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The Interaction of Fast Electrons with Light Atoms

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Abstract

A model is presented that describes the non-relativistic scattering of electrons from light atoms at energies above the single ionization threshold of the target. The simplest form of this approximation is considered, and application made to elastic collisions with hydrogen and helium atoms. This requires the numerical solution of a second order integro-differential equation, and a technique that achieves this is discussed.

Supplementing this model with a distorted wave approximation gives a description of the excitation of any target state. This is illustrated for the $1^1S \rightarrow 2^1S$, 2^3S and 2^1P transitions in helium and the 1s → 2s transition in hydrogen.

Differential, integrated and total cross-sections are presented in the energy range 50-200 eV for hydrogen and 50-500 eV for helium. In addition, the relative populations and phases of the magnetic sub-levels of the 2^1P state of helium, following excitation from the ground state, have been computed.

Finally, the use of dispersion relations as a consistency check on experimental data is demonstrated for electron-neon and positron-helium scattering.

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INTRODUCTION

The work presented here is concerned with a theoretical study of the scattering of electrons from atoms at non-relativistic velocities. By limiting the investigation to collisions with light atoms it is ensured that the total orbital and spin angular momenta are separately conserved, and the relevant dynamical equation is therefore that of Schrödinger.

The scattering of electrons at energies below the single ionization threshold of the target is adequately described by the close-coupling approximation. There is, however, no satisfactory model for the intermediate energy range, where the velocity of the electron is high, but not so great that its interaction with the target can be treated as a perturbation. Previous results in this intermediate region have been obtained for the most part by extending the range of application of the low and high energy approximations, and those relevant to the present work will be reviewed in Chapter 1. It is partly the object of this investigation to propose a model that will give an adequate description of scattering at intermediate energies, and this will be presented in Chapters 2 and 4. The applications to the particular cases of hydrogen and helium are considered in Chapters 3 and 5 for elastic and inelastic scattering respectively.

Of the measurable quantities that express the result of an electron-atom collision, we will calculate the ratio of the scattering amplitudes for the excitation of magnetic substates, the differential, the integrated and the total cross-sections. In assessing the merit of a particular approximation, it is essential to compare quantities that provide as fine a test as possible; this is well illustrated by the Born approximation which while predicting total cross-sections that agree favourably with experiment at certain energies, gives very poor values for the differential cross-section. However, the techniques required for the measurement of the ratio of scattering amplitudes for magnetic substate excitation are very new, and there is a corresponding lack of both data and theoretical predictions for this quantity. The present work will therefore concentrate mainly on the calculation of differential cross-sections.

It is also proposed to use conjectured analytic properties of the scattering amplitude to show how the consistency of experimental data may be assessed, and this will constitute Chapter 6.

All analysis shown will be for electron-hydrogen scattering, unless otherwise indicated, and we will work in atomic units throughout. Finally, since graphical and tabular representation of results serve different purposes, it is felt desirable to present the differential cross-sections of this work in both forms.

Chapter 1 Some Approximate Models of Scattering

1.1 The Second Order Potential Method

The dynamical equation for an electron, with co-ordinates $\underline{r}_{N+1}$, interacting with an atom whose N electrons have co-ordinates $\underline{r}_1 \ldots \underline{r}_N$ is, within the framework discussed in the Introduction

$$\left\{ \sum_{i=1}^{N+1}\left[-\frac{1}{2}\nabla_i^2+\frac{1}{r_i}\right]+\sum_{i>j}\frac{1}{r_{ij}}\right\}\Psi(\underline{r}_1\cdots\underline{r}_{N+1}) = E\Psi(\underline{r}_1\cdots\underline{r}_{N+1}) \qquad (1.1)$$

where $r_{ij} = |\underline{r}_i-\underline{r}_j|$, the nucleus has been taken as centre of mass, and a time-independent formulation has been assumed.

In particular, for scattering from the state $\phi_n(\underline{r}_1 \ldots \underline{r}_N)$ of say hydrogen, (1.1) is subject to the boundary conditions

$$\Psi(\underline{r}_1,\underline{r}_2) \underset{r_2\ \text{large}}{\sim} \delta_{nm}\,\phi_n(\underline{r}_1)\,e^{i\underline{k}_n\cdot\underline{r}_2}+\sum_m f_{mn}(\theta)\,\phi_m(\underline{r}_1)\,\frac{e^{ik_m r_2}}{r_2} \qquad (1.2)$$

$$\underset{r_1\ \text{large}}{\sim} \sum_m g_{mn}(\theta)\,\phi_m(\underline{r}_2)\,\frac{e^{ik_m r_1}}{r_1} \qquad (1.3)$$

where $f_{mn}(\theta)$, $g_{mn}(\theta)$ are the direct and exchange scattering amplitudes respectively. The range of m is over all possible channels, which are said to be open if $k_m^2>0$, and closed otherwise.

The total wave function may be expanded exactly as

$$\Psi(\underline{r}_1,\underline{r}_2) = \sum_m \phi_m(\underline{r}_1)\,F_m(\underline{r}_2) + \int d\underline{K}\,\phi_{\underline{K}}(\underline{r}_1)\,F_{\underline{K}}(\underline{r}_2) \qquad (1.4)$$

and equations for the coefficients $F_m(\underline{r})$ are found by substituting (1.4) into (1.1) giving

$$\left[\nabla^2 + k_m^2\right] F_m(\underline{r}_2) = 2\sum_{m'} V_{mm'}(\underline{r}_2)\, F_{m'}(\underline{r}_2) \qquad (1.5)$$

where

$$V_{mm'}(\underline{r}_2) = \int d\underline{r}_1\, \phi_m^*(\underline{r}_1)\left[\frac{1}{r_{12}} - \frac{1}{r_1}\right]\phi_{m'}(\underline{r}_1) \qquad (1.6)$$

and the sum over m' includes an integration over the continuum. The boundary condition

$$F_m(\underline{r}) \underset{r\to\infty}{\sim} \delta_{mn}\, e^{i\underline{k}_m\cdot\underline{r}} + f_{mn}(\theta)\,\frac{e^{ik_m r}}{r} \qquad (1.7)$$

follows immediately from (1.2).

Castillejo et al (1960) have shown that the coefficients $F_{\underline{K}}(\underline{r})$ in (1.4) are, unlike $F_m(\underline{r})$, discontinuous functions of $\underline{K}$. An appropriate choice for the path of integration over K, to avoid this singularity, then leads to the alternative boundary condition (1.3). Castillejo et al (1960) have also shown that these boundary conditions arise naturally when the total wave function is properly symmetrized:-

$$\Psi^{\pm}(\underline{r}_1,\underline{r}_2) = \sum_m \left[\phi_m(\underline{r}_1)F_m(\underline{r}_2) \pm \phi_m(\underline{r}_2)F_m(\underline{r}_1)\right] \qquad (1.8)$$

where the functions $F_m(\underline{r})$ are now continuous, for m in the continuum.

The approximation of the truncated eigenfunction expansion is obtained (Massey and Burhop 1969) on truncating the sum in (1.5) at some finite value $m' = M$. Alternatively, the expansion (1.4) may be truncated, and the resulting $\Psi(\underline{r}_1,\underline{r}_2)$ used as a trial function in the Kohn variational principle (Mott and Massey 1965). The best choice for the functions $F_m(\underline{r})$, in the sense that if the error in $\Psi(\underline{r}_1,\underline{r}_2)$ is to first order then the error in the scattering amplitude will be to second order, is then given by the solution of (1.5), subject to (1.7).

Note that the possibility of rearrangement does not arise in this approximation unless the trial function is properly symmetrized at the outset. In any case, the approximation is expected to be inadequate for applications at energies above the ionization threshold, since only a few of the infinitely many open channels are then taken into account. Mittleman (1960, 1961) has suggested that an effective potential may be introduced into (1.5) that partly makes allowance for those channels excluded from the expansion, the special case of truncation to one channel being considered. The generalization of this work to an arbitrary number of channels was made by Mittleman and Pu (1962). Subsequent workers (Mittleman 1970, Joachain and Mittleman 1971, Bransden and Coleman 1972, Alton et al 1972) have expressed this effective potential in configuration space, and illustrated different methods for its implementation.

Following Bransden and Coleman (1972) we adopt (1.5) for states $m \leq M$. This then becomes approximate when we choose to obtain $F_{m'}(\underline{r})$, for $m' > M$, from:-

$$\left[\nabla^2 + k_{m'}^2\right] F_{m'}(\underline{r}) = 2\sum_{m''=1}^{M} V_{m'm''}(\underline{r})\, F_{m''}(\underline{r}) \tag{1.9}$$

We introduce the free particle Green's function $G(k_n{}^2;\ \underline{r},\underline{r}')$ with outgoing wave boundary conditions satisfying the equation

$$\left[\nabla^2 + k_n^2\right] G(k_n^2; \underline{r}, \underline{r}') = \delta(\underline{r} - \underline{r}') \tag{1.10}$$

and we have explicitly,

$$G(k_n^2; \underline{r}, \underline{r}') = -\frac{1}{4\pi}\,\frac{e^{ik_n|\underline{r}-\underline{r}'|}}{|\underline{r}-\underline{r}'|} \tag{1.11}$$

(1.10) may now be used to solve (1.9) the solution of which, on substitution into (1.8), gives for $m \leqslant M$

$$\begin{aligned}\left[\nabla^2 + k_m^2\right] F_m(\underline{r}) = {} & 2\sum_{m'=1}^{M} V_{mm'}(\underline{r})\, F_{m'}(\underline{r}) \; + \\ & + 4\sum_{m'=1}^{M} \int d\underline{r}'\, K_{mm'}(\underline{r},\underline{r}')\, F_{m'}(\underline{r}')\end{aligned} \tag{1.12}$$

where

$$K_{mm'}(\underline{r},\underline{r}') = \sum_{m''=M+1}^{\infty} G(k_{m''}^2; \underline{r}, \underline{r}')\, V_{mm''}(\underline{r})\, V_{m''m'}(\underline{r}') \tag{1.13}$$

The infinite summation in (1.13) is now removed on replacing $k_{m''}^2$ by an average energy $\bar{k}^2$ and performing closure on the target states $\phi_{m''}(\underline{r}_1)$ to give

$$K_{mm'}(\underline{r},\underline{r}') = G(\bar{k}^2; \underline{r}, \underline{r}')\left\{V_{mm'}(\underline{r},\underline{r}') - \sum_{m''=1}^{M} V_{mm''}(\underline{r})\, V_{m''m'}(\underline{r}')\right\} \tag{1.14}$$

where

$$V_{mm'}(\underline{r},\underline{r}') = \int d\underline{x}\, \phi^*_m(\underline{x}) \left[\frac{1}{|\underline{r}-\underline{x}|} - \frac{1}{r}\right]\left[\frac{1}{|\underline{r}'-\underline{x}|} - \frac{1}{r'}\right] \phi_{m'}(\underline{x}) \qquad (1.15)$$

The non-local potential $K_{nm}(\underline{r},\underline{r}')$ is of second order in the interaction, and its introduction into the truncated eigenfunction expansion, together with the subsequent closure approximation, is the second order potential method of Bransden and Coleman (1972).

Referring to (1.9), it is noted that the consequence of the closure approximation is to replace $k^2_{m'}$, on the left hand side, by the constant $\bar{k}^2$. On setting $m' = \underline{K}$ and using (1.10) the continuum functions $F_{\underline{K}}(\underline{r})$ are found to be

$$F_{\underline{K}}(\underline{r}) = 2\int d\underline{r}'\, G(\bar{k}^2; \underline{r}, \underline{r}') \sum_{m''=1}^{M} V_{\underline{K}m''}(\underline{r}')\, F_{m''}(\underline{r}') \qquad (1.16)$$

and, by inspection, are continuous functions of $\underline{K}$. The boundary condition (1.3) is therefore replaced in this method by

$$\Psi(\underline{r}_1, \underline{r}_2) \underset{r_1 \to \infty}{\sim} 0 \qquad (1.17)$$

and to allow for exchange a reformulation using a symmetrized expansion of the form (1.8) is required.

1.2 The Close-Coupling Approximation

The equations of the previous section were derived in a configuration space, and are not tractable as they stand. The use of partial wave series, however, allows the equations to be expressed in a form amenable to numerical solution without further approximation. This will be illustrated here for the truncated eigenfunction expansion approximation, and the total wavefunction will also be symmetrized. When the truncation is physically chosen so that all the strongly coupled states associated with a particular transition are represented, in addition to those providing the main contribution to the polarizability of the atom, then we obtain the close-coupling approximation (Burke and Smith 1962).

In particular for electron-hydrogen scattering, let $\mathbf{r}_1$ and $(n\ell_1 m_1)$ be the co-ordinates and quantum numbers of the bound electron while those of the projectile are $\mathbf{r}_2$ and $(\ell_2 m_2)$. The expansion for the total wave function (1.4) may then be written

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = \sum_{\gamma} \frac{P_{n\ell_1}(r_1)}{r_1} Y_{\ell_1 m_1}(\hat{\mathbf{r}}_1) \frac{f_{\ell_2}(r_2)}{r_2} Y_{\ell_2 m_2}(\hat{\mathbf{r}}_2) \qquad (1.18)$$

where $Y_{\ell m}(\hat{\mathbf{r}})$ is a spherical harmonic (Schiff 1968) and γ denotes the set of quantum numbers $(n\ell_1 m_1 \ell_2 m_2)$. Following Percival and Seaton (1957) it is noted that our neglect of spin-orbit coupling ensures that the total orbital and spin angular momenta are constants of the motion. We transform therefore to the representation that is completely specified by the set $\Gamma \equiv (n\ell_1 \ell_2 LM)$, L and M being the quantum numbers of total orbital angular momentum, and also properly symmetrize the wave function to give

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = \sum_{\Gamma} \left[\frac{P_{n\ell_1}(r_1)}{r_1} \frac{f^{L}_{\ell_2}(r_2)}{r_2} \mathcal{Y}_{L\ell_1\ell_2 M}(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2) + (-1)^{S} \left\{ \mathbf{r}_1 \longleftrightarrow \mathbf{r}_2 \right\} \right] \qquad (1.19)$$

where the second term is obtained from the first on interchange of $\underline{r}_1$ and $\underline{r}_2$, S is the total spin and in the notation of Rose (1957)

$$\mathcal{Y}_{L\ell_1\ell_2M}(\hat{\underline{r}}_1,\hat{\underline{r}}_2) = \sum_{m_1m_2} C(\ell_1\ell_2L;m_1m_2M)Y_{\ell_1m_1}(\hat{\underline{r}}_1)Y_{\ell_2m_2}(\hat{\underline{r}}_2) \qquad (1.20)$$

$C(\ell_1\ell_2L;\ m_1m_2M)$ is the Clebsch-Gordon coefficient, with $M = m_1 + m_2$ and the triad $\ell_1\ell_2L$ satisfying the triangle inequalities. Percival and Seaton (1957) show that substitution of either equation (1.19) or its truncation into the Kohn variational principle (Mott and Massey 1965) leads to the radial equation for $f^L_\nu(r)$:-

$$\mathcal{L}_n f^L_\nu(r) = 2\sum_{\nu'} \left[V^L_{\nu\nu'}(r) - W^L_{\nu\nu'}(r)\right] f^L_{\nu'}(r) \qquad (1.21)$$

where $\nu \equiv (n\,\ell_1\,\ell_2)$ and

$$\mathcal{L}_n \equiv \frac{d^2}{dr^2} + k_n^2 - \frac{\ell_2(\ell_2+1)}{r^2} \qquad (1.22)$$

In their notation:-

$$V^L_{\nu\nu'}(r) = -\frac{\delta_{\nu\nu'}}{r} + \sum_\lambda f_\lambda(\ell_1\ell_2\ell_1'\ell_2'|L)y_\lambda(P_{n\ell_1}P_{n'\ell_1'}|r) \qquad (1.23)$$

and

$$W^L_{\nu\nu'}(r)f^L_{\nu'}(r) = (-1)^{1-S}\sum_\lambda g_\lambda(\ell_1\ell_2\ell_1'\ell_2'|L)P_{n'\ell_1'}(r) \times \left[y_\lambda(P_{n\ell_1}f^L_{\nu'}|r) + \delta_{\lambda 0}(\varepsilon_n+\varepsilon_{n'}-E)\Delta(P_{n\ell_1}|F^L_{\nu'})\right] \qquad (1.24)$$

where in general

$$y_\lambda(AB|r) = \int_0^\infty A^*(x)B(x)\frac{\min^\lambda(r,x)}{\max^{\lambda+1}(r,x)}\,dx \qquad (1.25)$$

and

$$\Delta(A|B) = \int_0^\infty A^*(x)B(x)\,dx \qquad (1.26)$$

with the coefficients f_λ and g_λ defined as

$$f_\lambda(l_1 l_2 l_1' l_2'|L) = \int d\hat{r}_1\, d\hat{r}_2\, Y_{Ll_1l_2M}(\hat{r}_1,\hat{r}_2)P_\lambda(\hat{r}_1\cdot\hat{r}_2)Y_{Ll_1'l_2'M}(\hat{r}_1,\hat{r}_2) \qquad (1.27)$$

$$= (-1)^{L-l_1-l_2}\, g_\lambda(l_1 l_2 l_2' l_1'|L) \qquad (1.28)$$

Finally, E is the total energy, ε_n the energy of the n^{th} state of the atom and $E - \varepsilon_n = \frac{1}{2} k_n^2$.

Burke and Schey (1962) show that, for electrons incident upon the ground state of an atom, (1.21) has the boundary condition

$$f_\nu^L(r) \underset{r\to\infty}{\sim} \sin\left(k_n r - l_2\frac{\pi}{2}\right)\delta_{\nu\nu_0} + T_{\nu\nu_0}^{LS}\, e^{i(k_n r - l_2\frac{\pi}{2})} \qquad (1.29)$$

where the partial wave amplitude $T_{\nu\nu_0}^{LS}$ is such that for the scattering amplitude we have

$$f_{\nu\nu_0}^S(\theta) = \sum_{L=0}^{\infty} \frac{1}{k_n}(2L+1)\,T_{\nu\nu_0}^{LS}\,P_L(\cos\theta) \qquad (1.30)$$

ν_0 being the quantum numbers of the incident channel. Equation (1.21) with a suitable truncation of the ν' summation is the close-coupling approximation, and Burke et al (1967) note that it has been most successful at energies where the channels excluded by the truncation are closed. A review of the applications of this model is given by Moiseiwitsch and Smith (1968).

1.3 Impact Parameter Approximation

In contrast to the previous section, the equations of Section 1.1 may be derived with additional approximation in an impact parameter space.

For an electron incident upon the i$^{\text{th}}$ state of a hydrogen atom, the total wave function is expanded as

$$\Psi(\underline{r}_1,\underline{r}_2) = \sum_n \phi_n(\underline{r}_1)\, e^{i\underline{k}_i\cdot\underline{r}_2}\, e^{i(\varepsilon_i-\varepsilon_n)Z/k_i}\, c_n(\underline{b},Z) \qquad (1.31)$$

where the projectile has incident wave vector $\underline{k}_i$ and coordinates $\underline{r}_2$ such that $\underline{r}_2 = Z\hat{\underline{k}}_i + \underline{b}$. Substituting (1.31) into the Schrodinger equation for the total system, the transition amplitudes $c_n(\underline{b},Z)$ are found to satisfy

$$\frac{\partial}{\partial Z} c_n(\underline{b},Z) = \frac{1}{ik_i}\sum_j V_{nj}(\underline{r}_2)\, e^{i(\varepsilon_n-\varepsilon_j)Z/k_i}\, c_j(\underline{b},Z) \qquad (1.32)$$

only after assuming:-

i) high velocity, such that

$$\frac{(\varepsilon_i-\varepsilon_n)^2}{k_i^2}\frac{\partial^2}{\partial Z^2} c_n(\underline{b},Z) \ll \frac{\partial}{\partial Z} c_n(\underline{b},Z) \qquad (1.33)$$

and ii) rectilinear propagation in the $\hat{\underline{k}}_i$ direction, so that

$$\underline{k}_i\cdot\underline{\nabla} = k_i\frac{\partial}{\partial Z} \qquad (1.34)$$

$V_{nj}(\underline{r})$ is defined in (1.6), and (1.32) is subject to the boundary condition

$$c_n(\underline{b}, -\infty) = \delta_{ni} \qquad (1.35)$$

In the notation of equation (1.1) the exact scattering amplitude for a particle colliding with a composite N-electron target and so causing an i → f atomic transition is (Bransden 1970)

$$f_{if}(\theta) = -\frac{1}{2\pi}\int e^{-i\underline{k}_f\cdot\underline{r}_{N+1}}\phi_f(\underline{r}_1\ldots\underline{r}_N)V(\underline{r}_1\ldots\underline{r}_{N+1})\Psi(\underline{r}_1\ldots\underline{r}_{N+1})d\underline{r}_1\ldots\underline{r}_{N+1} \qquad (1.36)$$

where $V(\underline{r}_1 \ldots \underline{r}_{N+1})$ is the projectile target interaction. Our semi-classical approximation to the scattering amplitude is therefore

$$f_{if}(\theta) = -\frac{1}{2\pi}\int d\underline{b}\,dz\, e^{i(\underline{k}_i-\underline{k}_f)\cdot\underline{r}_2}\sum_j V_{fj}(\underline{b},z)e^{i(\varepsilon_i-\varepsilon_j)\frac{z}{k_i}}c_j(\underline{b},z) \qquad (1.37)$$

for electron-hydrogen collisions.

At high energies Byron (1971) shows that $k_i - k_f \sim (\varepsilon_f - \varepsilon_i)/k_i$ and his approximation of $(\underline{k}_i - \underline{k}_f)\cdot\hat{\underline{k}}_i$ by $k_i - k_f$ allows us to write

$$e^{i(\underline{k}_i-\underline{k}_f)\cdot\underline{r}_2} \sim e^{i(\underline{k}_i-\underline{k}_f)\cdot\underline{b}}\, e^{i(\varepsilon_f-\varepsilon_i)\frac{z}{k_i}} \qquad (1.38)$$

After substitution of (1.38) into (1.37) and combination of the exponents in Z we recognize the summand as being that of (1.32) and obtain

$$\begin{aligned} f_{if}(\theta) &= -\frac{ik_i}{2\pi}\int d\underline{b}\, e^{i(\underline{k}_i-\underline{k}_f)\cdot\underline{b}}\int_{-\infty}^{\infty}dz\,\frac{\partial}{\partial z}c_f(\underline{b},z) \\ &= -\frac{ik_i}{2\pi}\int d\underline{b}\, e^{i(\underline{k}_i-\underline{k}_f)\cdot\underline{b}}\left[c_f(\underline{b},+\infty)-\delta_{if}\right] \end{aligned} \qquad (1.39)$$

where the boundary condition (1.35) has been used.

Both (1.32) and (1.39) can be simplified by making the decomposition of the surface element $d\underline{b}$ into $b\,db\,d\phi$. The ϕ dependence of the transition amplitudes is extracted on defining

$$a_n(b,z)\,e^{-im_n\phi} = c_n(\underline{b},z) \qquad (1.40)$$

Hence, (1.32) becomes

$$\frac{\partial}{\partial z}a_n(b,z) = \frac{1}{ik_i}\sum_j V_{nj}(b,z)\,e^{i(\varepsilon_n-\varepsilon_j)\frac{z}{k_i}}\,a_j(b,z) \qquad (1.41)$$

where

$$V_{nj}(\underline{b},z) = e^{i(m_j-m_n)\phi}\,V_{nj}(b,z) \qquad (1.42)$$

After substitution of (1.40) into (1.39) we take $\underline{\hat{b}}$ to be along the direction of the momentum transfer $\underline{q} = \underline{k}_i - \underline{k}_f$. The exponent $i(\underline{k}_i-\underline{k}_f).\underline{b}$ then becomes $i(k_i+k_f)b\sin\frac{\theta}{2}\cos\phi$ which at high energies $\sim 2ik_i b\sin\frac{\theta}{2}\cos\phi$, and using the integral representation for the Bessel function of the first kind:-

$$J_n(x) = \frac{(-i)^n}{2\pi}\int_0^{2\pi} e^{ix\cos\phi}\,e^{in\phi}\,d\phi \qquad (1.43)$$

we obtain finally

$$f_{if}(\theta) = (-i)^{m_f+1}k_i\int_0^{\infty}\left[a_f(b,+\infty)-\delta_{fi}\right]J_{m_f}\left(2k_i b\sin\frac{\theta}{2}\right)b\,db \qquad (1.44)$$

so agreeing with the expressions of McCarroll and Salin (1968) and Wilets and Wallace (1968).

The differential and total cross-sections, $\frac{d\sigma_{if}}{d\Omega}$ and Q_{if}, are defined by

$$Q_{if} = \int_0^{2\pi} d\phi \int_{-1}^{+1} d(\cos\theta)\, \frac{d\sigma_{if}(\theta,\phi)}{d\Omega} \tag{1.45a}$$

and

$$\frac{d\sigma_{if}}{d\Omega} = \frac{k_f}{k_i} \left| f_{if}(\theta,\phi) \right|^2 \tag{1.45b}$$

The impact parameter approximation to the total cross-section is therefore, in units of $a_0^{\,2}$,(Wilets and Wallace 1968)

$$Q_{if} = 2\pi \frac{k_f}{k_i} \int_0^{\infty} \left| a_f(b,+\infty) - \delta_{if} \right|^2 b\, db \tag{1.46}$$

Equation (1.41), after truncation to M channels, is the truncated eigenfunction expansion in the impact parameter approximation, and the second order potential method is now used, as before, to allow for the effect of the excluded states. Proceeding as in the development of (1.9) the transition amplitudes are then such that

$$\begin{aligned} \frac{\partial}{\partial z} a_n(b,z) = {} & \frac{1}{ik_i} \sum_{m=1}^{M} V_{nm}(b,z)\, e^{i(\varepsilon_n - \varepsilon_m)\frac{z}{k_i}}\, a_n(b,z) - \\ & - \frac{1}{k_i^2} \sum_{m=1}^{M} \int_{-\infty}^{z} dz'\, K_{nm}(z,z')\, a_m(b,z') \end{aligned} \tag{1.47}$$

where the second order potential is

$$\begin{aligned} K_{nm}(z,z') = {} & \left[V_{nm}(b,z\,;b,z') - \sum_{j=1}^{M} V_{nj}(b,z) V_{jm}(b,z') \right] \times \\ & \times \exp\left\{ \frac{i}{k_i}(\varepsilon_n - \bar{\varepsilon})\, z - \frac{i}{h_i}(\varepsilon_m - \bar{\varepsilon})\, z' \right\} \end{aligned} \tag{1.48}$$

and $\bar{\varepsilon} = E - \frac{1}{2}\bar{k}^2$ where E is the total energy.

The above formulation has been applied, with some success, to the scattering of electrons and protons from hydrogen and helium atoms by Bransden et al (1972), Sullivan et al (1972), Berrington et al (1973) and Begum et al (1973). However, their adoption of a semi-classical approximation, together with the neglect of exchange, limits applications to scattering at the higher intermediate energies. Furthermore, despite there being no reliable estimate for the range of applicability of their approximation, Bransden and co-workers presented results for electron energies as low as 50 eV.

A similar approach was proposed by Joachain and Mittleman (1971) who considered a one channel approximation to (1.12) by setting M=1, and in addition eikonalized the scattering wave function:-

$$F_1(\underline{r}) = e^{i\underline{k}_1.\underline{r}} \, e^{i\Lambda(\underline{b},z)} \tag{1.49}$$

Joachain and Mittleman (1971) made further approximations, however, to the resulting equation for the phase $\Lambda(\underline{b},Z)$, which results in their model being less satisfactory than that of Bransden and Coleman (1972).

1.4 The Born Series

It is convenient to define an integral operator $\tilde{G}_n$ such that

$$\tilde{G}_n Z(\underline{r}) = \int d\underline{r}' \, G(k_n^2 ; \underline{r}, \underline{r}') Z(\underline{r}') \tag{1.50}$$

for some function $Z(\underline{r})$, where $G(k_n^2; \underline{r}, \underline{r}')$ is defined by (1.10). Adopting the Einstein summation convention, whereby a term with a repeated index is summed over the full range of that index, the solution of (1.5) may be written compactly as

$$F_m(\underline{r}) = \delta_{mn}\psi_m(\underline{r}) + \tilde{G}_m U_{mm'} F_{m'}(\underline{r}) \tag{1.51}$$

where $\psi_m(\underline{r})$ is the plane wave solution to

$$\left[\nabla^2 + k_m^2\right]\psi_m(\underline{r}) = 0 \tag{1.52}$$

and $U_{mm'}(\underline{r}) = 2\,V_{mm'}(\underline{r})$

The Born series for the scattering function is generated by the iteration of (1.51), the terms being of successive powers in the interaction:-

$$F_m = \delta_{nm}\psi_m + \tilde{G}_m U_{mm'}\psi_{m'}\delta_{m'n} + \tilde{G}_m U_{mm'}\tilde{G}_{m'}U_{m'm''}\psi_{m''}\delta_{m''n} \tag{1.53}$$

Using the explicit form of the Green's function, (1.11), we have that as $r\to\infty$, for fixed r',

$$G(k_n^2;\underline{r},\underline{r}') \underset{r\to\infty}{\sim} -\frac{1}{4\pi}\frac{e^{ik_n r}}{r}\, e^{-i\underline{k}'_n\cdot\underline{r}'} \tag{1.54}$$

where the vector $\underline{k}'_n$ is of magnitude k_n and in the direction $\hat{\underline{r}}$. Substituting (1.54) in (1.50) we deduce

$$\tilde{G}_n z(\underline{r}) \underset{r\to\infty}{\sim} -\frac{1}{4\pi}\frac{e^{ik_n r}}{r}\int_0^\infty d\underline{r}'\, e^{-i\underline{k}'_n\cdot\underline{r}'}\, z(\underline{r}') \tag{1.55}$$

Equation (1.55) is now substituted into (1.53) and the resulting expression compared with the boundary condition (1.7) to give the Born series for the scattering amplitude

$$f_{mn}(\theta) = \sum_{n=1}^{\infty} \bar{f}_{Bn} \tag{1.56}$$

where, for example,

$$\bar{f}_{B1}(\theta) = -\frac{1}{2\pi}\int d\underline{r}\, e^{-i\underline{k}_m\cdot\underline{r}}\, V_{mn}(\underline{r})\, e^{i\underline{k}_n\cdot\underline{r}} \tag{1.57}$$

and

$$\bar{f}_{B2}(\theta) = -\frac{1}{2\pi}\int d\underline{r}_1\, d\underline{r}_2\, e^{-i\underline{k}_m\cdot\underline{r}_1} \sum_j V_{mj}(\underline{r}_1)\, G(k_j^2;\underline{r}_1,\underline{r}_2)\,\times \\ \times\, V_{jn}(\underline{r}_2)\, e^{i\underline{k}_n\cdot\underline{r}_2} \tag{1.58}$$

with $\cos\theta = \hat{\underline{k}}_m \cdot \hat{\underline{k}}_n$

The models in which the scattering amplitude is approximated by $\bar{f}_{B1}(\theta)$ and $[\bar{f}_{B1}(\theta) + \bar{f}_{B2}(\theta)]$ are called the first and second Born approximations respectively.

The polarization of an atom by an incoming electron results in an attractive interaction between them which, being of long range, affects only small angle scattering. At the intermediate energies this polarization potential dominates the elastic scattering in the forward direction, and its neglect by the first Born approximation leads to a characteristically flat maximum at $\theta=0$, in contrast to the experimentally observed sharp peak. Indeed, $\bar{f}_{B1}(0)$ is independent of energy for elastic collisions and equals 1 for hydrogen.

It should be noted from the work of Castillejo et al (1960) that the presence of the 2p state in the close-coupling approximation of Burke et al (1963) accounts for only 66% of the polarizability of the atom. The close-coupling results are therefore similarly defective in the forward direction for elastic scattering above the ionization threshold.

Regarding the second Born approximation, it is not possible to evaluate the integral (1.58) exactly and the simplification of Holt and Moiseiwitsch (1968) is to replace k_j^2 in the Green's function by an average energy $\bar{k}^2$ for all j higher than some value N; closure is then performed on the atomic states $\phi_j(\underline{r})$. This model includes the effect of polarization, and the results obtained show the expected peak in the forward direction. Doubts remain, however, as to the consistency of the approximation. Firstly, it is difficult to choose a value for $\bar{k}^2$ that is justified on physical grounds. Woollings and McDowell (1972) indicate that the best agreement with experiment is obtained with the choice of Holt et al (1971) where $\bar{k}^2$ is taken to be the energy of the lowest lying state not explicitly represented in the j summation in (1.58). Secondly, while the second Born amplitude includes all terms to second order in the potential, Kingston et al (1960) show that the corresponding differential cross-section excludes some fourth order terms. Thirdly, Byron and Joachain (1973) show that for k_i sufficiently large and denoting the momentum transfer by q

$$\bar{f}_{B2}(k_i, q) = \frac{A(q)}{k_i^2} + i\,\frac{B(q)}{k_i} \qquad (1.59)$$

for elastic scattering, while there is a further contribution of order $\overset{k^{-2}}{\cancel{\bar{k}^2}}$ from the term $\bar{f}_{B3}$. Thus the second Born approximation neglects some terms of order $\overset{k^{-2}}{\cancel{\bar{k}^2}}$ from both the scattering amplitude and the cross-section. Finally both first and second Born approximations neglect exchange and will therefore certainly be in error for energies less than 100 eV.

1.5 The Glauber Approximation

When the projectile-target interaction vanishes for Z larger than some finite value the exponent in (1.32) will always be small for sufficiently high energies. It is assumed therefore that

$$\frac{\partial}{\partial z} c_n(\underline{b}, z) = \frac{1}{ik_i} \sum_j V_{nj}(\underline{r}_2) c_j(\underline{b}, z) \tag{1.60}$$

This has the exact solution

$$c_n(\underline{b}, z) = \int d\underline{r}\, \phi_n^*(\underline{r}) \exp\left\{ \frac{1}{ik_i} \int_{-\infty}^{z} V(\underline{b}, z'; \underline{r})\, dz' \right\} \phi_i(\underline{r}) \tag{1.61}$$

which may be verified by substituting into (1.60) and performing closure of the j states.

The Glauber approximation (Glauber 1959) to the scattering amplitude is then, from (1.39),

$$f_{if}(\theta) = -\frac{ik_i}{2\pi} \int d\underline{b}\, d\underline{r}\, e^{i\underline{q}\cdot\underline{b}}\, \phi_f^*(\underline{r}) \left[e^{i\chi(\underline{b},\underline{r})} - 1 \right] \phi_i(\underline{r}) \tag{1.62}$$

where the Glauber phase $\chi(\underline{b},\underline{r})$ is

$$\chi(\underline{b}, \underline{r}) = -\frac{1}{k_i} \int_{-\infty}^{\infty} V(\underline{b}, z'; \underline{r})\, dz' \tag{1.63}$$

Franco (1968) puts $\underline{r} = \underline{s} + \xi\, \hat{\underline{k}}_i$, where $\underline{s}$ is the projection of $\underline{r}$ onto the plane containing $\underline{b}$, and finds this phase to be

$$\chi(\underline{b}, \underline{r}) = \frac{2}{k} \ln \frac{|\underline{b} - \underline{s}|}{b} \tag{1.64}$$

There are several undesirable features inherent in the Glauber approximation including the logarithmic divergence of the elastic cross-section in the forward direction, the selection rule $\Delta m \neq 0$ for s-p transitions, and the prediction of identical results for electron and positron scattering. The latter two deficiencies have been removed in a modification proposed by Byron (1971), but this results in a considerably more complex approximation.

The Glauber approximation shares with the first Born approximation the distinction of yielding differential and integrated cross-sections in closed, though complicated, analytic forms (Thomas and Gerjuoy 1971) for electron-hydrogen collisions. This no doubt accounts for the surprising amount of attention that it has received, even though there seems to be little possibility of it providing definitive cross-sections at the intermediate energies. The applications can be traced from the recent work of Franco (1973); in each case the effect of exchange has been neglected, very little work having been done on the evaluation of the Glauber exchange amplitude (Tenney and Yates 1972, Byron and Joachain 1972).

The expansion of the exponential in (1.62) allows the Glauber amplitude to be expressed as a power series in the interaction

$$f^{G}_{if}(\theta) = \sum_{n=1}^{\infty} \bar{f}_{Gn} \qquad (1.65)$$

where

$$\bar{f}_{Gn} = -\frac{ik_i}{2\pi}\frac{i^n}{n!}\int d\underline{b}\, d\underline{r}\, e^{i\underline{q}\cdot\underline{b}}\, \phi^*_f(\underline{r})\, \chi(\underline{b},\underline{r})\, \phi_i(\underline{r}) \qquad (1.66)$$

Expansion (1.65) is the Glauber eikonal series and provided that the Z axis has been chosen as the bisector of the scattering angle, the first term equals the first Born approximation $\bar{f}_{B1}$ (Glauber 1959, Byron et al 1973).

The rate of convergence of (1.65) has been investigated by Yates (1974) who finds it to be rapid for electron-hydrogen scattering at energies where the Glauber approximation itself is valid. This provides an alternative means for calculating the Glauber amplitude and is especially useful for collisions with complex atoms.

1.6 The Eikonal-Born Series

For sufficiently high energy k^2, each term in the Born series may be written for $n \geqslant 2$ as

$$\bar{f}_{B_n} \sim i^{n-1}\,\frac{A_n(q)}{k^{n-1}} + i^{n}\,\frac{B_n(q)}{k^{n}} \qquad (1.67)$$

and for scattering by Yukawa potentials Byron et al (1973) provide convincing evidence that the corresponding term in the Glauber eikonal series is

$$\bar{f}_{G_n} = i^{n-1}\,\frac{A_n(q)}{k^{n-1}} \qquad (1.68)$$

where $A_n(q)$ is identical with that of (1.67) for all momentum transfers q.

For electron-atom collisions, the long range forces present make the above relationships invalid for n=2 at small momentum transfers (Byron and Joachain 1973, 1974). However, it has been conjectured by Byron and Joachain (1973) that (1.67) and (1.68) are true for $n \geqslant 3$ at all momentum transfers, although this is not possible to demonstrate by direct computation. On the basis of this hypothesis, Byron and Joachain

(1973) suggest that the term $\bar{f}_{G3}$ ($=\mathrm{Re}\bar{f}_{B3}$) be added to the second Born amplitude so that all terms in the Born series for the scattering amplitude are included to order k^{-2}. The resulting Eikonal-Born series (EBS) approximation is then

$$f_{if}^{EBS}(\theta) = \bar{f}_{B1} + \mathrm{Re}\,\bar{f}_{B2} + \bar{f}_{G3} + i\,\mathrm{Im}\,\bar{f}_{B2} \qquad (1.69)$$

By combining this with the approximation of Ochkur (1964) for the exchange amplitude, the effect of exchange is also included to order k^{-2}.

The application of the EBS method to elastic electron-hydrogen and helium scattering has been made by Byron and Joachain (1973, 1973a, 1974) and gives agreement with differential cross-section measurements better than that of previous models. However, despite the success of this method, some reservations must be expressed. Firstly, as it is the differential cross-section that is compared with experiment, it would be more proper to demand consistency in this quantity, to a given order in k^{-1}, rather than in the scattering amplitude. The EBS method in fact, while working to order k^{-2} in $f_{if}(\theta)$, only includes two of six possible terms of order k^{-4} in the cross-section. From Table I of Byron and Joachain (1973) we can estimate that at 300 eV and 30^0 the inclusion of one of these neglected terms, $\mathrm{Im}\bar{f}_{B2}\ \mathrm{Im}\bar{f}_{G4}$, would lower their cross-section by 6%. There is always the possibility of cancellation between the excluded terms however, and further investigation into this is required. Secondly the Ochkur approximation is a high energy approximation to the Born-Oppenheimer exchange amplitude and we must question its use, as well as the adoption of the asymptotic expression (1.67), for energies as low as 50 eV. Finally, it is difficult to see how the method could be systematically improved to give consistency to higher orders in k^{-1}, in order to extend its application throughout the intermediate energy range.

1.7 The Distorted Wave Born Approximation

We consider now an exact expression for the scattering amplitude, known as the two potential formula (Rodberg and Thaler 1967 p321). This relationship may be approximated in a variety of ways, the most widely used form being known as the distorted wave Born approximation (DWBA). We derive this here for the case of electron-hydrogen scattering, and include the possibility of exchange by using the correctly symmetrized wave function for the total system, namely

$$\Psi_S(\underline{r}_1,\underline{r}_2) = \Psi(\underline{r}_1,\underline{r}_2) + (-1)^S\,\Psi(\underline{r}_2,\underline{r}_1) \qquad (1.70)$$

where $\underline{r}_1$ and $\underline{r}_2$ denote the space co-ordinates of the initially bound and incoming electron respectively.

Let H_0 be the unperturbed Hamiltonian with eigenstates $\Phi(\underline{r}_1,\underline{r}_2)$ and eigenvalue equal to the total energy E, then we have

$$\left[H_0 - E\right]\Phi(\underline{r}_1,\underline{r}_2) = 0 \qquad (1.71)$$

and

$$\left[H_0 + V - E\right]\Psi_S(\underline{r}_1,\underline{r}_2) = 0 \qquad (1.72)$$

where V is the projectile target interaction.

We next define the distorted wave $X(\underline{r}_1,\underline{r}_2)$ by

$$\left[H_0 + V_1 - E\right] X(\underline{r}_1,\underline{r}_2) = 0 \tag{1.73}$$

for some as yet unspecified potential V_1.

We further introduce the function $\xi(\underline{r}_1,\underline{r}_2)$ defined by

$$\Psi_S(\underline{r}_1,\underline{r}_2) = \Phi(\underline{r}_1,\underline{r}_2) + \xi(\underline{r}_1,\underline{r}_2) + (-1)^S \Psi(\underline{r}_2,\underline{r}_1) \tag{1.74}$$

which consequently is asymptotic to a superposition of products of outgoing waves and bound state wavefunctions.

Nor re-writing (1.72) as

$$\left[H_0 + V_1 - E\right] \Psi_S(\underline{r}_1,\underline{r}_2) = -(V - V_1)\Psi_S(\underline{r}_1,\underline{r}_2) \tag{1.75}$$

we substitute (1.74) in the above and invoke (1.71) to give

$$\left[H_0 + V_1 - E\right] \xi(\underline{r}_1,\underline{r}_2) = -(V - V_1)\Psi_S(\underline{r}_1,\underline{r}_2) - V_1 \Phi(\underline{r}_1,\underline{r}_2) +$$

$$- (-1)^S \left[H_0 + V_1 - E\right] \Psi(\underline{r}_2,\underline{r}_1) \tag{1.76}$$

Finally, we recall equation (1.73) and solve (1.76) by the technique described by Mott and Massey (1965 p75). From the boundary condition for $\xi(\underline{r}_1,\underline{r}_2)$ we then deduce the two potential formula for the scattering amplitude,

$$f_{if}(\theta) = -\frac{1}{2\pi}\int d\underline{r}_1 d\underline{r}_2\, X_f^{*-}(\underline{r}_1,\underline{r}_2)\left[V - V_1\right]\Psi_S^{+}(\underline{r}_1,\underline{r}_2) -$$

$$-\frac{1}{2\pi}\int d\underline{r}_1 d\underline{r}_2\, X_f^{*-}(\underline{r}_1,\underline{r}_2) V_1 \Phi_i(\underline{r}_1,\underline{r}_2) \tag{1.77}$$

This formula may be simplified by the judicious choice of V_1. Specifically, if we put

$$X_f(\underline{r}_1,\underline{r}_2) = \phi_f(\underline{r}_1)\chi_f(\underline{r}_2) \qquad (1.78)$$

and

$$\Phi_i(\underline{r}_1,\underline{r}_2) = \phi_i(\underline{r}_1)e^{i\underline{k}_i\cdot\underline{r}_2} \qquad (1.79)$$

then from (1.77) we see immediately that choosing V_1 to depend only on the co-ordinates $\underline{r}_2$ of the incoming electron causes the second integral in (1.77) to vanish for inelastic scattering, due to the orthogonality of the bound state wavefunctions $\phi_f(\underline{r}_1)$ and $\phi_i(\underline{r}_1)$. A suitable choice for V_1 is the static interaction potential between the projectile and atom in the final state, $V_{ff}(\underline{r}_2)$, and the two potential formula then becomes

$$f^S_{if}(\theta) = -\frac{1}{2\pi}\int d\underline{r}_1 d\underline{r}_2\, X_f^{*-}(\underline{r}_1,\underline{r}_2)\left[V - V_{ff}(\underline{r}_2)\right]\left[\Psi_i^+(\underline{r}_1,\underline{r}_2) + (-1)^S\,\Psi_i^+(\underline{r}_2,\underline{r}_1)\right] \qquad (1.80)$$

where it is stressed that the above is still exact.

We note that in the above derivation the imposition of incoming rather than outgoing wave boundary conditions on $\Psi_S(\underline{r}_1,\underline{r}_2)$ leads to the alternative two-potential formula:-

$$f_{if}(\theta) = -\frac{1}{2\pi}\int d\underline{r}_1 d\underline{r}_2\, \Psi_S^{*-}(\underline{r}_1,\underline{r}_2)\left[V - V_1\right]X_i^+(\underline{r}_1,\underline{r}_2) - \frac{1}{2\pi}\int d\underline{r}_1 d\underline{r}_2\, \Phi_f^*(\underline{r}_1,\underline{r}_2)V_1 X_i^+(\underline{r}_1,\underline{r}_2) \qquad (1.81)$$

which may be simplified in identical manner when V_1 is chosen this time to be the static potential in the initial state, V_{ii}, giving

$$f^S_{if}(\theta) = -\frac{1}{2\pi}\int d\underline{r}_1 d\underline{r}_2 \left[\Psi^-_f(\underline{r}_1,\underline{r}_2) + (-1)^S \Psi^-_f(\underline{r}_2,\underline{r}_1)\right]^* \left[V - V_{ii}(\underline{r}_2)\right] \chi^+_i(\underline{r}_1,\underline{r}_2) \qquad (1.82)$$

The generalization to the case where V_1 is chosen as a complex potential is given by Rodberg and Thaler (1967 p326).

The DWBA now consists simply of approximating $\Psi^+_i(\underline{r}_1,\underline{r}_2)$ in (1.80) by $\chi_i^+(\underline{r}_1,\underline{r}_2)$, or alternatively using $\chi_f^-(\underline{r}_1,\underline{r}_2)$ in place of $\Psi^-_f(\underline{r}_1,\underline{r}_2)$ in (1.82) to give, after some rearrangement,

$$f^{DWBA}_{if}(\theta) = -\frac{1}{2\pi}\int d\underline{r}_1 d\underline{r}_2\, \chi^{*-}_f(\underline{r}_1,\underline{r}_2) V \chi^+_i(\underline{r}_1,\underline{r}_2) - (-1)^S \frac{1}{2\pi}\int d\underline{r}_1 d\underline{r}_2\, \chi^{*-}_f(\underline{r}_1,\underline{r}_2)\left[V - V_1\right]\chi^+_i(\underline{r}_2,\underline{r}_1) \qquad (1.83)$$

where a) V_1 is $V_{ff}(\underline{r}_2)$ in which case V is the post interaction

or b) V_1 is $V_{ii}(\underline{r}_1)$ in which case V is the prior interaction.

The forms a) and b) are derived from (1.80) and (1.82) respectively. The first term in (1.83) is the direct scattering amplitude, while the second is the exchange amplitude.

The evaluation of (1.83) requires us to generate the function $\chi_\alpha(\underline{r}_2)$, where α is either i or f. Substituting (1.78) into (1.73) we deduce that it satisfies the equation

$$\left[\nabla^2 + k^2_\alpha\right]\chi_\alpha(\underline{r}_2) = 2V_{\alpha\alpha}(\underline{r}_2)\chi_\alpha(\underline{r}_2) \qquad (1.84)$$

This should, in principle, be solved with either outgoing or incoming wave boundary conditions. However, we note that in

(1.83) the complex conjugate of $\chi^-_f(\underline{r}_2)$ is required, and from the general relationship (Bransden 1970 p35)

$$\left[\Psi^-_{\underset{\sim}{k}}(\underline{r})\right]^* = \Psi^+_{-\underset{\sim}{k}}(\underline{r}) \qquad (1.85)$$

we conclude that (1.84) is solved with outgoing wave boundary conditions for α equal to both i and f.

The DWBA with its assumption that distortion in either the initial or final states is predominantly due to the static interaction, is expected to give good results for transitions between weakly coupled states. Excellent agreement with experiment has indeed been obtained by Madison and Shelton (1973) for excitation to the 2^1P level of helium.

Finally, we note that an expression similar to (1.83)has been obtained by Mott and Massey (1965 p420) from the truncated eigenfunction expansion, which they call the distorted wave approximation. This differs from the DWBA expression for the scattering amplitude by having V_1 equal to $k_i^2 - 2\varepsilon_f$, where ε_f is the energy of the bound state $\phi_f(\underline{r})$.

Chapter 2 Present Model of Elastic Scattering

2.1 Applicability

In this chapter we propose to expand the equations of the second-order potential method (1.12 and 1.13) in partial wave series. This avoids the uncertainty concerning the validity of the impact parameter approximation used in its previous applications, and also permits the effect of exchange to be included. In principle, the number of terms explicitly represented in the method can then be varied to give a general description of both elastic and inelastic scattering of charged particles by any light atom, at energies above the first ionization threshold. The resulting model however is very complicated and it is more expedient to consider first of all the simplest approximation of truncating (1.12) at M=1. This is called the one channel approximation and gives a description of elastic scattering only. It also restricts applications to scattering from atoms of low polarizability; hydrogen and the lighter inert gases for instance. For electron-alkali scattering, 98% of the high polarizability comes from the first excited p state (Bransden 1970 p227), and in this case at least a two-channel approximation is required.

Application of our model will be made therefore to electron scattering from hydrogen, for which the bound-state wavefunctions are known exactly, and from helium, this being the simplest of the inert gases. There are considerable problems in carrying out scattering experiments with atomic hydrogen, which is reflected in the scarcity of the data. The success of the present model will therefore be judged for the most part by comparison with the large number of electron-helium measurements that have been made. The analysis required will be illustrated as usual for the case of electron-hydrogen collisions.

2.2 Many Channel Partial Wave Formulation

The partial wave formulation of the second order potential method is most easily derived from the close-coupling equations (1.21). Choosing a value for ν, N say, such that states having $\nu > N$ are coupled only to those with $\nu \leq N$ we have

$$\mathcal{L}_n F^L_\nu(r) = 2\sum_{\nu'} VW_{\nu\nu'}(r)\, F^L_{\nu'}(r) \qquad \nu \leq N \qquad (2.1)$$

and

$$\mathcal{L}_n F^L_\nu(r) = 2\sum_{\nu'=1}^{N} VW_{\nu\nu'}(r)\, F^L_{\nu'}(r) \qquad \nu > N \qquad (2.2)$$

where the abbreviation

$$VW_{\nu\nu'}(r) = V_{\nu\nu'}(r) - W_{\nu\nu'}(r) \qquad (2.3)$$

has been introduced, and all other quantities are defined by equations (1.22) to (1.28).

Proceeding as in the development of (1.9) we introduce the free particle radial Green's function $g_\ell(k^2_n;r,r')$ satisfying outgoing wave boundary conditions, which is the solution of

$$\mathcal{L}_n g_\ell(k_n^2;r,r') = \delta(r-r') \qquad (2.4)$$

and is given explicitly by (Bransden 1970 p14)

$$g_\ell(k_n^2;r,r') = -ik_n rr'\, j_\ell(k_n r_<)\, h_\ell^{(1)}(k_n r_>) \qquad (2.5)$$

where $r_< = \min(r,r')$, $r_> = \max(r,r')$ and $j_\ell(x)$ and $h_\ell^{(1)}(x)$ are the spherical Bessel functions of the first and third kind defined by Abramowitz and Stegun (1965 p437). The solution of (2.2) is now expressed as

$$F^L_\nu(r) = 2\int_0^\infty dr'\, g_{\ell_2}(k_n^2; r, r') \sum_{\nu'=1}^{N} VW^L_{\nu\nu'}(r')\, F^L_{\nu'}(r') \qquad \nu > N \tag{2.6}$$

which on substitution into (2.1) gives for $\nu \leq N$

$$\begin{aligned} \mathcal{L}_n F^L_\nu(r) &= 2\sum_{\nu'=1}^{N} VW^L_{\nu\nu'}(r)\, F^L_{\nu'}(r) + \\ &+ 4\sum_{\nu'>N}^{\infty}\sum_{\nu''=1}^{N}\int_0^\infty dr'\, g_{\ell_2'}(k_{n'}^2; r, r')\, V^L_{\nu\nu'}(r)\, V^L_{\nu'\nu''}(r')\, F^L_{\nu''}(r') \end{aligned} \tag{2.7}$$

In obtaining (2.7) all exchange terms that are to second order in the potential, such as $V^L_{\nu\nu'}(r)$ $W^L_{\nu'\nu''}(r')$ and $W^L_{\nu\nu'}(r)$ x $W^L_{\nu'\nu''}(r')$, have been neglected. These terms correspond physically to exchange polarization effects which are generally considered to be small (Callaway et al 1968), particularly at the energies considered here.

Examining the ranges of the subscripts ν, ν' and ν'' in (2.7), it is seen that ν and ν'' are never equal to ν', and the Kronecker deltas in the definition (1.23) of $V^L_{\nu\nu'}(r)$ and $V^L_{\nu'\nu''}(r')$ are therefore always zero. This allows us to replace the product of potentials in (2.7) by $\bar{V}^L_{\nu\nu'}(r)$ $\bar{V}^L_{\nu'\nu''}(r')$ where

$$\begin{aligned} \bar{V}^L_{\nu\nu'}(r)\,\bar{V}^L_{\nu'\nu''}(r') &= \sum_{\lambda\lambda'} f_\lambda(\ell_1\ell_2\ell_1'\ell_2'|L)\, f_{\lambda'}(\ell_1'\ell_2'\ell_1''\ell_2''|L)\; \times \\ &\times\; y_\lambda(P_{n\ell_1} P_{n'\ell_1'}|r)\, y_{\lambda'}(P_{n'\ell_1'} P_{n''\ell_1''}|r') \end{aligned} \tag{2.8}$$

Furthermore, replacing $k_{n'}^2$ in the Green's function by an average energy $\bar{k}^2$ allows the closure of the $P_{n'\ell_1'}(x)$ states in (2.8) to be invoked, provided that the ν' summation in (2.7) is extended over all values. Specifically, we have

$$\sum_{\nu'=1}^{\infty} P_{n'\ell_1'}(r)\,P_{n'\ell_1'}(r') = \sum_{\ell_1'\ell_2'}\sum_{n'=\ell_1'+1}^{\infty} P_{n'\ell_1'}(r)\,P_{n'\ell_1'}(r') = \sum_{\ell_1'\ell_2'}\delta(r-r') \tag{2.9}$$

which allows us to write

$$\sum_{\nu'=1}^{\infty} y_\lambda(P_{n\ell_1},P_{n'\ell_1'}|r)\,y_{\lambda'}(P_{n'\ell_1'}\,P_{n''\ell_1''}|r') = \sum_{\ell_1'\ell_2'} Z_{\lambda\lambda'}(P_{n\ell_1},P_{n''\ell_1''}|r\,r') \tag{2.10}$$

where we have introduced the definition

$$Z_{\lambda\lambda'}(AB|rr') = \int_0^\infty A(t)\,B(t)\,\frac{\min^\lambda(r,t)}{\max^{\lambda+1}(r,t)}\,\frac{\min^{\lambda'}(r',t)}{\max^{\lambda'+1}(r',t)}\,dt \tag{2.11}$$

Finally then, the closure approximation together with the replacement given by (2.8) simplify (2.7) to the form:-

$$\begin{aligned} \mathcal{L}_n F_\nu^L(r) = {} & 2\sum_{\nu'=1}^{N} V\,W_{\nu\nu'}^L(r)\,F_{\nu'}^L(r) + 4\sum_{\nu''=1}^{N}\sum_{\ell_1'\lambda\lambda'\ell_2'} f_\lambda(\ell_1\ell_2\ell_1'\ell_2'|L)\,\times \\ & \times f_{\lambda'}(\ell_1'\ell_2'\ell_1''\ell_2''|L)\int_0^\infty dr'\,g_{\ell_2'}(\bar{k}^2;r,r')\,H_{n\ell_1,n''\ell_1''}^{\lambda\lambda'}(r,r')\,F_{\nu''}^L(r') \end{aligned} \tag{2.12}$$

for ν≤N, where

$$\begin{aligned} H_{n\ell_1,n''\ell_1''}^{\lambda\lambda'}(r,r') = {} & Z_{\lambda\lambda'}(P_{n\ell_1},P_{n''\ell_1''}|r\,r') - \\ & - \sum_{\nu'=1}^{N} y_\lambda(P_{n\ell_1}P_{n'\ell_1'}|r)\,y_{\lambda'}(P_{n'\ell_1'}\,P_{n''\ell_1''}|r') \end{aligned} \tag{2.13}$$

and all other quantities are defined in either this section, or in Section 1.2.

It is emphasized that (2.12) is equivalent to the second order potential equations in configuration space (1.12), except that the present method also includes all first order exchange terms in the channels $\nu < N$. In both formulations the introduction of the closure approximation necessitates a choice for the average energy $\bar{k}^2$.

2.3 The One Channel Approximation

Equation (2.12) simplifies considerably for the approximation of retaining one channel explicitly, so that N=1. The sets of quantum numbers ν and ν'' become $(10\ell_2)$ and $(10\ell_2'')$ respectively and (2.12) becomes

$$\mathcal{L}_1 F^L_{10\ell_2}(r) = 2VW^L_{10\ell_2 10\ell_2'}(r) F^L_{10\ell_2'}(r) + 4 \sum_{\ell_1' \lambda\lambda' \ell_2'} f_\lambda(0\ell_2\ell_1'\ell_2'|L) \times$$

$$\times f_{\lambda'}(\ell_1'\ell_2' 0\ell_2''|L) \int_0^\infty dr'\, g_{\ell_2'}(\bar{k}^2; r, r') H^{\lambda\lambda'}_{1010}(r, r') F^L_{10\ell_2''}(r) \qquad (2.14)$$

with

$$H^{\lambda\lambda'}_{1010}(r, r') = Z_{\lambda\lambda'}(\rho_{10}^2|rr') - y_\lambda(\rho_{10}^2|r) y_{\lambda'}(\rho_{10}^2|r') \times$$

$$\times \delta_{\ell_1' 0} \delta_{\ell_2' 0} \qquad (2.15)$$

In Appendix A it is shown that the angular coefficient $f_\lambda(0\ell_2\ell_1'\ell_2'|L)$ is given by

$$f_\lambda(0\ell_2\ell_1'\ell_2'|L) = (-1)^{\ell_2' - \ell_1'} \left(\frac{2\ell_2'+1}{2\ell_1'+1}\right)^{\frac{1}{2}} \delta_{\lambda\ell_1'} \delta_{\ell_2 L} \begin{pmatrix} \ell_1' & \ell_2' & L \\ 0 & 0 & 0 \end{pmatrix} \qquad (2.16)$$

where the notation for the Wigner 3-j symbol is that of Messiah (1964). The expression for the coefficient $f_\lambda(\ell_1'\ell_2' 0\ell_2''|L)$ follows immediately from (2.16) together with the relation (Percival and Seaton 1957)

$$f_\lambda(\ell_1'\ell_2'\ell_1''\ell_2''|L) = f_\lambda(\ell_1''\ell_2''\ell_1'\ell_2'|L) \qquad (2.17)$$

The appearance of the Kronecker delta $\delta_{\ell_2 L}$ in (2.16) is to be expected, since it expresses the fact that for collisions with the s state ($\ell_1=0$) of an atom, the total angular momentum L equals that of the incident particle, ℓ_2.

The coefficients $g_\lambda(0\ell_2 0\ell_2'|L)$ and $f_\lambda(0\ell_2 0\ell_2'|L)$ which are implicit in the term $VW^L_{10\ell_2,10\ell_2'}$ are easily found from (1.28) and (2.16) to be equal to $\delta_{\ell_2 L}\delta_{\ell_2\ell_2'}\delta_{\lambda 0}$

In a simplified notation therefore, in which ℓ denotes the incident angular momentum and the superscript S distinguishes between singlet and triplet solutions, equations (2.14) and (2.15) become

$$\left[\frac{d^2}{dr^2} + k_0^2 - \frac{\ell(\ell+1)}{r^2}\right] F_\ell^S(r) = 2V(r)F_\ell^S(r) +$$

$$+ 2\int_0^\infty \left[K_\ell^S(r,r') + h_\ell(r,r')\right] F_\ell^S(r')\,dr' \qquad (2.18)$$

where

$$V(r) = -\frac{1}{r} + y_0(P_{10}P_{10}|r) \qquad (2.19)$$

and the exchange and second order potential kernels equal

$$K_\ell^S(r,r') = \frac{(-1)^S}{2\ell+1} P_{10}(r)P_{10}(r')\left[\frac{\min^\ell(r,r')}{\max^{\ell+1}(r,r')} + \left(\epsilon_0 - \frac{k_0^2}{2}\right)\delta_{\ell 0}\right] \qquad (2.20)$$

and $$h_\ell(r,r') = -i\bar{k}rr'\sum_{\lambda=0}^{\infty}(2\lambda+1)j_\lambda(\bar{k}r_<)h_\lambda^{(1)}(\bar{k}r_>) \times 2$$

$$\times \sum_{n=0}^{\infty}\frac{1}{2n+1}\begin{pmatrix}\ell & \lambda & n\\ 0 & 0 & 0\end{pmatrix}^2 \left\{Z_{nn}(P_{10}^2|rr') - \delta_{n0}y_0(P_{10}^2|r)y_0(P_{10}^2|r')\right\}$$

$$(2.21)$$

ε_0 is the ground state of the atom and as usual $k_0^2 = 2(E - \varepsilon_0)$

For each value of λ, the number of terms in the n summation is finite, since the 3-j symbol vanishes unless n, ℓ and λ are such that $n+\ell+\lambda$ is even and $|\lambda - \ell| \leqslant n \leqslant \lambda + \ell$.

The boundary condition for (2.18) is, from (1.29)

$$F_\ell^S(r) \underset{r \to \infty}{\sim} \sin\left(k_0 r - \ell\frac{\pi}{2}\right) + T_\ell^S e^{i(k_0 r - \ell\frac{\pi}{2})} \qquad (2.22)$$

and on obtaining the partial wave amplitude T_ℓ^S the scattering amplitude $f^S(\theta)$ is calculated from (1.30). Finally on summing over the final and averaging over the initial spin states we obtain the differential cross-section for elastic electron-hydrogen scattering:-

$$\frac{d\sigma}{d\Omega} = \frac{1}{4}\left|f^0(\theta)\right|^2 + \frac{3}{4}\left|f^1(\theta)\right|^2 \qquad (2.23)$$

Comparing (2.18) with the work of John (1960) shows our one channel model to be the static exchange approximation with the addition of a non-local potential to account for the distortion of the atom and the loss of flux into the inelastic channels.

The many channel partial wave equations for electron-helium scattering are derived through a development identical to that of Section 2.2, but beginning with the close-coupling equations of Burke et al (1969) rather than those of (1.21). Specialising to the one channel case then gives, as before, the static exchange approximation with a non-local potential. However, Burke et al (1969) make the assumption that the reduction of the exchange kernel which is carried out when the bound state helium functions are exact, is still valid when approximate wave functions are used. This introduces an error which they suggest may be quite large for the S-wave phase shifts. An alternative procedure (Drukarev 1965 p127) is to anticipate that approximate helium wave functions must be used, and to reduce the exchange kernel in a manner consistent with this. We choose to use the form resulting from this latter method, rather than that of Burke et al (1969).

Defining the helium radial wave functions by

$$\phi_1(\underline{r}_1,\underline{r}_2) = \frac{P_{10}(r_1)}{r_1} Y_{00}(\hat{\underline{r}}_1)\frac{P_{10}(r_2)}{r_2} Y_{00}(\hat{\underline{r}}_2) \tag{2.24}$$

the one-channel equations for electron-helium scattering are therefore

$$\left[\frac{d^2}{dr^2} + k_0^2 - \frac{\ell(\ell+1)}{r^2}\right]F_\ell(r) = 2V(r)F_\ell(r) + 2\int_0^\infty \Big[K_\ell(r,r') + h_\ell(r,r')\Big]F_\ell(r')\,dr' \tag{2.25}$$

where the static potential and exchange kernel are now (Drukarev 1965)

$$V(r) = -\frac{2}{r} + 2y_0(P_{10}^2|r) \tag{2.26}$$

and

$$K_\ell(r,r') = -\frac{P_{10}(r)P_{10}(r')}{(2\ell+1)}\frac{\min^\ell(r,r')}{\max^{\ell+1}(r,r')} + q(r,r')\,\delta_{\ell 0} \tag{2.27}$$

with

$$q(r,r') = P_{10}(r')\Big\{-\frac{1}{2}V(r) - \frac{1}{2}V(r') + \frac{1}{r} + \frac{1}{r'} + \frac{1}{2}\frac{d^2}{dr^2} + E + \int_0^\infty P_{10}(x)\left[\frac{1}{2}\frac{d^2}{dx^2} + \frac{2}{x}\right]P_{10}(x)\,dx\Big\}P_{10}(r) + \frac{P_{10}(r)}{2}\frac{d^2}{dr'^2}P_{10}(r') \tag{2.28}$$

The second order potential $h_\ell(r,r')$ is equal to $\overset{2}{\cancel{4}}$ times that defined by (2.21), where the function $P_{10}(r)$ is now of course given by (2.24).

The reduction of the configuration space exchange kernel of Drukarev (1965) to the partial wave form of (2.27) is outlined in Appendix B, and the explicit expression for $q(r,r')$ is given for the case of $P_{10}(r)$ having the particular form $Nr\,(e^{-ar} + ce^{-br})$. Values for the parameters N, a, b and c have been given by Byron and Joachain (1966) and this approximation to the helium ground state wave function will be used in the application of our one channel model.

The partial wave amplitude T_ℓ and scattering amplitude $f(\theta)$ are obtained from the condition (2.22) and definition (1.30), the superscript S now being unnecessary as there is only one final total spin state. The differential cross-section for elastic electron-helium scattering is then

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 \qquad (2.29)$$

The evaluation of the integrals $y_0(P_{10}{}^2|r)$ and $z_{\ell\ell}(P_{10}{}^2|rr')$ is required in the present approximation in order that $h_\ell(r,r')$ may be calculated. While the former integral is easily expressible in analytic form, the latter requires closer examination. In general, $z_{\ell\ell}(P_{10}{}^2|rr')$ will be a linear combination of integrals of the form $M_\ell(\alpha|rr')$, where

$$M_\ell(\alpha|rr') = \int_0^\infty x^2 e^{-\alpha x}\,\frac{\min^\ell(r,x)}{\max^{\ell+1}(r,x)}\,\frac{\min^\ell(r',x)}{\max^{\ell+1}(r',x)}\,dx \qquad (2.30)$$

Introducing the notation $r_< = \min(r,r')$ and $r_> = \max(r,r')$ (2.30) is expressed as the sum of three integrals:-

$$M_\ell(\alpha|rr') = \frac{1}{(r_< r_>)^{\ell+1}}\int_0^{r_<} e^{-\alpha x} x^{2\ell+2}\,dx + \frac{r_<^{\ell}}{r_>^{\ell+1}}\int_{r_<}^{r_>} x\, e^{-\alpha x}\,dx$$

$$+ (r_< r_>)^{\ell}\int_{r_>}^{\infty} e^{-\alpha x} x^{-2\ell}\,dx \qquad (2.31)$$

$$= A_\ell(\alpha|rr') + B_\ell(\alpha|rr') + C_\ell(\alpha|rr') \qquad (2.32)$$

Recurrence relations for A_ℓ, B_ℓ and C_ℓ are obtained following integration by parts, and these are given in Appendix C together with their initial values. The expressions for $y_0(P_{10}^2|r)$ are presented in Appendix D.

Due to the complicated form of the second order potential, it will be useful to derive an asymptotic expression for $h_\ell(r,r')$ as $r_>$ becomes large. Examination of the defining equations for $z_{00}(P_{10}^2|rr')$ and $y_0(P_{10}^2|r)\, y_0(P_{10}^2|r')$ shows that for large $r_>$ these terms become equal. Furthermore, it is seen from Appendix C that $C_n(\alpha|rr')$ vanishes exponentially for large $r_>$, while $A_n(\alpha|rr')$ and $B_n(\alpha|rr')$ behave as $r_>^{-1-n}$. We have therefore that

$$z_{nn}(P_{10}^2|rr') \underset{r_> \to \infty}{\sim} \frac{S_n(r_<)}{r_>^{n+1}} \qquad (2.33)$$

where $S_n(r_<)$ is some function of $r_<$ that may be found from the recurrence relations for A_n and B_n, and the particular relationship between $z_{nn}(P_{10}^2|rr')$ and $M_n(\alpha|rr')$. Referring to equation (2.21), the leading term in the asymptotic expansion of $h_\ell(r,r')$ is thus of order $r_>^{-2}$, and arises from the $n=1$ contribution:-

$$h_\ell(r,r') = -i\bar{k}rr'\sum_{\lambda=\ell-1}^{\ell+1}(2\lambda+1)\,j_\lambda(\bar{k}r_<)\,h_\lambda^{(1)}(\bar{k}r_>)\,\frac{2}{3}\begin{pmatrix}1 & \lambda & \ell\\ 0 & 0 & 0\end{pmatrix}^2 \times$$

$$\times\,\frac{S_1(r_<)}{r_>^{2}} \quad + \quad O\left(r_>^{-4}\right) \tag{2.34}$$

Introducing explicit expressions for the 3-j symbols $\begin{pmatrix}1 & \ell\pm1 & \ell\\ 0 & 0 & 0\end{pmatrix}^2$ from Messiah (1964), (2.34) becomes

for $\ell=0$

$$h_0(r,r') \underset{r_>\to\infty}{\sim} -\frac{2i\bar{k}rr'}{3r_>^{2}}\,S_1(r_<)\,j_1(\bar{k}r_<)\,h_1^{(1)}(\bar{k}r_>) \tag{2.35}$$

and for $\ell\neq0$

$$h_\ell(r,r') \underset{r_>\to\infty}{\sim} -\frac{2i\bar{k}rr'}{3(2\ell+1)}\,\frac{S_1(r_<)}{r_>^{2}}\Big[\ell\, j_{\ell-1}(\bar{k}r_<)\,h_{\ell-1}^{(1)}(\bar{k}r_>)\,+$$

$$+\,(\ell+1)\,j_{\ell+1}(\bar{k}r_<)\,h_{\ell+1}^{(1)}(\bar{k}r_>)\Big] \tag{2.36}$$

To illustrate the calculation of $S_1(r_<)$ we consider electron-hydrogen scattering where, since $P_{10}(r) = 2re^{-r}$

$$Z_{11}(P_{10}^{2}|rr') = 4M_1(2|rr') \tag{2.37}$$

while from Appendix C

$$M_1(2|rr') \sim \frac{3}{4r_<^{2}} - \frac{3e^{-2r_<}}{4}\left(r_< + 2 + \frac{2}{r_<} + \frac{1}{r_<^{2}}\right) \tag{2.38}$$

and therefore from (2.33) we have

$$S_1(r_<) = \frac{3}{r_<^{2}} - 3e^{-2r_<}\left(r_< + 2 + \frac{2}{r_<} + \frac{1}{r_<^{2}}\right) \tag{2.39}$$

2.4 The Average Energy

The introduction of an average energy is an essential feature of the second order potential approximation. Although a value could be assigned to $\bar{k}^2$ on a purely phenomenological basis, the predictive nature of our model is ensured by requiring that $\bar{k}^2$ be chosen on theoretical grounds.

For an electron incident on the ground state of an atom, the force of longest range is that resulting from the polarization of the atom by the charged particle. Castillejo et al (1960) show that for large distances $\underline{r}$ from the atom, the electron then moves in a potential

$$U_p(r) = -\frac{\alpha_1}{r^4} + O(r^{-6}) \tag{2.40}$$

where α_1 is the dipole polarizability of the atom. Since this is also the potential resulting from the distortion of an atom by a static charge it is inferred that the adiabatic approximation, in which the projectile's velocity is neglected, is valid at sufficiently large distances from the atom.

Our choice for $\bar{k}^2$ will therefore be such that for large r equation (2.18) becomes

$$\left[\frac{d^2}{dr^2} + k_0^2 - \frac{\ell(\ell+1)}{r^2}\right] F_\ell^S(r) \underset{r\to\infty}{\sim} 2V(r)F_\ell^S(r) + U_p(r)F_\ell^S(r) \tag{2.41}$$

Since the exchange kernel vanishes exponentially at large distances, this is equivalent to the requirement that

$$2\int_0^\infty h_\ell^{AD}(r,r')F_\ell^S(r')\,dr' \underset{r\to\infty}{\sim} U_p(r)F_\ell^S(r) \tag{2.42}$$

where $h_\ell^{AD}(r,r')$ is the second order potential in the adiabatic approximation.

Now Bransden and Coleman (1972) give the free particle Green's function in the adiabatic approximation as

$$G^{AD}(k_n^2;\underline{r},\underline{r}') = \frac{\delta(\underline{r}-\underline{r}')}{2(\varepsilon_0-\varepsilon_n)} \qquad (2.43)$$

Also the partial wave expansion of $G(k_n^2;\underline{r},\underline{r}')$ is

$$G(k_n^2;\underline{r},\underline{r}') = \frac{1}{4\pi}\sum_{\ell=0}^{\infty}(2\ell+1)\frac{g_\ell(k_n^2;r,r')}{rr'}P_\ell(\cos\theta) \qquad (2.44)$$

which may be verified by substituting (2.44) into (1.10) to give (2.4).

Consequently substituting (2.44) into (2.43) and inverting the result allows us to deduce that

$$g_\ell^{AD}(k_n^2;r,r') = \frac{\delta(r-r')}{2(\varepsilon_0-\varepsilon_n)} \qquad (2.45)$$

where we have used

$$\delta(\underline{r}-\underline{r}') = \frac{\delta(r-r')}{rr'}\,\delta(\cos\theta-\cos\theta')\,\delta(\phi-\phi') \qquad (2.46)$$

Use of the adiabatic approximation to the radial Green's function (2.45) instead of (2.5) and proceeding as before with the derivation of the second order potential then gives

$$h_\ell^{AD}(r,r') = \frac{\delta(r-r')}{\varepsilon_0-\bar{\varepsilon}}\sum_{\lambda=0}^{\infty}(2\lambda+1)\sum_{n=0}^{\infty}\frac{1}{2n+1}\begin{pmatrix} n & \lambda & \ell \\ 0 & 0 & 0\end{pmatrix}^2 \times$$

$$\times\left\{Z_{nn}(\rho_{10}^2|rr') - y_0(\rho_{10}^2|r)\,y_0(\rho_{10}^2|r')\,\delta_{n0}\right\} \qquad (2.47)$$

We next note that the orthogonality condition of the 3-j symbols

$$\sum_{\ell_1} (2\ell_1+1) \begin{pmatrix} \ell_1 & \ell_2 & \ell_3 \\ m_1 & m_2 & M \end{pmatrix} \begin{pmatrix} \ell_1 & \ell_2 & \ell_3 \\ m_1' & m_2' & M \end{pmatrix} = \delta_{m_1 m_1'} \delta_{m_2 m_2'} \qquad (2.48)$$

allows the λ summation to be carried out, and therefore substituting (2.47) into (2.42) and integrating over r^1 gives the multipole expansion for $U_p(r)$:-

$$U_p(r) \underset{r\to\infty}{\sim} \frac{2}{(\varepsilon_0-\bar{\varepsilon})} \sum_{n=0}^{\infty} \frac{1}{2n+1} \left[Z_{nn}(\rho_{10}^2|rr) - y_0^2(\rho_{10}^2|r)\delta_{n0} \right] \qquad (2.49)$$

From the discussion at the end of the previous section we see that the monopole term in the above expansion vanishes, and the leading contribution to the polarization potential comes from the dipole term (n=1), in accord with the result of Castillejo et al (1960). In fact from (2.33) and (2.39) we find that for electron-hydrogen scattering

$$Z_{11}(\rho_{10}^2|rr) \underset{r\to\infty}{\sim} \frac{3}{r^4} \qquad (2.50)$$

and in this case it is concluded therefore that the average energy $\bar{k}^2$ must be chosen so that

$$\frac{2}{\varepsilon_0-\bar{\varepsilon}} = -\alpha_1 = -\frac{9}{2} \qquad (2.51)$$

where it is recalled that $k_0^2 + 2\varepsilon_0 = \bar{k}^2 + 2\bar{\varepsilon}$.

The calculation for electron-helium scattering proceeds in exactly the same way and it is found that $\bar{\varepsilon} - \varepsilon_0 = 1.13$, where we note however that this value now depends on the choice of wave function. To summarize therefore, the average energy is for hydrogen

$$\bar{k}^2 = k_0^2 - \frac{8}{9} \tag{2.52}$$

and for helium

$$\bar{k}^2 = k_0^2 - 2.26 \tag{2.53}$$

where k_0^2 is the energy in Rydbergs of the electron incident upon the ground state.

2.5 The Sasakawa-Austern Iteration

The present one channel model for elastic scattering requires the solution of a single second-order integro-differential equation. The close coupled equations of Burke and Schey (1962) despite containing integral terms can be reduced to a set of coupled differential equations. This is not possible in our case, however, due to the presence of the non-local potential. It is proposed therefore to adapt an iterative scheme introduced by Sasakawa (1963) and subsequently modified for applications in nuclear physics by Austern (1969) and Soper (1972).

The equation to be solved, (2.18), is written compactly as

$$\mathcal{L}_0 F_\ell(r) = \hat{U} F_\ell(r) \tag{2.54}$$

where $\hat{U}$ is an integral operator, and $\mathcal{L}_0^\ell$ is defined by (1.22). From (2.4) the solution of (2.54) satisfying outgoing wave boundary conditions is easily found to be

$$F_\ell(r) = S_\ell(k_0 r) + \int_0^\infty g_\ell(k_0^2; r, r') \hat{U} F_\ell(r') \, dr' \tag{2.55}$$

where we have written

$$S_\ell(k_0r) = k_0r\,j_\ell(k_0r) \underset{r\to\infty}{\sim} \sin\left(k_0r - \ell\frac{\pi}{2}\right) \tag{2.56}$$

this being the solution of $\mathcal{L}_0F_\ell(r) = 0$ that is regular at the origin. The function $e_\ell^+(x)$ is also introduced, given by

$$e_\ell^+(x) = ix\,h_\ell^{(1)}(x) \underset{r\to\infty}{\sim} e^{i(k_0r - \ell\frac{\pi}{2})} \tag{2.57}$$

so that the radial Green's function (2.5) may be re-written

$$g_\ell(k_0^2; r, r') = -\frac{1}{k_0} S_\ell(k_0r_<)\,e_\ell^+(k_0r_>) \tag{2.58}$$

Now substituting (2.58) into (2.55), and defining the coefficient T_ℓ by

$$T_\ell = -\frac{1}{k_0}\int_0^\infty S_\ell(k_0r)\,\hat{u}\,F_\ell(r)\,dr \tag{2.59}$$

together with the integral operator $\hat{P}$ by

$$\hat{P}F_\ell(r) = \frac{1}{k_0}\int_r^\infty \left\{e_\ell^+(k_0r)S_\ell(k_0r') - S_\ell(k_0r)e_\ell^+(k_0r')\right\}\hat{u}\,F_\ell(r')\,dr' \tag{2.60}$$

allows equation (2.55) to be expressed as

$$F_\ell(r) = S_\ell(k_0r) + T_\ell\,e_\ell^+(k_0r) + \hat{P}\,F_\ell(r) \tag{2.61}$$

In the limit as $r\to\infty$ $\hat{P}\,F_\ell(r)$ obviously vanishes, and on recalling the asymptotic forms (2.56) and (2.57) comparison of (2.61) with (1.29) shows that T_ℓ in fact is the partial wave amplitude.

An iterative solution of (2.61) has been proposed by Sasakawa (1963) and has been re-expressed by Austern (1969) in a form more suitable for numerical applications. In this method a zero-order trial solution is chosen as

$$F_\ell^{(0)}(r) = s_\ell(k_0 r) + T_\ell^{(0)} w_\ell^{(0)}(r) \tag{2.62}$$

where $T_\ell^{(0)}$ is as yet undetermined, and $w_\ell^{(0)}(r)$ is a function selected so that $w_\ell^{(0)}(r) \underset{r\to\infty}{\sim} e_\ell^+(k_0 r)$. Solving the above equation simultaneously with (2.59) gives for $T_\ell^{(0)}$

$$T_\ell^{(0)} = \frac{-\int_0^\infty s_\ell(k_0 r)\,\hat{u}\,s_\ell(k_0 r)\,dr}{k_0 + \int_0^\infty s_\ell(k_0 r)\,\hat{u}\,w_\ell^{(0)}(r)\,dr} \tag{2.63}$$

A solution $\bar{F}_\ell^{(1)}(r)$ may now be found satisfying the inhomogenous differential equation

$$\mathcal{L}_0 \bar{F}_\ell^{(1)}(r) = \hat{u}\,F_\ell^{(0)}(r) \tag{2.64}$$

which is however not a suitable first order solution since it is asymptotic to the same function as the zero order solution, namely $s_\ell(k_0 r) + T_\ell^{(0)} e_\ell^+(k_0 r)$. A new function $w_\ell^{(1)}(r)$ is therefore calculated such that

$$\bar{F}_\ell^{(1)}(r) = s_\ell(k_0 r) + T_\ell^{(0)} w_\ell^{(1)}(r) \tag{2.65}$$

and the first order solution taken to be

$$F_\ell^{(1)}(r) = s_\ell(k_0 r) + T_\ell^{(1)} w_\ell^{(1)}(r) \tag{2.66}$$

where $T_\ell^{(1)}$ is given by the right hand side of (2.63), but with $w_\ell^{(1)}(r)$ in place of $w_\ell^{(0)}(r)$. This process is continued until the value of $T_\ell^{(n)}$ from the n^{th} iterate agrees with $T_\ell^{(n-1)}$ to within a specified tolerance.

In actual computation by this method (2.64) will be solved numerically, and the requirement that the solution $\bar{F}_\ell^{(n)}(r)$ must give the same value for the partial wave amplitude $T_\ell^{(n-1)}$ as $F_\ell^{(n-1)}(r)$ provides an extremely useful check on the numerical accuracy, for each iterate.

Austern (1969) formulated the Sasakawa method in terms of standing wave boundary conditions, and chose the trial function $w_\ell^{(o)}$ to be

$$\begin{aligned} w_\ell^{(o)}(r) &= c_\ell(k_o r) \qquad \text{for} \quad r > r_o \\ &= N_\ell \, s_\ell(k_o r) \qquad \text{for} \quad r \leq r_o \end{aligned} \tag{2.67}$$

where $N_\ell = c_\ell(k_o r_o)/s_\ell(k_o r_o)$ and $c_\ell(x)$ is related to the spherical Bessel function of the second kind $y_\ell(x)$ according to

$$c_\ell(x) = -x\, y_\ell(x) \underset{x \to \infty}{\sim} \cos\left(x - \frac{\ell\pi}{2}\right) \tag{2.68}$$

This choice is well suited to applications in nuclear physics where in the surface - δ model it is assumed that the incoming particle interacts with the nuclear surface only; the parameter r_o is then taken to be the radius of this surface. There can be little justification however for adopting this for atomic collisions, particularly as it imposes a discontinuity in the derivatives of $w_\ell^{(o)}(r)$ which is undesirable for numerical work. We choose therefore the function

$$w_\ell^{(0)}(r) = \left[1 - \exp\left(-\frac{r}{r_0}\right)^{2\ell+1}\right] c_\ell(k_0 r) + i\, s_\ell(k_0 r) \tag{2.69}$$

which has the correct behaviour both at large r and near the origin where it is proportional to $r^{\ell+1}$.

2.6 Higher Partial Wave Corrections

In the partial wave formulation it is in principle necessary to solve the radial equations (2.18) for all values of ℓ such that the resulting T_ℓ gives a non-negligible contribution to the scattering amplitude. At the intermediate energies considered in this work a large number of partial waves are expected to contribute, which would require a prohibitively large amount of computer time. In any case the use of the present one channel approximation for higher partial waves would be unnecessarily wasteful as one would expect a semi-classical approach to be valid for the angular momentum states of large ℓ.

Now from (1.44) the elastic scattering amplitude $f^{IP}(\theta)$ in the impact parameter approximation to the second order potential method is

$$f^{IP}(\theta) = -ik_i \int_0^\infty \left[a_i(b,+\infty) - 1\right] J_0\left(2k_i b \sin\frac{\theta}{2}\right) b\, db \tag{2.70}$$

and using the expansion (Newton 1966 p586)

$$kb\, J_0\left(2kb \sin\frac{\theta}{2}\right) = \sum_{\ell=0}^{\infty} (2\ell+1) J_{2\ell+1}(2kb) P_\ell(\cos\theta) \qquad 2.71)$$

in (2.70) we find the partial wave amplitude to be

$$T_\ell^{IP} = -ik_i\int_0^\infty \left[a_i(b,+\infty) - 1\right] J_{2\ell+1}(2k_i b)\,db \qquad (2.72)$$

where as usual

$$f^{IP}(\theta) = \frac{1}{k_i}\sum_{\ell=0}^{\infty}(2\ell+1)T_\ell^{IP} P_\ell(\cos\theta) \qquad (2.73)$$

The transition amplitudes $a_f(b,+\infty)$ are tabulated for electron-hydrogen and helium scattering in unpublished supplements to the work of Bransden et al (1972) and Berrington et al (1973). It is proposed therefore to solve both the radial equations (2.18) and the integral (2.72) for only those ℓ up to a value, L say, where T_ℓ and T_ℓ^{IP} become equal. The contribution to the scattering amplitude of all partial waves with $\ell > L$ is then found immediately from

$$f^R(\theta) = f^{IP}(\theta) - \frac{1}{k_i}\sum_{\ell=0}^{L}(2\ell+1)T_\ell^{IP} P_\ell(\cos\theta) \qquad (2.74)$$

with $f^{IP}(\theta)$ computed from (2.70).

Chapter 3 Application to the elastic scattering of electrons from hydrogen and helium atoms

3.1 Numerical Methods

The second order potential $h_\ell(r,r')$ was evaluated from (2.21), and it was found that no more than thirty terms were required in the summation over λ. The generation of the integrals A_ℓ, B_ℓ and C_ℓ required for $z_{\ell\ell}(P_{10}{}^2|rr')$ was by the two term recurrence relations of Appendix C, those for A_ℓ and C_ℓ being inhomogenous. The latter can in general be unstable, in that a machine error in the initial value A_0 or C_0 is equivalent to introducing a fraction of the homogenous solution. Subsequent amplification of this error during recursion may then result in a considerable loss of significant figures from the required solution (Gautschi 1961).

Examination of the equations of Appendix C shows that the recurrence relation for C_ℓ is stable in the forward direction for all ℓ, while that for A_ℓ is stable up to a value $\ell = \alpha r_<$. For values of ℓ greater than this we use recurrence in the backward direction, the initial value of A_ℓ being chosen from the asymptotic expansion for large ℓ :-

$$A_\ell(\alpha|rr') \sim \frac{e^{-\alpha r_<}}{(2\ell+3)} \frac{r_<^{\ell+2}}{r_>^{\ell+1}} \left[1 + \frac{\alpha r_<}{2\ell+4} + \frac{\alpha^2 r_<^2}{(2\ell+4)(2\ell+5)} + \dots \right] \qquad (3.1)$$

The spherical Bessel functions were also generated by a combination of forward and backward recursion, the criteria for stability having been established by Corbato and Uretsky (1959).

Figure 1 shows a contour plot of Im $[h_0(r,r')/rr']$ for electron-hydrogen scattering, with $\bar{k} = 0.1$. This illustrates well the typically rapid variation of the kernel in the region of the origin, with comparatively smooth behaviour elsewhere. On the basis of this structure, it was decided that for r and r' greater than some value r_0 it would be sufficient to obtain $h_\ell(r,r')$ by interpolation in an array set up at the beginning of the computation. An empirical value of $1.2/k_0$ was used for r_0, and for r and $r'<r_0$ the kernel was evaluated each time it was required. In interpolating $h_\ell(r,r')$ it should be remembered that the kernel has discontinuous derivatives at $r=r'$, and interpolation should therefore be confined to points <u>either</u> in the region $r<r'$, <u>or</u> in the region $r>r'$. Finally, it is noted that from (2.35) we expect Im$[h_0(r,r')]$ to have zeroes at lines of constant r and r', corresponding to the zeroes of the function $j_1(\bar{k}r)$, for sufficiently large $r_>$; this is in fact clearly illustrated in figure 1.

The Sasakawa-Austern iteration described in Section 2.5 requires the solution of the differential equation

$$\frac{d^2y}{dx^2} = f(x)y(x) + g(x) \tag{3.2}$$

where the function g(x) arises from the integration over the second-order potential and exchange kernels and the wavefunction of the previous iterate. The integral with kernel $h_\ell(r,r')$, together with those required for the calculation of $T_\ell^{(n)}$, was evaluated by integrating over successive subintervals with the method of Clenshaw and Curtis (1960). As noted by Gentleman

(1972) this can be regarded as an expansion of the integrand either in a Chebyshev series or as a Fourier cosine transform, which is then integrated term by term.

In either case the N point quadrature formula obtained is

$$\int_{-1}^{+1} f(x)\,dx = \sum_{n=0}^{N}{}'' \left(\frac{a_n}{N}\right)\frac{2}{1-n^2} \qquad (3.3)$$

where the sum is over even values of n only, the symbol '' means that the first and last terms should be halved, and a_n is given by

$$a_n = 2\sum_{s=0}^{N}{}'' f\left(\cos\frac{\pi s}{N}\right)\cos\frac{\pi s n}{N} \qquad (3.4)$$

This particular method of integration was chosen because, as shown by Smith (1965), it requires fewer points to obtain a specified accuracy than any other method, with the exception of Gauss quadrature. Its advantage over the latter method is that there are reliable error estimates available for a given number of points, and moreover doubling the number of points requires less effort. The implementation of the technique was based on the work of O'Hara and Smith (1968) and Oliver (1972), from which the error estimates were also taken.

The integral over the exchange kernel requires the evaluation of $y_\ell(P_{10}F_\ell^{(n)}|r)$. This is calculated at the beginning of the $(n+1)^{th}$ iterate for the set of values $r_i=ih$, where h is some increment and i = 0, 1, 2..., and is most economically done using a step-by-step method. We use Simpson's rule (Davis and Rabinowitz 1967 p19) here, and subsequently interpolate in the array $y_\ell(P_{10}F_\ell^{(n)}|r_i)$ as required.

In evaluating semi-infinite integrals it is usual to replace the upper limit of infinity by some large finite value R, and then to sum the integrals over successive sub-intervals of this range. For the integral with the second order potential kernel, R was chosen as the point where the integrand had reached its asymptotic form; the integral from R to ∞ was then evaluated analytically. The integrand of the exchange term, being of short range, presented no difficulties.

The differential equation (3.2) was solved by the Numerov method (Melkanoff et al 1966) which replaces (3.2) by the algorithm

$$\left(1 - \frac{h^2}{12} f_{n+1}\right) y_{n+1} = \left(2 + \frac{5}{6} h^2 f_n\right) y_n - \left(1 - \frac{h^2}{12} f_{n-1}\right) y_{n-1} + \frac{h^2}{12}\left(g_{n+1} + 10\, g_n + g_{n-1}\right) \qquad (3.5)$$

where $h = x_{n+1} - x_n = x_n - x_{n-1}$ and y_{n+1} denotes $y(x_{n+1})$ with a similar abbreviation for $f(x_{n+1})$ and $g(x_{n+1})$. For integration out to 0.4 atomic units h was taken to be 0.02, this being increased to $0.15/k_0$ for $x > 0.4a_0$.

The Sasakawa-Austern iteration was found to converge rapidly for all angular momenta except $\ell=0$. Typically for electron-hydrogen scattering at 100 eV the criterion $\left[T_\ell^{(n)} - T_\ell^{(n-1)}\right] / T_\ell^{(n-1)} < 0.125\%$ was satisfied on the third iteration for $\ell \geq 4$ and the fourth iteration for $1 \leq \ell \leq 3$.

For the $\ell=0$ singlet case the convergence was improved using the technique of Burke and Seaton (1971) whereby the wavefunction at the n^th^ iterate is taken as the average of $F_\ell^{(n)}(r)$ and $F_\ell^{(n-1)}(r)$; at 100 eV however seven iterations were still necessary to obtain convergence. For energies less than 50 eV the triplet $\ell=0$ iteration did not converge at all, the difficulty being associated with the presence of the exchange integral. This was rectified by including only a small fraction of the exchange kernel on the first iterate; this fraction was then gradually increased on each successive iterate until before convergence was achieved it was equal to one.

The integrals (2.70) and (2.72) were evaluated by expressing them as a sum of an infinite series of definite integrals whose limits of integration are successive zeroes of the Bessel functions $J_{2\ell+1}(2kb)$ or $J_0(2kb\sin\frac{\theta}{2})$. Each integral was then computed by the method of Romberg (Davis and Rabinowitz 1967 p166). As each successive term in the series of integrals alternated in sign, it was found to be extremely useful to employ the Euler transformation (Davis and Rabinowitz 1967 p99) to speed up the convergence of the sum of these terms. As is usual in the calculation of semi-infinite integrals such as (2.70) and (2.72), the upper infinite limit is replaced by some finite R. This, of course, introduces an error which we may however bound by using the relations

$$\int_R^\infty f(b)J_{2\ell+1}(\lambda b)\,db \leq \frac{f(R)}{\lambda}\left[J_0(\lambda R)+2\sum_{p=1}^{\ell}J_{2p}(\lambda R)\right] \qquad (3.6)$$

and

$$\int_R^\infty g(b)J_0(\lambda b)\,db \leq g(R)\int_R^\infty J_0(\lambda b)\,db \qquad (3.7)$$

which, provided that f(b) and g(b) are positive decreasing in the range $R \leqslant b \leqslant \infty$, follow immediately from Bonnet's form of the second Mean Value Theorem (Whittaker and Watson 1963 p66). The integral on the right hand side of (3.7) is computed using the polynomial approximation of Hitchcock (Abramowitz and Stegun 1965 p481).

The solution of the radial equation (2.18) required approximately 5 minutes CPU time on an IBM 360/67, for each partial wave amplitude. At all energies considered it was found that satisfactory agreement with the impact parameter approximation to T_ℓ was obtained for $\ell > 7$.

3.2 Results

a) Partial Wave Amplitudes

The calculation of T_ℓ^{IP} that is required for the present model provides an opportunity for determining the validity of the impact parameter approximation used in previous applications. Since the latter neglects exchange, the second order potential radial equations (2.18) and (2.25) were first of all solved with the exchange kernel set equal to zero. The difference between the partial wave amplitude T_ℓ^D so obtained, and that calculated from (2.72) is then due to the semi-classical approximation alone.

Table I compares the values of $|T_\ell^D|^2$ with $|T_\ell^{IP}|^2$ for $\ell=0$ to 7, for electron-hydrogen scattering at 54.4, 100 and 200 eV, and the same quantities are tabulated in Table II for electron-helium collisions. It is clearly seen that for the case of helium the impact parameter approximation is very poor at 50 eV, the S wave value $|T_0^{IP}|^2$ being in error by 50%.

This error for $\ell=0$ decreases to 30% at 200 eV. On the other hand for hydrogen at 200 eV the error in $|T_0^D|^2$ is no greater than 10%. For energies greater than 50 eV $|T_\ell^{IP}|^2$ is seen to agree with the corresponding quantity in the partial wave treatment at $\ell=7$, for both hydrogen and helium.

Also included in table II are the values of $|T_\ell|^2$ for electron-helium scattering in our one channel model with exchange. As would be expected from its short range behaviour, comparison with $|T_\ell^D|^2$ shows that exchange has the greatest effect upon the S wave values, and for $\ell=7$ (where $|T_\ell^{IP}|^2 = |T_\ell^D|^2$) it can be considered negligible. It should be noted that even at 200 eV, where exchange has often been considered to be negligible in other models, $|T_0^D|^2$ is increased by 15% by the inclusion of this effect.

b) <u>Elastic Scattering of electrons on hydrogen</u>

In figures 2a) to 2c) we show the differential cross-sections predicted by the present model for elastic electron-hydrogen scattering at 54.4, 100 and 200 eV. They fall somewhat below the absolute 50 eV measurements of Teubner et al (1973), and those of Lloyd et al (1974) at 100 and 200 eV. However, from the discussion of Teubner et al (1973) it can be deduced that the error in both sets of data is up to ±35% in absolute value, and up to 10% in shape particularly at the larger angles; our results are not therefore inconsistent with the measurements. The degree of improvement achieved by replacing the approximations of Bransden et al (1972) with a full wave treatment and including exchange is striking, especially at 54.4 eV. Even at 200 eV there is a substantial correction at smaller angles, where the S wave partial wave amplitude has greatest effect.

Figure 2a) also shows the results of other theoretical work at 50 eV. The failure of the Born and close-coupling approximations to predict the forward peak, discussed in Section 1.4, is well illustrated. The EBS results of Byron and Joachain (1974) are quite different at small angles from those of the present work, but they are also within the error bounds on the data. Figures 2b) and 2c) show the EBS results of Byron and Joachain (1973) at 100 and 200 eV and it can be seen that as the energy increases their results become very close to ours, even for small angles. The work of Chen et al (1973), who consider the Glauber and Glauber-angle approximations, should also be mentioned. The latter is a modification of the Glauber approximation to account for trajectories other than straight lines, and gives results quite close to the present work, but slightly lower at small angles. In contrast the Glauber approximation predicts cross-sections that for angles greater than 15^{0} are very close to the results of Bransden et al (1973), this being shown in figure 2b) for 100 eV.

c) Elastic Scattering of electrons on helium

Figures 3a) to 3f) display the present electron-helium differential cross-section results at 50, 100, 200, 300, 400 and 500 eV. Comparison with experiment is hindered however by the conflicting nature of the available data, particularly at energies of 100 and 200 eV. To assess the reliability of the data, we note first of all that the absolute 500 eV measurements of Bromberg (1969) are generally regarded as being highly accurate, and it is expected that his recent data at 200, 300 and 400 eV (Bromberg 1974) is also good. This is confirmed by the good agreement found between the latter results, those of Jansen et al (1974) and to a lesser extent the data of Chamberlain et al (1970). This seems to indicate that the measurements of Crooks and Rudd (1972) are too high; indeed recent relative measurements by Sethuraman et al (1974) when normalized to Bromberg's at 500 eV and 60° suggest that those of Crooks and Rudd (1972) are consistently 20 to 25% too large in the range 30-150°.

Bearing in mind that the experimental situation still has to be satisfactorily resolved, it can be said that the agreement at small angles between our results and the data is very good. The extent to which we agree with the measurements of Bromberg (1969, 1974) at 400 and 500 eV is especially gratifying. At large angles our cross-sections fall consistently below those of Crooks and Rudd (1972) by at the most 30%. Figures 3d) and 3f) however, show that we are in good agreement with the large angle results of Sethuraman et al (1974) and Oda et al (1972), which are relative measurements normalized to the 500 eV values of Bromberg at 60° and 30° respectively.

Figures 3 also show the results of the impact parameter approximation to the second order potential method used by Berrington et al (1973). As in the case of scattering from hydrogen, it is seen that the effect of the semi-classical approximation in this energy region is considerable. Even at 500 eV the results of Berrington et al (1973) differ from ours by over 20% at the smaller angles.

At energies in the range 200-500 eV the EBS method gives results that lie very close, at small angles, to those of the present model and for this reason have not been displayed. As would be expected, the difference between the two methods begins to show at lower energies, and is clearly seen in figure 3b) for 100 eV. The cross-sections predicted by the EBS model for large angles have been calculated by Byron and Joachain (1973a), and from figures 3b), 3c) and 3e) it is seen that they are different from those of the present work at all energies and are in fact quite close to the data of Crooks and Rudd (1972). Figure 3c) also shows the result of the Glauber approximation (Byron and Joachain 1973a) which, as was found for electron-hydrogen scattering, lies close to the curve of the IP model.

For the sake of clarity, we have not shown the results of either the extended polarized potential approximation of LaBahn and Callaway (1969) or the second Born approximation of Holt et al (1971). While these models predict the expected peak in the forward direction, they both give differential cross-sections that differ in shape from the experimental curves at angles less than 30°. In particular, the agreement with Bromberg (1969) at 500 eV is poor.

From the partial wave amplitudes T_ℓ^D, we also calculated differential cross-sections in the present approximation with exchange neglected, and it was found that for energies greater than 200 eV the contribution from exchange is less than 10%.

d) Integrated and Total Cross-Sections

The elastic scattering amplitude in the forward direction is related to the total cross-section by

$$Q_{TOT} = \frac{4}{k_0} \operatorname{Im}\left[f(0)\right] \tag{3.8}$$

where Q_{TOT} is in units of πa_0^2. Equation (3.8) is known as the optical theorem, which we now use to calculate the total cross-section for electron-hydrogen and helium scattering from our knowledge of the scattering amplitude. In addition, we calculate the total elastic or integrated cross-section by

$$\sigma_{el} = \int \frac{d\sigma}{d\Omega} . d\Omega = 2\pi \int_{-1}^{+1} |f(\theta)|^2 \, d(\cos\theta) \tag{3.9}$$

These two quantities are tabulated in table III for electron-hydrogen scattering at 54.4, 100 and 200 eV, along with the values of Bransden et al (1972). It is seen that the two formulations of the second order potential method predict values for Q_{TOT} that agree quite well, despite the disparity between the results for integrated and differential cross-sections. This illustrates that to distinguish between theories, a more exacting test than a comparison of predicted total cross-sections is required.

In table IV integrated cross-sections for electron-helium scattering are seen to be in excellent agreement with the results of Vriens et al (1968) at 100-400 eV and with that of Bromberg (1969) at 500 eV. This very good agreement is also obtained in the extended polarization potential approximation of LaBahn and Callaway (1969), but is not found by either Holt et al (1971) or Berrington et al (1973) whose results are too high and low respectively.

Table V displays the present results for the real part of the forward scattering amplitude and Q_{TOT} for electron-helium scattering. The ratio of the imaginary to real parts of the scattering amplitude is seen to be in very poor agreement with the dispersion relation results of Bransden and McDowell (1970). This seems to be a result of Im $[f(0,k^2)]$ increasing too rapidly with decreasing k^2. In contrast the values for Re $[f(0,k^2)]$ obtained by Byron and Joachain (1973) with the EBS method are quite close to those of Bransden and McDowell (1970), but unfortunately the EBS values for Im $[f(0,k^2)]$ are not available. We have not included in Table V the results of the eikonal optical model of Byron and Joachain (1974a) which gives values for Re $[f(0,k^2)]$ agreeing to better than 1% with those of the present work.

The behaviour of Im $[f(0,k^2)]$ at low energies is reflected in an apparent divergence of the forward scattering intensity, in contrast to the dispersion relation results of Bransden and McDowell (1970) which indicate a fairly broad maximum at about 80 eV. This is shown in figure 4, which also illustrates that the same behaviour seems to be common to all methods that use an average excitation energy.

3.3 Discussion

The results obtained by the present model of elastic scattering clearly show the inadequacy of the impact parameter approximation used in previous applications of the second order potential method. Even at energies of 200 eV for hydrogen and 500 eV for helium there is still not satisfactory agreement between the two formulations. We suggest therefore that it is inaccurate to use a semi-classical approximation to the scattering amplitude for energies less than twenty times the single ionization threshold; within this energy region, its use is recommended as an approximation to the higher partial wave amplitudes. The present results also indicate that including the effect of exchange modifies differential cross-section by more than 10% for energies less than ten times the ionization threshold. Alton et al (1972) have carried out a partial wave treatment of the second order potential method for electron-hydrogen scattering at energies below 80 eV, with the neglect of exchange. We therefore expect an appreciable error in their results.

Over the energy and angular range considered, the present approximation gives agreement with differential cross-section measurements equalled only by the EBS results. However, the predictions of the two models differ, somewhat surprisingly, at large angles even at 400 eV. A possible reason for this discrepancy is that there are certain third order terms which the EBS method includes, but which are lacking from our one-channel model and may contribute to large angle scattering. Referring to (1.12), the present approximation for the configuration space elastic scattering function is the solution of

$$(\nabla^2 + k_0^2)F_0 = 2V_{00}F_0 + 4\sum_{m\neq 0} V_{0m}\tilde{G}_m V_{m0}F_0 \qquad (3.10)$$

where the integral operator $\tilde{G}_m$ is defined by (1.50). Recalling the definition of the plane wave $\psi(\underline{r})$ given by (1.52) the solution of (3.10) is

$$F_0 = \psi_0 + 2\tilde{G}_0 V_{00}F_0 + 4\tilde{G}_0\sum_{m\neq 0} V_{0m}\tilde{G}_m V_{m0}F_0 \qquad (3.11)$$

Iteration of the above equation then shows that the present approximation takes into account the third order terms $V_{on}\,V_{no}\,V_{oo}$, while neglecting those of the form $V_{on}\,V_{nm}\,V_{mo}$. Although the latter third order terms are included in the EBS method, we do not believe that this accounts for the large angle discrepancy between the two models. First of all, Byron and Joachain (1974a) remark that these terms are likely to affect small angle scattering only, and this has been confirmed by preliminary calculations by Vanderpoorten (1974) who found that adding the effect of the terms $V_{on}\,V_{nm}\,V_{mo}$ to the second order eikonal optical model altered the cross-section at wide angles by only 1%. Secondly, Bransden et al (1972) and Berrington et al (1973) found that their elastic scattering results were altered only at small angles on using a four channel rather than a one channel approximation. The significance of this is that the four channel model takes into account the additional third order terms $V_{on}\,V_{nm}\,V_{mo}$ where m is less than 4. We suggest therefore that the large angle discrepancy is more likely to be due to the failure of the EBS method to work to a consistent order k^{-4} in the differential cross-section.

In connection with the rapid increase of Im $[f(0,k^2)]$ for decreasing k^2, it is seen from (2.52) and (2.53) that when the energy of the incoming electron reaches the value $2(\bar{\varepsilon}-\varepsilon_0)$, the average energy $\bar{k}^2$ vanishes. This occurs at an energy below the ionization threshold for hydrogen, but at an energy of 30.7 eV for helium, and its effect on the scattering amplitude remains to be investigated. We note also that there is no justification for our use of the same value of average energy in both the real and imaginary parts of the second-order potential. A better approximation would be to supplement the work of Section 2.4 with a physical choice of $\bar{k}^2$ for Im $[h_\ell(r,r')]$ but whether this would remove the apparent divergence mentioned above remains in doubt.

Chapter 4 Present Model of Inelastic Scattering

4.1 A Distorted Wave Approximation

The description of the excitation of a light atom to an arbitrary state due to electron impact is contained within the many channel formulation of the second order potential method, provided that an appropriate number of channels are represented explicitly. In practice, the solution of equation (2.12) is a major computational task, even with N chosen to include only the n=1 and 2 levels. It is more appropriate therefore to consider an alternative description of inelastic scattering, but one which nevertheless utilizes the second order potential method.

Referring to (1.80), it is proposed to approximate the two potential formula by setting, for electron-hydrogen scattering,

$$\Psi_i^+(\underline{r}_1,\underline{r}_2) = \phi_i(\underline{r}_1)F_i^S(\underline{r}_2) \qquad (4.1)$$

where $F_i^S(\underline{r}_2)$ is the solution of the one channel approximation to the second order potential equations (1.12) and (1.14), and S is the total spin. This approximation is expected to be superior to the DWBA since it includes the effects of exchange, polarization and absorption on the distorted wave in the initial channel, $F_i^S(\underline{r}_2)$.

From the work of Section 1.7 it is seen that the present model of inelastic scattering therefore approximates the amplitude for direct scattering by

$$f_{if}^S(\theta) = -\frac{1}{2\pi}\int d\underline{r}_1 d\underline{r}_2\, \phi_f^*(\underline{r}_1)\chi_f^{-*}(\underline{r}_2)V\phi_i(\underline{r}_1)F_i^S(\underline{r}_2) \qquad (4.2)$$

while the expression for the exchange amplitude is

$$g^S_{if}(\theta) = -\frac{1}{2\pi}\int d\underline{r}_1 d\underline{r}_2\, \phi^*_f(\underline{r}_1)\, \chi^{-*}_f(\underline{r}_2)\left[V - V_{ff}(\underline{r}_2)\right] \times \qquad (4.3)$$

$$\times\ \phi_i(\underline{r}_2)\, F^S_i(\underline{r}_1)$$

where we emphasize that in (4.3) the potential V <u>must</u> be the post interaction

$$V = \frac{1}{|\underline{r}_1 - \underline{r}_2|} - \frac{1}{r_2} \qquad (4.4)$$

All other quantities in (4.2) and (4.3) have been defined previously in Section 1.7. The differential cross-section for excitation to the state f is then

$$\frac{d\sigma}{d\Omega} = \frac{1}{4}\frac{k_f}{k_i}\sum_{S=0}^{1}(2S+1)\left|f^S_{if}(\theta) + (-1)^S g^S_{if}(\theta)\right|^2 \qquad (4.5)$$

For electron-helium scattering the direct and exchange amplitudes are

$$f_{if}(\theta) = -\frac{1}{2\pi}\int d\underline{r}_1 d\underline{r}_2 d\underline{r}_3\, \phi^*_f(\underline{r}_1,\underline{r}_2)\, \chi^{-*}_f(\underline{r}_3)\, V \phi_i(\underline{r}_1,\underline{r}_2)\, F_i(\underline{r}_3) \qquad (4.6)$$

and

$$g_{if}(\theta) = -\frac{1}{2\pi}\int d\underline{r}_1 d\underline{r}_2 d\underline{r}_3\, \phi^*_f(\underline{r}_1,\underline{r}_2)\, \chi^{-*}_f(\underline{r}_3)\left[V - V_{ff}(\underline{r}_3)\right] \times$$

$$\times\ \phi_i(\underline{r}_2,\underline{r}_3)\, F_i(\underline{r}_1) \qquad (4.7)$$

where $\phi_n(\underline{r}_1,\underline{r}_2)$ is the bound wavefunction for the state n of helium, and the interaction is now

$$V = \frac{1}{|\underline{r}_1 - \underline{r}_3|} + \frac{1}{|\underline{r}_2 - \underline{r}_3|} - \frac{2}{r_3} \qquad (4.8)$$

$V_{ff}(\underline{r}_3)$ is the matrix element of the above interaction with respect to the state $\phi_f(\underline{r}_1,\underline{r}_2)$, and $\chi_f^-(\underline{r}_3)$ is defined by (1.84).

The differential cross-section for excitation to a singlet state of helium is then

$$\frac{d\sigma}{d\Omega}(1^1S \rightarrow n^1L) = \frac{k_f}{k_i}\left| f_{if}(\theta) - g_{if}(\theta)\right|^2 \qquad (4.9)$$

while for the spin forbidden transitions, which can only take place through electron exchange we have

$$\frac{d\sigma}{d\Omega}(1^1S \rightarrow n^3L) = \frac{3k_f}{k_i}\left| g_{if}(\theta)\right|^2 \qquad (4.10)$$

Since the one channel scattering function $F_i(\underline{r})$ is generated during the calculation of the elastic cross-sections for hydrogen and helium described in the previous chapter, the present model of inelastic scattering requires little extra effort in order to obtain excitation cross-sections. It is also apparent that transitions to any state f can be considered with approximately the same amount of computation; subject of course in the case of helium to the availability of accurate wave functions.

In common with the DWBA, the present model has the disadvantage that it represents the optically forbidden transitions more poorly than those that are allowed. This would be overcome to some extent if we were to use the second order potential approximation to the total wave function for the system, rather than the elastic scattering wave function. From Section 1.1 it is seen that the former is given by

$$\Psi_i(\underline{r}_1,\underline{r}_2) = \phi_i(\underline{r}_1)F_i(\underline{r}_2) + 2\sum_{n\neq i}\phi_n(\underline{r}_1) \times$$

$$\times \int d\underline{r}_2' \, G(\bar{k}^2;\underline{r}_2,\underline{r}_2')V_{ni}(\underline{r}_2')F_i(\underline{r}_2') \qquad (4.11)$$

We now extend the n summation over the infinite range, perform closure on the states $\phi_n(\underline{r})$ and substitute the result in (1.80), giving for example the direct amplitude as

$$f_{if}^{S}(\theta) = -\frac{1}{2\pi}\int d\underline{r}_2 \, \chi_f^{-*}(\underline{r}_2)V_{if}(\underline{r}_2)F_i^{S}(\underline{r}_2)$$

$$-\frac{1}{\pi}\int d\underline{r}_2 d\underline{r}_2' \, \chi_f^{-*}(\underline{r}_2)V_{if}(\underline{r}_2,\underline{r}_2')F_i^{S}(\underline{r}_2')G(\bar{k}^2;\underline{r}_2,\underline{r}_2')$$

$$+\frac{1}{\pi}\int d\underline{r}_2 d\underline{r}_2' \, \chi_f^{-*}(\underline{r}_2)V_{if}(\underline{r}_2)V_{ii}(\underline{r}_2')F_i^{S}(\underline{r}_2')G(\bar{k}^2;\underline{r}_2,\underline{r}_2') \qquad (4.12)$$

with $V_{nm}(\underline{r})$ and $V_{nm}(\underline{r},\underline{r}')$ defined by (1.6) and (1.15) respectively. Reference to (1.14) shows the one channel second order potential kernel $K_{nm}(\underline{r},\underline{r}')$ to be contained in (4.12), and the improved approximation to the direct scattering amplitude is therefore written more concisely as

$$f_{if}^{S(2)}(\theta) = f_{if}^{S(1)}(\theta) - \frac{1}{\pi}\int d\underline{r}_2 d\underline{r}_2' \, \chi_f^{-*}(\underline{r}_2)K_{if}(\underline{r}_2,\underline{r}_2')F_i^{S}(\underline{r}_2') \qquad (4.13)$$

where $f_{if}^{S(1)}(\theta)$ is our original distorted wave approximation given by (4.2). It is seen that the evaluation of $f_{if}^{S(2)}(\theta)$ is of a complexity intermediate between that of the solution of the many channel equations (2.12), and of the calculation of $f_{if}^{S(1)}(\theta)$.

In actual computation we work with radial rather than configuration space wave functions, and the angular momentum decomposition of the scattering amplitude must be made for each process under consideration. We will therefore require the following partial wave expansions for the distorted waves:-

$$\chi_f^{-*}(\underline{r}) = \sum_{\ell=0}^{\infty} (-i)^{\ell} (2\ell+1) \frac{x_\ell^{-*}(k_f r)}{k_f r} P_\ell(\hat{\underline{k}}_f \cdot \hat{\underline{r}}) \qquad (4.14)$$

and

$$F_i^S(\underline{r}) = \sum_{\ell=0}^{\infty} i^{\ell} (2\ell+1) \frac{f_\ell^S(k_i r)}{k_i r} P_\ell(\hat{\underline{k}}_i \cdot \hat{\underline{r}}) \qquad (4.15)$$

The elastic second order potential function $f_\ell^S(k_i r)$ is obtained from the solution of (2.18) and (2.25) for hydrogen and helium respectively, while the equation for the distorted wave $x_\ell^-(k_f r)$ is found on substituting (4.14) into (1.84) to be

$$\left[\frac{d^2}{dr^2} + k_f^2 - \frac{\ell(\ell+1)}{r^2}\right] x_\ell(k_f r) = 2\sum_{\ell_1=0}^{\infty} V_{ff}^{\ell\ell_1}(r)\, x_{\ell_1}(k_f r) \qquad (4.16)$$

where

$$V_{ff}^{\ell\ell_1}(r) = i^{\ell_1-\ell} \frac{(2\ell_1+1)}{2} \int_{-1}^{+1} d(\hat{\underline{k}}_f \cdot \hat{\underline{r}}) P_\ell(\hat{\underline{k}}_f \cdot \hat{\underline{r}}) V_{ff}(\underline{r}) P_{\ell_1}(\hat{\underline{k}}_f \cdot \hat{\underline{r}}) \qquad (4.17)$$

4.2 2s State Excitation of Hydrogen

We choose as our model of 1s→2s excitation of hydrogen the distorted wave approximation given by equations (4.2), (4.3) and (4.5).

Consider first of all the direct scattering amplitude. Since i and f are both s states, the matrix element $V_{fi}(\underline{r})$ has no angular dependence, and hence substituting the expansions (4.14) and (4.15) into (4.2) gives

$$f^S_{if}(\theta) = \frac{1}{k_i}\sum_{\ell=0}^{\infty}(2\ell+1)P_\ell(\cos\theta)\,t_\ell \tag{4.18}$$

where the direct partial wave amplitude t_ℓ is

$$t_\ell = -\frac{2}{k_f}\int_0^\infty dr\, x_\ell^{-*}(k_f r)\,V_{if}(r)\,f^S_\ell(k_i r) \tag{4.19}$$

Now comparing the expression for the distorted wave scattering amplitude given by (4.2) with that of the first Born approximation (1.57) and using the partial wave expansion of a plane wave

$$e^{\pm i\underline{k}.\underline{r}} = \sum_{\ell=0}^{\infty}(\pm i)^\ell(2\ell+1)\frac{s_\ell(kr)}{kr}P_\ell(\hat{\underline{k}}.\hat{\underline{r}}) \tag{4.20}$$

it is clear that the Born approximation to the partial wave amplitude t^B_ℓ is obtained by replacing $x^{-*}_\ell(k_f r)$ and $f^S_\ell(k_i r)$ in (4.19) by $s_\ell(k_f r)$ and $s_\ell(k_i r)$ respectively. Hence

$$t^B_\ell = -\frac{2}{k_f}\int_0^\infty dr\, s_\ell(k_f r)\,V_{if}(r)\,s_\ell(k_i r) \tag{4.21}$$

Since the above is much easier to compute than t_ℓ, the latter was calculated only for values of ℓ up to L for which $t_L = t_L^B$. The correction to the distorted wave amplitude for $\ell > L$ is then

$$f^R_{if}(\theta) = f^B_{if}(\theta) - \frac{1}{k_i}\sum_{\ell=0}^{L}(2\ell+1)P_\ell(\cos\theta)\,t^B_\ell \tag{4.22}$$

The Born scattering amplitude $f^{B}_{if}(\theta)$ is given by (1.57), and introducing the momentum transfer $\underline{q} = \underline{k}_i - \underline{k}_f$ the expansion (4.20) allows us to write, for s transitions

$$f^{B}_{if}(\theta) = -\frac{2}{q}\int_0^\infty dr\, r\, s_0(qr)\, V_{if}(r) \tag{4.23}$$

In particular using the expression for $V_{1s2s}(r)$ given in Appendix D, for 1s→2s transitions we have

$$f^{B}_{12}(\theta) = \frac{-8\sqrt{2}}{27q}\left[R_1\left(\tfrac{3}{2}\right) + \tfrac{3}{2}R_2\left(\tfrac{3}{2}\right)\right] \tag{4.24}$$

where

$$R_n(\lambda) = \int_0^\infty dr\, r^n s_0(qr)\, e^{-\lambda r} \tag{4.25}$$

with $R_0(\lambda) = \dfrac{q}{\lambda^2+q^2}$ and $R_n(\lambda) = -\dfrac{\partial}{\partial\lambda}R_{n-1}(\lambda)$

For the case of exchange scattering, the exchange partial wave amplitude g_ℓ is defined by

$$g^{S}_{if}(\theta) = \frac{1}{k_i}\sum_{\ell=0}^{\infty}(2\ell+1)P_\ell(\cos\theta)\, g_\ell \tag{4.26}$$

and from (4.3), (4.14) and (4.15) we find

$$g_\ell = \frac{-2}{k_f(2\ell+1)}\int_0^\infty dr\, f^{S}_\ell(k_i r)\left[\alpha(r)\, y_\ell(P_{10}x_\ell|r) - \delta_{\ell 0}\beta(r)\right] \tag{4.27}$$

where

$$\alpha(r) = P_{20}(r) \tag{4.28}$$

and

$$\beta(r) = P_{20}(r)\,\Delta\left(V_{2s2s} + \frac{1}{r}\,\middle|\,P_{10}\,x_0\right) \qquad (4.29)$$

The notation for $\Delta(A|B)$ and $y_\ell(AB|r)$ is that of (1.26) and (1.25) and we recall that $P_{n\ell}(r)$ is the radial part of the bound wavefunction $\phi_{n\ell m}(\underline{r}) = Y_{\ell m}(\hat{\underline{r}})\,P_{n\ell}(r)/r$. The function $V_{2s2s}^{\ell\ell'}(r)$ required for the generation of $x_\ell(k_f r)$ from equation (4.17) is equal to $\delta_{\ell\ell'}\,V_{2s2s}(r)$, and both this and $V_{1s1s}(r)$ are given in Appendix D.

The partial wave Born amplitude g_ℓ^B is obtained by replacing $f_\ell^S\,(k_i r)$ and $x_\ell(k_f r)$ by $s_\ell(k_i r)$ and $s_\ell(k_f r)$ in equations (4.27) to (4.29). As before the distorted wave amplitude g_ℓ was calculated for increasing ℓ until $g_L = g_L{}^B$. However, since the partial wave series for the exchange amplitude (4.26) is expected to converge much more rapidly than its direct counterpart (4.18), the contribution for $\ell > L$ was found merely by evaluating $g_\ell{}^B$ until convergence was achieved.

4.3 2^1S and 2^3S Excitation of Helium

For a description of the 2S excitation of helium we consider the approximations (4.6) and (4.7) to the scattering amplitudes. The partial wave expansion of $f_{if}(\theta)$ follows exactly as in the previous section to give a direct partial wave amplitude t_ℓ with exactly the same form as (4.19), but with $V_{1s2s}(r)$, $x_\ell^{-*}(k_f r)$ and $f_\ell\,(k_i r)$ appropriate to helium scattering. In other words $f_\ell\,(k_i r)$ is the solution of (2.25),

$x_\ell(k_f r)$ is the solution of (4.16) with $V^{\ell\ell_1}_{2s2s}(r) = \delta_{\ell\ell_1} V_{2s2s}(r)$, and $V_{2s2s}(r)$ together with $V_{1s2s}(r)$ are tabulated in Appendix D for the particular case of Hartree-Fock approximate wave functions.

The Born approximation to the direct amplitude is calculated easily by substitution of the helium form for $V_{1s2s}(r)$ into (4.23), and is as before a linear combination of the functions $R_n(\lambda)$ defined in (4.25). Its evaluation then allows the same technique to be used for the calculation of the higher partial wave correction as was used in the previous section.

For exchange scattering we introduce the following separation for the 2^1S and 2^3S wave functions

$$\phi_{200}(\underline{r}_1,\underline{r}_2) = \frac{P_{\bar{1}0}(r_1)}{r_1} Y_{00}(\hat{\underline{r}}_1)\frac{P_{20}(r_2)}{r_2} Y_{00}(\hat{\underline{r}}_2) \pm \{\underline{r}_1 \leftrightarrow \underline{r}_2\} \qquad (4.30)$$

where the + and - signs correspond to singlet and triplet states respectively. The corresponding expression for the ground state is that of (2.24).

The exchange amplitude for helium is then found to be given by (4.26) and (4.27), but in this case we have

$$\alpha(r) = P_{20}(r)\,\Delta(P_{10}|P_{\bar{1}0}) \pm \{P_{\bar{1}0} \leftrightarrow P_{20}\} \qquad (4.31)$$

and

$$\begin{aligned}\beta(r) = P_{20}(r)\Big[\Delta(P_{10}|P_{\bar{1}0})\,\Delta\big(V_{2s2s} + \tfrac{2}{r}\,\big|\,P_{10}x_0\big) \\ - \Delta(A\,|\,P_{10}x_0)\Big] \\ \pm \{P_{\bar{1}0} \leftrightarrow P_{20}\}\end{aligned} \qquad (4.32)$$

where we have put

$$A(r) = y_0(P_{10}P_{\bar{1}0}|r) \qquad (4.33)$$

The amplitude g_ℓ^B and the correction for the higher partial waves in (4.26) are found in the manner described in the previous section.

We also propose to investigate the importance of allowing for distortion in the final state by using a simplified distorted wave approximation in which $\chi_f^{-*}(\underline{r}_3)$ in (4.6) and (4.7) is replaced by the plane wave $e^{-i\underline{k}_f\cdot\underline{r}_3}$. This is equivalent to using $s_\ell(k_f r)$ instead of $x_\ell^{-*}(k_f r)$ in the partial wave amplitudes, giving

$$t_\ell = -\frac{2}{k_f}\int_0^\infty dr\, s_\ell(k_f r)\, V_{1s2s}(r)\, f_\ell(k_i r) \qquad (4.34)$$

and

$$g_\ell = \frac{-2}{k_f(2\ell+1)}\int_0^\infty dr\, f_\ell(k_i r)\left[\alpha(r)\, y_\ell(P_{10}s_\ell|r) - \delta_{\ell 0}\,\beta(r)\right] \qquad (4.35)$$

with $\alpha(r)$ as before and

$$\beta(r) = P_{20}(r)\left[\Delta(P_{10}|P_{\bar{1}0})\,\Delta\left(\tfrac{2}{r}\middle|P_{10}s_0\right) - \Delta(A|P_{10}s_0)\right] \pm \left\{P_{\bar{1}0} \longleftrightarrow P_{20}\right\} \qquad (4.36)$$

It is seen that this approximation greatly simplifies the exchange amplitude, since the two integrals in (4.36) that involve the final state wave function may be evaluated analytically, while the integral $y_\ell(P_{10}s_\ell|r)$ in (4.35) can be expressed in terms of recurrence relations. More precisely we have that $y_\ell(P_{10}s_\ell|r)$ is a combination of integrals of the form

$$M_\ell(kr) = \int_0^r x^{\ell+2}\, j_\ell(kx)\, e^{-\lambda x}\, dx \tag{4.37}$$

and

$$N_\ell(kr) = \int_r^\infty x^{1-\ell}\, j_\ell(kx)\, e^{-\lambda x}\, dx \tag{4.38}$$

From some basic recurrence relations for the spherical Bessel functions and their derivatives (Abramowitz and Stegun 1965 p439 10.1.19-10.1.24) it is not difficult to show that

$$(k^2+\lambda^2) M_\ell(kr) = 2k(\ell+1) M_{\ell-1}(kr) + e^{-\lambda r} r^{\ell+1} \times \left[kr\, j_{\ell+1}(kr) - \lambda r\, j_\ell(kr) - 2(\ell+1)\, j_\ell(kr) \right] \tag{4.39}$$

and

$$(k^2+\lambda^2) N_\ell(kr) = 2k\ell N_{\ell+1}(kr) + e^{-\lambda r} r^{1-\ell} \times \left[k\, j_{\ell-1}(kr) + \lambda\, j_\ell(kr) - \frac{2\ell}{r}\, j_\ell(kr) \right] \tag{4.40}$$

The initial values $M_0(kr)$, $N_0(kr)$ and $N_1(kr)$ are found trivially, that for $N_1(kr)$ requiring the computation of the exponential integral of the first kind with complex argument $E_1(z)$, (Abramowitz & Stegun 1965 p228).

4.4 2^1P Excitation of Helium

The partial wave decomposition of the direct and exchange amplitude is rather more complicated for the $1^1S \to 2^1P$ transition than that of the previous section, due to the non-zero angular momentum of the final atomic state. For this reason, we will consider the direct amplitude only, and use the simpler model discussed at the end of Section 4.3 in which we account for distortion only in the initial state. From (4.6) therefore the scattering amplitude for direct excitation to the 2^1P_m state of helium is

$$f_{1s2P_m}(\theta,\phi) = -\frac{1}{2\pi}\int d\underline{r}\, e^{-i\underline{k}_f\cdot\underline{r}}\, Y_{1m}(\hat{\underline{r}})\, V_{1s2P_m}(r)\, F_i(\underline{r}) \tag{4.41}$$

where the angular dependence of the matrix element $V_{1s2P_m}(\underline{r})$ has been separated out. Defining the partial wave amplitude t_ℓ^m by

$$f_{1s2P_m}(\theta,\phi) = \frac{1}{k_i}\sum_{\ell=0}^{\infty}(2\ell+1)\, t_\ell^m\, P_\ell^m(\cos\theta)\, e^{-im\phi} \tag{4.42}$$

where $P_\ell^m(x)$ is the Legendre function of the first kind, the usual expansion of the scattering wave functions in (4.41) gives

$$t_\ell^0 = \frac{i}{k_f}\sqrt{\frac{3}{\pi}}\sum_{\lambda=\ell\pm1}(\ell-\lambda)(2\lambda+1)\begin{pmatrix}\ell & \lambda & 1\\ 0 & 0 & 0\end{pmatrix}^2 A_{21}(\ell,\lambda) \tag{4.43}$$

and

$$t_\ell^1 = \frac{i}{k_f}\sqrt{\frac{3}{\pi}}\sum_{\lambda=\ell\pm1}\frac{(\ell-\lambda)(2\lambda+1)}{\sqrt{\ell(\ell+1)}}\begin{pmatrix}\ell & \lambda & 1\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}\ell & \lambda & 1\\ 0 & 1 & -1\end{pmatrix}A_{21}(\ell,\lambda)\left[1-\delta_{\ell 0}\right] \tag{4.44}$$

where we have written

$$A_{21}(\ell,\lambda) = \int_0^\infty dr\, S_\lambda(k_f r)\, V_{1s2P_m}(r)\, f_\ell(k_i r) \tag{4.45}$$

The differential cross section for 2^1P excitation is then

$$\frac{d\sigma}{d\Omega} = \frac{k_f}{k_i}\left\{\left|f_{1s2P_0}\right|^2 + 2\left|f_{1s2P_1}\right|^2\right\} \tag{4.46}$$

It follows from the work of Blatt and Biedenharn (1952) that the sum over the magnetic substates in (4.46) can be done algebraically after substitution of equation (4.42). The resulting expression then gives the differential cross-section in terms of the integral $A_{21}(\ell,\lambda)$ rather than the partial wave amplitudes, and in general for excitation to the $n\ell m$ state is

$$\frac{d\sigma}{d\Omega} = \frac{16\pi}{k_f k_i^3} \sum_{\substack{\ell_1\ell_2\\ \lambda_1\lambda_2}} A^*_{n\ell}(\lambda_1\lambda_2) A_{n\ell}(\ell_1\ell_2) \sum_L B_{n\ell}(\ell_1\ell_2\lambda_1\lambda_2|L) P_L(\cos\theta) \quad (4.47)$$

where

$$B_{n\ell}(\ell_1\ell_2\lambda_1\lambda_2|L) = \frac{i^{\ell_1+\lambda_1-\ell_2-\lambda_2}}{4\pi} (-1)^{\ell+L} (2\ell_1+1)(2\ell_2+1)(2\ell+1)(2\lambda_1+1)\times$$

$$\times(2\lambda_2+1)(2L+1)\begin{pmatrix}\lambda_1 & L & \ell_1\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}\ell_1 & \ell_2 & L\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}\lambda_1 & \lambda_2 & \ell\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}\ell_2 & \lambda_2 & L\\ 0 & 0 & 0\end{pmatrix}\begin{Bmatrix}\lambda_1 & L & \ell_1\\ \ell_2 & \ell & \lambda_2\end{Bmatrix} \quad (4.48)$$

While the alternative expression above is useful as a check on the numerical work involved in obtaining (4.46), we note that the loss of information regarding the excitation to magnetic sub-levels is undesirable. In particular, it prevents the calculation of the polarization fraction of impact radiation, which for $^1S \rightarrow {}^1P$ transitions is (Percival and Seaton 1958)

$$P_f = \frac{Q_0 - Q_1}{Q_0 + Q_1} \quad (4.49)$$

and of the parameters (Eminyan et al 1973)

$$\lambda(\theta) = \frac{I_0(\theta)}{I_0(\theta) + 2I_1(\theta)} \quad (4.50)$$

and

$$\chi(\theta) = \tan^{-1}\frac{\operatorname{Im} f_{1s2p_1}}{\operatorname{Re} f_{1s2p_1}} - \tan^{-1}\frac{\operatorname{Im} f_{1s2p_0}}{\operatorname{Re} f_{1s2p_0}} \quad (4.51)$$

where the differential and total cross-sections for excitation to the magnetic sub-level m have been denoted $I_m(\theta)$ and Q_m respectively. It is worth noting at this point that the expression given by Flannery (1970) for P_f is appropriate to hydrogen, and not helium. The values for P_f given by Flannery and Berrington et al (1973) are therefore incorrect.

The Born approximation to $f_{1s2P_m}(\theta)$ is used to obtain the higher partial wave correction in a manner identical to that of the previous two sections. From (1.57) we have that

$$f^{B}_{1s2P_m}(\theta) = \frac{2i}{q} Y^{*}_{1m}(\hat{q}) \int_0^\infty dr\, r\, s_1(qr) V_{1s2P_m}(r) \tag{4.52}$$

Substituting the expression for $V_{1s2P_m}(r)$ given in Appendix D into (4.52) the Born amplitude is easily expressed in terms of the function

$$S_\ell(\lambda) = \int_0^\infty dr\, r^n s_1(qr)\, e^{-\lambda r} \tag{4.53}$$

where we have

$$S_{-1}(\lambda) = 1 - \frac{\lambda}{q}\tan^{-1}\frac{q}{\lambda} \qquad S_0(\lambda) = \frac{1}{q}\tan^{-1}\frac{q}{\lambda} - \frac{\lambda}{q^2+\lambda^2}$$

$$S_1(\lambda) = \frac{2q^2}{(q^2+\lambda^2)^2} \quad \text{and} \quad S_n(\lambda) = -\frac{\partial}{\partial\lambda} S_{n-1}(\lambda) \quad \text{for } n>1 \tag{4.54}$$

Chapter 5 Application to the excitation of hydrogen and helium atoms by electrons

5.1 Numerical Methods

The evaluation of the direct matrix element (4.19) requires a single numerical integration, while for the exchange matrix elements (4.27) and (4.35) a double integration is necessary when distortion is included in the final state. These integrals were evaluated by a 4-point Gauss quadrature, and the accuracy checked by doubling the number of points in the suitably chosen subintervals.

When a plane wave is assumed for the final scattering state, the functions $M_\ell(kr)$ and $N_\ell(kr)$ required are generated by the recurrence relations (4.39) and (4.40), whose stability may be assessed in the manner of Gautschi (1961). It is found that recurrence for M_ℓ and N_ℓ is stable in the reverse and forward directions respectively. The exponential integral of complex argument was computed from its continued fraction representation by the algorithm of Beam (1960).

The solution of equation (4.16) in order to obtain the distorted wave in the final channel was by the method of Numerov, the algorithm being that of (3.5) with $g(x)=0$. A facility was incorporated whereby the step length was doubled every five steps whenever $(y_{n+3}-\bar{y}_{n+3})/y_{n+3}<\varepsilon$, where

$$\left(1-\frac{h^2}{12}f_{n+3}\right)y_{n+3}=\left(2+\frac{5h^2}{6}f_{n+2}\right)y_{n+2}-\left(1-\frac{h^2}{12}f_{n+1}\right)y_{n+1} \qquad (5.1)$$

$$\left(1-\frac{h^2}{3}f_{n+3}\right)\bar{y}_{n+3}=\left(2+\frac{10h^2}{3}f_{n+1}\right)y_{n+1}-\left(1-\frac{h^2}{3}f_{n-1}\right)y_{n-1} \qquad (5.2)$$

ε is a specified tolerance and all other quantities have been defined in (3.5). The alteration of h was only carried out, however, if it was consistent with generating at least thirty values of $x_\ell(k_f r)$ for each loop of the distorted wave.

5.2 Results

a) Generalized Oscillator Strengths

The calculations for helium made use of approximate target wave functions of the Hartree-Fock type, andit is important to have an estimate of the error introduced by this particular choice. This is conveniently done by using them to calculate the generalized oscillator strengths for 2^1S and 2^1P excitation, which are related to the first Born differential cross-section by

$$\mathcal{F}(1^1S \to n^1L) = \frac{q^2}{4}\left(k_i^2 - k_f^2\right)\left|f^B_{1SnL}(q)\right|^2 \qquad (5.3)$$

The resulting function of the momentum transfer q is then compared with that obtained by Bell et al (1969) using highly accurate many-parameter wave functions.

Figure 5 shows $\mathcal{F}(1^1S \to 2^1S)$ calculated with the 2^1S functions of Flannery (1970) and Byron and Joachain (1974b). While these wave functions give very close agreement with the "exact" results of Bell et al (1969) for small momentum transfers, for $q^2>4$ there is an increasing discrepancy between the Flannery and the exact values until at $q^2=16$ the former is 30% too high. In contrast, the Byron and Joachain wave function gives very good agreement with the exact oscillator strengths for all momentum transfers in the range considered.

Figure 5 also compares $\mathfrak{J}(1^1S\rightarrow 2^1P)$ obtained with the 2^1P function of Goldberg and Clogston (1939) and quoted by Flannery (1970), with the "exact" values of Bell et al (1969). In this case, there is good agreement for $q^2<2$, but there is a considerable disparity at large momentum transfers, with the Goldberg and Clogston value being more than 70% too large at $q^2=16$. The claim made by Flannery (1970) concerning the reliability of the 2^1S and 2^1P wave functions used by him would therefore seem to be misleading.

The above results are not surprising since the angular correlation between the bound electrons is a much more important effect for the 2^1P wave function than it is for the 2^1S (Vanderpoorten 1970). In the absence of a more reliable Hartree-Fock 2^1P function we will use the Goldberg and Clogston (1939) form together with the more satisfactory choice of Byron and Joachain (1974b) for the 2^1S. The ground state wave function in all the above calculations using Hartree-Fock functions was that of Byron and Joachain (1966).

b) $1^1S\rightarrow 2^3S$ Excitation of Helium

The energy region from 65.4 eV to 24.58 eV for electron-helium scattering is interesting in that it contains the thresholds of the doubly excited states. These produce narrow resonances (Smith et al 1973) which we will unfortunately not be able to predict with the present model. There is however an additional broad resonance, centred about 50 eV (Crooks et al 1972, Hall et al 1973) the effect of which is to give a very deep minimum in the differential cross-section for 2^3S excitation, and this we would hope to reproduce.

The results of the present approximation, in which the distortion in the initial state is by the static exchange and second order potentials and that in the final state is due to the static potential alone, are displayed in figures 6a) - 6d) for energies of 50, 81.63, 100 and 150 eV. In figure 6a) the present model is seen to reproduce the overall shape of the differential cross-section measurements at 50 eV quite well, although the minimum is not as pronounced as experiment would suggest, and in the forward direction our results are a factor of 2 smaller. Despite this, the present model gives results superior to those obtained by other calculations. We have also computed the DWBA, and a comparison of the two curves shows that including the second order and exchange potentials in the initial channel both accentuates the dip, and raises the cross-section in the forward and backward directions. Figure 6a) also shows that accounting only for distortion in the initial channel gives poor agreement with the data, but this is still to be preferred to the Born-Oppenheimer approximation which, although having a similar shape, is a factor of four larger, and is therefore not shown. Both the present results and the DWBA can be seen to be better than those of the first order many-body theory of Taylor (1974). Finally, the close coupling calculations of Ormonde and Golden (1973) while giving the deep minimum at 70° are a factor of 10 too small at 10°, and are not shown.

From figures 6b) - d) it is apparent that the present model predicts a second smaller minimum which begins to appear at 81.63 eV and is pronounced by 150 eV. This also appears, less conclusively, in the measurements at 100 and 150 eV, and the agreement between the data and our results at these energies is once again superior to that of other approximations.

At 100 eV we see that except in the forward direction, the DWBA again gives better results than the model of Taylor (1974). For both 81.63 eV and 100 eV we display the results of the recent plane wave approximation of Mathur and Rudge (1974) which although radically different from the Born-Oppenheimer values can not be considered as an improvement on the latter.

In table VI our calculated values for the total 2^3S cross-section in the present approximation, the DWBA and the Born-Oppenheimer approximation are presented. These are compared with the theoretical values of Mathur and Rudge (1974) and those of the Ochkur-Rudge approximation (Morrison and Rudge 1967) together with the data of Crooks and Rudd (1972), Vriens et al (1968a) and Suzuki and Takayanagi (1974). Our results agree quite well with the data, and we note that the approximation of Mathur and Rudge (1974) is for total cross-sections greatly superior to the Born-Oppenheimer approximation, although this is probably fortuitous.

c) $1^1S \rightarrow 2^1S$ Excitation of Helium

The differential cross-sections predicted by the present model of 2^1S excitation of helium, in which the direct and exchange matrix elements are evaluated with the elastic scattering function of Section 2.3 in the initial channel and the usual static distortion in the final channel, are presented in figures 7a) - 7d).

At 50 eV we see that our results are in fair agreement with the data, but fail to predict the minimum at 45^o and the rising cross-section in the backward direction shown by the measurements. They constitute a significant improvement over our DWBA results however. We show also the effect of taking a plane wave in the final channel and considering the direct scattering amplitude only. The resulting curve is in poor agreement with the data, but is little worse than the prediction of the Glauber approximation (Yates and Tenney 1972).

The first order many-body calculation of Taylor (1974) gives better agreement with the data than the present model, although it exhibits the same behaviour as ours in the forward and backward directions. This is somewhat surprising, as in the 2^3S case the many-body results were poorer. We also mention the recent work of Baye and Heenen (1974) whose second order diagonalization method gives results which are strongly peaked in the forward direction, follow the data of Crooks and Rudd to 60^o but then fail to predict the rising cross-section for angles larger than this.

The values given by the first Born approximation have not been shown on any of the figures 7a) to d), since it is well known that they give poor agreement with experiment (Rice at al 1972). Calculations were also performed at 50 eV using the 2^1S function of Flannery (1970), and it was found that the present results were altered by less than 5%.

Figure 7b) shows that at 81.63 eV there is again good agreement between the present results and experiment at small and large angles, with our model failing to predict the dip at 45°. As at 50 eV, the results are better than those of the DWBA, although they are inferior to those given by Taylor (1974) except at large angles. The coulomb projected Born approximation of Hidalgo and Geltman (1972) agrees well with the present results for angles up to 40°, but beyond this it decreases too rapidly. The results of both Baye and Heenen (1974) and Yates and Tenney (1972) lie below those of Hidalgo and Geltman and are not shown.

At 100 and 150 eV we see that the present results are in good agreement with the measurements at all angles. We display also at 100 eV the present results calculated from the direct scattering amplitude only, and see that the effect of exchange is considerable, especially at the larger angles.

The results of the impact parameter approximation to the second order potential method were unfortunately computed by Berrington et al (1973) only for angles up to 20°. From their unpublished transition amplitudes we therefore used (1.44) and (1.45) to obtain large angle values. The results of this calculation are shown at 100 eV as the curve IP, and it is seen that there is little agreement with the data of Crooks and Rudd (1972), although the model is seen to be superior to that of Hidalgo and Geltman (1972) at large angles. At 100 eV the Glauber approximation (Franco 1973) is again in poor agreement with both theory and experiment, and is not shown. We note that both Baye and Heenen (1974) and Berrington et al (1973) give a larger forward intensity than predicted by the other approximations considered.

In table VII we present our distorted wave results for the total 2^1S cross-section, together with those of Berrington et al (1973), Joachain and Vanderpoorten (1974) and the Born approximation. Comparison with experiment is difficult due to the conflicting nature of the data of Rice et al (1972) and Lassettre (1965) but it would seem that our results are too high, a result we would expect from inspection of the differential cross-sections.

Finally, we have calculated the distorted wave Born approximation to the direct partial wave amplitudes t_ℓ at 100 eV, using both the Byron and Joachain functions of Appendix D, and the configuration interaction wavefunctions of Vanderpoorten (1973). From the values given in table VIII it is apparent that the use of the more accurate 1^1S and 2^1S functions alters t_ℓ by less than 5%. We point out, however, that the exchange partial wave amplitudes g_ℓ are likely to be more sensitive to the choice of wavefunction.

d) $1^1S \rightarrow 2^1P$ Excitation of Helium

The results of the present calculation of the differential cross-sections for 2^1P excitation of helium at 50 and 100 eV are displayed in figures 8a) and 8b). We recall that for this particular transition our model considers the direct scattering amplitude only, and assumes a plane wave final state with second order potential distortion in the initial state. In view of the simplicity of this approximation, the agreement with experiment is surprisingly good for angles less than 40°; at the larger angles, however, the cross-sections decrease too rapidly. Nevertheless, we expect our large angle values to be better than those of Terebey (1974) who used the Glauber approximation. At 100 eV the latter small angle results have not been shown as they lie very close to ours.

We have also calculated, from the unpublished transition amplitudes of Berrington et al (1973), the large angle differential cross-sections predicted by theimpact parameter approximation to the second order potential method. These are also displayed in figures 8a) and 8b) andit is seen that this model gives quite good agreement with experiment at large angles. More significantly we see that for angles less than 40° the results are very close to those of our distorted wave approximation, even at $\theta=0$.

At 100 eV the results of Hidalgo and Geltman (1972) are shown, and are seen to reproduce the shape of the experimental curve quite poorly; they are in fact inferior to the results ofthe present model at small angles. Concerning other theoretical values not shown, we note that the DWBA of Madison and Shelton (1973) gives excellent agreement with the data of Crooks and Rudd (1972), while the results of Joachain and Vanderpoorten (1974) obtained by the eikonal distorted wave model of Chen et al (1972) are quite similar to those of our model, for angles less than 60°. The inadequacy of the first Born approximation and its variants has been clearly demonstrated by Truhlar et al (1970) and they have not therefore been considered.

In figures 9a) and 9b) we show the values predicted by the present distorted wave model for the quantity $\lambda(\theta)$, defined by (4.50), which is the fractional contribution to the differential cross-section of the magnetic substate m=0. These are compared with the data of Eminyan et al (1974) at 50 and 100 eV, and in addition to the experimental points we have of course that λ at $\theta=0^{0}$ must equal one. It is seen that our results are in good agreement with the measurements at both energies. At 50 eV the Born approximation gives values that lie very close to ours, but this is likely to be fortuitous as figure 9b) shows that there is no agreement at 100 eV. Of the other theoretical results available at these energies we see that both the many-body work of Taylor (1974) and the eikonal distorted wave model of Joachain and Vanderpoorten (1974a) are in very poor agreement with our results and the measurements. It is mentioned at this point that the measurements of Eminyan et al (1974) assume the axis of quantization to lie along the direction of the incident momentum; it would therefore be erroneous to include in figures 9a) and b) the results of theories that do not make this choice, such as that of Berrington et al (1973).

Figures 10a) and 10b) show the values of $\chi(\theta)$, the relative phase between the m=1 and m=0 scattering amplitudes, given by the present model at 50 and 100 eV. The agreement with the experimental results of Eminyan et al (1974) is very poor, which is rather surprising in view of the success with which our model predicted $\lambda(\theta)$. In contrast, we see that at 100 eV Joachain and Vanderpoorten (1974a) obtain much better agreement with the data using their eikonal distorted wave method, despite this giving poor values for $\lambda(\theta)$. However, Joachain and Vanderpoorten (1974a) find that on using a static rather than a Glauber distorting potential in their model (which is that of Joachain and Vanderpoorten 1974) there is a significant deterioration of the agreement. This is shown in figure 10b) where we see that their choice of a simpler distorting potential lowers the value of $\chi(\theta)$ at 45° by 15%.

e) <u>1s-2s Excitation of Hydrogen</u>

The present model of 2s excitation of hydrogen is described in Section 4.2 and at 100 and 200 eV gives results for the differential cross-sections which we show in figures 11a) and b). We also obtained DWBA results which at both energies are consistently higher than those of present method, but by no more than 10%, and for the sake of clarity these are therefore not shown. The effect of exchange was investigated by calculating the differential cross-sections from the direct amplitude (4.18) alone. It was found that at 100 eV the neglect of exchange increased the cross-section by 10% at 90°, while there was no change at small angles.

Figure 11 also shows the coulomb projected Born results of Geltman and Hidalgo (1971) and the distorted wave results of McDowell et al (1973), both of which fall considerably below the present results at 90° although all three approximations are in reasonable agreement in the forward direction. This behaviour is to be expected from the results for helium excitation where the coulomb projected Born results were also found to be much lower than those of the present model. Furthermore, the calculation of McDowell et al (1973) is very similar to our simplified model where we consider second order potential distortion in the initial channel only, and for helium this was found to give much smaller values than those of the more complete distorted wave model.

Figure 11a) also shows the results of the second order diagonalization method of Baye and Heenen (1974a) which show the same strong peak in the forward direction that has already been noted for ^1S excitation of helium. Other small angle results for 100 eV that are not shown are those of the Glauber approximation (Tai et al 1970) which lie between the present results and those of Baye and Heenen (1974a), and the eikonal distorted wave results of Joachain and Vanderpoorten (1973) which lie slightly lower than ours.

In table IX we show the results of our calculation of the total 1s→2s cross-section at 100 and 200 eV with both the present approximation and the DWBA. We also display the results of other calculations and from left to right the entries are in descending order of magnitude. It is seen immediately that the neglect by the DWBA of the polarization, absorption and exchange in the initial channel makes it a rather poor approximation for the total cross-section. On the other hand, the results of the present model seem quite satisfactory when compared with those of the other models.

5.3 Discussion

The distorted wave approximation proposed in Section 4.1 as a description of 2S excitation of helium gives good agreement with differential cross-section measurements over the entire angular range. In this respect it is superior to all other calculations that have been performed, with the exception of the work of Taylor (1974) in the 2^1S case. The present work when compared with the DWBA results shows that including the effect of the second order and exchange potentials on the distorted wave in the initial channel gives an improvement at 50 eV of up to 20% and 25% for the 2^3S and 2^1S cross-sections respectively. This improvement is, however, only 10% for the 2s excitation of hydrogen at 100 eV, but we should note that this 100 eV incident energy expressed as a multiple of the ionization threshold corresponds to an energy of nearly 200 eV for helium. It is therefore not surprising that we see less effect for hydrogen than for helium excitation with the particular energies chosen here.

Although the reliability of the 2^1S and 2^1P wavefunctions has been examined, no such assessment was made for the 2^3S function of Morse et at (1935). Although the latter is rather crude by recent standards, work of Joachain and Van den Eynde (1970) suggests that is is more important to use an accurate bound state wave function in the initial channel than in the final one. We do not expect, therefore, a serious error for 2^3S excitation from our choice of wave function.

The most serious deficiency in our model of s excitation is the neglect of s-p coupling, which has been shown by Berrington et al (1973) to have a considerable effect for helium ^1S excitation in the forward direction. Indeed we have seen here that for both hydrogen and helium the results of models that include s-p coupling (Baye and Heenen 1974a and Berrington et al 1973) are much more sharply peaked than those that do not. The former models however are both semi-classical approximations and fail to adequately reproduce the minimum that occurs for both 2^1S and 2^3S excitation at the lower energies, and we suggest that a full wave treatment with s-p coupling is necessary to show this effect.

The simpler distorted wave method that we have adopted for P excitation gives good results at the smaller angles, and the agreement in the forward direction with those of Berrington et al (1973) illustrates that 2^1S-2^1P coupling is in this case a small effect. On the basis of this alone, we therefore expect that the use of the more complete distorted wave model proposed for S excitation will give good results here also. This view is further substantiated by noting that the DWBA results of Madison and Shelton (1973) lie above the data for energies less than 100 eV; recalling the degree of improvement over the DWBA that we found for S excitation, we conclude that the more complete distorted wave model is likely to give excellent agreement with experiment for 2^1P excitation.

The success with which the experimental values of $\lambda(\theta)$ are reproduced by our simple model and to a lesser extent by the Born approximation makes us question whether this quantity will be of use in distinguishing between theories. The scarcity of both experimental and theoretical results makes it difficult to be more conclusive, but at this stage, it would seem that the evaluation of $\chi(\theta)$ is likely to be of more use, due to its apparent sensitivity.

Finally, we note that the computational procedure adopted here for the s transitions is to some extent wasteful, in that we calculate the distorted wave partial amplitude T_ℓ^{DW} until this becomes equal to the Born value T_ℓ^B for some value L. In every case, however, we found that the amplitude T_ℓ^{DW} becomes equal to the DWBA value T_ℓ^{DWBA} for $\ell < L$ and it would seem to be expedient therefore to use the three models (rather than only two) for different ranges of ℓ.

Chapter 6 The Use of Dispersion Relations in Atomic Scattering

6.1 Theory

The present investigation of electron-atom collisions has concentrated on obtaining the scattering amplitude $f(\theta,k^2)$ from either the asymptotic form of the scattered wave function, or from approximations to the two-potential formula. If, however, certain assumptions are made regarding the analytic structure of the function $\left[f(\theta,k^2)-f^B(\theta,k^2)\right]$, a third approach becomes available in that it is possible to write down a dispersion relation expressing the real part of $f(\theta,k^2)$ in terms of its imaginary part. For potential scattering for example it can be shown (Roman 1965 p210) that Re $f(\theta,k^2)$ is related to a Hilbert transform of Im $f(\theta,k^2)$, with an integration path that in general includes an unphysical region of the scattering amplitude.

Dispersion relations become of special interest for scattering in the forward direction since the Hilbert transform is then over the physical region only, and the optical theorem (equation 3.8) allows Im $f(0,k^2)$ to be replaced by the total cross-section. In particular Gerjuoy and Krall (1960, 1962) show that for electron-hydrogen and helium scattering this forward dispersion relation has the form

$$\mathrm{Re}\, f(0,k^2) = f^B(0,k^2) + \sum_j \frac{R_j(k^2)}{k_j^2 - k^2} + \frac{1}{4\pi}\, P\!\int_0^\infty \frac{Q_{TOT}(k'^2)\,k'\,dk'^2}{k'^2 - k^2} \qquad (6.1)$$

where the total cross-section is in units of πa_0^2, and the scattering amplitudes are of appropriate symmetry.

In deriving the above relationship, it is assumed that in the complex energy plane the function $\left[f(0,k^2)-f^B(0,k^2)\right]$ i) vanishes for large k^2, ii) has a branch cut along the positive real axis and iii) has poles on the negative real axis corresponding to bound eigen-states of the total Hamiltonian, the residues of which are $R_j(k^2)$.

The limiting case of (6.1) as k^2 tends to zero has been considered by Krall and Gerjuoy (1960) who deduce that

$$-A = f^B(0,0) + \sum_j \frac{R_j(0)}{k_j^2} + \frac{1}{4\pi} P\int_0^\infty \frac{Q_{TOT}(k'^2)\,dk'^2}{k'} \qquad (6.2)$$

where A denotes the scattering length. Equation (6.2) is an important sum rule, which must be satisfied by the total cross-section.

The utility of (6.1) and the optical theorem as a means of obtaining a theoretical value for the forward scattering intensity is rather limited. However, provided that total cross-section measurements have been made for all energies up to those for which the Born and Bethe approximations for $Q_{TOT}(k^2)$ become valid, equations (6.1) and (6.2) allow experimentally derived values of the forward intensity and scattering length to be computed. From these, the consistency of experimental data can then be estimated, as has been illustrated by the work of Gerjuoy and Krall (1960), Krall and Gerjuoy (1960) and Lawson et al (1966).

6.2 Applications

a) A consistency check of positron-helium measurements

Since the Born and Bethe approximation to the total cross-section is expected to be valid at 400 eV, the measurements of Canter et al (1973) in the range 2-400 eV in conjunction with the low energy results for $Q_{TOT}(k^3)$ of Canter et al (1972), Costello et al (1972), Jaduszliwer et al (1972) and Jaduszliwer and Paul (1973), make possible an analysis of positron-helium scattering using the equivalent of equations (6.1) and (6.2). Although the computation of the forward intensity is at present without interest, accurate calculations of both $f^B(0,k^2)$ and A have been made and it is proposed therefore to use the sum rule to check the consistency of the available data.

As there is no bound state of the positron helium system (Spruch 1969) equation (6.2) becomes

$$-A = f^{B}(0,0) + \frac{1}{4\pi}\int_0^\infty \frac{Q_{TOT}(k'^2)}{k'}\,dk'^2 \qquad (6.3)$$

where $f^B(0,0)$ is in this case the Born approximation to the direct amplitude only.

Humberston (1973) has obtained from the Kohn variational principle a value of -0.472 for the positron helium scattering length. Combining this with the Pekeris (1959) value for $f^B(0,0)$ -0.791 we deduce that the data for $Q_{TOT}(k^2)$ must be such that

$$\frac{1}{4\pi}\int_0^\infty \frac{Q_{TOT}(k^2)}{k}\,dk^2 = 1{\cdot}26 \qquad (6.4)$$

The integral was evaluated by first obtaining a least squares fit to the data which together with the Born-Bethe approximation gives the following analytic forms:-

i) For $2 \leq k^2 \leq 20$ eV

$$Q_{TOT}(k^2) = 0.883 - 7.5k - 8.97\,k^2 \ln k + 5.45\,k^2 + 1.44\,k^4 \qquad (6.5)$$

(5 parameters, 18 data points giving $\chi^2 = 12.4$)

ii) For $20 < k^2 \leq 400$ eV

$$Q_{TOT}(k^2) = \frac{1}{k^2}(26.7 - 12.2 \ln k - 68.9/k^2 + 63.9/k^4 - 21.3/k^6) \qquad (6.6)$$

(5 parameters, 14 data points giving $\chi^2 = 9.41$)

iii) For $k^2 > 400$ eV

$$Q_{TOT}(k^2) = (6.197 - 4.149/k^2 + 2.875/k^4 + 3.011 \ln k^2)/k^2 \qquad (6.7)$$

The analytic form for the low energy fit of (6.5) was suggested by the effective range formula of O'Malley (1963), and predicts a scattering length of ± 0.49, in good agreement with the value of Humberston (1973). In fact (6.5) gives values of $Q_{TOT}(k^2)$ for energies between 0 and 2 eV that agree well with those obtained from the variational phase shifts of Humberston (1974). The Born-Bethe approximation (6.7) is that of Kennedy (1968) and Inokuti et al (1967), this being the same for both electron and positron scattering.

Figure 12 shows the fitted values of $Q_{TOT}(k^2)$ together with those given by the Born-Bethe approximation. The inconsistency of the data is obvious even without the calculation of the left hand side of (6.4), as the measurements do not tend to the Born-Bethe values with increasing energy. However, making the interpolation shown we find that the evaluation of the left hand side of (6.4) gives the value 1.3 and the sum rule is satisfied to within 5%. In order to be consistent with (6.3) it therefore appears that positron-helium total cross-section measurements should reproduce the suggested interpolation of figure 12. This choice in fact seems to have been vindicated by the very recent experiments of Jaduszliwer et al (1974) and Coleman et al (1974) for energies up to 400 eV.

b) Extension of electron-neon data analysis

The use of the dispersion relation and sum rule of Section 6.1 is obviously limited to a consistency check of measurements of total cross-sections and scattering intensities near the forward direction. In general, to distinguish between alternative data sets we require an analysis in which a simultaneous best fit of parametrized phase shifts to the available measurement is attempted. However, in carrying out a data analysis of this type, the dispersion relation (6.1) can in principle be used to provide experimentally derived values of Re $f(0,k^2)$ as a supplement to the experimental data being fitted. This has been done for electron-helium scattering by Bransden and McDowell (1969, 1970) who were successful in being able to reject the differential cross-section data of Ramsauer and Kollath (1932) in favour of that of Gibson and Dolder (1969).

The extension of the phase shift analysis to electron scattering from neon and argon has been made by McDowell (1971), but without the use of the forward dispersion relation. Now the only difficulty in employing (6.1) for the case of neon, apart from some uncertainty regarding the total cross-section data of Normand (1930), lies in the evaluation of the Born scattering amplitude. It was decided therefore to calculate $f^B(0,k^2)$ for electron-neon scattering, to permit the extension of the work of McDowell (1971).

We choose the wavefunctions of Weber et al (1970) and Clementi (1965 Table 01-04) as two alternative choices for the ground state of neon. For these Hartree-Fock functions the calculation of the direct Born amplitude is then trivial, while unpublished work of Bransden and McDowell shows that the exchange amplitude reduces to a form requiring only one numerical integration.

The results of this computation show firstly the sensitivity of the Born exchange amplitude at zero energy to the choice of wavefunction. Specifically, it was found that the direct and exchange contributions to the Born amplitude $f^B(0,0)$ were 3.134 and 5.90 respectively for the function of Weber et al (1970), and 3.125 and 5.47 for that of Clementi (1965). This sensitivity of $f^B(0,0)$ has in fact been reported previously by Lawson et al (1966) for electron-helium scattering. For $k^2 \neq 0$ however we find that there is close agreement between the values of $f^B(0,k^2)$ predicted by the alternative wave functions.

Secondly our calculation shows that whichever value of $f^B(0,0)$ is adopted, it is impossible to satisfy the sum rule (6.2). Since there are no residue contributions for electron-neon scattering, then we expect that

$$f^B(0,0) = -A - \frac{1}{4\pi} P\int_0^\infty \frac{Q_{TOT}(k^2)\, dk^2}{k} \tag{6.8}$$

However, from the data of Normand (1930) together with the Bethe-Born approximation for $Q_{TOT}(k^2)$ the integral in (6.8) is found to be 4.12, while O'Malley (1963) gives for A the value 0.24. It is expected therefore that the difference between the Born direct and exchange amplitudes should be -4.36, which is obviously inconsistent with the values we have obtained.

Even allowing for the lack of reliability of the Normand data, it seems clear that for neon it is insufficient to use Hartree-Fock wave functions in the application of the forward dispersion relation. It is suggested therefore that the extension of the phase shift analysis of McDowell (1971) to incorporate the use of dispersion relations requires the evaluation of $f^B(0,k^2)$ by accurate configuration interaction wave functions.

CONCLUSIONS

A model has been presented that describes the scattering of electrons from light atoms at intermediate energies. A one channel approximation to this has been considered and application made to the elastic scattering from hydrogen and helium atoms. This gives agreement with measured differential cross-sections equalled only by the EBS method, but unlike ours the latter model is not amenable to systematic improvement. The results of this work also highlight the inadequacy of semi-classical approximations at intermediate energies.

The distorted wave approximation used for S excitation was found for helium to give good agreement with experiment. However, it failed to correctly reproduce, at lower energies, both the minimum and forward peak in the differential cross-section. This is attributed to the neglect of both s-p coupling, and polarization and absorption effects in the final channel. These deficiencies would not be present, however, in a second order potential approximation with the n= 2 levels represented explicitly. We expect therefore that this latter model will give excellent agreement with experiment.

It is concluded that the results of the present work provide sufficient justification for proceeding to an application of the many channel formulation of Section 2.2. In addition, the extension relevant to other light atoms such as sodium and lithium seems to be warranted. In this way, it is expected that definitive cross-sections will be obtained in the intermediate energy region, for excitation to states that the model explicitly represents. Furthermore, the utility of the distorted wave approximation as a supplement to the above method has been demonstrated.

The many channel second order potential method presented here will have even wider application when suitably modified to include channels that are closed. This will allow its use to be extended to energies below the single ionization threshold of the target. In addition for atoms other than hydrogen it will then be possible to represent doubly excited states, allowing the narrow shape resonances in the autoionization region to be studied. It is then forseeable that we would have a single model giving a good description of electron-atom scattering at all non-relativistic energies.

The result of the application of the dispersion relation and sum rule shows that they are valuable in establishing the consistency of experimental data. Their use is limited however, as they require total cross-section measurements to be available over a complete energy range. We have also seen that they are difficult to apply to complex atoms and in any case have no application to inelastic scattering.

Appendix A

The coefficients $f_\lambda(\ell_1\ell_2\ell_1'\ell_2'|L)$ and $g_\lambda(\ell_1\ell_2\ell_1'\ell_2'|L)$

The explicit form for the angular coefficients introduced in (1.27) and (1.28) is given by equation 36 of Percival and Seaton (1957). We write this as

$$f_\lambda(\ell_1\ell_2\ell_1'\ell_2'|L) = (-1)^{\ell_1+\ell_1'-L}\left[(2\ell_1+1)(2\ell_1'+1)(2\ell_2+1)(2\ell_2'+1)\right]^{\frac{1}{2}} \times$$

$$\times \begin{pmatrix} \ell_1 & \ell_1' & \lambda \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} \ell_2 & \ell_2' & \lambda \\ 0 & 0 & 0 \end{pmatrix}\begin{Bmatrix} \ell_1 & \ell_2 & L \\ \ell_2' & \ell_1' & \lambda \end{Bmatrix} \qquad (A.1)$$

where in order to exploit their symmetry properties, the Clebsch-Gordan and Racah coefficients of Percival and Seaton (1957) have been expressed in terms of Wigner 3-j and 6-j symbols defined by (Messiah 1964 Vol. II)

$$\begin{pmatrix} \ell_1 & \ell_2 & L \\ m_1 & m_2 & -M \end{pmatrix} = \frac{(-1)^{\ell_1-\ell_2+M}}{(2L+1)^{1/2}}\, C^{\ell_1\ell_2L}_{m_1m_2M} \qquad (A.2)$$

and

$$\begin{Bmatrix} \ell_1 & \ell_2 & \ell_3 \\ \ell_1' & \ell_2' & \ell_3' \end{Bmatrix} = (-1)^{\ell_1+\ell_2+\ell_1'+\ell_2'}\, W(\ell_1\ell_2\ell_2'\ell_1';\ell_3\ell_3') \qquad (A.3)$$

The 6-j symbol is invariant under an interchange of columns, and the interchange of any two momenta in the lower row with the corresponding pair in the top row. Therefore on noting that conservation of parity demands that

$$(-1)^{\ell_1+\ell_1'} = (-1)^{\ell_2+\ell_2'} \qquad (A.4)$$

it follows immediately from A.1 that

$$f_\lambda(\ell_1\ell_2\ell_1'\ell_2'|L) = f_\lambda(\ell_1'\ell_2'\ell_1\ell_2|L) \tag{A.5}$$

The properties of the 6-j symbol demand that the following triads satisfy the triangle inequalities:-

$$\text{i) } (\ell_1\ell_2L) \quad \text{ii) } (\ell_1\ell_1'\lambda) \quad \text{iii) } (\ell_2'\ell_2\lambda) \quad \text{iv) } (\ell_2'\ell_1'L) \tag{A.6}$$

where ii) and iii) are also implied by the 3-j symbols.

Consider the special case of $\ell_1=0$. We have that i) now gives $\ell_2=L$, ii) gives $\ell_1'=\lambda$ and the only triangle inequality is for $(\ell_2'L\ell_1')$. Equation (A.1) then reduces to

$$f_\lambda(0\ell_2\ell_1'\ell_2'|L) = (-1)^{\ell_2'-\ell_1'}\sqrt{\frac{2\ell_2'+1}{2\ell_1'+1}}\begin{pmatrix}\ell_2 & \ell_2' & \lambda\\ 0 & 0 & 0\end{pmatrix}\delta_{\ell_2L}\,\delta_{\ell_1'\lambda} \tag{A.7}$$

where we have used (Messiah 1964 p916)

$$\begin{Bmatrix} j & j' & 0\\ J & J' & g\end{Bmatrix} = \frac{(-1)^{j+J+g}\,\delta_{jj'}\,\delta_{JJ'}}{[(2j+1)(2J+1)]^{1/2}} \tag{A.8}$$

together with the symmetry of the 6-j symbol, and in addition (Messiah 1964 p910)

$$\begin{pmatrix} 0 & j & j'\\ 0 & 0 & 0\end{pmatrix} = \frac{(-1)^{-j}\,\delta_{jj'}}{\sqrt{(2j+1)}} \tag{A.9}$$

The coefficient $g_\lambda(\ell_1\ell_2\ell_1'\ell_2'|L)$ for the special case of $\ell_1=0$ is, from (1.28) and A.7)

$$g_\lambda(0\ell_2\ell_1'\ell_2'|L) = (-1)^{\ell_1'-\ell_2'}\sqrt{\frac{2\ell_1'+1}{2\ell_2'+1}}\begin{pmatrix}\ell_2 & \ell_1' & \lambda\\ 0 & 0 & 0\end{pmatrix}\delta_{\ell_2L}\,\delta_{\ell_2'\lambda} \tag{A.10}$$

Furthermore, on putting $\ell_1'=0$ we obtain from (A.7) and (A.9)

$$f_\lambda(0 l_2 0 l_2' | L) = \delta_{l_2 L} \delta_{l_2 l_2'} \delta_{\lambda 0} \qquad (A.11)$$

$$= g_\lambda(0 l_2 0 l_2' | L) \qquad (A.12)$$

thus agreeing with Percival and Seaton (1957 Table I).

Appendix B

The Static Exchange Approximation for Electron-Helium Scattering

We obtain the static exchange approximation from the Kohn variational principle, in the manner of Drukarev (1965 p122), except that we only make reductions that are consistent with the helium wave functions being approximate. This gives for the elastic scattering function $F(\underline{r})$

$$[\nabla^2 + k^2]F(\underline{r}) = 2V(\underline{r})F(\underline{r}) + 2\int W(\underline{r},\underline{r}')F(\underline{r}')\,d\underline{r}' \qquad (B.1)$$

where

$$\begin{aligned} W(\underline{r},\underline{r}') = &- \phi_{10}(\underline{r})\Big\{-\frac{1}{2}\nabla^2_{r'} - \frac{2}{r} - \frac{2}{r'} + \frac{1}{|\underline{r}-\underline{r}'|} - \frac{1}{2}k_0^2 - E_0 + \\ &+ \int \phi_{10}(\underline{r}'')\Big[-\frac{1}{2}\nabla^2_{r''} - \frac{2}{r''} + \frac{1}{|\underline{r}'-\underline{r}''|} + \frac{1}{|\underline{r}-\underline{r}''|}\Big]\phi_{10}(\underline{r}'')\,d\underline{r}''\Big\}\phi_{10}(\underline{r}') + \\ &+ \phi_{10}(\underline{r}')\frac{1}{2}\nabla^2_{r}\phi_{10}(\underline{r}) \end{aligned} \qquad (B.2)$$

and $\phi_{10}(\underline{r})$ is defined such that

$$\phi_1(\underline{r}_1,\underline{r}_2) = \phi_{10}(\underline{r}_1)\phi_{10}(\underline{r}_2) \qquad (B.3)$$

where $\phi_1(\underline{r}_1,\underline{r}_2)$ is given by (2.24). Equation (B.2) differs from (26.4) of Drukarev (1965 p127) in that we have not assumed the hermiticity of the Laplacian operator, this being only valid for exact wave functions.

We now make a partial wave decomposition of (B.1) by expanding

$$F(\underline{r}) = \sum_{\ell=0}^{\infty} \frac{(2\ell+1)}{2}\frac{f_\ell(r)}{r}P_\ell(\hat{\underline{k}}\cdot\hat{\underline{r}}) \qquad (B.4)$$

and

$$W(\underline{r},\underline{r}') = -\phi_{10}(r)\phi_{10}(r')\sum_{\lambda} P_{\lambda}(\hat{\underline{r}}\cdot\hat{\underline{r}}')\frac{\min^{\lambda}(r,r')}{\max^{\lambda+1}(r,r')} + q(r,r') \tag{B.5}$$

On substituting (B.4) and (B.5) into (B.1) and using

$$\int d\hat{\underline{r}}'\, P_{\ell'}(\hat{\underline{r}}'\cdot\hat{\underline{k}})\,P_{\lambda}(\hat{\underline{r}}\cdot\hat{\underline{r}}') = \frac{4\pi}{2\lambda+1}P_{\lambda}(\hat{\underline{r}}\cdot\hat{\underline{k}})\,\delta_{\lambda\ell'} \tag{B.6}$$

we obtain

$$\left[\frac{d^2}{dr^2} + k^2 - \frac{\ell(\ell+1)}{r^2}\right]f_{\ell}(r) = 2V(r)f_{\ell}(r) + 2\int_0^{\infty}K_{\ell}(r,r')f_{\ell}(r')\,dr' \tag{B.7}$$

where

$$K_{\ell}(r,r') = \frac{-1}{2\ell+1}P_{10}(r)P_{10}(r')\frac{\min^{\ell}(r,r')}{\max^{\ell+1}(r,r')} + q(r,r')\,\delta_{\ell 0} \tag{B.8}$$

and we have used (2.24) and (B.3) to replace $\phi_{10}(\underline{r})$. We note that

$$V(r) = 2\int d\underline{r}'\,\phi_{10}(\underline{r}')\frac{1}{|\underline{r}-\underline{r}'|}\phi_{10}(\underline{r}') - \frac{2}{r} \tag{B.9}$$

and comparing (B.5) to (B.2), use of (B.9) then gives for $q(r,r')$ the expression (2.28).

When $P_{10}(r)$ is chosen to have the form $Nr(e^{-ar} + ce^{-br})$ the derivatives in (2.28) are easily evaluated, and the integral over x gives a constant C_{10}, where

$$C_{10} = N^2\left\{a^2\left[\frac{1}{8a^3} + \frac{c}{(a+b)^3}\right] - (a-2)\left[\frac{1}{4a^2} + \frac{c}{(a+b)^2}\right] + cb^2\left[\frac{1}{(a+b)^3} + \frac{c}{8b^3}\right] - c(b-2)\left[\frac{1}{(a+b)^2} + \frac{c}{4b^2}\right]\right\} \tag{B.10}$$

Now introducing the function

$$D_{10}(r) = N\left[a(ar-2)e^{-ar} + cb(br-2)e^{-br}\right] \tag{B.11}$$

we can write the explicit form for q(r,r') as

$$q(r,r') = P_{10}(r')P_{10}(r)\left[\frac{1}{r} - \frac{V(r)}{2} + \frac{1}{r'} - \frac{V(r')}{2} + C_{10} + E\right] +$$

$$+ \frac{1}{2}P_{10}(r)D_{10}(r') + \frac{1}{2}P_{10}(r')D_{10}(r) \tag{B.12}$$

Choosing the parameters N, a, b and c to be those of Byron and Joachain (1966), the constant C_{10} is found to be

$$C_{10} = 1.9434 \tag{B.13}$$

Appendix C

Recurrence relations for the integral $M_\ell(\alpha|rr')$

We consider the integral $M_\ell(\alpha|rr')$ defined by (2.30)

Denoting

$$A_\ell(\alpha|rr') = \frac{1}{(r_< r_>)^{\ell+1}} \int_0^{r_<} e^{-\alpha x}\, x^{2\ell+2}\, dx \qquad (C.1)$$

then integration by parts gives for $\ell > 0$

$$A_\ell = \frac{(2\ell+1)(2\ell+2)}{\alpha^2 r_< r_>} A_{\ell-1} - \frac{e^{-\alpha r_<}}{\alpha}\left(\frac{r_<}{r_>}\right)^{\ell+1}\left(1 + \frac{2\ell+2}{\alpha r_<}\right) \qquad (C.2)$$

where the arguments of A_ℓ and $A_{\ell-1}$ are those of (C.1).

The initial value is

$$A_0 = \frac{2}{\alpha^3 r_< r_>} - \frac{e^{-\alpha r_<}}{\alpha r_>}\left(r_< + \frac{2}{\alpha} + \frac{2}{\alpha^2 r_<}\right) \qquad (C.3)$$

and $A_\ell(\alpha|0r') = 0$ for all ℓ.

Similarly we denote

$$B_\ell(\alpha|rr') = \frac{1}{r_>}\left(\frac{r_<}{r_>}\right)^{\ell} \int_{r_<}^{r_>} x\, e^{-\alpha x}\, dx \qquad (C.4)$$

and find that for $\ell > 0$

$$B_\ell(\alpha|rr') = \frac{r_<}{r_>} B_{\ell-1}(\alpha|rr') \qquad (C.5)$$

Equation (C.5) is solved subject to

$$B_0(\alpha|rr') = \frac{e^{-\alpha r_<}}{\alpha r_>}\left(r_< + \frac{1}{\alpha}\right) - \frac{e^{-\alpha r_>}}{\alpha r_>}\left(r_> + \frac{1}{\alpha}\right) \qquad (C.6)$$

and when $r_< = 0$

$$B_\ell = \delta_{\ell 0}\left[\frac{1}{\alpha^2 r_>} - \frac{e^{-\alpha r_>}}{\alpha}\left(1 + \frac{1}{\alpha r_>}\right)\right] \tag{C.7}$$

Finally, in writing

$$C_\ell(\alpha|rr') = (r_< r_>)^\ell \int_{r_>}^{\infty} x^{-2\ell} e^{-\alpha x}\, dx \tag{C.8}$$

we obtain for $\ell > 1$ the relation

$$C_\ell = \frac{\alpha^2 r_< r_>}{(2\ell-1)(2\ell-2)} C_{\ell-1} + \frac{r_> e^{-\alpha r_>}}{(2\ell-1)}\left(\frac{r_<}{r_>}\right)^\ell\left(1 - \frac{\alpha r_>}{2\ell-2}\right) \tag{C.9}$$

with the initial values

$$C_0(\alpha|rr') = \frac{1}{\alpha} e^{-\alpha r_>} \tag{C.10}$$

and

$$C_1(\alpha|rr') = r_< e^{-\alpha r_>} - \alpha r_< r_> E_1(\alpha r_>) \tag{C.11}$$

The exponential integral of the first kind, is defined as (Abramowitz and Stegun 1965 p228)

$$E_1(x) = \int_x^{\infty} e^{-t} t^{-1}\, dt \tag{C.12}$$

The integral $M_\ell(\alpha|rr')$ is now obtained from the sum of A_ℓ, B_ℓ and C_ℓ.

Appendix D

Wave functions and matrix elements of the interaction

1) Electron-hydrogen scattering

The normalized bound state wave function for hydrogen is written as

$$\phi_{n\ell m}(\underline{r}) = \frac{P_{n\ell}(r)}{r} Y_{\ell m}(\hat{\underline{r}}) \tag{D.1}$$

and in particular we have

$$P_{10}(r) = 2r e^{-r} \tag{D.2}$$

and

$$P_{20}(r) = \frac{1}{2\sqrt{2}}(2-r) r e^{-r/2} \tag{D.3}$$

From the above equations we obtain the following expressions for the matrix elements defined by (1.6):-

$$V_{1s1s}(\underline{r}) = -e^{-2r}\left(1+\frac{1}{r}\right) \tag{D.4}$$

$$V_{1s2s}(\underline{r}) = \frac{2\sqrt{2}}{27} e^{-3r/2}(3r+2) \tag{D.5}$$

and

$$V_{2s2s}(\underline{r}) = -\frac{e^{-r}}{8r}\left(r^3+2r^2+6r+8\right) \tag{D.6}$$

2) Electron-helium scattering

The normalized ground state function of helium is written as

$$\phi_{100}(\underline{r}_1, \underline{r}_2) = \frac{P_{10}(r_1)}{r_1} Y_{00}(\hat{\underline{r}}_1) \frac{P_{10}(r_2)}{r_2} Y_{00}(\hat{\underline{r}}_2) \tag{D.7}$$

while that for an excited state is

$$\phi_{nlm}(\mathbf{r}_1,\mathbf{r}_2) = \frac{P_{\bar{1}0}(r_1)}{r_1}Y_{00}(\hat{\mathbf{r}}_1)\frac{P_{nl}(r_2)}{r_2}Y_{lm}(\hat{\mathbf{r}}_2) \pm \left\{\mathbf{r}_1 \leftrightarrow \mathbf{r}_2\right\} \quad (D.8)$$

where the + and - signs correspond to singlet and triplet states respectively.

On adopting Hartree-Fock forms for (D.7) and (D.8) we have

$$P_{10}(r) = N_{10}\, r\left(e^{-ar} + c\, e^{-br}\right) \quad (D.9)$$

$$P_{\bar{1}0}(r) = r\, e^{-Zr} \quad (D.10)$$

$$P_{20}(r) = N_{20}\, r\left(e^{-pr} - c_1 r\, e^{-qr}\right) \quad (D.11)$$

and

$$P_{21}(r) = N_{21}\, r^2 e^{-sr} \quad (D.12)$$

The values of the parameters in the above radial functions are, for the

i) 1^1S state (Byron and Joachain 1966)

$a = 1.41$ $b = 2.61$ $c = 0.799$ $N_{10} = 2.6051$

ii) 2^1S state (Byron and Joachain 1974b)

$p = 0.865$ $q = 0.522$ $c_1 = 0.432784$ $N_{20} = 2.4705$

iii) 2^3S state (Morse et al 1935)

$p = 1.57$ $q = 0.611$ $c_1 = 0.34081$ $N_{20} = 4.20$

and iv) 2^1P state (Goldberg and Clogston 1939)

$s = 0.485$ $N_{21} = 0.7566$

with $Z = 2$ for all the above choices. For electron helium scattering the matrix element of the interaction is

$$V_{nm}(\underline{r}) = \int d\underline{r}_1 \, d\underline{r}_2 \, \phi_n^*(\underline{r}_1, \underline{r}_2) \left[\frac{1}{|\underline{r}_1 - \underline{r}|} + \frac{1}{|\underline{r}_2 - \underline{r}|} - \frac{2}{r} \right] \phi_m(\underline{r}_1, \underline{r}_2) \tag{D.13}$$

and in particular we have

$$V_{1s1s}(\underline{r}) = -N_{1s1s}\left[b_0(2,2a) + 2c\,b_0(2,a+b) + c^2 b_0(2,2b)\right] \tag{D.14}$$

$$\begin{aligned} V_{1s2s}(\underline{r}) = -N_{1s2s}\Big[& b_0(2,a+p) + c\,b_0(2,b+p) - c_1 b_0(3,a+q) - \\ & - c c_1 b_0(3,b+q)\Big] \end{aligned} \tag{D.15}$$

$$V_{1s2p}(\underline{r}) = -Y_{1m}(\hat{\underline{r}})\,N_{1s2p}\left[b_1(3,a+s) + c\,b_1(3,b+s) - \frac{\lambda_4}{r^2}\right] \tag{D.16}$$

and

$$\begin{aligned} V_{2s2s}(\underline{r}) = -N_{2s2s}\Big\{ & \lambda_1 b_0(2,2z) \pm \lambda_2\left[b_0(2,z+p) - c_1 b_0(3,z+q)\right] + \\ & + \lambda_3\left[b_0(2,2p) - 2c_1 b_0(3,p+q) + c_1^2 b_0(4,2q)\right]\Big\} \end{aligned} \tag{D.17}$$

where the + and - signs in (D.17) denote as usual singlet and triplet states.

Equations (D.14) to (D.17) have introduced the following constants:-

$$N_{1s1s} = 2N_{10}^2$$

$$N_{1s2s} = 4N_{10}^2 N_{20}\left[\frac{1}{(a+z)^3} + \frac{c}{(b+z)^3}\right]$$

$$N_{1s2p} = 8N_{10}^2 N_{21}\pi^{\frac{1}{2}}\left[\frac{1}{(a+z)^3} + \frac{c}{(b+z)^3}\right]$$

$$N_{2s2s} = 4N_{20}^2 \tag{D.18}$$

together with

$$\lambda_1 = \frac{1}{8p^3} - \frac{6c_1}{(p+q)^4} + \frac{3c_1^2}{8q^5}$$

$$\lambda_2 = \frac{2}{(p+z)^3} - \frac{6c_1}{(q+z)^4}$$

$$\lambda_3 = \frac{1}{8z^3}$$

$$\lambda_4 = \frac{8}{(a+s)^5} + \frac{8c}{(b+s)^5} \qquad (D.19)$$

and in addition we have the auxiliary function $b_L(n,\alpha)$ defined by

$$b_L(n,\alpha) = \frac{1}{2L+1}\int_r^\infty dx\, x^n e^{-\alpha x}\left[\frac{x^L}{r^{L+1}} - \frac{r^L}{x^{L+1}}\right] \qquad (D.20)$$

The particular functions required in equations (D.14) to (D.17) are:-

$$b_0(2,\alpha) = \frac{e^{-\alpha r}}{\alpha^2}\left[\frac{2}{\alpha r} + 1\right] \qquad (D.21)$$

$$b_0(3,\alpha) = \frac{e^{-\alpha r}}{\alpha^3}\left[\frac{6}{\alpha r} + 4 + \alpha r\right] \qquad (D.22)$$

$$b_0(4,\alpha) = \frac{e^{-\alpha r}}{\alpha^4}\left[\frac{24}{\alpha r} + 18 + 6\alpha r + \alpha^2 r^2\right] \qquad (D.23)$$

and

$$b_1(3,\alpha) = \frac{e^{-\alpha r}}{\alpha^3}\left[\frac{8}{\alpha^2 r^2} + \frac{8}{\alpha r} + 4 + \alpha r\right] \qquad (D.24)$$

Finally, the functions $y_o(P_{10}^2|r)$ that are required in this work are obtained from equations (2.19) and (D.4) for hydrogen and from (2.26) and (D.14) for helium, with $V(r) = V_{1s1s}(\underline{r})$.

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	54.4 eV		100 eV		200 eV	
ℓ	a	b	a	b	a	b
0	.269(0)	.391(0)	.237(0)	.295(0)	.191(0)	.213(0)
1	.540(1)	.736(1)	.528(1)	.670(1)	.533(1)	.611(1)
2	.157(1)	.188(1)	.153(1)	.202(1)	.182(1)	.205(1)
3	.611(2)	.696(2)	.548(2)	.552(2)	.694(2)	.767(2)
4	.268(2)	.309(2)	.246(2)	.266(2)	.294(2)	.314(2)
5	.126(2)	.147(2)	.126(2)	.134(2)	.135(2)	.142(2)
6	.615(3)	.718(3)	.697(3)	.750(3)	.711(3)	.720(3)
7	.315(3)	.367(3)	.404(3)	.435(3)	.409(3)	.403(3)

<u>Table I</u>

Electron-hydrogen elastic scattering:

$|T_\ell|^2$ in a) the impact parameter approximation

b) partial wave treatment without exchange

Note: The notation X(n) implies that the number X must be divided by 10^n

	50 eV			100 eV			200 eV		
ℓ	a	b	c	a	b	c	a	b	c
0	.362(0)	.762(0)	.880(0)	.361(0)	.605(0)	.713(0)	.353(0)	.464(0)	.536(0)
1	.680(1)	.114(o)	.196(0)	.654(1)	.962(1)	.148(0)	.710(1)	.963(1)	.124(0)
2	.150(1)	.218(1)	.299(1)	.157(1)	.194(1)	.273(1)	.183(1)	.221(1)	.289(1)
3	.399(2)	.499(2)	.591(2)	.499(2)	.592(2)	.726(2)	.581(2)	.651(2)	.813(2)
4	.119(2)	.125(2)	.136(2)	.197(2)	.218(2)	.246(2)	.232(2)	.244(2)	.286(2)
5	.386(3)	.348(3)	.362(3)	.840(3)	.880(3)	.945(3)	.108(2)	.110(2)	.122(2)
6	.148(3)	.111(3)	.114(3)	.381(3)	.376(3)	.392(3)	.559(3)	.556(3)	.594(3)
7	.633(4)	.409(4)	.411(4)	.193(3)	.173(3)	.177(3)	.300(3)	.300(3)	.313(3)

Table II

Electron helium elastic scattering:

a) and b) as for Table I

c) $|T_\ell|^2$ in partial wave treatment including exchange

Notation as for Table I

Energy (ev)	Integrated Cross-Section		Total Cross-Section	
	a	b	a	b
54.4	.609	1.03	3.72	4.02
100	.310	.445	2.37	2.46
200	.150	.185	1.42	1.43

Table III

Integrated and total cross-sections in units of πa_0^2 for electron-hydrogen scattering:

a) Impact parameter approximation of Bransden et al (1972)

b) Present results

Energy (ev)	Present Results	Experimental Results
50	1.82	-
100	.753	.762
200	.319	.308
300	.195	.190
400	.138	.142
500	.107	.108

Table IV

Integrated cross-section in units of πa_0^2 for electron-helium scattering. Experimental result at 500 eV that of Bromberg (1969), otherwise those of Vriens et al (1968).

Energy	Re $\left\{f(o,k^2)\right\}$			Total Cross-Section	
(eV)	a	b	c	a	b
50	1.85	1.88	-	3.06	1.59
100	1.67	1.91	1.91	1.92	1.13
200	1.44	1.71	1.54	1.13	.858
300	1.32	1.48	1.39	.810	.697
400	1.25	1.36	1.30	.636	.554
500	1.20	1.29	1.24	.533	.462

Table V

Real part of forward scattering amplitude and total cross-section (πa_o^2) for electron-helium scattering.

a) Present Results

b) Values adopted by Bransden and McDowell (1970)

c) Eikonal-Born Series results of Byron and Joachain (1973)

Table VI Total $1^1S \rightarrow 2^3S$ Cross-Sections (πa_0^2) for electron-helium scattering

BO - Born Oppenheimer; MOR - Morrison and Rudge (1967); MAR - Mathur and Rudge (1974)

CR - Crooks and Rudd (1972); VSM - Vriens et al (1968a); ST - Suzuki and Takayanagi (1974)

Notation as for Table I

ENERGY (eV)	BO	MOR	MAR	DWBA	PRESENT	CR	VSM	ST
50	3.33 (1)	2.07 (2)	1.25 (2)	8.03 (3)	9.14 (3)	9.5 (3)		3.5 (3)
81.63	6.13 (2)		4.24 (3)	3.46 (3)	3.16 (3)			
100	1.41 (2)	4.1 (3)	2.74 (3)	2.24 (3)	1.99 (3)	1.6 (3)	9.1 (4)	1.2 (3)
150	2.17 (3)			8.4 (4)	7.32 (4)		2.4 (4)	6.4 (4)

Table VII Total $1^1S \rightarrow 2^1S$ Cross-Sections (πa_0^2) for electron-helium scattering

JV - Joachain and Vanderpoorten (1974); BBC - Berrington et al (1973)

R - Rice et al (1972); L - Lassettre (1965)

Notation as for Table I

ENERGY (eV)	JV	BBC	PRESENT	BORN	R(50 eV) L(100 eV)
50	1.5 (2)	2.25 (2)	3.03 (2)	3.81 (2)	1.8 (2)
81.63			2.2 (2)		
100	1.35 (2)	1.54 (2)	1.88 (2)	2.25 (2)	2.1 (2)
150			1.35 (2)		

Table VIII Direct partial wave amplitudes for electron-helium $1^1S \rightarrow 2^1S$ excitation in the distorted wave Born approximation, with

a) Hartree-Fock wavefunctions (Byron and Joachain 1966, 1974b)

b) Configuration interaction wavefunctions (Vanderpoorten 1973)

Notation as for Table I

ℓ	Re t_ℓ^{DWBA}		Im t_ℓ^{DWBA}	
	a	b	a	b
0	-6.79 (2)	-6.90 (2)	4.84 (2)	4.99 (2)
1	3.65 (2)	3.78 (2)	7.11 (2)	7.22 (2)
4	1.76 (2)	1.83 (2)	5.81 (3)	5.89 (3)
6	5.67 (3)	5.92 (3)	1.03 (3)	1.04 (3)
7	3.09 (3)	3.24 (3)	4.22 (4)	4.20 (4)

Table IX   Total 1s → 2s Cross-Sections (πa_0^2) for electron-hydrogen scattering

GH - Geltman and Hidalgo (1971); DWPO - McDowell et al (1973);

BH - Baye and Heenen (1974a); SBC - Sullivan et al (1972)

Notation as for Table i

ENERGY (eV)	DWBA	GH	BORN	PRESENT	GLAUBER	DWPO	BH	SBC
100	5.91 (2)	5.82 (2)	5.77 (2)	5.4 (2)	5.05 (2)	5.01 (2)	4.76 (2)	4.0 (2)
200	2.97 (2)	2.96 (2)	2.95 (2)	2.83 (2)	2.84 (2)	2.75 (2)	2.68 (2)	2.64 (2)

Table X Present Differential Cross-Sections for Electron-Atom Elastic Scattering

Notation as for Table I

	HYDROGEN (a_o^2/Sr)			HELIUM (a_o^2/Sr)					
Angle	54.4 eV	100 eV	200 eV	50 eV	100 eV	200 eV	300 eV	400 eV	500 eV
0	9.69	6.72	4.81	5.59	4.46	3.24	2.64	2.30	2.09
5	7.38	3.88	1.81	4.98	3.52	2.08	1.45	1.12	.944(0)
10	4.61	2.10	.975(0)	4.08	2.50	1.25	.836(0)	.642(0)	.558(0)
15	2.88	1.24	.614(0)	3.32	1.75	.807(0)	.538(0)	.416(0)	.348(0)
20	1.86	.812(0)	.385(0)	2.66	1.23	.552(0)	.372(0)	.281(0)	.223(0)
25	1.25	.539(0)	.234(0)	2.12	.889(0)	.395(0)	.252(0)	.186(0)	.141(0)
30	.839(0)	.366(0)	.150(0)	1.67	.659(0)	.278(0)	.174(0)	.120(0)	.881(1)
40	.431(0)	.180(0)	.621(1)	1.04	.369(0)	.150(0)	.858(1)	.542(1)	.381(1)
50	.242(0)	.966(1)	.298(1)	.632(0)	.219(0)	.843(1)	.451(1)	.273(1)	.187(1)
60	.150(0)	.572(1)	.164(1)	.397(0)	.139(0)	.502(1)	.262(1)	.157(1)	.104(1)
70	.983(1)	.350(1)	.969(2)	.270(0)	.945(1)	.327(1)	.163(1)	.962(2)	.620(2)
80	.668(1)	.228(1)	.625(2)	.201(0)	.705(1)	.225(1)	.109(1)	.617(2)	.406(2)
90	.485(1)	.161(1)	.420(2)	.159(0)	.549(1)	.164(1)	.767(2)	.425(2)	.279(2)
100	.375(1)	.121(1)	.312(2)	.132(0)	.433(1)	.125(1)	.570(2)	.316(2)	.201(2)
120	.248(1)	.753(2)	.193(2)	.108(0)	.316(1)	.801(2)	.356(2)	.196(2)	.126(2)
140	.189(1)	.541(2)	.139(2)	.985(1)	.262(1)	.615(2)	.253(2)	.144(2)	.927(3)
160	.160(1)	.453(2)	.116(2)	.959(1)	.233(1)	.530(2)	.213(2)	.120(2)	.752(3)
180	.151(1)	.398(2)	.108(2)	.947(1)	.246(1)	.510(2)	.213(2)	.112(2)	.788(3)

Table XI **Present Differential Cross-Sections for Inelastic Electron-Atom Scattering**

Notation as for Table I	HELIUM $1^1S \rightarrow 2^1S$ (a_o^2/Sr)					HELIUM $1^1S \rightarrow 2^3S$ (a_o^2/Sr)			
Angle	50 eV	81.63 eV	100 eV	150 eV		50 eV	81.63 eV	100 eV	150 eV
0	.816(1)	.118(0)	.130(0)	.150(0)		.118(1)	.445(2)	.278(2)	.103(2)
10	.687(1)	.894(1)	.935(1)	.929(1)		.988(2)	.326(2)	.191(2)	.626(3)
20	.415(1)	.414(1)	.379(1)	.271(1)		.591(2)	.162(2)	.101(2)	.530(3)
30	.190(1)	.141(1)	.114(1)	.637(2)		.279(2)	.110(2)	.938(3)	.626(3)
40	.785(2)	.554(2)	.444(2)	.249(2)		.132(2)	.104(2)	.909(3)	.497(3)
50	.454(2)	.380(2)	.310(2)	.172(2)		.804(3)	.867(3)	.694(3)	.307(3)
60	.437(2)	.335(2)	.258(2)	.129(2)		.594(3)	.624(3)	.462(3)	.178(3)
70	.480(2)	.297(2)	.212(2)	.954(3)		.504(3)	.449(3)	.319(3)	.117(3)
80	.504(2)	.257(2)	.175(2)	.721(3)		.580(3)	.387(3)	.264(3)	.931(4)
90	.503(2)	.220(2)	.144(2)	.558(3)		.879(3)	.419(3)	.266(3)	.854(4)
100	.487(2)	.186(2)	.117(2)	.423(3)		.140(2)	.513(3)	.301(3)	.854(4)
110	.466(2)	.161(2)	.980(3)	.334(3)		.209(2)	.637(3)	.349(3)	.884(4)
120	.447(2)	.144(2)	.865(3)	.291(3)		.286(2)	.765(3)	.397(3)	.910(4)
130	.432(2)	.132(2)	.785(3)	.263(3)		.366(2)	.885(3)	.441(3)	.932(4)
140	.420(2)	.121(2)	.704(3)	.223(3)		.439(2)	.992(3)	.481(3)	.959(4)
150	.411(2)	.113(2)	.636(3)	.184(3)		.502(2)	.108(2)	.514(3)	.988(4)
160	.406(2)	.109(2)	.613(3)	.179(3)		.550(2)	.114(2)	.535(3)	.994(4)
170						.580(2)			

Table XI continued

Notation as for Table I	HYDROGEN 1s → 2s (a_o^2/Sr)		HELIUM $1^1S \rightarrow 2^1P$ (a_o^2/Sr)	
Angle	100 eV	200 eV	50 eV	100 eV
0	.785(0)	.862(0)	1.69	5.70
10	.447(0)	.291(0)	1.05	1.33
20	.110(0)	.320(1)	.384(0)	.188(0)
30	.233(1)	.465(2)	.121(0)	.281(1)
40	.757(2)	.110(2)	.370(1)	.506(2)
50	.413(2)	.616(3)	.122(1)	.148(2)
60	.258(2)	.475(3)	.475(2)	.751(3)
70	.162(2)	.267(3)	.234(2)	.493(3)
80	.105(2)	.130(3)	.140(2)	.341(3)
90	.753(3)	.847(4)	.963(3)	.245(3)
100	.534(3)	.718(4)	.717(3)	.192(3)
110	.402(3)	.651(4)	.555(3)	.158(3)
120	.335(3)	.415(4)	.432(3)	.126(3)
130			.341(3)	.102(3)
140			.280(3)	.925(4)
150			.243(3)	.909(4)
160			.218(3)	.844(4)
180			.191(3)	.653(4)

Figure Captions

Figure 1 Contour plot of $\mathrm{Im}\,[h_0(r,r')/rr']$ for electron-hydrogen scattering.

Figure 2 Differential cross-sections for elastic electron-hydrogen scattering at a) 54.4 b) 100 and c) 200 eV.
⊕ Teubner et al (1973); ○ Lloyd et al (1974); curve P, present results; IP, Bransden et al (1972); EBS, Byron and Joachain (1973, 1974); CC, Scott (1965); G, Glauber approximation of Chen et al (1973); B, Born approximation.

Figure 3 Differential cross-sections for elastic electron-helium scattering at a) 50 b) 100 c) 200 d) 300 e) 400 and f) 500 eV.
▽ Crooks and Rudd (1972); □ Vriens et al (1968); ⊕ Bromberg (1969, 1974); x Jansen et al (1974); ○ Chamberlain et al (1970); ▨ Sethuraman et al (1974); ◈ Oda et al (1972); curve P, present results; IP, Berrington et al (1973); EBS, Byron and Joachain (1973a); G, Glauber approximation of Byron and Joachain (1973a).

Figure 4 The differential cross-section in the forward direction for elastic electron-helium scattering.
Curve P, present results; IP, Berrington et al (1973); B2, Holt et al (1971); JM, Joachain and Mittleman (1971); DR, dispersion relation results of Bransden and McDowell (1970).

Figure 5 Generalized oscillator strengths for 2^1S and 2^1P excitation of helium from the ground state due to electron impact, with the wavefunctions of:-

○ Bell et al (1969); F, Flannery (1970); BJ, Byron and Joachain (1974b); GC, Goldberg and Clogston (1939).

Figure 6 Differential cross-sections for the $1^1S \rightarrow 2^3S$ excitation of helium by electron impact at a)50 b) 81.63 c) 100 and d) 150 eV.

∇ Crooks and Rudd (1972); ○ Hall et al (1973); ◉ Vriens et al (1968a); □ Suzuki and Takayanagi (1974); curve P, present results; DWBA, distorted wave Born approximation; DW-I, present direct cross-section with distortion in the initial state only; T, Taylor (1974); MR, Mathur and Rudge (1974); BO, Born-Oppenheimer approximation.

Figure 7 Differential cross-sections for the $1^1S \rightarrow 2^1S$ excitation of helium by electron impact at a) 50 b) 81.63 c) 100 and d) 150 eV.

∇ Crooks and Rudd (1972); ○ Rice et al (1972); ◉ Vriens et al (1968a); △ Opal and Beaty (1972) at 81.63 eV, Suzuki and Takayanagi (1974) at 150 eV; curve P, present results; DWBA, distorted wave Born approximation; DW-I, present direct cross-section with distortion in the initial state only; PD, present direct cross-section with both initial and final state distortion; T, Taylor (1974); IP, Berrington et al (1973); G, Glauber approximation of Yates and Tenney (1972); HG, Hidalgo and Geltman (1972).

Figure 8 Differential cross-sections for the $1^1S \rightarrow 2^1P$ excitation of helium by electron impact at a) 50 and b) 100 eV.

∇ Crooks and Rudd (1972); ◉ Vriens et al (1968a); ○ Hall et al (1973); I Chamberlain et al (1970); curve DW-I, present direct cross-section with initial state distortion only; IP, Berrington et al (1973); HG, Hidalgo and Geltman (1972); G, Glauber approximation of Terebey (1974).

Figure 9 The fractional contribution of the m=o substate to the $1^1S \rightarrow 2^1P$ differential cross-section for electron-helium scattering at a) 50 and b) 100 eV.

ɸ Eminyan et al (1974); curve P, present results; T, Taylor (1974); JV, Joachain and Vanderpoorten (1974a); B, Born approximation.

Figure 10 The relative phase between the m=1 and m=o scattering amplitudes for $1^1S \rightarrow 2^1P$ excitation of helium by a) 50 and b) 100 eV electrons.

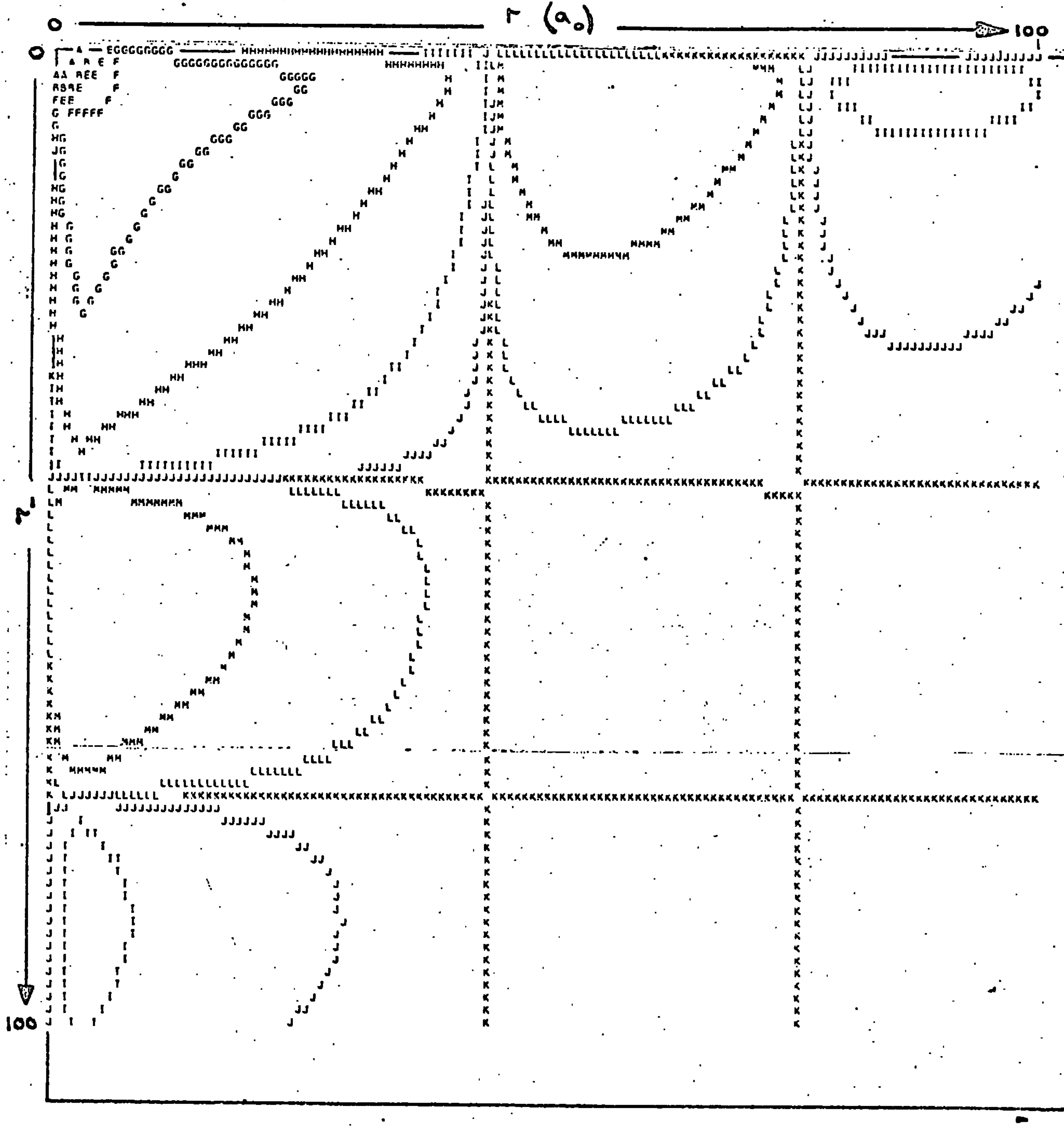
ɸ Eminyan et al (1974); curve P, present results; JV(1) and JV(2), Joachain and Vanderpoorten (1974a) using Glauber and static distorting potentials respectively.

Figure 11 Differential cross-sections for the 1s→2s excitation of hydrogen atoms by a) 100 and b) 200 eV electrons.

□ calculation of McDowell et al (1973); ∇ calculation of Geltman and Hidalgo (1971); curve P, present results; BH, Baye and Heenen (1974a).

Figure 12 Total cross-section for positron-helium scattering. curve e^++He, best fitto the data of Canter et al (1973); curve e^-+He, values of the electron-helium total cross-section of Bransden and McDowell (1969, 1970), equal to the Born-Bethe approximation for $k^2 > 20$ Rydbergs; - - - present suggested values for the positron-helium total cross-section.

Figure 1



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$B = 10^{-1}$

$C = 10^{-2}$

⋮

$J = 10^{-9}$

$K = 0$

$L = -10^{-9}$

$M = -10^{-8}$

⋮

Figure 2a

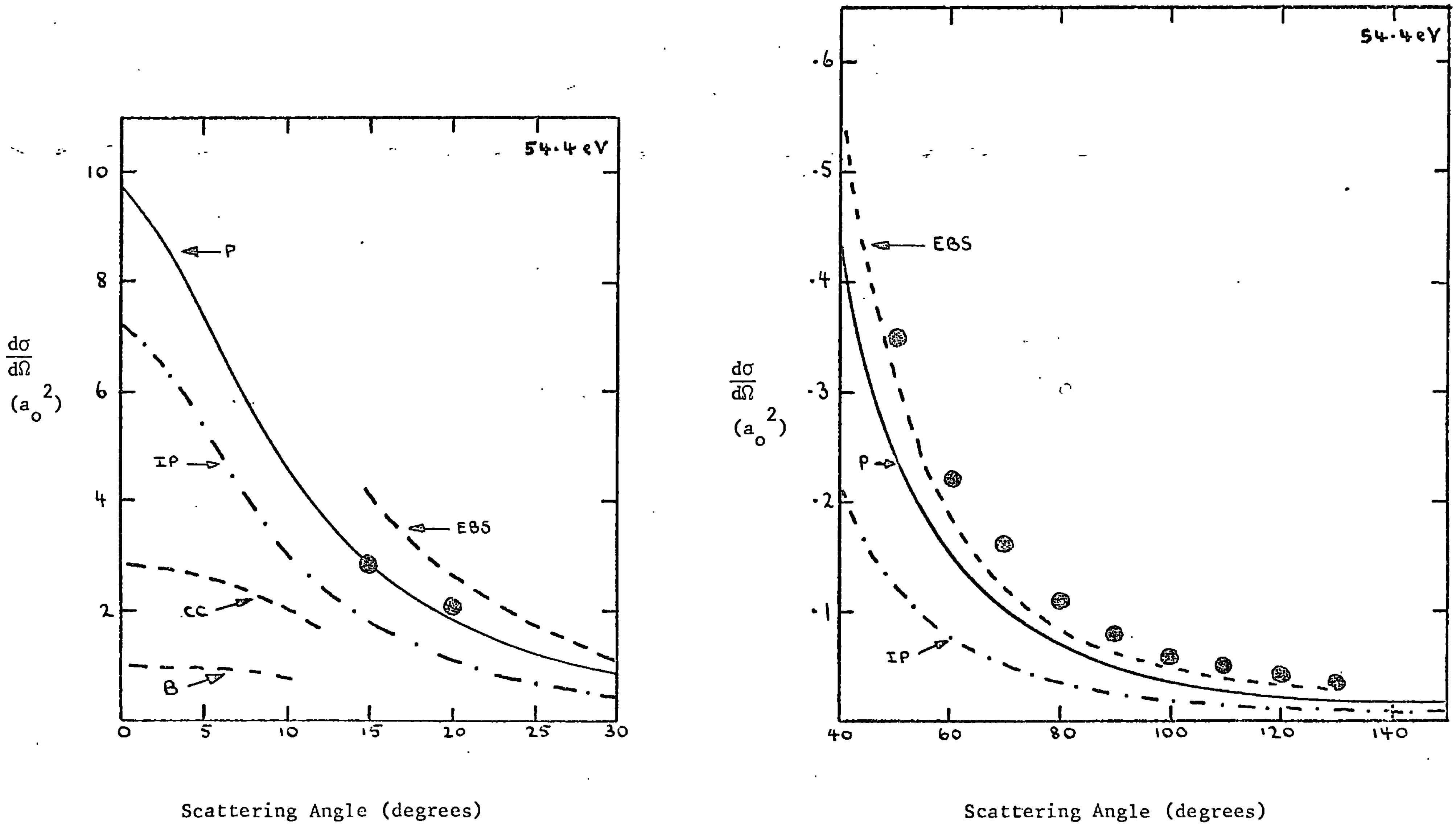
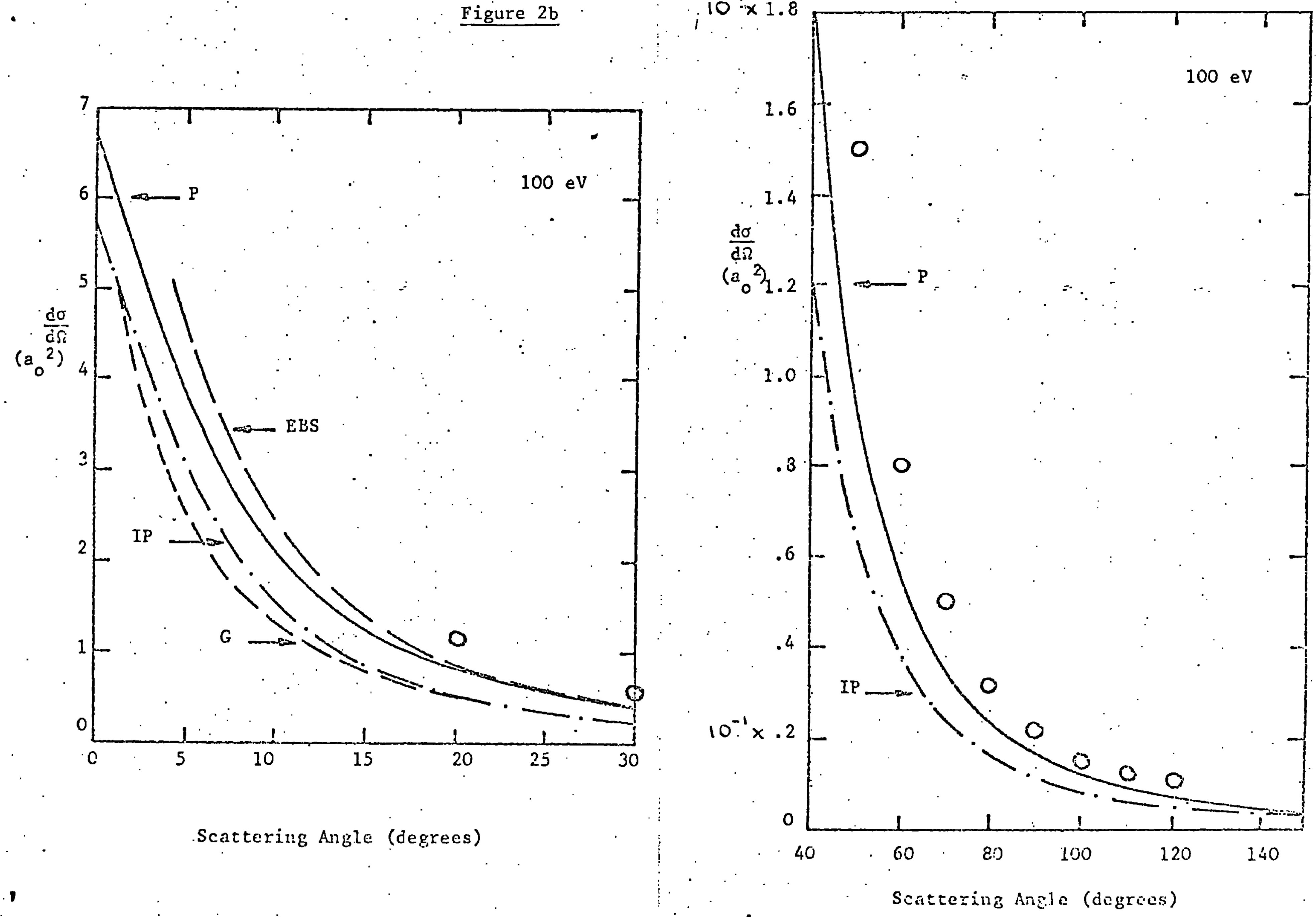

54·4 eV
dσ/dΩ (a_o^2)
10
8
6
4
2
P
IP
CC
B
EBS
0
5
10
15
20
25
30
Scattering Angle (degrees)
54·4 eV
dσ/dΩ (a_o^2)
·6
·5
·4
·3
·2
·1
EBS
P
IP
40
60
80
100
120
140
Scattering Angle (degrees)

Figure 2b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6
5
4
3
2
1
0
$\frac{d\sigma}{d\Omega}$
(a_o^2)
100 eV
P
EBS
IP
G
0
5
10
15
20
25
30
Scattering Angle (degrees)
10^{-1} x 1.8
1.6
1.4
1.2
1.0
.8
.6
.4
10^{-1} x .2
0
$\frac{d\sigma}{d\Omega}$
(a_o^2)
100 eV
P
IP
40
60
80
100
120
140
Scattering Angle (degrees)

Figure 2c

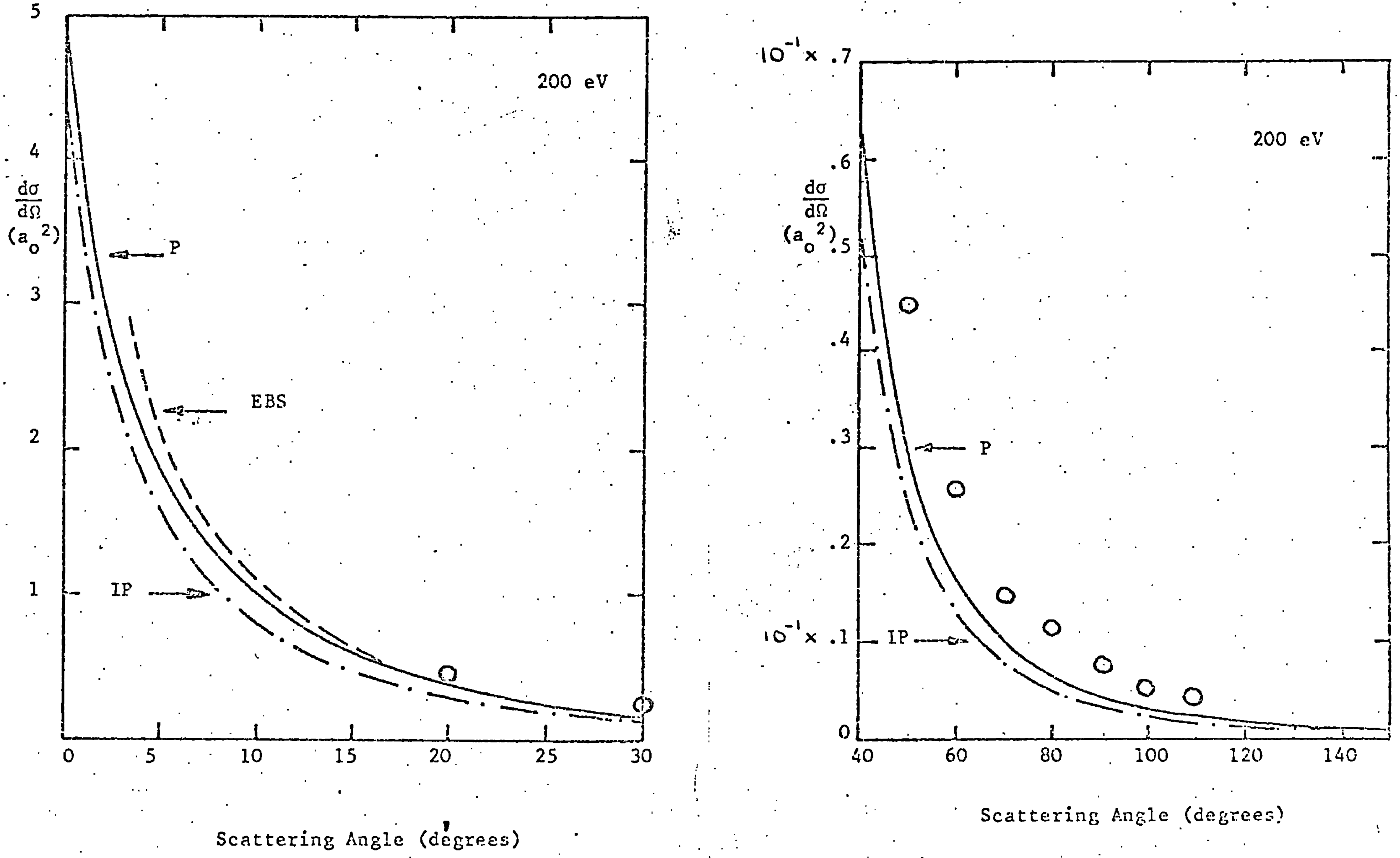
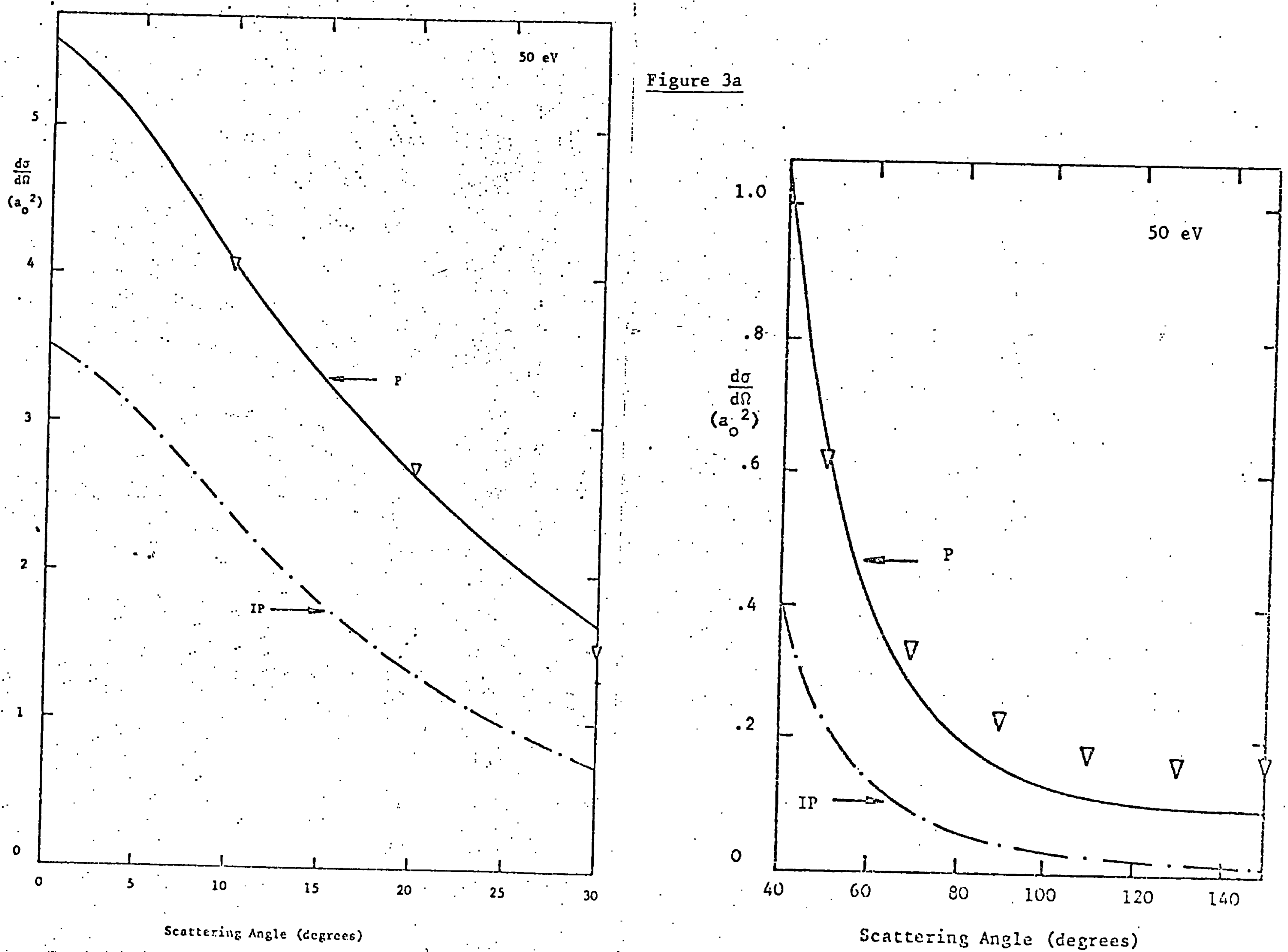

5
4
3
2
1
$\frac{d\sigma}{d\Omega}$ (a_o^2)
200 eV
P
EBS
IP
0
5
10
15
20
25
30
Scattering Angle (degrees)
10^{-1} x .7
.6
.5
.4
.3
.2
10^{-1} x .1
0
$\frac{d\sigma}{d\Omega}$ (a_o^2)
200 eV
P
IP
40
60
80
100
120
140
Scattering Angle (degrees)

Figure 3a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$\frac{d\sigma}{d\Omega}$ (a_o^2)
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1
2
3
4
5
P
IP
0
5
10
15
20
25
30
Scattering Angle (degrees)
50 eV
$\frac{d\sigma}{d\Omega}$ (a_o^2)
0
.2
.4
.6
.8
1.0
P
IP
40
60
80
100
120
140
Scattering Angle (degrees)

Figure 3b

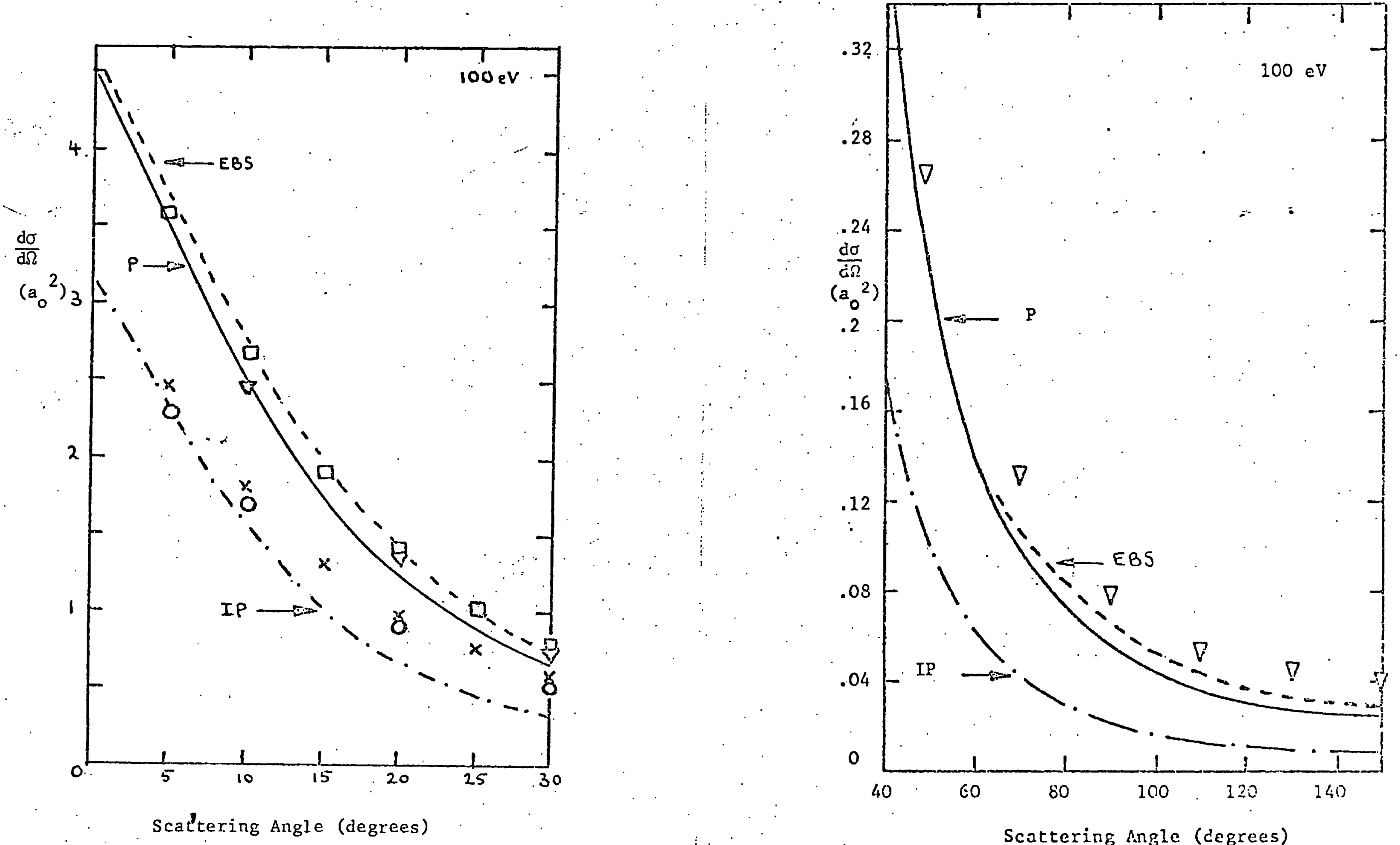

100 eV
EBS
P
IP
$\frac{d\sigma}{d\Omega}$ (a_o^2)
0
1
2
3
4
0
5
10
15
20
25
30
Scattering Angle (degrees)
100 eV
P
EBS
IP
$\frac{d\sigma}{d\Omega}$ (a_o^2)
0
.04
.08
.12
.16
.2
.24
.28
.32
40
60
80
100
120
140
Scattering Angle (degrees)

Figure 3c

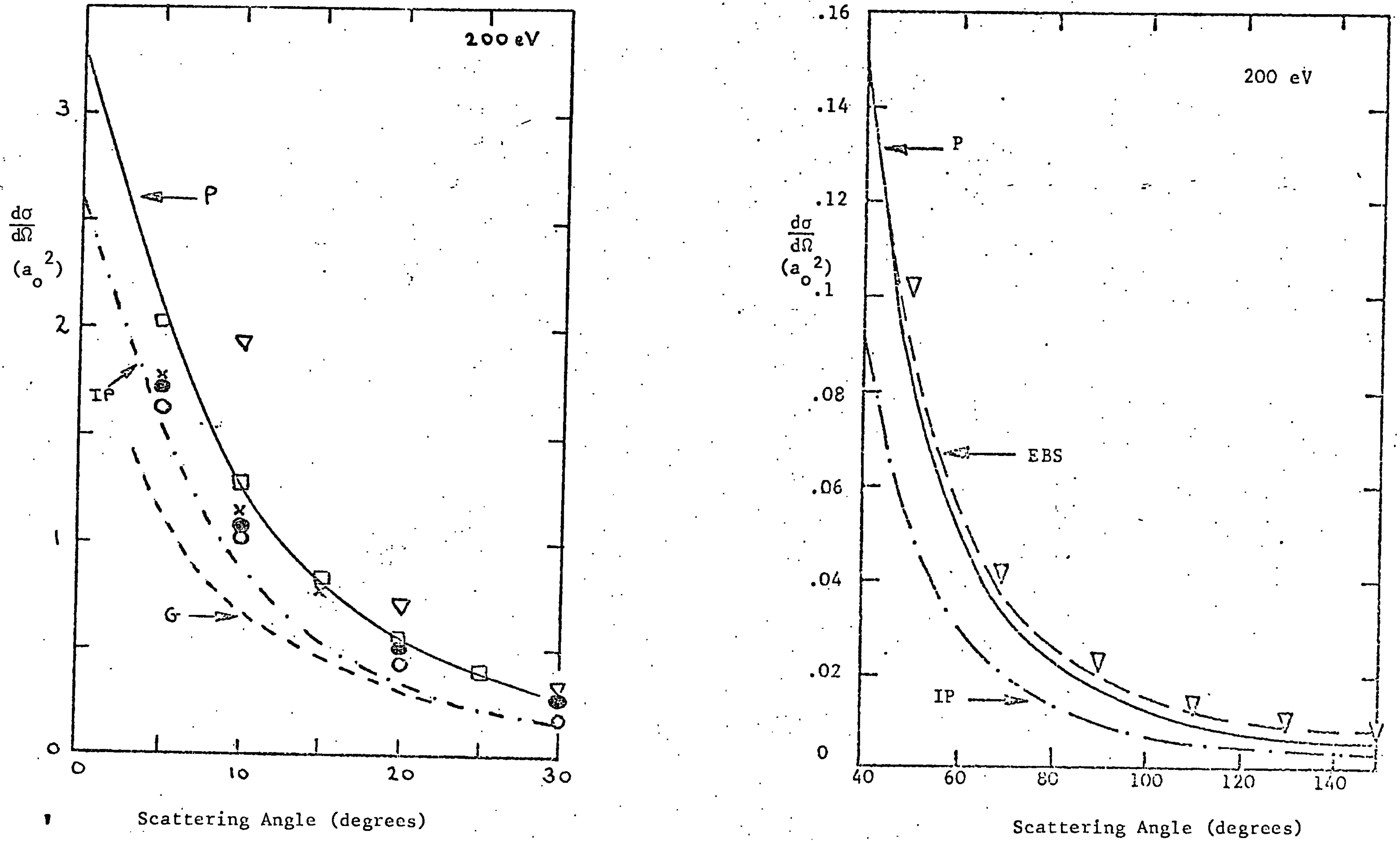

200 eV
$\frac{d\sigma}{d\Omega}$ (a_o^2)
3
2
1
0
P
IP
G
0
10
20
30
Scattering Angle (degrees)
200 eV
$\frac{d\sigma}{d\Omega}$ (a_o^2)
.16
.14
.12
.1
.08
.06
.04
.02
0
P
EBS
IP
40
60
80
100
120
140
Scattering Angle (degrees)

Figure 3d

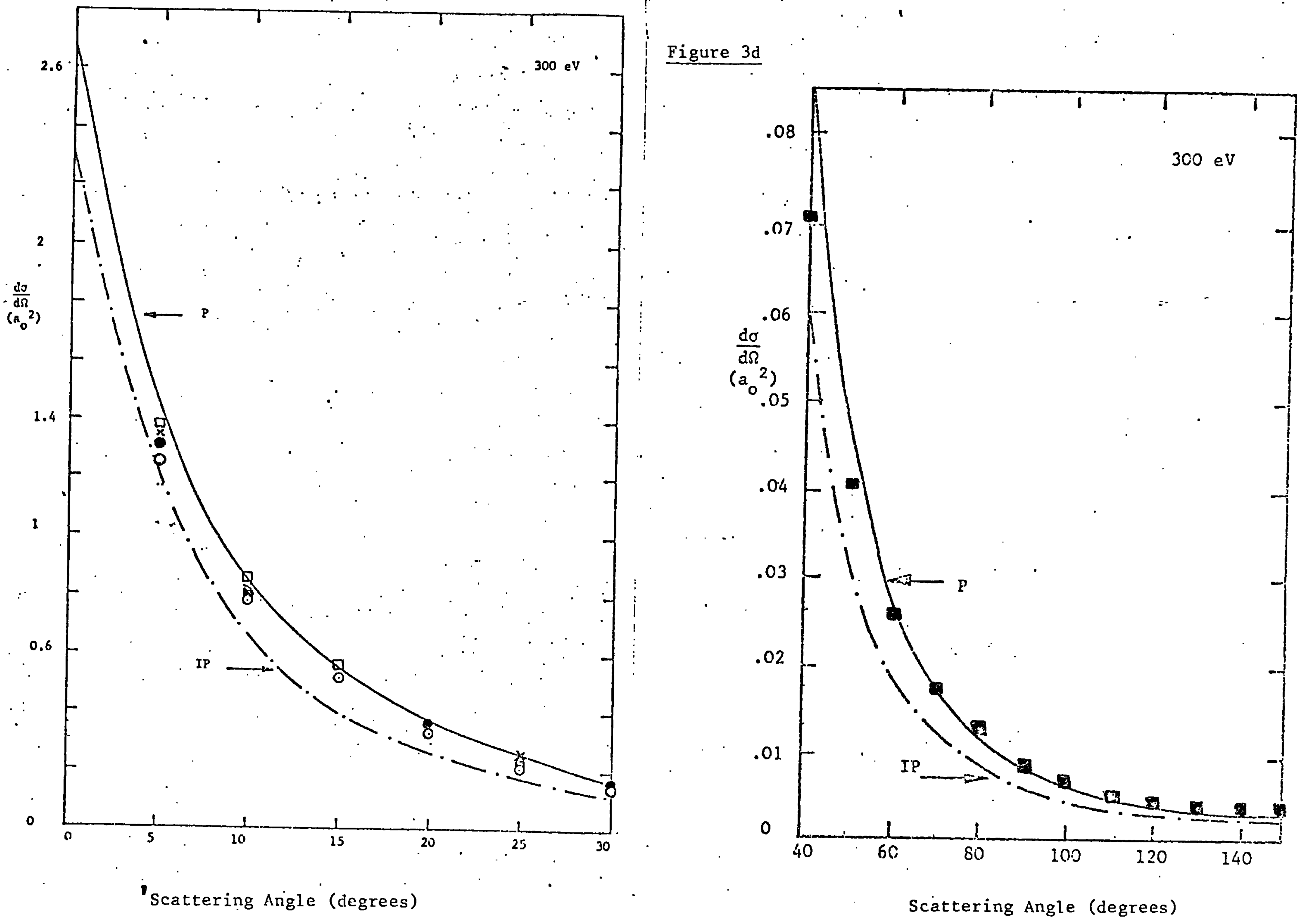

2.6
2
$\frac{d\sigma}{d\Omega}$ (a_o^2)
1.4
1
0.6
0
300 eV
P
IP
0
5
10
15
20
25
30
Scattering Angle (degrees)
.08
.07
.06
.05
.04
.03
.02
.01
0
300 eV
P
IP
40
60
80
100
120
140
Scattering Angle (degrees)

Figure 3e

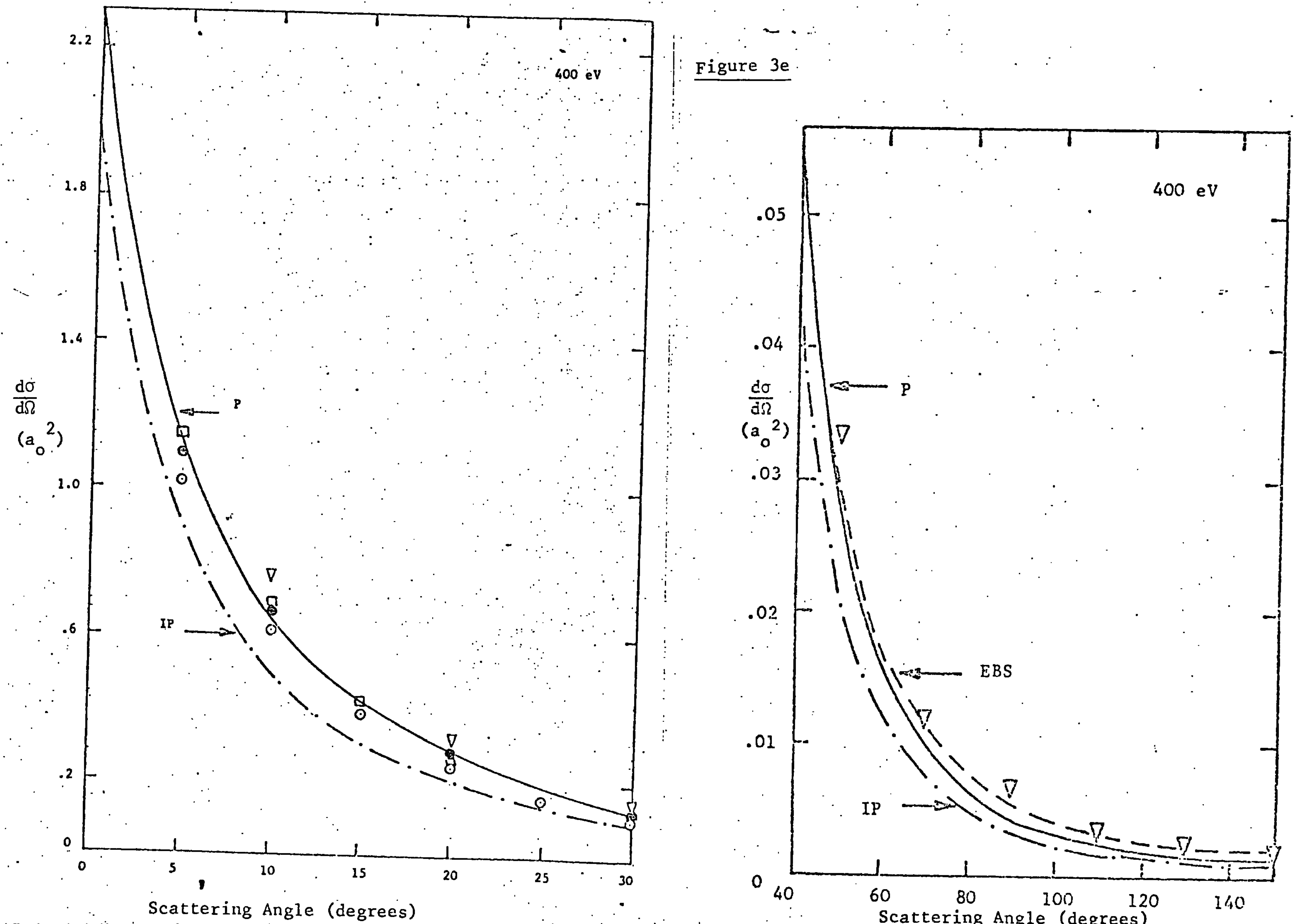

2.2
1.8
1.4
1.0
.6
.2
0
$\frac{d\sigma}{d\Omega}$
(a_o^2)
400 eV
P
IP
0
5
10
15
20
25
30
Scattering Angle (degrees)
.05
.04
.03
.02
.01
0
$\frac{d\sigma}{d\Omega}$
(a_o^2)
400 eV
P
EBS
IP
40
60
80
100
120
140
Scattering Angle (degrees)

Figure 3f

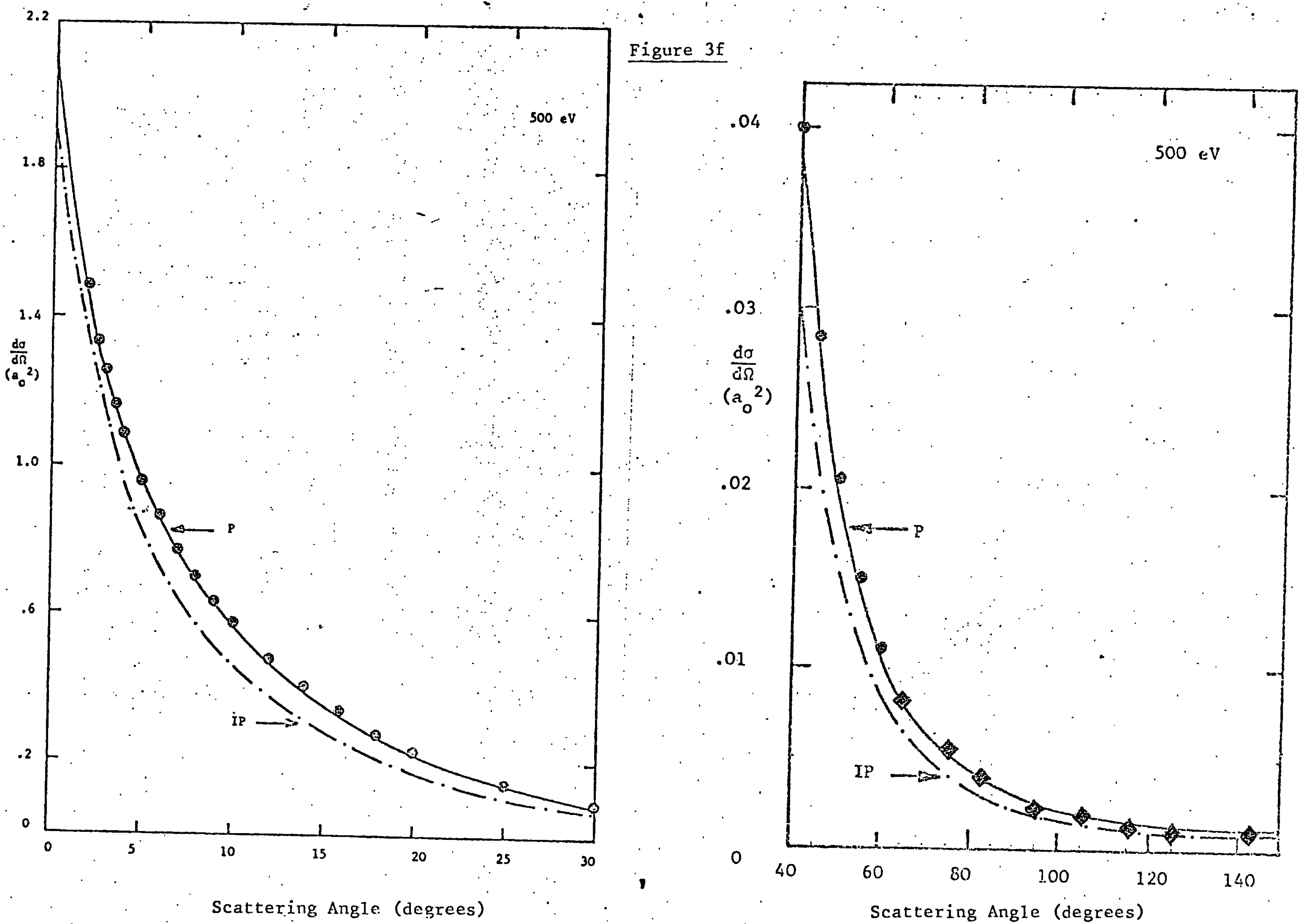
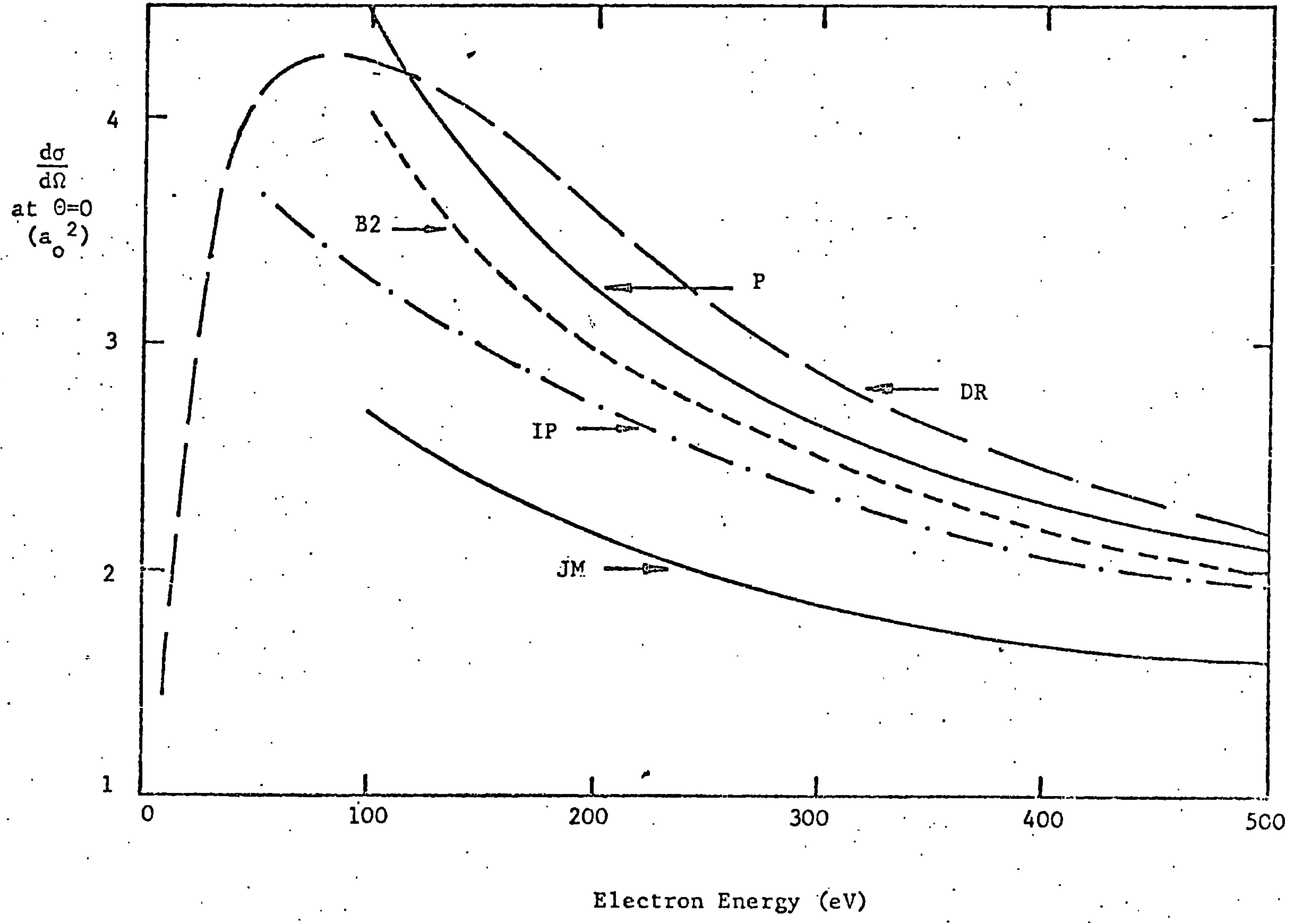
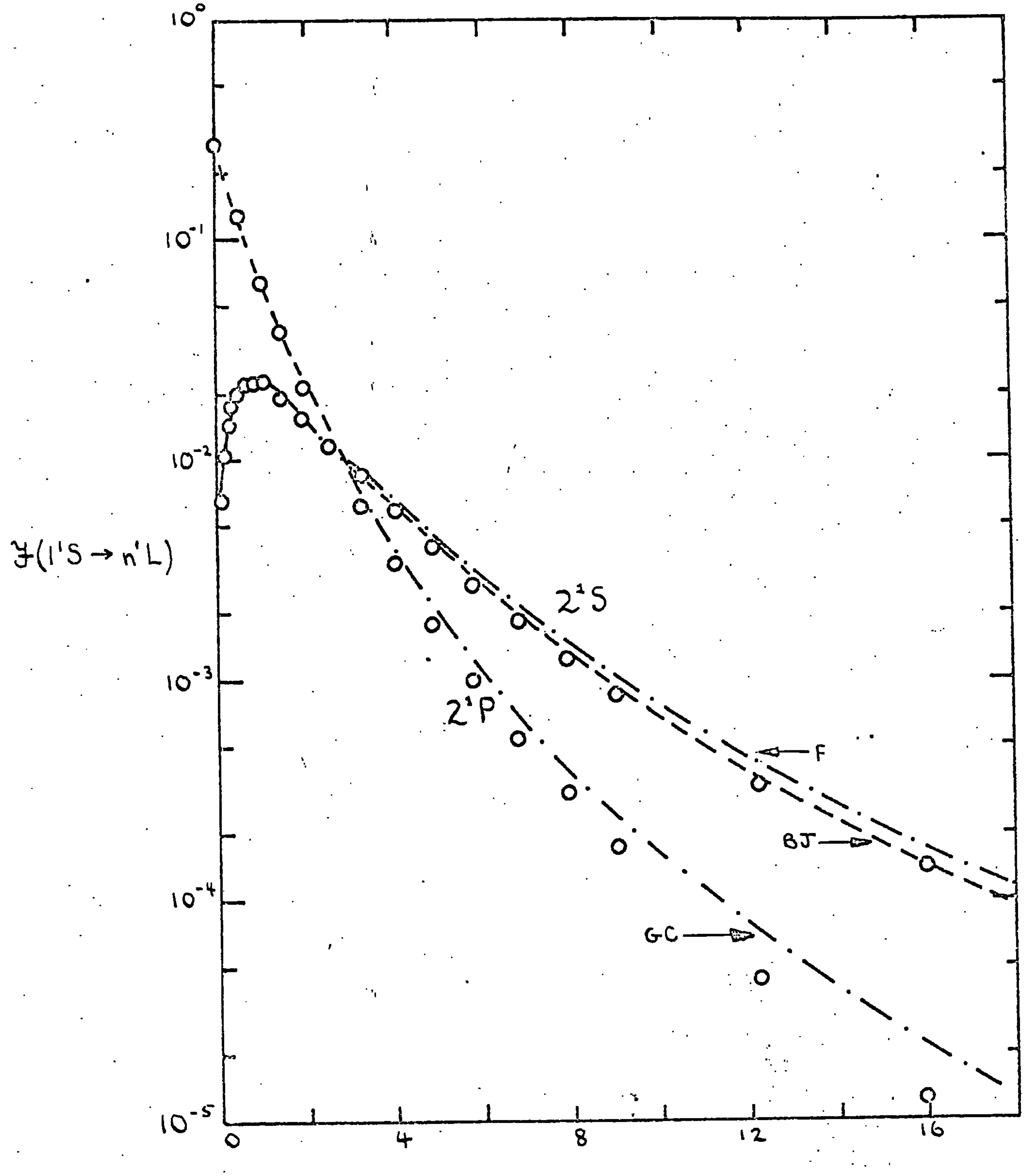

2.2
1.8
1.4
1.0
.6
.2
0
$\frac{d\sigma}{d\Omega}$ (a_o^2)
500 eV
P
IP
0
5
10
15
20
25
30
Scattering Angle (degrees)
.04
.03
.02
.01
0
$\frac{d\sigma}{d\Omega}$ (a_o^2)
500 eV
P
IP
40
60
80
100
120
140
Scattering Angle (degrees)

Figure 4



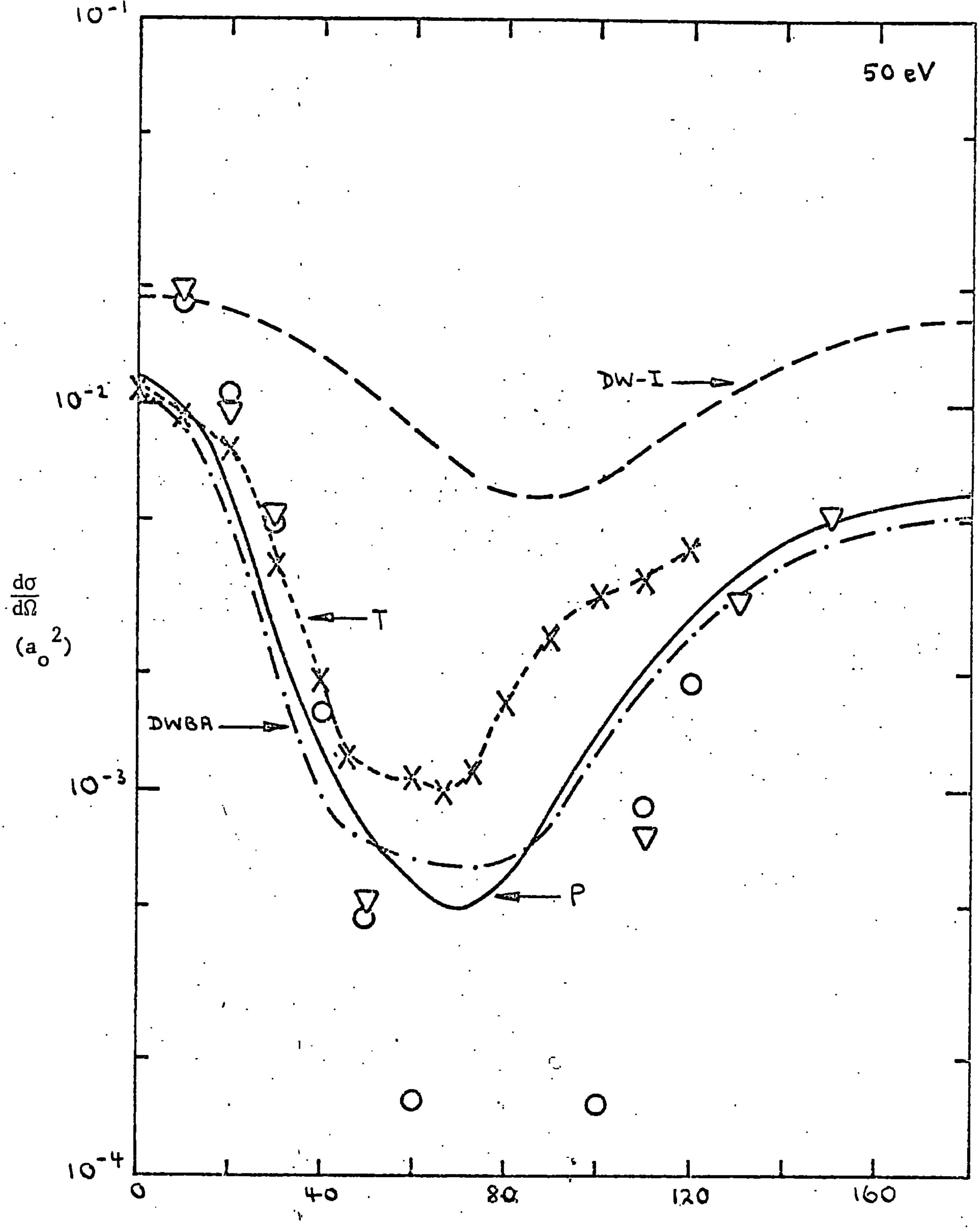
$\frac{d\sigma}{d\Omega}$ at Θ=0 $(a_o{}^2)$
4
3
2
1
0
100
200
300
400
500
Electron Energy (eV)
B2
P
DR
IP
JM

Figure 5



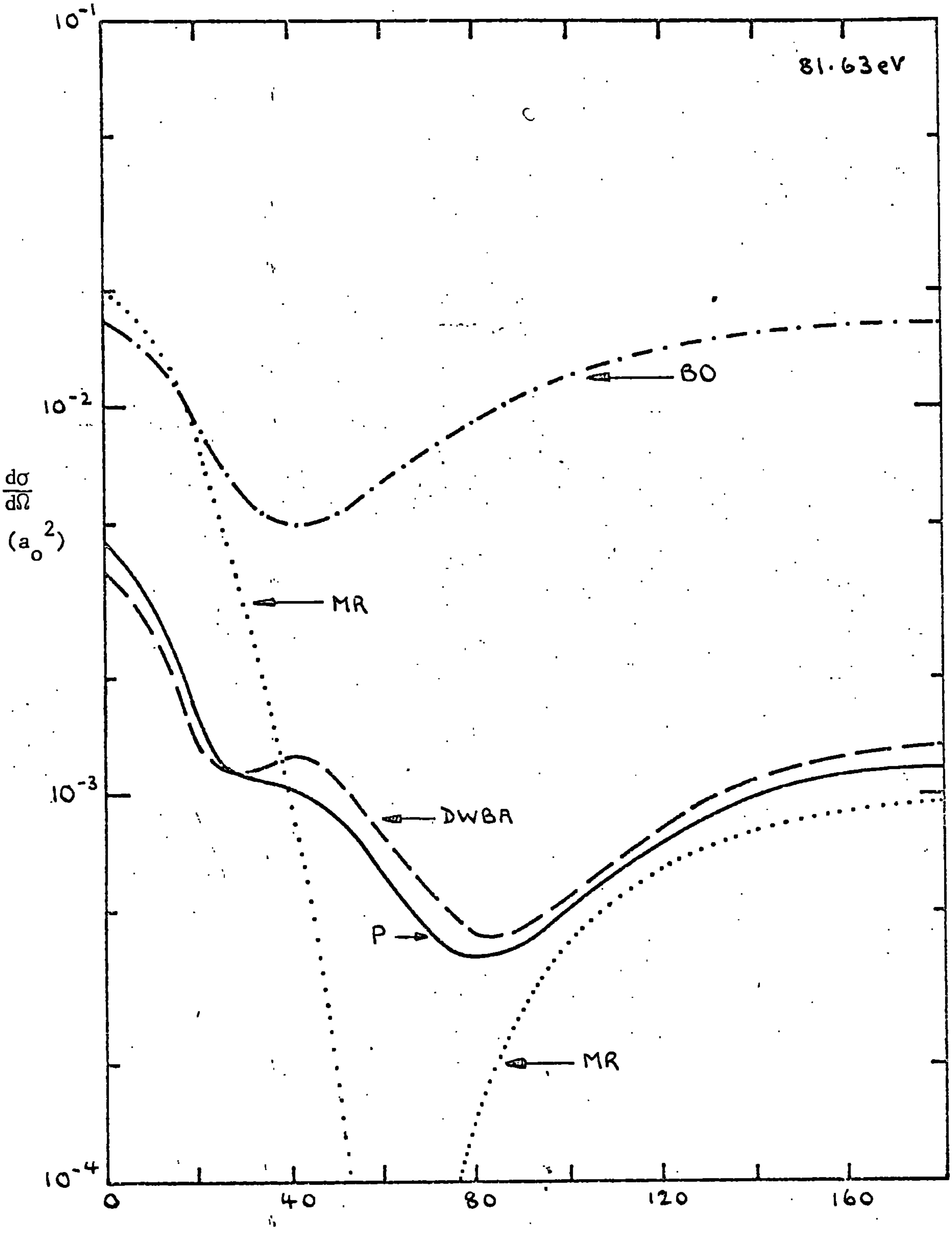
(qa_o^2)

Figure 6a



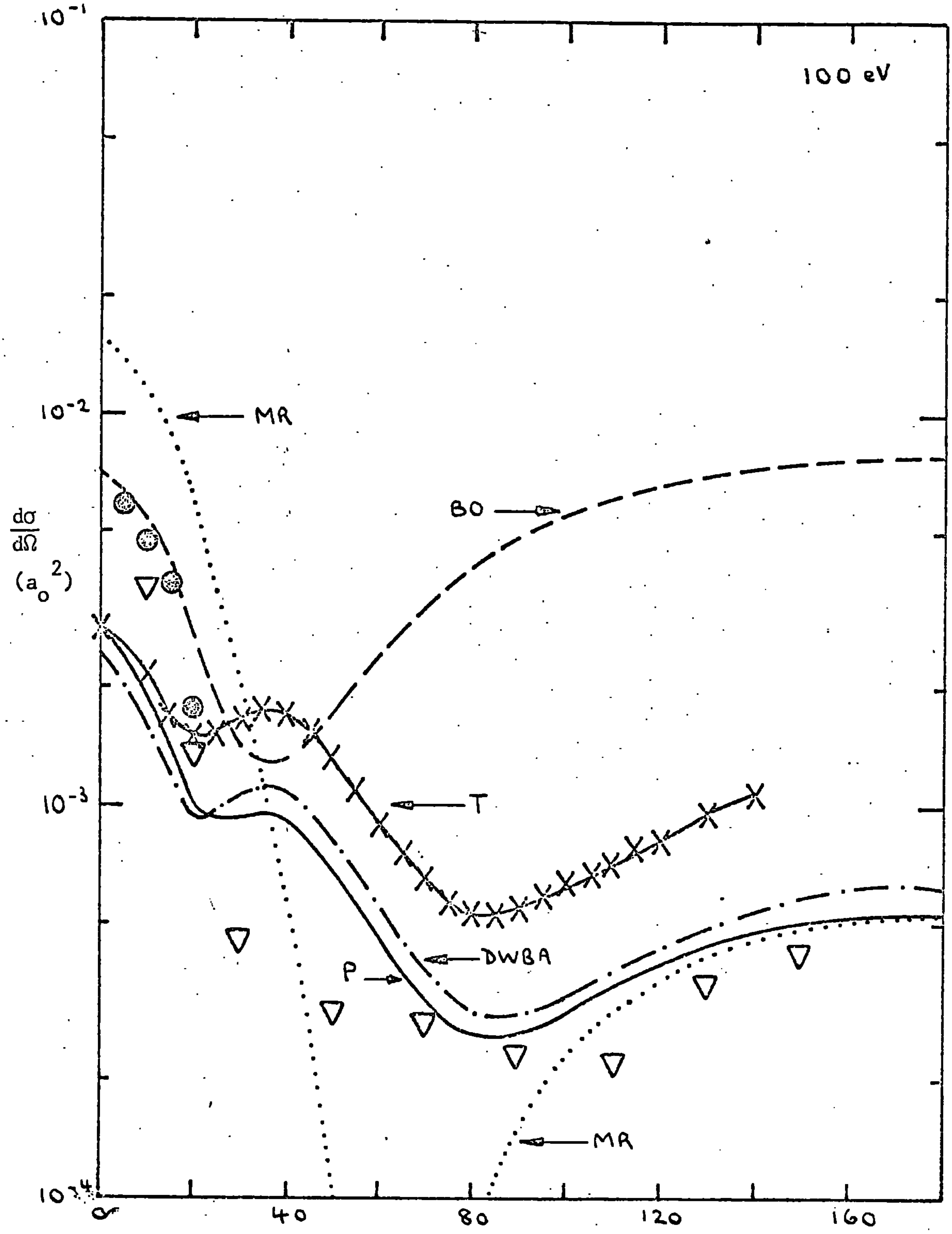
Scattering Angle (degrees)

Figure 6b



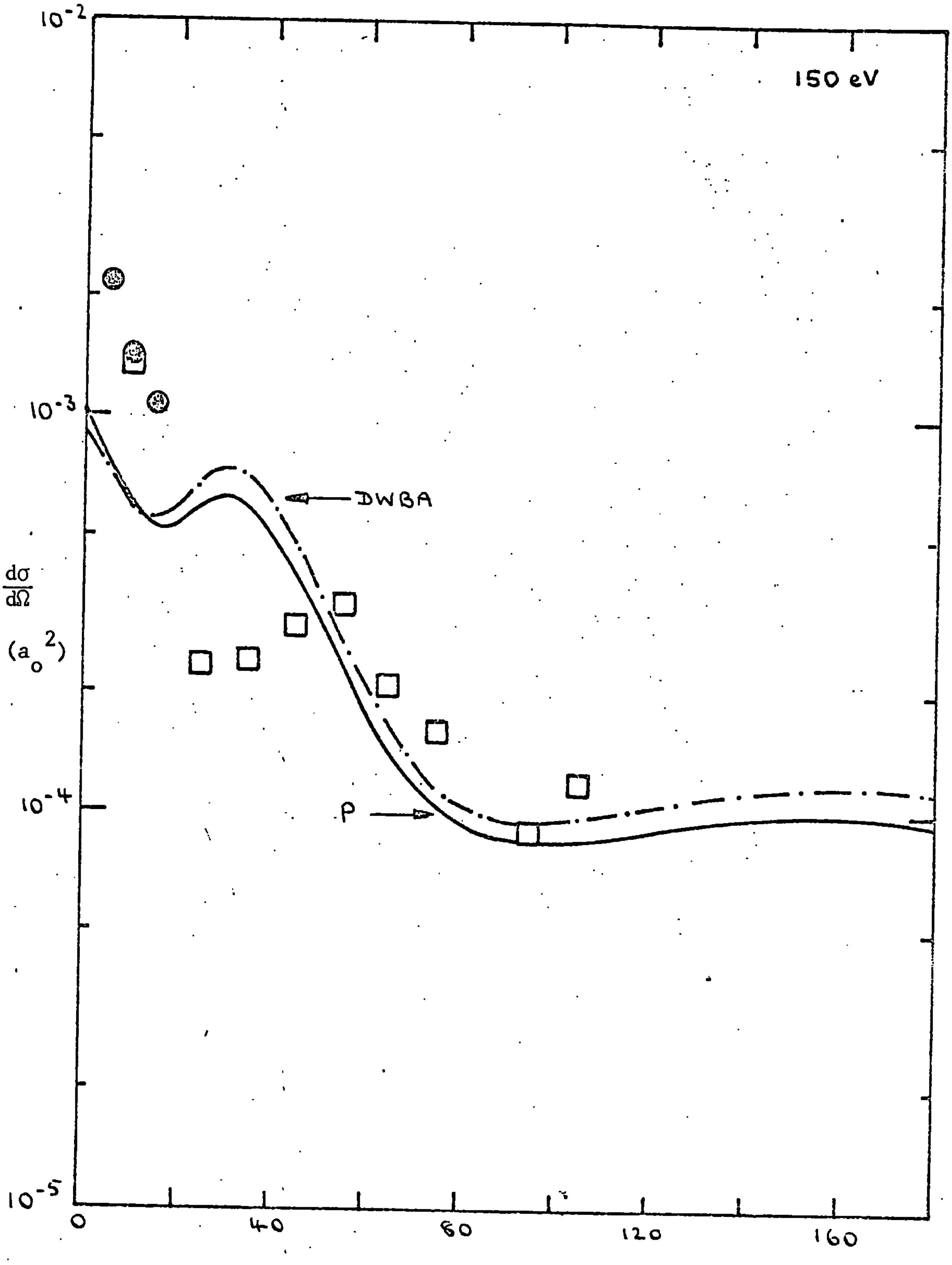
Scattering Angle (degrees)

Figure 6c



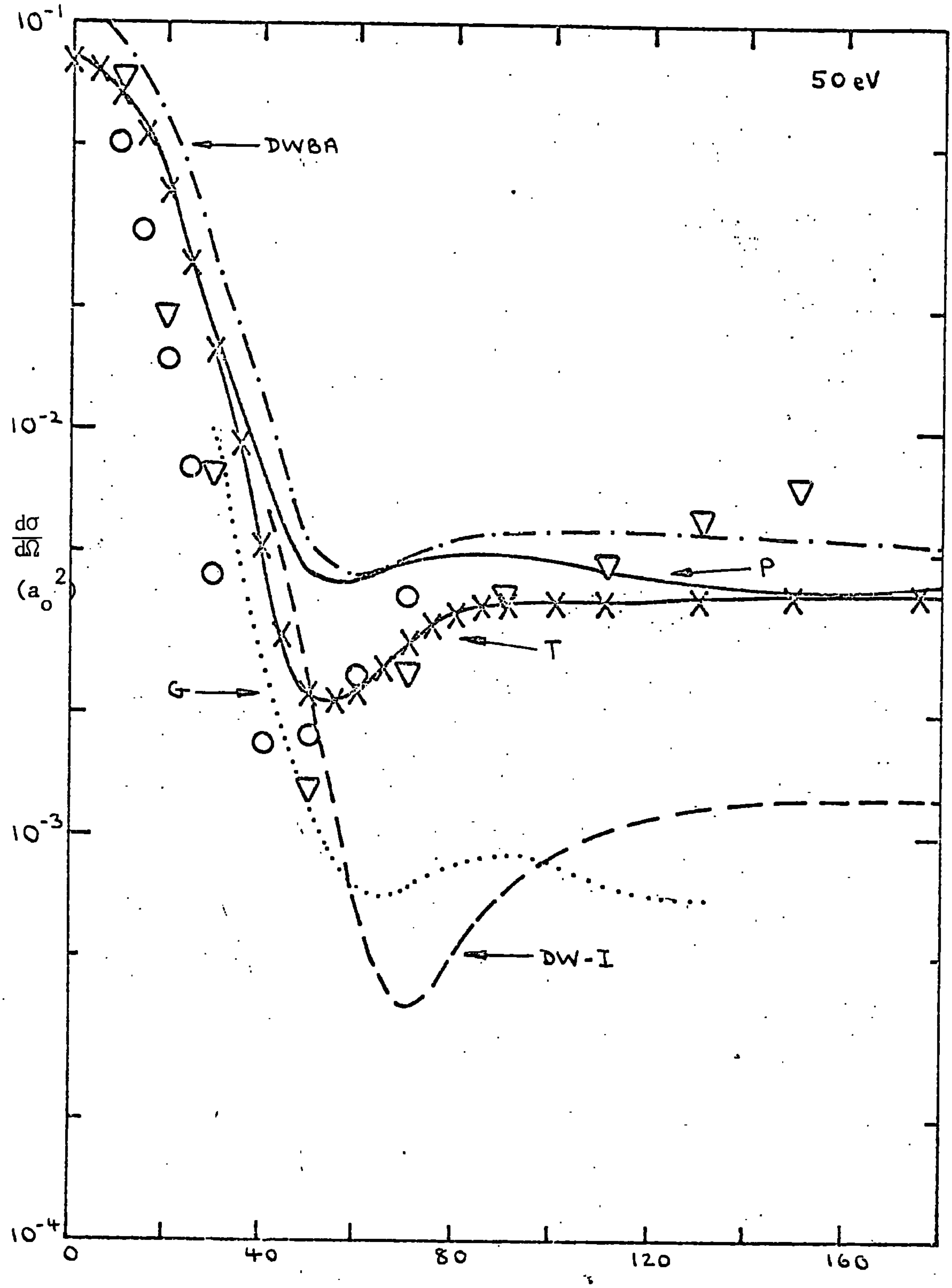
Scattering Angle (degrees)

Figure 6d



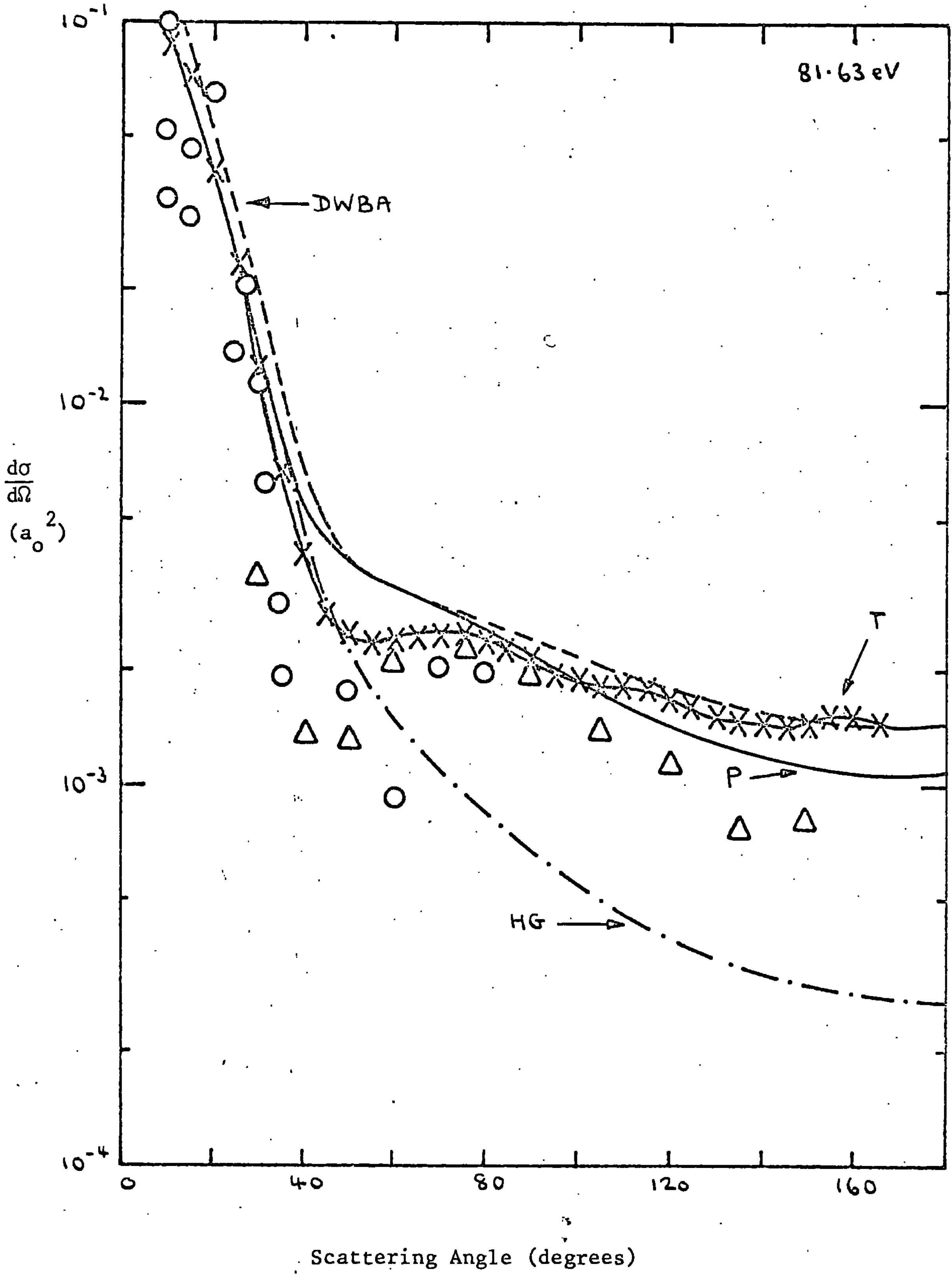
Scattering Angle (degrees)

Figure 7a



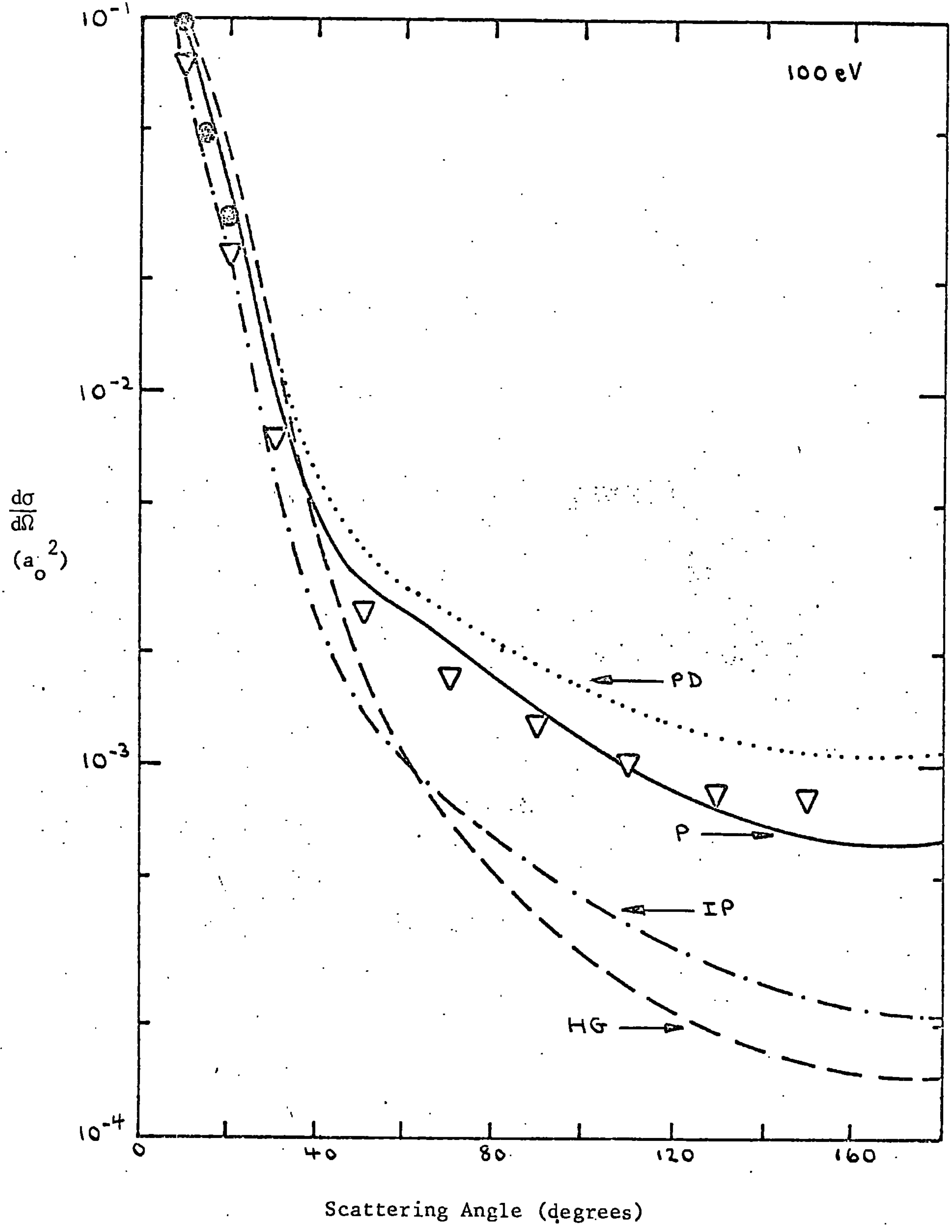
Scattering Angle (degrees)

Figure 7b



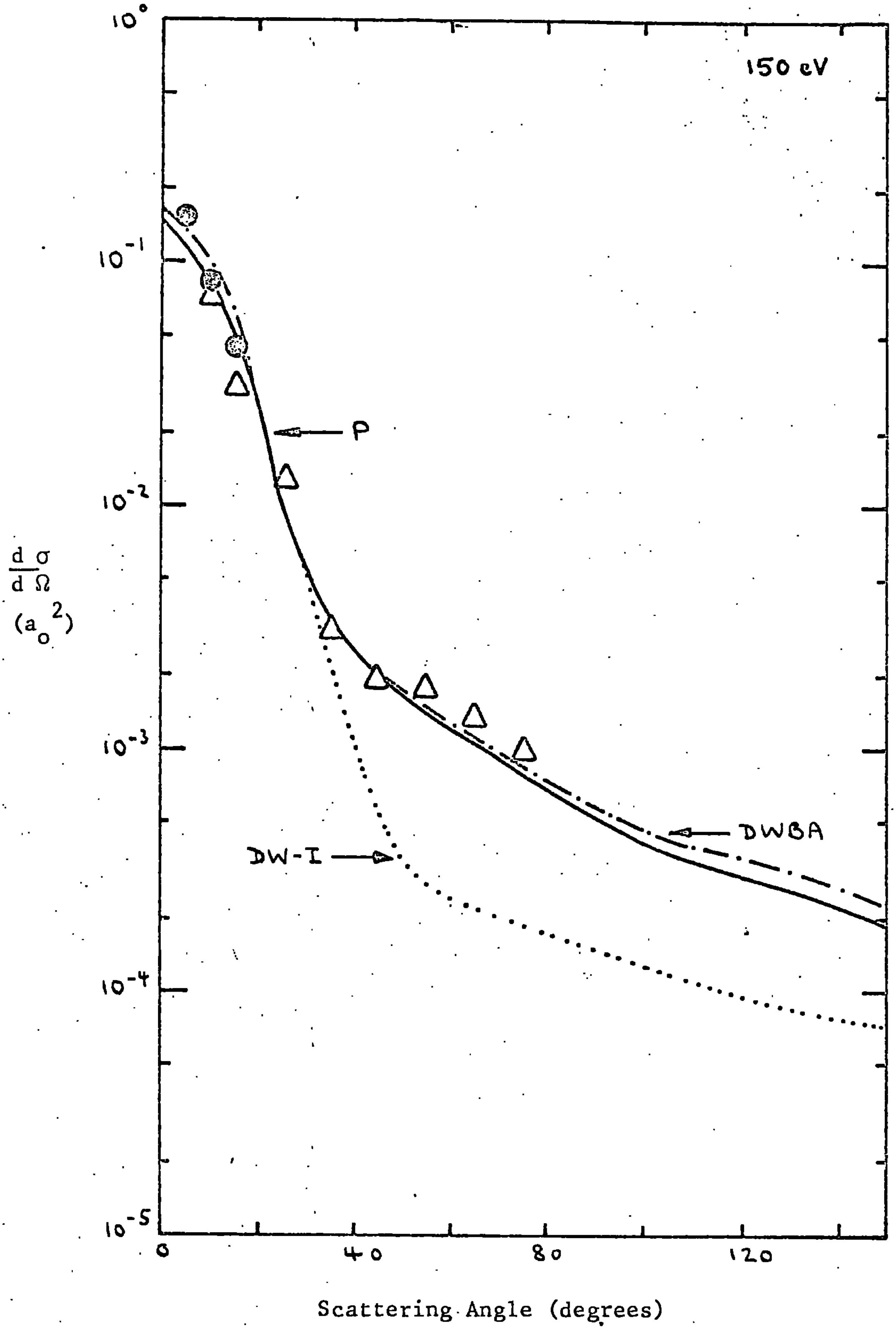
81·63 eV
DWBA
T
P
HG
10^{-1}
10^{-2}
10^{-3}
10^{-4}
$\frac{d\sigma}{d\Omega}$ (a_o^2)
0
40
80
120
160
Scattering Angle (degrees)

Figure 7c



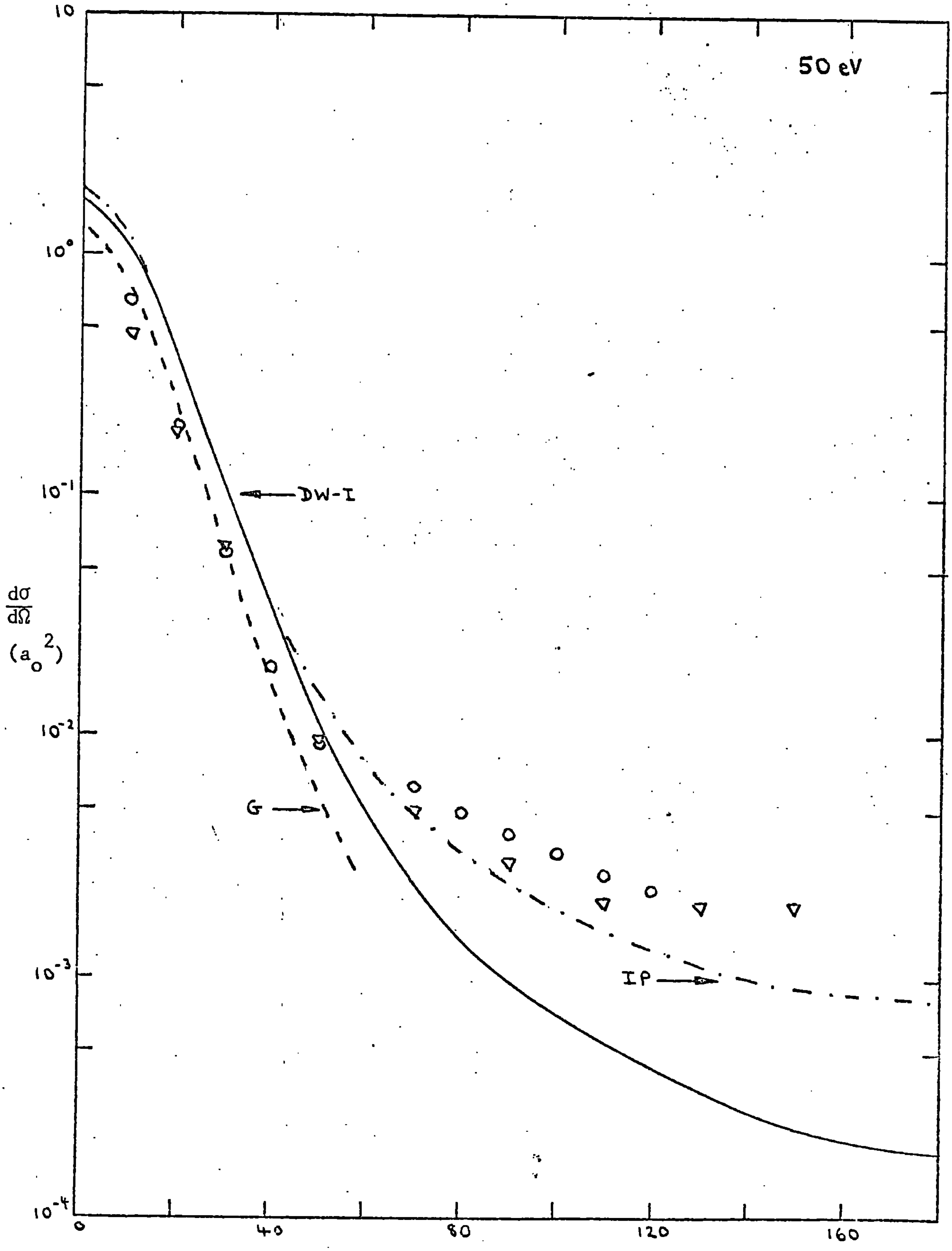
10^{-1}
10^{-2}
10^{-3}
10^{-4}
100 eV
$\frac{d\sigma}{d\Omega}$
(a_o^2)
PD
P
IP
HG
0
40
80
120
160
Scattering Angle (degrees)

Figure 7d



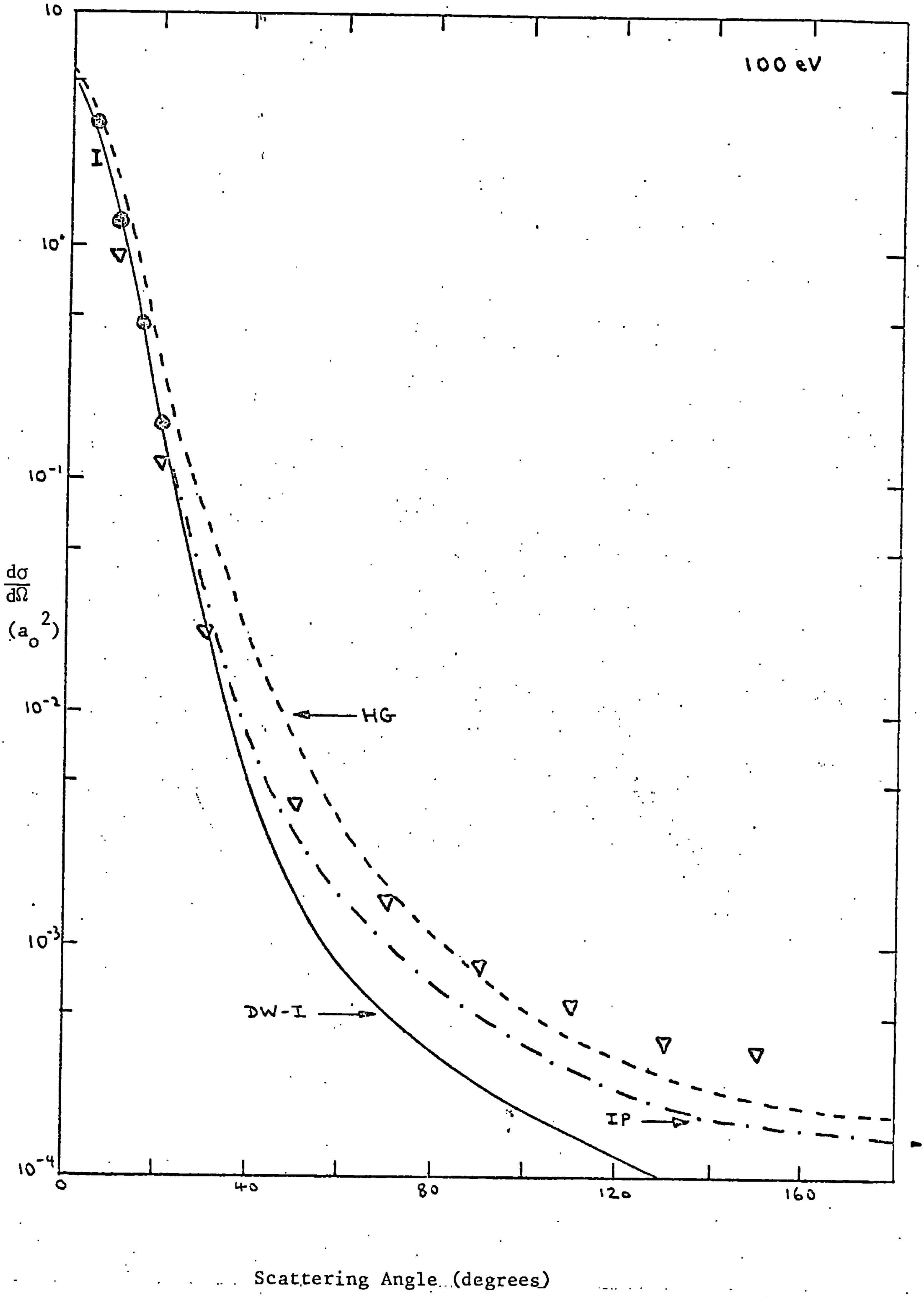
150 eV
P
DWBA
DW-I
10°
10⁻¹
10⁻²
10⁻³
10⁻⁴
10⁻⁵
$\frac{d\sigma}{d\Omega}$ (a_o^2)
0
40
80
120
Scattering Angle (degrees)

Figure 8a



$\frac{d\sigma}{d\Omega}$ $(a_o{}^2)$

Scattering Angle (degrees)



10
10°
10⁻¹
10⁻²
10⁻³
10⁻⁴
dσ/dΩ
(a_o^2)
100 eV
I
HG
DW-I
IP
0
40
80
120
160
Scattering Angle (degrees)

Figure 8b

Figure 9a

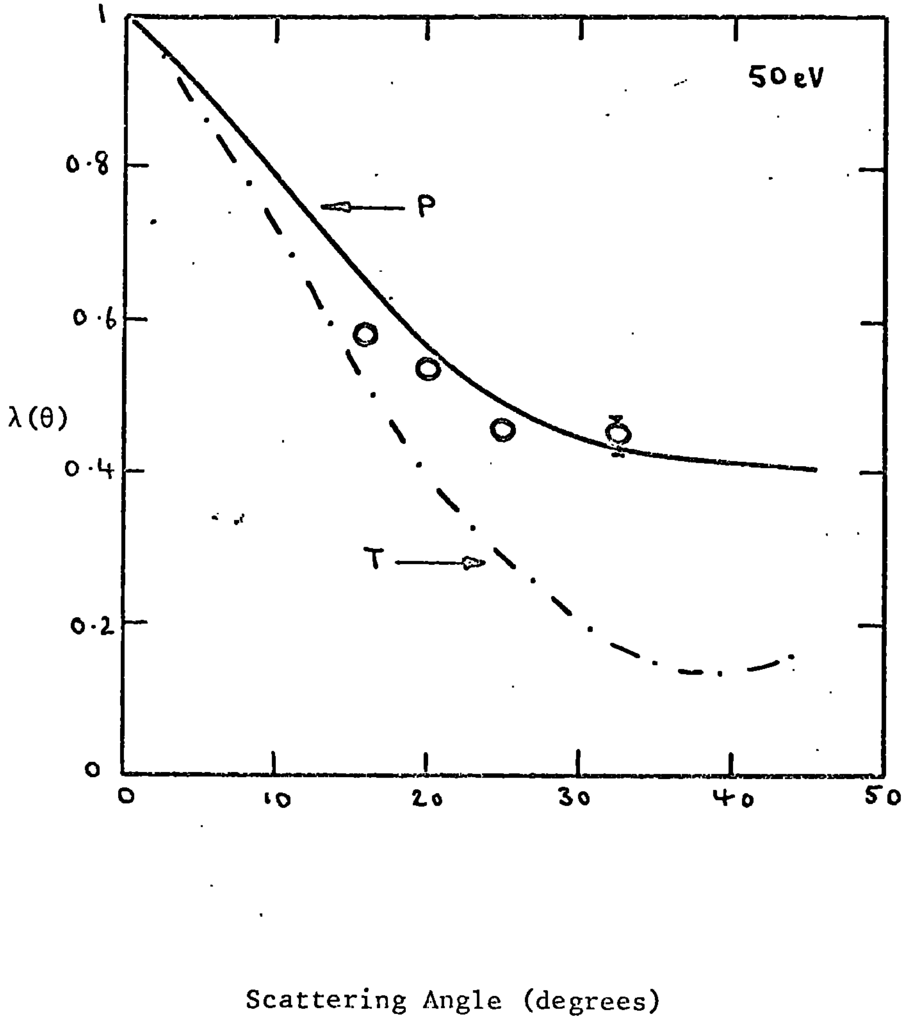


Figure 9b

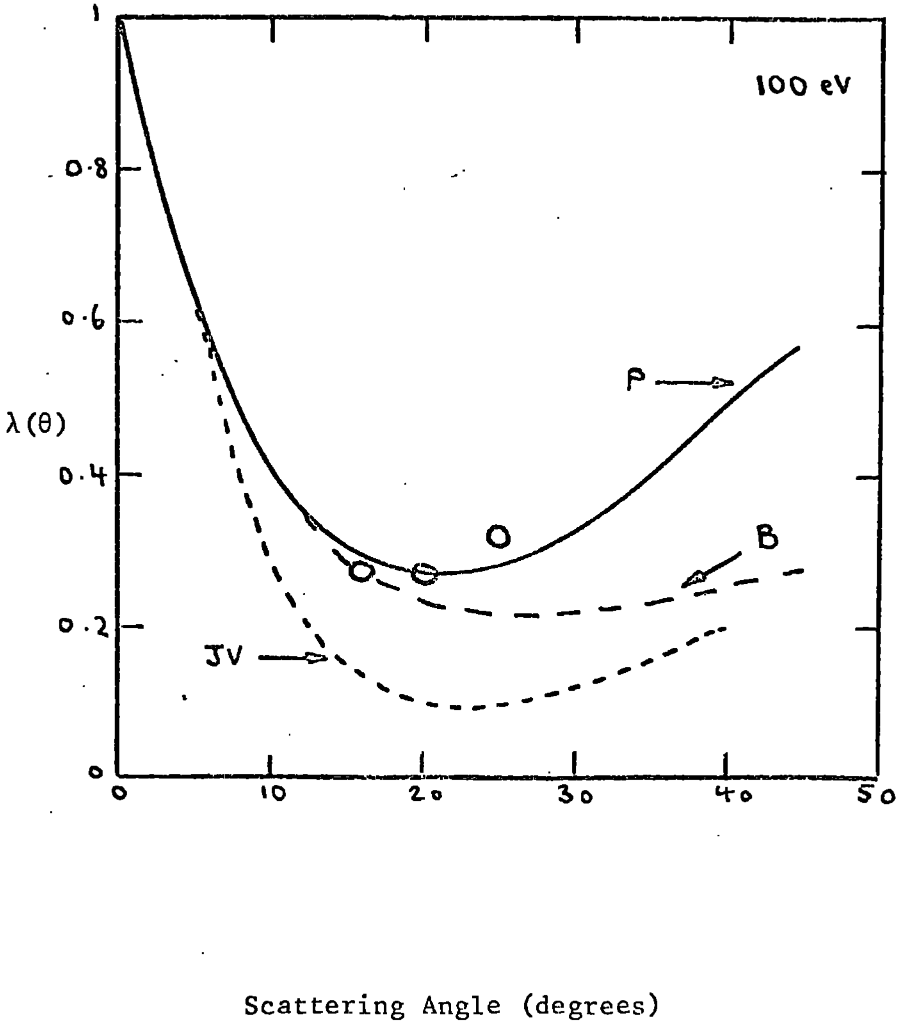


Figure 10a

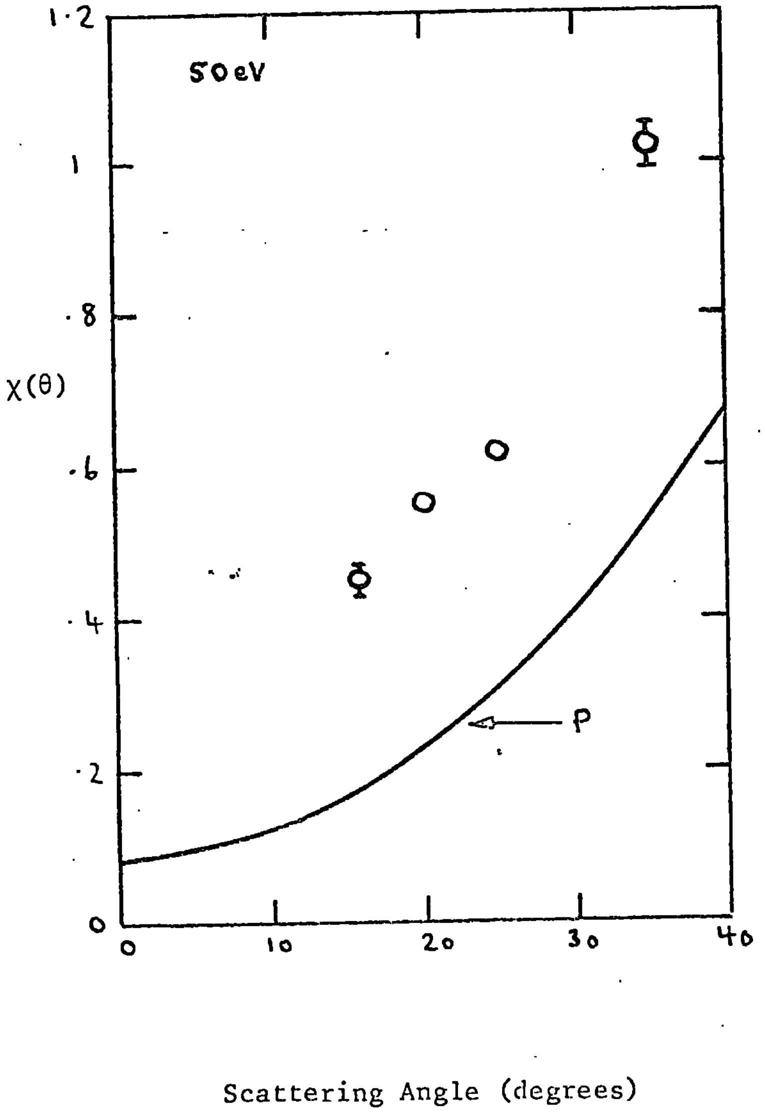


Figure 10 b

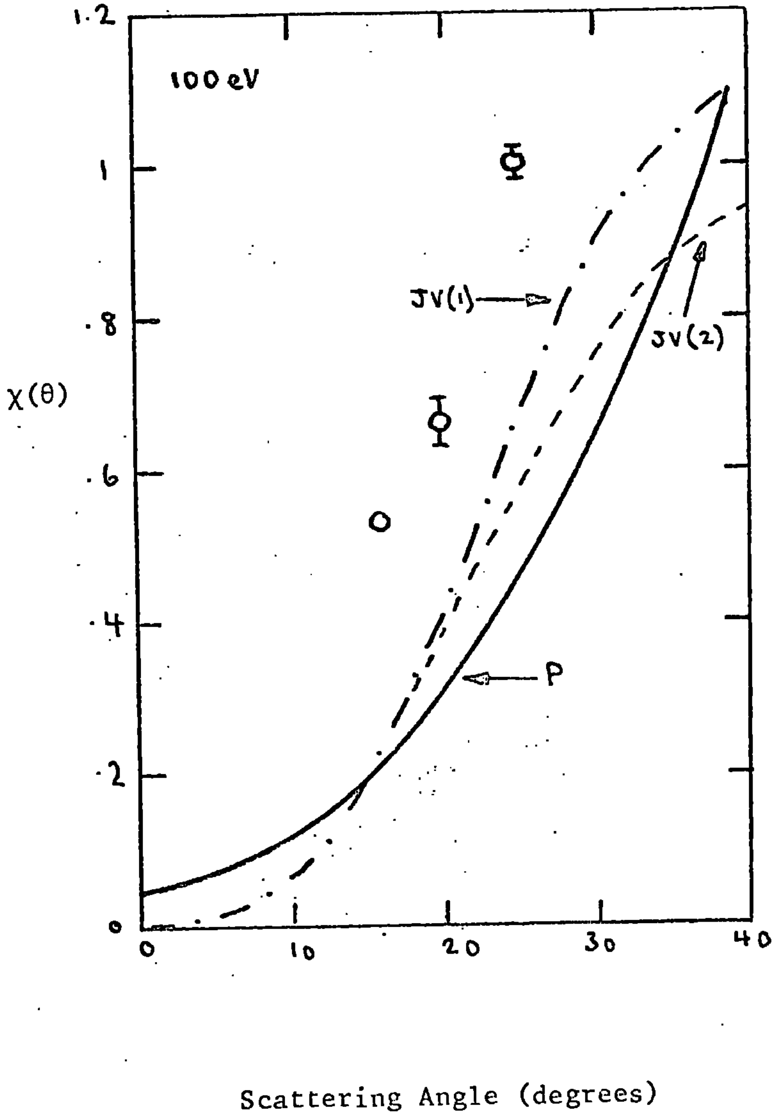


Figure 11a

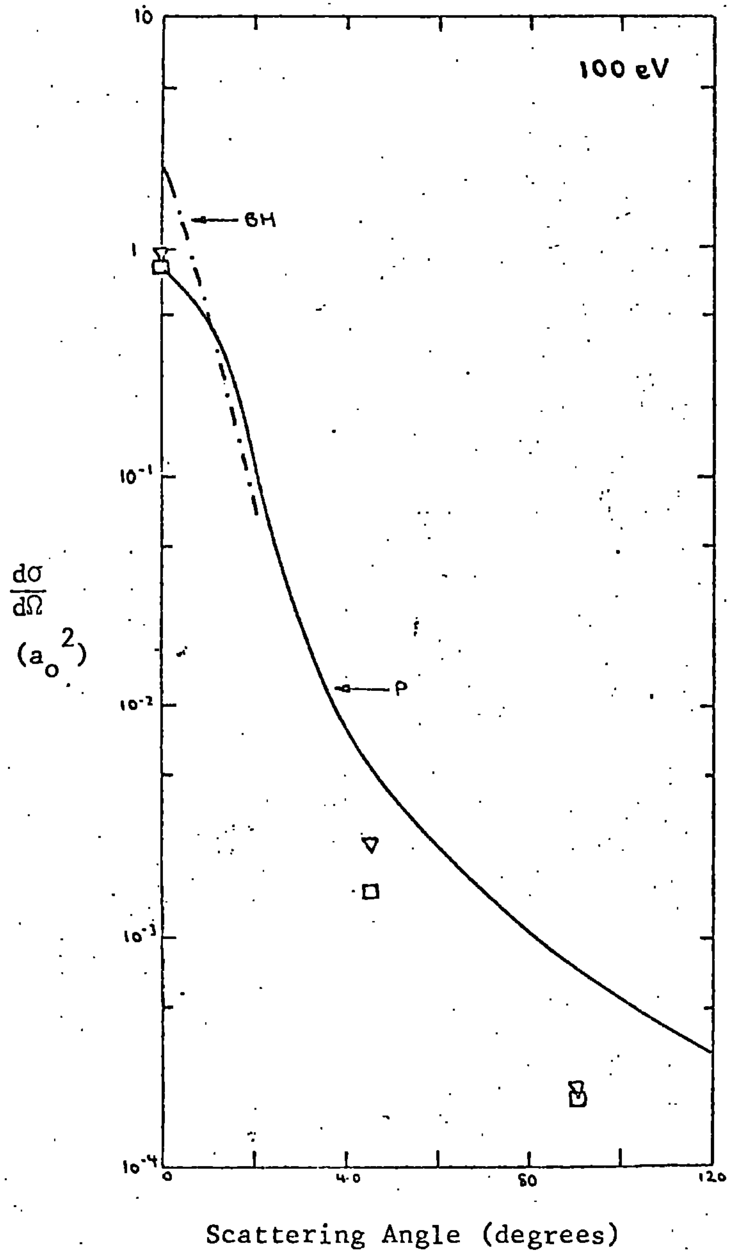


Figure 11 b

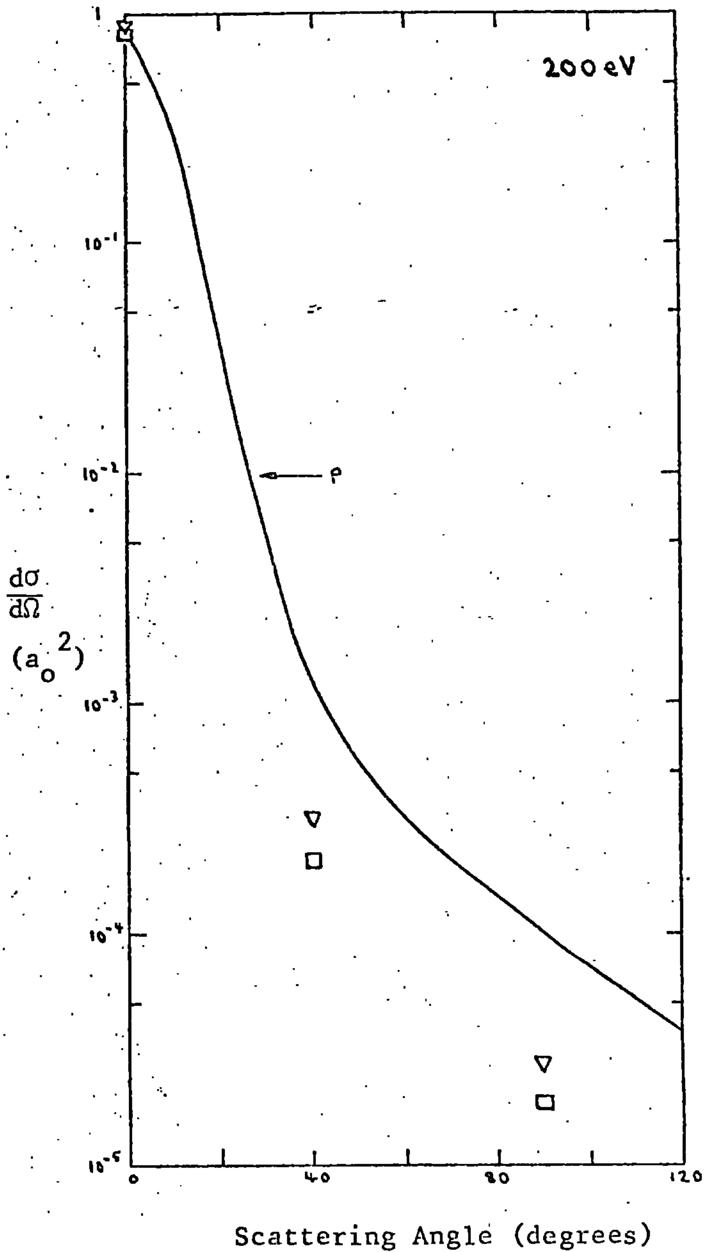
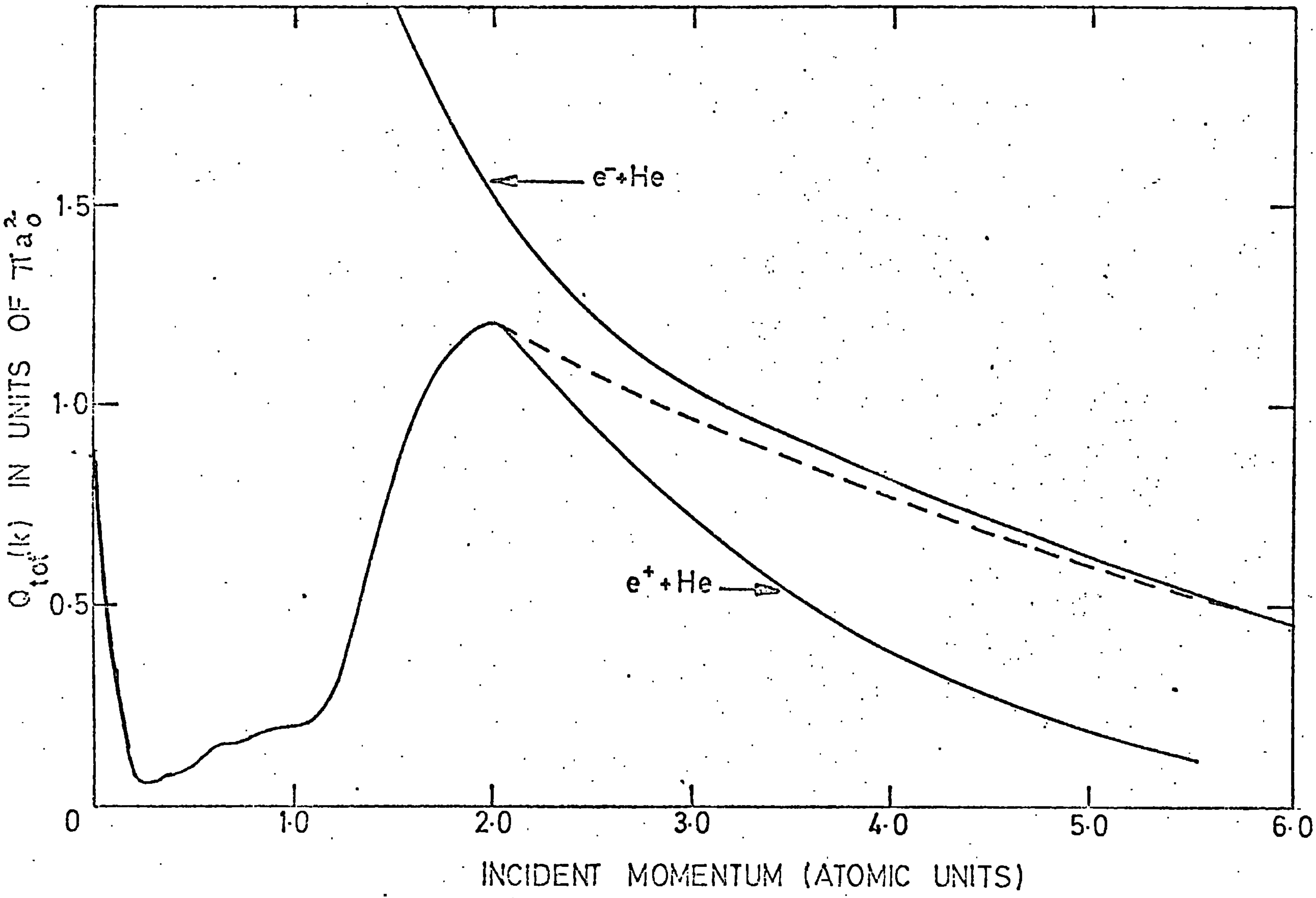


Figure 12


$Q_{tot}(k)$ IN UNITS OF πa_o^2
0
0·5
1·0
1·5
1·0
2·0
3·0
4·0
5·0
6·0
INCIDENT MOMENTUM (ATOMIC UNITS)
$e^- + He$
$e^+ + He$