DIFFERENTIAL CROSS SECTIONS FOR CHARGE

TRANSFER USING SCREENED COULOMB POTENTIALS

IN THE EIKONAL APPROXIMATION

by

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I would like to dedicate this work to my mother who has labored to provide me with my education. And most importantly, I would like to thank my loving wife who has provided for my health and emotional well being and shares with me in a dream.

CHAPTER 1

INTRODUCTION

Charge transfer or, sometimes, electron capture is a type of re-
arrangement collision. This is depicted in the reaction,

$$A + (e + B) \rightarrow (A + e) + B,$$
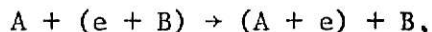
where A represents the projectile system, B the target system, and e the
transferred electron. Due to the Coulomb interactions influencing the
projectile's path, the projectile will scatter at various angles depend-
ing on the impact parameter, see Figure 1. Looking at many scattering
events corresponding to various impact parameters, an angular distribu-
tion will arise. Calculation of the charge transfer angular distributions
from the K shell by proton impact is presented in this thesis.

Thus far, charge transfer calculations yield non rigorous total
cross sections for K shell capture. The most extensively used method for
determining electron capture cross sections is the first Born approxima-
tion or, simply, the Born approximation. This method is used for its
simplicity and not necessarily for its validity. It is known that the
second Born term dominates at very high energies[1] and second order calcu-
lations are now being pursued. In this presentation, the simplicity of
the first order calculation is retained while viewing the differential
cross section for charge transfer.

Examination of the differential cross section can give a deeper
understanding of the charge transfer process. The perturbing potential
for charge transfer is still somewhat unclear. Since the differential

Figure 1. Scattering of an ion from an atomic target, where ρ is the impact parameter and θ is the scattering angle.

A (projectile)

θ

ρ

B (target)

z
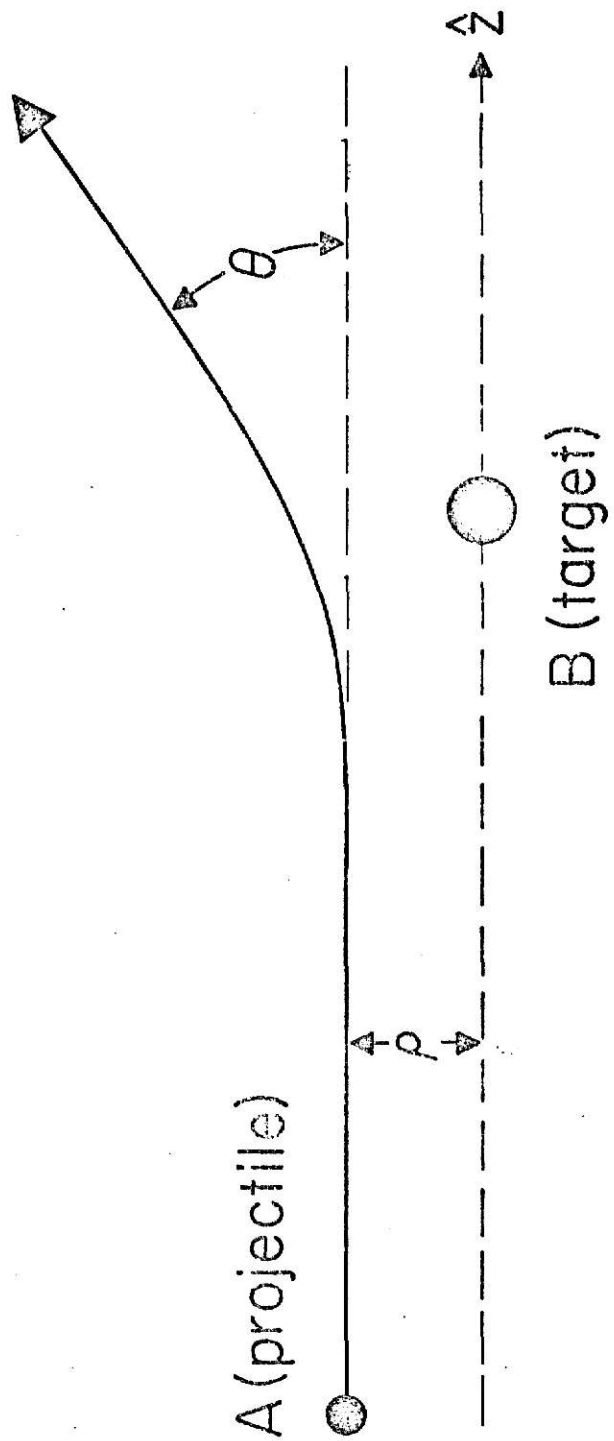
cross section is sensitive to how the Hamiltonian is broken up, detailed information of the charge transfer process is possible. Thus, calculations of angular distributions could lend credance to ideas as to how the Hamiltonian for charge transfer should be broken up in first order perturbation theory.

One of the first charge transfer calculations was done by Brinkman and Kramers[2] in 1930. Their calculation was performed adhering to the point of view that the relevant interaction potential was between the projectile and (captured) electron[3]. It is argued that the internuclear interaction, which is largely responsible for the path of the projectile, contributes little to the total capture cross section for heavy particles. For most capture cross sections, the resulting BK total cross sections were typically too large by a factor[4] of 2 to 10.

Another first order calculation was performed by Jackson and Schiff[5] in 1953 for the special case of protons incident upon hydrogen. The potential used in the JS calculation was the full interaction, that is, the BK potential and the internuclear (or core) potential. Including the "core" term had the effect of reducing the total cross section over a range of energies thus giving much better agreement with experiment. However, when the JS method was applied to other systems of higher nuclear charge, total calculated cross sections were found to disagree with experiment by as much as several orders of magnitude.[6,7]

The success of the JS approach was later partially explained by Bates[8] in 1958. Taking into account the nonorthogonality of the initial and final state wave functions, Bates was able to demonstrate that a JS like core term with unit nuclear charge originates from the average electron interaction. This tends to account for the relative success of the

JS method for protons on hydrogen, and suggests an alternate method for targets of nuclear charge greater than one.

At the present time, some believe that the Bates calculation offers the most complete picture for viewing charge transfer to first order. Nevertheless, only various approximations for the Bates method of charge exchange have been used resulting in total cross sections that tend to agree with experiment.[9,10] The success of these approximations in predicting total cross sections tend to indicate that the Bates approach is superior to that of BK or JS.

Taking advantage of the heavy projectile mass, it is often useful to study the charge transfer process by means of the impact parameter treatment. A transformation from the wave picture over to an impact parameter picture is presented in appendix 1. This impact parameter formalism was used by Belkic and Salin[11] in 1976 for the angular distributions for charge transfer.

The impact parameter formalism used in Belkic and Salin's calculation employs an eikonal phase so as to include the internuclear potential together with the Brinkman-Kramers method. Justification for the use of the eikonal phase within the impact parameter treatment is made in Chapter 2. By including the internuclear potential in the eikonal phase, Belkic and Salin were able to get improved agreement at wide angles with the differential cross section for electron capture from argon by 6 MeV protons observed by Cocke,[12] et al., in 1976, see Figure 2. Using the BK probability amplitude for capture which is calculated in a straight-line impact-parameter version of the BK approximation Belkic and Salin were able to obtain a better angular distribution than the BK calculation which took into account no contributions of the internuclear repulsion.

Figure 2. Differential cross section in laboratory system

for capture of K-shell electrons from argon by 6 MeV protons.

The curve marked BK represents the Brinkman-Kramers approxi-

mation; and CBK, the Coulomb Brinkman-Kramers approximation.

Experimental data are those of Cocke, et al., (1976). Figure

taken from Belkic and Salin, J. Phys. B: Atom. Molec. Phys.

9, L397 (1976).

$p + Ar \longrightarrow H + Ar^+$
6 MeV

BK

CBK

$\dfrac{d\sigma}{d\Omega}$ (cm^2/ster.-atom)

10^{-17}

10^{-18}

10^{-19}

θ (°)

0   0.04   0.08   0.12   0.16

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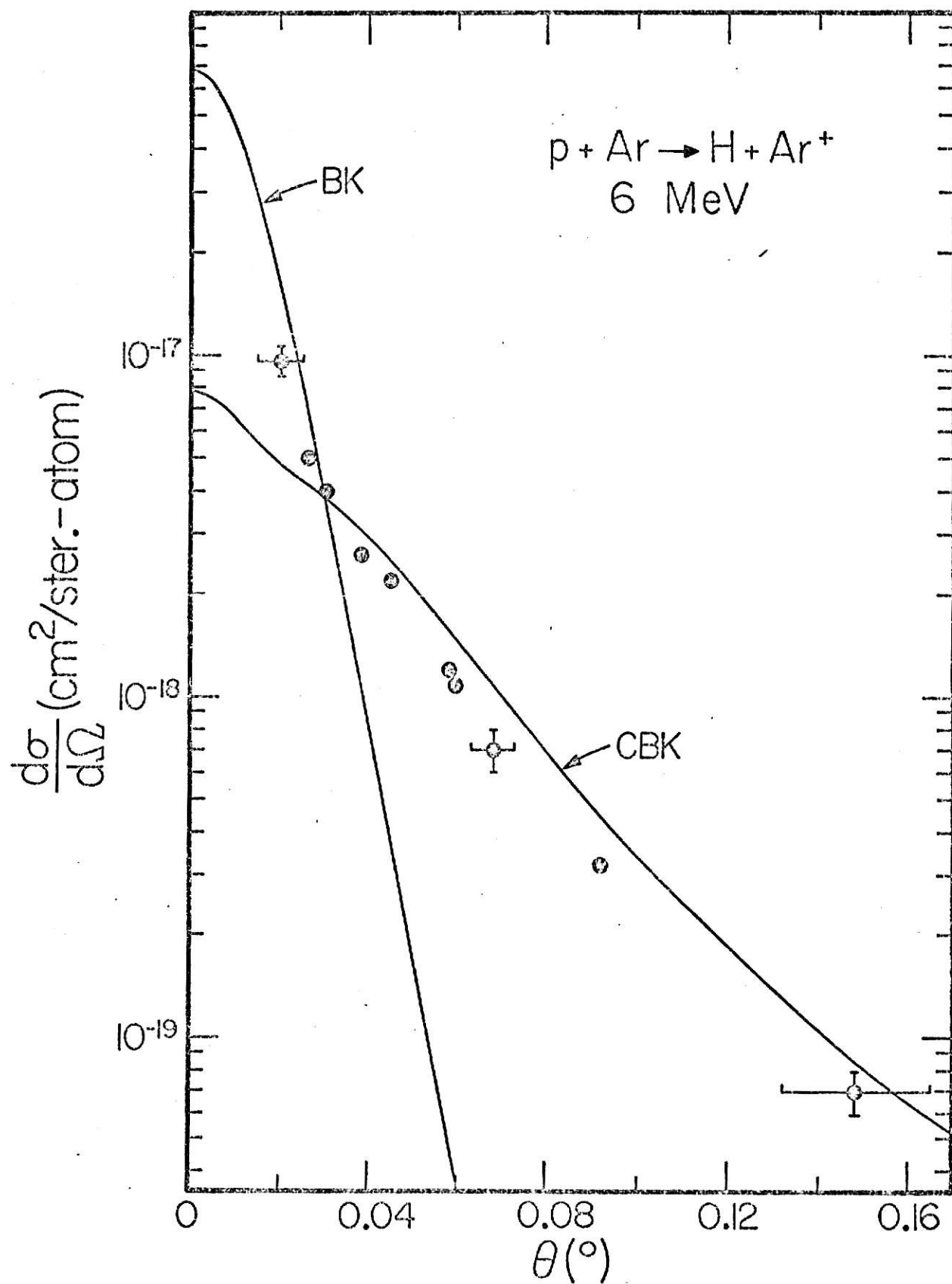
Note that their results are in good agreement at large angles (i.e. small impact parameters) but may give poor agreement at the forward angles (i.e. large impact parameters). Data for protons on helium support this trend, suggesting that the scattering potential is too strong at large impact parameters.

One of the limitations of the Belkic and Salin calculation is the omission of the screening effects by the electrons at large impact parameters. We include the effects of screening by the electrons in an approximate manner. For p + H and p + He, the internuclear potential is represented by the static potential (cf. Chapter 2) which is introduced into the eikonal phase within the BK method. Hence, it will be referred to as the Static Brinkman-Kramers (SBK) approximation. For p + Ar which is mathematically more complex, a screened Coulomb potential is incorporated in the eikonal phase as an approximation for the static potential. This Screened Coulomb Brinkman-Kramers calculation will be referred to as the SCBK approximation.

Application of the eikonal impact parameter treatment of charge transfer is made for three specific cases. The relatively simple system of protons incident upon hydrogen is presented first. This is followed by protons incident on helium. Then finally, the more complex system of protons on argon is examined. The two later cases are compared with recently gathered experimental differential cross sections for charge transfer.

CHAPTER 2

THEORY

2.1   The Differential Cross Section

The differential cross section is defined as

$$\frac{d\sigma}{d\Omega} \equiv \frac{\text{Number of particles per unit time scattered into a solid angle}}{\text{Number of particles incident on the target per unit area per unit time}} \quad .$$

This can be written symbolically as,

$$\frac{d\sigma}{d\Omega} = \frac{\omega/d\Omega_f}{I} \quad . \tag{2.1}$$

The incident flux, I, can be given as,

$$I = \frac{\text{velocity of incident particle}}{\text{unit volume}}$$

$$= \frac{k_i \hbar}{\mu_i L^3} \tag{2.2}$$

where $\hbar k_i$ is the magnitude of the relative initial momentum, μ_i is the initial reduced mass of the system, and L^3 is the volume of a cube of length, L.   The transition probability per unit time,[13] ω, is given by,

$$\omega = \frac{2\pi}{\hbar} \rho_f |<\phi_f|H'|\psi>|^2, \tag{2.3}$$

where ρ_f is the density of final states and $<\phi_f|H'|\psi>$ is the transition matrix element for a transition from all possible states, ψ, into the

final state, ϕ_f, under the perturbing Hamiltonian, H'. The density of final states, ρ_f, is given by,

$$\rho_f = \frac{\mu_f k_f d\Omega_f L^3}{(2\pi)^3 \hbar^2} , \qquad (2.4)$$

where μ_f is the reduced mass of the final system, $\hbar k_f$ is the magnitude of the final relative momentum, $d\Omega_f$ is the solid angle subtended by the detector, and L^3 is the volume. Combining eq. 2.1, 2.2, 2.3 and 2.4, the differential cross section becomes,

$$\frac{d\sigma}{d\Omega} = \frac{\mu_i \mu_f L^6}{(2\pi)^2 \hbar^4} \left(\frac{k_f}{k_i}\right) |<\phi_f|H'|\Psi>|^2 \qquad (2.5)$$

It is now convenient to introduce atomic units ($e^2 = \hbar = m_e = 1$), where e is the electron charge and m_e is the electron mass. A few basic units are given below;

$$\text{unit length} = a_o = \frac{\hbar^2}{m_e e^2} = 5.29 \cdot 10^{-9} \text{ cm}$$

$$\text{unit energy} = \frac{m_e e^4}{\hbar^2} = 27.2 \text{ eV}$$

$$\text{unit time} = \frac{\hbar^3}{m_e e^4} = 2.42 \cdot 10^{-17} \text{ sec.}$$

Atomic units will be used unless stated otherwise.

The differential cross section given in atomic units is,

$$\frac{d\sigma}{d\Omega} = \frac{\mu_i \mu_f}{(2\pi)^2} \left(\frac{k_f}{k_i}\right) |<\phi_f|H'|\Psi>|^2 , \qquad (2.6)$$

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where the wave functions are normalized to the unit volume, L^3. As yet, all we have done is to have re-written the definition of differential cross section into a form that can be used for calculation.

2.2 The Hamiltonian

Charge transfer is not a well understood atomic process. In our quest toward understanding the charge transfer process, approximations for both the wave functions and the perturbing Hamiltonian are made. However, in making approximations for the wave functions, difficulties arise from the fact that the wave functions are not described in the same basis set (i.e., nonorthogonal wave functions are used). In addition, it is a general practice to consider only one electron target atoms in charge transfer.

The Hamiltonian for a charged projectile incident upon a multi-electron target (assuming two body interactions) is given by,

H = Total Kinetic Energy + Total Potential Energy

$$= \frac{P^2}{2M_a} + \frac{Z_a Z_b e^2}{R} - \sum_{j=1}^{Z_b} \frac{Z_a e^2}{|\vec{R} - \vec{r}_j|}$$

$$+ \sum_{j=1}^{Z_b} \left(\frac{P_j^2}{2m_e} - \frac{Z_b e^2}{r_i} \right) + \sum_{k>j}^{Z_b} \frac{e^2}{|\vec{r}_k - \vec{r}_j|} \qquad (2.7)$$

where Z_a and M_a are the charge and mass of the incident projectile with momentum P, Z_b is the charge of the target nucleus, R represents the projectile coordinate and $\vec{r}_1 \ldots \vec{r}_{Z_b}$ the set of coordinates of the target electrons measured from the target nucleus, and P_j is the momentum of the jth electron. By adding then subtracting the average projectile electron potential (i.e.,

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$$\bar{V}_e^j \equiv \langle \phi_i \mid \frac{-Z_a e^2}{|\vec{R}-\vec{r}_j|} \mid \phi_i \rangle \tag{2.8}$$

where ϕ_i is the initial bound state wave function for the jth electron),
the Hamiltonian in eq. 2.7 takes the form,

$$H = \frac{P^2}{2M_a} + V_s(R) + H' + H_o' + H_o, \tag{2.9}$$

where $V_s(R)$ is the static potential[15] given by

$$V_s(R) \equiv \frac{Z_a Z_b e^2}{R} + \sum_{j=1}^{Z_b} \bar{V}_e^j \tag{2.10}$$

or

$$V_s(R) \equiv Z_a \left| \frac{Z_b e^2}{R} + \sum_{j=1}^{Z_b} \frac{\rho(\vec{r}_j)}{|\vec{R}-\vec{r}_j|} d\vec{r}_j \right| ,$$

where (r_j) is the charge density for the jth electron H' is the electron
capture potential prescribed by Bates[8], i.e.,

$$H' \equiv \frac{-Z_a e^2}{|\vec{R}-\vec{x}|} + \langle \phi_i \mid \frac{Z_a e^2}{|\vec{R}-\vec{x}|} \mid \phi_i \rangle \tag{2.11}$$

where $\vec{x}$ is the coordinate of the captured electron measured from the target
nucleus; H_o' is the Hamiltonian that describes the initial bound state
of the electron to be captured, i.e.,

$$H_o' \equiv \frac{P_e^2}{2m_e} - \frac{Z_b e^2}{x} + V(\vec{x}), \tag{2.11A}$$

where P_e is the momentum of the captured electron and $V(\vec{x})$ is the effective
potential between the captured electron and the spectator electrons, i.e.,

$$V(\vec{x}) \simeq \sum_{k=1}^{Z_b} {}' \frac{e^2}{|\vec{r}_k-\vec{x}|} , \tag{2.11B}$$

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where the prime indicates the restricted sum $r_k \neq x$; and H_o is the

Hamiltonian for the spectator electrons which is given by

$$H_o \equiv \sum_{j=1}^{Z_b-1} \left[\frac{P_j^2}{2m_e} - \frac{Z_b e^2}{r_j} + V(\vec{r}_j) - \bar{V}_e^j \right] , \qquad (2.11C)$$

where the summation is over all the spectator electrons and $V(\vec{r}_j)$ is

the effective potential between the spectator electrons (cf. eq. 2.11B).

To retain the simplicity of the one electron atom, the effects due to

the spectator electrons, eq.2.11C, are ignored[14] in the development to

follow. This is done so that simple hydrogenic wave functions can be

used to describe the bound state of the captured electron. Note that

in this fashion of breaking up the Hamiltonian, both the static potential

and the electron capture potential of Bates are directly related.

The perturbation to the one electron Hamiltonian is separable

into two categories: the perturbation for electron capture and the

perturbation responsible for scattering of the projectile. Both are

needed for the differential cross section. The perturbation for the

capture process is the Bates potential, eq. 2.11. The "scattering"

perturbation is the static potential given by eq. 2.10. We choose to

treat these two processes separately.

2.3 The Eikonal Phase

We can treat the scattering process within the eikonal approxima-

tion. As an introduction to the eikonal approximation, let us consider

the scattering of a particle from the central potential, $V(R)$. The time

independent Schrödinger equation for such a process is

$$\left[-\frac{\nabla^2}{2\mu} + V(R) \right] \psi = \frac{k^2}{2\mu} \psi, \tag{2.12}$$

where μ is the reduced mass and k is the momentum of the projectile.

Assuming our wave function to be of the form,

$$\psi = e^{i\vec{k}\cdot\vec{R}} \Phi(R) \tag{2.13}$$

and substituting into eq. 2.12 we get

$$\left[\frac{k^2}{2\mu} \Phi(R) - \frac{\nabla^2}{2\mu} \Phi(R) - \frac{2i\vec{k}\cdot\vec{\nabla}\Phi(R)}{2\mu} + V(R)\Phi(R) \right]$$

$$X \ e^{i\vec{k}\cdot\vec{R}} = \frac{k^2}{2\mu} \Phi(R) \ e^{i\vec{k}\cdot\vec{R}} . \tag{2.14}$$

Equation 2.14 reduces to

$$-\frac{\nabla^2}{2\mu} \Phi(R) - \frac{i\vec{k}\cdot\vec{\nabla}\Phi(R)}{\mu} + V(R)\Phi(R) = 0. \tag{2.15}$$

Assuming $\Phi(R)$ to vary slowly over many wavelengths of the incident projectile,[16] i.e.

$$\nabla^2 \Phi(R) \ll \vec{k}\cdot\vec{\nabla}\Phi(R), \tag{2.16}$$

choosing $\vec{k}$ along the $\hat{z}$ direction, and solving eq. 2.15 for $\Phi(R)$ we get

$$\Phi(R) = \left[\exp \frac{-\mu i}{k} \int_{-\infty}^{\infty} V(R) dz \right]. \tag{2.17}$$

Noting that $R = \sqrt{\rho^2 + z^2}$ where ρ is the impact parameter, our projectile

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wave function (eq. 2.13) is

$$\psi \approx \exp(i\vec{k}_i \cdot \vec{R}_i + 2i\delta(\rho)), \qquad\qquad (2.18)$$

where

$$\delta(\rho) \equiv \frac{-i}{v} \int_0^\infty V(R) \, dz, \qquad\qquad (2.19)$$

and $\mu v = k$.

2.4   The Eikonal Impact Parameter Method

McCarroll and Salin[17] (1968) present a method for evaluation of the differential cross section (Appendix 1) where the wave picture is formally transformed into an impact parameter picture. The results of this method were then modified by Belkic and Salin (1976) so as to include scattering from the internuclear potential in an eikonal phase. The internuclear potential used by Belkic and Salin appears to be too strong at the large impact parameters which suggests that screening of the electrons is important for angular distributions. Here the eikonal impact parameter method used by Belkic and Salin is presented in a general form so that the screening effects are properly taken into account.

The differential cross section (eq. A1. 38) is obtained by McCarroll and Salin by evaluating the transition matrix. The transition matrix, T_{if}, is given by either of the two equivalent expressions,[18]

$$T_{if} = \langle \phi_f | V_f | \psi_i \rangle \qquad\qquad (2.20)$$

or

$$T_{if} = \langle \phi_i | V_i | \psi_f \rangle, \qquad\qquad (2.21)$$

where the subscripts i and f are used to denote initial and final conditions. The first of the two expressions for the transition matrix is evaluated in Appendix 1. Since the single electron charge transfer process is time reversible, the perturbation is given by some appropriate interaction potential between the captured electron and the projectile either before or after the collision indicated by V_i and V_f respectively.

It has already been mentioned that the choice of the static potential in the eikonal phase corresponds to use of the Bates potential, i.e.

$$V_f \approx \frac{Z_b e^2}{x} - <\phi_i | \frac{Z_b e^2}{x} | \phi_i>. \qquad (2.22)$$

The Bates potential has two desirable features that the BK and JS potentials lack. First, the orthogonality of the wave functions ϕ_i and ϕ_f are maintained. Second, the choice of a zero point energy has no effect on the total or differential cross sections as it should.[8] However, the Bates calculation is difficult computationally. For this reason, the BK potential is adopted at this point for computational convenience, i.e.

$$V_f = \frac{Z_b e^2}{x}. \qquad (2.23)$$

One consequence of using the BK potential is failure of our calculation to produce correctly normalized distributions. It is well known that the BK results generally lie above observed results for total cross sections.[4]

The general form for the eikonal impact parameter method used by Belkic and Salin is presented. Using the BK potential in the evaluation of the probability amplitude (cf. Appendix 2), the differential cross section (eq. A1.38) takes the form,

$$\frac{d\sigma}{d\Omega} = \left| i\mu v \int_0^\infty \rho d\rho J_0(\eta\rho) \exp(2i\delta(\rho)) b_{BK}(\rho) \right|^2, \qquad (2.24)$$

where μ is the reduced mass, v is the velocity of the incident projectile, η is the momentum transfer, J_0 is the zero order Bessel function of the first kind, $\delta(\rho)$ is the eikonal phase (eq. 2.19) for the static potential, and $b_{BK}(\rho)$ is the Brinkman-Kramers probability amplitude (eq. A2.30) for the capture of an electron at the impact parameter, ρ. In eq. 2.24, the probability amplitude (eq. A1.37) is separable into the BK probability amplitude times an overall phase (eq. A2.8). The BK probability amplitude given by McGuire and Cocke[19] is

$$b_{BK}(\rho) = \left(\frac{2in_a}{v}\right) \left(\frac{Z_a Z_b}{n_a n_b}\right)^{5/2} \left(\frac{\rho^2}{\gamma}\right) K_2\left(\gamma^{\frac{1}{2}}\rho\right), \qquad (2.25)$$

where Z_a and Z_b are the charges of the respective nuclei A and B, n_a and n_b are the principle quantum numbers of the bound electron to the respective nuclei A and B, K_2 is the second order Bessel function of the third kind, and

$$\gamma = \frac{Z_b^2}{n_b^2} + \left(\frac{v}{2} + \frac{1}{2v}\left(\frac{Z_a^2}{n_a^2} - \frac{Z_b^2}{n_b^2}\right)\right)^2. \qquad (2.26)$$

Upon specification of the eikonal phase, the integration over impact parameters gives the differential cross section for charge transfer of an electron from the state n_b to state n_a.

CHAPTER 3

APPLICATIONS AND RESULTS

3.1 The Static Brinkman-Kramers Approximation

Use of the static potential (eq. 2.10) in the calculation of the eikonal phase (eq. 2.19) with the BK probability amplitude (eq. 2.25) defines the Static Brinkman-Kramers (SBK) approximation. The static potential for hydrogen and helium like targets is easily evaluated in the independent electron approximation. The form of the eikonal phase using the static potential is now presented.

The average electron-projectile interaction potential (eq. 2.8) using hydrogenic wave functions is readily evaluated for the K shell. The initial wave function[20] is

$$\phi_i = \left(\frac{Z^*}{a_o}\right)^{3/2} 2 \exp\left(-\frac{Z^* r}{a_o}\right) \frac{1}{2\sqrt{\pi}} P_o(\cos\theta), \tag{3.1}$$

where Z^* ($Z^* = Z_b$ for a one electron atom) is the effective nuclear charge seen by the bound electrons, and P_o is the Legendre polynomial. The projectile-electron interaction potential[21] is

$$-\frac{Z_a}{|\vec{R} - \vec{r}|} = \frac{-Z_a}{r_>} \sum_{\ell=o}^{\infty} \left(\frac{r_<}{r_>}\right)^\ell P_\ell(\cos\theta), \tag{3.2}$$

where R is the internuclear separation distance and r is the electron tar-get separation distance ($r_<$ and $r_>$ refer to the lesser and greater of the two distances). From eq. 3.1 and eq. 3.2, the average projectile – 1s electron interaction potential is

$$\bar{V}_e = \frac{-Z_a}{\pi} \left(\frac{Z^*}{a_o}\right)^3 \int_0^\infty r^2 \, dr \, \exp\left(-\frac{2Z^* r}{a_o}\right) \frac{1}{r_>}$$

$$X \sum_{\ell=0}^\infty \left(\frac{r_<}{r_>}\right)^\ell \int_{-1}^1 P_\ell(\cos\theta) P_o(\cos\theta) P_o(\cos\theta) d(\cos\theta) \int_0^{2\pi} d\phi. \qquad (3.3)$$

Upon integration over ϕ and noting that $P_o(\cos\theta) = 1$, eq. 3.3 reads

$$\bar{V}_e = -2Z_a \left(\frac{Z^*}{a_o}\right)^3 \int_0^\infty r^2 dr \, \exp\left(-\frac{2Z^* r}{a_o}\right) \frac{1}{r_>}$$

$$X \sum_{\ell=0}^\infty \left(\frac{r_<}{r_>}\right)^\ell \int_{-1}^1 P_\ell(\cos\theta) P_o(\cos\theta) d(\cos\theta). \qquad (3.4)$$

Using the orthogonality of Legendre polynomials,[22]

$$\int_{-1}^1 P_\ell(x) P_o(x) dx = 2\delta_{\ell o}, \qquad (3.5)$$

the summation vanished except for the $\ell = 0$ term. This reduces eq. 3.4 to,

$$\bar{V}_e = -\frac{Z_a}{2} \int_0^\infty \frac{x^2 e^{-x}}{x_>} \, dx, \qquad (3.6)$$

where $x = 2Z^* \frac{r}{a_o}$ and

$$x_> = \begin{cases} R & \text{if } x < \dfrac{2Z^* R}{a_o} \\[3mm] r & \text{if } x > \dfrac{2Z^* R}{a_o} \ . \end{cases} \qquad (3.7)$$

Since[23]

$$\int_t^\infty x e^{-x} dx = e^{-t}(t + 1) \qquad (3.8)$$

and

$$\int x^2 e^{-x} dx = e^{-x}(-x^2 - 2x - 2), \qquad (3.9)$$

eq. 3.6 is evaluated as

$$\overline{V}_e = -\frac{Z_a}{R} + Z_a \left(\frac{1}{R} + \frac{Z^*}{a_o}\right) \exp\left(-\frac{2Z^* R}{a_o}\right). \qquad (3.10)$$

This is precisely the expression that Bassel and Gerjouy[9](1960) obtained for the average electron interaction for protons on hydrogen ($Z^* = Z_a = 1$). Hence, the static potential (eq. 2.10) for $Z_b \leq 2$ is

$$Z_a Z_b \left[\frac{1}{R} - \frac{1}{R} + \left(\frac{1}{R} + \frac{Z^*}{a_o}\right) \exp\left(-\frac{2Z^* R}{a_o}\right)\right]. \qquad (3.11)$$

The eikonal phase for the static potential in eq. 3.11 is

$$\delta(\rho) = -\frac{Z_a Z_b}{v} \int_o^\infty \left(\frac{1}{R} + \frac{Z^*}{a_o}\right) \exp\left(\frac{-2Z^* R}{a_o}\right) dz. \qquad (3.12)$$

Letting $q = \frac{2Z^*}{a_o}$ and noting $R = \sqrt{\rho^2 + z^2}$, we have

$$\int_o^\infty (\rho^2 + z^2)^{-\frac{1}{2}} \exp(-q(\rho^2 + z^2)^{\frac{1}{2}}) dz \qquad (3.13)$$

which is evaluated to be $K_o(\rho q)$ which is the zero-order modified Bessel function of the third kind.[24] Since

$$\frac{\partial}{\partial q} \frac{e^{-qR}}{R} = -e^{-qR}, \qquad (3.14)$$

we have

$$\int_o^\infty \exp(-q(\rho^2 + z^2)^{\frac{1}{2}}) dz = -\frac{\partial}{\partial q} K_o(\rho q). \qquad (3.15)$$

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Letting $p = \rho q$, we have[25]

$$-\rho \frac{\partial}{\partial p} K_o(p) = \rho \, K_1(p), \tag{3.16}$$

where K_1 is the first order Bessel function of the third kind. The eikonal phase for the static potential is,

$$\delta(\rho) = -\frac{Z_a Z_b}{v} \left[K_o\left(\frac{2Z^*\rho}{a_o}\right) + \frac{Z^*\rho}{a_o} K_1\left(\frac{2Z^*\rho}{a_o}\right) \right]. \tag{3.17}$$

Appendix 3 contains a computer program for the calculation of the differential cross section (eq. 2.24) for the static potential in the eikonal phase (eq. 3.17)

3.2 Screened Coulomb Brinkman-Kramers Approximation

For targets with more than two electrons, the static potential contains terms that arise from electrons in shells and subshells other than the K shell. For this reason, there are a multitude of additional terms to be evaluated to obtain the total static potential. To simplify matters, we can approximate the screening of the electrons by the screened Coulomb potential,

$$V(R) = \frac{Z_a Z_b}{R} \exp\left(-\frac{R}{r_o}\right), \tag{3.18}$$

where r_o is an appropriate screening radius. For atom-atom collisions, an expression for the screening radius exists in the literature, given by,[26,27]

$$r_o = a_o / (Z_a^{2/3} + Z_b^{2/3})^{1/2}. \tag{3.19}$$

Making use of eq. 3.13, the eikonal phase (eq. 2.10) for a screened Coulomb potential (eq. 3.18) is

$$\delta(\rho) = -\frac{Z_a Z_b}{v} K_o \left[\frac{\rho}{r_o}\right] . \tag{3.20}$$

Use of the screened Coulomb potential in the eikonal phase with the BK probability amplitude defines the Screened Coulomb Brinkman-Kramers (SCBK) approximation.

The limiting cases for screening give the results of Brinkman and Kramers and the results of Belkic and Salin. When the screening radius is zero the screened Coulomb potential vanishes, i.e.

$$\frac{Z_a Z_b}{R} \exp\left(-\frac{R}{r_o}\right) \xrightarrow[r_o \to o]{} 0. \tag{3.21}$$

This corresponds to the calculation of Brinkman and Kramers. When the screening radius is infinite the screened Coulomb potential reduces to the Coulomb potential, i.e.

$$\frac{Z_a Z_b}{R} \exp\left(-\frac{R}{r_o}\right) \xrightarrow[r_o \to \infty]{} \frac{Z_a Z_b}{R} . \tag{3.22}$$

This is the potential used by Belkic and Salin to obtain the Coulomb Brinkman-Kramers (CBK) approximation.

Appendix 4 contains a program for the calculation of the differential cross section (eq. 2.24) using the screened Coulomb potential in the eikonal phase (eq. 3.20).

3.3 Protons on Hydrogen

We can now test the effects of screening of the internuclear poten-

tial by the target electrons in the charge transfer process. Consider the simplest possible system of a proton incident upon atomic hydrogen, i.e.

$$p + H \rightarrow H + p .$$
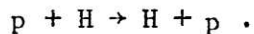
In viewing this reaction, we compare the differential cross section of SCBK, for several screening radii, with SBK.

There are several interesting features of SCBK and SBK. In figure 3, a comparison of the differential cross sections versus angle is presented for protons incident upon atomic hydrogen at 50 keV. There are three distinct curve shapes (solid lines). The screened Coulomb Brinkman-Kramers calculation reduces to the Brinkman-Kramers calculation and the Coulomb Brinkman-Kramers calculation of Belkic and Salin in the limiting cases of screening parameters. The total cross sections from all the differential cross sections in figure 3 are identical. Finally, the shape of SCBK is not sensitive to reasonable choices of the screening parameter.

There are three distinct shapes for the differential cross section indicated by the solid curves in figure 3. The BK angular distribution is peaked in the forward direction and falls off rapidly at the larger angles, for the BK calculation takes into account no internuclear interaction. On the other hand, the CBK calculation takes into account the full internuclear interaction i.e. $V(R) = \frac{1}{R}$, where R is the internuclear separation distance. As a result, the curve marked CBK shows that the capture process at the larger angles is orders of magnitude above the BK results due to inclusion of the internuclear repulsion within the eikonal phase. Recalling the discussion of figure 2, the SBK calculation gives the desired results of following BK at the forward angles ($\theta < \frac{m_e}{m_p}$) and CBK at large

Figure 3.   The differential cross section for electron capture

by 50 keV protons incident on atomic hydrogen is shown.   The curve

marked BK is the Brinkman-Kramers approximation, CBK is the

Coulomb Brinkman-Kramers approximation, SBK is the Static Brinkman-

Kramers approximation, and SCBK the Screened Coulomb Brinkman-

Kramers approximation.

$p + H \rightarrow H + p$
50 keV

BK ($r_o = 0$)

CBK ($r_o = \infty$)

SCBK ($r_o = 1$)

SBK

SCBK ($r_o = .7$)

$\frac{d\sigma}{d\Omega}$ (cm²/ster.)

θ (degrees)
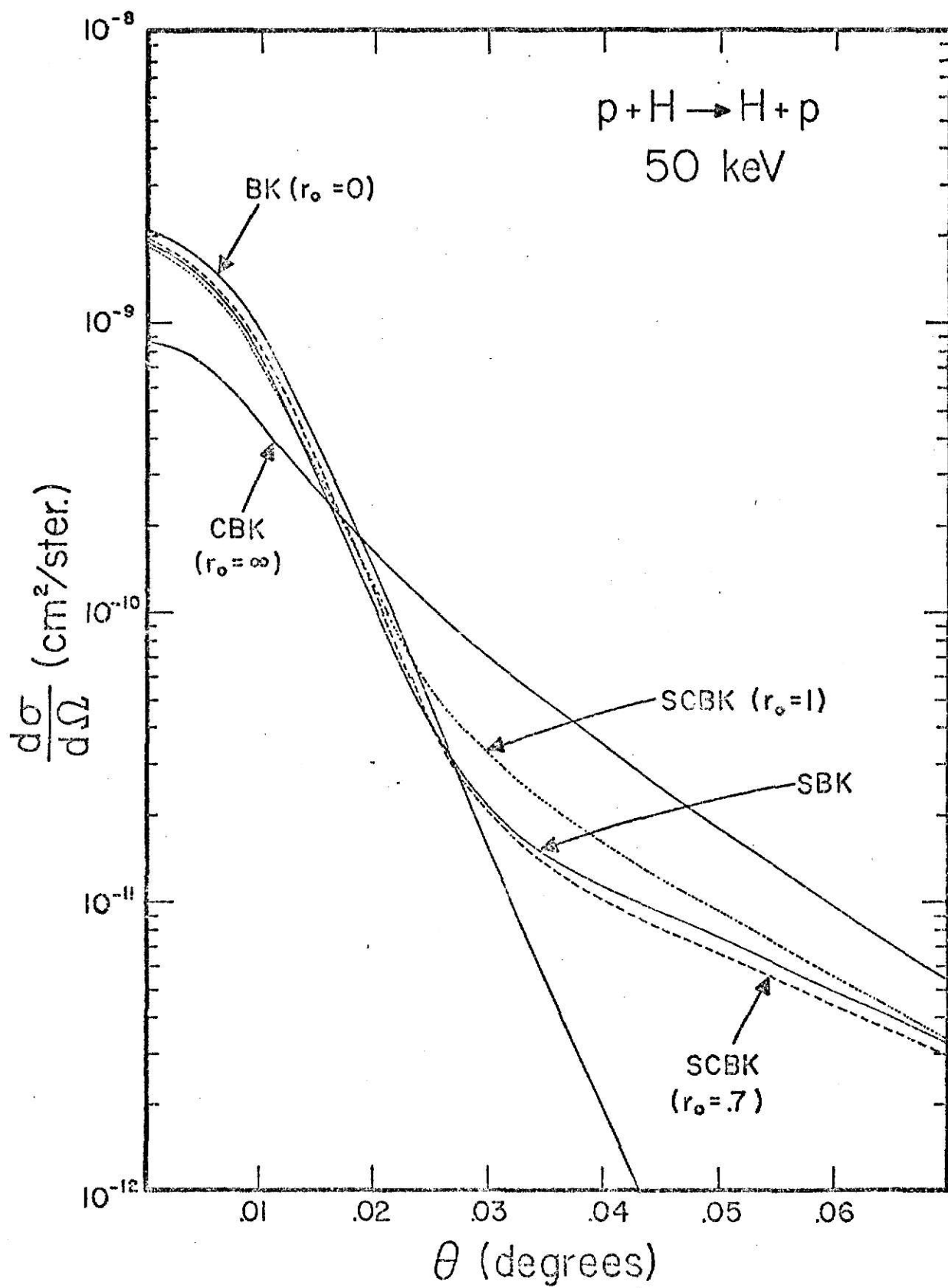
angles ($\theta > \frac{m_e}{m_p}$, where m_e is the mass of the electron and m_p is the projectile mass). The charge parameters used are $Z_a = Z_b = Z^* = 1$.

The SCBK calculation reduces to BK and CBK in the limiting cases for screening parameters. The BK curve in figure 3 is obtained by choosing the screening radius in SCBK to be 10^{-2}, cf. eq. 3.21. The CBK curve is obtained by choosing the screening radius in SCBK to be 10^2, cf. eq. 3.22. There were difficulties in choosing extreme values for the screening parameter due to the Bessel function subroutines. However, it is noted that in atomic dimensions $10^{-2} \approx 0$ and $10^2 \approx \infty$. This serves as a check on the SCBK program.

The total integrated cross sections for BK, CBK, and SBK are identical. This is because the eikonal phase appears as an overall phase in the probability amplitude (eq. A2.8), i.e.

$$\sigma_{Total} = 2\pi \int |b(\rho)|^2 \rho d\rho \qquad (3.23)$$

$$= 2\pi \int |b_{BK}(\rho)|^2 \rho d\rho$$

$$= \sigma_{BK},$$

where $b(\rho)$ is the probability amplitude (eq. A2.8), $b_{BK}(\rho)$ is the BK probability amplitude (eq. 2.9), ρ is the impact parameter, σ_{Total} is the total cross section, and σ_{BK} is the BK total cross section. The total integrated cross sections BK, SBK, and CBK are in agreement with the closed form expression for the total BK cross section of $2.96 \cdot 10^{-16}$ cm^2. This serves as a check on the various integration techniques used in the SBK and SCBK computer programs.

The shape of SCBK is not sensitive to reasonable choices of the

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screening parameter. That is, the SCBK calculation for screening radii

on the order the K shell radius (dotted and dashed curves in figure 3)

retains the two region shape of the SBK calculation. For the Bohr screen-

ing radius (eq. 3.19), the SCBK calculation (dashed line) closely follows

that of SBK. This indicates that the screened Coulomb potential with Bohr

screening is a good approximation to the static potential.

3.4   Protons on Helium

Although the angular distribution for protons incident on atomic

hydrogen is easiest to treat theoretically, it is difficult to measure

experimentally simply because hydrogen is diatomic. A comparison with

observed differential cross sections is necessary to check the screening

effects of the electrons on the internuclear potential in the SBK approxi-

mation. For these reasons we choose to consider the charge transfer pro-

cess,

$$p + He \rightarrow H + He^{+}.$$
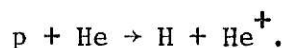
Data for this reaction exists at 293 keV observed by Bratton,[28] et al.,

(1977).

The differential cross section for 293 keV protons incident on helium

is compared with the normalized theoretical predictions of BK, CBK, and

SBK (cf. figure 4). The fact that the theoretical predictions must be

reduced by a factor of 3.55 to agree with the observed cross section of

$9.4 \cdot 10^{-19}$ cm^2/atom indicates a poor asumption has been made. The charge

parameters used in the SBK calculation are $Z_a = 1$, $Z_b = 2$ and $Z^* = 1.618$.

We believe the weakest assumption made is use of the BK probability ampli-

tude in our calculation, for it is well known that the BK results generally

lie above the observed total cross sections. Nevertheless, we are testing

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Figure 4. Differential cross section in laboratory system for capture of K-shell electrons from helium by 293 keV protons. The curve marked BK represents the normalized Brinkman-Kramers approximation; CBK, the normalized Coulomb Brinkman-Kramers approximation, and SBK, the normalized Static Brinkman-Kramers approximation. Each theoretical curve has been reduced by a factor of 3.55 normalizing total cross sections to observed results of $9.4 \cdot 10^{-19}$ cm^2/atom. Experimental data are those of Bratton, et al., (1977).
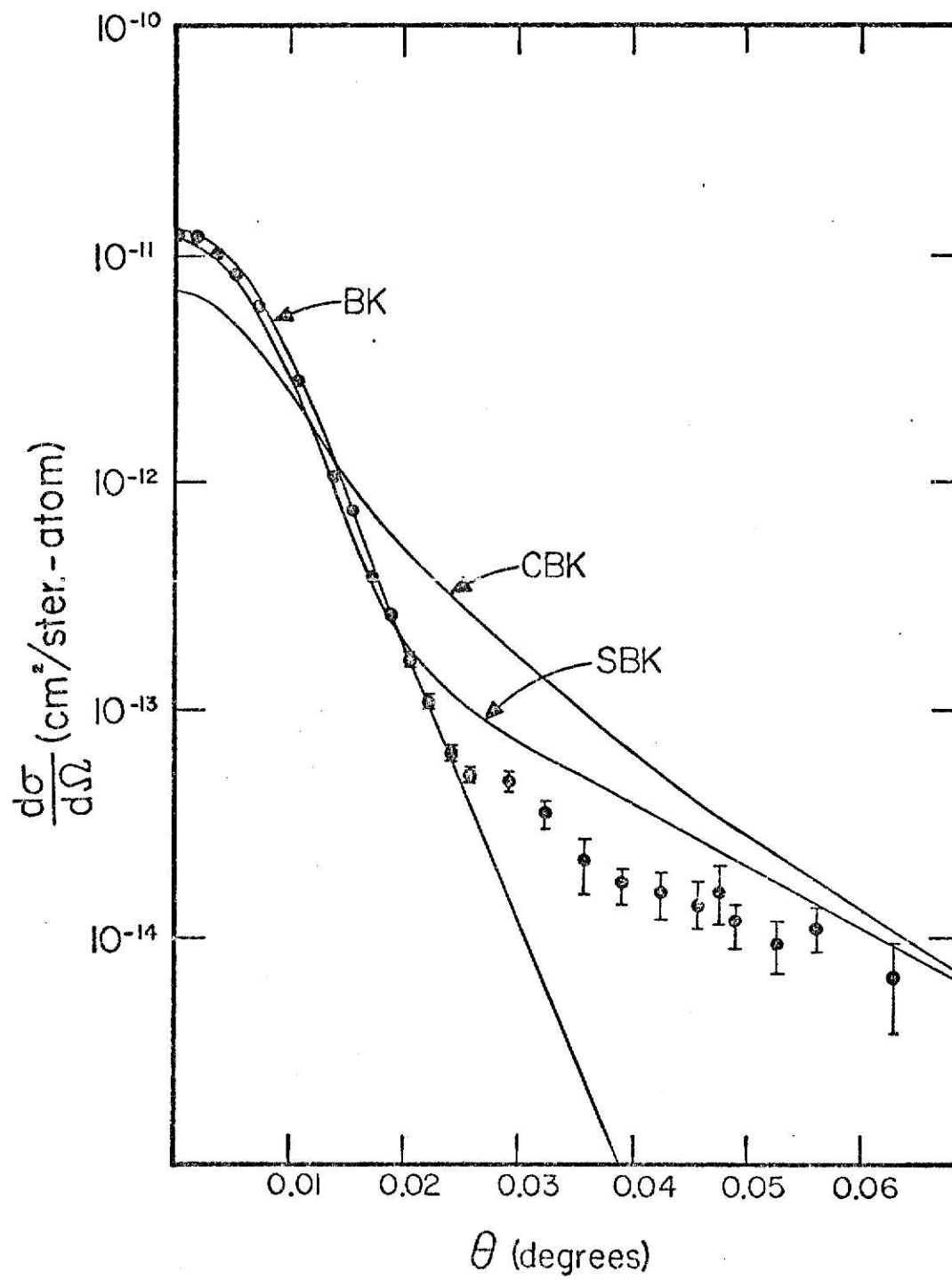
the screening effects on the differential cross section and not the BK approximation. Hence, when comparing our predictions with data, normalization is unavoidable when the BK probability amplitude is used.

There is evidence that a normalization factor is justified for bringing the SBK approximation into close agreement with observation. A recent close coupling calculation of the Bates probability amplitude by Lin[10] indicates the Bates probability amplitude exhibits the same impact parameter dependence as the BK probability amplitude times a constant factor. In addition, the total cross section from this calculation is in agreement with that observed by Bratton, et al., (1977). Another justification of the normalization of SBK is witnessed in a plot of the laboratory angle $\theta_{\frac{1}{2}}$ where the scattering distribution falls to half the maximum intensity as a function of the projectile energy,[29] cf. figure 5. A normalization factor is not an issue in the calculation of $\theta_{\frac{1}{2}}$ since we are considering a ratio of intensities.

SBK gives a better fit to the data than CBK or BK. Referring to figure 4, it is seen that the SBK calculation features two regions, the forward angle region where BK gives a reasonable fit to the data and the large angle region where CBK gives reasonable fit to the data. Referring to figure 5, it is seen that the SBK approximation is superior to CBK in its agreement with data. This is because CBK follows the angular distribution at large angles whereas $\theta_{\frac{1}{2}}$ is calculated at the forward angle region where CBK is in poor agreement. A similar argument can be given as to why BK and SBK agree in the calculation of $\theta_{\frac{1}{2}}$. However, it should be noted that the BK approximation does not give good agreement for large angle capture as witnessed in the angular distribution in figure 4.

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Figure 5. The laboratory angle $\theta_{\frac{1}{2}}$ where the scattering dis-

tribution falls to half the maximum intensity as a function

of the projectile energy. The curve marked BK represents

results using the Brinkman-Kramers approximation; SBK using

the Static Brinkman-Kramers approximation; and CBK the Coulomb

Brinkman-Kramers approximation. Experimental data are due to

(o) Wittkower and Gilbody[30](1967), and (Δ) Bratton,[31] (1977).

$p + He \rightarrow H + He^+$

CBK

BK

SBK

ENERGY (keV)

$\theta_{1/2}^{LAB}$ (MILLIRADIANS)
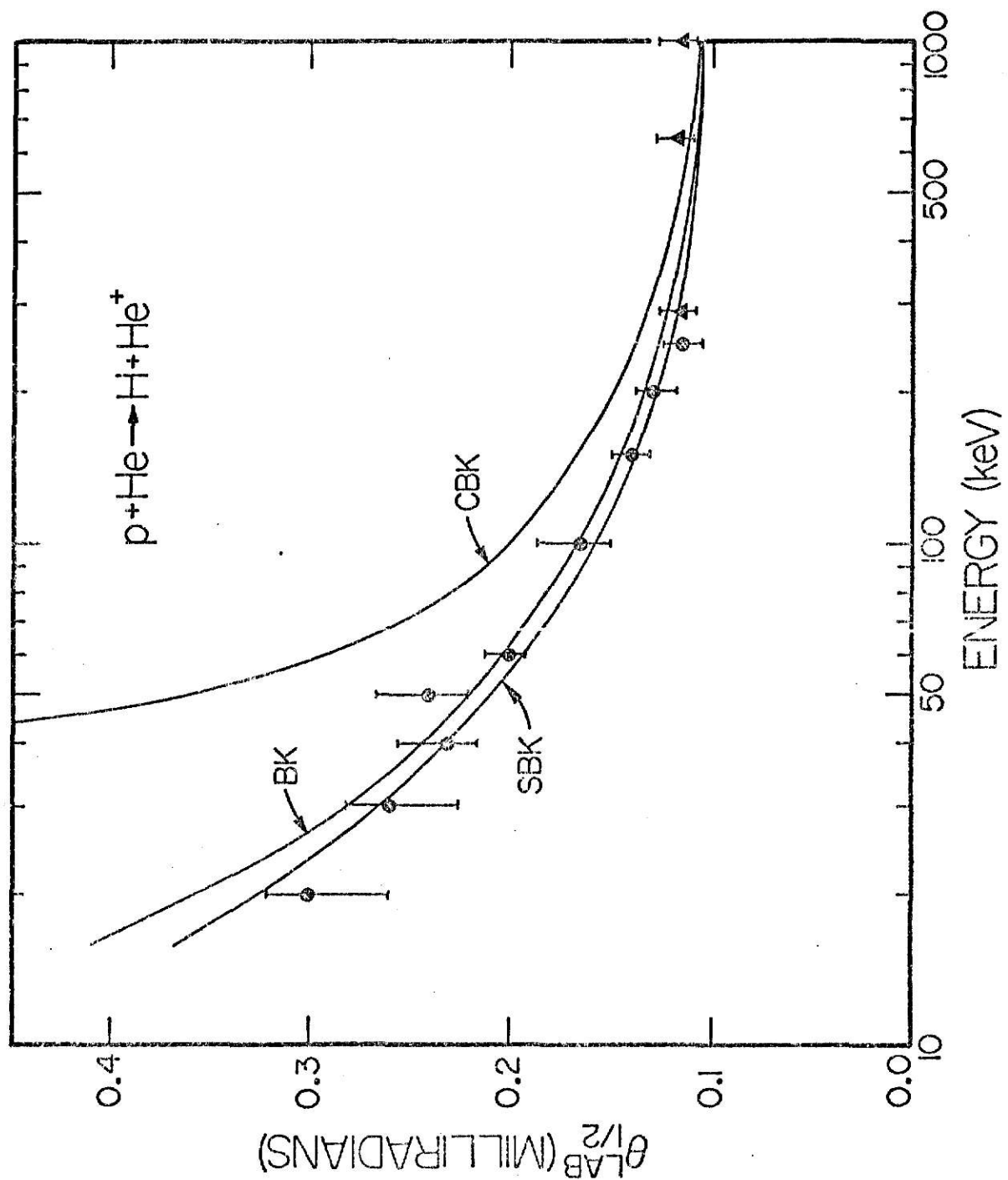
3.5   Protons on Argon

In considering the reaction of protons incident on helium, a nor-
malization factor was introduced to bring the BK, CBK, and SBK calcula-
tions into agreement with the experimental total cross section.   For the
reaction

$$p + Ar \rightarrow H + Ar^+,$$
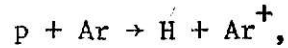
the BK total cross section is in close agreement with the data at a pro-
jectile energy of 6 MeV.   For this reaction, we compare the SCBK approxi-
mation to the data without normalization.

Using hydrogenic wave functions as before and charge parameters
$Z_a = 1$ and $Z_b = Z^* = 18$, we calculate BK, CBK and SCBK, cf. figure 6.
These are precisely the results obtained by Belkic and Salin for the BK
and CBK approximations in figure 2.   The SCBK results are obtained for
Bohr screening which corresponds to the SBK approximation.   The total
cross section for BK (i.e. all curves) is $1.78 \cdot 10^{-23}$ cm^2/atom which
compares with the experimental results[32] of $(1.68 \pm 0.9) \times 10^{-23}$ cm^2/atom.
Again the screened Coulomb Brinkman-Kramers approximation is in better
agreement with the data than either BK or CBK at both the large and small
angles.

Figure 6. Differential cross section in laboratory system for the capture of K-shell electrons from argon by 6 MeV protons. The curve marked BK is the Brinkman-Kramers approximation; CBK, the Coulomb Brinkman-Kramers approximation, and SCBK the Screened Coulomb Brinkman-Kramers approximation. Experimental data are those of Cocke, et al., (1976).

$p + Ar \longrightarrow H + Ar^+$

6 MeV

BK

SCBK

CBK

$\frac{d\sigma}{d\Omega}$ (cm²/ster.- atom)

10^{-17}

10^{-18}

10^{-19}

0   .02   .04   .06   .08   .10   .12   .14   .16

θ (degrees)
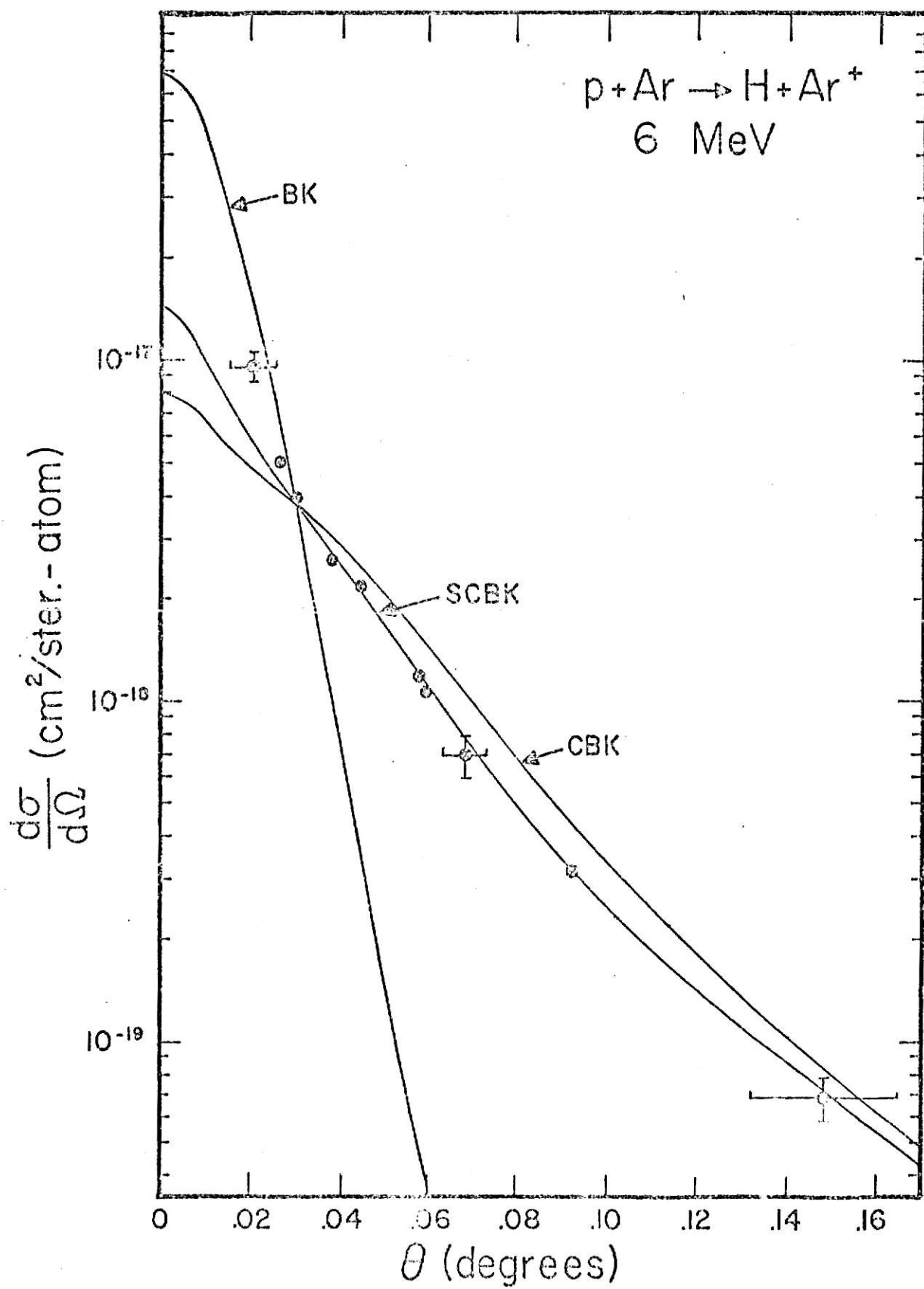
CHAPTER 4

CONCLUSION

The role of the internuclear potential in angular distributions has been examined. Using the eikonal method of McCarroll and Salin, the effective internuclear potential is represented by the static potential. The shape of the angular distribution using this static potential gives improved agreement with observed results of Bratton, et al., over that obtained by Belkic and Salin using an unscreened Coulomb potential and much better agreement than Brinkman and Kramers which takes into account no internuclear repulsion.

As a consequence of choosing the static potential to represent the effective internuclear potential, the electron capture potential is found to be the potential prescribed by Bates. Although the Brinkman-Kramers potential is used to approximate the Bates electron capture potential, the shape of the differential cross section in the Static Brinkman-Kramers (SBK) approximation exhibits two distinct regions in the differential cross section corresponding to observation by Bratton, et al. In contrast to other methods, the SBK approximation has no node in the differential cross section. Since the static potential and the Bates potential are intimately related, the SBK results reinforce use of the Bates potential.

However, our SBK approximation suffers from various limitations. Possible improvements in our calculation include:

    i)   use of the Bates potential in calculating the electron capture probability amplitude,

    ii) use of better wave functions to describe the bound electron, and

iii)   taking into account second order effects.

Other effects are probably less important than these although they may
contribute to a total understanding of charge transfer.

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APPENDIX 1

The Transition Matrix

The form of the transition matrix developed in this section closely
follows that outlined by McCarroll and Salin (1968). Related results have
previously been given by Schiff[33](1954) and Glauber[34](1958). From this
development the validity of the expressions for the transition matrix, and
hence the differential cross section, is clearly shown.

Consider the charge transfer process,

$$A + (e + B) \rightarrow (A + e) + B.$$

A diagram of the position vectors for this reaction is given in Figure 7.
This diagram is used extensively in the steps to follow. In addition,
some vector relations corresponding to the diagram are used:

$$\vec{x} = \vec{r}_2 - \vec{r}_1 \qquad (A1.1)$$

$$\vec{s} = \vec{r}_2 - \vec{r}_3 \qquad (A1.2)$$

$$\vec{R} = \vec{r}_3 - \vec{r}_1 = \vec{x} - \vec{s} \qquad (A1.3)$$

$$\vec{r} = \tfrac{1}{2}(\vec{x} + \vec{s}). \qquad (A1.4)$$

Letting m_a be the mass of the projectile and m_b be the mass of the target,
the following vector quantities are defined from the reduced mass rela-
tions for the respective electron-nucleus systems:

$$\vec{r}_1 + \vec{s} = \frac{m_b}{m_b + 1} \vec{x} \qquad (A1.5)$$

and

Figure 7. The coordinates for the charge transfer process

A + (e +B) → (A + e) + B.

$$A + (e + B) \longrightarrow (A + e) + B$$

e (electron)

$\vec{x}$

$\vec{s}$

center of
mass
(B + e)

$\vec{r}_1$

$\vec{r}_f$

center of
mass
(A + e)

B
(target)

$\vec{R}$

$\vec{r}_1$

$\vec{r}_2$

A
(projectile)

$\vec{r}_3$

$\hat{\rho}$

$\hat{z}$
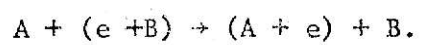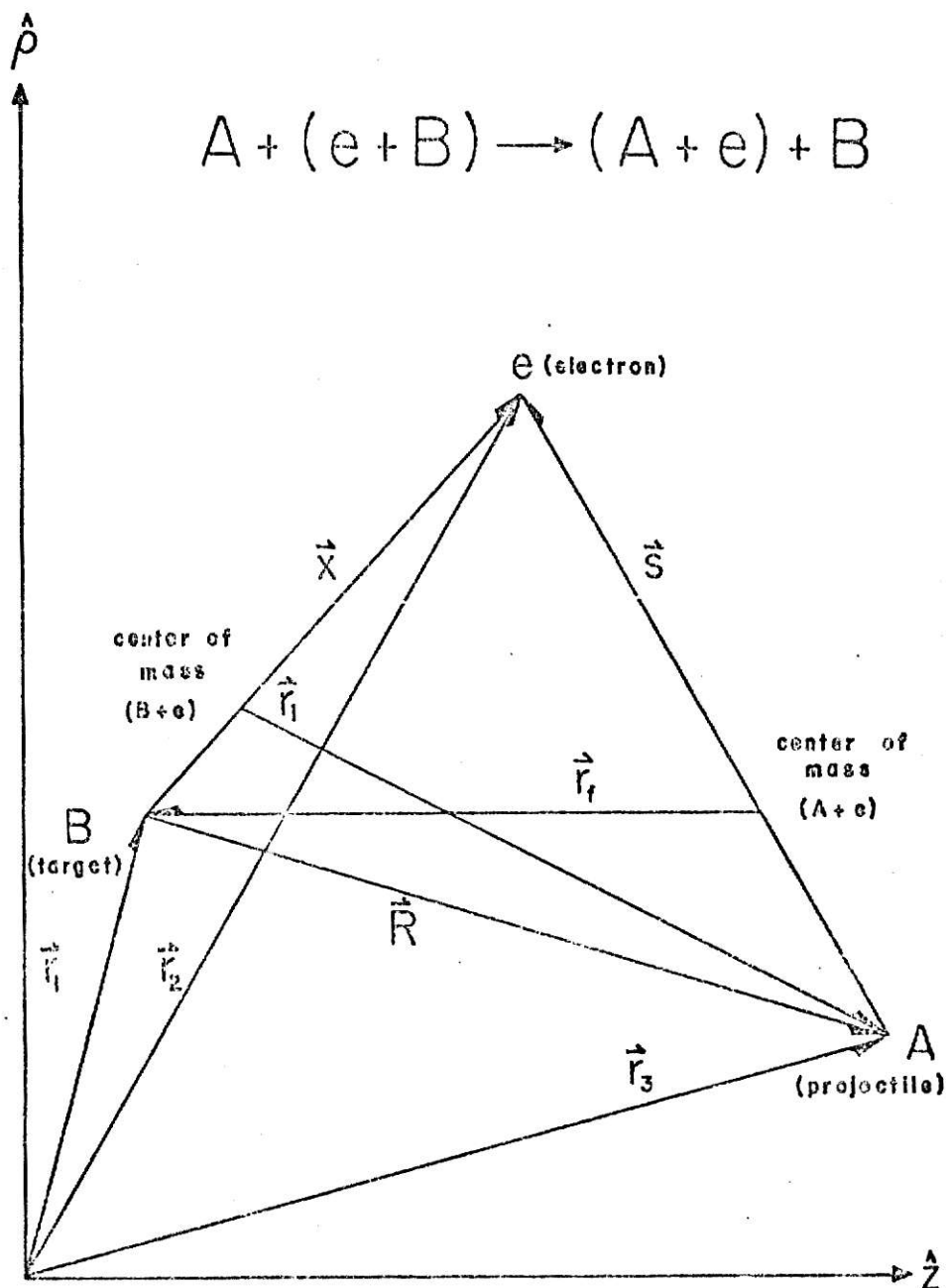
$$\vec{r}_f + \vec{x} = \frac{m_a}{m_a + 1} \; \vec{s}. \tag{A1.6}$$

Upon substitution for $\vec{x}$ and $\vec{s}$ (eq. A1.1 and eq. A1.2) eq. A1.5 and A1.6 become,

$$\vec{r}_i = \vec{r}_3 - \frac{m_b \vec{r}_1 + \vec{r}_2}{m_b + 1} \tag{A1.7}$$

$$\vec{r}_f = \vec{r}_1 - \frac{m_a \vec{r}_3 + \vec{r}_2}{m_a + 1}. \tag{A1.8}$$

A two state wave expansion of the total wave function within the independent electron model is

$$\Psi = \phi_b(\vec{x}) F(\vec{r}_i) + \phi_a(\vec{s}) G(\vec{r}_f), \tag{A1.9}$$

where $\phi_a(\vec{s})$ and $\phi_b(\vec{x})$ are the bound state functions of the active electron around nuclei A and B, respectively. The asymptotic conditions on Ψ are

$$F(\vec{r}_i) \xrightarrow[\vec{r}_i \to \infty]{} \exp(i\vec{k}_i \cdot \vec{r}_i) + O(\frac{1}{r_i})$$

and

$$G(\vec{r}_f) \xrightarrow[\vec{r}_i \to \infty]{} O(\frac{1}{r_f}). \tag{A1.11}$$

The scattered waves are shown to fall off as $\exp(ikr)/r$, i.e. $O(\frac{1}{r})$.

It is now of relative importance to introduce the quantities,

$$F(\vec{r}_i) \equiv \exp(-i\vec{k}_i \cdot \vec{r}_i) F(\vec{r}_i) \tag{A1.12}$$

and

$$G(\vec{r}_f) \equiv \exp(i\vec{k}_i \cdot \vec{r}_f) G(\vec{r}_f). \tag{A1.13}$$

This phase transformation is made for later simplification in the transition matrix.

The transition matrix (eq. 2.18) is now given by,

$$T_{if} \equiv \langle \phi_f | V_f | \Psi_i \rangle$$

$$= \langle \phi_a(\vec{s}) \exp(-i\vec{k}_f \cdot \vec{r}_f) | V_f | \Psi_i \rangle, \tag{A1.14}$$

where Ψ is given by eq. A1.9. Substitution of $F(\vec{r}_i)$ and $G(\vec{r}_f)$ from eqs. A1.12 and A1.13 gives,

$$\Psi = \exp(i\vec{k}_i \cdot \vec{r}_i) L(\vec{x}, \vec{r}_i), \tag{A1.15}$$

where

$$L(\vec{x}, \vec{r}_i) = \phi_b(\vec{x}) F(\vec{r}_i) + \phi_b(\vec{s}) G(\vec{r}_f) \exp\left[-i\vec{k}_i \cdot (\vec{r}_f + \vec{r}_i)\right]. \tag{A1.16}$$

It then follows that the transition matrix is given by,

$$T_{if} = \int d\vec{R} \int d\vec{r} \phi_a^*(\vec{s}) \exp\left[i(\vec{k}_f \cdot \vec{r}_f + \vec{k}_i \cdot \vec{r}_i)\right] V_f L(\vec{x}, \vec{r}_i) \tag{A1.17}$$

Modification of the exponential phase in eq. A1.17 is needed. Consider,

$$\vec{k}_f \cdot \vec{r}_f + \vec{k}_i \cdot \vec{r}_i = \vec{k}_i \cdot \vec{r}_f - \vec{k}_i \cdot \vec{r}_f + \vec{k}_f \cdot \vec{r}_f + \vec{k}_i \cdot \vec{r}_i$$

$$= (\vec{k}_f - \vec{k}_i) \cdot \vec{r}_f + \vec{k}_i \cdot (\vec{r}_i + \vec{r}_f) \tag{A1.18}$$

$$= -\vec{n} \cdot \vec{r}_f + \vec{k}_i \cdot (\vec{r}_i + \vec{r}_f), \tag{A1.19}$$

where the definition,

$$\vec{\eta} \equiv \vec{k}_i - \vec{k}_f, \tag{A1.20}$$

is used. Utilizing eq. A1.3 and eq. A1.6 (also see diagram) it follows

$$-\vec{r}_f \approx \vec{R}, \tag{A1.21}$$

since $m_a \gg 1$. Combining eq. A1.19 and eq. A1.21, the phase is

$$\vec{k}_f \cdot \vec{r}_f + \vec{k}_i \cdot \vec{r}_i \approx \vec{\eta} \cdot \vec{R} + \vec{k}_i \cdot (\vec{r}_i + \vec{r}_f). \tag{A1.22}$$

Noting that

$$\vec{R} = z\hat{z} + \vec{\rho}, \tag{A1.23}$$

where $\hat{z}$ is chosen to be $(2k_i)^{-1}(\vec{k}_i + \vec{k}_f)$ and $\vec{\rho}$ is the plane of impact parameters perpendicular to $\vec{z}$, eq. A1.22 becomes

$$\vec{k}_f \cdot \vec{r}_f + \vec{k}_i \cdot \vec{r}_i \approx \vec{\eta} \cdot \vec{z} + \vec{\eta} \cdot \vec{\rho} + \vec{k}_i \cdot (\vec{r}_i + \vec{r}_f). \tag{A1.24}$$

However, it is observed

$$\vec{\eta} \cdot \vec{z} = \frac{k_i^2 - k_f^2}{2k_i} \ z. \tag{A1.25}$$

From conservation of energy, we have

$$\frac{k_i^2}{2\mu_i} + \varepsilon_i = \frac{k_f^2}{2\mu_f} + \varepsilon_f, \tag{A1.26}$$

where ε_i and ε_f are the initial and final binding energies of the electrons to the respective nuclei B and A. Combining eq. A1.25 with eq.

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A1.26 and noting that

$$\mu \equiv \mu_i = \frac{(m_b + 1)m_a}{m_a + m_b + 1} \approx \frac{(m_a + 1)m_b}{m_a + m_b + 1} = \mu_f, \qquad (A1.27)$$

we get

$$\vec{\eta} \cdot \vec{z} = -\frac{\varepsilon_f - \varepsilon_i}{v} z, \qquad (A1.28)$$

where $\mu v = k_i$ is used. Defining $\Delta E \equiv \varepsilon_f - \varepsilon_i$ and substituting eq. A1.28 into eq. A1.24, the phase takes the form

$$\vec{k}_f \cdot \vec{r}_f + \vec{k}_i \cdot \vec{r}_i \approx \vec{\eta} \cdot \vec{\rho} + \vec{k}_i \cdot (\vec{r}_i \cdot \vec{r}_f) + \frac{\Delta E}{v} z. \qquad (A1.29)$$

Replacing the phase in the transition matrix (eq. A1.17) by eq. A1.29, we obtain

$$T_{if} \approx \int \exp(i\vec{\eta} \cdot \vec{\rho}) d\vec{\rho} \int_{-\infty}^{\infty} dz \int d\vec{r} \phi_a^{\,*}(\vec{s}) \exp(i\xi) V_f L(\vec{x}, \vec{r}_i), \qquad (A1.30)$$

where

$$\xi \equiv \vec{k}_i \cdot (\vec{r}_i + \vec{r}_f) + \frac{\Delta E}{v} z. \qquad (A1.31)$$

Considering only s state to s state electron capture gives our system cylindrical symmetry. Hence, the integration over the plane of impact parameters becomes

$$d\vec{\rho} = \rho d\rho d\alpha \qquad (A1.32)$$

and

$$\vec{\eta} \cdot \vec{\rho} = \eta\rho\cos\alpha, \qquad (A1.33)$$

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where α is the azmuthal angle. The integral,

$$\int_0^{2\pi} \exp(i\eta\rho\cos\alpha)d\alpha \qquad\qquad (A1.34)$$

is the evaluated[35] to be,

$$2\pi J_0(\eta\rho), \qquad\qquad (A1.35)$$

where J_0 is the zero order Bessel function of the first kind. Using the result of eq. A1.35, the transition matrix (eq. A1.30) becomes

$$T_{if} \approx -i2\pi v \int_0^\infty \rho d\rho J_0(\eta\rho)b(\rho), \qquad\qquad (A1.36)$$

where

$$b(\rho) = \frac{i}{v}\int_{-\infty}^\infty dz \int d\vec{r} \phi_a^*(\vec{s})\exp(i\xi)V_f L(\vec{x}, \vec{r}_i). \qquad\qquad (A1.37)$$

It follows immediately (eq. A1.36 and eq. 2.6) that the differential cross section is given by,

$$\frac{d\sigma}{d\Omega} \approx \left| -i\mu v \int_0^\infty \rho d\rho J_0(\eta\rho)b(\rho) \right|^2. \qquad\qquad (A1.38)$$

In arriving at eq. A1.38 near elastic scattering, i.e. $k \equiv k_i \approx k_f$, is assumed.

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APPENDIX 2

The Brinkman Kramers Probability Amplitude

The probability that a projectile will capture an electron at a given impact parameter, ρ, is

$$\text{Probability} = |b(\rho)|^2, \tag{A2.1}$$

where $b(\rho)$ is the probability amplitude. From appendix 1, the probability amplitude is given by

$$b(\rho) = \frac{-i}{v} \exp(2i\delta(\rho)) \int_{-\infty}^{\infty} dz \int d\vec{r}\, \phi_a^*(\vec{s}) \exp(i\xi) \frac{Z_b}{x} \phi_b(\vec{x}), \tag{A2.2}$$

where the BK potential (eq. 2.23) and the projectile wave function (eq. 2.18) are used. Note in the eikonal phase, we have $\vec{k}_i || \hat{z}$. In the probability amplitude (eq. A1.37), we have $\vec{k}_i + \vec{k}_f || \hat{z}$. For small angle scattering, $\vec{k}_i$ is approximately parallel to $\vec{k}_i + \vec{k}_f$.

Using the definitions of the reduced mass (eq. A1.27) and the vector relations (eq. A1.3 - eq. A1.6), the phase (eq. A1.31) becomes

$$\xi = (f + g)\vec{v}\cdot\vec{r} + \tfrac{1}{2}(g - f)\vec{v}\cdot\vec{R} + \frac{\Delta E}{v} z, \tag{A2.3}$$

where

$$f \equiv - \frac{m_a}{(m_a + 1)} \frac{(m_b + 1)}{(m_a + m_b + 1)} \tag{A2.4}$$

and

$$g \equiv - \frac{m_a}{m_a + m_b + 1}. \tag{A2.5}$$

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Noting that

$$v_z \, \hat{z} \approx \vec{v} \qquad\qquad\qquad (A2.6)$$

and that within $O(\frac{1}{\mu})$

$$f + g \approx -1, \qquad\qquad\qquad (A2.7)$$

the probability amplitude (eq. A2.2) becomes

$$b(\rho) = -b_{BK}(\rho) \exp(2i\delta(\rho)), \qquad\qquad (A2.8)$$

where

$$b_{BK}(\rho) = \frac{i}{v} \int_{-\infty}^{\infty} dz \, \exp(i(\frac{v}{2}(g - f) \, z + \frac{\Delta E}{v} z))$$

$$X \int d\vec{r} \phi_a^*(\vec{s}) \frac{Z_b}{x} \phi_b(\vec{x}) \exp(-i\vec{v}\cdot\vec{r}) \qquad (A2.9)$$

Following the Fourier transform method of McDowell and Coleman,[36] the probability amplitude for symmetric charge capture ($Z_a = Z_b \equiv Z$ and $m_a = m_b \equiv M$) is

$$b_{BK}(\rho) = \frac{i}{v} \int_{-\infty}^{\infty} dz \, \exp(i\frac{\Delta E}{v} z) \int d\vec{r} \phi_a^*(\vec{s}) \frac{Z_b}{x} \, \phi_b(\vec{x}) \exp(-i\vec{v}\cdot\vec{r}). \qquad (A2.10)$$

By performing the Fourier transforms on

$$f_a(\vec{k}) \equiv \int \phi_a(\vec{s}) \exp(-i\vec{k}\cdot\vec{s}) d\vec{s} \qquad\qquad (A2.11)$$

and

$$g_b(\vec{K}) \equiv \int \phi_b(\vec{x}) \frac{Z_b}{x} \exp(-i\vec{K}\cdot\vec{x}) d\vec{x} \qquad\qquad (A2.12)$$

to give

$$\phi_a(\vec{s}) = (2\pi)^{-3} \int f_a(\vec{k}) \exp(i\vec{k}\cdot\vec{s}) d\vec{k} \qquad (A2.13)$$

and

$$\frac{Z_b}{x} \phi_b(\vec{x}) = (2\pi)^{-3} \int g_b(\vec{K}) \exp(i\vec{K}\cdot\vec{x}) d\vec{K}, \qquad (A2.14)$$

eq. A2.10 is

$$b_{BK}(\rho) = \frac{i}{v} (2\pi)^{-6} \int_{-\infty}^{\infty} dz \, \exp(i\frac{\Delta E}{v} z) \int d\vec{K} \int d\vec{k} f_a(\vec{k})^* g_b(\vec{K})$$

$$\times \int d\vec{r} \, \exp(i(\vec{K}\cdot\vec{x} - \vec{k}\cdot\vec{s} - \vec{v}\cdot\vec{r})). \qquad (A2.15)$$

From eq. A1.3 and eq. A1.4,

$$\vec{x} = \vec{r} + \tfrac{1}{2} \vec{R} \qquad (A2.16)$$

and

$$\vec{s} = \vec{r} - \tfrac{1}{2} \vec{R}, \qquad (A2.17)$$

the integration over $\vec{r}$ reduces eq. A2.15 to

$$b_{BK}(\rho) = \frac{i}{v} (2\pi)^{-3} \int_{-\infty}^{\infty} dz \, \exp(i \frac{\Delta E}{v} z) \exp(\frac{i}{2} \vec{v}\cdot\vec{R})$$

$$\times \int d\vec{k} f_a(\vec{k})^* g_b(\vec{k} + \vec{v}) \exp(i\vec{k}\cdot\vec{R}). \qquad (A2.18)$$

Recalling that

$$\vec{R} = \rho\hat{\rho} + z\hat{z} \qquad (A2.19)$$

and choosing

$$\vec{k} = k_x\hat{x} + k_y\hat{y} + k_z\hat{z} \qquad (A2.20)$$

such that $\hat{x}||\hat{\rho}$, the BK probability amplitude (eq. A2.18) is

$$b_{BK}(\rho) = \frac{1}{v} \, (2\pi)^{-3} \int_{-\infty}^{\infty} dk_x \int_{-\infty}^{\infty} dk_y \int_{-\infty}^{\infty} dk_z \, f_a(k_x, \, k_y, \, k_z)^*$$

$$X \; g_b(k_x, \, k_y, \, k_z + v) \exp(i\rho k_x) \int_{-\infty}^{\infty} dz \, \exp(iz(\frac{v}{2} + k_z)). \qquad (A2.21)$$

At this time, we further limit our development of the BK probability amplitude to consider K shell to K shell capture. The 1s wave function in momentum space is

$$f_a(k) = \frac{8\pi^{\frac{1}{2}} Z_a^{5/2}}{(k^2 + Z_a^2)^2} \qquad (A2.22)$$

which gives

$$g_b(\vec{k} + \vec{v}) = \frac{4\pi^{\frac{1}{2}} Z_b^{5/2}}{((\vec{k} + \vec{v})^2 + Z_b^2)}. \qquad (A2.23)$$

Completing the integration over $\vec{z}$ and substituting eq. A2.22 and eq. A2.23, eq. A2.21 is

$$b_{BK}(\rho) = \frac{i8Z^5}{\pi v} \int_{-\infty}^{\infty} dk_x \int_{-\infty}^{\infty} dk_y \, \exp(i\rho k_x) (k_x^2 + k_y^2 + \beta)^{-3}, \qquad (A2.24)$$

where

$$\beta = \frac{v^2}{4} + z^2. \qquad (A2.25)$$

Integrating over k_y, eq. A2.24 reduces to

$$b_{BK}(\rho) = \frac{i6Z^5}{v} \int_{0}^{\infty} \frac{\cos(\rho k_x)}{(k_x^2 + \beta)^{5/2}} \, dk_x. \qquad (A2.26)$$

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The last integration, eq. A2.26 is

$$b_{BK}(\rho) = \left(\frac{2i}{v}\right) z^5 \left[\frac{\rho^2}{\beta}\right] K_2 \left(\beta^{\frac{1}{2}}\rho\right), \qquad (A2.27)$$

where K_2 is the second-order modified Bessel function of the third kind. This corresponds to the transition probability amplitude calculated in a straight-line impact parameter method given by Belkic and Salin as,

$$b_{BK}(\rho) = \left(\frac{2i}{v}\right) \left(Z_a Z_b\right)^{5/2} \left[\frac{\rho^2}{\gamma_o}\right] K_2 \left(\gamma_o^{\frac{1}{2}}\rho\right), \qquad (A2.28)$$

where

$$\gamma_o = Z_b^2 + \left[\frac{v}{2} + \frac{\Delta E}{v}\right]^2. \qquad (A2.29)$$

An even more general expression given by McGuire and Cocke is given as,

$$b_{BK}(\rho) = \left(\frac{2i n_a}{v}\right) \left(\frac{Z_a Z_b}{n_a n_b}\right)^{5/2} \left(\frac{\rho^2}{\gamma}\right) K_2 \left(\gamma^{\frac{1}{2}}\rho\right), \qquad (A2.30$$

where

$$\gamma = \frac{Z_b^2}{n_b^2} + \left[\frac{v}{2} + \frac{1}{2v}\left(\frac{Z_a^2}{n_a^2} - \frac{Z_b^2}{n_b^2}\right)\right]^2 \qquad (A2.31)$$

and

$$\Delta E = \frac{1}{2}\left(\frac{Z_a^2}{n_a^2} - \frac{Z_b^2}{n_b^2}\right). \qquad (A2.32)$$

The principal quantum numbers are indicated by n_a and n_b for the respective nuclei A and B. The probability amplitude in eq. A2.30 is justified[19]

only when there is a one-to-one correspondence between the angle and
impact parameter, in contrast to eq. A2.28.

APPENDIX 3

The computer program for the calculation of the differential cross section for the static potential in the eikonal phase, cf. Section 3.1, is listed.

```
//WATFIV   JOB (5228O4023,DMB0S4N8),'S.R.ROGERS',TIME=(,59)
// EXEC WATFIV
//SYSIN    DD *
$JOB          ,TIME=(,59),PAGES=15
C COMPUTES DIFFERENTIAL CRCSS SECTION FCR SCREENED COULOMB BRINKMAN -
C KRAMER'S APPROXIMATION FOR ELECTRON CAPTURE.  INCLUDES EIKONAL
C PHASE AND CAPTURE PROBABILITY WORKED OUT IN THEORY BY STEVEN R.
C ROGERS AND JAMES H. MC GUIRE, KANSAS STATE UNIVERSITY.
C
C HYDROGEN (1S) TC HYCROGEN (1S) STATES
C
      IMPLICIT REAL*8(A-H,O-Z)
      REAL*8 MA,MB,NA,NB,KC,MU
      REAL*8 LAB
      COMMON COEF,XBAR,KC,THETA,RO,THETAD,ETA
      DIMENSION XW(100,10)
      EXTERNAL FOFY
      EXTERNAL GOFY
      PI=3.14159265358S8
      ICRDER=12
      NUMBER=ICRDER/4
C
C READ IN GAUSS LEGENDRE WEIGHTS AND ABCISSA ARRAY, XW
C
      READ 10, ((XW(I,J),J=1,4),I=1,NUMBER)
   10 FORMAT (4D20.14)
C
C READ IN INCIDENT ENERGY OF PROJECTILE IN ELECTRON VCLTS
C
      READ 1, EINC
    1 FORMAT (D20.14)
      PRINT 3, EINC
    3 FORMAT ('1',20X,'SCREENED COULCMB BRINKMAN KRAMERS APPROXIMATION'
     1    //21X,'ENERGY (IN ELECTRON VOLTS)= ',1PD11.4/ )
C
C READ IN PROJECTILE(A)-TARGET(B) CHARGE AND MASS (ELECTRON MASS = 1)
C
```

```
      READ 2, ZA,ZB,MA,MB
    2 FORMAT (4D20.14)
C
C PRINCIPLE QUANTUM NUMBERS OF PROJECTILE-ELECTRON SYSTEM (NA) AND TARGET-
C ELECTRON SYSTEM (NB)
C
      NB=1.
      NA=1.
C
C ENERGY IN RYDBERGS
C
      RYDB=13.6D0
      EINC=EINC/RYDB
C
      VO=(EINC/MA)**0.5D0
      MU=MA*MB/(MA+MB)
      KO=VO*MU
      ZABAR=ZA/NA
      ZBBAR=ZB/NB
C
C LIMITS OF INTEGRATION FOR DIFFERENTIAL CROSS SECTIONS
C
      AA=1.D-10  /ZBBAR
      BB=.1D0    /ZEBAR
      CC=1.      /ZEBAR
      DD=2.      /ZEBAR
      EE=5.      /ZEBAR
      FF=10.  /ZBBAR
C
      SBAR=VO/ ZBBAR*(1.-(ZBBAR**2-ZABAR**2)/VO**2)
      XBAR=ZBBAR*(1.+SBAR**2/4.)**.5D0
      C1=NA*32*PI*(ZBBAR*ZABAR)**2.5D0
      COEF=KO*C1/(16*VO*PI*XBAR**2)
C
C AO IS THE RADIUS OF THE FIRST BOHR ORBIT, RO IS SCREENING PARAMETER
C
      AC=1.
```

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```
      RO=AO/2/ZB
      PRINT 21, RO
   21 FORMAT (' ',20X,'SCREENING RADIUS (IN AO)    = ',1PD11.4//)
      PRINT 11,ZA,MA,NA,ZB,MB,NB
   11 FORMAT (' ',15X,'CHARGE',13X,'MASS (ELECTRON MASS = 1)',5X,'PRINCI
     1PLE QUANTUM NO.'//1X,'PROJECTILE',5X,'ZA = ',F10.0,4X,'MA = ',
     2F10.0,14X,'NA = ',F10.0//1X,'TARGET',9X,'ZB = ',F10.4,4X,'MB = ',
     3F10.0,14X,'NB = ',F10.0/)
      BETA=(VO**4+2*VO**2*(ZBBAR**2+ZABAR**2)+(ZBBAR**2-ZABAR**2)**2)
     1/(4*VO**2)
      CLOSED=2**8*(ZA*ZB)**5/(5*VO**2*NA**3*NB**5*BETA**5)
C
C
C     THE NUCLEAR CHARGE OF THE NUCLEUS IS 1 FOR HYDROGEN.
C
      ETA=2.*ZA*ZB/VO
      THETAM=0.
      THETA=0.
      THETAD=0.
      SCBK=0.
      ORK=0.
      TAU=0.
      TAU=MA/MB
      PRINT 101
  101 FORMAT (' ', 8X,'THETA',20X,'THETA',21X,'DIFFERENTIAL CROSS SECTIO
     1NS',9X,'RUNNING TOTAL CROSS SECTIONS'/6X,'(IN RADIANS)',13X,
     2'(IN DEGREES)',21X,'(IN PI*AO**2/RADIAN)',21X,'(IN PI*AO**2)'//
     353X,'BRINKMAN KRAMERS',9X,'SCREENED COULOMB',9X,'B-K.',9X,'SCBK'//
     442X,'(C.M.)',7X,'(LAB)',7X,'(C.M.)',7X,'(LAB)',7X,'(C.M.)',
     557X,'(LAB)',7X,'(C.M.)',7X,'(LAB)',7X,'(C.M.)',7X,'(C.M.)'//)
      DO 50 ITER=1,50
      THETAS=PI/1.D6
      THETAM=THETA
C
C OUTPUT SCALING TO COVER WIDEST RANGE OF VALUES OF ANGLE
C
      IF (THETAD-2.D-2) 75,76,76
```

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```
   75 THETA=(THETA+THETAS)*1.3D0
      GO TO 77
   76 THETAS=5.D-5
      IF (THETAD.GT.6.D-2) THETAS=THETAS*4.
      THETA=THETA+THETAS
   77 THETAD=THETA*180.D0/PI
      LAB=(1.+2.*TAU*DCOS(THETA)+TAU**2)**1.5D0/DABS(1.+TAU*DCOS(THETA))
      THETA1=DARCCS((DCOS(THETA)+TAU)/(1.+2.*TAU*DCOS(THETA)+
     1TAU**2)**.5D0)
      THETD1=THETA1*180./PI
      DTHETA=THETA-THETAM
      A2=VC**2*((1.D0-(ZBBAR**2-ZABAR**2)/VC**2)**2+4.*MU**2*THETA**2)/4
      HTHETA=C1*MU/(2.D0**.5D0*PI*(ZBBAR**2+A2)**3)
      DQCBK=HTHETA**2
      DCCBKL=DQCBK*LAB
      GCCBK=DGCCBK*THETA*DTHETA
      CBK=DBK+QCBK
      FOFY1=0.
      GOFY2=0.
      IF (THETAD.GT.0.3) GO TO 86
C
C FOFY IS THE REAL PART OF F(THETA)
C
      CALL SSIGMA (FOFY,AA,BB,CC,DD,EE,FF,5,XW,NUMBER,1,FOFY1)
C
C GOFY IS THE IMAGINARY PART OF F(THETA)
C
   86 CALL SSIGMA (GOFY,AA,BB,CC,DD,EE,FF,5,XW,NUMBER,2,GOFY2)
      DIFCRS=(FOFY1**2+GOFY2**2)*2
      DIFCRL=DIFCRS*LAB
      SCREEN=DIFCRS*THETA*DTHETA
      SCBK=SCBK+SCREEN
      PRINT 22,THETA,THETA1,THETAD,THETD1,DQCBK,DQCBKL,DIFCRS,DIFCRL,
     1CBK,SCBK
   22 FORMAT (' ',1PD11.4,4(2X,1PD10.4,2X,1PD11.5),2X,1PD11.5)
      IF (THETAD.GE.2.) GO TO 51
   50 CONTINUE
```

```
   51 PRINT 88
   88 FORMAT ('0','TOTAL CROSS SECTIONS IN UNITS OF PI*AO**2')
      PRINT 44, CLOSED,OBK,SCBK
   44 FORMAT (' ','CLOSED FORM BK = ',1PD20.13,'; INTEGRAL VALUE BK = ',
     1 1PD20.13,'; SCREENED COULOMB BK = ',1PD20.13)
      STOP
      END
C
C SUBROUTINE FOR GETTING FUNCTION INTO INTEGRATION ROUTINE
C
      DOUBLE PRECISION FUNCTION FOFY (B)
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*8 KO
      COMMON COEF,XBAR,KO,THETA,RO,THETAD,ETA
      CALL BESK (XBAR*B,2,BK2,IER2)
      IF (IER2.NE.0) PRINT 6, IER2
    6 FORMAT (' ','IEP FOR BESK 2 IS ',I2)
      CALL BESK (B/RO,0,BKO,IERO)
      IF (IERO.NE.0) PRINT 7, IERO
    7 FORMAT (' ','IER FOR BESK 0 IS ',I2)
      CALL BESK (B/RO,1,BK1,IER1)
      IF (IER1.NE.0) PRINT 10, IER1
   10 FORMAT (' ', IER FOR BESK 1 IS ',I2)
      CALL BESJO (KO*THETA*B,BJ,IER)
      IF (IER.NE.0) PRINT 8, IER
    8 FORMAT (' ','IER FOR BESJ IS ',I2)
      FOFY=COEF*B**3*DSIN(ETA*(BKO+B/RO/2*BK1))*BK2*BJ
      RETURN
      END
C
      DOUBLE PRECISION FUNCTION GOFY (B)
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*8 KO
      COMMON COEF,XBAR,KO,THETA,RO,THETAD,ETA
      CALL BESK (XBAR*B,2,BK2,IER2)
      IF (IER2.NE.0) PRINT 6, IER2
    6 FORMAT (' ','IER FOR BESK 2 IS ',I2)
```

```
      CALL BESK (B/RC,0,BK0,IERO)
      IF (IER0.NE.0) PRINT 7, IERO
    7 FORMAT (' ','IER FOR BESK 0 IS ',I2)
      CALL BESK (B/R0,1,BK1,IER1)
      IF (IER1.NE.0) PRINT 10, IER1
   10 FORMAT (' ','IER FOR BESK 1 IS ',I2)
      CALL BESJ0 (KO*THETA*B,BJ,IER)
      IF (IER.NE.0) PRINT 8, IER
    8 FORMAT (' ','IER FOR BESJ IS ',I2)
      GOFY=COEF*B**3*DCOS(ETA*(BK0+B/RO/2*BK1))*BK2*BJ
      RETURN
      END
```

```
      SUBROUTINE BESK                                          BESK   40
                                                               BESK   50
C     COMPUTE THE K BESSEL FUNCTION FOR A GIVEN ARGUMENT AND ORDERBESK 60
C                                                              BESK   70
C     USAGE                                                    BESK   80
C        CALL BESK(X,N,BK,IER)                                 BESK   90
C                                                              BESK  100
C     DESCRIPTION OF PARAMETERS                                BESK  110
C        X  -THE ARGUMENT OF THE K BESSEL FUNCTION DESIRED     BESK  120
C        N  -THE ORDER OF THE K BESSEL FUNCTION DESIRED        BESK  130
C        BK -THE RESULTANT K BESSEL FUNCTION                   BESK  140
C        IER-RESULTANT ERROR CODE WHERE                        BESK  150
C           IER=0  NO ERROR                                    BESK  160
C           IER=1  N IS NEGATIVE                               BESK  170
C           IER=2  X IS ZERO OR NEGATIVE                       BESK  180
C           IER=3  X .GT. 170, MACHINE RANGE EXCEEDED          BESK  190
C           IER=4  BK .GT. 10**70                              BESK  200
C                                                              BESK  210
C     REMARKS                                                  BESK  220
C        N MUST BE GREATER THAN OR EQUAL TO ZERO               BESK  230
C                                                              BESK  240
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED            BESK  250
C        NONE                                                  BESK  260
C                                                              BESK  270
```

```
C     METHOD                                                          BESK 280
C     COMPUTES ZERO ORDER AND FIRST ORDER BESSEL FUNCTIONS USING      BESK 290
C     SERIES APPROXIMATIONS AND THEN COMPUTES N TH ORDER FUNCTION     BESK 300
C     USING RECURRENCE RELATION.                                      BESK 310
C     RECURRENCE RELATION AND POLYNOMIAL APPROXIMATION TECHNIQUE      BESK 320
C     AS DESCRIBED BY A.J.M.HITCHCOCK,'POLYNOMIAL APPROXIMATIONS      BESK 330
C     TO BESSEL FUNCTIONS OF ORDER ZERO AND ONE AND TO RELATED        BESK 340
C     FUNCTIONS', M.T.A.C., V.11,1957,PP.86-88, AND G.N. WATSON,      BESK 350
C     'A TREATISE ON THE THEORY OF BESSEL FUNCTIONS', CAMBRIDGE       BESK 360
C     UNIVERSITY PRESS, 1958, P. 62                                   BESK 370
C     .......                                                         BESK 380
C     .......                                                         BESK 390
C     .......                                                         BESK 400
      SUBROUTINE BESK(X,N,BK,IER)                                     BESK 410
      IMPLICIT REAL*8(A-H,O-Z)                                        BESK 415
      REAL*8 KC                                                       BESK 420
      COMMON COEF,XBAR,KO,THETA,RO,THETAD,ETA                         BESK 430
      DIMENSION T(12)                                                 BESK 440
      BK=.0                                                           BESK 450
      IF(N)10,11,11                                                   BESK 460
   10 IER=1                                                           BESK 470
      RETURN                                                          BESK 480
   11 IF(X)12,12,20                                                   BESK 490
   12 IER=2                                                           BESK 500
      RETURN                                                          BESK 510
   20 IF(X-170.0)22,22,21                                             BESK 520
   21 IER=3                                                           BESK 530
      RETURN                                                          BESK 540
   22 IER=0                                                           BESK 550
   25 IF(X-1.)36,36,25                                                BESK 560
   25 A=DEXP(-X)                                                      BESK 570
      B=1./X                                                          BESK 580
      C=DSQRT(B)                                                      BESK 590
      T(1)=B                                                          BESK 600
      DO 26 L=2,12                                                    BESK 610
   26 T(L)=T(L-1)*B
      IF(N-1)27,29,27
```

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```
C
C     COMPUTE K0 USING POLYNOMIAL APPROXIMATION                          BESK 620
C                                                                        BESK 630
                                                                         BESK 640
   27 G0=A*(1.2533141-.1566642*T(1)+.0881128*T(2)-.0913095*T(3)         BESK 650
     2+.1344596*T(4)-.2299850*T(5)+.3792410*T(6)-.5247277*T(7)           BESK 660
     3+.5575368*T(8)-.4262633*T(9)+.2184518*T(10)-.0668097*T(11)         BESK 670
     4+.0091893*T(12))*C                                                 BESK 680
      IF(N)20,28,29                                                      BESK 690
   28 BK=G0                                                              BESK 700
      RETURN                                                             BESK 710
C                                                                        BESK 720
C     COMPUTE K1 USING POLYNOMIAL APPROXIMATION                          BESK 730
C                                                                        BESK 740
   29 G1=A*(1.2533141+.4699927*T(1)-.1468583*T(2)+.1280427*T(3)         BESK 750
     2-.1736432*T(4)+.2847618*T(5)-.4594342*T(6)+.6283381*T(7)           BESK 760
     3-.6632295*T(8)+.5050239*T(9)-.2581304*T(10)+.0788001*T(11)         BESK 770
     4-.0108241*T(12))*C                                                 BESK 780
      IF(N-1)20,30,31                                                    BESK 790
   30 BK=G1                                                              BESK 800
      RETURN                                                             BESK 810
C                                                                        BESK 820
C     FROM K0,K1 COMPUTE KN USING RECURRENCE RELATION                    BESK 830
C                                                                        BESK 840
   31 DO 35 J=2,N                                                        BESK 850
      GJ=2.*(DFLOAT(J)-1.)*G1/X+G0                                       BESK 860
      IF(GJ-1.0E70)33,33,32                                              BESK 870
   32 IER=4                                                              BESK 880
      GO TO 34                                                           BESK 890
   33 G0=G1                                                              BESK 900
   35 G1=GJ                                                              BESK 910
   34 BK=GJ                                                              BESK 920
      RETURN                                                             BESK 930
   36 B=X/2.                                                             BESK 940
      A=.5772157+DLOG(B)                                                 BESK 950
      C=B*B                                                              BESK 960
      IF(N-1)37,43,37                                                    BESK 970
C                                                                        BESK 980
```

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```
C
C     COMPUTE K0 USING SERIES EXPANSION
C
37    G0=-A
      X2J=1.
      FACT=1.
      HJ=.0
      DO 40  J=1,6
      RJ=1./DFLOAT(J)
      X2J=X2J*C
      FACT=FACT*RJ*RJ
      HJ=HJ+RJ
40    G0=G0+X2J*FACT*(HJ-A)
      IF(N)43,42,43
42    BK=G0
      RETURN
C
C     COMPUTE K1 USING SERIES EXPANSION
C
43    X2J=R
      FACT=1.
      HJ=1.
      G1=1./X+X2J*(.5+A-HJ)
      DO 50  J=2,8
      X2J=X2J*C
      RJ=1./DFLOAT(J)
      FACT=FACT*RJ*RJ
      HJ=HJ+RJ
50    G1=G1+X2J*FACT*(.5+(A-HJ)*DFLOAT(J))
      IF(N-1)31,52,31
52    BK=G1
      RETURN
      END
C     SUBROUTINE BESJ0 (X,BJ,IER)
C     COMPUTES THE J-ZERO BESSEL FUNCTION
C
C     USAGE: CALL BESJ0 (X,BJ,IER)
C
```

```
BESK 990
BESK1000
BESK1010
BESK1020
BESK1030
BESK1040
BESK1050
BESK1060
BESK1070
BESK1080
BESK1090
BESK1100
BESK1110
BESK1120
BESK1130
BESK1140
BESK1150
BESK1160
BESK1170
BESK1180
BESK1190
BESK1200
BESK1210
BESK1220
BESK1230
BESK1240
BESK1250
BESK1260
BESK1270
BESK1280
BESK1290
BESK1300
```

```
      SUBROUTINE BESJO (X,BJ,IER)
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*8 KO
      COMMON COEF,XBAR,KO,THETA,RO,THETAO,ETA
      VALUE1=X/3.DO
      VALUE2=3.DO/X
      IF (X+3.) 50,100,100
   50 IER=1
      RETURN
  100 IER=0
      IF (X-3.) 150,150,200
  150 BJ=1.DO-2.2499997DO*(VALUE1)**2+1.2656208DO*(VALUE1)**4-
     1.3163866DO*(VALUE1)**6+.0444479DO*(VALUE1)**8-.0039444DO*(VALUE1)
     2**10+.0002100DO*(VALUE1)**12
      RETURN
  200 FO=.79788456DO-.00000077DO*(VALUE2)-.00552740DO*(VALUE2)**2
     1-.00009512DO*(VALUE2)**3+.00137237DO*(VALUE2)**4-.00072805DO*
     2(VALUE2)**5+.00014476DO*(VALUE2)**6
      THETAO=X-.78539816DO-.04166397DO*(VALUE2)-.00003954DO*(VALUE2)**2
```

```
      1+.0026262573D0*(VALUE2)**3-.0005412500*(VALUE2)**4-.0002933300*   SIGMA 01
      2(VALUE2)**5+.0001355800*(VALUE2)**6                               SIGMA 02
      BJ=F0*DCOS(THETA0)/X**.5D0                                         SIGMA 03
      RETURN                                                             SIGMA 04
      END                                                                SIGMA 05
C SUBROUTINE SSIGMA                                                      SIGMA 06
C                                                                        SIGMA 07
C     COMPUTE THE INTEGRAL OF THE FUNCTION (Y) USING GAUSS              SIGMA 08
C     LEGENDRE INTEGRATION TECHNIQUE.                                    SIGMA 09
C                                                                        SIGMA 10
C USAGE                                                                  SIGMA 11
C     CALL SSIGMA (FOFY,A,B,C,D,E,F,N,XW,NUMBER,INVERT,SSUM)            SIGMA 12
C                                                                        SIGMA13A
C DESCRIPTION OF PARAMETERS                                             SIGMA13B
C     A-F ARE POINTS OF INTEGRATION                                     SIGMA13C
C     N- NUMBER OF INTERVALS TO INTEGRATE                               SIGMA13D
C     XW - GAUSS LEGENDRE WEIGHTS AND ABCISSA ARRAY                     SIGMA 14
C     NUMBER - ORDER OF THE LEGENDRE POLYNOMIAL USED/4                  SIGMA 15
C     INVERT - SWITCHES THE FUNCTION IN THE INTEGRATION SUBROUTINE      SIGMA 16
C              FFOM FOFY (1) TO GOFY (2)                                SIGMA 17
C     SSUM - THE RESULTING INTEGRAL VALUE                               SIGMA 18
C                                                                        SIGMA 19
C REMARKS                                                                SIGMA 20
C     ORDER MUST BE DIVISIBLE BY 4                                      SIGMA 21
C                                                                        SIGMA 22
C SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                         SIGMA 23
C     DOUBLE PRECISION FUNCTION FOFY (Y)                                SIGMA 24
C     IMPLICIT REAL*8(A-H,O-Z)                                          SIGMA 25
C     FOFY = FUNCTION TO BE INTEGRATED                                  SIGMA 26
C     RETURN                                                             SIGMA 27
C     END                                                                SIGMA 28
C                                                                        SIGMA 29
C MUST PRECEDE MAIN PROGRAM
C     IMPLICIT REAL*8(A-H,O-Z)
C     DIMENSION XW(100,10)
C     EXTERNAL FOFY
C
```

```
C MUST PRECEDE SUBROUTINE SSIGMA                                          SIGMA 30
C A-F, N, AND NUMBER                                                      SIGMA 31
CC                                                                        SIGMA 32
CC   READ IN GAUSS LEGENDRE WEIGHTS AND ABCISSA ARRAY, XW                 SIGMA 33
CC                                                                        SIGMA34A
C    READ 10, ((XW(I,J),J=1,4),I=1,NUMBER)                                SIGMA34B
C 10 FORMAT (4D20.14)                                                     SIGMA34C
C                                                                         SIGMA34D
C                                                                         SIGMA35A
C .................................................................       SIGMA35B
      SUBROUTINE SSIGMA (FOFY,AA,BB,C,D,E,F,N,XW,NUMBER,INVERT,SSUM)      SIGMA35C
      IMPLICIT REAL*8(A-H,O-Z)                                            SIGMA35D
      REAL*8 KO
      COMMON.COEF,XBAR,KC,THETA,RO,THETAD,ETA
      DIMENSION XW(100,10)
      A=AA                                                                SIGMA 36
      B=BB                                                                SIGMA 37
      SSUM=0.                                                             SIGMA 38
      M=0                                                                 SIGMA 39
   30 M=M+1                                                               SIGMA 40
      NEG=1                                                               SIGMA 41
   40 I=0                                                                 SIGMA 42
   50 DO 100 IX=1,NUMBER                                                  SIGMA 43
      J=-1                                                                SIGMA 44
      I=I+1                                                               SIGMA 45
      DO 100 JX=1,2                                                       SIGMA 46
      J=J+2                                                               SIGMA47A
      K=J+1                                                               SIGMA47R
      Y=(B-A)/2.DO*XW(I,J)*NEG+(B+A)/2.DO                                 SIGMA47C
      IF (INVERT-1) 1,1,2                                                 SIGMA47D
    1 TOFY=FOFY(Y)                                                        SIGMA47E
      GO TO 3                                                             SIGMA47F
    2 TOFY=GOFY(Y)                                                        SIGMA 48
    3 CONTINUE                                                            SIGMA 49
      SUM=(B-A)/2.DO*XW(I,K)*TOFY                                         SIGMA 50
  100 SSUM=SSUM+SUM                                                       SIGMA 51
      IF (NEG) 200,200,150
  150 NEG=NEG-2
```

```
      GO TO 40                                                          SIGMA  52
200   GO TO (220,270,320,370,420),M                                     SIGMA  53
220   CONTINUE                                                          SIGMA  54
      IF (M-N) 260,420,420                                              SIGMA  56
260   A=B                                                               SIGMA  57
      B=C                                                               SIGMA  58
      GO TO 30                                                          SIGMA  59
270   CONTINUE                                                          SIGMA  60
      IF (M-N) 310,420,420                                              SIGMA  62
310   A=C                                                               SIGMA  63
      B=D                                                               SIGMA  64
      GO TO 30                                                          SIGMA  65
320   CONTINUE                                                          SIGMA  66
      IF (M-N) 360,420,420                                              SIGMA  68
360   A=D                                                               SIGMA  69
      B=E                                                               SIGMA  70
      GO TO 30                                                          SIGMA  71
370   CONTINUE                                                          SIGMA  72
      IF (M-N) 410,420,420                                              SIGMA  74
410   A=E                                                               SIGMA  75
      B=F                                                               SIGMA  76
      GO TO 30                                                          SIGMA  77
420   CONTINUE                                                          SIGMA  78
      RETURN                                                            SIGMA  80
      END                                                               SIGMA  81
$ENTRY
9.8156063424671 9E-014.7175336386511 8E-029.0411725637047 5E-011.0693932599531 8E-01
7.6990267419430 5E-011.6007822854334 6E-015.8731795428661 7E-012.0316742672306 6E-01
3.6783149898180 0E-012.3349253653835 5E-011.2523340851146 9E-012.4914704581340 3E-01
50.               E 3.
1.0000000 0     E 00 1.000     E 00 1836.     E 00 1836.     E 00
/*
```

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APPENDIX 4

The main program for the Screened Coulomb Brinkman-Kramers approximation is listed, cf. Section 3.2. The three subroutines not listed are identical to those used in Appendix 3.

```
//WATFIV   JOB (52304028,DMBOS4N8),'S.R.ROGERS',TIME=(,59)
// EXEC WATFIV
//SYSIN   DD *
$JOB            ,TIME=(,59),PAGES=15
C CCMPUTES DIFFERENTIAL CROSS SECTION FOR SCREENED COULOMB BRINKMAN -
C KRAMER'S APPROXIMATION FOR ELECTRON CAPTURE.  INCLUDES EIKONAL
C PHASE AND CAPTURE PROBABILITY WORKED OUT IN THEORY BY STEVEN R.
C ROGERS AND JAMES +. MC GUIRE, KANSAS STATE UNIVERSITY.
C
C ARGON (1S) TO HYDROGEN (1S) STATES
C
C
      IMPLICIT REAL*8(A-H,O-Z)
      REAL*8 MA,MB,NA,NB,KO,MU
      REAL*8 LAB
      COMMON COEF,XBAR,KO,THETA,RO,THETAD,ETA
      DIMENSION XW(100,10)
      EXTERNAL FOFY
      EXTERNAL GOFY
      PI=3.141592653589B
      IORDER=12
      NUMBER=IORDER/4
C
C READ IN GAUSS LEGENDRE WEIGHTS AND ABCISSA ARRAY, XW
C
      READ 10, ((XW(I,J),J=1,4),I=1,NUMBER)
   10 FORMAT (4D20.14)
C
C READ IN INCIDENT ENERGY OF PROJECTILE IN ELECTRON VOLTS
C
      READ 1, EINC
    1 FORMAT (D20.14)
      PRINT 3, EINC
    3 FORMAT ('1',20X,'SCREENED COULOMB BRINKMAN KRAMERS APPROXIMATION'
     1 //21X,'ENERGY (IN ELECTRON VOLTS)= ',1PD11.4/ )
C
C READ IN PROJECTILE(A)-TARGET(B) CHARGE AND MASS (ELECTRON MASS = 1)
C
```

```
      READ 2, ZA,ZB,MA,MB
    2 FORMAT (4D20.14)
C
C  PRINCIPLE QUANTUM NUMBERS OF PROJECTILE-ELECTRON SYSTEM (NA) AND TARGET-
C  ELECTRON SYSTEM (NB)
C
      NB=1.
      NA=1.
C
C  ENERGY IN RYDBERGS
C
      RYDB=13.6D0
      EINC=EINC/RYDB
C
      VO=(EINC/MA)**0.500
      MU=MA*MB/(MA+MB)
      KO=VO*MU
      ZABAR=ZA/NA
      ZBBAR=ZB/NB
C
C  LIMITS OF INTEGRATION FOR DIFFERENTIAL CROSS SECTIONS
C
      AA=1.D-10  /ZBBAR
      BB=.1D0    /ZBBAR
      CC=1.      /ZBBAR
      DD=2.      /ZBBAR
      EE=5.      /ZBBAR
      FF=10.     /ZBBAR
C
      SBAR=VO/ ZBBAR*(1.-(ZBBAR**2-ZABAR**2)/VO**2)
      XBAR=ZBBAR*(1.+SBAR**2/4.)**.5D0
      C1=NA*32*PI*(ZBBAR*ZABAR)**2.5D0
      COEF=KO*C1/(16*VO*PI*XBAR**2)
C
C  AO IS THE RADIUS OF THE FIRST BOHR ORBIT, RO IS SCREENING PARAMETER
C
      AC=1.
```

```
      RO=1.
      RC=1.D-2
      RC=1.D2
      RC=AO/(ZA**(2.DO/3.DO)+ZB**(2.DO/3.DO))**.5DO
      PRINT 21, RC
   21 FORMAT (' ',20X,'SCREENING RADIUS (IN AO)    = ',1PD11.4//)
      PRINT 11,ZA,MA,NA,ZB,MB,NB
   11 FORMAT (' ',15X,'CHARGE',13X,'MASS (ELECTRON MASS = 1)',5X,'PRINCI
     1PLE QUANTUM NO.'//1X,'PROJECTILE',5X,'ZA = ',F10.0,4X,'MA = ',
     2F10.0,14X,'NA = ',F10.0//1X,'TARGET',9X,'ZB = ',F10.4,4X,'MB = ',
     3F10.0,14X,'NB = ',F10.0/)
      BETA=(VO**4+2*VO**2*(ZBBAR**2+ZABAR**2)+(ZBBAR**2-ZABAR**2)**2)
     1/(4*VO**2)
      CLOSED=2**8*(ZA*ZB)**5/(5*VO**2*NA**3*NB**5*BETA**5)
      ETA=2.*ZA*ZB/VO
      THETAM=0.
      THETA=0.
      THETAD=0.
      SCBK=0.
      CBK=0.
      TAU=0.
      TAU=MA/MB
      PRINT 101
  101 FORMAT (' ', 8X,'THETA',20X,'THETA',21X,'DIFFERENTIAL CROSS SECTIO
     1NS',9X,'RUNNING TOTAL CROSS SECTIONS'/6X,'(IN RADIANS)',13X,
     2'(IN DEGREES)',21X,'(IN PI*AO**2/RADIAN)',21X,'(IN PI*AO**2)'//
     353X,'BRINKMAN KRAMERS',9X,'SCREENED COULOMB',9X,'B.K.',9X,'SCBK'//
     442X,'(C.M.)',7X,'(LAB)',7X,'(C.M.)',7X,'(LAB)',7X,'(C.M.)',7X,
     557X,'(LAB)',7X,'(C.M.)',7X,'(LAB)',7X,'(C.M.)',7X,'(C.M.)'//)
      DO 50 ITER=1,50
      THETAS=PI/1.D6
      THETAM=THETA
C
C OUTPUT SCALING TO COVER WIDEST RANGE OF VALUES OF ANGLE
C
      IF (THETAD-2.D-2) 75,76,76
   75 THETA=(THETA+THETAS)*1.3DO
```

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```
      GO TO 77
   76 THETAS=5.D-5
      IF (THETAD.GT.6.D-2) THETAS=THETAS*4.
      THETA=THETA+THETAS
   77 THETAD=THETA*18C.DO/PI
      LAB=(1.+2.*TAU*DCOS(THETA)+TAU**2)**1.5D0/CABS(1.+TAU*DCOS(THETA))
      THETA1=DARCOS((DCOS(THETA)+TAU)/(1.+2.*TAU*DCOS(THETA)+
     1TAU**2)**.5C0)
      THETD1=THETA1*18O./PI
      DTHETA=THETA-THETAM
      A2=VO**2*((1.DO-(ZBBAR**2-ZABAR**2)/VC**2)**2+4*MU**2*THETA**2)/4
      HTHETA=C1*MU/(2.DO**.5DO*PI*(ZBBAR**2+A2)**3)
      DQCBK=HTHETA**2
      DQCBKL=DQCBK*LAB
      QOBK=DQCBK*THETA*DTHETA
      CBK=OBK+QCBK
      FOFY1=0.
      GOFY2=0.
      IF (THETAD.GT.0.3) GO TO 86
C
C FOFY IS THE REAL PART OF F(THETA)
C
      CALL SSIGMA (FOFY,AA,BB,CC,DC,EE,FF,5,XW,NUMBER,1,FOFY1)
C
C GOFY IS THE IMAGINARY PART OF F(THETA)
C
      CALL SSIGMA (GOFY,AA,BB,CC,DC,EE,FF,5,XW,NUMBER,2,GOFY2)
   86 DIFCRS=(FOFY1**2+GOFY2**2)*2
      DIFCRL=DIFCRS*LAB
      SCREEN=DIFCRS*THETA*DTHETA
      SCBK=SCBK+SCREEN
      PRINT 22,THETA,THETA1,THETAD,THETD1,DQCBK,DQOBKL,DIFCRS,DIFCRL,
     1CBK,SCBK
   22 FORMAT (' ',1PD11.4,4(2X,1PD1C.4,2X,1PD11.5),2X,1PD11.5)
      IF (THETAD.GE.2.) GO TO 51
   50 CONTINUE
   51 PRINT 88
```

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```
88 FORMAT ('0','TOTAL CROSS SECTIONS IN UNITS OF PI*AO**2')
   PRINT 44, CLOSED,OBK,SCBK
44 FORMAT (' ','CLOSED FORM BK = ',1PD20.13,'; INTEGRAL VALUE BK = ',
  11PD20.13,'; SCREENED CCULOMB BK = ',1PD20.13)
   STOP
   END
C
C SUBROUTINE FOR GETTING FUNCTION INTO INTEGRATION ROUTINE
C
   DOUBLE PRECISION FUNCTION FOFY (B)
   IMPLICIT REAL*8 (A-H,O-Z)
   REAL*8 KO
   COMMON COEF,XRAR,KO,THETA,RO,THETAD,ETA
   CALL BESK (XBAR*B,2,BK2,IER2)
   IF (IER2.NE.0) PRINT 6, IER2
6  FORMAT (' ','IER FOR BESK 2 IS ',I2)
   CALL BESK (B/RO,0,BKO,IERO)
   IF (IERO.NE.0) PRINT 7, IERO
7  FORMAT (' ','IER FOR BESK 0 IS ',I2)
   CALL BESJO (KO*THETA*B,BJ,IER)
   IF (IER.NE.0) PRINT 8, IER
8  FORMAT (' ','IER FOR BESJ IS ',I2)
   FOFY=COEF*B**3*DSIN (ETA *BKO)*BK2 *BJ
   RETURN
   END
C
   DOUBLE PRECISION FUNCTION COFY (B)
   IMPLICIT REAL*8 (A-H,O-Z)
   REAL*8 KO
   COMMON COEF,XBAR,KO,THETA,RO,THETAD,ETA
   CALL BESK (XPAR*B,2,BK2,IER2)
   IF (IER2.NE.0) PRINT 6, IER2
6  FORMAT (' ','IER FOR BESK 2 IS ',I2)
   CALL BESK (B/RO,0,BKO,IERO)
   IF (IERO.NE.0) PRINT 7, IERO
7  FORMAT (' ','IER FOR BESK 0 IS ',I2)
   CALL BESJO (KO*THETA*B,BJ,IER)
```

```
      IF (IER.NE.0) PRINT 8, IER
    8 FORMAT (' ',' IER FOR BESJ IS ',I2)
   9000 Y=COEF*B**3*DCCS (ETA  *BKO)*BK2 *BJ
      RETURN
      END
C
C     SUBROUTINE BESK                                      BESK  40
C                                                          BESK  50

             . . .

$ENTRY
9.8156063424671 9E-014.717533638651 18E-029.0411725637 0475E-011.0693932599 5318E-01
7.6960267419 4305E-011.6007832854 3346E-015.8731795428 6617E-012.0315742672 3066E-01
3.5783149899 8130E-012.3349253653 6355E-011.2523340851 1469E-012.4914704581 3403E-01
6.0           E 6
1.00000000    E 00 18.00    E 00     1836.    E 00    73440.    E 00
/*
```

DIFFERENTIAL CROSS SECTIONS FOR CHARGE

TRANSFER USING SCREENED COULOMB POTENTIALS

IN THE EIKONAL APPROXIMATION

by

STEVEN RAY ROGERS

B.A., University of Northern Colorado, 1975

———————————

AN ABSTRACT OF A MASTER'S THESIS

submitted in partial fulfillment of the

requirements for the degree

MASTER OF SCIENCE

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Manhattan, Kansas

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The effects of electronic screening of the internuclear potential in charge transfer is considered. By studying the differential cross section, the role of the internuclear potential is examined. Using the eikonal method of McCarroll and Salin (1968), the effective internuclear potential is represented by the static potential. The differential cross section for capture of K-shell electrons from helium by 293 keV protons observed by Bratton, et al., (1977), are compared with the theoretical predictions of Brinkman and Kramers (BK), Belkic and Salin (CBK), and myself (SBK). The shape of the observed differential cross section is in closer agreement to SBK, which uses the static potential, than BK, which uses no potential, or CBK, which uses the full Coulomb potential. The SBK differential cross section yields an improvement over CBK for the capture of K-shell electrons from argon by 6 MeV protons observed by Cocke, et al., (1976). Both CBK and SBK show marked improvements over BK.