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THE APPLICATION OF SECOND ORDER POTENTIALS TO THE SCATTERING OF CHARGED PARTICLES FROM HELIUM

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ABSTRACT

This work is concerned with a theoretical description of the scattering of charged particles from a helium target, at non - relativistic velocities.

Using a truncated atomic eigenfunction expansion it is necessary at high energies to make some allowance for all the channels not explicitly included in the expansion. This is done by constructing a second order potential matrix. The method is applied to the scattering by helium atoms of electrons between 50 ev. and 1000 ev., and results are presented for elastic scattering and the 2'S and 2'P excitations. It is found that the inclusion of the couplings between these channels and the inclusion of second order terms in the potential, leads to cross sections which are in significantly better agreement with the experimental data.

By reversing the sign of the potential, a comparison is made between positron and electron scattering at the same energy.

THE APPLICATION OF SECOND ORDER POTENTIALS TO THE SCATTERING OF CHARGED PARTICLES FROM HELIUM

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PART I

GENERAL FORMALISM

Chapter 1

INTRODUCTION

The interaction between a charged particle and an atom can be studied in two ways: experimentally, where a beam of particles of definite energy and momentum is scattered from atoms in a target, and theoretically, as in this thesis, where one tries to predict the results of such an experiment. To simplify the problem, we can assume that both the beam and target densities are so low that interactions between the particles in the beam and multiple scattering processes can be ignored.

Let us consider, then, a single interaction between the particle beam and an atom. The forces involved are electromagnetic in origin and so become small at large distances. This implies that at large separations ($\underline{R}$), both before and after the collision, the atom and particle can be considered independently; and we know that an unperturbed atom will stay in the same "eigenstate" indefinitely. Also, since we can specify the initial momentum ($\underline{k}_0$) of the particles, Heisenberg's uncertainty principle forbids their localisation in space or time. So each particle can be represented in free space by the plane wave, $\exp(i\underline{k}_o.\underline{R})$. However, during the collision the wave will be scattered and dispersed. The dispersion occurs because energy can sometimes be transferred to the atom to excite one or more of its electrons. The final structure of the particle wave, then, depends on the final state of the atom as well as the nature of the potentials experienced.

Since both initially and finally the atom is in a stationary state, let us use the set of all possible atomic eigenstates as a basis for describing the combined particle - atom system. Thus in Chapter 2 we expand the total wavefunction Ψ, in terms of the eigenfunctions, $|\phi_n\rangle$, of the unperturbed atom;

$$\Psi = \sum_{n=o}^{\infty} F_n(\underline{R})\,|\phi_n\rangle \ . \qquad (1\text{-}1)$$

The coefficients of the expansion, $F_n(\underline{R})$, are related to the probability of finding the atom in its n-th state, and so will tend to stationary values at large separations, $\underline{R}$. For example before the collision, if the atom is originally in its n=o state, then the $F_{n\neq o}(\underline{R})$ are zero for large $\underline{R}$, since we know that the atom is definitely not in any of these states. After the collision the $F_n(\underline{R})$ take on non-zero values for the open (energetically allowable) channels, and in Chapter 3 we show how their assymptotic form is related to the excitation cross sections which are experimentally observed.

Using the expansion (1-1) in Shrödinger's wave equation, we find we have to solve an infinite set of coupled differential equations for the scattering amplitudes. In the close coupling approximation (Bransden,1970,ch.5) the expansion is truncated to include only the open channels. This is useful at low energies where there may only be a few open channels, but it is not practicable above the ionization threshold where an infinite number of channels are open.

At much higher energies, the collision time will be short compared with typical atomic transition times. So only the initial and final channels need be included in the expansion (1-1), since the coupling to intermediate states during the collision will be small. This is Born's first approximation (Mott and Massey, 1965, ch.16). An additional assumption is that the potential due to the atom is so weak that the initial plane wave of the particle is scarcely altered by the collision. This, however, is a high energy approximation. The energy range we are interested in, then, lies below the range of validity of the Born approximation, but above the ionization threshold. For electron scattering from helium, this is between about 50ev. and 1000ev.

It is well known that the Born approximation does not predict the strong forward elastic scattering peak found experimentally, even at energies as high as 700 ev. for electrons incident on helium (Mott and Massey, 1965, ch.16). Moreover, this discrepancy persists even when elaborate atomic wavefunctions are used; for example, the calculations of Kim and Inokuti (1968) who used a 20 term Hylleraas wavefunction for helium (see Vriens et al.,1968a). For an accurate description of the process, therefore, we need to find the cause of this forward peak.

Massey and Mohr (1934) show that allowance must be made for the following processes during collision:

1. Scattering by the static field of the atom.
2. Distortion of the incident and scattered particle waves.
3. Electron exchange or transfer.

4. Polarization; the disturbance of the atom by the field of the incident particle.

The Born approximation takes account of the first process and distorted waves can easily be incorporated to take care of the second. However, at the energies we are interested in (above 100ev. for electron-helium scattering), neither distortion (Massey and Mohr,1934) nor electron exchange (Khare and Moiseiwitsch,1965) is responsible for the peak in the forward direction.

The fourth effect, polarization, arises from the interaction of the charged particle with the neutral atom. The particle sees an asymmetric charge distribution which gives rise to a potential which, whilst not pure Coulombic, is nevertheless still long range. The effect on the atom is to distort the energy levels so that interference occurs between the inelastic channels. Massey and Mohr (1934) found that by considering the contribution from the second order Born term and so making an allowance for these intermediate states, non-local terms arose in the potential which greatly increased the scattering in the forward direction. There are two ways of introducing these contributions.

Firstly, let us examine the partial wave treatment of scattering. Expanding the scattering function F($\underline{R}$) in a series of Legendre polynomials, we may write

$$F(\underline{R}) = \frac{1}{R}\sum_{L=0}^{\infty} f_L(R)\, P_L(\cos\Theta) \qquad (1\text{-}3)$$

Using this in Schrödinger's equation, we obtain the radial equation (McDowell and Coleman,1970, ch.5),

$$\left[d^2/dR^2 + k_0^{\,2} - V_{oo}(\underline{R}) - L(L+1)/R^2\right] f_L(R) = 0. \qquad (1\text{-}4)$$

So far we have neglected both exchange and polarization. Now, in the adiabatic limit, first order perturbation theory yields a long range potential in the entrance channel which, for electron scattering, is of the form

$$V_p(\underline{R}) \underset{R \to \infty}{\sim} -\tfrac{1}{2}\alpha_1/R^4 \qquad (1\text{-}5)$$

where α_1 is the dipole polarizability (Bransden,1970, ch.5). To allow for polarization then, a potential with this asymptotic form can be added to the static potential $V_{oo}(\underline{R})$ in (1-4), and the radial equation solved for each partial wave (eg.,Khare and Moiseiwitsch,1965). In considering the elastic scattering of electrons from helium, LaBahn and Callaway (1969) included non-adiabatic corrections to allow for the finite velocity of the particle beam. However the method becomes too involved at high energies because of the large number of phase shifts which have to be computed (100 at 500 ev. and away from the forward direction).

Secondly, at high energies it is more natural to introduce these polarization effects as contributions from second order terms in the potential. In chapter 4 we show that we can explicitly include a few strongly coupled states in a truncated expansion, as in the close coupling method, and then take into account those states not explicitly included by constructing a second order potential matrix. Coupled integro-differential equations then arise for the scattering amplitudes instead of the ordinary differential equations of the close coupling method. The second order potentials can be evaluated in a closure approximation and so depend on a parameter, the "average energy" of the states not explicitly included in the expansion. In Chapter 5 we show that this parameter can be fixed so that the correct long range potential is obtained in the entrance channel. Thus the method combines the characteristics of the close coupling and polarized orbital methods.

In Chapter 6 we examine the asymptotic expansion of the second order potential, particularly in the case of scattering from ground state hydrogen or helium atoms. It is shown that the leading term is related to the forward elastic scattering amplitude given by the first Born approximation. Thus we obtain a simple prescription for the average energy parameter: if all the states above the ground state are averaged, it is just the ratio of the Born amplitude and the dipole polarizability.

Other theoretical methods, for example the Second Born and Glauber approximations have been applied to helium scattering. The relation of these to our method is discussed in Chapter 7.

In part II of this thesis we apply the second order potential method to the scattering of charged particles, mainly electrons, from helium atoms initially in their ground state. In Chapter 8 we describe the wavefunctions used, and show the sensitivity of the elastic cross sections to the choice of the average energy.

We solve the coupled equations in the elastic, 2's and 2'p channels at several energies between 50ev. and 1000ev. The angular distributions and total cross sections obtained in each channel are compared, in Chapters 9, 11 and 12, with those of other methods and with the available experimental data. Chapter 10 examines the forward elastic scattering amplitudes and cross sections in detail. We compare the scattering of electrons with that of positrons at the same energy in Chapter 13.

Finally, the numerical methods used are outlined in Chapter 14, and in Chapter 15 we summarise the conclusions of the work.

Chapter 2

A TRUNCATED EIGENFUNCTION EXPANSION

The usefulness of atomic eigenfuncion expansions has been well established, particularly in the development of the Born series (Mott and Massey, 1933). In this chapter we follow the procedure of Bransden and Coleman (1972) by adopting an impact parameter formulation. Although we are mainly concerned with electron scattering, the method is equally applicable to the scattering of heavier particles such as protons (Bransden, Coleman and Sullivan, 1972). Atomic units, defined in Appendix I, will be used throughout.

The total wavefunction of the combined projectile - atom system, $\Psi(\underline{R},\underline{r})$, can be expanded in terms of the eigenfunctions of the unperturbed atom, $\left|\phi_n(\underline{r})\right\rangle$;

$$\Psi(\underline{R},\underline{r}) = \sum_{n=0}^{\infty} F_n(\underline{R}) \left|\phi_n(\underline{r})\right\rangle \qquad (2\text{-}1)$$

where $\underline{r}$ represents the internal coordinates of the atom and $\underline{R}$ the position vector of the projectile, with the nucleus of the atom as origin. The entrance channel is taken as $n=0$; in this thesis only scattering from atoms initially in their ground state will be examined.

The summation over n in equation (2-1) includes an integration over continuum states. Although $\Psi(\underline{R},\underline{r})$ as defined here is not symmetrised, Castillejo et al.(1960) show that electron exchange can be described by the expansion (2-1) provided the boundary conditions are chosen correctly, and allowance is made for the exchange singularity in the continuum integrand. However, at the energies we are interested in (above 100 ev. for electrons incident on helium atoms), we can ignore exchange.

The coefficients $F_n(\underline{R})$, which we show in chapter 3 to be related asymptotically to the excitation cross sections, are obtained by solving Shrödinger's equation for $\Psi(\underline{R},\underline{r})$;

$$(H - E)\,\Psi(\underline{R},\underline{r}) = 0. \tag{2-2}$$

Here, H is the total Hamiltonian of the system,

$$H = -\tfrac{1}{2}\nabla_{\underline{R}}^{2} + V(\underline{R},\underline{r}) + H'(\underline{r}) \tag{2-3}$$

with $V(\underline{R},\underline{r})$ the potential between projectile and atom, and $H'(\underline{r})$ the Hamiltonian of the unperturbed atom, whose eigenvalues are ϵ_n;

$$(H'(\underline{r}) - \epsilon_n)\left|\phi_n(\underline{r})\right\rangle = 0. \tag{2-4}$$

Since the initial energy of the atom is ϵ_o, the total energy $E = \epsilon_o + T$, where T is the initial kinetic energy of the projectile. So the Shrödinger equation (2-2) and (2-3) becomes, with the eigenfunction expansion (2-1),

$$\sum_{m=o}^{\infty}\left(-\tfrac{1}{2}\nabla_{\underline{R}}^{2} + V(\underline{R},\underline{r}) + H'(\underline{r}) - \epsilon_o - T\right) F_m(\underline{R})\left|\phi_m(\underline{r})\right\rangle = 0 \tag{2-5}$$

or, using (2-4),

$$\sum_{m=o}^{\infty} (-\tfrac{1}{2}\nabla_{\underline{R}}^{2} + V(\underline{R},\underline{r}) + \epsilon_m - \epsilon_o - T)\, F_m(\underline{R}) \left|\phi_m(\underline{r})\right\rangle = 0 \tag{2-6}$$

Multiplying (2-6) by $\left\langle\phi_n(\underline{r})\right|$ and thereby integrating over the atomic coordinates, $\underline{r}$, we get

$$\sum_{m=o}^{\infty} (-\tfrac{1}{2}\nabla_{\underline{R}}^{2} + \epsilon_m - \epsilon_o - T)\, F_m(\underline{R}) \left\langle\phi_n(\underline{r})\middle|\phi_m(\underline{r})\right\rangle = -\sum_{m=o}^{\infty} V_{nm}(\underline{R})\, F_m(\underline{R}) \tag{2-7}$$

$$\text{where}\quad V_{nm}(\underline{R}) = \left\langle\phi_n(\underline{r})\middle|V(\underline{R},\underline{r})\middle|\phi_m(\underline{r})\right\rangle \tag{2-8}$$

Since the atomic eigenfunctions form a complete orthonormal set,

$$\left\langle\phi_n(\underline{r})\middle|\phi_m(\underline{r})\right\rangle = \delta_{nm} . \tag{2-9}$$

Equation (2-7) thus reduces to

$$(\tfrac{1}{2}\nabla_{\underline{R}}^{2} + \tfrac{1}{2}k_n^{2})\, F_n(\underline{R}) = \sum_{m=o}^{\infty} V_{nm}(\underline{R})\, F_m(\underline{R}) \tag{2-10}$$

$$\text{where}\quad \tfrac{1}{2}k_n^{2} = T + \epsilon_o - \epsilon_n \tag{2-11}$$

Let us now use an impact parameter representation for $F_n(\underline{R})$ and set

$$F_n(\underline{R}) = \exp(i\underline{k}_o\cdot\underline{R})\, f_n(\underline{b},Z) \tag{2-12}$$

where Z is the component of $\underline{R}$ in the direction of incidence, $\hat{\underline{k}}_o$, and $\underline{b}$ is the impact parameter vector such that

$$\underline{R} = Z\hat{\underline{k}}_o + \underline{b} . \tag{2-13}$$

Differentiating (2-12) twice we find

$$\nabla_{\underline{R}}^{2}F_n(\underline{R}) = -k_o^{2}\, F_n(\underline{R}) + 2i\underline{k}_o\exp(i\underline{k}_o\cdot\underline{R})\nabla_{\underline{R}} f_n(\underline{b},Z) + \exp(i\underline{k}_o\cdot\underline{R})\, \nabla_{\underline{R}}^{2}\, f_n(\underline{b},Z) \tag{2-14}$$

Assuming the velocity is high enough that $\nabla_{\underline{R}}^2 f_n(\underline{b},Z)$ is negligible compared with $\underline{k}_o.\nabla_{\underline{R}}\, f_n(\underline{b},Z)$ (cf. Wilets and Wallace, 1968, in the limit of infinite target mass), we can reduce (2-14) to

$$(\tfrac{1}{2}\nabla_{\underline{R}}^2 + \tfrac{1}{2}k_n^2)\, F_n(\underline{R}) = (\epsilon_o - \epsilon_n)\, \exp(i\underline{k}_o.\underline{R})\, f_n(\underline{b},Z) + i\underline{k}_o \exp(i\underline{k}_o.\underline{R})\, \nabla_{\underline{R}}\, f_n(\underline{b},Z) \qquad (2\text{-}15)$$

since, from (2-11), $\tfrac{1}{2}k_o^2 - \tfrac{1}{2}k_n^2 = \epsilon_n - \epsilon_o$. (2-16)

Comparing (2-15) with equation (2-10) we find,

$$i\underline{k}_o.\nabla_{\underline{R}}\, f_n(\underline{b},Z) = (\epsilon_n - \epsilon_o)\, f_n(\underline{b},Z) + \sum_{m=o}^{\infty} V_{nm}(\underline{R})\, f_m(\underline{b},Z). \qquad (2\text{-}17)$$

If the velocities are sufficiently high to assume straight line trajectories, then

$$\hat{\underline{k}}_o = \hat{\underline{Z}} \quad \text{and} \quad \underline{b}.\underline{k}_o = 0,$$

where $\underline{b}$ is the classical impact parameter (the closest distance of approach to the atom) as in figure 2a, and $\underline{Z} = \underline{k}_o t$ in atomic units, where t is the time. So,

$$\underline{k}_o.\underline{R} = k_o Z \quad \text{and} \quad \underline{k}_o.\nabla_{\underline{R}} = k_o \frac{\partial}{\partial Z}. \qquad (2\text{-}18)$$

Thus equation (2-15) becomes,

$$ik_o \frac{\partial}{\partial Z} f_n(\underline{b},Z) = (\epsilon_n - \epsilon_o)\, f_n(\underline{b},Z) + \sum_{m=o}^{\infty} V_{nm}(\underline{R})\, f_m(\underline{b},Z) \qquad (2\text{-}19)$$

In practice it is better to remove the oscillatory term by making the substitution,

$$f_n(\underline{b},Z) = \exp(i(\epsilon_o - \epsilon_n)Z/k_o)\, a_n(b,Z) \qquad (2\text{-}20)$$

in which case (2-19) becomes,

$$\frac{\partial}{\partial Z}\, a_n(b,Z) = \frac{1}{ik_o} \sum_{m=o}^{\infty} V_{nm}(\underline{R}) \exp(i(\epsilon_n - \epsilon_m)Z/k_o)\, a_m(b,Z). \tag{2-21}$$

These coupled equations are to be solved with the boundary conditions,

$$a_n(b,-\infty) = \delta_{no}. \tag{2-22}$$

This infinite set of coupled differential equations cannot, in general, be solved. However, it may be a good approximation to assume that only a few low lying states are strongly coupled. Thus we can truncate the series (2-21) at a suitable level, as in the close coupling approximation (Bransden, 1970, ch.5). A better approximation is to make some allowance for the states not included explicitly in the truncated expansion, and this is the basis of the second order potential method which we describe in chapter 4.

Figure

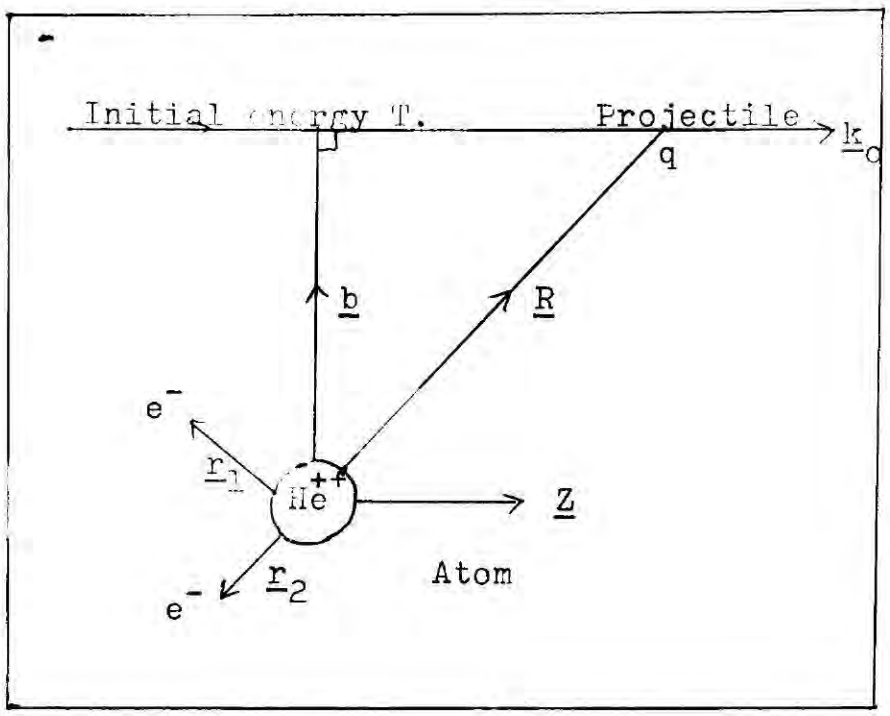

Figure 2a. Kinematics in the scattering of charged particles from helium.

Chapter 3

THE SCATTERING AMPLITUDE AND CROSS SECTION

It is now necessary to show how the amplitudes $F_n(\underline{R})$ of the eigenfunction expansion used in Chapter 2 are related to the cross sections for excitation to the n-th atomic state.

We know that the interaction between target and projectile becomes negligible at large separations. So asymptotically the amplitudes of the expansion (2-1) must, from the physics, represent an incident plane wave, $\exp(i\underline{k}_o.\underline{R})$, in the entrance channel, and outgoing spherical waves, $\exp(ik_nR)/R$ in each open channel. Thus

$$F_n(\underline{R}) \underset{R\to\infty}{\sim} \exp(i\underline{k}_o.\underline{R})\,\delta_{no} + f_{no}(\Theta,\Phi)\exp(ik_nR)/R \tag{3-1}$$

McDowell and Coleman (1970,ch.5) show that this asymptotic form is only valid for potentials which fall off faster than 1/R as R tends to infinity. Thus Coulomb potentials must be "screened", as for example in the potential due to a neutral atom.

The outgoing spherical waves have in general some angular distribution given by $f_n(\Theta,\Phi)$, but there should be no interference between these waves well away from the interaction region. Because of the analogy with Fraunhoffer diffraction in optics, let us use the construction of Wilets and Wallace (1968) who place a screen at a distance Z_0 beyond the interaction, as in figure 3a. The volume enclosed by this screen and a hemisphere at infinity is assumed to be free of interactions between the projectile and target. Since we know our complete wavefunction can be written as a linear combination of $F_n(\underline{R})|\emptyset_n\rangle$, and if the outgoing spherical wave associated with $F_n(\underline{R})$ is $U(\underline{R})$, then in the interaction-free enclosure, $U(\underline{R})$ must be a solution of the free particle wave equation. This is given by equation (2-10) with the potential $V(\underline{R},\underline{r}) = 0$;

$$(\tfrac{1}{2}\nabla_{\underline{R}}^2 + \tfrac{1}{2}k_n^2)\, U(\underline{R}) = 0 . \qquad (3\text{-}2)$$

If there exists another function, $W(\underline{R})$, satisfying the same wave equation in the enclosure, then we may use Green's Theorem (Born and Wolf, 1965) which converts a volume integral to an integral over the surface bounding the enclosure:

$$\int (U\nabla^2 W - W\nabla^2 U)\, d\tau = \int \hat{\underline{n}}.(U\nabla W - W\nabla U)\, dS . \qquad (3\text{-}3)$$

Since the functions $U(\underline{R})$ and $W(\underline{R})$ are both solutions of (3-2), the left-hand integral in (3-3) vanishes.

To find the function at a particular point P inside our enclosure, we place a sphere round the point to exclude it from our region (see figure 3a). Born and Wolf (1965) show that its contribution to the surface integral in (3-3) is just $4\pi U(\underline{R})$, where $\underline{R}$ is the vector joining the point to the screen. So (3-3) becomes,

$$U(\underline{R}) = \frac{1}{4\pi}\int \hat{\underline{n}}.(U\nabla W - W\nabla U)\, dS. \qquad (3\text{-}4)$$

In (3-4) we need only consider the surface integral over the Fraunhoffer screen, since the functions U and W vanish on the infinite hemisphere.

At large $\underline{R}$ a solution to the wave equation (3-2) is just the spherical wave

$$W(\underline{R}) = \exp(ik_n(R-x))/R, \qquad (3\text{-}5)$$

where $x = b \cos \Phi \sin \Theta$, from figure 3a.

The functions W and U in the kernel of equation (3-4) have to be evaluated on the screen. We know that physically the scattering must be independent of the direction of the impact parameter $\underline{b}$, since the scattering is cylindrically symmetric. Thus we can define our functions in terms of R', the projection of the impact parameter on an axis fixed on the screen, as in figure 3b. Since $\hat{\underline{x}} = \hat{\underline{R}}$, we find

$$\hat{\underline{n}} \cdot \nabla_{\underline{R}'} W(R) = \hat{\underline{n}} \cdot \hat{\underline{x}} \frac{\partial}{\partial x} W(R)$$

or, using (3-5),

$$= -ik_n \hat{\underline{n}} \cdot \hat{\underline{R}} \exp(ik_n(R-x))/R \ . \qquad (3\text{-}6)$$

Substituting (3-5) and (3-6) into equation (3-4),

$$U(\underline{R}) = -\frac{1}{4\pi R} \exp(ik_n R) \int \exp(-ik_n b \sin \Theta \cos \Phi)\, \hat{\underline{n}} \cdot \qquad (3\text{-}7)$$
$$\left[\nabla_{\underline{R}'} U(R') + ik_n \hat{\underline{R}}\, U(R') \right] dS \ .$$

To find U(R') we must examine the eigenfunction expansion of the total wavefunction in equation (2-1), which, with the substitutions (2-12) and (2-20), is

$$\Psi(\underline{R},\underline{r}) = \sum_{n=0}^{\infty} a_n(\underline{b},Z) \exp(iKZ)\, \phi_n(r,\theta,\phi) \qquad (3\text{-}8)$$

In (3-8), $K = k_o - (\epsilon_o - \epsilon_n)/k_o$. In a high energy approximation, we can use K instead of k_n in equations (3-5) to (3-7), and in so doing still make some allowance for the difference in energy between the initial and final atomic states.

Although the initial state can be assumed to be an s-state, the final state, $\phi_n(r,\theta,\phi)$ may have a non - zero magnetic quantum number, m. We can take out the dependence of the function on the direction of $\underline{b}$, since we know the reaction is independent of this, by making the transformation $\phi = \phi' - \Phi$ (see figure 3b). So our function $F_n(\underline{R})$, defined by (2-1), can be rewritten as

$$F_n(\underline{R}) = a_n(|b|) \exp(iKZ) \exp(-im\Phi). \tag{3-9}$$

This includes the incident plane wave, $\delta_{no} \exp(ik_o . Z)$, which must be subtracted out to get the spherical wave contribution, $U(R')$, before we can substitute into equation (3-7);

$$U(\underline{R}) \underset{R \to \infty}{\sim} - \frac{1}{4\pi R} \exp(iKR) \int dS \exp(-iKb \sin\Theta \cos\Phi)$$

$$\underline{\hat{n}} . \left[\nabla_{\underline{R}'} (a_n(b) - \delta_{no}) \exp(iKZ) \exp(-im\Phi) \right.$$

$$\left. + iKR (a_n(b) - \delta_{no}) \exp(iKZ_o) \exp(-im\Phi) \right]. \tag{3-10}$$

Now $\underline{\hat{n}} . \nabla_{\underline{R}'} \exp(iKZ) = iK \exp(iKZ_o)$, and $\underline{\hat{n}} . \underline{\hat{R}} = \cos\Theta$.

$$\text{So, } U(\underline{R}) \underset{R \to \infty}{\sim} - \frac{1}{4\pi R} \exp(iKZ_o) \exp(iKR)$$

$$\times \int dS \exp(-iKb \sin\Theta \cos\Phi)(1 + \cos\Theta)$$

$$\times \left[a_n(b) - \delta_{no} \right] \exp(-im\Phi). \tag{3-11}$$

From figure 3b we have the element of area on the screen, $dS = b.db.d\Phi$. Also we note that $1 + \cos\Theta = 2\cos^2\frac{1}{2}\Theta$. So (3-11) becomes,

$$U(\underline{R}) \underset{R\to\infty}{\sim} -iK\exp(iKZ_o)[\exp(iKR)/R]\cos^2\tfrac{1}{2}\Theta$$

$$X\int_0^\infty b\,db[a_n(b) - \delta_{no}]\int_0^{2\pi}\frac{d\Phi}{2\pi}\exp(-iKb\sin\Theta\cos\Phi) \qquad (3\text{-}12)$$

$$X\exp(-im\Phi)$$

Making the transformation $\Phi = \pi/2 - \Phi'$, the right hand integral reduces to a standard form (Watson, 1922, p.20);

$$(-i)^m\int_0^{2\pi}\frac{d\Phi'}{2\pi}\exp[i(m\Phi' - Kb\sin\Theta\sin\Phi')] = (-i)^m J_m(Kb\sin\Theta) \qquad (3\text{-}13)$$

where $J_m(x)$ is the m-th order Bessel function. So (3-12) becomes,

$$U(\underline{R}) \underset{R\to\infty}{\sim} (-i)^{m+1}K\cos^2\tfrac{1}{2}\Theta[\exp(iK(R+Z_o))/R]$$

$$X\int_0^\infty b\,db[a_n(b) - \delta_{no}]J_m(Kb\sin\Theta). \qquad (3\text{-}14)$$

Since the asymptotic form of our scattering functions is given by (3-1), we have the following identity for the spherical wave,

$$U(\underline{R}) \equiv f_n(\Theta,\Phi)\exp(iK(R+Z_o))/R. \qquad (3\text{-}15)$$

By comparing (3-15) with (3-14), we find a relation for the scattering amplitude, $f_n(\Theta,\Phi)$. The approximation is a small angle one; Wilets and Wallace explain that the extension to large angle scattering is usually effected by replacing the $\sin\Theta$ by $2\sin\frac{1}{2}\Theta$ in (3-14), and by ignoring the factor $\cos^2\frac{1}{2}\Theta$. So

$$f_n(\Theta,\Phi) = (-i)^{m+1}K\int_0^\infty bdb[a_n(b) - \delta_{no}]\, J_m(2Kb\sin\tfrac{1}{2}\Theta). \tag{3-16}$$

If the incident beam has unit density, then its flux (number of particles crossing a unit area / second) is just the initial velocity, v_o. The differential cross section, $\sigma_n(\Theta)$, for excitation to the n-th atomic state is defined as (McDowell and Coleman, 1970, ch.1);

$$\sigma_n(\Theta) = \frac{\text{Flux through } d\Omega \text{ in the n-th channel at R}}{\text{Incident flux.}}$$

With the asymptotic form of (3-1), the outgoing spherical waves in each channel contribute

$$\left|f_n(\Theta,\Phi)\right|^2 R^{-2}\, v_n\, R^2\, d\Omega \qquad (v_n = \text{final velocity})$$

to the flux through a solid angl $d\Omega$. So

$$\sigma_n(\Theta) = \frac{v_n}{v_o}\left|f_n(\Theta,\Phi)\right|^2 \qquad (a_o^2). \tag{3-17}$$

Integrating over the solid angle, $d\Omega = \sin\Theta d\Theta d\Phi$, we have the total excitation cross section

$$Q(0,n) = 2\int_0^\pi \sigma_n(\Theta)\sin\Theta d\Theta \qquad (\pi a_o^2). \tag{3-18}$$

Noticing that most of the contribution to the angular integration in (3-18) comes from the forward directions, we can use the known properties of the Bessel function (Watson, 1922, p.453) to rewrite the total cross section as an integral over the impact parameter; using equations (3-16) and (3-17),

$$Q(0,n) = 2\frac{v_n}{v_o}\int_0^\infty bdb\left|a_n(b) - \delta_{no}\right|^2 \qquad (\pi a_o^2) \tag{3-19}$$

Figures

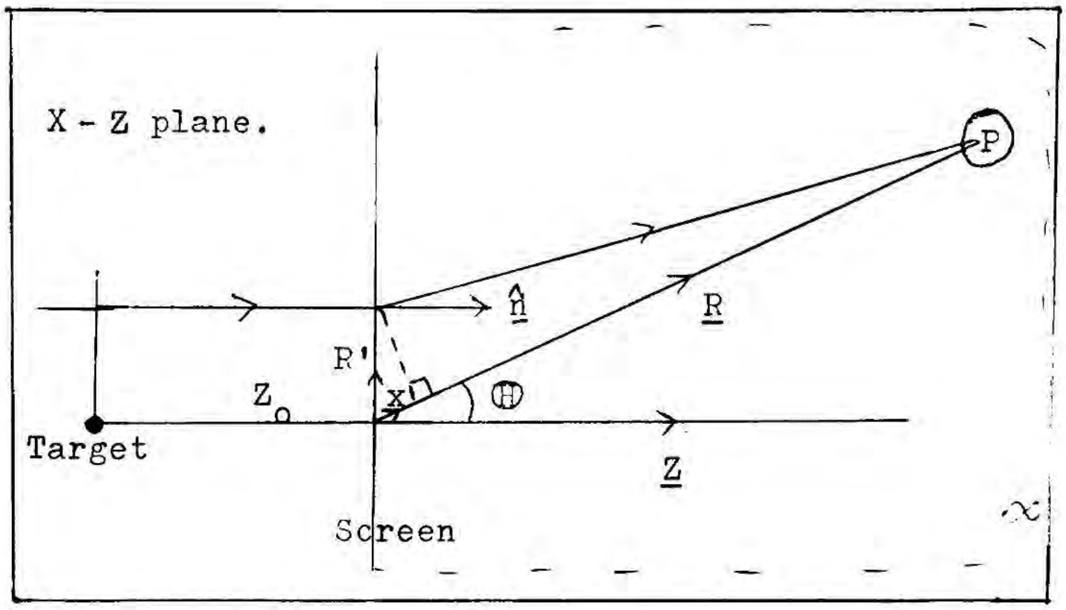

Figure 3a. The analogy with Fraunhoffer scattering.

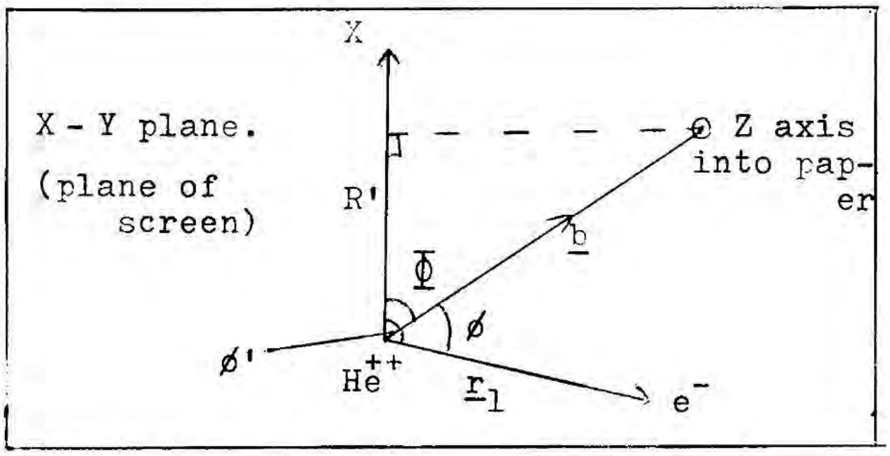

Figure 3b. The axial angles defined in equation (3-9).

Chapter 4

THE SECOND ORDER POTENTIAL METHOD

The truncated eigenfunction expansion introduced at the end of chapter 2 depends on a few low - lying states being more strongly coupled than the higher states. It was mentioned in chapter 1 that the close coupling method is very useful below the ionization threshold when only a limited number of channels are open. However, at higher energies, some allowance must be made for the effect of the channels not explicitly included.

Assuming the first N channels are strongly coupled, we can truncate the expansion (2-21) at the N-th state, and make an approximation for the higher states so as to include only the couplings to the first N channels; let

$$\frac{\partial}{\partial Z} a_n(b,Z) \underset{n>N}{\sim} \frac{1}{ik_o} \sum_{j=o}^{N} V_{nj}(Z) \exp(i(\epsilon_n - \epsilon_j)Z/k_o)\, a_j(b,Z) \tag{4-1}$$

Integrating, $$a_n(b,Z) = \frac{1}{ik_o} \sum_{j=o}^{N} \int_{-\infty}^{Z} dZ' V_{nj}(Z') \exp(i(\epsilon_n - \epsilon_j)Z'/k_o)\, a_j(b,Z') \tag{4-2}$$

Substituting this into the expansion (2-21) for the states above N, we find;

$$\frac{\partial}{\partial Z} a_n(b,Z) = \frac{1}{ik_o} \sum_{m=o}^{N} V_{nm}(Z) \exp(i(\epsilon_n - \epsilon_m) Z/k_o) a_m(b,Z)$$

$$- \frac{1}{k_o^2} \sum_{m=N+1}^{\infty} \sum_{j=o}^{N} \int_{-\infty}^{Z} dZ' V_{nm}(Z) V_{mj}(Z') \exp(i(\epsilon_n - \epsilon_m) Z/k_o)$$

$$\text{X} \exp(i(\epsilon_m - \epsilon_j) Z'/k_o) a_j(Z') \qquad (4-3)$$

By defining a second order potential matrix,

$$K_{nm}^{N}(Z,Z') = \sum_{j=N+1}^{\infty} V_{nj}(Z) V_{jm}(Z') \exp(i(\epsilon_n - \epsilon_j) Z/k_o) \text{ X } \exp(-i(\epsilon_m - \epsilon_j) Z'/k_o) \qquad (4-4)$$

we get the following N+1 coupled equations,

$$\frac{\partial}{\partial Z} a_n(b,Z) = \frac{1}{ik_o} \sum_{m=o}^{N} V_{nm}(Z) \exp(i(\epsilon_n - \epsilon_m) Z/k_o) a_m(b,Z)$$

$$- \frac{1}{k_o^2} \sum_{m=o}^{N} \int_{-\infty}^{Z} dZ' K_{nm}^{N}(Z,Z') a_m(b,Z') \qquad (4-5)$$

with the boundary conditions given by 2-22);

$$a_n(b,-\infty) = \delta_{no} . \qquad (4-6)$$

The infinite summation which defines the $K_{nm}^{N}(Z,Z')$ in equation (4-4) cannot be evaluated as it stands. However, at high incident energies ($T \gg \epsilon_n$), the energies ϵ_n of the levels above, say, M, can be averaged to a single energy ($\bar{\epsilon}$) which can now be taken outside the summation. So equation (4-4) can be rewritten as;

$$K_{nm}^{N}(Z,Z') = \sum_{j=N+1}^{M} \exp\left[(i(\epsilon_n - \epsilon_j) Z - (\epsilon_m - \epsilon_j) Z')/k_o\right] V_{nj}(Z) V_{jm}(Z')$$

$$+ \exp\left[(i(\epsilon_n - \bar{\epsilon}) Z - (\epsilon_m - \bar{\epsilon}) Z')/k_o\right] \sum_{j=M+1}^{\infty} V_{nj}(Z) V_{jm}(Z') \qquad (4-7)$$

The summation on the right of (4-7) can be written as,

$$\sum_{j=M+1}^{\infty} V_{nj}(Z)V_{jm}(Z') = \sum_{j=o}^{\infty} V_{nj}(Z)V_{jm}(Z') - \sum_{j=o}^{M} V_{nj}(Z)V_{jm}(Z') \qquad (4\text{-}8)$$

and we know from the definition of $V_{nm}(Z)$, equation (2-8), that

$$\sum_{j=o}^{\infty} V_{nj}(Z)V_{jm}(Z') = \sum_{j=o}^{\infty} \left\langle \phi_n(\underline{r}) \middle| V(\underline{R},\underline{r}) \middle| \phi_j(\underline{r}) \right\rangle \left\langle \phi_j(\underline{r}') \middle| V(\underline{R}',\underline{r}') \middle| \phi_m(\underline{r}') \right\rangle . \qquad (4\text{-}9)$$

Since our original expansion (2-1) is complete, we can use closure (McDowell and Coleman, 1970, ch.4) on the wavefunctions $\phi_n(\underline{r})$:

$$\sum_{j=o}^{\infty} \left| \phi_j(\underline{r}) \right\rangle \left\langle \phi_j(\underline{r}') \right| = \delta(\underline{r}-\underline{r}'). \qquad (4\text{-}10)$$

So $$\sum_{j=o}^{\infty} V_{nj}(Z)V_{jm}(Z') = \left\langle \phi_n(\underline{r}) \middle| V(\underline{R},\underline{r})V(\underline{R}',\underline{r}) \middle| \phi_m(\underline{r}) \right\rangle$$

$$= U_{nm}(Z,Z') . \qquad (4\text{-}11)$$

Using equations (4-8) and (4-11), we can rewrite (4-7) as

$$K^N_{nm}(Z,Z') = \sum_{j=N+1}^{M} \exp\left[(i(\epsilon_n - \epsilon_j)Z - (\epsilon_m - \epsilon_j)Z')/k_o\right] V_{nj}(Z)V_{jm}(Z')$$

$$+\exp\left[(i(\epsilon_n - \bar{\epsilon})Z - (\epsilon_m - \bar{\epsilon})Z')/k_o\right]$$

$$\times \left[U_{nm}(Z,Z') - \sum_{j=o}^{M} V_{nj}(Z)V_{jm}(Z') \right] \qquad (4\text{-}12)$$

As we shall see later, the $K_{nm}(Z,Z')$ are generally very difficult to calculate. So let us consider the simpler, if less consistent, method of allowing the higher states to couple only to the initial state, so that equation (4-1) is replaced by

$$\frac{\partial}{\partial Z} a_n(b,Z) \underset{n>N}{\sim} \frac{1}{ik_o} V_{no}(Z)\, a_o(b,Z) \exp(i(\epsilon_n - \epsilon_o)Z/k_o) \qquad (4\text{-}13)$$

Using this in (2-21), and proceding as before, we find equations (4-3) and (4-4) become;

$$\frac{\partial}{\partial Z} a_n(b,Z) = \frac{1}{ik_o} \sum_{m=o}^{N} V_{nm}(Z)\exp(i(\epsilon_n - \epsilon_m)Z/k_o)a_m(b,Z)$$

$$- \frac{1}{k_o^2} \int_{-\infty}^{Z} dZ' \; K_{no}(Z,Z') \; a_o(Z') \qquad (4\text{-}14)$$

with $$K_{no}(Z,Z') = \sum_{j=N+1}^{\infty} V_{nj}(Z)V_{jo}(Z')\exp(i(\epsilon_n - \epsilon_j)Z/k_o)\exp(-i(\epsilon_o - \epsilon_j)Z'/k_o) \qquad (4\text{-}15)$$

In the applications to scattering from a helium target, we use this equation for elastic scattering (n=0) only;

$$\frac{\partial}{\partial Z} a_o(b,Z) = \frac{1}{ik_o} \sum_{m=o}^{N} V_{om}(Z)\exp(i(\epsilon_o - \epsilon_m)Z/k_o)a_m(b,Z)$$

$$- \frac{1}{k_o^2} \int_{-\infty}^{Z} dZ' \; K_{oo}(Z,Z') \; a_o(b,Z') \qquad (4\text{-}16)$$

where, from (4-12),

$$K_{oo}(Z,Z') = \sum_{j=N+1}^{M} \exp\left[i(\epsilon_o - \epsilon_j)(Z-Z')/k_o\right] V_{oj}(Z)V_{jo}(Z')$$

$$+ \exp\left[i(\epsilon_o - \bar{\epsilon})(Z-Z')/k_o\right]\left[U_{oo}(Z,Z') - \sum_{j=o}^{M} V_{oj}(Z)V_{jo}(Z')\right] \qquad (4\text{-}17)$$

For the inelastic channels we shall ignore the integral term and use

$$\frac{\partial}{\partial Z} a_n(b,Z) = \frac{1}{ik_o} \sum_{m=o}^{N} V_{nm}(Z)a_m(b,Z)\exp(i(\epsilon_n - \epsilon_m)Z/k_o) \qquad (4\text{-}18)$$

We shall also be investigating the importance of different couplings, so for future reference we note the following equations for the elastic and inelastic amplitudes;

$$\frac{\partial}{\partial Z} a_o(b,Z) = \frac{1}{ik_o} V_{oo}(Z) a_o(b,Z) - \frac{1}{k_o^2} \int_{-\infty}^{Z} dZ' K_{oo}(Z,Z') a_o(b,Z') \tag{4-19}$$

and

$$\frac{\partial}{\partial Z} a_n(b,Z) = \frac{1}{ik_o} V_{no}(Z) \exp(i(\epsilon_n - \epsilon_o)Z/k_o) a_o(b,Z) + \frac{1}{ik_o} V_{nn}(Z) a_n(b,Z). \tag{4-20}$$

The single channel approximation (4-19) differs from equation (4-16) by the negect of the back couplings from the inelastic channels; and the distorted wave approximation (4-20) differs from equation (4-18) by the neglect of intercoupling between the inelastic channels.

Chapter 5

A CHOICE OF THE AVERAGE ENERGY

In chapter 4 we used a closure approximation on the states not included in the truncated expansion. This involved defining an average energy $\bar{\epsilon}$ of these states, and we now examine a particular choice of the value of this parameter.

The success of the polarized orbital approximation at low energies (see, eg.,Bransden, 1970, ch.5), where a suitable non - local potential is introduced into the single channel equation (1-4), leads us to choose the average energy in such a way that the effective potential in the incident channel has the correct asymptotic behaviour in the adiabatic limit. This is given by first order perturbation theory (Bransden, 1970, ch.5) as;

$$\mathrm{Re}\left[V^{eff}(R) \right] \underset{R \to \infty}{\sim} -\tfrac{1}{2}\alpha_1 R^{-4} + O(R^{-6}) \qquad (5\text{-}1)$$

where α_1 is the dipole polarizability.

Examining our wavefunction (2-1) and the Shrödinger equation it satisfies (2-2), we see that the effective potential in the elastic channel must come from,

$$(\tfrac{1}{2}\nabla_{\underline{R}}^2 + \tfrac{1}{2}\underline{k}_0^2)\, F_0(\underline{R}) .$$

Making the substitution $F_o(\underline{R}) = \exp(ik_oZ)a_o(b,Z)$ as in chapter 1, we see from equation (2-15) that

$$(\tfrac{1}{2}\nabla_{\underline{R}}^2 + \tfrac{1}{2}k_o^2)\,F_o(\underline{R}) = ik_o\exp(ik_oZ)\,\frac{\partial}{\partial Z}\,a_o(b,Z). \tag{5-2}$$

Now $(\partial/\partial Z)\,a_o(b,Z)$ is given by equation (4-5), but we know that asymptotically the $a_n(b,Z)$ tend to the boundary conditions (4-6). So

$$\frac{\partial}{\partial Z}\,a_o(b,Z) \underset{Z\to-\infty}{\sim} \frac{1}{ik_o}V_{oo}(Z)a_o(b,Z) - \frac{1}{k_o^2}\int_{-\infty}^{Z}dZ'K_{oo}(Z,Z')a_o(b,Z')$$

$$\underset{Z\to-\infty}{\sim} \frac{1}{ik_o}V_{oo}(Z)a_o(b,Z) - \frac{1}{ik_o}V_p(Z)a_o(b,Z) \tag{5-3}$$

where we have integrated the kernel by parts, assuming that $a_o(b,Z')$ is fairly constant in the range $[-\infty,Z]$ when $Z \to -\infty$; and have defined a potential $V_p(\underline{R})$ such that

$$V_p(Z) = \frac{1}{ik_o}\int_{-\infty}^{Z}dZ'\;K_{oo}(Z,Z'). \tag{5-4}$$

Using (5-3) in (5-2), we find that the equation satisfied by $F_o(\underline{R})$ for large $\underline{R}$ is (cf.Bransden, 1970, ch.5),

$$(\tfrac{1}{2}\nabla_{\underline{R}}^2 + \tfrac{1}{2}k_o^2)\,F_o(\underline{R}) \underset{R\to\infty}{\sim} V_{oo}(\underline{R})F_o(\underline{R}) + V_p(\underline{R})F_o(\underline{R}). \tag{5-5}$$

If the atom is initially in an s-state, the $V_{oo}(\underline{R})$ will vanish exponentially as $R \to \infty$ (this is shown for a helium target in appendix 2). So the long range potential comes from the second order term (5-4). From equation (4-12) we have,

$$K_{oo}^{N}(Z,Z') = \sum_{j=N+1}^{M} V_{oj}(Z)V_{jo}(Z')\exp[i(\epsilon_o - \epsilon_j)(Z-Z')/k_o]$$

$$+ \exp[i(\epsilon_o - \bar{\epsilon})(Z-Z')/k_o]\,[U_{oo}(Z,Z') - \sum_{j=o}^{M} V_{oj}(Z)V_{jo}(Z')] \tag{5-6}$$

By defining $\alpha(Z') = U_{oo}(Z,Z') - V_{oo}(Z)V_{oo}(Z')$

$$\text{and } \beta_j(Z') = V_{oj}(Z)V_{jo}(Z') , \tag{5-7}$$

equation (5-6) reduces to

$$K_{oo}^{N}(Z,Z') = [\alpha(Z') - \sum_{j=1}^{M}\beta_j(Z')]\exp[i(\epsilon_o - \bar{\epsilon})(Z - Z')/k_o]$$

$$+ \sum_{j=N+1}^{M}\beta_j(Z')\exp[i(\epsilon_o - \epsilon_j)(Z - Z')/k_o] \tag{5-8}$$

Since the potentials must vanish at infinity, we have $\alpha(-\infty) = \beta_j(-\infty) = 0$. So integrating $K_{oo}^{N}(Z,Z')$ in (5-8) by parts, we find

$$\int_{-\infty}^{Z} dZ' K_{oo}^{N}(Z,Z') = -ik_o[\alpha(Z) - \sum_{j=1}^{M}\beta_j(Z)]/(\bar{\epsilon} - \epsilon_o)$$

$$- \sum_{j=N+1}^{M} ik_o\beta_j(Z)/(\epsilon_j - \epsilon_o) \tag{5-9}$$

where the derivatives of $\alpha(Z)$ and $\beta_j(Z)$ have been ignored, since we are only interested in the real part of the effective potential, as defined by (5-4). So

$$\mathrm{Re}[V_p(\underline{R})] \underset{R \to \infty}{\sim} -[\alpha(Z) - \sum_{j=1}^{M}\beta_j(Z)]/(\bar{\epsilon} - \epsilon_o) - \sum_{j=N+1}^{M}\beta_j(Z)/(\epsilon_j - \epsilon_o)$$

$$\underset{R \to \infty}{\sim} -\Big[[a - \sum_{j=1}^{M} b_j]/(\bar{\epsilon} - \epsilon_o) - \sum_{j=N+1}^{M} b_j/(\epsilon_j - \epsilon_o)\Big].R^{-4}, \tag{5-10}$$

if $\quad \alpha(Z) \equiv U_{oo}(Z,Z) - V_{oo}(Z)V_{oo}(Z) \sim a\, R^{-4}$

$$\text{and} \quad \beta_j(Z) \equiv |V_{oj}(Z)|^2 \sim b_j R^{-4}. \tag{5-11}$$

So for $\mathrm{Re}[V_p(\underline{R})]$ to have the form (5-1), the average energy $\bar{\epsilon}$ must be chosen so that

$$\bar{\epsilon} - \epsilon_o = [a - \sum_{j=1}^{M} b_j] / [\tfrac{1}{2}\alpha_1 - \sum_{j=N+1}^{M} b_j/(\epsilon_j - \epsilon_o)]. \tag{5-12}$$

Note that in the derivation of (5-12), we have considered the general case of coupling the high channels to the N+1 low-lying, strongly coupled, states. If only the coupling to the initial state is considered, as in equation (4-13), then $N = 0$ and (5-12) becomes;

$$\bar{\epsilon} - \epsilon_o = [a - \sum_{j=1}^{M} b_j] / [\tfrac{1}{2}\alpha_1 - \sum_{j=1}^{M} b_j/(\epsilon_j - \epsilon_o)]. \tag{5-13}$$

If we average all the atomic states above the ground state, then $M = 0$ and (5-13) reduces to

$$\bar{\epsilon} - \epsilon_o = 2a/\alpha_1 . \tag{5-14}$$

Chapter 6

THE ASYMPTOTIC EXPANSION OF THE SECOND ORDER POTENTIAL

Having decided in chapter 5 to choose the average energy so that the correct long range potential is obtained in the elastic channel, we now examine the potentials in order to find a simple presciption for this parameter. We assume that the target atom is either hydrogen or helium, and the atomic electrons are initially in their ground (1's) state.

The potential on a particle, charge q, approaching a neutral atom whose atomic number is A, can be written as (Mott and Massey, 1965, ch.16);

$$V(\underline{R},\underline{r}) = q\sum_{i=1}^{A}\left[\frac{1}{R} - \frac{1}{|\underline{R}-\underline{r}_i|}\right]. \qquad (6\text{-}1)$$

The ground state wavefunction for hydrogen and helium can be written in the seperable form $u(r_1)$ and $u(r_1)u(r_2)$ respectively, where r_1 and r_2 represent the positions of each atomic electron, with respect to the nucleus of the atom. So let

$$|\emptyset_o(\underline{r})\rangle = \prod_{k=1}^{A} u(r_k)\ , \qquad (6\text{-}2)$$

where $u(r_k)$ is the spherically symmetric hydrogen - like wavefunction, normalised so that,

$$\left\langle \phi_o(\underline{r}) \middle| \phi_o(\underline{r}) \right\rangle = 1 = \int d\underline{r}_k \left| u(r_k) \right|^2. \tag{6-3}$$

The first order potential, $V_{oo}(\underline{R})$, defined by (2-8), becomes, with this groundstate wavefunction;

$$V_{oo}(\underline{R}) = \left\langle \phi_o(\underline{r}) \middle| V(\underline{R},\underline{r}) \middle| \phi_o(\underline{r}) \right\rangle$$

using (6-1) and (6-2),

$$= q\sum_{i=1}^{A} \prod_k \int d\underline{r}_k \left| u(r_k) \right|^2 \left[\frac{1}{R} - \frac{1}{|\underline{R} - \underline{r}_i|} \right]$$

$$= q\sum_{i=1}^{A} \int d\underline{r}_i \left| u(r_i) \right|^2 \left[\frac{1}{R} - \frac{1}{|\underline{R} - \underline{r}_i|} \right] \prod_{k\neq i} \int d\underline{r}_k \left| u(r_k) \right|^2 \tag{6-4}$$

Because of the normalisation condition (6-3), the right hand integral is unity. So,

$$V_{oo}(\underline{R}) = qA \int d\underline{r} \left| u(r) \right|^2 \left[\frac{1}{R} - \frac{1}{|\underline{R} - \underline{r}|} \right]. \tag{6-5}$$

Similarly, the second order potential in the elastic channel, defined in equation (4-11), becomes;

$$U_{oo}(\underline{R},\underline{R}') = \left\langle \phi_o(\underline{r}) \middle| V(\underline{R},\underline{r}) V(\underline{R}',\underline{r}) \middle| \phi_o(\underline{r}) \right\rangle$$

using (6-1) and (6-2),

$$= q^2 \sum_{i=1}^{A} \sum_{j=1}^{A} \prod_k \int d\underline{r}_k \left| u(r_k) \right|^2 \left[\frac{1}{R} - \frac{1}{|\underline{R} - \underline{r}_i|} \right] \left[\frac{1}{R'} - \frac{1}{|\underline{R}' - \underline{r}_j|} \right]$$

$$= q^2 \sum_{i=1}^{A} \int d\underline{r}_k \left| u(r_k) \right|^2 \left[\frac{1}{R} - \frac{1}{|\underline{R} - \underline{r}_i|} \right] \left[\frac{1}{R'} - \frac{1}{|\underline{R}' - \underline{r}_i|} \right] \prod_{k\neq i} \int d\underline{r}_k \left| u(r_k) \right|^2 \tag{6-6}$$

$$+ q^2 \sum_{i=1}^{A} \sum_{j\neq i}^{A} \int d\underline{r}_i \left| u(r_i) \right|^2 \left[\frac{1}{R} - \frac{1}{|\underline{R} - \underline{r}_i|} \right] \int d\underline{r}_j \left| u(r_j) \right|^2 \left[\frac{1}{R'} - \frac{1}{|\underline{R}' - \underline{r}_j|} \right]$$

$$\times \prod_{k\neq i,j} \int d\underline{r}_k \left| u(r_k) \right|^2$$

Because of (6-3), the two right hand integrals are unity. So (6-6) can be rewritten as,

$$U_{oo}(\underline{R},\underline{R}') = q^2 A\int d\underline{r}\,|u(r)|^2\left\{\frac{1}{R}\left[\frac{1}{R'} - \frac{1}{|\underline{R}'-\underline{r}|}\right] + \frac{1}{R'}\left[\frac{1}{R} - \frac{1}{|\underline{R}-\underline{r}|}\right] - \frac{1}{RR'} + \frac{1}{|\underline{R}-\underline{r}|}\frac{1}{|\underline{R}'-\underline{r}|}\right\} \qquad (6\text{-}7)$$

$$+\; q^2 A(A-1)\int d\underline{r}\,|u(r)|^2\left[\frac{1}{R} - \frac{1}{|\underline{R}-\underline{r}|}\right]\int d\underline{r}\,|u(r)|^2\left[\frac{1}{R'} - \frac{1}{|\underline{R}'-\underline{r}|}\right]$$

Substituting in the first order potentials from (6-5), we find

$$U_{oo}(\underline{R},\underline{R}') - V_{oo}(\underline{R})V_{oo}(\underline{R}') = \frac{-1}{A}\left[V_{oo}(\underline{R}) - \frac{Aq}{R}\right]\left[V_{oo}(\underline{R}') - \frac{Aq}{R'}\right]$$

$$+\; q^2 A\int d\underline{r}\,|u(r)|^2\frac{1}{|\underline{R}-\underline{r}|}\frac{1}{|\underline{R}'-\underline{r}|} \qquad (6\text{-}8)$$

Examining the asymptotic behaviour of (6-8) by letting $R,R'\rightarrow\infty$, we find that the first order potential, $V_{oo}(\underline{R})$ vanishes exponentially. To show this, we note that by expanding the $1/|\underline{R}-\underline{r}|$ in (6-5) in terms of spherical harmonics (Messiah, 1961-2) we have

$$\frac{1}{4\pi}\int d\Omega\left[\frac{1}{R} - \frac{1}{|\underline{R}-\underline{r}|}\right] = \frac{1}{R} - \gamma_0(R,r) \qquad (6\text{-}9)$$

where $$\gamma_0(R,r) = \begin{cases} 1/R\,, & r<R \\ 1/r\,, & r>R\,. \end{cases}$$

So for a spherically symmetric u(r), (6-5) becomes,

$$V_{oo}(\underline{R}) = 4\pi\int_R^{\infty} r^2 dr\; u(r)^2\left[\frac{1}{R} - \frac{1}{r}\right]. \qquad (6\text{-}10)$$

Now u(r) is a hydrogen-like wavefunction, of exponential form, so integrating (6-10) we find that $V_{oo}(\underline{R})$ must contain terms which vanish exponentially as $R\rightarrow\infty$.

The long range behaviour of $U_{oo}(\underline{R},\underline{R}')$ must therefore arise from the remaining terms in (6-8). Thus,

$$U_{oo}(\underline{R},\underline{R}') - V_{oo}(\underline{R})V_{oo}(\underline{R}') \underset{R,R'\to\infty}{\sim} - q^2A/R^2 + q^2A\int d\underline{r}\ u(r)^2 \frac{1}{|\underline{R}-\underline{r}|}^2 \qquad (6\text{-}11)$$

From appendix 3, equation (A3-), we have immediately that

$$\int d\underline{r}\ u(r)^2 \frac{1}{|\underline{R}-\underline{r}|}^2 = \sum_{L=0}^{\infty} R^{-(2L+2)}\ \frac{4\pi}{2L+1}\int_0^{\infty} dr\,|u(r)|^2\, r^{2L+2}\ . \qquad (6\text{-}12)$$

when L=0,

$$\frac{4\pi}{R^2}\int_0^{\infty} dr\ r^2|u(r)|^2 = \frac{1}{R^2}\int d\underline{r}\,|u(r)|^2 = 1/R^2, \qquad (6\text{-}13)$$

since the u(r) is spherically symmetric. This term therefore cancels with the $1/R^2$ term in (6-11). So the dominant term is $L=1$;

$$U_{oo}(\underline{R},\underline{R}') - V_{oo}(\underline{R})V_{oo}(\underline{R}') \underset{R,R'\to\infty}{\sim} - \frac{4\pi}{3}\ q^2A\,R^{-4}\int_0^{\infty} dr\ r^4|u(r)|^2 + O(R^{-6}). \qquad (6\text{-}14)$$

Let us now look at the first Born approximation to the forward scattering amplitude for the spherically symmetric potential, $V_{oo}(\underline{R})$. From Mott and Massey (1965, ch.16);

$$f_{B1}(\Theta = 0) = -2\int_0^{\infty} R^2 dR\ V_{oo}(\underline{R}) \qquad (6\text{-}15)$$

substituting $V_{oo}(\underline{R})$ from equation (6-5), and integrating over $d\Lambda$, using equation (6-9), we find

$$f_{B1}(0) = -8\pi qA\int_0^{\infty} R^2 dR\int_0^{\infty} r^2 dr\,|u(r)|^2\left[\frac{1}{R} - \gamma_0(R,r)\right]. \qquad (6\text{-}16)$$

Reversing the order of integration;

$$= -8\pi qA\int_0^{\infty} r^2 dr\,|u(r)|^2\int_0^{r} R^2 dR\left[\frac{1}{R} - \frac{1}{r}\right]. \qquad (6\text{-}17)$$

The right hand integral = $r^2/6$. So (6-17) becomes

$$f_{B1}(0) = -\frac{4\pi}{3}\,qA\int_0^\infty dr\; r^4\,|u(r)|^2 . \tag{6-18}$$

Comparing this with (6-14), we see that $f_{B1}(0)$ is just the leading coefficient in the asymptotic expansion of the second order potential in the elastic channel.

So,for electron scattering;

$$U_{00}(\underline{R},\underline{R}') - V_{00}(\underline{R})V_{00}(\underline{R}') \underset{R,R'\to\infty}{\sim} f_{B1}(0).R^{-4} + O(R^{-6}). \tag{6-19}$$

Comparing this with equation (5-14), we see that the average energy of the atomic states above the ground state is just the ratio of the first Born amplitude and the atomic polarizability;

$$\bar{\epsilon} - \epsilon_0 = f_{B1}(\Theta=0)/\tfrac{1}{2}\alpha_1 \tag{6-20}$$

The values of these parameters are shown in table I for electron scattering from helium and hydrogen, using the polarizabilities given by Bransden (1970, ch.5).

Table I

Values of the parameters defined by equation (6-20) for hydrogen and helium targets, in atomic units.

Atom	α_1	$f_{B1}(0)$	$\bar{\epsilon} - \epsilon_0$	$\bar{\epsilon}$
H	9/2	1.00	4/9	-1/18
He	1.39	0.79	1.14	-1.76

Chapter 7

A COMPARISON WITH PREVIOUS WORK

In part II of this thesis we apply the second order potential method to the scattering of charged particles from helium atoms. Other theoretical techniques have been applied to this process. We now take a look at the more important of these, specifically to determine the differences and simularities with our method.

The Born series in an impact parameter formulation can be derived from the eigenfunction expansion introduced in chapter 2 (Bates, 1961). Putting $a_n(b,Z) = \delta_{no}$ on the right hand side of the coupled equations (2-21), we have the first Born approximation, B1;

$$\text{B1:} \qquad \frac{\partial}{\partial Z} a_n(b,Z) = \frac{1}{ik_o} V_{no}(Z) \exp\left[i(\epsilon_n - \epsilon_o) Z/k_o \right] \tag{7-1}$$

Integrating (7-1) and substituting the resulting $a_n(b,Z)$ into the right hand summation of (2-21) again, we get the second Born approximation, B2;

$$\text{B2:} \qquad \frac{\partial}{\partial Z} a_n(b,Z) = \frac{1}{ik_o} V_{no}(Z) \exp\left[i(\epsilon_n - \epsilon_o) Z/k_o \right] - \frac{1}{k_o^2} \int_{-\infty}^{Z} dZ' \sum_{j=o}^{\infty} V_{nj}(Z) V_{jo}(Z') \exp\left[i(\epsilon_n - \epsilon_j) Z/k_o - i(\epsilon_o - \epsilon_j) Z'/k_o \right] \tag{7-2}$$

Because of the inclusion of coupling to intermediate states, B2 is expected to be an improvement over B1 at lower energies (cf. chapter 1). In order to compare B2 with our method, let us integrate (7-1) for $a_o(b,Z)$;

$$a_o(b,Z) = 1 + \frac{1}{ik_o}\int_{-\infty}^{Z} dZ' \, V_{oo}(Z') . \qquad (7\text{-}3)$$

Using this in (7-2) we find B2 can be rewritten as;

B2: $$\frac{\partial}{\partial Z} a_n(b,Z) = \frac{1}{ik_o} V_{no}(Z) a_o(b,Z) \exp\left[i(\epsilon_n - \epsilon_o)Z/k_o\right] - \frac{1}{k_o^2}\int_{-\infty}^{Z} dZ' \, K_{no}(Z,Z') , \qquad (7\text{-}4)$$

where the $K_{no}(Z,Z')$ is identical with our second order potential matrix,defined in equation (4-15), and can therefore be evaluated in a closure approximation as in chapter 5. Different choices of the average energy parameter have been made; this is discussed later for scattering from a helium target.

Comparing (7-4) with our integro - differential equation (4-14), we see that the essential assumption in the second Born approximation is the replacement of $a_o(b,Z')$ by unity in the integral term. This can only be a good approximation at large impact parameters and high energies, where we expect $a_n(b,Z) \sim \delta_{no}$. Moreover, as can be seen from the coupled equations (2-21), our method is unitary (Bransden and Coleman, 1971) in that

$$\sum_{n=o}^{\infty} \left| a_n(b,Z) \right|^2 = 1 \qquad (7\text{-}5)$$

This, however, is not true for the amplitudes given by the Born approximations above.

Since the Born series assumes a weak scattering potential, it would be inconsistent to allow for the possibility of a few strongly coupled channels as in our equations (4-16,18). We shall see later that such couplings can be important in inelastic scattering; for example, in the excitation He(1'S → 2'S) by electron impact, the inclusion of the 2'S - 2'P coupling (which is of long range) significantly increases the differential cross section at small angles.

Let us now look at the method of Joachain and Mittleman (1971) who, in examining elastic electron - helium scattering, used a unitary eikonalised scattering function;

$$F_o(\underline{R}) = \exp(ik_oZ)\exp[\,i\Lambda(b,Z)\,]. \qquad (7\text{-}6)$$

Their expression for the $\Lambda(b,Z)$ is,

$$\Lambda(b,Z) = -\frac{1}{k_o}\int_{-\infty}^{Z} V_{oo}(Z')dZ' + \frac{i}{k_o^2}\int_{-\infty}^{Z} dZ'\int_{-\infty}^{Z'} dZ''K_{oo}(Z',Z''). \qquad (7\text{-}7)$$

where the $K_{oo}(Z',Z'')$ is given by (4-15). This yields on differentiation;

$$\frac{\partial}{\partial Z}\exp[\,i\Lambda(b,Z)\,] = \frac{1}{ik_o}\exp[i\Lambda(b,Z)]V_{oo}(Z)$$
$$- \frac{1}{k_o^2}\exp[i\Lambda(b,Z)]\int_{-\infty}^{Z} dZ'K_{oo}(Z,Z'). \qquad (7\text{-}8)$$

Comparing (7-8) with our single channel equation (4-19), using the identity,

$$a_o(b,Z) \doteq \exp[\,i\,\Lambda(b,Z)\,], \qquad (7\text{-}9)$$

we see that the integral term still does not explicitly depend on $a_o(b,Z')$ as in our method. In evaluating the second order potential, Joachain and Mittleman (1971) assumed a polarization potential with the simple form (cf.chapter 1);

$$V_p(\underline{R}) = -\alpha_1/(R^2 + d^2)^2 \qquad (7\text{-}10)$$

where d is a phenomenological cut - off parameter.

In the Glauber approximation (Glauber, 1959) the complete wavefunction is eikonalised;

$$\Psi(\underline{R},\underline{r}) = \exp(ik_o Z)\exp[\,i\chi(\underline{b},\underline{r})\,] \qquad (7\text{-}11)$$

where
$$\chi(\underline{b},\underline{r}) = \frac{1}{k_o}\int_{-\infty}^{\infty} V(\underline{R},\underline{r})\, dZ\,. \qquad (7\text{-}12)$$

This was applied to electron - helium scattering by Franco (1970) and in his notation the scattering amplitude is given by;

$$f_n(H) = -\frac{ik_o}{2\pi}\int d\underline{b}\, \exp(i\underline{k}_o\cdot\underline{b})\, b_n(\underline{b}) \qquad (7\text{-}13)$$

where
$$b_n(\underline{b}) = \left\langle \phi_n(\underline{r}) \middle| \exp[-i\chi(\underline{b},\underline{r})] - 1 \middle| \phi_o(\underline{r}) \right\rangle \qquad (7\text{-}14)$$

Expanding the exponential, assuming $\chi(\underline{b},\underline{r})$ is small, we have;

$$\exp[-\chi(\underline{b},\underline{r})] - 1 = -i\chi(\underline{b},\underline{r}) - \chi(\underline{b},\underline{r})^2 + i\chi(\underline{b},\underline{r})^3 + \ldots.. \qquad (7\text{-}15)$$

Substituting (7-12) into this expansion, (7-14) becomes,

$$b_n(\underline{b}) = \frac{1}{ik_o}\int_{-\infty}^{\infty} dZ\, V_{no}(Z) - \frac{1}{k_o^2}\int_{-\infty}^{\infty} dZ \int_{-\infty}^{\infty} dZ'\, U_{no}(Z,Z') + \frac{i}{k_o^3}\int_{-\infty}^{\infty} dZ \int_{-\infty}^{\infty} dZ' \int_{-\infty}^{\infty} dZ''\, W_{no}(Z,Z',Z'') + \ldots.. \qquad (7\text{-}16)$$

where

$$V_{no}(Z) = \left\langle \phi_n(\underline{r}) \middle| V(\underline{R},\underline{r}) \middle| \phi_o(\underline{r}) \right\rangle$$

$$U_{no}(Z,Z') = \left\langle \phi_n(\underline{r}) \middle| V(\underline{R},\underline{r})V(\underline{R}',\underline{r}) \middle| \phi_o(\underline{r}) \right\rangle \qquad (7\text{-}17)$$

$$W_{no}(Z,Z',Z'') = \left\langle \phi_n(\underline{r}) \middle| V(\underline{R},\underline{r})V(\underline{R}',\underline{r})V(\underline{R}'',\underline{r}) \middle| \phi_o(\underline{r}) \right\rangle \quad \text{etc.}$$

Using closure (cf.equation (4-8)) to insert a complete set of states in each term, we find;

$$U_{no}(Z,Z') = \sum_{m=o}^{\infty} V_{nm}(Z)V_{mo}(Z')$$

$$W_{no}(Z,Z',Z'') = \sum_{m=o}^{\infty} \sum_{j=o}^{\infty} V_{nm}(Z)V_{mj}(Z')V_{jo}(Z'') \qquad \text{etc.} \tag{7-18}$$

By making the identity, $b_n(\underline{b}) = a_n(b,\infty)$, equation (7-13) is similar to our equation (3-16) for the scattering amplitude. Comparing equation (7-16) with our single channel (N = 0) version of equation (4-14) for the $a_n(b,\infty)$, we see that Glauber theory takes into account all the possible sequencies of transition between the excited states, whereas our method only includes the terms $V_{no}(Z)$ and $U_{no}(Z,Z')$ from the perturbation expansion (7-18). On the other hand, the Glauber method omits the factor $\exp[i(\epsilon_o - \epsilon_n)(Z - Z')/k_o]$ which allows for the change in energy of the projectile in an intermediate state, and omits the time ordering introduced by the finite upper integration limit in our equation (4-14).

PART II

APPLICATIONS TO THE SCATTERING FROM A HELIUM TARGET

Chapter 8

THE HELIUM WAVEFUNCTIONS AND AVERAGE ENERGY

We now apply the second order potential method to the scattering of electrons from a helium target.

The helium atom possesses two electrons, and initially both are assumed to be in their ground (1s) state. In a collision with a charged particle, either or both electrons can be excited, depending on the kinetic energy of the projectile. At the energies we have in mind (50 ev. to 1000 ev. for electron scattering), the following processes are important, and much interest, both theoretical and experimental (eg.Chamberlain et al.,1970) has been shown in them;

$$\begin{aligned} e^- + \mathrm{He}(1s,1s) &\longrightarrow e^- + \mathrm{He}(1s,1s) \\ e^- + \mathrm{He}(1s,1s) &\longrightarrow e^- + \mathrm{He}(1s,2s) \qquad (8\text{-}1) \\ e^- + \mathrm{He}(1s,1s) &\longrightarrow e^- + \mathrm{He}(1s,2p). \end{aligned}$$

The third process includes scattering to each of the magnetic substates, represented by $2p_o$ and $2p_{\pm 1}$.

To be both in a 1s state, the electrons must have anti - parallel spins because of the Pauli exclusion principle (eg. Dicke and Wittke, 1960). Since, by ignoring electron exchange, there is no mechanism for changing the spin orientation, only the singlet (spins antiparallel) states of helium are available for excitation. By convention, the final helium states in the above processes (8-1) are denoted by 1'S, 2'S and 2'P respectively.

In part I of this thesis, we showed how the cross sections for each process can be calculated from the solutions of the coupled integro - differential equations (4-14). To calculate the matrix elements involved in these equations, we need the unperturbed wavefunctions of the helium atom. For the ground state, He(1'S), we use the three parameter Hartree - Fock function of Byron and Joachain (1966):

$$|1'S\rangle = \frac{N_o}{\pi} u(r_1)u(r_2)$$

where $u(r) = \exp(-ar) + c.\exp(-br)$

$$\begin{aligned} N_o &= 1.6966 \\ a &= 1.41 \\ b &= 2.61 \\ c &= 0.799 \end{aligned} \qquad (8\text{-}2)$$

It is generally recognised (eg. Mott and Massey, 1965) that the choice of wavefunction does not greatly affect the final cross sections; an indication of this is that the elastic first Born amplitude in the forward direction, $f_{B1}(\Theta = 0)$, calculated from (8-4) is 0.792 au.; the value given by Kim and Inokuti (1968), who used a 20 term Hylleraas wavefuction, is 0.791 au.

The He(2'S) wavefunction we use is the Cohen and McEachran (1967) unrestricted Hartree - Fock function, curve - fitted to the following simple analytical form (Flannery, 1970):

$$|2'S\rangle = \frac{N_1}{\pi}\left[v_0(r_1)v_1(r_2) + v_0(r_2)v_1(r_1)\right]$$

where $v_0(r) = \exp(-2r)$

$v_1(r) = \exp(-pr) - c_1 r.\exp(-qr)$ (8-3)

$N_1 = 0.70640/(1 + (0.007322)^2)^{\frac{1}{2}}$

$p = 1.1946$

$q = 0.4733$

$c_1 = 0.26832$

This particular choice of parameters rendered the 2'S function orthogonal to the ground state (8-2).

For He(2'P) we use the function of Goldberg and Clogston (1939):

$$|2'P_m\rangle = \frac{N_2}{\pi^{1/2}}\left[w_0(r_1)w_2(\underline{r}_2) + w_0(r_2)w_2(\underline{r}_1)\right]$$

where $w_0(r) = \exp(-2r)$

$w_2(\underline{r}) = r.\exp(-sr)\ Y_{1,m}(r)$ (8-4)

$N_2 = 0.37831.$

$s = 0.485$

$Y_{1,m}$ is a spherical harmonic (Messiah, 1961)

These wavefunctions are use to calclate the potential matrix elements, $V_{nm}(Z)$, defined by equation (2-8), between the 1'S, 2'S, $2'P_0$ and $2'P_{\pm1}$ channels; the results are shown in appendix 2. In appendix 3 we calculate the second order potential in the elastic channel, $U_{oo}(Z,Z')$, defined by (4-11).

The excitation energies for helium ($\epsilon_m - \epsilon_o$) also required by the coupled equations (4-14) are (from Martin, 1960),

$\epsilon_{2'S} - \epsilon_{1'S} = 0.7577$ au.

$\epsilon_{2'P} - \epsilon_{1'S} = 0.7799$ au. (8-5)

In chapter 5 we showed how the average energy ($\bar{\epsilon} - \epsilon_0$) can be chosen so that the correct long range potential is obtained in the elastic channel. Replacing all the atomic levels above the ground state by an average energy, we find from Table I, chapter 6, that for helium, $\bar{\epsilon} - \epsilon_0 = 1.14$ au. Bransden, Coleman and Sullivan (1971) showed that the total elastic cross sections for hydrogen were relatively insensitive to the choice of the average energy. In table II we find this is true also for helium; the total cross section for 500 ev. electrons is reduced by less than 3% when $\bar{\epsilon} - \epsilon_0$ is set to zero (in chapter 14 we show that the error in these numbers is about 2%).

Table II

The sensitivity of the total elastic cross section for electron - helium scattering at 500 ev. to the choice of average energy, $\bar{\epsilon}$.

$\bar{\epsilon} - \epsilon_0$ (au.)	0.0'	1.14'	1.34"	Bromberg (1969)
$Q_{el}/\pi a_0^2$	0.084	0.086	0.088	0.108

' Averaging all states above ground state

" Replacing the 2'S and 2'P states by their exact energy.

Table II also shows the cross section obtained using the exact energies for the 2'S and 2'P channels, as in equation (4-7). This gives rise to a new average energy which can be calculated from equation (5-13) for the remaining states; for a helium target this is $\bar{\epsilon} - \epsilon_0 = 1.34$; this method is used for the remainder of this thesis. The experimental cross section shown was estimated by Bromberg (1969) from his measurements of the differential cross section from 2^o to 60^o at 500 ev.

In figure 8a we show the effect of the average energy on the elastic angular distribution for 500 ev. electrons, using the single channel approximation of equation (4-16). Since the average energy belongs to the second order potential, which we know to be of long range, the greatest effect is seen at large impact parameters, and therefore at small angles. This agrees qualitatively with Joachain and Mittleman (1971) (described in chapter 7) who also found a variation of $\bar{\epsilon}$ in their imaginary potential only significantly affected elastic scattering at large impact parameters. Moreover, if $\bar{\epsilon} - \epsilon_0$ is increased, physically we would expect the effect of the second order potential to be diminished, and so reduce the scattering in the forward directions. This is also shown in figure 8a. Qualitatively this agrees with the second Born approximation (chapter 7) of Woollings and McDowell (1972), who used a larger effective energy than Holt et al. (1971a,b) and so decreased the forward scattering amplitude.

Figure Caption

Figure 8a. Effect of varying the average energy on the elastic scattering of 500 ev. electrons from helium.

Curve 0. $\bar{\epsilon} - \epsilon_o = 0.0$ au.

Curve 1. $\bar{\epsilon} - \epsilon_o = 1.14$ au.

Curve 3. $\bar{\epsilon} - \epsilon_o = 3.0$ au.

Curve E. Exact energies used for the 2'S and 2'P states, with a new average energy (see text) of $\bar{\epsilon} - \epsilon_o = 1.34$ au.

I Experimental data from Bromberg (1969).

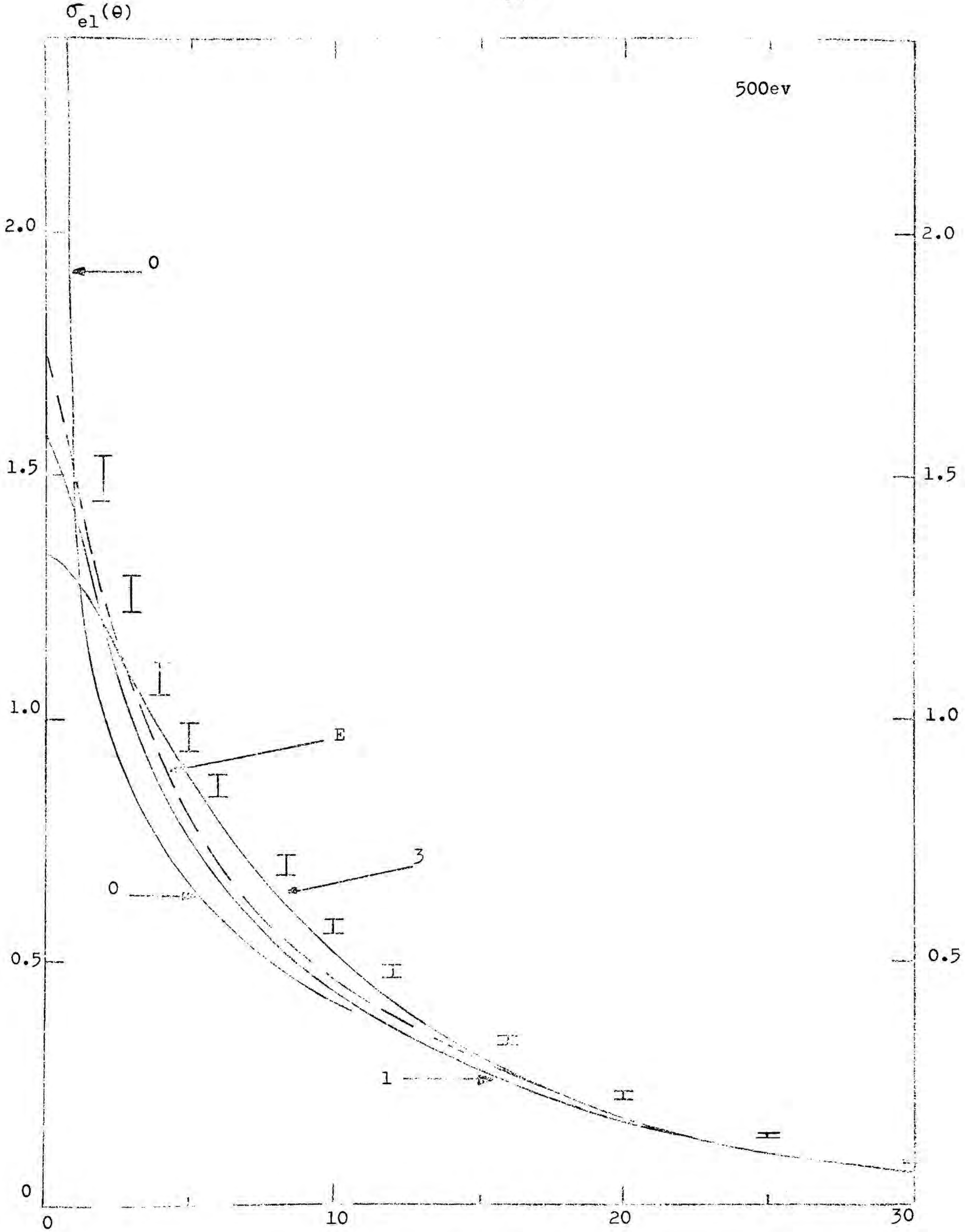
$\sigma_{el}(\theta)$
500ev
2.0
1.5
1.0
0.5
0
0
E
3
0
1
0
10
20
30
Scattering angle (degrees).

Figure 8a

Chapter 9

ELASTIC SCATTERING OF ELECTRONS

We now procede by solving the coupled equations (4-16) and (4-18); that is, with the full static coupling between the 1'S, 2'S and 2'P states and the second order term in the elastic channel. The resulting $a_n(b,Z)$ at $Z = +\infty$ are then integrated over impact parameters as in equations (3-16 to 19) to obtain the total and differential cross sections; the whole procedure being repeated for different energies.

Our total cross sections for elastic electron scattering are compared in table III with the results obtained by omitting the second order term (the four channel static approach of Flannery, 1970), the first Born results (B1) of Bell et al. (1969), the second Born results (B2) of Holt et al. (1971a), and the experimental results of Vriens et al. (1968a) and Bromberg (1969).

Table III

Total cross sections for the elastic scattering of electrons from helium (in units of πa_o^2)

Energy (ev)	B1	B2	Static	Present results	Experimental[a]
50	0.714	-	0.557	0.813	-
100	0.412	0.893	0.351	0.415	0.495
200	0.223	0.352	0.200	0.215	0.248
300	0.152	0.211	0.139	0.147	0.170
400	0.115	0.149	0.107	0.107	0.130
500	0.093	0.115	0.087	0.088	0.108[b]
1000	0.047	-	0.045	0.045	-

[a] Vriens et al. (1968a) renormalised to Chamberlain et al.(1970)

[b] Bromberg (1969)

In figure 9a we show the effect of various degrees of coupling on the elastic differential cross sections at 300 ev. Keeping the second order term in the elastic channel, we see that the inclusion of the back couplings from the 2'S and 2'P channels to the ground state, as in equation (4-16), only increases the small angle scattering, since the s-p coupling is of long range. However, the inclusion of the 2'S,2'P inter-couplings, as in equation (4-18), is seen to have no effect in elastic scattering.

Also shown in figure 9a are the results of the eikonal approximation of Joachain and Mittleman (1971), who fixed their polarization potential cut-off parameter (equation (7-10)) to give the best fit to the experimental data of Chamberlain et al.(1970) at 5^{o}, the Glauber approximation of Franco (1971) (described in chapter 7), and the second Born approximations of Holt et al. (1971a) and Woollings and McDowell (1972), who used a much larger value for the average energy.

In chapter 7 it was shown that the essential assumption in the second Born approximation is the replacement of $a_0(b,Z')$ by unity in the integral term in equation (4-19). Comparison with our results shows that this is accurate only for large impact parameters, and this accounts for the agreement of the second Born cross sections of Holt et al. (1971a) with our results at small angles, but not at large.

Figures 9b,c and d show that our differential cross sections for the elastic scattering of electrons between 100 ev. and 1000 ev. agree well with the experimental data. Less significance can be attached to our results at 50 ev. as our model is a high energy approximation and electron exchange, important at low energies, has been ignored. By 1000 ev. (see figure 9d) our results are becoming quite close to those of the first Born approximation.

Figure Captions

Figure 9a. Differential cross sections for the elastic scattering of electrons at 300 ev: comparison of models.

Curve (1). Our results with no coupling between the states, but with the second order term in the elastic channel, using equations (4-19) and (4-20).

Curve (2). Our results with the back coupling from the 2'S and 2'P channels to the ground state, and the second order term in the elastic channel, using equations (4-16)and (4-20).

Curve (3). Our results with the full static coupling between the 1'S,2'S and 2'P states and the second order term in the elastic channel, using equations (4-16)and(4-18).

Curve B1. First Born approximation.

Curve B2. Second Born approximation (Holt et al., 1971a).

Curve SB2. Second Born approximation (Woollings and McDowell,1972).

Figure Captions continued...

Curve JM.	Eikonal approximation of Joachain and Mittleman (1971).
Curve G.	Glauber approximation of Franco (1970).
Curve S.	Four channel coupling, but without the second order term.
I	Chamberlain et al. (1970).
⊙	Vriens et al. (1968a), renormalised at 5° to Chamberlain et al. (1970).

Figures 9b,c,d. Differential cross sections for the elastic scattering of electrons at (b) 50 ev and 100 ev, (c) 200 ev and 400 ev, (d) 500 ev and 1000 ev. Curves (3), B1 and B2 are as in figure 9a.

⊙	Vriens et al. (1968a), renormalised at 5° to Chamberlain et al. (1970).
▽	Opal and Beaty (1972).
X	Hughes et al. (1932).
⊗	Bransden and McDowell (1972), using dispersion relations.
I	Bromberg (1969) at 500 ev , otherwise Chamberlain et al. (1970).

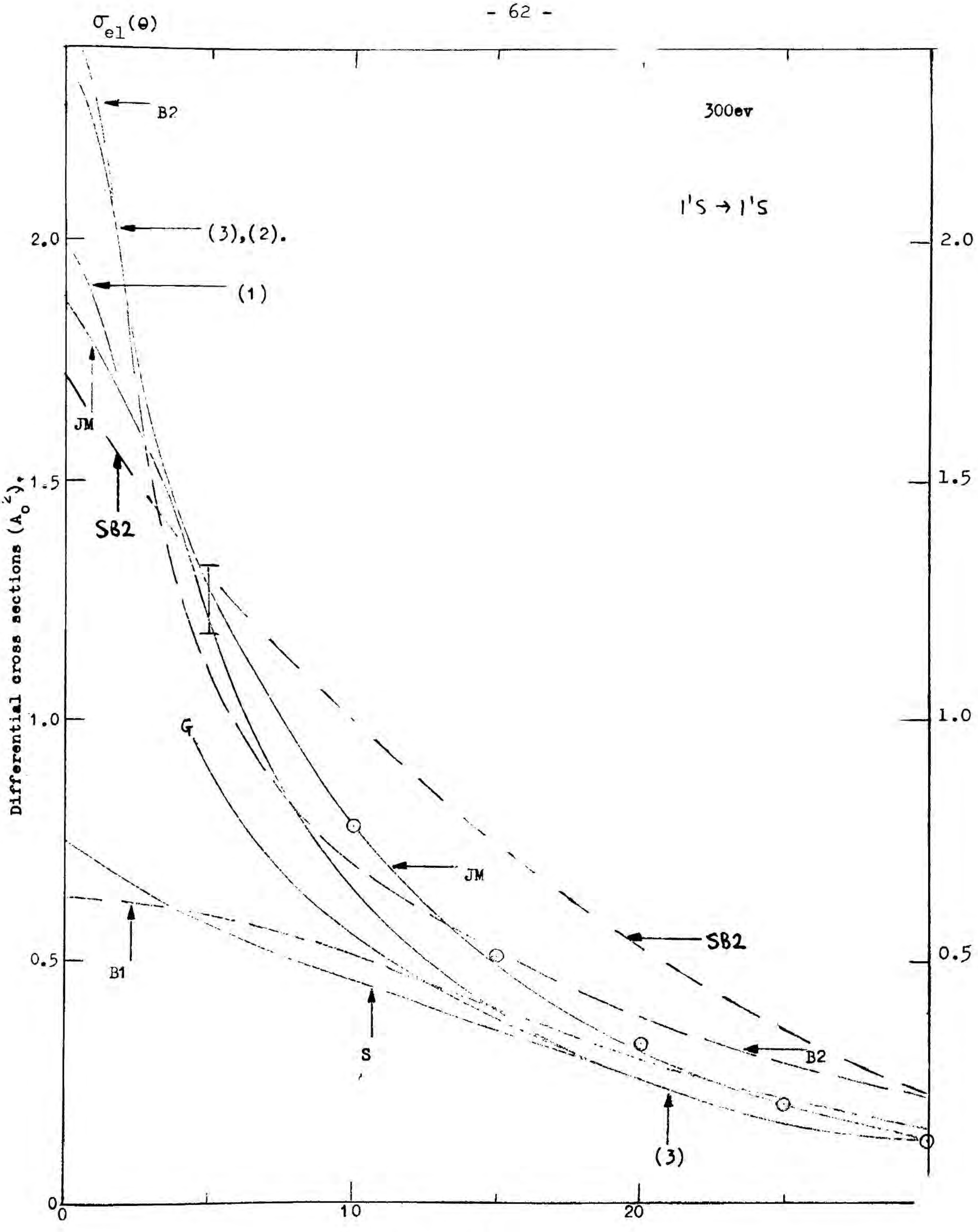
$\sigma_{el}(\theta)$
Differential cross sections (A_o^2).
300ev
1'S → 1'S
B2
(3),(2).
(1)
JM
SB2
G
JM
SB2
B2
B1
S
(3)
2.0
1.5
1.0
0.5
0
0
10
20
Scattering angle (degrees).

Figure 9a

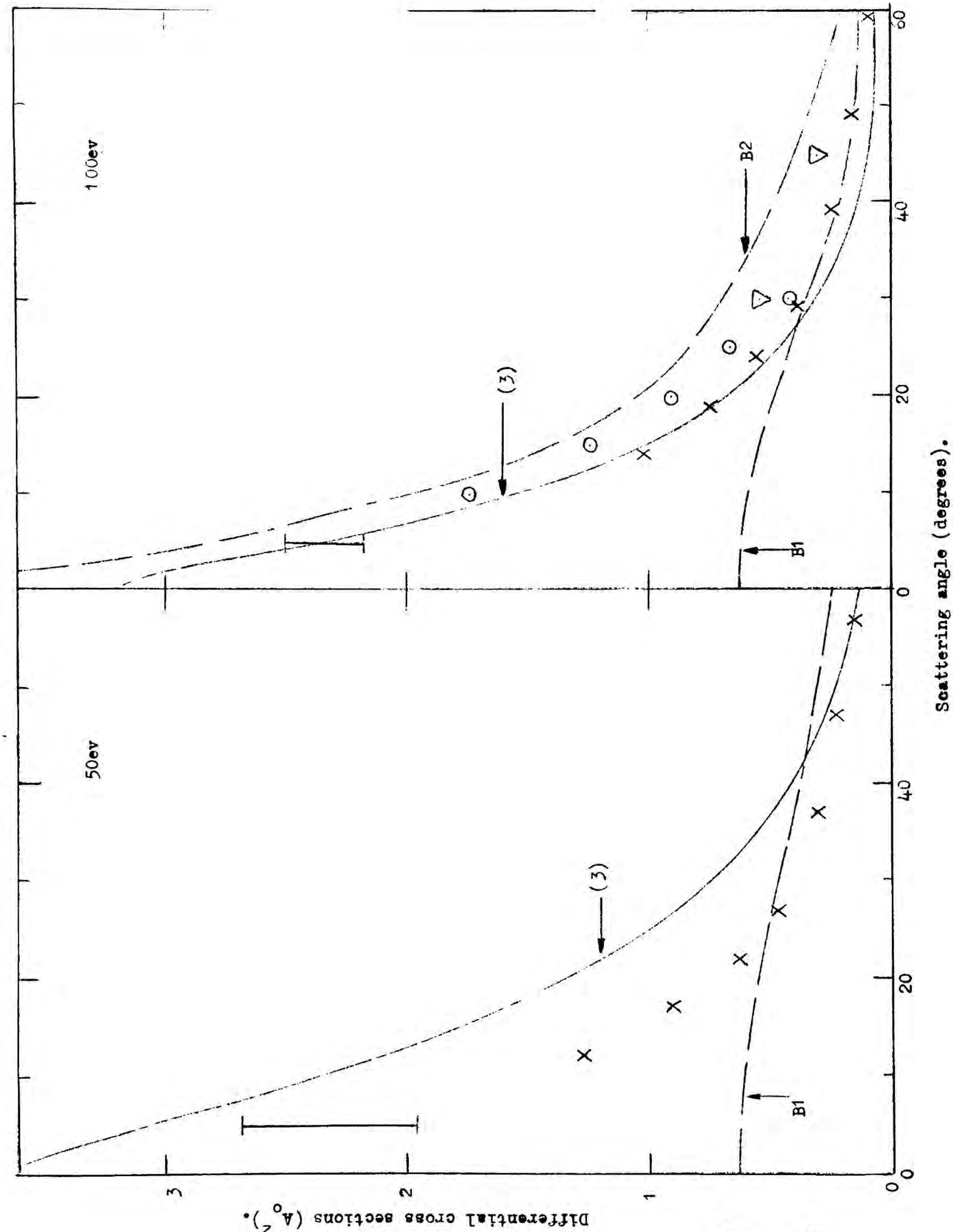
100ev
50ev
(3)
(3)
B1
B1
B2
0
20
40
60
0
20
40
0
1
2
3
Scattering angle (degrees).
Differential cross sections (A_o^2).

Figure 9b

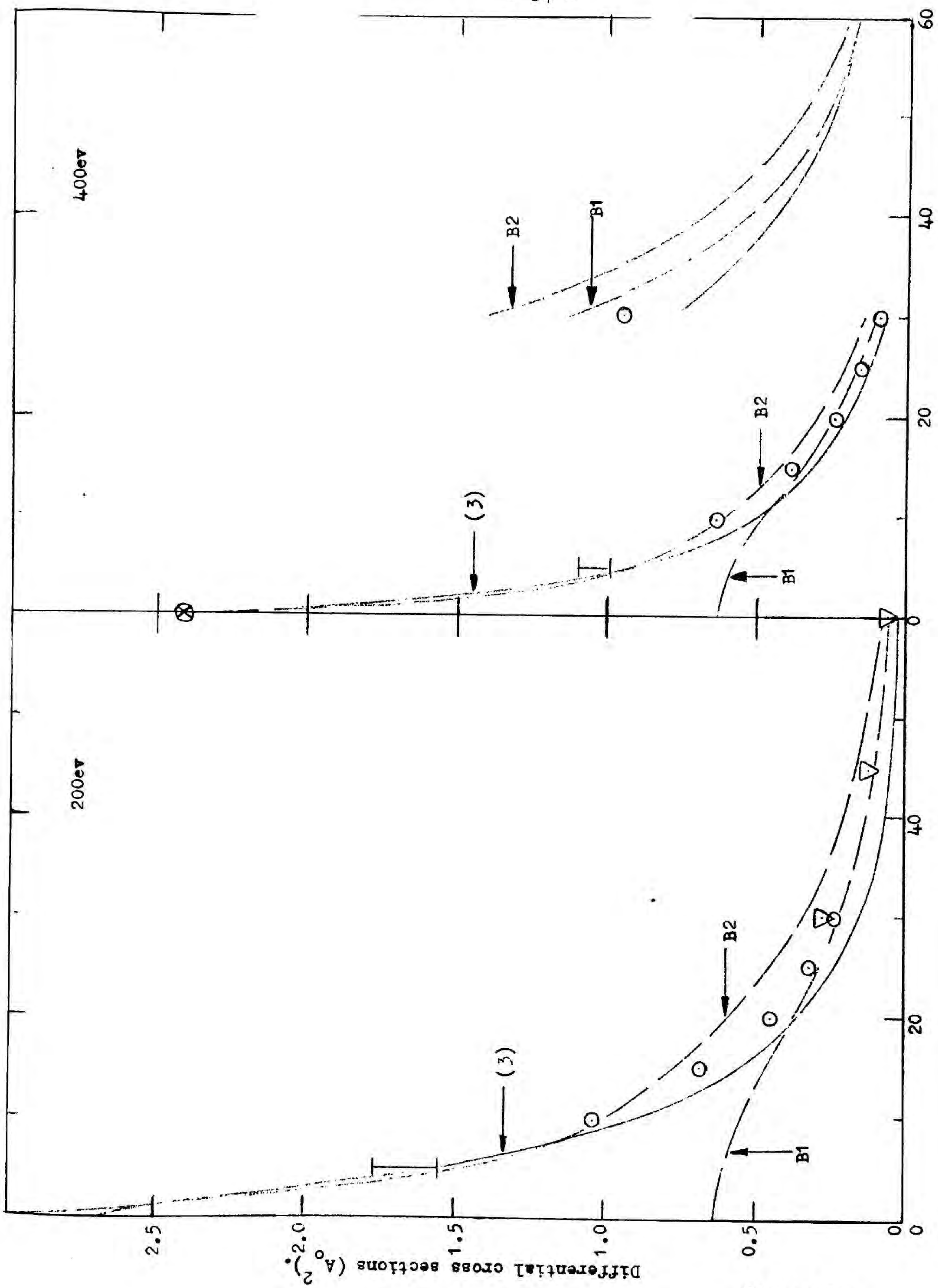
200ev
400ev
(3)
B1
B2
(3)
B1
B2
B2
B1
Differential cross sections (A$_o^2$).
Scattering angle (degrees).
0
0.5
1.0
1.5
2.0
2.5
0
20
40
0
20
40
60

Figure 9c.

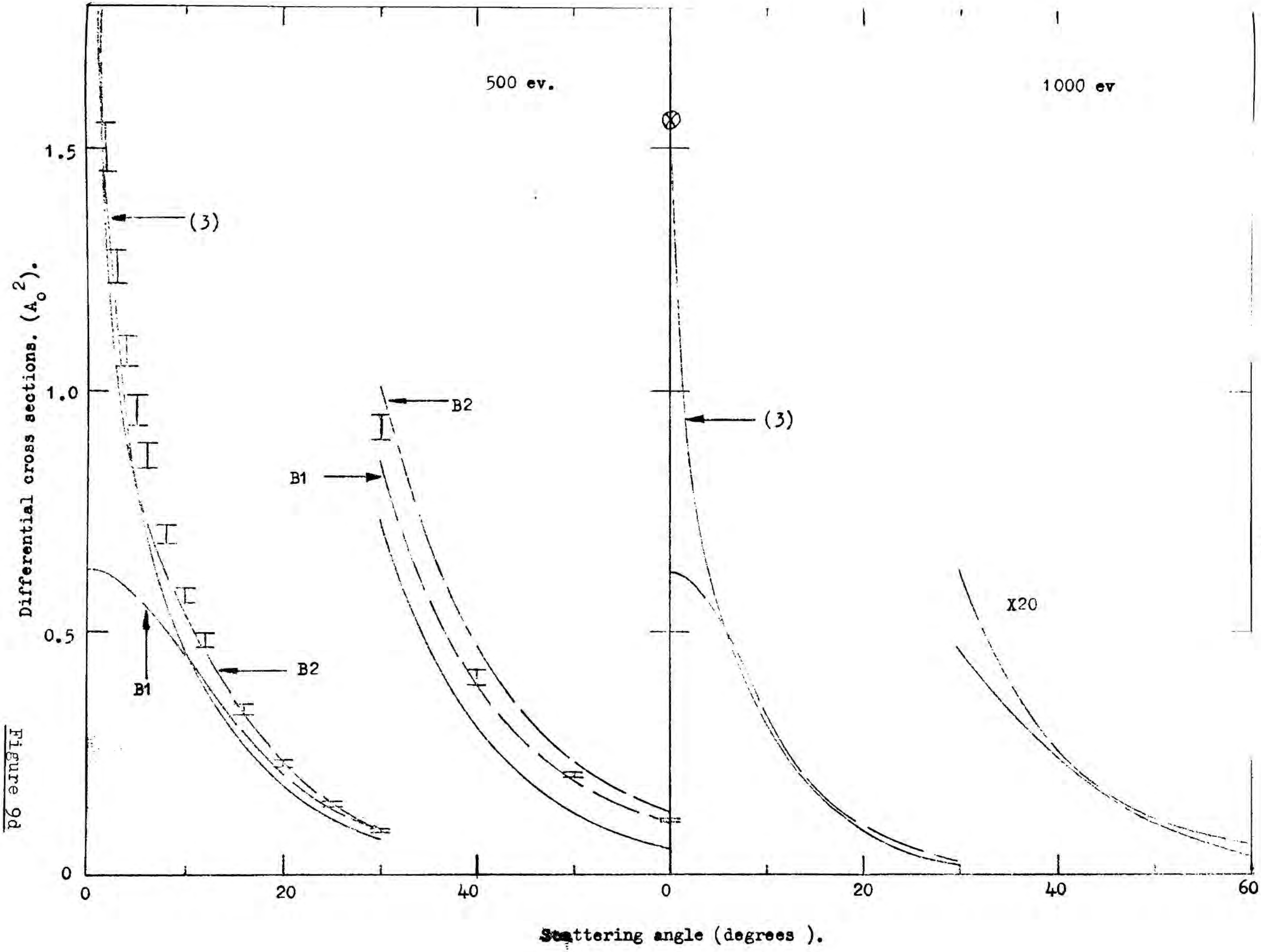
500 ev.
1000 ev
(3)
B1
B2
B1
B2
(3)
X20
1.5
1.0
0.5
0
0
20
40
0
20
40
60
Differential cross sections. (A_o^2).
Scattering angle (degrees).

Figure 9d

Chapter 10

FORWARD ELASTIC SCATTERING

As was mentioned in chapter 1, one test of our method must be in the forward directions, where the first Born approximation, by neglecting the long range polarization terms in the potential, completely underestimates elastic scattering (Mott and Massey, 1965, ch.5).

Although no experimental data exists for electron scattering at zero angles, differential cross sections have been measured down to 5° by Vriens et al. (1968a) at several energies, and to 2° at 500 ev. by Bromberg (1969). Bransden and McDowell (1970) fitted the Bromberg data to parametric forms for the elastic cross section $\sigma(\theta)$, and extrapolated this data and the data of Vriens et al. to zero angle. The forms used were

$$\sigma(\theta) = (A_1 + \theta A_2)^{-A_3} + A_4 + A_5\theta \qquad (10\text{-}1)$$

$$\sigma(\theta) = A_1 \exp\left[-(A_2\theta + A_3\theta^2)\right] + A_4 + A_5\theta . \qquad (10\text{-}2)$$

The first form would be accurate if short - range forces dominated the scattering cross section at small angles, the second form if long - range inverse power law potentials dominated. (10-1) gives us the lower, and (10-2) the upper, bound on the extrapolated forward elastic cross sections, as shown on figure 10a. The crosses on this graph represent Bromberg's procedure of a linear extrapolation of $\log(\sigma(\theta))$ to $\theta = 0$; this is not based on any particular model. Our cross sections are consistent with these extrapolations above 200 ev. The second Born results of Holt et al. (1971b) are in better agreement with the data, though this may be due to the choice of the effective energy. Holt et al. used the energy of the 3'S state, giving $\bar{\epsilon} - \epsilon_0 = 0.84$ au., compared with our 1.34 (chapter 8), and as in figure 8a the main effect of this is to slightly increase the forward scattering. Notice that the eikonal approximation of Joachain and Mittleman (1971) under - estimates the scattering in the forward direction.

Bransden and McDowell (1969) show that, since no bound states of the electron - helium system exists, the real part of the forward elastic amplitude, $\mathrm{Re}(f(0,k^2))$, satisfies the dispersion relation;

$$\mathrm{Re}\, f(0,k^2) = f^D_{B1}(0,k^2) - f^E_{B1}(0,k^2) + \frac{1}{4\pi} P \int_0^\infty dk'^2 \, \frac{k' Q_{TOT}(k'^2)}{(k'^2 - k^2)} \qquad (10\text{-}3)$$

together with the optical theorem;

$$\mathrm{Im}\, f(0,k^2) = \frac{k}{4} Q_{TOT}(k^2) \qquad (10\text{-}4)$$

where f^D_{B1} and f^E_{B1} are the direct and exchange amplitudes calculated in the first Born approximation. Woollings(1972) has recently shown that similar equations exist for the second Born amplitude, but no applications have so far been reported.

The total cross section, Q_{TOT}, for electron - helium scattering was deduced from the experimental data of Normand (1930) below 100 ev., and above 300 ev. from that given by the first Born approximation; the intermediate region being represented by an empirical formula. In this way Bransden and McDowell (1970) used (10-3) and (10-4) to evaluate the forward elastic cross sections. These are shown in the energy range of figure 10a to lie well above our present results for forward scattering, though at 1000 ev., (see figure 9d) we only differ by about 7%.

Our values for the real part of the forward elastic scattering amplitude, Re(f(0)), are displayed in table IV (overleaf). These are shown to be from 30% to 10% smaller than the dispersion relation (DR) results of Bransden and McDowell (1970), but are in better agreement with the DR results than either the lower values given by the eikonal approximation of Joachain and Mittleman (1971) and the Pade approximation of Garibotti and Massaro (1971), or the very high values given by the second Born approximation of Holt et al. (1971b).

Using the optical theorem (10-4) we can calculate the total cross section, Q_{TOT}, from the imaginary part of the forward scattering amplitude. Our results are compared in Table V with the experimental/theoretical results quoted by Bransden and McDowell (1970) (BM). The agreement, however, is not good at low energies.

Table IV

The real part of the forward elastic amplitude for electron - helium scattering (in units of a_0).

Energy (ev)	B2	DR	Pade	JM	Present results
50	-	-	-	-	1.48
100	2.93	1.91	-	1.01	1.39
200	2.25	1.71	-	1.00	2.28
300	1.96	1.48	1.31	1.00	1.22
400	1.79	1.36	0.99	0.97	1.15
500	1.68	1.29	0.95	0.99	1.13
1000	-	1.12	-	-	1.02

Table V

The total cross section, Q_{TOT}, for electrons incident on helium (in units of πa_0^2).

Energy (ev)	BM	Present results
50	1.59	2.52
100	1.13	1.69
200	0.86	1.07
300	0.70	0.80
400	0.55	0.62
500	0.46	0.53
1000	0.26	0.30

Figure Caption

Figure 10a. Elastic differential cross sections in the forward direction.

Curve (3).	Present results.
Curve B2.	Second Born approximation (Holt et al., 1971a).
Curve JM.	Eikonal approximation of Joachain and Mittleman (1971).
Curve DR.	Dispersion relation results of Bransden and McDowell (1970).
$\overset{\circ}{\underset{\circ}{\times}}$	Extrapolations of the data to zero angle by Bransden and McDowell (1970).

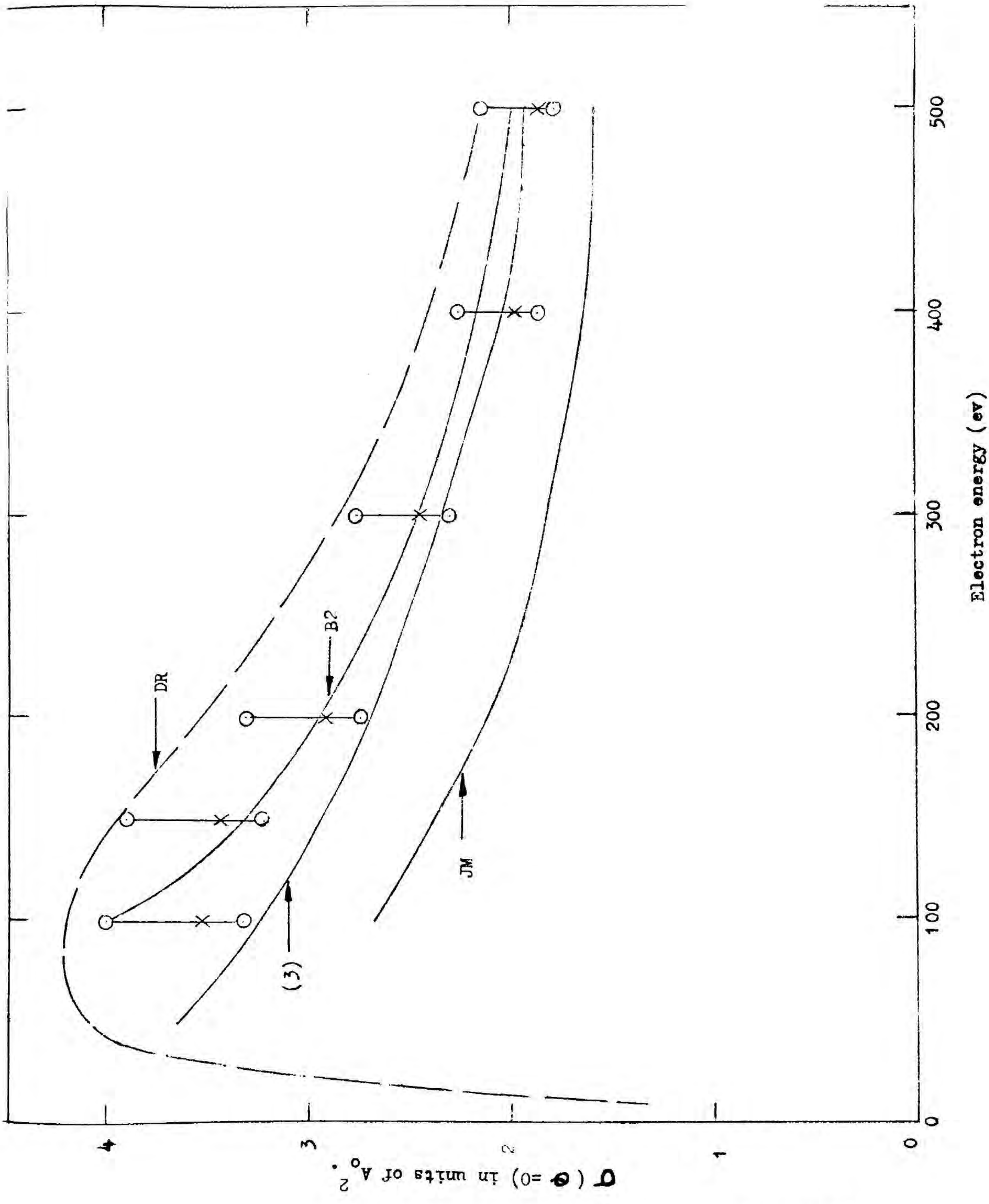
DR
B2
(3)
JM
0
100
200
300
400
500
Electron energy (ev)
0
1
2
3
4
σ (Θ=0) in units of A_o^2.

Figure 10a

Chapter 11

THE 2'S EXCITATION OF HELIUM BY ELECTRONS

Our total cross sections, evaluated with the full static coupling between the 1'S, 2'S and 2'P states and the second order term in the elastic channel, are shown in table VI for the 2'S excitation. These are compared with the first Born cross sections (B1) of Bell et al. (1969), the second Born results (SB2) of Woollings and McDowell (1972), and the results using the four channel static approach of Flannery (1970), that is, without the second order term. Our results are in good agreement with the experimental data shown in table VI, particularly with that of Vriens et al. (1968b). Notice that at all energies our total cross sections are lowered by the inclusion of the second order term.

Figure 11a shows the effects of various approximations on the differential cross sections for the 2'S excitation by 300 ev electrons. The inclusion of the second order term has little effect on the static approximation, though there is a marked discrepancy when the inter-coupling between the 2'S and 2'P states is omitted. This shows the importance of the 2'S-2'P coupling in the 2'S excitation angular distributions, and by ignoring this coupling the Born results are too low in the forward direction.

Figures 11b, c and d show the 2'S excitation differential cross sections for a range of energies, significant improvement being made over the Born results. In figure 11c we show the simplified second Born results of Woollings and McDowell (1972). Although we saw in figure 9b that their elastic differential cross sections were too large, they improved upon the 2'S and 2'P excitation results of Holt et al., who found nearly the same angular distribution as that calculated from the first Born approximation.

In all our graphs the first Born differential cross sections for the 2'S and 2'P excitations were deduced from the generalised oscillator strengths calculated by Kim and Inokuti (1968).

Table VI

Total cross sections in units of $10^{-3}\pi a_o^2$ for the 2'S excitation of helium by electrons

Energy (ev)	B1	SB2	Static	Present results	Experimental	
50	38.1	-	31.0	22.5	(18±9)[c]	-
100	22.5	-	18.2	15.4	-	21.0[b]
200	11.8	10.4	10.2	9.26	6.7[a]	11.2
300	7.97	7.28	7.07	6.64	5.3	7.6
400	6.03	5.64	5.43	5.20	4.7	5.7
500	4.85	4.57	4.40	4.24	-	-
1000	2.45	-	2.27	2.23	-	-

[a] Vriens et al. (1968b) renormalised to Chamberlain et al. (1970)
[b] Lassettre (1965). [c] Rice et al. (1972) at 55.5 ev.

Figure Captions

Figure 11a. Differential cross sections for the 2'S excitation of helium by 300 ev electrons. Comparison of models.

Curve (1).	Our results with no coupling between the states, but with the second order term in the elastic channel, using equations (4-19) and (4-20).
Curve (2).	Our results with the back coupling from the 2'S and 2'P channels to the ground state, and the second order term in the elastic channel, using equations (4-16) and (4-20).
Curve (3).	Our results with the full static coupling between the 1'S, 2'S and 2'P states and the second order term in the elastic channel, using equations (4-16) and (4-18).
Curve S.	Four channel coupling, but without the second order term.
Curve B1.	First Born approximation.
Curve B2.	Second Born approximation (Holt et al., 1971a).
I	Chamberlain et al. (1970).
O	Vriens et al. (1968 b), renormalised at 5° to Chamberlain et al. (1970).

Figure Captions continued...

Figures 11b,c,d. Differential cross sections for the 2'S excitation of helium by electrons at (b) 50 ev and 100 ev, (c) 200 ev and 400 ev, (d) 500 ev and 1000 ev. Curves (3), S, and B1 are as in figure 11a.

Curve SB2.	Second Born approximation (Woollings and McDowell, 1972).
⊙	Vriens et al. (1968b), renormalised at 5° to Chamberlain et al. (1970).
△	Lassettre et al. (1964) at 417 ev and 511 ev.
I	Chamberlain et al.(1970).
X	Rice et al. (1972) at 55.5 ev.

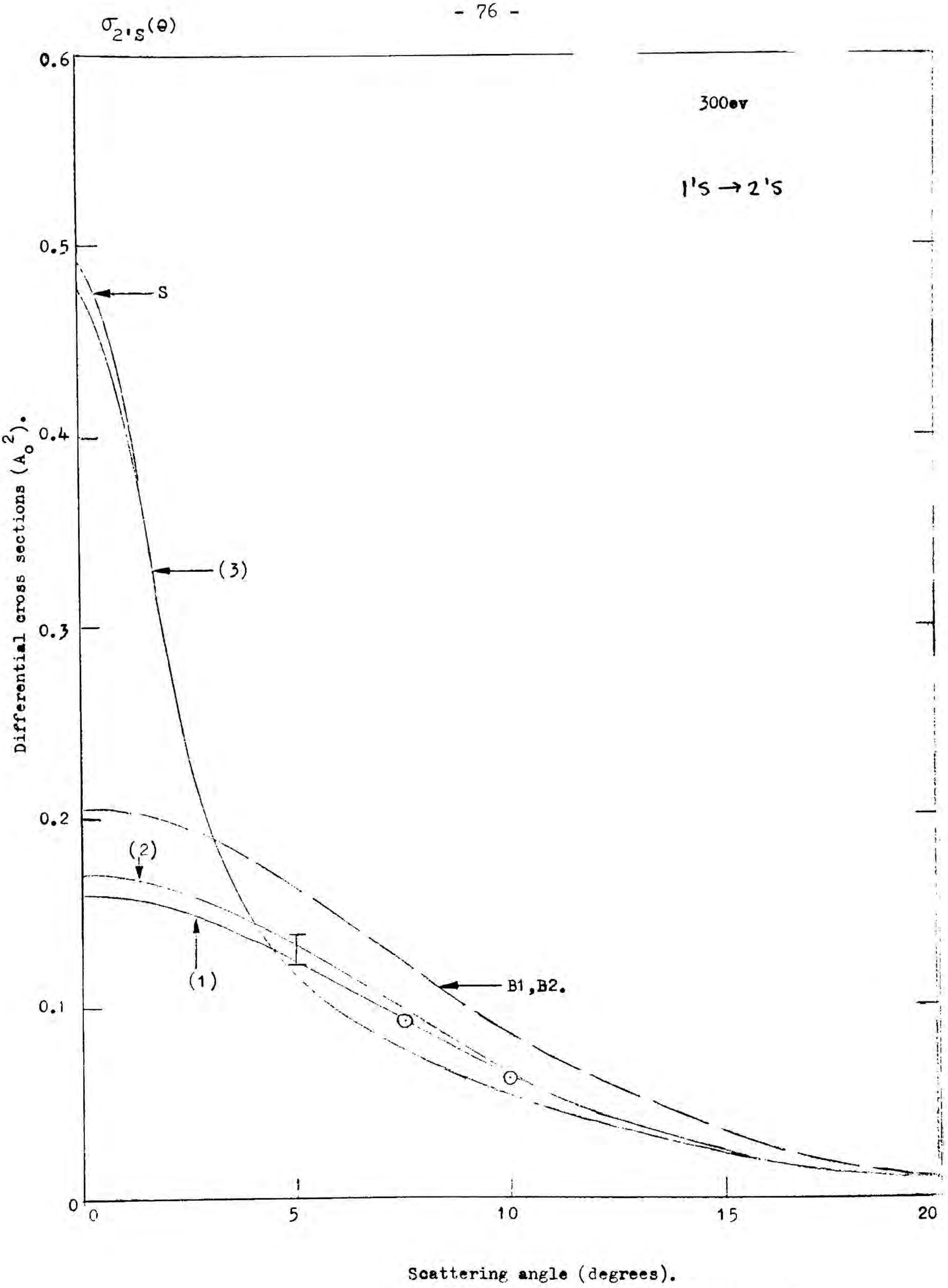
$\sigma_{2'S}(\theta)$
0.6
0.5
0.4
0.3
0.2
0.1
0
300ev
1'S → 2'S
S
(3)
(2)
(1)
B1,B2.
0
5
10
15
20
Differential cross sections (A_0^2).
Scattering angle (degrees).

Figure 11a

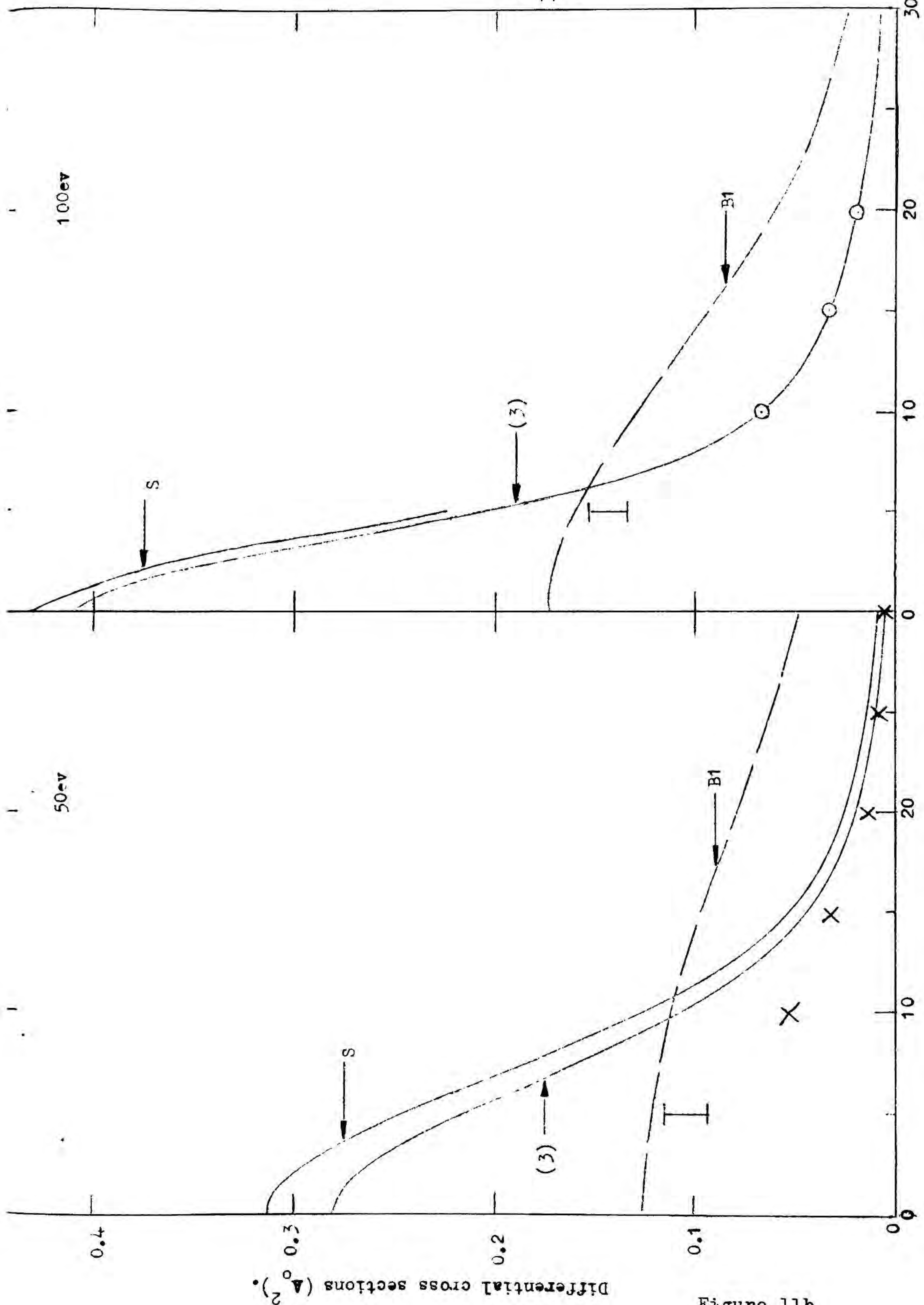
50ev
100ev
S
(3)
B1
S
(3)
B1
0
10
20
0
10
20
30
0
0.1
0.2
0.3
0.4
Scattering angle (degrees).
Differential cross sections (A$_o$^{2}).

Figure 11b

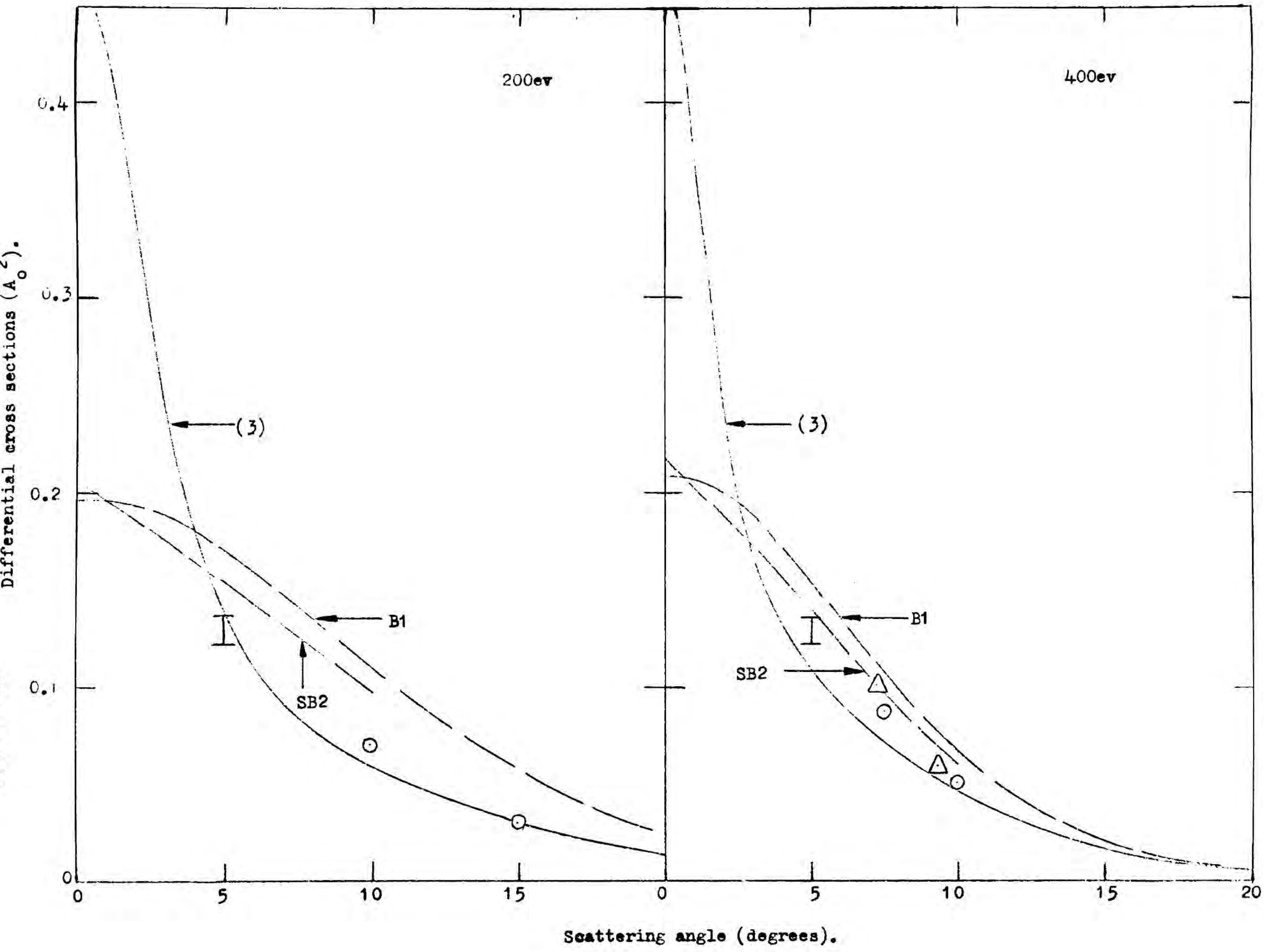
200ev
400ev
Differential cross sections (A_o^2).
Scattering angle (degrees).
0.4
0.3
0.2
0.1
0
0
5
10
15
0
5
10
15
20
(3)
B1
SB2
(3)
B1
SB2

Figure 11c.

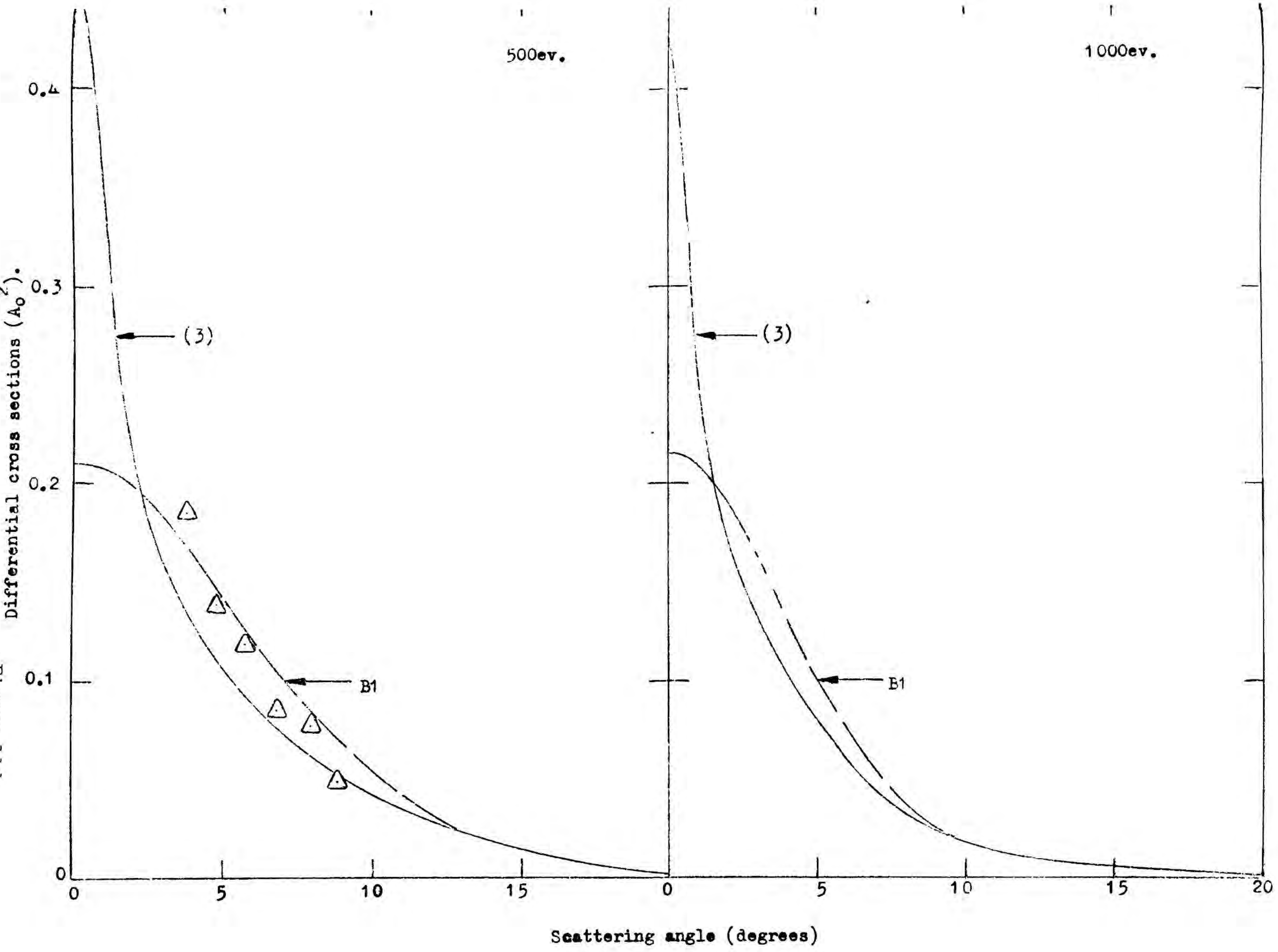
500ev.
1000ev.
(3)
(3)
B1
B1
Differential cross sections (A_o^2).
0.4
0.3
0.2
0.1
0
0
5
10
15
0
5
10
15
20
Scattering angle (degrees)

Figure 11d

Chapter 12

THE 2'P EXCITATION OF HELIUM BY ELECTRONS

Table VII shows the results with the full static coupling between the 1'S, 2'S and 2'P states, and the second order term in the elastic channel. This is compared with the results using the four channel static approach of Flannery (1970) and the first Born results of Bell et al. (1969). Only below 100ev does the effect of the second order term become noticeable.

Table VII

Total cross sections in units of πa_0^2 for the 2'P excitation of helium by electrons.

Energy (ev)	Born	Static	Present Results
50	0.169	0.232	0.215
100	0.148	0.161	0.155
200	0.107	0.107	0.105
300	0.0841	0.0830	0.0822
400	0.0699	0.0685	0.0681
500	0.0602	0.0584	0.0581
1000	0.0367	0.0362	0.0362

A large amount of reliable data has recently become available on the total excitation cross sections for the 2'P state (see Donaldson et al.,1972). This is displayed in figure 12a together with our total cross sections. Although there appears to be a maximum in the experimental data between 60ev (Moustafa Moussa et al., 1969) and 85 ev (Donaldson et al.,1972), our results show a steep rise below 100 ev and further investigation is required in this energy region.

Figure 12b shows the effect of various approximations on the differential cross sections for the 2'P excitation by 300 ev electrons, where it is shown that the inclusion of back-coupling to the ground state as in equation (4-16) has a small effect on the angular distribution. The strong 1'S-2'P coupling completely swamps any effect similar to that observed in the 2'S excitation, where omission of the 2'S-2'P coupling altered the results considerably.

Figures 12c, 12d and 12e show the 2'P excitation differential cross sections for a range of energies. Again significant improvement is made over the Born results.

Flannery (1970) noticed that the effect of the four-channel couplings is to reduce the percentage polarization of emitted radiation, Pe, as compared to the first Born approximation. Using the equation derived by Percival and Seaton (1958), we calculate Pe with our results shown in table VIII, and find that The addition of the second order term causes a slight increase over the results using the static approach of Flannery (1970).

Table VIII

Percentage polarization, Pe, of radiation following excitation of He (2'P) by electrons.

Energy (ev)	Static	Present Results
50	3.14	3.59
100	-0.15	-0.03
200	-3.10	-3.01
300	-4.31	-4.24
400	-5.80	-5.35
500	-6.51	-6.45
1000	-7.63	-7.63

Figure Captions

Figure 12a. Total cross sections for the 1'S 2'P excitation of helium by electron impact.

Curve (3).	Our results with full static coupling between the 1'S, 2'S and 2'P states and the second order term in the elastic channel, using equations (4-16) and (4-18).
Curve S.	Four channel coupling, but without the second order term.
Curve B1.	First Born approximation.
Curve B2.	Second Born approximation (Holt et al.,1971a).
Curve SB2.	Second Born approximation (Woollings and McDowell, 1972).
⊙	Van Eck and de Jongh (1970).
X	Moustaffa Moussa et al. (1969).
|	Donaldson et al. (1972).

Figure 12b. Differential cross section for the 2'P excitation of helium by 300 ev electrons: comparison of models.

Curves S, B1 and B2 are as in figure 12a.

Curve (1).	Our results with no coupling between the states, but with the second order term in the elastic channel, using equations (4-19) and (4-20).

Figure Captions continued...

Curve (2).	Our results with the back coupling from the 2'S and 2'P channels to the ground state, and the second order term in the elastic channel, using equations (4-16) and (4-20).
Curve (3).	Our results with the full static coupling between the 1'S,2'S and 2'P states and the second order term in the elastic channel, using equations (4-16) and (4-18).
I	Chamberlain et al.(1970).
Θ	Vriens et al. (1968b), renormalised at 5° to Chamberlain et al. (1970).

Figures 12c,d,e. Differential cross sections for the 2'P excitation of helium by electrons at (c) 50 ev and 100 ev, (d) 200 ev and 400 ev, (e) 500 ev and 1000 ev. Curves (3), B1 and SB2 are as in figure 12a.

⊙	Vriens et al. (1968b), renormalised at 5° to Chamberlain et al. (1970).
△	Lassettre et al. (1964) at 511 ev.
I	Chamberlain et al. (1970).
X	Truhlar et al. (1970) at 55.5 ev, as renormalised by Rice et al. (1972).

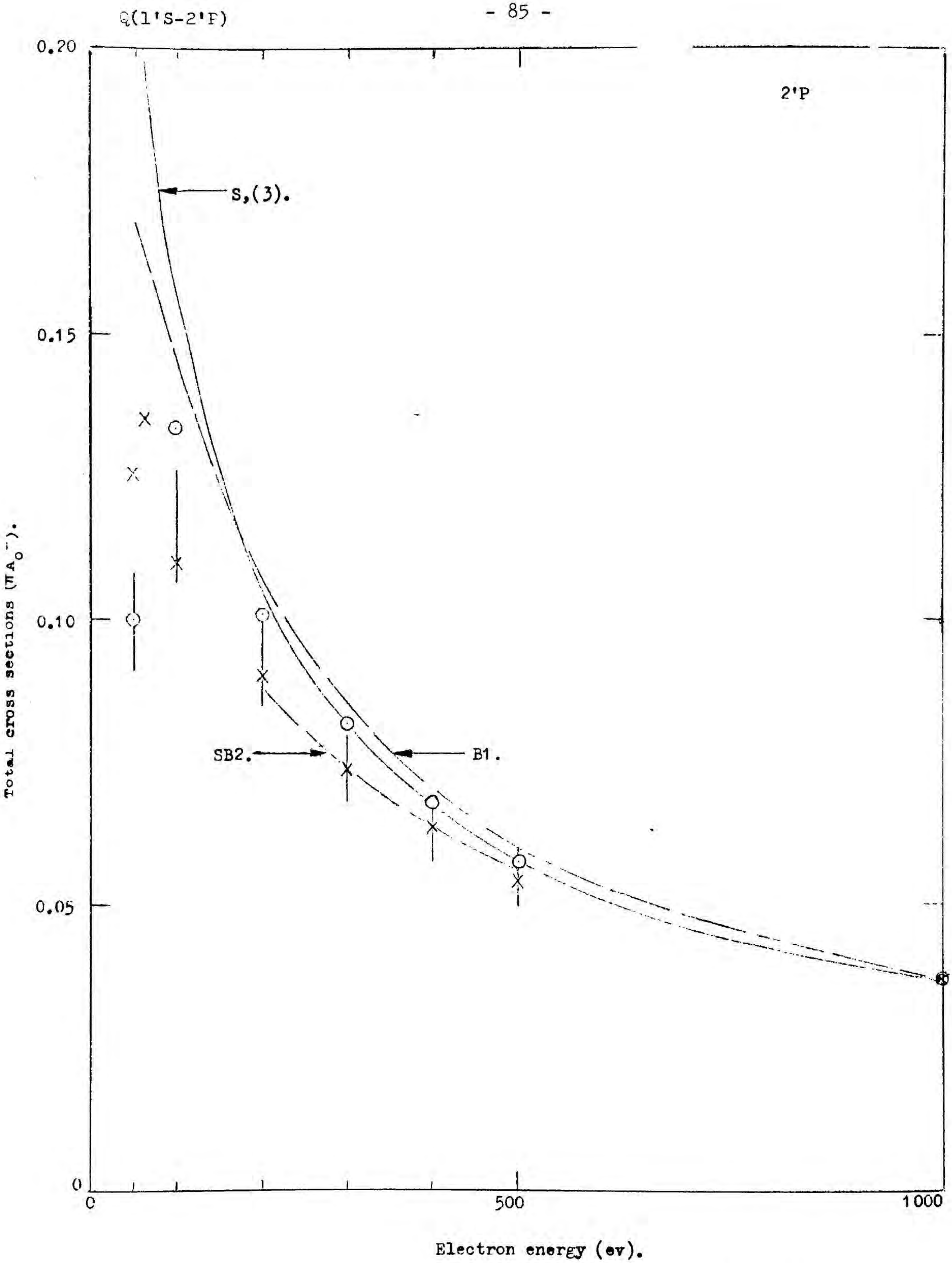
Q(1'S-2'P)
2'P
S,(3).
SB2.
B1.
0.20
0.15
0.10
0.05
0
0
500
1000
Total cross sections (πa_0^2).
Electron energy (ev).

Figure 12a

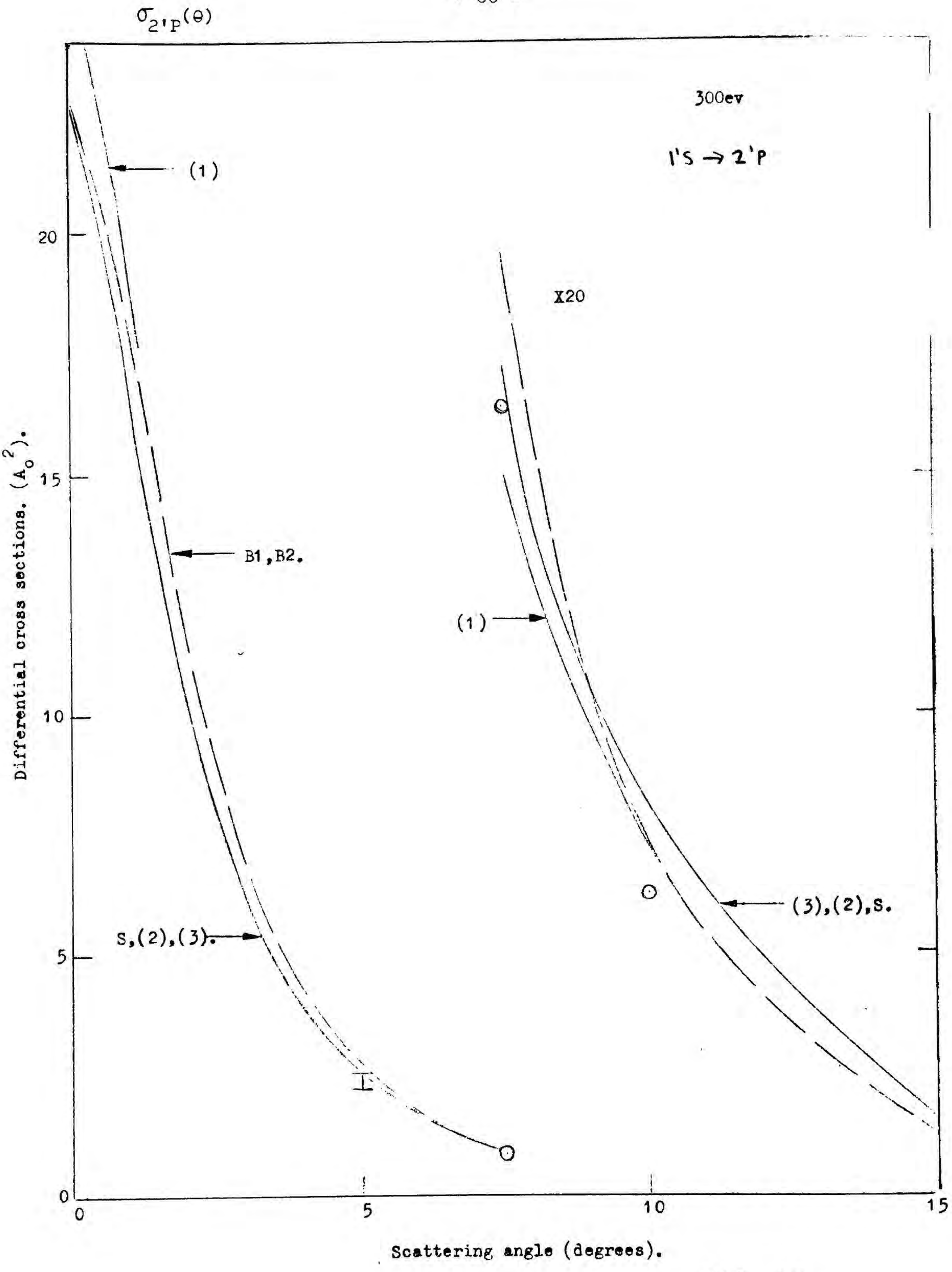
σ2'P(θ)
300ev
1'S → 2'P
(1)
20
X20
15
B1,B2.
(1)
10
(3),(2),S.
S,(2),(3).
5
0
0
5
10
15
Differential cross sections. (Ao2).
Scattering angle (degrees).

Figure 12b

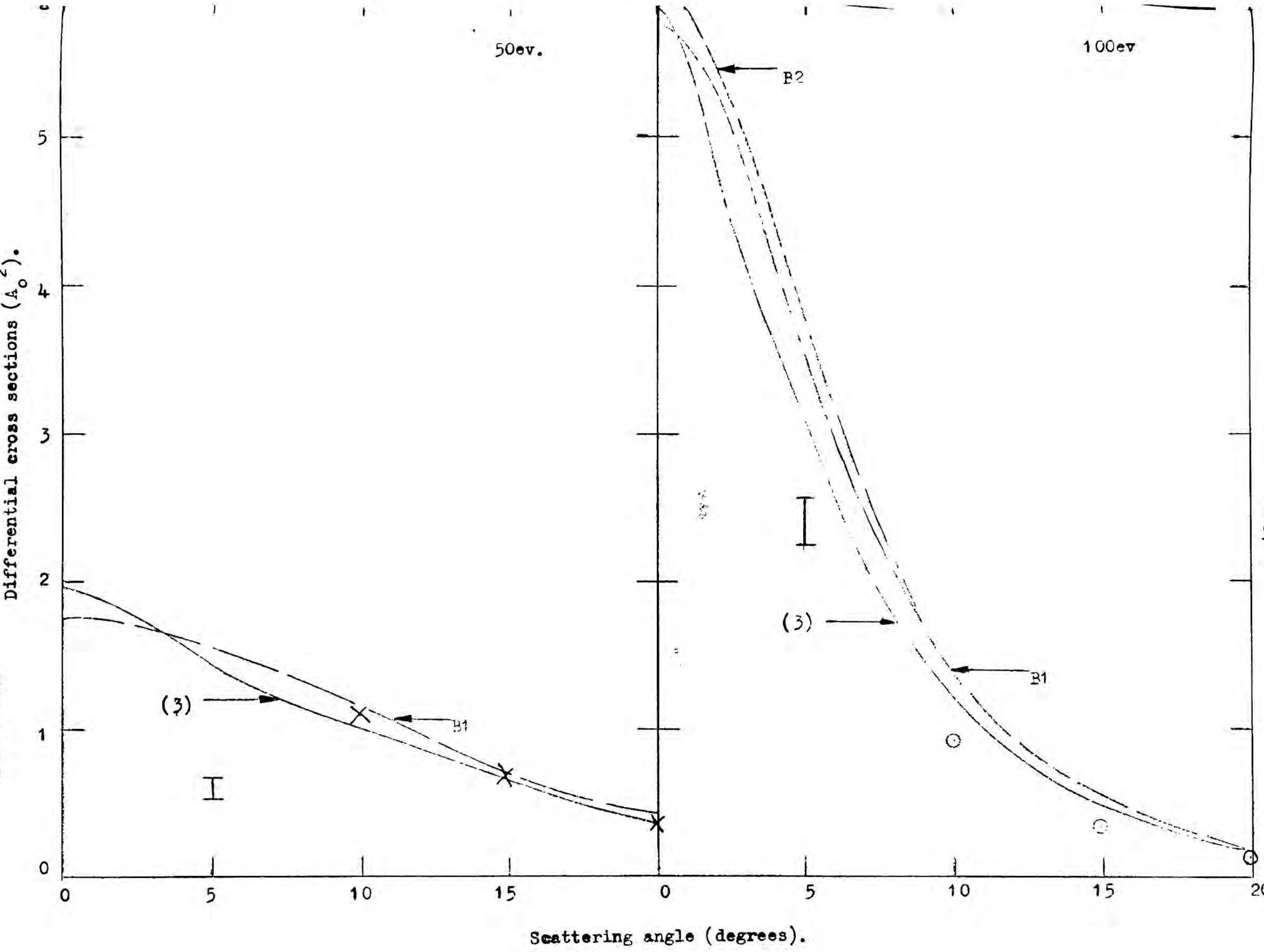
Differential cross sections (A_o^2).
50ev.
100ev
B2
B1
(3)
(3)
B1
0
1
2
3
4
5
0
5
10
15
0
5
10
15
20
Scattering angle (degrees).

Figure 12c

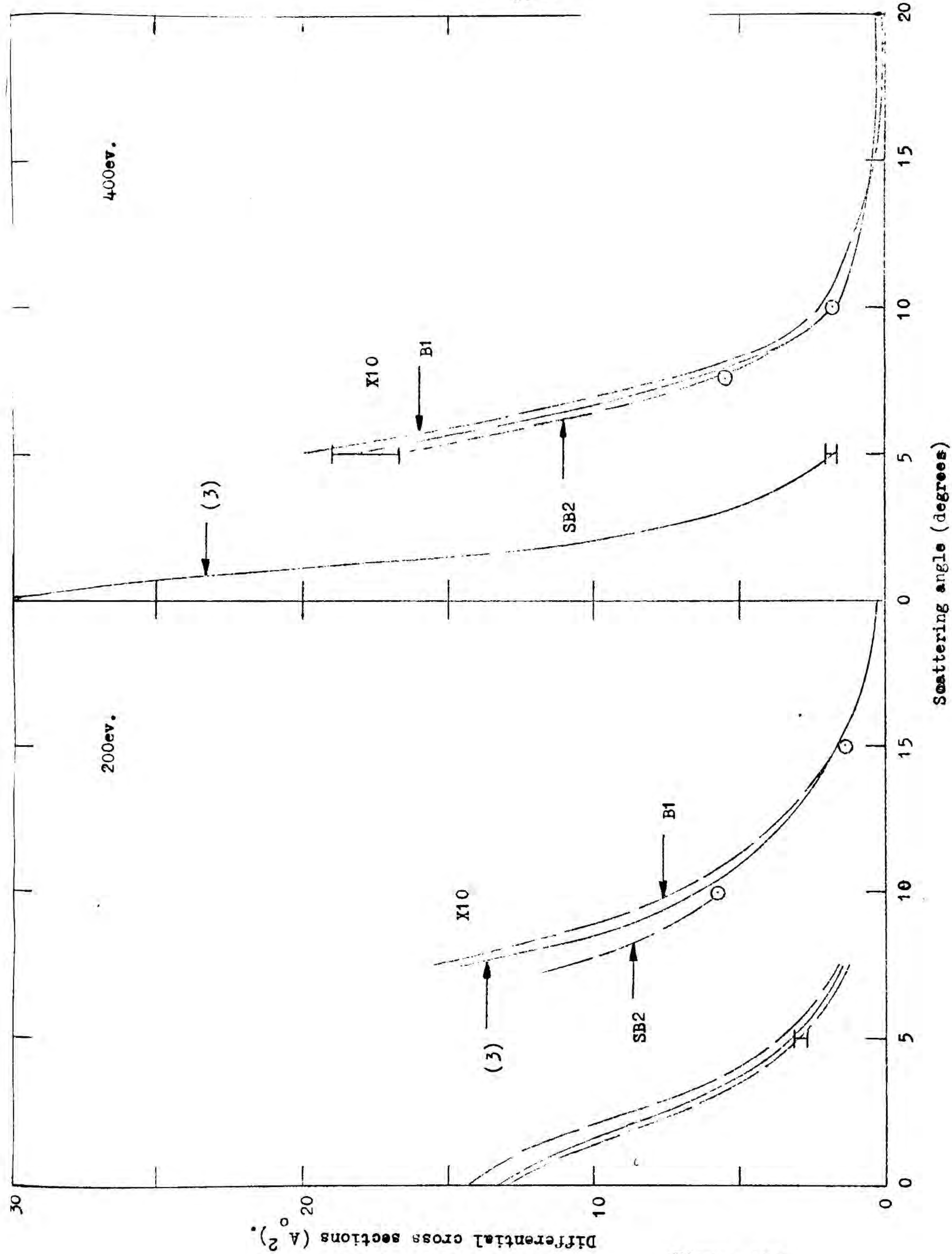
400ev.
200ev.
X10
X10
B1
B1
SB2
SB2
(3)
(3)
0
5
10
15
20
0
5
10
15
Scattering angle (degrees)
0
10
20
30
Differential cross sections ($\overset{o}{A}{}^2$).

Figure 12d

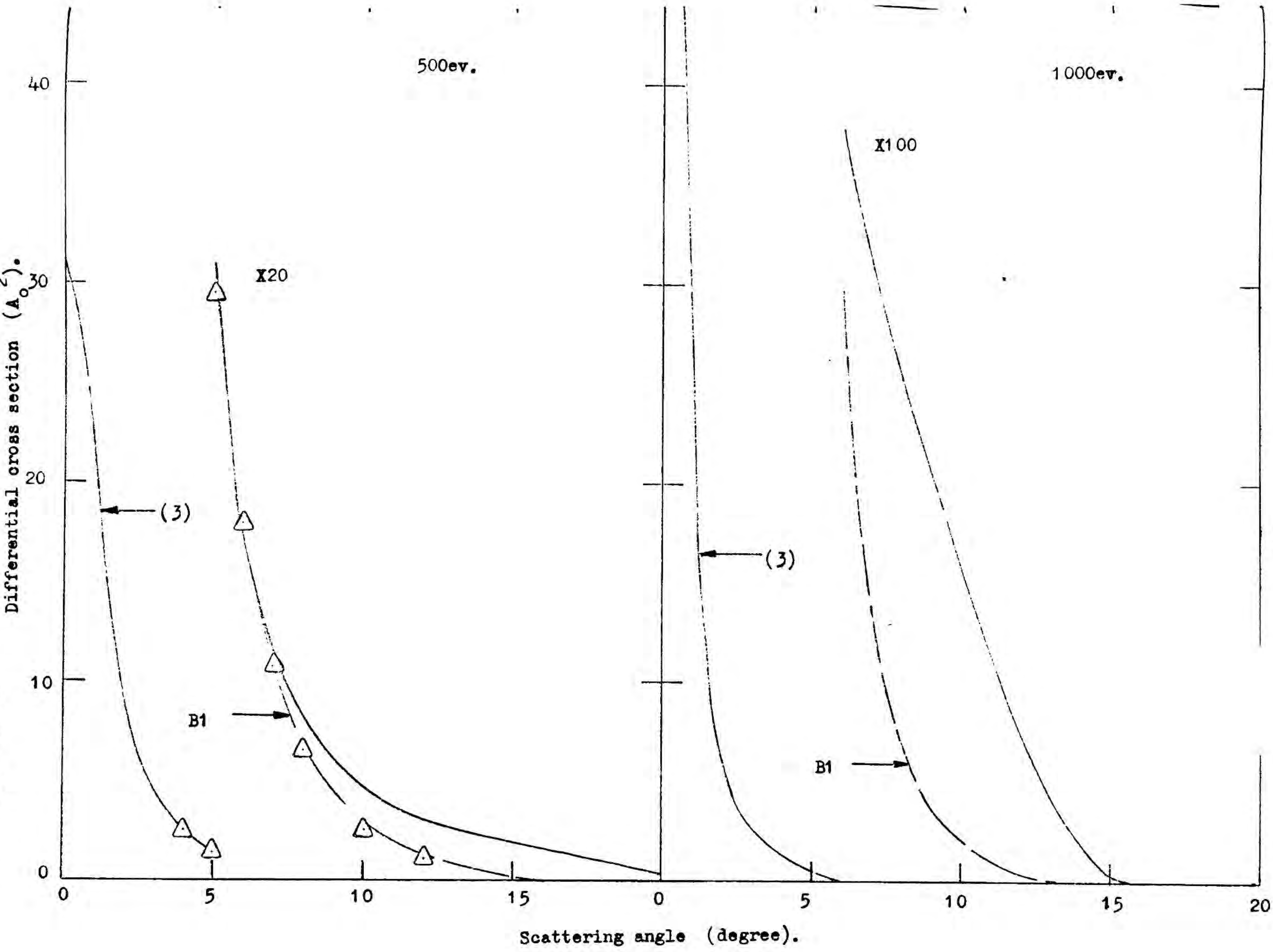
500ev.
1000ev.
X20
X100
(3)
(3)
B1
B1
Differential cross section (A_o^2).
Scattering angle (degree).
0
10
20
30
40
0
5
10
15
0
5
10
15
20

Figure 12e

Chapter 13

THE SCATTERING OF POSITRONS FROM HELIUM

By reversing the sign of the potential we can compare the scattering of electrons with that of positrons in the same approximation. At a fixed energy, the cross sections given by the first Born and the static approximations are unaffected by the change in sign, but figure 13a shows that the inclusion of the second order term at 300 ev. causes a significant difference in the angular distributions, particularly for elastic scattering where the forward peak is almost absent for positrons.

In table IX we compare the total cross sections for electron and positron scattering from helium at 300 ev. with the first Born (B1) and static approximations. As would be expected, the change in sign reverses the effect of the second order term; for example, in the elastic scattering of electrons the cross section is increased when the second order potential is included in the elastic channel, whereas in positron scattering it is decreased. We see that at this energy, although elastic scattering is reduced, the 2'S and 2'P excitations of helium are increased by positron impact. Because of the reduction in the imaginary part of the forward elastic amplitude, the optical theorem (equation (10-4)) predicts a smaller total cross section (Q_{TOT}) for positrons.

Table IX

A comparison of electron and positron scattering from helium atoms at 300 ev: total cross sections, in units of πa_0^2.

Process	B1	Static	Present results:	
			electrons	positrons
$1'S \rightarrow 1'S$	0.152	0.139	0.147	0.133
$1'S \rightarrow 2'S$	0.0080	0.0071	0.0066	0.0090
$1'S \rightarrow 2'P_0$	-	0.023	0.023	0.030
$1'S \rightarrow 2'P_1$	-	0.030	0.030	0.026
$1'S \rightarrow \sum_m 2'P_m$	0.084	0.083	0.082	0.083
$1'S \rightarrow 2'S + 2'P$	0.092	0.090	0.089	0.092
$1'S \rightarrow 1'S + 2'S + 2'P$	0.243	0.229	0.236	0.225
Q_{TOT}	0.0	0.229	0.803	0.784

It must be noted that by ignoring charge transfer and exchange, no allowance has been made for the possibility of positronium formation.

Figure Captions

Figures 13a and 13b. Comparison of electron and positron scattering from helium at 300 ev, differential cross sections for (a) elastic scattering, (b)the 2'S and 2'P excitations.

Curves (e^-) and (e^+).	Present results for e^- and e^+ respectively.
Curve S	Four channel coupling, but without the second order term.
Curve B1	First Born approximation.

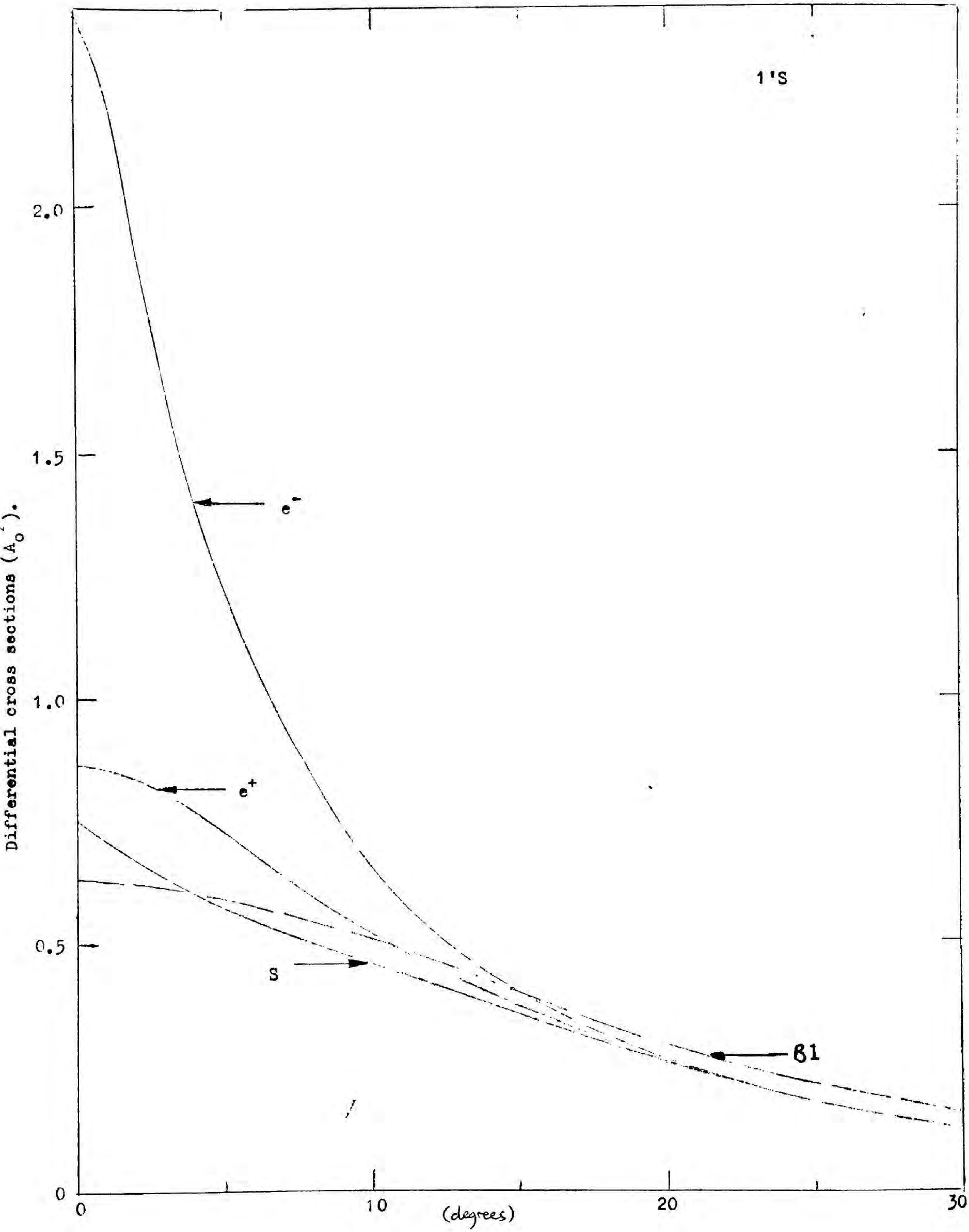
1'S
Differential cross sections (A_o^2).
2.0
1.5
1.0
0.5
0
e^-
e^+
S
B1
0
10
20
30
(degrees)

Figure 13a

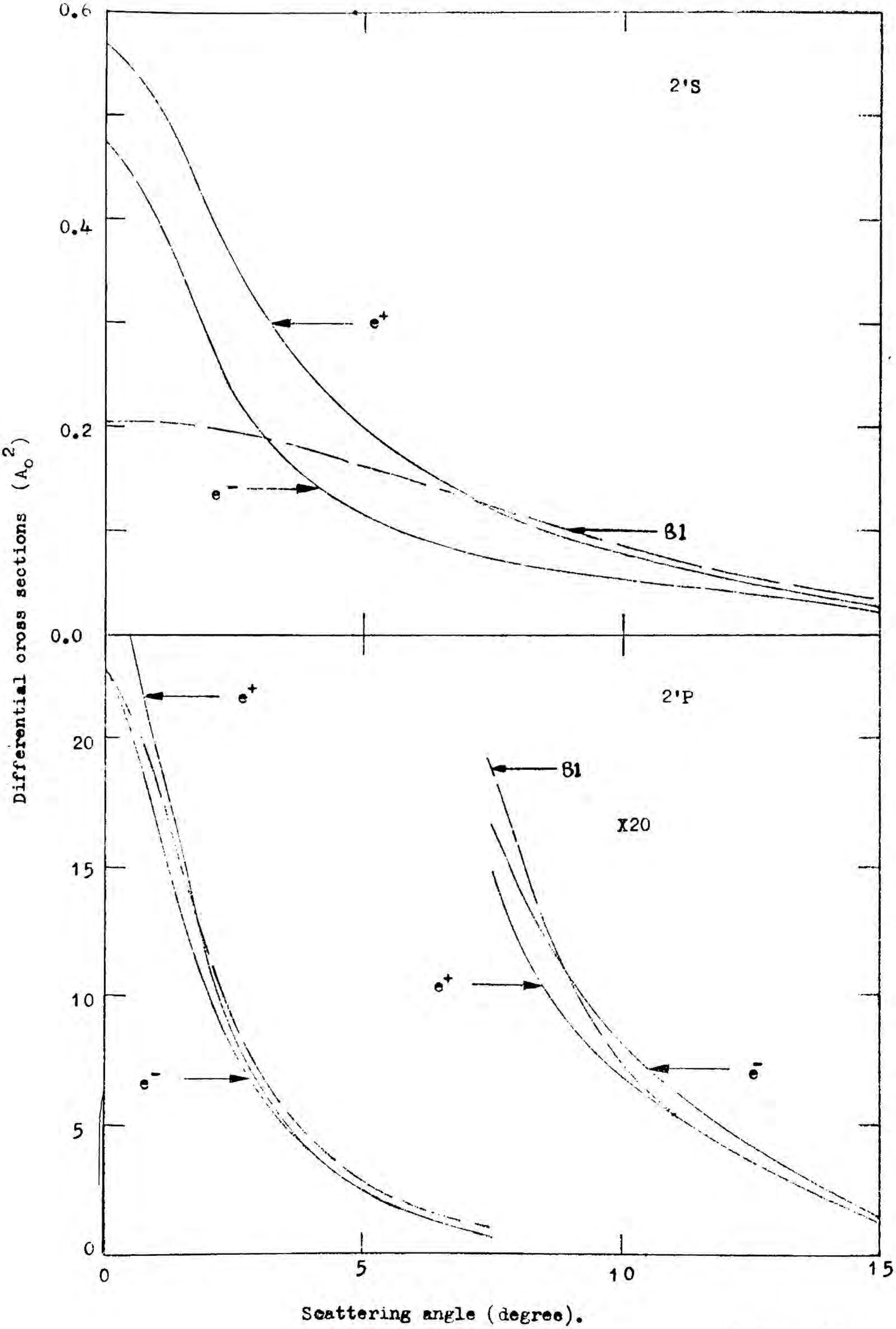
0.6
0.4
0.2
0.0
2'S
e+
e−
B1
Differential cross sections (A0 2)
20
15
10
5
0
2'P
e+
B1
X20
e+
e−
e−
0
5
10
15
Scattering angle (degree).

Figure 13b

Chapter 14

NUMERICAL METHODS

The kernel of the second order potential in the elastic channel (see equation (6-8)) was evaluated by a method due to Coleman in appendix 3. A one - dimensional integral resulted which must be solved numerically. This was done using Simpson's rule and halving the step-length until convergence was reached:

$$\text{Simpson's rule;} \int_{x}^{x+2h} y = \frac{h}{3}\left(y_1 + 4y_2 + y_3\right) + O(h^5) \qquad (14\text{-}1)$$

where $y_1 = y(x)$, $y_2 = y(x+h)$ etc.

For speed, at large Z the asymptotic expansion was used for evaluating the second order potential, as in chapter 6.

Coupling the 1'S, 2'S and 2'P channels for electron - helium scattering, as in chapters 9 to 13, required solving four coupled integro - differential equations,(4-16 to 20),as two of the three magnetic substates of the 2'P state give equal amplitudes (cf. Flannery, 1970) and the number of equations involved are consequently reduced by one. A Fortran program was written to solve the equations for the four $a_n(b,Z)$ simultaneously in a step-by-step iterative procedure. At each stage, the 5-point equations of Milne (1953) were used;

$$\begin{aligned} y_2 &= y_1 + \frac{h}{720}(251y_1' + 646y_2' - 264y_3' + 106y_4' - 19y_5') \\ y_3 &= y_1 + \frac{h}{90}(29y_1' + 124y_2' + 24y_3' + 4y_4' - y_5') \\ y_4 &= y_1 + \frac{3h}{80}(9y_1' + 34y_2' + 24y_3' + 14y_4' - y_5') \\ y_5 &= y_1 + \frac{2h}{45}(7y_1' + 32y_2' + 12y_3' + 32y_4' + 7y_5') \end{aligned} \qquad (14\text{-}2)$$

where y' represents the derivative of y. These equations were iterated to convergence.

The integration from the lower boundary in the elastic channel in (4-16) was carried out by grouping the stored values of $a_0(b,Z')$ in groups of five and using (Milne, 1953),

$$\int_x^{x+4h} y = \frac{4h}{3}(2y_2 - y_3 + 2y_4) \qquad +O(h^5), \qquad (14\text{-}3)$$

this is of the same order of accuracy as Simpson's rule (14-1), but faster since the kernel only needs to be evaluated at three points in every four steps.

The step-length was adjusted automatically after every five steps in order to keep the error in the iteration of (14-2) between preset bounds. The programs were run to give an error of less than 1% in the $a_n(b,\infty)$.

The $a_n(b,\infty)$ were calculated for suitably spaced impact parameters, b. The final integration over b, as specified by equations (3-16 to 19), was performed using Simpson's rule. The Bessel functions required by (3-16) were computed from an algorithm given by Abramowitz and Stegun (1964). The error in the resulting cross sections was about 2%.

Chapter 15

CONCLUSIONS

The importance of including a few stongly coupled channels, and the importance of making some allowance for all possible intermediate states, had both been recognised and seperately taken care of in the close coupling and polarized orbital approximations respectively. Our second order potential method includes both effects in a consistent way and is valid in a wide energy range. The results are significantly better than those obtained without allowance for the channels not explicitly included, and, as was shown by Sullivan et al.(1972), our method lends itself to systematic improvement by the addition of further first and second order coupling, as in equation (4-5). Sullivan et al. (1972), however, found only a small alteration in electron-hydrogen scattering when the complete second order potential matrix was evaluated between the four coupled channels.

In table X we summarise the results of chapters 9 to 13 for electron - helium scattering. Starting with the four channel coupled equations (as in Flannery, 1970) we show the effect of including the second order term in the elastic channel, and the effect of the first order inelastic couplings.

Table X

The effect of different couplings between the 1'S, 2'S and 2'P channels in electron-helium scattering, summarised from chapters 9 to 13.

Comparison of models.	Elastic scattering.	2'S excitation.	2'P excitation.
Inclusion of second order elastic term in the four channel calculation; using equations (4-16) and (4-18)	Large peak in forward direction. Increase in total cross section below 300 ev.	Slight reduction in forward scattering below 300 ev. Reduction in total cross section.	Little effect on angular distributions. Slight reduction in total cross sections below 100 ev.
Neglect of 2'S, 2'P intercouplings at 300 ev; using equations (4-16) and (4-20)	No significant effect.	Considerable reduction in forward scattering below 5^{o}, slight increase in larger angle scattering.	No significant effect.
Neglect of back coupling from the 2'S and 2'P channels to the ground state at 300 ev.; using (4-19) and (4-20)	Slight decrease in forward scattering below 5^{o}.	Further slight reduction in forward scattering below 2^{o}.	Slight reduction in forward scattering below 5^{o}, but slight increase in larger angle scattering.

Finally, we do not expect our approximations to be valid at low energies because of the imact parameter assumption of staight line projectile trajectories (chapter 2), and the non - allowance of charge exchange.

APPENDIX 1,2 and 3

APPENDIX 1

ATOMIC UNITS

Throughout this thesis atomic units are used in the equations and for the resulting cross sections. The following identities define atomic units (eg. Bransden, 1970);

$$e = m_e = h/2\pi = 1, \qquad \text{(A1-1)}$$

where $-e$ and m_e are the charge and mass of the electron, and h Planck's constant. This yields a value for the Bohr radius of the hydrogen, $a_o = 1$ au.

The conversion factor for energies, which are normally quoted in electron Volts (ev) is,

$$1 \text{ ev.} = 27.3 \text{ au.} \qquad \text{(A1-2)}$$

In atomic units the velocity of light is 137; table XI displays the velocities corresponding to the projectile energies in our results. It can be seen that we are well in the non-relativistic ($v \ll c$) region.

Table XI

Electron velocities, corresponding to the energies used, in au.

Energy (ev.)	50	100	200	300	400	500	1000
Velocity (au)	1.19	2.71	3.83	4.69	5.41	6.05	8.56

APPENDIX 2

THE FIRST ORDER POTENTIALS FOR HELIUM

The matrix elements are defined in equation (2-8) as,

$$V_{nm}(\underline{R}) = \langle \phi_n(\underline{r}) | V(\underline{R},\underline{r}) | \phi_m(\underline{r}) \rangle \qquad \text{(A2-1)}$$

Now $\underline{r}$ represents the collective coordinates of the atom. Since helium has two electrons, each can be represented by the vectors $\underline{r}_1$ and $\underline{r}_2$. So (A2-1) becomes;

$$V_{nm}(\underline{R}) = \int d\underline{r}_1 \int d\underline{r}_2 \; \phi^*_n(\underline{r}_1,\underline{r}_2) V(\underline{R},\underline{r}_1,\underline{r}_2) \phi_m(\underline{r}_1,\underline{r}_2) \qquad \text{(A2-2)}$$

The potential for helium is just, from equation (6-1),

$$V(\underline{R},\underline{r}_1,\underline{r}_2) = q\left[\frac{2}{R} - \frac{1}{|\underline{R} - \underline{r}_1|} - \frac{1}{|\underline{R} - \underline{r}_2|}\right] \qquad \text{(A2-3)}$$

where q is the charge on the projectile.

Using the mutually orthogonal analytic helium wavefunctions described in chapter 8, we find the following matrix elements for electron scattering:

$$\langle 1'S | V(\underline{R},\underline{r}) | 1'S \rangle = -N_{oo}\left[b_o(2,2a) + 2cb_o(2,a+b) + c^2 b_o(2,2b) \right]$$

$$\langle 1'S | V(\underline{R},\underline{r}) | 2'S \rangle = -N_{o1}\left[b_o(2,a+p) + cb_o(2,b+p) - c, b_o(3,a+q) \right.$$
$$\left. - cc, b_o(3,b+q) \right]$$

$$\langle 2'S|V(\underline{R},\underline{r})|2'S\rangle = -N_{11}[\lambda_1(2+1/R)\exp(-4R) + \lambda_2(b_0(2,p+2) - c_1 b_0(3,q+2))$$
$$+ b_0(2,2p) - 2c_1 b_0(3,p+q) + c_1^2 b_0(4,2q)]$$

$$\langle 1'S|V(\underline{R},\underline{r})|2'P_m\rangle = -N_{02}[b_1(3,a+s) + cb_1(3,b+s) - \lambda_3/R^3]$$

$$\langle 2'S|V(\underline{R},\underline{r})|2'P_m\rangle = -N_{12}[b_1(3,p+s) - c_1 b_1(4,q+s) + \tfrac{1}{2}\lambda_2 b_1(3,s+2) - \lambda_4/R^2]$$

$$\langle 2'P_m|V(\underline{R},\underline{r})|2'P_m\rangle = -N_{22}[\lambda_5(2+1/R)\exp(-4R) + b_0(4,2s) + \beta_m(b_2(4,2s)$$
$$- \lambda_6/R^3)]$$

$$\langle 2'P_0|V(\underline{R},\underline{r})|2'P_{\pm 1}\rangle = -N_{23}[b_2(4,2s) - \lambda_6/R^3] \qquad \text{(A2-4)}$$

where $N_{00} = 8N$

$N_{01} = 32NN_1[2/(a+2)^3 + 2c/(b+2)^3]$

$N_{11} = N_1^2$

$N_{02} = 32NN_2\pi^{1/2}Y_{1,m}(\hat{\underline{R}})[2/(a+2)^3 + 2c/(b+2)^3]$

$N_{12} = N_1N_2\pi^{1/2}Y_{1,m}(\hat{\underline{R}})$

$N_{22} = \tfrac{1}{4}N_2^2$

$N_{23} = (9/32)^{\frac{1}{2}}N_2^2(8\pi/15)^{\frac{1}{2}}Y_{2,\pm1}(\hat{\underline{R}})$

$N_{34} = -\tfrac{3}{8}N_2^2(32\pi/15)^{\frac{1}{2}}Y_{2,2}(\hat{\underline{R}})$ (A2-5)

and $\lambda_1 = 2/(2p)^3 - 12c_1/(p+q)^4 + 24c_1^2/(2q)^5$

$\lambda_2 = 64[2/(p+2)^3 - 6c_1/(q+2)^4]$

$\lambda_3 = 8/(a+s)^5 + 8c/(b+s)^5$

$$\lambda_4 = 8/(p+s)^5 - 40c,/(q+s)^6 + 4\lambda_2/(s+2)^5$$

$$\lambda_5 = 24/(2s)^5$$

$$\lambda_6 = 144/(2s)^7 \qquad \text{(A2-6)}$$

$$\beta_0 = (16\pi/5)^{\frac{1}{2}} Y_{2,0}(R), \qquad \beta_{\pm 1} = -\tfrac{1}{2}(16-/5)^{\frac{1}{2}} Y_{2,\pm 1}(R)$$

and the values of the wavefunction parameters are as in chapter 8.

The functions $b_L(n,\alpha)$ are defined by

$$b_L(n,\alpha) = \frac{1}{2L+1} \int_R^\infty dr\ (r^{n+L}/R^{L+1} - R^L r^{n-L-1}) \exp(-\alpha R) \qquad \text{(A2-7)}$$

and this integral is easily calculable. Note that from (2-13) and (2-18),

$$R^2 = b^2 + Z^2 . \qquad \text{(A2-8)}$$

APPENDIX 3

THE SECOND ORDER POTENTIAL IN THE ELASTIC CHANNEL

The matrix element $U_{nm}(\underline{R},\underline{R}')$, defined by (4-11), is evaluated in the elastic channel in chapter 6 for electron-helium scattering. This reduces to equation (6-8);

$$U_{00}(\underline{R},\underline{R}') - V_{00}(\underline{R})V_{00}(\underline{R}') = -\tfrac{1}{2}\left[V_{00}(\underline{R}) + 2/R\right]\left[V_{00}(\underline{R}') + 2/R'\right] + 2\int d\underline{r}\, |u(r)|^2 \frac{1}{|\underline{R}-\underline{r}|}\frac{1}{|\underline{R}'-\underline{r}|} .$$

Using u(r) from the helium ground state wacefunction defined in equation (8-2), the integral term becomes

$$8N\left[\, C(2,2a) + 2cC(2,a+b) + c^2C(2,2b)\,\right]$$

where $$C(2,\alpha) = \frac{1}{4\pi}\int d\underline{r}\, \frac{1}{|\underline{R}-\underline{r}|}\frac{1}{|\underline{R}'-\underline{r}|}\exp(-\alpha r).$$

Writing each $1/|\underline{R}-\underline{r}|$ in terms of spherical harmonics and using orthogonality and the addition theorem (Messiah, 1961) we find,

$$\frac{1}{4\pi}\int \frac{1}{|\underline{R}-\underline{r}|}\frac{1}{|\underline{R}'-\underline{r}|}\, d\Omega = \sum_{L=0}^{\infty} \frac{1}{2L+1}\, \gamma_L(R,r)\, \gamma_L(R',r) P_L(\cos\hat{RR'})$$

where $$\gamma_L(R,r) = \begin{cases} r^L/R^{L+1} \; ; & r < R \\ R^L/r^{L+1} \; ; & r > R \end{cases} \qquad \text{(A3-1)}$$

The radial integral in $C(2,\alpha)$ after using (A3-1), has been evaluated by Coleman (1971) and can be reduced to the one-dimensional integral;

$$C(2,\alpha) = \frac{1}{\alpha S}\int_{0}^{r} dt\, \frac{(1+St)\exp(-St) - (1+S/t)\exp(-S/t)}{(t^4 - 2t^2\cos(\widehat{RR'}) + 1)^{\frac{1}{2}}}$$

where $S = \alpha(RR')^{\frac{1}{2}}$

$$r = (R/R')^{\frac{1}{2}}, \quad R' \geqslant R \qquad \text{(A3-1)}$$

since $R^2 = b^2 + Z^2$, from (A2-8); $\cos(\widehat{RR'}) = (ZZ' + b^2)/RR'$.

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