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**IONIZATION OF ATOMS BY ELECTRON IMPACT**

A Thesis submitted to the  
Faculty of Science  
for the degree of  
Doctor of Philosophy

in

the University of Durham

by

Dionysius Gregory Economides, B.Sc. (London), M.Sc. (London)



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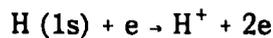
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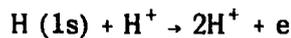
## ABSTRACT

In Chapter I of this thesis a short review of the quantal theory of ionizing collisions is presented, with particular regard to recent theoretical developments. A brief discussion is given of quantal and classical approximations and their predictions compared with experimental data, and a brief outline of some useful empirical formulae.

The impulse approximation is derived in Chapter II and the evaluation of cross sections for the processes

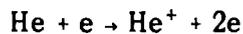


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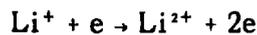


is described in detail. The results obtained for the above processes are presented and are compared with the results obtained by other authors.

In Chapter III the evaluation of cross sections for the processes



and



in which both He and  $\text{Li}^+$  are initially in their ground states is described in detail. An open shell two-parameter wave function has been used for the ground state of the target. The cross sections obtained using both the length and velocity formulations of the Born approximation are in excellent agreement with experiment at energies higher than 25 times threshold and approach the Bethe limit (within 3%) at energies higher than 50 times threshold. The evaluation of cross sections with Hylleraas type correlated wave functions for the ground state of the target forms the subject of Chapter IV. Cross sections are calculated in the length formulation of the Born approximation, for the processes studied in Chapter III and the results obtained are presented and are compared with the length and velocity formulation results obtained in the latter Chapter.

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CHAPTER I  
REVIEW OF THE THEORY OF THE IONIZATION OF ATOMS  
BY ELECTRON IMPACT

1. Introduction

In recent years considerable experimental and theoretical work has been devoted to the study of ionization cross sections of atoms or ions by electron impact. The interpretation of a wide variety of physical phenomena demands an accurate evaluation of these cross sections. Examples of such phenomena arise in the fields of thermonuclear research, plasma physics, shock waves through gases, in the study of stellar atmospheres and the solar corona. During the last few years considerable progress has been made towards obtaining accurate ionization cross sections. On the experimental side a great deal of work has been carried out in which single or multiple ionization cross sections of atoms or ions initially in their ground states have been measured. This work has been the subject of a review by Kieffer and Dunn (1966). Although there exists a considerable amount of experimental data these are far from exhaustive. Many species require investigation and difficulties arise in the experimental determination of ionization cross sections from excited states. In these cases recourse has been made to theoretical studies. On the theoretical side a great deal of work has been devoted to the basic formulation of the problem and it is found that the theory of ionizing collisions differs quite appreciably from the theory of collisions involving excitation. A number of new approximate quantal methods have been investigated but even so quantal calculations are rather lengthy and not yet as accurate as could be wished. Alternative approaches have therefore been pursued in order to obtain reasonably accurate estimates in a very simple way. These approaches arise through the use of classical rather than quantal methods and from devising

semi-empirical formulae which may be used to estimate as yet unmeasured or uncalculated data.

## 2. The Quantum Theory of Ionizing Collisions

Several very extensive review articles concerned with ionizing collisions have so far been published by Bates, Fundamirsky, Leech, and Massey (1950), Massey (1956), Veldre (1965) and Rudge (1968). In this Chapter a short review of the quantum theory of ionizing collisions is presented, with particular regard to recent theoretical developments. A brief discussion is given of quantal and classical approximations and their predictions compared with experimental data, as well as a brief outline of some useful empirical formulae. The discussion throughout this Chapter is confined to the theory of ionization of atoms or ions by electron impact but applies with very little modification to the case of ionization by other structureless charged particles.

### 2.1 Exchange in ionizing collisions

The treatment of exchange in ionizing collisions differs in several respects from the treatment appropriate to elastic collisions and bound-state excitation and the most important features may be seen from consideration of the simplest case of ionization of atomic hydrogen by electron impact. Suppose that the incident electron and the atomic electron are distinguishable by having opposite spins. In the case of excitation one may define a direct cross-section proportional to  $|f(n, \underline{k}_n)|^2$ , for the process in which the atomic electron is excited to state  $n$  and the incident electron is scattered with relative momentum  $\underline{k}_n$ , and an exchange cross section proportional to  $|g(n, \underline{k}_n)|^2$ , for the process in which the incident electron is captured in state  $n$  and the atomic electron is ejected with relative momentum  $\underline{k}_n$ . For the case of ionizing collisions one may similarly define a cross section, proportional to  $|f(\underline{k}, \underline{k}_f)|^2$ , for the process in which the incident electron is scattered with final

relative momentum  $\underline{k}_f$  and an 'exchange' cross section, proportional to  $|g(\underline{k}, \underline{k}_f)|^2$ , for the process in which the incident electron has final relative momentum  $\underline{k}$  and the atomic electron has final relative momentum  $\underline{k}_f$ . Clearly  $f(\underline{k}, \underline{k}_f)$  and  $g(\underline{k}_f, \underline{k})$ , the direct and exchange ionization scattering amplitudes, describe the same physical process and so they must be proportional to each other. Peterkop (1961) was the first to show that, when normalization and phase factors are suitably defined

$$f(\underline{k}, \underline{k}_f) = g(\underline{k}_f, \underline{k}) . \quad (2.1)$$

For excitation of state  $n$  of atomic hydrogen the total cross section is proportional to

$$|f(n, \underline{k}_n)|^2 + |g(n, \underline{k}_n)|^2 \quad (2.2)$$

for distinguishable electrons having opposite spins and to

$$\frac{1}{4} \{ |f(n, \underline{k}_n) + g(n, \underline{k}_n)|^2 + 3 |f(n, \underline{k}_n) - g(n, \underline{k}_n)|^2 \} \quad (2.3)$$

for indistinguishable electrons having random spins. In the case of ionization we have, using (2.1), that the cross sections are proportional to

$$|f(\underline{k}, \underline{k}_f)|^2 + |f(\underline{k}_f, \underline{k})|^2 \text{ (opposite spins)} \quad (2.4)$$

$$\frac{1}{4} \{ |f(\underline{k}, \underline{k}_f) + f(\underline{k}_f, \underline{k})|^2 + 3 |f(\underline{k}, \underline{k}_f) - f(\underline{k}_f, \underline{k})|^2 \} \text{ (random spins).} \quad (2.5)$$

The total ionization cross section, defined in terms of the number of ions produced, may be obtained by integrating over  $\underline{k}_f$  and  $\underline{k}$ , subject to the condition  $k_f > k$  (or  $k_f < k$ ), or by integrating over all  $\underline{k}_f, \underline{k}$  and dividing the result by two.

In the case of approximations for excitation  $g$  is taken to be zero when exchange is neglected. One then considers only the case for which the incident electron has a final energy which is larger than the (negative) final energy of the atomic electron.

For ionization one cannot, because of (2.1) put  $g = 0$ .

## 2.2 Threshold laws for single ionization

The problem which has received most of the attention in recent ionization studies has been the behaviour of the ionization cross section near threshold. This problem

has been the subject of investigations by (among others) Wannier (1953), by Geltman (1956), by Rudge and Seaton (1964), by Temkin (1966) and by Peterkop (1969).

By a classical approach, involving certain statistical-mechanical arguments, Wannier (1953) found that the threshold law for single ionization of an atom or ion has the form

$$Q \propto (E - I)^{1.127} \quad (2.6)$$

where  $Q$  is the total ionization cross section,  $E$  the total energy of the system and  $I$  the ionization potential of the atom or ion. A disadvantage of Wannier's result or of anyone else's from an experimental point of view is that there is no way of knowing how far above threshold this power law is supposed to be valid. From a theoretical point of view, it appears more desirable to approach this problem within the conventional framework of the quantum theory of inelastic collisions so that all approximations made may be clearly delineated. In their attempt to put the problem of the ionization of atomic hydrogen by electron impact on a rigorous theoretical footing Rudge and Seaton (1964), largely independently of Peterkop (1961), have derived an asymptotic form of the wave function. This asymptotic form can be used to determine a phase factor which must be known in order that an independently derived relation between direct and exchange ionization amplitudes be of use. Further, this asymptotic form is, in the important region of configuration space, proportional to the complex conjugate of a function  $\Phi$ , a product of two Coulomb waves whose charges are functions of the velocities of the outgoing particles. This is the underlying basis upon which the latter have deduced that for ionization of hydrogenic systems

$$Q \propto (E - I) \quad (2.7)$$

near threshold. The work of Rudge and Seaton (1964) has been criticized by Temkin (1966) who points out inadequacies in the above asymptotic form, and shows by means of a simple model that the neglect of certain terms which must be made in deriving it

is not justified. The two arguments taken together, he argues, indicate that the asymptotic form is not correct. This in turn has obvious negative implications about the aforementioned phase factor and about the validity of a linear law at threshold; he proposes an asymptotic form of the wave function which he argues is more acceptable, albeit less explicit, than the above. He then derives a  $3/2$  power law for the simple model and infers that this is the correct result for e-H ionization threshold behaviour. Geltman (1956) obtains a linear threshold law on assuming that both of the electrons in the final state move in the unscreened field of the nucleus, but gives no justification for this assumption.

Vinkalns and Gailitis (1967) have carried out a classical analysis of near threshold ionization of atomic hydrogen, similar to the work of Wannier, and deduced that there is a departure from linearity of about 1%.

In the case of detachment from negative ions the only Coulomb potential operating in the final state is the repulsion between the two free electrons or, for detachment by positron impact, there is a Coulomb attraction between the two free particles. The threshold laws deduced in this case are Rudge (1964), Hart, Grey and Guier (1957)

$$Q \propto (E - I)^{3/2} \quad (2.8)$$

for detachment from a negative ion by a particle which is positively charged and

$$Q \propto (E - I)^{3/2} \exp[-\gamma(E - I)^{-1/2}] \quad (2.9)$$

where  $\gamma$  is a constant, for detachment from a negative ion by a negatively charged particle.

Theoretically little has been predicted as to how far above threshold these threshold laws are supposed to be valid. For example the linear law states that at threshold the first derivative of the ionization cross section does not vanish but does not state what the relative magnitudes of the first to higher derivatives are in the

near-threshold region. All treatments ignore recoil of the target nucleus, i.e. they put the mass of the proton  $M_p = \infty$

### 2.3 Multiple ionization

Owing to the numerical difficulty of a full quantal calculation little theoretical work has been done on multiple ionization. Geltman (1956) carried out calculations for the double ionization of Helium by electron impact taking into account only the s-wave; both continuum electrons were represented as Coulomb waves belonging to charge  $z$ , with  $z$  the charge of the ion core. The final state of the atom was represented by the product of these two Coulomb waves and a delta function,  $\delta(\underline{k}_1 + \underline{k}_2)$  where  $\underline{k}_1$  and  $\underline{k}_2$  are the relative momenta of the two continuum electrons. The insertion of the delta function being based on the assumption that the dominant contribution to the cross section will arise from states in which the two ejected electrons take asymptotic directions just opposite to each other as a result of their mutual repulsion. Since s-waves only were included the calculations are only useful very near threshold, where the cross section behaves like  $(E - I)^2$ . This Geltman showed was in agreement with experimental data and inferred an  $(E - I)^n$  threshold law for n-tuple ionization. Using what is essentially a form of the Bethe approximation Mittleman (1966) and Byron and Joachain (1966) derived expressions for the ratio of the single to double ionization cross section valid at high energies. Mittleman (1966), using a Hartree-Fock function for the initial state of helium, finds a ratio  $Q_{\text{single}}/Q_{\text{double}} = 198$ . However, Byron and Joachain (1966) show that this ratio is strongly dependent on the form assumed for the initial and final state wave functions. (See also McDowell and Coleman (1969) for a more detailed criticism).

### 3. Quantal Approximations

The most salient features of the various quantal approximations which have been used may be discussed for the particular case of the ionization of atomic hydrogen.

### 3.1 Wave functions

Let  $\underline{r}_i$  denote the position vector of the  $i$  th electron relative to the nucleus, taken as a fixed origin,  $\underline{k}_i$  the momentum of the incident electron, and  $\underline{k}_f$  and  $\underline{k}$  the momenta of the continuum electrons in the final state.

The total Hamiltonian of the system is written as  $H$ , and in general for an electron colliding with an  $N$ -electron atomic system, neglecting spin-orbit and like interactions, is (in atomic units)

$$H = \sum_{i=1}^{N+1} H_i + \sum_{i>j} r_{ij}^{-1} \quad (3.1)$$

where  $H_i$  the single-electron Hamiltonian is

$$H_i = -\frac{1}{2} \nabla_i^2 - z/r_i \quad (3.2)$$

and

$$r_{ij} = |\underline{r}_i - \underline{r}_j|$$

Bound-state hydrogenic eigenfunctions are written  $\psi_\alpha(\underline{r})$  and satisfy the equation

$$H \psi_\alpha(\underline{r}) = E_\alpha \psi_\alpha(\underline{r}) \quad (3.3)$$

They are taken to be orthonormal with  $\alpha$  denoting collectively the quantum numbers  $n, l, m$ .  $\alpha = i$  and  $\alpha = f$  will be taken to refer to the initial and final states of the atom respectively. The continuum eigenfunctions satisfy

$$H \psi(\underline{z}, \underline{k}, \underline{r}) = \frac{1}{2} k^2 \psi(\underline{z}, \underline{k}, \underline{r}) \quad (3.4)$$

and are normalized such that

$$\int \psi(\underline{z}, \underline{k}, \underline{r}) \psi^*(\underline{z}, \underline{k}', \underline{r}) d\underline{r} = \delta(\underline{k} - \underline{k}') \quad (3.5)$$

The continuum solutions are not uniquely defined through the normalization condition (3.5). Integral expressions for the ionization amplitude involve a particular solution of (3.4) defined by

$$\psi(\underline{z}, \underline{k}, \underline{r}) = (2\pi)^{-3/2} \chi(\underline{z}, -\underline{k}, \underline{r}) \quad (3.6)$$

where

$$\chi(z, -\underline{k}, \underline{r}) = [2\pi\gamma / (1 - e^{-2\pi\gamma})]^{1/2} \exp[i\eta(\gamma)] \exp(-i\underline{k} \cdot \underline{r}) {}_1F_1[i\gamma, 1, i(kr + \underline{k} \cdot \underline{r})] \quad (3.7)$$

and

$$\gamma = z/k, \quad \eta(\gamma) = \arg \Gamma(1 - i\gamma)$$

and where  ${}_1F_1(a, c, x)$  is the confluent hypergeometric function.

Asymptotically

$$\chi(z, -\underline{k}, \underline{r}) \underset{r \rightarrow \infty}{\sim} \exp[-i(\underline{k} \cdot \underline{r} + \gamma \ln |kr + \underline{k} \cdot \underline{r}|)] + [f(\theta)/r] \cdot \exp i(kr + \gamma \ln 2kr), \quad (3.8)$$

where  $\cos \theta = -\hat{\underline{k}} \cdot \hat{\underline{r}}$  and

$$f(\theta) = \frac{\gamma \Gamma(1 - i\gamma) \exp\{2i\gamma \ln[\sin(\theta/2)]\}}{2k \Gamma(1 + i\gamma) \sin^2(\theta/2)} \quad (3.9)$$

### 3.2 Cross section expressions

Considering the particular case of the ionization of atomic hydrogen we let one of the continuum electrons be ejected with momentum  $\underline{k}_f$  in the solid angle  $d\hat{\underline{k}}_f$  and the other with momentum  $\underline{k}$  in the solid angle  $d\hat{\underline{k}}$ , and let the energy of one of them, no matter which, be in the range  $d\epsilon$ . The differential cross section is

$$I(\underline{k}_f, \underline{k}) d\hat{\underline{k}}_f d\hat{\underline{k}} d\epsilon, \quad (3.10)$$

where

$$\begin{aligned} I(\underline{k}_f, \underline{k}) &= \frac{k_f k}{4 k_i} \{ |f(\underline{k}_f, \underline{k}) + f(\underline{k}, \underline{k}_f)|^2 + 3 |f(\underline{k}_f, \underline{k}) - f(\underline{k}, \underline{k}_f)|^2 \} \\ &= \frac{k_f k}{k_i} \{ |f(\underline{k}_f, \underline{k})|^2 + |f(\underline{k}, \underline{k}_f)|^2 - \operatorname{Re} f^*(\underline{k}_f, \underline{k}) f(\underline{k}, \underline{k}_f) \}, \end{aligned} \quad (3.11)$$

where  $\operatorname{Re}$  denotes the real part.

The cross section for ejection of an electron with energy  $\epsilon$  in the range  $d\epsilon$  is  $\sigma(\epsilon) d\epsilon$  where

$$\sigma(\epsilon) = \int d\hat{\underline{k}}_f d\hat{\underline{k}} I(\underline{k}_f, \underline{k}), \quad (3.12)$$

and where  $\epsilon = \frac{1}{2} k^2$  or  $\frac{1}{2} k_f^2$ . Since  $E = \frac{1}{2} (k_f^2 + k^2)$  is constant,  $\sigma(\epsilon) = \sigma(E - \epsilon)$ .

The total cross section for production of ejected electrons is

$$Q = \int_0^E \sigma(\epsilon) d\epsilon \quad (3.13)$$

### 3.3 Born approximations

For atomic hydrogen Born's method consists in making the approximations

$$\begin{aligned} \Psi_i(\underline{r}_1, \underline{r}_2) &= \psi_i(\underline{r}_2) e^{i \underline{k}_i \cdot \underline{r}_1} , \\ \Psi_f(\underline{r}_1, \underline{r}_2) &= \frac{1}{(2\pi)^{3/2}} \chi^*(1, -\underline{k}, \underline{r}_2) e^{i \underline{k}_f \cdot \underline{r}_1} . \end{aligned} \quad (3.14)$$

This gives for the Born ionization scattering amplitude

$$\begin{aligned} f_B(\underline{k}_f, \underline{k}) &= -\frac{1}{2\pi} \iint \Psi_i(\underline{r}_1, \underline{r}_2) (H - E) \Psi_f^*(\underline{r}_1, \underline{r}_2) d\underline{r}_1 d\underline{r}_2 \\ &= -\frac{1}{(2\pi)^{3/2}} \iint \psi_i(\underline{r}_2) e^{i \underline{k}_i \cdot \underline{r}_1} \left( \frac{1}{r_1} - \frac{1}{r_{12}} \right) \chi^*(1, -\underline{k}, \underline{r}_2) e^{i \underline{k}_f \cdot \underline{r}_1} d\underline{r}_1 d\underline{r}_2 . \end{aligned} \quad (3.15) \quad / \psi$$

The choice of the functions  $\Psi_i$  and  $\Psi_f$  of Eq. (3.14) is not a serious defect at high energies, but at low energies it gives rise to substantial errors in the cross section and an incorrect threshold behaviour.

Neglect of exchange has been treated quite differently in work on ionizing collisions from what it has been in problems of excitation of discrete energy levels. Referring to Eq. (3.11) it is seen that neglecting exchange means that all terms involving  $f(\underline{k}, \underline{k}_f)$  should be excluded to give

$$Q[\text{Born (ii)}] = \frac{k_f}{\pi k_i} \int_0^{E/2} k d\left(\frac{1}{2}k^2\right) \iint d\underline{\hat{k}}_f d\underline{\hat{k}} |f_B(\underline{k}_f, \underline{k})|^2 \quad (3.16)$$

An expression frequently used has been

$$Q[\text{Born (i)}] = \frac{k_f}{\pi k_i} \int_0^E k d\left(\frac{1}{2}k^2\right) \iint d\underline{\hat{k}}_f d\underline{\hat{k}} |f_B(\underline{k}_f, \underline{k})|^2 \quad (3.17)$$

If we are dealing with ionization involving distinguishable particles then Equation (3.17) is the right expression to use. In the case of ionization by electron impact with random spin orientations, (3.17) would correspond to neglecting only the interference term of (3.11) while retaining the  $|f(\underline{k}, \underline{k}_f)|^2$  term. This procedure is obviously inconsistent and Eq. (3.16) is the more acceptable definition. The procedure followed in order to get Eq. (3.16) is analogous to that used for excitation in the Born approximation, in which one puts  $g = 0$ . Results were obtained in the two approximations for the cases of ionization of atomic hydrogen [ Rudge and Seaton (1965) ] from its ground state. When these are compared with the mean of the experimental measurements of Fite and Brackmann (1958), Boksenberg (1960), and Rothe et al (1963) it is seen that the Born (ii) approximation is superior to Born (i). Sloan (1965) made use of both forms of the Born approximation to evaluate cross sections for the ionization of Helium from its ground state by electron impact. His results when compared with the observed results of Smith (1930) show once again that the main features are the same as for hydrogen, with Born (ii) approximation being superior to Born (i).

In the case of ionization of a hydrogenic positive ion of nuclear charge  $z$  by electron impact, the appropriate expression for  $f_B$  is

$$f_B(\underline{k}_f, \underline{k}) = \frac{1}{(2\pi)^{5/2}} \int \psi_i(\underline{r}_2) \times (z-1, \underline{k}_i, \underline{r}_1) \left( \frac{1}{r_1} - \frac{1}{r_{12}} \right) \times (z, -\underline{k}, r_2) \times (z-1, -\underline{k}_f, \underline{r}_1) d\underline{r}_1 d\underline{r}_2 . \quad (3.18)$$

The name Coulomb – Born approximation is appropriate to this case in order to distinguish it from calculations where plane waves have been used to describe the incident and scattered electrons. The latter treatment is unsatisfactory at low energies but at higher energies becomes equal to (3.18).

Calculations in the Born (i) approximation have been reported in recent years by Omidvar (1965) for ionization of hydrogen from an initial state with principal quantum numbers  $n = 1$  (1) 10; for  $\text{He}^+$  in the 1s and 2s states by Burke and Taylor (1965); for helium in the ground state by Peach (1965) and by Dalgarno and McDowell (1956), the latter authors calculating also cross sections for excited states of helium with  $(n, l) = 2p, 3p, 4p, 3d, 4d$ ; for Li by McDowell et al (1965) and Peach (1965); for Be by Peach (1965); for Ne by Inokuti (1962). Cross sections for inner-shell ionization of Ni, Ag, and Hg in the Born approximation neglecting relativistic effects have been calculated by Burhop (1940). Arthurs and Moiseiwitsch (1958) have calculated cross sections for inner-shell ionization of Ni including relativistic effects, and Perlman (1960) has in similar fashion calculated inner-shell ionization of Ni and Hg.

The Born (ii) approximation has been used for ionization of the species indicated by the following authors: H (1s) Rudge and Seaton (1965); H (2s),  $\text{He}^+$  (1s), and  $\text{He}^+$  (2s) Rudge and Schwartz (1966a);  $\text{Fe}^{\text{XV}}$  and  $\text{Fe}^{\text{XVI}}$  Rudge and Schwartz (1966b); H, He, Li, Be Peach (1965); Na, Mg Peach (1966a); B, C, N, O, F, Ne, Al, Si, P, S, Cl, Ar Peach (1968); Na Bates et al (1965); He,  $\text{Li}^+$  Economides and McDowell (1969).

Additional approximations are involved in the description of the bound-state wave functions and the wave functions for the ejected electron, in all the calculations of ionization of nonhydrogenic systems.

### 3.4 The Bethe approximation

The Bethe approximation [ Bethe (1930)] is a further approximation to those already made in the Born approximation, and gives the form of the Born in the limit of very high impact velocities. The main features of the approximation may be seen by examining the case of atomic hydrogen. Performing the integration in (3.15) with respect to  $r_1$  gives

$$f_{\text{Born}}(\underline{k}_f, \underline{k}) = - \frac{2}{(2\pi)^{3/2} p^2} \int \psi_i(\underline{r}) e^{i \underline{p} \cdot \underline{r}} \chi(1, -\underline{k}, \underline{r}) d\underline{r}, \quad (3.19)$$

where  $\underline{p} = \underline{k}_i - \underline{k}_f$ . Expanding  $e^{i \underline{p} \cdot \underline{r}}$  as a power series, using the orthogonality condition, and assuming  $p$  is small, we have that

$$f_{\text{Bethe}}(\underline{k}_f, \underline{k}) = - \frac{2i}{(2\pi)^{3/2} p} \int \psi_i(\underline{r}) r \cos \theta \chi(1, -\underline{k}, \underline{r}) d\underline{r}, \quad (3.20)$$

where  $\hat{\underline{p}}$  is taken as the axis of quantization, and  $\cos \theta = \hat{\underline{p}} \cdot \hat{\underline{r}}$ . Now transforming the  $\hat{\underline{k}}_f$  integration of (3.16) to one over  $p$  gives the ionization cross section as

$$Q_{\text{Bethe}} = \frac{1}{\pi^3 k_i^2} \int_0^{E/2} k d\left(\frac{1}{2}k^2\right) \int_{p_{\min}}^{p_{\max}} \frac{dp}{p} \int d\hat{\underline{k}} | \langle i | r \cos \theta | -\underline{k} \rangle |^2, \quad (3.21)$$

where we define the notation

$$\langle i | r \cos \theta | -\underline{k} \rangle = \int \psi_i(\underline{r}) r \cos \theta \chi(1, -\underline{k}, \underline{r}) d\underline{r},$$

and where  $p_{\min} = k_i - k_f$  and  $p_{\max} = k_i + k_f$ . Since (3.20) is valid only for small values of  $p$ ,  $p_{\max}$  may be taken to be  $\tau(k_i + k_f)$ , where  $\tau$  is a constant less than unity, to give

$$Q_{\text{Bethe}} = \frac{1}{\pi^3 k_i^2} \int_0^{E/2} k \ln \left| \frac{\tau(k_i + k_f)}{k_i - k_f} \right| d\left(\frac{1}{2}k^2\right) \int d\hat{\underline{k}} | \langle i | r \cos \theta | -\underline{k} \rangle |^2. \quad (3.22)$$

Since the main contribution to the cross section comes from the region where  $k$  is small, we make the additional approximation by writing

$$\begin{aligned} k_i - k_f &\simeq 2I/(k_i + k_f) \\ &\simeq I/k_i, \end{aligned} \quad (3.23)$$

and (3.22) becomes

$$Q_{\text{Bethe}} = \frac{1}{\pi^3 k_i^2} \ln \left( \frac{2\tau k_i^2}{I} \right) \int_0^{E/2} | \langle i | r \cos \theta | -\underline{k} \rangle |^2 dk. \quad (3.24)$$

Writing  $E_i = \frac{1}{2} k_i^2$ , (3.24) takes the form

$$Q = A \ln E_i/E_i + B/E_i \quad (3.25)$$

where

$$A = \frac{1}{2\pi^3} \int_0^{E/2} | \langle i | r \cos \theta | -k \rangle |^2 dk$$

$$B = A \ln (4r/I) + \text{const.} \quad (3.26)$$

The additional constant in (3.26) arises from the terms which have been neglected in approximating (3.19) by (3.20). The constant A thus depends on the optical properties of the atom and can easily be evaluated, but the constant B depends on a full Born calculation since it is determined through the cut-off parameter  $r$  and the neglected terms. If we now use sum rules proved by Bethe (1930) and average over the  $m$  states, for large  $E$  the constant A may be written

$$A = \frac{4}{3} [ \langle r_{nl}^2 \rangle - \sum_{n'} | \frac{l+1}{2l+1} (R_{n,l}^{n', l+1})^2 + \frac{1}{2l+1} (R_{n,l}^{n', l-1})^2 | ] , \quad (3.27)$$

where

$$\psi_i(\mathbf{r}) = R_{nl}(r) Y_{lm}(\hat{\mathbf{r}}) , \quad (3.28)$$

$$R_{nl}^{n'l'} = \int_0^\infty r^3 R_{nl}(r) R_{n'l'}(r) dr , \quad (3.29)$$

and

$$\langle r_{nl}^2 \rangle = \int_0^\infty r^4 R_{nl}(r) R_{nl}(r) dr . \quad (3.30)$$

Alternatively, if  $\bar{f}_{n'l',nl}$  is the average oscillator strength defined by Bethe and Salpeter (1957) then we may write

$$A = 4 [ \frac{1}{3} \langle r_{nl}^2 \rangle - \sum_{n'} \frac{\bar{f}_{n'l',nl}}{2|E_n - E_{n'}|} ] . \quad (3.31)$$

The sums over  $n'$  in both (3.27) and (3.31) include  $n = n'$ .

An equivalent method may be used [Seaton (1962b)] to derive Bethe's approximation for ionization of ions. His method consists in replacing  $(\frac{1}{r_1} - \frac{1}{r_{12}})$  in (3.18) by  $-\frac{r_2}{r_1^2} P_1(\hat{r}_1, \hat{r}_2)$ . The essential difference that results is in the Gaunt factor  $\ln \left\{ r \frac{(k_i + k_f)}{k_i - k_f} \right\}$  which appears in (3.26). This is modified due to the charge on the ion, and appropriate Gaunt factor formulae are in this case given by Grant (1958).

In the case of complex atoms the appropriate formula for A is

$$A = 4 \left[ \frac{1}{3} \langle (\sum_i r_i)^2 \rangle - \sum_{n'l'} \frac{\bar{f}_{n'l', nl}}{2|E_n - E_{n'}|} \right] \quad (3.32)$$

In the case of hydrogen A decreases with l increasing for given n Bethe (1930), and Kingston (1965b) shows that when averaged over l is proportional to n. For  $H^-$  it follows from (3.32) that the constant A corresponding to the total detachment cross section is  $\frac{4}{3} \langle (r_1 + r_2)^2 \rangle$  and is large. In the case of the alkali metals on the other hand the dominant contribution to the sum over oscillator strengths in (3.32) comes from the resonance levels and in these cases A may be expected to be small.

Seaton (1959) expressed Equation (3.22) in the form

$$Q_{\text{Bethe}} = \frac{I_H}{\pi \alpha E} \int_0^{E/2 - I} \frac{a(w)}{I + W} \ln \left( \frac{4E}{I + W} \right) dw, \quad (3.33)$$

where  $a(w)$  is the photo-detachment cross section for photon energy  $(W + I)$ ,  $W$  the energy of the ejected electron,  $I_H$  the threshold ionization potential of hydrogen and  $\alpha$  the fine-structure constant. Seaton (1959) using Bethe's approximation derived a functional relation between the cross sections for electron impact ionization  $Q(E)$  and photo-detachment  $a(w)$  which may be used to give reasonable estimates of ionization cross sections. He considers two atoms, A and B, for which the photo-detachment cross sections  $a_A, a_B$  are such that

$$a_A(I_A x) / a_A(0) = a_B(I_B x) / a_B(0) \quad (3.34)$$

Then from (3.33) and (3.34)

$$I_A Q_A(I_A \epsilon) / a_A(0) = I_B Q_B(I_B \epsilon) / a_B(0) \quad (3.35)$$

Bethe's approximation (3.33) is valid for large values of  $\epsilon = E/I$ . For values of  $\epsilon$  which are not large (3.33) is expected to give similar percentage errors for  $Q_A$  and  $Q_B$  and that the functional relation (3.35) will remain a useful approximation. This approximation has been used by Seaton (1959) to calculate ionization cross sections for Ne, O, and N, and McDowell and Williamson (1963) have used the Bethe approximation, Equation (3.33), to calculate electron detachment cross section for  $H^-$  by electron impact.

### 3.5 The Born-Oppenheimer approximation

The Born-Oppenheimer approximation assumes that the relative phases of the direct and exchange amplitudes are the same for all  $\underline{k}_f$  and  $\underline{k}$ . Further it assumes that the slower electron screens one unit of nuclear charge from the faster electron. One disadvantage in the latter approximation arises from the lack of orthogonality between initial and final states which tends to give an unphysically large cross section close to threshold. This lack of orthogonality means that if a constant were added to the Hamiltonian (which corresponds to a null force), the cross section calculated in this approximation would change, and this is clearly absurd [Schiff (1952)]. Exchange is taken into account in this approximation by adopting expression (3.10) for the differential cross section. Burke and Taylor (1965) show that the method is much better in the case of ionization of positive ions than it is for neutral species. The Born-Oppenheimer approximation has been used by Geltman (1960) for  $H^-$ , by Malik and Trefftz (1961) for  $O^{4+}$ , by Trefftz (1963) for  $O^{5+}$ , and by Burke and Taylor (1965) for evaluating the ionization cross sections of H (1s), H (2s),  $He^+(1s)$  and  $He^+(2s)$ .

### 3.6 The Born-Exchange approximation

The Born-exchange approximation is an alternative to the Born-Oppenheimer approximation which makes use of the relation between the exact direct and exchange scattering amplitudes. This method is an improvement over the Born-Oppenheimer approximation in that there are no orthogonality difficulties. Making use of Eq. (2.1) for the magnitudes of the respective amplitudes and introducing a phase factor into the relationship, the approximation is

$$g_{\text{B.E.}}(\underline{k}_f, \underline{k}) = e^{i \tau(\underline{k}_f, \underline{k})} f_{\text{Born}}(\underline{k}, \underline{k}_f) \quad (3.36)$$

The method suffers from the inaccuracies inherent in adopting the Born approximation for  $f(\underline{k}_f, \underline{k})$  and these are likely to be greatest where  $k > k_f$ , that is the region where (3.36) is applied. Three possible choices which have been made for this phase factor are: (1) Peterkop (1962) defined

$$\tau_1(\underline{k}_f, \underline{k}) = \arg \{ f(\underline{k}_f, \underline{k}) / f(\underline{k}, \underline{k}_f) \}, \quad (3.37)$$

which gives the smallest cross section in any approximation for  $f$ , since it allows for maximum interference; (2) Peterkop (1962), Geltman, Rudge, and Seaton (1963), and Sloan (1965) defined

$$\tau_2(\underline{k}_f, \underline{k}) = \arg [ \Gamma(1 - iz/k_f) / \Gamma(1 - iz/k) ], \quad (3.38)$$

where  $z$  is the net charge on the new ion produced; (3) the third choice, which is useful when partial-wave expansions are used, has been described by Burgess and Rudge (1963) and by Rudge and Schwartz (1966a).

The Born-exchange approximation with various choices of the phase factor has been used by Peterkop (1962) and Geltman, Rudge, and Seaton (1963) for ionization of H (1s), by Rudge and Schwartz (1966a, b) for H (2s), He<sup>+</sup>(1s), He<sup>+</sup>(2s), Fe<sup>XV</sup>, and Fe<sup>XVI</sup>, by Sloan (1965) for He (1s<sup>2</sup>), and by Peach (1966b) for ionization of He, Li, Be, Na, and Mg from their ground states.

The results of Peterkop (1962) and Geltman, Rudge, and Seaton (1963) for ionization of H (1s) and those of Sloan (1965) for He (1s<sup>2</sup>) show that the Born-exchange approximation gives substantial improvement over Born calculations.

### 3.7 The Born-Ochkur approximation

The Born-Ochkur approximation retains the Born approximation for the direct scattering amplitude but selects an alternative expression for the exchange scattering amplitude. Different formulae have been proposed, the first given by Ochkur (1964) appropriate to excitation problems and the second, by Ochkur (1965) appropriate to ionization problems. Rudge (1965) modified the expression of Ochkur for excitation and derived a third formula, by a different argument, which he shows to be obtainable from a variational principle while Ochkur's is not.

Ochkur (1964) and (1965) argues that the deficiencies of the calculations using the Born-Oppenheimer approximation are not due to the fact that the method is essentially bad, but due to an incorrect extrapolation into the low energy region. In the derivation of the Born-Oppenheimer formula, as in the derivation of the Born formula, the incident and scattered electrons are both described by plane waves. This is correct at high energies, and it is obvious Ochkur argues, that if we consider this condition to be satisfied and expand the Born-Oppenheimer expression for the exchange scattering amplitude in a series in inverse powers of  $k_i$  or  $k_f$ , then only the leading term of this series will have a real meaning. The remaining terms he discards because they are of higher order of smallness. In the case of excitation he obtains, by this procedure, the result that for neutral species

$$g_{\text{Och}}^{(1)} = \frac{p^2}{k_i^2} f_{\text{Born}} \quad (3.39)$$

Extending his analysis to the ionization case Ochkur (1965) obtains the result

$$g_{\text{Och}}^{(2)}(\underline{k}_f, \underline{k}) = \frac{p^2}{|\underline{k}_i - \underline{k}|^2} f_{\text{Born}}(\underline{k}_f, \underline{k}), \quad (3.40)$$

which he further simplifies by replacing  $|\underline{k}_i - \underline{k}|^2$  by  $(k_i^2 - k^2)$  to give a third approximation

$$g_{\text{Och}}^3(\underline{k}_f, \underline{k}) = \frac{p^2}{(k_i^2 - k^2)} f_{\text{Born}}(\underline{k}_f, \underline{k}). \quad (3.41)$$

The derivation of Ochkur's results is of an ad hoc nature and is not clear why his method is a marked improvement over the Born-Oppenheimer approximation. The  $1/r$  term which appears in the Born-Oppenheimer approximation is simply discarded in this approach. The discarded term gives a large contribution to the cross section due to the non orthogonality of the initial and final states and this might probably account for some of the improvement, but in the problem of proton-hydrogen atom, charge transfer, for example, the neglect of this term leads to worse results rather than an improvement.

The Born-Ochkur approximation Equation (3.41) has been applied by Ochkur (1965) for ionization of H (1s); the Born-Ochkur method Eq. (3.39) has been used by Prasad (1965) for H (1s), H (2s), and H (2p), by Peach (1966b) for ionization of He, Li, Be, Na and Mg from their ground states, and by Peach (1968) for ionization of B, C, N, O, F, Ne, Al, Si, P, S, Cl and Ar from their ground states.

A comparison of the results of Ochkur (1965) with the Born (ii) results of Rudge and Seaton (1965) and experimental data shows that the Born-Ochkur method is a marked improvement over the Born.

### 3.8 The distorted-wave Born-Oppenheimer method

Apart from the question of phase of the amplitude, the most drastic approximation used in evaluating the scattering amplitude has been the form assumed for  $\Psi_i(\underline{r}_1, \underline{r}_2)$ .

Burke and Taylor (1965) have carried out calculations in which the initial state is represented in the form

$$\Psi_i(\underline{r}_1, \underline{r}_2) = [1 + (-1)^S P_{12}] \sum_{nl_1} \psi_{nl_1}(\underline{r}_2) F_{nl_1}(\underline{r}_1), \quad (3.42)$$

where  $\psi_{nl_1}(\underline{r}_2)$  are hydrogenic eigenfunctions and the sum over  $nl_1$  in (3.42) goes over 1s, 2s and 2p states.  $F_{nl_1}(\underline{r}_1)$  are determined through the Hartree-Fock equations

$$\int \psi_{nl_1}^*(\underline{r}_2) (H - E) \Psi_i(\underline{r}_1, \underline{r}_2) d\underline{r}_2 = 0, \quad (3.43)$$

and the operator  $[1 + (-1)^S P_{12}]$  explicitly symmetrizes or anti-symmetrizes the solution according to the total spin  $S$ . The final state was chosen as in the Born-Oppenheimer approximation. A comparison of this approximation with the Born, Born-exchange approximation, and experiment for ionization from the ground state shows that, despite the much greater complexity of Eq. (3.43), there is little improved agreement with experiment, which indicates that a better description of the final state is also necessary. In the case of ionization from the 2s state, Burke and Taylor find that the effects of close coupling in the initial state are of much greater importance. Similar work to that of Burke and Taylor (1965) has been carried out by Veldre and Vinkalns (1963).

### 3.9 Improved final-state approximation

This approximation has been described by Rudge and Schwartz (1966) and applied by them to ionization of H (1s). The method consists in adopting the approximations

$$\begin{aligned} \Psi_i(\underline{r}_1, \underline{r}_2) &= \psi_i(\underline{r}_2) e^{i \underline{k}_i \cdot \underline{r}_1}, \\ \Psi_f(\underline{r}_1, \underline{r}_2) &= \frac{1}{(2\pi)^3} \chi^*(z_e - \underline{k}_f, \underline{r}_1) \chi^*(1, -\underline{k}, \underline{r}_2), \end{aligned} \quad (3.44)$$

with

$$z_e = 1 - \frac{k_f}{|\underline{k}_f - \underline{k}|}. \quad (3.45)$$

With this choice a linear-threshold behaviour is obtained but, in order to evaluate the cross section, one more integration is needed than in the previous approximations. A little improvement is obtained in the agreement between theory and experiment in the case where exchange is neglected. However, at higher energies than 1.5 times threshold there is a discrepancy between theory and experiment and this discrepancy increases with inclusion of exchange. This they argue might be due to choice of effective charges.

### 3.10 Geltman approximation

In this approximation both continuum electrons are represented as Coulomb waves belonging to charge  $z$ , with  $z$  the charge on the new ion produced. The method of Geltman (1956) was adopted by Trefftz (1963) and by Malik and Trefftz (1961) in considering the ionization of  $O^{4+}$  and  $O^{5+}$ . A linear-threshold behaviour is obtained in this way but the cross section is over-estimated at low energies. This approximation has been examined in great detail by Veldre and Vinkalns (1963) both including and excluding exchange.

### 3.11 Plane-wave approximation

In this approximation plane waves are used to describe both continuum electrons, one of these being orthogonalized to the ground state of the atom. This approximation has been used by Michael (1963) in considering the ionization of hydrogen and cesium. A threshold behaviour like  $E^2$  is obtained, which gives results which are too low at low energies, while it over-estimates in the region of the maximum of the cross section. The approximation is very poor.

### 3.12 Impulse approximation

This approximation forms the subject of Chapter II.

## 4. Classical Approximations

The application of classical mechanics to describe ionizing collisions involves

three basic approximations. These are:

- (1) The initial state of the system is described quantumly.
- (2) The collision is described in terms of Newtonian Laws of motion.
- (3) In the simplest case of ionization of hydrogen by electron impact the equations of motion are further simplified by treating the three-body problem as though it were a sum of two-body collisions.

#### 4.1 The Thomson theory

Thomson (1912), in the earliest treatment of ionizing collisions, considered classically the ionization of an atom of mass  $m_2$  and charge  $z_2e$  by a particle of mass  $m_1$  and charge  $z_1e$  with the assumption that the atomic electron is at rest. The energy transfer  $\Delta E$  in the course of a Coulomb collision in which the incident particle has speed  $v$  and impact parameter  $b$  relative to the atomic electron is

$$\Delta E = \frac{2\mu^2 v^2 \sin^2 \frac{\theta}{2}}{m_2} \quad (4.1)$$

where  $\theta$  is the angle between the initial and final relative velocities and

$\mu = m_1 m_2 / (m_1 + m_2)$  is the reduced mass. Expressing (4.1) in terms of  $b$  we get

$$\Delta E = \frac{2\mu^2 v^2 z_1^2 z_2^2 e^4}{m_2 [z_1^2 z_2^2 e^4 + b^2 v^4 \mu^2]} \quad (4.2)$$

The Thomson expression for the cross section is given by

$$Q = 2\pi \int_0^{b_{\max}} b \, db, \quad (4.3)$$

with  $b_{\max}$  chosen so that  $\Delta E = I$ , the ionization potential.

The cross section for an energy transfer  $\Delta E = I$ , in the case of a collision between two free electrons, is

$$Q = \frac{\pi e^4}{E_i} \left( \frac{1}{I} - \frac{1}{E_i} \right) (\text{cm}^2) .$$

In terms of the Bohr radius,  $a_0 = \hbar^2/me^2$ , and the hydrogen ionization potential,  $I_H = me^4/2\hbar^2$ , this gives

$$Q = 4 \left( \frac{I_H}{I} \right)^2 \left( \frac{1}{x} \right) \left( 1 - \frac{1}{x} \right) (\pi a_0^2) , \quad (4.4)$$

where  $E_i = \frac{1}{2} m_i v^2$  and  $x = E_i/I$ . We have assumed in deriving (4.4) that only one electron was available to be removed from the atom. In the case of ionization from a shell of  $n$  equivalent electrons (4.4) must be multiplied by  $n$ . The first prediction of Thomson's theory is that ionization cross sections obey a scaling law expressed by saying that

$$\bar{Q}(x) = \left( \frac{I}{I_H} \right)^2 \frac{Q}{n} \quad (4.5)$$

is a universal function of  $n$ . It is referred to as the reduced ionization cross section. This result is useful and a comparison with experimental data for H, He and  $\text{Na}^+$  shows that for these species at low and intermediate energies the prediction is in good agreement with data. However, (4.4) does not give the correct shape of the ionization curve. Bethe's theory shows that at high energies the cross section behaves like  $A \ln E_i/E_i + B/E_i$ , but in (4.4) there is no logarithmic dependence. This is a severe drawback, because at high energies the logarithmic term is the dominant. Thomson's theory for ionization by other particles, for example, protons or alpha particles gives for the cross section the Thomson formula

$$Q = (4 I_H^2 z_1^2 z_2^2 / v^4) \left[ \frac{2v^2}{I} - \left( \frac{1 + m_1}{m_1} \right)^2 \right] . \quad (4.6)$$

This formula predicts a threshold where

$$\frac{1}{2} m_1 v^2 = \frac{I (1 + m_1)^2}{4 m_1}, \quad (4.7)$$

which is only correct for electrons with  $m_1 = 1$ . The correct expression for the threshold energy is

$$\frac{1}{2} \frac{m_1 m_2}{m_1 + m_2} v^2 = I, \quad (4.8)$$

so that for ionization of atomic hydrogen by proton impact, for example, at threshold  $v^2 \simeq 4I/m_2$ , while in Thomson's theory  $v^2 \simeq I/2$ . Equation (4.6) shows that the cross section for ionization by proton impact, for example, approaches from above the cross section for ionization by an electron having the same velocity, as the velocity increases. This result may be derived from quantal expressions for the ionization cross section, but Thomson was the first to deduce this relationship.

#### 4.2 The classical methods of Gryzinski and others

Interest in the classical methods appeared to have lapsed for many years but the publication of Gryzinski's work [Gryzinski (1959)] dramatically revived it. Essentially this was an independent reworking of the calculation of Williams (1927) and Thomas (1927). Gryzinski used the results of Chandrasekhar (1941) and Chandrasekhar and Williamson (1941), who calculated the energy transfer between two colliding particles moving arbitrarily with respect to one another under an inverse square law force. Scattering in Gryzinski's calculation is considered in the centre of mass frame of the incident and struck electrons followed by transformation to a frame at rest relative to the nucleus. In the course of his calculation Gryzinski made the simplifying approximation of replacing the true relative speed of the electrons  $v = |\underline{v}_1 - \underline{v}_2|$  by its average value  $(v_1^2 + v_2^2)^{1/2}$ . This approximation was later removed by Ochkur and Petrun'kin (1963) and by Stabler (1964). Defining  $E_2$  to be the initial

kinetic energy of the atomic electron, introducing another reduced variable  $y = E_2/I$ , and assuming the distribution of electron velocities to be isotropic, Stabler's result for the ionization cross section is

$$Q = 4n \left(\frac{I_H}{I}\right)^2 \frac{1}{x} \left\{ 1 + \frac{2y}{3} - \frac{1}{x-y} \right\} \quad x \geq y + 1$$

$$- \frac{8n}{3} \left(\frac{I_H}{I}\right)^2 \frac{1}{x} \left\{ \frac{(x-1)^3}{y} \right\}^{1/2} \quad 1 \leq x \leq y + 1 \quad (4.9)$$

With the additional approximation mentioned above and taking  $y = 1$ , Gryzinski's result for the ionization cross section is

$$Q = 4n \left(\frac{I_H}{I}\right)^2 \left(\frac{x}{x+1}\right)^{3/2} \frac{1}{x} \left(\frac{5}{3} - \frac{2}{x}\right) \quad x \geq 2$$

$$- \frac{16\sqrt{2}n}{3} \left(\frac{I_H}{I}\right)^2 \left(\frac{x}{x+1}\right)^{3/2} \frac{1}{x} \left(1 - \frac{1}{x}\right)^{1/2} \quad 1 \leq x \leq 2. \quad (4.10)$$

A comparison of the Gryzinski-Stabler classical theory Eq. (4.9) with experimental data for H(1s) shows that far from improving the Thomson theory it actually makes it worse. The subsidiary approximation made by Gryzinski to give (4.10) suffers like (4.9) from the following defects:

- (a) The shape of the ionization curve is still in error at high energies.
- (b) The low energy behaviour of the cross section is like  $(x-1)^{3/2}$  rather than  $(x-1)$ , as given quantumly and in the Thomson theory.

The position of the maximum given by (4.9) is incorrect, though for hydrogen the position of the maximum given by (4.10) is more correct and numerical values are in better accord at intermediate energies.

One may conclude that neither (4.9) nor (4.10) represents an appreciable improvement over the Thomson theory.

In order to force a logarithmic dependence in the ionization cross section Gryzinski reconsidered the problem in a series of papers (1965 a, b, c) by assuming a continuous velocity distribution for the atomic electron. An empirical distribution function was chosen so that on averaging over this distribution, a logarithmic dependence would be obtained. He introduced the following distribution function for the atomic electron:

$$f(v) = a v^{-3} \exp(-\beta/v), \quad (4.11)$$

where  $a$  and  $\beta$  are constants. This is completely at variance with any quantal velocity distribution; the fact that it yields an infinite kinetic energy also leads to difficulties. Burgess and Percival (1968) point out whom we quote: "We feel that it could not be accepted by any who interpret atomic structure according to quantum mechanics in the final analysis." By averaging over the distribution (4.11) Gryzinski obtains

$$Q = 4\pi \left(\frac{I_H}{I}\right)^2 \left(\frac{1}{x}\right) \left(\frac{x-1}{x+1}\right)^{3/2} \left[1 + \frac{2}{3}\left(1 - \frac{1}{2x}\right) \ln \{2.7 + (x-1)^{1/2}\}\right]. \quad (4.12)$$

Eq. (4.12) again has an incorrect form at threshold. There is now a logarithmic term, but the coefficient multiplying it is in general incorrect, the correct factor being given by (3.27). The choice of the velocity distribution (4.11) is made in an arbitrary fashion which is simply an ad hoc device for obtaining the logarithmic term of (4.12).

Gryzinski (1965 d) reconsidered the problem of velocity distribution for the atomic electron. He argues that the correct velocity distribution is that for an electron of a Bohr atom in which it has only radial motion, corresponding to a degenerate line ellipse. The velocity distribution is in this case

$$f(v) = \frac{4}{\pi} v_n^{-3} (v^2 + v_n^2)^{-2}, \quad (4.13)$$

where  $\frac{1}{2} v_n^2 = |E_n|$ , and where  $E_n$  is the energy at the initial state with principal quantum number  $n$ . Kingston (1964 a, b, 1966 a, b) has applied the Gryzinski (1959) theory and the corrected form of this theory to electron impact ionization from the ground state and several excited states of hydrogen. He gives cross sections obtained from putting  $E_i = I$  and from averaging over the proper quantum mechanical velocity distribution, and compares them with Born approximation results. Prasad and Prasad (1963) have used the Gryzinski (1959) theory with  $E_i = I$ , to calculate ionization cross sections for several atoms and diatomic molecules by electron and proton impact. McDowell (1966) and Vriens (1967) have worked out the theory for a binary encounter between an incident proton and an initially bound electron with non-zero  $E_i$ , to first order in  $m_e/m_p$ . McDowell gives the ionization cross section, and Vriens the quantity  $dQ(\Delta E)/d(\Delta E)$  which is then integrated to give excitation or ionization cross sections.

Fock (1935) has shown that the momentum distribution for the level  $n$  of the quantal H atom is independent of  $n$  and is given by

$$\rho(\underline{p}) = \frac{8 p_C^5}{\pi^2 (p^2 + p_C^2)^3}, \quad (4.14)$$

where the classical momentum  $p_C$  is given by

$$p_C^2 = 2m_e I, \quad (4.15)$$

and where  $m_e$  is the mass of the bound electron. Abrines and Percival (1966 a, b) and Mapleton (1966) show that the result (4.14) is obtained also from the classical micro-canonical distribution provided that an integration is performed over the classical angular momentum. However, if such an integration is not effected, then, for a degenerate line ellipse, Mapleton (1966) shows that the Gryzinski result (4.13) is obtained. Abrines and Percival (1966), Percival and Valentine (1966), and Abrines, Percival and Valentine (1966) integrated the classical equations of motion exactly

thus discarding the binary encounter approximation. The initial momentum distribution was taken to be that given by (4.14) and a Monte Carlo calculation was performed to average over initial classical states of the system. Percival and Valentine (1966) show that for proton impact ionization of hydrogen the result of removing the binary encounter approximation is to reduce the cross section by a factor of 2 at its maximum. A comparison of the results of Abrines et al. (1966) for electron impact ionization of hydrogen with experimental data shows a quite reasonable agreement. The agreement with experiment is not nearly so good as for protons at low incident electron velocities; this disagreement is due in part at least to the quantum mechanical interference between direct and exchange scattering, which is shown to be important by the binary encounter theories.

#### 4.3 The exchange-classical approximation

In order to improve the Thomson theory Burgess (1963) and (1964) argues that certain features of the quantal treatment must be introduced into the approximation. The first of these features is that exchange must be incorporated in the approximation. This in a purely classical treatment is obviously impossible but the Thomson cross section expression makes a good starting point for a semi-classical modification of the theory. Including exchange means that the Thomson cross section expression, Eq. (4.3), is replaced by

$$Q = \frac{8}{k_i^2} \int_0^{\frac{1}{2}(\frac{1}{2}k_i^2 - I)} \left\{ \frac{1}{k_f^4} + \frac{1}{(2I + k^2)^2} - \frac{1}{k_f^2(2I + k^2)} \cos \left[ \frac{1}{k_i} \ln \left( \frac{2I + k^2}{k_f^2} \right) \right] \right\} d \left( \frac{1}{2}k^2 \right), \quad (4.16)$$

with the usual energy relation

$$\frac{1}{2} k_i^2 - \frac{1}{2} k_f^2 = \frac{1}{2} k^2 + I,$$

and where the upper limit of integration has been chosen to be in agreement with

quantal theory. However the integrand in (4.16) is not symmetric, i.e., the relationship  $f(\underline{k}_f, \underline{k}) = g(\underline{k}, \underline{k}_f)$  is not satisfied [ Burgess (1963) ]. If integration in (4.16) is extended over the full range of energy and a factor of  $\frac{1}{2}$  is introduced, which is an equivalent procedure in a quantal treatment, then (4.16) diverges. In order to get over this difficulty Burgess (1963) made use of a procedure similar to the one employed by De la Rippelle (1949). The expression (4.16) is then replaced by one which is symmetric in  $k_f$  and  $k$ . This expression is given by

$$Q = \frac{2}{(k_i^2 + 2I)} \int_0^{\frac{1}{2}(k_i^2 - I)} \left\{ \frac{1}{(2I + k_f^2)^2} + \frac{1}{(2I + k^2)^2} - \frac{1}{(2I + k_f^2)(2I + k^2)} \cos \left[ \frac{1}{(2I + k_i^2)^{1/2}} \ln \left( \frac{2I + k^2}{2I + k_f^2} \right) \right] \right\} dk^2. \quad (4.17)$$

Assuming the argument of the cosine is constant and equal to  $\gamma$ , then (4.17) becomes

$$Q = 4 \left( \frac{IH}{I} \right)^2 \frac{1}{(x + 1)} \left\{ 1 - \frac{1}{x} - \cos \left[ \gamma \ln \left( \frac{x}{1 + x} \right) \right] \right\}. \quad (4.18)$$

Burgess (1964) and Vriens (1966) assume the atomic electron to have an initial kinetic energy. This complicates the analysis and the results of these authors do not coincide. Vriens (1966), on carrying through the procedure of Burgess (1964), obtains

$$Q = 4 \left( \frac{IH}{I} \right)^2 \frac{1}{(x + \frac{T}{I})} \left\{ 1 - \frac{1}{x} + \frac{2}{3} \gamma \left( 1 - \frac{1}{x^2} \right) - \frac{\cos(\gamma \ln x)}{1 + x} \right\}, \quad (4.19)$$

where  $T$  is the gain in kinetic energy of the incident electron.

Expressions (4.18) and (4.19) are a substantial improvement in the theory in that they remove one of the major defects of the Thomson expression. However they do not represent the correct high energy behaviour.

#### 4.4 Exchange-classical impact parameter (ECIP) approximation

If the influence of the nucleus may be ignored the close electron-electron

encounters have been treated exactly in the previous sections. On the other hand in the impact parameter method Alder et al.(1965) and Seaton (1962b), the distant collisions are treated in a good approximation. Burgess (1963) and (1964) in his efforts to improve the Thomson theory suggested combining the previous theory with an impact-parameter formulation. Calculations by Burgess (1964) indicate considerable success for this method. The treatment is elegant in that the correct behaviour at low and high energies is obtained while at the same time the quantitative predictions are profoundly sound. Unfortunately the method does not produce any simple formula such as those obtained previously.

#### 5. Empirical Formulae For Ionization Cross Sections

In using empirical formulae to calculate ionization cross sections certain criteria must be met, these being:

- (a) To give a good fit to the known data at all energies.
- (b) To predict variations in the ionization cross sections for members of iso-electronic sequences.
- (c) To give the variations in the ionization cross sections as a function of the quantum numbers of the initial state.

A multitude of empirical formulae have appeared in the literature many of which are only of limited usefulness and have been superseded by the formulae we discuss below.

The latest and most extensive list of formulae for ionization cross sections and for reaction rates for ionization has been compiled by Lötzt (1967). Lötzt writes the ionization cross section in the form

$$Q = \zeta_1 \frac{a \ln (E/I_1)}{I_1 E} \quad \text{if} \quad I_1 \leq E < I_2$$

$$= \sum_{j=1}^N \zeta_j \frac{a \ln (E/I_j)}{I_j E} = \zeta \frac{a \ln (E/I)}{I E} \quad \text{if} \quad E > I_N \quad (5.1)$$

The expression (5.1) applies to an atom or ion containing several shells of electrons, the  $I_j$  being successive ionization potentials;  $a$  is a fixed constant, and the  $\zeta_j$  are numbers, the relevant values of which Lötzt tabulates for the three energy regions of the ionization curve. For the high energy part of the ionization curve the  $\zeta_j$  are equal to the number of electrons in each shell. The constants are determined from experimental data and apply to ionization from the ground state.

The expression (5.1) is derived from a very successful formula of Drawin (1961), who writes the reduced cross section of Eq. (4.7) in the form

$$\bar{Q}(x) = 2.66 f_1 \left(\frac{x-1}{x}\right) \ln (1.25 f_2 x) \quad (5.2)$$

where  $x$  is the reduced energy and  $f_1$  and  $f_2$  are constants which, in the absence of further data, Drawin recommends be taken equal to unity. Expression (5.2) has a linear behaviour near the threshold region and its form at high energies agrees with the Bethe theory. It gives a very reasonable estimate of the ionization cross section for a large number of species from their ground states but with the choice  $f_1 = f_2 = 1$  it is less accurate for ionization from excited states.

Percival (1966) gives formulae for the average cross section for ionization from excited states of hydrogen and hydrogenic positive ions. The formula of Percival for the average ionization cross section from an initial state of hydrogen with principal quantum number  $n$  is

$$\begin{aligned} \bar{Q}(x) &= (x - 1) (1.19 \ln x + 5.26) / (x^2 + 1.67 x + 3.57) && \text{if } n = 1 \\ &= (x - 1) \left\{ \frac{1.28}{n} \ln \left( \frac{x}{n^2} \right) + 6.67 \right\} / (x^2 + 1.67 x + 3.57) && \text{if } n \geq 2 . \end{aligned} \quad (5.3)$$

For large  $x$  and large  $n$ , (5.3) gives

$$Q(x) \sim \frac{6.67}{x} ,$$

a form which derives from the Gryzinski or exchange-classical approximations when the initial kinetic energy of the bound electron is taken to be equal to  $I$ . It has been shown by Abrines and Percival (1966b) that for large  $n$ , the classical and quantal cross sections are equal when expressed in terms of the reduced energy, and calculations performed by Abrines, Percival and Valentine (1966) are in accord with the exchange-classical results at high energies. The reduced ionization cross section of hydrogenic positive ions, Percival (1966) writes

$$\bar{Q}(z, x) = 1 + \frac{2.3}{\left(1 - \frac{1}{z^2}\right) + 2(x-1)^2} \bar{Q}(1, x) , \quad (5.4)$$

where  $z$  is the nuclear charge.

For positive ions the reduced ionization cross sections are greater than for the neutral member of the given isoelectronic sequence as a result of the focusing of the incident electron beam by the attractive Coulomb field of the ion. If we denote by  $z_i$  the initial charge on the ion, then a factor of focusing  $F$  can be defined by

$$F = 1 + \frac{z_i}{x^{1/2}} , \quad (5.5)$$

and the reduced ionization cross section for the isoelectronic sequence can be written

$$\bar{Q}(z_i, x) = F \bar{Q}(0, x) . \quad (5.6)$$

In the case of the hydrogen isoelectronic series expressions (5.4) and (5.6) give a good representation of the variation of the reduced cross section with  $z$ .

## CHAPTER II

### THE IMPULSE APPROXIMATION

#### 1. Introduction

Fermi (1936) was the first to make an explicit study of an impulse approximation in discussing the effect of molecular binding on neutron scattering by protons in hydrogen molecules. Chew (1950) introduced the term "impulse approximation" in connection with nucleon-deuteron scattering. Studies of this approximation were subsequently made by Chew and Wick (1952) and by Ashkin and Wick (1952) and the approximation generalised by Chew and Goldberger (1952) within the framework of the formal theory of scattering.

The basic assumption of the impulse approximation is that the effects of the binding potential of the target can be neglected during the collision, except insofar as it determines the initial state of the system. This neglect of the effects of the binding potential is termed the impulse hypothesis, in analogy with the treatment of impulsive reactions in classical mechanics, where the motion of the target is neglected for the very short time during which the impulsive force acts.

In the present Chapter our primary aim is to reconsider the approximation used by Akerib and Borowitz (1961). In view of this we shall restrict our attention to a model problem in which the effects of the interaction between the projectile and the target nucleus are neglected, this essentially being the model considered by Akerib and Borowitz. In the case of electron impact the possibility of exchange is consistently excluded.

#### 2. Notation

Atomic units are used ( $e$ , the electron charge,  $m$ , the mass of the electron, and  $\hbar$ , Planck's constant divided by  $2\pi$ , are taken as the fundamental units and therefore

have the value unity);  $E$  denotes the total positive energy of the system in these units. Cross section expressions and cross sections are expressed in units of  $\pi a_0^2$ , where  $a_0$  is the first Bohr radius of atomic hydrogen ( $\pi a_0^2$  is  $8.806 \times 10^{-17}$  cm<sup>2</sup>).

Throughout this Chapter we shall be concerned with collisions between a structureless particle 1 and an hydrogen atom consisting of a nucleus 2 and an electron 3.

The masses and charges of the particles 1 and 2 are denoted by  $M_1$ ,  $M_2$  and  $z_1$ ,  $z_2$  respectively and  $\underline{r}_1$ ,  $\underline{r}_2$ ,  $\underline{r}_3$  are the position vectors of the three particles with respect to some arbitrary fixed origin  $O$ . The relative co-ordinates  $\underline{R}$ ,  $\underline{x}$  and  $\underline{r}$  are defined by

$$\underline{R} = \underline{r}_1 - \underline{r}_2, \quad \underline{x} = \underline{r}_3 - \underline{r}_1, \quad \underline{r} = \underline{r}_3 - \underline{r}_2 . \quad (2.1)$$

If the position vector of particle 1 with respect to the centre of mass of 2 and 3 is denoted by  $\underline{\sigma}$  and that of the centre mass of 1 and 3 with respect to 2 by  $\underline{\rho}$  then

$$\underline{\sigma} = a \underline{r} - \underline{x}, \quad \underline{\rho} = \underline{r} - b \underline{x} , \quad (2.2)$$

where the dimensionless quantities  $a$  and  $b$  are defined by

$$a = \frac{M_2}{M_2 + 1} \quad b = \frac{M_1}{M_1 + 1} . \quad (2.3)$$

The position vector,  $\underline{G}$ , of the centre of mass of the system with respect to the origin  $O$  is given by

$$\underline{G} = \frac{1}{M} (M_1 \underline{r}_1 + M_2 \underline{r}_2 + \underline{r}_3) , \quad (2.4)$$

where  $M = M_1 + M_2 + 1$ .

In the centre-of-mass frame of reference the Hamiltonian of the system is

$$H = H_0 + V_{12} + V_{13} + V_{23} , \quad (2.5)$$

where  $V_{ij}$  is the potential acting between particles  $i$  and  $j$ , and  $H_0$  is the kinetic energy operator.

With the use of Equations (2.1) – (2.3) the kinetic energy operator can be expressed in the alternative forms

$$H_0 = -\frac{1}{2\mu} \nabla_{\underline{\sigma}}^2 - \frac{1}{2a} \nabla_{\underline{r}}^2 \quad (2.6)$$

$$= -\frac{1}{2\mu'} \nabla_{\underline{\rho}}^2 - \frac{1}{2b} \nabla_{\underline{x}}^2$$

where

$$\mu = \frac{M_1 M_2}{M} (M_2 + 1) \quad , \quad \mu' = \frac{M_1 M_2}{M} (M_1 + 1) \quad (2.7)$$

At infinite separation of the target and projectile before the collision the Hamiltonian of the system is

$$H_i = H_0 + V_{23} \quad (2.8)$$

Let  $\phi_i(\underline{r})$  and  $\epsilon_i$  be the wave function and corresponding eigen energy of state  $i$  of the system (2 + 3). Then  $\phi_i(\underline{r})$  satisfies the equation

$$\left\{ -\frac{1}{2a} \nabla_{\underline{r}}^2 + V_{23}(\underline{r}) \right\} \phi_i(\underline{r}) = \epsilon_i \phi_i(\underline{r}) \quad (2.9)$$

If  $\underline{k}_i$  is the initial relative momentum of the colliding systems, the wave function  $\psi_i$  of the initial unperturbed state of the system is given by

$$\psi_i = e^{i \underline{k}_i \cdot \underline{\sigma}} \phi_i(\underline{r}) \quad (2.10)$$

and satisfies the Schrödinger equation

$$H_i \psi_i = E \psi_i \quad (2.11)$$

where

$$E = \frac{1}{2\mu} k_i^2 + \epsilon_i \quad (2.12)$$

The form of the final unperturbed wave function  $\psi_f$  depends on the type of transition

considered. The normalization has been chosen so that  $\psi_i$  represents a projectile beam of unit density.

The wave function  $\Psi_i$  of the system, in the presence of the perturbing potential  $V_i$ , satisfies the equation

$$(H - E) \Psi_i = 0. \quad (2.13)$$

This may be written as

$$(E - H_i) \Psi_i = V_i \Psi_i, \quad (2.14)$$

where

$$V_i = V_{i2} + V_{i3}. \quad (2.15)$$

Equation (2.14) is equivalent to the integral equation

$$\Psi_i^\pm = \psi_0 + (E - H_i \pm i\epsilon)^{-1} V_i \Psi_i^\pm. \quad (2.16)$$

In (2.16)  $\epsilon$  is a small positive quantity which is allowed to go to zero when all the relevant integrations have been carried out, and  $\psi_0$  is any solution of (2.11) determined from the boundary conditions imposed on the relevant solution of (2.14).  $\Psi_i^+$  and  $\Psi_i^-$  are solutions of (2.14) obtained from (2.16) with the former solution containing outgoing scattered waves and the latter containing ingoing scattered waves. The wave function which describes the colliding systems in the presence of all their interactions and which evolves from the state  $\psi_i$  is

$$\Psi_i^+ = \psi_i + (E - H_i + i\epsilon)^{-1} V_i \Psi_i^+. \quad (2.17)$$

If A and B are two operators for which inverse operators  $A^{-1}$  and  $B^{-1}$  exist, then

$$A^{-1} = B^{-1} + B^{-1} (B - A) A^{-1} \quad (2.18a)$$

$$= B^{-1} + A^{-1} (B - A) B^{-1}. \quad (2.18b)$$

Writing

$$G_i^\pm = (E - H_i \pm i\epsilon)^{-1} \quad (2.19)$$

we have that the Green's functions operators

$$G^{\pm} = (E - H \pm i \epsilon)^{-1} \quad (2.20)$$

satisfy the integral equations

$$G^{\pm} = G_i^{\pm} + G^{\pm} V_i G_i^{\pm} \quad (2.21a)$$

$$= G_i^{\pm} + G_i^{\pm} V_i G^{\pm} . \quad (2.21b)$$

By operating on both sides of (2.17) with  $G^+ V_i$  and making use of (2.21a) we obtain

$$\begin{aligned} G^+ V_i \Psi_i^+ &= G^+ V_i \psi_i + G^+ V_i G_i^+ V_i \Psi_i^+ \\ &= G^+ V_i \psi_i + (G^+ - G_i^+) V_i \Psi_i^+ . \end{aligned} \quad (2.22)$$

It follows that

$$G^+ V_i \psi_i = G_i^+ V_i \Psi_i^+ , \quad (2.23)$$

and

$$\Psi_i^+ = (1 + G^+ V_i) \psi_i . \quad (2.24)$$

## 2.1 Formal derivation of the impulse approximation

The wave function for the three-particle system, corresponding to an initial state  $\psi_i$  and outgoing wave boundary conditions is

$$\Psi_i^+ = \Omega^+ \psi_i , \quad (2.25)$$

where

$$\Omega^+ = 1 + G^+ V_i , \quad (2.26)$$

The three-body scattering operator  $\Omega^+$  is expanded in terms of the simpler two-body operators  $\omega_{ij}^+$  defined below; from this expansion the impulse approximation will be derived.

Let  $\chi_m$  belong to the complete set of free-particle wave functions satisfying the the Schrödinger equation

$$(H_0 - E_m) \chi_m = 0 . \quad (2.27)$$

The two-body operators  $\omega_{ij}^+$  ( $i, j = 1, 2, 3, i \neq j$ ) are defined by the equation

$$\begin{aligned}\omega_{ij}^+(m) \chi_m &= [1 + (E_m - H_0 - V_{ij} + i\epsilon)^{-1} V_{ij}] \chi_m \\ &= \psi_m^+(ij) \quad .\end{aligned}\tag{2.28}$$

It is clear that the function  $\psi_m^+(ij)$  satisfies the equation

$$(H_0 + V_{ij} - E) \psi_m^+(ij) = 0\tag{2.29}$$

provided that

$$\begin{aligned}\lim_{\epsilon \rightarrow 0^+} \epsilon \psi_m^+(ij) &= 0 \quad .\end{aligned}\tag{2.30}$$

It has been shown by Mapleton (1961) that the condition (2.30) is not satisfied when  $V_{ij}$  is a Coulomb potential and in that case (2.29) will be taken as the equation defining  $\psi_m^+(ij)$ .

Taking  $A = E_m - H_0 - V_{ij} + i\epsilon$  and  $B = E - H + i\epsilon$  and making use of the operator identity (2.18b) gives

$$\begin{aligned}G^+ &\equiv (E - H + i\epsilon)^{-1} = (E_m - H_0 - V_{ij} + i\epsilon)^{-1} \\ &+ G^+ [E_m - E + V_{12} + V_{13} + V_{23} - V_{ij}] (E_m - H_0 + V_{ij} + i\epsilon)^{-1}\end{aligned}\tag{2.31}$$

and therefore

$$G^+ V_{ij} = b_{ij}^+(m) + G^+ [E_m - E + V_{12} + V_{13} + V_{23} - V_{ij}] b_{ij}^+(m) ,\tag{2.32}$$

where the operators  $b_{ij}^+$  are defined by

$$b_{ij}^+(m) = \omega_{ij}^+(m) - 1 \quad ,\tag{2.33}$$

where the plane wave basis  $\chi_m$  is understood. Operating on  $\psi_i$  and making use of the fact that

$$\begin{aligned}(E_m - E) \langle \chi_m | \psi_i \rangle &= \langle E_m \chi_m | \psi_i \rangle - \langle \chi_m | E \psi_i \rangle \\ &= - \langle \chi_m | V_{23} | \psi_i \rangle\end{aligned}\tag{2.34}$$

we obtain

$$\begin{aligned}
G^+ V_{ij} \psi_i &= \sum_m G^+ V_{ij} \chi_m \langle \chi_m | \psi \rangle \\
&= \sum_m [b_{ij}^+ (m) + G^+ \{E_m - E + V_{12} + V_{13} + V_{23} - V_{ij} | b_{ij}^+ (m)\}] \chi_m \langle \chi_m | \psi_i \rangle \\
&= \{b_{ij}^+ + G^+ [V_{23}, b_{ij}^+] + G^+ (V_{12} + V_{13} - V_{ij}) b_{ij}^+ | \psi_i \rangle, \tag{2.35}
\end{aligned}$$

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

$$b_{ij}^+ = \sum_m b_{ij}^+ (m) | \chi_m \rangle \langle \chi_m | . \tag{2.36}$$

Combination of (2.26), (2.35) and the definition of  $V_i$  gives

$$\Omega^+ = (\omega_{12}^+ + \omega_{13}^+ - 1) + G^+ [V_{23}, (b_{12}^+ + b_{13}^+)] + G^+ (V_{12} b_{13}^+ + V_{13} b_{12}^+), \tag{2.37}$$

where

$$\omega_{ij}^+ = b_{ij}^+ + 1 . \tag{2.38}$$

The transition matrix element is given by

$$T_{if} = \langle \psi_f | V_f | \Psi_i^+ \rangle \tag{2.39a}$$

$$= \langle \Psi_f^- | V_i | \psi_i \rangle \tag{2.39b}$$

where  $V_f$  is the perturbation in the final state and

$$\Psi_f^- = (1 + G^- V_f) \psi_f . \tag{2.40}$$

From a combination of Equations (2.25), (2.37) and (2.39a) we have that

$$\begin{aligned}
T_{if} &= \langle \psi_f | V_f | (\omega_{12}^+ + \omega_{13}^+ - 1) \psi_i \rangle \\
&+ \langle \psi_f | V_f | G^+ [V_{23}, (b_{12}^+ + b_{13}^+)] \psi_i \rangle \\
&+ \langle \psi_f | V_f | G^+ (V_{12} b_{13}^+ + V_{13} b_{12}^+) \psi_i \rangle . \tag{2.41}
\end{aligned}$$

The neglect of the effects of the binding potential means that the commutator involving the potential  $V_{23}$  will vanish. This simplified (2.41) but some additional approximation must be made before one can evaluate  $T_{if}$ . The third term in (2.41) arises from multiple scattering and it vanishes if  $V_{12}$  is zero. When the projectile is a heavy particle, the contribution to  $T_{if}$  from the potential  $V_{12}$  is expected to be

of the order of  $1/M$  compared with the contributions from other potentials, and therefore negligible. For a more detailed discussion the reader is referred to Bransden (1965) or McDowell and Coleman (1969). In applications of the theory it is customary to make the additional approximation of neglecting  $V_{i2}$  in  $V_f$  and of replacing  $\omega_{i2}^+$  by unity. Thus we obtain

$$T_{if}^{IMP} = \langle \psi_f | V_f | \omega_{i3}^+ \psi_i \rangle, \quad (2.42)$$

which is called the "post" form of the approximation.

By expanding  $\Psi_f^-$  in terms of the operators

$$\omega_{ij}^- \equiv \sum_m \omega_{ij}^-(m) | \chi_m \rangle \langle \chi_m |$$

where

$$\omega_{ij}^-(m) = [1 + (E - H_0 - V_{ij} - i\epsilon)^{-1} V_{ij}] \chi_m$$

we obtain the "prior" form of the approximation. In general the cross sections obtained from the post and prior forms are not equal and their difference is called the post-prior discrepancy.

## 2.2 Reduction of the transition matrix element

In this section the transition matrix element given by (2.42) is reduced to a form suitable for computation. The processes considered are:

$$H(1s) + \left\{ \begin{matrix} e \\ H^+ \end{matrix} \right\} \rightarrow H^+ + e + \left\{ \begin{matrix} e \\ H^+ \end{matrix} \right\}. \quad (2.43)$$

In the impulse approximation the cross section for the processes (2.43) is given by

$$Q = \frac{\mu}{4\pi^3} \left( \frac{k_f}{k_i} \right) \int_0^{k_{\max}} k^2 dk \iint d\hat{k} d\hat{k}_f | T_{if}^{IMP} |^2 (\pi a_0^2), \quad (2.44)$$

where the vectors  $\underline{k}$  and  $\underline{k}_f$  are as defined in Chapter I. Transforming the  $\hat{k}_f$  integration of (2.44) to one over  $p$ , defined in Chapter I, gives the ionization cross section as

$$\begin{aligned}
Q &= \frac{\mu^2}{2\pi^2 k_i^2} \int_0^{k_{\max}} dk \int_{p_{\min}}^{p_{\max}} p |T_{if}^{\text{IMP}}|^2 dp \\
&= \frac{\mu^2}{2\pi^2 k_i^2} \int_0^{k_{\max}} dk \int_{p_{\min}}^{p_{\max}} p |I_{12} + I_{13}|^2 dp, \quad (2.45)
\end{aligned}$$

where

$$I_{ij} = \langle \psi_f | V_{ij} | \omega_{13}^+ \psi_i \rangle \quad (2.46)$$

with  $V_{12} = \frac{z_1}{R}$  and  $V_{13} = -\frac{z_1}{x}$ . In accordance with the definition (2.28) of the operator  $\omega_{13}^+$ , the wave function  $\omega_{13}^+ \psi_i$  can be written as

$$\begin{aligned}
\omega_{13}^+ \psi_i &= \sum_m \omega_{13}^+ \chi_m \langle \chi_m | \psi_i \rangle \\
&= \sum_m \psi_m^+(13) \langle \chi_m | \psi_i \rangle, \quad (2.47)
\end{aligned}$$

and a convenient set of plane wave solutions of (2.27) is

$$\chi_m = (2\pi)^{-3} \exp [i(\underline{K} \cdot \underline{x} + \underline{t} \cdot p)] \quad ; \quad (2.48)$$

the energy  $E_m$  is then given by

$$E_m = \frac{1}{2} \left( \frac{K^2}{b} + \frac{t^2}{\mu} \right), \quad (2.49)$$

and the summation over  $m$  in (2.47) implies integration over all values of  $\underline{K}$  and  $\underline{t}$ . With  $i = 1$  and  $j = 3$ , (2.29) becomes

$$\left( \frac{1}{2\mu} \nabla_{\underline{t}}^2 + \frac{1}{2b} \nabla_{\underline{x}}^2 + \frac{z_1}{x} + E_m \right) \psi_m^+(13) = 0. \quad (2.50)$$

This equation is satisfied by

$$\psi_m^+(13) = N(K) \chi_m {}_1F_1 \left[ \frac{i\alpha}{K}, 1, i(Kx - \underline{K} \cdot \underline{x}) \right] \quad (2.51)$$

with  $\alpha = bz_1$  and

$$N(K) = e^{\pi\alpha/2K} \Gamma \left( 1 - \frac{i\alpha}{K} \right). \quad (2.52)$$

Using Eqs. (2.2), (2.10) and (2.48) it follows that

$$\begin{aligned} \langle \chi_m | \psi_i \rangle &= (2\pi)^{-3} \int \int d\underline{x} d\underline{r} \psi_{1s}(\underline{r}) \exp[-i(\underline{K} \cdot \underline{x} + \underline{t} \cdot \underline{\rho} - \underline{k}_i \cdot \underline{\sigma})] \\ &= G_{1s}(\underline{a}\underline{k}_i - \underline{t}) \delta(\underline{k}_i + \underline{K} - \underline{b}\underline{t}), \end{aligned} \quad (2.53)$$

where

$$G_{1s}(\underline{u}) = \int e^{i\underline{u} \cdot \underline{r}} \psi_{1s}(\underline{r}) d\underline{r}.$$

Substitution of (2.51) and (2.53) in (2.47) gives

$$\begin{aligned} \omega_{1s}^+ \psi_i &= (2\pi)^{-3} \int \int d\underline{K} d\underline{t} N(\underline{K}) \exp[i(\underline{K} \cdot \underline{x} + \underline{t} \cdot \underline{\rho})] {}_1F_1\left[\frac{i\underline{a}}{\underline{K}}, 1, i(\underline{K}\underline{x} - \underline{K} \cdot \underline{x})\right] \\ &\quad \times G_{1s}(\underline{a}\underline{k}_i - \underline{t}) \delta(\underline{k}_i + \underline{K} - \underline{b}\underline{t}) \\ &= (2\pi b)^{-3} \int d\underline{K} N(\underline{K}) \exp(-i\underline{k}_i \cdot \underline{k}_i) {}_1F_1\left[\frac{i\underline{a}}{\underline{K}}, 1, i(\underline{K}\underline{x} - \underline{K} \cdot \underline{x})\right] \\ &\quad \times G_{1s}\left\{\underline{k}_i\left(a - \frac{1}{b}\right) - \frac{1}{b}\underline{K}\right\} \exp\left[\frac{i}{b}(\underline{k}_i + \underline{K}) \cdot \underline{r}\right], \end{aligned} \quad (2.54)$$

the final result being obtained by performing the  $\underline{t}$  integration and noting that

$$\delta(\alpha \underline{t}) = \alpha^{-3} \delta(\underline{t}).$$

With

$$\psi_f = e^{i\underline{k}_f \cdot \underline{\sigma}} \phi_f(\underline{r}) \quad (2.55)$$

we have, using Eqs. (2.42), (2.54), (2.55) and the definition of  $I_{ij}$ , that

$$\begin{aligned} I_{1s} &= (2\pi b)^{-3} \int \int d\underline{x} d\underline{r} e^{-i\underline{k}_f \cdot \underline{\sigma}} \phi_f^*(\underline{r}) V_{1s} \int d\underline{K} N(\underline{K}) e^{-i\underline{k}_i \cdot \underline{x}} \\ &\quad \times {}_1F_1\left[\frac{i\underline{a}}{\underline{K}}, 1, i(\underline{K}\underline{x} - \underline{K} \cdot \underline{x})\right] G_{1s}\left\{\left(a - \frac{1}{b}\right)\underline{k}_i - \frac{1}{b}\underline{K}\right\} e^{\frac{i}{b}(\underline{k}_i + \underline{K}) \cdot \underline{r}}. \end{aligned} \quad (2.56)$$

since  $V_{1s} = -\frac{Z_1}{x}$ , (2.56) gives

$$I_{13} = -(2\pi b)^{-3} z_1 \int d\mathbf{K} N(\mathbf{K}) G_{1s} \left( -\frac{1}{\mu} \mathbf{k}_i - \frac{1}{b} \mathbf{K} \right) G_f^* \left[ -\frac{1}{b} (\mathbf{k}_i + \mathbf{K}) + a \mathbf{k}_f \right] I(-\mathbf{p}, \mathbf{K}) \quad (2.57)$$

where

$$I(\mathbf{p}, \mathbf{K}) = \int d\mathbf{x} \frac{1}{x} e^{i\mathbf{p} \cdot \mathbf{x}} \left[ F_1 \frac{ia}{K}, 1, i(\mathbf{Kx} - \mathbf{K} \cdot \mathbf{x}) \right] \quad (2.58)$$

The evaluation of  $I(\mathbf{p}, \mathbf{K})$  is discussed in Appendix A. Substituting (A.9) in (2.57) we obtain

$$I_{13} = -\frac{z_1}{2\pi^2 b^3 p^2} \int d\mathbf{K} N(\mathbf{K}) G_{1s} \left( -\underline{v} - \frac{1}{b} \mathbf{K} \right) G_f^* \left( -\underline{v} - \frac{1}{b} \mathbf{K} - a \mathbf{p} \right) \times \left[ \frac{(-\underline{p} + \mathbf{K})^2 - K^2}{p^2} \right]^{-\frac{ia}{K}}, \quad (2.59)$$

where  $\underline{v} = \frac{1}{\mu} \mathbf{k}_i$ .

If the interaction between the projectile and the target nucleus,  $V_{12}$ , is neglected and if it is assumed that the ejected electron is adequately represented by a plane wave

$$\phi_f(\mathbf{r}) = (2\pi)^{-3/2} e^{i\mathbf{k} \cdot \mathbf{r}} \quad (2.60)$$

then (2.45) becomes

$$Q = \frac{1}{2\pi^2 v^2} \int_0^{k_{\max}} dk \int_{p_{\min}}^{p_{\max}} p |I_{13}|^2 dp, \quad (2.61)$$

and

$$G_f^* \left( -\underline{v} - \frac{1}{b} \mathbf{K} - a \mathbf{p} \right) (2\pi)^{-3/2} \int e^{i \left( \underline{v} + \frac{1}{b} \mathbf{K} + a \mathbf{p} - \mathbf{k} \right) \cdot \mathbf{r}} d\mathbf{r} = (2\pi)^{3/2} \delta \left( \underline{v} + \frac{1}{b} \mathbf{K} + a \mathbf{p} - \mathbf{k} \right) \quad (2.62)$$

Substituting (2.62) in (2.59) we obtain

$$I_{11} = - \left(\frac{2}{\pi}\right)^{1/2} \frac{Z_1}{p^2} N(K) G_{1S}(a \underline{p} - \underline{k}) \left[1 - \frac{2}{p^2} \underline{p} \cdot \underline{K}\right]^{-\frac{i\alpha}{K}}, \quad (2.63)$$

where  $\underline{K} = \underline{b}\underline{k} - \underline{a}\underline{p} - \underline{b}\underline{v}$ . The Fourier transform of the initial state is easily evaluated; since  $\phi_{1S}(\underline{r}) = \pi^{-1/2} e^{-r}$  we have that

$$\begin{aligned} G_{1S}(a \underline{p} - \underline{k}) &= \pi^{-1/2} \int e^{i(a \underline{p} - \underline{k}) \cdot \underline{r}} e^{-r} d\underline{r} \\ &= \frac{8 \pi^{1/2}}{[1 + (a \underline{p} - \underline{k})^2]^2} \end{aligned} \quad (2.64)$$

Substituting (2.64) and (2.52) in (2.63) gives

$$I_{11} = -8 \sqrt{2} \frac{Z_1}{p^2} e^{\frac{\pi\alpha}{2K}} \left[ \frac{\pi\alpha}{K \sinh\left(\frac{\pi\alpha}{K}\right)} \right]^{1/2} [1 + (a \underline{p} - \underline{k})^2]^{-2} \left[1 - \frac{2}{p^2} \underline{p} \cdot \underline{K}\right]^{-\frac{i\alpha}{K}} e^{i\eta}, \quad (2.65)$$

where  $\eta = \arg \Gamma\left(1 - \frac{i\alpha}{K}\right)$ .

An undesirable consequence of the use of a plane wave to describe the ejected electron is the lack of orthogonality between the initial and final unperturbed wave functions. In the Bethe approximation (Chap. I, 3.4), the dipole term provides the major contribution to the ionization cross section which for large incident energies  $E_i$  takes the form

$$Q = A \ln E_i/E_i + B/E_i.$$

However, if non-orthogonal wave functions are used the monopole term does not vanish and the resulting cross section tends to a finite (non-zero) value as  $E_i \rightarrow \infty$ . This difficulty can be circumvented by using a Coulomb wave or, more simply, the function

$$\begin{aligned} \phi_f(\underline{r}) &= (2\pi)^{-3/2} [e^{i \underline{k} \cdot \underline{r}} - \langle e^{i \underline{k} \cdot \underline{r}} | \phi_{1S}(\underline{r}) \rangle \phi_{1S}(\underline{r})] \\ &= (2\pi)^{-3/2} \left[ e^{i \underline{k} \cdot \underline{r}} - \frac{8}{(1+k^2)^2} e^{-r} \right] \end{aligned} \quad (2.66)$$

for the ejected electron. Substituting (2.66) in (2.56) the simple expression (2.65) is

replaced by

$$I_{13}' = I_{13} + \frac{64 \sqrt{2} z_1}{\pi^{3/2} b^3 (1+k^2)^2 p^2} \int d\underline{K} N(K) [1 + (\underline{v} + \frac{1}{b}\underline{K})^2]^{-2} [1 + (\underline{V} + \frac{1}{b}\underline{K} + a\underline{p})^2]^{-2} \times [1 - \frac{2}{p^2} \underline{p} \cdot \underline{K}]^{-\frac{ia}{K}} \quad (2.67)$$

where the first term,  $I_{13}$ , on the right hand side of (2.67) is given by (2.65).

Further reduction of (2.67) in closed form has not proved possible, and it's evaluation, like the evaluation of the corresponding expression obtained by using a Coulomb wave to describe the ejected electron, presents a formidable computational task. In order to obtain cross sections one must therefore make some approximation which reduces the integral to a form suitable for computation.

The Born approximation transition amplitude with expression (2.66) taken to represent the ejected electron is

$$T_{if}^{\text{Born}'} = \iint d\underline{x} d\underline{r} \psi_i V_{13} \psi_f^* = -\frac{z_1}{2^{3/2} \pi} \iint d\underline{x} d\underline{r} e^{i\underline{p} \cdot \underline{\sigma}} \frac{1}{x} [e^{-i\underline{k} \cdot \underline{r}} - \frac{8}{(1+k^2)^2} e^{-r}] e^{-r} \quad (2.68)$$

Performing the  $\underline{x}$  and  $\underline{r}$  integrations of (2.68) we obtain

$$T_{if}^{\text{Born}'} = -\frac{8 \sqrt{2} z_1}{p^2} \left[ \frac{1}{\{1 + (a\underline{p} - \underline{k})^2\}^2} - \frac{16}{(1+k^2)^2 (4+a^2 p^2)^2} \right] \quad (2.69)$$

To examine the effect of using the wave function given by (2.66) we noted that the Born and impulse approximations agree in the high energy limit and therefore made the approximation of replacing the second term on the r.h.s. of Eq. (2.67) by the second term on the r.h.s. of Eq. (2.69), having ascribed to it the phase of  $I_{13}$ , i.e. we put

$$\begin{aligned} & \frac{64 \sqrt{2} z_1}{\pi^{3/2} b^3 (1+k^2)^2 p^2} \int d\underline{k} N(K) [1 + (\underline{v} + \frac{1}{b} \underline{K})^2]^{-2} [1 + (\underline{v} + \frac{1}{b} \underline{K} + a p)^2]^{-2} [1 - \frac{2}{p^2} p \cdot \underline{K}]^{-\frac{ia}{K}} \\ &= \frac{128 \sqrt{2} z_1}{p^2 (1+k^2)^2 (4+a^2 p^2)^2} [1 - \frac{2}{p^2} p \cdot (\underline{b}\underline{k} - \underline{a}b\underline{p} - \underline{b}\underline{v})]^{-\frac{ia}{|\underline{b}\underline{k} - \underline{a}b\underline{p} - \underline{b}\underline{v}|}} e^{i\eta} \end{aligned} \quad (2.70)$$

With this additional approximation the expression (2.67) is replaced by

$$\begin{aligned} I_{11}^{(I)} = & - \frac{8 \sqrt{2} z_1}{p^2} \left[ e^{\frac{\pi a}{2K}} \left| \frac{\pi a}{K \sinh(\frac{\pi a}{K})} \right|^{1/2} \frac{16}{(1+k^2)^2 (4+a^2 p^2)^2} \right] \\ & \times [1 - \frac{2}{p^2} p \cdot \underline{K}]^{-\frac{ia}{K}} e^{i\eta} \end{aligned} \quad (2.71)$$

with  $\underline{K} = \underline{b}\underline{k} - \underline{a}b\underline{p} - \underline{b}\underline{v}$ .

Substituting (2.71) in (2.61) we obtain

$$Q_I = \frac{64 z_1^2}{\pi^2 v^2} \int_0^{k_{\max}} d\underline{k} \int_{p_{\min}}^{p_{\max}} \frac{dp}{p^3} \left[ e^{\frac{\pi a}{2K}} \left| \frac{\pi a}{K \sinh(\frac{\pi a}{K})} \right|^{1/2} \frac{16}{(1+k^2)^2 (4+a^2 p^2)^2} \right] \quad (2.72)$$

The Born approximation cross section is given by

$$Q^{\text{Born}} = \frac{1}{2\pi^2 v^2} \int_0^{k_{\max}} d\underline{k} \int_{p_{\min}}^{p_{\max}} p |T_{if}^{\text{Born}}|^2 dp \quad (2.73)$$

Substituting (2.69) in (2.73) and integrating over  $\underline{k}$  we obtain

$$\begin{aligned} Q^{\text{Born}'} = & \frac{256}{\pi v^2} \int_0^{k_{\max}} k^2 dk \int_{p_{\min}}^{p_{\max}} \frac{dp}{p^3} \frac{1 + 2(a^2 p^2 + k^2) + (a^2 p^2 - k^2)^2 + \frac{16}{3} a^2 p^2 k^2}{\{1 + 2(a^2 p^2 + k^2) + (a^2 p^2 - k^2)^2\}^3} \\ & - \frac{32}{(1+k^2)^2 (4+a^2 p^2)^2 \{1 + 2(a^2 p^2 + k^2) + (a^2 p^2 - k^2)^2\}} \\ & + \frac{256}{(1+k^2)^4 (4+a^2 p^2)^4} \end{aligned} \quad (2.74)$$

If the ejected electron is represented by a Coulomb wave, Eq. (3.7) of Chap. I, 3.1, the ionization cross section in the Born approximation (Mott and Massey 1965 p. 490) is given by

$$Q^{\text{Born}} = \frac{2^{11}}{v^2} \int_0^{k_{\text{max}}} dk \int_{p_{\text{min}}}^{p_{\text{max}}} \frac{dp}{p} \frac{k}{(1 - e^{-2\pi/k})} \exp \left[ -\frac{2}{k} \arctan \left( \frac{2k}{1 + p^2 - k^2} \right) \right] \times \frac{[p^2 + \frac{1}{3}(1 + k^2)]}{[(1 + p^2 - k^2)^2 + 4k^2] [1 + 2(p^2 + k^2) + (p^2 - k^2)^2]} \quad (2.75)$$

The limits of integration are given by

$$p_{\text{min}} = k_i - k_f, \quad p_{\text{max}} = k_i + k_f \quad (2.76)$$

The equation of conservation of energy is

$$\frac{1}{2\mu} k_i^2 + \epsilon_i = \frac{1}{2\mu} k_f^2 + \frac{1}{2} k^2 \quad (2.77)$$

Using (2.76) together with the equation of conservation of energy (2.77) we find that

$$p_{\text{min}} = \frac{(I + k^2)}{v [1 + \{1 - \frac{(I + k^2)}{\mu v^2}\}^{1/2}]} \quad (2.78)$$

$$p_{\text{max}} = \mu v [1 + \{1 - \frac{(I + k^2)}{\mu v^2}\}^{1/2}] \quad (2.79)$$

and

$$k_{\text{max}} = (\mu v^2 - I)^{1/2} \quad (2.80)$$

where  $I (= -2\epsilon_i)$  is the ionization potential of hydrogen in Rydbergs.

Cross sections have been calculated for the processes (2.43) in the impulse and Born approximations by performing the integrations in (2.70), (2.74) and (2.75). The numerical methods employed are discussed in Section 3 and the results are presented and discussed in Section 4.

### 3. Numerical Methods

The integrations were carried out using a frame of reference Oxy z with the z-axis along  $\hat{p}$  and such that the xz-plane is the plane of  $\underline{p}$  and  $\underline{k}$ . Spherical polar co-ordinates in this frame are denoted by  $(k, \nu, \phi)$ . The calculation of ionization cross sections in the impulse approximation involves the numerical evaluation of a four-dimensional integral, namely, the integrals with respect to  $\phi, \nu, p$  and  $k$  in (2.70). The evaluation of ionization cross sections in the Born approximation involves the numerical evaluation of a double integral, namely, the integral with respect to  $p$  and the final integration over  $k$  in (2.74) and (2.75).

First we describe the method used to evaluate the expression (2.70). The integrand in this expression is a well-behaved function of the four variables  $\phi, \nu, p$  and  $k$ , with no singularities within the range of integration. In our frame of reference  $\underline{v}$  can be written in the form

$$\underline{v} = v (\sin \delta, 0, \cos \delta) . \quad (3.1)$$

Making use of the equation of conservation of energy, the equation defining  $p$ , and Eq. (3.1) we can write  $K$  in the form

$$K^2 = b^2 \left[ (a+1) k^2 + \left(a + \frac{1}{\mu}\right) a p^2 + v^2 + a I - k \cos \nu \left\{ (2a + \frac{1}{\mu}) p^2 + I + k^2 / p \right. \right. \\ \left. \left. - k \sin \nu \cos \phi \left\{ (p^2 - p_{\min}^2) \cdot (2\mu v - p_{\min})^2 - p^2 \right\}^{1/2} / \mu p \right\} \right] . \quad (3.2)$$

Repeated Gaussian integration formulae of various orders were used to evaluate the integrals over the variables  $\phi, \nu, p$  and  $k$  in the following order: (a)  $\phi, \nu, p, k$ ; (b)  $\nu, \phi, p, k$ ; (c)  $p, \phi, \nu, k$ . As a result of tests carried out for the  $\phi, \nu, p$ , and  $k$  integrations it was decided to split the range of integration in the following way:

- (1) The range  $(0, \pi)$  for the  $\phi$  and  $\nu$  integrations was split into four parts,  $(0, \frac{\pi}{4})$ ,  $(\frac{\pi}{4}, \frac{\pi}{2})$ ,  $(\frac{\pi}{2}, \frac{3\pi}{4})$ ,  $(\frac{3\pi}{4}, \pi)$ ;
- (2) the range  $(a, b)$  for the  $p$  and  $k$  integrations was split

into sixteen parts,  $(a, a + t)$ ,  $(a + t, a + 2t)$ ,  $(a + 2t, a + 8t)$  and  $(a + 8t, b)$  where  $t = \frac{1}{16}(b - a)$ . Gaussian quadratures of order 4, 6, 8 and 12 were in turn applied to each part. In the case of proton impact the range of integration was truncated at  $p = 15$  and  $k = 15$  because the integrand becomes negligible for large values of  $p$  and  $k$ . A very good agreement was obtained between the different methods, and the indications are that the cross section values obtained are at least accurate to three significant figures.

The integrals over the variables  $p$  and  $k$  in (2.74) and (2.75) were evaluated using (a) the Simpson integration formula, the steplength being chosen on the basis of the observed behaviour of  $|T_{if}^{\text{Born}}|^2$  as a function of  $p$  and  $k$ , and (b) Gaussian formulae of order 4, 6, 8 and 12. The agreement between the results obtained, using the Gaussian integration formulae and Simpson's formula, is better than four significant figures. The Born cross sections were obtained using the Born (1) approximation (Chap. I, 3.3, Eq. 3.17).

#### 4. Results

Cross sections for the processes (2.43) are given in Tables 1 and 2. In these Tables  $Q_I$  denotes the cross sections obtained with the use of Eq. (2.72),  $Q_B^{(1)}$  denotes Born (i) cross sections with Coulomb wave for the ejected electron and  $Q_B^{(2)}$  denotes Born (i) cross sections with wave function (2.66) for the ejected electron. The results are also presented graphically in Figs 1 and 2, to allow comparison with experiment and with other approximations. In Fig. 1 we display the results for the process  $e + H(1s) \rightarrow e + H^+ + e$  and in Fig. 2 the results for the process  $H^+ + H(1s) \rightarrow H^+ + H^+ + e$ .

The present approximation over-estimates the true electron impact ionization cross section at all energies in excess of 1.5 times threshold, a result which is in

striking contrast with that obtained by Akerib and Borowitz (1961). At high energies, as mentioned previously,  $Q_I \rightarrow Q_B$  but the approach to the limit is very slow, the ratio  $Q_I/Q_B$  being approximately 2.54 at an incident energy of 45 rydbergs.

For proton impact the present approximation grossly over-estimates the ionization cross section at all energies in excess of 25 kev. Again at high energies  $Q_I \rightarrow Q_B$  but the approach to the limit is extremely slow, the ratio  $Q_I/Q_B$  being approximately 4.9 at an incident energy of 750 kev.

The present model, which is identical with the non-exchange approximation of Akerib and Borowitz (1961), leads to results which are incompatible with experiment and with the predictions of the Born (i) approximation. Furthermore, a drawback of the model, in the case of electron impact, is that it does not seem possible to include exchange in a logical way in view of the fact that  $V_{12}$  is taken to be identically zero.

## 5. Conclusions

We conclude that the agreement with experiment obtain by Akerib and Borowitz for electron impact ionization is fortuitous. The indications are that the impulse approximation will not give good results if  $I_{11}$  (Eq. 2.67) is evaluated without a further approximation. The computational effort required to evaluate (2.45) when the ejected electron is described by a Coulomb wave is not, in our view, justified until the validity of the impulse approximation is better understood.

Table 1

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

E (Ryd)	$Q_I$	$Q_B^{(1)}$	$Q_B^{(2)}$
2	1.025	1.016	0.466
3	1.391	1.195	0.864
4	1.499	1.145	1.066
6	1.483	0.958	1.138
8	1.389	0.804	1.071
10	1.287	0.690	0.983
12	1.192	0.604	0.901
16	1.034	0.484	0.766
20	0.916	0.406	0.666
30	0.715	0.293	0.506
40	0.586	0.233	0.411
45	0.538	0.212	0.377

Table 2

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

E (kev)	$Q_I$	$Q_B^{(1)}$	$Q_B^{(2)}$
5	0.153	0.667	0.237
10	0.818	1.625	0.479
15	2.276	2.149	0.718
20	3.984	2.377	0.960
25	5.521	2.445	1.178
50	8.782	2.122	1.716
100	7.542	1.448	1.653
200	4.692	0.873	1.226
300	3.320	0.631	0.965
400	2.559	0.497	0.801
500	2.078	0.412	0.687
750	1.413	0.291	0.514
1000	1.070	0.227	0.415

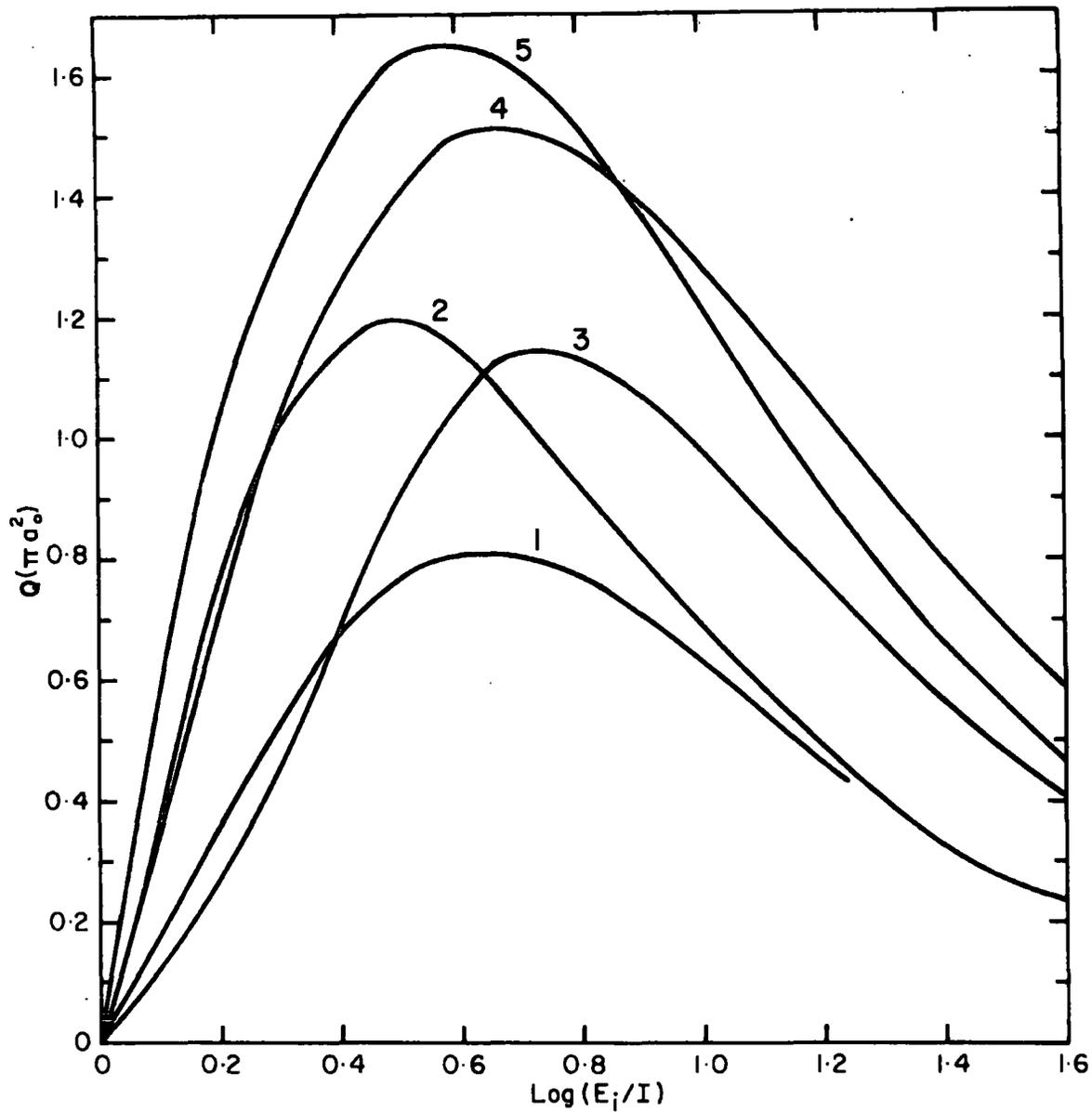


Fig.1 Cross section for  $H(1S) + e \rightarrow H^+ + 2e$

1: Experiment, Fite and Brackmann (1958)

2:  $Q_B^{(1)}$ , 3:  $Q_B^{(2)}$ , 4:  $Q_I$ , 5: Veldre & Vinkeln (1963)

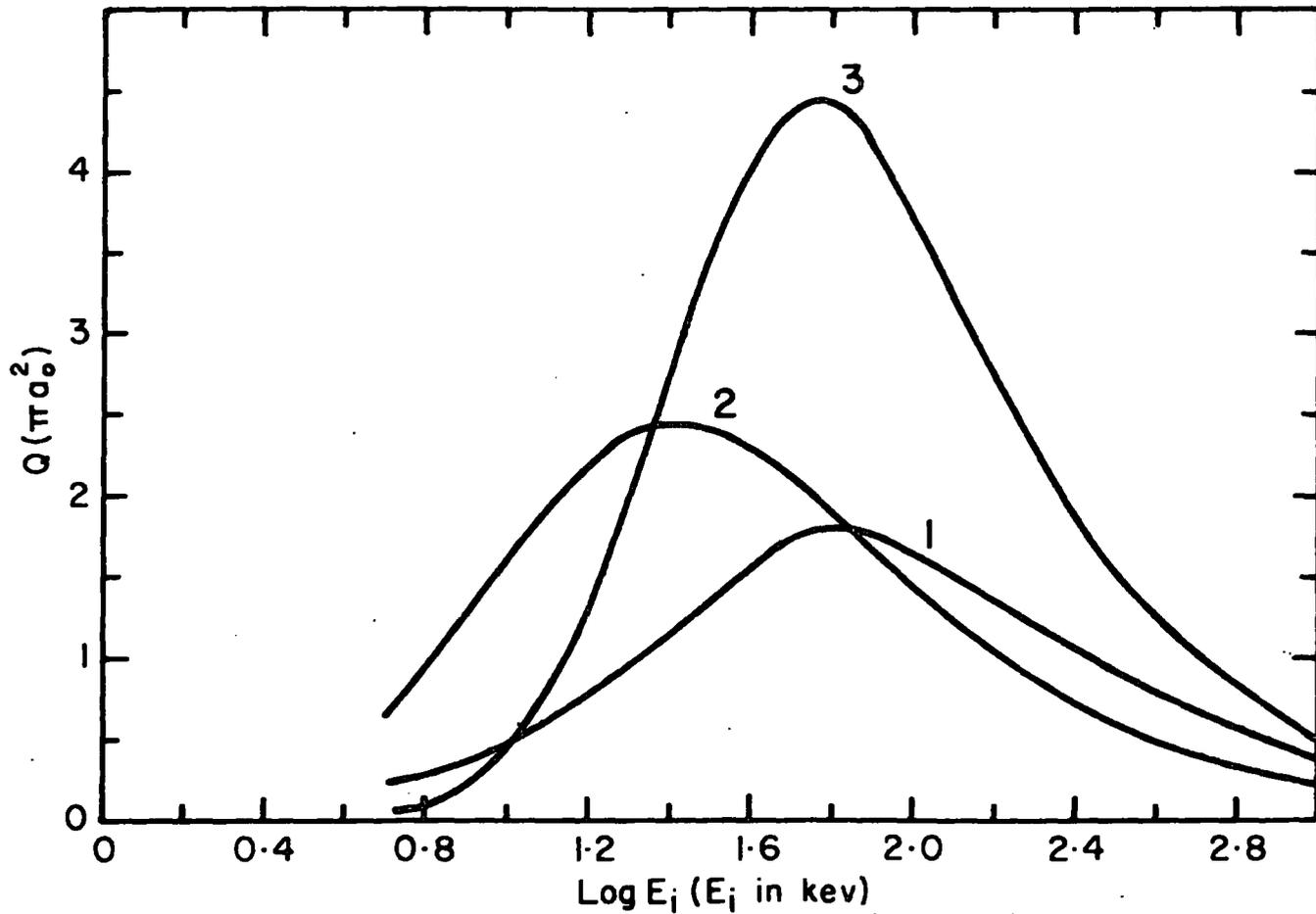


Fig.2 Cross sections for  $\text{H}(1\text{S}) + \text{H}^+ \rightarrow 2\text{H}^+ + e$   
 1:  $Q_B^{(2)}$ , 2:  $Q_B^{(1)}$ , 3:  $Q_I$  divided by 2

## CHAPTER III

### IONIZATION OF He AND Li<sup>+</sup> BY ELECTRON IMPACT

#### 1. Introduction

Cross sections are evaluated, in the Born (ii) approximation (Chap. I, 3.3, Eq. 3.16), for the processes



in which both Helium and Li<sup>+</sup> are initially in their ground states.

For ionization of Helium by electron impact there are several sets of theoretical results (Massey and Mohr 1933, Erskine 1954, Sloan 1964, Peach 1965, Inokuti and Kim 1969) and experimental results (Smith 1930, Rapp and Golden 1965, Schram et al, 1965, Gaudin and Hagemann 1967). The results of Smith and Rapp and Golden differ very slightly over the energy range covered by Rapp and Golden, but the difference between these two sets of experimental measurements and those of Schram et al, and Gaudin and Hagemann is quite appreciable. The calculations of Erskine and Sloan agree well with experiment at energies between 500 ev and 1 kev. Erskine used a one-parameter function for the 1s state and solved for one electron in the average field of He<sup>+</sup> for  $l = 1$  which gives the largest contribution to the total cross section. Sloan made use of a polarized orbital for the ejected electron. Peach has used a Hartree-Fock wave function for the initial bound states, together with an undistorted Coulomb function for the ejected electron.

For ionization of Li<sup>+</sup> by electron impact the only theoretical results available are an unpublished evaluation of the Bethe limit by Kim and Inokuti (1969) and an unpublished Coulomb-Born calculation by Moores (1969). Two independent sets of experimental results are available (Lineberger et al 1966, Peart and Dolder 1968, and

Peart and Dolder 1969). The experimental measurements of both these groups are compatible in the energy range in common.

Two experiments have also been carried out on electron impact detachment from the isoelectronic system  $H^-$  (Dance et al. 1967, Tisone and Branscomb 1968) together with several theoretical calculations for this process, in particular a Born calculation by Bely and Schwartz (1969), a Bethe-Born calculation McDowell and Williamson (1963), and a sum rule evaluation of the Bethe limit Inokuti and Kim (1968). These three theoretical estimates of the cross section are in agreement with each other and with the Dance et al experiment, but are in disagreement with the Tisone and Branscomb experiment. It is therefore of interest to extend the earlier Born calculations for He to higher energies to test whether the Bethe asymptotic limit is approached correctly, and to get some estimate of the reliability of the computed cross section by using alternative formulations, and to extend the work to  $Li^+$

## 2. Reduction of the Matrix Element

The Born (ii) cross section for the ionization of a two-electron atom by electrons incident with energy  $\frac{1}{2} k_i^2$  (Chap. I, 3.3, Eq. 3.16)

$$Q(k_i^2) = \frac{1}{k_i^2} \int_0^{\epsilon_{\max}} k \, d\epsilon \int d\hat{k} \int_{p_{\min}}^{p_{\max}} |f(\underline{k}, \underline{p})|^2 dp^2 (\pi a_0^2), \quad (2.1)$$

where  $\epsilon = \frac{1}{2} k^2$  and  $\epsilon_{\max} = \frac{1}{2} (\frac{1}{2} k_i^2 - I)$ . All other quantities are defined as in Chapters I and II. The matrix element  $f(\underline{k}, \underline{p})$  is (Chap. I, 3.3, Eq. 3.15)

$$f_{\underline{k}}(\underline{k}, \underline{p}) = - \frac{2}{p^2} \sum_{j=1}^2 \int e^{i \underline{p} \cdot \underline{r}_j} \psi_0(\underline{r}_1, \underline{r}_2) \psi_{\underline{k}}^*(\underline{r}_1, \underline{r}_2) d\underline{r}_1 d\underline{r}_2 \quad (2.2)$$

$\psi_0(\underline{r}_1, \underline{r}_2)$  and  $\psi_{\underline{k}}(\underline{r}_1, \underline{r}_2)$  being the wave functions of the ground and final states respectively.

If the wave functions are exact, then

$$\Psi_0 (\nabla_1^2 + \nabla_2^2) \Psi_{\underline{k}}^* - \Psi_{\underline{k}}^* (\nabla_1^2 + \nabla_2^2) \Psi_0 = -2(I + \epsilon) \Psi_{\underline{k}}^* \Psi_0. \quad (2.3)$$

Substituting (2.3) in (2.2) gives

$$f(\underline{k}, \underline{p}) = \frac{2}{p^2(I + \epsilon)} [p^2 \int e^{i \underline{p} \cdot \underline{r}_1} \Psi_0 \Psi_{\underline{k}}^* d\underline{r}_1 d\underline{r}_2 - 2ip \int e^{i \underline{p} \cdot \underline{r}_1} \Psi_0 \frac{\partial}{\partial z_1} \Psi_{\underline{k}}^* d\underline{r}_1 d\underline{r}_2]. \quad (2.4)$$

Substituting (2.2) in (2.4) we obtain

$$f_v(\underline{k}, \underline{p}) = - \frac{8i}{p(k^2 + p^2 + 2I)} \int e^{i \underline{p} \cdot \underline{r}_1} \Psi_0 \frac{\partial}{\partial z_1} \Psi_{\underline{k}}^* d\underline{r}_1 d\underline{r}_2. \quad (2.5)$$

This alternative expression for the amplitude was first derived by Bates et al. (1950). The expressions (2.2) and (2.5) are equivalent for exact wave functions but not, in general, if approximate wave functions are used. Their difference is, in a weak sense, a test of the accuracy of the approximate wave functions used. Following Chandrasekhar (1945), we call (2.2) and (2.5) the length and velocity forms of  $f(\underline{k}, \underline{p})$ , respectively. Kennedy and Kingston (1968) made use of expressions similar to (2.2) and (2.5) in their work on the excitation of the 2 'P state of Helium, while McDowell (1969) has also studied both forms in a Born calculation of electron impact ionization of Li.

For the ground state we use an open shell two-parameter wave function, the variational parameters being given by Silverman et al (1960). The parameters used are listed in Table 1, together with the corresponding value of the ionization potentials. We write the initial and final wave functions as

$$\Psi_0(\underline{r}_1, \underline{r}_2) = N [e^{-\alpha r_1 - \beta r_2} + e^{-\alpha r_2 - \beta r_1}], \quad (2.6)$$

$$\Psi_{\underline{k}}(\underline{r}_1, \underline{r}_2) = \frac{1}{\sqrt{2}} [\psi_{1s}(z, \underline{r}_1) \psi_{\underline{k}}(\underline{r}_2) + \psi_{1s}(z, \underline{r}_2) \psi_{\underline{k}}(\underline{r}_1)], \quad (2.7)$$

where N is a normalization constant. Here z is the charge of the target nucleus,

$\psi_{1s}(z, \underline{r}) = \left(\frac{z^3}{\pi}\right)^{1/2} e^{-zr}$ , and the function  $\psi_{\underline{k}}(\underline{r})$  for the ejected electron of momentum  $\underline{k}$  may be written

$$\psi_{\underline{k}}(\underline{r}) = \frac{1}{(2\pi)^{3/2} k^{1/2}} \sum_{l=0}^{\infty} (2l+1) i^l e^{-i(\sigma_l + \eta_l)} r^{-1} u_l(k, r) P_l(\hat{\underline{k}} \cdot \hat{\underline{r}}), \quad (2.8)$$

where  $P_l(x)$  is the  $l$ th Legendre polynomial, and the radial function  $u_l(k, r)$  is regular at the origin, with asymptotic form

$$u_l(k, r) \underset{r \rightarrow \infty}{\sim} \frac{1}{k^{1/2}} \sin \left[ kr + \frac{(z-1)}{k} \ln(2kr) - \frac{1}{2} l \pi + \sigma_l + \eta_l \right] \quad (2.9)$$

where  $\sigma_l = \arg \Gamma \left[ l + 1 - i \frac{(z-1)}{k} \right]$  while  $\eta_l$  is the non-Coulomb part of the phase shift.

Table 1

Parameters used in evaluating the matrix element

	$z$	$a$	$\beta$	$I$
He	2	2.183171	1.188530	0.8756614 1.74513229
Li <sup>+</sup>	3	3.294909	2.078981	2.748748 5.497496

The final state wave function  $\Psi_{\underline{k}}(\underline{r}_1, \underline{r}_2)$  is automatically orthogonal to the ground state function  $\Psi_0(\underline{r}_1, \underline{r}_2)$  for  $l > 0$ ; for  $l = 0$  we orthogonalize the ground and final state wave functions by writing the latter in the form

$$\Psi_{\underline{k}}(\text{Orthogonalized}) = \Psi_{\underline{k}}(\underline{r}_1, \underline{r}_2) - \langle \Psi_0 | \Psi_{\underline{k}} \rangle \Psi_0(\underline{r}_1, \underline{r}_2) \quad (2.10)$$

The orthogonality factor  $\langle \Psi_0 | \Psi_{\underline{k}} \rangle$  in Eq. (2.10) is given by

$$\langle \Psi_0 | \Psi_{\underline{k}} \rangle = \iint d\underline{r}_1 d\underline{r}_2 \Psi_0^*(\underline{r}_1, \underline{r}_2) \Psi_{\underline{k}}(\underline{r}_1, \underline{r}_2)$$

which, with the use of Eqs. (2.6), (2.7) and (2.8), we can easily reduce to the form

$$\langle \Psi_0 | \Psi_{\underline{k}} \rangle = \frac{16 z^{3/2} N e^{-i(\sigma_0 + \eta_0)}}{k^{1/2}} \int_0^{\infty} r u_0(k, r) \left[ \frac{e^{-\alpha r}}{(z + \beta)^3} + \frac{e^{-\beta r}}{(z + \alpha)^3} \right] dr \quad (2.11)$$

Substituting (2.6) and (2.10) in (2.2) gives

$$f_L(\underline{k}, \underline{p}) = -\frac{4}{p^2} \iint \left[ \frac{1}{\sqrt{2}} \{ \psi_{1s}^*(z, \underline{r}_2) \psi_{\underline{k}}^*(\underline{r}_1) + \psi_{1s}^*(z, \underline{r}_1) \psi_{\underline{k}}^*(\underline{r}_2) \} - \psi_0 \psi_{\underline{k}}^* \psi_0^*(\underline{r}_1, \underline{r}_2) \right] \times e^{i \underline{p} \cdot \underline{r}_1} \psi_0(\underline{r}_1, \underline{r}_2) d\underline{r}_1 d\underline{r}_2$$

$$= I_1 + I_2 + I_3, \quad (2.12)$$

where

$$I_1 = -\frac{2\sqrt{2}}{p^2} \iint \psi_{1s}^*(z, \underline{r}_2) \psi_{\underline{k}}^*(\underline{r}_1) e^{i \underline{p} \cdot \underline{r}_1} \psi_0(\underline{r}_1, \underline{r}_2) d\underline{r}_1 d\underline{r}_2, \quad (2.13)$$

$$I_2 = -\frac{2\sqrt{2}}{p^2} \iint \psi_{1s}^*(z, \underline{r}_1) \psi_{\underline{k}}^*(\underline{r}_2) e^{i \underline{p} \cdot \underline{r}_1} \psi_0(\underline{r}_1, \underline{r}_2) d\underline{r}_1 d\underline{r}_2, \quad (2.14)$$

and

$$I_3 = \frac{4}{p^2} \langle \psi_0 | \psi_{\underline{k}} \rangle^* \iint \psi_0^*(\underline{r}_1, \underline{r}_2) e^{i \underline{p} \cdot \underline{r}_1} \psi_0(\underline{r}_1, \underline{r}_2) d\underline{r}_1 d\underline{r}_2. \quad (2.15)$$

The integrations were carried out in a frame of reference Oxy z with the z-axis along  $\hat{p}$ . In this frame the spherical polar co-ordinates of  $\underline{r}_1$ ,  $\underline{r}_2$  and  $\underline{k}$  are denoted by  $(r_1, \theta_1, \phi_1)$ ,  $(r_2, \theta_2, \phi_2)$  and  $(k, \nu, \phi)$  respectively.

Substituting (2.6) and (2.8) in (2.13) and making use of the expansion

$$e^{i \underline{p} \cdot \underline{r}} = \sum_{n=0}^{\infty} (2n+1) i^n j_n(pr) P_n(\hat{p} \cdot \hat{r}) \quad (2.16)$$

where  $j_n(pr)$  is the n th spherical Bessel function of the first kind we obtain, after performing the integrations with respect to  $\underline{r}_2$ ,  $\theta_1$ , and  $\phi_1$ , the result

$$I_1 = -\frac{32 z^{3/2} N}{p^2 k^{1/2}} \sum_{l=0}^{\infty} (2l+1) e^{i(\sigma_l + \eta_l)} P_l(\cos \nu) \int_0^{\infty} r u_l(k, r) j_l(pr) \left[ \frac{e^{-\alpha r}}{(z+\beta)^3} + \frac{e^{-\beta r}}{(z+\alpha)^3} \right] dr. \quad (2.17)$$

In a similar manner we obtain

$$I_2 = -\frac{32 z^{3/2} N}{p^2 k^{1/2}} e^{i(\sigma_0 + \eta_0)} \int_0^{\infty} r u_0(k, r) \left[ \frac{(z+\alpha) e^{-\beta r}}{(z+\alpha)^2 + p^2} + \frac{(z+\beta) e^{-\alpha r}}{(z+\beta)^2 + p^2} \right] dr, \quad (2.18)$$

and

$$I_3 = \frac{1024 z^{3/2} \pi^2 N^2}{p^2 k^{1/2}} e^{i(\sigma_0 + \eta_0)} \left[ \frac{a}{\beta^3 (4a^2 + p^2)^2} + \frac{8}{(a + \beta)^2 ((a + \beta)^2 + p^2)^2} + \frac{\beta}{a^3 (4\beta^2 + p^2)^2} \right] \\ \times \int_0^\infty r u_0(k, r) \left[ \frac{e^{-ar}}{(z + \beta)^3} + \frac{e^{-\beta r}}{(z + a)^3} \right] dr \quad (2.19)$$

Substitution of (2.17), (2.18) and (2.19) in (2.12) gives

$$f_L(\underline{k}, p) = - \frac{32 z^{3/2} N^\infty}{p^2 k^{1/2}} \sum_{l=0}^{\infty} (2l+1) e^{i(\sigma_l + \eta_l)} P_l(\cos \nu) \left[ \int_0^\infty r u_l(k, r) j_l(pr) \left| \frac{e^{-ar}}{(z + \beta)^3} + \frac{e^{-\beta r}}{(z + a)^3} \right| dr \right. \\ \left. + \delta_{l,0} \int_0^\infty r u_0(k, r) \left| \frac{(z + a) e^{-\beta r}}{((z + a)^2 + p^2)^2} + \frac{(z + \beta) e^{-ar}}{((z + \beta)^2 + p^2)^2} \right| dr \right] \\ - 32 \pi^2 N^2 \left\{ \frac{a}{\beta^3 (4a^2 + p^2)^2} + \frac{8}{(a + \beta)^2 ((a + \beta)^2 + p^2)^2} + \frac{\beta}{a^3 (4\beta^2 + p^2)^2} \right\} \\ \times \delta_{l,0} \int_0^\infty r u_0(k, r) \left| \frac{e^{-ar}}{(z + \beta)^3} + \frac{e^{-\beta r}}{(z + a)^3} \right| dr \Big] \\ = - \frac{32 z^{3/2} N^\infty}{p^2 k^{1/2}} \sum_{l=0}^{\infty} (2l+1) e^{i(\sigma_l + \eta_l)} P_l(\cos \nu) V_l^{(L)}(k, p) \quad (2.20)$$

Expression (2.20) gives the required ionization scattering amplitude in the length formulation of the Born approximation. Substituting (2.20) in (2.1) and performing the integration with respect to  $\underline{k}$  yields the result

$$Q_L(k_i^2) = \frac{2^{13} z^3 \pi N^2}{k_i^2} \sum_{l=0}^{\infty} (2l+1) \int_0^{k_{\max}} k dk \int_{p_{\min}}^{p_{\max}} \frac{dp}{p^3} |V_l^{(L)}(k, p)|^2 (\pi a_0^2) \quad (2.21)$$

Substitution of (2.10) in (2.5) gives

$$f_V(\underline{k}, p) = - \frac{4\sqrt{2} i}{p(k^2 + p^2 + 2I)} \iint d\underline{r}_1 d\underline{r}_2 e^{i\underline{p} \cdot \underline{r}_1} \Psi_0(\underline{r}_1, \underline{r}_2) \left[ \psi_{1s}^*(z, \underline{r}_2) \frac{\partial}{\partial z_1} \psi_{\underline{k}}^*(\underline{r}_1) + \psi_{\underline{k}}^*(\underline{r}_2) \frac{\partial}{\partial z_1} \psi_{1s}^*(z, \underline{r}_1) \right. \\ \left. - \sqrt{2} \langle \Psi_0 | \psi_{\underline{k}} \rangle^* \frac{\partial}{\partial z_1} \Psi_0^*(\underline{r}_1, \underline{r}_2) \right] \quad (2.22)$$

The differential operator  $\frac{\partial}{\partial z}$  is in spherical polar co-ordinates given by

$$\frac{\partial}{\partial z} \equiv \cos \theta \frac{\partial}{\partial r} - \frac{\sin \theta}{r} \frac{\partial}{\partial \theta} \quad (2.23)$$

With the use of (2.23) we have that

$$\begin{aligned} \frac{\partial}{\partial z_1} \psi_{\underline{k}}^* (\underline{r}_1) &= \frac{1}{(2\pi)^{3/2} k^{1/2} l} \sum_{l=0}^{\infty} (2l+1) (-i)^l e^{i(\sigma_l + \eta_l)} \left[ \frac{\cos \theta_1}{r_1} \left| \frac{du_l}{dr_1} (k, r_1) - \frac{u_l(k, r_1)}{r_1} P_l(\hat{\underline{k}} \cdot \hat{\underline{r}}_1) \right. \right. \\ &\quad \left. \left. - \frac{u_l(k, r_1)}{r_1^2} \sin \theta_1 \frac{\partial}{\partial \theta_1} P_l(\hat{\underline{k}} \cdot \hat{\underline{r}}_1) \right] \end{aligned} \quad (2.24)$$

and

$$\frac{\partial}{\partial z_1} \psi_{1s}(z, \underline{r}_1) = -\left(\frac{z^3}{\pi}\right)^{1/2} \cos \theta_1 e^{-zr_1} \quad (2.25)$$

Substituting (2.24) and (2.25) in (2.22) gives

$$f_v(k, p) = J_1 + J_2 + J_3 \quad (2.26)$$

where

$$\begin{aligned} J_1 &= -\frac{2z^{3/2} Ni}{\pi^2 p k^{1/2} (k^2 + p^2 + 2I) l} \sum_{l=0}^{\infty} (2l+1) (-i)^l e^{i(\sigma_l + \eta_l)} \iint d\underline{r}_1 d\underline{r}_2 e^{i\underline{p} \cdot \underline{r}_1} e^{-zr_2} (e^{-\alpha r_1 - \beta r_2} + e^{-\alpha r_2 - \beta r_1}) \\ &\quad \times \left[ \frac{\cos \theta_1}{r_1} \left| \frac{du_l}{dr_1} (k, r_1) - \frac{u_l(k, r_1)}{r_1} P_l(\hat{\underline{k}} \cdot \hat{\underline{r}}_1) - \frac{u_l(k, r_1)}{r_1^2} \sin \theta_1 \frac{\partial}{\partial \theta_1} P_l(\hat{\underline{k}} \cdot \hat{\underline{r}}_1) \right] \end{aligned} \quad (2.27)$$

$$\begin{aligned} J_2 &= \frac{2z^{3/2} Ni}{\pi^2 p k^{1/2} (k^2 + p^2 + 2I) l} \sum_{l=0}^{\infty} (2l+1) (-i)^l e^{i(\sigma_l + \eta_l)} \iint d\underline{r}_1 d\underline{r}_2 e^{i\underline{p} \cdot \underline{r}_1} e^{-zr_1} (e^{-\alpha r_1 - \beta r_2} + e^{-\alpha r_2 - \beta r_1}) \cos \theta \\ &\quad \times \frac{u_l(k, r_2)}{r_2} P_l(\hat{\underline{k}} \cdot \hat{\underline{r}}_2) \end{aligned} \quad (2.28)$$

and

$$\begin{aligned}
J_1 &= -\frac{8\langle \Psi_0 | \Psi_k \rangle^* N^2 i}{p(k^2 + p^2 + 2I)} \int \int d\underline{r}_1 d\underline{r}_2 e^{i p \cdot \underline{r}_1} (e^{-\alpha r_1 - \beta r_2} + e^{-\alpha r_2 - \beta r_1}) (\alpha e^{-\alpha r_1 - \beta r_2} + \beta e^{-\alpha r_2 - \beta r_1}) \cos \theta_1 \\
&= -\frac{8\langle \Psi_0 | \Psi_k \rangle^* N^2 i}{p(k^2 + p^2 + 2I)} \int \int d\underline{r}_1 d\underline{r}_2 e^{i p \cdot \underline{r}_1} \cos \theta_1 [\alpha e^{-2(\alpha r_1 + \beta r_2)} + (\alpha + \beta) e^{-(\alpha + \beta)(r_1 + r_2)} + \beta e^{-2(\alpha r_2 + \beta r_1)}]
\end{aligned} \tag{2.29}$$

When the  $\underline{r}_2$  integration of (2.27) is carried out we obtain

$$\begin{aligned}
J_1 &= -\frac{16z^{1/2} Ni}{\pi p k^{1/2} (k^2 + p^2 + 2I)} \sum_{\ell=0}^{\infty} (2\ell+1) (-i)^\ell e^{i(\sigma_\ell + \eta_\ell)} \int d\underline{r}_1 e^{i p \cdot \underline{r}_1} \left[ \frac{e^{-\alpha r_1}}{(z+\beta)^3} + \frac{e^{-\beta r_1}}{(z+\alpha)^3} \right] \\
&\times \left[ \frac{\cos \theta_1}{r_1} \left\{ \frac{d u_\ell}{d r_1}(k, r_1) - \frac{u_\ell(k, r_1)}{r_1} \right\} P_\ell(\hat{\underline{k}} \cdot \hat{\underline{r}}_1) - \frac{u_\ell(k, r_1)}{r_1^2} \sin \theta_1 \frac{\partial}{\partial \theta_1} P_\ell(\hat{\underline{k}} \cdot \hat{\underline{r}}_1) \right],
\end{aligned}$$

which with the use of the addition formula for the Legendre polynomials

$$P_n(\hat{\underline{k}} \cdot \hat{\underline{r}}) = P_n(\cos \theta) P_n(\cos \nu) + 2 \sum_{m=1}^n \frac{(n+m)!}{(n+m)!} P_n^m(\cos \theta) P_n^m(\cos \nu) \cos m(\phi_1 - \phi) \tag{2.30}$$

becomes

$$\begin{aligned}
J_1 &= -\frac{16z^{1/2} Ni}{\pi p k^{1/2} (k^2 + p^2 + 2I)} \sum_{\ell=0}^{\infty} (2\ell+1) (-i)^\ell e^{i(\sigma_\ell + \eta_\ell)} \int d\underline{r}_1 e^{i p \cdot \underline{r}_1} \left[ \frac{e^{-\alpha r_1}}{(z+\beta)^3} + \frac{e^{-\beta r_1}}{(z+\alpha)^3} \right] \\
&\times \left[ \frac{\cos \theta_1}{r_1} \left\{ \frac{d u_\ell}{d r_1}(k, r_1) - \frac{u_\ell(k, r_1)}{r_1} \right\} \{ P_\ell(\cos \theta_1) P_\ell(\cos \nu) + 2 \sum_{m=1}^{\ell} \frac{(\ell-m)!}{(\ell+m)!} P_\ell^m(\cos \theta_1) P_\ell^m(\cos \nu) \right. \\
&\quad \times \cos m(\phi_1 - \phi) \} \\
&+ \frac{u_\ell(k, r_1)}{r_1^2} \sin^2 \theta_1 \{ P_\ell(\cos \nu) \frac{d}{d(\cos \theta_1)} P_\ell(\cos \theta_1) + 2 \sum_{m=1}^{\ell} \frac{(\ell-m)!}{(\ell+m)!} P_\ell^m(\cos \nu) \frac{d}{d(\cos \theta_1)} P_\ell^m(\cos \theta_1) \} \\
&\quad \times \cos m(\phi_1 - \phi) \} \\
&= -\frac{32z^{1/2} Ni}{p k^{1/2} (k^2 + p^2 + 2I)} \sum_{\ell=0}^{\infty} (2\ell+1) (-i)^\ell e^{i(\sigma_\ell + \eta_\ell)} P_\ell(\cos \nu) \int_0^\infty r_1^2 dr_1 \int_{-1}^1 d(\cos \theta_1) \left[ \frac{e^{-\alpha r_1}}{(z+\beta)^3} + \frac{e^{-\beta r_1}}{(z+\alpha)^3} \right] \\
&\times e^{i p \cdot \underline{r}_1} \left[ \frac{\cos \theta_1}{r_1} \left\{ \frac{d u_\ell}{d r_1}(k, r_1) - \frac{u_\ell(k, r_1)}{r_1} \right\} P_\ell(\cos \theta_1) + \frac{u_\ell(k, r_1)}{r_1^2} \sin^2 \theta_1 \frac{d}{d(\cos \theta_1)} P_\ell(\cos \theta_1) \right].
\end{aligned}$$

We have obtained the last result by performing the integration over  $\phi$ .

Using (2.16) and the recurrence formulae

$$(1 - z^2) \frac{dP_n(z)}{dz} = n P_{n-1}(z) - n z P_n(z) \quad (2.31)$$

$$(2n + 1) z P_n(z) = (n + 1) P_{n+1}(z) + P_{n-1}(z) \quad (2.32)$$

the above expression for  $J_1$  reduces, after the integration over  $\theta$ , has been performed, to the form

$$J_1 = - \frac{64 z^{3/2} N}{pk^{1/2} (k^2 + p^2 + 2I)} \sum_{l=0}^{\infty} e^{i(\sigma_l + \eta_l)} P_l(\cos \nu) \int_0^{\infty} dr_1 \left[ \frac{e^{-\alpha r_1}}{(z + \beta)^3} + \frac{e^{-\beta r_1}}{(z + \alpha)^3} \right] \\ \times [l(l+1) j_{l+1}(pr_1) + l(l-1) j_{l-1}(pr_1)] u_l(k, r_1) - [l(l+1) j_{l+1}(pr_1) - l j_{l-1}(pr_1)] \\ \times \frac{d}{dr_1} [r_1 u_l(k, r_1)] .$$

Now integrating by parts the term, in the above expression, which contains the derivative of the radial function  $u_l(k, r_1)$  and making use of the recurrence formulae

$$n j_n(z) - z \frac{d}{dz} j_n(z) = z j_{n+1}(z) \quad (2.33)$$

$$z j_{n-1}(z) + z j_{n+1}(z) = (2n + 1) j_n(z) \quad (2.34)$$

we obtain

$$J_1 = - \frac{64 z^{3/2} N}{pk^{1/2} (k^2 + p^2 + 2I)} \sum_{l=0}^{\infty} (2l+1) e^{i(\sigma_l + \eta_l)} P_l(\cos \nu) \int_0^{\infty} dr_1 u_l(k, r_1) [pr j_l(pr) \\ \times \left\{ \frac{e^{-\alpha r}}{(z + \beta)^3} + \frac{e^{-\beta r}}{(z + \alpha)^3} \right\} - \frac{1}{p} [l(l+1) j_l(pr) - pr j_{l-1}(pr)] \left\{ \frac{\alpha e^{-\alpha r}}{(z + \beta)^3} + \frac{\beta e^{-\beta r}}{(z + \alpha)^3} \right\}] . \quad (2.35)$$

The  $\underline{r}_1$  and  $\underline{r}_2$  integrations of (2.28) can quite easily be carried out and the latter expression then reduces to the form

$$J_2 = -\frac{64 z^{3/2} N}{k^{1/2}(k^2+p^2+2I)} e^{i(\sigma_0+\eta_0)} \int_0^\infty r u_0(k,r) \left[ \frac{e^{-\alpha r}}{\{(z+\beta)^2+p^2\}^2} + \frac{e^{-\beta r}}{\{(z+\alpha)^2+p^2\}^2} \right] dr. \quad (2.36)$$

Performing the integrations over  $\underline{r}_1$  and  $\underline{r}_2$  in (2.29) we obtain

$$J_1 = \frac{64 \pi^2 N^2 \langle \Psi_0 | \Psi_{\underline{k}} \rangle^*}{(k^2+p^2+2I)} \left[ \frac{\alpha}{\beta^3(4\alpha^2+p^2)^2} + \frac{8}{(\alpha+\beta)^2\{( \alpha+\beta)^2+p^2\}^2} + \frac{\beta}{\alpha^3(4\beta^2+p^2)^2} \right]. \quad (2.37)$$

Substituting (2.35), (2.36) and (2.37) in (2.26) and making use of (2.11) we obtain

$$f_V(\underline{k}, \underline{p}) = -\frac{64 z^{3/2} N}{k^{1/2}(k^2+p^2+2I)} \sum_{l=0}^{\infty} (2l+1) e^{i(\sigma_l+\eta_l)} P_l(\cos \nu) V_l^{(v)}(\underline{k}, \underline{p}) \quad (2.38)$$

where

$$\begin{aligned} V_l^{(v)}(\underline{k}, \underline{p}) = & \int_0^\infty r u_l(k, r) \left[ j_l(pr) - \delta_{l,0} A(p) \left\{ \frac{e^{-\alpha r}}{(z+\beta)^3} + \frac{e^{-\beta r}}{(z+\alpha)^3} \right\} \right. \\ & - \frac{1}{r p^2} \{(l+1) j_l(pr) - pr j_{l-1}(pr)\} \left\{ \frac{\alpha e^{-\alpha r}}{(z+\beta)^3} + \frac{\beta e^{-\beta r}}{(z+\alpha)^3} \right\} \\ & \left. + \delta_{l,0} z \left\{ \frac{e^{-\alpha r}}{(z+\beta)^2+p^2} + \frac{e^{-\beta r}}{(z+\alpha)^2+p^2} \right\} \right] dr, \end{aligned} \quad (2.39)$$

and where

$$A(p) = 16 \pi^2 N^2 \left[ \frac{\alpha}{\beta^3(4\alpha^2+p^2)^2} + \frac{8}{(\alpha+\beta)^2\{( \alpha+\beta)^2+p^2\}^2} + \frac{\beta}{\alpha^3(4\beta^2+p^2)^2} \right].$$

Expression (2.38) gives the ionization scattering amplitude in the velocity formulation of the Born approximation. Substituting (2.38) in (2.1) and integrating over  $\hat{\underline{k}}$  we obtain

$$Q_V(k_i^2) = \frac{2^{1/2} z^{3/2} \pi N^2}{k_i^2} \sum_{l=0}^{\infty} (2l+1) \int_0^{k_{\max}} k dk \int_{p_{\min}}^{p_{\max}} \frac{p dp}{(k^2+p^2+2I)^2} |V_l^{(v)}(\underline{k}, \underline{p})|^2 (\pi a_0^2). \quad (2.40)$$

### 3. The Method of Polarized Orbitals

Sloan (1964), following Temkin and Lamkin (1961), takes the total wave function for scattering by an hydrogen-like ion to be of the form

$$\Psi_{\underline{k}}(\underline{r}_1, \underline{r}_2) = (1 \pm P_{12}) \psi_{\underline{k}}(\underline{r}_1) [\psi_{1S}(z, \underline{r}_2) + \psi^{\text{pol}}(\underline{r}_1, \underline{r}_2)] , \quad (3.1)$$

where  $P_{12}$  permutes  $\underline{r}_1$  and  $\underline{r}_2$ , and the upper and lower signs correspond respectively to singlet and triplet scattering. The 'static' problem is to determine  $\psi^{\text{pol}}(\underline{r}_1, \underline{r}_2)$ , an approximation to the first-order perturbation of the ground state function  $\psi_{1S}(z, \underline{r}_2)$  by a stationary electron at  $\underline{r}_1$ . Generalizing the methods of Temkin (1959) to an arbitrary nuclear charge  $z$  and using atomic units Sloan obtains

$$\psi^{\text{pol}}(\underline{r}_1, \underline{r}_2) = - \frac{1}{(\pi z)^{1/2}} \frac{\epsilon(r_1, r_2)}{r_1^2} e^{-zr} \left( \frac{1}{2} z r_2^2 + r_2 \right) \cos \theta_{12} , \quad (3.2)$$

where

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

$\theta_{12} = \arccos(\underline{r}_1 \cdot \underline{r}_2)$ . For  $r_1 > r_2$  and  $r_1 \rightarrow \infty$ ,  $\psi^{\text{pol}}(\underline{r}_1, \underline{r}_2)$  is the dipole contribution to the first-order perturbation of  $\psi_{1S}(z, \underline{r}_2)$ .

The variational principle used by Sloan implies that  $\Psi_{\underline{k}}(\underline{r}_1, \underline{r}_2)$  satisfies the equation

$$\int \psi_{1S}^*(z, \underline{r}_2) (H - E) \Psi_{\underline{k}}(\underline{r}_1, \underline{r}_2) d\underline{r}_2 = 0 , \quad (3.3)$$

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 result of using (3.3) with  $\Psi_{\underline{k}}(\underline{r}_1, \underline{r}_2)$  given by (3.1) is to obtain integro-differential equations for the scattering wave functions. Thus, replacing  $\psi_{\underline{k}}(\underline{r})$  by the expansion (2.8) we find that the radial function  $u_l(k, r)$  satisfies the integro-differential equation

$$\begin{aligned} & \left[ \frac{d^2}{dr^2} + k^2 + \frac{2(z-1)}{r} + 2\left(z + \frac{1}{r}\right) e^{-2zr} - \frac{l(l+1)}{r^2} \right] u_l(k, r) = -\frac{\beta(zr)}{(zr)^4} u_l(k, r) \pm \frac{8z^3}{(2l+1)} e^{-zr} \\ & \times \left[ r^{-l} I(l+1, r) + r^{l+1} \{ I(-l, \infty) - I(-l, r) - \frac{1}{2} \delta_{l,0} (z^2 + k^2) I(-l+1, \infty) \} \right] \\ & \mp \frac{4ze^{-zr}}{(2l+1)} \left[ \delta_{l,1} \left\{ -\frac{1}{2} z(z^2+k^2) r^3 + (z^2-k^2) r^2 \right\} J(-l, r) + 2\left(\frac{1}{2} z r^3 + r^2\right) \left\{ \frac{l}{(2l-1)} r^{l-1} J(-l-1, r) \right. \right. \\ & \qquad \qquad \qquad \left. \left. + \frac{(l+1)}{(2l+3)} r^{l+1} J(-l-3, r) \right\} \right] \\ & \pm \frac{4}{3} \frac{z\delta}{l,1} e^{-2zr} \left[ \left( \frac{3}{2} z^2 r^2 + \frac{1}{2} zr - 3 \right) u_l(k, r) - \left( \frac{1}{2} zr^2 + r \right) \frac{du_l(k, r)}{dr} \right] , \end{aligned} \quad (3.4)$$

where

$$\beta(x) = \frac{9}{2} - \frac{2}{3} e^{-2x} \left( x^5 + \frac{9}{2} x^4 + 9x^3 + \frac{27}{2} x^2 + \frac{27}{2} x + \frac{27}{4} \right) , \quad (3.5)$$

$$I(m, r) = \int_0^r e^{-zx} u_l(k, x) x^m dx , \quad (3.6)$$

$$J(m, r) = \int_r^\infty e^{-zx} u_l(k, x) x^m dx . \quad (3.7)$$

The direct polarization potential has the property

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

where  $\alpha = 9/2z^4$  is the dipole polarizability.

The exchange polarization approximation is obtained if on the right-hand side of equation (3.4) the terms in the two final square brackets are omitted. The exchange approximation [Morse and Allis (1933); Seaton (1957)] is obtained by omitting  $\psi^{\text{pol}}(\underline{r}_1, \underline{r}_2)$

from the total wave function (3.1).

In the present work we have taken  $u_l(k, r)$  to be a solution of the integro-differential equation

$$\left[ \frac{d^2}{dr^2} + k^2 + \frac{2(z-1)}{r} + 2A_1 \left( z + \frac{1}{r} \right) e^{-2zr} - \frac{l(l+1)}{r^2} + A_2 \frac{\beta(zr)}{(zr)^4} \right] u_l(k, r) = \frac{8z^3 A_1}{(2l+1)} e^{-zr} \times [r^{-l} I(l+1, r) + r^{l+1} \{ I(-l, \infty) - I(-l, r) - \frac{1}{2l, 0} (z^2 + k^2) I(-l+1, \infty) \}] , \quad (3.8)$$

where  $A_1$ ,  $A_2$ , and  $A_3$  are constants whose function is to switch on or off the terms which they multiply.

### 3.1 The normalization of the continuum wave functions

In this section the amplitude of the solution of (3.8) is examined in the asymptotic region and adjusted so that (2.9) is satisfied. This is easily achieved by means of the Strömrgren method (cf. Bates and Seaton, 1949). In the asymptotic region the radial part  $u_l(k, r)$  of the continuum orbital satisfies an equation of the form

$$\frac{d^2}{dr^2} u_l(k, r) + \lambda(k, r) u_l(k, r) = 0 \quad (3.9)$$

which, as can easily be verified, is satisfied by

$$u_l(k, r) = C \zeta^{-1/2} \sin \{ \phi(r) + \delta \} , \quad (3.10)$$

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

$$\zeta^2 = \lambda(k, r) + \zeta^{1/2} \frac{d^2}{dr^2} (\zeta^{-1/2}) . \quad (3.11)$$

This equation can be solved by iteration; the convergence is very rapid – indeed it is usually only necessary to replace  $\zeta$  in the second term by  $\lambda(k, r)$ . As  $r \rightarrow \infty$ ,  $\lambda(k, r)$  tends to  $k^2$ , so that the asymptotic amplitude of (3.10) is simply  $C k^{-1/2}$ . The determination of the multiplying constant  $C$  involved in any particular solution of

(3.9) can be carried out in the following manner: choosing two radial distances  $r_1$  and  $r_2$ , and introducing

$$a = \frac{1}{2} \int_{r_1}^{r_2} \zeta dr, \quad a_1 = \zeta_1^{1/2} u_l(k, r_1), \quad a_2 = \zeta_2^{1/2} u_l(k, r_2) \quad (3.12)$$

it can easily be shown that

$$C = \frac{1}{2} [(a_1 + a_2)^2 \sec^2 a + (a_1 - a_2)^2 \operatorname{cosec}^2 a]^{1/2} \quad (3.13)$$

Since  $\zeta$  is known from (3.11), this can easily be evaluated.

### 3.2 The solution of the continuum integro-differential equation

It is convenient to write (3.8) in the form

$$\frac{d^2}{dr^2} u_l(k, r) = f_l(k, r) u_l(k, r) + g_l(r) \int_0^r e^{-zx} u_l(k, x) \left\{ r^{-l} x^{l+1} - r^{l+1} x^{-l} \right\} dx + r^{l+1} a g_l(r) \quad (3.14)$$

where

$$f_l(k, r) = \frac{l(l+1)}{r^2} - k^2 - \frac{2(z-1)}{r} - 2A_1 \left(z + \frac{1}{r}\right) e^{-2zr} - A_2 \frac{\beta(zr)}{(zr)^4} \quad (3.15)$$

$$g_l(r) = \frac{8z^3 A_3}{(2l+1)} e^{-zr} \quad (3.16)$$

$$a = \int_0^\infty e^{-zx} u_l(k, x) x^{-l} \left\{ 1 - \frac{1}{2l+1} x(z^2 + k^2) \right\} dx \quad (3.17)$$

Following Percival and Marriott [Marriott (1958)] if we define  $X_l(k, r)$ ,  $Y_l(k, r)$  as solutions of the equations

$$\frac{d^2}{dr^2} X_l(k, r) = f_l(k, r) X_l(k, r) + g_l(r) \int_0^r e^{-zx} X_l(k, x) \left\{ r^{-l} x^{l+1} - r^{l+1} x^{-l} \right\} dx \quad (3.18)$$

$$\frac{d^2}{dr^2} Y_l(k, r) = f_l(k, r) Y_l(k, r) + g_l(r) \int_0^r e^{-zx} Y_l(k, x) \left\{ r^{-l} x^{l+1} - r^{l+1} x^{-l} \right\} dx + r^{l+1} g_l(r) \quad (3.19)$$

then clearly

$$u_l(k, r) = X_l(k, r) + a Y_l(k, r) \quad (3.20)$$

is a particular solution of (3.14). Substituting (3.20) in (3.17) we obtain

$$a = \frac{\int_0^\infty e^{-zx} X_l(k, x) x^{-l} \{1 - \frac{1}{2} \delta_{l,0} x (z^2 + k^2)\} dx}{1 - \int_0^\infty e^{-zx} Y_l(k, x) x^{-l} \{1 - \frac{1}{2} \delta_{l,0} x (z^2 + k^2)\} dx} \quad (3.21)$$

The non-iterative method that was used for the solution of (3.18) and (3.19) is described in Appendix B. In this Appendix we also describe the numerical methods used for the evaluation of the exchange integrals  $I(m, r)$ , the radial integrals in (2.20) and (2.39) and the integrals over the variables  $p$  and  $k$  in (2.21) and (2.40).

#### 4. Results

Although we have calculated cross sections in the Born (ii) approximation using both (2.21) and (2.40) for the following set of values for  $A_1$ ,  $A_2$  and  $A_3$ ,

- (i)  $A_1 = A_2 = A_3 = 0$  ,
- (ii)  $A_1 = A_3 = 1, A_2 = 0$  ,
- (iii)  $A_1 = A_2 = A_3 = 1$  ,

we shall only present results for the case (ii). Case (i) corresponds to the work of Peach (1965), and (iii) to that of Sloan (1964). Cross sections obtained in case (ii) and case (iii) differ by less than 0.1%. Repeating the previous calculations of Sloan (1964) and Peach (1965) provided a good test of our computer program; good agreement was obtained in all cases. The method used for obtaining the phase shifts for scattering by ionized helium is that of Burgess (1963).

Calculated partial wave cross sections  $Q_l(k_1^2)$ ,

$$Q(k_1^2) = \sum_{l=0}^4 Q_l(k_1^2) ,$$

are presented in Tables 2 – 5. The s-wave results ( $l = 0$ ) depend on the orthogonalization procedure adopted, and may be significantly in error. However, the agreement of both sets of results with Bethe's sum rule at energies in excess of 50 times threshold indicates that this error cannot be greater than 10% of the s-wave contribution in this energy range. As expected, the dipole contribution dominates and the convergence of the partial wave sum is rapid for  $l \geq 1$  at all energies.

In our analysis we neglect the fact that the incident electron, in the case of  $\text{Li}^+ \rightarrow \text{Li}^{2+}$ , should be represented by a Coulomb wave and not a plane wave. However, the total cross sections obtained for process (1.2) are in excellent agreement with the values obtained by Moores (1969, private communication) using a Coulomb-Born approximation, at energies as low as five times threshold.

The length and velocity formulations yield results for the total cross section differing by less than 9% for He and less than 6% for  $\text{Li}^+$  at all energies. It is therefore judged unlikely that the true Born cross section (i.e. the cross section computed with exact wave functions) would differ from the mean of our results by more than 10%.

Our results for the total cross section for processes (1.1) and (1.2) are presented in Tables 6 and 7 respectively. In the latter table we also present the results of Moores for comparison.

In Fig. 1 we compare our calculated cross sections for He with the experimental measurements of Golden and Rapp (1964) and of Smith (1930), and with the Bethe asymptotic results (derived from sum rules) of Inokuti and Kim (1969). They give

$$Q(E_i) \underset{E_i \rightarrow \infty}{=} \frac{4}{E_i} [A \ln E_i + B] (\pi a_0^2)$$

with

$$A = 0.489 , \quad B = 0.036 + 2 \ln 2$$

to within 1% for  $E_i \geq 50$ . Our length calculations agree with this result to within 3% for  $E_i > 1$  kev. The velocity formulation results appear to be low, compared with experiment, but are in good agreement with the data of Smith within his estimated errors. A fit to our length results of the form

$$Q(E_i) = \frac{4}{E_i} [A \ln E_i + B] (\pi a_0^2)$$

yields

$$A = 0.480 , \quad B = 0.758 .$$

A fit to our velocity results of the above form gives

$$A = 0.428 , \quad B = 0.743 .$$

In Fig. 2 we compare our results for ionization of  $\text{Li}^+$  with the experimental results of Peart and Dolder (1968, 1969). The results of Lineberger et al are consistent with those shown. Kim and Inokuti [private communication, (1969)] find that for process (1.2) at impact velocity  $v$  cm sec<sup>-1</sup>, the Bethe limit is

$$Q(E_i) = \frac{4}{E_i} [A \ln \left( \frac{\beta^2}{1 - \beta^2} \right) - \beta^2 + B] (\pi a_0^2)$$

where

$$\beta = \frac{v}{c}, \quad A = 0.1445 , \quad B = 1.552 \pm 0.058 .$$

For  $E_i > 50$  our length results agree with the results of Kim and Inokuti to within 4%, while our velocity results are approximately 6% lower, though both are compatible with experiment. We note that in both cases (He and  $\text{Li}^+$ ) a plot of  $E_i Q(E_i)$  vs  $\ln E_i$  has a linear region in the neighbourhood of  $E_i = 10$  with a slope substantially larger than the one finally attained. A fit to our length results of the form

$$Q(E_i) = \frac{4}{E_i} [A \ln \left( \frac{\beta^2}{1 - \beta^2} \right) - \beta^2 + B] (\pi a_0^2)$$

gives

$$A = 0.1513 \quad , \quad B = 1.5636 .$$

A similar fit to our velocity results gives

$$A = 0.1414 \quad , \quad B = 1.4753 .$$

In Fig. 3 we compare our results for ionization of  $\text{Li}^+$  with the results of Moores. Both our length and our velocity results are in excellent agreement with the values obtained by Moores, at energies as low as five times threshold.

In order to explain the origin of the results presented in Tables 8 - 13, we write

$$Q_L(k_i^2) = \sum_{\ell=0}^{\infty} \int_0^{k_{\max}^{(L)}} \sigma_{\ell}^{(L)}(k^2) d\left(\frac{1}{2}k^2\right) ,$$

$$Q_V(k_i^2) = \sum_{\ell=0}^{\infty} \int_0^{k_{\max}^{(V)}} \sigma_{\ell}^{(V)}(k^2) d\left(\frac{1}{2}k^2\right) ,$$

where

$$\sigma_{\ell}^{(L)}(k^2) = \int_{p_{\min}}^{p_{\max}} |I_{\ell}^{(L)}(k, p)|^2 dp ,$$

$$\sigma_{\ell}^{(V)}(k^2) = \int_{p_{\min}}^{p_{\max}} |I_{\ell}^{(V)}(k, p)|^2 dp ,$$

with

$$I_{\ell}^{(L)}(k, p) = \left\{ \frac{2^{13} z^3 \pi (2\ell + 1)^{1/2}}{p^3} \right\} \frac{N}{k_i} V_{\ell}^{(L)}(k, p) ,$$

$$I_{\ell}^{(V)}(k, p) = \{ 2^{13} z^3 \pi (2\ell + 1) p \}^{1/2} \frac{N}{k_i (k^2 + p^2 + 2I)} V_{\ell}^{(V)}(k, p) .$$

A sample of our calculated results for the quantities  $I_1^{(L)}(k, p)$  and  $I_1^{(v)}(k, p)$ , for the process  $\text{He} + e \rightarrow \text{He}^+ + 2e$ , are presented in Tables 8 and 9, and illustrated in Fig. 4. A similar sample for the process  $\text{Li}^+ + e \rightarrow \text{Li}^{2+} + 2e$  are presented in Tables 10 and 11 and illustrated in Fig. 6. A sample of our calculated results for the differential cross sections  $\sigma_1^{(L)}(k^2)$  and  $\sigma_1^{(v)}(k^2)$  are presented in Table 12 and illustrated in Fig. 6, for the process  $\text{He} + e \rightarrow \text{He}^+ + 2e$ , and in Table 13 and Fig. 7 for the process  $\text{Li}^+ + e \rightarrow \text{Li}^{2+} + 2e$ .

The excellent agreement obtained between our Born (ii) calculations for He and for  $\text{Li}^+$  and experiment, and with the sum rule limits indicates that the similar agreement of Bely and Schwartz's (1969) and McDowell and Williamson's (1963) calculations for  $\text{H}^-$  detachment with the experimental results of Dance et al. (1967) is not accidental. We believe it substantially reinforces Bely and Schwartz's conclusion that their calculation is incompatible with the Tisone-Branscomb experiment.

## 5. Conclusions

Using a partial wave expansion for the ejected electron we have calculated cross sections for electron impact ionization of the ground state of He and  $\text{Li}^+$  in the Born (ii) approximation at energies from threshold to 9 kev. Cross sections calculated with an open shell two-parameter wave function for the ground state of the target in both the length and velocity formulations are in reasonable agreement. In both cases the calculated cross sections are in agreement with experiment at impact energies in excess of 25 times threshold. They approach the Bethe asymptotic limit correctly. We conclude that electron impact ionization of two-electron systems is well described by the first Born approximation at energies in excess of 25 times threshold. This implies that in the case of  $\text{H}^-$ , the Dance et al. experiment is to be preferred to that of Tisone and Branscomb, in agreement with the conclusions of Bely and Schwartz.

Table 2

Born (ii) approximation (Length formulation) partial cross sections  $Q$  ( $\pi a_0^2$ )  
for electron impact ionization of the ground state of Helium

$E_i$ (ev)	$Q_0$	$Q_1$	$Q_2$	$Q_3$	$Q_4$
40	.445 (-1)†	.193	.282 (-1)	.267 (-2)	.238 (-3)
60	.600 (-1)	.344	.595 (-1)	.830 (-2)	.121 (-2)
80	.599 (-1)	.397	.725 (-1)	.120 (-1)	.221 (-2)
100	.562 (-1)	.408	.760 (-1)	.140 (-1)	.294 (-2)
125	.507 (-1)	.398	.748 (-1)	.149 (-1)	.352 (-2)
150	.456 (-1)	.379	.711 (-1)	.151 (-1)	.385 (-2)
200	.375 (-1)	.338	.624 (-1)	.143 (-1)	.407 (-2)
300	.271 (-1)	.272	.483 (-1)	.120 (-1)	.386 (-2)
400	.211 (-1)	.226	.387 (-1)	.101 (-1)	.347 (-2)
600	.145 (-1)	.171	.275 (-1)	.745 (-2)	.278 (-2)
800	.110 (-1)	.139	.211 (-1)	.587 (-2)	.228 (-2)
1000	.886 (-2)	.117	.172 (-1)	.482 (-2)	.192 (-2)
2000	.447 (-2)	.683 (-1)	.880 (-2)	.252 (-2)	.105 (-2)
3000	.299 (-2)	.492 (-1)	.591 (-2)	.170 (-2)	.718 (-3)
4000	.225 (-2)	.389 (-1)	.445 (-2)	.128 (-2)	.544 (-3)
5000	.180 (-2)	.323 (-1)	.356 (-2)	.103 (-2)	.438 (-3)
6000	.150 (-2)	.277 (-1)	.297 (-2)	.860 (-3)	.366 (-3)
7000	.129 (-2)	.243 (-1)	.255 (-2)	.740 (-3)	.315 (-3)
8000	.113 (-2)	.217 (-1)	.223 (-2)	.648 (-3)	.276 (-3)
9000	.101 (-2)	.196 (-1)	.198 (-2)	.577 (-3)	.246 (-3)

† The numbers in brackets denote the power of 10 by which the entry should be multiplied.

Table 3

Born (ii) approximation (Velocity formulation) partial cross sections  $Q$  ( $\pi a_0^2$ )  
for electron impact ionization for the ground state of Helium

$E_i$ (ev)	$Q_0$	$Q_1$	$Q_2$	$Q_3$	$Q_4$
40	.419 (-1)†	.174	.259 (-1)	.231 (-2)	.197 (-3)
60	.571 (-1)	.311	.554 (-1)	.741 (-2)	.105 (-2)
80	.573 (-1)	.360	.684 (-1)	.110 (-1)	.198 (-2)
100	.539 (-1)	.369	.723 (-1)	.131 (-1)	.270 (-2)
125	.487 (-1)	.360	.716 (-1)	.142 (-1)	.330 (-2)
150	.439 (-1)	.343	.683 (-1)	.144 (-1)	.365 (-2)
200	.360 (-1)	.305	.603 (-1)	.138 (-1)	.392 (-2)
300	.261 (-1)	.245	.467 (-1)	.117 (-1)	.377 (-2)
400	.202 (-1)	.204	.375 (-1)	.983 (-2)	.340 (-2)
600	.139 (-1)	.154	.266 (-1)	.730 (-2)	.273 (-2)
800	.106 (-1)	.125	.205 (-1)	.576 (-2)	.225 (-2)
1000	.851 (-2)	.106	.166 (-1)	.473 (-2)	.189 (-2)
2000	.430 (-2)	.614 (-1)	.852 (-2)	.247 (-2)	.104 (-2)
3000	.287 (-2)	.442 (-1)	.572 (-2)	.167 (-2)	.709 (-3)
4000	.216 (-2)	.349 (-1)	.431 (-2)	.126 (-2)	.537 (-3)
5000	.173 (-2)	.289 (-1)	.346 (-2)	.101 (-2)	.432 (-3)
6000	.144 (-2)	.248 (-1)	.288 (-2)	.844 (-3)	.362 (-3)
7000	.124 (-2)	.218 (-1)	.247 (-2)	.725 (-3)	.311 (-3)
8000	.109 (-2)	.195 (-1)	.216 (-2)	.636 (-3)	.273 (-3)
9000	.966 (-3)	.176 (-1)	.192 (-2)	.567 (-3)	.243 (-3)

† The numbers in brackets denote the power of 10 by which the entry should be multiplied.

Table 4

Born (ii) approximation (Length formulation) partial cross sections  $Q$  ( $\pi a_0^2$ )  
for electron impact ionization of the ground state of  $\text{Li}^+$

$E_i$ (ev)	$Q_0$	$Q_1$	$Q_2$	$Q_3$	$Q_4$
83	.857 (-3)†	.266 (-2)	.338 (-3)	.173 (-4)	.551 (-6)
98	.283 (-2)	.105 (-1)	.154 (-2)	.109 (-3)	.593 (-5)
125	.524 (-2)	.237 (-1)	.405 (-2)	.405 (-3)	.360 (-4)
150	.635 (-2)	.324 (-1)	.599 (-2)	.723 (-3)	.828 (-4)
175	.686 (-2)	.381 (-1)	.742 (-2)	.102 (-2)	.138 (-3)
200	.703 (-2)	.417 (-1)	.839 (-2)	.126 (-2)	.193 (-3)
260	.682 (-2)	.451 (-1)	.950 (-2)	.165 (-2)	.309 (-3)
400	.563 (-2)	.429 (-1)	.930 (-2)	.194 (-2)	.463 (-3)
600	.427 (-2)	.364 (-1)	.780 (-2)	.183 (-2)	.519 (-3)
800	.338 (-2)	.310 (-1)	.649 (-2)	.162 (-2)	.508 (-3)
1000	.279 (-2)	.270 (-1)	.550 (-2)	.143 (-2)	.477 (-3)
1400	.205 (-2)	.215 (-1)	.418 (-2)	.114 (-2)	.409 (-3)
2000	.147 (-2)	.166 (-1)	.304 (-2)	.856 (-3)	.327 (-3)
3000	.989 (-3)	.122 (-1)	.208 (-2)	.599 (-3)	.240 (-3)
4000	.745 (-3)	.973 (-2)	.158 (-2)	.459 (-3)	.188 (-3)
5000	.597 (-3)	.814 (-2)	.127 (-2)	.371 (-3)	.154 (-3)
6000	.499 (-3)	.703 (-2)	.106 (-2)	.311 (-3)	.130 (-3)
7000	.428 (-3)	.620 (-2)	.914 (-3)	.268 (-3)	.113 (-3)
8000	.375 (-3)	.556 (-2)	.801 (-3)	.235 (-3)	.994 (-4)
9000	.333 (-3)	.505 (-2)	.713 (-3)	.209 (-3)	.887 (-4)

† The numbers in brackets denote the power of 10 by which the entry should be multiplied.

Table 5

Born (ii) approximation (Velocity formulation) partial cross sections  $Q$  ( $\pi a_0^2$ )  
for electron impact ionization of the ground state of  $\text{Li}^+$

$E_i$ (ev)	$Q_0$	$Q_1$	$Q_2$	$Q_3$	$Q_4$
83	.834 (-3)†	.250 (-2)	.328 (-3)	.159 (-4)	.483 (-6)
98	.276 (-2)	.981 (-2)	.148 (-2)	.998 (-4)	.515 (-5)
125	.513 (-2)	.222 (-1)	.388 (-2)	.371 (-3)	.316 (-4)
150	.625 (-2)	.304 (-1)	.576 (-2)	.668 (-3)	.738 (-4)
175	.676 (-2)	.358 (-1)	.715 (-2)	.947 (-3)	.124 (-3)
200	.694 (-2)	.392 (-1)	.812 (-2)	.119 (-2)	.177 (-3)
260	.675 (-2)	.424 (-1)	.925 (-2)	.158 (-2)	.290 (-3)
400	.558 (-2)	.404 (-1)	.912 (-2)	.188 (-2)	.446 (-3)
600	.422 (-2)	.342 (-1)	.766 (-2)	.180 (-2)	.509 (-3)
800	.335 (-2)	.291 (-1)	.639 (-2)	.160 (-2)	.500 (-3)
1000	.276 (-2)	.254 (-1)	.542 (-2)	.141 (-2)	.471 (-3)
1400	.203 (-2)	.202 (-1)	.411 (-2)	.112 (-2)	.405 (-3)
2000	.145 (-2)	.156 (-1)	.299 (-2)	.847 (-3)	.324 (-3)
3000	.979 (-3)	.114 (-1)	.205 (-2)	.593 (-3)	.239 (-3)
4000	.737 (-3)	.913 (-2)	.155 (-2)	.454 (-3)	.187 (-3)
5000	.591 (-3)	.764 (-2)	.125 (-2)	.367 (-3)	.153 (-3)
6000	.494 (-3)	.659 (-2)	.105 (-2)	.308 (-3)	.130 (-3)
7000	.423 (-3)	.582 (-2)	.899 (-3)	.265 (-3)	.112 (-3)
8000	.371 (-3)	.521 (-2)	.788 (-3)	.232 (-3)	.987 (-4)
9000	.330 (-3)	.473 (-2)	.702 (-3)	.207 (-3)	.881 (-4)

† The numbers in brackets denote the power of 10 by which the entry should be multiplied.

Table 6

Born (ii) approximation cross sections  $Q$  ( $\pi a_0^2$ )  
for electron ionization of the ground state of He

$E_i$ (ev)	$Q$ (Length)	$Q$ (Velocity)
40	.268	.244
60	.473	.432
80	.544	.498
100	.557	.511
125	.542	.498
150	.514	.473
200	.456	.419
300	.363	.333
400	.300	.275
600	.223	.205
800	.179	.164
1000	.150	.137
2000	.851 (-1)†	.777 (-1)†
3000	.605 (-1)	.551 (-1)
4000	.474 (-1)	.431 (-1)
5000	.391 (-1)	.356 (-1)
6000	.334 (-1)	.304 (-1)
7000	.292 (-1)	.265 (-1)
8000	.260 (-1)	.236 (-1)
9000	.234 (-1)	.213 (-1)

† The numbers in brackets denote the power of 10 by which the entry should be multiplied.

Table 7

Born (ii) approximation (Length and Velocity formulations) and Coulomb-Born approximation (Moore, 1969) cross sections  $Q$  ( $\pi a_0^2$ ) for electron impact ionization of the ground state of  $\text{Li}^+$

$E_i$ (ev)	Q (Length)	Q (Velocity)	$E_i$ (ev)	Q (Coulomb-Born)
83	.387 (-2)†	.368 (-2)†	85.05	.123 (-1)†
98	.149 (-1)	.142 (-1)	94.5	.219 (-1)
125	.334 (-1)	.316 (-1)	113.4	.371 (-1)
150	.455 (-1)	.432 (-1)	170.1	.595 (-1)
175	.536 (-1)	.508 (-1)	226.8	.655 (-1)
200	.590 (-1)	.556 (-1)	302.4	.650 (-1)
260	.634 (-1)	.603 (-1)	378.0	.613 (-1)
400	.602 (-1)	.574 (-1)	453.6	.570 (-1)
600	.508 (-1)	.484 (-1)	755.6	.434 (-1)
800	.430 (-1)	.410 (-1)	944.5	.370 (-1)
1000	.372 (-1)	.354 (-1)	1511.2	.261 (-1)
1400	.292 (-1)	.278 (-1)	2266.8	.186 (-1)
2000	.223 (-1)	.212 (-1)	3000.0	.150 (-1)
3000	.161 (-1)	.153 (-1)	5000.0	.977 (-2)
4000	.127 (-1)	.121 (-1)	15000.0	.386 (-2)
5000	.105 (-1)	.100 (-1)	25000.0	.261 (-2)
6000	.903 (-2)	.857 (-2)		
7000	.792 (-2)	.751 (-2)		
8000	.707 (-2)	.670 (-2)		
9000	.639 (-2)	.606 (-2)		

† The numbers in brackets denote the power of 10 by which the entry should be multiplied.

Table 8

$I_1(k, p)$  for electron impact ionization of the ground state of He

$k = 0.949 (-1)^\dagger$  a.u.

$p$	$I_1^{(L)}(k, p)$	$I_1^{(V)}(k, p)$
0.190	0.101 (1)†	0.929
0.402	0.653	0.604
0.679	0.428	0.400
0.891	0.309	0.291
0.100 (1)	0.258	0.245
0.122 (1)	0.182	0.173
0.149 (1)	0.113	0.108
0.170 (1)	0.781 (-1)	0.747 (-1)
0.210 (1)	0.398 (-1)	0.375 (-1)
0.337 (1)	0.575 (-2)	0.516 (-2)
0.503 (1)	0.788 (-3)	0.700 (-3)
0.630 (1)	0.234 (-3)	0.212 (-3)
0.709 (1)	0.121 (-3)	0.111 (-3)
0.879 (1)	0.355 (-4)	0.337 (-4)
0.110 (2)	0.944 (-5)	0.919 (-5)
0.127 (2)	0.398 (-5)	0.392 (-5)

† The numbers in brackets denote the power of 10 by which the entry should be multiplied.

Table 9

$I_1(k, p)$  for electron impact ionization of the ground state of He

$k = 0.555$  a. u.

$p$	$I_1^{(L)}(k, p)$	$I_1^{(V)}(k, p)$
.213	.756	.717
.424	.519	.492
.700	.368	.349
.911	.284	.270
.102 (1)†	.245	.233
.123 (1)	.181	.173
.151 (1)	.119	.113
.172 (1)	.842 (-1)	.804 (-1)
.212 (1)	.443 (-1)	.419 (-1)
.338 (1)	.665 (-2)	.602 (-2)
.504 (1)	.923 (-3)	.826 (-3)
.630 (1)	.275 (-3)	.250 (-3)
.709 (1)	.142 (-3)	.132 (-3)
.878 (1)	.419 (-4)	.398 (-4)
.110 (2)	.112 (-4)	.109 (-4)
.127 (2)	.470 (-5)	.464 (-5)

† The numbers in brackets denote the power of 10 by which the entry should be multiplied.

Table 10

$I_1(k, p)$  for electron impact ionization of the ground state of  $\text{Li}^+$

$k = 0.906 (-1)^\dagger$  a.u.

$p$	$I_1^{(L)}(k, p)$	$I_1^{(V)}(k, p)$
.482	0.206	0.197
.685	0.168	0.161
.949	0.135	0.130
.115 (1)	0.115	0.111
.126 (1)	0.106	0.102
.146 (1)	0.908 (-1)	0.877 (-1)
.173 (1)	0.733 (-1)	0.709 (-1)
.193 (1)	0.617 (-1)	0.598 (-1)
.230 (1)	0.441 (-1)	0.429 (-1)
.352 (1)	0.141 (-1)	0.136 (-1)
.510 (1)	0.336 (-2)	0.319 (-2)
.632 (1)	0.126 (-2)	0.119 (-2)
.707 (1)	0.721 (-3)	0.682 (-3)
.869 (1)	0.246 (-3)	0.235 (-3)
.108 (2)	0.745 (-4)	0.721 (-4)
.124 (2)	0.337 (-4)	0.330 (-4)

† The numbers in brackets denote the power of 10 by which the entry should be multiplied.

Table 11

$I_1(k, p)$  for electron impact ionization of the ground state of  $\text{Li}^+$

$k = .109 (1)^\dagger$  a.u.

$p$	$I_1^{(L)}(k, p)$	$I_1^{(V)}(k, p)$
.578	.139	.136
.777	.119	.116
.104 (1)	.101	.978 (-1)
.124 (1)	.894 (-1)	.868 (-1)
.134 (1)	.841 (-1)	.816 (-1)
.154 (1)	.747 (-1)	.725 (-1)
.180 (1)	.635 (-1)	.616 (-1)
.200 (1)	.555 (-1)	.538 (-1)
.237 (1)	.421 (-1)	.409 (-1)
.357 (1)	.151 (-1)	.147 (-1)
.513 (1)	.386 (-2)	.370 (-2)
.632 (1)	.148 (-2)	.141 (-2)
.707 (1)	.858 (-3)	.816 (-3)
.866 (1)	.297 (-3)	.284 (-3)
.107 (2)	.910 (-4)	.883 (-4)
.123 (2)	.414 (-4)	.406 (-4)

† The numbers in brackets denote the power of 10 by which the entry should be multiplied.

Table 12

Differential cross sections  $\sigma_1$  ( $k^2$ ), in units of  $\pi a_0^2$ , for  $\text{He} + e \rightarrow \text{He}^+ + 2e$

$E_i = 600 \text{ ev}$			$E_i = 800 \text{ ev}$		
$k$	$\sigma_1^{(L)}$ ( $k^2$ )	$\sigma_1^{(V)}$ ( $k^2$ )	$k$	$\sigma_1^{(V)}$ ( $k^2$ )	$\sigma_1^{(V)}$ ( $k^2$ )
.200 (-1)†	.348	.298	.232 (-1)	.282	.241
.949 (-1)	.343	.295	.110	.276	.238
.193	.328	.284	.224	.261	.226
.268	.311	.271	.311	.243	.212
.308	.301	.263	.357	.232	.204
.383	.278	.246	.444	.210	.186
.480	.247	.221	.557	.180	.162
.555	.223	.200	.644	.157	.142
.695	.178	.163	.807	.118	.109
.114 (1)	.761 (-1)	.702 (-1)	.133 (1)	.422 (-1)	.386 (-1)
.173 (1)	.228 (-1)	.204 (-1)	.201 (1)	.105 (-1)	.915 (-2)
.218 (1)	.921 (-1)	.805 (-2)	.253 (1)	.377 (-2)	.326 (-2)
.246 (1)	.531 (-1)	.462 (-2)	.286 (1)	.205 (-2)	.178 (-2)
.306 (1)	.176 (-2)	.155 (-2)	.355 (1)	.619 (-3)	.552 (-3)
.384 (1)	.518 (-3)	.475 (-3)	.446 (1)	.178 (-3)	.166 (-3)
.444 (1)	.223 (-3)	.209 (-3)	.516 (1)	.746 (-4)	.712 (-4)

† The numbers in brackets denote the power of 10 by which the entry should be multiplied.

Table 13

Differential cross sections  $\sigma_1$  ( $k^2$ ), in units of  $\pi a_0^2$ , for  $Li^+ + e \rightarrow Li^{2+} + 2e$

$E_i = 600 \text{ ev}$			$E_i = 800 \text{ ev}$		
$k$	$\sigma_1^{(L)}$ ( $k^2$ )	$\sigma_1^{(V)}$ ( $k^2$ )	$k$	$\sigma_1^{(L)}$ ( $k^2$ )	$\sigma_1^{(V)}$ ( $k^2$ )
.191 (-1)†	.267 (-1)	.248 (-1)	.224 (-1)	.224 (-1)	.208 (-1)
.907 (-1)	.266 (-1)	.247 (-1)	.106	.223 (-1)	.207 (-1)
.184	.263 (-1)	.244 (-1)	.216	.219 (-1)	.203 (-1)
.256	.258 (-1)	.240 (-1)	.300	.214 (-1)	.199 (-1)
.294	.256 (-1)	.238 (-1)	.345	.211 (-1)	.196 (-1)
.365	.249 (-1)	.232 (-1)	.429	.204 (-1)	.190 (-1)
.459	.240 (-1)	.224 (-1)	.539	.193 (-1)	.180 (-1)
.530	.232 (-1)	.216 (-1)	.623	.184 (-1)	.172 (-1)
.664	.214 (-1)	.201 (-1)	.780	.165 (-1)	.156 (-1)
.101 (1)	.152 (-1)	.144 (-1)	.128 (1)	.105 (-1)	.999 (-2)
.165 (1)	.839 (-2)	.796 (-2)	.194 (1)	.495 (-2)	.469 (-2)
.208 (1)	.500 (-2)	.472 (-2)	.245 (1)	.263 (-2)	.247 (-2)
.235 (1)	.357 (-2)	.336 (-2)	.276 (1)	.172 (-2)	.165 (-2)
.292 (1)	.173 (-2)	.162 (-2)	.343 (1)	.763 (-3)	.712 (-3)
.367 (1)	.685 (-3)	.644 (-3)	.431 (1)	.273 (-3)	.257 (-3)
.424 (1)	.348 (-3)	.330 (-3)	.498 (1)	.132 (-3)	.126 (-3)

† The numbers in brackets denote the power of 10 by which the entry should be multiplied.

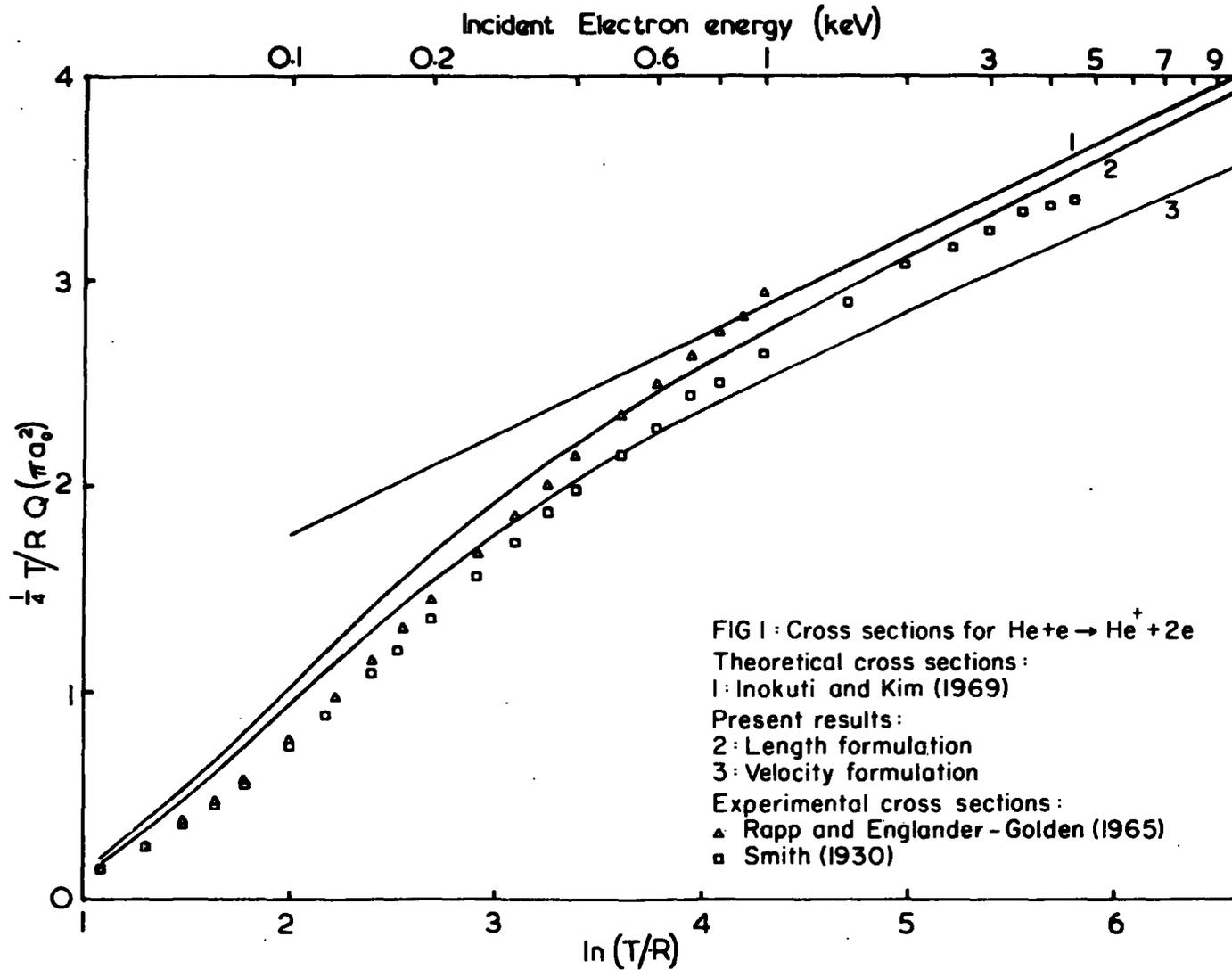


Fig. 1.

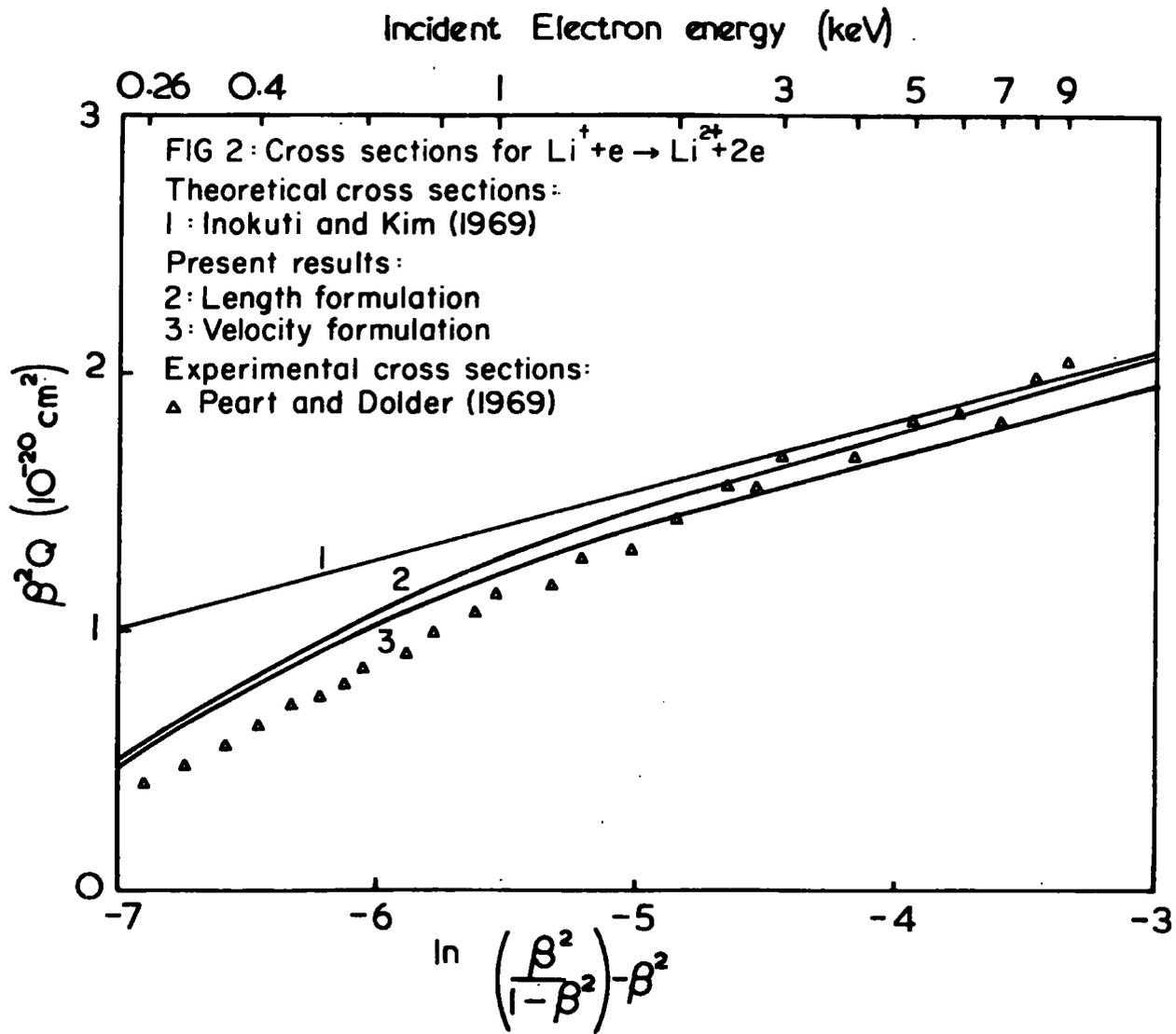
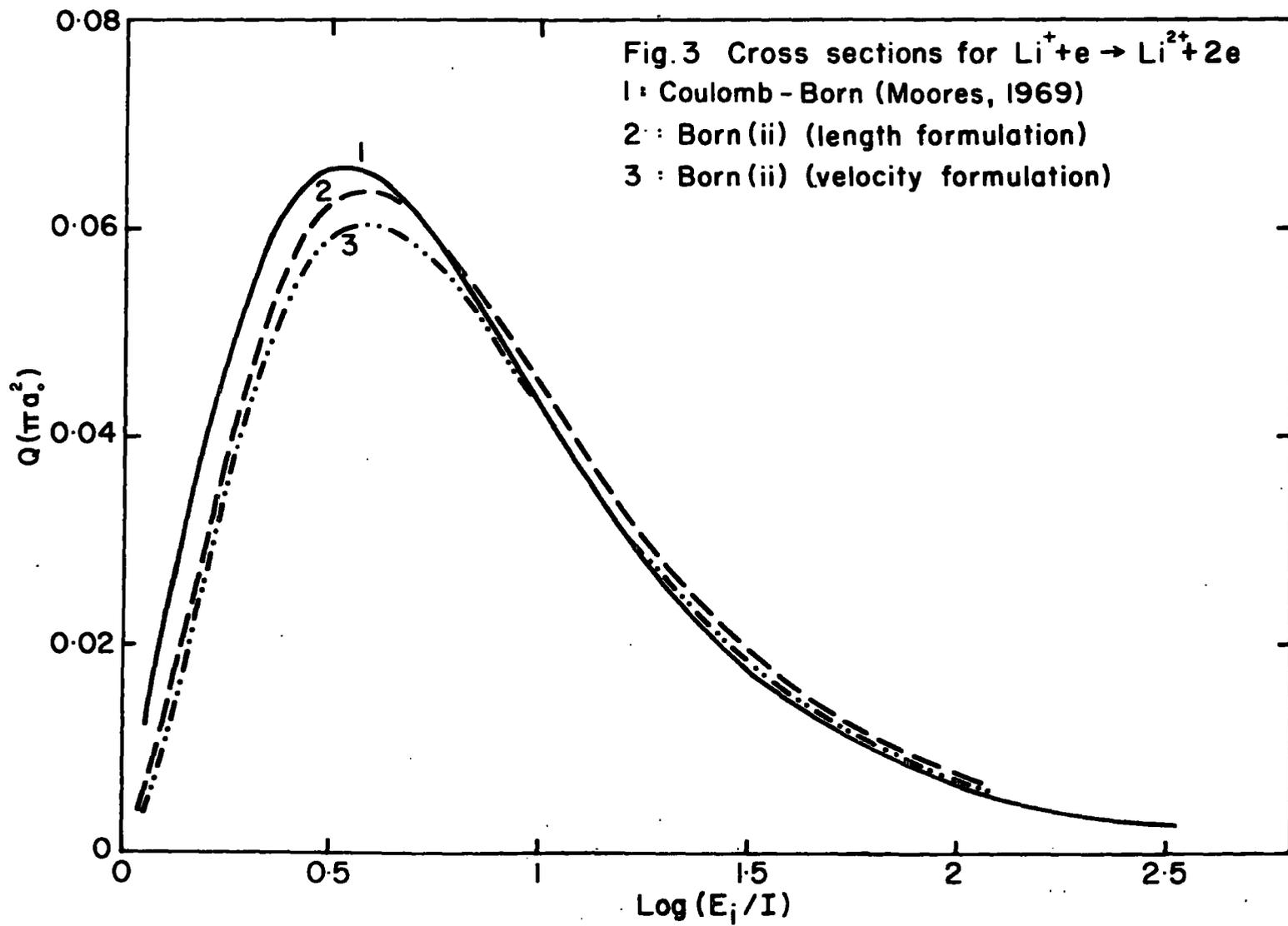
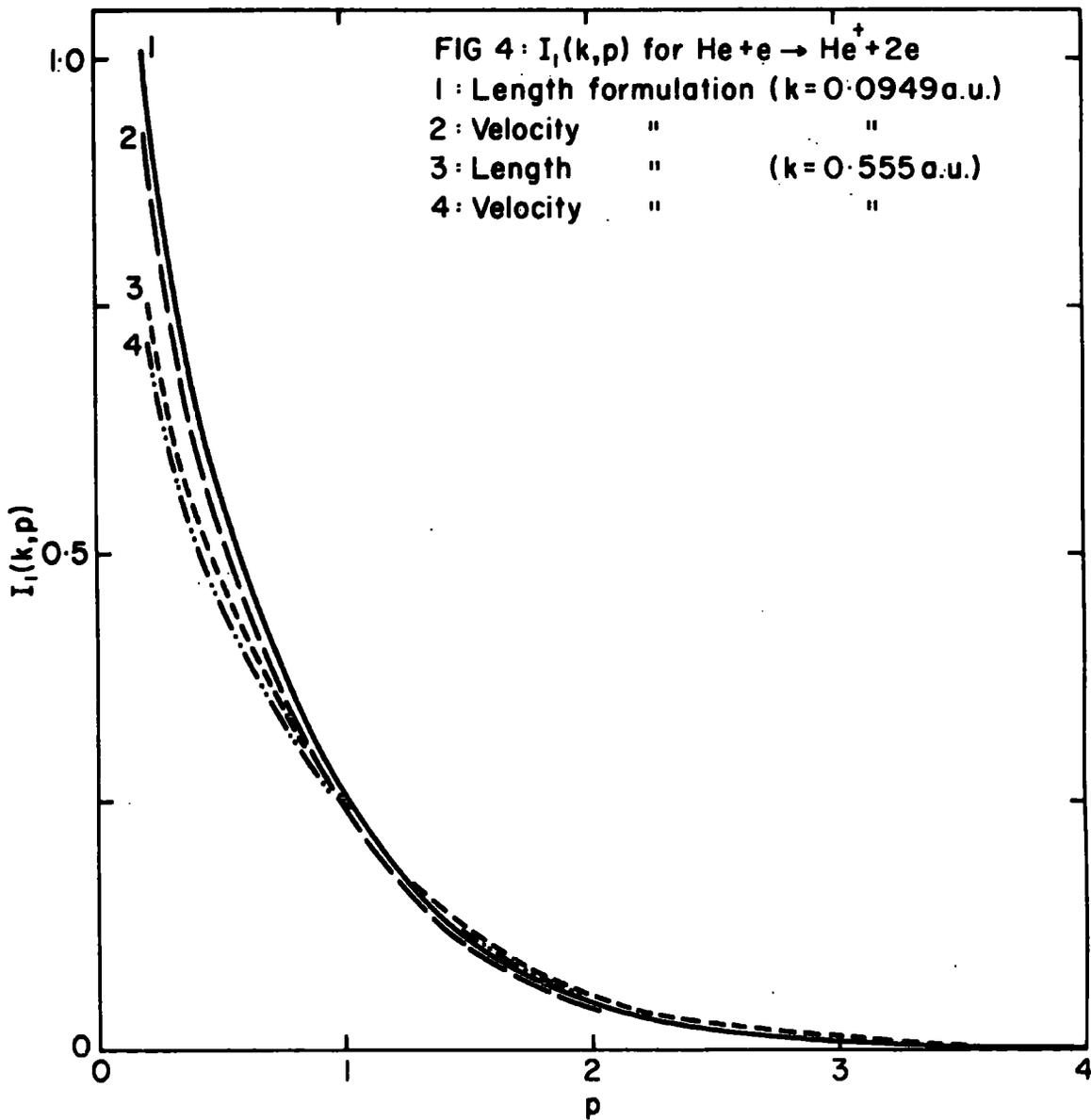
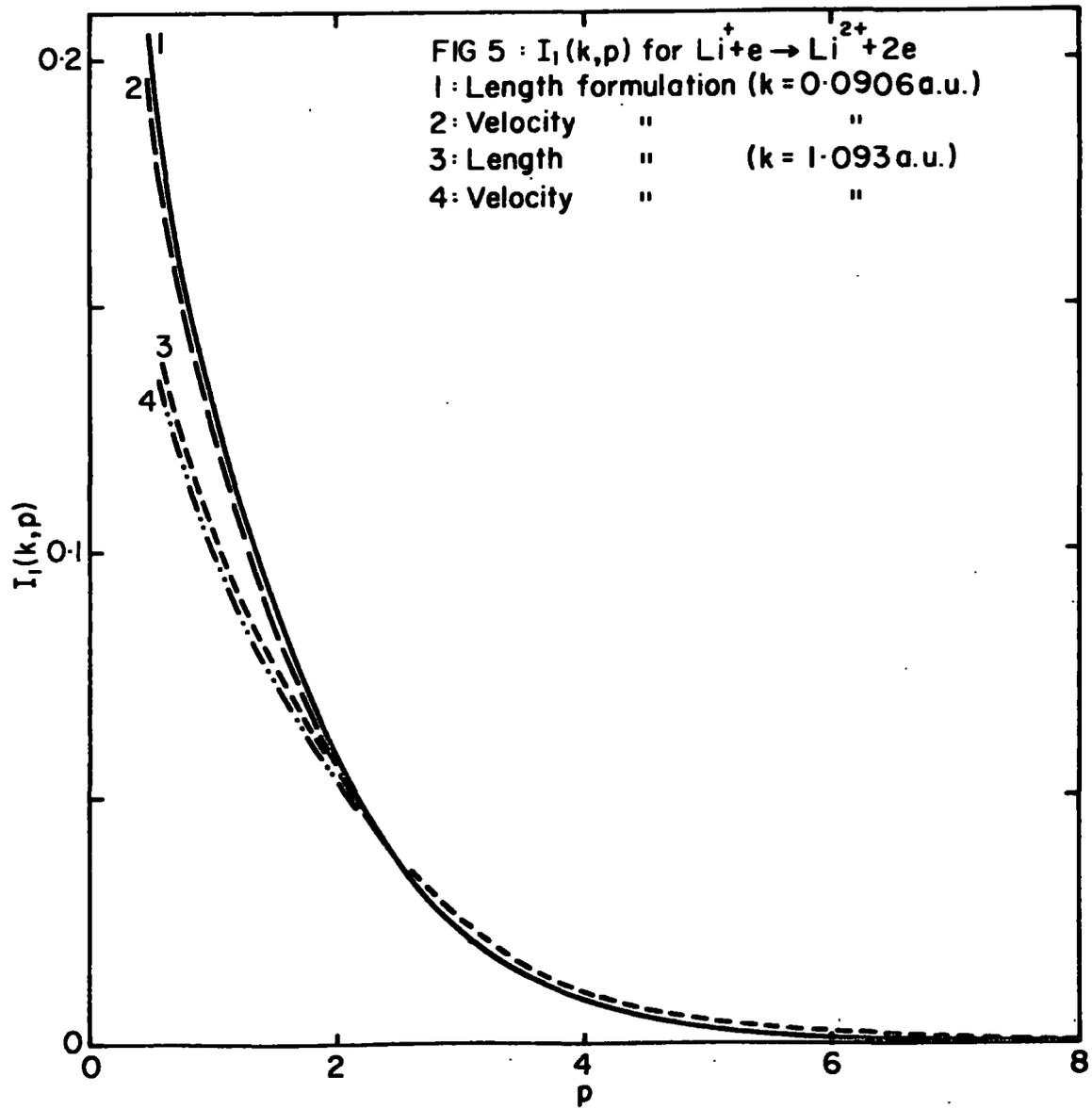
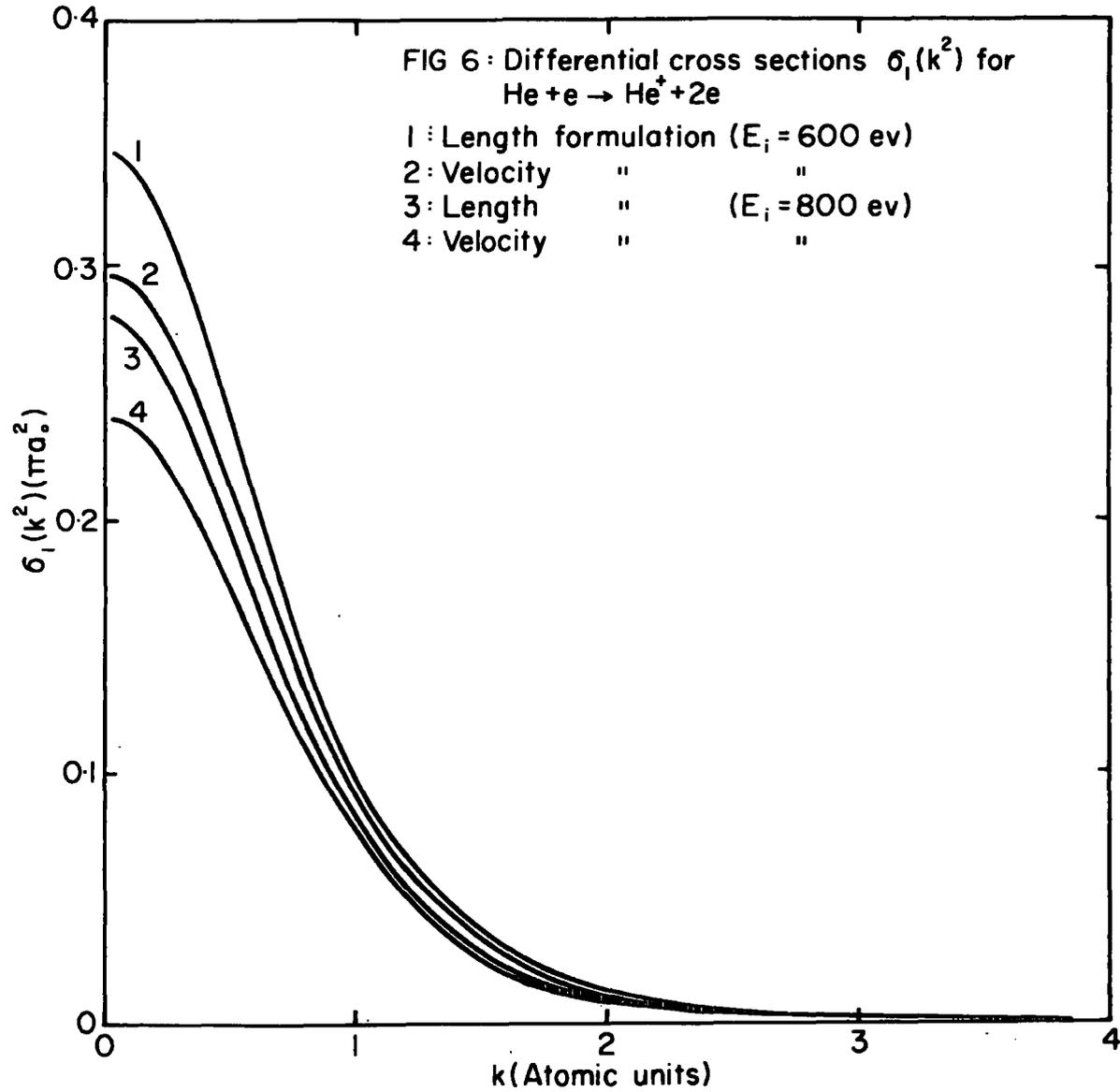


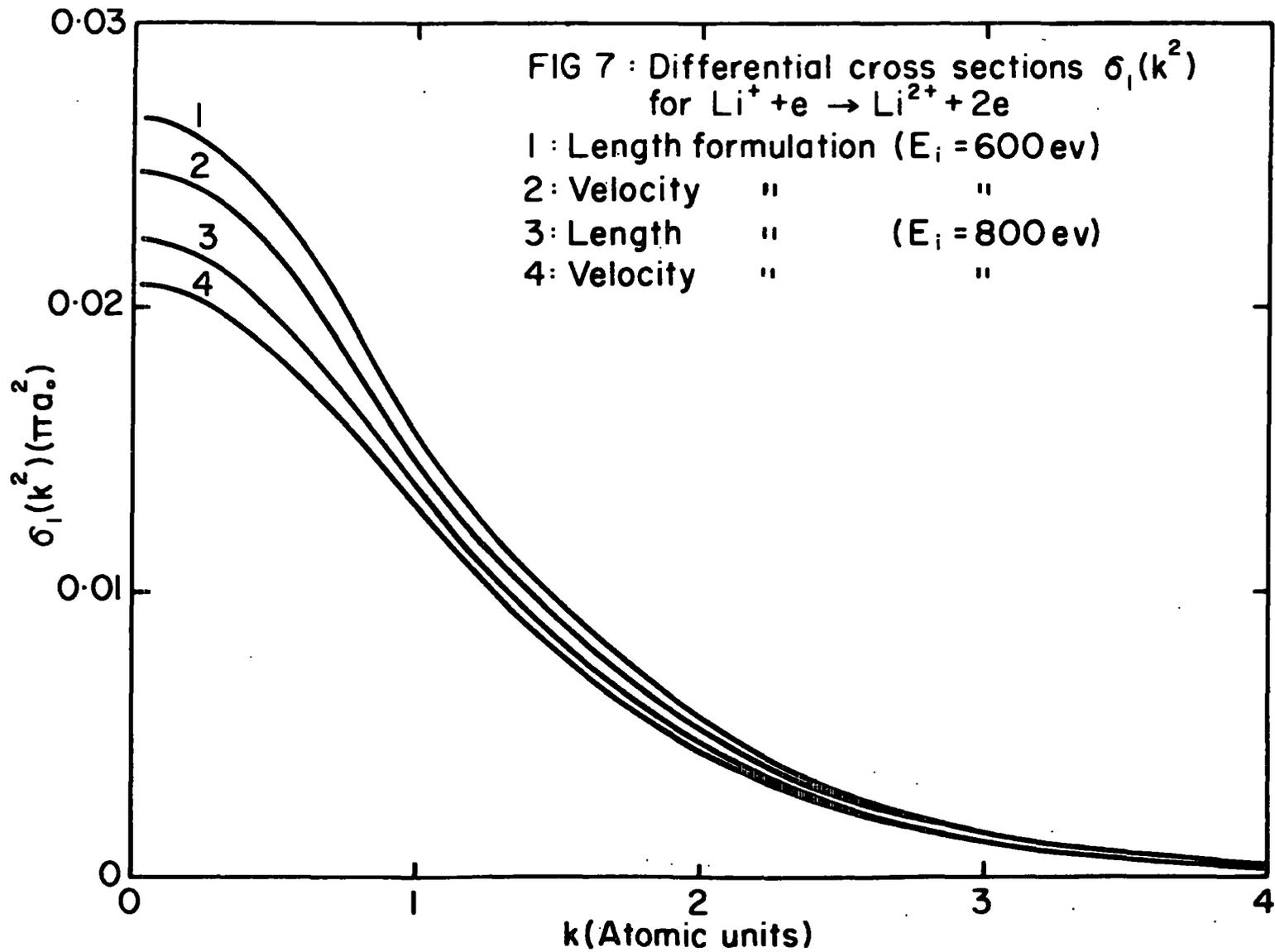
Fig. 2.











## CHAPTER IV

### IONIZATION OF He AND Li<sup>+</sup> BY ELECTRON IMPACT

#### (WITH A HYLLERAAS CORRELATED WAVE FUNCTION FOR THE GROUND STATE)

##### 1. Introduction

The effect of the interaction between the continuum electron and the core can only be fully obtained if the trial function defining the initial bound state depends explicitly on the distance  $r_{12}$  between the core and the continuum electrons. Such wave functions have been obtained for two-electron systems by a number of authors but correlation has never been allowed for in previous calculations for the ionization of He by electron impact. It is therefore of interest to reconsider the processes (cf. Chap. III)



using a Hylleraas type correlated wave function for the ground state of the target, in order to test the reliability of the computed cross section. Again, a partial wave expansion is used for the ejected electron, the radial functions used being continuum Hartree-Fock.

The partial wave cross sections  $l = 0$  and  $l = 1$  are calculated in the length formulation of the Born (ii) approximation (Chap. I, 3.3, Eq. 3.16. ). It is found that the correlated wave function used predicts the dipole oscillator strength for the transition (1.1) in satisfactory agreement with experiment and gives partial wave cross sections intermediate between the length and velocity results, obtained with an open-shell two-parameter wave function for the ground state of the target, and presented in Chapter III.

## 2. Reduction of the Matrix Element

We adopt the same notation as that used in the previous Chapters. All quantities not defined in the present Chapter are as defined in Chapter III. For the ground state we use a Hylleraas type correlated wave function, the variational parameters being given by Green et al.(1954). The parameters used are listed in Table 1, together with the corresponding value of the ionization potential. We write the initial wave function as

$$\Psi_0(\underline{r}_1, \underline{r}_2) = N [e^{-a r_1 - \beta r_2} + e^{-a r_2 - \beta r_1}] [1 + c r_{12}], \quad (2.1)$$

where N is a normalization constant.

Table 1

Parameters used in evaluating the matrix element

	z	a	$\beta$	c	I
He	2	1.436	2.208	0.2924	1.80284
Li <sup>+</sup>	3	2.362	3.299	0.2770	5.55436

The orthogonality factor  $\langle \Psi_0 | \Psi_{\underline{k}} \rangle$  is given by

$$\begin{aligned} \langle \Psi_0 | \Psi_{\underline{k}} \rangle &= \frac{N}{\sqrt{2}} \iint d\underline{r}_1 d\underline{r}_2 [e^{-a r_1 - \beta r_2} + e^{-a r_2 - \beta r_1}] [\psi_{1s}(z, \underline{r}_2) \psi_{\underline{k}}(\underline{r}_1) + \psi_{1s}(z, \underline{r}_1) \psi_{\underline{k}}(\underline{r}_2)] \\ &\quad \times (1 + c r_{12}) \\ &= \sqrt{2} N \iint d\underline{r}_1 d\underline{r}_2 [e^{-a r_1 - \beta r_2} + e^{-a r_2 - \beta r_1}] \psi_{1s}(z, \underline{r}_2) \psi_{\underline{k}}(\underline{r}_1) (1 + c r_{12}) \\ &= I_1 + I_2, \end{aligned} \quad (2.2)$$

where

$$I_1 = \sqrt{2} N \iint d\underline{r}_1 d\underline{r}_2 [e^{-a r_1 - \beta r_2} + e^{-a r_2 - \beta r_1}] \psi_{1s}(z, \underline{r}_2) \psi_{\underline{k}}(\underline{r}_1), \quad (2.3)$$

and

$$I_2 = \sqrt{2} c N \iint d\underline{r}_1 d\underline{r}_2 [e^{-a r_1 - \beta r_2} + e^{-a r_2 - \beta r_1}] \psi_{1s}(z, \underline{r}_2) \psi_{\underline{k}}(\underline{r}_1) r_{12}. \quad (2.4)$$

The  $\underline{r}_1$  integration of (2.3) can easily be carried out to give

$$I_1 = 8 (2\pi z^3)^{1/2} N \int d\underline{r}_1 \left[ \frac{e^{-\alpha r_1}}{(z + \beta)^3} + \frac{e^{-\beta r_1}}{(z + \alpha)^3} \right] \psi_{\underline{k}}(\underline{r}_1) .$$

Making use of the partial wave expansion for  $\psi_{\underline{k}}(\underline{r}_1)$  and integrating over  $\underline{r}_1$  we obtain

$$I_1 = \frac{16 z^{3/2} N}{k^{1/2}} e^{-i(\sigma_0 + \eta_0)} \int_0^\infty r u_0(k, r) \left[ \frac{e^{-\alpha r}}{(z + \beta)^3} + \frac{e^{-\beta r}}{(z + \alpha)^3} \right] dr . \quad (2.5)$$

With the use of the expansion

$$\frac{1}{r_{12}} = \frac{1}{r_>} \sum_{n=0}^{\infty} \left( \frac{r_{<}}{r_>} \right)^n P_n(\cos \theta_{12}) \quad (2.6)$$

where  $r_{<} =$  the smaller of  $r_1$  and  $r_2$ ,  $r_> =$  the larger of  $r_1$  and  $r_2$ , we write

$$\begin{aligned} r_{12} &= (r_1^2 + r_2^2 - 2r_1 r_2 \cos \theta_{12}) \frac{1}{r_>} \sum_{n=0}^{\infty} \left( \frac{r_{<}}{r_>} \right)^n P_n(\cos \theta_{12}) \\ &= (r_1^2 + r_2^2) \frac{1}{r_>} \sum_{n=0}^{\infty} \left( \frac{r_{<}}{r_>} \right)^n P_n(\cos \theta_{12}) \\ &\quad - \frac{2r_1 r_2}{r_>} \sum_{n=0}^{\infty} \left( \frac{r_{<}}{r_>} \right)^n \frac{1}{(2n+1)} [(n+1) P_{n+1}(\cos \theta_{12}) + n P_{n-1}(\cos \theta_{12})] . \end{aligned} \quad (2.7)$$

Substituting (2.7) in (2.4) and integrating over  $\underline{r}_2$  gives

$$I_2 = 4\sqrt{2} \pi c N \int d\underline{r}_1 \psi_{\underline{k}}(\underline{r}_1) \int_0^\infty r_2^2 \psi_{1s}(z, \underline{r}_2) [e^{-\alpha r_1 - \beta r_2} + e^{-\alpha r_2 - \beta r_1}] \left[ \frac{(r_1^2 + r_2^2)}{r_>} - \frac{2r_1 r_2 r_{<}}{3r_>^2} \right] .$$

Again with the aid of the expansion for  $\psi_{\underline{k}}(\underline{r}_1)$  we obtain, after we perform the integration over  $\underline{r}_1$ , the result

$$I_2 = \frac{8 z^{3/2} c N}{k^{1/2}} e^{-i(\sigma_0 + \eta_0)} \int_0^\infty r_1 u_0(k, r_1) I(r_1) dr_1 , \quad (2.8)$$

where

$$\begin{aligned}
I(r_1) &= \int_0^\infty r_1^2 e^{-zr_2} [e^{-ar_1 - \beta r_2} + e^{-ar_2 - \beta r_1}] \left[ \frac{(r_1^2 + r_2^2)}{r_2} - \frac{2r_1 r_2 r_2}{3r_2^2} \right] dr_2 \\
&= \frac{1}{r_1} \int_0^{r_1} e^{-zr_2} [e^{-ar_1 - \beta r_2} + e^{-ar_2 - \beta r_1}] (r_2^4 + 3r_1^2 r_2^2) dr_2 \\
&+ \int_{r_1}^\infty e^{-zr_2} [e^{-ar_1 - \beta r_2} + e^{-ar_2 - \beta r_1}] (3r_2^3 + r_1^2 r_2) dr_2 .
\end{aligned}$$

The  $r_2$  integration can now be performed to give

$$\begin{aligned}
I(r_1) &= \frac{2}{r_1} \left[ 4 \left\{ \frac{e^{-ar_1}}{(z+\beta)^3} + \frac{e^{-\beta r_1}}{(z+a)^3} \right\} + \left\{ \frac{e^{-ar_1}}{(z+\beta)^3} + \frac{e^{-\beta r_1}}{(z+a)^3} \right\} r_1^2 \right. \\
&\quad \left. - 4 \left\{ \frac{1}{(z+\beta)^3} + \frac{1}{(z+a)^3} \right\} e^{-(z+a+\beta)r_1} - \left\{ \frac{1}{(z+\beta)^4} + \frac{1}{(z+a)^4} \right\} r_1 e^{-(z+a+\beta)r_1} \right] . \quad (2.9)
\end{aligned}$$

Substituting (2.9) in (2.8) we obtain

$$\begin{aligned}
I_2 &= \frac{16 z^{3/2} c N}{k^{1/2}} e^{-i(\sigma_0 + \eta_0)} \int_0^\infty u_0(k, r) [4 \{T_s(r) - T_s(0) e^{-(z+a+\beta)r}\} \\
&\quad + r \{r T_s(r) - T_s(0) e^{-(z+a+\beta)r}\}] dr , \quad (2.10)
\end{aligned}$$

$$\text{where } T_n(r) = \frac{e^{-ar}}{(z+\beta)^n} + \frac{e^{-\beta r}}{(z+a)^n} .$$

Substitution of (2.5) and (2.10) in (2.2) yields

$$\begin{aligned}
\langle \Psi_0 | \Psi_{\underline{k}} \rangle &= \frac{16 z^{3/2} N}{k^{1/2}} e^{-i(\sigma_0 + \eta_0)} \int_0^\infty u_0(k, r) [4c \{T_s(r) - T_s(0) e^{-(z+a+\beta)r}\} \\
&\quad + r \{1 + cr\} T_s(r) - cr T_s(0) e^{-(z+a+\beta)r}] dr . \quad (2.11)
\end{aligned}$$

The matrix element is

$$\begin{aligned}
f(k, p) &= -\frac{4}{p^2} \int \int d\underline{r}_1 d\underline{r}_2 \psi_{\underline{k}}^* \text{ (Orthogonalized) } e^{i \underline{p} \cdot \underline{r}_1} \psi_0(\underline{r}_1, \underline{r}_2) \\
&= -\frac{4}{p^2} \int \int d\underline{r}_1 d\underline{r}_2 \left[ \frac{1}{\sqrt{2}} \{ \psi_{1s}^*(z, \underline{r}_2) \psi_{\underline{k}}^*(\underline{r}_1) + \psi_{1s}^*(z, \underline{r}_1) \psi_{\underline{k}}^*(\underline{r}_2) \} - \langle \psi_0 | \psi_{\underline{k}} \rangle^* \psi_0^*(\underline{r}_1, \underline{r}_2) \right] \\
&\quad \times e^{i \underline{p} \cdot \underline{r}_1} \psi_0(\underline{r}_1, \underline{r}_2) \\
&= J_1 + J_2,
\end{aligned}$$

where

$$J_1 = -\frac{2\sqrt{2}N}{p^2} \int \int d\underline{r}_1 d\underline{r}_2 \{ \psi_{1s}^*(z, \underline{r}_2) \psi_{\underline{k}}^*(\underline{r}_1) + \psi_{1s}^*(z, \underline{r}_1) \psi_{\underline{k}}^*(\underline{r}_2) \} e^{i \underline{p} \cdot \underline{r}_1} [e^{-a r_1 - \beta r_2} + e^{-a r_2 - \beta r_1}] [1 + c r_{12}], \quad (2.12)$$

and

$$J_2 = \frac{4 \langle \psi_0 | \psi_{\underline{k}} \rangle^* N^2}{p^2} \int \int d\underline{r}_1 d\underline{r}_2 e^{i \underline{p} \cdot \underline{r}_1} [e^{-2(a r_1 + \beta r_2)} + 2 e^{-(a + \beta)(r_1 + r_2)} + e^{-2(a r_2 + \beta r_1)}] [1 + 2c r_{12} + c^2 r_{12}^2]. \quad (2.13)$$

We write

$$J_1 = -\frac{2\sqrt{2}N}{p^2} [J_{11} + J_{12}], \quad (2.14)$$

$$J_2 = \frac{4 \langle \psi_0 | \psi_{\underline{k}} \rangle^* N^2}{p^2} [J_{21} + J_{22}], \quad (2.15)$$

where

$$J_{11} = \int \int d\underline{r}_1 d\underline{r}_2 \{ \psi_{1s}^*(z, \underline{r}_2) \psi_{\underline{k}}^*(\underline{r}_1) + \psi_{1s}^*(z, \underline{r}_1) \psi_{\underline{k}}^*(\underline{r}_2) \} [e^{-a r_1 - \beta r_2} + e^{-a r_2 - \beta r_1}] e^{i \underline{p} \cdot \underline{r}_1}, \quad (2.16)$$

$$J_{12} = c \int \int d\underline{r}_1 d\underline{r}_2 \{ \psi_{1s}^*(z, \underline{r}_2) \psi_{\underline{k}}^*(\underline{r}_1) + \psi_{1s}^*(z, \underline{r}_1) \psi_{\underline{k}}^*(\underline{r}_2) \} [e^{-a r_1 - \beta r_2} + e^{-a r_2 - \beta r_1}] e^{i \underline{p} \cdot \underline{r}_1} r_{12}, \quad (2.17)$$

$$J_{21} = \int \int d\underline{r}_1 d\underline{r}_2 [e^{-2(a r_1 + \beta r_2)} + 2 e^{-(a + \beta)(r_1 + r_2)} + e^{-2(a r_2 + \beta r_1)}] e^{i \underline{p} \cdot \underline{r}_1}, \quad (2.18)$$

$$J_{22} = c \int \int d\underline{r}_1 d\underline{r}_2 [e^{-2(a r_1 + \beta r_2)} + 2 e^{-(a + \beta)(r_1 + r_2)} + e^{-2(a r_2 + \beta r_1)}] e^{i \underline{p} \cdot \underline{r}_1} (2r_{12} + c r_{12}^2). \quad (2.19)$$

In Chapter III the integral  $J_{11}$  has been reduced to a form suitable for computation and the integral  $J_{21}$  evaluated in closed form. In this section we describe the reduction of  $J_{12}$  to a computable form and evaluate  $J_{22}$  in closed form. It is convenient to write

$$J_{12} = c [J_{121} + J_{122}] , \quad (2.20)$$

where

$$J_{121} = \int \int d\underline{r}_1 d\underline{r}_2 \psi_{1s}^* (z, \underline{r}_2) \psi_{\underline{k}}^* (\underline{r}_1) [e^{-\alpha r_1 - \beta r_2} + e^{-\alpha r_2 - \beta r_1}] e^{i \underline{p} \cdot \underline{r}_1} r_{12} , \quad (2.21)$$

$$J_{122} = \int \int d\underline{r}_1 d\underline{r}_2 \psi_{1s}^* (z, \underline{r}_1) \psi_{\underline{k}}^* (\underline{r}_2) [e^{-\alpha r_1 - \beta r_2} + e^{-\alpha r_2 - \beta r_1}] e^{i \underline{p} \cdot \underline{r}_1} r_{12} . \quad (2.22)$$

Use is made of the relation (2.7) and integration over  $\hat{r}_2$  is effected to yield, from (2.21), the result

$$J_{121} = 4(\pi z^3)^{1/2} \int d\underline{r}_1 \psi_{\underline{k}}^* (\underline{r}_1) e^{i \underline{p} \cdot \underline{r}_1} \int_0^\infty r_2^2 \left[ \frac{(r_1^2 + r_2^2)}{r_>} - \frac{2r_1 r_2 r_{\leq}}{3r_>^2} \right] [e^{-\alpha r_1 - \beta r_2} + e^{-\alpha r_2 - \beta r_1}] e^{-z r_2} dr_2 .$$

Now use is made of the expansion for  $\psi_{\underline{k}} (\underline{r}_1)$ , the Legendre polynomial expansion for  $e^{i \underline{p} \cdot \underline{r}_1}$  (Chap. III, 2, Eq. 2.16) and integration over  $\underline{r}_1$  is effected to give

$$J_{121} = 4 \left( \frac{2z^3}{k} \right)^{1/2} \sum_{\ell=0}^{\infty} (2\ell+1) e^{i(\sigma_\ell + \eta_\ell)} P_\ell (\cos \nu) \int_0^\infty r_1 u_\ell (k, r_1) j_\ell (pr_1) dr_1 \int_0^\infty r_2^2 \left[ \frac{(r_1^2 + r_2^2)}{r_>} - \frac{2r_1 r_2 r_{\leq}}{3r_>^2} \right] \times [e^{-\alpha r_1 - \beta r_2} + e^{-\alpha r_2 - \beta r_1}] e^{-z r_2} dr_2 ,$$

which with the use of (2.9) we can write in the form

$$J_{121} = 8 \left( \frac{2z^3}{k} \right)^{1/2} \sum_{\ell=0}^{\infty} (2\ell+1) e^{i(\sigma_\ell + \eta_\ell)} P_\ell (\cos \nu) \int_0^\infty u_\ell (k, r) j_\ell (pr) [4 \{T_s(r) - T_s(0) e^{-(z+\alpha+\beta)r}\} + r \{r T_s(r) - T_s(0) e^{-(z+\alpha+\beta)r}\}] dr . \quad (2.23)$$

Performing the  $\hat{r}_1$  integration of (2.22) yields

$$J_{122} = 4(\pi z^3)^{1/2} \sum_{n=0}^{\infty} i^n \int d\underline{r}_2 \psi_{\underline{k}}^* (\underline{r}_2) \int_0^\infty r_1^2 j_n (pr_1) e^{-z r_1} [e^{-\alpha r_1 - \beta r_2} + e^{-\alpha r_2 - \beta r_1}] \times \frac{r_{\leq}^n}{r_{>}^{n+1}} [r_1^2 + r_2^2 - 2 r_1 r_2 \left\{ \frac{n}{2n-1} \frac{r_>}{r_{<}} + \frac{n+1}{2n+3} \frac{r_{\leq}}{r_>} \right\}] P_n (\cos \theta_2) dr_1 .$$

Replacement of  $\psi_{\underline{k}}^* (\underline{r}_2)$  by its expansion and integration over  $\underline{r}_2$  leads to the expression

$$J_{122} = 4 \left( \frac{2z^3}{k} \right)^{1/2} \sum_{\ell=0}^{\infty} e^{i(\sigma_\ell + \eta_\ell)} P_\ell (\cos \nu) \int_0^\infty r u_\ell (k, r) I_\ell (p, r) dr , \quad (2.24)$$

where

$$\begin{aligned}
 I_L(p, r_2) &= \int_0^\infty r_1^2 j_L(pr_1) e^{-zr_1} [e^{-ar_1 - \beta r_2} + e^{-ar_2 - \beta r_1}] \frac{r_<}{r_>^{L+1}} [r_1^2 + r_2^2 - 2r_1 r_2] \left[ \frac{r_>}{2L-1} + \frac{L+1}{2L+3} \frac{r_<}{r_>} \right] dr_1 \\
 &= \int_0^{r_2} \frac{r_1^{L+2}}{r_2^{L+1}} \left[ \frac{r_1^2}{2L+3} - \frac{r_2^2}{2L-1} \right] [e^{-ar_1 - \beta r_2} + e^{-ar_2 - \beta r_1}] j_L(pr_1) dr_1 \\
 &\quad + \int_{r_2}^\infty \frac{r_2^L}{r_1^{L-1}} \left[ \frac{r_2^2}{2L+3} - \frac{r_1^2}{2L-1} \right] [e^{-ar_1 - \beta r_2} + e^{-ar_2 - \beta r_1}] j_L(pr_1) dr_1 .
 \end{aligned}$$

It is convenient to write this as

$$\begin{aligned}
 I_L(p, r_2) &= \int_0^\infty \frac{r_1^{L+2}}{r_2^{L+1}} \left[ \frac{r_1^2}{2L+3} - \frac{r_2^2}{2L-1} \right] [e^{-ar_1 - \beta r_2} + e^{-ar_2 - \beta r_1}] j_L(pr_1) dr_1 \\
 &\quad + \int_{r_2}^\infty \left[ \frac{r_2^{L+2}}{(2L+3)r_1^{L-1}} - \frac{r_2^L}{(2L-1)r_1^{L-3}} + \frac{r_1^{L+2}}{(2L-1)r_2^{-1}} - \frac{r_1^{L+4}}{(2L+3)r_2^{L+1}} \right] \\
 &\quad \times [e^{-ar_1 - \beta r_2} + e^{-ar_2 - \beta r_1}] j_L(pr_1) dr_1 . \tag{2.25}
 \end{aligned}$$

Substituting (2.23) and (2.24) in (2.20) we obtain

$$\begin{aligned}
 J_{12} &= 8 \left( \frac{2z^3}{k} \right)^{1/2} c \sum_{l=0}^\infty (2l+1) e^{i(\sigma_l + \eta_l)} P_l(\cos \nu) \int_0^\infty u_l(k, r) [j_l(pr)] 4(T_3(r) - T_3(o)) e^{-(z+a+\beta)r} \\
 &\quad + r (rT_3(r) - T_3(o)) e^{-(z+a+\beta)r} \Big| + \frac{1}{2(2l+1)} r I_L(p, r) \Big| dr . \tag{2.26}
 \end{aligned}$$

Using the relation (2.7) and performing the  $\hat{r}_2$  integration of (2.19) we obtain

$$\begin{aligned}
 J_{22} &= 4\pi c \int d\underline{r}_1 \int_0^\infty r_2^2 [e^{-2(ar_1 + \beta r_2)} + 2e^{-(a+\beta)(r_1 + r_2)} + e^{-2(ar_2 + \beta r_1)}] e^{i \underline{p} \cdot \underline{r}_1} \\
 &\quad \times \left[ \frac{2(r_1^2 + r_2^2)}{r_>} - \frac{4r_1 r_2 r_<}{3r_>^2} + c(r_1^2 + r_2^2) \right] dr_2 .
 \end{aligned}$$

Now integrating over  $\hat{r}_1$  we get

$$\begin{aligned}
 J_{22} &= 16\pi^2 c \int_0^\infty r_1^2 j_0(pr_1) dr_1 \int_0^\infty r_2^2 [e^{-2(ar_1 + \beta r_2)} + 2e^{-(a+\beta)(r_1 + r_2)} + e^{-2(ar_2 + \beta r_1)}] \\
 &\quad \times \left[ \frac{2(r_1^2 + r_2^2)}{r_>} - \frac{4r_1 r_2 r_<}{3r_>^2} + c(r_1^2 + r_2^2) \right] dr_2 .
 \end{aligned}$$

Subdividing the range of the  $r_2$  integration into sub-ranges  $(0, r_1)$  and  $(r_1, \infty)$ , integrating over  $r_2$  and then over  $r_1$  gives

$$\begin{aligned}
 J_{22} = 8\pi^2 \left\{ \frac{1}{a^5(4\beta^2 + p^2)} + \frac{64}{(\alpha + \beta)^5(\alpha + \beta)^2 + p^2} + \frac{1}{\beta^5(4\alpha^2 + p^2)} \right\} \\
 + 6c \left\{ \frac{\beta}{a^5(4\beta^2 + p^2)^2} + \frac{32}{(\alpha + \beta)^4(\alpha + \beta)^2 + p^2} + \frac{\alpha}{\beta^5(4\alpha^2 + p^2)^2} \right\} \\
 + 2 \left\{ \frac{(12\beta^2 - p^2)}{\alpha^3(4\beta^2 + p^2)^3} + \frac{16(3(\alpha + \beta)^2 - p^2)}{(\alpha + \beta)^3((\alpha + \beta)^2 + p^2)^3} + \frac{(12\alpha^2 - p^2)}{\beta^3(4\alpha^2 + p^2)^3} \right\} \\
 + 24c \left\{ \frac{\beta(4\beta^2 - p^2)}{\alpha^2(4\beta^2 + p^2)^4} + \frac{8((\alpha + \beta)^2 - p^2)}{(\alpha + \beta)^2((\alpha + \beta)^2 + p^2)^4} + \frac{\alpha(4\alpha^2 - p^2)}{\beta^2(4\alpha^2 + p^2)^4} \right\} \\
 - \left( \frac{1}{a^5} \frac{64}{(\alpha + \beta)^5} \frac{1}{\beta^5} \right) \frac{1}{(4(\alpha + \beta)^2 + p^2)} - 2 \left( \frac{1}{a^4} \frac{32}{(\alpha + \beta)^4} \frac{1}{\beta^5} \right) \frac{(\alpha + \beta)}{(4(\alpha + \beta)^2 + p^2)} \Bigg\} . \quad (2.27)
 \end{aligned}$$

Use of (2.26), (2.27) and the results of Chapter III for the integrals  $J_{11}$  and  $J_{21}$

gives

$$f(k, p) = - \frac{32 z^{\frac{3}{2}} N \sum_{l=0}^{\infty} (2l+1) e^{i(\sigma_l + \eta_l)} P_l(\cos \nu) V_l(k, p)}{p^2 k^{\frac{1}{2}} l^{\frac{1}{2}}} , \quad (2.28)$$

where

$$\begin{aligned}
 V_l(k, p) = \int_0^{\infty} u_l(k, r) \left[ |j_l(pr) - \delta_{l,0} A(p)| \{4c(T_3(r) - T_3(0)) e^{-(z + \alpha + \beta)r} \right. \\
 \left. + r(1 + cr) T_3(r) - cr T_4(0) e^{-(z + \alpha + \beta)r} \right. \\
 \left. + \delta_{l,0} r \left\{ \frac{(z + \alpha) e^{-\beta r}}{((z + \alpha)^2 + p^2)^2} + \frac{(z + \beta) e^{-\alpha r}}{((z + \beta)^2 + p^2)^2} \right\} \right. \\
 \left. + \frac{c}{2(2l+1)} r |I_l(p, r)| \right] dr , \quad (2.29)
 \end{aligned}$$

with

$$A(p) = 32 \pi^2 N^2 \left[ \frac{\beta}{\alpha^3 (4\beta^2 + p^2)^2} + \frac{8}{(\alpha + \beta)^2 \{(\alpha + \beta)^2 + p^2\}^2} + \frac{\alpha}{\beta^3 (4\alpha^2 + p^2)^2} \right] + 2c N^2 J_{22} \quad (2.30)$$

For  $\ell = 0$  the integral  $I_\ell(p, r)$  has been evaluated in closed form; for  $\ell > 0$  one more integration is needed than in the calculations described in Chapter III, since the integral of the form

$$\int_a^\infty x(r) dr$$

occurring in (2.25) cannot be evaluated in closed form, with the result that the time of computation increases considerably. In view of this and of the fact that the dipole contribution dominates we have restricted ourselves to the calculation of cross sections for the partial waves  $\ell = 0$  and  $\ell = 1$ . The numerical methods used for the evaluation of these cross sections are described in Appendix B

### 3. Results

Calculated partial wave cross sections  $Q_\ell$  ( $\ell = 0, 1$ ), in the length formulation of the Born approximation, are given in Tables 2 and 3. Again, the s-wave results ( $\ell = 0$ ), because of the orthogonalization procedure adopted, may be significantly in error.

The analysis neglects the fact that in the case of ionization of an hydrogenic positive ion of nuclear charge  $z$  by electron impact, the incident electron should be represented by a Coulomb wave belonging to charge  $z - 1$ , and not a plane wave. However, the partial wave cross sections obtained in the case of  $\text{Li}^+ \rightarrow \text{Li}^{2+}$  indicate that the total cross sections would be in excellent agreement with the values obtained by Moores (1969), private communication, using a Coulomb-Born approximation, at energies as low as five times threshold.

The length results obtained with the wave function (2.1) for the ground state are intermediate between the length and velocity results presented in the previous Chapter.

Our results for the total cross section ( $\sum_{l=2}^4 Q_l$  being the result obtained, in the length formulation, with a two-parameter wave function for the ground state of the target) are presented in Table 4 and illustrated in Figs. 1 and 2. In these two figures we compare the length results obtained with the wave function (2.1) for  $\Psi_0$  with the length and velocity results obtained with a simple two-parameter wave function for the ground state.

Sample results for the quantity  $I_1^{(L)}(k, p)$  (for two ejected electron energies) and the differential cross section  $\sigma_1^{(L)}(k^2)$  (for two impact energies) for the process  $\text{He} + e \rightarrow \text{He}^+ + 2e$ , obtained with the two-parameter and three-parameter wave function for  $\Psi_0$ , are presented in Tables 5 and 6 respectively and illustrated in Figs. 3 and 4 respectively.

A fit to our helium results of the form

$$Q(E_i) = \frac{4}{E_i \rightarrow \infty} \frac{4}{E_i} [A \ln E_i + B]$$

gives

$$A = 0.488 \quad , \quad B = 0.536 \quad .$$

A fit to our  $\text{Li}^+$  results of the form

$$Q(E_i) = \frac{4}{E_i \rightarrow \infty} \frac{4}{E_i} [A \ln \left( \frac{\beta^2}{1 - \beta^2} \right) - \beta^2 + B]$$

gives

$$A = 0.157 \quad , \quad B = 1.564 \quad .$$

#### 4. Conclusions

We have calculated partial wave cross sections ( $l = 0, 1$ ) for electron impact ionization of He and  $\text{Li}^+$  in the Born (ii) approximation at energies from threshold to 9 keV. The results obtained reinforce our conclusions of the previous Chapter that electron impact ionization of two-electron systems is well described by the first Born approximation at energies above 25 times threshold.

Table 2

Cross sections  $Q_l$  ( $\pi a_0^2$ ) for  $\text{He} + e \rightarrow \text{He}^+ + 2e$  calculated with  
the three-parameter correlated wave function for  $\Psi_0$

$E_i$ (ev)	$Q_0$	$Q_1$
40	0.383 (-1)†	0.156
60	0.555 (-1)	0.297
80	0.572 (-1)	0.352
100	0.544 (-1)	0.367
125	0.496 (-1)	0.362
150	0.449 (-1)	0.347
200	0.371 (-1)	0.312
300	0.269 (-1)	0.253
400	0.209 (-1)	0.212
600	0.144 (-1)	0.161
800	0.109 (-1)	0.130
1000	0.880 (-2)	0.110
2000	0.445 (-2)	0.645 (+1)
3000	0.298 (-2)	0.465 (-1)
4000	0.225 (-2)	0.366 (-1)
5000	0.181 (-2)	0.304 (-1)
6000	0.151 (-2)	0.260 (-1)
7000	0.130 (-2)	0.231 (-1)
8000	0.114 (-2)	0.206 (-1)
9000	0.102 (-2)	0.186 (-1)

† The numbers in brackets denote the power of 10 by which the entry should be multiplied.

Table 3

Cross sections  $Q_l$  ( $\pi a_0^2$ ) for  $\text{Li}^+ + e \rightarrow \text{Li}^{2+} + 2e$  calculated with the three-parameter correlated wave function for the ground state

$E_i$ (ev)	$Q_0$	$Q_1$
83	0.732 (-3)†	0.211 (-2)
98	0.268 (-2)	0.920 (-2)
125	0.512 (-2)	0.216 (-1)
150	0.628 (-2)	0.299 (-1)
175	0.681 (-2)	0.355 (-1)
200	0.700 (-2)	0.391 (-1)
260	0.680 (-2)	0.427 (-1)
400	0.559 (-2)	0.410 (-1)
600	0.421 (-2)	0.349 (-1)
800	0.333 (-2)	0.298 (-1)
1000	0.274 (-2)	0.260 (-1)
2000	0.145 (-2)	0.160 (-1)
3000	0.991 (-3)	0.118 (-1)
4000	0.769 (-3)	0.941 (-2)
5000	0.633 (-3)	0.788 (-2)
6000	0.526 (-3)	0.681 (-2)
7000	0.458 (-3)	0.601 (-2)
8000	0.413 (-3)	0.539 (-2)
9000	0.365 (-3)	0.490 (-2)

† The numbers in brackets denote the power of 10 by which the entry should be multiplied.

Table 4

Cross sections  $Q_l$  ( $\pi a_0^2$ ) for electron ionization of the ground state of He and  $\text{Li}^+$

He		$\text{Li}^+$	
$E_i$ (ev)	$\sum_{l=0}^4 Q$	$E_i$ (ev)	$\sum_{l=0}^4 Q$
40	.224	83	.309 (-2)
60	.422	98	.111 (-1)
80	.496	125	.312 (-1)
100	.514	150	.429 (-1)
125	.505	175	.508 (-1)
150	.481	200	.563 (-1)
200	.429	260	.610 (-1)
300	.344	400	.583 (-1)
400	.286	600	.495 (-1)
600	.212	800	.417 (-1)
800	.170	1000	.361 (-1)
1000	.143	2000	.217 (-1)
2000	.813 (-1)†	3000	.157 (-1)
3000	.578 (-1)	4000	.124 (-1)
4000	.451 (-1)	5000	.103 (-1)
5000	.372 (-1)	6000	.884 (-2)
6000	.317 (-1)	7000	.776 (-2)
7000	.280 (-1)	8000	.694 (-2)
8000	.249 (-1)	9000	.628 (-2)
9000	.224 (-1)		

† The numbers in brackets denote the power of 10 by which the entry should be multiplied.

Table 5

$I_i^{(L)}(k, p)$  for electron impact ionization of the ground state of He calculated with the three-parameter correlated wave function for the ground state

$k = .949 (-1)^\dagger$ a.u.		$k = .555$ a.u.	
$p$	$I_i^{(L)}(k, p)$	$p$	$I_i^{(L)}(k, p)$
.194	.936	.217	.729
.406	.606	.428	.499
.682	.397	.704	.350
.894	.289	.915	.268
.101 (1)†	.242	.103 (1)	.231
.122 (1)	.172	.124 (1)	.172
.150 (1)	.107	.151 (1)	.113
.171 (1)	.741 (-1)	.172 (1)	.802 (-1)
.210 (1)	.370 (-1)	.212 (1)	.417 (-1)
.337 (1)	.461 (-2)	.338 (1)	.556 (-2)
.503 (1)	.497 (-3)	.504 (1)	.641 (-3)
.630 (1)	.128 (-3)	.630 (1)	.172 (-3)
.709 (1)	.620 (-4)	.709 (1)	.852 (-4)
.879 (1)	.166 (-4)	.878 (1)	.236 (-4)
.110 (2)	.419 (-5)	.110 (2)	.607 (-5)
.127 (2)	.173 (-5)	.127 (2)	.253 (-5)

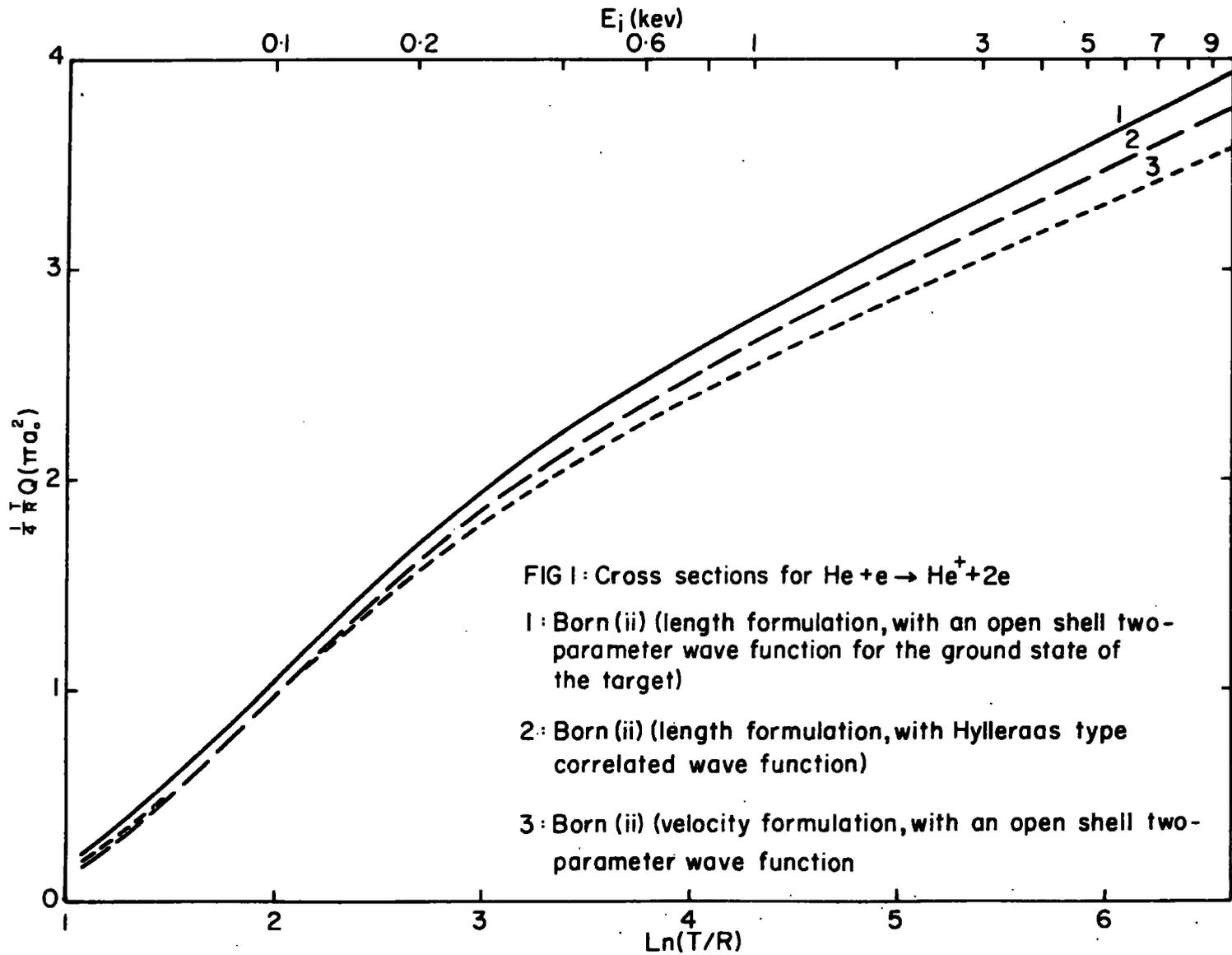
† The numbers in brackets denote the power of 10 by which the entry should be multiplied.

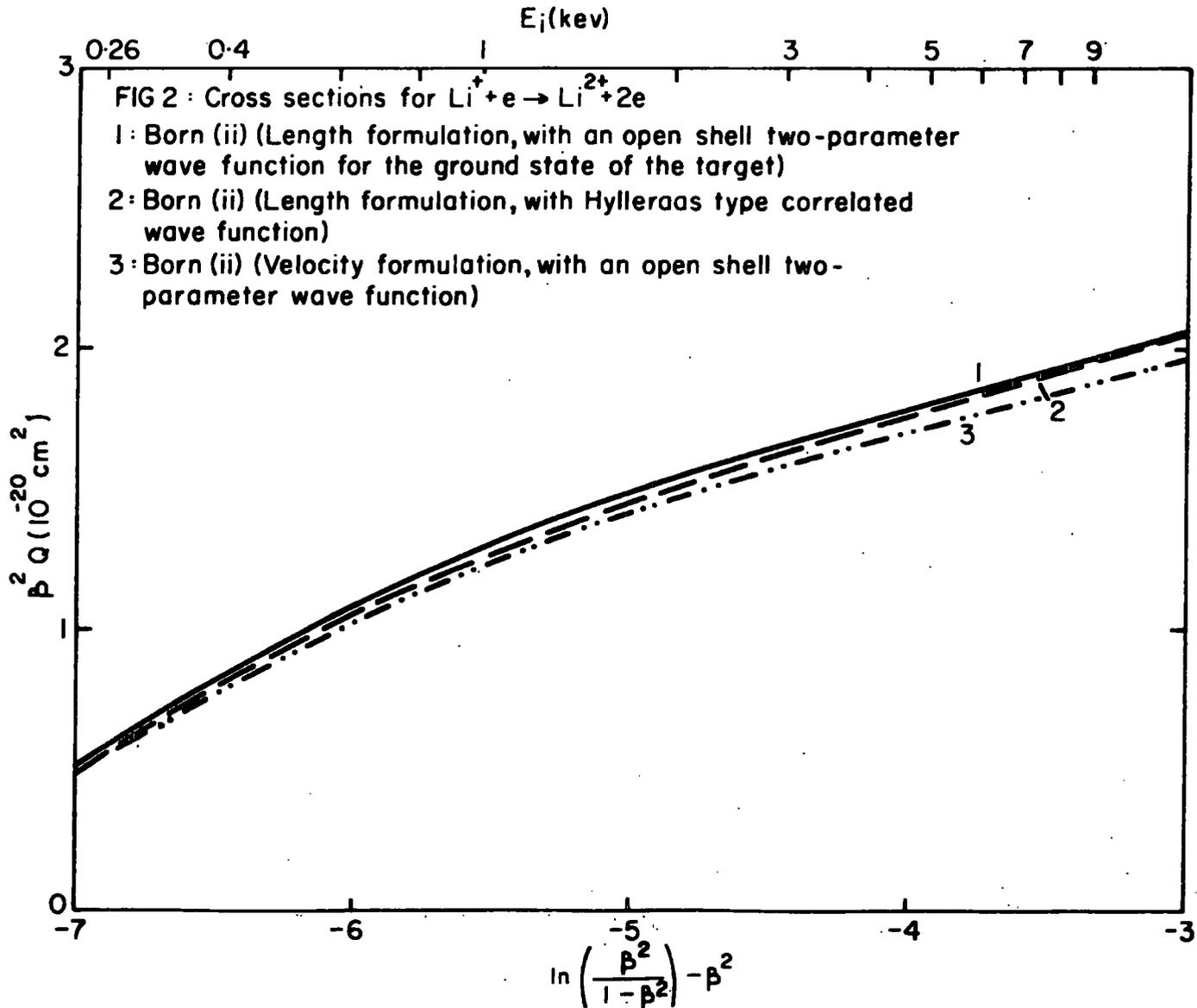
Table 6

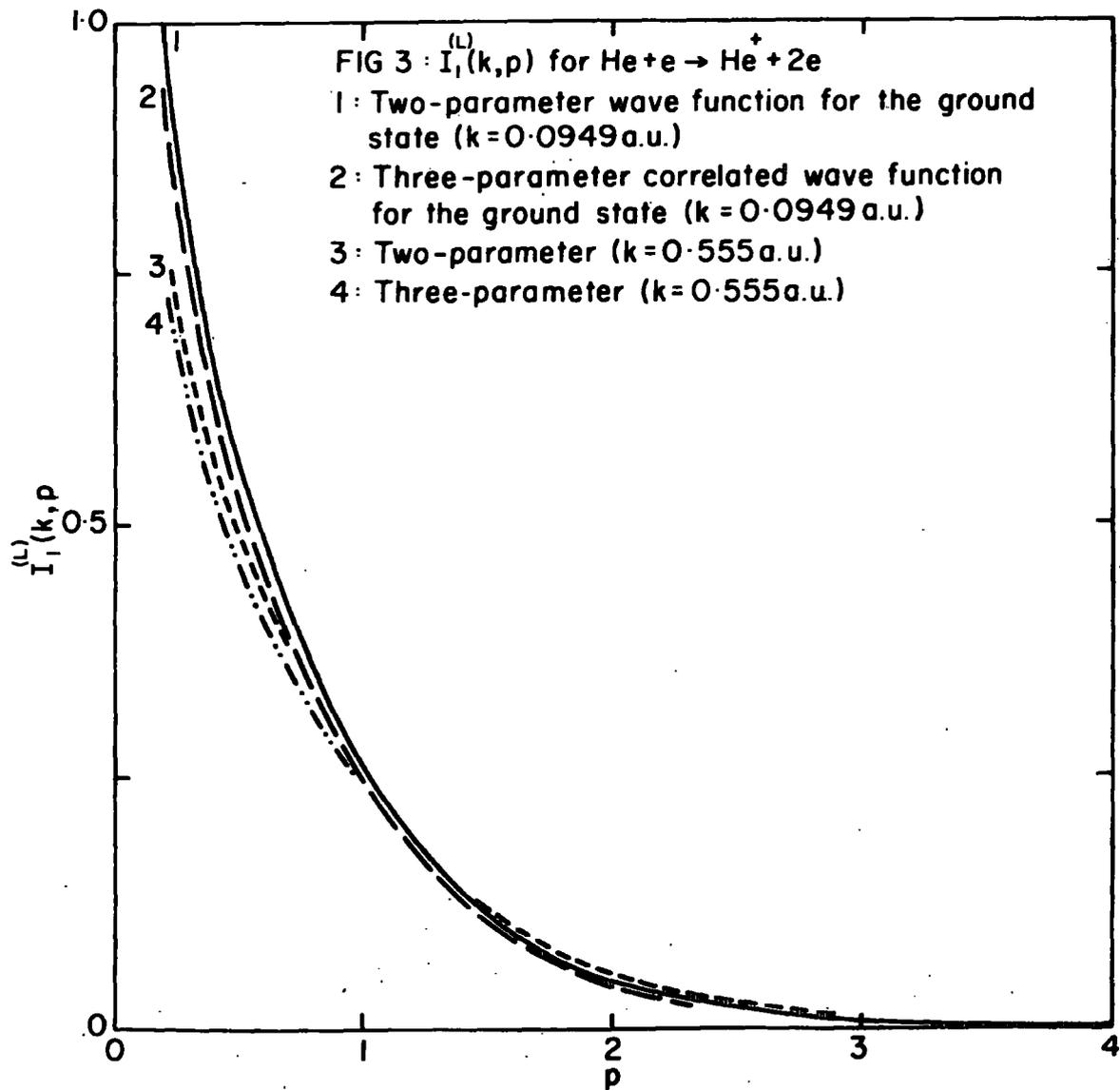
Differential cross section  $\sigma_1^{(L)}(k^2)$ , in units of  $\pi a_0^2$ , for  $\text{He} + e \rightarrow \text{He}^+ + 2e$   
calculated with the three-parameter correlated wave function for the ground state

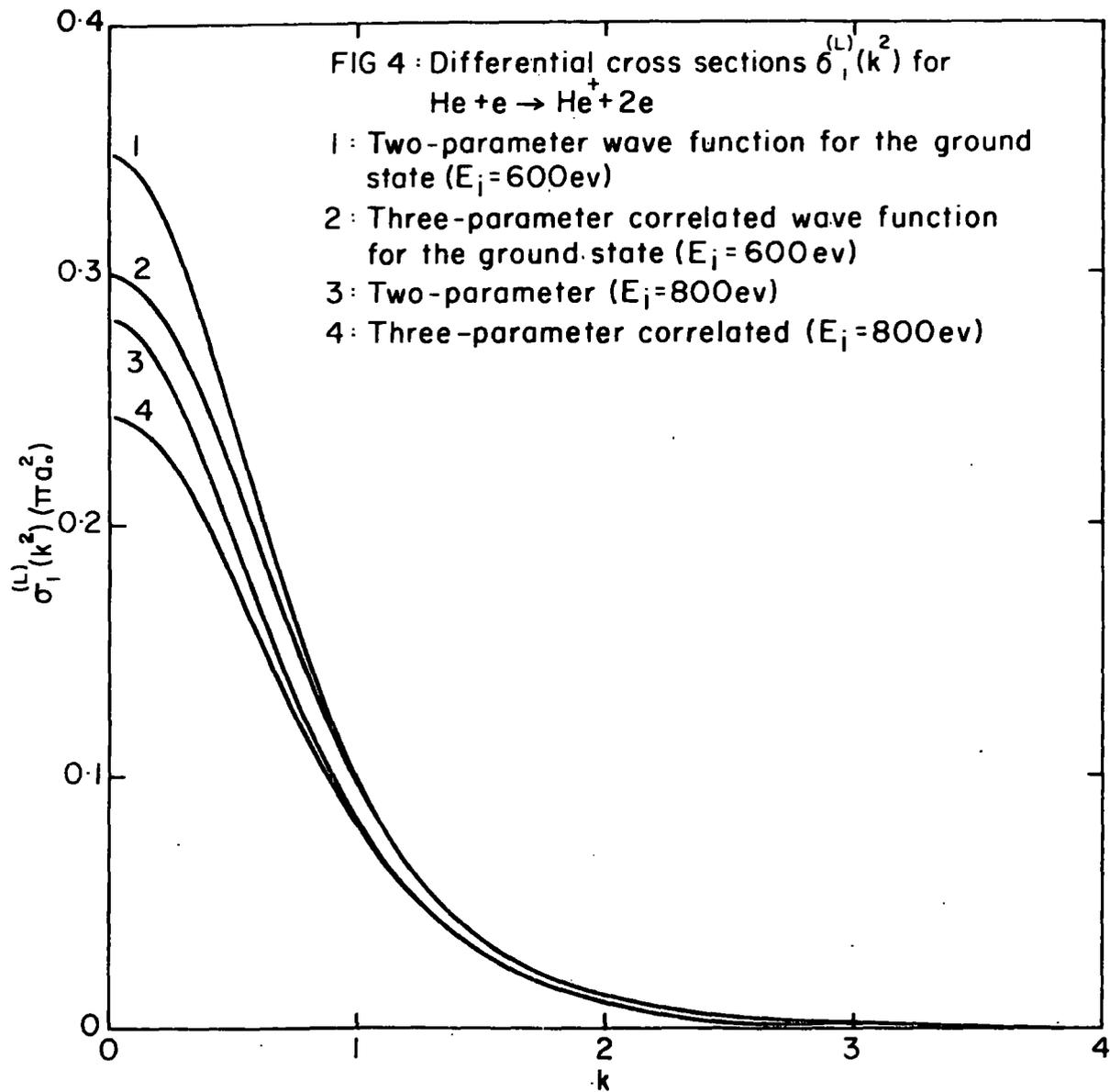
$E_i = 600 \text{ ev}$		$E_i = 800 \text{ ev}$	
$k$	$\sigma_1^{(L)}(k^2)$	$k$	$\sigma_1^{(L)}(k^2)$
.200 (-1)†	.299	.232 (-1)	.243
.949 (-1)	.296	.110	.239
.193	.285	.224	.228
.267	.273	.310	.215
.307	.265	.357	.207
.382	.249	.444	.189
.480	.224	.555	.165
.555	.204	.644	.146
.695	.167	.806	.113
.114 (1)	.740 (-1)	.133 (1)	.411 (-1)
.173 (1)	.220 (-1)	.201 (1)	.994 (-2)
.218 (1)	.872 (-2)	.253 (1)	.352 (-2)
.246 (1)	.500 (-2)	.285 (1)	.191 (-2)
.306 (1)	.166 (-2)	.355 (1)	.585 (-3)
.384 (1)	.495 (-3)	.446 (1)	.171 (-3)
.444 (1)	.216 (-3)	.515 (1)	.730 (-4)

† The numbers in brackets denote the power of 10 by which the entry should be multiplied.









## APPENDIX A. EVALUATION OF $I(p, K)$

The integral  $I(p, K)$  defined by (2.58) is evaluated by considering the limit, as  $\beta \rightarrow 0$ , of the expression

$$J(\alpha, \beta) = \int dx e^{-\beta x} e^{i p \cdot x} \frac{1}{x} {}_1F_1\left[\frac{i\alpha}{K}, 1, i(Kx - K \cdot x)\right]. \quad (A.1)$$

A method due to Nordsieck (1954) will be described and the limit as  $\beta \rightarrow 0$  will be examined in detail.

The method begins with the standard contour integral representation of the confluent hypergeometric function

$${}_1F_1(a, 1, z) = \frac{1}{2\pi i} \int_C e^{tz} t^{a-1} (t-1)^{-a} dt. \quad (A.2)$$

In (A.2)  $C$  is any closed contour which starts at the origin and encircles the point  $t = 1$  once in the positive sense (Erdelyi 1953, Vol. 1 p. 272). In this equation all powers have their principal values. Substituting (A.2) in (A.1) gives

$$J(\alpha, \beta) = \frac{1}{2\pi i} \int_C dt t^{\frac{i\alpha}{K} - 1} (t-1)^{-\frac{i\alpha}{K}} u(t), \quad (A.3)$$

where

$$u(t) = \int e^{i p \cdot x} \frac{1}{x} e^{-\beta x} e^{i t(Kx - K \cdot x)} dx. \quad (A.4)$$

The change in the order of integration implied in (A.3) is allowed provided  $u(t)$  converges uniformly with respect to  $t$ . A sufficient condition for uniform convergence is that the inequality

$$\beta + 2K \operatorname{Im} t > 0 \quad (A.5)$$

be satisfied for all  $t$  within and on  $C$ . We shall assume that the contour  $C$  has been chosen to satisfy this condition.

The integral in (A.4) is easily evaluated and we obtain

$$u(t) = \frac{4\pi}{\beta^2 + p^2 - 2t(\underline{p} \cdot \underline{K} + i\beta K)}$$

which, on substitution in (A.3), gives

$$J(\alpha, \beta) = \frac{2}{i} \int_C t^{\frac{i\alpha}{K} - 1} (t-1)^{-\frac{i\alpha}{K}} \frac{dt}{\beta^2 + p^2 - 2t(\underline{p} \cdot \underline{K} + i\beta K)} \quad (A.6)$$

The integrand in (A.6) has a simple pole at

$$t = t_0 \equiv \frac{\beta^2 + p^2}{2(\underline{p} \cdot \underline{K} + i\beta K)} \quad (A.7)$$

and, since

$$\beta + 2K \operatorname{Im} t_0 = -\frac{\beta(1 - \cos^2 \nu) p^2}{\beta^2 + p^2 \cos^2 \nu} < 0$$

where  $\cos \nu = \hat{\underline{p}} \cdot \hat{\underline{K}}$ , this pole lies outside the contour C. Applying Cauchy's theorem to the region outside C we obtain

$$\begin{aligned} J(\alpha, \beta) &= \frac{\pi t_0^{\frac{i\alpha}{K} - 1} (t_0 - 1)^{-\frac{i\alpha}{K}}}{(\underline{K} \cdot \underline{p} + i\beta K)} \\ &= \frac{4\pi}{\beta^2 + p^2} \left[ \frac{q^2 - (\underline{K} + i\beta)^2}{\beta^2 + p^2} \right]^{-\frac{i\alpha}{K}}, \end{aligned} \quad (A.8)$$

where  $\underline{q} = \underline{p} - \underline{K}$ .

From (A.7) we have that

$$\operatorname{Re} t_0 = \frac{(\beta^2 + p^2)(\underline{K} \cdot \underline{p})}{2[(\underline{K} \cdot \underline{p}^2) + \beta^2 K^2]}$$

$$\text{Im } t_0 = - \frac{\beta K (\beta^2 + K^2)}{2 [(K \cdot p)^2 + \beta^2 K^2]} .$$

It follows that for  $\beta \neq 0$  the point  $t = t_0$  lies below the real axis and that it moves up to the real axis as  $\beta \rightarrow 0$ .

In considering the phase of the quantity

$$\begin{aligned} r &= q^2 - (K - i\beta)^2 \\ &= (\beta^2 + p^2) \left( \frac{t_0 - 1}{t_0} \right) , \end{aligned}$$

in the limit as  $\beta \rightarrow 0$ , two distinct cases arise:

(i) If  $K > q$ , then, when  $\beta = 0$ ,

$$\text{Re } t_0 = \frac{(K + q)^2}{2 [K^2 + K \cdot q]} < 1$$

and therefore, as  $\beta \rightarrow 0$ ,  $t_0$  approaches the real axis between 0 and 1 from below. It follows that

$$\arg t_0 = 0 (\beta)$$

and

$$\arg (t_0 - 1) = -\pi + 0 (\beta) .$$

(ii) We now suppose  $K < q$ . If  $\underline{p} \cdot \underline{K} > 0$  it follows that  $\text{Re } t_0 > 1$  whereas, if  $\underline{p} \cdot \underline{K} < 0$ ,  $\text{Re } t_0 < 0$ . Thus, when  $K < q$ ,  $t_0$  and  $t_0 - 1$  have the same phase.

Therefore we have that

$$\begin{aligned} \arg r &= -\pi + 0 (\beta) & K > q \\ &= 0 (\beta) & K < q . \end{aligned}$$

Thus

$$\begin{aligned} I(\underline{p}, \underline{K}) &= \lim_{\beta \rightarrow 0} J(\alpha, \beta) \\ &= \frac{4\pi}{p^2} \left[ \frac{(\underline{p} + \underline{K})^2 - K^2}{p^2} \right]^{-\frac{i\alpha}{K}} A(p) , \end{aligned} \tag{A.9}$$

where

$$A(p) = 1$$

$$= \exp(-\pi u_i / K)$$

$$| \underline{p} + \underline{K} | > K$$

$$| \underline{p} + \underline{K} | < K .$$

## APPENDIX B. NUMERICAL METHODS

In this Appendix we describe the numerical methods used for the evaluation of cross sections for the processes (1.1) and (1.2) of Chapter III.

We require the solution to equation (3.14) which is regular at the origin and such that

$$u_l(k, 0) = 0 \quad (\text{B.1})$$

and

$$u_l(k, r) \underset{r \rightarrow \infty}{\sim} \frac{1}{k^{1/2}} \sin \left[ kr + \frac{(z-1)}{k} \ln(2kr) - \frac{1}{2} \ell \pi + \sigma_l + \eta_l \right]. \quad (\text{B.2})$$

The boundary condition (B.1) is satisfied if  $X_l(k, r)$  and  $Y_l(k, r)$  are the solutions of equations (3.18) and (3.19) respectively which are finite at the origin and such that

$$X_l(k, 0) = Y_l(k, 0) = 0. \quad (\text{B.3})$$

We therefore assume solutions in the form

$$X_l(k, r) = \sum_{n=0}^{\infty} a_n^{(l)} r^{n+\sigma}, \quad (\text{B.4})$$

$$Y_l(k, r) = \sum_{n=0}^{\infty} b_n^{(l)} r^{n+\rho}, \quad (\text{B.5})$$

where  $a_0^{(l)} \neq 0$ ,  $b_0^{(l)} \neq 0$  are arbitrary and  $\sigma, \rho$ , the remaining  $a_n^{(l)}$ 's and  $b_n^{(l)}$ 's are to be determined. Near the origin  $f_l(k, r)$  and  $g_l(r)$  are given by

$$f_l(k, r) = \frac{\ell(\ell+1)}{r^2} \left( \frac{z_0}{r} + z_1 + z_2 r + z_3 r^2 + O(r^3) \right), \quad (\text{B.6})$$

$$g_l(r) = \frac{2A_1'}{(2\ell+1)} \left| 1 - zr + \frac{1}{2} z^2 r^2 + O(r^3) \right|, \quad (\text{B.7})$$

where  $z_0 = -2(z-1+A_1)$ ,  $z_1 = (2A_1 z - k^2)$ ,  $z_2 = \frac{8A_2 z}{15}$ ,  $z_3 = -\frac{2z^2}{3}(2A_1 z + A_2)$  and

and  $A_1' = 4z^3 A_1$ . Substitution of (B.4), (B.6) and (B.7) in (3.18) yields

$$\sum_{n=0}^{\infty} (n+\sigma)(n+\sigma-1) a_n^{(l)} r^{n+\sigma-2} \left[ \frac{l(l+1)}{r^2} + \frac{z_0}{r} + z_1 + z_2 r + z_3 r^2 + 0(r^3) \right] \sum_{n=0}^{\infty} a_n^{(l)} r^{n+\sigma}$$

$$- 2A_3 \sum_{n=0}^{\infty} a_n^{(l)} \left[ \frac{r^{n+\sigma+2}}{(n+\sigma+l+2)(n+\sigma-l+1)} + 0(r^{n+\sigma+3}) \right]$$

We are thus led to the following equations: for  $n = 0$ ,

$$[\sigma(\sigma-1) - l(l+1)] a_0^{(l)} = 0, \quad (B.8)$$

for  $n = 1$ ,

$$[\sigma(\sigma+1) - l(l+1)] a_1^{(l)} = z_0 a_0^{(l)}, \quad (B.9)$$

for  $n = 2$ ,

$$[(\sigma+1)(\sigma+2) - l(l+1)] a_2^{(l)} = z_0 a_1^{(l)} + z_1 a_0^{(l)}, \quad (B.10)$$

for  $n = 3$ ,

$$[(\sigma+2)(\sigma+3) - l(l+1)] a_3^{(l)} = z_0 a_2^{(l)} + z_1 a_1^{(l)} + z_2 a_0^{(l)}, \quad (B.11)$$

for  $n = 4$ ,

$$[(\sigma+3)(\sigma+4) - l(l+1)] a_4^{(l)} = z_0 a_3^{(l)} + z_1 a_2^{(l)} + z_2 a_1^{(l)} + (z_3 - \frac{A_3}{2l+3}) a_0^{(l)}, \quad (B.12)$$

Since  $a_0^{(l)} \neq 0$ , we have, from (B.8), that

$$\sigma(\sigma-1) - l(l+1) = 0. \quad (B.13)$$

The roots of this equation are:

$$\sigma = l+1, \quad \sigma = -l. \quad (B.14)$$

From the recurrence relations (B.9), (B.10), .., we can determine the remaining  $a_n^{(l)}$ 's in terms of  $a_0^{(l)}$ . The condition that  $X_l(k, 0) = 0$  requires that we take  $\sigma = l+1$ . We

therefore have that

$$X_l(k, r) = r^{l+1} [a_0^{(l)} + a_1^{(l)} r + a_2^{(l)} r^2 + a_3^{(l)} r^3 + a_4^{(l)} r^4 + 0(r^5)]. \quad (B.15)$$

In a similar manner we obtain

$$Y_l(k, r) = r^{l+1} [b_0^{(l)} + b_1^{(l)} r + b_2^{(l)} r^2 + b_3^{(l)} r^3 + b_4^{(l)} r^4 + 0(r^5)]. \quad (B.16)$$

If we write

$$E_l(k, r) = \int_0^r e^{-zx} x^{l+1} X(k, x) dx, \quad (B.17)$$

$$F_L(k, r) = \int_0^r e^{-zx} x^{-L} X_L(k, x) dx, \quad (B.18)$$

$$G_L(k, r) = \int_0^r e^{-zx} x^{L+1} Y_L(k, x) dx, \quad (B.19)$$

and

$$H_L(k, r) = \int_0^r e^{-zx} x^{-L} Y_L(k, x) dx, \quad (B.20)$$

then (3.18) and (3.19) can be put in the form

$$\frac{d^2 X_L(k, r)}{dr^2} = f_L(k, r) X_L(k, r) + C_L(k, r), \quad (B.21)$$

$$\frac{d^2 Y_L(k, r)}{dr^2} = f_L(k, r) Y_L(k, r) + D_L(k, r), \quad (B.22)$$

where

$$C_L(k, r) = g_L(r) [r^{-L} E_L(k, r) - r^{L+1} F_L(k, r)], \quad (B.23)$$

and

$$D_L(k, r) = g_L(r) [r^{-L} G_L(k, r) - r^{L+1} \{H_L(k, r) - 1\}]. \quad (B.24)$$

With the use of equations (B.15) – (B.20) we obtain

$$E_L(k, r) = r^{2L+3} \left[ \frac{a_0^{(L)}}{(2L+3)} + \left| \frac{a_1^{(L)} - za_0^{(L)}}{(2L+4)} \right| r + \left| \frac{a_2^{(L)} - za_1^{(L)} + \frac{1}{2}z^2 a_0^{(L)}}{(2L+5)} \right| r^2 + O(r^3) \right], \quad (B.25)$$

$$F_L(k, r) = r^2 \left[ \frac{a_0^{(L)}}{2} + \left| \frac{a_1^{(L)} - za_0^{(L)}}{3} \right| r + \left| \frac{a_2^{(L)} - za_1^{(L)} + \frac{1}{2}z^2 a_0^{(L)}}{4} \right| r^2 + \left| \frac{a_3^{(L)} - za_2^{(L)} + \frac{1}{2}z^2 a_1^{(L)} - \frac{1}{6}z^3 a_0^{(L)}}{5} \right| r^3 + O(r^4) \right], \quad (B.26)$$

$$G_L(k, r) = r^{2L+3} \left[ \frac{b_0^{(L)}}{(2L+3)} + \left| \frac{b_1^{(L)} - zb_0^{(L)}}{(2L+4)} \right| r + \left| \frac{b_2^{(L)} - zb_1^{(L)} + \frac{1}{2}z^2 b_0^{(L)}}{(2L+5)} \right| r^2 + O(r^3) \right], \quad (B.27)$$

$$H_L(k, r) = r^2 \left[ \frac{b_0^{(L)}}{2} + \left| \frac{b_1^{(L)} - zb_0^{(L)}}{3} \right| r + \left| \frac{b_2^{(L)} - zb_1^{(L)} + \frac{1}{2}z^2 b_0^{(L)}}{4} \right| r^2 + \left| \frac{b_3^{(L)} - zb_2^{(L)} + \frac{1}{2}z^2 b_1^{(L)} - \frac{1}{6}z^3 b_0^{(L)}}{5} \right| r^3 + O(r^4) \right]. \quad (B.28)$$

Use of equations (B.23) – (B.28) yields

$$C_l(k,r) = -2A_1 \cdot e^{-zr} r^{l-3} \left[ \frac{a_0^{(l)}}{2(2l+3)} + \frac{a_1^{(l)} - za_0^{(l)}}{3(2l+4)} \{ r \} + \frac{a_2^{(l)} - za_1^{(l)} + \frac{1}{2}z^2 a_0^{(l)}}{4(2l+5)} \{ r^2 + 0(r^4) \} \right] \quad (B.29)$$

$$D_l(k,r) = -2A_1 \cdot e^{-zr} r^{l+1} \left[ -\frac{1}{(2l+1)} + \frac{b_0^{(l)}}{2(2l+3)} r^2 + \frac{b_1^{(l)} - zb_0^{(l)}}{3(2l+4)} \{ r^3 \} + \frac{b_2^{(l)} - zb_1^{(l)} + \frac{1}{2}z^2 b_0^{(l)}}{4(2l+5)} \{ r^4 + 0(r^5) \} \right] \quad (B.30)$$

The coefficients  $a_0^{(l)}$  and  $b_0^{(l)}$  in the starting series (B.15) and (B.16) respectively were arbitrarily chosen to be

$$a_0^{(l)} - b_0^{(l)} = 1 \quad (B.31)$$

The integro-differential equations (B.21) and (B.22) were then integrated outward from the origin and used to evaluate the transformation factor  $a$  defined by (3.21). The integrating routine employed Numerov's method and a seven-point Newton-Cotes formula of open type. If we write

$$a_j = 1 - \frac{1}{12} h^2 f_j \quad (B.32)$$

$$\beta_j = 2 + \frac{5}{6} h^2 f_j \quad (B.33)$$

where  $h$  is the integration step-length and  $f_j = f(r_j)$ , then Numerov's formula applied to (B.21) and (B.22) gives

$$X_{j+1} = \frac{1}{a_{j+1}} \{ \beta_j X_j - a_{j-1} X_{j-1} + \frac{1}{12} h^2 \{ C_{j+1} + 10C_j + C_{j-1} \} \} \quad (B.34)$$

$$Y_{j+1} = \frac{1}{a_{j+1}} \{ \beta_j Y_j - a_{j-1} Y_{j-1} + \frac{1}{12} h^2 \{ D_{j+1} + 10D_j + D_{j-1} \} \} \quad (B.35)$$

The seven-point Newton-Cotes formula (Abramowitz and Stegun, 1965) applied to the exchange integral in (B.17) gives

$$E_{j+1} = E_{j-5} + 0.3h [11P_{j-4} - 14P_{j-3} + 26P_{j-2} - 14P_{j-1} + 11P_j] , \quad (\text{B.36})$$

where

$$P_j = e^{-zr_j} r_j^{-1} X_j , \quad (\text{B.37})$$

with similar expressions for the other exchange integrals. Thus  $E_{j+1}$  as obtained from (B.36) involves only preceding values of  $X$  and the solution may be built up step by step.

To commence the integration routine six starting values are required and these may be obtained by means of the series expansions at the origin (formulae (B.15), (B.16) and (B.25) – (B.30) ).

The radial integrals in (2.20) and (2.39) were evaluated with the use of the Simpson integration formula. The range of integration was truncated at  $r = 12$  because the integrand becomes negligible for large values of  $r$ . Examination of the results obtained by varying the step-length showed that it was unnecessary to carry the integration farther.

Because of the spherical Bessel function  $j_l(pr)$  occurring in the integrand it was feared that some error might be incurred in the numerical work when  $pr$  was small ( $pr < 0.6$ ). For values of  $pr < 0.6$  the evaluation of  $j_l(pr)$  was therefore carried out by two different methods. The first method consisted in making use of the recurrence relation (2.34) and the formulae

$$j_0(z) = \frac{\sin z}{z} \quad (\text{B.38})$$

$$j_1(z) = \frac{\sin z}{z^2} - \frac{\cos z}{z} \quad (\text{B.39})$$

to generate  $j_l(z)$  in terms of  $\sin z$  and  $\cos z$  which were then evaluated with the use of library sub-programs built in the compiler. The second method consisted in making use of the series

$$j_l(z) = \frac{z^l}{1.3.5 \dots (2l+1)} \left[ 1 - \frac{\frac{1}{2} z^2}{1! (2l+3)} + \frac{(\frac{1}{2} z^2)^2}{2! (2l+3)(2l+5)} - \dots \right] \quad (\text{B.40})$$

The two methods gave identical results. We therefore concluded that the first method was quite satisfactory.

The final integrals over the variables  $p$  and  $k$  were evaluated by Gaussian quadrature, the range  $(a, b)$  being split, on the basis of the observed behaviour of  $V(k, p)$  as a function of  $p$  and  $k$ , into subranges  $(a, a+t)$ ,  $(a+t, a+2t)$ ,  $(a+2t, a+8t)$ , and  $(a+8t, b)$  where  $t = \frac{1}{16}(b-a)$ . Quadratures of order 4, 8, and 12 were found to be adequate for the energy range between threshold and 1 keV, between 1 keV and 5 keV and between 5 keV and 9 keV respectively.

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