SEMICLASSICAL COULOMB APPROXIMATION

WITH APPLICATION TO SINGLE AND DOUBLE

K-SHELL IONIZATION IN ION-ATOM COLLISIONS

by

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CHAPTER 1

INTRODUCTION

Full understanding of the collision mechanisms of ions and atoms has
not been accomplished, neither in atomic physics nor in the application of
related fields to atomic physics. The three body collision problem has
not been fully solved in atomic physics. Furthermore, much of the research
currently conducted in atomic physics deals with collisions between atomic
many-particle systems which are inherently more complex than the three body
problem.

Atomic ionization, induced by ion-atom collisions, is important in
many physical phenomena. For example, an ion-atom collision can result
in the ejection of an inner shell electron of a target atom. This results
in higher energy electrons of the target atom cascading down to fill the
vacancy and the subsequent release of energy in the form of x-rays. This
process has broad applications, viz., trace element analysis[1], x-ray
astronomy[2], and laser technology[3]. Also, ion-atom collisions will result
in some energy loss of the projectile by collisional energy loss or by
bremsstrahlung[4]. This process adversely affects some fusion reactions for
generating energy.

One central, basic question of atomic theory concerns the yet
unsolved problem of three charged particles. A systematic method of
addressing this problem has yet to be realized, due in part to the obscurity
of the features of the collision process in a full quantum treatment. This
is analogous to the gravitational three-body problem, as yet unsolved
analytically but approximated numerically. Thus, many techniques
(perturbation theory, variation methods, asymptotic forms, effective
potential, close coupling equations, series expansions, etc.) are required
to build the physical picture.

The problem may be stated simply. An ion-atom collision consists of a nonrelativistic ionic projectile that passes near a target atom. The force considered here is the coulombic force of repulsion or attraction. Often, the collisions have well defined projectile energies, charge states and inpact parameters. The study of the results after collision reveals information concerning the target structure and the forces of interaction between the ion and the atom, as well as many body effects, such as multiple ionization, in many electron systems.

One quantity measured in ion-atom collisions is the total cross sectional area for ionizing an atomic target. This quantity is proportional to the probability that a target electron in some initial state will obtain enough energy from the collision to escape into the continuum. There is also a total cross section for multiple ionization of the target, which is sometimes more difficult to detect and to calculate. The target and projectile may be left in excited states after collision, emitting either photons or electrons. These photon or electron emissions may be either directly or indirectly caused by the collision. Observation of these phenomena adds to the basis of what is currently known about the collision mechanisms.

Some theoretical methods for calculating single ionization cross sections are available. These include, in chronological order, (a) the plane-wave Born approximation, PWBA, introduced[5] by Henneberg in 1933, (b) the semiclassical Coulomb approximation, SCA, by Bang and Hansteen[6] in 1959, and (c) the classical binary encounter approximation, BEA, by Gryzinski[7] 1965. Perhaps, the SCA method is the most useful, since the physical picture is clear and the unitarity constraint (namely that the probability may not exceed unity) is easily tested. Unfortunately, few details of the application of the SCA theory to direct Coulomb ionization are available in the literature.

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For many-electron targets, the independent electron approximation[8-10] is used in the calculations of single and multiple ionization cross sections. The independent electron approximation occurs when the target electrons are assumed to interact independently with the projectile, so during the collision the interaction between the projectile and a given target electron neither affects nor depends on the other target electrons. The SCA method is an appropriate theory that may be applied within the independent electron approximation. The time-dependent perturbation (SCA) theory for the Coulombic interaction between the projectile and ionized electron is developed in Chapter 2 for single, independent ionizations. Double ionization in the independent electron approximation is treated in Chapter 3 where the multi-electron transition probability for ionization is simply a product of independent binomial distributions of single ionization probabilities.

In Chapter 4, single K-shell ionization data[11] of O and F is compared to the independent electron approximation using the SCA method. Double K-shell ionization cross sections using both BEA and SCA for the independent electron predictions are also compared. Ratios of double K-shell ionization to single K-shell ionization are compared to experimental data to determine an overall fit.

Thus, this thesis will develop the theory of the independent electron using the SCA theory. The details of SCA calculations for direct Coulomb ionizations, not available in the current literature, are documented here. Finally, SCA theory is used to predict various inner shell ionization cross sections, and these results are compared to experimental observations.

CHAPTER 2

THEORY FOR SINGLE IONIZATION

Now, let us consider the ionization of a single atomic electron by a charged, heavy particle. The semiclassical Coulomb approximation (SCA) is an appropriate theory, when the target atom has a high nuclear charge (Z_2e) and the projectile has a low nuclear charge (Z_1e). The Coulomb interaction between the projectile and the atomic nucleus is treated as a time-dependent perturbation of the target atom.

The projectile has an assumed velocity such that its path is viritually undeflected, so the projectile's velocity remains viritually constant. Such an assumption means that energy is not conserved. With the projectile at constant velocity and the target atom fixed, the ionized electron goes from a negative energy to a positive energy into the continuum. In reality, the amount of energy lost by the projectile is normally so small that its velocity is viritually the same, and the basic assumption is reasonably valid.

The ionized electrons considered here are in the 1S state and scattered into final continuum states by the pure Coulomb potential. In spherical coordinates, the particular solutions to the hydrogenic radial equation[12] are the spherical Coulomb functions[13], sometimes called the radial Coulomb functions[14], which form the total wave expansion of the hydrogenic eigen-functions in the continuum. Only the first four spherical Coulomb functions from S to F are considered significant in this paper for the calculation of these probabilies used to evaluate total ionization cross sections.

The system will have the reference frame fixed on the atom's nucleus at A, the projectile at P with velocity v and the electron at E. Let the

position vectors x and r be the positions where E and P are from A, and

R(t) the position vector of E from P. While assuming a straight line

trajectory for the projectile, the impact parameter becomes $\rho = |\vec{\rho}|$.
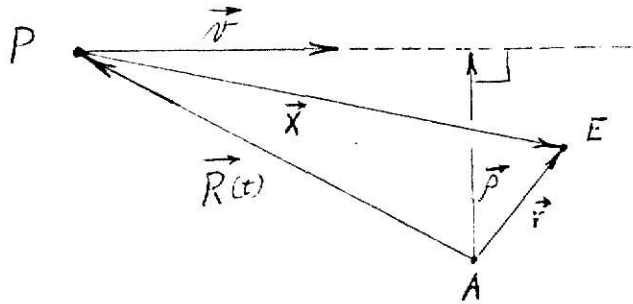
The energy Hamiltonian of the independent electron is $H_{el} = H_o + V(r,t)$

where $H_o = -\dfrac{\hbar}{2m_e}\nabla_r^2 - \dfrac{Z_2 e^2}{r}$, the hydrogenic Hamiltonian.

The Coulomb potential term is

$$V(\vec{r}, t) = \frac{Z_1 Z_2 e^2}{|\vec{R}(t)|} - \frac{Z_1 e^2}{|\vec{X}|} = \frac{Z_1 Z_2 e^2}{|\vec{\rho} + \vec{v}t|} - \frac{Z_1 e^2}{|\vec{r} - \vec{R}(t)|} .$$

From Schrodinger's equation,

$$H_{el}\, \psi_n(\vec{r}, t) = i\hbar\, \frac{\partial}{\partial t}\psi_n(\vec{r}, t) .$$

Thus,

$$\left(-\frac{\hbar^2}{2m_e}\nabla_r^2 - \frac{Z_2 e^2}{r}\right)\psi_n + \left(\frac{Z_1 Z_2 e^2}{R(t)} - \frac{Z_1 e^2}{X}\right)\psi_n = \left(i\hbar\frac{\partial}{\partial t}\right)\psi_n$$

At $t \to \infty$, the time-dependent interaction term will disappear so that the Schrodinger equation reduces to the hydrogenic equation. As $t \to \infty$, separation of variables implies $\psi'_n(\vec{r}, t) = \phi(r) \, e^{-i \frac{E_n}{\hbar} t}$. Let $\phi_n \, e^{i \frac{E_n}{\hbar} t} \equiv \Phi_n(\vec{r})$. The set $\left\{ \Phi_n(\vec{r}) \right\}$ forms a complete orthonormal basis set of hydrogenic eigenfunctions for the electron of nucleus A. Thus, one can choose $\psi_n(\vec{r}, t) = \sum_\kappa a_{n\kappa}(t) \, \Phi_\kappa(\vec{r})$, which sums over the discrete bound states and the continuum. At $t \to -\infty$, $a_{nn} = 1$ and $a_{nm} = 0$ for all $m \neq n$. Thus, the electron is assumed to be in some unperturbed hydrogenic state before any interaction is involved. Else, the initial condition is just a sum of unperturbed hydrogenic states. (The 1S state will be assumed in the later development.) It is interesting to note that

$$\lim_{t \to \infty} \left\langle \Phi_m \middle| \psi_n(\vec{r}, t) \right\rangle = \lim_{t \to \infty} \left\langle \Phi_m \middle| \sum_\kappa a_{n\kappa} \Phi_\kappa \right\rangle = \lim_{t \to \infty} \sum_\kappa a_{n\kappa} \left\langle \Phi_m \middle| \Phi_\kappa \right\rangle$$

$$= \lim_{t \to \infty} \sum_\kappa a_{n\kappa}(t) \, \delta_{m\kappa} = \lim_{t \to \infty} a_{nm}(t) = a_{nm}(\infty).$$

This is simply the contribution of the Φ_m state to $\psi_n(\vec{r}, t)$ as $t \to \infty$. To determine the transition to the m state from the n state as $t \to \infty$, the probability $P_{n,m}(\rho, \vec{v}) = \left| a_{nm}(+\infty) \right|^2$ for given ρ and $\vec{v}$ for the projectile.

Using the Schrodinger equation and assuming weak interactions, first-order time-dependent perturbation theory obtains these equations (Cf. Appendix 1).

$$a_{mn}(t) = \delta_{nm} - \frac{i}{\hbar} \int_{-\infty}^{t} V_{mn} \, e^{i \omega_{mn} t'} dt'$$

$$V_{mn}(r, t) = \int \Phi_m^* \, \frac{-Z_i e^2}{X} \, \Phi_n \, d\vec{r}$$

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So, $\dfrac{1}{X} = \dfrac{1}{|\vec{r} - \vec{R}(t)|} = \dfrac{1}{2\pi^2} \int \dfrac{d\vec{q}}{q^2} e^{i\vec{q}\cdot(\vec{r} - \vec{R}(t))}$

where $\vec{q}$ is an arbitrary momentum transfer vector of the transform.

Consider $i \neq f$ as $t \to \infty$, then

$$a_{if} = \dfrac{i Z_1 e^2}{2\pi^2} \int dt \int \dfrac{d\vec{q}}{q^2} e^{-i\vec{q}\cdot\vec{R}} e^{i\omega_{if}t} \int \phi_f^* \phi_i\, e^{i\vec{q}\cdot\vec{r}}\, d\vec{r}.$$

Define the last integral as the generalized form factor[15], $\iota(\vec{q}\cdot\vec{k})$. Now,

$\vec{q}\cdot\vec{R}(t) = \vec{q}\cdot(\vec{\rho} + \vec{v}t) = q_0 vt + \vec{q}_\perp \cdot \vec{\rho}$ where q_0 is parallel to $\vec{v}$ and $\vec{q}_\perp$

is perpendicular to $\vec{v}$ but not necessarily to $\vec{\rho}$. Consequently,

$q = \sqrt{q_c^2 + q_\perp^2}$. From Appendix 2, the coefficient a_{if} can be determined

with a given impact parameter and momentum, $\vec{k}$.

$$a_{if}(\rho, k) = \dfrac{16\pi Z_1 e^2}{v\, \hbar} e^{-\frac{\pi\eta}{2}} \left(\dfrac{Z_2}{a_c}\right)^{3/2} \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} Y_\ell^{m*}(\theta_k, \phi_k) \left[\dfrac{(2\ell+1)(\ell-m)!}{(\ell+m)!}\right]^{1/2} \dfrac{(2k)^\ell}{(2\ell+1)!}$$

$$\times \left| \Gamma(\ell+1-i\eta) \right| i^m \int J_m(q_\perp \rho) P_\ell^m\left(\dfrac{\omega/v}{\sqrt{\frac{\omega^2}{v^2}+q_\perp^2}}\right) \dfrac{q_\perp}{\frac{\omega^2}{v^2}+q_\perp^2} \iota_\ell\left(\sqrt{\frac{\omega^2}{v^2}+q_\perp^2}, k\right) dq_\perp$$

To obtain the probability for ionization, simply determine $\int \left| a_{if}(\rho, k)\right|^2 dE$.

Since we are using mutually orthogonal eigenfunctions, the cross terms reduce

the double summation to diagonal terms. The only problem left is to express

the generalized form factor, $\iota_\ell(q,k)$, for each partial wave.

Originally, the K-shell electron is assumed to be in the hydrogenic

1S state, $\phi_i = \dfrac{1}{\sqrt{\pi}}\left(\dfrac{Z_2}{a_o}\right)^{3/2} e^{-\frac{Z_2 r}{a_o}}$. The final wave states of the continuum

hydrogenic eigenfunctions are the spherical Coulomb waves, which form the

total radial wave expansion.

$$\phi_f = e^{-\frac{\pi\eta}{2}} \sum_{\ell=0}^{\infty} i^\ell (2kr)^\ell \dfrac{|\Gamma(\ell+1+i\eta)|}{(2\ell)!} e^{ikr} P_\ell(\cos\theta)$$

$$\times {}_1F_1\left[\ell+1+i\eta, 2\ell+2, -2ikr\right] \qquad \text{where} \quad \eta = -\dfrac{Z_2}{a_o k} \quad .$$

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With this, the generalized form factor can be expanded into a summation (Appendix 2),

$$\mathcal{U}(\vec{q}\cdot\vec{k}) = \int \phi_f^* \phi_i \, e^{i\vec{q}\cdot\vec{r}} \, d\vec{r}$$

$$= 16 \left(\frac{\pi Z_2}{a_c}\right)^{3/2} e^{-\frac{\pi\eta}{2}} \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} (2k)^{\ell} \frac{|\Gamma(\ell+1-i\eta)|}{(2\ell+1)!} Y_\ell^{m*}(\Theta_k, \phi_k) Y_\ell^{m}(\Theta_q, \phi_q) \, \mathcal{U}_\ell(q,k)$$

The individual $\mathcal{U}_\ell$ terms ($\ell = 0$ through 3) for the S, P, D and F spherical Coulomb functions are derived in Appendices 3 through 6 respectively. Each integral of $\mathcal{U}_\ell(q,k)$ can be evaluated analytically in terms of Gaussian hypergeometric functions.

Now, let us calculate the probability using the value of $\mathcal{U}(\vec{q}\cdot\vec{k})$.

$$\int |a_{if}(\rho,k)|^2 \, dE = \int |a_{if}(\rho,k)|^2 \, k \, dk \, d\Omega_k =$$

$$= \left(\frac{16\pi Z_1}{v^2\hbar}\right)^2 e^{-\pi\eta} \, v^4 \left(\frac{Z_2}{a_c}\right)^3 \left| \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} (i)^m \left[\frac{(2\ell+1)(\ell-m)!}{(\ell+m)!}\right]^{1/2} \frac{(2k)^{\ell}}{(2\ell+1)!} |\Gamma(\ell+1-i\eta)| \right.$$

$$\left. \times Y_\ell^{m*}(\Theta_k, \phi_k) \int \frac{J_m(q_\perp \rho) P_\ell^{in}\left(\omega/v \Big/ \sqrt{q_\perp^2 + \frac{\omega^2}{v^2}}\right)}{q_\perp^2 + \frac{\omega^2}{v^2}} \mathcal{U}_\ell(q,k) \, q_\perp \, dq_\perp \right|^2 d\Omega_k \, k \, dk$$

Note that

$$\int Y_\ell^{m*}(\Theta_k, \phi_k) \, Y_{\ell'}^{m'}(\Theta_k, \phi_k) \, d\Omega_k = \delta_{\ell\ell'} \, \delta_{mm'}$$

$$\int |a_{if}(\rho,k)|^2 \, dE = \left(\frac{16\pi Z_1}{v^2\hbar}\right)^2 e^{-\pi\eta} \, v^4 \left(\frac{Z_2}{a_c}\right)^3 \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \frac{(2\ell+1)(\ell-m)!}{(\ell+m)!} \frac{(2k)^{2\ell}}{[(2\ell+1)!]^2}$$

$$\times |\Gamma(\ell+1-i\eta)|^2 \int \left\{ \int J_m(q_\perp \rho) P_\ell^{in}\left(\frac{\omega/v}{\sqrt{\frac{\omega^2}{v^2}+q_\perp^2}}\right) \frac{q_\perp}{q_\perp^2 + \frac{\omega^2}{v^2}} \mathcal{U}_\ell(q,k) \right\}^2 k \, dk$$

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It is assumed that the series expansion can be truncated at $\ell = 3$, making the probability at a given ρ reduce to

$$\int |a_{\lambda f}(\rho, N)|^2 \, dE = \left(\frac{16 \pi z_1}{v^2 \hbar}\right)^2 e^{-\pi \eta} 4 \left(\frac{z_2}{a_o}\right)^3 \sum_{\ell=0}^{3} \sum_{m=-\ell}^{\ell} \frac{(2\ell+1)(\ell-m)!}{(\ell+m)!} \frac{2 k^{2\ell}}{[(2\ell+1)!]^2}$$

$$\times |\Gamma(\ell+1-i\eta)|^2 \int_{\kappa}^{\infty} \left\{ \int_c^{\infty} J_m(q_\perp \rho) P_\ell^m\left(\frac{\omega/v}{\sqrt{q_\perp^2 + \frac{\omega^2}{v^2}}}\right) \frac{q_\perp \, dq_\perp}{q_\perp^2 + \frac{\omega^2}{v^2}} \mathcal{L}_\ell(\varepsilon, N) \right\}^2 k \, dk$$

This is the general expression for the ionization probability. This is the basic expression for full SCA calculations widely used in the literature Expressions for the generalized form factor $\mathcal{L}_\ell(q, k)$ are given in Appendicies 3-6.

It is sometimes useful to consider the low energy limit when the expression for this amplitude simplifies considerably. Hence, let us consider this limiting form for this ionization probability. In the low energy limit the spherical S wave Coulomb function, which is the lowest energy eigenfunction in the continuum, will overwhelm the other spherical Coulomb functions in magnitude.

$$V_{1s,s} = \langle \phi_s | \frac{z_1 e^2}{|\vec{r} - \vec{R}|} | \phi_{1s} \rangle = -z_1 e^2 \int \left(\frac{z_2}{a_o}\right)^{3/2} \frac{2 e^{-\frac{z_2 r}{a_o}}}{\sqrt{4\pi}} e^{-\frac{\eta \pi}{2}} \left\{ |\Gamma(1+i\eta)| e^{ikr} {}_1F_1(1+i\eta, 2, -2ikr) \right\}^* \frac{r^2}{|\vec{r} - \vec{R}|} \, dr$$

$$a_{1s \to s} = \frac{8i \sqrt{\pi} z_1 e^2}{v^2 \hbar} e^{-\frac{\pi}{2}} \left(\frac{z_2}{a_o}\right)^{3/2} |\Gamma(1-i\eta)|$$

$$\times \int J_o(\rho q_\perp) \frac{q_\perp}{\left(\frac{\omega^2}{v^2} + q_\perp^2\right)^{3/2}} \frac{1}{2i} \left\{ \frac{\left(1 - \frac{2ik}{\lambda_1}\right)^{-1+i\eta}}{\lambda_1^2} - \frac{\left(1 - \frac{2ik}{\lambda_2}\right)^{-1+i\eta}}{\lambda_2^2} \right\} dq_\perp \quad .$$

In the low energy limits for protons on H at $k \ll q$ and nominally $l \ll q$, the $\left\{ \quad \right\}$ term approaches $\frac{8i}{q^3}$ (Appendix 7).

Also, $\int_i^\infty \frac{\chi_\perp^{m+1} J_m(q_\perp \rho)}{(q^2)^{\mu+1}} = \frac{\rho^\mu q_\mu^{m-\mu}}{\Gamma(\mu+1) 2^\mu} \mathcal{K}_{m-\mu}(\rho q_\mu)$ from Erdelyi et al.[16]

Using this limit,

$$a_{1s \to s} \simeq \frac{8i\sqrt{\pi}}{v\hbar} Z_1 e^2 e^{-\frac{\pi n}{2}} \left(\frac{Z_2}{a_o}\right)^{3/2} |\Gamma(1-in)| \frac{8i}{2i} \int \frac{\chi_\perp J(q_\perp \rho)}{q^3 q^2} dq_\perp$$

$$= \frac{32 i e^2 \sqrt{\pi} Z_1 Z_2^{3/2}}{v\hbar a_o^{3/2}} e^{-\frac{\pi n}{2}} |\Gamma(1-in)| \frac{\rho^2}{8 q_\mu^2} \mathcal{K}_{-2}(q_\mu \rho) \quad \& \quad \mathcal{K}_{(-2)} = \mathcal{K}_2$$

$$|a_{1s \to s}|^2 = \frac{16 e^4 \pi Z_1^2 Z_2^3}{\hbar^2 v^2 a_o^3} e^{-\pi n} |\Gamma(1-in)|^2 \frac{\rho^4}{q_\mu^4} \left[\mathcal{K}_2(\rho q_\mu)\right]^2$$

$$= \frac{16 e^4 \pi Z_1^2 Z_2^3}{\hbar^2 v^2 a_o^3} \frac{n\pi}{\sinh(n\pi)} \frac{\rho^4 v^4}{\omega^4} \left[\mathcal{K}_2(\rho q_\mu)\right]^2$$

$$= \frac{16 \pi^2 e^4 Z_1^2 Z_2^3}{\hbar^2 a_o^3} \frac{n}{\sinh(n\pi)} \frac{\rho^4 v^4}{\omega^4} \left[\mathcal{K}_2(\rho q_\mu)\right]^2$$

In Bang and Hansteen (1958), $\frac{d\sigma_K}{dE_f} = Z_1^2 \frac{M_1}{E_1} \frac{e^4}{\hbar^2} \frac{Z_2^2}{2 a_o^2} |N_i|^2 |N_f|^2 \frac{\rho^4}{q_\mu^4} \left[\mathcal{K}_2(\rho q_\mu)\right]^2$

N_i and $N_f^{o,k}$ are energy normalization constants, which are listed by Alder and Winther[17] as

$$N_{\ell,\lambda} = e^{-\frac{n\pi}{2}} \frac{|\Gamma(1+\ell+in)|}{(2\ell+1)!} i^\ell \qquad (eq.\ 9,\ p.\ 6)$$

So, $|N_i|^2 = \frac{4 Z_2^3}{a_o^3}$ and $|N_f|^2 = e^{-n\pi} \frac{n\pi}{\sinh(n\pi)}$

$$\frac{d\sigma_K}{dE_f} = \frac{Z_1^2 M_1 e^4}{\hbar^2 \frac{1}{2} M_1 v^2} \frac{Z_2^2 4}{2 a_o^2} \frac{e^{-n\pi} Z_2^3 n\pi}{\sinh(n\pi) a_o^3} \frac{\rho^4}{q_\mu^4} \left[\mathcal{K}_2(\rho q_\mu)\right]^2$$

$$= \frac{e^4}{\hbar^2} \frac{4\pi Z_2^5 Z_1^2}{a_o^5} e^{-n\pi} \frac{n}{\sinh(n\pi)} \frac{\rho^4 v^{-2}}{\omega^4} \left[\mathcal{K}_2(\rho q_\mu)\right]^2$$

where $n = \frac{-Z_2}{a_o K}$ and $q_\mu^2 = \frac{\omega^4}{v^4}$

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This corresponds[18] to the result given without detail in Bang and Hansteen, and used [19, 20] for applications at low energies.

THEORETICAL DEVELOPMENT OF

DOUBLE K-SHELL IONIZATION

To formulate the amplitude for ionization of independent K-shell
electrons, appropriate sections of the basic theory established by McGuire
and Weaver[9] are covered. The full Hamiltonian for the system being
considered becomes

$$\mathcal{H} = \frac{p^2}{2M} - \frac{Z_1 Z_2 e^2}{R} + \sum_{j=1}^{Z_2} \frac{Z_1 e^2}{|\vec{R}-\vec{r_j}|} + \sum_{j=1}^{Z_2} \left(\frac{p_j^2}{2m} + \frac{Z_2 e^2}{r_j} - \sum_{k>j}^{Z_2} \frac{e^2}{|\vec{r_k}-\vec{r_j}|} \right) \quad .$$

Due to the presence of the interelectron interactions, $e^2/|\vec{r_k}-\vec{r_j}|$, complete
commutativity is impossible between separate terms of the Hamiltonian. As
an established practice, an effective potential $V(\vec{r_j})$ approximates the
interelectron term, $\sum_{k} e^2/|\vec{r_k}-\vec{r_j}|$. Thus,

$$\mathcal{H} = \frac{p^2}{2M} + \sum_{j=1}^{Z_1} \left(\frac{Z_1 e^2}{|\vec{R}-\vec{r_j}|} - \frac{Z_1 e^2}{R} \right) + \sum_{j=1}^{Z_2} \left(\frac{p_j^2}{2m} + \frac{Z_1 e^2}{r_j} + V(\vec{r_j}) \right)$$

$$= \frac{p^2}{2M} + \sum_{j=1}^{Z_2} V\left(\vec{R}, \vec{r_1}, ..., \vec{r_{Z_2}} \right) + \mathcal{H}_T$$

$$= \frac{p^2}{2M} + \sum_{j=1}^{Z_2} \mathcal{H}_j \left(\vec{R}, \vec{r_1}, ..., \vec{r_{Z_2}} \right)$$

where $\mathcal{H}_T$ and $\mathcal{H}_j$ now become sums of single-particle Hamiltonians.

To reduce ψ in $\mathcal{H}\psi = i\hbar \frac{\partial \psi}{\partial t}$ as a product wave function, three
assumptions are introduced. First, the initial asymptotic wave function
is assumed as a product of wave functions. Second, $\frac{p^2}{2M}$ is assumed to
commute with the separate terms of the Hamiltonian. Third, the spin terms

are assumed to be negligible[10], which is not stated in the original paper. In the first assumption, coorelations between the target's wave functions are ignored due to the approximation of an effective potential. The second assumption approximates how the projectile moves classically. The last assumption is quantatively correct when considering heavy projectiles. Initially, the asymptotic wave function $\psi_i(\vec{R}, \vec{r}_1, ..., \vec{r}_{Z_2}) = \phi_i(\vec{R}) \prod_{j=1}^{Z_2} \phi_{i,j}(\vec{r}_j)$ where $\vec{R} = \vec{\rho} + \vec{\pi F} t$ for the initial wave packet $\phi_i(\vec{R})$ and where $\phi_{i,j}(\vec{r}_j)$ are bounded one-electron wavefunctions. The evolution operator $\Omega(t_1, t_2)$ in the Heisenberg picture factors into a product of single-electron evolution operators.

$$\Omega(t_1, t_2) = \mathcal{T} e^{-\frac{i}{\hbar} \int_{t_1}^{t_2} \mathcal{H}(t) dt}$$

$$= \mathcal{T} e^{-\frac{i}{\hbar} \int_{t_1}^{t_2} \frac{p^2}{2M} dt} \prod_{j=1}^{Z_2} \mathcal{T} e^{-\frac{i}{\hbar} \int_{t_1}^{t_2} \mathcal{H}_j(t) dt}$$

$$= \Omega_p(t_1, t_2) \prod_{j=1}^{Z_2} \Omega_j(t_1, t_2)$$

where $\mathcal{T}$ is the time-ordering operator. Note that $[\mathcal{H}_j(t_1), \mathcal{H}_j(t_2)] = 0$ only if $t_1 = t_2$. At any point in time,

$$\Omega(-\infty, t) \psi_i = \Omega_p(-\infty, t) \phi_i(\vec{R}) \prod_{j=1}^{Z_2} \Omega_{i,j}(-\infty, t) \phi_i(\vec{r}_j)$$

The amplitude $a_{if}(t)$ that the evolution operator developes ψ_i into a particular ψ_f state is calculated by $a_{if}(t) = \langle \psi_f | \Omega(-\infty, t) | \psi_i \rangle$. If ψ_f are orthonormal eigenfunctions of the asymptotic Hamiltonian, then

$$a_{if}(t) = \left\langle \phi_f(\vec{R}) \prod_{j=1}^{Z_2} \phi_{f,i}(\vec{r}_j) \middle| \Omega(-\infty, t) \middle| \phi_i(\vec{R}) \prod_{j=1}^{Z_2} \phi_{i,j}(\vec{r}_j) \right\rangle$$

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Since the evolution operator is a product of single-electron terms, then

$$a_{if}(t) = \left\langle \phi_f(\vec{R}) \left| \Omega_p(-\infty, t) \right| \phi_i(\vec{R}) \right\rangle$$

$$\times \prod_{j=1}^{Z_2} \left\langle \phi_{i,i}(\vec{r_i}) \left| \Omega_j(-\infty, t) \right| \phi_{i,j}(\vec{r_i}) \right\rangle$$

$$= \prod_{j=c}^{Z_2} a_{if,j}(t)$$

where $a_{if,c}(t) = \left\langle \phi_f(\vec{R}) \left| \Omega_p \right| \phi_i(\vec{R}) \right\rangle$ and where $a_{if,j}(t)$ is the single electron probability amplitude. A nonorthonormal basis of eigenfunctions ψ_f can be chosen, which will still produce the same result of a product of single-electron probability amplitudes. The probability for the transition from an initial state ψ_i for given impact parameter $\vec{\rho}$ to a final state ψ_f is the square of the amplitude

$$|a_{if}(t=+\infty)|^2 = |a_{if}(\rho, k)|^2 \;,$$ where k is the momentum of the ionized electron. The total cross section for a uniform beam is calculated by integrating the probability over the impact parameter of the projectile,

$$\sigma_{if} = \int 2\pi\rho \, d\rho \, |a_{if}(\rho, k)|^2 \;.$$

The cross section for ionization of a single electron in this approximation is

$$\sigma_{if,s} = \int 2\pi\rho \, d\rho \, |a_{if,s}|^2 \sum_{f}^{Z_2} \prod_{j \neq s} |a_{if,j}(\rho)|^2 = \int 2\pi\rho \, d\rho \, |a_{if,s}|^2 \;.$$

One-to-one correspondence between impact parameter and scattering angle of the projectile is assumed in this classical[21] model. So, summing over scattering angles is the same as summing differential cross sections over impact parameters.

Assuming unitarity for each single electron, then $\left| a_{\mathscr{F},j}(\rho,k) \right|^2$ is the probability that the j th electron is scattered into the continuum final state $\mathscr{F}$, and $1 - \left| a_{i\mathscr{F},j}(\rho,k) \right|^2$ is scattered into a final state other than $\mathscr{F}$.

The probability for ionizing an electron in the K-shell into the continuum is $P_K = \int d\mathscr{F} \left| a_{i\mathscr{F}}(\rho,k) \right|^2$. The probability for not producing a vacancy is $1 - P_K$.

If single electron vacancies are identical in an atomic shell of N electrons, there are $\binom{N}{n}$ ways to produce n vacancies with a probability of $\binom{N}{n} P (1-P)^{N-n}$.

To remove k electrons from the K-shell, the effective total cross section

$$\sigma_k = \int 2\pi\rho \, d\rho \binom{2}{k} \left(P_K \right)^k \left(1 - P_K \right)^{2-k}$$

In this work, $P_K \approx \sum_{\mathscr{F}=S,P,D,F} \left| a_{K\mathscr{F}}(\rho,k) \right|^2$ and the total cross sections for single and double ionizations are

$$\sigma_1 = 2\pi \int \rho \, 2 \, P_K \left(1 - P_K \right) d\rho$$

and

$$\sigma_2 = 2\pi \int \rho \, P_K^2 \, d\rho \ .$$

These expressions together with the SCA expressions for $P_K (\rho)$ given in Chapter 2 are used to evaluate cross sections for single and double ionization in the next chapter.

CHAPTER 4

RESULTS OF CALCULATIONS

As discussed earlier, single and double K-shell ionization data of O and F are evaluated and compared separately to H^+ and He^+ projectiles. BEA and SCA calculations for both single and double K-shell ionizations are compared on each graph. BEA single and double K-shell ionizations were provided[22] by McGuire. Total SCA ionization cross sections were obtained from Hansteen, Johnsen and Kochbach[23]. The total cross sections were calculated by numerically integrating the integrals by the retangular rule

$$\sigma_1 = 4\pi \int \rho \, P_K \left(1 - P_K\right) d\rho$$

$$\sigma_2 = 2\pi \int \rho \, P_K^2 \, d\rho$$

where the probabilities are dependent on the impact parameter ρ and the energy of the projectile.

The first figure shows single K-shell ionization for both H^+ and He^+ projectiles on O. BEA overestimates slightly for the H^+ while SCA underestimates slightly. With He^+, both theories slightly underestimate but BEA is a little closer.

Single K-shell ionization for both H^+ and He^+ on F is plotted on figure 2. For H^+, BEA overestimates the cross section but has the right shape while SCA is closer in the lower energy range and further away in the upper range. With He^+, SCA is nominally closer than BEA.

Figure 1. Cross sections for single K-shell ionization as a function of projectile energy for H^+ and He^+ incident on O. The theoretical curves, BEA and SCA, are represented by solid lines. The data points are due to Richard, et al.

Figure 2. Cross sections for single K-shell ionization as a function of projectile energy for H^+ and He^+ indicent on F. The theoretical curves, BEA and SCA, are represented by solid lines. The data points are due to Richard, et al.

Figure 3. Cross sections for double K-shell ionization as a function of projectile energy for H^+ and He^+ incident on O. The theoretical curves, BEA and SCA, are represented by solid lines. The data points are due to Richard, et al.
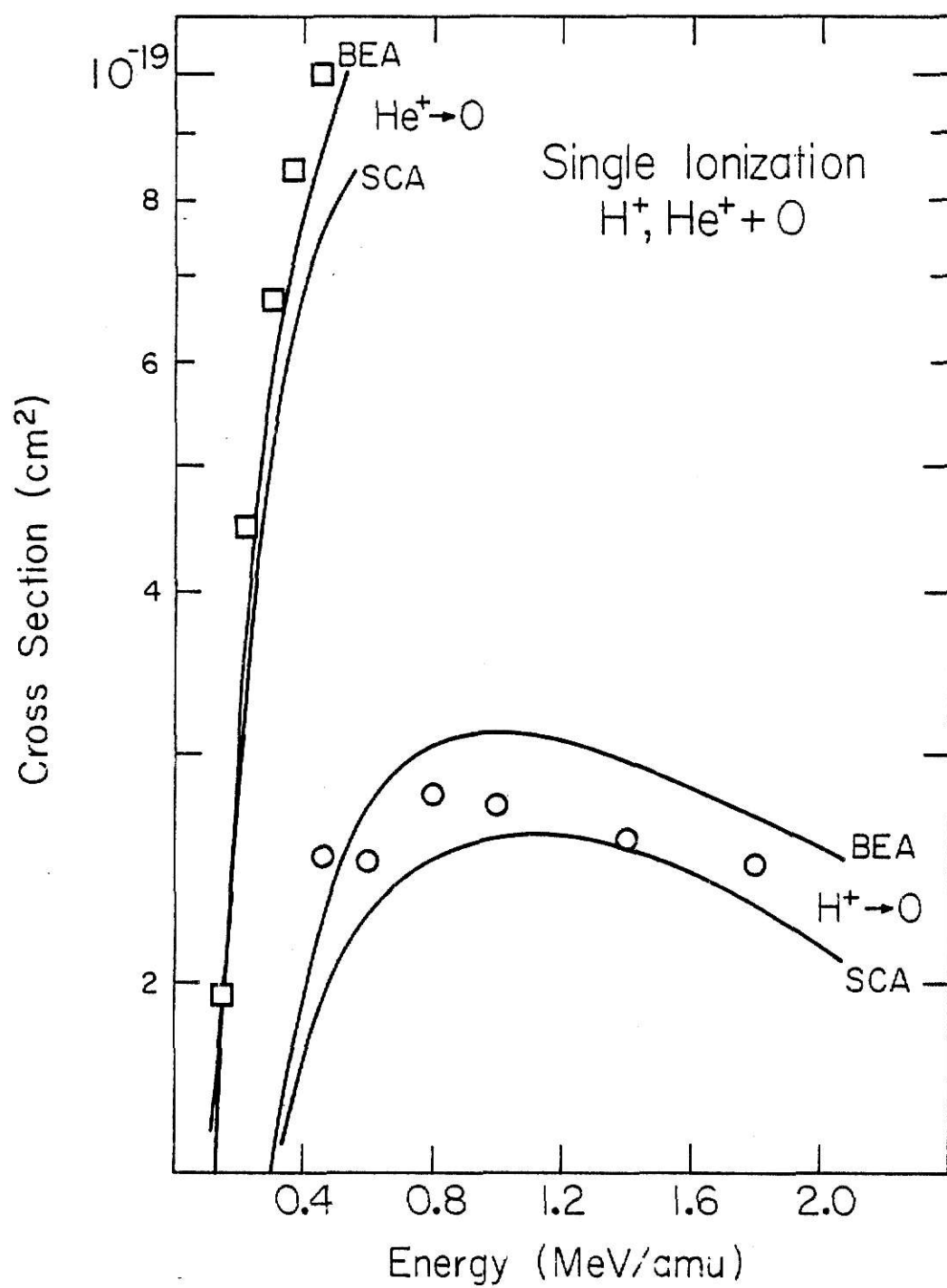
Figure 4. Cross sections for double K-shell ionization as a function of projectile energy for H^+ and He^+ incident on F. The theoretical curves, BEA and SCA, are represented by solid lines. The data points are due to Richard, et al.
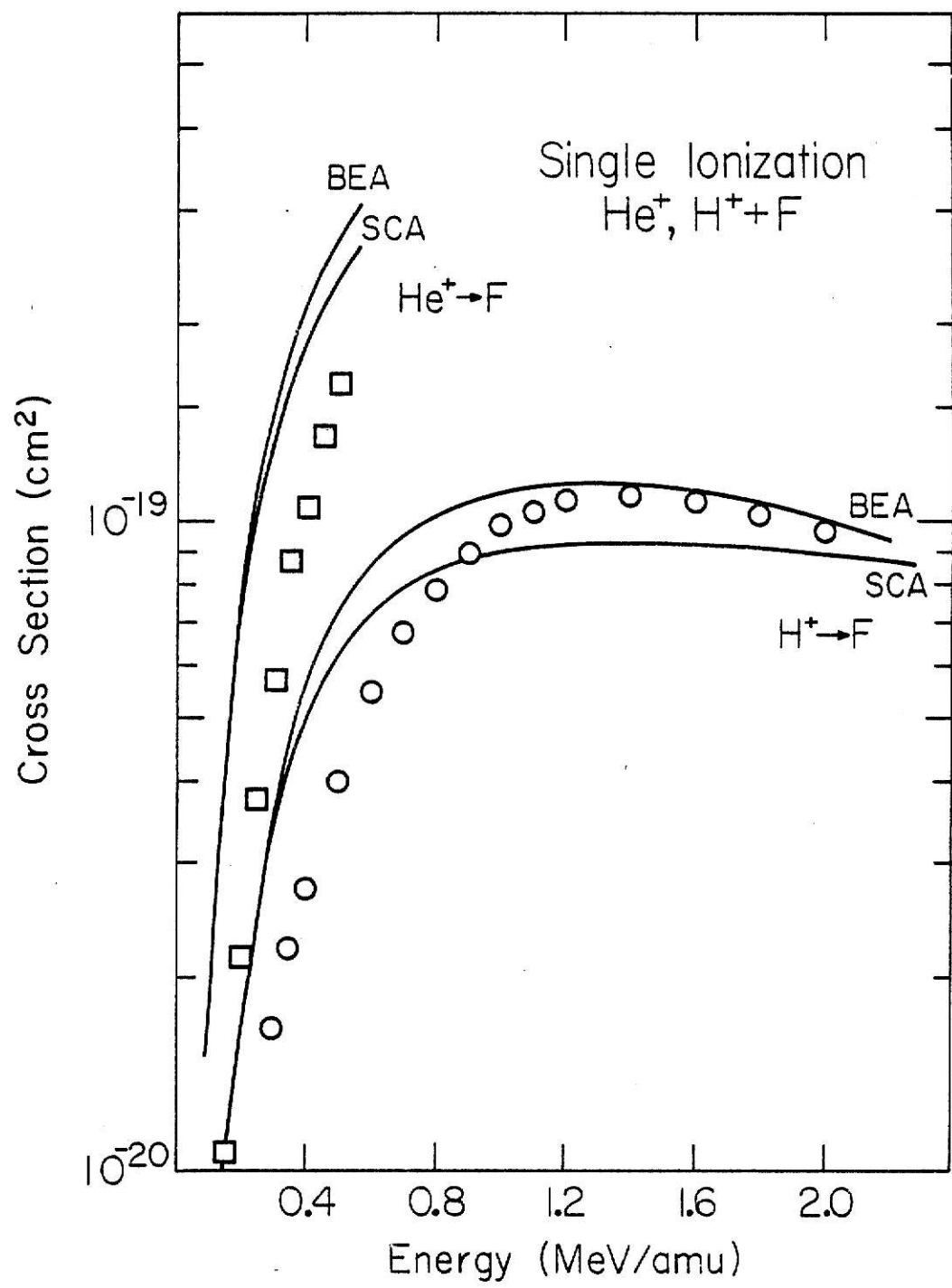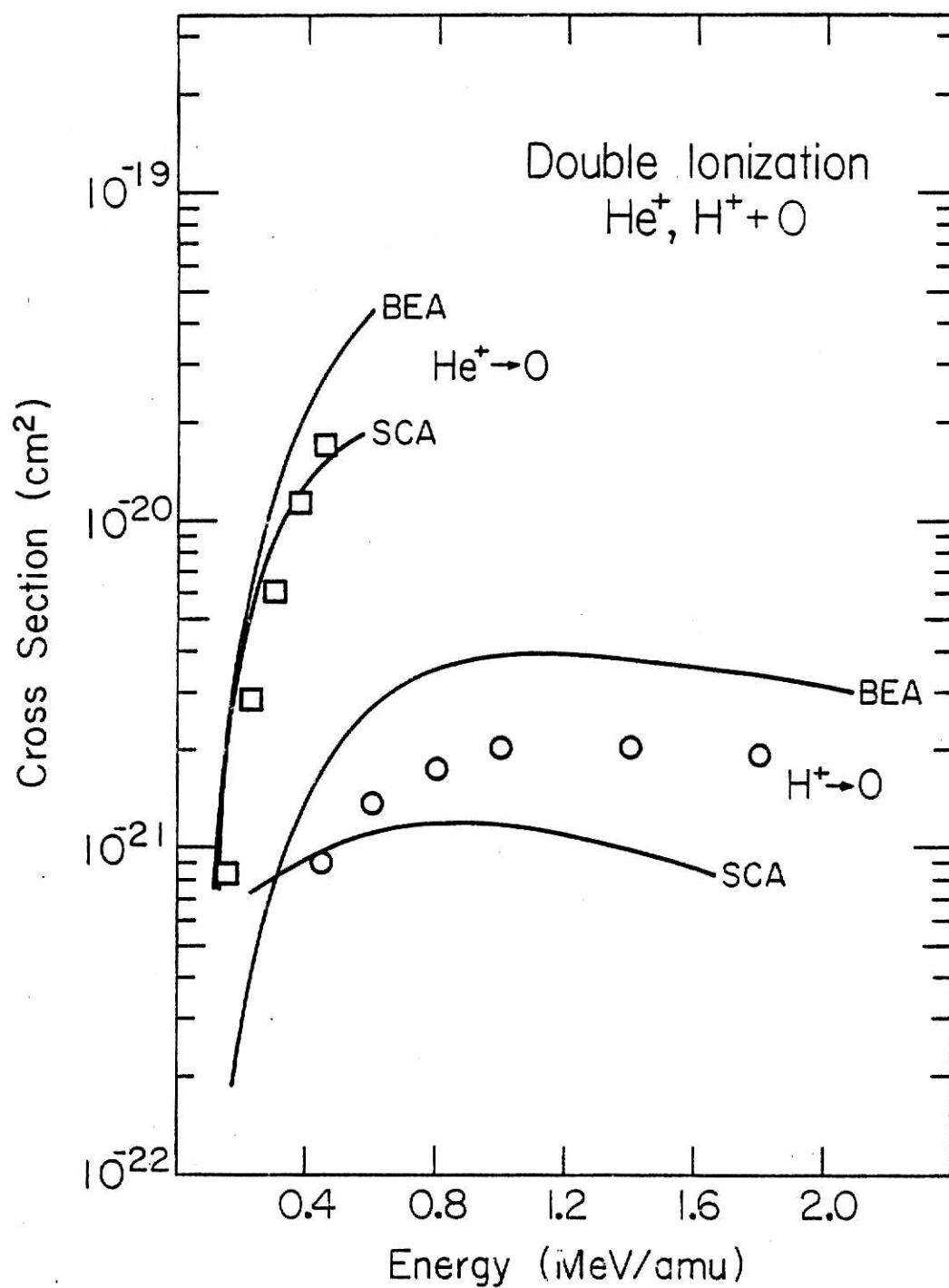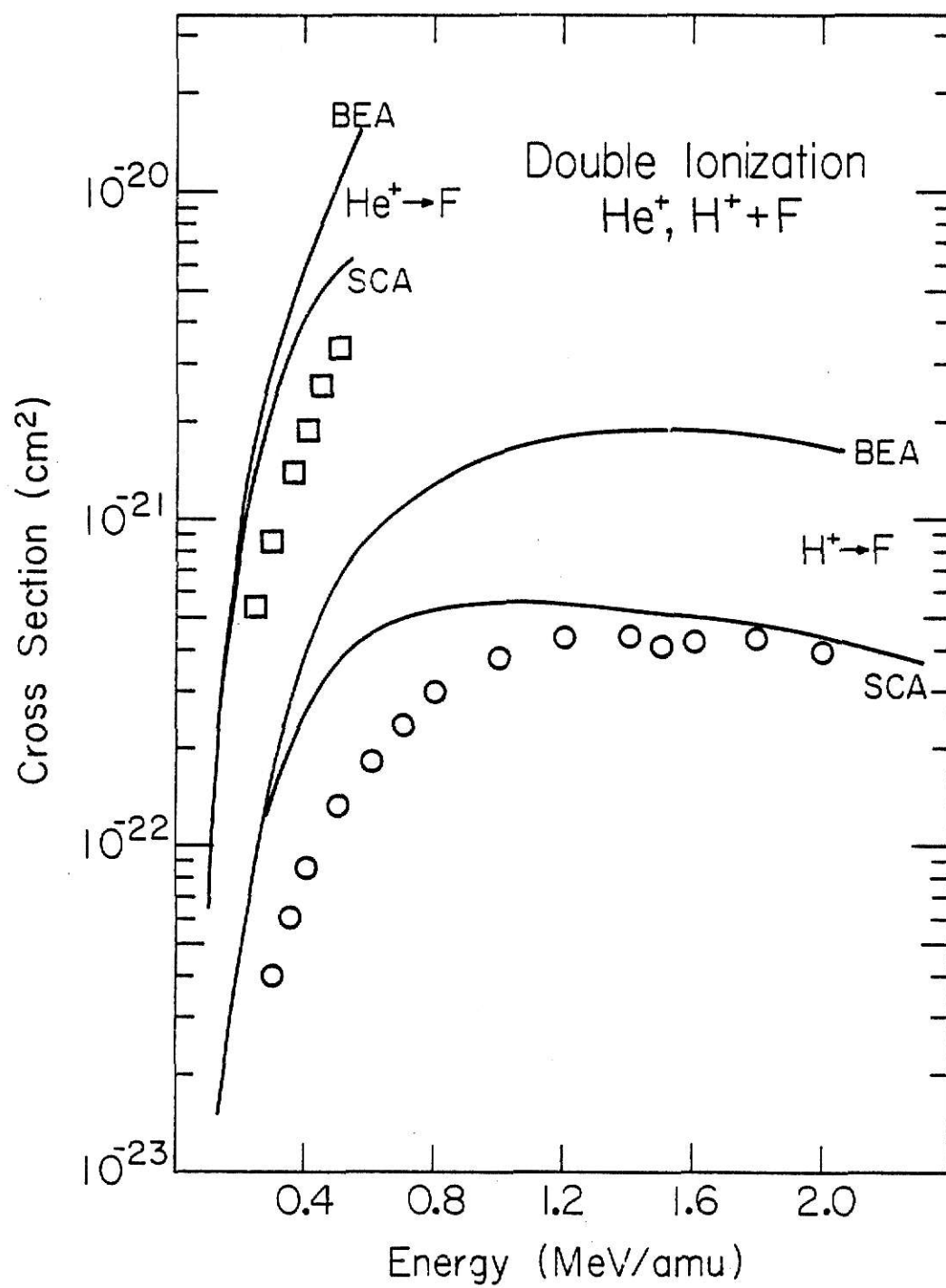
The double K-shell ionization for O is shown in figure 3. Again as in the single ionization case using H^+, BEA overestimates the data but has the slightly better shaped curve for the O target while SCA crosses the data curve. For the He^+ projectile, again, SCA appears to fit closer to the data.

For the double K-shell ionization using F as the target, figure 4 is shown. Here, SCA seems to approximate the experimental data better than BEA for both H^+ and He^+.

As a check to see whether BEA or SCA matched better despite any bias, the ratio $\sigma_{double\ K} / \sigma_{single\ K}$ was taken for both projectiles for the O target (figure 5) and for the F target (figure 6). In all but one case, SCA gave a closer fit than BEA to the experimental data.

Also note that comparisons between theory and experiments tend to be somewhat different for double ionization than for single ionization. The theory sometimes tends to be comparatively lower for double ionization, for example, as compared to data. Thus, in practice, comparing multiple as well as single ionization cross sections to experiment tends to give a more complete picture of the relationship between theory and experiment.

Figure 5. Ratio of double to single K-shell ionization cross sections as a function of projectile energy for H^+, He^+ on O. Theory and data correspond to figures 1 and 3.

Double to Single
K-Shell Ionization
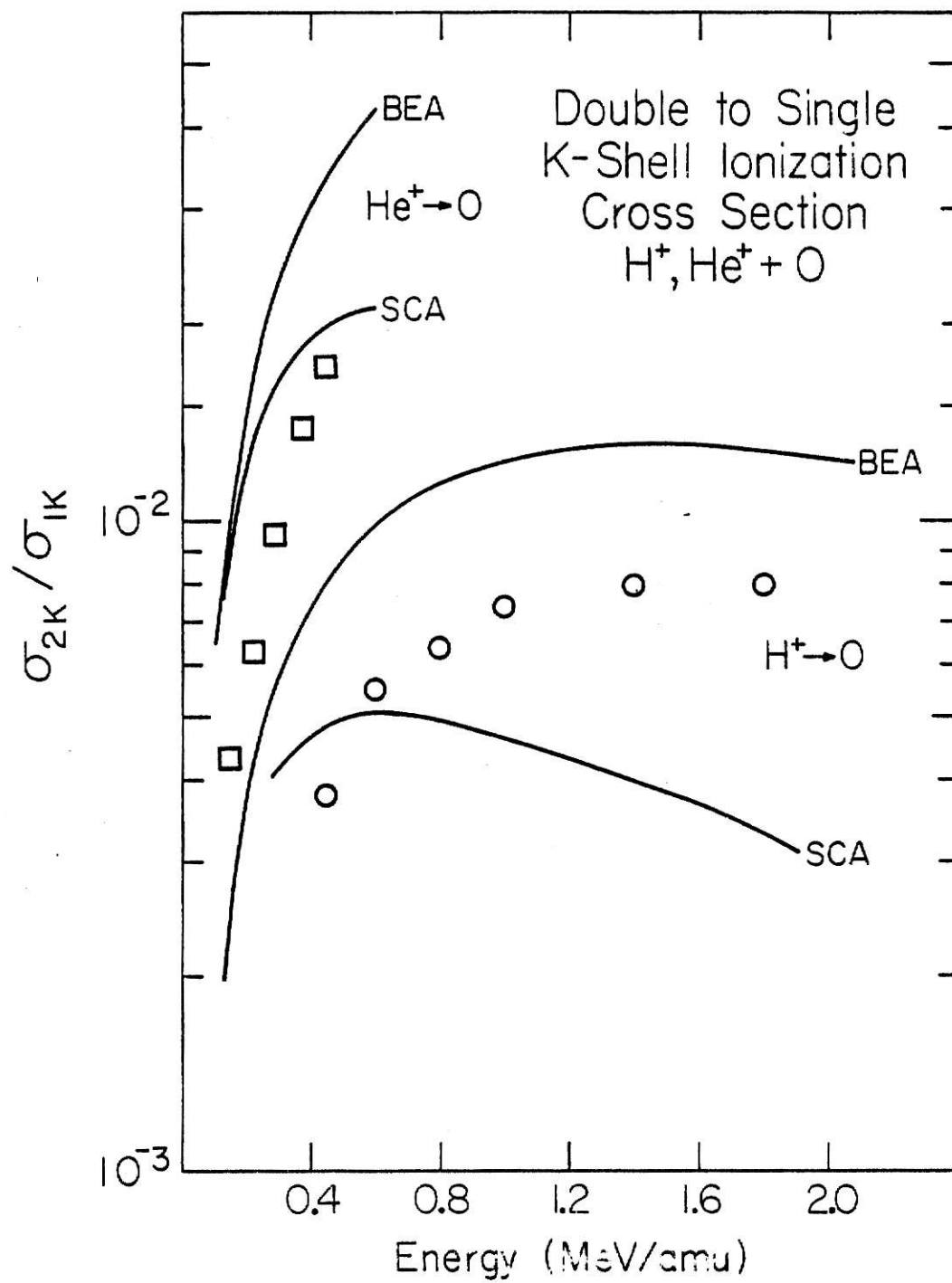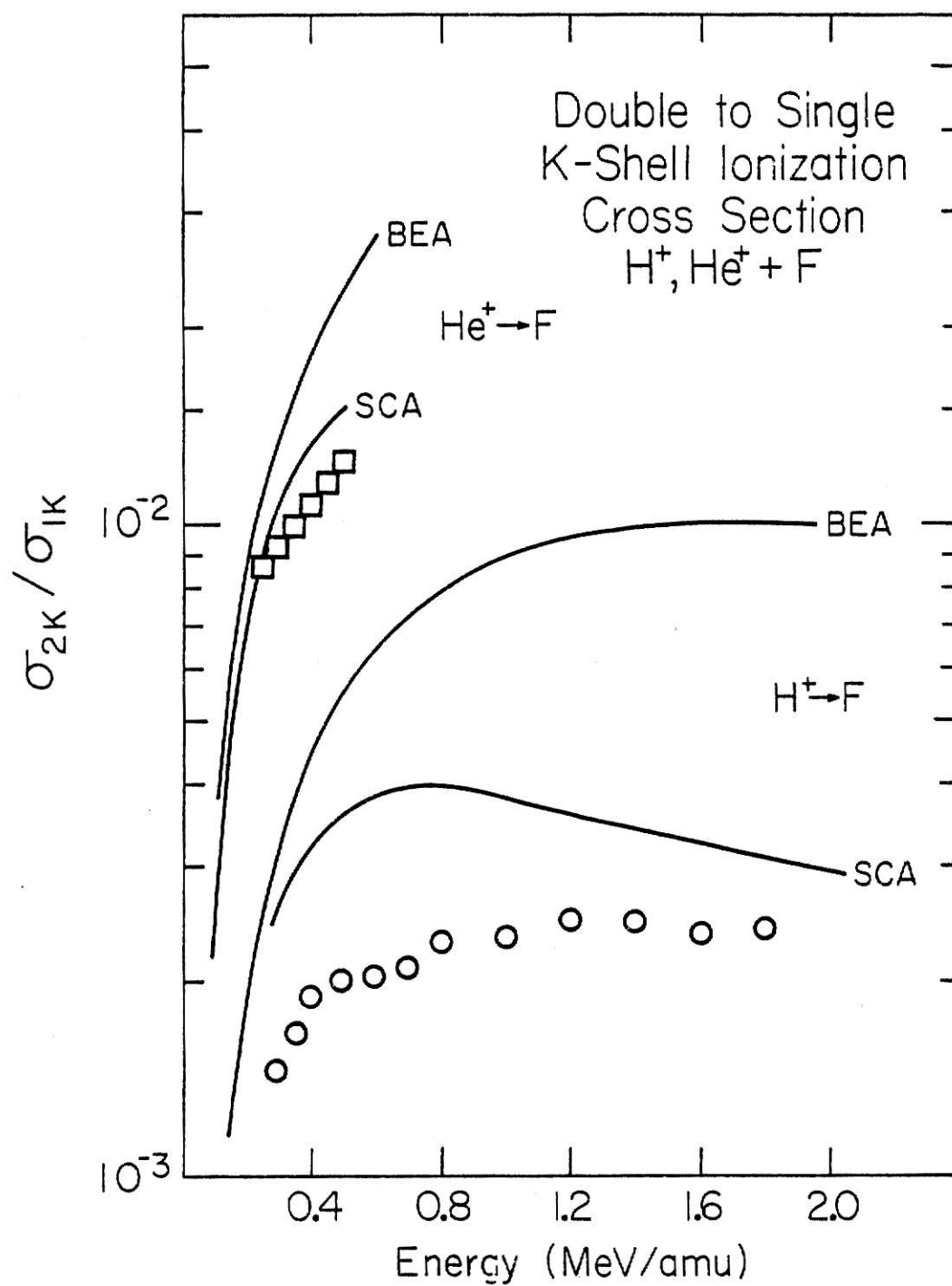Cross Section
$H^+, He^+ + O$

Figure 6. Ratio of double to single K-shell ionization cross sections as a function of projectile energy for H^+, He^+ on F. Theory and data correspond to figures 2 and 4.

Double to Single
K-Shell Ionization
Cross Section
$H^+, He^+ + F$

CHAPTER 5

CONCLUSION

Ever since its inception the SCA approximation has been widely used
as an appropriate tool for studying and analyzing collisions of ions with
multiple electron systems. Unfortunately, this tool has not be thoroughly
documented in the literature.

Only when the approximations are clearly detailed can the nature of
the invoked approximations, both physically and mathematically, be well
understood. For example, the SCA approximation simplifies at low projectile
velocities to a form that is both simple and convenient to use. But, the
constraints involved in this low energy limit are not entirely clear in
the present literature. In this thesis, the semiclassical approximation
for direct coulomb ionization has been developed explicitly. Derivation
of the useful low energy limit has been presented as well as a detailed
development of the full SCA probability amplitude.

Not only is the SCA approximation useful in single ionization studies,
but it is also applicable for multiple ionization studies within the
independent electron approximation. Theoretically, a more complete
physical picture of ion-atom collisions should be obtained from both
single and multiple ionization cross sections. This is true in principle
because single and multiple ionization emphasize different regions of
impact parameter space. In practice, this has been illustrated in this
thesis by applying SCA to single and double K-shell ionization. Further-
more the SCA approximation has been compared to the BEA model for both
single and double K-shell ionization to achieve a fuller picture of the

ionization process. In our opinion, SCA gives a better fit to the data than BEA.

Now that SCA is defined more clearly, one may now concentrate more confidently on the deviations of single ionization from SCA theory in both total cross section and impact parameter studies. Furthermore, once single ionization theory is well defined, then it may be possible to seek corrections to the independent electron approximation and, thus, look toward a more generalized solution of the many electron problem in the theory of ion-atom collisions.

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APPENDIX 1: Derivation of the Potential Term and Probability Coefficient

Using the expansion of $\Psi_n'(\vec{r}, t)$ and Schrodinger's equation,

$$\left(\frac{\hbar^2}{2m_e}\nabla_r^2 + \frac{\bar{z}_1 e^2}{X} + \frac{Z_2 e^2}{r} - \frac{Z_1 Z_2 e^2}{R} + i\hbar\frac{\partial}{\partial t}\right)\sum_k a_{nk}(t)\, \Phi_k(\vec{r}) = 0 = \left(i\hbar\frac{\partial}{\partial t} - \mathcal{H}_{el}\right)\Psi_n(\vec{r}, t).$$

Take the limit as $t \rightarrow \infty$ of the inner product using $\Phi_m(\vec{r})$.

$$\int \Phi_m^*\left(-\mathcal{H}_{el} + i\hbar\frac{\partial}{\partial t}\right)\sum_k a_{nk}(t)\, \Phi_k\, d\vec{r} = \int \Phi_m^*\left(-\mathcal{H}_c - V(\vec{r}, t) + i\hbar\frac{\partial}{\partial t}\right)\sum_k a_{nk}(t)\, \Phi_k\, d\vec{r}$$

$$= \int \Phi_m^*\left(-\mathcal{H}_c\right)\left(\sum_k a_{nk}(t)\, \Phi_k\right) d\vec{r} + \int \Phi_m^*\left(-V(\vec{r}, t)\right)\sum_k a_{nk}(t)\, \Phi_k\, d\vec{r}$$

$$+ i\hbar\int \Phi_m^*\sum \frac{\partial a_{nk}(t)}{\partial t}\, \Phi_k\, d\vec{r} + i\hbar\int \Phi_m^*\sum a_{nk}(t)\frac{\partial \Phi_k}{\partial t}\, d\vec{r}$$

$$= \int \Phi_m^*\left[\sum_k a_{nn}(t)(-E_k)\Phi_k\right] d\vec{r} - \int \Phi_m^* V(\vec{r}, t)\left(\sum a_{nk}\Phi_k\right) d\vec{r}$$

$$+ i\hbar\sum_k \dot{a}_{nk}(t)\int \Phi_m^*\Phi_k\, d\vec{r} + i\hbar\sum_k a_{nk}(t)\int \Phi_m^*\Phi_k\left(\frac{-iE_k}{\hbar}\right)e^{-\frac{iE_k t}{\hbar}}\, d\vec{r}$$

$$= \sum a_{nn}(t)\delta_{mk}(-E_k) - \sum_k a_{nk}(t)\int \phi_m^* e^{i\frac{E_m t}{\hbar}} V(\vec{r}, t)\, \phi_n\, e^{-\frac{iE_k t}{\hbar}}\, d\vec{r}$$

$$+ i\hbar\, \dot{a}_{nk}(t)\delta_{mk} + \sum a_{nk}(t)E_k\delta_{nm}.$$

Thus, $\quad i\hbar\, \dot{a}_{nm}(t) = \sum_k a_{nk}(t)\int \phi_m^* V(\vec{r}, t)\, \phi_n\, e^{i\left(\frac{E_m - E_k}{\hbar}\right)t}\, d\vec{r}$

or $\quad i\hbar \, \dot{a}_{nm}(t) = \sum_{\kappa \neq m} a_{n\kappa}(t) \, V_{m\kappa} \, e^{i \omega_{m\kappa} t}$

where $\quad \omega_{mn} = \dfrac{E_m - E_\ell}{\hbar}$. $\quad V_{n\kappa}$ can be rewritten as

$$V_{m\kappa} = e^2 \int \Phi_m^* \left(\frac{Z_1 Z_2}{R} - \frac{Z_1}{X} \right) \Phi_\kappa \, d\vec{r} \, dt = \frac{Z_1 Z_2 e^2}{R} \int \Phi_m^* \Phi_\kappa \, d\vec{r} \, dt - e^2 \int \Phi_m^* \frac{Z_1}{X} \Phi_\kappa \, d\vec{r} \, dt$$

$$= \frac{e^2 Z_1 Z_2}{R} \delta_{m\kappa} - \int \Phi_m^* \frac{Z_1 e^2}{X} \Phi_\kappa \, d\vec{r} \, dt \underset{\substack{\approx \, t \to \infty \\ R \to \infty}}{\approx} -Z_1 e^2 \int \Phi_m^* \frac{1}{X} \Phi_\kappa \, d\vec{r} \, dt$$

$$= V_{m\kappa} \quad \text{if} \quad R \neq R(\vec{r}).$$

If we have a moving nonrelativistic projectile where the transitions are rare, $a_{nn}(t) \approx 1$.

With weak interactions where the transitions are rare, the main contributions from the m to the n state will be the k = n term in the summation. Other contributions would involve multiple transitions, such as k to j then to n, which are very improbable under weak transitions.

$$a_{mn}(t) \approx \delta_{nm} - \frac{i}{\hbar} \sum_{\kappa \neq m} a_{n\kappa}(t) \int \phi_m^* \, V(\vec{r}, t) \, \phi_\kappa \, e^{i \frac{(E_m - E_\kappa)t}{\hbar}} \, d\vec{r} \, dt$$

$$\approx \delta_{nm} - \frac{i}{\hbar} a_{nn}^{\,1}(t) \int \phi_m^* \, V(\vec{r}, t) \, \phi_n \, e^{i \frac{(E_m - E_n)t}{\hbar}} \, d\vec{r} \, dt$$

$$\approx \delta_{nm} - \frac{i}{\hbar} \int_{-\infty}^{t} V_{mn} \, e^{i \omega_{mn} t} \, dt$$

which is first order perturbation theory.

APPENDIX 2:   Derivation of the Generalized Probability Coefficient

Starting with equation

$$a_{if} = \frac{i Z_1 e^2}{\hbar \, 2 \pi^2} \int dt \int \frac{d\vec{q}}{q^2} \, e^{-i \vec{q} \cdot \vec{R}} e^{i \omega_{if} t} \int \phi_f^* \phi_i \, e^{i \vec{q} \cdot \vec{r}} \, d\vec{r}$$

where

$$\vec{q} \cdot \vec{R} = \vec{q} \cdot (\vec{\rho} + \vec{r} t) = q_r \, v t + \vec{q}_\perp \cdot \vec{\rho} \quad \text{as } q_r \parallel v \text{ and } q_\perp \perp v$$

then

$$\frac{1}{2 \pi} \int_0^\infty e^{i(-q_r \, v + \omega) t} \, dt \; = \; \delta(-q_r \, v + \omega)$$

$$\delta(f(x)) = \left| \frac{d \, f(x)}{dx} \right|^{-1} \delta(x - x_c) \qquad \text{with } f(x_c) = 0$$

$$\delta(-q_r \, v + \omega) = \left| \frac{d(-q_r \, v + \omega)}{d q_r} \right|^{-1} \delta\left(q - \frac{\omega}{v}\right) = \frac{1}{v} \, \delta\left(q_c - \frac{\omega}{v}\right)$$

$$a_{if} = \frac{i Z_1 e^2}{v \pi \hbar} \int \frac{e^{-i q_\perp \, \rho \cos \phi_\ell}}{q^2} \; q_\perp \, dq_\perp \, dq_r \, d\phi_q \; \delta\left(q_c - \frac{\omega}{v}\right) \ell(\vec{q} \cdot \vec{R})$$

Now figure $\ell(\vec{q} \cdot \vec{R}) = \int \phi_f^* \phi_i \, e^{i \vec{q} \cdot \vec{r}} \, d\vec{r}$.

Initially $\phi_i = \phi_{1S} = \frac{1}{\sqrt{\pi}} \left(\frac{Z_2}{a_o}\right)^{3/2} e^{-\frac{Z_2 r}{a_o}}$

and in the continuum hydrogenic eigenfunctions

$$\phi_f = e^{-\frac{\pi \eta}{2}} \sum_{\ell=0}^\infty i^\ell (2kr)^\ell \frac{|\Gamma(\ell+1+i\eta)|}{(2\ell)!} e^{ikr} P_\ell(\cos\theta) \, {}_1F_1(\ell+1+i\eta, 2\ell+2, -2ikr)$$

where $\eta = -\frac{Z_2}{k \, a_o}$ and k is the momentum of the ejected elctron.

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Now, $\mathcal{A}(\vec{q}\cdot\vec{k}) = \int \sum_\ell f^*(r) P_\ell(\cos\theta_r) \frac{1}{\sqrt{\pi}} \left(\frac{Z_2}{a_0}\right)^{3/2} e^{-\frac{Z_2 r}{a_0}} e^{iqr\cos\gamma} r^2\, dr\, d\Omega_r$

where $f^*(r) = e^{-\frac{\pi\eta}{2}} (-i2k)^\ell e^{-ikr} r^\ell \frac{|\Gamma(\ell+1-i\eta)|}{(2\ell)!} \,{}_1F_1(\ell+1+i\eta, 2\ell+2, 2ikr)$

then, $\mathcal{A}(\vec{q}\cdot\vec{k}) = \left(\frac{Z_2}{a_0}\right)^{3/2} \frac{1}{\sqrt{\pi}} \sum_\ell \int f^*(r) e^{-\frac{Z_2 r}{a_0}} r^2\, dr \int P_\ell(\cos\theta_r) e^{iqr\cos\gamma}\, d\Omega_r$

as[24, 25] $P_\ell(\cos\theta_r) = \frac{4\pi}{2\ell+1} \sum_{m=-\ell}^{\ell} Y_\ell^{m*}(\theta_k, \phi_k) Y_\ell^m(\theta_r, \phi_r)$

and

$$e^{iqr\cos\gamma} = 4\pi \sum_{\ell'=0}^{\infty} \sum_{m=-\ell'}^{\ell'} i^{\ell'} j_{\ell'}(qr) Y_{\ell'}^{m'}(\theta_q, \phi_q) Y_{\ell'}^{m'*}(\theta_r, \phi_r)$$

Then

$\mathcal{A}(\vec{q}\cdot\vec{k}) = \left(\frac{Z_2}{a_0}\right)^{3/2} \frac{1}{\sqrt{\pi}} \sum_\ell \int f^*(r) e^{-\frac{Z_2 r}{a_0}} r^2\, dr \int \sum_{\ell'=0}^{\infty} \sum_{m=-\ell'}^{\ell'} 16\pi^2 i^{\ell'} j_{\ell'}(qr)$

$\times \sum_{m=-\ell}^{\ell} \frac{1}{2\ell+1} Y_\ell^{m*}(\theta_k, \phi_k) Y_{\ell'}^{m'}(\theta_q, \phi_q) Y_{\ell'}^{m'*}(\theta_r, \phi_r) Y_\ell^m(\theta_r, \phi_r)\, d\Omega_r$

$= 16 \left(\frac{\pi Z_2}{a_0}\right)^{3/2} \sum_\ell \int f^*(r) e^{-\frac{Z_2 r}{a_0}} r^2\, dr \sum_{\ell'=0}^{\infty} \sum_{m'=-\ell'}^{\ell'} i^{\ell'} \frac{j_{\ell'}(qr)}{2\ell+1} Y_\ell^{m*}(\theta_k, \phi_k) Y_{\ell'}^{m'}(\theta_q, \phi_q) \delta_{\ell\ell'} \delta_{mm'}$

$= 16 \left(\frac{\pi Z_2}{a_0}\right)^{3/2} \sum_{\ell=0}^{\infty} \int e^{-\frac{\pi\eta}{2}} (-2ik)^\ell e^{-ikr} r^{\ell+2} \frac{|\Gamma(\ell+1-i\eta)|}{2\ell!}$

$\times \,{}_1F_1(\ell+1-i\eta, 2\ell+2, 2ikr) e^{-\frac{Z_2 r}{a_0}}\, dr$

$\times \sum_{m=-\ell}^{\ell} i^\ell \frac{j_\ell(qr)}{2\ell+1} Y_\ell^{m*}(\theta_k, \phi_k) Y_\ell^m(\theta_q, \phi_q)$

So that

$$\mathcal{U}(\vec{q}\cdot\vec{K}) = 16\left(\frac{\pi Z_2}{a_o}\right)^{3/2} e^{-\frac{\pi n}{2}} \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} (2k)^{\ell} \frac{|\Gamma(\ell+1-in)|}{2\ell!} \frac{Y_{\ell}^{m*}(\theta_k,\phi_k) Y_{\ell}^{m}(\theta_q,\phi_q)}{2\ell+1}$$

$$\times \int e^{-ikr} e^{-\frac{Z_2 r}{a_o}} r^{\ell+2} {}_1F_1(\ell+1-in, 2\ell+2, 2ikr) j_{\ell}(qr) \, dr$$

$$\mathcal{U}(\vec{q}\cdot\vec{K}) = 16\left(\frac{\pi Z_2}{a_o}\right)^{3/2} e^{-\frac{\pi n}{2}} \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} (2k)^{\ell} \frac{|\Gamma(\ell+1-in)|}{(2\ell+1)!} Y_{\ell}^{m*}(\theta_k,\phi_k) Y_{\ell}^{m}(\theta_q,\phi_q) \mathcal{U}_{\ell}(q,k) \quad .$$

Substituting in $\mathcal{U}(\vec{q}\cdot\vec{K})$,

$$a_{if} = \frac{i Z_1 e^2}{v \pi \hbar} \int \frac{e^{-i q_z \rho \cos\phi_q}}{q^2} q_{\perp} \, dq_{\perp} \, dq_z \, d\phi_q \, \delta\left(q_z - \frac{\omega}{v}\right)$$

$$\times 16\left(\frac{\pi Z_2}{a_o}\right)^{3/2} e^{-\frac{\pi n}{2}} \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} (2k)^{\ell} \frac{|\Gamma(\ell+1-in)|}{(2\ell+1)!} Y_{\ell}^{m*}(\theta_k,\phi_k) Y_{\ell}^{m}(\theta_q,\phi_q) \mathcal{U}_{\ell}(q,k)$$

where[26, 27]

$$Y_{\ell}^{m}(\theta_q,\phi_q) = (-1)^m \left[\frac{(2\ell+1)(\ell-m)!}{4\pi(\ell+m)!}\right]^{\frac{1}{2}} P_{\ell}^{m}(\cos\theta_q) e^{im\phi_q}$$

Then $$a_{if} = \frac{\sqrt{\pi} \, i Z_1 e^2 \, 16}{v \hbar} e^{-\frac{\pi n}{2}} \left(\frac{Z_2}{a_o}\right)^{3/2} \int \frac{e^{-i q_z \rho \cos\phi_q}}{q^2} q_{\perp} \, dq_{\perp} \, dq_z \, d\phi_q \, \delta\left(q_z - \frac{\omega}{v}\right)$$

$$\times \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} (-1)^m \left[\frac{(2\ell+1)(\ell-m)!}{(\ell+m)!}\right]^{\frac{1}{2}} P_{\ell}^{m}(\cos\phi_q) e^{im\phi_q} (2k)^{\ell} \frac{|\Gamma(\ell+1-in)|}{(2\ell+1)!} Y_{\ell}^{m*}(\theta_k,\phi_k) \mathcal{U}_{\ell}(q,k)$$

hence,

$$a_{if} = \frac{8i Z_1 e^2 e^{-\frac{\pi n}{2}}}{v \hbar} \left(\frac{Z_2}{a_o}\right)^{3/2} \int \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \frac{e^{-i q_z \rho \cos\phi_q + im\phi_q}}{q^2} q_{\perp} \, dq_{\perp} \, dq_z \, d\phi_q \, \delta\left(q_z - \frac{\omega}{v}\right)$$

$$\times Y_{\ell}^{m*}(\theta_k,\phi_k)(-1)^m \left[\frac{(2\ell+1)(\ell-m)!}{(\ell+m)!}\right]^{\frac{1}{2}} P_{\ell}^{m}(\cos\theta_q)(2k)^{\ell} \frac{|\Gamma(\ell+1-in)|}{(2\ell+1)!} \mathcal{U}_{\ell}(q,k)$$

$$\times \left\{\int_{-\pi}^{\pi} e^{-i q_{\perp} \rho \cos\phi_q} \cos m\phi_q \, d\phi_q + i\int_{-\pi}^{\pi} e^{-i q_{\perp} \rho \cos\phi_q} \sin m\phi_q \, d\phi_q\right\} \quad .$$

Note that
$$\int_{-\pi}^{0} e^{-i q_\perp \rho \cos\phi_q} \sin m\phi_q \, d\phi_q = -\int_{0}^{\pi} e^{-i q_\perp \rho \cos\phi_q} \sin m\phi_q \, d\phi_q$$

as $\quad \sin(-m\phi) = -\sin m\phi \quad$, making the imaginary integral zero.

With[28, 29]
$$\int_{-\pi}^{\pi} e^{-i q_\perp \rho \cos\phi_q} \cos m\phi_q \, d\phi_q = 2\int_{0}^{\pi} e^{-i q_\perp \rho \cos\phi_q} \cos m\phi_q \, d\phi_q$$

$$= 2(i)^m \pi J_m(-q_\perp \rho) = 2(-i)^m \pi J_m(q_\perp \rho) .$$

Hence,
$$a_{if} = \frac{8i Z_1 e^2 e^{-\frac{\pi\eta}{2}}}{v \hbar} \left(\frac{Z_2}{a_o}\right)^{3/2} \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \int 2(-i)^m \pi J_m(q_\perp \rho) \frac{q_\perp}{q^2} \, dq_\perp \, \delta(q_z - \tfrac{\omega}{v}) \, dq_z$$

$$\times (-1)^m \left[\frac{(2\ell+1)(\ell-m)!}{(\ell+m)!}\right]^{1/2} P_\ell^m(\cos\theta_q)(2k)^\ell \frac{|\Gamma(\ell+1-i\eta)|}{(2\ell+1)!} \mathcal{U}_\ell(q,k) Y_\ell^{m*}(\theta_k,\phi_k)$$

$$a_{if} = \frac{16 \pi Z_1 e^2 e^{-\frac{\pi\eta}{2}}}{v \hbar} \left(\frac{Z_2}{a_o}\right)^{3/2} \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} Y_\ell^{m*}(\theta_k,\phi_k) \left[\frac{(2\ell+1)(\ell-m)!}{(\ell+m)!}\right]^{1/2} \frac{(2k)^\ell}{(2\ell+1)!}$$

$$\times |\Gamma(\ell+1-i\eta)|(i)^m \int \frac{J_m(q_\perp \rho) q_\perp}{q_\perp^2 + \frac{\omega^2}{v^2}} P_\ell^m\left(\frac{\omega/v}{\sqrt{q_\perp^2 + \frac{\omega^2}{v^2}}}\right) \mathcal{U}_\ell(q,k) \, dq_\perp$$

Each individual $\mathcal{U}_\ell(q,k)$ for $\ell = 0, 1, 2$ and 3 is evaluated explicitly in Appendices 3-6 respectively.

APPENDIX 3: Derivation of $\mathcal{L}_c(q, k)$ Term

Using the expression[30],

$$\mathcal{L}_\ell(q, k) = \int e^{-\left(\frac{Z_2}{a_0} + ik\right)r} {}_1F_1(\ell+1-in, 2\ell+2, 2ikr) \, f_\ell(qr) \, r^{\ell+2} \, dr$$

Now, compute $\mathcal{L}_c(q, k)$ using $f_c(qr) = \dfrac{\sin qr}{qr}$.

$$\mathcal{L}_c(q, k) = \int e^{-\left(\frac{Z_2}{a_0} + ik\right)r} r^2 \left[\frac{e^{iqr} - e^{-iqr}}{qr(2i)} \right] {}_1F_1(1-in, 2, 2ikr) \, dr$$

$$= \int \frac{e^{-\left(\frac{Z_2}{a_0} + i(k-q)\right)r}}{2iq} \, r \, {}_1F_1(1-in, 2, 2ikr) \, dr$$

$$- 1 \int \frac{e^{-\left(\frac{Z_2}{a_0} + i(k+q)\right)r}}{2iq} \, r \, {}_1F_1(1-in, 2, 2ikr) \, dr$$

Let $\lambda_1 = \dfrac{Z_2}{a_0} + i(k-q)$ and $\lambda_2 = \dfrac{Z_2}{a_0} + i(k+q)$

so that

$$\mathcal{L}_c(q, k) = \frac{1}{2iq} \left\{ \frac{\Gamma(2) \, {}_2F_1\left(1-in, 2, 2, \frac{2ik}{\lambda_1}\right)}{\lambda_1^2} - \frac{\Gamma(2) \, {}_2F_1\left(1-in, 2, 2, \frac{2ik}{\lambda_2}\right)}{\lambda_2^2} \right\}$$

as[31-33]

$$\int_0^\infty e^{-\mu x} x^{\sigma-1} \, {}_mF_n(a_1, ..., a_m; b_1, ..., b_n; \lambda x) \, dx =$$

$$= \Gamma(b_n) \, \mu^{-\sigma} \, {}_{m+1}F_n\left(a_1, ..., a_m; \sigma; b_1, ..., b_n; \frac{\lambda}{\mu}\right)$$

where

$$m < n \quad \mathcal{R}e \, \sigma > 0, \ \mathcal{R}e \, \mu > 0$$
$$m = n \quad \mathcal{R}e \, \mu > \mathcal{R}e \, \lambda .$$

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APPENDIX 4: Derivation of $\mathcal{U}_1(q,k)$ Term

Here consider

$$\mathcal{U}_1(q,k) = \int e^{-\left(\frac{Z_2}{a_0}+ik\right)r} \,_1F_1(2-i\eta, 4, 2ikr)\, f_1(qr)\, r^3\, dr$$

as $f_1(qr) = \dfrac{\sin qr}{(qr)^2} - \dfrac{\cos qr}{qr}$.

$$\mathcal{U}_1(q,k) = \int e^{-\left(\frac{Z_2}{a_0}+ik\right)r} \,_1F_1(2-i\eta, 4, 2ikr)\left[\frac{\sin qr}{(qr)^2} - \frac{\cos qr}{qr}\right] r^3\, dr$$

$$= \int e^{-\left(\frac{Z_2}{a_0}+ik\right)r}\left[\frac{e^{iqr}-e^{-iqr}}{2i(qr)^2} - \frac{e^{iqr}+e^{-iqr}}{2qr}\right] \,_1F_1(2-i\eta, 4, 2ikr)\, r^3\, dr$$

$$= \frac{1}{2iq^2}\int_0^\infty \left(e^{-\left(\frac{Z_2}{a_0}+i(k-q)\right)r} - e^{-\left(\frac{Z_2}{a_0}+i(k+q)\right)r}\right) r \,_1F_1(2-i\eta, 4, 2ikr)\, dr$$

$$+ \frac{-1}{2q}\int_0^\infty \left(e^{-\left(\frac{Z_2}{a_0}+i(k-q)\right)r} + e^{-\left(\frac{Z_2}{a_0}+i(k+q)\right)r}\right) r^2 \,_1F_1(2-i\eta, 4, 2ikr)\, dr$$

$$\mathcal{U}_1(q,k) = \frac{1}{2iq^2}\left\{\frac{\Gamma(2)\,_2F_1\left(2-i\eta, 2, 4, \frac{2ik}{\lambda_1}\right)}{\lambda_1^2} - \frac{\Gamma(2)\,_2F_1\left(2-i\eta, 2, 4, \frac{2ik}{\lambda_2}\right)}{\lambda_2^2}\right\}$$

$$+ \frac{-1}{2q}\left\{\frac{\Gamma(3)\,_2F_1\left(2-i\eta, 3, 4, \frac{2ik}{\lambda_1}\right)}{\lambda_1^3} + \frac{\Gamma(3)\,_2F_1\left(2-i\eta, 3, 4, \frac{2ik}{\lambda_2}\right)}{\lambda_2^3}\right\}$$

where $\lambda_1 = \dfrac{Z_2}{a_0} + i(k-q)$ and $\lambda_2 = \dfrac{Z_2}{a_0} + i(k+q)$

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Using the Gaussian Hypergeometric properly[34],

$$\left(2b-c-bz+az\right)\,{}_2F_1\left(a,b,c;z\right)=\left(b-c\right)\,{}_2F_1\left(a,b-1,c,z\right)+b(1-z)\,{}_2F_1\left(a,b+1,c,z\right),$$

$$_2F_1\left(2-in,3,4,\frac{2ik}{\lambda}\right)=\frac{-{}_2F_1\left(2-in,2,4,\frac{2ik}{\lambda}\right)+3\left(1-\frac{2ik}{\lambda}\right){}_2F_1\left(2-in,4,4,\frac{2ik}{\lambda}\right)}{2-(1+in)\frac{2ik}{\lambda}}\,.$$

$$\mathcal{L}_1(q,k)=\frac{{}_2F_1\left(2-in,2,4,\frac{2ik}{\lambda_1}\right)}{2iq^2\lambda_1^2}-\frac{{}_2F_1\left(2-in,2,4,\frac{2ik}{\lambda_2}\right)}{2iq^2\lambda_2^2}$$

$$+\frac{-2}{2q}\left\{\frac{-{}_2F_1\left(2-in,2,4,\frac{2ik}{\lambda_1}\right)+3\left(1-\frac{2ik}{\lambda_1}\right){}_2F_1\left(2-in,4,4,\frac{2ik}{\lambda_1}\right)}{\lambda_1^3\left(2-(1+in)\frac{2ik}{\lambda_1}\right)}\right\}$$

$$+\frac{-2}{2q}\left\{\frac{-{}_2F_1\left(2-in,2,4,\frac{2ik}{\lambda_2}\right)+3\left(1-\frac{2ik}{\lambda_2}\right){}_2F_1\left(2-in,4,4,\frac{2ik}{\lambda_2}\right)}{\lambda_2^3\left(2-(1+in)\frac{2ik}{\lambda_2}\right)}\right\}$$

Now, compare the coefficients of ${}_2F_1\left(2-in,2,4,\frac{2ik}{\lambda_1}\right)$.

$$\frac{1}{2iq^2\lambda_1^2}+\frac{1}{q\lambda_1^3\left(2+(1+in)\frac{2ik}{\lambda_1}\right)}=\frac{1}{q\lambda_1^2}\left[\frac{1}{2iq}+\frac{1}{2\lambda_1-(1+in)2ik}\right]$$

$$=\frac{1}{q\lambda_1^2}\left[\frac{1}{2iq}+\frac{1}{2\frac{Z_2}{a_0}+i2k-2iq-2ik+2nk}\right]$$

$$=\frac{1}{q\lambda_1^2}\left[\frac{1}{2iq}+\frac{1}{-2iq}\right]=c\quad\text{as}\quad n=-\frac{Z_2}{a_0k}.$$

Likewise, compare the coefficients of ${}_2F_1\left(2-in,2,4,\frac{2ik}{\lambda_2}\right)$.

$$-\frac{1}{2iq^2\lambda_2^2}+\frac{1}{\lambda_2^3\left(2-(1+in)\frac{2ik}{\lambda_2}\right)}=\frac{1}{q\lambda_2^2}\left[\frac{1}{-2iq}+\frac{1}{2\lambda_2-(1+in)2ik}\right]$$

$$=\frac{1}{q\lambda_2^2}\left[\frac{-1}{2iq}+\frac{1}{2\frac{Z_2}{a_0}+i2k+2iq-2ik+2nk}\right]=0.$$

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Thus,

$$\ell_1(q,k) = -\left[\frac{3\left(1-\frac{2ik}{\lambda_1}\right){}_2F_1\left(2-in,4,4,\frac{2ik}{\lambda_1}\right)}{q\,\lambda_1^3\left(2-(1+in)\frac{2ik}{\lambda_1}\right)} + \frac{3\left(1-\frac{2ik}{\lambda_2}\right){}_2F_1\left(2-in,4,4,\frac{2ik}{\lambda_2}\right)}{q\,\lambda_2^3\left(2-(1+in)\frac{2ik}{\lambda_2}\right)}\right].$$

APPENDIX 5: Derivation of $\mathcal{L}_2(q,k)$ Term

Here consider

$$\mathcal{L}_2(q,k) = \int e^{-\left(\frac{z_2}{a_0} + ik\right)r} \, {}_1F_1(3-in, 6, 2ikr) \, j_2(qr) \, r^4 \, dr$$

as $\quad j_2(qr) = \left(\frac{3}{(qr)^3} - \frac{1}{qr}\right) \sin qr - \frac{3}{(qr)^2} \cos qr$.

One has

$$\mathcal{L}_2(q,k) = \int \left\{\left(\frac{3}{(qr)^3} - \frac{1}{qr}\right) \sin qr - \frac{3 \cos qr}{(qr)^2}\right\} e^{-\left(\frac{z_2}{a_0} + ik\right)r} \, r^4 \, {}_1F_1(3-in, 6, 2ikr) \, dr$$

$$= \int \frac{3}{q^3} \, \frac{e^{+iqr} - e^{-iqr}}{2i} \, e^{-\left(\frac{z_2}{a_0} + ik\right)r} \, r \, {}_1F_1(\,,\,) \, dr$$

$$+ \int -\frac{r^3}{q} \, \frac{e^{iqr} - e^{-iqr}}{2i} \, e^{-\left(\frac{z_2}{a_0} + ik\right)r} \, {}_1F_1(\,,\,) \, dr + \int \frac{-3r^2}{q^2} \, \frac{e^{iqr} + e^{-iqr}}{2} \, e^{-\left(\frac{z_2}{a_0} + ik\right)r} \, {}_1F_1(\,,\,) \, dr$$

$$= \frac{3}{2iq^3} \int e^{-\left(\frac{z_2}{a_0} + i(k-q)\right)r} \, r \, {}_1F_1(\,,\,) \, dr - \frac{3}{2iq^3} \int e^{-\left(\frac{z_2}{a_0} + i(k+q)\right)r} \, r \, {}_1F_1(\,,\,) \, dr$$

$$+ \frac{-1}{2iq} \int e^{-\left(\frac{z_2}{a_0} + i(k-q)\right)r} \, r^3 \, {}_1F_1(\,,\,) \, dr + \frac{1}{2iq} \int e^{-\left(\frac{z_2}{a_0} + i(k+q)\right)r} \, r^3 \, {}_1F_1(\,,\,) \, dr$$

$$+ \frac{-3}{2q^2} \int e^{-\left(\frac{z_2}{a_0} + i(k-q)\right)r} \, r^2 \, {}_1F_1(\,,\,) \, dr - \frac{3}{2q^2} \int e^{-\left(\frac{z_2}{a_0} + i(k+q)\right)r} \, r^2 \, {}_1F_1(\,,\,) \, dr$$

$$= \frac{3}{2iq^3} \, \frac{\Gamma(2) \, {}_2F_1\left(3-in, 2, 6, \frac{2ik}{\lambda_1}\right)}{\lambda_1^2} - \frac{3}{2iq^3} \, \frac{\Gamma(2) \, {}_2F_1\left(3-in, 2, 6, \frac{2ik}{\lambda_2}\right)}{\lambda_2^2}$$

$$+ \frac{-\Gamma(4)}{2iq} \, \frac{{}_2F_1\left(3-in, 4, 6, \frac{2ik}{\lambda_1}\right)}{\lambda_1^4} + \frac{\Gamma(4)}{2iq} \, \frac{{}_2F_1\left(3-in, 4, 6, \frac{2ik}{\lambda_2}\right)}{\lambda_2^4}$$

$$+ \frac{-3\Gamma(3)}{2q^2} \, \frac{{}_2F_1\left(3-in, 3, 6, \frac{2ik}{\lambda_1}\right)}{\lambda_1^3} - \frac{3\Gamma(3)}{2q^2} \, \frac{{}_2F_1\left(3-in, 3, 6, \frac{2ik}{\lambda_2}\right)}{\lambda_2^3}$$

where $\lambda_1 = \dfrac{z_2}{c_i} + i(k-q)$, $\lambda_2 = \dfrac{z_2}{c_i} + i(k+q)$ and $\eta = -\dfrac{z_2}{c_i k}$.

Thus,

$$
\begin{aligned}
\mathcal{l}_2(q,k) = {} & \frac{3}{2iq^3}\left(\frac{{}_2F_1\left(3-in,\,2,\,6,\,\frac{2ik}{\lambda_1}\right)}{\lambda_1^2} - \frac{{}_2F_1\left(3-in,\,2,\,6,\,\frac{2ik}{\lambda_2}\right)}{\lambda_2^2} \right) \\[2mm]
& + \frac{3}{iq}\left(-\frac{{}_2F_1\left(3-in,\,4,\,6,\,\frac{2ik}{\lambda_1}\right)}{\lambda_1^4} + \frac{{}_2F_1\left(3-in,\,4,\,6,\,\frac{2ik}{\lambda_2}\right)}{\lambda_2^4} \right) \\[2mm]
& + \frac{-3}{q^2}\left(\frac{{}_2F_1\left(3-in,\,3,\,6,\,\frac{2ik}{\lambda_1}\right)}{\lambda_1^3} + \frac{{}_2F_1\left(3-in,\,3,\,6,\,\frac{2ik}{\lambda_2}\right)}{\lambda_2^3} \right) .
\end{aligned}
$$

APPENDIX 6: Derivation of $\mathcal{U}_3(q,k)$ Term

Here consider

$$\mathcal{U}_3(q,k) = \int e^{-\left(\frac{z_2}{a_0}+ik\right)r} {}_1F_1(4-in,\, 8,\, 2ikr)\, j_3'(qr)\, r^5\, dr$$

where

$$j_3'(qr) = \left[\frac{15}{(qr)^4} - \frac{6}{(qr)^2}\right]\sin qr + \left[\frac{1}{qr} - \frac{15}{q^3 r^3}\right]\cos qr$$

so that

$$\mathcal{U}_3(q,k) = \int \left(\left[\frac{15}{(qr)^4} - \frac{6}{(qr)^2}\right]\frac{e^{iqr}-e^{-iqr}}{2i} + \left[\frac{1}{qr} - \frac{15}{q^3 r^3}\right]\frac{e^{iqr}+e^{-iqr}}{2}\right)$$

$$\times\; e^{-\left(\frac{z_2}{a_0}+ik\right)r} {}_1F_1(4-in,\,8,\,2ikr)\, r^5\, dr\;.$$

$$\mathcal{U}_3(q,k) = \int \frac{15}{2iq^4} e^{-\left(\frac{z_2}{a_0}+i(k-q)\right)r} r\, {}_1F_1(\,,\,)\,dr + \int \frac{-15}{2iq^4} e^{-\left(\frac{z_2}{a_0}+i(k+q)\right)r} r\, {}_1F_1(\,,\,)\,dr$$

$$+ \int \frac{-6}{2iq^2} e^{-\left(\frac{z_2}{a_0}+i(k-q)\right)r} r^3\, {}_1F_1(\,,\,)\,dr + \int \frac{6}{2iq^2} e^{-\left(\frac{z_2}{a_0}+i(k+q)\right)r} r^3\, {}_1F_1(\,,\,)\,dr$$

$$+ \int \frac{1}{2q} e^{-\left(\frac{z_2}{a_0}+i(k-q)\right)r} r^4\, {}_1F_1(\,,\,)\,dr + \int \frac{1}{2q} e^{-\left(\frac{z_2}{a_0}+i(k+q)\right)r} r^4\, {}_1F_1(\,,\,)\,dr$$

$$+ \int \frac{-15}{2q^3} e^{-\left(\frac{z_2}{a_0}+i(k-q)\right)r} r^2\, {}_1F_1(\,,\,)\,dr + \int \frac{-15}{2q^3} e^{-\left(\frac{z_2}{a_0}+i(k+q)\right)r} r^2\, {}_1F_1(\,,\,)\,dr$$

$$\mathcal{U}_3(q,k) =$$

$$\frac{15}{2iq^4}\left(\frac{\Gamma(2)\, {}_2F_1\left(4-in,2,8,\frac{2ik}{\lambda_1}\right)}{\lambda_1^2} - \frac{\Gamma(2)\, {}_2F_1\left(4-in,2,8,\frac{2ik}{\lambda_2}\right)}{\lambda_2^2}\right)$$

$$+ \frac{-6}{2iq^2}\left(\frac{\Gamma(4)\, {}_2F_1\left(4-in,4,8,\frac{2ik}{\lambda_1}\right)}{\lambda_1^4} - \frac{\Gamma(4)\, {}_2F_1\left(4-in,4,8,\frac{2ik}{\lambda_2}\right)}{\lambda_2^4}\right)$$

$$+ \frac{1}{2q}\left(\frac{\Gamma(5)\, {}_2F_1\left(4-in,5,8,\frac{2ik}{\lambda_1}\right)}{\lambda_1^5} + \frac{\Gamma(5)\, {}_2F_1\left(4-in,5,8,\frac{2ik}{\lambda_2}\right)}{\lambda_2^5}\right) \;+$$

$$+ \frac{-15}{2q^3}\left(\frac{\Gamma(3)\ _2F_1\left(4-in,3,8,\frac{2ik}{\lambda_1}\right)}{\lambda_1^3} + \frac{\Gamma(3)\ _2F_1\left(4-in,3,8,\frac{2ik}{\lambda_2}\right)}{\lambda_2^3}\right)$$

Thus,

$$\ell_3(q,k) = \frac{15}{2iq^4}\left(\frac{_2F_1\left(4-in,2,8,\frac{2ik}{\lambda_1}\right)}{\lambda_1^2} - \frac{_2F_1\left(4-in,2,8,\frac{2ik}{\lambda_2}\right)}{\lambda_2^2}\right)$$

$$+ \frac{18}{iq^2}\left(\frac{-\ _2F_1\left(4-in,4,8,\frac{2ik}{\lambda_1}\right)}{\lambda_1^4} + \frac{_2F_1\left(4-in,4,8,\frac{2ik}{\lambda_2}\right)}{\lambda_2^4}\right)$$

$$+ \frac{12}{q}\left(\frac{_2F_1\left(4-in,5,8,\frac{2ik}{\lambda_1}\right)}{\lambda_1^5} + \frac{_2F_1\left(4-in,5,8,\frac{2ik}{\lambda_2}\right)}{\lambda_2^5}\right)$$

$$+ \frac{15}{q^3}\left(-\frac{_2F_1\left(4-in,3,8,\frac{2ik}{\lambda_1}\right)}{\lambda_1^3} - \frac{_2F_1\left(4-in,3,8,\frac{2ik}{\lambda_2}\right)}{\lambda_2^3}\right)$$

APPENDIX 7:   Approximation of $\mathcal{L}(q,k)$ for Low Energy

Now consider

$$\mathcal{L}_{is \to s}(q,k) = \frac{1}{2iq} \left\{ \frac{{}_2F_1\left(1-in, 2, 2, \frac{2ik}{\lambda_1}\right)}{\lambda_1^2} - \frac{{}_2F_1\left(1-in, 2, 2, \frac{2ik}{\lambda_2}\right)}{\lambda_2^2} \right\}$$

with $\quad {}_2F_1(a, 2, 2, z) = (1-z)^{-a}, \quad 1-in = 1 + \frac{i}{k}, \quad \lambda_1 = 1 + i(k-q),$

$\lambda_2 = 1 + i(k+q) \quad$ and $\quad z_1 = z_2 = 1,$

Now,

$$\frac{\left(1 - \frac{2ik}{1+i(k-q)}\right)^{-1-\frac{i}{k}}}{\left[1 + i(k-q)\right]^2} - \frac{\left(1 - \frac{2ik}{1+i(k+q)}\right)^{-1-\frac{i}{k}}}{\left[1 + i(k+q)\right]^2} \underset{k \ll q}{\sim} \frac{\left(1 - \frac{2ik}{1-iq}\right)^{-\frac{i}{k}}}{1-q^2-2iq} - \frac{\left(1 - \frac{2ik}{1+iq}\right)^{-\frac{i}{k}}}{1-q^2+2iq}$$

$$= \frac{\left[1 + \left(\frac{-i}{k}\right)\left(\frac{-2ik}{1-iq}\right) + \ldots\right]}{1-q^2-2iq} - \frac{\left[1 + \left(\frac{-i}{k}\right)\left(\frac{-2ik}{1+iq}\right) + \ldots\right]}{1-q^2+2iq} \sim \frac{1 - \frac{2}{1-iq}}{1-q^2-2iq} - \frac{1 - \frac{2}{1+iq}}{1-q^2+2iq}$$

$$= \frac{1-iq-2}{(1-iq)^3} - \frac{1+iq-2}{(1+iq)^3} = \frac{8qi(q^2-1)}{(q^2+1)^3} \underset{1 \ll q}{\sim} \frac{8i}{q^3}$$

So,

$$\mathcal{L}(q,k) \simeq \frac{8i}{q^3} .$$

SEMICLASSICAL COULOMB APPROXIMATION

WITH APPLICATION TO SINGLE AND DOUBLE

K-SHELL IONIZATION IN ION-ATOM COLLISIONS

by

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ABSTRACT

The probability amplitude for direct Coulomb ionization in the semiclassical Coulomb approximation is derived in full detail, including the low energy limit. This SCA approximation is used within the independent electron approximation to evaulate both single and double K-Shell ionization cross sections for H^+ and He^+ incident on 0 and F. Results are compared to both the binary encounter approximation (BEA) and recent observations.