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MULTIPLE ELECTRON CAPTURE AT HIGH VELOCITIES

USING THE BATES POTENTIAL IN THE

INDEPENDENT ELECTRON APPROXIMATION

by

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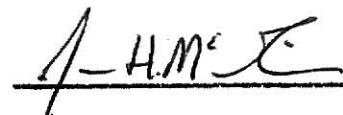
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CHAPTER 1

INTRODUCTION

Since the atom is a microscopic quantity, its properties
cannot be determined using macroscopic measuring devices
directly. One way to investigate the atom is to probe it
with a particle that is of the same relative size. In an
atom-ion collision, this particle is a fast moving ionic
projectile. It is incident upon the target atom to be
investigated, usually at some known energy, trajectory
and charge state. As the projectile passes near the atom,
it is deflected from its original path. At the same time
some of the electronic properties of the atom and the ion
may be altered. Studying the results of the collision
reveals information about the structure of the target and
the forces of interaction between the two systems.

The quantity that is measured in an atom-ion collision
is the total cross section. It is proportional to the
probability that if the projectile is in a particular
initial state, its interaction with the target will cause
a transition into a particular final state. Two transitions
of interest are excitation of a projectile electron into a
higher energy level, and ionization of a projectile electron
into the continuum. Extensive work has been done in the
calculation of both excitation and ionization cross sections.
It has been shown that there is another type of transition
that occurs. This is known as electron capture or charge
transfer.

Electron capture is a rearrangement collision in which one or more electrons initially bound to the target atom are, upon collision, transferred to the projectile. This process is believed to be significant in many aspects of physical research as well as in the study of the structure of the atom. One such aspect is astrophysics. Since multiply charged ions are present in the interstellar medium, along with neutral hydrogen and helium atoms, if charge capture reactions are rapid at the thermal energies of the medium, they play an important role in reducing the fractional abundance of such ions.[1] Then charge capture must be included in calculations of models to be compared with observed physical conditions of the interstellar medium.

Louisell et. al.[2] have applied charge transfer to the development of an x-ray laser. The process they propose invloves passing a beam of bare nuclei through a target and capturing electrons into a particular excited state. Then population inversion will cause the stimulated emission of x-rays of a particular wavelength. Sweeping the ions along a foil at speeds near that of light will cause the radiation emitted from the first ions to stimulate radiation from the inverted ions arriving along the foil later. Hence charge transfer could provide a mechanism for pumping of the required excited-state population.

The role of charge exchange in nuclear fusion studies is discussed by Crandall et. al.[3] It is significant in such properties as charge-state distribution, resistivity and energy transfer. It is believed that charge transfer

between multicharged impurities and neutral particles injected into a plasma may be instrumental in stopping the injected beam at the outer edge of the plasma, thus destroying the needed plasma heating. Klinger et. al.[4] emphasize the need for the charge transfer process in the ion source extraction region of heavy-ion accelerators. This process, in which atoms are repeatedly stripped of electrons while being accelerated, has opened new possibilities in the design of high energy, heavy-ion accelerators.

Since the range of application of multiple charge capture is so broad, it is important to develop a suitable formalism for the collision process. Much work has been done in the calculation of first order single charge capture cross sections. Since the transition matrix is too complicated to solve exactly, one must approximate the initial and final wave functions and the perturbing potential used. Several attempts have been made to calculate single capture cross sections that closely agree with those experimentally measured.

Oppenheimer[5], in 1928, and Brinkman and Kramers[6], in 1930, calculated cross sections for a single K-shell electron of hydrogen captured into the K-shell of a proton. They used the product of a plane wave and a bound state hydrogen wave function for their initial and final wave functions. This is the first Born approximation. They argued that the internuclear potential should not have an appreciable effect on the probability of charge capture since its only effect seems to be a slight deflection of the projectile. Their total interaction potential, then, is the Coulomb

attraction between the projectile ion and the electron to
be captured. When compared to experiment, their results
seem to have the right shape, but are too large by a factor
of four near incident energies of 100 KeV, and even larger
at smaller energies.

Jackson and Schiff[7], in 1953, and Bates and Dalgarno,[8]
in 1952, used the sum of the projectile-electron and the
projectile-target nucleus potentials as the perturbing potential
in their calculations. They argued that since charge capture
is a three body problem involving non-orthogonal initial and
final states, the internuclear term is not negligible.
Combining this with the first Born wave functions, they
obtained cross sections for protons on hydrogen that were
in better agreement with experiment than those of Oppenheimer
and Brinkman and Kramers.

A distorted wave Born approximation[9] is used by Bassel
and Gerjuoy[10] in an attempt to reconcile the problem of
whether or not to include the internuclear potential. The
result of their use of the total interaction potential
(electron-projectile and nuclear-nuclear interactions) and
the plane wave limit to the distorted wave Born approximation
in the transition matrix turns out to be the same as using
the plane wave Born approximation wave functions combined
with the difference between the instantaneous and average
interaction potentials. This does not depend on the inter-
nuclear term directly. Their total cross sections for
charge capture of a single electron from the ground state
of the hydrogen atom to the ground state of the incident

proton is in best agreement with experiment of the three procedures presented.

Bates[11], in 1958, approaches the problem from a different point of view. He recognizes that the inclusion of the dubious internuclear potential does in fact improve agreement with experiment, but explains that the reason for the inclusion is unsatisfactory. The internuclear potential should have little effect on the total cross section especially for fast moving projectiles. He shows that one needs rather to be concerned with the problems of the non-orthogonality of the initial and final states and with the incongruous fact that the choice of the zero point potential alters the total cross sections. His final results are very similar to those of Bassel and Gerjuoy but the physical interpretation for his calculations is a bit more palatable.

First order calculations have been extended to single capture involving arbitrary projectile and target charge states as well as capture into higher energy levels for a wide variety of incident energies. A summary of these results for hydrogen targets has been compiled by Tawara and Russek.[12] More general results are reviewed by Betz.[13]

Only recently has any attempt been made to develop a formalism to calculate multiple capture cross sections. It is known that double charge capture is the dominant process for resonant systems at low energies. In the case of alpha particles on helium, double capture cross sections are almost an order of magnitude larger than single capture cross sections at energies of about 10 KeV.[14] Crandall et. al.[3] have shown

that in this energy range, double capture is also the dominant process for C^{+4} on helium.

Even though multiple charge transfer is accepted as an important process, and a great deal of experimental data for multiple capture is available, few theoretical calculations have been attempted because the interaction is too complicated to be dealt with using previously developed techniques. Gerasimenko[15] has calculated double capture cross sections by protons from helium using the first Born approximation. His results are two orders of magnitude higher than experimental values. Roy et. al.[16] used an impact parameter formalism[17] to calculate the same cross sections. They too get poor agreement with experiment. Biswas et. al.[18] investigate an integral approximation to the three state close-coupling formalism for protons on helium. They get excellent agreement with experiment for incident energies from 5 KeV to 1 MeV. This agreement is not well understood, however, since their method is the wave treatment counterpart to the impact treatment of Roy et. al. and one would expect similar results. C. D. Lin[19] uses a three state close-coupling formalism too, and replaces the interelectron Coulomb interaction by a monopole term with a screening charge. He extends the calculation to higher charge states, and gets good agreement with experiment.

It is the purpose of this thesis to present a different approach to the calculation of multiple charge transfer cross sections. The independent electron approximation developed by Mc Guire and Weaver[20] for atomic scattering by

heavy particles will be applied to the case of charge transfer. In this approximation, the full wave function for the scattering system is expressed as a product of single electron wave functions, and the cross sections for multiple electron transfer are expressed as products of single electron probabilities. This approximation is independent of the perturbation theory one chooses to use. This means that all the techniques considered when dealing with single charge capture are applicable to the problem of multiple charge transfer in this independent electron approximation.

The Bates-Born approximation is used to calculate cross sections for single charge capture from the ground state of helium atoms to the ground state of alpha particles in the incident energy range of 0 to 1000 KeV. This calculation is compared to experiment and the discrepancies noted. Then charge capture cross sections are calculated for the same system. The discrepancies here are compared to those for single capture in order to test the validity of the independent electron approximation.

CHAPTER 2

CROSS SECTIONS

In a scattering experiment, a target is bombarded by a monoenergetic beam of particles of known incident flux. A detector with a finite detecting area is placed at a particular angle with respect to the direction of the incident beam. It counts the number of particles deflected into that angle per unit time. This number normalized by the incident flux, I, is known as the differential cross section. Symbolically,

$$\frac{d\sigma}{d\Omega} = \frac{d N(\theta, \phi)}{I} \; .$$

Classically, the particles approach the scattering center at a distance b from its center, and are scattered through an angle, θ. The distance, b, is known as the impact parameter, and θ is referred to as the scattering angle. Since the detector has a finite area, particles scattered into angles from θ to $\theta + d\theta$ will be detected. The total number of particles counted per second is then,

$$dN(\theta, \phi) = I \, b \, db \, d\phi$$

and the classical differential cross section is

$$\frac{d\sigma}{d\Omega} = \frac{b \, db \, d\phi}{d\Omega} = b \frac{db}{d(\cos \theta)}$$

The particles of concern here can be thought of quantum

mechanically as waves. In order to define a quantum mechanical differential cross section, one assumes that the motion of the particles involved in the scattering process may be described by the Hamiltonian

$$H = H_o + V_i,$$

where V_i is effective over only a finite range. The incident partical flux may be visualized as the superposition of plane waves. The scattering center may be regarded as the source of spherical waves. The simplest expression for the incident wave is a normalized plane wave

$$\Psi_{in} = A e^{i \vec{k}_i \cdot \vec{r}},$$

where $\vec{k}_i$ is the initial momentum of the system, $\vec{r}$ is the position vector of the incident beam, μ_i is the reduced mass of the initial system, and A is the normalizing amplitude such that the intensity of the incident beam is

$$I = |\Psi_{in}|^2 \cdot \frac{\hbar k_i}{\mu_i} = \frac{\hbar k_i}{\mu_i}.$$

Asymptotically, the final wave function may be expressed as the superposition of the incident plane wave and some angular dependent amplitude times a spherical wave.

$$\Psi_{out} = A e^{i \vec{k}_i \cdot \vec{r}} + f(\theta) \frac{e^{i \vec{k}_i \cdot \vec{r}}}{r}.$$

The intensity of the beam scattered at an angle θ is

$$N(\theta) = \left| f(\theta) \frac{e^{i \vec{k}_i \cdot \vec{r}}}{r} \right|^2 \cdot \frac{\hbar k_i}{\mu_i} = |f(\theta)|^2 \frac{\hbar k_i}{\mu_i r^2}.$$

Then the number of particles scattered into the detector

of area, $r^2 d\Omega$ is

$$dN(\theta, \phi) = |f(\theta)|^2 \cdot \frac{\hbar k_i}{\mu_i} \, d\Omega.$$

Hence the quantum mechanical differential cross section is

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

and $f(\theta)$ is known as the scattering amplitude.

If the perturbation, V_i, is effective over only a finite range, one may assume it is small in comparison with H_o and may solve the Schrödinger equation for the system

$$H\Psi = i\hbar \frac{\partial \Psi}{\partial t},$$

using time-dependent perturbation theory.[21] The resulting transition rate from an initial state Ψ_i to a final state Ψ_f is

$$w_{if} = \frac{2\pi}{\hbar} \, \rho_f \, |\langle \Psi_f | V_i | \Psi_i \rangle|^2.$$

For a system with final momentum $\vec{k}_f$, and final reduced mass μ_f in a volume L^3, the density of final states is

$$\rho_f = \frac{\mu_f k_f L^3}{8\pi^3 \hbar^2} \, d\Omega.$$

The quantity $\langle \Psi_f | V_i | \Psi_i \rangle$ will be referred to as the transition matrix element or transition matrix and will be denoted by T_{if}. Then

$$w_{if} = \frac{\mu_f k_f L^3}{4\pi^2 \hbar^3} \, |T_{if}|^2 \, d\Omega.$$

Since the transition rate is equivalent to the number of particles detected per unit time, the differential cross

section may be expressed as

$$\frac{d\sigma}{d\Omega} = \frac{w_{if}}{I \, d\Omega} .$$

Since the incident flux was shown above to be

$$I = \frac{\hbar k_i}{\mu_i L^3} ,$$

the differential cross section may be expressed in terms of the transition matrix as follows

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 = \mu_i \mu_f \left(\frac{k_f}{k_i}\right) \left(\frac{L^3}{2\pi \hbar^2}\right)^2 |T_{if}|^2 .$$

In order to simplify the coefficient of the differential scattering cross section, atomic units will be adopted here and will be used throughout the rest of the paper unless otherwise specified. In atomic units, e, the charge on the electron, is taken to be one unit of charge. The mass of the electron, m_e, is one unit of mass. Plancks constant divided by 2π, $\hbar$, is one unit of energy times time. In this system, the differential cross section is

$$\frac{d\sigma}{d\Omega} = \frac{\mu_i \mu_f}{4 \pi^2} \left(\frac{k_f}{k_i}\right) |T_{if}|^2 .$$

A total cross section may be obtained by integration of the differential cross section over all possible scattering angles.

$$\sigma = \int_\Omega \frac{d\sigma}{d\Omega} \, d\Omega = \int_0^{2\pi} \int_{-1}^1 \frac{d\sigma}{d\Omega} \, d(\cos\theta) \, d\phi .$$

Classically, the total cross section is

$$\sigma = 2\pi \int_0^\infty P(b) \, b \, db$$

where P(b) is the probability that a particle incident at an impact parameter b will be scattered into an angle θ.

For transition matrix elements independent of the azimuthal angle φ.

$$\sigma = \frac{\mu_i \mu_f}{2\pi} \left(\frac{k_f}{k_i}\right) \int_{-1}^{1} |T_{if}(\theta)|^2 \, d(\cos\theta) \qquad \text{in units of } a_0^2.$$

Two other common forms in which the total scattering cross section is given are

$$\sigma = \frac{\mu_i \mu_f}{2\pi^2} \left(\frac{k_f}{k_i}\right) \int_{-1}^{1} |T_{if}(\theta)|^2 \, d(\cos\theta) \qquad \text{in units of } \pi a_0^2$$

and

$$\sigma = (8.79735 \times 10^{-17}) \frac{\mu_i \mu_f}{2\pi^2} \left(\frac{k_f}{k_i}\right) \int_{-1}^{1} |T_{if}(\theta)|^2 \, d(\cos\theta) \quad \text{in units of } cm^2.$$

It has proved useful[22,23] to obtain an expression for total cross sections that depends quantum mechanically on impact parameter rather than scattering angle. This is accomplished by expanding the transition matrix in partial waves. That is,

$$T_{if}(\theta) = \left(\frac{\pi^2}{\mu_i \mu_f \, k_i \, k_f}\right)^{1/2} \sum_{\ell=0}^{\infty} (2\ell+1) \, a_\ell \, P_\ell(\cos\theta).$$

Then

$$\sigma = \frac{\pi}{k_i k_f} \sum_{\ell=0}^{\infty} (2\ell+1) |a_\ell|^2,$$

where a_1 is the 1th probability amplitude and $P_1(\cos\theta)$ is the 1th order Legendre polynomial. Multiplying both sides of the above expression for T_{if} by $P_{1'}(\cos\theta)$ and integrating over all angles, one finds that

$$a_\ell = \left(\frac{\mu_i \mu_f k_i k_f}{4\pi^2}\right)^{1/2} \int_{-1}^{1} T_{if}(\theta)\, P_\ell(\cos\theta)\, d(\cos\theta).$$

For heavy projectiles, large values of l dominate, and the only non-zero probability amplitudes are those for l on the order of k_i times b. Also for large l, $P_l(\cos\theta)$ may be approximated as the zeroth order Bessel function with argument l times θ. Then P(b) becomes

$$P(b) = |a_\ell|^2 = \frac{\mu_i \mu_f k_i k_f}{4\pi^2} \left| \int_{-1}^{1} T_{if}(\theta)\, J_0(k_i b\theta)\, d(\cos\theta) \right|^2.$$

One may now compute cross sections by integration over impact parameter or scattering angle provided the transition matrix element can be evaluated for the system of interest.

CHAPTER 3

APPROXIMATIONS

3.1 The Independent Electron Approximation.

In the independent electron approximation[20] to be
described below, the target atom is treated as a collection
of electrons which independently interact with the projectile.
During the time of collision, the interaction between the
projectile and a given electron neither affects nor depends
on the other target electrons. The non-participating electronic
wave functions are not used in the calculation. One approach
to multi-electron transitions is to calculate single
transition probabilities then to use the product of these
single probabilities to calculate multiple transition
probabilities.

Consider a particle of charge Z_1, incident on a target
with Z_2 electrons. The wave function for the full system,
$\Psi(\vec{R}, \vec{r}_1, \vec{r}_2, \ldots \vec{r}_{Z_2})$, is a solution of the Schrödinger equation

$$H \Psi = i \frac{\partial}{\partial t} \Psi.$$

Here, $\vec{R}$ is the projectile position vector and $\vec{r}_1$, $\vec{r}_2, \ldots \vec{r}_{Z_2}$
are the target electron coordinates. The full Hamiltonian is

$$H = \frac{p^2}{2\mu_i} + \frac{Z_1 Z_2}{R} - \sum_{j=1}^{Z_2} \frac{Z_1}{|\vec{R} - \vec{r}_j|} + \sum_{j=1}^{Z_2} \left\{ \frac{p_j^2}{2} - \frac{Z_2}{r_j} + \sum_{\ell > j}^{Z_2} \frac{1}{|\vec{r}_j - \vec{r}_\ell|} \right\}$$

$$= KE + V_c + \sum_{j=1}^{Z_2} V_{ej} + H_T,$$

where $KE = \frac{P^2}{2\mu_i}$, is the initial kinetic energy of the system,

$V_c = \frac{Z_1 Z_2}{R}$, is the Coulomb attraction between the

projectile and the target nucleus,

$V_{ej}^i = \frac{-Z_1}{|\vec{R} - \vec{r}_j|}$, is the Coulomb repulsion between the

projectile and the target electrons,

and $H_T = \sum_{j=1}^{Z_2} \left\{ \frac{P_j^2}{2} - \frac{Z_2}{r_j} + \sum_{k>j}^{Z_2} \frac{1}{|\vec{r}_j - \vec{r}_k|} \right\}$, is the Hamiltonian

of the unperturbed

target atom.

The perturbing potential, then, is

$$V_i = \frac{Z_1 Z_2}{R} - \sum_{j=1}^{Z_2} \frac{Z_1}{|\vec{R} - \vec{r}_j|} = V_c - \sum_{j=1}^{Z_2} V_{ej}^i.$$

In order that the electrons be uncorrelated, the full

wave function must reduce to a product wave function. This

is done by making two assumptions. First assume that the

total asymptotic wave functions, initially and finally,

are product wave functions. That is

$$\Psi_i (\vec{R}, \vec{r}_1, \vec{r}_2, \cdots \vec{r}_{Z_2}) = \Psi_i (\vec{R}) \prod_{j=1}^{Z_2} \phi_j^i (r_j)$$

and

$$\Psi_f (\vec{R}, \vec{r}_1, \vec{r}_2, \cdots \vec{r}_{Z_2}) = \Psi_f (\vec{R}) \prod_{j=1}^{Z_2} \phi_j^f (r_j).$$

For this to be true, correlations in the target wave function

are ignored. This corresponds to the replacement of the term

$\sum_{k>j}^{Z_2} \frac{1}{|\vec{r}_j - \vec{r}_k|}$ by an effective potential $\sum_{j=1}^{Z_2} V_j(r_j)$, so that H_T

is the sum of single electron terms.

The second approximation is that $\frac{p^2}{2\mu_i}$ commutes with all other terms in the full Hamiltonian, H. This treats the projectile motion classically. It also guarantees that Ψ_i evolves as a product wave function because the evolution operator, $\Omega(t_1, t_2)$,[24] factors into a product of single particle terms. For example, in the Heisenberg picture, with T the time ordering operator,

$$\Omega(t_1, t_2) = T\exp\left\{-i\int_{t_1}^{t_2} H(t)\,dt\right\}$$

$$= T\exp\left\{-i\int_{t_1}^{t_2}\left(\frac{p^2}{2\mu_i} + V_c(R) + \sum_{j=1}^{z_a}(V_{ej} + H_{jT})\right)dt\right\}$$

$$= T\exp\left\{-i\int_{t_1}^{t_2}\left(\frac{p^2}{2\mu_i} + V_c\right)dt\right\}\prod_{j=1}^{z_a} T\exp\left\{-i\int_{t_1}^{t_2} V_{ej}\,dt\right\}$$

$$= \Omega_p(t_1, t_2)\prod_{j=1}^{z_a}\Omega_j(t_1, t_2).$$

This is due to the fact that exp(A+B+C+...) = $e^A e^B e^C$... if and only if the commutation relations, $[A,B]$, $[B,C]$, $[A,C]$ etc. are zero.

The probability amplitude, A^{if}, corresponds to the projection of the vector $\Omega(-\infty,\infty)|\Psi_i\rangle$ representing the full state evolved from $|\Psi_i\rangle$, onto a particular final state $\langle\Psi_f|$. This becomes a product of single electron probability amplitudes, a_j^{if}, in the independent electron approximation provided Ψ_f and Ψ_i are orthogonal. That is

$$A^{if} = \left\langle \psi_f(\vec{R})\prod_{j=1}^{z_a}\phi_j^f(\vec{r}_j)\,\middle|\,\Omega(-\infty,\infty)\,\middle|\,\psi_i(\vec{R})\prod_{j=1}^{z_a}\phi_j^i(\vec{r}_j)\right\rangle$$

$$= \left\langle \psi_f(\vec{R})\,\middle|\,\Omega_p\,\middle|\,\psi_i(\vec{R})\right\rangle\prod_{j=1}^{z_a}\left\langle\phi_j^f(\vec{r}_j)\,\middle|\,\Omega_j\,\middle|\,\phi_j^i(\vec{r}_j)\right\rangle$$

$$= \prod_{j=0}^{z_a} a_j^{if},$$

where j = 0 corresponds to the internuclear term.

If one isolates a particular transition, s, and sums over other electron activity, the total cross section is

$$\sigma = 2\pi \int_0^\infty |a_s^{if}|^2 \, \overset{z_a}{\underset{j \neq s}{\Pi}} \sum_f |a_j^{if}|^2 \, b \, db$$

$$= 2\pi \int_0^\infty |a_s^{if}|^2 \, b \, db,$$

since $\sum_f |a_j^{if}|^2 = 1$, according to conservation of electron probability.

3.2 The Bates-Born Approximation.

The next step in the calculation of multi-electron capture cross sections is to find an appropriate method for calculating single electron probability amplitudes. If one were to follow the accepted procedure for calculating the transition matrix in the wave picture and the first Born approximation, when dealing with ionization or excitation, one would choose the initial wave function to be the product of the unperturbed bound state wave function of the target and a plane wave dependent on the initial relative momentum of the system and its corresponding relative position vector. That is

$$\Psi_i = \phi_i(\vec{r}_{ae}) e^{i\vec{k}_i \cdot \vec{R}_i} .$$

Similarly one would choose the fianl wave function of the system to be the asymptotic final wave function which is the product of the final bound state wave function and a plane wave dependent upon the final relative momentum and its corresponding relative position vector. Hence

$$\Psi_f = \phi_f(\vec{r}_{ie}) e^{i\vec{k}_f \cdot \vec{R}_f} .$$

In both Ψ_i and Ψ_f, the translational motion of the electron is neglected because it is attached to a moving nucleus. These wave functions along with V_i, when inserted into the transition matrix, should lead to cross sections for single electron capture.

Bates[11] points out, however, that if one were to add to V_i, any constant function of R, the transition matrix,

hence the cross section, would be altered. This is not acceptable since the choice of the zero point potential should not affect the outcome of the calculation. This ambiguity arises because, using the above method, one has ignored the fact that in charge capture, ϕ_i and ϕ_f are not orthogonal. This non-orthogonality would also rule out the application of this independent electron approximation to charge transfer.

Bates accounts for the non-orthogonality of the initial and final states by expressing his full wave function as the sum of Ψ_i, Ψ_f and a term, T, orthogonal to both ϕ_i and ϕ_f. This is equivalent to a Gram-Schmidt orthogonalization of the initial state vector $\langle \Psi_i |$ to the final state vector $| \Psi_f \rangle$ at each internuclear separation $\vec{R}$. That is

$$| \Psi_f \rangle \rightarrow | O\Psi_f \rangle = \frac{| \Psi_f \rangle - | \Psi_i \rangle \langle \Psi_i | \Psi_f \rangle}{1 - |\langle \Psi_f | \Psi_i \rangle|^2} .$$

Implicit in this expression for $| O\Psi_f \rangle$ is the neglection of all terms not involving the initial and final bound states. Backcoupling is neglected. This assumes that the amplitude of the scattered wave is much much smaller than the amplitude of the initial wave. Bates also assumes that for sufficiently high velocities the perturbation of the atomic eigen-energies, δ, is small.

Having made these assumptions, $| \Psi_f \rangle$ is replaced in the transition matrix by $| O\Psi_f \rangle$, and one obtains the result

$$T_{if} = \left\langle \Psi_i \left| \frac{V_i - U_i}{1 - |S|^2} \right| \Psi_f \right\rangle ,$$

where

$$U_i = \langle \phi_i | V_i | \phi_i \rangle$$

is the average interaction potential, and

$$|S|^2 = |\langle \Psi_f | \Psi_i \rangle|^2.$$

Since $|S|^2 \ll 1$ for high velocities[25], it will be neglected in this calculation. The transition matrix that will be evaluated is

$$T_{if} = \langle \Psi_f | V_i - U_i | \Psi_i \rangle.$$

This approximation will be referred to as the Bates-Born version of first order perturbation theory. It is equivalent to the expression used by Bassel and Gerjuoy[10] in their plane wave limit to the distorted wave Born approximation. Note that since the effective perturbing potential is now the difference between the instantaneous and average interaction potentials, there is no longer any dependence of the transition matrix on the choice of the zero point potential.

3.3 Application to Multiple Electron Capture.

Combining the Bates-Born approximation with the independent electron approximation, one may now deal with the problem of multiple charge capture. Without them the initial and final asymptotic wave functions are not orthogonal and the evolution of the initial system does not remain an uncorrelated product of single electron wave functions. Since one expresses $|\Psi_f\rangle$ as $|O\Psi_f\rangle$, such that

$$\langle \Psi_i | O \Psi_f \rangle = \delta_{if},$$

all assumptions made in Section 3.1 are true and the probability amplitude does reduce to the product of single electron probability amplitudes.

$$A^{if} = \prod_{j=0}^{Z_a} a_j^{if}.$$

Since $P_j(b) = \left| a_j^{if} \right|^2$, the probability for charge capture of the jth electron is $P_j(b)$, and the probability of not capturing the kth electron is $1 - P_k(b)$. The cross section for capture of the sth electron is

$$\sigma = 2\pi \int_0^\infty P_s(b) \prod_{j \ne s}^{Z_a} (1 - P_j(b)) b\,db.$$

As an example, let $P_1 = P_2 = P$ be the probability of the capture of a single electron from a helium atom. Then the single capture cross section is

$$\sigma_1 = 2\pi \int_0^\infty \left\{ P_1(b)(1-P_2(b)) + P_2(b)(1-P_1(b)) \right\} b\,db$$

$$= 4\pi \int_0^\infty P(b)(1-P(b)) b\,db.$$

The cross section for double capture from helium is

$$\sigma_2 = 2\pi \int_0^\infty P_1(b)P_2(b)\,b\,db$$

$$= 2\pi \int_0^\infty P^2(b)\,b\,db.$$

CHAPTER 4

CALCULATION OF SINGLE TRANSITION PROBABILITIES

In order to calculate multiple charge capture cross sections, from the ground state of the target into the ground state of the projectile in the Bates-Born and independent electron approximations, one needs to evaluate the transition matrix for single charge capture. This was shown in Section 3.2 to be

$$T_{if} = \langle \Psi_f | V_i - U_i | \Psi_i \rangle .$$

Before this can be solved, the system must be defined and some relationships developed. Assume the incident projectile has mass M_1, charge Z_1 and incident velocity $\vec{v}_i$. The target has mass M_2 and effective charge Z_2. The electron is initially bound to the target and has mass 1 and charge 1 in accordance with atomic units.

The initial reduced mass of the system is μ_i and the final reduced mass of the system is μ_f where

$$\mu_i = \frac{M_1(M_2+1)}{M_1+M_2+1} \qquad \text{and} \qquad \mu_f = \frac{M_2(M_1+1)}{M_1+M_2+1} .$$

The reduced mass of the target initially is a. The final reduced mass of the projectile is b, where

$$a = \frac{M_1}{M_1+1} \qquad \text{and} \qquad b = \frac{M_2}{M_2+1} .$$

The coordinate system chosen to describe the interaction is

shown in Figure 1. Here $\vec{R}$ is the vector from the projectile to the target nucleus. The coordinates from the projectile to the electron and from the target to the electron are $\vec{r}_{1e}$ and $\vec{r}_{2e}$ respectively. The coordinate from the center of mass of the initial target atom to the projectile is $\vec{R}_i$, and the coordinate from the center of mass of the final projectile atom to the target nucleus is $\vec{R}_f$. Then

$$\vec{R}_i = b\vec{r}_{2e} - \vec{r}_{1e} \qquad \text{and} \qquad \vec{R}_f = a\vec{r}_{1e} - \vec{r}_{2e}.$$

The initial relative momentum of the system is $\vec{k}_i$. $\vec{k}_i = \mu_i \vec{v}_{relative}$, but $\vec{v}_{relative} = \vec{v}_i$ since initially the target nucleus is assumed stationary. The final relative momentum of the stsrem is $\vec{k}_f$. Let the initial and final binding energies of the system be BE_i amd BE_f respectively. Then since the energy of the system must be conserved,

$$k_f = \left\{ \mu_f \left[k_i^2 / \mu_i + 2(BE_f - BE_i) \right] \right\}^{1/2}.$$

The center of mass scattering angle, θ, defined as the angle between the initial and final center of mass momenta, is the same angle as that between the initial and final relative momenta, hence, one may define θ as

$$\theta = \cos^{-1} \left\{ \frac{\vec{k}_i \cdot \vec{k}_f}{k_i k_f} \right\}.$$

A normalized hydrogenic wave function for an atom of charge Z and electron positioned a distance r from the nucleus is

$$u(r) = \left[\frac{Z^3}{\pi} \right]^{1/2} e^{-Zr}.$$
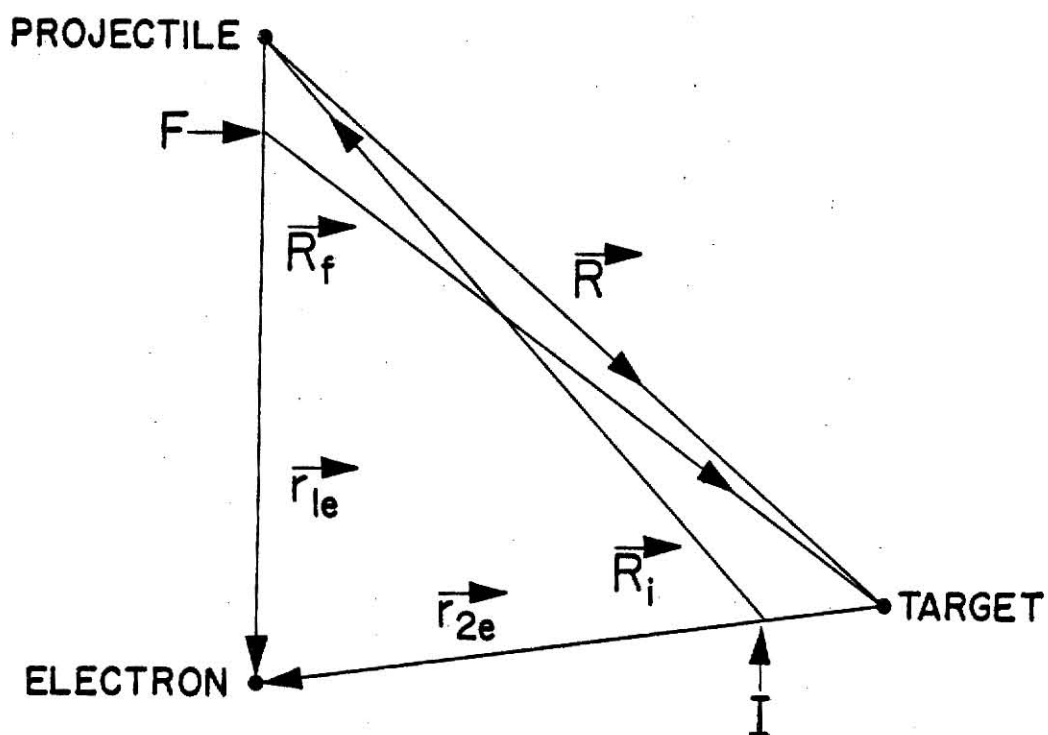
FIGURE 1.

The coordinates for charge capture.

I is the center of mass of the target and electron.

F is the center of mass of the projectile and electron.

The initial wave function of the system is then

$$\Psi_i = e^{i\vec{k}_i \cdot \vec{R}_i} u(r_{2e}) = \left[\frac{z_2^3}{\pi}\right]^{1/2} e^{i\vec{k}_i \cdot \vec{R}_i} e^{-Z_2 r_{2e}} .$$

The final wave function is

$$\Psi_f = e^{-i\vec{k}_f \cdot \vec{R}_f} u(r_{1e}) = \left[\frac{z_1^3}{\pi}\right]^{1/2} e^{-i\vec{k}_f \cdot \vec{R}_f} e^{-Z_1 r_{1e}} .$$

The difference between the instantaneous and average potentials in terms of the system defined above is

$$V_i - U_i = V_i - \int d\vec{r}_{2e} \, u(r_{2e}) \, V_i \, u(r_{2e}) .$$

This has been evaluated in Appendix 1. To order of M_2^{-1}, the resulting potential is

$$V_i - U_i = Z_1 \left\{ \frac{1}{R} - \frac{1}{r_{1e}} - \left[\frac{1}{R} + Z_2\right] e^{-2Z_2 R} \right\} .$$

Then

$$T_{if} = \int d\vec{r}_{1e} \int d\vec{r}_{2e} \, u^*(r_{1e}) \, e^{i\vec{k}_f \cdot \vec{R}_f} (V_i - U_i) \, e^{i\vec{k}_i \cdot \vec{R}_i} u(r_{2e})$$

$$= \int d\vec{r}_{1e} \int d\vec{r}_{2e} \, u^*(r_{1e}) e^{-i(\vec{k}_i - a\vec{k}_f) \cdot \vec{r}_{1e}} (V_i - U_i) u(r_{2e}) e^{i(b\vec{k}_i - \vec{k}_f) \cdot \vec{r}_{2e}} .$$

Let $\vec{A} = \vec{k}_i - a\vec{k}_f$ and $\vec{B} = b\vec{k}_i - \vec{k}_f$. Then

$$T_{if} = \int d\vec{r}_{1e} \int d\vec{r}_{2e} \, u^*(r_{1e}) \, e^{-i\vec{A} \cdot \vec{r}_{1e}} (V_i - U_i) \, u(r_{2e}) \, e^{i\vec{B} \cdot \vec{r}_{2e}} .$$

$$= IBK + IJS + IBG.$$

IBK is the transition matrix used by Brinkman and Kramers in their single capture cross section calculation.

$$IBK = -Z_1 \int d\vec{r}_{1e} \int d\vec{r}_{2e} \; u^*(r_{1e}) \; e^{-i\vec{A}\cdot\vec{r}_{1e}} \frac{1}{r_{1e}} u(r_{2e}) \; e^{i\vec{B}\cdot\vec{r}_{2e}} .$$

This has been evaluated by many authors[6,23,26] and is found to be

$$IBK = -32\,\pi\,(Z_1 Z_2)^{5/2} \, (Z_1{}^2 + A^2)^{-1} \, (Z_2{}^2 + B^2)^{-2} ,$$

where $A^2 = |\vec{A}|^2$ and $B^2 = |\vec{B}|^2$. Jackson and Schiff use the sum of IBK and IJS in their transition matrix, where

$$IJS = Z_1 \int d\vec{r}_{1e} \int d\vec{r}_{2e} \; u^*(r_{1e}) \; e^{-i\vec{A}\cdot\vec{r}_{1e}} \; \frac{1}{R} \; u(r_{2e}) \; e^{i\vec{B}\cdot\vec{r}_{2e}} .$$

The transition matrix used in the approximation of Bassel and Gerjuoy is the sum of IBK, IJS and IBG, where

$$IBG = -Z_1 \int d\vec{r}_{1e} \int d\vec{r}_{2e} u^*(r_{1e}) e^{-\vec{A}\cdot\vec{r}_{1e}} \left[\frac{1}{R} + Z_2\right] e^{-2Z_2 R} u(r_{2e}) e^{i\vec{B}\cdot\vec{r}_{2e}} .$$

IBG and IJS will be evaluated in Appendix 2. Due to the complexity of their results, they will not be repeated in the text of this thesis.

CHAPTER 5

RESULTS

Since the calculation of double electron capture
cross sections, in the independent electron approximation
used, is explicitly dependent on the scattering amplitudes
used when calculating single capture cross sections, it is
imperative that one verify that these amplitudes are correct.
Hence, the first calculation made was an attempt to reproduce
the differential cross sections computed by Bassel and Gerjuoy
for single capture from hydrogen into protons incident
at an energy of 25 KeV. Agreement would guarantee the correct
expressions for IBK, IJS and IBG, except for the charge
dependence. One could then assume the algebra that is
included in Appendix 2 but omitted from the Bassel and Gerjuoy
paper is accurate. The computer program used in the calc-
ulation is presented in Appendix 4. The comparison to the
results of Bassel and Gerjuoy is shown in Figure 2.

Unfortunately, the comparison was not successful. The
differential cross sections for the Jackson and Schiff
approximation is identical to present results. The Bassel
and Gerjuoy curve, however, differs appreciably as Λ increases.
The algebra has been rechecked a number of times, and the
computer program has been carefully reexamined. The final
conclusion reached is that the results presented by Bassel
and Gerjuoy differ from present results.

Luckily, the discrepancies in the angular distributions
do not affect the total cross sections appreciably. This

FIGURE 2

Differential electron capture cross sections

for protons on hydrogen at 25 KeV.

——————, present and Bassel and Gerjuoy calculations

in the Jackson and Schiff approximation.

----------, present calculation in the Bassel and

Gerjuoy approximation.

-.-.-.-.-, Bassel and Gerjuoy calculation in the

Bassel and Gerjuoy approximation.

DIFFERENTIAL CROSS SECTIONS IN $(4\pi^2 a_0^3/\text{Sr})$

$\lambda = (2M \sin\theta/2)^2$
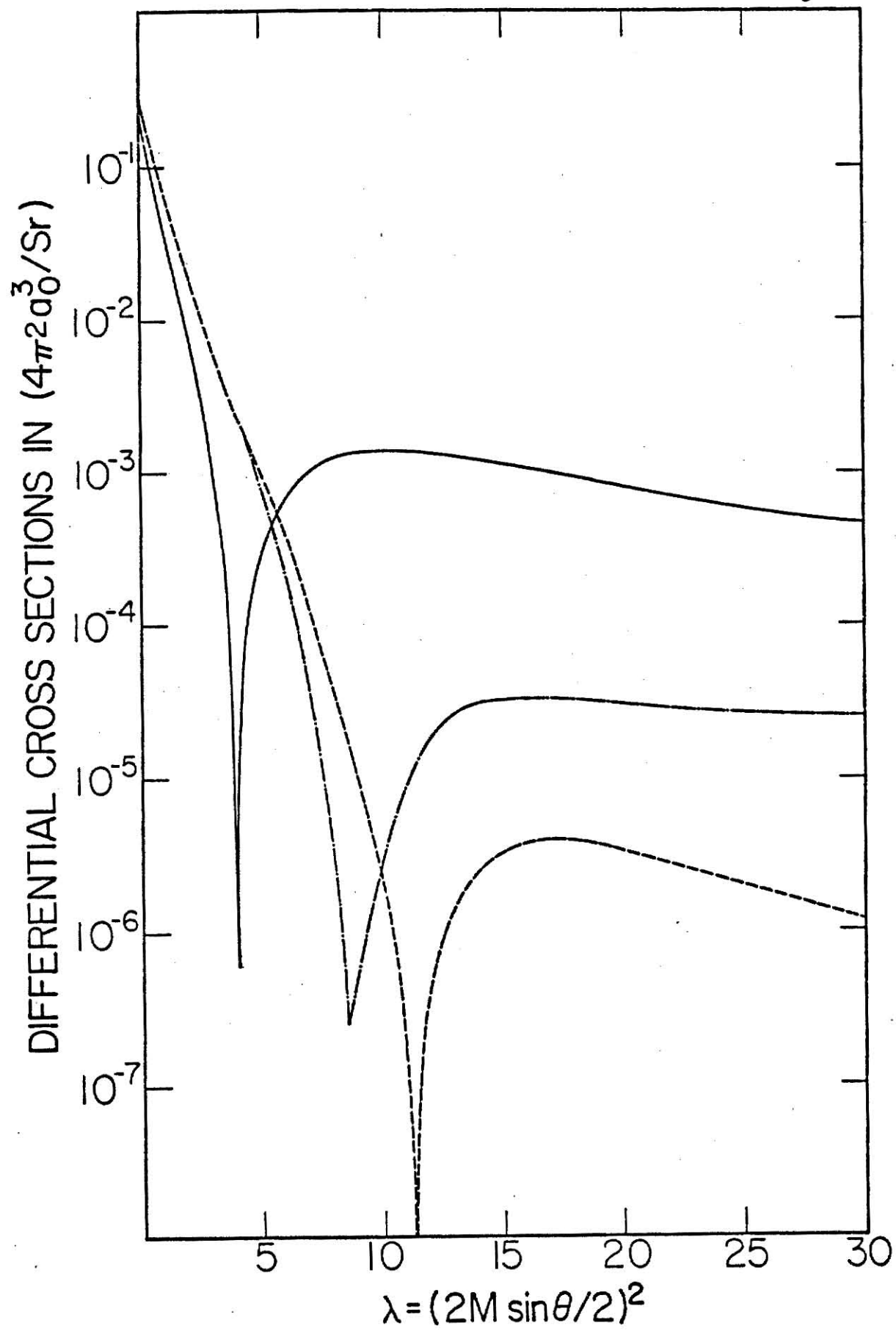
is due to the fact that the error occurs after the differential
cross section has fallen off more than two orders of magnitude.
This causes error of less than one per cent in their total
cross section calculation. This can be seen in Figure 3.
Here the total cross sections for 25 KeV protons incident
on hydrogen are presented for the Brinkman and Kramers,
the Jackson and Schiff and the Bassel and Gerjuoy approx-
imations as calculated by both the author and by Bassel and
Gerjuoy. Only three curves are shown because these results
are identical to one another.

After a careful check of the charge dependence of the
transition matrix, single charge capture cross sections were
computed for the capture of electrons from the ground state
of helium to the ground state of alpha particles. This
calculation was made for incident energies from 0 to 1,000
KeV. The masses used are $M_1 = M_2 = 7344.0$, which is four
times the mass of a proton in atomic units. The charge on the
projectile is $Z_1 = 2.0$. The effective charge on the target
due to screening of the nucleus by the electrons present is
$Z_2 = 1.618$. The initial and final binding energies used
are the ionization energies for a helium atom, 24.587, and for
He^+, 54.4, respectively.

These resulting cross sections are presented in Figure
4 where they are compared to the experimental results compiled
by Barnett et. al.[14] for capture to all energy levels. At
high velocities, when the projectile electron velocity is
much greater than the velocity of the orbiting electron, the
capture cross sections are inversely proportional to n^3

FIGURE 3

Total single capture cross sections

for protons on hydrogen.

——————, Brinkman and Kramers approximation.

— — — — —, Jackson and Schiff approximation.

—.—.—.—, Bassel and Gerjuoy approximation.

$H^+ + H \longrightarrow H + H^+$

CROSS SECTIONS IN CM^2

ENERGY (KeV)

FIGURE 4

Total single electron capture cross sections
from helium atoms by alpha particle projectiles.

•   , Experimental data of Barnett et. al.

————————, Theoretical results from present calculation.

SINGLE CAPTURE CROSS SECTIONS IN CM^2

ENERGY (KeV)

He^{++} + He $\rightarrow$ He^{+}
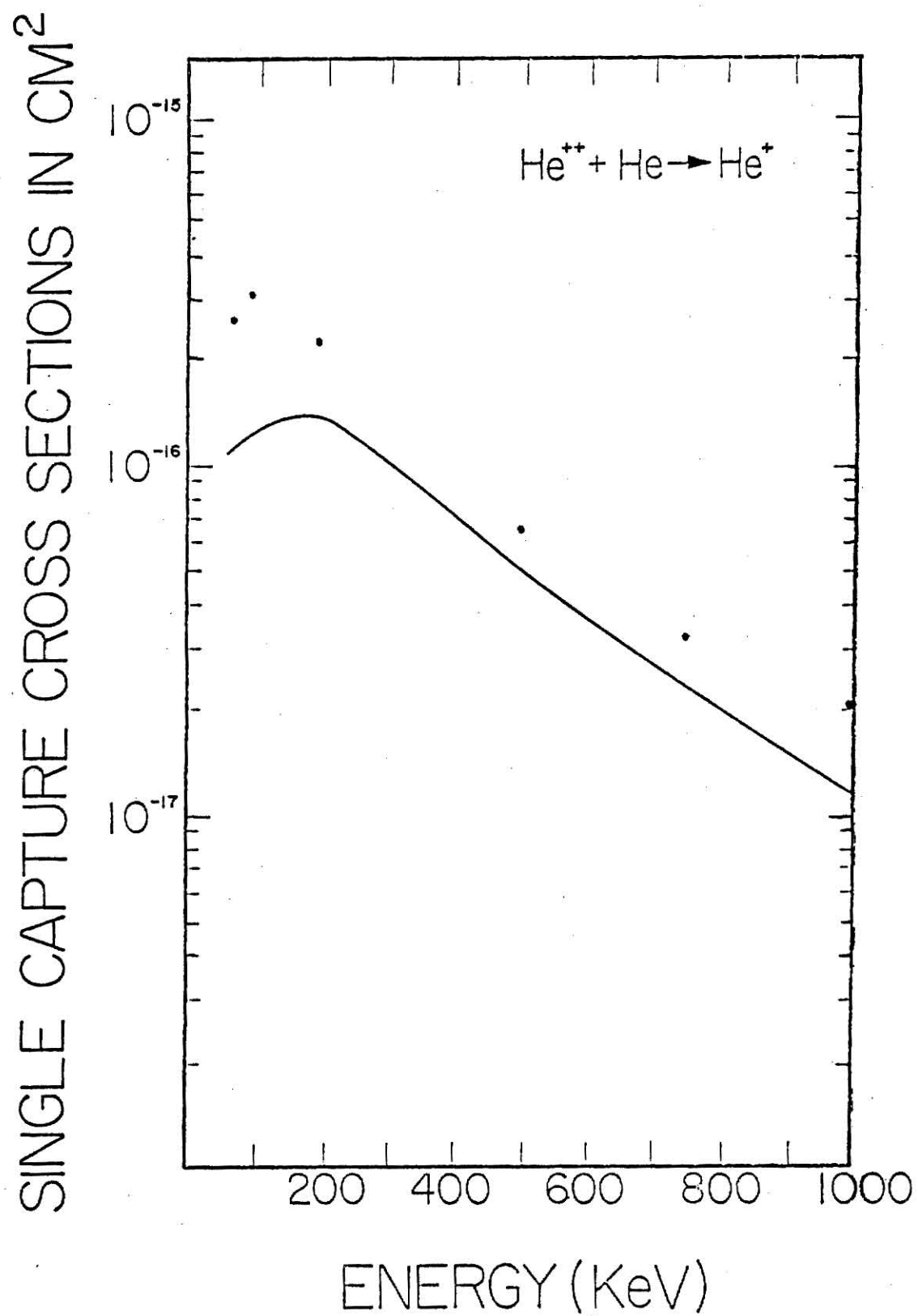
where n is the principle quantum number.[26] Then one expects
that twenty per cent of the experimental result is due to
capture into higher energy levels. Multiplying the present
result by 1.2 would result in excellent agreement with
experiment for higher energies.

For smaller incident energies the comparison becomes
less and less agreeable. This is expected for any number of
reasons. First the percentage of higher level transitions
increases.[27] The significance of the omitted backcoupling
and $|S|^2$ term becomes larger and larger as the energy decreases.
Finally, there is persuasive evidence that the second order
Born calculation becomes appreciable and may even dominate
as the energy becomes small.[28,29]

The computer program used to compute both the single
and double capture cross sections is presented in Appendix 3.
The square of the probability amplitude for single capture
is the basis for double capture in accordance with the
independent electron approximation. The results of this
calculation, in which the same parameters were used, is
shown in Figure 5. The experimental data to which it is
compared is also a composit by Barnett et. al.[14] A comparison
shows the theoretical calculation falls farther below the
data than for the case of single capture. This is expected
since the percentage of higher level transitions is twice as
large for this case. That is only 60% of the total transitions
are attributed to 1s to 1s capture. Also some disagreement
may be due to the use of the single capture binding energy.
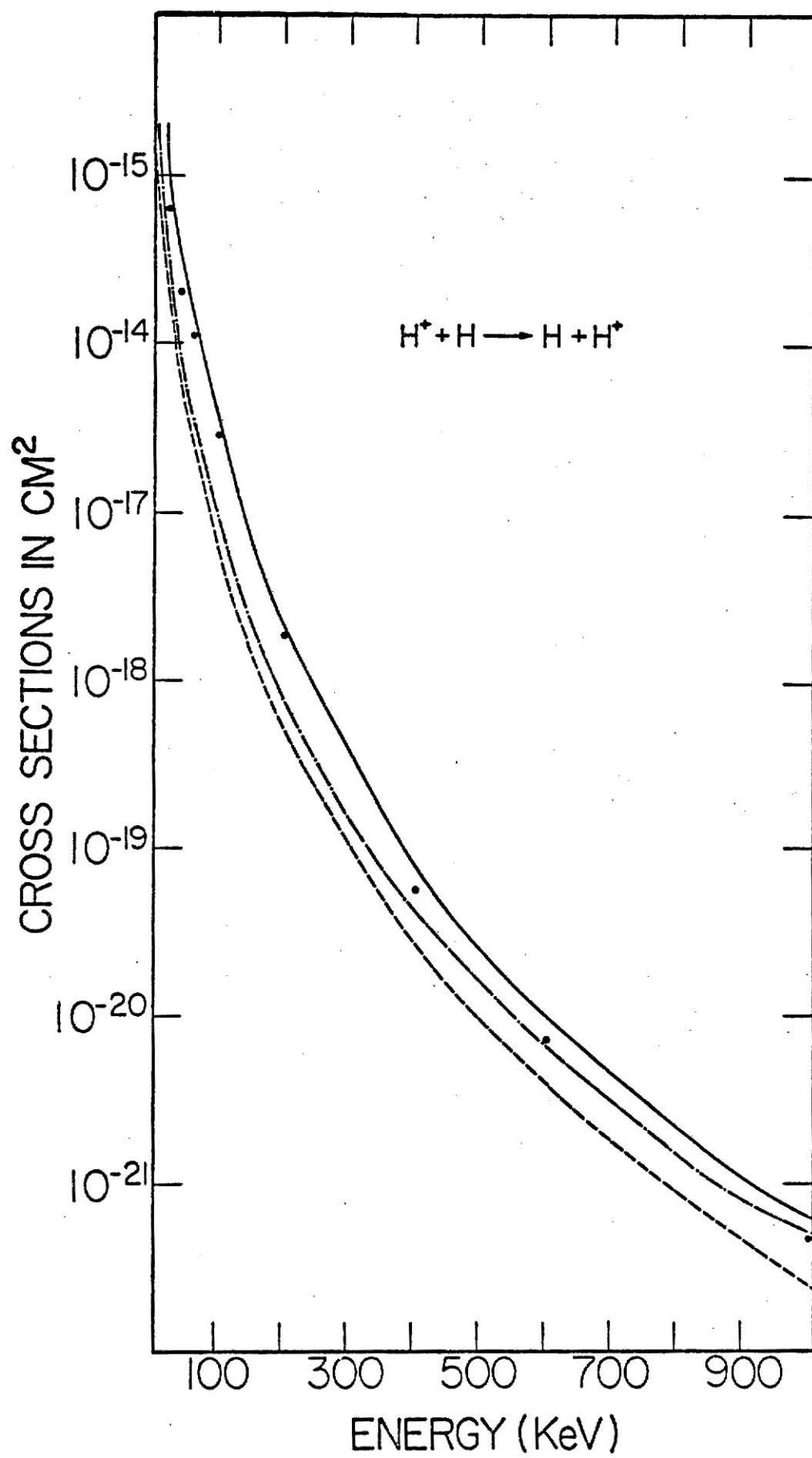This corresponds to the assumption that the collision process

FIGURE 5

Total double electron capture cross sections
from helium atoms by alpha particle projectiles.

, Experimental data of Barnett et. al.
————, Theoretical results from present calculation.
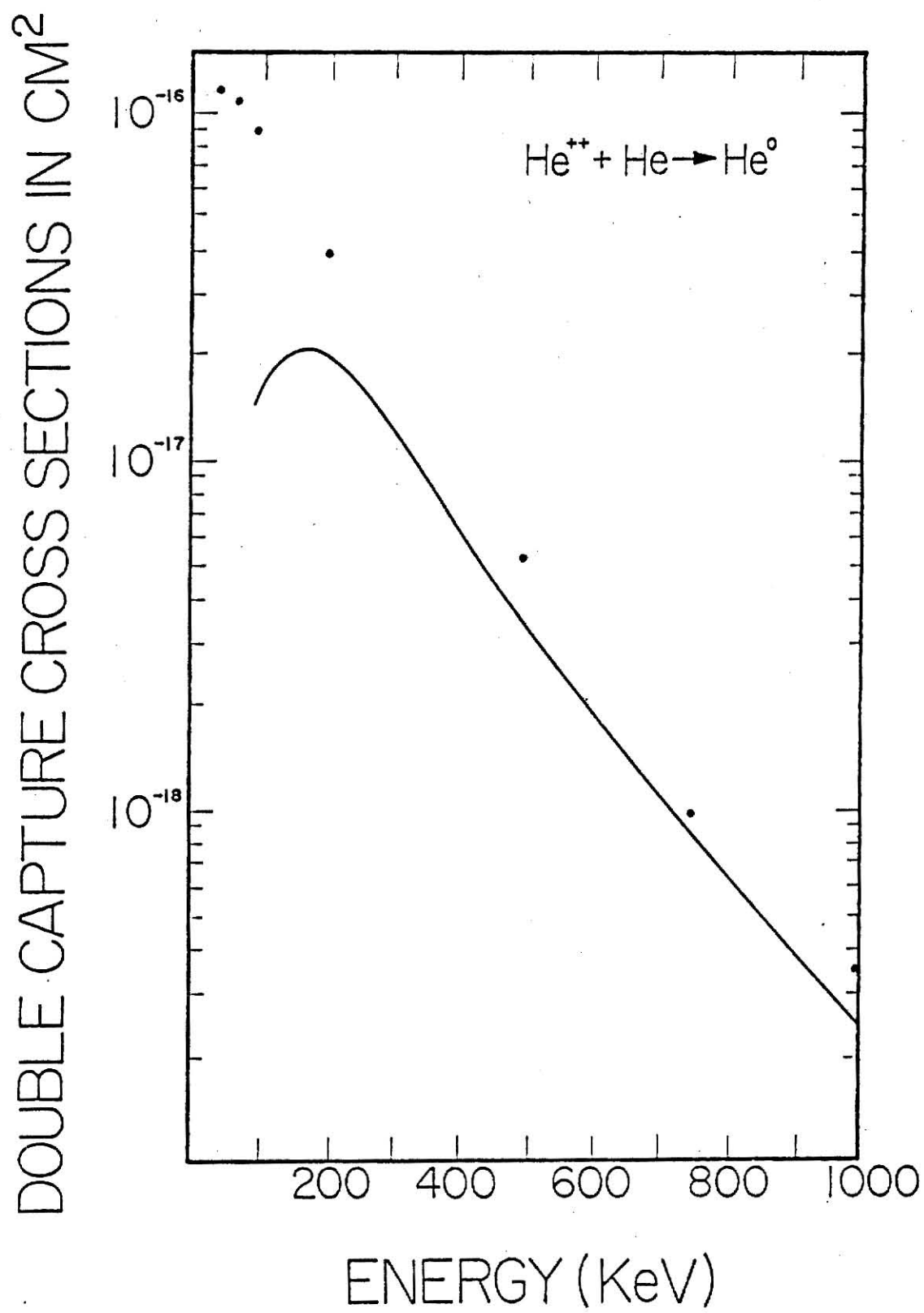
occurs too quickly to allow the target atom to readjust after the first electron has been captured.

Then the agreement with experiment achieved for the double charge capture process does follow the same pattern as that for single capture. It is good at high energies and falls farther below the data as the energy decreases. One may then conclude that the independent electron approximation used is a valid one.

Several calculations have been made for K-shell to K-shell capture for this system using the close-coupling technique. The results of one approximation using three state, two center atomic expansion[19] are compared to the present results in Figure 6. Here it can be seen that agreement with experiment is comparable or even better than the close-coupling calculation at energies above 600 KeV, but worse for low energies. This is attributed to an inadequacy in the single capture calculation rather than the breakdown of the independent electron approximation.

FIGURE 6

Total double electron capture cross sections
from helium atoms by alpha particles.

, Experimental data of Barnett et. al.

————, Theoretical results from present calculation.

—·—·—·—, Theoretical results from Lin.

$He^{++} + He \rightarrow He^{o}$
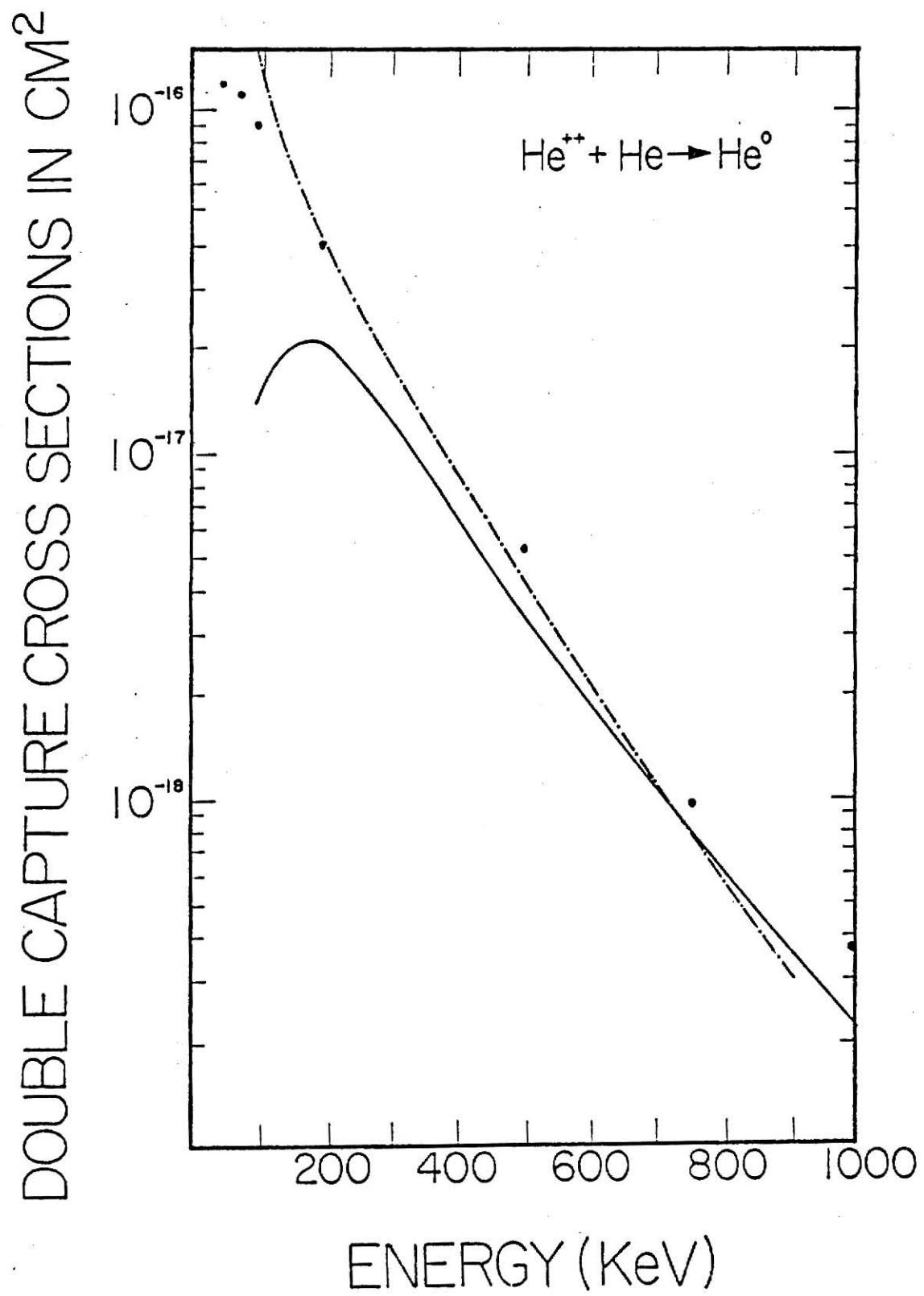
CHAPTER 6

CONCLUSION

The independent electron approximation of McGuire
and Weaver has been tested for double charge capture from
the ground state of a helium atom into the ground state of
an alpha particle of high incident energy. The difference
between the instantaneous and the average interaction
potential was used as the perturbing potential as in the
approximation of Bates. The wave functions used were those
dictated by the first Born approximation.

The resulting cross sections for double capture were
compared to experimental results and the discrepancies were
noted. These differences turned out to follow the same
trend as the comparison made for single capture. This led
to the conclusion that the discrepancies were due to the
weaknesses in the probability amplitude computed. Then the
independent electron approximation has passed the test and
has been deemed a worthwhile approximation to use when
dealing with the complicated reaction of multiple charge
transfer.

Since it has proven to be worthwhile, a thorough
investigation into the limitations of the approximation
would be advantageous. For example, the comutator terms
that were neglected could be evaluated to see if they are
truly as small as rough estimates indicate. The choice of

the effective inter-electron interaction potential could
be investigated to see if there is a better way of expres-
sing it than the one used.

The applications of the approximation are numerous.
Cross sections for higher target and projectile charge states
are a minor perturbation of the calculation already done.
Capture of more than two electrons is obtainable. Capture
into higher energy levels could be computed as well for
multiple charge transfer. Computations could be made com-
bining multiple charge capture and multiple ionization cross
sections. The second Born terms could be computed for
multiple charge transfer as well.

These calculations among others are now conceivable
in a simple way since this independent electron approximation
has been shown to give results that are in reasonable agreement
with experiment and with theoretical results that are much
more complicated to compute.

APPENDIX 1

THE DIFFERENCE BETWEEN THE INSTANTANEOUS AND AVERAGE POTENTIALS

In order to arrive at the form of the Bates potential used in this calculation, the exact form of the interaction potential is evaluated here. The result is then approximated to order M_2^{-1}, where M_2 is the target mass, in order that its use may be facilitated.

$$V_i = \frac{Z_1 Z_2}{R} - \frac{Z_1}{r_{1e}} .$$

$$U_i = \left\langle u(r_{2e}) \mid V_i \mid u(r_{2e}) \right\rangle$$

$$= \left\langle u(r_{2e}) \left| - \frac{Z_1}{r_{1e}} \right| u(r_{2e}) \right\rangle + \left\langle u(r_{2e}) \left| \frac{Z_1 Z_2}{R} \right| u(r_{2e}) \right\rangle$$

$$= \qquad U_{i1} \qquad + \qquad U_{i2} \qquad .$$

$$u(r_{2e}) = \left(\frac{Z_2^3}{\pi} \right)^{1/2} e^{-Z_2 r_{2e}} .$$

Generally, using a standard expansion in terms of Spherical Harmonics, $Y_{lm}(\theta, \phi)$,

$$\left| \vec{r} - \vec{R} \right|^{-1} = \sum_{l,m} \frac{4\pi}{2l+1} \frac{r_<^l}{r_>^{l+1}} Y_{lm}^*(\theta', \phi') Y_{lm}(\theta, \phi) .$$

where $r_<$ is the lesser of r and R and

$r_>$ is the greater of r and R.

Since only 1s to 1s transitions are of concern, $l = m = 0$, and $Y_{00}(\theta, \phi) = 1/\sqrt{4\pi}$,

$$\left| \vec{r} - \vec{R} \right|^{-1} = \frac{4\pi}{r_>} Y_{00}^*(\theta', \phi') Y_{00}(\theta, \phi) = \frac{1}{r_>}$$

Then specifically, $\left| \vec{r}_{1e} \right|^{-1} = \left| \vec{R}_i - b\vec{r}_{2e} \right|^{-1} = 1/r_>$ where

$b = M_2/(M_2 + 1)$ and $r_>$ is the greater of R and br_{2e}. Then

$$U_{i1} = -Z_1 \int_0^{2\pi} \int_{-1}^{1} \int_0^{\infty} \frac{r_{2e}^2}{r_>} \left(\frac{Z_2^3}{\pi} \right) e^{-2Z_2 r_{2e}} \, dr_{2e} d(\cos\theta) d\phi$$

$$= -4Z_1 Z_2^3 \int_0^{\infty} \frac{r_{2e}^2}{r_>} e^{-2Z_2 r_{2e}} \, dr_{2e},$$

where $\qquad r_> = R_i$ if $br_{2e} < R_i$

or $\qquad r_> = br_{2e}$ if $br_{2e} > R_i$.

Let $2Z_2 r_{2e} = x$. Then

$$r_{2e} = \frac{x}{2Z_2} \quad , \quad dr_{2e} = \frac{dx}{2Z_2}$$

and $\quad x_> = R_i$ if $\frac{bx}{2Z_2} < R_i$ or $x_> = \frac{bx}{2Z_2}$ if $\frac{bx}{2Z_2} > R_i$.

Then

$$U_i = -4Z_1 Z_2^3 \int_0^{\infty} \left(\frac{1}{2Z_2} \right)^2 \frac{x^2}{x_>} e^{-x} \left(\frac{1}{2Z_2} \right) dx$$

$$= -\frac{Z_1}{2} \left\{ \int_0^{\left(\frac{2Z_2}{b} \right) R_i} \frac{x^2}{R_i} e^{-x} \, dx + \int_{\left(\frac{2Z_2}{b} \right) R_i}^{\infty} \frac{2Z_2}{b} x e^{-x} \, dx \right\}$$

$$= -Z_1 \left\{ \frac{1}{R_i} - e^{-(2Z_2 R_i)/b} \left(\frac{Z_2}{b} + \frac{1}{R_i} \right) \right\} .$$

Similarly $\left| \vec{R} \right|^{-1} = \left| \vec{R}_i + g\vec{r}_{2e} \right|^{-1} = 1/r_>$ where $g = 1/(M_2 + 1)$

and $r_>$ is the greater of R and gr_{2e}.

Then

$$U_{i2} = Z_1 Z_2 \iiint\limits_{0 \ -1 \ 0}^{2\pi \ 1 \ \infty} \frac{r_{2e}^2}{r_>} \left(\frac{Z_2^3}{\pi}\right) e^{-2Z_2 r_{2e}} \, dr_{2e} d(\cos\theta) d\phi$$

$$= 4Z_1 Z_2^4 \int\limits_0^\infty \frac{r_{2e}^2}{r_>} e^{-2Z_2 r_{2e}} \, dr_{2e}$$

This is the same integral as evaluated in U_{i1} except for the constant $-Z_2$, and now

$$r_> = R_i \text{ if } gr_{2e} < R_i \quad \text{or} \quad r_> = gr_{2e} \text{ if } gr_{2e} > R_i \quad .$$

So that with b replaced by g,

$$U_{i2} = Z_1 Z_2 \left\{ \frac{1}{R_i} - e^{-(2Z_2 R_i)/g} \left(\frac{1}{R_i} + \frac{Z_2}{g}\right) \right\}$$

Then the average interaction potential is

$$U_i = U_{i1} + U_{i2}$$

$$= Z_1 Z_2 \left\{ \frac{1}{R_i} - e^{-2Z_2(M_2+1)R_i} \left(\frac{1}{R_i} + Z_2(M_2+1)\right) \right\}$$

$$-Z_1 \left\{ \frac{1}{R_i} - e^{-2Z_2 R_i(M_2+1)/M_2} \left(\frac{1}{R_i} + \frac{Z_2(M_2+1)}{M_2}\right) \right\} .$$

Now, since $M_2 \gg 1$, the exponential, $\exp\left[-Z_2(M_2+1)R_i\right]$ is very small and the term containing it may be neglected altogether from the expression for U_i. To order of M_2^{-1}, the quantity $(M_2+1)/M_2$ is approximately equal to one. For large M_2, R_i is approximately equal to R. With these three approximates all on the order of M_2^{-1} included, the expression for U_i becomes

$$U_i = \frac{Z_1 Z_2}{R} - \frac{Z_1}{R} + Z_1 \, e^{-2Z_2 R} \left[\frac{1}{R} + Z_2 \right] .$$

Then the instantaneous minus the average potential is

$$V_i - U_i = \frac{Z_1 Z_2}{R} - \frac{Z_1}{r_{1e}} - \frac{Z_1 Z_2}{R} + \frac{Z_1}{R} - Z_1 \, e^{-2Z_2 R} \left(\frac{1}{R} + Z_2 \right)$$

$$= Z_1 \left\{ \frac{1}{R} - \frac{1}{r_{1e}} - e^{-2Z_2 R} \left(\frac{1}{R} + Z_2 \right) \right\} .$$

This is indeed the potential given as the Bates potential in Chapter 3.

APPENDIX 2

CALCULATION OF THE PIECES OF THE TRANSITION
MATRIX CALLED IJS AND IBG

In this appendix the integral forms of IJS and IBG will be reduced to closed form expressions. In their integral form they are

$$IJS = Z_1 \int d\vec{r}_{1e} \int d\vec{r}_{2e} \ u^*(r_{1e}) \ e^{-i\vec{A} \cdot \vec{r}_{1e}} \frac{1}{R} u(r_{2e}) \ e^{+i\vec{B} \cdot \vec{r}_{2e}}$$

and

$$IBG = -Z_1 \int d\vec{r}_{1e} \int d\vec{r}_{2e} u^*(r_{1e}) e^{-i\vec{A} \cdot \vec{r}_{1e}} \left(\frac{1}{R} + Z_2\right) e^{-2Z_2 R} u(r_{2e}) e^{i\vec{B} \cdot \vec{r}_{2e}} \ .$$

Note that

$$\left(\frac{1}{R} + Z_2\right) e^{-2Z_2 R} = \left(1 - Z_2 \frac{\partial}{\partial(2Z_2)}\right) \frac{1}{R} \ e^{-2Z_2 R}$$

Let $2Z_2 = y$. Then

$$IBG = -Z_1 \left(1 - Z_2 \frac{\partial}{\partial y}\right) \int d\vec{r}_{1e} \int d\vec{r}_{2e} \ u^*(r_{1e}) e^{-i\vec{A} \cdot \vec{r}_{1e}} \frac{1}{R} e^{-yR} u(r_{2e}) e^{i\vec{B} \cdot \vec{r}_{2e}}$$

and IJS is a special case of IBG. That is

$$IJS = \lim_{y \to 0} -IBG \ .$$

Hence evaluation of the integral

$$I = \int d\vec{r}_{1e} \int d\vec{r}_{2e} \ u^*(r_{1e}) \ e^{-i\vec{A} \cdot \vec{r}_{1e}} \frac{1}{R} e^{-yR} u(r_{2e}) \ e^{i\vec{B} \cdot \vec{r}_{2e}}$$

gives both closed form expressions sought.

The Fourier transform of e^{-yR}/R is[30]

$$F\left(\frac{e^{-yR}}{R}\right) = \frac{1}{2\pi^2}\int d\vec{p}\ (p^2+y^2)^{-1}\ e^{i\vec{p}\cdot\vec{R}}$$

$$= \frac{1}{2\pi^2}\int d\vec{p}\ (p^2+y^2)^{-1}\ e^{i\vec{p}\cdot\vec{r}_{2e}}\ e^{-i\vec{p}\cdot\vec{r}_{1e}}$$

since $\vec{R} = \vec{r}_{2e} - \vec{r}_{1e}$. Then

$$I = \frac{1}{2\pi^2}\int d\vec{p}(p^2+y^2)^{-1}\int d\vec{r}_{1e} u^*(r_{1e})e^{-i(\vec{A}+\vec{p})\cdot\vec{r}_{1e}}\int d\vec{r}_{2e}u(r_{2e})e^{i(\vec{B}+\vec{p})\cdot\vec{r}_{2e}}$$

The Fourier transform of the wave function $u(r)$ is

$$\phi_o(\vec{K}) = \int e^{i\vec{K}\cdot\vec{r}}\ u(r)d\vec{r}.$$

For a ground state hydrogenic bound state wave function of charge Z,[7]

$$\phi_o(\vec{K}) = 8\pi^{1/2}Z^{5/2}\left[Z^2+K^2\right]^{-2}.$$

so that

$$I = \frac{1}{2\pi^2}\int d\vec{p}(p^2+y^2)^{-1}\ \phi_o^*(\vec{A}+\vec{p})\ \phi_o(\vec{B}+\vec{p})$$

$$= \frac{32}{\pi}(Z_1Z_2)^{5/2}\int d\vec{p}(p^2+y^2)^{-1}\left[Z_1^2+(A+p)^2\right]^{-2}\left[Z_2^2+(B+p)^2\right]^{-2}.$$

Let $a = Z_1$, $b = Z_2$ and recall $y = 2Z_2$. Then

$$I = \frac{8}{\pi}(Z_1Z_2)^{5/2}\frac{1}{ab}\frac{\partial}{\partial a}\frac{\partial}{\partial b}\int d\vec{p}\left\{(p^2+y^2)\left[a^2+(A+p)^2\right]\left[b^2+(B+p)^2\right]\right\}^{-1}.$$

The integral

$$I' = \int d\vec{p}\left\{(p^2+y^2)\left[a^2+(A+p)^2\right]\left[b^2+(B+p)^2\right]\right\}^{-1}$$

has been evaluated by Lewis[31] to be

$$I' = \pi^2(\beta-\alpha\gamma)^{-1/2}\ln\left\{\frac{\beta+(\beta^2-\alpha\gamma)^{1/2}}{\beta-(\beta^2-\alpha\gamma)^{1/2}}\right\}.$$

where

$$\alpha\gamma = \left[(A-B)^2 + (a+b)^2\right]\left[(a+y)^2 + A^2\right]\left[(b+y)^2 + B^2\right]$$

and

$$\beta = y\left[(A-B)^2 + (a+b)^2\right] + b(A^2+a^2+y^2) + a(B^2+b^2+y^2).$$

For the calculation of interest, $\alpha\gamma$ is greater than β so that

$$I' = i\pi^2(\alpha\gamma-\beta^2)^{-1/2}\ln\frac{1 + \frac{i}{\beta}(\alpha\gamma-\beta^2)^{1/2}}{1 - \frac{i}{\beta}(\alpha\gamma-\beta^2)^{1/2}} \quad .$$

Let $x = \frac{1}{\beta}(\alpha\gamma-\beta^2)^{1/2}$.

$$I = \frac{i\pi^2}{x}\ln\left\{\frac{1+ix}{1-ix}\right\}.$$

Using the identities[32]

$$\tanh^{-1}(ix) = -i\tan^{-1}(x)$$

and

$$\tanh^{-1}(ix) = \frac{1}{2}\ln\left\{\frac{1+ix}{1-ix}\right\},$$

$$\ln\left\{\frac{1+ix}{1-ix}\right\} = -2i\tan^{-1}(x) \quad .$$

Then
$$I' = \frac{i\pi^2}{x}(-2i\tan^{-1}(x))$$

$$= \frac{2\pi^2}{x}\tan^{-1}(x)$$

$$= 2\pi^2(\alpha\gamma-\beta^2)^{-1/2}\tan^{-1}\left\{\frac{(\alpha\gamma-\beta^2)^{1/2}}{\beta}\right\},$$

and $\quad I = 16\pi (z \cdot z_a)^{5/2} \frac{1}{ab} \frac{\partial}{\partial a} \frac{\partial}{\partial b} (\alpha\gamma - \beta^2)^{-1/2} \tan^{-1}\left(\frac{(\alpha\gamma - \beta^2)^{-1/2}}{\beta}\right).$

Let $\quad t = \alpha\gamma - \beta^2 \quad$ and $\quad z = \tan^{-1}(t^{1/2}/\beta)$

Then

$\frac{\partial}{\partial a} \frac{\partial}{\partial b} (t^{-\frac{1}{2}} z) = \frac{\partial}{\partial a} t^{-1/2} \frac{\partial}{\partial b} z + t^{-1/2} \frac{\partial^2 z}{\partial a \partial b} + \frac{\partial z}{\partial a} \frac{\partial t^{-1/2}}{\partial b} + z \frac{\partial^2}{\partial a \partial b} t^{-1/2}.$

$\qquad = -\frac{1}{2} t^{-3/2} \frac{\partial t}{\partial a} \frac{\partial z}{\partial b} + t^{-\frac{1}{2}} \frac{\partial^2 z}{\partial a \partial b} - \frac{1}{2} t^{-\frac{3}{2}} \frac{\partial z}{\partial a} \frac{\partial t}{\partial b} + z \frac{\partial^2}{\partial a \partial b} t^{-1/2}.$

$\frac{\partial t}{\partial a} = \frac{\partial \alpha\gamma}{\partial a} - 2\beta \frac{\partial \beta}{\partial a}.$

$\frac{\partial t}{\partial b} = \frac{\partial \alpha\gamma}{\partial b} - 2\beta \frac{\partial \beta}{\partial b}.$

$\frac{\partial z}{\partial a} = (1 + t/\beta^2)^{-1} \left[\frac{t^{-1/2}}{2\beta} \frac{\partial t}{\partial a} - \frac{t^{1/2}}{\beta^2} \frac{\partial \beta}{\partial a} \right]$

$\qquad = \frac{\beta^2}{\beta^2 + \alpha\gamma - \beta^2} \left[\frac{1}{2\beta t^{1/2}} \frac{\partial \alpha\gamma}{\partial a} - \frac{1}{t^{1/2}} \frac{\partial \beta}{\partial a} - \frac{t^{1/2}}{\beta^2} \frac{\partial \beta}{\partial a} \right]$

$\qquad = \frac{\beta^2}{\alpha\gamma} \left[\frac{1}{2\beta t^{1/2}} \frac{\partial \alpha\gamma}{\partial a} - \frac{1}{t^{1/2}} \frac{\partial \beta}{\partial a} - \frac{t^{1/2}}{\beta^2} \frac{\partial \beta}{\partial a} \right]$

$\qquad = \frac{\beta}{2\alpha\gamma t^{1/2}} \frac{\partial \alpha\gamma}{\partial a} - \frac{\beta^2}{\alpha\gamma t^{1/2}} \frac{\partial \beta}{\partial a} - \frac{t^{1/2}}{\alpha\gamma} \frac{\partial \beta}{\partial a}.$

$\frac{\partial z}{\partial b} = \frac{\beta}{2\alpha\gamma t^{1/2}} \frac{\partial \alpha\gamma}{\partial b} - \frac{\beta^2}{\alpha\gamma t^{1/2}} \frac{\partial \beta}{\partial b} - \frac{t^{1/2}}{\alpha\gamma} \frac{\partial \beta}{\partial b}.$

$\frac{\partial^2}{\partial a \partial b} t^{-1/2} z = \frac{\partial}{\partial a} \left[-\frac{1}{2} t^{-3/2} z \frac{\partial t}{\partial b} + t^{-1/2} \frac{\partial z}{\partial b} \right]$

$\qquad = \frac{\partial}{\partial a} \left[-\frac{z}{2t^{3/2}} \frac{\partial \alpha\gamma}{\partial b} + \frac{\beta z}{t^{3/2}} \frac{\partial \beta}{\partial b} + \frac{\beta}{2\alpha\gamma t} \frac{\partial \alpha\gamma}{\partial b} - \frac{\beta^2}{\alpha\gamma t} \frac{\partial \beta}{\partial b} - \frac{1}{\alpha\gamma} \frac{\partial \beta}{\partial b} \right]$

$\qquad = -\frac{z}{2t^{3/2}} \frac{\partial}{\partial a} \left(\frac{\partial \alpha\gamma}{\partial b}\right) + \frac{\partial \alpha\gamma}{\partial b} \left[-\frac{1}{2t^{3/2}} \frac{\partial z}{\partial a} + \frac{3z}{4t^{5/2}} \frac{\partial t}{\partial a} \right] + \frac{\beta z}{t^{3/2}} \frac{\partial}{\partial a} \left(\frac{\partial \beta}{\partial b}\right)$

$\qquad + \frac{\partial \beta}{\partial b} \left[\frac{z}{t^{3/2}} \frac{\partial \beta}{\partial a} + \frac{\beta}{t^{3/2}} \frac{\partial z}{\partial a} - \frac{3\beta z}{2t^{5/2}} \frac{\partial t}{\partial a} \right] + \frac{\beta}{2\alpha\gamma t} \frac{\partial}{\partial a} \left(\frac{\partial \alpha\gamma}{\partial b}\right)$

$\qquad + \frac{\partial \alpha\gamma}{\partial b} \left[\frac{1}{2\alpha\gamma t} \frac{\partial \beta}{\partial a} - \frac{\beta}{2\alpha\gamma^2 t} \frac{\partial \alpha\gamma}{\partial a} - \frac{\beta}{2\alpha\gamma t^2} \frac{\partial t}{\partial a} \right] - \frac{\beta^2}{\alpha\gamma t} \frac{\partial}{\partial a}\left(\frac{\partial \beta}{\partial b}\right) - \frac{1}{\alpha\gamma} \frac{\partial}{\partial a}\left(\frac{\partial \beta}{\partial b}\right)$

$\qquad + \frac{\partial \beta}{\partial b} \left[-\frac{2\beta}{\alpha\gamma t} \frac{\partial \beta}{\partial a} + \frac{\beta^2}{\alpha\gamma^2 t} \frac{\partial \alpha\gamma}{\partial a} + \frac{\beta^2}{\alpha\gamma t^2} \frac{\partial t}{\partial a} \right] + \frac{1}{\alpha\gamma^2} \frac{\partial \alpha\gamma}{\partial a} \frac{\partial \beta}{\partial b}.$

$$\frac{\partial^2}{\partial a \partial b}\, t^{-1/2}\, z$$

$$= \frac{\partial}{\partial a}\left(\frac{\partial \gamma}{\partial b}\right)\left[-\frac{z}{2t^{3/2}} + \frac{\beta}{2\alpha\gamma t}\right] + \frac{\partial}{\partial a}\left(\frac{\partial \beta}{\partial b}\right)\left[\frac{\beta z}{t^{3/2}} - \frac{\beta^2}{\alpha\gamma t} - \frac{1}{\alpha\gamma}\right] + \frac{1}{\alpha\gamma^2}\frac{\partial \gamma}{\partial a}\frac{\partial \beta}{\partial b}$$

$$+ \frac{\partial \gamma}{\partial b}\left[-\frac{\beta}{4\alpha\gamma t^2}\frac{\partial \gamma}{\partial a} + \frac{\beta^2}{2\alpha\gamma t^2}\frac{\partial \beta}{\partial a} + \frac{1}{2\alpha\gamma t}\frac{\partial \beta}{\partial a} + \frac{3z}{4t^{5/2}}\frac{\partial \gamma}{\partial a} - \frac{3\beta z}{2t^{5/2}}\frac{\partial \beta}{\partial a}\right]$$

$$+ \frac{\partial \beta}{\partial b}\left[\frac{z}{t^{3/2}}\frac{\partial \beta}{\partial a} + \frac{\beta^2}{2\alpha\gamma t^2}\frac{\partial \gamma}{\partial a} - \frac{\beta^3}{\alpha\gamma t^2}\frac{\partial \beta}{\partial a} - \frac{\beta}{\alpha\gamma t}\frac{\partial \beta}{\partial a} - \frac{3\beta z}{2t^{5/2}}\frac{\partial \gamma}{\partial a} + \frac{3\beta^2 z}{t^{5/2}}\frac{\partial \beta}{\partial a}\right]$$

$$+ \frac{\partial \gamma}{\partial b}\left[\frac{1}{2\alpha\gamma t}\frac{\partial \beta}{\partial a} - \frac{\beta}{2\alpha\gamma^2 t}\frac{\partial \gamma}{\partial a} - \frac{\beta}{2\alpha\gamma t^2}\frac{\partial \gamma}{\partial a} + \frac{\beta^2}{\alpha\gamma t^2}\frac{\partial \beta}{\partial a}\right]$$

$$+ \frac{\partial \beta}{\partial b}\left[-\frac{2\beta}{\alpha\gamma t}\frac{\partial \beta}{\partial a} + \frac{\beta^2}{\alpha\gamma^2 t}\frac{\partial \gamma}{\partial a} + \frac{\beta^2}{\alpha\gamma t^2}\frac{\partial \gamma}{\partial a} - \frac{2\beta^3}{\alpha\gamma t^2}\frac{\partial \beta}{\partial a}\right].$$

$$= \frac{\partial}{\partial a}\left(\frac{\partial \beta}{\partial b}\right)\left[-\frac{1}{\alpha\gamma} - \frac{\beta^2}{\alpha\gamma t} + \frac{\beta z}{t^{3/2}}\right] + \frac{\partial}{\partial a}\left(\frac{\partial \gamma}{\partial b}\right)\left[\frac{\beta}{2\alpha\gamma t} - \frac{z}{2t^{3/2}}\right]$$

$$+ \frac{\partial \beta}{\partial a}\frac{\partial \beta}{\partial b}\left[-\frac{3\beta^3}{\alpha\gamma t^2} - \frac{3\beta}{\alpha\gamma t} + \frac{3\beta^2 z}{t^{5/2}} + \frac{z}{t^{3/2}}\right]$$

$$+ \frac{\partial \gamma}{\partial a}\frac{\partial \gamma}{\partial b}\left[-\frac{3\beta}{4\alpha\gamma t^2} - \frac{\beta}{2\alpha\gamma^2 t} + \frac{3z}{4t^{5/2}}\right]$$

$$+ \frac{\partial \gamma}{\partial a}\frac{\partial \beta}{\partial b}\left[\frac{1}{\alpha\gamma^2} + \frac{\beta^2}{\alpha\gamma^2 t} + \frac{3\beta^2}{2\alpha\gamma t^2} - \frac{3\beta z}{2t^{5/2}}\right]$$

$$+ \frac{\partial \gamma}{\partial b}\frac{\partial \beta}{\partial a}\left[\frac{3\beta^2}{2\alpha\gamma t^2} + \frac{1}{\alpha\gamma t} - \frac{3\beta z}{2t^{5/2}}\right].$$

Since they will be used repeatedly, the following quantities will be represented by symbols:

$$rp = -\frac{1}{\alpha\gamma} - \frac{\beta^2}{\alpha\gamma t} + \frac{\beta z}{t^{3/2}},$$

$$ap = \frac{\beta}{2\alpha\gamma t} - \frac{z}{2t^{3/2}},$$

$$gp = -\frac{3\beta^3}{\alpha\gamma t^2} - \frac{3\beta}{\alpha\gamma t} + \frac{3\beta^2 z}{t^{5/2}} + \frac{z}{t^{3/2}},$$

$$pp = -\frac{3\beta}{4\alpha\gamma t^2} - \frac{\beta}{2\alpha\gamma^2 t} + \frac{3z}{4t^{5/2}},$$

$$op = \frac{3\beta^2}{2\alpha\gamma t^2} + \frac{1}{\alpha\gamma t} - \frac{3\beta z}{2t^{3/2}}$$

and bp $= \frac{1}{\alpha\gamma^2} + \frac{\beta^2}{\alpha\gamma^2 t} + \frac{3\beta^2}{2\alpha\gamma t^2} - \frac{3\beta z}{2\gamma t^{5/2}}$.

Note that $\frac{1}{\alpha\gamma^2} + \frac{\beta^2}{\alpha\gamma^2 t} = \frac{t+\beta^2}{\alpha\gamma^2 t} = \frac{\alpha\gamma - \beta^2 + \beta^2}{\alpha\gamma^2 t} = \frac{\alpha\gamma}{\alpha\gamma^2 t} = \frac{1}{\alpha\gamma t}$,
so that bp = op, and

$$I = 16\pi(Z_1 Z_2)^{5/2} \frac{1}{ab} \left\{ \frac{\partial}{\partial a}\left(\frac{\partial\beta}{\partial b}\right)(rp) + \frac{\partial}{\partial a}\left(\frac{\partial\alpha\gamma}{\partial b}\right)(ap) + \frac{\partial\beta}{\partial a}\frac{\partial\beta}{\partial b}(gp) \right.$$

$$\left. + \frac{\partial\alpha\gamma}{\partial a}\frac{\partial\alpha\gamma}{\partial b}(pp) + \left(\frac{\partial\alpha\gamma}{\partial a}\frac{\partial\beta}{\partial b} + \frac{\partial\alpha\gamma}{\partial b}\frac{\partial\beta}{\partial a}\right)(op) \right\}.$$

Here the calculations of IJS and IBG must part company, since the definitions of $\alpha\gamma$ and β are different in the two cases. The term IJS will be completed first. It has the same form as I above except that the expressions for $\alpha\gamma$ and β are in the limit where y = 0. That is

$$\alpha\gamma' = \left[(\vec{A}-\vec{B})^2 + (a+b)^2\right]\left[A^2+a^2\right]\left[B^2+b^2\right] \text{ and}$$

$$\beta' = b(A^2+a^2) + a(B^2+b^2) .$$

The partial derivatives of these with respect to a and b needed for the equation for I are:

$$\frac{\partial\alpha\gamma'}{\partial a} = 2a\left[(\vec{A}-\vec{B})^2 + (a+b)^2\right]\left[B^2+b^2\right] + 2(a+b)\left[A^2+a^2\right]\left[B^2+b^2\right]$$

$$\frac{\partial\alpha\gamma'}{\partial b} = 2b\left[(A-B)^2 + (a+b)^2\right]\left[A^2+a^2\right] + 2(a+b)\left[A^2+a^2\right]\left[B^2+b^2\right]$$

$$\frac{\partial\beta'}{\partial a} = 2ab + B^2 + b^2$$

$$\frac{\partial\beta'}{\partial b} = 2ab + A^2 + a^2$$

$$\frac{\partial}{\partial a}\left(\frac{\partial\beta'}{\partial b}\right) = 2(a+b)$$

$$\frac{\partial}{\partial a}\left(\frac{\partial\alpha\gamma'}{\partial b}\right) = 4ab\left[(\vec{A}-\vec{B})^2+(a+b)^2\right] + 4b(a+b)\left[A^2+a^2\right] + 4a(a+b)\left[B^2+b^2\right] .$$

Also for the term IJS, with

$$t' = \alpha\gamma' - \beta'^2 \qquad \text{and} \qquad z' = \tan^{-1}\left(t'^{1/2}/\beta'\right),$$

$$rp' = -\frac{1}{\alpha\gamma'} - \frac{\beta'^2}{\alpha\gamma't'} + \frac{\beta'z'}{t'^{5/2}},$$

$$ap' = \frac{\beta'}{2\alpha\gamma't'} - \frac{z'}{2t'^{3/2}},$$

$$gp' = -\frac{3\beta'^3}{\alpha\gamma'^2 t'^2} - \frac{3\beta'}{\alpha\gamma't'} + \frac{3\beta'^2 z'}{t'^{5/2}} + \frac{z'}{t'^{3/2}},$$

$$pp' = -\frac{3\beta'}{4\alpha\gamma't'^2} - \frac{\beta'}{2\alpha\gamma'^2 t'} + \frac{3z'}{4t'^{5/2}}$$

$$\text{and } op' = \frac{3\beta'^2}{2\alpha\gamma't'^2} + \frac{1}{\alpha\gamma't'} - \frac{3\beta'z'}{2t'^{5/2}}$$

Then with the quantities defined as above,

$$IJS = 16\pi\, Z_1 (Z_1 Z_2)^{5/2} \frac{1}{ab} \left\{ \frac{\partial}{\partial a}\left(\frac{\partial\beta'}{\partial b}\right)(rp') + \frac{\partial}{\partial a}\left(\frac{\partial\alpha\gamma'}{\partial b}\right)(ap') \right.$$

$$+ \frac{\partial\beta'}{\partial a}\frac{\partial\beta'}{\partial b}(gp') + \frac{\partial\alpha\gamma'}{\partial a}\frac{\partial\alpha\gamma'}{\partial b}(pp')$$

$$\left. + \left(\frac{\partial\alpha\gamma'}{\partial a}\frac{\partial\beta'}{\partial b}\right) + \frac{\partial\alpha\gamma'}{\partial b}\frac{\partial\beta'}{\partial a}(op') \right\}.$$

The expression for IBG is a great deal more complicated due to the presence of the partial with respect to y.

$$IBG = -16\pi\, Z_1 (Z_1 Z_2)^{5/2} \frac{1}{ab}\left(1 - Z_2\frac{\partial}{\partial y}\right)\left\{ \frac{\partial}{\partial a}\left(\frac{\partial\beta}{\partial b}\right)(rp) + \frac{\partial}{\partial a}\left(\frac{\partial\alpha\gamma}{\partial b}\right)(ap) \right.$$

$$\left. + \frac{\partial\beta}{\partial a}\frac{\partial\beta}{\partial b}(gp) + \frac{\partial\alpha\gamma}{\partial a}\frac{\partial\alpha\gamma}{\partial b}(pp) + \left[\left(\frac{\partial\alpha\gamma}{\partial a}\frac{\partial\beta}{\partial b}\right) + \left(\frac{\partial\alpha\gamma}{\partial b}\frac{\partial\beta}{\partial a}\right)\right](op) \right\}$$

$$= 16\pi (Z_1 Z_2)^{5/2} \left\{ \frac{\partial}{\partial a}\left(\frac{\partial\beta}{\partial b}\right)\left[\frac{\partial}{\partial y}(rp) - \frac{1}{Z_2}(rp)\right] + (rp)\frac{\partial}{\partial y}\left(\frac{\partial}{\partial a}\frac{\partial\beta}{\partial b}\right) \right.$$

$$+ \frac{\partial}{\partial a}\left(\frac{\partial\alpha\gamma}{\partial b}\right)\left[\frac{\partial}{\partial y}(ap) - \frac{1}{Z_2}(ap)\right] + (ap)\frac{\partial}{\partial y}\left(\frac{\partial}{\partial a}\frac{\partial\alpha\gamma}{\partial b}\right)$$

$$+ \frac{\partial\beta}{\partial a}\frac{\partial\beta}{\partial b}\left[\frac{\partial}{\partial y}(gp) - \frac{1}{Z_2}(gp)\right] + (gp)\frac{\partial}{\partial y}\left(\frac{\partial\beta}{\partial a}\frac{\partial\beta}{\partial b}\right)$$

$$+ \frac{\partial\alpha\gamma}{\partial a}\frac{\partial\alpha\gamma}{\partial b}\left[\frac{\partial}{\partial y}(pp) - \frac{1}{Z_2}(pp)\right] + (pp)\frac{\partial}{\partial y}\left(\frac{\partial\alpha\gamma}{\partial a}\frac{\partial\alpha\gamma}{\partial b}\right)$$

$$+ \left(\frac{\partial \alpha\gamma}{\partial a} \frac{\partial \beta}{\partial b} + \frac{\partial \alpha\gamma}{\partial b} \frac{\partial \beta}{\partial a} \right) \left[\frac{\partial}{\partial y} (op) - \frac{1}{z_2} (op) \right] + (op) \frac{\partial}{\partial y} \left(\frac{\partial \alpha\gamma}{\partial a} \frac{\partial \beta}{\partial b} + \frac{\partial \alpha\gamma}{\partial b} \frac{\partial \beta}{\partial a} \right).$$

Recall that

$$\alpha\gamma = \left[(\vec{A} - \vec{B})^2 + (a+b)^2 \right] \left[A^2 + (a+y)^2 \right] \left[B^2 + (b+y)^2 \right]$$

and

$$\beta = y \left[(\vec{A} - \vec{B})^2 + (a+b)^2 \right] + b(A^2 + a^2 + y^2) + a(B^2 + b^2 + y^2)$$

The partial derivatives needed above are given below.

$$\frac{\partial \beta}{\partial b} = 2y(a+b) + A^2 + a^2 + y^2 + 2ab$$

$$\frac{\partial \beta}{\partial a} = 2y(a+b) + B^2 + b^2 + y^2 + 2ab$$

$$\frac{\partial}{\partial a}\left(\frac{\partial \beta}{\partial b} \right) = 2y + 2a + 2b$$

$$\frac{\partial}{\partial y}\left(\frac{\partial}{\partial a} \frac{\partial \beta}{\partial b} \right) = 2$$

$$\frac{\partial}{\partial y}\left(\frac{\partial \beta}{\partial a} \right) = 2(a+b+y)$$

$$\frac{\partial}{\partial y}\left(\frac{\partial \beta}{\partial b} \right) = 2(a+b+y)$$

$$\frac{\partial \alpha\gamma}{\partial a} = 2(a+y)\left[(\vec{A}-\vec{B})^2 + (a+b)^2 \right]\left[B^2 + b^2 + y^2 \right] + 2(a+b)\left[A^2 + (a+y)^2 \right]\left[B^2 + (b+y)^2 \right]$$

$$\frac{\partial \alpha\gamma}{\partial b} = 2(b+y)\left[(\vec{A}-\vec{B})^2 + (a+b)^2 \right]\left[A^2 + a^2 + y^2 \right] + 2(a+b)\left[A^2 + (a+y)^2 \right]\left[B^2 + (b+y)^2 \right]$$

$$\frac{\partial}{\partial a}\left(\frac{\partial \alpha\gamma}{\partial b} \right) = 4(a+y)(b+y)\left[(\vec{A}-\vec{B})^2 + (a+b)^2 \right] + 4(a+b)(b+y)\left[A^2 + (a+y)^2 \right]$$
$$+ 4(a+y)(a+b)\left[B^2 + (b+y)^2 \right] + 2\left[A^2 + (a+y)^2 \right]\left[B^2 + (b+y)^2 \right].$$

$$\frac{\partial}{\partial y}\left(\frac{\partial}{\partial a} \frac{\partial \alpha\gamma}{\partial b} \right) = 4\left[a+b+2y \right]\left[(\vec{A}-\vec{B})^2 + (a+b)^2 \right] + 16(a+b)(a+y)(b+y)$$
$$+ 4\left[a+2b+y \right]\left[A^2 + (a+y)^2 \right] + 4(2a+b+y)\left[A^2 + (a+y)^2 \right]$$

$$\frac{\partial}{\partial y}\left(\frac{\partial \alpha\gamma}{\partial a} \right) = 4(a+y)(b+y)\left[(\vec{A}-\vec{B})^2 + (a+b)^2 \right] + 2\left[(\vec{A}-\vec{B})^2 + (a+b)^2 \right]\left[B^2 + (b+y)^2 \right]$$
$$+ 4(a+b)(a+y)\left[B^2 + (b+y)^2 \right] + 4(a+b)(b+y)\left[A^2 + (a+y)^2 \right]$$

$$\frac{\partial}{\partial y}\left(\frac{\partial \alpha \gamma}{\partial b}\right) = 4(a+y)(b+y)\left[(\vec{A}-\vec{B})^2 + (a+b)^2\right] + 2\left[(\vec{A}-\vec{B})^2 + (a+b)^2\right]\left[A^2 + (a+y)^2\right]$$
$$+ 4(a+b)(a+y)\left[B^2 + (b+y)^2\right] + 4(a+b)(b+y)\left[A^2 + (a+y)^2\right]$$

$$\frac{\partial t}{\partial y} = \frac{\partial}{\partial y}(\alpha\gamma - \beta^2) = \frac{\partial \alpha\gamma}{\partial y} - 2\beta\frac{\partial\beta}{\partial y}$$

$$\frac{\partial \alpha\gamma}{\partial y} = 2(b+y)\left[(\vec{A}-\vec{B})^2 + (a+b)^2\right]\left[A^2 + (a+y)^2\right] + 2(a+y)\left[(\vec{A}-\vec{B})^2 + (a+b)^2\right]\left[B^2 + (b+y)^2\right]$$

$$\frac{\partial\beta}{\partial y} = \left[(\vec{A}-\vec{B})^2 + (a+b)^2\right] + 2by + 2ay$$

$$\frac{\partial z}{\partial y} = \frac{\beta^2}{\alpha\gamma}\left[\frac{1}{2\beta t^{1/2}}\frac{\partial t}{\partial y} - \frac{t^{1/2}}{\beta}\frac{\partial\beta}{\partial y}\right] = \frac{\beta}{2\alpha\gamma t^{1/2}}\frac{\partial\alpha\gamma}{\partial y} - \frac{\beta^2}{\alpha\gamma t^{1/2}}\frac{\partial\beta}{\partial y} - \frac{t^{1/2}}{\alpha\gamma}\frac{\partial\beta}{\partial y}$$

$$\frac{\partial}{\partial y}(rp) = \frac{\partial \alpha\gamma}{\partial y}\left[\frac{1}{\alpha\gamma^2} + \frac{\beta^2}{\alpha\gamma^2 t} + \frac{3\beta^2}{2\alpha\gamma t^2} - \frac{3\beta z}{2t^{5/2}}\right]$$
$$+ \frac{\partial\beta}{\partial y}\left[-\frac{3\beta}{\alpha\gamma t} - \frac{3\beta^3}{\alpha\gamma t^2} + \frac{z}{t^{5/2}} + \frac{3\beta^2 z}{t^{5/2}}\right].$$

$$\frac{\partial}{\partial y}(ap) = \frac{\partial \alpha\gamma}{\partial y}\left[-\frac{\beta}{2\alpha\gamma^2 t} - \frac{3\beta}{4\alpha\gamma t^2} + \frac{3z}{4t^{5/2}}\right]$$
$$+ \frac{\partial\beta}{\partial y}\left[\frac{1}{\alpha\gamma t} + \frac{3\beta^2}{2\alpha\gamma t^2} - \frac{3\beta z}{2t^{5/2}}\right]$$

$$\frac{\partial}{\partial y}(gp) = \frac{\partial \alpha\gamma}{\partial y}\left[\frac{3\beta^3}{\alpha\gamma^2 t^2} + \frac{3\beta}{\alpha\gamma^2 t} - \frac{15\beta^2 z}{2t^{7/2}} + \frac{15\beta^3}{2\alpha\gamma t^3} - \frac{3z}{2t^{5/2}} + \frac{7\beta}{2\alpha\gamma t^2}\right]$$
$$+ \frac{\partial\beta}{\partial y}\left[-\frac{19\beta^2}{\alpha\gamma t^2} - \frac{15\beta^4}{\alpha\gamma t^3} + \frac{9\beta z}{t^{5/2}} + \frac{15\beta^3 z}{t^{7/2}} - \frac{4}{\alpha\gamma t}\right]$$

$$\frac{\partial}{\partial y}(pp) = \frac{\partial \alpha\gamma}{\partial y}\left[\frac{5\beta}{4\alpha\gamma^2 t^2} + \frac{\beta}{\alpha\gamma^3 t} + \frac{15\beta}{8\alpha\gamma t^3} - \frac{15z}{8t^{7/2}}\right]$$
$$+ \frac{\partial\beta}{\partial y}\left[-\frac{3}{2\alpha\gamma t^2} - \frac{15\beta^2}{4\alpha\gamma t^3} - \frac{1}{2\alpha\gamma^2 t} - \frac{\beta^2}{\alpha\gamma^2 t^2} + \frac{15\beta z}{4t^{7/2}}\right]$$

$$\frac{\partial}{\partial y}(op) = \frac{\partial \alpha\gamma}{\partial y}\left[-\frac{3\beta^2}{2\alpha\gamma^2 t^2} - \frac{1}{\alpha\gamma^2 t} - \frac{1}{\alpha\gamma t^2} + \frac{15\beta z}{4t^{7/2}} - \frac{15\beta^2}{4\alpha\gamma t^3}\right]$$
$$+ \frac{\partial\beta}{\partial y}\left[\frac{13\beta}{2\alpha\gamma t^2} - \frac{3z}{2t^{5/2}} - \frac{15\beta^2 z}{2t^{7/2}} + \frac{15\beta^3}{2\alpha\gamma t^3}\right].$$

APPENDIX 3

A computer program that calculates single and double charge
capture cross sections from the ground state of a target
atom into the ground state of a projectile. These are given
in units of a_o^2, πa_o^2 and cm^2, in the approximations of
Brinkman and Kramers, Jackson and Schiff, and Bassel and
Gerjuoy.

```
C     PROGRAM BY TERRY C. THEISEN, KANSAS STATE UNIVERSITY, NOV. 1978.
C     COMPUTATION OF SINGLE AND DOUBLE ELECTRON CAPTURE CROSS SECTIONS
C     IN THE BRINKMAN AND KRAMERS, THE JACKSON AND SCHIFF AND THE
C     BASSEL AND GERJUOY APPROXIMATIONS.
C
C     M1 IS THE MASS OF THE PROJECTILE IN ATOMIC UNITS
C     Z1 IS THE CHARGE OF THE PROJECTILE IN ATOMIC UNITS
C     M2 IS THE MASS OF THE TARGET IN ATOMIC UNITS
C     Z2 IS THE CHARGE OF THE TARGET IN ATOMIC UNITS
C     BEI IS THE BINDING ENERGY OF THE INITIAL SYSTEM.
C     BEF IS THE BINDING ENERGY OF THE FINAL SYSTEM.
C     BIA IS THE INITIAL BINDING ENERGY IN ATOMIC UNITS.
C     BFA IS THE FINAL BINDING ENERGY IN ATOMIC UNITS.
C     ENERGY IS THE ENERGY OF THE INCIDENT PARTICLE IN ELECTRON VOLTS.
C     V IS THE VELOCITY OF THE INCIDENT PARTICLE
C     KI IS THE MOMENTUM OF THE INCIDENT PARTICLE.
C     KF IS THE MOMENTUM OF THE TARGET AFTER CAPTURE.
C     THE INITIAL AND FINAL REDUCED MASSES ARE MUI AND MUF RESPECTIVELY.
C     THETA IS THE SCATTERING ANGLE
C     TTHETA IS THE SCATTERING AMPLITUDE
C     B IS THE IMPACT PARAMETER
C     BJ IS THE VALUE OF THE ZEROTH ORDER BESSEL FUNCTION WHOSE
C         ARGUMENT IS: K*B*THETA
C     AL IS THE PROBABILITY AMPLITUDE
C     PB IS THE PROBABILITY AMPLITUDE SQUARED
C
C     BK DENOTES THE BRINKMAN KRAMERS APPROXIMATION.
C     JS DENOTES THE SUM OF THE JACKSON AND SHIFF AND THE BK
C         APPROXIMATIONS.
C     BG DENOTES THE SUM OF THE JS AND THE BASSEL AND GERJUOY
C         APPROXIMATIONS.
C
      IMPLICIT REAL*8 (A-H,O-Z)
```

```
      REAL*8 KI,KF,MUI,MUF,M1,M2,IEK,IJS,IBG
      READ 10,M1,Z1,M2,Z2
   10 FORMAT (4F10.0)
      READ 12,BEI,BEF
   12 FORMAT (2F10.0)
    5 READ 20,ENERGY
   20 FORMAT (F15.0)
      IF (ENERGY.LE.0) STOP
      PRINT 15,M1,Z1,M2,Z2
   15 FORMAT ('1',7X,'CALCULATION CF TCTAL CROSS SECTICNS',
     1//8X,'M1=',F11.5,10X,'Z1=',F8.5//8X,'M2=',F11.5,10X,'Z2=',F8.5//)
      PRINT 50,ENERGY
   50 FORMAT('0','THE INCIDENT ENERGY IN EV IS: ',F10.1//)
      PRINT 23
   23 FORMAT ('0',5X,'B',10X,'P(B)BK',11X,'P(B)JS',11X,'P(B)BG')
      PI=3.1415926
      AQ=5.29177150-9
      RYDB=13.6058
      E=ENERGY/RYDB
      EIA=BEI/(2.0*RYDB)
      BFA=BEF/(2.0*RYDB)
      SBK1=0.0
      SJS1=0.0
      SBG1=C.0
      SBK4=0.0
      SJS4=0.0
      SBG4=0.0
      B=-0.0499
      CB=0.C5
      DO 40 J=1,50
      B=B+CB
      THET1=C.0
      THET2=3.0*Z2/M2
      THET3=27.5/M2
      THET4=3.1405926
      CThET1=(THET2-ThET1)/25.
      DThET2=(ThET3-ThET2)/25.
```

```fortran
      DTHET3=(THET4-THET3)/25.
      CALL AL(M1,M2,Z1,Z2,E,BIA,BFA,THET1,DTHET1,B,ALEK1,ALJS1,ALBG1)
      CALL AL(M1,M2,Z1,Z2,E,BIA,BFA,THET2,DTHET2,B,ALEK2,ALJS2,ALBG2)
      CALL AL(M1,M2,Z1,Z2,E,BIA,BFA,THET3,DTHET3,B,ALEK3,ALJS3,ALBG3)
      ALBK=ALBK1+ALBK2+ALBK3
      ALJS=ALJS1+ALJS2+ALJS3
      ALBG=ALBG1+ALBG2+ALBG3
      PBBK=ALBK**2
      PBJS=ALJS**2
      PBBG=ALBG**2
      PRINT 25,B,PBBK,FBJS,PBBG
   25 FORMAT (' ',1PD10.3,1P3D17.7)
      CC=B*CE*2.0
      SBK1=SBK1+CC*PBBK
      SJS1=SJS1+CC*PBJS
      SEG1=SEG1+CC*PBBG
      SBK4=SBK4+CC*PBBK**2
      SJS4=SJS4+CC*PBJS**2
      SEG4=SEG4+CC*PBBG**2
   40 CONTINUE
      SBK1=SBK1*2.0
      SJS1=SJS1*2.0
      SBG1=SBG1*2.0
      SBK2=SBK1*PI
      SJS2=SJS1*PI
      SEG2=SEG1*PI
      SBK3=SBK2*AO**2
      SJS3=SJS2*AO**2
      SBG3=SBG2*AO**2
      SBK5=SBK4*PI
      SJS5=SJS4*PI
      SBG5=SBG4*PI
      SBK6=SBK5*AC**2
      SJS6=SJS5*AO**2
      SEG6=SEG5*AO**2
      PRINT 80
   80 FORMAT (//,'0','TOTAL SINGLE CAPTURE',10X,'IN',15X,'IN',15X,'IN')
```

```
      PRINT 82
   82 FORMAT ('0',4X,'CROSS SECTIONS',10X,'PI*A0**2',10X,'A0**2',11X,
     1'CM**2')
      PRINT 84,SBK1,SBK2,SBK3
   84 FORMAT ('0',1X,'BRINKMAN KRAMERS',5X,1P3D17.7)
      PRINT 86,SJS1,SJS2,SJS3
   86 FORMAT ('0',1X,'JACKSON AND SCHIFF',3X,1P3D17.7)
      PRINT 88,SBG1,SBG2,SBG3
   88 FORMAT ('0',1X,'BASSEL AND GERJUOY',3X,1P3D17.7)
      PRINT 90
   90 FORMAT (//'0','TOTAL DOUBLE CAPTURE',10X,'IN',15X,'IN',15X,'IN')
      PRINT 92
   92 FORMAT ('0',4X,'CROSS SECTIONS',10X,'IN','PI*AC**2',10X,'AC**2',11X,
     1'CM**2')
      PRINT 94,SBK4,SBK5,SBK6
   94 FORMAT ('0',1X,'BRINKMAN KRAMERS',5X,1P3D17.7)
      PRINT 96,SJS4,SJS5,SJS6
   96 FORMAT ('0',1X,'JACKSON AND SCHIFF',3X,1P3D17.7)
      PRINT 98,SBG4,SBG5,SBG6
   98 FORMAT ('0',1X,'BASSEL AND GERJUOY',3X,1P3D17.7)
      GO TO 5
      END
C.........................................................
C
C     SUBROUTINE AL CALCULATES THE SQUARE ROOT OF THE PROBABILITY
C     AMPLITUDE WHICH IS THE INTEGRAL OF THE PRODUCT OF THE SCATTERING
C     AMPLITUDE, THE J0 BESSEL FUNCTION, SIN(THETA), AND A CONSTANT OVER
C     A GIVEN THETA INTERVAL.
C     M1, M2, Z1, AND Z2 ARE THE MASSES AND CHARGES OF THE PROJECTILE
C     AND THE TARGET, RESPECTIVELY. E IS THE ENERGY OF THE PROJECTILE
C     IN RYDBERGS.
C
      SUBROUTINE AL(M1,M2,Z1,Z2,E,E1A,BFA,THETA,CTHETA,B,AL3K,ALJS,ALBG)
      IMPLICIT REAL*8 (A-H,O-Z)
```

```
REAL*8 KI,KF,MUI,MUF,M1,M2,IBK,IJS,IBG
AC=5.2917715C-9
PI=3.1415926
V=(E/M1)**.5
MLI=(M1*(M2+1.))/(M1+M2+1.)
MUF=(M2*(M1+1.))/(M1+M2+1.)
W=M1/(M1+1.)
XA=M2/(M2+1.)
KI=MUI*V
KF=(MUF*(KI**2/MUI-2.0*(BIA-EFA)))**0.5
Y=2.*Z2
C=16.*PI*(Z1*Z2)**2.5
C3=(MUI*MUF*KI*KF)**0.5/(2.*PI)
ALBK=0.00
ALJS=0.00
ALBG=0.00
DC 30 J=1,25
THETA=THETA+CTI-ETA
ASQ=KI**2+(W*KF)**2-2.0*KI*KF*W*DCOS(THETA)
BSQ=KF**2+(XA*KI)**2-2.0*KI*KF*XA*DCOS(THETA)
AMNBSC=ASQ+BSQ+2.*KI*KF*CCCS(TI-ETA)*(W*XA+1.0)
   1   -2.*(W*KF**2+XA*KI**2)
P=AMNBSQ+(Z1+Z2)**2
QJS=ASC+Z1**2
RJS=BSQ+Z2**2
AGJS=P*QJS*RJS
BTAJS=Z2*QJS+Z1*RJS
TJS=AGJS-BTAJS**2
ZJS=CATAN(TJS**.5/ETAJS)
REDJS=-1./AGJS -BTAJS**2/(AGJS*TJS) +BTAJS*ZJS/TJS**1.5
AGUAJS=BTAJS/(2.*AGJS*TJS) -ZJS/(2.*TJS**1.5)
GRJS=-(3.*BTAJS**3)/(AGJS*TJS**2)-3.*BTAJS/(AGJS*TJS)
   1   +(3.*BTAJS**2*ZJS)/TJS**2.5 +ZJS/TJS**1.5
FNKJS=-3.*BTAJS/(4.*AGJS*TJS**2) -BTAJS/(2.*AGJS**2*TJS)
   1   +3.*ZJS/(4.*TJS**2.5)
CRJS=3.*BTAJS**2/(2.*AGJS*TJS**2) +1./(AGJS*TJS) -3.*BTAJS*ZJS/
   1   (2.*TJS**2.5)
```

```
      BJSA=2.*Z1*Z2+RJS
      EJSB=2.*Z1*Z2+CJS
      AGJSA=2.*Z1*RJS*P+2.*(Z1+Z2)*QJS*RJS
      AGJSB=2.*Z2*QJS*P+2.*(Z1+Z2)*QJS*RJS
      AAGJSB=4.*Z1*Z2*P+4.*Z2*(Z1+Z2)*QJS+2.*Z1*(Z1+Z2)*RJS
      IHK=(-32.*PI*(Z1+Z2)**2.5)/(CJS**2*RJS)
      IJS=(C./Z2)*(2.*(Z1+Z2)*REDJS +AAGJSB*AGUAJS +BJSA*BJSB*GRJS)
     1  +AGJSA*AGJSB*PNKJS +(AGJSA*EJSB+AGJSB*EJSA)*CRJS)
      G=ASQ+(Z1+Y)**2
      R=ESG+(Z2+Y)**2
      AG=P*G*R
      BTA=Y*P+Z2*(CJS+Y**2)+Z1*(RJS+Y**2)
      T=AG-BTA**2
      Z=CATAN(T**.5/ETA)
      REC=-1./AG  -BTA**2/(AG*T) +BTA*Z/T**1.5
      AGUA=ETA/(2.*AG*T)  -Z/(2.*T**1.5)
      GR=-3.*BTA**3/(AG*T**2) -3.*BTA/(AG*T) +(3.*ETA**2*Z)/T**2.5
     1  +Z/T**1.5
      PNK=-3.*BTA/(4.*AG*T**2)  -ETA/(2.*AG**2*T) +3.*Z/(4.*T**2.5)
      QR=3.*BTA**2/(2.*AG*T**2) +1./(AG*T)  -3.*ETA*Z/(2.*T**2.5)
      AGY=2.*(Z2+Y)*P*Q  +2.*(Z1+Y)*P*R
      EY=P+2.*Y*(Z1+Z2)
      REDY=AGY*(1./AG**2 +BTA**2/(AG**2*T)  -3.*BTA*Z/(2.*T**2.5)
     1  +3.*BTA**2/(2.*AG*T**2)) +BY*(-3.*BTA/(AG*T)  -3.*BTA*Z/T**2.5
     2  /(AG*T**2) +Z/T**1.5 +3.*ETA**2*Z/T**2.5)
      AGUAY=AGY*(-BTA/(2.*AG**2*T) +3.*Z/(4.*T**2.5)  -3.*BTA/(4.*
     1  AG*T**2)) +BY*(1./(AG*T) +3.*BTA**2/(2.*AG*T**2)  -3.*
     2  BTA*Z/(2.*T**2.5))
      GRY=AGY*((3.*BTA**2/AG**2 +BTA**2/AG**2)*(BTA/T**2)+(3.*BTA/AG**2)/T
     1  -(15.*BTA**2/T**2)*(Z/(2.*T**1.5))+(15.*BTA**2/(2.*AG*T))*
     3  (BTA/T**2)-(3./(2.*T))*(Z/(2.*T))*(Z/T**1.5)+(7.*ETA/(2.*T**2))/AG)
     4  +BY*(-(15.*BTA**2/(AG*T))*(ETA/T**2)+(5.*ETA/T**1.5)*(Z/T)
     5  +(15.*BTA**2/T**2)*(BTA/T**1.5)-(19.*ETA**2/T**2)/AG
     6  -4./(AG*T))
      PNKY=AGY*((5.*BTA/AG**2)/(4.*T**2)+(BTA/AG**2)/(AG*T)-(15./T**2)
     1  *(Z/(8.*T**1.5))+(15./(8.*AG*T))*(ETA/T**2))
     2  +BY*(-(3./AG)/(2.*T**2)-1./(2.*AG**2*T)-(BTA**2/AG**2)/T**2
```

```fortran
3    +(15.*BTA/T**2)*(Z/(4.*T**1.5))-(15.*ETA**2/T**3)/(4.*AG))
ORY=AGY*(-(3.*BTA/T**2)*(Z/(2.*AG**2))/T**2-1./(AG**2*T)-1./(AG*T**2)
1    +(15.*BTA/T**2)*(Z/(4.*T**1.5))-(15.*BTA**2/(4.*T**2))/(AG*T)))
2    +BY*(-(3./(2.*T))*(Z/(T**1.5))-(15.*BTA/T**2)*(Z/(2.*T**1.5))
3    +(15.*BTA**2/(2.*T**2))*(ETA/(AG*T)))+(13.*BTA/T**2)/(2.*AG)))
BA=2.*Y*(Z1+Z2)+2.*Z1*Z2+RJS+Y**2
BB=2.*Y*(Z1+Z2)+2.*Z1*Z2+QJS+Y**2
ABB=Y+Z1+Z2
AGA=2.*(Z1+Y)*P*R+2.*(Z1+Z2)*Q*R
AGB=2.*(Z2+Y)*P*Q+2.*(Z1+Z2)*Q*R
YAGA=4.*(Z1+Y)*(Z2+Y)*P*R+4.*P*R+4.*(Z1+Y)*(Z1+Z2)*R+4.*(Z1+Z2)*
1    (Z2+Y)*C
YAGB=4.*(Z1+Y)*(Z2+Y)*P+2.*P*Q+4.*(Z1+Y)*(Z1+Z2)*R+4.*(Z1+Z2)*
1    (Z2+Y)*C
AAGB=4.*(Z1+Z2)*(Z2+Y)*Q+4.*(Z1+Y)*(Z2+Y)*F+4.*(Z1+Z2)*(Z1+Y)*R
1    +2.*Q*R
YAAGB=4.*ABB*(Q+P+R)+4.*(Z2*C+Z1*R+Y*P)+16.*(Z1+Z2)*(Z1+Y)*(Z2+Y)
IBG=C*(2.*ABB*(REDY-RED/Z2)+AAGB*(AQUAY-AQUA/Z2)+BA*EB*(GRY-GR/
1    Z2)+AGA*ACE*(PNKY-PNK/Z2)+(AGA*EB+ACE*EA)*(QRY-QR/Z2)
2    +2.*RED+YAAGB*AQUA+2.*ABB*(6A+EB)*GR+(AGA*YAGE+AGE*YAGA)
3    *FNK+(2.*ABB*(AGA+AGB)+EA*YAGB+BB*YAGA)*CR)
TTBK=IBK
TTJS=IBK+IJS
TTBG=IBK+IJS+IBG

C
C    CALCULATION OF THE ZEROTH-ORDER BESSEL FUNCTION USING THE
C    FORMULAS OF ABRAMOWITZ AND STEGUN, PAGES 369 AND 370. EQUATIONS
C    9.4.1 AND9.4.3.
C
X=KI*THETA*B
VAL1=X/3.CO
VAL2=3.D0/X
IF (X+3.) 50,100,100
50 IER=1
GC TC 17
100 IER=0
```

```
      IF (X-3.) 150,150,200
150 BJ=1.D0-2.2495570D0*(VAL1)**2 +1.2656208D0*(VAL1)**4
   1   -.3163866D0*(VAL1)**6 +.0444479D0*(VAL1)**8
   2   -.0039444D0*(VAL1)**10 +.0021000D0*(VAL1)**12
      GO TO 17
200 F0=.7978845600 -.0000077D0*(VAL2) -.0055274D0*(VAL2)**2
   2   -.00009512D0*(VAL2)**3 +.0013723700*(VAL2)**4
   2   -.0007280500*(VAL2)**5 +.0014476D0*(VAL2)**6
      THETA0=X -.7853581600 -.0416635700*(VAL2) -.0003954D0*(VAL2)**2
   1   +.0026257300*(VAL2)**3 -.0005412500*(VAL2)**4
   2   -.0002933300*(VAL2)**5 +.0001355800*(VAL2)**6
      BJ=F0*DCOS(THETA0)/X**.5E0
17 CONTINUE
      CTHETA=C3*BJ*DSIN(THETA)*DTHETA
      ALBK=ALBK+TTBK*CTHETA
      ALJS=ALJS+TTJS*CTHETA
      ALBG=ALBG+TTBG*CTHETA
30 CONTINUE
      RETURN
      END
C..............................................................
C
C
$ENTRY
0.0
/*
```

APPENDIX 4

This computer program computes single charge capture
differential cross sections in $\pi a_o{}^2$ for the approximations
of Brinkman and Kramers, Jackson and Schiff, and Bassel
and Gerjuoy.

```
C      CALCULATION CF DSIGMA/DOMEGA IN THE BRINKMAN KRAMERS, JACKSON AND
C      SHIFF, AND THE BASSEL AND GERJUOY APPROXIMATIONS.
C
C
       IMPLICIT REAL*8 (A-H,C-Z)
       REAL*8 K,MUI,MUF,M1,M2,IBK,IJS,IBG
       READ 10,M1,Z1,M2,Z2
  10   FORMAT (4F10.0)
       PRINT 15,M1,Z1,M2,Z2
  15   FORMAT ('1',8X,'DIFFERENTIAL CROSS SECTICNS IN PI*A0**2.',
      1//8X,'M1=',F11.5,10X,'Z1=',F8.5//3X,'M2=',F11.5,10X,'Z2=',F8.5//)
       PRINT 32
  32   FORMAT ('0',2X,'THETA',6X,'LAMECA',10X,'IBK',14X,'IJS',14X,'IBG',
      1 10X,'(DSIGMA/COMEGA)BK',1X,'(DSIGMA/DOMEGA)JS',1X,'(DSIGMA/DOMEGA
      2 )BG')
  5    READ 20,ENERGY
  20   FORMAT (F15.0)
       IF (ENERGY.LE.0) STOP
       RYDB=13.6058
       E=ENERGY/RYDB
       PI=3.1415926
       THET1=0.0
       THET2=.0029832
       THET3=PI/2.
       THET4=PI-.001
       DTHET1=(THET2-THET1)/30.
       DTHET2=(THET3-THET2)/30.
       DTHET3=(THET4-THET3)/30.
       CALL DIFCS(M1,M2,Z1,Z2,E,THET1,DTHET1,CSOBK1,DSCJS1,CSCBG1)
       CALL DIFCS(M1,M2,Z1,Z2,E,THET2,DTHET2,CSCEK2,CSCJS2,CSCBG2)
       CALL DIFCS(M1,M2,Z1,Z2,E,THET3,DTHET3,DSCBK3,DSCJS3,CSCBG3)
       PRINT 50,ENERGY
  50   FORMAT(//'0','THE INCIDENT ENERGY IN EV IS: ',F10.1//)
       GC TO 5
       END
C
C
```

```
C     SUBROUTINE DIFCS CALCULATES THE DIFFERENTIAL CROSS SECTION IN
C     PI*A0**2 FOR A GIVEN THETA AND A GIVEN DTHETA.
C     THE BRINKMAN KRAMERS DIFF CROSS SECTION IS DENOTED BY DSDOBK.
C     THE JACKSON AND SCHIFF DIFF CROSS SECTION IS DENOTED BY DSDOJS.
C     THE BASSEL AND GERJUOY DIFF CROSS SECTION IS DENOTED BY DSDOBG.
C     M1, M2, Z1, AND Z2 ARE THE MASSES AND CHARGES OF THE PROJECTILE
C     AND TARGET, RESPECTIVELY.  E IS THE ENERGY OF THE PROJECTILE IN
C     RYDBERGS.
C
C
      SUBROUTINE DIFCS(M1,M2,Z1,Z2,E,THETA,DTHETA,DSDOBK,DSDOJS,DSDOBG)
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*8 K,MUI,MUF,M1,M2,IBK,IJS,IBG
      PI=3.1415926
      A0=5.2917715D-9
      MUI=(M1*(M2+1.))/(M1+M2+1.)
      MUF=(M2*(M1+1.))/(M1+M2+1.)
      V=(E/M1)**.5
      K=MUI*V
      W=M1/(M1+1.)
      X=M2/(M2+1.)
      Y=2.*Z2
      C=16.*PI*(Z1*Z2)**2.5
      C2=MUI*MUF/(4.*PI**3)
      DO 30 J=1,30
      THETA=THETA+DTHETA
      ALAMBD=(2.*M1*DSIN(THETA/2.))**2
      ASQ=K**2*(1.+W**2-2.*W*DCOS(THETA))
      BSQ=K**2*(1.+X**2-2.*X*DCOS(THETA))
      AMNBSQ=K**2*((W-1.)**2+(X-1.)**2+2.*(W*X-W-X+1.)*DCOS(THETA))
      P=AMNBSQ+(Z1+Z2)**2
      CJS=ASQ+Z1**2
      RJS=BSQ+Z2**2
      AGJS=P*CJS*RJS
      BTAJS=Z2*CJS+Z1*RJS
```

```
TJS=AGJS-BTAJS**2
ZJS=CATAN(TJS**.5/BTAJS)
REDJS=-1./AGJS -BTAJS**2/(AGJS*TJS) +BTAJS*ZJS/TJS**1.5
AQUAJS=BTAJS/(2.*AGJS*TJS) -ZJS/(2.*TJS**1.5)
GRJS=-(3.*BTAJS**3)/(AGJS**2*TJS**2)-3.*BTAJS/(AGJS*TJS**1.5)
1    +(3.*BTAJS**2*ZJS)/TJS**2.5 +ZJS/(2.*AGJS**2*TJS))
PNKJS=-3.*ETAJS/(4.*AGJS*TJS**2) -BTAJS/(2.*AGJS**2*TJS)
1    +3.*ZJS/(4.*TJS**2.5)
CRJS=3.*BTAJS**2/(2.*AGJS*TJS**2) +1./(AGJS*TJS) -3.*ETAJS*ZJS/
1    (2.*TJS**2.5)
BJSA=2.*Z1*Z2+RJS
EJSB=2.*Z1*Z2+QJS
AGJSA=2.*Z1*RJS*P+2.*(Z1+Z2)*QJS*RJS
AGJSB=2.*Z2*QJS*P+2.*(Z1+Z2)*QJS*RJS
AAGJSB=4.*Z1*Z2*P+4.*Z2*(Z1+Z2)*QJS+2.*QJS*RJS+4.*Z1*(Z1+Z2)*RJS
IBK=(-22.*PI*(Z1+Z2)**2.5)/(GJS**2*RJS)
IJS=C*(2*(Z1+Z2)*REDJS +AAGJSA*BJSB*AQUAJS +BJSA*EJSE*GRJS +AGJSA*AGJSB
1    *PNKJS +(AGJSA*BJSB*AGJSB*EJSA)*CRJS)
G=ASQ+(Z1+Y)**2
R=BSQ+(Z2+Y)**2
AG=P*G*R
BTA=Y*P+Z2*(QJS+Y**2)+Z1*(RJS+Y**2)
T=AG-BTA**2
Z=DATAN(T**.5/ETA)
RED=-1./AG -BTA**2/(AG*T) +BTA*Z/T**1.5
AQUA=BTA/(2.*AG*T) -Z/(2.*T**1.5)
GR=-3.*BTA**3/(AG*T**2) -3.*BTA/(AG*T) +(3.*ETA**2*Z)/T**2.5
1    +Z/T**1.5
FNK=-3.*BTA/(4.*AG*T**2) -ETA/(2.*AG**2*T) +3.*Z/(4.*T**2.5)
QR=3.*BTA**2/(2.*AG*T**2) +1./(AG*T) -3.*ETA*Z/(2.*T**2.5)
AGY=2.*(Z2+Y)*P*Q +2.*(Z1+Y)*P*R
BY=P+2.*Y*(Z1+Z2)
REDY=AGY*(1.-/AG**2 +BTA**2/(2.*AG*T**2)) +BY*(-3.*BTA/(AG*T) -3.*BTA**3
1    +3.*BTA**2/(2.*AG*T**2)) +Z/T**1.5 +3.*ETA**2*Z/T**2.5) -3.*ETA*Z/(2.*T**2.5)
2    /(AG*T**2) +Z/(4.*T**2.5) +3.*Z/(4.*T**2.5) -3.*BTA/(2.*AG*T**2.5)
AQUAY=AGY*(-BTA/(2.*AG**2*T) +3.*Z/(4.*T**2.5) +3.*BTA**2/(2.*AG*T**2.5)  -3.*
1    AG*T**2)) +BY*(1./(AG*T) +3.*BTA**2/(2.*AG*T**2) -3.*
```

```fortran
2     BTA*Z/(2.*T**2.5))
  GRY=AGY*(3.*BTA**3/(AG**2*T**2) +3.*BTA/(AG**2*T)  -15.*BTA**2*Z/
 1    (2.*T**3.5) +15.*BTA**3/(2.*AG*T**2)) -2.*Z/(2.*T**2.5)
 2    +7.*BTA/(2.*AG*T**2)) +BY*(-15.*BTA**4/(AG*T**3) +5.*ETA*Z/
 3    T**2.5 +15.*BTA**3*Z/T**3.5 -19.*BTA**2/(AG**2*T**2) -4./(AG*T))
  PNKY=AGY*(15.*BTA/(4.*AG**2*T**2)) +BTA/(8.*AG*T**3)) -15.*Z/(8.*T**3.5)
 1    +15.*BTA/(8.*AG*T**3)) +BY*(-3./(2.*AC*T**2) -1./(2.*AG**2*T))
 2    -ETA**2/(AG**2*T**2) +15.*BTA*Z/(4.*T**3.5) -15.*BTA**2/
 3    (4.*AG*T**3))
  ORY=AGY*(-3.*BTA**2/(2.*AG**2*T**2) -1./(AC**2*T) -1./(AG*T**2)
 1    +15.*BTA*Z/(4.*T**3.5) -15.*BTA**2/(4.*AG*T**3)) +BY*(-3.*Z/(
 2    2.*T**2.5) -15.*ETA**2*Z/(2.*T**3.5 +15.*BTA**3/(2.*AG*T**2)/(
 3    +13.*BTA/(2.*AG*T**2))
  BA=2.*Y*(Z1+Z2)+2.*Z1*Z2*RJS+Y**2
  BB=2.*Y*(Z1+Z2)+2.*Z1*Z2*CJS+Y**2
  AEB=Y+Z1+Z2
  AGA=2.*(Z1+Y)*P*R+2.*(Z1+Z2)*Q*R
  AGB=2.*(Z2+Y)*P*Q+2.*(Z1+Z2)*Q*R
  YAGA=4.*(Z1+Y)*(Z2+Y)*P*R+4.*(Z1+Y)*(Z1+Z2)*R+4.*(Z1+Z2)*
 1    (Z2+Y)*G
  YAGB=4.*(Z1+Y)*(Z2+Y)*P+2.*P*Q+4.*(Z1+Y)*(Z2+Y)*F+4.*(Z1+Y)*R
 1    (Z2+Y)*C
  AAGB=4.*(Z1+Z2)*(Z2+Y)*G+4.*(Z2*G+Z1*R+Y*P)+16.*(Z1+Z2)*(Z1+Y)*(Z2+Y)
 1    +2.*Q*R
  YAAGB=4.*ABB*(G+P+R)+4.*(Z2*G+Z1*R+Y*P)+16.*(Z1+Z2)*(Z1+Y)*(Z2+Y)
  IBG=C*(2.*ABB*(REDY-RED/Z2) +AAGB*(AQUAY-AQUA/Z2) +BA*BB*(GRY-GR/
 1    Z2) +AGA*AGB*(PNKY-PNK/Z2) +(AGA*BB+AGB*EA)*(ORY-OR/Z2)
 2    +2.*RED +YAAGB*AQUA +2.*ABB*(BA+EB)*CR +(AGA*YAGE+AGB*YAGA)
 3    *PNK +(2.*ABB*(AGA+AGB)+EA*YAGB+BB*YAGA)*CR)
  TTEK=IBK
  TIJS=IBK+IJS
  TTBG=IBK+IJS+IBG
  DSDCBK=C2*TTEK**2
  CSCCJS=C2*TTJS**2
  CSCOEG=C2*TTBG**2
  PRINT 40,THETA,ALAMBD,IBK,IJS,IBG,DSCCEK,CSCCJS,CSCOEG
40 FORMAT ('0',F11.7,F11.4,1P6D17.7)
```

```
      30 CONTINUE
         RETURN
         END
C    ...........................................................
C
$ENTRY
1836.0     1.0       1836.0     1.0
25000.
0.0
/*
```

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MULTIPLE ELECTRON CAPTURE AT HIGH VELOCITIES

USING THE BATES POTENTIAL IN THE

INDEPENDENT ELECTRON APPROXIMATION

by

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B.A., Colorado State University, 1976

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Cross sections are calculated in the independent electron approximation using the Bates-Born approximation. Based on the independent electron approximation, where electrons in a multi-electron atom are uncorrelated, the probability for capture of two electrons is the product of the probabilities of capture of two single electrons. Probability amplitudes for single electron capture are computed using the difference between the instantaneous and average interaction potentials. This choice has been made because it eliminates the dependence of the probability amplitude on the choice of the zero point potential and it effectively orthogonalizes the initial and final wave functions used in the transition matrix.

Agreement with the literature is obtained for capture of a single electron for protons incident on hydrogen. The technique is then used to calculate single and double charge capture cross sections from the K-shell of helium atoms to the K-shell of alpha particles for incident energies of 0 to 1,000 KeV. These results are compared to experiment and previous calculations and reasonable agreement is obtained.