Alternatively the order of the angular loops within the program may be interchange

Prior to the calculation of angular dependent quantities we calculate any constant or purely energy dependent quantities. This part of the computation is performed by the subroutine PREANG 1.

PREANG 1

This subroutine in turn calls the subroutine USZERO and EXPOWER. The first of these generates the particular examples of the integrals $\int_0^\infty R_{nl} r\, u_\lambda(r, k_s) dr$ required in the calculations. The "s" state integrals of this type, corresponding to $l=\lambda=0$ appear in equation (4.42) while the "p" state counterparts, corresponding to $l=\lambda=1$, appear in (4.30). The second subroutin EXPOWER calculates the various combinations of "s" state parameters within the summation sign of (4.42). PREANG 1 combines the results from these two subroutines to obtain the expression (4.42) apart from the multiplicative constant.

As previously mentioned in chapter 4 the calculations of the triple differential cross section performed by this program used the Peterkop form of the exchange amplitude, obtained by a simple interchange of momentum vectors in the expression for the direct amplitude. Hence the coding for exchange terms is exactly analogous to that for the terms appearing in the direct amplitude.

The order in which the angular dependent quantities are computed depends on which scattering angle is to remain fixed. If θ_f, the scattering angle of the fast electron, remains fixed then the next subroutine called by TRIPLE 3 is ANGFDEP. This subroutine calculates most of the terms in the direct amplitude, using, for this purpose the subroutines SONE, PONE, ULINTS and FORMF.

Because a particular multiplicative constant may be common to several expressions it is of course logical to multiply by the constant after the expressions have been combined. Hence various quantities calculated in the program may differ from the actual expressions referenced through the absence of such multiplicative constants.

The subroutines SONE and PONE calculate the expressions F_{1B}^{S} (equation (4.25)) and F_{1B}^{P} (equation (4.30)) respectively. The subroutine ULINTS generates the momentum transfer dependent integrals appearing in the Legendre Polynomial expansion for F_{1A} given by equation (4.20). We have restricted the expansion to its first seven terms, including an appropriate correction for the discarded terms at a later stage. In common with other subroutines performing numerical integrations ULINTS uses the Simpson Rule. However since preliminary investigations indicated that the particular integrals to be evaluated were frequently amenable to the use of Gauss-

Laguerre Quadrature due allowance for the use of this method has been made. Each integral is first calculated by Gauss-Laguerre Quadrature. The pivotal points for the quadrature are then slightly modified and the calculation repeated. If the two results satisfy a suitable convergence condition the Simpson Rule integration is not activated. Otherwise the integration is performed in the usual way. We do not attempt the same proceedure for the corresponding exchange terms since Gauss-Laguerre Quadrature has proved to be unsuitable for these.

Finally the subroutine FORMF and its associated subroutines calculate the form factor defined by equation (4.31). Apart from instigating the calculation of the quantities described, subroutine ANGFDEP uses the results of SONE together with the appropriate phase factors to compute the real and imaginary parts of F_{1B}^{S}. Also the form factor is combined with the overlap integral (4.42), calculated by PREANG 1, to give (to within a multiplicative constant) the second term inside the brackets of (4.9). In the event of the roles of the two scattering angles being interchanged, so that θ_s remains fixed while θ_f varies, then the routine ANGFDEP is replaced by ANGSDEP. This generates exchange terms which are exactly analogous to the direct terms obtained from ANGFDEP.

Having completed the calculation of the appropriate direct or exchange terms the main program now enters the angular loop corresponding to the variable scattering angle. Control then passes to whichever of the two subroutines ANGFDEP and ANGSDEP depends on the variable angle and the corresponding calculations are performed as previously described. By this stage sufficient information has been generated to determine, within a multiplicative constant, the real and imaginary parts of the direct and exchange amplitudes and this is done by the subroutines RIMFD and RIFEXCH respectively. Because of the form of the exchange amplitude used in our model these two subroutines have identical structures. Hence we shall only describe the function of the first of these two subroutines. The purpose of the subroutine RIMFD is purely to collate information previously obtained and to set the values of the parameters for subroutine RIPARTS to which control next passes. The calculation of the quantity F_{1B}^{P}, defined by equation (4.30), has already been made apart from the inclusion of the phase factor and the Legendre Polynomial of order one. This calculation is now completed, the final expression being split into its real and imaginary parts (denoted by ONEPRE and ONEPIM respectively). The next step in the calculations is to extract the real and imaginary parts of F_{1A} (equation (4.20)). The integrals appearing in this series expansion have been previously generated by the subroutine ANGFDEP and it only remains to premultiply them by the appropriate Legendre functions and use the phase factors to separate out the real and imaginary parts. Following this the real and imaginary parts of F_1 (defined by equation (4.10)) are obtained from the appropriate combinations of the real and imaginary parts of F_{1A}, F_{1B}^{S} and F_{1B}^{P}. The penultimate step in the evaluation of the real and imaginary parts of the direct amplitude is to include the contributions arising from the second term in equation (4.9). This is easily achieved through the use of the appropriate phase factor since the magnitude of this term is already known. Finally the subroutine RIPARTS modifies the real part of the direct amplitude by making a correction for the higher order terms neglected through the truncation of the series expansion appearing in equation (4.20) (see appendix B). This correction is provided by the subroutine HIGHPW, and is obtained by replacing the radial functions $u_l(k_s,r)/r$ appearing in the relevant integrals by Spherical Bessel functions for which the integrals may be evaluated in closed analytic form. The integrals that result from the Spherical Bessel function replacement in the first seven terms of the expansion (4.20) are calculated by the subroutine CALBES 2. These are expressible in terms of Legendre functions of the second kind and their derivatives (see appendix B) which are generated by the subroutine DIVPOL 2 using the various recurrence relations that exist between the functions. The information thus generated is used by HIGHPW to calculate the first seven terms of the modified form of (4.20) the sum of which is denoted by SUMA.

The Spherical Bessel function replacement corresponds to a plane wave representation of the slow electron for which the quantity F_{1A} may be evaluated without recourse to the expansion (4.20). This calculation is performed by the subroutine BESRES, the result being denoted by BORNRES. The correction to the direct scattering amplitude is obtained by subtracting SUMA from BORNRES. Since both of these quantities are real the correction only affects the real part of the direct scattering amplitude. After the corrected amplitude has been calculated control is returned to the main program and from there to RIFEXCH which performs the corresponding calculations for the exchange amplitude. Finally these amplitudes are combined according to equations (1.99) and (1.106) by the subroutine XSECT3 so giving the triple differential cross section.

If so desired the program allows for the suppression of all exchange calculations through an appropriate option parameter. The output from the program can be obtained in punched card form in addition to the standard printout. This option is included to provide data cards for other programs performing further analysis.

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