COMPARISONS BETWEEN THE BORN APPROXIMATION AND A DISTORTED WAVE BORN APPROXIMATION FOR 1S-2S EXCITATION BY ELECTRON IMPACT IN HYDROGENIC TARGETS

by

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B.S., The University of Southern Colorado, 1974

A MASTER'S THESIS

submitted in partial fulfillment of the

requirements for the degree

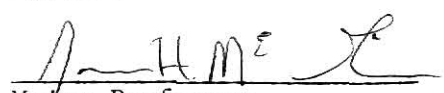
MASTER OF SCIENCE

Department of Physics

KANSAS STATE UNIVERSITY
Manhattan, Kansas

1976

Approved:



Major Professor

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CHAPTER 1

INTRODUCTION

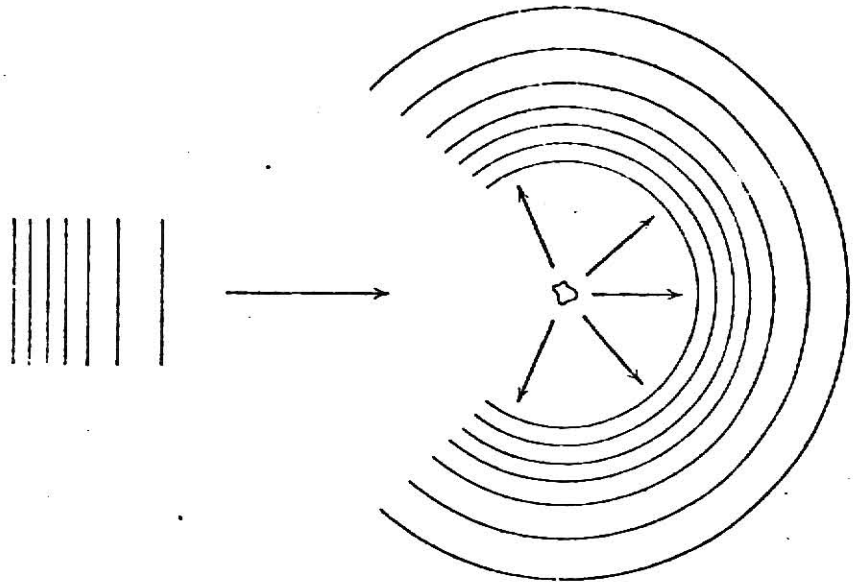
Since the inception of atomic physics one of the major problems has been to observe the workings of small objects such as the atom. One basic method of examining atomic structure is through scattering experiments. That is, if the object to be observed cannot be investigated directly, perhaps it can be probed indirectly by hurling many small objects at it and determining how the incident particles are affected. We thus use the incident particles to interact with the electron cloud of the target atom, and by increasing or decreasing the velocity and charge of the projectiles we can probe more or less deeply into the atom. Since the atom has structure, the incoming projectiles can deposit mass-energy and momentum into the target. Thus the initial and final target states may be different, and so we need to consider all combinations of initial and final states to get a complete picture of the scattering process. This thesis is concerned with a particular method of approximating the scattering probability in the situation where the target atom is in its ground state initially and in its first excited state finally.

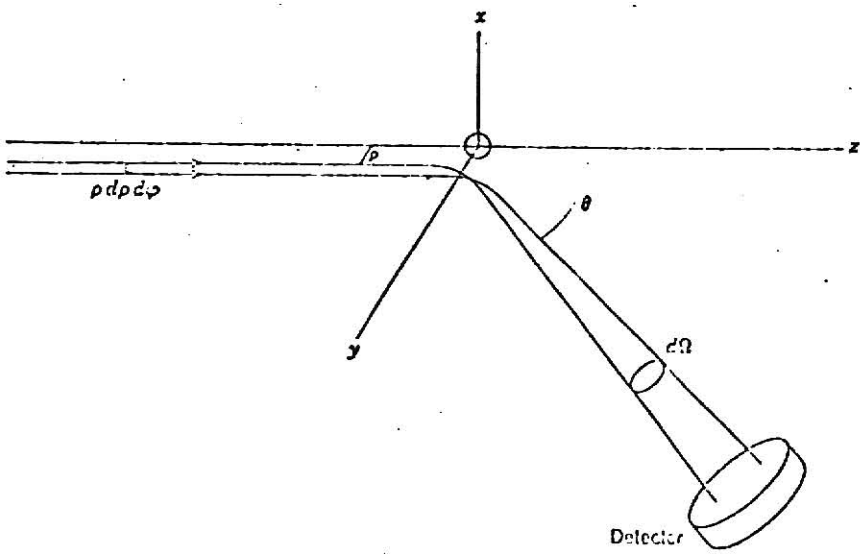
Since the projectile mass, and target size are so small we require the use of quantum mechanics. In quantum mechanics we can envision the incident projectile beam as an incoming plane wave, and the scattered beam as an outgoing spherical wave. (See Fig. 1(a).) The quantity which is most often used in scattering theory is the differential cross section $\frac{d\sigma}{d\Omega}$. The

Figure 1.

(a) The scattering process may be represented by an incoming plane wave and an outgoing scattered spherical wave. (This Fig. was taken from reference 14.)

(b) Scattering through an angle θ of a classical particle beam incident at impact parameter ρ and azimuth ϕ. (This Fig. was taken from reference 14.)




x
z
ρ
ρdρdφ
θ
y
dΩ
Detector

differential cross section is the number of events recorded by the detector (at angles θ, ϕ) per unit solid angle and time normalized to the incident flux. The differential $d\sigma$ has units of area, and it can be seen to be the area which, when placed at right angles to the incident beam, is traversed by as many particles as are scattered into the unit solid angle centered on the direction characterized by θ and ϕ. (See Fig. 1(b).) For a given projectile and target, $\frac{d\sigma}{d\Omega}$ depends primarily on the angle (θ) between the incident beam and the detector, and on the projectile energy. The angular dependence of $\frac{d\sigma}{d\Omega}$ gives us information about the structure of the target.

Under certain conditions it can be shown that (See Chap. II.) the differential cross section for a particle being scattered from an initial state ψ_i to a final state ψ_f is proportional to the square of the matrix element $|\langle\Phi_f|V|\psi_i\rangle|$, where $H = H_o + V$ is the total Hamiltonian, and ψ_i and Φ_f are defined by

$$H\psi_i = E\psi_i \quad ,$$

$$H_o\Phi_f = E\Phi_f \quad .$$

The total Hamiltonian can be broken up into H_o and V in several different ways. The choice of which way to divide up H depends on the existence of known solutions for Φ_f, and on the difficulty of the resultant calculation. As long as the exact ψ_i and Φ_f are known the choice of H_o and V will not affect the value of the matrix element. Only in a few cases do we know

the exact form of ψ_i, and so we are forced to make an approximate choice for ψ_i. Once an approximate ψ_i is selected, the choice of H_o and V can influence the resultant matrix element.

The (plane wave) Born approximation results from choosing V to be the total interaction between the incident projectile and the target, and approximating ψ_i by the product of a plane wave and an appropriate bound state wave function. This choice of H_o and V causes ϕ_f also to be a plane wave times a bound state wave function, and thus ψ_i and ϕ_f are orthogonal. This orthogonality causes the contribution to the matrix element from the nuclear interaction to vanish. (See Chap. 2.) The Born approximation has for a long time been a useful tool in the high energy regime, where the incident projectile velocity is greater than the orbital velocity of the atomic electrons. The simple form of the Born approximation has rendered many of the problems of atomic physics tractable, and it has been gainfully employed in excitation, ionization, and charge transfer.

There has of course been a continual search for ways to improve the Born approximation while retaining the simplicity of the Born calculation. One particular motivation for the approximation which we use here is that the Born approximation fails to accurately fit experimental data for electrons impacting on hydrogen. Figure 2 shows a plot of $\frac{d\sigma}{d\Omega}$ versus θ for the 1S-2S, 2P transitions at 200 eV. The Born approximation curve fits the data well at small values of θ, but is several orders of magnitude too small at larger angles. (The curve denoted by DWBA is due to the approximation which we shall later introduce and use.) Note that the total Born cross section will still be in agreement with the data since the discrepancy

Figure 2.

Differential cross sections, for (1S-2S, 2P) excitation of hydrogen by electron impact. (200 eV) The broken curve is the Born approximation, the solid curve is the DWBA, and the dots are from the experiment of Williams[38] normalized at 21° to the DWBA. (This Fig. was taken from reference 2.)

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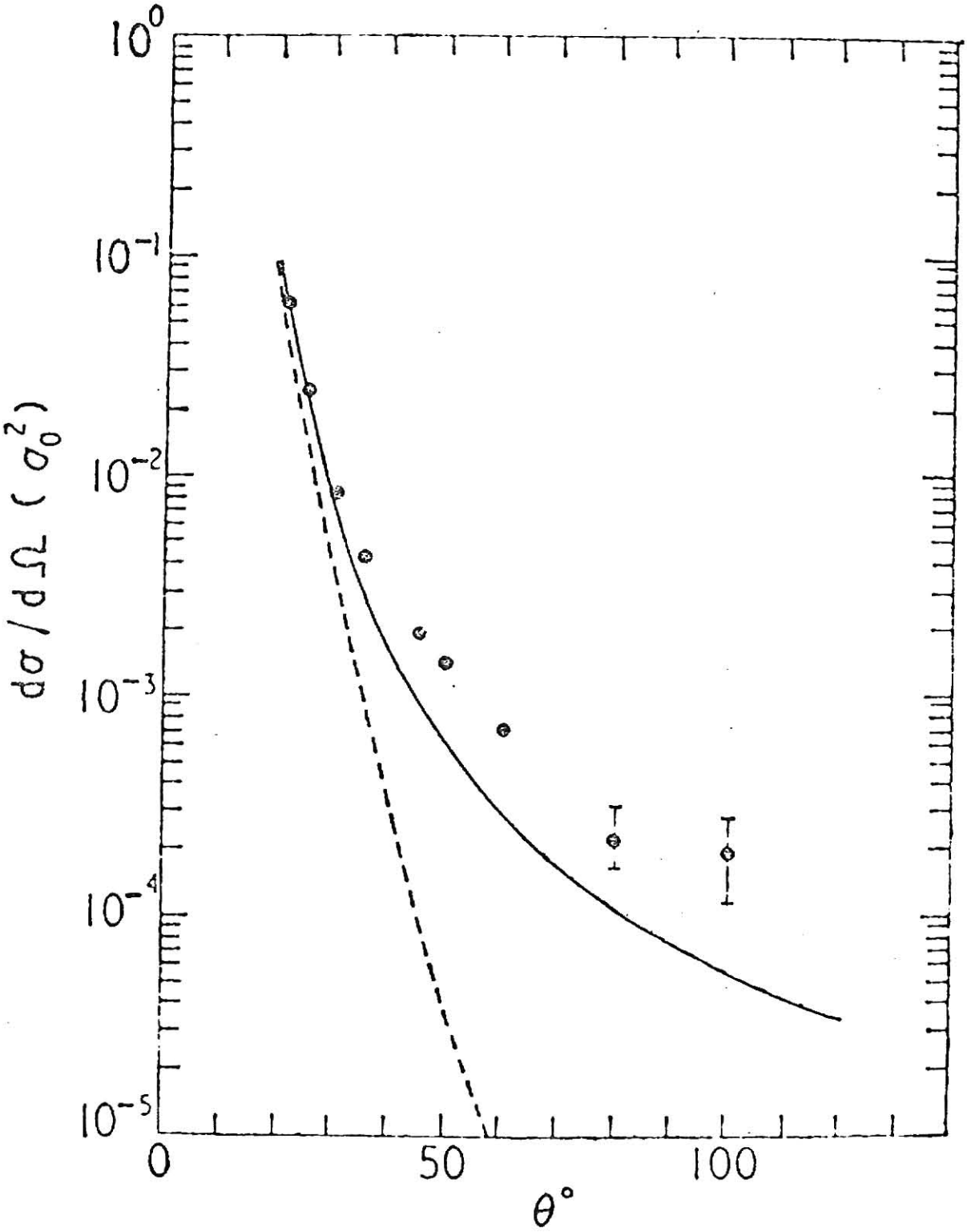

10^0
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
$d\sigma / d\Omega\ (\sigma_0^2)$
0
50
100
$\theta°$

at large angles does not greatly influence the total cross section. This is because the curves fall so rapidly that the large angle contributions are small. Physically, we expect large angle scattering to result from the interaction of the projectile with a relatively massive object, in this case, the nucleus. In the Born approximation the contribution to the matrix element from the projectile-nucleus interaction vanishes, so we have an explanation for the discrepancies in Fig. 2.

We thus wish to include the projectile-nucleus interaction in a manner which retains much of the simplicity of the Born approximation. One way to do this is to choose the perturbing potential, V, to contain only the interaction between the projectile and the atomic electrons, thus H_o contains the projectile-nucleus interaction. This changes ϕ so that it becomes a Coulomb wave (rather than a plane wave) multiplied by an appropriate bound state wave function. We can still approximate ψ_i by a plane wave times a bound state wave function as in the Born calculation. We will refer to this calculation as a (Coulomb) distorted wave Born approximation, or DWBA. Since in the Born approximation the projectile-nucleus term does not contribute, the only difference between the Born approximation and the DWBA is that in the DWBA a Coulomb wave function appears in the final state rather than a plane wave function. It should be noted that since there are many ways of breaking up the Hamiltonian into H_o and V, there are many approximations which could claim the title of DWBA. The calculation which we use is only a particular form of the DWBA.

Recently, Geltman[1] applied the DWBA to the problem of proton-hydrogen charge transfer. By using the DWBA he was able to include the proton-proton interaction in the unperturbed part of the problem. Geltman and Hidalgo[2-5] subsequently applied the approximation to hydrogen and helium excitation and ionization by fast electrons. Junker[6] extended the technique by varying the amount of nuclear interaction included in H_o, thus taking into account screening of the nuclear potential by the atomic electrons. Junker has used his modified calculation to compute excitation cross sections of fast electrons on hydrogen. Stauffer and Morgan[7,8] have similarly generalized the DWBA by changing the amount of nuclear interaction in H_o, and they have applied their method to calculate cross sections for the excitation of sublevels of hydrogen.

This thesis will be concerned with the excitation of any hydrogenic atom from 1S to 2S energy levels by electron impact in the high velocity regime. We will be using the DWBA described above and all equations and results will be written in atomic units unless otherwise noted. (In atomic units $\hbar = e = m_e = 1$.) We do not take into account the effect of exchange, which is small for incident energies greater than 100 eV.[6]

A possible testing ground for our DWB calculation is the momentum transfer cross section. The momentum transfer cross section is just the regular cross section multiplied by a weighting factor which is an increasing function of θ. Thus the large angle portion of the differential cross section is amplified. It turns out that momentum transfer cross sections can be used to calculate certain plasma transport properties.[9,10,11]

Recall that one of the advantages of the Born approximation is its relative simplicity. In particular the Born approximation obeys a useful scaling relation. If excitation cross sections of hydrogenic atoms (one electron, atomic number Z) are calculated, and if $Z\sigma$ is plotted against a scaled energy, $E_{inc}/|E_{1S} - E_{2S}|$, then the curve is found to be independent of Z. We are thus led to check the DWBA for a similar scaling law.

My contribution to this work consists of the following: evaluation of the 1S-2S DWBA matrix element from the general formula of Golden, Junker, and McGuire,[12] construction of a computer program to calculate the differential cross section and the total cross section, application of the calculation to the momentum transfer cross section, elucidation of a scaling relation in the atomic number of the target Z_b.

In Chapter 2 we exhibit in detail the theory involved in deriving an expression for the scattering cross section. We also discuss the approximation leading to the Born and DWB calculations. In Chapter 3 we display the details of the DWB calculation and put the equations derived in Chapter 2 in a form convenient for programming. We then discuss the computer code which we use to do the calculations. In Chapter 4 we present our results in graphical form, and discuss their meaning. Chapter 5 contains concluding remarks and discussion. The appendix contains a copy of the computer code.

CHAPTER 2

THEORY

In the previous chapter we discussed our aims and motivations. Before we set up the actual DWB calculation we must build the theoretical foundations. We first define and discuss the concept of a scattering cross section, both classically and quantum mechanically. We then use a time dependent approach in the interaction picture to derive an expression for the differential scattering cross section in terms of the transition matrix T. With the T matrix in hand we discuss the Born and DWB approximations and their regions of validity. The Born approximation is developed by iterating an integral Green's function equation, and the distorted wave Born approximation is achieved through the introduction of a two potential formalism followed again by iterating a Green's function equation.[13]

Classically, the differential cross section is the area within which the projectile must strike so that a certain final configuration of target and projectile will occur. In order to define the differential cross section, consider a given initial flux (I_o) of particles incident on a scattering center. (See Figs. 1(a,b).) The differential scattering cross section is defined by

$$\frac{d\sigma}{d\Omega} = \frac{I(\theta,\phi)}{I_o} \quad , \tag{2.1}$$

where $d\Omega \equiv$ the solid angle subtended by the detector, $I(\theta,\phi) \equiv$ the number

of events recorded per unit solid angle and time at (θ,ϕ) by the detector, and $I_o \equiv$ the number of incident particles per unit area and time.

It is clear from the definition above that $\frac{d\sigma}{d\Omega}$ has the units of area. Since $I_o d\sigma = I(\theta,\phi)d\Omega$ it can be seen that $d\sigma$ represents the area which, when placed at right angles to the incident beam, is traversed by as many particles as are scattered into the unit solid angle in the direction characterized by θ and ϕ.[14]

Classically, we can show that[15]

$$\frac{d\sigma}{d\Omega} = \frac{\rho}{\sin\theta}\left|\frac{d\rho}{d\theta}\right|, \qquad (2.2)$$

where ρ is the impact parameter, and θ is the scattering angle. (See Fig. 1(b), Chap. 1.) The classical differential cross section is determined by the relationship between the scattering angle and the impact parameter. This classical result is reasonable as long as the de Broglie wavelength of the incident particle is much smaller than the size of the scatterer. If the de Broglie wavelength of the incident particle is on the order of or larger than the size of the scatterer, then we must consider the problem quantum mechanically.

One can approach quantum mechanical scattering theory in at least two ways. In the time independent or stationary state approach one considers a monoenergetic beam of particles with a constant flux striking the target area. In this thesis we consider the more formal time dependent approach in which one considers two systems of particles which come together, interact, and separate.[13,16] The total time involved in the scattering

experiment can be broken up into three periods. In the first period ($t \lesssim -\infty$) the two noninteracting systems are created. In the second period ($-t_c \leq t \leq t_c$) the two systems interact and may thereby be altered. In the third period ($t \gtrsim +\infty$) the scattered wave packet is detected in a region where the two systems have ceased interacting. The final two systems may be different from the initial systems due to processes such as excitation, ionization, or charge transfer.

Time dependent quantum mechanics can be expressed in several different pictures. In the Schrödinger picture the wave functions carry the time dependence while the operators representing observables are time independent. The Heisenberg picture places the time dependence in the observables and uses time independent wave functions. The picture to be used here is called the interaction picture, and its time dependence is contained both in the wave functions and in the operators. (I will define the interaction picture in terms of the Schrödinger picture.) In the Schrödinger picture the time development of the wave function, $\psi(t)$, is determined by

$$i\frac{\partial\psi(t)}{\partial t} = H\psi(t) \quad , \tag{2.3}$$

where H is the total Hamiltonian. Thus

$$\psi(t) = e^{-iH(t - t_o)}\psi(t_o) \quad , \tag{2.4}$$

where $\psi(t_o)$ is the wave function at some time t_o. The time dependence

is completely contained in the unitary exponential operator $e^{-iH(t - t_o)}$. We next break up the Hamiltonian into two parts, $H = H_o + V$, where H_o is called the unperturbed Hamiltonian and V is called the perturbation. As we will see later, the motivations for the way in which H_o and V are chosen are to make the perturbing potential (V) small, and to choose H_o so that its exact eigenfunctions are known. We can now define the wave function in the interaction picture as

$$\psi_I(t) \equiv e^{iH_o t} \psi(t) \quad . \tag{2.5}$$

If we differentiate Eq. (2.5) and use Eq. (2.4), we get

$$i\frac{\partial \psi_I(t)}{\partial t} = -H_o e^{iH_o t} \psi(t) + ie^{iH_o t} \frac{\partial \psi(t)}{\partial t}$$

$$= e^{iH_o t}(-H_o + H)\psi(t) = e^{iH_o t} V e^{-iH_o t}(e^{iH_o t} \psi(t))$$

$$= V(t)\, \psi_I(t) \quad , \tag{2.6}$$

where $V(t) \equiv e^{iH_o t} V e^{-iH_o t}$ is the perturbation potential in the interaction picture. Note that both $\psi_I(t)$ and V(t) are time dependent. Equation (2.6) is the interaction picture equivalent of Eq. (2.3). The equation corresponding to Eq. (2.4) can be derived from Eq. (2.5) and Eq. (2.4) as follows:

$$\psi_I(t) = e^{iH_o t}\psi(t) = e^{iH_o t}e^{-iH(t - t_o)}\psi(t_o)$$

$$= e^{iH_o t}e^{-iH(t - t_o)}e^{-iH_o t_o}\psi_I(t_o)$$

$$= U(t, t_o)\,\psi_I(t_o) \quad , \tag{2.7}$$

where

$$U(t, t_o) \equiv e^{iH_o t}e^{-iH(t - t_o)}e^{-iH_o t_o} \tag{2.8}$$

is the operator which determines the time development of the system in the interaction picture. Some useful properties of the causal operator $U(t, t_o)$ are:

$$U(t, t) = 1 \quad , \tag{2.9}$$

$$U(0, t) = e^{iHt}e^{-iH_o t} \quad , \tag{2.10}$$

$$U(t, t')\,U(t', t_o) = U(t, t_o) \tag{2.11}$$

$$U^{+}(t, t_o) = e^{iH_o t_o}e^{iH(t - t_o)}e^{-iH_o t} = U(t_o, t). \tag{2.12}$$

Equations (2.9), (2.10), and (2.11) are the result of direct substitution from Eq. (2.8). Equation (2.12) is the result of elementary properties

of quantum mechanical operators.[17] We can also combine Eqs. (2.9), (2.11), and (2.12) to show that $U(t, t_o)$ is a unitary operator, since $U^+(t, t_o)U(t, t_o) = U(t_o, t)U(t, t_o) = U(t_o, t_o) = 1$, and thus $U^+(t, t_o) = U^{-1}(t, t_o)$. From Eqs. (2.6) and (2.7) we can obtain

$$i\frac{\partial \psi_I}{\partial t} = i\frac{\partial U(t, t_o)}{\partial t}\ \psi_I(t_o) = V(t)U(t, t_o)\psi_I(t_o) \ , \qquad (2.13)$$

so that

$$i\frac{\partial U(t, t_o)}{\partial t} = V(t)U(t, t_o) \quad , \qquad (2.13)$$

which is the equation of motion of $U(t, t_o)$. Integrating Eq. (2.13) yields

$$U(t, t_o) = 1 - i\int_{t_o}^{t} V(t')U(t', t_o)dt' \quad ,$$

where the constant has been evaluated with the help of Eq. (2.9).

Recall in our earlier discussion of scattering that there were three important time periods ($t \simeq -\infty$, $-t_c \leq t \leq t_c$, $t \simeq +\infty$). With the above formalism we can now write $\psi_I(+\infty)$ in terms of $\psi_I(-\infty)$, and we obtain

$$\psi_I(+\infty) = S\psi_I(-\infty) \quad , \qquad (2.14)$$

where

$$S \equiv \lim_{\substack{t_o \to -\infty \\ t \to +\infty}} U(t, t_o) \quad . \qquad (2.15)$$

If at time t_o the systems are separated such that there is no interaction between them, then[13]

$$\psi(t_o) = e^{-iE_i t_o}\psi_i \quad , \tag{2.16}$$

where ψ_i is an eigenfunction of H_o and E_i is the corresponding eigenenergy. According to Eq. (2.5),

$$\psi_I(t_o) = e^{iH_o t_o} e^{-iE_i t_o}\psi_i$$

$$= e^{iE_i t_o} e^{-iE_i t_o}\psi_i = \psi_i \quad ,$$

and since t_o is some time when the interaction V is zero, we can choose $t_o = -\infty$. Thus we have

$$\psi_I(-\infty) = \psi_i \quad . \tag{2.17}$$

The final state of the scattered projectile will be some superposition of the eigenstates of H_o. The probability amplitude for the transition from ψ_i to some final state ψ_f is the matrix element S_{if} which is given by

$$S_{if} = \langle\psi_f|S|\psi_i\rangle$$

$$= \lim_{\substack{t_o \to -\infty \\ t \to +\infty}} \langle\psi_f|U(t, t_o)|\psi_i\rangle$$

$$= \lim_{\substack{t_o \to -\infty \\ t \to +\infty}} \langle U(0, t)\psi_f|U(0, t_o)\psi_i\rangle \quad , \tag{2.18}$$

where Eqs. (2.11) and (2.12) have been used in the last step. The S_{if} are called the components of the scattering matrix S. To evaluate the matrix element S_{if} we need to examine the expression $\lim_{t \to \pm\infty} U(0, t)\psi_a$, where ψ_a is an eigenfunction of H_o. The evaluation of the above limits is not straightforward. Due to the fact that we are using single states with a specific energy, rather than wave packets, we may create oscillations in the function as the limit is taken.[18] We thus need to construct a mathematical device which dampens these oscillations. One such device which has been used by Gell-Mann and Goldberger[19] is to define the limits of a function f(t) as $t \to \pm\infty$ by

$$\lim_{t \to -\infty} f(t) \equiv \lim_{\varepsilon \to 0^+} \varepsilon \int_{-\infty}^{0} e^{\varepsilon t'} f(t')dt' \quad , \tag{2.19a}$$

and

$$\lim_{t \to +\infty} f(t) \equiv \lim_{\varepsilon \to 0^+} \varepsilon \int_{0}^{\infty} e^{-\varepsilon t'} f(t')dt' \quad . \tag{2.19b}$$

(Note: To simplify notation, whenever ε appears the limit will be implicitly assumed.) If the limits exist in the normal sense, no oscillations, then the above expressions yield the expected values, since

$$\lim_{t \to -\infty} f(t) = \lim_{\varepsilon \to 0^+} \varepsilon \int_{-\infty}^{0} e^{\varepsilon t'} f(t')dt'$$

$$= \lim_{\varepsilon \to 0^+} \varepsilon \left[\frac{e^{\varepsilon t'}}{\varepsilon} f(t') \Bigg|_{-\infty}^{0} - \int_{-\infty}^{0} \frac{f'(t')e^{\varepsilon t'} dt'}{\varepsilon} \right]$$

$$= \lim_{\varepsilon \to 0^+} [f(0)] - \lim_{\varepsilon \to 0^+} \int_{-\infty}^{0} f'(t')e^{\varepsilon t'}dt'$$

$$= f(0) - f(0) + f(-\infty) = f(-\infty) \ .$$

In a similar manner we can derive the expected result for Eq. (2.19(b)). If we introduce the Møller operator Ω^+, defined by

$$\Omega^+ = \lim_{t \to -\infty} U(0,t) \quad , \tag{2.20}$$

then

$$\lim_{t \to -\infty} U(0,t)\psi_a = \Omega^+\psi_a = \lim_{\varepsilon \to 0^+} \varepsilon \int_{-\infty}^{0} e^{\varepsilon t'} e^{iHt'} e^{-iE_a t'} \psi_a dt'$$

$$= \lim_{\varepsilon \to 0^+} \frac{i\varepsilon}{E_a - H + i\varepsilon} \psi_a \ . \tag{2.21}$$

By definition $(E_a - H_o)\psi_a = 0$, so that

$$\Omega^+\psi_a = \lim_{\varepsilon \to 0^+} \frac{1}{E_a - H + i\varepsilon} (i\varepsilon + E_a - H_o)\psi_a \equiv \psi_a^+ \ , \tag{2.22}$$

and

$$\psi_a^+ = \left(\frac{i\varepsilon + E_a - H}{i\varepsilon + E_a - H}\right)\psi_a + \frac{1}{i\varepsilon + E_a - H} V\psi_a$$

$$= \psi_a + \lim_{\varepsilon \to 0^+} \frac{1}{i\varepsilon + E_a - H} V\psi_a$$

$$= \psi_a + G^+ V\psi_a \quad ,$$

where $G^+ \equiv \lim_{\varepsilon \to 0^+} [i\varepsilon + E_a - H]^{-1}$ is the outgoing Green's function for the total Hamiltonian. In this form ψ_a^+ can be recognized as a continuum wave function of the total Hamiltonian, with energy E_a, which satisfies outgoing wave boundary conditions.[20] Similarly we can define

$$\Omega^- \equiv \lim_{t \to +\infty} U(0,t) \quad , \tag{2.24}$$

and

$$\Omega^- \psi_a \equiv \psi_a^- \quad , \tag{2.25}$$

with the result

$$\psi_a^- = \psi_a + \lim_{\varepsilon \to 0^+} \frac{1}{E_a - H - i\varepsilon} V\psi_a \quad . \tag{2.26}$$

Thus ψ_a^- is the continuum eigenfunction of H with energy E_a which satisfies incoming wave conditions.[20] From Eqs. (2.23) and (2.26), we have

$$\psi_a^{\pm} = \psi_a + G^{\pm} V\psi_a \quad . \tag{2.27}$$

We wish to write $G^{\pm}V\psi_a$ in terms of $\psi_a^{\pm}$. To do this we will need the use of the following operator identities:

$$P^{-1} = Q^{-1} + P^{-1}(Q - P)Q^{-1} \quad , \tag{2.28a}$$

$$= Q^{-1} + Q^{-1}(Q - P)P^{-1} \quad , \tag{2.28b}$$

where P and Q are operators whose inverses exist. This pair of identities can be easily verified, since

$$P^{-1}(Q - P)Q^{-1} = (P^{-1}Q\ Q^{-1} - P^{-1}P\ Q^{-1}) = P^{-1} - Q^{-1} \quad ,$$

and

$$Q^{-1}(Q - P)P^{-1} = (Q^{-1}Q\ P^{-1} - Q^{-1}P\ P^{-1}) = P^{-1} - Q^{-1} \quad .$$

If we define $G_o^{\pm} \equiv [E - H_o \pm i\varepsilon]^{-1}$ and set $P^{\pm} = E - H \pm i\varepsilon$, $Q^{\pm} = E - H_o \pm i\varepsilon$, then we can apply Eq. (2.28(b)) (since the required inverses exist) and we get

$$G^{\pm} = G_o^{\pm} + G_o^{\pm}(E - H_o \pm i\varepsilon - (E - H \pm i\varepsilon))G^{\pm}$$

$$= G_o^{\pm} + G_o^{\pm}\ V\ G^{\pm} \quad . \tag{2.29}$$

If we now operate on both sides of Eq. (2.27) with $G_o^{\pm}V$, then

$$G_o^{\pm}V\psi_a^{\pm} = G_o^{\pm}V\psi_a + G_o^{\pm}VG^{\pm}V\psi_a$$

$$= G_o^{\pm}V\psi_a + (G^{\pm} - G_o^{\pm})V\psi_a \quad ,$$

which implies that

$$G_o^{\pm}V\psi_a^{\pm} = G^{\pm}V\psi_a \quad . \tag{2.30}$$

If we substitute Eq. (2.30) into Eq. (2.27), we obtain

$$\psi_a^{\pm} = \psi_a + G_o^{\pm} V \psi_a^{\pm} = \psi_a + \lim_{\varepsilon \to 0^+} \left[\frac{1}{E_a - H_o \pm i\varepsilon} \right] V \psi_a^{\pm} \quad . \qquad (2.31)$$

This is called the Lippmann-Schwinger equation.

Recall that the elements of the scattering matrix were defined by

$$S_{if} = \lim_{\substack{t_o \to -\infty \\ t \to +\infty}} \langle U(0,t)\psi_f | U(0,t_o)\psi_i \rangle$$

$$= \langle \Omega^- \psi_f | \Omega^+ \psi_i \rangle = \langle \psi_f^- | \psi_i^+ \rangle$$

$$= \langle \psi_f^+ | \psi_i^+ \rangle + \langle \psi_f^- - \psi_f^+ | \psi_i^+ \rangle$$

$$= \delta_{if} + \langle \psi_f^- - \psi_f^+ | \psi_i^+ \rangle \quad , \qquad (2.32)$$

where the δ function, $\delta_{if} = \langle \psi_f^+ | \psi_i^+ \rangle$, is a Dirac delta function over the energies, and a Kronecker delta function over the other (discrete) quantum numbers. From Eq. (2.27), we obtain

$$\psi_f^- - \psi_f^+ = G^- V\psi_f - G^+ V\psi_f = \lim_{\varepsilon \to 0^+} \left(\frac{1}{E_f - H - i\varepsilon} - \frac{1}{E_f - H + i\varepsilon} \right) V\psi_f .$$

Thus Eq. (2.32) becomes

$$S_{if} = \delta_{if} + \lim_{\varepsilon \to 0^+} \left\langle \left(\frac{1}{E_f - H - i\varepsilon} - \frac{1}{E_f - H + i\varepsilon} \right) V \psi_f \middle| \psi_i^+ \right\rangle$$

$$= \delta_{if} + \lim_{\varepsilon \to 0^+} \left\langle \psi_f \middle| V \left(\frac{1}{E_f - H + i\varepsilon} - \frac{1}{E_f - H - i\varepsilon} \right) \psi_i^+ \right\rangle$$

$$= \delta_{if} + \lim_{\varepsilon \to 0^+} \left(\frac{1}{E_f - E_i + i\varepsilon} - \frac{1}{E_f - E_i - i\varepsilon} \right) \langle \psi_f | V | \psi_i^+ \rangle$$

$$= \delta_{if} + \lim_{\varepsilon \to 0^+} \left(\frac{-2i\varepsilon}{(E_f - E_i)^2 + \varepsilon^2} \right) \langle \psi_f | V | \psi_i^+ \rangle \quad , \tag{2.33}$$

for Hermitian V and H. Using the well known limit[21]

$$\lim_{\varepsilon \to 0^+} \left(\frac{\varepsilon}{(E_f - E_i)^2 + \varepsilon^2} \right) = \pi \delta(E_f - E_i) \quad ,$$

we can write Eq. (2.33) as

$$S_{if} = \delta_{if} - 2\pi i \delta(E_f - E_i) \langle \psi_f | V | \psi_i^+ \rangle$$

$$= \delta_{if} - 2\pi i \delta(E_f - E_i) T_{if} \quad , \tag{2.34a}$$

where

$$T_{if} \equiv \langle \psi_f | V | \psi_i^+ \rangle \tag{2.35}$$

defines the elements of the transition matrix T. We can also express S_{if} in the form

$$S_{if} = \langle\psi_f^-|\psi_i^+\rangle = \langle\psi_f^-|\psi_i^-\rangle + \langle\psi_f^-|\psi_i^+ - \psi_i^-\rangle \quad , \tag{2.36}$$

which leads, in the same manner as above, to

$$S_{if} = \delta_{if} - 2\pi i\delta(E_f - E_i)\langle\psi_f^-|V|\psi_i\rangle \quad . \tag{2.34b}$$

Comparing Eqs. (2.34(a)) and (2.34(b)), we see that when $E_i = E_f$,

$$\langle\psi_f|V|\psi_i^+\rangle = \langle\psi_f^-|V\psi_i\rangle \quad . \tag{2.38}$$

We now have an expression for S_{if} which is useable. However, $|S_{if}|^2$ is the total probability (for all time) that a transition occurs from state ψ_i to state ψ_f. To get a transition probability per unit time we need to differentiate. Define the transition probability per unit time as

$$W_{if} = \lim_{t_o \to -\infty} \frac{\partial}{\partial t} |\langle\psi_f|U(t,t_o)|\psi_i\rangle|^2 \tag{2.39}$$

$$= \frac{d}{dt} |\langle\psi_f|\psi_I(t)\rangle|^2 \tag{2.40}$$

$$= \langle\psi_f| \frac{\partial}{\partial t} \psi_I(t)\rangle^* \langle\psi_f|\psi_I(t)\rangle + \text{c.c.} \quad , \tag{2.41}$$

where c.c. will be used to denote the complex conjugate of the first term in the expression. In order to simplify the first term in Eq. (2.41) we need the identity

$$\psi_I(0) = \psi_i^+ \quad . \tag{2.42}$$

We can derive Eq. (2.42) by starting with Eq. (2.7)

$$\psi_I(0) = U(0,-\infty)\psi_I(-\infty) = \Omega^+\psi_i = \psi_i^+ \quad .$$

We now simplify $\langle\psi_f| \frac{\partial}{\partial t} \psi_I(t)\rangle$ to obtain

$$\begin{aligned}
\langle\psi_f| \frac{\partial}{\partial t} \psi_I(t)\rangle &= -i\langle\psi_f|e^{iH_o t} V e^{-iH_o t} \psi_I(t)\rangle \\
&= -i\langle\psi_f|e^{iH_o t} V e^{-iH_o t} U(t,0)\psi_I(0)\rangle \\
&= -i\langle\psi_f|e^{iH_o t} V e^{-iH_o t} e^{iH_o t} e^{-iHt} \psi_I(0)\rangle \\
&= -i\langle\psi_f|e^{iH_o t} V e^{-iHt} \psi_i^+\rangle \\
&= -ie^{i(E_f - E_i)t} T_{if} \quad , \qquad (2.43)
\end{aligned}$$

and by simplifying $\langle\psi_f|\psi_I(t)\rangle$ we obtain

$$\begin{aligned}
\langle\psi_f|\psi_I(t)\rangle &= \langle\psi_f|e^{iH_o t} e^{-iHt} \psi_i^+\rangle \\
&= e^{i(E_f - E_i)t} \langle\psi_f|\psi_i^+\rangle \\
&= e^{i(E_f - E_i)t} \left(\langle\psi_f|\psi_i\rangle + \lim_{\varepsilon \to 0^+} \langle\psi_f|\frac{1}{E_i - H_o + i\varepsilon} V\psi_i^+\rangle\right) \\
&= e^{i(E_f - E_i)t} \left(\delta_{if} + \frac{1}{E_i - E_f + i\varepsilon} T_{if}\right) \quad . \qquad (2.44)
\end{aligned}$$

We substitute Eqs. (2.43) and (2.44) into Eq. (2.41), so that

$$W_{if} = \lim_{\varepsilon \to 0^+} \left[iT^*_{if} e^{-i(E_f - E_i)t} e^{i(E_f - E_i)t} \left(\delta_{if} + \frac{1}{E_i - E_f + i\varepsilon} T_{if} \right) + C.C. \right]$$

$$= \lim_{\varepsilon \to 0^+} \left[\left(iT^*_{ii} \delta_{if} + \frac{i}{E_i - E_f + i\varepsilon} |T_{if}|^2 \right) + C.C. \right]$$

$$= 2\, \mathrm{Im}(T_{ii}) \delta_{if} + \lim_{\varepsilon \to 0^+} |T_{if}|^2 \left(\frac{i}{E_i - E_f + i\varepsilon} - \frac{i}{E_i - E_f - i\varepsilon} \right)$$

$$= 2\, \mathrm{Im}(T_{ii}) \delta_{if} + 2\pi \delta(E_f - E_i) |T_{if}|^2 \quad , \tag{2.45}$$

where the last expression results from taking the same limit as in Eq. (2.33). The Dirac delta function, δ_{if}, is due to the fact that W_{if} is the transition probability to a single continuum state. This singularity can be removed by considering the transition probability to some set of states centered at $E = E_f$, with the density of these states being denoted by $\rho(E)$. ($\rho(E) \equiv$ the number of states with energies in the range E to E + dE per unit solid angle). If ψ_i does not belong to such a set of states, then the transition probability from ψ_i to the set of states is given by

$$w_{if} \equiv \int_{E_f - \Delta E}^{E_f + \Delta E} W_{if} \rho(E)\, dE\, d\Omega$$

$$= 2\pi \rho(E_f) |T_{if}|^2 d\Omega \quad , \tag{2.46}$$

where $E_i = E_f$.

An expression for $\rho(E)$ can be obtained by considering a free particle in a box with periodic boundary conditions. The eigenvalues of such a system are given (in atomic units) by[22]

$$E = \frac{\pi^2}{8u\ell^2}\,(n_x^{\,2} + n_y^{\,2} + n_z^{\,2}) \quad , \tag{2.47}$$

where u ≡ the mass of the particle, 2ℓ ≡ the dimension of the box, and $n_x, n_y, n_z = 1,2,3, \ldots$. Thus there is a one-to-one correspondence between ordered triplets in n_i and eigenstates. Now consider a 3-dimensional n-space, whose coordinates are given by (n_x, n_y, n_z). For every point in n-space whose coordinates are positive integers, there exists an eigenstate in the box, so that the density of states in n-space is one per unit volume. All of the eigenstates with energy E or less will be contained in the sphere of radius n in n-space, where

$$n = (n_x^{\,2} + n_y^{\,2} + n_z^{\,2})^{\frac{1}{2}} = \left(\frac{8u\ell^2}{\pi^2}\,E\right)^{\frac{1}{2}} \quad . \tag{2.48}$$

We can count up all such states ($n_i > 0$) by determining the volume of the sphere in one octant of n-space. We have

$$\int_0^E N(E)\,dE = \left(\frac{1}{8}\right)\frac{4}{3}\,\pi n^3 \quad . \tag{2.49}$$

Of course we are making an approximation by using the discrete distribution of states as if it were continuous, but for sufficiently high energies the error is small.[23] Thus we have

$$N(E)\,dE = \left(\frac{1}{8}\right)4\pi n^2\,dn \quad , \tag{2.50}$$

but $n^2 = \left(\frac{8u\ell^2}{\pi^2}\,E\right)$, and $dn = \frac{1}{2}\left(\frac{8u\ell^2}{\pi^2}\right)^{\frac{1}{2}} E^{-\frac{1}{2}}\,dE$, so that

$$N(E)dE = \frac{4\sqrt{2E}\,(u\ell^2)^{3/2}}{\pi^2}\,dE \quad .$$

We obtain $\rho(E)$ by dividing $N(E)$ by the volume of the well and the total solid angle (4π), and thus

$$w_{if} = \frac{uk_f}{4\pi^2}\,|T_{if}|^2\,d\Omega \quad .$$

But w_{if} is just the probability per unit time that a transition occurs to some set of states near ψ_f, and so

$$w_{if} = \frac{\#\text{of detections per unit time}}{\#\text{of particles}} = \frac{I_o \frac{d\sigma}{d\Omega}}{N}$$

$$= \frac{\frac{N}{V}\frac{k_i}{u}\frac{d\sigma}{d\Omega}}{N} = \frac{k_i}{u}\frac{d\sigma}{d\Omega} \quad ,$$

where I_o is the incident flux, ($I_o = \frac{N}{V}\frac{k_i}{u}$), N is the number of incident particles, and V is a unit volume.

Thus we have

$$\frac{d\sigma}{d\Omega} = \frac{u}{k_i}\,w_{if} = \frac{u^2k_f}{4\pi^2k_i}\,|T_{if}|^2 \quad ,$$

and the total cross section is given by

$$\sigma = \frac{u^2k_f}{4\pi^2k_i}\int |T_{if}|^2 d\Omega \quad .$$

We now have an expression for the differential cross section which involves integrating a term containing ψ_f, the perturbing potential V, and

ψ_i^+. The integration itself does not pose a problem since it can always be done numerically if analytic techniques fail. Expressions for ψ_f and V are no problem since the Hamiltonian was broken up so that the ψ_f's were known. The problem is how to determine ψ_i^+, the solution to the total Hamiltonian. Since we know that

$$\psi_a^{\pm} = \psi_a + \lim_{\varepsilon \to 0^+} \frac{1}{E_a - H \pm i\varepsilon} V \psi_a = \psi_a + G^+ V \psi_a ,$$

we essentially need to solve a Green's function equation. Unfortunately exact solutions for $\psi_a^{\pm}$ are not in general available, and we are forced to approximate $\psi_i^{\pm}$. One of the easiest method of approximating $\psi_i^{\pm}$ is by taking Eq. (2.31) and iterating it, which yields

$$\begin{aligned} \psi_a^{\pm} &= \psi_a + G_o^{\pm} V \psi_a + G_o^{\pm} V \, G_o^{\pm} V \psi_a + \ldots \\ &= \sum_{n=0}^{\infty} (G_o^{\pm} V)^n \psi_a \quad , \end{aligned} \tag{2.57}$$

and thus

$$T_{if} = \langle \psi_f | V | \psi_i \rangle + \langle \psi_f | V \, G_o^+ V | \psi_i \rangle + \ldots \quad .$$

If only the first (n = 0) term is retained, $\psi_a^{\pm} \simeq \psi_a$ and the result is the first Born approximation

$$T_{if}^B = \langle \psi_f | V | \psi_i \rangle \quad .$$

Since H may be split up into H_o and V in very many way there are many different expansions which have the same form as Eq. (2.57). In many cases

only the first Born approximation is calculated, primarily because higher order terms are difficult to calculate.[24] It is thus important to consider in what situations the first Born approximation is meaningful.

We can get an estimate of the validity of the first Born approximation at high energies by making a crude approximation of the second Born term,[25]

$$\langle\psi_f|VG_o^+V|\psi_i\rangle = \langle\psi_f|V\,\frac{1}{E_i - H_o + i\varepsilon}\,V|\psi_i\rangle$$

$$\simeq \frac{1}{E_i}\langle\psi_f|V^2|\psi_i\rangle \ ,$$

so that the ratio

$$\left|\frac{T_{if}^{(2)}}{T_{if}^{(1)}}\right| \approx \frac{1}{Ei}\left|\frac{\langle\psi_f|V^2|\psi_i\rangle}{\langle\psi_f|V|\psi_i\rangle}\right| \ ,$$

provides a rough estimate for the error in the first Born approximation. The expression above seems to indicate that at sufficiently high energies the ratio will become small, implying that the first Born approximation becomes adequate. It can in fact be shown that for two particle collisions the Born series converges to its first term at sufficiently high energies, however in more complicated collisions the Born series may diverge.[25,26,27]

The distorted wave Born approximation is one of many methods which have arisen in hopes of improving the Born approximation. As we mentioned in Chapter 1 the DWBA attempts to put more of the interaction into the unperturbed part of the Hamiltonian, thus making the perturbing potential (V) smaller. It is thus hoped that an iterated DWB series would converge

more rapidly than a corresponding Born series.[28]

Consider the splitting up of the total Hamiltonian H in two different ways $H = H_i + V_i = H_f + V_f$. This is particularly convenient for rearrangement collisions, where H_i is the initial unperturbed Hamiltonian and H_f is the final unperturbed Hamiltonian. From Eq. (2.27) we can write

$$\psi_i^+ = \psi_i + \lim_{\varepsilon \to 0^+} \frac{1}{E - H + i\varepsilon} (H - H_i)\psi_i \quad , \qquad (2.59)$$

and

$$\psi_f^- = \psi_f + \frac{1}{E - H - i\varepsilon} (H - H_f)\psi_f \quad , \qquad (2.60)$$

since $V_i = H - H_i$, $V_f = H - H_f$, and where $E_i = E_f = E$. Let H' be a Hamiltonian which contains the kinetic energy terms of H and perhaps some interaction terms also. Define

$$\chi_i^+ \equiv \psi_i + \frac{1}{E - H' + i\varepsilon} (H' - H_i)\psi_i \quad , \qquad (2.61)$$

$$\chi_f^- \equiv \psi_f + \frac{1}{E - H' - i\varepsilon} (H' - H_f)\psi_f \quad . \qquad (2.62)$$

Using the above two expressions, we can write

$$\psi_i^+ = \chi_i^+ + \frac{1}{E - H + i\varepsilon} (H - H_i)\psi_i - \frac{1}{E - H' + i\varepsilon} (H' - H_i)\psi_i \quad . \qquad (2.63)$$

With the operator identity, $P^{-1} = Q^{-1} + Q^{-1}(Q - P)P^{-1}$, (from Eq. (2.28(b)) we can obtain

$$\frac{1}{E - H' + i\varepsilon} = \frac{1}{E - H + i\varepsilon}\left(1 + (E - H + i\varepsilon - E + H' - i\varepsilon)\frac{1}{E - H' + i\varepsilon}\right)$$

$$= \frac{1}{E - H + i\varepsilon}\left(1 - (H - H')\frac{1}{E - H' + i\varepsilon}\right) \quad , \tag{2.65}$$

where $P = E - H' + i\varepsilon$ and $Q = E - H + i\varepsilon$. We can now use Eq. (2.65) to write ψ_i^+ as

$$\psi_i^+ = \chi_i^+ + \frac{1}{E - H + i\varepsilon}\{H - H_i - (1 - (H - H')\frac{1}{E - H' + i\varepsilon})(H' - H_i)\}\psi_i$$

$$= \chi_i^+ + \frac{1}{E - H + i\varepsilon}\{(H - H')(1 + \frac{1}{E - H' + i\varepsilon}(H' - H_i))\}\psi_i$$

$$= \chi_i^+ + \frac{1}{E - H + i\varepsilon}(H - H')\chi_i^+ \quad . \tag{2.66}$$

Similarly we can obtain

$$\psi_f^- = \chi_f^- + \frac{1}{E - H - i\varepsilon}(H - H')\chi_f^- \quad . \tag{2.67}$$

We now have

$$T_{if} = \langle\psi_f|V_f|\psi_i^+\rangle = \langle\psi_f|H - H_f|\psi_i^+\rangle \quad , \tag{2.68a}$$

$$= \langle\psi_f^-|H - H_i|\psi_i\rangle \tag{2.68b}$$

and we define

$$T'_{if} \equiv \langle \psi_f | H' - H_f | \chi_i^+ \rangle \quad , \tag{2.69a}$$

$$\equiv \langle \chi_f^- | H' - H_i | \psi_i \rangle \quad , \tag{2.69b}$$

so that

$$T_{if} - T'_{if} = \langle \psi_f | H - H_f | \psi_i^+ \rangle - \langle \psi_f | H' - H_f | \chi_i^+ \rangle$$

$$= \langle \psi_f | H - H_f | \chi_i^+ \rangle + \langle \psi_f | (H - H_f) \frac{1}{E - H + i\varepsilon} (H - H') \chi_i^+ \rangle - \langle \psi_f | H' - H_f | \chi_i^+ \rangle$$

$$= \langle \psi_f | H - H' | \chi_i^+ \rangle + \langle \psi_f | (H - H_f) \frac{1}{E - H + i\varepsilon} (H - H') | \chi_i^+ \rangle$$

$$= \left\langle \left(1 + \frac{1}{E - H - i\varepsilon} (H - H_f) \right) \psi_f | (H - H') \chi_i^+ \right\rangle$$

$$= \langle \psi_f^- | (H - H') | \chi_i^+ \rangle \quad . \tag{2.70}$$

Finally, we can write

$$T_{if} = T'_{if} + \langle \psi_f^- | H - H' | \chi_i^+ \rangle \quad . \tag{2.71a}$$

Similarly from the alternate Eqs. (2.68(b)) and (2.69(b)), we get

$$T_{if} = T'_{if} + \langle \chi_f^- | H - H' | \psi_i^+ \rangle \quad , \tag{2.71b}$$

so that

$$\langle \psi_f^- | H - H' | \chi_i^+ \rangle = \langle \chi_f^- | H - H' | \psi_i^+ \rangle \quad .$$

Now suppose we split up the Hamiltonian into three pieces $H = H_i + U_i + W_i = H_f + U_f + W_f$, where H_i and H_f are the unperturbed Hamiltonians and U_i and U_f are arbitrary potentials, and define

$$H' = H_i + U_i \quad . \tag{2.72a}$$

With the above choices, we have

$$T_{if} = \langle\psi_f|H' - H_f|\chi_i^+\rangle + \langle\psi_f^-|H - H'|\chi_i^+\rangle$$

$$= \langle\psi_f|H_f + V_f - W_i - H_f|\chi_i^+\rangle + \langle\psi_f^-|H - H'|\chi_i^+\rangle$$

$$= \langle\psi_f|V_f - W_i|\chi_i^+\rangle + \langle\psi_f^-|W_i|\chi_i^+\rangle \quad . \tag{2.73a}$$

If we alternatively define

$$H' = H_f + U_f \tag{2.72b}$$

we derive in the same manner

$$T_{if} = \langle\chi_f^-|V_i - W_f|\psi_i\rangle + \langle\chi_f^-|W_f|\psi_i^+\rangle \quad . \tag{2.73b}$$

These are exact expressions for T_{if}, but once again we have expressions containing a solution to the total Hamiltonian (ψ_f^-, ψ_i^+) which in most cases is not known exactly. The DWBA is achieved by approximating ψ_f^- by χ_f^-, which yields

$$T_{if}^{DWB} = \langle \psi_f | V_f - W_i | \chi_i^+ \rangle + \langle \chi_f^- | W_i | \chi_i^+ \rangle \quad , \tag{2.74a}$$

or using the alternate forms we obtain

$$T_{if}^{DWB} = \langle \chi_f^- | V_i - W_f | \psi_i \rangle + \langle \chi_f^- | W_f | \chi_i^+ \rangle \tag{2.74b}$$

where we have approximated ψ_i^+ by χ_i^+. As in the Born approximation we can derive an iterated series to get a DWBA expansion

$$\psi_i^{\pm} = \sum_{n=0}^{\infty} [G'^{\pm}(H - H')]^n \chi_i^{\pm} \quad , \tag{2.75}$$

where $G'^{\pm} = \dfrac{1}{E - H' \pm i\varepsilon}$. Equation (2.75) is the DWB series for both forms of T_{if}^{DWB}, but it must be remembered that for Eq. (2.74(b)) H' and χ are not the same as the H' and χ in (2.74(a)).

As in the Born approximation the convergence of the DWB series is a sufficient condition that $T_{if}^{DWB} \to T_{if}$. Arguments similar to those used for the Born approximation lead us to believe that the DWBA is a high energy approximation which works best for small perturbing potentials. In fact, since the perturbing potential used in the DWBA is smaller than in the corresponding Born calculation, we expect that the DWBA series converges more rapidly than the Born series. However, the basic convergence problems of the Born approximation are retained in the DWBA.[29,30]

In the next chapter we will apply the approximations explained here to the particular problem of high energy electrons incident on hydrogenic atoms, which will also serve to illustrate the utility of the theory presented here.

CHAPTER 3

APPLICATIONS

In this chapter we take the general results of the theory presented in Chapter 2 and apply them specifically to the problem at hand by writing out the Hamiltonian and choosing U_i and U_f. Once the particular form of T_{if}^{DWB} is determined, it is then manipulated algebraically and put into a form which is usable by the computer. The computer code is then discussed, and finally the momentum transfer cross section is defined.

The Hamiltonian for the interaction between an incident particle Z_a and a hydrogenic atom with atomic number Z_b is given (in the center of mass) by[2,6] (See Fig. 3).

$$H = -\frac{1}{2}\nabla_R^2 + \frac{Z_a Z_b}{R} - \frac{1}{2}\nabla_b^2 - \frac{Z_b}{r_b} - \frac{Z_a}{r_a} \quad , \tag{3.1}$$

where $-\frac{1}{2}\nabla_R^2$ is the projectile kinetic energy,

$\frac{Z_a Z_b}{R}$ is the projectile-nucleus interaction,

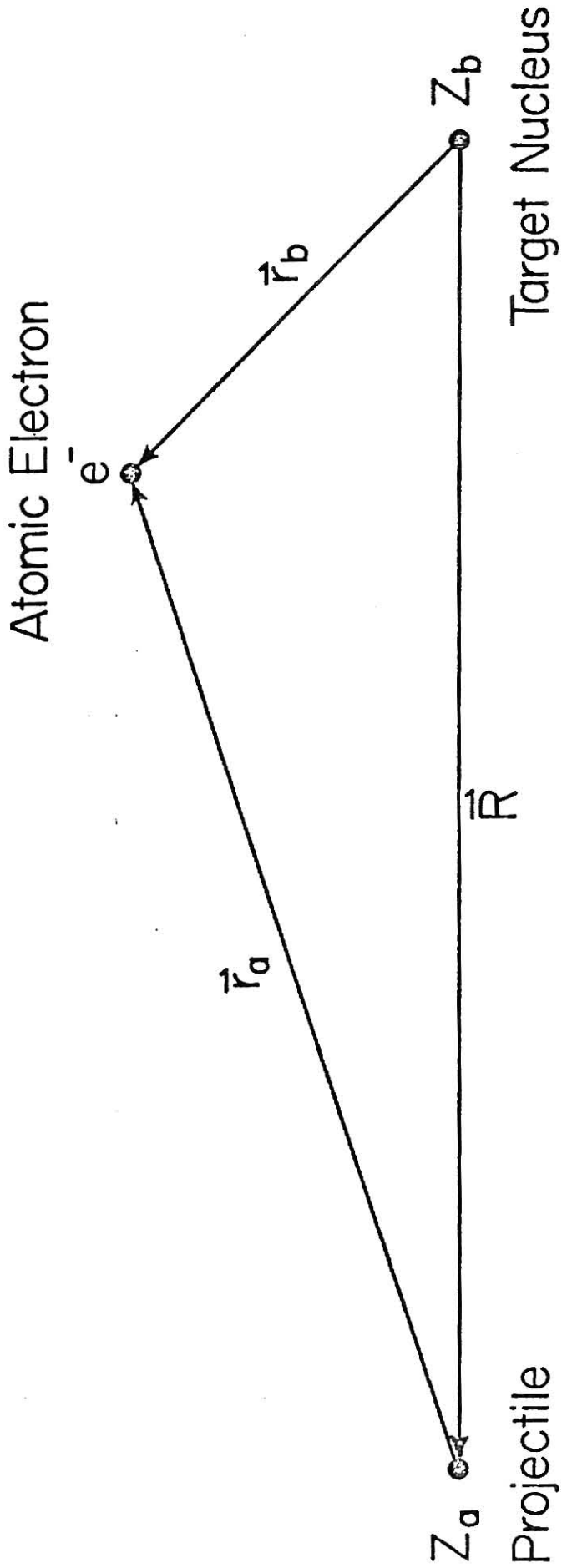
$-\frac{1}{2}\nabla_b^2$ is the (atomic) electron kinetic energy,

$-\frac{Z_b}{r_b}$ is the interaction between the atomic electron and the nucleus,

and $-\frac{Z_a}{r_a}$ is the interaction between the projectile and the atomic electron. Recall that in our previous discussion the choice of U_i and U_f were nearly

Figure 3.

Diagram depicting the radial variables, and notation used for the three particles.


Atomic Electron
e^-
$\vec{r}_b$
Z_b
Target Nucleus
$\vec{R}$
$\vec{r}_a$
Z_a
Projectile

arbitrary, we now take advantage of the arbitrariness to choose U_f in a manner which causes one of the terms in the two potential formula to vanish. We define

$$H_i = H_f = -\frac{1}{2}\nabla_R^2 - \frac{1}{2}\nabla_b^2 - \frac{Z_b}{r_b} \quad , \tag{3.2}$$

$$U_i = 0 \quad , \quad W_i = \frac{Z_a Z_b}{R} - \frac{Z_a}{r_a} \quad , \tag{3.3}$$

$$U_f = \frac{Z_a Z_b}{R} \quad , \quad W_f = -\frac{Z_a}{r_a} \quad . \tag{3.4}$$

With the choices above Eq. (2.74(b)) becomes

$$\begin{aligned} T_{if}^{DWB} &= \langle \chi_f^- | V_i - W_f | \psi_i \rangle + \langle \chi_f^- | W_f | \chi_i^+ \rangle \\ &= \langle \chi_f^- | \frac{Z_a Z_b}{R} | \psi_i \rangle + \langle \chi_f^- | -\frac{Z_a}{r_a} | \chi_i^+ \rangle \quad , \end{aligned} \tag{3.5}$$

and where

$$H_i \psi_i = E\psi_i \quad , \quad H_f \psi_f = E\psi_f \quad , \tag{3.6}$$

$$(H_i + U_i)\chi_i = E\chi_i = H_i \chi_i \quad , \tag{3.7}$$

$$(H_f + U_f)\chi_f = E\chi_f \quad . \tag{3.8}$$

Thus ψ_i, ψ_f and χ_i consist of a plane wave times a bound state hydrogenic wave function[6], and χ_f satisfies the following differential equation

$$(-\frac{1}{2}\nabla_R^2 - \frac{1}{2}\nabla_b^2 - \frac{Z_b}{r_b} + \frac{Z_a Z_b}{R})\chi_f^- = E\chi_f^- \quad , \tag{3.9}$$

whose solution is a hydrogenic wave function times a Coulomb wave function[2]

$$\chi_f^-(\vec{R},\vec{r}_b) = \psi_{2S}(r_b)\chi_f^-(\vec{R})$$

$$= \psi_{2S}(r_b)e^{i\vec{k}_f\cdot\vec{R}} e^{-\frac{\pi\alpha}{2}} \Gamma(1 - i\alpha)\,{}_1F_1[i\alpha,1,-i(k_fR+\vec{k}_f\cdot\vec{R})] \quad , \tag{3.10}$$

where $\alpha \equiv \frac{Z_a Z_b}{k_f}$, and $\psi_{2S}(r_b) = \frac{Z_b^{3/2}}{2\sqrt{2\pi}}[1 - \frac{Z_b r_b}{2}]e^{-\frac{Z_2 r_b}{2}}$.

We can also write out χ_i^+ as

$$\chi_i^+ = e^{i\vec{k}_i\cdot\vec{R}}\psi_{1S} = e^{i\vec{k}_i\cdot\vec{R}}(\frac{Z_b^{3/2}}{\sqrt{\pi}})\, e^{-Z_b r_b} \quad . \tag{3.11}$$

For convenience of notation we define

$$\vec{q} = \vec{k}_i - \vec{k}_f \quad , \qquad \lambda = 3/2\ Z_b \quad , \tag{3.12}$$

so that we can write T_{if}^{DWB} as

$$T_{if}^{DWB} = \langle\chi_f^-|\frac{Z_a Z_b}{R}|\psi_i\rangle + \langle\chi_f^-|W_f|\chi_i^+\rangle$$

$$= \langle\psi_{2S}(r_b)\chi_f^-(\vec{R})|\frac{Z_a Z_b}{R}|e^{i\vec{k}_i\cdot\vec{R}}\psi_{1S}(r_b)\rangle + \langle\chi_f^-|W_f|\chi_i^+\rangle$$

$$= \langle\chi_f^-|W_f|\chi_i^+\rangle \quad ,$$

since the integration over $\vec{r}_b$ in the first term vanishes due to orthogonality. Thus noting in Eq. (3.3) that $U_i = 0$ corresponding to a projectile plane wave we have

$$T_{if}^{DWB} = C \int d\vec{r} \int d\vec{R}\, e^{i\vec{q}\cdot\vec{R}-\lambda r_b} \left(\frac{1}{r_a}\right) {}_1F_1[-i\alpha,1,i(k_f R+\vec{k}_f\cdot\vec{R})]\left[1-\frac{Z_b r_b}{2}\right] , \quad (3.13)$$

where $C = \dfrac{Z_b{}^3 Z_a}{2\pi\sqrt{2}}\, e^{-\pi\alpha/2}\Gamma(1+i\alpha)$, and where the $d\vec{r}$ integration can either be over $d\vec{r}_a$ or $d\vec{r}_b$. Note that if we set $\alpha=0$, then $\chi_f^-(\vec{R}) = e^{i\vec{k}_f\cdot\vec{R}}$ and thus $T_{if}^{DWB} \xrightarrow[\alpha\to 0]{} T_{if}^{B}$. This gives us a convenient means for calculating the Born approximation. We can write Eq. (3.13) as

$$T_{if}^{DWB} = \frac{Z_b{}^3 Z_a}{2\pi\sqrt{2}}\, e^{-\frac{\pi\alpha}{2}}\, \Gamma(1+i\alpha)\left[1+\frac{Z_b}{2}\frac{\partial}{\partial\lambda}\right] I(\lambda,\vec{q}), \quad (3.14)$$

where

$$I(\lambda,\vec{q}) = \int d\vec{r} \int d\vec{R}\, e^{i\vec{q}\cdot\vec{R}} \left(\frac{1}{r_a}\right) e^{-\lambda r_b}\, {}_1F_1[-i\alpha,1,i(k_f R+\vec{k}_f\cdot\vec{R})]. \quad (3.15)$$

Thus calculating T_{if}^{DWB} is reduced to the problem of doing the $d\vec{r}$ and $d\vec{R}$ integrations. The problem is that there are three interrelated vectors ($\vec{R}$, $\vec{r}_a$, $\vec{r}_b$) only two of which are linearly independent. However, if we can choose a coordinate system such that the volume element $d\vec{r}$ contains an r_a term, the r_a dependence would be cancelled out, and the integration would be made easier. Consider the equations of transformation to ellipsoidal coordinates[31,32]

$$r_a = \frac{R}{2}(\varepsilon+\eta) \quad , \quad r_b\sin\theta_b = \frac{R}{2}\left[(\varepsilon^2-1)(1-\eta^2)\right]^{1/2} \quad ,$$

$$r_b = \frac{R}{2}(\varepsilon-\eta) \quad , \quad r_b\cos\theta_b = \frac{R}{2}\left[\varepsilon\eta-1\right] \quad ,$$

$$1 \le \varepsilon \le \infty \quad , \quad -1 \le \eta \le 1 \quad ,$$

$$d\vec{r} = \frac{R}{2} r_a r_b\, d\varepsilon\, d\eta\, d\theta \quad ,$$

then

$$I(\lambda,\vec{q}) = \int d\vec{R} e^{i\vec{q}\cdot\vec{R}} {}_1F_1[-i\alpha,1,i(k_f R+\vec{k}_f\cdot\vec{R})\ \frac{R^2}{4}\int (\varepsilon-\eta)e^{\frac{-\lambda R(\varepsilon-\eta)}{2}} d\varepsilon\ d\eta\ d\phi$$

$$= \frac{\pi}{2}\int d\vec{R} e^{i\vec{q}\cdot\vec{R}} {}_1F_1[-i\alpha,1,i(k_f R+\vec{k}_r\cdot\vec{R})]R^2\int (\varepsilon-\eta)e^{\frac{-\lambda R(\varepsilon-\eta)}{2}} d\varepsilon\ d\eta. \quad (3.16)$$

We choose to do the ε integration first so we are faced with two integrals of the form

$$\int_1^\infty \varepsilon\ e^{\frac{-\lambda R\varepsilon}{2}} d\varepsilon = \frac{2e^{-R/2}}{\lambda R}\left(1+\frac{2}{\lambda R}\right), \quad (3.17)$$

and

$$\int_1^\infty e^{\frac{-\lambda R\varepsilon}{2}} d\varepsilon = \frac{2e^{-\lambda R/2}}{\lambda R}. \quad (3.18)$$

Substituting Eqs. (3.17) and (3.18) into Eq. (3.16) yields

$$I(\lambda,\vec{q}) = \frac{\pi}{2}\int d\vec{R}\ e^{i\vec{q}\cdot\vec{R}}\ R^2\ {}_1F_1[-i\alpha,1,i(k_f R+\vec{k}_f\cdot\vec{R})]\int_{-1}^{1} d\eta\ \frac{2e^{\frac{-\lambda R(1-\eta)}{2}}}{\lambda R}\left[1+\frac{2}{R}-\eta\right].$$

The η integrals have the form

$$\int_{-1}^{1} \eta\ d\eta\ e^{\lambda R\eta/2} = \frac{2}{\lambda R}\left[e^{\lambda R/2}\left(1-\frac{2}{\lambda R}\right)+e^{-\lambda R/2}\left(1+\frac{2}{\lambda R}\right)\right], \quad (3.19)$$

and

$$\int_{-1}^{1} d\eta\ e^{\lambda R\eta/2} = \frac{2}{\lambda R}\left[e^{\lambda R/2}-e^{-\lambda R/2}\right], \quad (3.20)$$

so that

$$I(\lambda,\vec{q}) = \frac{2\pi}{\lambda^2}\int d\vec{R}\, e^{i\vec{q}\cdot\vec{R}}\,{}_1F_1[-i\alpha,1,i(k_fR+\vec{k}_f\cdot\vec{R})][(1+\frac{2}{\lambda R})(1-e^{-\lambda R})-(1-\frac{2}{\lambda R})-e^{-\lambda R}(1+\frac{2}{\lambda R})]$$

$$= \frac{2\pi}{\lambda^2}\int d\vec{R}\, e^{i\vec{q}\cdot\vec{R}}\,{}_1F_1[-i\alpha,1,i(k_fR+\vec{k}_f\cdot\vec{R})][\frac{4}{\lambda R} - e^{-\lambda R}(2+\frac{4}{\lambda R})] \quad . \quad (3.21)$$

We can write $I(\lambda,\vec{q})$ in a particularly convenient form using[33,34]

$$J \equiv \int \frac{e^{-\omega R}}{R}\, e^{i\vec{q}\cdot\vec{R}}\,{}_1F_1[-i\alpha,1,i(k_fR+\vec{k}_f\cdot\vec{R})]d\vec{R}$$

$$= \frac{4\pi}{(\omega^2+q^2)^{1+i\alpha}}\,[k_i^2 - k_f^2 - 2i\omega k_f + \omega^2]^{i\alpha} \quad , \quad (3.21)$$

and noting that

$$\frac{dJ}{d\omega} = 4\pi\left[\frac{-2\omega(1+i\alpha)}{(\omega^2+q^2)} + \frac{i\alpha(2\omega - 2ik_f)}{(k_i^2-k_f^2-2i\omega k_f+\omega^2)}\right]\frac{(k_i^2-k_f^2-2i\omega k_f+\omega^2)^{i\alpha}}{(\omega^2+q^2)^{1+i\alpha}} \quad , (3.22)$$

so that we can write

$$I(\lambda,\vec{q}) = \frac{2\pi}{\lambda^2}\left[\frac{4}{\lambda}(J(\omega=0) - J(\omega=\lambda)) + 2\,\frac{\partial J}{\partial\omega}\Big|_{\omega=\lambda}\right] \quad . \quad (3.23)$$

Substituting Eqs. (3.21) and (3.22) into Eq. (3.23), we obtain

$$I(\lambda,\vec{q}) = \left[\frac{4\pi}{\lambda}\right]^2\left[\frac{2}{\lambda}(CA) + 2(CB)(CC)\right] \quad , \quad (3.24)$$

where

$$CA = \frac{(k_i^2 - k_f^2)^{i\alpha}}{q^2 + 2i\alpha} - \frac{(k_i^2 - k_f^2 - 2i\lambda k_f + \lambda^2)^{i\alpha}}{(\lambda^2 + q^2)^{1 + i\alpha}} ,$$

$$CB = (\lambda^2 + q^2)^{-1-i\alpha}(k_i^2 - k_f^2 - 2i\lambda k_f + \lambda^2)^{i\alpha} ,$$

$$CC = \frac{-(1 + i\alpha)\lambda}{\lambda^2 + q^2} + \frac{i\alpha(\lambda - ik_f)}{k_i^2 - k_f^2 - 2i\lambda k_f + \lambda^2} .$$

Recall from Eq. (3.14) that T_{if}^{DWB} is given by

$$T_{if}^{DWB} = \frac{Z_b^3 Z_a}{2\pi\sqrt{2}} e^{-\pi\alpha/2} \Gamma(1 + i\alpha) \left[1 + \frac{Z_b}{2} \frac{\partial}{\partial\lambda}\right] I(\lambda,\vec{q}) .$$

Since the expression for the differential cross section contains $|T_{if}^{DWB}|^2$, we square the above expression, to obtain

$$|T_{if}^{DWB}|^2 = \frac{Z_b^6 Z_a^2}{8\pi^2} e^{-\pi\alpha} |\Gamma(1 + i\alpha)|^2 \left|\left[1 + \frac{Z_b}{2} \frac{\partial}{\partial\lambda}\right] I(\lambda,\vec{q})\right|^2$$

$$= \frac{Z_b^6 Z_a^2}{8\pi^2} e^{-\pi\alpha} \frac{\pi\alpha}{\sinh\pi\alpha} \left|\left[1 + \frac{Z_b}{2} \frac{\partial}{\partial\lambda}\right] I(\lambda,\vec{q})\right|^2 , \qquad (3.25)$$

since[35] $|\Gamma(1 + i\alpha)|^2 = \pi\alpha/\sinh(\pi\alpha)$.

Equation (3.25) is the expression that we wish to evaluate on the computer. To get the differential cross section we just need to multiply $|T_{if}^{DWB}|^2$ by $(u^2 k_f/4\pi^2 k_i)$, and we can then get the total cross section by numerical integration. However, the form of Eq. (3.25) must be modified so that it can be conveniently programmed. The expression for $I(\lambda,\vec{q})$ is complicated and must be broken down into bite sized chunks, which will contain complex numbers taken to complex powers. A complex number is

stored in the computer as an ordered pair (i.e. a+ib → (a,b)) so that the complex terms must be written in a form such that the real and imaginary parts are evident. An easy way of doing this is to express each complex term as an exponential, $e^{a}e^{i\theta}$ where a and θ are real, then the real and imaginary parts are easily determined. This solves the problem of having to take a complex number to a complex power since

$$(e^{a}e^{i\theta})^{1 + i\alpha} = e^{a-\theta\alpha}\ e^{i(a\alpha + \theta)} \quad .$$

We must also determine an expression for $\frac{\partial I(\lambda,\vec{q})}{\partial \lambda}$. The three above mentioned steps are simple but tedious, and I will thus not display them here. The appendix, which contains a copy of the coding used in the program, also contains Eq. (3.25) in its computer digestible form.

The computer code consists of two parts, a subprogram which computes $|T_{if}|^2$ and a main program which does the numerical integration. The numerical integration technique used is that of Gauss Legendre quadrature using five weighting factors.[36,37] The program was checked out by comparing our results with those of Junker, Geltman and Hidalgo.

Once we have a program for $\frac{d\sigma}{d\Omega}$ it is easy to compute a higher moment of the cross section such as the momentum transfer cross section. The momentum transfer differential cross section is defined by

$$\frac{d\sigma_M}{d\Omega} \equiv (1 - \frac{k_f}{k_i}\cos\theta)\ \frac{d\sigma}{d\Omega} \quad , \tag{3.26}$$

where θ is the scattering angle, and the total momentum transfer cross section is given by

$$\sigma_M = \int_{4\pi} (1 - \frac{k_f}{k_i} \cos\theta) \frac{d\sigma}{d\Omega} \, d\Omega \quad . \tag{3.27}$$

It is clear that $\frac{d\sigma_M}{d\Omega}$ is just the change in the Z-component of momentum of the projectile (normalized to k_i) times the differential cross section. As we mentioned in Chapter 1, the effect of the $(1 - (k_f/k_i)\cos\theta)$ term is to amplify $\frac{d\sigma}{d\Omega}$ at large angles. This can be easily seen by looking at the two extremes, $\theta \simeq 0°$, $\theta \simeq 180°$, for if $\theta \simeq 0°$, then $(1 - \frac{k_f}{k_i} \cos\theta) \simeq 1 - \frac{k_f}{k_i} \simeq 0$, and if $\theta \simeq 180°$, then $(1 - \frac{k_f}{k_i} \cos\theta) \simeq 1 + \frac{k_f}{k_i} \simeq 2$. This is why momentum transfer cross sections provide a good testing ground for comparison of σ^{DWBA} and σ^{Born}. Momentum transfer cross sections appear in the calculation of various plasma transport properties such as diffusion and electrical conductivity, and may thus be useful in plasma physics.[9,10]

CHAPTER 4

RESULTS

Our motivation for using the DWBA is that the Born approximation does not yield correct angular distributions. Figure 2 (Chap. 1) shows that $d\sigma^{Born}/d\Omega$ is several orders of magnitude too low at large angles (for 200 eV incident energy). Physically we expect large angle scattering to be caused by collisions between the projectile electron and the nucleus, but the projectile-nucleus interaction does not contribute in the Born approximation due to orthogonal initial and final states. We are thus led to the DWB calculation in which the projectile-nucleus interaction is treated in the unperturbed part of the problem. As expected, Fig. 2 shows that $d\sigma^{DWBA}/d\Omega$ provides a better fit to the data at large angles. Figures 4 and 5 show how the Born and DWB angular distributions change with projectile energy. (Note that Z = 1 since we are presently considering only hydrogen targets). In both figures the curves tend to become more sharply peaked around $\theta = 0^{o}$, as the projectile energy increases. As the projectile velocity is increased it is deflected through a smaller angle. Figure 6 is a plot of σ^{Born} and σ^{DWBA} as a function of the scaled energy $E_{inc}/|E_{2S} - E_{1S}|$. ($|E_{2S} - E_{1S}| = 10.2$ eV). The DWBA and Born curves both approach the same high energy limit, but they have very different low energy behavior. This is because in the DWB calculation the projectile-nucleus interaction is treated in the unperturbed part of the problem so that the nuclear Coulomb potential is effective very far away from the nucleus. Figure 6 shows that

Figure 4.

Born differential cross sections for (1S-2S) excitation of hydrogenic atoms by electron impact at various energies.

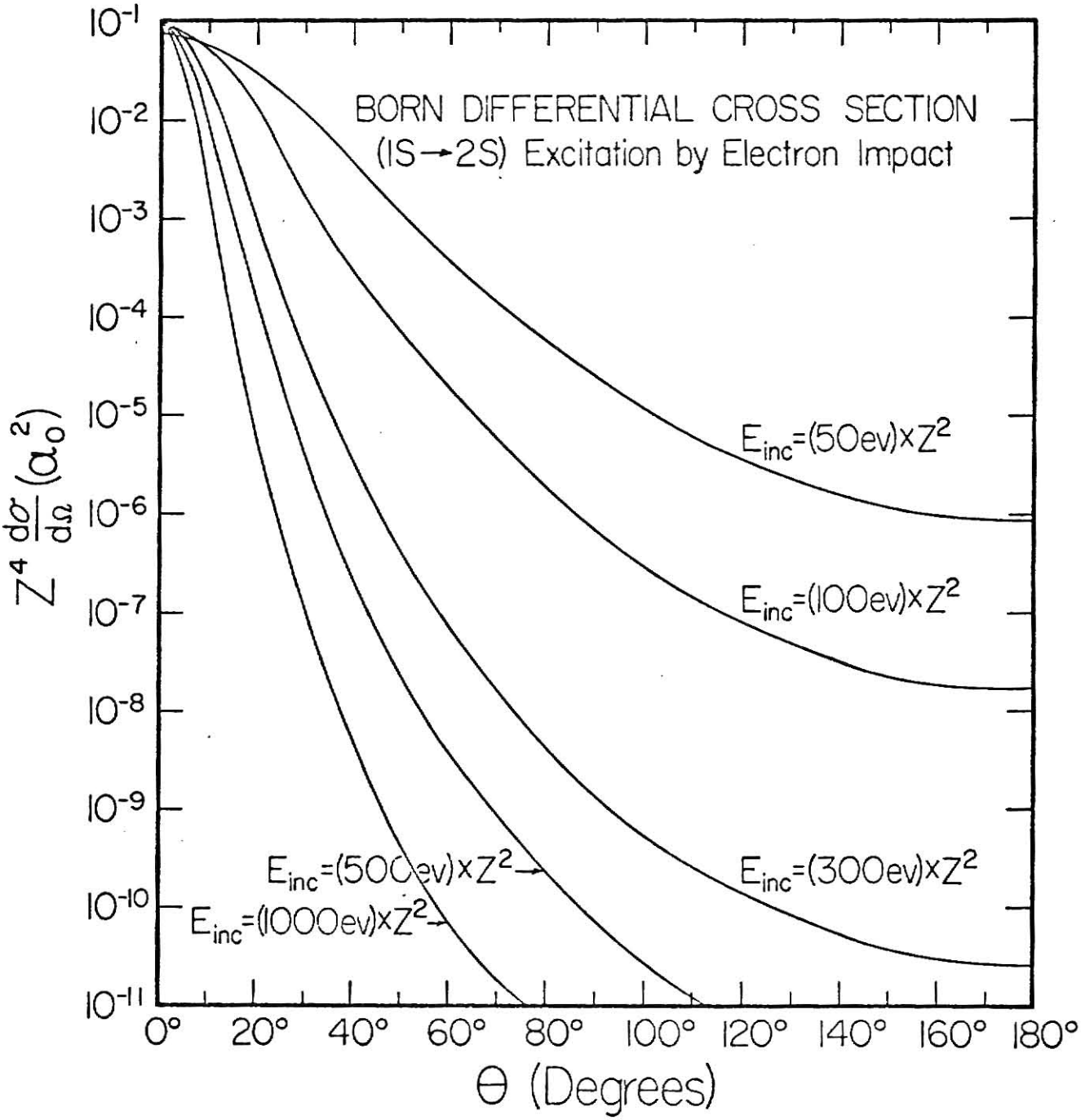

BORN DIFFERENTIAL CROSS SECTION
(1S→2S) Excitation by Electron Impact
E_{inc}=(50ev)×Z^2
E_{inc}=(100ev)×Z^2
E_{inc}=(300ev)×Z^2
E_{inc}=(500ev)×Z^2
E_{inc}=(1000ev)×Z^2
$Z^4 \frac{d\sigma}{d\Omega} (a_o^2)$
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
10^{-8}
10^{-9}
10^{-10}
10^{-11}
0° 20° 40° 60° 80° 100° 120° 140° 160° 180°
Θ (Degrees)

Figure 5.

DWB differential cross sections for (1S-2S) excitation of hydrogenic atoms by electron impact at various energies.

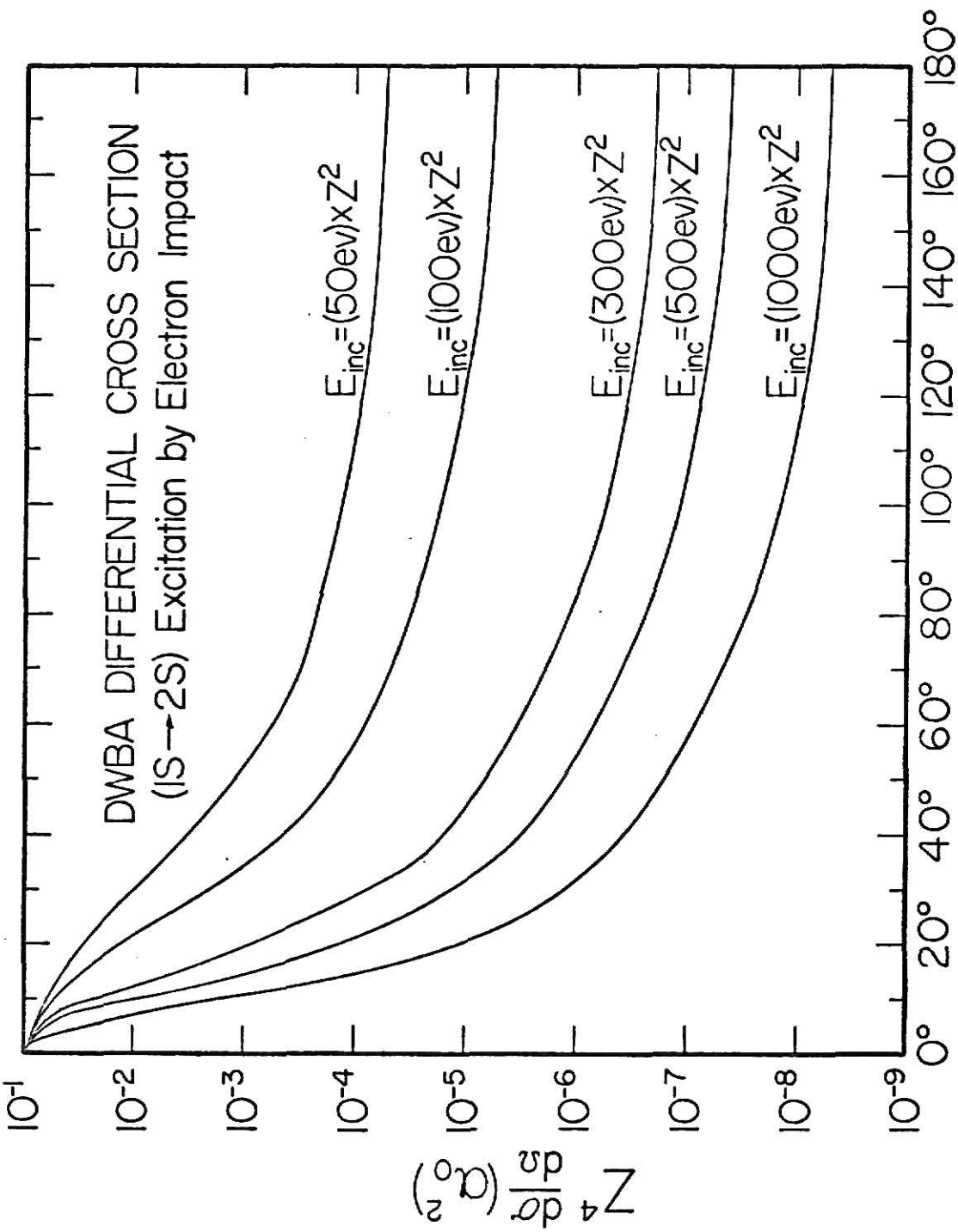
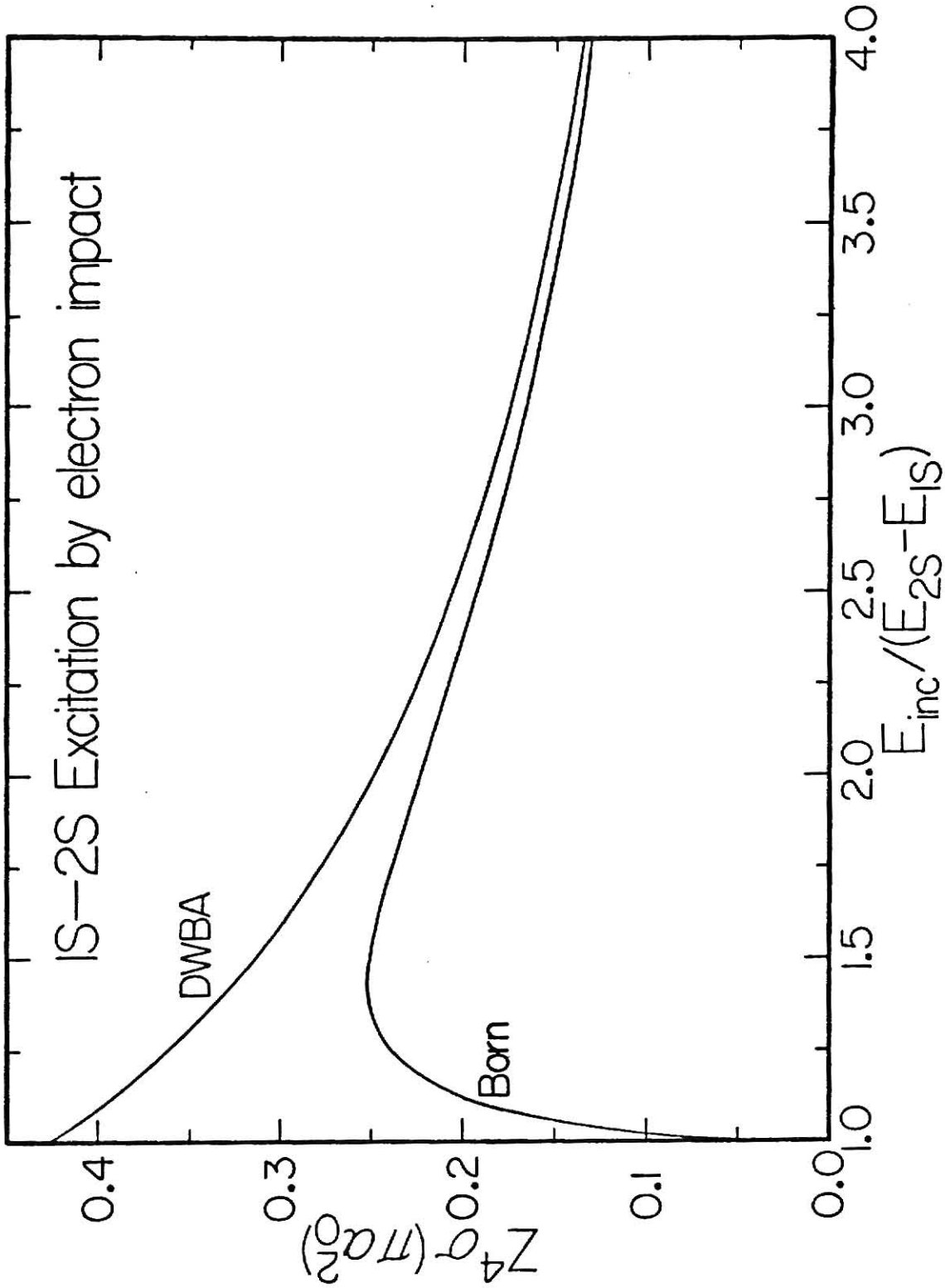

DWBA DIFFERENTIAL CROSS SECTION
(1S→2S) Excitation by Electron Impact
E_{inc}=(50ev)xZ²
E_{inc}=(100ev)xZ²
E_{inc}=(300ev)xZ²
E_{inc}=(500ev)xZ²
E_{inc}=(1000ev)xZ²
$Z^4 \frac{d\sigma}{d\Omega}(a_o^2)$
10⁻¹
10⁻²
10⁻³
10⁻⁴
10⁻⁵
10⁻⁶
10⁻⁷
10⁻⁸
10⁻⁹
0°
20°
40°
60°
80°
100°
120°
140°
160°
180°
Θ (Degrees)

Figure 6.

Total Born and DWB cross sections for (1S-2S) excitation of hydrogenic atoms by electron impact as a function of the scaled energy $E_{inc}/|E_{2S} - E_{1S}|$.


1S–2S Excitation by electron impact
DWBA
Born
$Z^4\sigma/(\pi a_0^2)$
$E_{inc}/(E_{2S}-E_{1S})$
0.0
0.1
0.2
0.3
0.4
1.0
1.5
2.0
2.5
3.0
3.5
4.0

despite the large differences between Born and DWB angular distributions, the total cross sections agree to within 10% at incident energies greater than 25 eV. The reason for this is that the vertical scale in Fig. 2 is sharply logarithmic and thus most of the total cross section is summed up in the first few degrees where the Born and DWB approximations agree. If the difference between Born and DWB is to be seen, the contribution from large angles must be more heavily weighted than the contribution from small angles. In the last chapter, we saw that the effect of the $(1 - \frac{k_f}{k_i}\cos\theta)$ term in the momentum transfer cross section was to weight large angles more heavily. Figures 7 and 8 are plots of the differential cross sections and differential momentum transfer cross sections in the Born and DWB approximations at 100 eV and 500 eV respectively. From these two figures we can see the enhancement at large angles in the momentum transfer cross section. The limiting values of $\frac{d\sigma_M}{d\Omega}$ $(\theta \to 0^o)$ are much less than $\frac{d\sigma}{d\Omega}$ $(\theta \to 0^o)$ so that the total momentum transfer cross sections will also be smaller than the corresponding total cross sections. We note that as the projectile energy increases the momentum transfer differential cross sections also tend to be more peaked, for the same reason as above.

In plasma physics it is the total momentum transfer cross section which is useful. We thus wish to compare DWB and Born total momentum transfer cross sections, and note any differences. Figure 9 shows how the momentum transfer cross sections (DWB and Born) vary with the scaled energy $E_{inc}/|E_{2S} - E_{1S}|$. Figure 9 has the same general shape as Fig. 6 (total cross section), but the momentum transfer curves have a smaller amplitude. In order to compare the DWB and Born calculations more

Figure 7.

Differential cross sections and momentum transfer cross sections in the Born and DWB approximations for (1S-2S) excitation of hydrogenic atoms by electron impact at 100 eV. The dashed curves are for the momentum transfer cross sections.

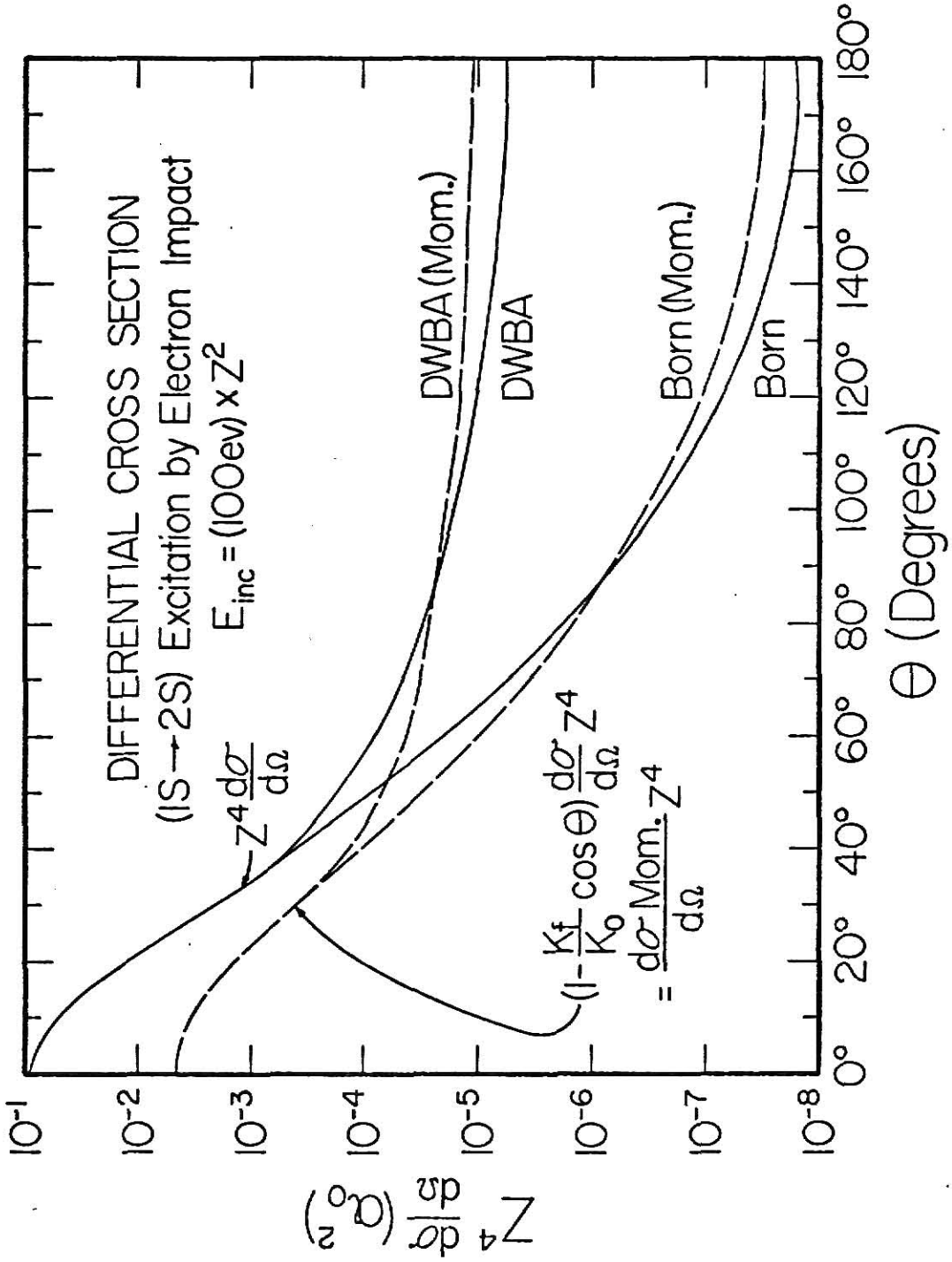

DIFFERENTIAL CROSS SECTION
(1S→2S) Excitation by Electron Impact
E_{inc} = (100ev) x Z^2
$Z^4 \frac{d\sigma}{d\Omega}$
DWBA (Mom.)
DWBA
Born (Mom.)
Born
$(1-\frac{K_f}{K_o}\cos\theta)\frac{d\sigma}{d\Omega}Z^4$
$= \frac{d\sigma\ \text{Mom.}}{d\Omega} Z^4$
$Z^4 \frac{d\sigma}{da}(a_o^2)$
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
10^{-8}
0°
20°
40°
60°
80°
100°
120°
140°
160°
180°
Θ (Degrees)

Figure 8.

Differential cross sections and momentum transfer cross sections in the Born and DWB approximations for (1S-2S) excitation of hydrogenic atoms by electron impact at 500 eV. The dashed curves are for the momentum transfer cross sections.

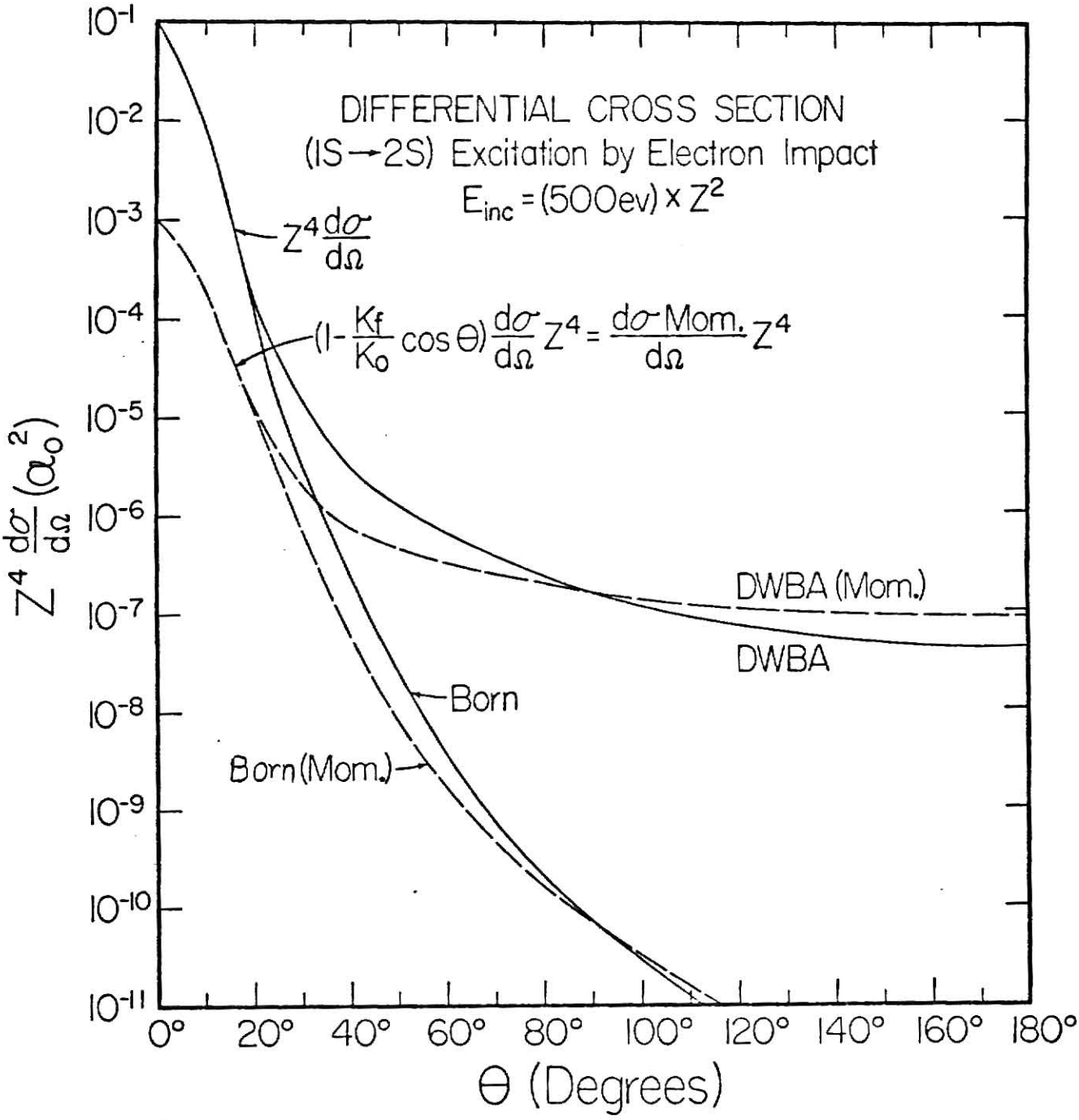
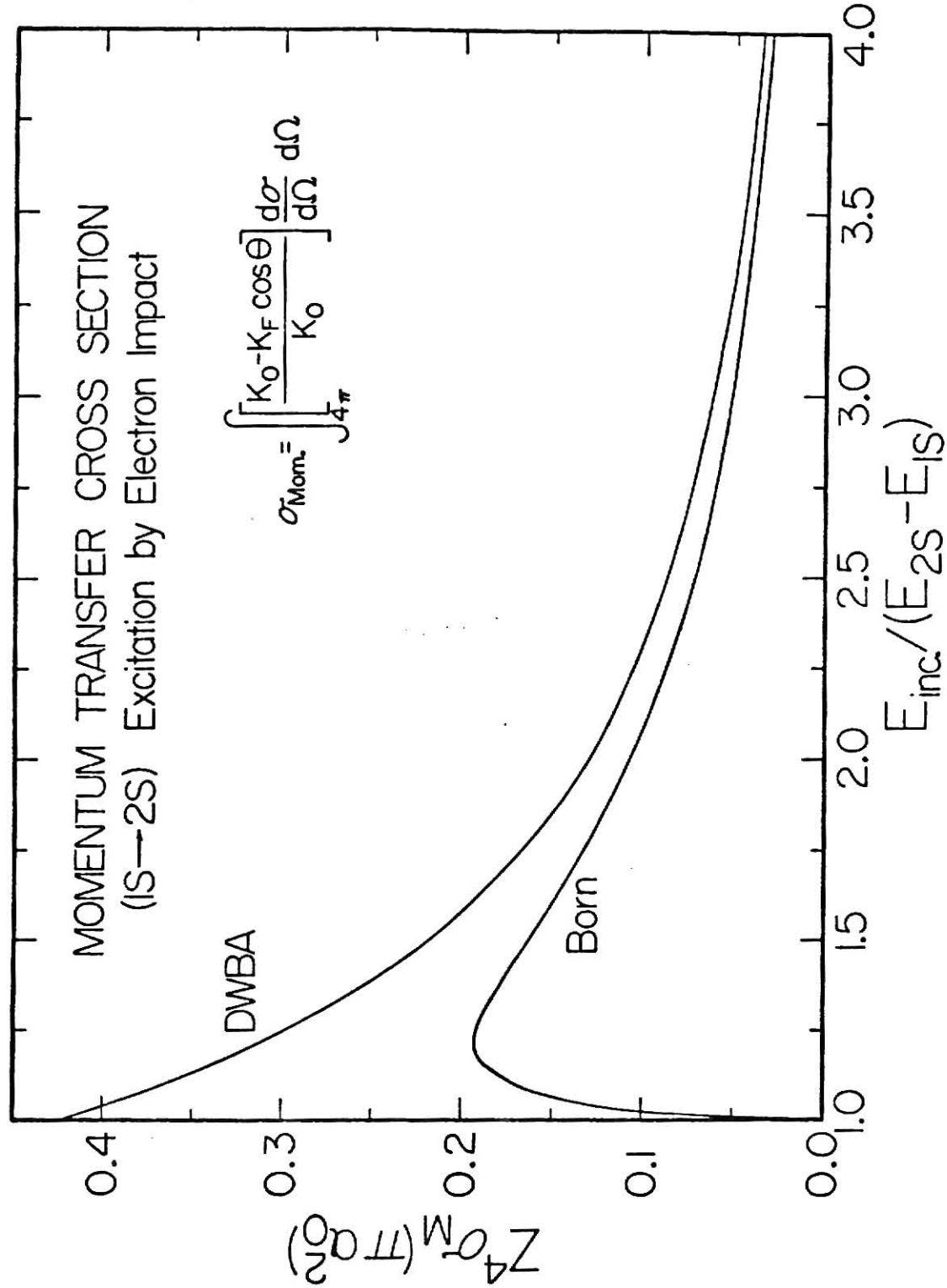

DIFFERENTIAL CROSS SECTION
(1S→2S) Excitation by Electron Impact
$E_{inc} = (500ev) \times Z^2$
$Z^4 \frac{d\sigma}{d\Omega}$
$(1 - \frac{K_f}{K_o} \cos\theta) \frac{d\sigma}{d\Omega} Z^4 = \frac{d\sigma_{Mom.}}{d\Omega} Z^4$
DWBA (Mom.)
DWBA
Born
Born (Mom.)
$Z^4 \frac{d\sigma}{d\Omega} (a_o^2)$
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
10^{-8}
10^{-9}
10^{-10}
10^{-11}
0°
20°
40°
60°
80°
100°
120°
140°
160°
180°
θ (Degrees)

Figure 9.

Total Born and DWB momentum transfer cross sections for (1S-2S) excitation of hydrogenic atoms by electron impact as a function of the scaled energy $E_{inc}/|E_{2S} - E_{1S}|$.

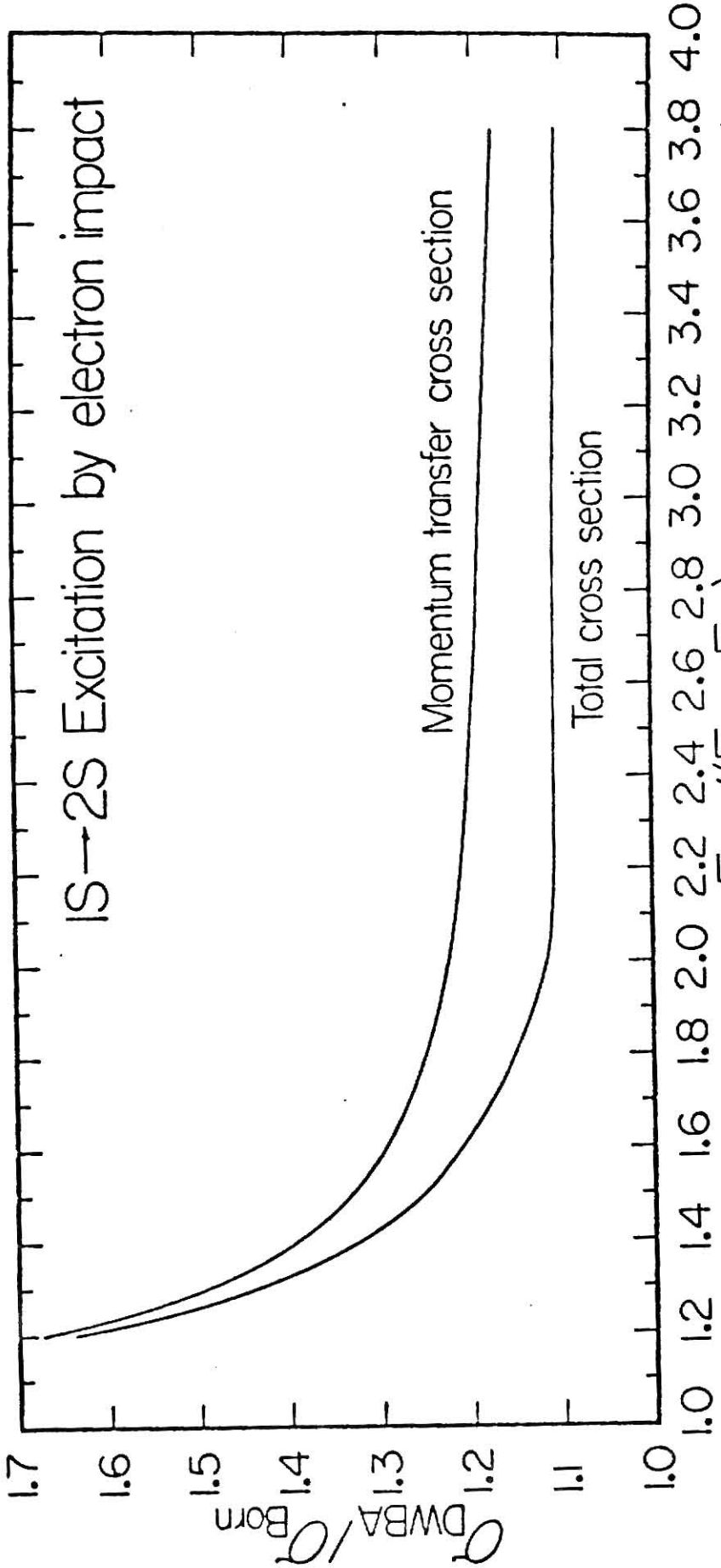

MOMENTUM TRANSFER CROSS SECTION
(1S—2S) Excitation by Electron Impact
$\sigma_{Mom.} = \int_{4\pi} \left[\frac{K_0 - K_F \cos\theta}{K_0}\right] \frac{d\sigma}{d\Omega} d\Omega$
DWBA
Born
$Z^4\sigma_M(\pi a_0^2)$
$E_{inc}/(E_{2S}-E_{1S})$
0.0
0.1
0.2
0.3
0.4
1.0
1.5
2.0
2.5
3.0
3.5
4.0

clearly we have plotted the ratio $\sigma^{DWB}/\sigma^{Born}$ against the scaled energy for both regular and momentum transfer cross sections in Fig. 10. The height of the top curve tells us how much larger σ_M^{DWBA} is than σ_M^{Born}, and the bottom curve tells us how much larger σ^{DWBA} is than σ^{Born}. The difference in height of the two curves gives us an idea of how much difference there is between σ_M and σ. Since both the Born and DWB are high energy approximations, we expect that the curves are not reliable for incident velocities below the mean velocity of a 1S electron. The energy of a 1S electron is 13.6 eV, which yields a scaled energy of about 1.3. (Note that this is the same scaled energy at which σ and σ_M have a maximum value, in Figs. 6 and 9). In the range of scaled energies from about 1.6 to 2.6 Fig. 10 yields about 30% to 20% difference between σ_M^{DWBA} and σ_M^{Born}.

In Chapter 1 we also expressed an interest in certain scaling laws In particular if one considers $Z^4\sigma^{Born}$, where σ^{Born} is the Born calculated cross section for excitation of a hydrogenic target of atomic number Z, then one finds that $Z^4\sigma^{Born}$ is independent of Z at the scaled energy $E_{inc}/|E_{2S} - E_{1S}|$. The utility of such a scaling relation is clear. If we calculate cross sections at all energies for Z = 1, we can easily obtain the cross section for any hydrogenic (Z = n) target at any energy by a simple multiplication. What we wish to determine is whether or not the DWB calculations and the momentum transfer cross sections scale in the same manner. Figure 4 shows that at each scaled energy the Born differential cross sections scale as Z^{-4}, and Fig. 5 shows that at each scaled energy the DWB differential cross sections also scale as Z^{-4}. Clearly σ^{Born} and σ^{DWB} must also scale similarly as is shown in Fig. 6.

Figure 10.

The ratio of $\sigma^{DWB}/\sigma^{Born}$ plotted against the scaled energy $E_{inc}/|E_{2S} - E_{1S}|$ for both regular and momentum transfer cross sections.


IS→2S Excitation by electron impact
Momentum transfer cross section
Total cross section
Q_{DWBA}/Q_{Born}
$E_{inc}/(E_{2S}-E_{1S})$
1.0
1.1
1.2
1.3
1.4
1.5
1.6
1.7
1.0
1.2
1.4
1.6
1.8
2.0
2.2
2.4
2.6
2.8
3.0
3.2
3.4
3.6
3.8
4.0

Figures 11 and 12 show that the Born and DWB calculated momentum transfer differential cross sections scale as Z^{-4} at each scaled energy and Fig. 9 verifies the scaling law for the corresponding total momentum transfer cross sections. In other words, all of the calculated cross sections scale in the same manner.

For our hydrogen-like wavefunctions the scaling relation above follows from the DWBA matrix element: $T_{if}^{DWBA} = \langle \chi_f^- | W_f | \chi_i^+ \rangle = \iint (\chi_f^-)^* W_f \chi_i^+ d\vec{R} d\vec{r}_b$. If we scale $R \propto \frac{1}{Z}$, and $v \propto Z$ (corresponding to our scaled energy, $E \propto Z^2$), then $\chi_f^- \propto Z^{3/2}$, $W_f \propto Z$, $\chi_i^+ \propto Z^{3/2}$, $d\vec{R} \propto Z^{-3}$ and $d\vec{r}_b \propto Z^{-3}$ so that $T_{if}^{DWBA} \propto \frac{Z^4}{Z^6} = Z^{-2}$, which yields $\frac{d\sigma}{d\Omega} \propto |T_{if}^{DWBA}|^2 \propto Z^{-4}$, in accord with our results.

Figure 11.

Born differential momentum transfer cross section for (1S-2S) excitation of hydrogenic atoms by electron impact at various energies.

BORN DIFFERENTIAL CROSS SECTION (1S→2S) Excitation by Electron Impact

$$\frac{d\sigma_m}{d\Omega} = \left(1 - \frac{K_f}{K_o}\right)\cos\theta \frac{d\sigma}{d\Omega}$$

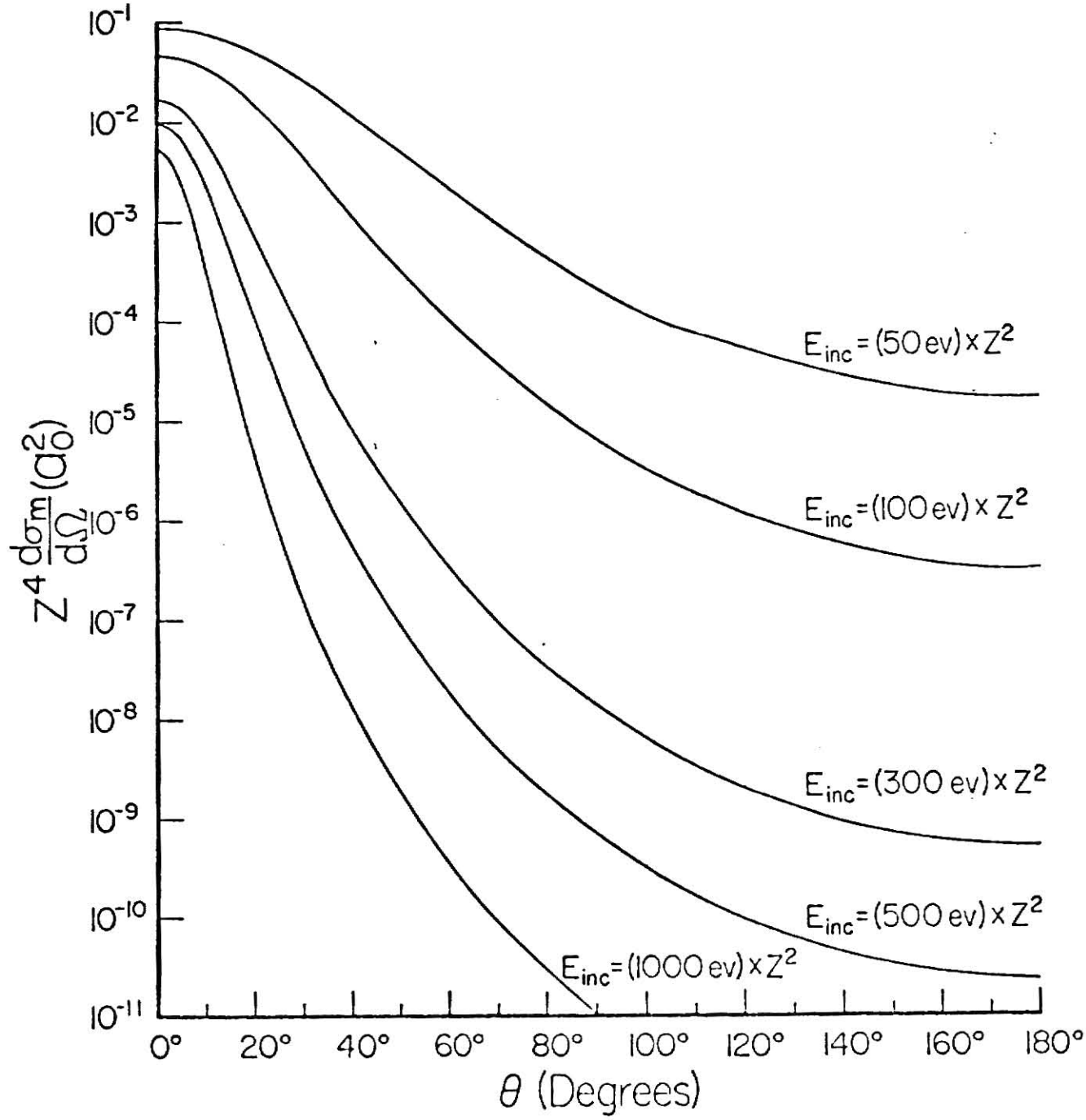
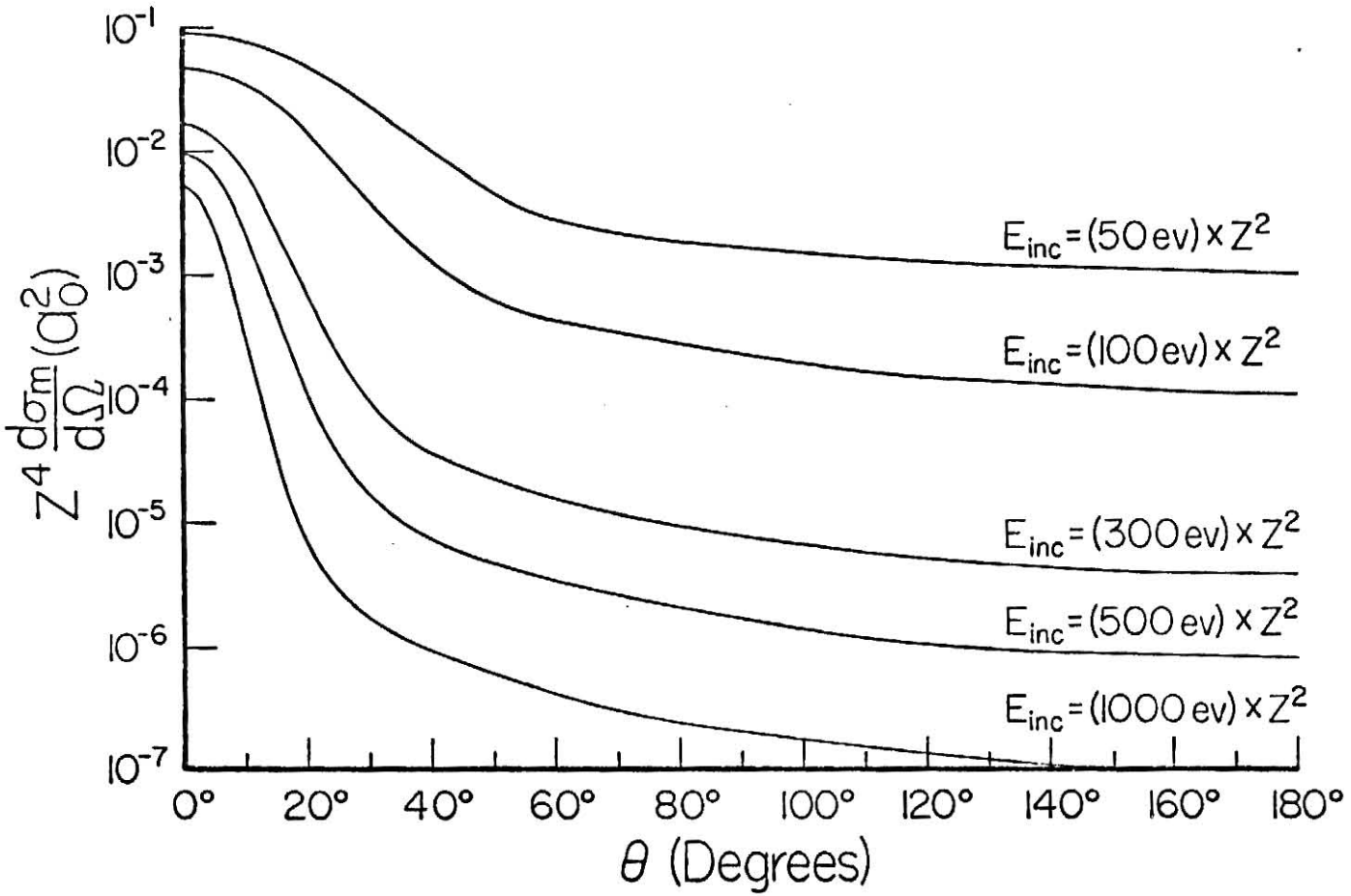


Figure 12.

DWB differential momentum transfer cross sections for (1S-2S) excitation of hydrogenic atoms by electron impact at various energies.

DWBA MOMENTUM TRANSFER CROSS SECTION (1S→2S) Excitation by Electron Impact

$$\frac{d\sigma_m}{d\Omega} = \left(1 - \frac{K_f}{K_o}\right)\cos\theta \frac{d\sigma}{d\Omega}$$



CHAPTER 5

CONCLUSIONS

The Born approximation is a widely used calculation in scattering theory. One reason for this usefulness is that the calculation yields reliable total cross sections in the high energy region while retaining a reasonably simple form. However we see that for incident energies in the region around 200 eV the differential cross sections predicted by the Born approximation for electrons on hydrogen (1S - 2S and 2P excitation) are too small at large angles. We thus choose to use a modified Born (DWB) technique in which the projectile-nucleus interaction is taken into account by using a Coulomb wave for the final outgoing wave function rather than a plane wave. This results in angular distributions which more nearly fit the data.

We find that momentum transfer cross sections, which may be useful in plasma physics, tend to weight more heavily the large angle portion of the angular distribution, and thus present us with a convenient testing ground for comparing Born and DWB approximations. The comparison shows that the DWB calculation is as much as 30% greater than the corresponding Born calculation.

We also know that a particular manifestation of the simplicity of the Born approximation is the existence of a scaling relation in Z. That is, if the Born cross sections for hydrogenic targets of different atomic number are calculated as a function of a scaled incident energy $(E_{inc}/|E_{2S} - E_{1S}|)$, then these cross sections are proportional to Z^{-4}.

We check the differential and total cross sections (both regular and momentum transfer), and find that in the DWBA the same scaling relation is maintained.

There are several directions which could be taken to continue the work done here. The present computer code can easily be adjusted to do corresponding calculations using incident protons. The calculation could also be extended to excitation and ionization. It would also be possible, after some additional algebra, to use Coulomb waves for the initial state as well as the final state.

APPENDIX

After the algebraic manipulations and simplifications mentioned in Chapter 3, the expression for the DWBA differential cross section becomes

$$\frac{d\sigma^{DWB}}{d\Omega} = \frac{u^2 k_f}{4\pi^2 k_i} |T_{if}^{DWB}|^2 ,$$

$$= \frac{u^2 k_f}{32\pi^3 k_i} e^{-\pi\alpha} \left(\frac{\alpha}{\sinh(\pi\alpha)}\right) \left|\left[1 + \frac{Z_b}{2} \frac{\partial}{\partial\lambda}\right] I(\lambda,\vec{q})\right|^2 ,$$

where $I(\lambda,\vec{q}) = \left[\frac{4\pi}{\lambda}\right]^2 \left[\frac{2}{\lambda}(CA) + 2(CB)\ (CC)\right]$,

$$CA = \frac{(k_i^2 - k_f^2)^{i\alpha}}{q^2 + 2i\alpha} - \frac{(k_i^2 - k_f^2 - 2i\lambda k_f + \lambda^2)^{i\alpha}}{(\lambda^2 + q^2)^{1 + i\alpha}} ,$$

$$= e^{i\alpha(\theta_k - 2\theta_q) - 2\theta_q} - e^{+i\alpha(\beta - \theta_\lambda) - \alpha\theta_\rho - \theta_\lambda} ,$$

$$CB = (\lambda^2 + q^2)^{-1-i\alpha} (k_i^2 - k_f^2 - 2i\lambda k_f + \lambda^2)^{i\alpha} ,$$

$$= e^{-\theta_\lambda - \alpha\theta_\rho - i\alpha(\theta_\lambda - \beta)} ,$$

$$CC = \frac{-(1 + i\alpha)\lambda}{\lambda^2 + q^2} + \frac{i\alpha(\lambda - ik_f)}{k_i^2 - k_f^2 - 2i\lambda k_f + \lambda^2} ,$$

$$= -(1 + i\alpha)\lambda e^{-\theta_\lambda} + i\alpha(\lambda - ik_f) e^{-i\theta_\rho - \beta} ,$$

where we have defined

$$k_i^2 - k_f^2 = e^{\theta_k} , \qquad \theta_k = \ln(k_i^2 - k_f^2) ,$$

$$q = e^{\theta_q} \qquad\qquad q = \ell n q$$

$$k_i^2 - k_f^2 - 2i\lambda k_f + \lambda^2 = \rho e^{i\theta_\rho}\ ,\ \rho = [(e^{\theta_k}+\lambda^2)^2 + 4\lambda^2 k_f^2]^{1/2} = e^{\beta},\ \beta = \ell n \rho$$

$$\theta_\rho = \tan^{-1}\left[\frac{-2\lambda k_f}{e^{\theta_k} + \lambda^2}\right]$$

$$(\lambda^2 + q^2) = e^{\theta_\lambda} \qquad\qquad \theta_\lambda = \ell n(\lambda^2 + q^2)$$

and

$$\frac{dI}{d\lambda} = \left\{ \begin{array}{l} -\frac{2}{\lambda} I + \left[\frac{4\pi}{\lambda}\right]^2\left[\frac{-2}{\lambda^2}(CA) + \frac{2}{\lambda}(CB)(CE - CD - E)\right] \\ \\ + \left[\frac{4\pi}{\lambda}\right]^2\left[-2(CC)(CB)(CE - CD - E) + 2(CB)(CF - CH - C\,(F - \frac{iE}{\alpha}))\right] \end{array} \right\} ,$$

where

$$CD = (2k_f^2 + \lambda^2 + e^{\theta_k})e^{-2\beta}(2i\alpha\lambda)$$

$$CE = 2\lambda e^{-\theta_\lambda}(1 + i\alpha)$$

$$E = \frac{2k_f\alpha}{1 + 4\lambda^2 k_f^2/(e^{\theta_k} + \lambda^2)^2}\left(\frac{1}{e^{\theta_k} + \lambda^2} - \frac{2\lambda^2}{(e^{\theta_k} + \lambda^2)^2}\right) ,$$

$$CF = i\alpha e^{-i\theta_\rho - \beta}$$

$$CG = \alpha(k_f + i\lambda)e^{-i\theta_\rho - \beta}$$

$$F = \frac{2\lambda}{\rho^2}\left(\lambda^2 + e^{\theta k} + 2k_f^2\right),$$

$$CH = (1 + i\alpha)e^{-\theta_k}\left[1 - \frac{2\lambda^2}{\lambda^2 + q^2}\right]$$

What follows is a copy of the computer code used.

```
      $JOB
      C       NUMERICAL INTEGRATION VIA GAUSS LEGENDRE QUADRATURE
     1        IMPLICIT REAL (A-H), COMPLEX (C)
     2        DIMENSION Z(5), W(5),THET(11)
     3        COMMON ZA,ZB,Z1,Z2,M1,M2,ED,VO,KO,KF,M,DE,L,E1,E5,AL
     4        REAL L,M,KO,KF
     5        READ (5,23) Z1,Z2,ZA,ZB,M1,M2
      C       Z1,Z2,AND ZB ARE THE NUCLEAR CHARGE
      C       ZA IS THE PROJECTILE CHARGE
      C       M1 IS THE PROJECTILE MASS
      C       M2 IS THE TARGET MASS
     6     23 FORMAT (6F10.5)
      C       READ IN TOLERANCE, STATES ONE TWO
     7        READ (5,11) T,ST1,ST2
     8     11 FORMAT (3F10.5)
     9        DO 3 J=1,5
      C       READ IN PTS AT WHICH TO EVALUATE FUNCTION
    10        READ (5,2) Z(J),W(J)
    11      2 FORMAT (2F20.15)
    12      3 CONTINUE
      C       READ IN ANGLES AT WHICH TO EVALUATE
      C       DIFFERENTIAL CROSS SECTIONS
    13        READ (5,901) IOTA
    14    901 FORMAT (I8)
    15        IF (IOTA.EQ.0) GO TO 902
    16        DO 903 IA=1,IOTA
    17        READ (5,904) THET(IA)
    18    904 FORMAT (F10.5)
    19    903 CONTINUE
    20    902 CONTINUE
    21     12 READ (5,9) E                                          SUBPROG
      C       E IS THE INCIDENT ENERGY
    22      9 FORMAT (F10.5)
    23        IF (E.LE.0) GO TO 16
    24        WRITE (6,10)
    25     10 FORMAT (1H1)
    26        RYDB=13.605
    27        IABC=0
    28        PI=3.1415926
    29        A=(M1*M2)/(M1+M2)
    30        DE=(ZA*ZB/2.)*(1./(ST1*ST1)-1./(ST2*ST2))*(2.*RYDB)
      C       THE FOLLOWING CARD SHOULD BE DELETED
      C       WHEN THE ENERGY OF THE INCIDENT PARTICLE
      C       IS READ IN, IN EV RATHER THAN AS A SCALED ENERGY
    31        E=E*DE
    32        SE=E/DE                                              SCALED E
    33        WRITE (6,21) ZA,ZB,M1,M2,E
    34     21 FORMAT (' ZA=',F4.1,3X,'ZB=',F4.1,3X,'M1=',1PE10.2,3X,'M2=',1PE10.
           2,3X,'INCIDENT ENERGY=',1PE15.4)
    35        WRITE (6,25) ST1,ST2,DE,SE
    36     25 FORMAT (////' STATE 1 =',F4.1,3X,'STATE 2 =',F4.1,3X,'THE ENERGY D
           IFFERENCE BETWEEN STATES=',1PE12.4,3X,'E/(E2S-E1S)= ',1PE10.2////)
      C       CHANGE EV TO ATOMIC UNITS
    37        ED=E/(2.*RYDB)
    38        VO=SQRT(2.*E/M)
    39        KO=M*VO
    40        DE=DE/(2.*RYDB)
    41        KF=SQRT(KO*KO-2.*M*DE)
    42        IF (IOTA.EQ.0) GO TO 905
    43        L=1
```

```
      DO 906 IAM=1,IOTA
      THE=TH*T(IAM)/57.29577951
      D=SQRT(KO**KO+KF**KF-(COS(THE))*2.*KO*KF)
      AL=(ZA*ZB**M)/KF
C     ATOMIC UNITS FOR DIFFERENTIAL
C     CROSS SECTIONS, A.U. **2 UNITS FOR TOTAL
      DUMMY=F(J)*PI
      DUMMY=DUMMY*M**M*KF/(4*Q*PI*PI*KO)
      AL=)
      DUMM2=F(J)*PI
      DUMM2 =DUMM2*M**M*KF/(4*Q*PI*PI*KO)
      WRITE (6,937) Q,THET(IAM),DUMM2,DUMMY
  937 FORMAT (' ',3X,' Q=',1PE12.4,8X,'THETA=',1PE12.4,8X,'F(BORN)**2='
     C,1PE12.4,8X,'F(COUL.)**2=',1PE12.4)
  906 CONTINUE
  909 CONTINUE
C     A AND B ARE MIN AND MAX PTS OF INTEGRATION
      DO 909 J1=1,2
      AL=)
      IF (J1.EQ.2) AL=(ZA*ZB**M)/KF
      A=KO-KF
      QINT =KO*KF
      B=AMIN1(QINT,KO+KF)
C     N EQUALS NUMBER OF SUBINTERVALS INTO
C     WHICH INTEGRATION INTERVAL IS BROKEN
      N=2
  104 AREA1=0
C     H EQUALS SUBINTERVAL DISTANCE
    4 AREA2=0
      H=(B-A)/N
      C=A
C     LOOP TO SUM OVER ALL SUBINTERVALS
      DO 6 I=1,N
      SUM=)
      D=C
      C=C+H
C     LOOP TO APPROXIMATE INTEGRAL IN THE SUBINTERVAL,
C     USING THE FIVE POINTS AND WEIGHT FACTORS ABOVE
      DO 5 L=1,5
      SUM=SUM+W(L)*F((Z(L)*(C-D)+C+D)/2)
      IF (L.NE.5) GO TO 103
      IF (QI/EF.LT.100000.0) GO TO 103
C     IABC=1 MEANS THAT QINT WILL
C     BE REDUCED BY .5
      IABC=1
  103 CONTINUE
    5 CONTINUE
      AREA=((C-D)/2.)*SUM
      AREAL=AREA*(M**M/(2.*PI*K)*KO))
    6 AREA2=AREA2+AREA
      AREA3=AREA2*(M**M/(2.*PI*KO*KO))
      IF (J1.EQ.2) GO TO 909
      WRITE (6,910) N,H,T,AREA3,AREAL
  910 FORMAT (' N=',I2,3X,'H=',1PE12.4,8X,'T=',1PE9.3,8X,'TOTAL CROSS
     C SECTION(BORN)=',1PE12.4,4X,'LAST INTERVAL =',1PE12.4)
      IF (IABC.EQ.0) GO TO 555
C INTEGRATION INTERVAL TOO LARGE, DECREASE Q BY .5
      QINT=QINT-.5
      B=AMIN1(QINT,KO+KF)
      WRITE (6,105)
```

```
      105  FORMAT (///' INTEGRATION INTERVAL TOO LARGE, DECREASING Q BY .5')
           IABC=0
           GO TO 106
       555 GO TO 911
       900 WRITE (6,912) N,M,I,AREA3,AREAL
       912 FORMAT (//' N=',I2,3X,'M=',1PE12.4,3X,'T=',1PE9.3,3X,'TOTAL CROSS
          CSECTION (BARNS)=',1PE12.4,4X,'LAST INTERVAL =',1PE12.4)
           IF (IABC.EQ.0) GO TO 911
      C INTEGRATION INTERVAL TOO LARGE, DECREASE Q BY .5
           QINT=QINT-.5
           I=SMIN1(QINT,KO*KE)
           WRITE (6,106)
      106  FORMAT (///' INTEGRATION INTERVAL TOO LARGE, DECREASING Q BY .5')
           IABC=0
           GO TO 106
       911 CONTINUE
      C    CHECK TO SEE IF DIFFERENCE BETWEEN TWO CONSECUTIVE ESTIMATES
      C    OF INTEGRAL IS LESS THAN TOLERANCE T
           IF(ABS(AREA2-AREAL))/AREA2.LT.T) GO TO 8
           AREA1=AREA2
           N=N+1
           GO TO 4
         8 CONTINUE
       999 CONTINUE
           GO TO 12
        16 CONTINUE
           WRITE (6,13)
           STOP
           END
      C    SUBPROGRAM TO COMPUTE TIFSQ
      C     COMPUTING TIF
      C    SEE REFERENCES FOR DEFINITION OF VARIABLES

           FUNCTION F(Q)
           IMPLICIT REAL (K,M), COMPLEX (C)
           COMMON ZA,Z3,Z1,Z2,M1,M2,E0,V0,KO,KE,M,DE,L,E1,F5,AL
           REAL LAM,COS,C
           PI=3.1415926
           VE=SE/4
           LAM=Z1+(Z2/2.)
           TK=ALOG(KO*KO-KE*KE)
           TQ=AL*Q
           ROE=SQRT((EXP(TK)+LAM*LAM)**2+4.*LAM*LAM*KE*KE)
           BETA=ALOG(ROE)
           TROE=ATAN2((-2.)*LAM*KE,EXP(TK)+LAM*LAM)
           TLAM=ALOG(LAM*LAM+0*0)
           CA=CMPLX(COS(AL*TK-2.*AL*TQ),SIN(AL*TK-2.*AL*TQ))/EXP(2.*TQ)
           CB=CMPLX(COS(AL*BETA-AL*TLAM),SIN(AL*BETA-AL*TLAM))/EXP(AL*TROE+
          CTLAM)
           CA=CA-CB
           CC=1.*(AL/ROE)*CMPLX(KE*COS(TROE)+LAM*SIN(TROE),LAM*COS(TROE)-KE*
          CSIN(TROE))-(LAM/EXP(TLAM))*CMPLX(1.,AL)
           CI=(((4.*PI)/LAM)**2*((2./LAM)*CA+2.*CC*CB))
           D=(4.*LAM*LAM*KE)/((EXP(TK)+LAM*LAM)**2)
           E123=(1./(1.+D*KE))*(2.*KE/(EXP(TK)+LAM*LAM)-D)
           E=(AL/(1.+D*KE))*(2.*KE/(EXP(TK)+LAM*LAM)-D)
           CJ=CMPLX(0.,(2.*AL*LAM*(2.*KE*KE+EXP(TK)+LAM*LAM))/(ROE*ROE))
           CF=(2.*LAM/(LAM*LAM+Q*Q))*CMPLX(1.,AL)
           CG=(1./ROE)*CMPLX(AL*SIN(TROE),AL*COS(TROE))
           CG=(1.*AL*EXP(-BETA))*CMPLX(KE*COS(TROE)+LAM*SIN(TROE),LAM*COS(
```

```
                CTA*E)-KE*SIN(TKDE))
  140           B=(2.*(LAM*(2.*KE*KE+EXP(TK)+LAM*LAM))/(RDE*RDE)
  141           CH=(1.-2.*LAM*LAM/(LAM*LAM+Q*Q))*EXP(-TLAM)*CMPLX(1.,AL)
  142           C1=((-2.)*C1/LAM)+(4.*PI/LAM)**2*((-2.)*CA/(LAM*LAM)-CB*(2./LAM)*
                C(*,*)-CE)+LAM*CC*(E*CD-CE)*(2./LAM)+CB+2.*CB*(CF+CG*((-F)+(E123)*
                C(),,1,1)-CH))
          C     3.*8570*4/3 IS A NORMALIZATION
          C     FACTOR OF (PI)**(Z)**3/2 WHICH WAS LEFT OUT EARLIER
  143           CK=(1.+C1+(7272.)*CJ)/(4.9857*5E75)
  144           TIFSQ=CDSQRT(CK)*CK
          C     AL=) FOR THE FIRST BORN APPROXIMATION
  145           IF (AL.EQ.0.) GO TO 50
  146           TIFSQ=TIFSQ*((Z1*Z2)**3)*ZA*ZA*AL*PI/(SINH(AL*PI)*EXP(AL*PI))
  147           GO TO 51
  148        50 TIFSQ=TIFSQ*((Z1*Z2)**3)*ZA*ZA
  149        51 F=TIFSQ
  150           F=F*E/21                                              REGULAR
          C     CHANGE RADIANS TO DEGREES
  151           THETA=(ARCOS((KO*KO+KE*KE-Q*Q)/(2.*KO*KE)))*(57.29577951)
  152           FTH=TIFSQ*(KE**4/(4.*PI*PI*PI*KO))
  153           IF (L.NE.1) GO TO 101
  154           FI=FTH
  155        101 CONTINUE
  156           IF (L.NE.5) GO TO 102
  157           FS=FTH
  158        102 CONTINUE
  159           RETURN
  160           END

        $ENTRY
```

ACKNOWLEDGEMENTS

I dedicate this work to my parents, Edward and Agnes Simony. Their love has reached across five hundred miles to encourage me.

I would like to express my profound appreciation to my major professor, Jim McGuire, for his help and guidance. He has provided me with a working model of a theoretical atomic physicist. I am grateful to Dr. J. E. Golden and Professor B. R. Junker for their notes and suggestions. I would also like to thank my peers here at Kansas State University for their comments and suggestions.

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COMPARISONS BETWEEN THE BORN APPROXIMATION AND A DISTORTED WAVE BORN APPROXIMATION FOR 1S-2S EXCITATION BY ELECTRON IMPACT IN HYDROGENIC TARGETS

by

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AN ABSTRACT OF A MASTER'S THESIS

submitted in partial fulfillment of the

requirements for the degree

MASTER OF SCIENCE

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1976

Cross sections for 1S - 2S excitation of hydrogenic targets have been computed in the Born approximation and the DWBA as a function of the charge, Z, of the target and the velocity, V, of the projectile. We compare the Born and DWB calculations in three areas: angular distributions, momentum transfer cross sections, and scaling laws. When the Born and DWB differential cross sections for 1S - 2S, 2P excitation are compared with experimental data, it is found that the Born results are several orders of magnitude too small at large angles (for 200 eV incident energy). The DWBA fits the data much better at large angles, and both approximations agree with the data at small angles. We exploit the difference in angular distributions by comparing Born and DWB calculated momentum transfer cross sections. Momentum transfer cross sections may be used in plasma physics to calculate certain transport properties, and they have the affect of amplifying the large angle portion of the angular distribution. We find that the Born and DWB momentum transfer cross sections differ by as much as 25% at high velocities. When $Z^4\sigma^{Born}$ is plotted against a scaled energy, $E_{inc}/|E_{1S} - E_{2S}|$, the resultant curve is independent of Z (for hydrogenic targets). We find that in the DWBA the differential and total cross sections also scale in the same way, and that the momentum transfer cross sections obey the same scaling relation in both Born and DWB.