Craig D. Conticchio ANALYTICAL CROSS SECTIONS FOR MOMENTUM TRANSFER TO INNER SHELL ELECTRONS (Under the direction of Dr. G. Lapicki) Department of Physics, East Carolina University, May 2011

The Plane Wave Born Approximation (PWBA), the most prevalent First Born Approximation (FBA), serves as input into theories well beyond the scope of the PWBA. Using Mathematica's advanced symbolic programming capabilities and integrated C++ code, algorithms are designed and developed that generate analytical formulas for electron excitation and ionization of atomic constituents of biological materials ranging from hydrogen to argon. Singly-differential cross sections with respect to momentum transfer, obtained here analytically, can be integrated over energy transfer with its zeroth and higher powers to yield cross sections, stopping power, and straggling; they provide input for studies of energy deposition in biomedical media by Monte Carlo or other techniques. Mathematica's existing subroutines and functions do not analytically integrate products of non-trivial functions that are the core of the plane wave framework of the FBA toward calculations for the ionizing and/or excitation interactions. Computational procedures and programs developed here in Mathematica overcome this obstacle, and result in cross sections, differential with respect to the momentum transfer, for excitation and ionization of 1s, 2s, 2p, 3s, 3p, and 3d screened hydrogenic states of said biological constituents.

ANALYTICAL CROSS SECTIONS FOR MOMENTUM TRANSFER
TO INNER SHELL ELECTRONS

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DEDICATION

To my late wife Helen Lynn Kite and late son Bryson Joseph Conticchio.

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LIST OF UNITS AND SYMBOLS

Atomic Units

Quantity	Unit	Value in the SI system
Length	$a_0 = 4\pi\varepsilon_0 \frac{\hbar^2}{m_e e^2}$	5.29×10^{-11} m
Area	a_0^2	2.80×10^{-21} m^2
Wavenumber	$\frac{1}{a_0}$	1.89×10^{10} m^{-1}
Momentum	$\frac{\hbar}{a_0}$	1.99×10^{-24} kg $\cdot$ m/s
Energy	$\frac{1}{4\pi\varepsilon_0}\frac{e^2}{a_0}$	4.36×10^{-18} kg $\cdot$ m^2 / s^2
Velocity	$v_0 = \frac{1}{4\pi\varepsilon_0}\frac{e^2}{\hbar}$	2.19×10^{6} m/s
Time	$\tau_0 = 4\pi\varepsilon_0 \frac{\hbar a_0}{e^2}$	2.42×10^{-17} s
Planck's constant	$\hbar = h / 2\pi$	1.055×10^{-34} kg $\cdot$ m^2/s
Electron mass	m_e	9.109×10^{-31} kg
Electron charge	e	1.602×10^{-19} C

Symbols and Definitions

E_1 = Kinetic energy of projectile ion in MeV = 1.6 x 10^{-13} J

M_1 = Mass of projectile ion in atomic mass units

M_2 = Mass of target atom in atomic mass units

$M = \frac{M_1 M_2}{M_1 + M_2} =$ Reduced mass of projectile ion-target atom system

v_1 = Projectile ion's velocity

$v_{2s} = \frac{Z_{2s}}{n}$ = Electron velocity in the S subshell of the target atom

q = Momentum transfer of the ejected electron

$Q = (qa_{2s})^2 = \frac{q^2}{Z_{2s}^2} =$ Dimensionless square of the momentum transfer

ΔE = Energy transfer to the ejected electron

$W = \frac{\Delta E}{\frac{1}{2} Z_{2s}^2} = k^2 + \frac{1}{n^2} =$ Dimensionless energy transferred to ejected electron

$k^2 = W - \frac{1}{n^2}$ where k is the momentum of the ejected electron

Z_1 = Charge of the projectile's nucleus

Z_{2s} = Screened (effective) charge as seen by electron in the target's subshell S

$\eta_s = \frac{2E_1}{M_1} / Z_{2s}^2 = \frac{v_1^2}{Z_{2s}^2}$ = Scaled square of the velocity of the projectile ion

$U_{2s} = \frac{1}{2}\frac{Z_{2s}^2}{n^2} - V_{2s}$ = Observed binding energy of the target's S-subshell

$\theta_s = U_{2s}\left(\frac{1}{2}\frac{Z_{2s}^2}{n^2}\right)^{-1}$ = Observed binding energy scaled by hydrogenic binding energy

$\sigma_s = (2j+1)4\pi\left(\frac{Z_1}{Z_{2s}^2}\right)^2 \frac{f_s(\eta_s, \theta_s)}{\eta_s}$ = Cross section for S subshell ionization in a_0^2 units

f_s = Dimensionless cross section

CHAPTER 1: INTRODUCTION

1.1 General Problem Description

Ultimately, we wish to calculate, in an analytical framework, differential ionization cross sections for transition from an initially filled subshell (S = K, $L_{1,2,3}$, $M_{1,2,3,4,5}$) to a final state in which S-electrons are excited to unoccupied states or ionized into the continuum following a particular momentum transfer. Such cross sections can be calculated within the confines of the plane wave Born approximation (PWBA) that – with explanation of symbols, reasons, and justifications discussed in Chapter 2 - we choose for our analytical foundation.

The integral over Q in the following equation (derived in section 2.2 p.24) is called the "excitation function" [see Eq. 7.2 in [1] and note the upper limit of integration substitution from infinity in [1] to a finite $Q_{\max}$].

$$I\left(\eta_s, W\right) = \int_{Q_{\min}}^{Q_{\max}} \left|F_{Ws}\left(Q\right)\right|^2 Q^{-2} dQ \qquad \textbf{(1.1.1)}$$

This $I\left(\eta_s, W\right)$ is the energy distribution of ejected electrons and obtaining an analytical expression for this energy distribution is at the very heart of this work. It is the springboard for several theoretically valuable quantities such as cross section$\left[\int_{W_{\min}}^{W_{\max}} I\left(\eta_s, W\right) dW\right]$, stopping power$\left[\int_{W_{\min}}^{W_{\max}} WI\left(\eta_s, W\right) dW\right]$, straggling$\left[\int_{W_{\min}}^{W_{\max}} W^2 I\left(\eta_s, W\right) dW\right]$, and other moments of that energy distribution (1.1.1) in studies of penetration of charged particles through matter. We will develop an analytical expression for the indefinite integral,

$$\int \left|F_{Ws}\left(Q\right)\right|^2 Q^{-2} dQ \qquad \textbf{(1.1.2)}$$

to yield cross sections with any momentum transfer to S-shell electrons. After the integration of Eq. (1.1.2) we can evaluate the result over a definite range $(Q_{\min}, Q_{\max})$. Then after numerical integration of $I(\eta_s, W)$ over *W*, we obtain cross sections, σ_s, for direct ionization of a given shell S = K, $L_{1,2,3}$, $M_{1,2,3,4,5}$. These σ_s are derived and compared with ionization cross section provided by previous fully numerical calculations tabulated by Khandelwhal, Choi, and Merrzbacher [2] as well as tabulated and/or obtained from the code of Liu and Cipolla [3].

1.2 Rationale and Significance

Our analytical approach in evaluating Eq. (1.1.2) provides insight, transparency, and accuracy that a numerical approach may not. One can determine limiting behavior of the resulting functions, and analyze their properties over the full range of parameters depending on application of interest. We can determine the reliability and accuracy of the analytically obtained ionization cross sections by comparing results to existing fully numerical results. If found equally or more accurate our cross sections could be used to supplement the current cross section database for use in various ion transport models.

1.3 General Strategy

In this work *Mathematica* is used extensively. *Mathematica* is computational software utilized in technical computation across a myriad of disciplines [4]. Our analytical build up and evaluation uses an integral approach in the PWBA. Even with advanced symbolic-analytical capabilities, *Mathematica* cannot integrate the simplified yet still complex integrands resulting from the PWBA quantum analysis of ionizing projectile bombarding target electrons described by screened hydrogenic wave functions. We will establish a process that uses several mathematical techniques and *Mathematica's* built in algorithms to break up these integrands into sub-parts that are manageable and ultimately integrable. In this divide-and-conquer process, we can fragment integrands that commonly occur in our analysis and then recombine their individual generic solutions. The indefinite integral equation (1.1.2) is a linear combination of these all-purpose “generic integrals”. They can be called upon to calculate differential ionization cross sections with respect to any momentum transfer specific to the subshell (S = K, $L_{1,2,3}$, $M_{1,2,3,4,5}$).

CHAPTER 2: BACKGROUND

2.1 History and Terminology

Atomic and nuclear physicists have studied inner-shell ionization of targets by inelastic collisions with heavy incident charged particles for many decades, particularly with regard to characteristic x-ray production. Applications in many interdisciplinary areas of research including ecological, biological, bio-medical, aeronautics and more have accelerated a renewed urgency in this field. Investigation of inner-shell excitation and ionization offers unique insight into energy loss processes by charged projectiles through matter. These processes involve cross sections, stopping power, straggling, and other energy transfer quantities. Inner-shell ionizations produce the secondary electrons that are often examined via track studies as e.g., Monte Carlo simulations. These studies are most pertinent to radiation phenomena in microdosimetry and health physics research.

Quite commonly, calculation of the ionization cross section via direct Coulomb excitation has been done, using the PWBA as a foundation, for all K, L, and M shells. In the PWBA framework, incident-inelastically scattered charged particles are described by plane waves, assumed to be bare, as their electronic make-up is ignored. Additionally, since the works of Bethe (K-Shell) [5], Walske (L-Shell) [6], and Choi (M-Shell) [7], screened hydrogenic wave functions are often used to describe the target's electrons.

In this work, we will use atomic units throughout as listed and defined in the "List of Symbols and Abbreviations" on page vii. Our notation associated with the projectile ion will include a subscript "1" and with target atom a subscript "2".

2.2 Theoretical Framework

Within the PWBA framework, we make several limiting assumptions and approximations:

- Incident and inelastically scattered projectile ion are described by plane waves within the FBA.
- A projectile ion acts as a bare charged point particle given by the charge of its nucleus.
- A projectile mass is significantly heavier than the electron mass.
- Screened hydrogenic wave functions describe the target's atomic electrons.
- An electron is removed from an inner shell into unoccupied states (excitation) and the continuum state (ionization) of the target.
- The Coulomb force is the only force of interaction between the projectile's nucleus of charge Z_1 and the target's nucleus charge Z_2 and its electrons.

Starting with the Schrödinger equation,

$$H\Psi = E\Psi \text{,} \qquad \textbf{(2.2.1)}$$

where the Hamiltonian H consist of the entire system to be studied, we let the heavy charged projectile having a Coulomb interaction with the target atom be described by the following Hamiltonian,

$$H = \frac{1}{2M}\nabla_{\vec{R}}^2 + H_2 + Z_1\left[\frac{Z_2}{R} - \sum_{i=1}^{Z_2}\frac{1}{\left|\vec{R}-\vec{r}_i\right|}\right]. \qquad \textbf{(2.2.2)}$$

Here $\vec{R}$ and $\vec{r}_i$ are position vectors for the projectile and the target electrons in the frame of the target nucleus. The first term in Eq. (2.2.2) is the kinetic energy of the projectile in the center of mass of the projectile and target nuclei $M^{-1} = M_1^{-1} + M_2^{-1}$. The second term is the Hamiltonian H_2

of the target atom. Lastly, the third term accounts for the projectile-target interaction potential *V*. We assume the projectile ion to be non-relativistic, which limits its kinetic energy E_1, divided by its mass M_1 to 50 MeV/amu or less. The electronic configuration of the target is determined via the Schrödinger equation

$$H_2\psi_2\left(\vec{r}_1,\vec{r}_2,...,\vec{r}_{Z_2}\right)=E_2\psi\left(\vec{r}_1,\vec{r}_2,...,\vec{r}_{Z_2}\right). \qquad \textbf{(2.2.3)}$$

Neglecting electron spin and nuclear effects, we take

$$H_2=\sum_{i=1}^{Z_2}\left[-\frac{1}{2}\nabla_{\vec{r}_i}^2-\frac{Z_2}{r_i}+\sum_{j=1}^{i-1}\frac{1}{\left|\vec{r}_i-\vec{r}_j\right|}\right]. \qquad \textbf{(2.2.4)}$$

When solving Eq. (2.2.3) with Eq. (2.2.4) we choose antisymetric product of screened hydrogenic wave functions.

Next, we introduce the single-electron approximation by setting the atomic Hamiltonian as

$$H_2=\sum_{i=1}^{Z_2}H_2^i\left(\vec{r}_i\right) \qquad \textbf{(2.2.5)}$$

where

$$H_2^i\phi_i\left(\vec{r}_i\right)=E_2^i\phi_i\left(\vec{r}_i\right) \qquad \textbf{(2.2.6)}$$

With ϕ_i and E_2^i being the single-electron eigenfunction and eigenvalue of the single-electron Hamiltonian H_2^i. In this treatment,

$$H_2^i=-\frac{1}{2}\nabla_{\vec{r}_i}^2+V\left(\vec{r}_i\right) \qquad \textbf{(2.2.7)}$$

In the Hartree approximation the interaction potential, the so-called Hartree potential is

$$V\left(\vec{r}_i\right)=\sum_{k\neq i}\int\left|\phi_k\left(\vec{r}\right)\right|^2\frac{d^3r}{\left|\vec{r}-\vec{r}_i\right|}-\frac{Z_2}{r_i} \qquad \textbf{(2.2.8)}$$

and due to other electrons and nucleus of the target. The Hartree potential can be simplified with the help of a central field approximation. Replace $V\left(\vec{r}_i\right)$ with its average over all angles of $\vec{r}_i$; thus making it spherically symmetric. Now the single-electron wave functions $\phi_{nlm}\left(r_i\right)$ can be separated into products of their radial part R_{nl} and of spherical harmonics Y_{lm},

$$\phi_{nlm}\left(r_i\right) = R_{nl}\left(r_i\right) Y_{lm}\left(\theta_i, \phi_i\right) \tag{2.2.9}$$

with quantum numbers *n, l,* and *m*. Linear combinations of cross sections, based on these functions, form cross sections for ionization of inner subshell S to be identified by a triple of quantum numbers {n, l, j} as $\mathrm{K} = \{1,0,1/2\}$, $\mathrm{L}_{1,2,3} = \{2,0,1/2\},\{2,1,1/2\},\{2,1,3/2\}$, and $\mathrm{M}_{1,2,3,4,5} = \{3,0,1/2\},\{3,1,1/2\},\{3,1,3/2\},\{3,2,3/2\},\{3,2,5/2\}$.

In the hydrogrenic approximation the atomic Hamiltonian Eq. (2.2.7) is

$$H_2^i = -\frac{1}{2}\nabla_{\vec{r}_i}^2 - \frac{Z_2}{r_i} \tag{2.2.10}$$

and the single electron approximation (2.2.6) has exact analytical solutions given as hydrogenic wavefunctions

$$\phi_{nlm}^H\left(r_i\right) = R_{nl}^H\left(r_i\right) Y_{lm}\left(\theta_i, \phi_i\right) \tag{2.2.11}$$

with negative energies

$$E_2^H = -\frac{1}{2}\frac{Z_2^2}{n^2} \tag{2.2.12}$$

and the continuum of positive energies $\frac{1}{2}k^2$ with substitution, $n = i\frac{Z_2}{k}$, where k is the momentum of an electron ejected into the continuum. We can obtain screened hydrogenic (SH) wavefunctions, $\phi_{nlm}^{SH}\left(r_i\right)$, by reduction of Z_2 in Eq. (2.2.11) by appropriate Slater's screening constant [8]. The result, Z_{2s}, is the effective atomic charge as seen by an electron in an inner shell (K, $L_{1,2,3}$, $M_{1,2,3,4,5}$) of a screened hydrogenic atom. Z_2 is replaced with:

$Z_{2K} = Z_2 - 0.3$ for K shell (n = 1)

$Z_{2L} = Z_2 - 4.15$ for L shell (n = 2, l = 0,1)

$Z_{2M} = Z_2 - 11.25$ for M_1, M_2, and M_3 subshells (n = 3, l = 0,1)

$Z_{2M} = Z_2 - 21.15$ for M_4 and M_5 subshells (n = 3, l = 2)

The hydrogenic binding energy, $\frac{1}{2}\frac{Z_{2s}^2}{n^2}$, is reduced by a constant potential V_{2s} to match the observed binding energy U_{2s}

$$U_{2s} = \frac{1}{2}\frac{Z_{2s}^2}{n^2} - V_{2s} . \qquad \textbf{(2.2.13)}$$

Using SH wave functions to analytically represent S-subshell atomic electrons provides significant simplicity and clarity while maintaining a suitable model. The suitability of this choice of wave functions can be confirmed by comparing their generalized oscillator strengths (GOS), which are proportional to the differential cross sections, with those of competing wave functions such as Hartree-Fock, correlated, etc. Irrespective of the collision regime, differential ionization cross sections calculated with realistic correlated wave functions would be just about the same as cross sections obtained with analytically simple and yet, in this sense, very accurate wave functions of the target atom – the screened hydrogenic wave functions. Our choice of SH wave functions is well justified when differential cross sections are integrated over all energy transfers (i.e., to obtain the total ionization cross section σ_s) are considered. SH wave functions are especially well suited for a description of the inner-most shells of heavy elements [9].

To get to the heart of the matter, Eqs. (1.1.1) and (1.1.2), we provide a customary primer of collision physics. The doubly differential cross section with respect to the energy transfer *dE* and to solid scattering angle $d\Omega_k$ of the ionized electron, already integrated over momentum transfer *q*, is written as

$$\frac{d^2\sigma}{dEd\Omega_k} = \frac{(2\pi)^2}{v_1^2}\int_{q_{\min}}^{q_{\max}} \left|T_{f_i}\right|^2 qdq. \qquad \textbf{(2.2.14)}$$

where v_1 is the projectile velocity. The transition amplitude T_{f_i} from initial state ϕ_i to final state ϕ_f is

$$T_f = \left\langle \phi_f \left|V\right| \psi_i^{(+)} \right\rangle. \qquad \textbf{(2.2.15)}$$

The complete Hamiltonian is $H = H_0 + V$ where

$$H_0\phi_{i,f} = E_{i,f}\phi_{i,f'}. \qquad \textbf{(2.2.16)}$$

We cannot determine $\psi_i^{(+)}$ exactly. Therefore, we can choose H_0 and approximate $\psi_i^{(+)}$. The Born expanded transition amplitude is

$$T_{f_i} = \sum_{N=1}^{\infty} T_{f_i}^{(N)}, \qquad \textbf{(2.2.17)}$$

where

$$T_{f_i}^{(1)} = \left\langle \phi_f \left|V\right| \phi_i \right\rangle \qquad \textbf{(2.2.18)}$$

is the transition amplitude in the first Born approximation (FBA). There are two choices for H_0 which do

a) $H_0 = -\frac{1}{2M}\nabla_R^2 + H_2\left(\vec{r}_1, \vec{s}_1; \ldots; \vec{r}_{Z_2}, \vec{s}_{Z_2}\right) + \frac{Z_1 Z_2}{R}$

or do not

b) $H_0 = -\frac{1}{2M}\nabla_R^2 + H_2\left(\vec{r}_1, \vec{s}_1; ...; \vec{r}_{Z_2}, \vec{s}_{Z_2}\right)$

include the Coulomb repulsion between the nuclei of the projectile ion and target. With choice a) the incoming ion is represented by a Coulomb wave function and with choice b) by a plane wave function. Within the FBA of equation (2.2.18) and our choice of the plane wave function for the description of the projectile, one is lead to the PWBA. Owing to the orthogonality of atomic orbitals, whose antisymmetrized product designates the electronic configuration of the target atom, the PWBA transition amplitude is

$$T_{f_i}^{PWBA} = \left\langle \phi_f^{PWBA} \left| V \right| \phi_i^{PWBA} \right\rangle \qquad \textbf{(2.2.19)}$$

which with V from the third term in Eq. (2.2.2)

$$V = \frac{Z_1 Z_2}{R} - \sum_{j=1}^{Z_2} \frac{Z_1}{\left|\vec{R} - \vec{r}_j\right|} \qquad \textbf{(2.2.20)}$$

is reduced to the calculation of

$$T_{\vec{k}nlm}^{PWBA} = \frac{1}{(2\pi)^3} \iint d^3R d^3r e^{i\left(\vec{K}_i - \vec{K}_f\right)\vec{R}} \phi_k^{SH*}(\vec{r}) \frac{Z_1}{\left|\vec{R} - \vec{r}\right|} \phi_{nlm}^{SH}(\vec{r}) \qquad \textbf{(2.2.21)}$$

where $\vec{K}_i$ and $\vec{K}_f$ are the initial and final momenta of the projectile and $\vec{k}$ is the momentum of the ejected electron. Using Bethe's integral [10],

$$\int d^3R \frac{e^{i\vec{q}\vec{R}}}{\left|\vec{R} - \vec{r}\right|} = \frac{4\pi}{q^2} e^{i\vec{q}\vec{r}} \qquad \textbf{(2.2.22)}$$

$T_{\vec{k}nlm}^{PWBA}$ of (2.2.21) can be further reduced to

$$T_{\vec{k}nlm}^{PWBA} = \frac{2Z_1}{(2\pi)^2 q^2} F_{\vec{k}nlm}^{SH}(\vec{q}) \qquad \textbf{(2.2.23)}$$

where $F_{\vec{k}nlm}^{SH}(\vec{q})$ is defined by

$$F_{\vec{k}nlm}^{SH}\left(\vec{q}\right) \equiv \int d^3r\ e^{i\vec{q}\vec{r}} \phi_{\vec{k}}^{SH*}\left(\vec{r}\right) \phi_{nlm}^{SH}\left(\vec{r}\right) . \qquad \textbf{(2.2.24)}$$

Generally, literature represents ionization cross sections in terms of atomic form factors. After integration of Eq. (2.2.14) with respect to the solid angle $d\Omega_k$, but before integration over the momentum transfer *q*, the atomic form factors depend on energy transfer ΔE.

$$\left|F_{\Delta Enlm}\left(\vec{q}\right)\right|^2 = \int d\Omega_k \left|F_{\vec{k}nlm}\left(\vec{q}\right)\right|^2 . \qquad \textbf{(2.2.25)}$$

Integration of Eq. (2.2.25) over the momentum and energy transfers becomes universal in dimensionless variables. They are the dimensionless square of the momentum transfer *Q* and the dimensionless energy transfer *W* such that

$$Q = \left(qa_{2s}\right)^2 = \frac{q^2}{Z_{2s}^2} \qquad \textbf{(2.2.26)}$$

amd

$$W = \frac{\Delta E}{\frac{1}{2}Z_{2s}^2} = k^2 + \frac{1}{n^2}, \qquad \textbf{(2.2.27)}$$

where $a_{2s} = n^2 / Z_{2s}$ is the radius of an electron in the n^{th} orbit of a screened hydrogenic atom. To gain a sense of the relative speed of a collision, it is useful to scale the square of the projectile ion velocity $v_1^2 = 2E_1 / M_1$ to the square of the electron's velocity $v_{2s} = Z_{2s} / n$ in the ground state (*n* = 1) of a screened hydrogenic atom as the dimensionless η_s

$$\eta_s = \frac{2E_1}{M_1} / Z_{2s}^2 = \frac{v_1^2}{Z_{2s}^2} . \qquad \textbf{(2.2.28)}$$

For historical reasons, as these variables were introduced in Bethe [5] and Livingston and Bethe [11] to analyze just the K-shell data, both q^2 and ΔE are scaled to the ground state (with *n* =1) of screened hydrogenic atom. Furthermore, it is natural to scale the binding energy U_{2s} of Eq. (2.2.13) to the hydrogenic binding energy, $\frac{1}{2}\frac{Z_{2s}^2}{n^2}$ in terms of the dimensionless θ_s

$$\theta_s = U_{2s}\left(\frac{1}{2}\frac{Z_{2s}^2}{n^2}\right)^{-1}. \qquad \textbf{(2.2.29)}$$

With the introduction of these dimensionless universal variables the PWBA cross section in atomic units of a_0^2 for S-subshell ionization is expressed as

$$\sigma_s^{PWBA} = (2j+1)4\pi\left(\frac{Z_1}{Z_{2s}^2}\right)^2 \frac{f_s(\eta_s,\theta_s)}{\eta_s}, \qquad \textbf{(2.2.30)}$$

where

$$f_s(\eta_s,\theta_s) = \int_{W_{\min}}^{W_{\max}} dW \int_{Q_{\min}}^{Q_{\max}} \frac{dQ}{Q^2}\left|F_{W,s}(Q)\right|^2. \qquad \textbf{(2.2.31)}$$

The function $\left|F_{W,s}(Q)\right|^2$ in equation (2.2.31) is called the "form factor" and results from the transition between the bound state and final state of the electron. The integration over Q in equation (2.2.31) leads us back to the "excitation function" from Eq. (1.1.1) which we have now derived as promised. The first integral over Q in Eq. (2.2.31) gives the energy distribution of ejected electrons. The second integral over W gives the total ionization cross section for S-subshells [1].

CHAPTER 3: PROCEDURE AND PROGRESSION

3.1 Problem Revisited

Recall the excitation function described in Eq. (1.1.1)

$$I\left(\eta_s, W\right) = \int_{Q_{\min}}^{Q_{\max}} \left|F_{Ws}\left(Q\right)\right|^2 Q^{-2} dQ \quad .$$

Again, this integral equation is at the very foundation of our work. For the K shell (1s) where *n* = 1 the integrand is

$$I_{1s}(Q,k) = \frac{2^7 \exp\left(-\frac{2}{k}\tan^{-1}\left(Q-k^2+1, 2k\right)\right)}{\left(1-\exp\left(-\frac{2\pi}{k}\right)\right)\left(\left(Q-k^2+1\right)^2+4k^2\right)^3}\left(1+\frac{k^2+1}{3Q}\right) \qquad \textbf{(2.3.1)}$$

where, instead of the traditional $\left(\frac{2k}{Q-k^2+1}\right)$, *the argument of the inverse tangent function is expressed as* $\left(Q-k^2+1, 2k\right)$ *throughout this work for Mathematica to take the* $\tan^{-1}$ *in the proper quadrant.*

This is the simplest of expressions to be integrated and yet the integration has never been done analytically and is always evaluated numerically. Our initial attempts to integrate analytically by hand met the same fate. We tried to use Mathematica’s symbolic integration algorithm but as shown below it simply returns an unevaluated integral

In[84]:= I1[Q_, k_] := $\frac{2^7\,\mathrm{Exp}\left[\frac{-2}{k}\,\mathrm{ArcTan}[Q-k^2+1,\,2k]\right]}{\left(1-\mathrm{Exp}\left[-\frac{2\pi}{k}\right]\right)\left((Q-k^2+1)^2+(2)^2 k^2\right)^3} * \left(1+\frac{k^2+1}{3Q}\right)$

In[85]:= Integrate[I1[Q, k], Q]

Out[85]= $\frac{128\int \frac{e^{-\frac{2\,\mathrm{ArcTan}[1-k^2+Q,\,2k]}{k}}\left(1+\frac{1+k^2}{3Q}\right)}{\left(4k^2+(1-k^2+Q)^2\right)^3}\,dQ}{1-e^{-\frac{2\pi}{k}}}$

The crux of the problem is the Q^{-1} terms. However, as detailed below and through a good bit of trial and error we discovered a way to evaluate this type of integral analytically. In short, we distribute the first product through the second. The resulting first term will be integrable but we then focus our attention on the second term with the Q^{-1} dependence.

3.2 Specific Processes and Progressions

The integrand in Eq. (2.2.31) and Eq. (1.1.2) can be written as a product of two factors such that

$$\frac{1}{Q^2}\left|F_{W,s}(Q)\right|^2 = A_n(Q,k)\,S_{nl}(Q,k) \qquad \textbf{(2.4.1)}$$

n is the principal quantum number and note that the form of $A_n(Q,k)$ is the same for all subshells of each shell

$$A_n(Q,k) = \frac{2^7\exp\left(-\frac{2}{k}\tan^{-1}\left(Q-k^2+\frac{1}{n^2},\frac{2k}{n}\right)\right)}{n^3\left(1-\exp\left(-\frac{2\pi}{k}\right)\right)\left(\left(Q-k^2+\frac{1}{n^2}\right)^2+\left(\frac{2}{n}\right)^2 k^2\right)^{2n+1}}. \qquad \textbf{(2.4.2)}$$

The second factors, $S_{nl}(Q,k)$ in Eq. (2.4.1), different for each shell S, provided for K shell by Merzbacher and Lewis [1] and for L and M by Liu and Cipolla [3], are shown below and in Appendix A. They are polynomials in Q (defined in Eq.(2.2.26)) with indices from -1 and higher.

The coefficients are polynomials in k (related to energy transfer defined in Eq.(2.2.27)). For example, for K shell with $\{n,l\}$ = {0,1} = 1s,

$$S_{1s}\left(Q,k\right)=1+\frac{k^2+1}{3Q}. \qquad \textbf{(2.4.3)}$$

The first term of which has Q index 0 and k polynomial coefficient 1 and the second term has Q index -1 and k polynomial coefficient $\frac{k^2+1}{3}$.

For L_1 subshell {2,0} = 2s,

$$\begin{aligned}S_{2s}\left(Q,k\right)&=Q^4-\left(\frac{8}{3}+\frac{11}{3}k^2\right)Q^3+\left(\frac{41}{24}+6k^2+\frac{14}{3}k^4\right)Q^2+\\&\left(\frac{5}{48}-\frac{31}{24}k^2-\frac{10}{3}k^4-2k^6\right)Q+\left(\frac{47}{3840}-\frac{41}{120}k^4-\frac{2}{3}k^6-\frac{1}{3}k^8\right)Q^0+\\&\left(\frac{1}{768}+\frac{17}{768}k^2+\frac{7}{48}k^4+\frac{11}{24}k^6+\frac{2}{3}k^8+\frac{1}{3}k^{10}\right)Q^{-1}.\end{aligned} \qquad \textbf{(2.4.4)}$$

For $L_{2,3}$ subshells {2,1} = 2p,

$$\begin{aligned}S_{2p}\left(Q,k\right)&=\frac{9}{4}Q^3-\left(\frac{3}{4}+3k^2\right)Q^2+\left(\frac{19}{32}-\frac{3}{4}k^2-\frac{1}{2}k^4\right)Q+\\&\left(\frac{107}{960}+\frac{41}{48}k^2+\frac{113}{60}k^4+k^6\right)Q^0+\left(\frac{11}{3072}+\frac{3}{64}k^2+\frac{7}{32}k^4+\frac{5}{12}k^6+\frac{1}{4}k^8\right)Q^{-1}.\end{aligned} \qquad \textbf{(2.4.5)}$$

Formulas for the M subshells are more cumbersome. To generate $S_{3s}\left(Q,k\right), S_{3p}\left(Q,k\right)$, and $S_{3d}\left(Q,k\right)$, we use a handy matrix equation given by Liu and Cipolla [3].

$$S_{3l}\left(Q,k\right)=\frac{1}{Q}\sum_{i=0}^{i_{\max}}\sum_{j=0}^{j_{\max}}C_{ij}^{(3l)}k^{2i}Q^j \qquad \textbf{(2.4.6)}$$

Choi [7] provides the coefficients $C_{ij}^{(nl)}$. The actual values of these $C_{ij}^{(nl)}$ and calculations resulting in the $S_{3l}\left(Q,k\right)$ functions are included in Appendix A.

3.3 Problem Solution Protocol

To evaluate Eq.(1.1.2), $\int \left|F_{Ws}(Q)\right|^2 Q^{-2} dQ$, we call its integrand

$$I_{nl}(Q,k) = A_n(Q,k)\, S_{nl}(Q,k) \qquad \textbf{(2.5.1)}$$

Once $S_{nl}(Q,k)$ are defined as already listed for particular {*n*, *l*} subshells, they are multiplied by $A_n(Q,k)$ of equation (2.4.2) for the corresponding {*n*}-shell. For example for the K shell

$$I_{1s}(Q,k) = \frac{2^7 e^{-\frac{2\tan^{-1}\left(-k^2+Q+1,2k\right)}{k}}}{\left(1-e^{-\frac{2\pi}{k}}\right)\left(\left(-k^2+Q+1\right)^2+4k^2\right)^3}\left(\frac{k^2+1}{3Q}+1\right) \qquad \textbf{(2.5.2)}$$

The integral of this integrand over a definite range of Q is the excitation function Eq. (1.1.1) for the K shell. The integrations of this and similar integrands $I_{2s}(Q,k) = A_2(Q,k) * S_{2s}(Q,k)$ $I_{3s}(Q,k) = A_3(Q,k) * S_{3s}(Q,k)$ with respect to Q are extremely difficult to solve analytically. Any direct attempts were fruitless. Many attempts were made using various techniques such as; series expansions, ordinary variable replacements, etc. It was hypothesized that the root of the problem stemmed from the product of Q^{-1} and $A_n(Q,k)$. Finally, a combination of techniques was uncovered and provided analytical solutions for the integrals for all shells K through M.

The complete process for the K shell follows these steps:

- Start with Eq. (2.3.1)

$$I_{1s}(Q,k) = \frac{2^7}{\left(1-\exp\left(-\frac{2\pi}{k}\right)\right)} \frac{e^{-\frac{2\tan^{-1}\left(-k^2+Q+1,2k\right)}{k}}}{\left(\left(-k^2+Q+1\right)^2+4k^2\right)^3}\left(1+\frac{k^2+1}{3Q}\right) \qquad \textbf{(2.5.3)}$$

- For clarity and computationally less overhead remove the factor

$$\frac{2^7}{\left(1-\exp\left(-\frac{2\pi}{k}\right)\right)}$$

since it is constant with respect to Q.

- Then distribute $I_{1s}(Q,k)$ into two terms

$$I_{1s}\left(Q,k\right)=\frac{e^{-\frac{2\tan^{-1}(-k^2+Q+1,2k)}{k}}}{((-k^2+Q+1)^2+4k^2)^3}+\frac{e^{-\frac{2\tan^{-1}(-k^2+Q+1,2k)}{k}}}{((-k^2+Q+1)^2+4k^2)^3}\left(\frac{1+k^2}{3Q}\right) \quad \textbf{(2.5.4)}$$

The first term is directly integrable.

- Integrate the *first term* in (2.5.4) over Q

$$I1ag(Q,k)=\int\frac{e^{-\frac{2\tan^{-1}(-k^2+Q+1,2k)}{k}}}{((-k^2+Q+1)^2+4k^2)^3}dQ$$

$$=\frac{e^{-\frac{2\tan^{-1}\left(-k^2+Q+1,2k\right)}{k}}}{128\left(4k^2+1\right)}\left(\frac{32\left(-k^2+Q+2\right)}{\left(\left(-k^2+Q+1\right)^2+4k^2\right)^2}+\frac{12\left(-k^2+Q+3\right)}{\left(k^2+1\right)\left(\left(-k^2+Q+1\right)^2+4k^2\right)}+\frac{3}{k^2+1}\right) \quad \textbf{(2.5.5)}$$

This is the first part of our solution. Set it aside as to combine it with the following parts later. If we attempt to symbolically integrate the second term of (2.5.4) *Mathematica will simply return the expression unevaluated. Therefore, use the following process to challenge the second terms faulty integrability.*

- Decompose the second term inverse polynomial factor into its partial fraction equivalent.

$$\frac{(k^2+1)}{3}e^{-\frac{2\tan^{-1}\left(-k^2+Q+1,2k\right)}{k}}\frac{1}{Q\left(\left(-k^2+Q+1\right)^2+4k^2\right)^3}$$

$$\frac{\left(k^2+1\right)}{3}e^{-\frac{2\tan^{-1}\left(-k^2+Q+1,2k\right)}{k}}\left(\begin{array}{l}\frac{1}{\left(k^2+1\right)^6 Q}+\frac{2k^2-Q-2}{\left(k^2+1\right)^6\left(k^4-2k^2Q+2k^2+Q^2+2Q+1\right)}+\\ \frac{2k^2-Q-2}{\left(k^2+1\right)^4\left(k^4-2k^2Q+2k^2+Q^2+2Q+1\right)^2}+\\ \frac{2k^2-Q-2}{\left(k^2+1\right)^2\left(k^4-2k^2Q+2k^2+Q^2+2Q+1\right)^3}\end{array}\right) \quad \textbf{(2.5.6)}$$

The middle two terms of result are directly integrable.

- Let the middle two terms of equation (2.5.6) be

$$I1ba\left(Q,k\right)=\frac{(k^2+1)}{3}e^{-\frac{2\tan^{-1}\left(-k^2+Q+1,2k\right)}{k}}\left(\begin{array}{l}\frac{2k^2-Q-2}{\left(k^2+1\right)^4\left(k^4-2k^2Q+2k^2+Q^2+2Q+1\right)^2}+\\ \frac{2k^2-Q-2}{\left(k^2+1\right)^2\left(k^4-2k^2Q+2k^2+Q^2+2Q+1\right)^3}\end{array}\right)$$

- Integrate *I1ba (Q, k)*

$$I1bg\left(Q,k\right)=\int I1ba\left(Q,k\right)dQ=$$

$$\frac{-\left(e^{-\frac{2\tan^{-1}\left(-k^2+Q+1,2k\right)}{k}}\left(\begin{array}{l}-3k^6-16k^4+53k^2+\frac{32\left(k^2+1\right)^3\left(k^4-k^2(Q+8)+2Q+3\right)}{\left(k^4-2k^2(Q-1)+(Q+1)^2\right)^2}+\\ \frac{4\left(3k^8+k^6(7-3Q)-k^4(16Q+165)+k^2(53Q+61)+18Q+38\right)}{k^4-2k^2(Q-1)+(Q+1)^2}+18\end{array}\right)\right)}{(384(k^2+1)^3(4k^4+5k^2+1))} \quad \textbf{(2.5.7)}$$

Now there are three pieces to our collective solution since together they are integrable. However, the outer two terms of result (2.5.6) *are left to deal with.*

- Distribute the outer two terms in (2.5.6) and integrate term by term as two functions.

$$I1ar1(Q,k)=\frac{e^{-\frac{2\tan^{-1}\left(-k^2+Q+1,2k\right)}{k}}}{3\left(k^2+1\right)^5 Q} \quad \textbf{(2.5.8)}$$

$$I1ar2(Q,k)=\frac{e^{-\frac{2\tan^{-1}\left(-k^2+Q+1,2k\right)}{k}}\left(2k^2-Q-2\right)}{3\left(k^2+1\right)^5\left(k^4-2k^2Q+2k^2+Q^2+2Q+1\right)} \quad \textbf{(2.5.9)}$$

Mathematica cannot directly integrate these two expressions. Of the two integrands I1ar2(Q,k) can be analytically integrated by substitution.

- The variable replacement process will be repeated in many places so a subroutine is developed for the task. It is called SubForInt[input, variable, substituting variable, its definition]

  The code and usage examples are included in Appendix B

- Go back to *I1ar2(Q,k)* from equation (2.5.9) and do the following substitutions:

  let $x=-\frac{2\tan^{-1}(-k^2+Q+1,2k)}{k}$, then

$$I1ar4(x,k)=\frac{e^x\left(k^2+2k\cot\left(\frac{kx}{2}\right)-1\right)}{12\left(k^2+1\right)^5}$$

The integrand in this form is now directly integrable.

- Integrate *I1ar4(x,k)*

$$\int I1ar4(x,k)\,dx=$$

$$\frac{e^x\left((k-i)\left(-2ik\,{}_2F_1\left(1,-\frac{i}{k};\frac{k-i}{k};e^{ikx}\right)+k^2-1\right)-2ke^{ikx}\,{}_2F_1\left(1,\frac{k-i}{k};2-\frac{i}{k};e^{ikx}\right)\right)}{12(k-i)^6(k+i)^5} \quad \textbf{(2.5.10)}$$

where the symbol ${}_2F_1$ *stands for Hypergeometric functions.*

- Now reverse the substitution and return to the variable Q

$$I1ar6(Q,k)=\frac{e^{-\frac{2\tan^{-1}\left(-k^2+Q+1,2k\right)}{k}}\left((k-i)\left(-2ik\,{}_2F_1\left(1,-\frac{i}{k};\frac{k-i}{k};e^{-2i\tan^{-1}\left(-k^2+Q+1,2k\right)}\right)+k^2-1\right)-2ke^{-2i\tan^{-1}\left(-k^2+Q+1,2k\right)}\,{}_2F_1\left(1,\frac{k-i}{k};2-\frac{i}{k};e^{-2i\tan^{-1}\left(-k^2+Q+1,2k\right)}\right)\right)}{12(k-i)^6(k+i)^5} \quad \textbf{(2.5.11)}$$

Again put this partial solution aside to combine with the previous partial solutions I1ag(Q,k) and I1bg(Q,k).

- With this last result, the only remaining piece and most difficult, is the integration of the function *I1ar1(Q,k)* of equation (2.5.8)

$$I1ar1(Q,k)=\frac{\mathrm{e}^{-\frac{2\tan^{-1}(-k^2+Q+1,2k)}{k}}}{3(k^2+1)^5 Q} \quad \textbf{(2.5.12)}$$

- To integrate this and similar functions *Mathematica* code is developed to permute factors of an integrand into combinational pairs that can be *attempted* to integrate by parts via:

$$\int udv=uv-\int vdu$$

The code is in Appendix B. Suffice to say for now that the usage format for IntegrateParts[ ] is:

```
IntegrateParts[factor1, factor2, factor3, factor4,
 integration variable]
```

one can input from two to four factors into IntegrateParts[ ].

- Use the code and defined function to integrate *I1ar1(Q,k)* from (2.5.8); the input/output for this calculation can be found in Appendix B

$$\int \frac{e^{-\frac{2\tan^{-1}\left(-k^2+Q+1,2k\right)}{k}}}{Q} dQ = -4\int \frac{e^{-\frac{2\tan^{-1}\left(-k^2+Q+1,2k\right)}{k}} \log(Q)}{\left(-k^2+Q+1\right)^2+4k^2} dQ + e^{-\frac{2\tan^{-1}\left(-k^2+Q+1,2k\right)}{k}} \log(Q) \quad \textbf{(2.5.13)}$$

the second is ready to be added to the collective solution

$$I1ag7\left(Q,k\right) = \frac{1}{3\left(1+k^2\right)^5} e^{-\frac{2\tan^{-1}\left(-k^2+Q+1,2k\right)}{k}} \log(Q) \qquad \textbf{(2.5.14)}$$

- Now work with the integral term from (2.5.13). To handle this difficult expression integrate by substitution. To do so utilize the SubForInt[] function again.

- Let $x = -\frac{2\tan^{-1}\left(-k^2+Q+1,2k\right)}{k}$

  Then $-4\frac{e^{-\frac{2\tan^{-1}\left(-k^2+Q+1,2k\right)}{k}} \log(Q)}{\left(-k^2+Q+1\right)^2+4k^2} = -e^x \log\left(k^2 - 2k\cot\left(\frac{kx}{2}\right) - 1\right)$

- Next let $\xi = \frac{kx}{2}$

  Then

$$-e^x \log\left(k^2 - 2k\cot\left(\frac{kx}{2}\right) - 1\right) = -\frac{2e^{\frac{2\xi}{k}} \log(k^2 - 2k\cot(\xi) - 1)}{k} \qquad \textbf{(2.5.15)}$$

Result (2.5.15) i*s still not in an integrable form. However, the following derivation will get it closer:*

$$
-\frac{2e^{\frac{2\xi}{k}}\log\left(k^2-2k\cot(\xi)-1\right)}{k}=
$$

$$
-\frac{2e^{\frac{2\xi}{k}}\log\left(\frac{-\sin(\xi)+k^2\sin(\xi)-2k\cos(\xi)}{\sin(\xi)}\right)}{k}= \qquad \textbf{(2.5.16)}
$$

$$
-\frac{2}{k}e^{\frac{2\xi}{k}}\log\left(-\sin(\xi)+k^2\sin(\xi)-2k\cos(\xi)\right)+-\frac{2}{k}e^{\frac{2\xi}{k}}\log\left(\sin(\xi)\right)
$$

This result shows two terms to integrate the second term of result (2.5.16) *is directly integrable.*

- Integrate the second term of result (2.5.16) directly to get

$$
\frac{2}{3k(k^2+1)^5}\int e^{\frac{2\xi}{k}}\log(\sin(\xi))d\xi=
$$

$$
\frac{e^{\frac{2\xi}{k}}\left(ik\,{}_2F_1\left(1,-\frac{i}{k};\frac{k-i}{k};e^{2i\xi}\right)+\frac{ke^{2i\xi}\,{}_2F_1\left(1,\frac{k-i}{k};2-\frac{i}{k};e^{2i\xi}\right)}{k-i}+2\log(\sin(\xi))\right)}{6\left(k^2+1\right)^5} \qquad \textbf{(2.5.17)}
$$

- Reverse the substitutions. Result (2.5.17) becomes another part of our collective solution

$$
I1ag9(Q,k)=
$$

$$
\frac{e^{-\frac{2\tan^{-1}\left(-k^2+Q+1,2k\right)}{k}}\left(\begin{array}{l} ik\,{}_2F_1\left(1,-\frac{i}{k};\frac{k-i}{k};e^{-2i\tan^{-1}\left(-k^2+Q+1,2k\right)}\right)+ \\ \frac{ke^{-2i\tan^{-1}\left(-k^2+Q+1,2k\right)}\,{}_2F_1\left(1,\frac{k-i}{k};2-\frac{i}{k};e^{-2i\tan^{-1}\left(-k^2+Q+1,2k\right)}\right)}{k-i}+ \\ 2\log\left(-\sin\left(\tan^{-1}\left(-k^2+Q+1,2k\right)\right)\right) \end{array}\right)}{6\left(k^2+1\right)^5} \qquad \textbf{(2.5.18)}
$$

This is the result of integrating the second term of result (2.5.16) *only.*

- Next integrate by parts the first term of result (2.5.16) via the IntegrateParts[] function. The *Mathematica* input/output for this calculation can be found in Appendix B.

$$\int -\frac{2e^{\frac{2\xi}{k}}\log\left(\left(k^2-1\right)\sin(\xi)-2k\cos(\xi)\right)}{k}d\xi = \int \frac{e^{\frac{2\xi}{k}}\left(\left(k^2-1\right)\cos(\xi)+2k\sin(\xi)\right)}{\left(k^2-1\right)\sin(\xi)-2k\cos(\xi)}d\xi - e^{\frac{2\xi}{k}}\log\left(\left(k^2-1\right)\sin(\xi)-2k\cos(\xi)\right) \qquad \textbf{(2.5.19)}$$

and once again, there is one term to be added to the collective solution and yet another integral to evaluate.

- Reverse the substitutions in the second term of result (2.5.19).

$$I1ag10\left(Q,k\right) = -\frac{e^{-\frac{2\tan^{-1}\left(-k^2+Q+1,2k\right)}{k}}\log\left(-\frac{2kQ}{\sqrt{k^4-2k^2(Q-1)+(Q+1)^2}}\right)}{3\left(k^2+1\right)^5} \qquad (2.5.20)$$

- Manipulate the integrand of first term of result (2.5.19) to obtain an integrable form. Divide numerator and denominator of the integrand by k^2-1,

$$\frac{e^{\frac{2\xi}{k}}\left(\left(k^2-1\right)\cos(\xi)+2k\sin(\xi)\right)}{\left(k^2-1\right)\sin(\xi)-2k\cos(\xi)}$$

by k^2-1,

$$\frac{e^{\frac{2\xi}{k}}\left(\frac{2k\sin(\xi)}{k^2-1}+\cos(\xi)\right)}{\sin(\xi)-\frac{2k\cos(\xi)}{k^2-1}},$$

Let $\phi = \tan^{-1}(k^2-1,2k)$ so that $\tan\left(\phi\right)=\frac{2k}{k^2-1}$ then:

$$\frac{e^{\frac{2\xi}{k}}(\cos(\xi)+\tan(\phi)\sin(\xi))}{-\tan(\phi)\cos(\xi)+\sin(\xi)}=$$

$$\frac{e^{\frac{2\xi}{k}}(\cos(\phi)\cos(\xi)+\sin(\phi)\sin(\xi))}{\sin(\phi)\cos(\xi)-\cos(\phi)\sin(\xi)}=$$

$$\frac{e^{\frac{2\xi}{k}}\cos(\phi-\xi)}{\sin(\phi-\xi)}=$$

$$e^{\frac{2\xi}{k}}\cot(\phi-\xi);\text{let } y=\phi-\xi,\text{then}$$

$$=e^{\frac{2(\phi-y)}{k}}\cot(y) \qquad \textbf{(2.5.21)}$$

which is now in a form that is analytically integrable and results Hypergeometric functions that are later converted to Incomplete Beta Functions.

- Integrate result (2.5.21)

$$\int e^{\frac{2(\phi-y)}{k}}\cot(y)dy=$$
$$\frac{1}{2}i\Gamma\left(\frac{i+k}{k}\right)\left(k\,{}_2\tilde{F}_1\left(1,\frac{i}{k};\frac{i+k}{k};e^{2iy}\right)+ie^{2iy}\,{}_2\tilde{F}_1\left(1,\frac{i+k}{k};2+\frac{i}{k};e^{2iy}\right)\right)e^{-\frac{2(y-\phi)}{k}} \qquad \textbf{(2.5.22)}$$

Here Γ *is the Gamma function and* ${}_2\tilde{F}_1$ *is the Regularized Hypergeometric Function*

- Reverse the substitutions to return to variables (Q,k),

$$I1ag11(Q,k)=$$
$$\frac{1}{6\left(k^2+1\right)^5}i\Gamma\left(\frac{k+i}{k}\right)e^{-\frac{2\tan^{-1}\left(-k^2+Q+1,2k\right)}{k}} \qquad \textbf{(2.5.23)}$$
$$\left(\begin{array}{l} k\,{}_2\tilde{F}_1\left(1,\frac{i}{k};\frac{k+i}{k};\exp\left(2i\left(\tan^{-1}\left(k^2-1,2k\right)+\tan^{-1}\left(-k^2+Q+1,2k\right)\right)\right)\right)+ \\ i\exp\left(2i\left(\tan^{-1}\left(-k^2+Q+1,2k\right)+\tan^{-1}\left(k^2-1,2k\right)\right)\right) \\ {}_2\tilde{F}_1\left(1,\frac{k+i}{k};2+\frac{i}{k};\exp\left(2i\left(\tan^{-1}\left(k^2-1,2k\right)+\tan^{-1}\left(-k^2+Q+1,2k\right)\right)\right)\right) \end{array}\right)$$

With that we have the final part to our collective solution.

- Add all partial solutions.

$$IQTest(Q,k) =$$
$$I1ag(Q,k) + I1bg(Q,k) + I1ag6(Q,k) + I1ag7(Q,k) + I1ag9(Q,k) + I1ag10(Q,k) + I1ag11(Q,k)$$

$$\frac{1}{384\left(k^2+1\right)^5} e^{-\frac{2\tan^{-1}\left(-k^2+Q+1,2k\right)}{k}}$$
$$((128(k^4-2k^2(Q-1)+(Q+1)^2)^2\log(-\sin(\tan^{-1}(-k^2+Q+1,2k)))+$$
$$128(k^4-2k^2(Q-1)+(Q+1)^2)^2\log(Q)-$$
$$128(k^4-2k^2(Q-1)+(Q+1)^2)^2\log\left(-\frac{2kQ}{\sqrt{k^4-2k^2(Q-1)+(Q+1)^2}}\right)+$$
$$\left(3k^6+13k^4+33k^2-41\right)Q^4-4\left(3k^8+7k^6+7k^4-75k^2+50\right)Q^3+$$
$$\left(k^2+1\right)^3\left(3k^8+4k^6+10k^4+276k^2+11\right)+$$
$$2\left(9k^{10}+15k^8+34k^6+6k^4+309k^2-181\right)Q^2-$$
$$4\left(k^2+1\right)\left(3k^{10}+4k^8+10k^6+20k^4-181k^2+64\right)Q\Big)/$$
$$\left(k^4-2k^2(Q-1)+(Q+1)^2\right)^2+64i\Gamma\left(\frac{i+k}{k}\right)$$
$$\left(k\,{}_2\tilde{F}_1\left(1,\frac{i}{k};\frac{i+k}{k};\exp\left(2i\left(\tan^{-1}\left(k^2-1,2k\right)+\tan^{-1}\left(-k^2+Q+1,2k\right)\right)\right)\right)+\right.$$
$$i\exp\left(2i\left(\tan^{-1}\left(-k^2+Q+1,2k\right)+\tan^{-1}\left(k^2-1,2k\right)\right)\right) \qquad \textbf{(2.5.24)}$$
$$\left.{}_2\tilde{F}_1\left(1,\frac{i+k}{k};2+\frac{i}{k};\exp\left(2i\left(\tan^{-1}\left(k^2-1,2k\right)+\tan^{-1}\left(-k^2+Q+1,2k\right)\right)\right)\right)\right)\Bigg).$$

After the restoration of the prefactor $2^7/\left(1-e^{\frac{-2\pi}{k}}\right)$ the function $IQTest(Q,k)$ is the result of the indefinite integral of $I_{1s}(Q,k)$ in equation (2.3.1). That is, the evaluation of $\int\left|F_{Ws}(Q)\right|^2 Q^{-2}dQ$ for the 1s subshell. With any value of *k*, one can evaluate this result on any range of *Q*.

For example, with $k = 2$ we take $\left(10^{-4},10^4\right)$ for limits over *Q:*

$$\frac{2^7}{1-e^{\frac{-2\pi}{2}}}\left(IQTest\left(10^4,2\right)-IQTest\left(10^{-4},2\right)\right)=0.0661398+1.62542\times10^{-15}i.$$

We compare this solution to *Mathematica's* numerical solution. In this particular case.

```
NIntegrate[2^7/(1 - Exp[-2π/2]) * I1[Q, 2], {Q, 10^-4, 10^4}]
```

```
0.0661398
```

.

The result is exactly the same as the real part of our evaluation above. Its miniscule imaginary part is inherent in such a calculation; the absolute value is exactly 0.0661398. In this manner, our analytical solution can be tested against the numerical solution for any value of k and over any interval of Q.

At this point, it is important to note that this long and complicated procedure is for the **K-Shell** evaluation only. We still needed to find solutions to L and M shell integrals as well.

3.4 Generic Integrals Method

We realized that throughout the shells and subshells there would be integrands of the form

$$I_{nl}\left(Q,k\right)_p = A_n\left(Q,k\right)S_{nl}(Q,k)_p = \left(\frac{e^{(x_n)}}{\left(d_n\right)^{2n+1}}C_p\left(k\right)Q^{p-2}\right) \qquad \textbf{(2.6.1)}$$

where each $S_{nl}\left(Q,k\right)_p$ represents one term of the function $S_{nl}\left(Q,k\right)$ and $p=1,2,3,...,p_{\max}$ is the term number.

$$x_n = -\frac{2}{k}\tan^{-1}\left[Q-k^2+\frac{1}{n^2},\frac{2k}{n}\right] \qquad \textbf{(2.6.2)}$$

and

$$d_n = \left(Q-k^2+\frac{1}{n^2}\right)^2+\left(\frac{2}{n}\right)^2 k^2 \qquad \textbf{(2.6.3)}$$

and $C_p(k)$ are constants in *k* which we will associated with each term $S_{nl}(Q,k)_p$. We wish to determine a “generic integral” for each subshell {*n*, *l*} and term number *p*. Then we can sum those evaluated integrals for the solution of the entire state {*n*,*l*}.

$$\begin{aligned} IQ_{nl}(Q,k) &= \int A_n(Q,k)\sum_{p=1}^{p_{\max}} S_{nl}(Q,k)_p dQ = \int \frac{e^{(x_n)}}{(d_n)^{2n+1}}\sum_{p=1}^{p_{\max}}\left(C_p(k)Q^{p-2}\right)dQ \\ &= \sum_{p=1}^{p_{\max}}\int A_n(Q,k)S_{nl}(Q,k)_p\, dQ = \sum_{p=1}^{p_{\max}} C_p(k)\int \frac{e^{(x_n)}}{(d_n)^{2n+1}}Q^{p-2}dQ \end{aligned} \quad \textbf{(2.6.4)}$$

For example the K-shell integrand $A_1(Q,k)S_{1s}(Q,k)$ was

$$\frac{\mathrm{e}^{-\frac{2\tan^{-1}(-k^2+Q+1,2k)}{k}}}{((-k^2+Q+1)^2+4k^2)^3}+\frac{\mathrm{e}^{-\frac{2\tan^{-1}(-k^2+Q+1,2k)}{k}}}{((-k^2+Q+1)^2+4k^2)^3}\left(\frac{1+k^2}{3Q}\right)$$

which in generic form would be

$$\frac{e^{x_1}}{d_1^3}Q^0+\frac{\left(1+k^2\right)}{3}\frac{e^{x_1}}{d_1^3}Q^{-1}$$

and the integration of which can be represented by

$$\begin{aligned} IQ_{1s}(Q,k) &= \sum_{p=1}^{2}\int A_2(Q,k)S_{1s}(Q,k)_p\, dQ \\ &= \sum_{p=1}^{2} C_p(k)\int \frac{e^{(x_1)}}{(d_1)^3}Q^{p-2}dQ \\ &= C_1(k)\int \frac{e^{(x_1)}}{(d_1)^3}Q^{-1}dQ + C_2(k)\int \frac{e^{(x_1)}}{(d_1)^3}Q^{0}dQ \end{aligned}$$

In this case, $C_2(k)=1$ and $C_1(k)=\left(1+k^2\right)/3$. As mentioned in earlier we found that the Q^{-1} generic integrals were the "tricky" ones resulting in hypergeometric functions and/or incomplete beta functions and required the use of the procedure outlined in Section 3.3 above. A full listing of the “generic integrals” can be found in APPENDIX C..

With these generic integrals in hand we wrote *Mathematica* code that for a given $\{n,l,j\}$ selects the proper product $A_n(Q,k)\,S_{nl}(Q,k)_p$, term by term pulling the associated generic integral, and summing those selected generic integrals. Output is the solution $IQ\left[Q,k,\{n,l,j\}\right]$ or more concisely $IQ_{nl}(Q,k)$ to the corresponding integral Eq.(1.1.2). For instance to generate the solution for K-shell $IQ\left[Q,k,\{1,0,0\}\right]$ the code would automatically use the generic integrals $gi10(Q,k)$ and $gi1i1(Q,k)$ such that,

$$I_{1s}(Q,k)=\frac{\mathrm{e}^{-\frac{2\tan^{-1}(-k^2+Q+1,2k)}{k}}}{((-k^2+Q+1)^2+4k^2)^3}+\frac{\mathrm{e}^{-\frac{2\tan^{-1}(-k^2+Q+1,2k)}{k}}}{((-k^2+Q+1)^2+4k^2)^3}\left(\frac{1+k^2}{3Q}\right)$$

$$\begin{aligned}IQ_{1s}(Q,k)&=\int I_{1s}(Q,k)dQ\\&=\int\frac{e^{x_1}}{d_1^3}Q^0+\frac{\left(1+k^2\right)}{3}\frac{e^{x_1}}{d_1^3}Q^{-1}dQ\\&=gi10(Q,k)+\frac{\left(1+k^2\right)}{3}gi1i1(Q,k)\end{aligned}$$

This again gives us the solution to Eq. (1.1.2), albeit in a much less intensive manner. The generated $IQ_{nl}(Q,k)$ can be multiplied by the proper pre-factors (those stripped earlier for clarity) and numerically integrated over *k* (or the scaled variable of integration *W*) to get the total cross sections as defined in Eq.(2.2.30) and Eq. (2.2.31).

Later each individual $IQ\left[Q,k,\{n,l,j\}\right]$ would be "compacted" into a more transparent form. That is, they are "compacted" into a clear polynomial in *Q* (with coefficient polynomials in *k*) multiplied by the exponential factor. A full listing of the resulting $IQ\left[Q,W,\{n,l,j\}\right]$ can be found in Appendix D, where $W=k^2+1/n^2$.

3.5 Comparisons and Verification

To further determine the validity of this method we verify the values of f_s from Merzbacher, Choi, and Khandelwal [2] and [12]. In these works values of $f_s(\eta_s, \theta_s)$ are tabulated for K and L shells, over a range of η's (0.005 to 10.0) and a range of θ's (0.64 to 0.95, or 0.24 to 0.78 in the revised paper [12]). The revised work corrects the error of [2] for the $S_{2l}(Q,k)$ functions for the L shell. We used the above-mentioned "Generic Integrals" and associated *Mathematica* code to reproduce these tables. That is, the tables for the K shell in [2] paper and the tables for the L shells in [12].

Comparative results are outstanding and typically within .02% of the published data. We find a larger divergence corresponding to larger values of θ_s and at smaller values of η_s (low energy). Samples of the comparative results are shown in the following figures.

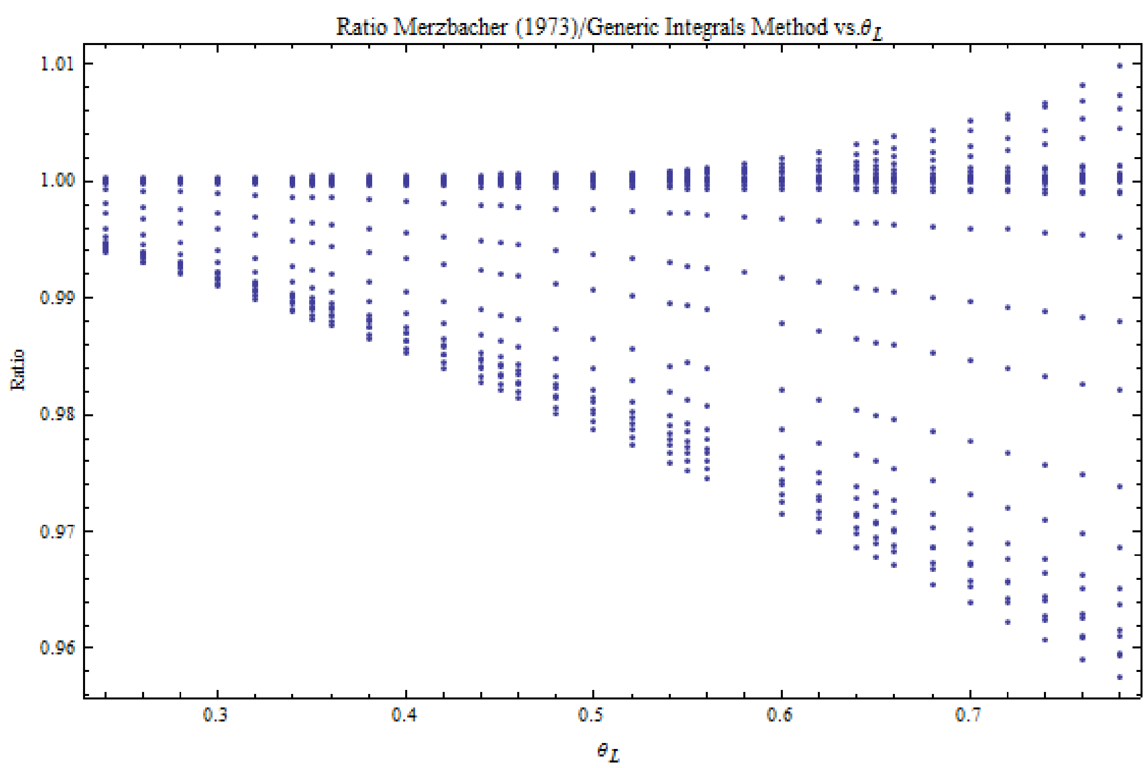

Figure 1. Merzbacher et. al [12]/Generic Integrals Method vs θ_L for L_1 Shell

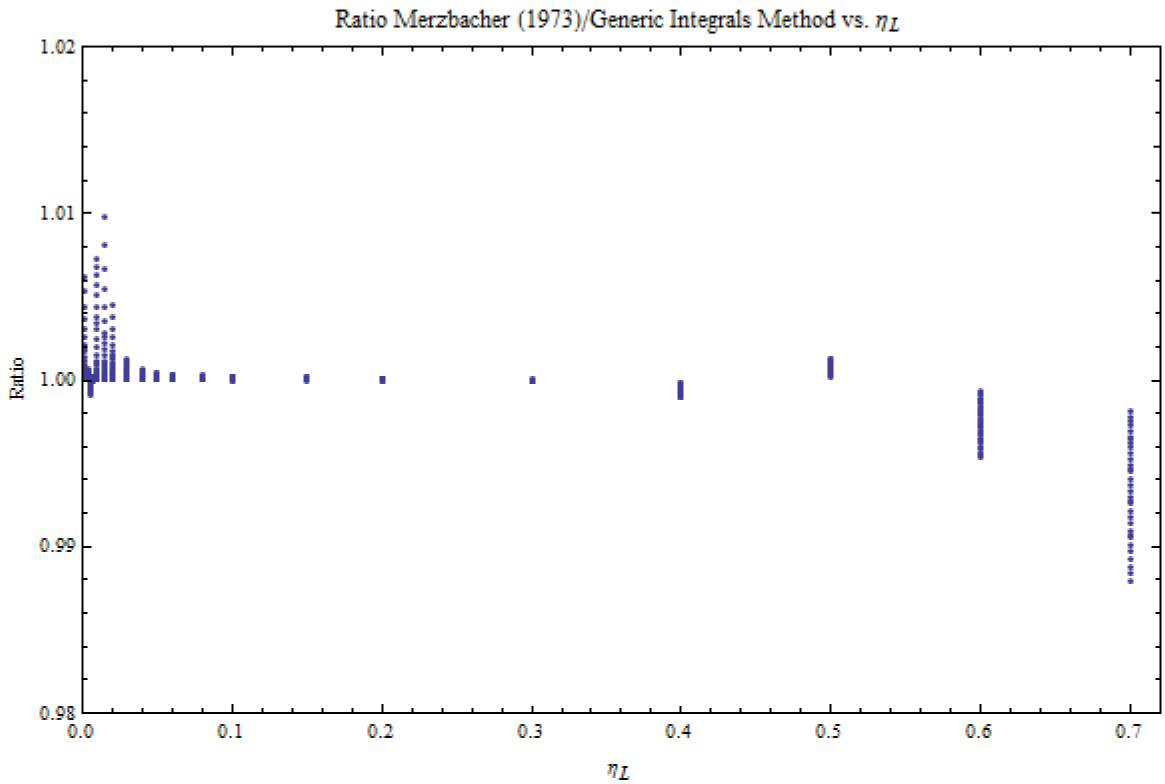

Figure 2. Merzbacher et. al [2]/Generic Integrals Method vs η_L for L_1 Shell.

Liu and Cipolla [3] provide for exact limits of Q and C++ code (ISICS) that calculates ionization and x-ray production cross sections using the so-called ECPSSR theory [13]. In their work (and in the code) they compare the PWBA cross sections to the ECPSSR theory. We can run their program and extract the PWBA cross sections for various elements. Then use the extracted data for comparison with cross sections calculated in our code.

This code was written utilizing the afore-mentioned generic integrals method that given $M_1, M_2, Z_1, Z_2, E_1(\min\ to\ \max), U_{2s}$ and $\{n, l, j\}$ will calculate cross sections in the scaled values of Liu and Cipolla.

Usage for program the ModelCS[ ]:

ModelCS[$M_1, M_2, Z_1, Z_2, E_{1\min}, E_{1\max}, inc., List[U_{2s}], List[\{n,l,j\}]]$: *where* $E_{1\min}$ and $E_{1\max}$ *give the range of energies we wish to calculate and inc is the step by which we increase the energy variable. All other variables have been previously defined. However,* $List[U_{2s}]$ *means a list of binding energies associated with a list of quantum triples,* $List[\{n,l,j\}]$.

A sample of results directly from *Mathematica* output:

H on Au:

ModelCS$\left[\mathbf{1.00797, 196.967, 1, 79, 1, 1, .01,}\right.$
$\{\{\mathbf{8.0725\,10^4}\}, \{\mathbf{1.4353\,10^4}\}, \{\mathbf{1.3734\,10^4}\}, \{\mathbf{1.1919\,10^4}\}, \{\mathbf{3.4249\,10^3}\}, \{\mathbf{3.1478\,10^3}\}, \{\mathbf{2.7430\,10^3}\},$
$\{\mathbf{2.2911\,10^3}\}, \{\mathbf{2.2057\,10^3}\}\}, \{\{\mathbf{1, 0, \frac{1}{2}}\}, \{\mathbf{2, 0, \frac{1}{2}}\}, \{\mathbf{2, 1, \frac{1}{2}}\}, \{\mathbf{2, 1, \frac{3}{2}}\}, \{\mathbf{3, 0, \frac{1}{2}}\},$
$\left.\{\mathbf{3, 1, \frac{1}{2}}\}, \{\mathbf{3, 1, \frac{3}{2}}\}, \{\mathbf{3, 2, \frac{3}{2}}\}, \{\mathbf{3, 2, \frac{5}{2}}\}\}\right]$

$\left\{\left\{1, 0, \frac{1}{2}\right\}, \left\{2, 0, \frac{1}{2}\right\}, \left\{2, 1, \frac{1}{2}\right\}, \left\{2, 1, \frac{3}{2}\right\}, \left\{3, 0, \frac{1}{2}\right\}, \left\{3, 1, \frac{1}{2}\right\}, \left\{3, 1, \frac{3}{2}\right\}, \left\{3, 2, \frac{3}{2}\right\}, \left\{3, 2, \frac{5}{2}\right\}\right\}$

{80725., 14353., 13734., 11919., 3424.9, 3147.8, 2743., 2291.1, 2205.7}

	n	l	j	E1 (MeV)	U2s (eV)	σs (barn)
Cross Section Table	1	0	$\frac{1}{2}$	1	80725.	0.0000913192
	2	0	$\frac{1}{2}$	1	14353.	1.61957
	2	1	$\frac{1}{2}$	1	13734.	3.353
	2	1	$\frac{3}{2}$	1	11919.	16.0589
	3	0	$\frac{1}{2}$	1	3424.9	1089.44
	3	1	$\frac{1}{2}$	1	3147.8	1707.07
	3	1	$\frac{3}{2}$	1	2743.	5697.55
	3	2	$\frac{3}{2}$	1	2291.1	9107.45
	3	2	$\frac{5}{2}$	1	2205.7	15259.2

Figure 3. Sample output from ModelCS program is summarized in Table 1.

Table 1. Summary of input and output in the ModelCS calculation of K, L, and M shell ionization cross sections of gold by 1 MeV protons

Subshell	$\{n,l,j\}$	E_1 (MeV)	U_{2s} (eV)	σ_s (barn)
K	{1,0,1/2}	1	8.0725 x 10^4	9.13192 x 10^{-5}
L_1	{2,0,1/2}	1	1.4353 x 10^4	1.61957
L_2	{2,1,1/2}	1	1.3734 x 10^4	3.35300
L_3	{2,1,3/2}	1	1.1919 x 10^4	1.60589 x 10^1
M_1	{3,0,1/2}	1	3.4249 x 10^3	1.08944 x 10^3
M_2	{3,1,1/2}	1	3.1478 x 10^3	1.70707 x 10^3
M_3	{3,1,3/2}	1	2.7430 x 10^3	5.69755 x 10^3
M_4	{3,2,3/2}	1	2.2911 x 10^3	9.10745 x 10^3
M_5	{3,2,5/2}	1	2.2057 x 10^3	1.52592 x 10^4

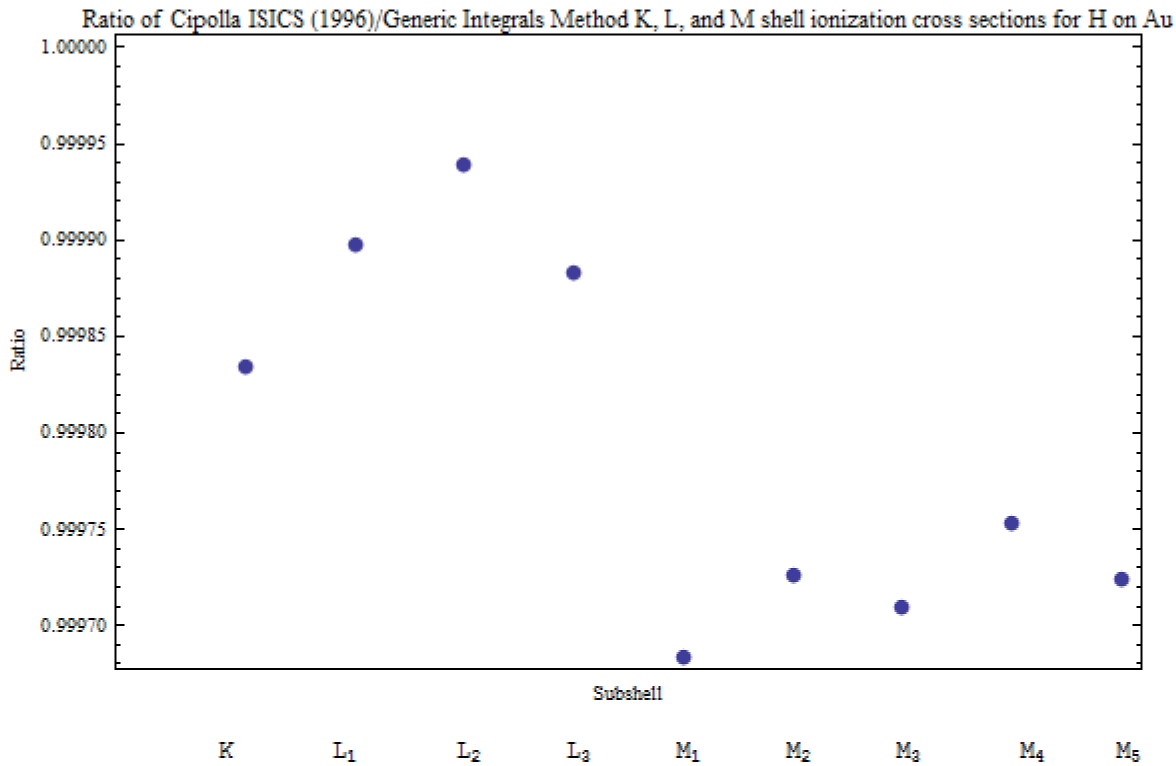

Figure 4. Ratio of this Cipolla ISICS PWBA [3]/Generic Integrals Method ionization cross sections for 1 MeV Protons on Gold (Z_2 = 79)

Table 2. Summary of K, L, and M shell ionization cross sections of nickel by 1 MeV protons

Subshell	$\{n, l, j\}$	E_1 (MeV)	U_{2s} (eV)	σ_s (barn)
K	{1,0,1/2}	1	8332.8	31.6614
L_1	{2,0,1/2}	1	1008.1	64522.9
L_2	{2,1,1/2}	1	871.9	74336.1
L_3	{2,1,3/2}	1	854.9	154831
M_1	{3,0,1/2}	1	111.8	3.30484×10^6
M_2	{3,1,1/2}	1	68.1	8.32143×10^6
M_3	{3,1,3/2}	1	68.1	1.66429×10^7
M_4	{3,2,3/2}	1	3.6	3.92946×10^9
M_5	{3,2,5/2}	1	3.6	5.89419×10^9

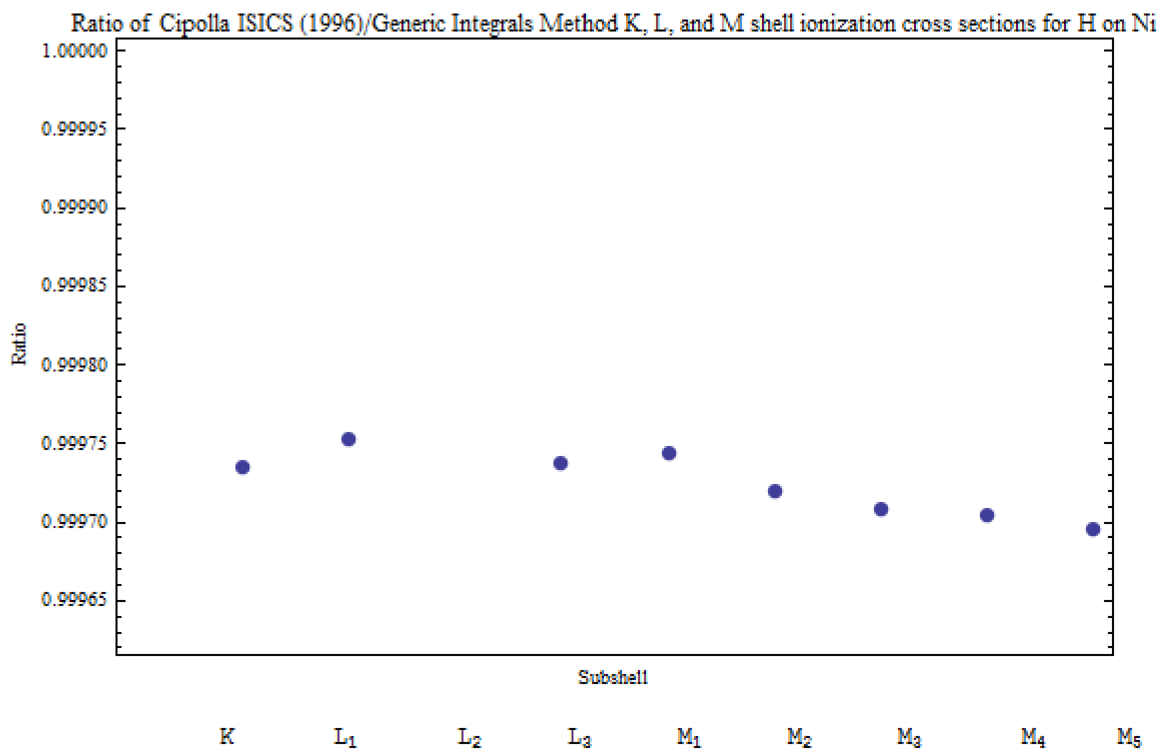

Figure 5. Ratio of this Cipolla ISICS PWBA [3]/Generic Integrals Method ionization cross sections for 1MeV Protons on Nickel (Z_2 = 28)

Table 3. Summary of K, L, and M shell ionization cross sections of germanium by 1 MeV protons

Subshell	$\{n, l, j\}$	E_1 (MeV)	U_{2s} (eV)	σ_s (barn)
K	{1,0,1/2}	1	1.1103 x 10^4	7.98435
L_1	{2,0,1/2}	1	1.4143 x 10^3	2.65481 x 10^4
L_2	{2,1,1/2}	1	1.2478 x 10^3	2.98266 x 10^4
L_3	{2,1,3/2}	1	1.2167 x 10^3	6.32591 x 10^4
M_1	{3,0,1/2}	1	1.8000 x 10^2	1.61714 x 10^6
M_2	{3,1,1/2}	1	1.2790 x 10^2	2.97174 x 10^6
M_3	{3,1,3/2}	1	1.2080 x 10^2	6.52253 x 10^6
M_4	{3,2,3/2}	1	2.8700 x 10^1	7.80248 x 10^7
M_5	{3,2,5/2}	1	2.8700 x 10^1	1.17037 x 10^8

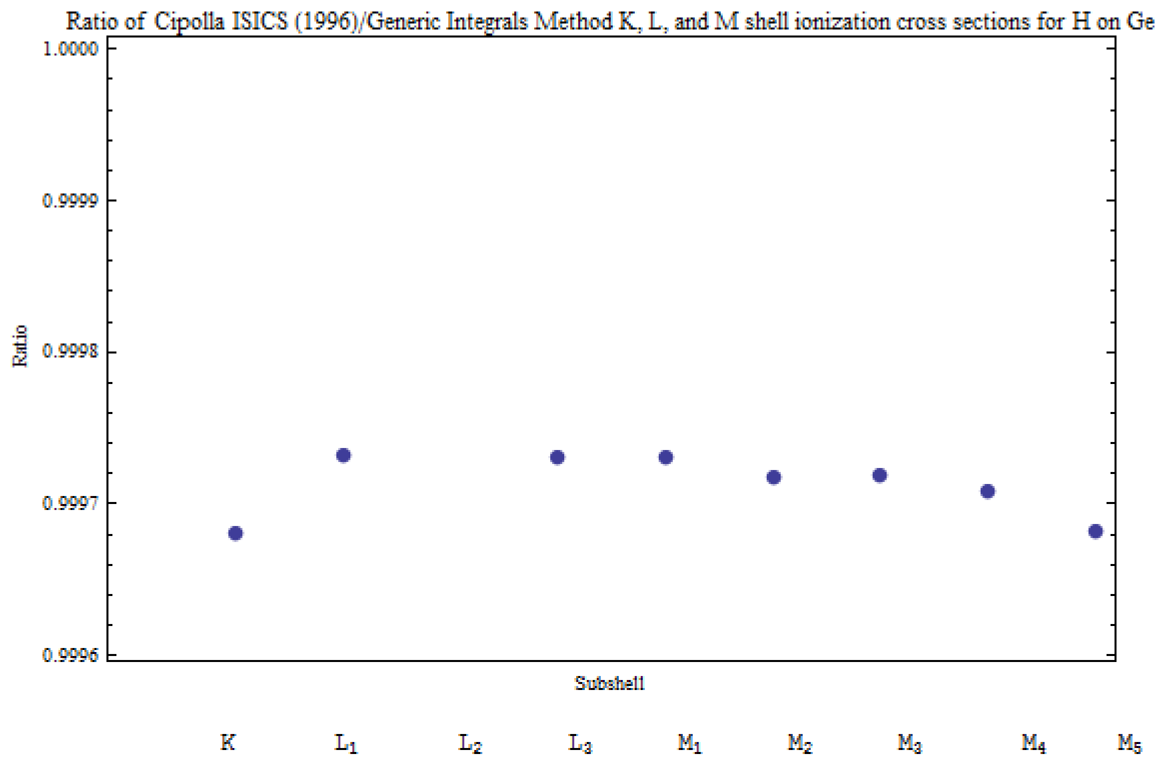

Figure 6. Ratio of this Cipolla ISICS PWBA [3]/Generic Integrals Method ionization cross sections for 1MeV Protons on Germanium (Z_2 = 32)

Table 4. Summary of K, L, and M shell ionization cross sections of samarium by 1 MeV protons

Subshell	$\{n, l, j\}$	E_1 (MeV)	U_{2s} (eV)	σ_s (barn)
K	{1,0,1/2}	1	4.6834 x 10^4	2.70987 x 10^{-3}
L_1	{2,0,1/2}	1	7.7368 x 10^3	1.47108 x 10^1
L_2	{2,1,1/2}	1	7.3118 x 10^3	6.81062 x 10^1
L_3	{2,1,3/2}	1	6.7162 x 10^3	2.03852 x 10^2
M_1	{3,0,1/2}	1	1.7228 x 10^3	1.51218 x 10^4
M_2	{3,1,1/2}	1	1.5407 x 10^3	1.84053 x 10^4
M_3	{3,1,3/2}	1	1.4198 x 10^3	4.54013 x 10^4
M_4	{3,2,3/2}	1	1.1060 x 10^3	7.75420 x 10^4
M_5	{3,2,5/2}	1	1.0802 x 10^3	1.23050 x 10^5

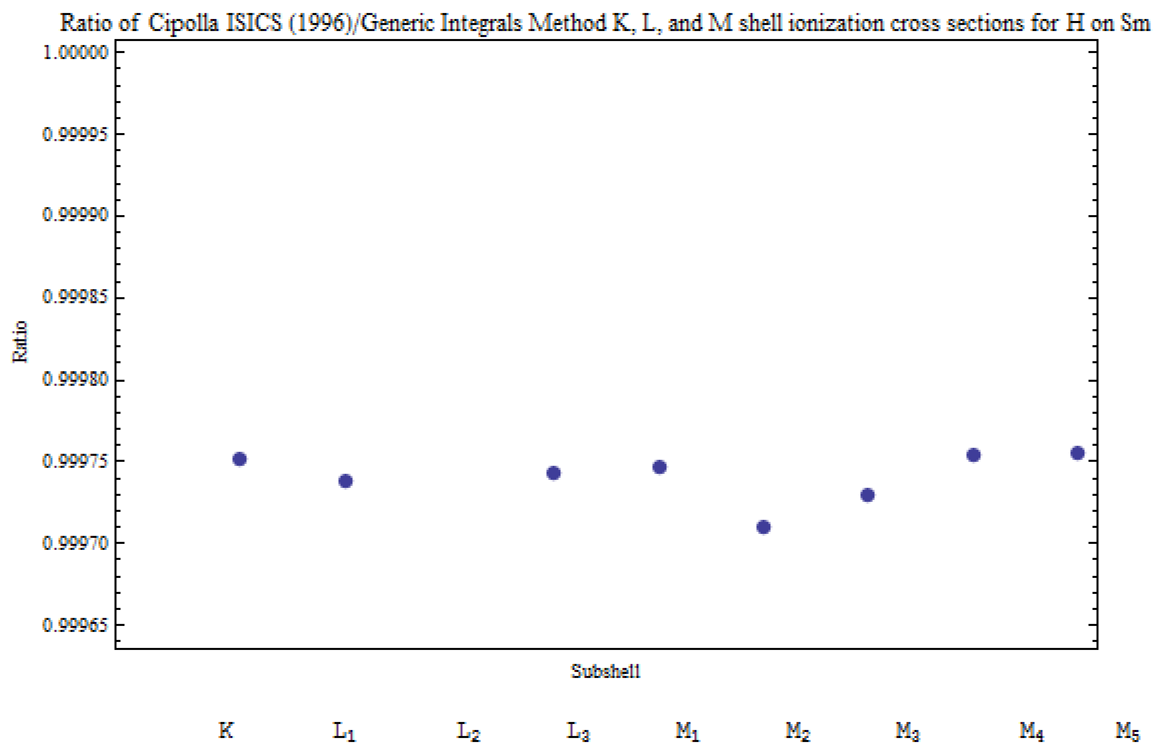

Figure 7. Ratio of this Cipolla ISICS PWBA [3]/Generic Integrals Method ionization cross sections for 1MeV Protons on Samarium (Z_2 = 62)

CHAPTER 4: CONCLUSIONS

4.1 Results

We set out to calculate differential ionization cross sections analytically. In doing so, we determined that the major hurdle was to analytically evaluate the integral equation (1.1.1)

$$I\left(\eta_s, W\right) = \int_{Q_{\min}}^{Q_{\max}} \left|F_{Ws}\left(Q\right)\right|^2 Q^{-2} dQ$$

which gives the energy distribution of ejected electrons. Numerical evaluations of $I\left(\eta_s, W\right)$ are found across the literature dating back to the work of Bethe in the 1930's. However, to this day, no analytical solution exists. We developed a process to analytically solve the indefinite form of this integral and evaluate it over any limits of *Q*. Results were exact functions of *Q* and *W* that one can utilize as a firm basis in further calculations of cross sections, stopping power, straggling, and other moments.

The next step is to take a second integral of our analytical functions over the full range of transferred energy to obtain total cross sections. We found that our foundation provided excellent agreement with our numerical calculations as well existing numerical calculations of [2, 3, 12].

4.2 Strengths, Weaknesses, Limitations

The assumptions made within the PWBA framework outlined in Chapter 2 certainly restrict the applicability of numerical and analytical analysis, at least with regard to incident energies, charge of projectiles, and target atoms. At very low projectile energies, PWBA ionization cross sections for inner shell ionization disagree with experiment by orders of magnitude [7, 9]. However, results based on screened hydrogenic wave functions of target electrons are in good agreement with experiment when compared to K shell ionization cross sections and realistically for L shell within the restrictions that $Z_2 \geq 30$ and for projectile energies such that $Z_1 / v_1 >> 1$, $Z_1 << Z_2$, and $v_1 >> v_{2s}$. The application of direct Coulomb excitation may be out of the reach of the PWBA framework, particularly for projectile energies less than 1 MeV/amu. [7].

4.3 Prospect of Future Work

Our analytical solutions and their generic build up may have many future applications. What follows are a few thoughts. Our choice of screened hydrogenic wave functions is one of many. A tremendous benefit of screened hydrogenic wave functions vs. Hartree-Slater and correlated wavefunctions is that clarity and transparent analytical calculations are, in the case of correlated, problematic if not completely prevented due to the mutual influence of configuration interaction and spin coupling in heavy atoms. An extension of this work can be to determine if one could produce *A(Q,k)* and *S(Q,k)* type functions resulting from other, less limiting, wave functions and find their analytical solutions via our generic integrals method. Some suggest more accurate calculations may be obtained using Hartree-Fock wave functions [2, 9]. Another extension of this work is to develop a similar process to analytically integrate our generically composed solutions over *W*.

It is important to note that beyond the PWBA, corrections can be made for energy loss (E), Coulomb deflection (C), perturbed stationary state (PSS), and relativistic (R) effects collectively known as ECPSSR theory [13]. These corrections have been done with analytical functions that were incorporated into the ECPSSR by appropriate scaling of the PWBA. One may exploit these corrections in the context of our work.

Finally, one might apply the singly differential cross section, $d\sigma / dW$, for calculation of energy spectra in biological material in a way similar to which it was done for water in 2003 [14] for comparison with data of Toburen [15]. Reference [14] in shown in APPENDIX E.

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APPENDIX A: CIPOLLA MATRICES

Sample Mathematica calculation of the $S_s(Q,k)$ *functions using the generating matrix given by Liu and Cipolla* [3]. *As well as the* $S_{3l}(Q,k)$ *functions.*

For $C_{ij}^{(3n)}$ = M1trix:

$$
\mathbf{M1trix} = \{
$$

$$
\left\{\frac{49}{3^{19}}, \frac{3073}{3^{19}}, \frac{3100}{3^{16}}, \frac{5324}{3^{14}}, \frac{17054}{3^{13}}, \frac{1294}{3^{9}}, \frac{1676}{3^{8}}, \frac{1300}{3^{7}}, \frac{59}{3^{4}}, \frac{1}{3}\right\},
$$

$$
\left\{\frac{433}{3^{18}}, \frac{9256}{5*3^{17}}, \frac{-4828}{5*3^{13}}, \frac{-140008}{5*3^{13}}, \frac{-167942}{5*3^{11}}, \frac{-33656}{5*3^{8}}, \frac{-31036}{5*3^{7}}, \frac{-296}{3^{4}}, \frac{-5}{3}, 0\right\},
$$

$$
\left\{\frac{17644}{5*7*3^{15}}, \frac{8908}{3^{15}}, \frac{62516}{5*3^{13}}, \frac{194444}{5*7*3^{10}}, \frac{60956}{5*3^{9}}, \frac{21524}{5*3^{7}}, \frac{76}{3^{3}}, \frac{4}{3}, 0, 0\right\},
$$

$$
\left\{\frac{1444}{5*3^{12}}, \frac{69368}{5*3^{13}}, \frac{328148}{5*3^{11}}, \frac{360592}{5*3^{9}}, \frac{146164}{5*3^{7}}, \frac{1544}{3^{4}}, \frac{28}{3}, 0, 0, 0\right\},
$$

$$
\left\{\frac{-1030}{3^{12}}, \frac{-561554}{5*3^{11}}, \frac{-166468}{3^{9}}, \frac{-406676}{5*3^{7}}, \frac{-4910}{3^{4}}, \frac{-98}{3}, 0, 0, 0, 0\right\},
$$

$$
\left\{\frac{29954}{5*3^{9}}, \frac{138616}{3^{9}}, \frac{456844}{5*3^{7}}, \frac{248}{3}, \frac{154}{3}, 0, 0, 0, 0, 0\right\},
$$

$$
\left\{\frac{-4588}{3^{7}}, \frac{-16348}{3^{6}}, \frac{-4924}{3^{4}}, \frac{-140}{3}, 0, 0, 0, 0, 0, 0\right\},
$$

$$
\left\{\frac{3460}{3^{6}}, \frac{1912}{3^{4}}, \frac{76}{3}, 0, 0, 0, 0, 0, 0, 0\right\},
$$

$$
\left\{\frac{-103}{3^{3}}, \frac{-23}{3}, 0, 0, 0, 0, 0, 0, 0, 0\right\},
$$

$$
\{1, 0, 0, 0, 0, 0, 0, 0, 0, 0\}
$$

$$
\};
$$

sM1a = $\sum_{i=0}^{9}\sum_{j=0}^{9}$ **M1trix[[j + 1, i + 1]] * k^(2 i) * Q^j**

$$\frac{49}{1162261467}+\frac{3073\,k^{2}}{1162261467}+\frac{3100\,k^{4}}{43046721}+\frac{5324\,k^{6}}{4782969}+\frac{17054\,k^{8}}{1594323}+\frac{1294\,k^{10}}{19683}+\frac{1676\,k^{12}}{6561}+\frac{1300\,k^{14}}{2187}+\frac{59\,k^{16}}{81}+$$
$$\frac{k^{18}}{3}+\frac{433\,Q}{387420489}+\frac{9256\,k^{2}\,Q}{645700815}-\frac{4828\,k^{4}\,Q}{7971615}-\frac{140008\,k^{6}\,Q}{7971615}-\frac{167942\,k^{8}\,Q}{885735}-\frac{33656\,k^{10}\,Q}{32805}-\frac{31036\,k^{12}\,Q}{10935}-$$
$$\frac{296\,k^{14}\,Q}{81}-\frac{5\,k^{16}\,Q}{3}+\frac{17644\,Q^{2}}{502211745}+\frac{8908\,k^{2}\,Q^{2}}{14348907}+\frac{62516\,k^{4}\,Q^{2}}{7971615}+\frac{194444\,k^{6}\,Q^{2}}{2066715}+\frac{60956\,k^{8}\,Q^{2}}{98415}+$$
$$\frac{21524\,k^{10}\,Q^{2}}{10935}+\frac{76\,k^{12}\,Q^{2}}{27}+\frac{4\,k^{14}\,Q^{2}}{3}+\frac{1444\,Q^{3}}{2657205}+\frac{69368\,k^{2}\,Q^{3}}{7971615}+\frac{328148\,k^{4}\,Q^{3}}{885735}+\frac{360592\,k^{6}\,Q^{3}}{98415}+$$
$$\frac{146164\,k^{8}\,Q^{3}}{10935}+\frac{1544\,k^{10}\,Q^{3}}{81}+\frac{28\,k^{12}\,Q^{3}}{3}-\frac{1030\,Q^{4}}{531441}-\frac{561554\,k^{2}\,Q^{4}}{885735}-\frac{166468\,k^{4}\,Q^{4}}{19683}-\frac{406676\,k^{6}\,Q^{4}}{10935}-$$
$$\frac{4910\,k^{8}\,Q^{4}}{81}-\frac{98\,k^{10}\,Q^{4}}{3}+\frac{29954\,Q^{5}}{98415}+\frac{138616\,k^{2}\,Q^{5}}{19683}+\frac{456844\,k^{4}\,Q^{5}}{10935}+\frac{248\,k^{6}\,Q^{5}}{3}+\frac{154\,k^{8}\,Q^{5}}{3}-\frac{4588\,Q^{6}}{2187}-$$
$$\frac{16348\,k^{2}\,Q^{6}}{729}-\frac{4924\,k^{4}\,Q^{6}}{81}-\frac{140\,k^{6}\,Q^{6}}{3}+\frac{3460\,Q^{7}}{729}+\frac{1912\,k^{2}\,Q^{7}}{81}+\frac{76\,k^{4}\,Q^{7}}{3}-\frac{103\,Q^{8}}{27}-\frac{23\,k^{2}\,Q^{8}}{3}+Q^{9}$$

sM1b = sM1a * Q^-1 // Distribute

$$\frac{433}{387420489}+\frac{9256\,k^{2}}{645700815}-\frac{4828\,k^{4}}{7971615}-\frac{140008\,k^{6}}{7971615}-\frac{167942\,k^{8}}{885735}-\frac{33656\,k^{10}}{32805}-\frac{31036\,k^{12}}{10935}-\frac{296\,k^{14}}{81}-\frac{5\,k^{16}}{3}+$$
$$\frac{49}{1162261467\,Q}+\frac{3073\,k^{2}}{1162261467\,Q}+\frac{3100\,k^{4}}{43046721\,Q}+\frac{5324\,k^{6}}{4782969\,Q}+\frac{17054\,k^{8}}{1594323\,Q}+\frac{1294\,k^{10}}{19683\,Q}+\frac{1676\,k^{12}}{6561\,Q}+$$
$$\frac{1300\,k^{14}}{2187\,Q}+\frac{59\,k^{16}}{81\,Q}+\frac{k^{18}}{3\,Q}+\frac{17644\,Q}{502211745}+\frac{8908\,k^{2}\,Q}{14348907}+\frac{62516\,k^{4}\,Q}{7971615}+\frac{194444\,k^{6}\,Q}{2066715}+\frac{60956\,k^{8}\,Q}{98415}+$$
$$\frac{21524\,k^{10}\,Q}{10935}+\frac{76\,k^{12}\,Q}{27}+\frac{4\,k^{14}\,Q}{3}+\frac{1444\,Q^{2}}{2657205}+\frac{69368\,k^{2}\,Q^{2}}{7971615}+\frac{328148\,k^{4}\,Q^{2}}{885735}+\frac{360592\,k^{6}\,Q^{2}}{98415}+$$
$$\frac{146164\,k^{8}\,Q^{2}}{10935}+\frac{1544\,k^{10}\,Q^{2}}{81}+\frac{28\,k^{12}\,Q^{2}}{3}-\frac{1030\,Q^{3}}{531441}-\frac{561554\,k^{2}\,Q^{3}}{885735}-\frac{166468\,k^{4}\,Q^{3}}{19683}-\frac{406676\,k^{6}\,Q^{3}}{10935}-$$
$$\frac{4910\,k^{8}\,Q^{3}}{81}-\frac{98\,k^{10}\,Q^{3}}{3}+\frac{29954\,Q^{4}}{98415}+\frac{138616\,k^{2}\,Q^{4}}{19683}+\frac{456844\,k^{4}\,Q^{4}}{10935}+\frac{248\,k^{6}\,Q^{4}}{3}+\frac{154\,k^{8}\,Q^{4}}{3}-\frac{4588\,Q^{5}}{2187}-$$
$$\frac{16348\,k^{2}\,Q^{5}}{729}-\frac{4924\,k^{4}\,Q^{5}}{81}-\frac{140\,k^{6}\,Q^{5}}{3}+\frac{3460\,Q^{6}}{729}+\frac{1912\,k^{2}\,Q^{6}}{81}+\frac{76\,k^{4}\,Q^{6}}{3}-\frac{103\,Q^{7}}{27}-\frac{23\,k^{2}\,Q^{7}}{3}+Q^{8}$$

sM1c = Collect[sM1b, Q]

$$\frac{433}{387420489}+\frac{9256\,k^2}{645700815}-\frac{4828\,k^4}{7971615}-\frac{140008\,k^6}{7971615}-\frac{167942\,k^8}{885735}-\frac{33656\,k^{10}}{32805}-\frac{31036\,k^{12}}{10935}-\frac{296\,k^{14}}{81}-\frac{5\,k^{16}}{3}+\frac{\frac{49}{1162261467}+\frac{3073\,k^2}{1162261467}+\frac{3100\,k^4}{43046721}+\frac{5324\,k^6}{4782969}+\frac{17054\,k^8}{1594323}+\frac{1294\,k^{10}}{19683}+\frac{1676\,k^{12}}{6561}+\frac{1300\,k^{14}}{2187}+\frac{59\,k^{16}}{81}+\frac{k^{18}}{3}}{Q}+$$
$$\left(\frac{17644}{502211745}+\frac{8908\,k^2}{14348907}+\frac{62516\,k^4}{7971615}+\frac{194444\,k^6}{2066715}+\frac{60956\,k^8}{98415}+\frac{21524\,k^{10}}{10935}+\frac{76\,k^{12}}{27}+\frac{4\,k^{14}}{3}\right)Q+$$
$$\left(\frac{1444}{2657205}+\frac{69368\,k^2}{7971615}+\frac{328148\,k^4}{885735}+\frac{360592\,k^6}{98415}+\frac{146164\,k^8}{10935}+\frac{1544\,k^{10}}{81}+\frac{28\,k^{12}}{3}\right)Q^2+$$
$$\left(-\frac{1030}{531441}-\frac{561554\,k^2}{885735}-\frac{166468\,k^4}{19683}-\frac{406676\,k^6}{10935}-\frac{4910\,k^8}{81}-\frac{98\,k^{10}}{3}\right)Q^3+$$
$$\left(\frac{29954}{98415}+\frac{138616\,k^2}{19683}+\frac{456844\,k^4}{10935}+\frac{248\,k^6}{3}+\frac{154\,k^8}{3}\right)Q^4+$$
$$\left(-\frac{4588}{2187}-\frac{16348\,k^2}{729}-\frac{4924\,k^4}{81}-\frac{140\,k^6}{3}\right)Q^5+\left(\frac{3460}{729}+\frac{1912\,k^2}{81}+\frac{76\,k^4}{3}\right)Q^6+\left(-\frac{103}{27}-\frac{23\,k^2}{3}\right)Q^7+Q^8$$

Which results in the $S_{3s}(Q,k)$ factor,

$$\mathbf{S_{3s}(Q,k)} =$$
$$\left(\frac{433}{387420489}+\frac{9256\,k^2}{645700815}-\frac{4828\,k^4}{7971615}-\frac{140008\,k^6}{7971615}-\frac{167942\,k^8}{885735}-\frac{33656\,k^{10}}{32805}-\frac{31036\,k^{12}}{10935}-\frac{296\,k^{14}}{81}-\frac{5\,k^{16}}{3}\right)+$$
$$\frac{\frac{49}{1162261467}+\frac{3073\,k^2}{1162261467}+\frac{3100\,k^4}{43046721}+\frac{5324\,k^6}{4782969}+\frac{17054\,k^8}{1594323}+\frac{1294\,k^{10}}{19683}+\frac{1676\,k^{12}}{6561}+\frac{1300\,k^{14}}{2187}+\frac{59\,k^{16}}{81}+\frac{k^{18}}{3}}{Q}+$$
$$\left(\frac{17644}{502211745}+\frac{8908\,k^2}{14348907}+\frac{62516\,k^4}{7971615}+\frac{194444\,k^6}{2066715}+\frac{60956\,k^8}{98415}+\frac{21524\,k^{10}}{10935}+\frac{76\,k^{12}}{27}+\frac{4\,k^{14}}{3}\right)Q+$$
$$\left(\frac{1444}{2657205}+\frac{69368\,k^2}{7971615}+\frac{328148\,k^4}{885735}+\frac{360592\,k^6}{98415}+\frac{146164\,k^8}{10935}+\frac{1544\,k^{10}}{81}+\frac{28\,k^{12}}{3}\right)Q^2+$$
$$\left(-\frac{1030}{531441}-\frac{561554\,k^2}{885735}-\frac{166468\,k^4}{19683}-\frac{406676\,k^6}{10935}-\frac{4910\,k^8}{81}-\frac{98\,k^{10}}{3}\right)Q^3+$$
$$\left(\frac{29954}{98415}+\frac{138616\,k^2}{19683}+\frac{456844\,k^4}{10935}+\frac{248\,k^6}{3}+\frac{154\,k^8}{3}\right)Q^4+\left(-\frac{4588}{2187}-\frac{16348\,k^2}{729}-\frac{4924\,k^4}{81}-\frac{140\,k^6}{3}\right)Q^5+$$
$$\left(\frac{3460}{729}+\frac{1912\,k^2}{81}+\frac{76\,k^4}{3}\right)Q^6+\left(-\frac{103}{27}-\frac{23\,k^2}{3}\right)Q^7+Q^8$$

Similar Calculations give for $S_{3p}\left(Q,k\right)$ $S_{3d}\left(Q,k\right)$

$$S_{3p}(Q,k) = \left(\frac{448}{71744535} + \frac{9760\,k^2}{43046721} + \frac{79456\,k^4}{23914845} + \frac{67648\,k^6}{2657205} + \frac{32768\,k^8}{295245} + \frac{8992\,k^{10}}{32805} + \frac{224\,k^{12}}{729}\right) +$$
$$\frac{\frac{152}{1162261467} + \frac{2992\,k^2}{387420489} + \frac{2800\,k^4}{14348907} + \frac{1456\,k^6}{531441} + \frac{12320\,k^8}{531441} + \frac{784\,k^{10}}{6561} + \frac{784\,k^{12}}{2187} + \frac{400\,k^{14}}{729} + \frac{8\,k^{16}}{27}}{Q} +$$
$$\left(\frac{2384}{55801305} - \frac{83984\,k^2}{23914845} - \frac{276608\,k^4}{2657205} - \frac{2098912\,k^6}{2066715} - \frac{592\,k^8}{135} - \frac{5776\,k^{10}}{729} - \frac{32\,k^{12}}{9}\right) Q +$$
$$\left(\frac{25664}{7971615} + \frac{40768\,k^2}{885735} + \frac{255808\,k^4}{295245} + \frac{197056\,k^6}{32805} + \frac{3328\,k^8}{243} + \frac{128\,k^{10}}{27}\right) Q^2 +$$
$$\left(\frac{14048}{295245} + \frac{25744\,k^2}{59049} + \frac{5296\,k^4}{10935} - \frac{656\,k^6}{729} + \frac{80\,k^8}{9}\right) Q^3 + \left(-\frac{1088}{2187} - \frac{32608\,k^2}{6561} - \frac{11936\,k^4}{729} - \frac{256\,k^6}{9}\right) Q^4 +$$
$$\left(\frac{4880}{2187} + \frac{10640\,k^2}{729} + \frac{800\,k^4}{27}\right) Q^5 + \left(-\frac{320}{81} - \frac{128\,k^2}{9}\right) Q^6 + \frac{8\,Q^7}{3}$$

$$S_{3d}(Q,k) = \left(\frac{37504}{1937102445} + \frac{473504\,k^2}{645700815} + \frac{263648\,k^4}{23914845} + \frac{660544\,k^6}{7971615} + \frac{283328\,k^8}{885735} + \frac{18784\,k^{10}}{32805} + \frac{3616\,k^{12}}{10935}\right) +$$
$$\frac{\frac{176}{1162261467} + \frac{8816\,k^2}{1162261467} + \frac{6800\,k^4}{43046721} + \frac{2800\,k^6}{1594323} + \frac{17680\,k^8}{1594323} + \frac{2288\,k^{10}}{59049} + \frac{16\,k^{12}}{243} + \frac{80\,k^{14}}{2187}}{Q} +$$
$$\left(\frac{656}{1240029} + \frac{690352\,k^2}{71744535} + \frac{318688\,k^4}{7971615} - \frac{218912\,k^6}{2066715} - \frac{76928\,k^8}{98415} - \frac{7184\,k^{10}}{10935}\right) Q +$$
$$\left(\frac{3968}{2657205} - \frac{124096\,k^2}{1594323} - \frac{579392\,k^4}{885735} - \frac{33344\,k^6}{19683} - \frac{7744\,k^8}{10935}\right) Q^2 +$$
$$\left(-\frac{87952}{2657205} + \frac{222224\,k^2}{885735} + \frac{297776\,k^4}{98415} + \frac{16496\,k^6}{10935}\right) Q^3 + \left(\frac{5632}{32805} - \frac{26464\,k^2}{19683} + \frac{6176\,k^4}{10935}\right) Q^4 +$$
$$\left(\frac{208}{2187} - \frac{16\,k^2}{9}\right) Q^5 + \frac{512\,Q^6}{729}$$

APPENDIX B: INTEGRATION SUB-ROUTINES

IntegrateParts and SubForInt Mathematica programs used throughout this work.

```
IntegrateParts[f___, x_] :=
 {
  t = {f};
  If[Length[{f}] == 2,
    {
     p = Permutations [{f}];
     Print["Permutations are ", p, "\n",
      "********************************************************************************
        *****"];
     Do[
      u[i] = p[[i, 1]] // Simplify;
      dv[i] = p[[i, 2]] // Simplify;
      v[i] = Integrate[dv[i], x] // Simplify;
      du[i] = D[u[i], x] // Simplify;
      newint[i] = u[i] * v[i] - Integrate[v[i] * du[i], x] // Simplify;
      Print["p = ", i, "\n"
        "u = ", u[i], "\n"
        "dv = ", dv[i], "\n"
             "v = ", v[i], "\n"
              "du = ", du[i], "\n"
               ];
      Print["∫ u dv = u v - ∫ v du\n",
        "=>  ∫ ", u[i] * dv[i], " = ", newint[i]];
      Print[
       "*******************************************************************************
         ******"],
      {i, 1, Length[p]}
     ]
    }
   ]
   If[Length[{f}] == 3,
    {
     p = Permutations [{f}];
     p2 = Drop[p, {1, 6, 2}];
     Print["Permutations are ", p2, "\n",
      "********************************************************************************
        *****"]
```

```
Do[
  u[i] = p2[[i, 1]] // Simplify;
  dv[i] = (p2[[i, 2]] * p2[[i, 3]]) // Simplify;
  v[i] = Integrate[dv[i], x] // Simplify;
  du[i] = D[u[i], x] // Simplify;
  newint[i] = u[i] * v[i] - Integrate[v[i] * du[i], x] // Simplify;
  Print["p = ", i, "\n"
    "u = ", u[i], "\n"
      "dv = ", dv[i], "\n"
       "v = ", v[i], "\n"
        "du = ", du[i], "\n"
         ];
  Print["∫ u dv = u v - ∫ v du\n",
      "=>  ∫ ", u[i] * dv[i], " = ", newint[i]];
  Print[
   "***********************************************************************************************
     **"],
  {i, 1, 3}
 ]
 Do[
  u2[i] = (p2[[i, 2]] * p2[[i, 3]]) // Simplify;
  dv2[i] = p2[[i, 1]] // Simplify;
  v2[i] = Integrate[dv2[i], x] // Simplify;
  du2[i] = D[u2[i], x] // Simplify;
  newint2[i] = u2[i] * v2[i] - Integrate[v2[i] * du2[i], x] // Simplify;
  Print["p2 = ", i, "\n"
    "u2 = ", u2[i], "\n"
      "dv2 = ", dv2[i], "\n"
       "v2 = ", v2[i], "\n"
        "du2 = ", du2[i], "\n"
         ];
  Print["∫ u2 dv2 = u2 v2 - ∫ v2 du2\n",
      "=>  ∫ ", u2[i] * dv2[i], " = ", newint2[i]];
  Print[
   "***********************************************************************************************
     **"],
  {i, 1, 3}
 ]
 }
]
```

```
If[Length[{f}] == 4,
 {
  p = Permutations[{f}];
  p2 = Take[p, {1, 19, 6}];
  p3 = {p[[1]], p[[3]], p[[9]]};
  Print["Permutations are ", p2, "\n",
    "*****************************************************************************************
      ***"]
   Do[
    u[i] = p2[[i, 1]] // Simplify;
    dv[i] = (p2[[i, 2]] * p2[[i, 3]] * p2[[i, 4]]) // Simplify;
    v[i] = Integrate[dv[i], x] // Simplify;
    du[i] = D[u[i], x] // Simplify;
    newint[i] = u[i] * v[i] - Integrate[v[i] * du[i], x] // Simplify;
    Print["p = ", i, "\n"
      "u = ", u[i], "\n"
        "dv = ", dv[i], "\n"
          "v = ", v[i], "\n"
            "du = ", du[i], "\n"
              ];
    Print["∫ u dv = u v - ∫ v du\n",
        "=>  ∫ ", u[i] * dv[i], " = ", newint[i]];
    Print[
     "************************************************************************************
       ****"],
    {i, 1, Length[p2]}
   ]
   Do[
    u2[i] = (p2[[i, 2]] * p2[[i, 3]] * p2[[i, 4]]) // Simplify;
    dv2[i] = p2[[i, 1]] // Simplify;
    v2[i] = Integrate[dv2[i], x] // Simplify;
    du2[i] = D[u2[i], x] // Simplify;
    newint2[i] = u2[i] * v2[i] - Integrate[v2[i] * du2[i], x] // Simplify;
    Print["p2 = ", i, "\n"
      "u2 = ", u2[i], "\n"
        "dv2 = ", dv2[i], "\n"
          "v2 = ", v2[i], "\n"
            "du2 = ", du2[i], "\n"
              ];
    Print["∫ u2 dv2 = u2 v2 - ∫ v2 du2\n",
        "=>  ∫ ", u2[i] * dv2[i], " = ", newint2[i]];
    Print[
     "************************************************************************************
       ****"],
    {i, 1, Length[p2]}
   ]
```

```
Do[
    u3[i] = (p3[[i, 1]] * p3[[i, 2]]) // Simplify;
    dv3[i] = (p3[[i, 3]] * p3[[i, 4]]) // Simplify;
    v3[i] = Integrate[dv3[i], x] // Simplify;
    du3[i] = D[u3[i], x] // Simplify;
    newint3[i] = u3[i] *v3[i] - Integrate[v3[i] * du3[i], x] // Simplify;
    Print["p3 = ", i, "\n"
      "u3 = ", u3[i], "\n"
        "dv3 = ", dv3[i], "\n"
          "v3 = ", v3[i], "\n"
            "du3 = ", du3[i], "\n"
              ];
    Print["∫ u3 dv3 = u3 v3 - ∫ v3 du3\n",
        "=>  ∫ ", u3[i] * dv3[i], " = ", newint3[i]];
    Print[
     "*************************************************************************************
       ****"],
    {i, 1, Length[p3]}
   ]
   Do[
    u4[i] = (p3[[i, 3]] * p3[[i, 4]]) // Simplify;
    dv4[i] = (p3[[i, 1]] * p3[[i, 2]]) // Simplify;
    v4[i] = Integrate[dv4[i], x] // Simplify;
    du4[i] = D[u4[i], x] // Simplify;
    newint4[i] = u4[i] *v4[i] - Integrate[v4[i] * du4[i], x] // Simplify;
    Print["p4 = ", i, "\n"
      "u4 = ", u4[i], "\n"
        "dv4 = ", dv4[i], "\n"
          "v4 = ", v4[i], "\n"
            "du4 = ", du4[i], "\n"
              ];
    Print["∫ u4 dv4 = u4 v4 - ∫ v4 du4\n",
        "=>  ∫ ", u4[i] * dv4[i], " = ", newint4[i]];
    Print[
     "*************************************************************************************
       ****"],
    {i, 1, Length[p3]}
   ]
   }
  ]

 }
```

Here we integrate $I1ar1(Q,k) = \dfrac{e^{-\frac{2\,\mathrm{ArcTan}\left[1-k^2+Q,2k\right]}{k}}}{3\left(1+k^2\right)^5 Q}$

```
IntegrateParts[e^(-2 ArcTan[1-k^2+Q, 2 k]/k), 1/Q, Q]
```

$$\mathtt{IntegrateParts}\left[e^{-\frac{2\,\mathrm{ArcTan}\left[1-k^2+Q,2\,k\right]}{k}},\ \frac{1}{Q},\ Q\right]$$

In this example factor1$=\exp\left[-2ArcTan\left[2k/Q+k^2+1\right]/k\right]$, *factor2*$=Q^{-1}$. *There are no further Q dependent factors and hence we can omit factors 3 and 4. The coefficient polynomial in k* $1/3\left(1+k^2\right)^5$ *is constant with respect to this integration and is removed for clarity.*

Resulting output for this example is:

Permutations are $\left\{\left\{e^{-\frac{2\,\mathrm{ArcTan}\left[1-k^2+Q,2\,k\right]}{k}},\ \frac{1}{Q}\right\},\ \left\{\frac{1}{Q},\ e^{-\frac{2\,\mathrm{ArcTan}\left[1-k^2+Q,2\,k\right]}{k}}\right\}\right\}$

****

p = 1

$$u = e^{-\frac{2\,\mathrm{ArcTan}\left[1-k^2+Q,2\,k\right]}{k}}$$

$$dv = \frac{1}{Q}$$

$$v = \mathrm{Log}[Q]$$

$$du = \frac{4\,e^{-\frac{2\,\mathrm{ArcTan}\left[1-k^2+Q,2\,k\right]}{k}}}{4\,k^2+\left(1-k^2+Q\right)^2}$$

$$\int u\ dv = u\ v - \int v\ du$$

$$\Rightarrow\ \int \frac{e^{-\frac{2\,\mathrm{ArcTan}\left[1-k^2+Q,2\,k\right]}{k}}}{Q} = -4\int \frac{e^{-\frac{2\,\mathrm{ArcTan}\left[1-k^2+Q,2\,k\right]}{k}}\,\mathrm{Log}[Q]}{4\,k^2+\left(1-k^2+Q\right)^2}\,dQ + e^{-\frac{2\,\mathrm{ArcTan}\left[1-k^2+Q,2\,k\right]}{k}}\,\mathrm{Log}[Q]$$

$p = 2$

$u = \frac{1}{Q}$

$dv = e^{-\frac{2\,\mathrm{ArcTan}[1-k^2+Q,2k]}{k}}$

$v = \int e^{-\frac{2\,\mathrm{ArcTan}[1-k^2+Q,2k]}{k}}\,dQ$

$du = -\frac{1}{Q^2}$

$\int u\,dv = u\,v - \int v\,du$

$$\Rightarrow \int \frac{e^{-\frac{2\,\mathrm{ArcTan}[1-k^2+Q,2k]}{k}}}{Q} = \frac{\int e^{-\frac{2\,\mathrm{ArcTan}[1-k^2+Q,2k]}{k}}\,dQ}{Q} + \int \frac{\int e^{-\frac{2\,\mathrm{ArcTan}[1-k^2+Q,2k]}{k}}\,dQ}{Q^2}\,dQ$$

This output shows two permutations, the second of which is useless. The first permutation however, results in one integral term that can be managed and one integrated term.

Here is another example calculation used in the progression above.

$\mathrm{IntegrateParts}\left[\frac{-2}{k}\,e^{\frac{2\xi}{k}},\ \mathrm{Log}[-\mathrm{Sin}[\xi]+k^2\,\mathrm{Sin}[\xi]-2\,k\,\mathrm{Cos}[\xi]],\ \xi\right]$

Permutations are $\left\{\left\{-\frac{2\,e^{\frac{2\xi}{k}}}{k},\ \mathrm{Log}[-2\,k\,\mathrm{Cos}[\xi]-\mathrm{Sin}[\xi]+k^2\,\mathrm{Sin}[\xi]]\right\},\right.$

$\left.\left\{\mathrm{Log}[-2\,k\,\mathrm{Cos}[\xi]-\mathrm{Sin}[\xi]+k^2\,\mathrm{Sin}[\xi]],\ -\frac{2\,e^{\frac{2\xi}{k}}}{k}\right\}\right\}$

****
***

The first permutation is useless so we will omit it here. Results of the second permutation are p = 2

$$u = \text{Log}\left[-2\,k\,\text{Cos}[\xi] + \left(-1+k^2\right)\text{Sin}[\xi]\right]$$

$$dv = -\frac{2\,e^{\frac{2\xi}{k}}}{k}$$

$$v = -e^{\frac{2\xi}{k}}$$

$$du = \frac{\left(-1+k^2\right)\text{Cos}[\xi] + 2\,k\,\text{Sin}[\xi]}{-2\,k\,\text{Cos}[\xi] + \left(-1+k^2\right)\text{Sin}[\xi]}$$

$$\int u\ dv = u\ v - \int v\ du$$

$$\Rightarrow \int -\frac{2\,e^{\frac{2\xi}{k}}\ \text{Log}\left[-2\,k\,\text{Cos}[\xi] + \left(-1+k^2\right)\text{Sin}[\xi]\right]}{k} =$$

$$\int \frac{e^{\frac{2\xi}{k}}\left(\left(-1+k^2\right)\text{Cos}[\xi] + 2\,k\,\text{Sin}[\xi]\right)}{-2\,k\,\text{Cos}[\xi] + \left(-1+k^2\right)\text{Sin}[\xi]}\,d\xi - e^{\frac{2\xi}{k}}\ \text{Log}\left[-2\,k\,\text{Cos}[\xi] + \left(-1+k^2\right)\text{Sin}[\xi]\right]$$

****
**

We conclude that

$$\int -\frac{2\,e^{\frac{2\xi}{k}}\ \text{Log}[-2\,k\,\text{Cos}[\xi] + (-1+k^2)\,\text{Sin}[\xi]]}{k}\,d\xi =$$

$$\int \frac{e^{\frac{2\xi}{k}}\ ((-1+k^2)\,\text{Cos}[\xi] + 2\,k\,\text{Sin}[\xi])}{-2\,k\,\text{Cos}[\xi] + (-1+k^2)\,\text{Sin}[\xi]}\,d\xi - e^{\frac{2\xi}{k}}\ \text{Log}\left[-2\,k\,\text{Cos}[\xi] + \left(-1+k^2\right)\text{Sin}[\xi]\right]$$

Integration by substitution sub-routine.

```
SubForInt[in_, x_, u_, sb_] :=
 {nin = in / D[sb, x] /. sb → u; xsb = Solve[u == sb, x][[1, 1]];
   nin /. xsb}[[1]]
```

The subroutine requires the user to input the integrand (in), the original variable (x), the substituting variable (u), and its definition (sb).

A simple usage example: $\int \sin[x^2 - 1]dx$

```
SubForInt[Sin[x^2 - 1], x, q, x^2 - 1]
```

$$-\frac{\text{Sin}[q]}{2\sqrt{1+q}}$$

APPENDIX C: LIST OF SIMPLIFIED GENERIC INTEGRALS

for n = 1 the generic integrals are

$$\int \frac{e^{-\frac{2\,\mathrm{ArcTan}[1-k^2+Q,2k]}{k}}}{(4k^2+(1-k^2+Q)^2)^3} * Q^{-1}\,dQ = \mathrm{gi1i1}[Q,k]$$

$$\mathrm{gi1i1}[Q\_,k\_] := \frac{1}{(1+k^2)^6} e^{-\frac{2}{k}\mathrm{ArcTan}[1-k^2+Q,2k]} \Big(\big(-298-1195k^2-989k^4+1273k^6+2283k^8+991k^{10}+89k^{12}+19k^{14}+3k^{16}+ (-640-2008k^2+476k^4+1172k^6-872k^8-240k^{10}-52k^{12}-12k^{14})\,Q+ (-596-1622k^2+1602k^4-172k^6+320k^8+66k^{10}+18k^{12})\,Q^2+ (-272-752k^2+884k^4-212k^6-52k^8-12k^{10})\,Q^3+(-50-167k^2+91k^4+19k^6+3k^8)\,Q^4\big) / \big((1+4k^2)\,(4k^2+(1-k^2+Q)^2)^2\big) - 64\left(e^{2i\,\mathrm{ArcTan}[-(1+k^2)^2+(-1+k^2)\,Q,2kQ]}\right)^{-\frac{i}{k}} \left(\mathrm{Beta}\left[e^{-2i\,\mathrm{ArcTan}[-(1+k^2)^2+(-1+k^2)\,Q,2kQ]},1-\frac{i}{k},0\right]+\mathrm{Beta}\left[e^{2i\,\mathrm{ArcTan}[-(1+k^2)^2+(-1+k^2)\,Q,2kQ]},1+\frac{i}{k},0\right]\right)\Big)$$

$$\int \frac{e^{-\frac{2\,\mathrm{ArcTan}[1-k^2+Q,2k]}{k}}}{(4k^2+(1-k^2+Q)^2)^3} * Q^{0}\,dQ = \mathrm{gi10}[Q,k]$$

$$\mathrm{gi10}[Q\_,k\_] := e^{-\frac{2}{k}\mathrm{ArcTan}[1-k^2+Q,2k]} \big(103+104k^2-2k^4+3k^8+(128-28k^2+24k^4-12k^6)\,Q+(78-48k^2+18k^4)\,Q^2+(24-12k^2)\,Q^3+3Q^4\big) / \big((1+k^2)\,(1+4k^2)\,(4k^2+(1-k^2+Q)^2)^2\big)$$

for n = 2 the generic integrals

$$\int \frac{e^{-\frac{2\,\mathrm{ArcTan}\left[\frac{1}{4}-k^2+Q,\,k\right]}{k}}}{\left(k^2+\left(\frac{1}{4}-k^2+Q\right)^2\right)^5} * Q^{-1}\, dQ = \mathrm{gi2i1}[Q,\, k]$$

$$\mathrm{gi2i1}[Q\_,\, k\_] := \frac{1}{(1+4k^2)^{10}}\, e^{-\frac{2\,\mathrm{ArcTan}\left[\frac{1}{4}-k^2+Q,\,k\right]}{k}}$$

$$\Bigg(\Bigg(-\frac{1230135}{2048}-\frac{26572247\,k^2}{1024}-\frac{119497353\,k^4}{256}-\frac{285026127\,k^6}{64}-\frac{357978345\,k^8}{16}-\frac{119309859\,k^{10}}{4}+$$

$$337387491\,k^{12}+2443402452\,k^{14}+8099649648\,k^{16}+15289222848\,k^{18}+15935800576\,k^{20}+$$

$$7364692992\,k^{22}+507334656\,k^{24}+562544640\,k^{26}+845217792\,k^{28}+790364160\,k^{30}+330301440\,k^{32}+$$

$$\Big(-9216-\frac{5552841\,k^2}{16}-\frac{39763717\,k^4}{8}-\frac{66128347\,k^6}{2}-83889132\,k^8+121582976\,k^{10}+719312672\,k^{12}-$$

$$2812412544\,k^{14}-21367605248\,k^{16}-45909659648\,k^{18}-35674152960\,k^{20}-2732752896\,k^{22}-$$

$$2139881472\,k^{24}-4095737856\,k^{26}-5001707520\,k^{28}-2642411520\,k^{30}\Big)\,Q+$$

$$\Big(-\frac{2409783}{32}-\frac{39286231\,k^2}{16}-\frac{107556087\,k^4}{4}-108972470\,k^6-31270368\,k^8+710069872\,k^{10}+$$

$$2183823040\,k^{12}+15550778368\,k^{14}+65845159936\,k^{16}+89370292224\,k^{18}+8091844608\,k^{20}+$$

$$4186570752\,k^{22}+9239003136\,k^{24}+14202961920\,k^{26}+9248440320\,k^{28}\Big)\,Q^2+$$

$$\Big(-\frac{802371}{2}-11254450\,k^2-89512626\,k^4-154123864\,k^6+383132832\,k^8+869012352\,k^{10}-$$

$$1631368192\,k^{12}-40111271936\,k^{14}-129617903616\,k^{16}-14978580480\,k^{18}-5510922240\,k^{20}-$$

$$13232504832\,k^{22}-24442306560\,k^{24}-18496880640\,k^{26}\Big)\,Q^3+$$

$$\Big(-\frac{5858433}{4}-\frac{71310609\,k^2}{2}-193696198\,k^4+97245512\,k^6+512744480\,k^8+1846364928\,k^{10}+$$

$$4817118208\,k^{12}+118959869952\,k^{14}+18175229952\,k^{16}+5318737920\,k^{18}+13744865280\,k^{20}+$$

$$28901376000\,k^{22}+23121100800\,k^{24}\Big)\,Q^4+$$

$$\Big(-3651504-79741904\,k^2-281255904\,k^4+859931008\,k^6-1627944960\,k^8+10465509376\,k^{10}-$$

$$68518035456\,k^{12}-14505934848\,k^{14}-3773300736\,k^{16}-11415846912\,k^{18}-24442306560\,k^{20}-$$

$$18496880640\,k^{22}\Big)\,Q^5+$$

$$\Big(-5959192-123899696\,k^2-310638528\,k^4+1918132224\,k^6-6086930432\,k^8+24924659712\,k^{10}+$$

$$7249494016\,k^{12}+2225602560\,k^{14}+7862747136\,k^{16}+14202961920\,k^{18}+9248440320\,k^{20}\Big)\,Q^6+$$

$$\Big(-5746560-122748928\,k^2-339125760\,k^4+2202277888\,k^6-4689551360\,k^8-2043183104\,k^{10}-$$

$$1492254720\,k^{12}-3820486656\,k^{14}-5001707520\,k^{16}-2642411520\,k^{18}\Big)\,Q^7+$$

$$\Big(-2485216-58726336\,k^2-270391552\,k^4+567628800\,k^6+566849536\,k^8+622903296\,k^{10}+$$

$$872742912\,k^{12}+790364160\,k^{14}+330301440\,k^{16}\Big)\,Q^8\Bigg)\Big/\left((1+k^2)\,(1+9k^2)\,(1+16k^2)\left(k^2+\left(\frac{1}{4}-k^2+Q\right)^2\right)^4\right)-$$

$$8388608\left(e^{2i\,\mathrm{ArcTan}\left[-\left(\frac{1}{4}+k^2\right)^2+\left(-\frac{1}{4}+k^2\right)Q,\,kQ\right]}\right)^{-\frac{i}{k}}$$

$$\left(\mathrm{Beta}\left[e^{-2i\,\mathrm{ArcTan}\left[-\left(\frac{1}{4}+k^2\right)^2+\left(-\frac{1}{4}+k^2\right)Q,\,kQ\right]},\,1-\frac{i}{k},\,0\right]+\mathrm{Beta}\left[e^{2i\,\mathrm{ArcTan}\left[-\left(\frac{1}{4}+k^2\right)^2+\left(-\frac{1}{4}+k^2\right)Q,\,kQ\right]},\,1+\frac{i}{k},\,0\right]\right)\Bigg)$$

$$\int \frac{e^{-\frac{2\,\text{ArcTan}\left[\frac{1}{4}-k^2+Q,\,k\right]}{k}}}{\left(k^2+\left(\frac{1}{4}-k^2+Q\right)^2\right)^5} * Q^0\, dQ = \text{gi20}[Q,\,k]$$

gi20[Q_, k_] :=

$$e^{-\frac{2\,\text{ArcTan}\left[\frac{1}{4}-k^2+Q,\,k\right]}{k}} \left(\frac{556403}{16384}+\frac{109009\,k^2}{256}+\frac{362523\,k^4}{256}+\frac{8185\,k^6}{8}+\frac{5\,k^8}{32}+21\,k^{10}-105\,k^{12}+1260\,k^{16}+\left(256+\frac{164493\,k^2}{128}+\frac{16107\,k^4}{16}+\frac{347\,k^6}{8}+42\,k^8-1050\,k^{10}+5040\,k^{12}-10080\,k^{14}\right) Q+\left(\frac{294259}{256}+\frac{2513\,k^2}{4}+\frac{24031\,k^4}{16}-5082\,k^6+14385\,k^8-30240\,k^{10}+35280\,k^{12}\right) Q^2+\left(\frac{54831}{16}-\frac{58485\,k^2}{8}+19824\,k^4-44940\,k^6+75600\,k^8-70560\,k^{10}\right) Q^3+\left(\frac{224805}{32}-24675\,k^2+60585\,k^4-100800\,k^6+88200\,k^8\right) Q^4+\left(9870-38010\,k^2+75600\,k^4-70560\,k^6\right) Q^5+\left(9135-30240\,k^2+35280\,k^4\right) Q^6+\left(5040-10080\,k^2\right) Q^7+1260\,Q^8\right) \Big/ \left(\left(1+k^2\right)\left(1+4\,k^2\right)\left(1+9\,k^2\right)\left(1+16\,k^2\right)\left(k^2+\left(\frac{1}{4}-k^2+Q\right)^2\right)^4\right)$$

$$\int \frac{e^{-\frac{2\,\text{ArcTan}[\frac{1}{4}-k^2+Q,\,k]}{k}}}{\left(k^2+\left(\frac{1}{4}-k^2+Q\right)^2\right)^5} * Q^1\, dQ = \text{gi21}[Q, k]$$

gi21[Q_, k_] :=

$$e^{-\frac{2\,\text{ArcTan}[\frac{1}{4}-k^2+Q,\,k]}{k}} \left(-2-\frac{426637\,k^2}{16384}-\frac{30767\,k^4}{256}-\frac{57317\,k^6}{256}-\frac{1031\,k^8}{8}+\frac{5\,k^{10}}{32}+21\,k^{12}-105\,k^{14}+1260\,k^{18}+\left(256\,k^2+\frac{164493\,k^4}{128}+\frac{16107\,k^6}{16}+\frac{347\,k^8}{8}+42\,k^{10}-1050\,k^{12}+5040\,k^{14}-10080\,k^{16}\right)Q+\left(\frac{294259\,k^2}{256}+\frac{2513\,k^4}{4}+\frac{24031\,k^6}{16}-5082\,k^8+14385\,k^{10}-30240\,k^{12}+35280\,k^{14}\right)Q^2+\left(\frac{54831\,k^2}{16}-\frac{58485\,k^4}{8}+19824\,k^6-44940\,k^8+75600\,k^{10}-70560\,k^{12}\right)Q^3+\left(\frac{224805\,k^2}{32}-24675\,k^4+60585\,k^6-100800\,k^8+88200\,k^{10}\right)Q^4+\left(9870\,k^2-38010\,k^4+75600\,k^6-70560\,k^8\right)Q^5+\left(9135\,k^2-30240\,k^4+35280\,k^6\right)Q^6+\left(5040\,k^2-10080\,k^4\right)Q^7+1260\,k^2\,Q^8\right) \Big/ \left(\left(1+k^2\right)\left(1+4\,k^2\right)\left(1+9\,k^2\right)\left(1+16\,k^2\right)\left(k^2+\left(\frac{1}{4}-k^2+Q\right)^2\right)^4\right)$$

$$\int \frac{e^{-\frac{2\,\text{ArcTan}[\frac{1}{4}-k^2+Q,\,k]}{k}}}{\left(k^2+\left(\frac{1}{4}-k^2+Q\right)^2\right)^5} * Q^2\, dQ$$

gi22[Q_, k_] :=

$$e^{-\frac{2\,\text{ArcTan}[\frac{1}{4}-k^2+Q,\,k]}{k}} \left(\frac{42037}{262144}+\frac{43473\,k^2}{16384}+\frac{278631\,k^4}{16384}+\frac{3335\,k^6}{64}+\frac{38025\,k^8}{512}+\frac{1149\,k^{10}}{32}+\frac{71\,k^{12}}{32}+6\,k^{14}-\frac{375\,k^{16}}{4}+180\,k^{18}+1260\,k^{20}+\left(-\frac{42037\,k^2}{2048}-\frac{44909\,k^4}{256}-\frac{28479\,k^6}{64}-\frac{4853\,k^8}{16}+40\,k^{10}-63\,k^{12}-420\,k^{14}+3600\,k^{16}-10080\,k^{18}\right)Q+\left(\frac{42037}{4096}+\frac{43473\,k^2}{256}+\frac{80167\,k^4}{64}+\frac{12759\,k^6}{16}+\frac{7235\,k^8}{8}-3297\,k^{10}+10380\,k^{12}-25200\,k^{14}+35280\,k^{16}\right)Q^2+\left(\frac{7833}{256}+\frac{54309\,k^2}{128}+\frac{40953\,k^4}{16}-\frac{39039\,k^6}{8}+14079\,k^8-34770\,k^{10}+65520\,k^{12}-70560\,k^{14}\right)Q^3+\left(\frac{32115}{512}+\frac{25065\,k^2}{32}+\frac{129315\,k^4}{32}-16920\,k^6+\frac{93945\,k^8}{2}-88200\,k^{10}+88200\,k^{12}\right)Q^4+\left(\frac{705}{8}+\frac{8565\,k^2}{8}+5115\,k^4-27840\,k^6+65520\,k^8-70560\,k^{10}\right)Q^5+\left(\frac{1305}{16}+1035\,k^2+5130\,k^4-25200\,k^6+35280\,k^8\right)Q^6+\left(45+630\,k^2+3600\,k^4-10080\,k^6\right)Q^7+\left(\frac{45}{4}+180\,k^2+1260\,k^4\right)Q^8\right) \Big/ \left(\left(1+k^2\right)\left(1+4\,k^2\right)\left(1+9\,k^2\right)\left(1+16\,k^2\right)\left(k^2+\left(\frac{1}{4}-k^2+Q\right)^2\right)^4\right)$$

$$\int \frac{e^{-\frac{2\,\text{ArcTan}\left[\frac{1}{4}-k^2+Q,\,k\right]}{k}}}{\left(k^2+\left(\frac{1}{4}-k^2+Q\right)^2\right)^5} * Q^3\, dQ = \text{gi23}[Q,\,k]$$

gi23[Q_, k_] :=

$$e^{-\frac{2\,\text{ArcTan}\left[\frac{1}{4}-k^2+Q,\,k\right]}{k}} \Bigg(-\frac{7833}{524288}-\frac{85641 k^2}{262144}-\frac{47631 k^4}{16384}-\frac{218769 k^6}{16384}-\frac{33735 k^8}{1024}-\frac{20793 k^{10}}{512}-\frac{291 k^{12}}{16}+\frac{123 k^{14}}{32}-\frac{177 k^{16}}{8}-\frac{165 k^{18}}{4}+540 k^{20}+1260 k^{22}+$$

$$\left(\frac{7833 k^2}{4096}+\frac{54309 k^4}{2048}+\frac{1035 k^6}{8}+\frac{7995 k^8}{32}+\frac{1185 k^{10}}{8}+\frac{63 k^{12}}{4}-168 k^{14}+600 k^{16}+720 k^{18}-10080 k^{20}\right) Q+$$

$$\left(-\frac{7833}{8192}-\frac{85641 k^2}{4096}-\frac{103095 k^4}{512}-\frac{89541 k^6}{128}-\frac{15993 k^8}{32}+\frac{27 k^{10}}{4}-\frac{789 k^{12}}{2}+3210 k^{14}-15120 k^{16}+35280 k^{18}\right) Q^2+$$

$$\left(\frac{2611}{512}+\frac{20801 k^2}{128}+\frac{144423 k^4}{128}+\frac{19679 k^6}{16}-\frac{7807 k^8}{8}+4284 k^{10}-16110 k^{12}+45360 k^{14}-70560 k^{16}\right) Q^3+$$

$$\left(\frac{10705}{1024}+\frac{163185 k^2}{512}+\frac{3705 k^4}{2}-\frac{20305 k^6}{32}-\frac{14715 k^8}{4}+\frac{43695 k^{10}}{2}-63000 k^{12}+88200 k^{14}\right) Q^4+$$

$$\left(\frac{235}{16}+\frac{7085 k^2}{16}+\frac{19355 k^4}{8}-2700 k^6-9180 k^8+45360 k^{10}-70560 k^{12}\right) Q^5+$$

$$\left(\frac{435}{32}+\frac{6675 k^2}{16}+\frac{4875 k^4}{2}-2040 k^6-15120 k^8+35280 k^{10}\right) Q^6+\left(\frac{15}{2}+240 k^2+1650 k^4+720 k^6-10080 k^8\right) Q^7+$$

$$\left(\frac{15}{8}+\frac{255 k^2}{4}+540 k^4+1260 k^6\right) Q^8\Bigg) \Big/ \left(\left(1+k^2\right)\left(1+4k^2\right)\left(1+9k^2\right)\left(1+16k^2\right)\left(k^2+\left(\frac{1}{4}-k^2+Q\right)^2\right)^4\right)$$

$$\int \frac{e^{-\frac{2\,\mathrm{ArcTan}\left[\frac{1}{4}-k^2+Q,\,k\right]}{k}}}{[\ldots]} * Q^4\, dQ = \mathrm{gi24}[Q,\,k]$$

$$\mathrm{gi24}[Q\_,\,k\_] := e^{-\frac{2\,\mathrm{ArcTan}\left[\frac{1}{4}-k^2+Q,\,k\right]}{k}}$$

$$\Bigg(\frac{6423}{4194304}+\frac{2859\,k^2}{65536}+\frac{69093\,k^4}{131072}+\frac{28503\,k^6}{8192}+\frac{219501\,k^8}{16384}+\frac{945\,k^{10}}{32}+\frac{8631\,k^{12}}{256}+\frac{261\,k^{14}}{16}-\frac{351\,k^{16}}{64}-$$
$$39\,k^{18}+\frac{381\,k^{20}}{2}+1080\,k^{22}+1260\,k^{24}+$$
$$\left(-\frac{6423\,k^2}{32768}-\frac{16449\,k^4}{4096}-\frac{65967\,k^6}{2048}-\frac{7899\,k^8}{64}-\frac{13575\,k^{10}}{64}-\frac{867\,k^{12}}{8}-\frac{219\,k^{14}}{4}+84\,k^{16}+906\,k^{18}-\right.$$
$$\left.3600\,k^{20}-10080\,k^{22}\right)Q+$$
$$\left(\frac{6423}{65536}+\frac{2859\,k^2}{1024}+\frac{144609\,k^4}{4096}+\frac{13899\,k^6}{64}+\frac{76155\,k^8}{128}+\frac{1713\,k^{10}}{4}-\frac{1383\,k^{12}}{8}+996\,k^{14}-3261\,k^{16}+35280\,k^{20}\right)$$
$$Q^2+\left(-\frac{2141}{4096}-\frac{41201\,k^2}{2048}-\frac{29245\,k^4}{128}-\frac{3857\,k^6}{4}-\frac{4177\,k^8}{4}+\frac{3547\,k^{10}}{4}-2646\,k^{12}+3312\,k^{14}+\right.$$
$$\left.15120\,k^{16}-70560\,k^{18}\right)Q^3+$$
$$\left(\frac{44961}{8192}+\frac{37885\,k^2}{256}+\frac{141747\,k^4}{128}+\frac{25575\,k^6}{16}-\frac{35957\,k^8}{16}+5715\,k^{10}-5130\,k^{12}-25200\,k^{14}+88200\,k^{16}\right)Q^4+$$
$$\left(\frac{987}{128}+\frac{26279\,k^2}{128}+\frac{23501\,k^4}{16}+\frac{10325\,k^6}{8}-6660\,k^8+10242\,k^{10}+15120\,k^{12}-70560\,k^{14}\right)Q^5+$$
$$\left(\frac{1827}{256}+\frac{1551\,k^2}{8}+\frac{23199\,k^4}{16}+1578\,k^6-8511\,k^8+35280\,k^{12}\right)Q^6+$$
$$\left(\frac{63}{16}+\frac{897\,k^2}{8}+942\,k^4+1956\,k^6-3600\,k^8-10080\,k^{10}\right)Q^7+\left(\frac{63}{64}+30\,k^2+\frac{591\,k^4}{2}+1080\,k^6+1260\,k^8\right)Q^8\Bigg)\Bigg/$$
$$\left(\left(1+k^2\right)\left(1+4\,k^2\right)\left(1+9\,k^2\right)\left(1+16\,k^2\right)\left(k^2+\left(\frac{1}{4}-k^2+Q\right)^2\right)^4\right)$$

for n = 3 the generic integrals are

$$\int \frac{e^{-\frac{2\,\mathrm{ArcTan}\left[\frac{1}{9}-k^2+Q,\frac{2k}{3}\right]}{k}}}{\left(\frac{4k^2}{9}+\left(\frac{1}{9}-k^2+Q\right)^2\right)^7} * Q^{-1}\, dQ = \mathrm{gi3i1}[Q,k]$$

gi3i1[Q_, k_] :=

$$\frac{1}{(1+9k^2)^{14}} e^{-\frac{2\,\mathrm{ArcTan}\left[\frac{1}{9}-k^2+Q,\frac{2k}{3}\right]}{k}}$$

$$\Bigg(\Bigg(-\frac{1037663134}{2187}-\frac{54262536991\,k^2}{729}-\frac{142578443075\,k^4}{27}-\frac{2013971369059\,k^6}{9}-6277476508977\,k^8-$$
$$121158290714769\,k^{10}-1589114982108015\,k^{12}-12524766106763205\,k^{14}-149078840821434 81\,k^{16}+$$
$$1083717809333232282\,k^{18}+16809168344807748294\,k^{20}+146811361172584894002\,k^{22}+$$
$$871461285631327019430\,k^{24}+3644612762991560011710\,k^{26}+10608096139325860837122\,k^{28}+$$
$$20433271143079689484662\,k^{30}+23312774968505181944532\,k^{32}+11966977442540110957965\,k^{34}+$$
$$6206891752029071437 47\,k^{36}+15824333275570151072 73\,k^{38}+7748579956601914066395\,k^{40}+$$
$$2848320878258602819363 5\,k^{42}+703471041441740330258 85\,k^{44}+1042519813114131644685 75\,k^{46}+$$
$$702105180260537638257 75\,k^{48}+$$
$$\Bigg(-23003136-\frac{29594947976\,k^2}{9}-\frac{618162235988\,k^4}{3}-7437014691540\,k^6-169780270433400\,k^8-$$
$$2501901474621552\,k^{10}-22485308571670428\,k^{12}-90392435336176164\,k^{14}+286424202527096544\,k^{16}+$$
$$2783478576580776720\,k^{18}-4894156652054207608 8\,k^{20}-93441102936200986903 2\,k^{22}-$$
$$741995419737698405870 4\,k^{24}-342867351151884069118 08\,k^{26}-955724232910184256610 80\,k^{28}-$$
$$149088086463667464535464\,k^{30}-100752141382914914996256\,k^{32}-532412450971703659533 6\,k^{34}-$$
$$722138521242582847479 6\,k^{36}-420708591864808669535 40\,k^{38}-195917526822270972647160\,k^{40}-$$
$$597364640911232741650320\,k^{42}-1063795727667481270087500\,k^{44}-842526216312645165909300\,k^{46}\Bigg)Q+$$
$$\Bigg(-\frac{5801834300}{9}-\frac{249081312830\,k^2}{3}-4510920634434\,k^4-134919839041524\,k^6-2408853341505888\,k^8-$$
$$25460394137585802\,k^{10}-136576206350145018\,k^{12}-20141323438441392\,k^{14}+$$
$$470198025465973423 2\,k^{16}+54784814023354299372\,k^{18}+791288663388954954012\,k^{20}+$$
$$898851481371585135885 6\,k^{22}+614750633632808317810 08\,k^{24}+242348394562972394974812\,k^{26}+$$
$$509885181651270561051996\,k^{28}+445468729679675907437520\,k^{30}+257522838365352467670 12\,k^{32}+$$
$$18208217394463136404158\,k^{34}+109234928636153705842470\,k^{36}+631267016501216923107660\,k^{38}+$$
$$2356930054283365317098160\,k^{40}+5008350285858501819571950\,k^{42}+4633894189719548412501150\,k^{44}\Bigg)$$
$$Q^2+\Bigg(-\frac{38280045328}{3}-1460209478032\,k^2-67391239797540\,k^4-1618810134457788\,k^6-$$
$$21496404173101884\,k^8-147867813320570820\,k^{10}-310924619415248400\,k^{12}+$$
$$2223265390431411600\,k^{14}+14771137162541022000\,k^{16}-141609321560838486960\,k^{18}-$$
$$4969473202774583317944\,k^{20}-60146027682933473430408\,k^{22}-362952259229275678882440\,k^{24}-$$
$$1074734903483159771588472\,k^{26}-1237834046469906131314896\,k^{28}-808979292088180884684 00\,k^{30}-$$
$$34836548952346664793120\,k^{32}-182466749754625675122720\,k^{34}-1282383548205010989970500\,k^{36}-$$
$$5802283363993743520057500\,k^{38}-14510173725384444523993500\,k^{40}-15446313965731828041670500\,k^{42}\Bigg)$$
$$Q^3+\Bigg(-188858752254-19039266645597\,k^2-733163910051087\,k^4-13636683170492679\,k^6-$$
$$125080720990841295\,k^8-455650224647712660\,k^{10}+668158930359205380\,k^{12}+$$
$$11745473470107565140\,k^{14}+86735666213731319760\,k^{16}+180930665504845603161 0\,k^{18}+$$
$$35894411028922142919294\,k^{20}+35042576334719647937398 2\,k^{22}+1530315596233816320891942\,k^{24}+$$
$$2372306369843356254214524\,k^{26}+176373485429344923124980\,k^{28}+558965640056705203069 80\,k^{30}+$$
$$221838814747457055288630\,k^{32}+1862385491862812368302075\,k^{34}+10110078196701149217296025\,k^{36}+$$
$$29137364980812311987696625\,k^{38}+34754206422896613093758625\,k^{40}\Bigg)Q^4+$$
$$\Bigg(-2129130961344-189068190768432\,k^2-5990282486458776\,k^4-82069516393224552\,k^6-$$
$$451530384395023296\,k^8-347907900988091520\,k^{10}+5852089353544491744\,k^{12}+$$
$$34103899300406009760\,k^{14}-132964253745948764352\,k^{16}-1104153476407216644067 2\,k^{18}-$$
$$2125095179052702946857 12\,k^{20}-1523777511314514528338544\,k^{22}-3271449850900910640931392\,k^{24}-$$
$$277466664059896886346240\,k^{26}-747217395306247069005 12\,k^{28}-209039355745991291357280\,k^{30}-$$
$$2080575811774530535512960\,k^{32}-13414605965317294479972720\,k^{34}-43249679104049118516677400\,k^{36}-$$
$$55606730276634580950013800\,k^{38}\Bigg)Q^5+$$
$$\Bigg(-18342648731880-1448464006144476\,k^2-37446685923351420\,k^4-347283153649330560\,k^6-$$

$$\int \frac{e^{-\frac{2\,\text{ArcTan}\left[\frac{1}{9}-k^2+Q,\frac{2k}{3}\right]}{k}}}{\left(\frac{4k^2}{9}+\left(\frac{1}{9}-k^2+Q\right)^2\right)^7} * Q^0\, dQ = \text{gi30}[Q, k]$$

$$\text{gi30}[Q\_, k\_] := e^{-\frac{2\,\text{ArcTan}\left[\frac{1}{9}-k^2+Q,\frac{2k}{3}\right]}{k}}$$

$$\left(\frac{180451625}{10077696}+\frac{120731945 k^2}{139968}+\frac{914149907 k^4}{62208}+\frac{134972035 k^6}{1296}+\frac{429065747 k^8}{1536}+\frac{6049405 k^{10}}{32}+\right.$$
$$\frac{20907 k^{12}}{128}-\frac{31185 k^{14}}{16}+\frac{3007125 k^{16}}{512}+\frac{7577955 k^{18}}{64}-\frac{341007975 k^{20}}{256}+\frac{27621645975 k^{24}}{512}+$$
$$\left(384+\frac{110184151 k^2}{10368}+\frac{17729239 k^4}{192}+\frac{34702063 k^6}{128}+\frac{3026199 k^8}{16}+\frac{107703 k^{10}}{64}-\frac{1136025 k^{12}}{32}+\right.$$
$$\left.\frac{22012155 k^{14}}{64}-\frac{22733865 k^{16}}{16}-\frac{1023023925 k^{18}}{128}+\frac{9207215325 k^{20}}{64}-\frac{82864937925 k^{22}}{128}\right) Q+$$
$$\left(\frac{108788009}{20736}+\frac{21199145 k^2}{288}+\frac{65733107 k^4}{256}+\frac{3084675 k^6}{16}-\frac{1443123 k^8}{128}-\frac{307395 k^{10}}{2}+\right.$$
$$\left.\frac{434830275 k^{12}}{128}-\frac{613814355 k^{14}}{16}+\frac{74680746525 k^{16}}{256}-\frac{46036076625 k^{18}}{32}+\frac{911514317175 k^{20}}{256}\right) Q^2+$$
$$\left(\frac{88286935}{1728}+\frac{28179855 k^2}{128}+\frac{1372305 k^4}{4}-\frac{40451895 k^6}{32}+\frac{308192445 k^8}{32}-\frac{4235836275 k^{10}}{64}+\right.$$
$$\left.\frac{3144851325 k^{12}}{8}-\frac{60358411575 k^{14}}{32}+\frac{414324689625 k^{16}}{64}-\frac{1519190528625 k^{18}}{128}\right) Q^3+$$
$$\left(\frac{190792305}{512}-\frac{31413195 k^2}{32}+\frac{1036994805 k^4}{128}-\frac{830247165 k^6}{16}+\frac{76568018175 k^8}{256}-\frac{47627447175 k^{10}}{32}+\right.$$
$$\left.\frac{766244919825 k^{12}}{128}-\frac{138108229875 k^{14}}{8}+\frac{13672714757625 k^{16}}{512}\right) Q^4+$$
$$\left(\frac{33330825}{16}-\frac{986225625 k^2}{64}+\frac{3379487265 k^4}{32}-\frac{39349433475 k^6}{64}+\frac{11889811395 k^8}{4}-\right.$$
$$\left.\frac{723277914975 k^{10}}{64}+\frac{966757609125 k^{12}}{32}-\frac{2734542951525 k^{14}}{64}\right) Q^5+$$
$$\left(\frac{1151693235}{128}-\frac{744604245 k^2}{8}+\frac{83641257315 k^4}{128}-\frac{55296337635 k^6}{16}+\frac{1740163696425 k^8}{128}-\right.$$
$$\left.\frac{580054565475 k^{10}}{16}+\frac{6380600220225 k^{12}}{128}\right) Q^6+$$
$$\left(\frac{957348315}{32}-\frac{22443376725 k^2}{64}+\frac{18891841815 k^4}{8}-\frac{338620919175 k^6}{32}+\frac{966757609125 k^8}{32}-\right.$$
$$\left.\frac{2734542951525 k^{10}}{64}\right) Q^7+$$
$$\left(\frac{38609680725}{512}-\frac{56493654525 k^2}{64}+\frac{1326862030725 k^4}{256}-\frac{138108229875 k^6}{8}+\frac{13672714757625 k^8}{512}\right) Q^8+$$
$$\left(\frac{2235496725}{16}-\frac{186531362325 k^2}{128}+\frac{414324689625 k^4}{64}-\frac{1519190528625 k^6}{128}\right) Q^9+$$
$$\left(\frac{46036076625}{256}-\frac{46036076625 k^2}{32}+\frac{911514317175 k^4}{256}\right) Q^{10}+\left(\frac{9207215325}{64}-\frac{82864937925 k^2}{128}\right) Q^{11}+$$
$$\left.\frac{27621645975 Q^{12}}{512}\right) \Big/ \left(\left(1+k^2\right)\left(1+4k^2\right)\left(1+9k^2\right)\left(1+16k^2\right)\left(1+25k^2\right)\left(1+36k^2\right)\left(\frac{4k^2}{9}+\left(\frac{1}{9}-k^2+Q\right)^2\right)^6\right)$$

$$\int \frac{e^{-\frac{2\,\mathrm{ArcTan}\left[\frac{1}{9}-k^2+Q,\frac{2k}{3}\right]}{k}}}{\left(\frac{4k^2}{9}+\left(\frac{1}{9}-k^2+Q\right)^2\right)^7} * Q^1\,dQ = \mathrm{gi31}[Q,k]$$

$$\mathrm{gi31}[Q\_,k\_] := e^{-\frac{2\,\mathrm{ArcTan}\left[\frac{1}{9}-k^2+Q,\frac{2k}{3}\right]}{k}} \Bigg(-\frac{32}{81}-\frac{181847767k^2}{10077696}-\frac{45321943k^4}{139968}-\frac{178818541k^6}{62208}-\frac{16731517k^8}{1296}-\frac{120253895k^{10}}{4608}-\frac{504195k^{12}}{32}+$$

$$\frac{20907k^{14}}{128}-\frac{31185k^{16}}{16}+\frac{3007125k^{18}}{512}+\frac{7577955k^{20}}{64}-\frac{341007975k^{22}}{256}+\frac{27621645975k^{26}}{512}+$$

$$\left(384k^2+\frac{110184151k^4}{10368}+\frac{17729239k^6}{192}+\frac{34702063k^8}{128}+\frac{3026199k^{10}}{16}+\frac{107703k^{12}}{64}-\frac{1136025k^{14}}{32}+\right.$$

$$\left.\frac{22012155k^{16}}{64}-\frac{22733865k^{18}}{16}-\frac{1023023925k^{20}}{128}+\frac{9207215325k^{22}}{64}-\frac{82864937925k^{24}}{128}\right)Q+$$

$$\left(\frac{108788009k^2}{20736}+\frac{21199145k^4}{288}+\frac{65733107k^6}{256}+\frac{3084675k^8}{16}-\frac{1443123k^{10}}{128}-\frac{307395k^{12}}{2}+\right.$$

$$\left.\frac{434830275k^{14}}{128}-\frac{613814355k^{16}}{16}+\frac{74680746525k^{18}}{256}-\frac{46036076625k^{20}}{32}+\frac{911514317175k^{22}}{256}\right)Q^2+$$

$$\left(\frac{88286935k^2}{1728}+\frac{28179855k^4}{128}+\frac{1372305k^6}{4}-\frac{40451895k^8}{32}+\frac{308192445k^{10}}{32}-\frac{4235836275k^{12}}{64}+\right.$$

$$\left.\frac{3144851325k^{14}}{8}-\frac{60358411575k^{16}}{32}+\frac{414324689625k^{18}}{64}-\frac{1519190528625k^{20}}{128}\right)Q^3+$$

$$\left(\frac{190792305k^2}{512}-\frac{31413195k^4}{32}+\frac{1036994805k^6}{128}-\frac{830247165k^8}{16}+\frac{76568018175k^{10}}{256}-\right.$$

$$\left.\frac{47627447175k^{12}}{32}+\frac{766244919825k^{14}}{128}-\frac{138108229875k^{16}}{8}+\frac{13672714757625k^{18}}{512}\right)Q^4+$$

$$\left(\frac{33330825k^2}{16}-\frac{986225625k^4}{64}+\frac{3379487265k^6}{32}-\frac{39349433475k^8}{64}+\frac{11889811395k^{10}}{4}-\right.$$

$$\left.\frac{723277914975k^{12}}{64}+\frac{966757609125k^{14}}{32}-\frac{2734542951525k^{16}}{64}\right)Q^5+$$

$$\left(\frac{1151693235k^2}{128}-\frac{744604245k^4}{8}+\frac{83641257315k^6}{128}-\frac{55296337635k^8}{16}+\frac{1740163696425k^{10}}{128}-\right.$$

$$\left.\frac{580054565475k^{12}}{16}+\frac{6380600220225k^{14}}{128}\right)Q^6+$$

$$\left(\frac{957348315k^2}{32}-\frac{22443376725k^4}{64}+\frac{18891841815k^6}{8}-\frac{338620919175k^8}{32}+\frac{966757609125k^{10}}{32}-\right.$$

$$\left.\frac{2734542951525k^{12}}{64}\right)Q^7+$$

$$\left(\frac{38609680725k^2}{512}-\frac{56493654525k^4}{64}+\frac{1326862030725k^6}{256}-\frac{138108229875k^8}{8}+\frac{13672714757625k^{10}}{512}\right)Q^8+$$

$$\left(\frac{2235496725k^2}{16}-\frac{186531362325k^4}{128}+\frac{414324689625k^6}{64}-\frac{1519190528625k^8}{128}\right)Q^9+$$

$$\left(\frac{46036076625k^2}{256}-\frac{46036076625k^4}{32}+\frac{911514317175k^6}{256}\right)Q^{10}+\left(\frac{9207215325k^2}{64}-\frac{82864937925k^4}{128}\right)Q^{11}+$$

$$\frac{27621645975k^2Q^{12}}{512}\Bigg) \Bigg/ \left(\left(1+k^2\right)\left(1+4k^2\right)\left(1+9k^2\right)\left(1+16k^2\right)\left(1+25k^2\right)\left(1+36k^2\right)\left(\frac{4k^2}{9}+\left(\frac{1}{9}-k^2+Q\right)^2\right)^6\right)$$

$$\int \frac{e^{-\frac{2\,\text{ArcTan}\left[\frac{1}{9}-k^2+Q,\,\frac{2k}{3}\right]}{k}}}{\left(\frac{4k^2}{9}+\left(\frac{1}{9}-k^2+Q\right)^2\right)^7} * Q^2\, dQ = \text{gi32}[Q, k]$$

$$\begin{aligned}
&\text{gi32}[Q_, k_] := \\
&e^{-\frac{2\,\text{ArcTan}\left[\frac{1}{9}-k^2+Q,\,\frac{2k}{3}\right]}{k}} \\
&\Bigg(\frac{9889819}{816293376}+\frac{4581403\,k^2}{7558272}+\frac{42328297\,k^4}{3359232}+\frac{29337397\,k^6}{209952}+\frac{109405375\,k^8}{124416}+\frac{1174829\,k^{10}}{384}+ \\
&\quad \frac{23828573\,k^{12}}{4608}+\frac{5733\,k^{14}}{2}+\frac{46683\,k^{16}}{512}-\frac{202095\,k^{18}}{128}+\frac{4691115\,k^{20}}{512}+\frac{2066715\,k^{22}}{32}-\frac{651015225\,k^{24}}{512}+ \\
&\quad \frac{279006525\,k^{26}}{128}+\frac{27621645975\,k^{28}}{512}+ \\
&\quad \left(-\frac{9889819\,k^2}{839808}-\frac{17598599\,k^4}{46656}-\frac{1297241\,k^6}{288}-\frac{41801351\,k^8}{1728}-\frac{20908693\,k^{10}}{384}-\frac{1096083\,k^{12}}{32}+\right. \\
&\qquad \frac{1269\,k^{14}}{2}-\frac{742365\,k^{16}}{32}+\frac{35527815\,k^{18}}{128}-\frac{101269035\,k^{20}}{64}-\frac{93002175\,k^{22}}{32}+\frac{7533176175\,k^{24}}{64}- \\
&\qquad \left.\frac{82864937925\,k^{26}}{128}\right) Q + \\
&\quad \left(\frac{9889819}{1679616}+\frac{4581403\,k^2}{15552}+\frac{88216993\,k^4}{10368}+\frac{145495981\,k^6}{1728}+\frac{67724001\,k^8}{256}+\frac{6149253\,k^{10}}{32}-\right. \\
&\qquad \frac{874989\,k^{12}}{64}-\frac{1903905\,k^{14}}{32}+\frac{556668045\,k^{16}}{256}-\frac{1804242195\,k^{18}}{64}+\frac{30411711225\,k^{20}}{128}- \\
&\qquad \left.\frac{82864937925\,k^{22}}{64}+\frac{911514317175\,k^{24}}{256}\right) Q^2 + \\
&\quad \left(\frac{8026085}{139968}+\frac{71894095\,k^2}{31104}+\frac{34774375\,k^4}{576}+\frac{267952915\,k^6}{1152}+\frac{9689915\,k^8}{32}-\frac{60753375\,k^{10}}{64}+\right. \\
&\qquad \frac{236738295\,k^{12}}{32}-\frac{3354803325\,k^{14}}{64}+\frac{20746374075\,k^{16}}{64}-\frac{209657903175\,k^{18}}{128}+\frac{383633971875\,k^{20}}{64}- \\
&\qquad \left.\frac{1519190528625\,k^{22}}{128}\right) Q^3 + \\
&\quad \left(\frac{1927195}{4608}+\frac{16075535\,k^2}{1152}+\frac{175140205\,k^4}{512}-\frac{11401065\,k^6}{16}+\frac{1623199095\,k^8}{256}-\frac{2654482185\,k^{10}}{64}+\right. \\
&\qquad \left.\frac{62893253925\,k^{12}}{256}-\frac{2531725875\,k^{14}}{2}+\frac{2723196686175\,k^{16}}{512}-\frac{2071623448125\,k^{18}}{128}+\frac{13672714757625\,k^{20}}{512}\right) Q^4 + \\
&\quad \left(\frac{112225}{48}+\frac{4279925\,k^2}{64}+\frac{50530815\,k^4}{32}-\frac{378649485\,k^6}{32}+\frac{2691303975\,k^8}{32}-\frac{2029678155\,k^{10}}{4}+\right. \\
&\qquad \left.\frac{81591841485\,k^{12}}{32}-\frac{324112579875\,k^{14}}{32}+\frac{911514317175\,k^{16}}{32}-\frac{2734542951525\,k^{18}}{64}\right) Q^5 + \\
&\quad \left(\frac{1292585}{128}+\frac{8290485\,k^2}{32}+\frac{191051595\,k^4}{32}-\frac{2257677765\,k^6}{32}+\frac{33860369655\,k^8}{64}-\frac{94317294645\,k^{10}}{32}+\right. \\
&\qquad \left.\frac{389958119775\,k^{12}}{32}-\frac{1095658623675\,k^{14}}{32}+\frac{6380600220225\,k^{16}}{128}\right) Q^6 + \\
&\quad \left(\frac{1074465}{32}+\frac{52172505\,k^2}{64}+\frac{588758625\,k^4}{32}-\frac{17097014655\,k^6}{64}+\frac{62970739335\,k^8}{32}-\frac{602189083125\,k^{10}}{64}+\right. \\
&\qquad \left.\frac{911514317175\,k^{12}}{32}-\frac{2734542951525\,k^{14}}{64}\right) Q^7 + \\
&\quad \left(\frac{43332975}{512}+\frac{263187225\,k^2}{128}+\frac{23327471475\,k^4}{512}-\frac{22165518375\,k^6}{32}+\frac{2311941068325\,k^8}{512}-\right. \\
&\qquad \left.\frac{2071623448125\,k^{10}}{128}+\frac{13672714757625\,k^{12}}{512}\right) Q^8 + \\
&\quad \left(\frac{2508975}{16}+\frac{513234225\,k^2}{128}+\frac{5638687425\,k^4}{64}-1209028275\,k^6+\frac{383633971875\,k^8}{64}-\frac{1519190528625\,k^{10}}{128}\right) Q^9 + \\
&\quad \left(\frac{51667875}{256}+\frac{361675125\,k^2}{64}+\frac{16089376275\,k^4}{128}-\frac{82864937925\,k^6}{64}+\frac{911514317175\,k^8}{256}\right) Q^{10} + \\
&\quad \left(\frac{10333575}{64}+\frac{651015225\,k^2}{128}+\frac{7533176175\,k^4}{64}-\frac{82864937925\,k^6}{128}\right) Q^{11} + \\
&\quad \left(\frac{31000725}{512}+\frac{279006525\,k^2}{128}+\frac{27621645975\,k^4}{512}\right) Q^{12}\Bigg) \Big/ \\
&\left((1+k^2)\,(1+4k^2)\,(1+9k^2)\,(1+16k^2)\,(1+25k^2)\,(1+36k^2)\left(\frac{4k^2}{9}+\left(\frac{1}{9}-k^2+Q\right)^2\right)^6\right)
\end{aligned}$$

$$\int \frac{e^{-\frac{2\,\mathrm{ArcTan}\left[\frac{1}{9}-k^2+Q,\frac{2k}{3}\right]}{k}}}{\left(\frac{4k^2}{9}+\left(\frac{1}{9}-k^2+Q\right)^2\right)^7} * Q^3\, dQ = \mathrm{gi33}[Q, k]$$

gi33[Q_, k_] :=

$$e^{-\frac{2\,\mathrm{ArcTan}\left[\frac{1}{9}-k^2+Q,\frac{2k}{3}\right]}{k}}$$

$$\Bigg(-\frac{1605217}{3673320192}-\frac{6933229 k^2}{272097792}-\frac{1801411 k^4}{2834352}-\frac{266258483 k^6}{30233088}-\frac{123493201 k^8}{1679616}-\frac{46490311 k^{10}}{124416}-$$
$$\frac{11440009 k^{12}}{10368}-\frac{7625851 k^{14}}{4608}-\frac{217989 k^{16}}{256}-\frac{18783 k^{18}}{512}-\frac{44307 k^{20}}{64}+\frac{6834375 k^{22}}{512}-\frac{10333575 k^{24}}{256}-$$
$$\frac{539412615 k^{26}}{512}+\frac{837019575 k^{28}}{128}+\frac{27621645975 k^{30}}{512}+$$
$$\left(\frac{1605217 k^2}{3779136}+\frac{14378819 k^4}{839808}+\frac{3209635 k^6}{11664}+\frac{34529773 k^8}{15552}+\frac{15918035 k^{10}}{1728}+\frac{6739247 k^{12}}{384}+\right.$$
$$\frac{41763 k^{14}}{4}-\frac{29295 k^{16}}{32}-\frac{98901 k^{18}}{64}+\frac{17616285 k^{20}}{128}-\frac{26867295 k^{22}}{16}+\frac{390609135 k^{24}}{64}+$$
$$\left.\frac{4185097875 k^{26}}{64}-\frac{82864937925 k^{28}}{128}\right) Q +$$
$$\left(-\frac{1605217}{7558272}-\frac{6933229 k^2}{559872}-\frac{12282887 k^4}{31104}-\frac{86775635 k^6}{15552}-\frac{15007553 k^8}{432}-\frac{66394297 k^{10}}{768}-\right.$$
$$\frac{3517341 k^{12}}{64}-\frac{114237 k^{14}}{8}+\frac{9544311 k^{16}}{128}+\frac{46419075 k^{18}}{256}-\frac{1312364025 k^{20}}{128}+\frac{8686403145 k^{22}}{64}-$$
$$\left.\frac{64450507275 k^{24}}{64}+\frac{911514317175 k^{26}}{256}\right) Q^2 +$$
$$\left(\frac{1605217}{629856}+\frac{19228537 k^2}{69984}+\frac{228511237 k^4}{31104}+\frac{412053359 k^6}{5184}+\frac{294559715 k^8}{1152}+\frac{1890163 k^{10}}{8}-\right.$$
$$\frac{26804025 k^{12}}{64}+\frac{113408505 k^{14}}{32}-\frac{1788845715 k^{16}}{64}+\frac{6313814325 k^{18}}{32}-\frac{148834480725 k^{20}}{128}+$$
$$\left.\frac{322252536375 k^{22}}{64}-\frac{1519190528625 k^{24}}{128}\right) Q^3 +$$
$$\left(\frac{385439}{20736}+\frac{77755121 k^2}{41472}+\frac{46661395 k^4}{1152}+\frac{149959429 k^6}{512}-\frac{32337567 k^8}{128}+\frac{840108105 k^{10}}{256}-\right.$$
$$\frac{368352765 k^{12}}{16}+\frac{38075221665 k^{14}}{256}-\frac{217738758825 k^{16}}{256}+\frac{2064183274125 k^{18}}{512}-\frac{1795406988375 k^{20}}{128}+$$
$$\left.\frac{13672714757625 k^{22}}{512}\right) Q^4 +$$
$$\left(\frac{22445}{216}+\frac{2876035 k^2}{288}+\frac{11405923 k^4}{64}+\frac{5839101 k^6}{8}-\frac{90154377 k^8}{16}+\frac{733852953 k^{10}}{16}-\right.$$
$$\left.\frac{9964026675 k^{12}}{32}+\frac{14051595285 k^{14}}{8}-\frac{125757541035 k^{16}}{16}+\frac{801027733275 k^{18}}{32}-\frac{2734542951525 k^{20}}{64}\right) Q^5 +$$
$$\left(\frac{258517}{576}+\frac{5351619 k^2}{128}+\frac{41132091 k^4}{64}+\frac{58682043 k^6}{64}-\frac{1986187959 k^8}{64}+\frac{9693276075 k^{10}}{32}-\right.$$
$$\left.\frac{127540427175 k^{12}}{64}+\frac{605313956205 k^{14}}{64}-\frac{966757609125 k^{16}}{32}+\frac{6380600220225 k^{18}}{128}\right) Q^6 +$$
$$\left(\frac{23877}{16}+136962 k^2+\frac{123753987 k^4}{64}-\frac{29612709 k^6}{32}-\frac{7523990775 k^8}{64}+\frac{19722661245 k^{10}}{16}-\right.$$
$$\left.\frac{456994087515 k^{12}}{64}+\frac{801027733275 k^{14}}{32}-\frac{2734542951525 k^{16}}{64}\right) Q^7 +$$
$$\left(\frac{962955}{256}+\frac{176787765 k^2}{512}+\frac{309879675 k^4}{64}-\frac{2912460705 k^6}{512}-\frac{87618382425 k^8}{256}+\frac{1652927656275 k^{10}}{512}-\right.$$
$$\left.\frac{1795406988375 k^{12}}{128}+\frac{13672714757625 k^{14}}{512}\right) Q^8 +$$
$$\left(\frac{55755}{8}+\frac{41512905 k^2}{64}+\frac{1246076055 k^4}{128}-\frac{65445975 k^6}{16}-\frac{46966098375 k^8}{64}+\frac{322252536375 k^{10}}{64}-\right.$$
$$\left.\frac{1519190528625 k^{12}}{128}\right) Q^9 +$$
$$\left(\frac{1148175}{128}+\frac{219301425 k^2}{256}+\frac{1862110215 k^4}{128}+\frac{762617835 k^6}{32}-\frac{64450507275 k^8}{64}+\frac{911514317175 k^{10}}{256}\right) Q^{10} +$$
$$\left(\frac{229635}{32}+\frac{22733865 k^2}{32}+\frac{1804242195 k^4}{128}+\frac{4185097875 k^6}{64}-\frac{82864937925 k^8}{128}\right) Q^{11} +$$
$$\left(\frac{688905}{256}+\frac{142603335 k^2}{512}+\frac{837019575 k^4}{128}+\frac{27621645975 k^6}{512}\right) Q^{12}\Bigg) \Big/$$
$$\left((1+k^2)\,(1+4k^2)\,(1+9k^2)\,(1+16k^2)\,(1+25k^2)\,(1+36k^2)\left(\frac{4k^2}{9}+\left(\frac{1}{9}-k^2+Q\right)^2\right)^6\right)$$

$$\int \frac{e^{-\frac{2\,\mathrm{ArcTan}\left[\frac{1}{9}-k^2+Q,\frac{2k}{3}\right]}{k}}}{\left(\frac{4k^2}{9}+\left(\frac{1}{9}-k^2+Q\right)^2\right)^7} * Q^4\, dQ = \mathrm{gi34}[Q, k]$$

gi34[Q_, k_] :=

$$e^{-\frac{2\,\mathrm{ArcTan}\left[\frac{1}{9}-k^2+Q,\frac{2k}{3}\right]}{k}}$$

$$\Bigg(\frac{385439}{22039921152}+\frac{3342029\,k^2}{2754990144}+\frac{1873723\,k^4}{51018336}+\frac{21577097\,k^6}{34012224}+\frac{51789811\,k^8}{7558272}+\frac{19991561\,k^{10}}{419904}+\frac{90797\,k^{12}}{432}+\frac{961591\,k^{14}}{1728}+\frac{197137\,k^{16}}{256}+\frac{24663\,k^{18}}{64}-\frac{3987\,k^{20}}{32}+\frac{60507\,k^{22}}{64}+\frac{1089855\,k^{24}}{128}-\frac{10792845\,k^{26}}{64}-\frac{2066715\,k^{28}}{8}+\frac{837019575\,k^{30}}{64}+\frac{27621645975\,k^{32}}{512}+$$

$$\left(-\frac{385439\,k^2}{22674816}-\frac{9899165\,k^4}{11337408}-\frac{46873093\,k^6}{2519424}-\frac{14768065\,k^8}{69984}-\frac{42141631\,k^{10}}{31104}-\frac{8288483\,k^{12}}{1728}-\frac{1051015\,k^{14}}{128}-\frac{73173\,k^{16}}{16}-\frac{139455\,k^{18}}{128}+\frac{990711\,k^{20}}{64}-\frac{8868285\,k^{22}}{128}-\frac{29622915\,k^{24}}{32}+\frac{1791841905\,k^{26}}{128}-\frac{837019575\,k^{28}}{64}-\frac{82864937925\,k^{30}}{128}\right)Q+$$

$$\left(\frac{385439}{45349632}+\frac{3342029\,k^2}{5668704}+\frac{35761153\,k^4}{1679616}+\frac{1032607\,k^6}{2592}+\frac{240665011\,k^8}{62208}+\frac{4080163\,k^{10}}{216}+\frac{31223407\,k^{12}}{768}+\frac{401607\,k^{14}}{16}-\frac{1027161\,k^{16}}{256}+\frac{2827791\,k^{18}}{32}-\frac{262210365\,k^{20}}{256}+\frac{194960115\,k^{22}}{32}+\frac{3540282795\,k^{24}}{256}-\frac{9207215325\,k^{26}}{16}+\frac{911514317175\,k^{28}}{256}\right)Q^2+$$

$$\left(-\frac{385439}{3779136}-\frac{91630925\,k^2}{7558272}-\frac{87273431\,k^4}{209952}-\frac{300502855\,k^6}{46656}-\frac{236096093\,k^8}{5184}-\frac{47319445\,k^{10}}{384}-\frac{1368181\,k^{12}}{16}-\frac{26325\,k^{14}}{32}+\frac{13401855\,k^{16}}{64}-\frac{540156195\,k^{18}}{128}+\frac{1817561025\,k^{20}}{32}-\frac{35392494375\,k^{22}}{64}+\frac{230180383125\,k^{24}}{64}-\frac{1519190528625\,k^{26}}{128}\right)Q^3+$$

$$\left(\frac{385439}{124416}+\frac{931867\,k^2}{3888}+\frac{424945321\,k^4}{62208}+\frac{130906931\,k^6}{1728}+\frac{405319309\,k^8}{1536}+\frac{2178099\,k^{10}}{16}+\frac{68439465\,k^{12}}{128}-\frac{165355425\,k^{14}}{32}+\frac{23635750995\,k^{16}}{512}-\frac{2903734575\,k^{18}}{8}+\frac{597166965675\,k^{20}}{256}-\frac{690541149375\,k^{22}}{64}+\frac{13672714757625\,k^{24}}{512}\right)Q^4+$$

$$\left(\frac{22445}{1296}+\frac{6518275\,k^2}{5184}+\frac{27725803\,k^4}{864}+\frac{50581165\,k^6}{192}+\frac{130347\,k^8}{2}-\frac{5168205\,k^{10}}{32}+\frac{135246267\,k^{12}}{16}-\frac{3181680405\,k^{14}}{32}+\frac{12890101455\,k^{16}}{16}-\frac{308971825785\,k^{18}}{64}+\frac{635297857425\,k^{20}}{32}-\frac{2734542951525\,k^{22}}{64}\right)Q^5+$$

$$\left(\frac{258517}{3456}+\frac{562723\,k^2}{108}+\frac{15693573\,k^4}{128}+\frac{5877179\,k^6}{8}-\frac{175763637\,k^8}{64}+\frac{42337323\,k^{10}}{8}+\frac{4000318245\,k^{12}}{64}-\frac{6789158775\,k^{14}}{8}+\frac{742200757515\,k^{16}}{128}-\frac{193351521825\,k^{18}}{8}+\frac{6380600220225\,k^{20}}{128}\right)Q^6+$$

$$\left(\frac{7959}{32}+\frac{1086855\,k^2}{64}+\frac{6109341\,k^4}{16}+1755810\,k^6-\frac{59529897\,k^8}{4}+\frac{989803395\,k^{10}}{32}+\frac{5904604755\,k^{12}}{16}-\frac{32866968645\,k^{14}}{8}+\frac{635297857425\,k^{16}}{32}-\frac{2734542951525\,k^{18}}{64}\right)Q^7+$$

$$\left(\frac{320985}{512}+\frac{2740185\,k^2}{64}+\frac{122478615\,k^4}{128}+\frac{257046615\,k^6}{64}-\frac{11951200485\,k^8}{256}+\frac{3069071775\,k^{10}}{64}+\frac{195769578375\,k^{12}}{128}-\frac{690541149375\,k^{14}}{64}+\frac{13672714757625\,k^{16}}{512}\right)Q^8+$$

$$\left(\frac{18585}{16}+\frac{10343655\,k^2}{128}+\frac{119384685\,k^4}{64}+\frac{1161519345\,k^6}{128}-\frac{2963439675\,k^8}{32}-\frac{15882704775\,k^{10}}{128}+\frac{230180383125\,k^{12}}{64}-\frac{1519190528625\,k^{14}}{128}\right)Q^9+$$

$$\left(\frac{382725}{256}+\frac{3444525\,k^2}{32}+\frac{678877605\,k^4}{256}+\frac{554568525\,k^6}{32}-\frac{25104387105\,k^8}{256}-\frac{9207215325\,k^{10}}{16}+\frac{911514317175\,k^{12}}{256}\right)Q^{10}+$$

$$\left(\frac{76545}{64}+\frac{11558295\,k^2}{128}+\frac{77846265\,k^4}{32}+\frac{1407432915\,k^6}{64}-\frac{837019575\,k^8}{64}-\frac{82864937925\,k^{10}}{128}\right)Q^{11}+$$

$$\left(\frac{229635}{512}+\frac{1148175\,k^2}{32}+\frac{274873095\,k^4}{256}+\frac{837019575\,k^6}{64}+\frac{27621645975\,k^8}{512}\right)Q^{12}\Bigg)\Bigg/$$

$$\left((1+k^2)(1+4k^2)(1+9k^2)(1+16k^2)(1+25k^2)(1+36k^2)\left(\frac{4k^2}{9}+\left(\frac{1}{9}-k^2+Q\right)^2\right)^6\right)$$

We have computed generic integrals for $n = 4$ as well. However, they are not used in this work and are therefore omitted.

APPENDIX D: LIST OF $IQ_{nl}\left(Q,W\right)$ FUNCTIONS

The linear combinations of "generic integrals" for each subshell are presented here. Note that these can be expressed in terms incomplete Beta functions instead of Hypergeometric functions. These have been so simplified from Hypergeometric to incomplete Beta functions.

IQ10[W,Q]----1s

IQ10[W_, Q_] :=

$$\frac{1}{W^5}\, e^{-\frac{2\,\text{ArcTan}[2+Q-W,\,2\sqrt{-1+W}]}{\sqrt{-1+W}}} \left(\frac{1}{\left((Q-W)^2+4Q\right)^2} \left(Q^4\left(-\frac{64}{3}+\frac{16\,W}{3}+\frac{4\,W^2}{3}+W^3\right) + Q^3\left(-\frac{512}{3}+\frac{320\,W}{3}-\frac{16\,W^2}{3}+\frac{20\,W^3}{3}-4\,W^4\right) + Q^2\left(-\frac{1024}{3}+256\,W-64\,W^2+\frac{128\,W^3}{3}-20\,W^4+6\,W^5\right) + Q\left(-\frac{1024\,W}{3}+256\,W^2+\frac{64\,W^3}{3}-32\,W^4+\frac{44\,W^5}{3}-4\,W^6\right) - \frac{256\,W^3}{3}+\frac{256\,W^4}{3}+\frac{16\,W^5}{3}-\frac{8\,W^6}{3}+W^7\right) - \frac{64}{3}\left(e^{2\,i\,\text{ArcTan}[Q(-2+W)-W^2,\,2Q\sqrt{-1+W}]}\right)^{-\frac{i}{\sqrt{-1+W}}} \left(\text{Beta}\left[e^{-2\,i\,\text{ArcTan}[Q(-2+W)-W^2,\,2Q\sqrt{-1+W}]},\,1-\frac{i}{\sqrt{-1+W}},\,0\right] + \text{Beta}\left[e^{2\,i\,\text{ArcTan}[Q(-2+W)-W^2,\,2Q\sqrt{-1+W}]},\,1+\frac{i}{\sqrt{-1+W}},\,0\right]\right)\right)$$

IQ20[W,Q]----2s

$$IQ20[W\_, Q\_] := \frac{1}{W^6} e^{-\frac{4\,\mathrm{ArcTan}[1+2Q-2W,\sqrt{-1+4W}]}{\sqrt{-1+4W}}}$$

$$\Bigg(\frac{1}{((Q-W)^2+Q)^4}\Bigg(Q^8\left(-1+\frac{2W}{3}+\frac{2W^2}{3}+\frac{W^3}{3}+W^4\right)+Q^7\left(-4+\frac{32W}{3}-\frac{20W^2}{3}-\frac{10W^3}{3}+\frac{10W^4}{3}-8W^5\right)+$$

$$Q^6\left(-6+28W-56W^2+\frac{115W^3}{3}+21W^4-\frac{86W^5}{3}+28W^6\right)+$$

$$Q^5\left(-4+\frac{80W}{3}-\frac{292W^2}{3}+\frac{532W^3}{3}-\frac{308W^4}{3}-74W^5+\frac{250W^6}{3}-56W^7\right)+$$

$$Q^4\left(-1+\frac{26W}{3}-\frac{170W^2}{3}+\frac{575W^3}{3}-315W^4+\frac{496W^5}{3}+131W^6-\frac{380W^7}{3}+70W^8\right)+$$

$$Q^3\left(-8W^2+\frac{166W^3}{3}-190W^4+\frac{988W^5}{3}-\frac{2818W^6}{15}-\frac{374W^7}{3}+\frac{334W^8}{3}-56W^9\right)+$$

$$Q^2\left(-W^3-\frac{37W^4}{3}+\frac{262W^5}{3}-\frac{961W^6}{5}+\frac{743W^7}{5}+\frac{193W^8}{3}-\frac{170W^9}{3}+28W^{10}\right)+$$

$$Q\left(-2W^5-\frac{26W^6}{3}+\frac{248W^7}{5}-\frac{1054W^8}{15}-\frac{50W^9}{3}+\frac{46W^{10}}{3}-8W^{11}\right)-\frac{23W^7}{15}-\frac{26W^8}{15}+\frac{218W^9}{15}+$$

$$\frac{5W^{10}}{3}-\frac{5W^{11}}{3}+W^{12}\Bigg)-\left(2+\frac{8}{3}W\right)\left(e^{2i\,\mathrm{ArcTan}[-Q+2QW-2W^2,Q\sqrt{-1+4W}]}\right)^{-\frac{2i}{\sqrt{-1+4W}}}$$

$$\left(\mathrm{Beta}\left[e^{-2i\,\mathrm{ArcTan}[-Q+2QW-2W^2,Q\sqrt{-1+4W}]},1-\frac{2i}{\sqrt{-1+4W}},0\right]+\right.$$

$$\left.\mathrm{Beta}\left[e^{2i\,\mathrm{ArcTan}[-Q+2QW-2W^2,Q\sqrt{-1+4W}]},1+\frac{2i}{\sqrt{-1+4W}},0\right]\right)\Bigg)$$

IQ21[W,Q]----2p

$$\text{IQ21}[W\_,Q\_]:=\frac{1}{W^7}e^{-\frac{4\,\text{ArcTan}[1+2Q-2W,\sqrt{-1+4W}]}{\sqrt{-1+4W}}}$$

$$\left(\frac{1}{((Q-W)^2+Q)^4}\left(Q^8\left(-\frac{2}{3}+\frac{W}{3}+\frac{2W^2}{3}+W^4+3W^5\right)+Q^7\left(-\frac{8}{3}+\frac{20W}{3}-\frac{8W^2}{3}-\frac{16W^3}{3}+6W^4+10W^5-24W^6\right)+\right.\right.$$

$$Q^6\left(-4+18W-\frac{100W^2}{3}+14W^3+\frac{101W^4}{3}+7W^5-86W^6+84W^7\right)+$$

$$Q^5\left(-\frac{8}{3}+\frac{52W}{3}-\frac{184W^2}{3}+\frac{308W^3}{3}-28W^4-48W^5-110W^6+250W^7-168W^8\right)+$$

$$Q^4\left(-\frac{2}{3}+\frac{17W}{3}-\frac{110W^2}{3}+120W^3-\frac{535W^4}{3}+83W^5-8W^6+253W^7-380W^8+210W^9\right)+$$

$$Q^3\left(-\frac{16W^2}{3}+36W^3-\frac{358W^4}{3}+\frac{626W^5}{3}-132W^6+\frac{266W^7}{5}-262W^8+334W^9-168W^{10}\right)+$$

$$Q^2\left(-\frac{2W^3}{3}-\frac{25W^4}{3}+\frac{181W^5}{3}-\frac{382W^6}{3}+\frac{491W^7}{5}-\frac{469W^8}{15}+137W^9-170W^{10}+84W^{11}\right)+$$

$$Q\left(-\frac{4W^5}{3}-\frac{10W^6}{3}+\frac{122W^7}{3}-\frac{208W^8}{5}+\frac{74W^9}{15}-34W^{10}+46W^{11}-24W^{12}\right)-\frac{2W^7}{3}+\frac{13W^8}{15}+$$

$$\left.\frac{176W^9}{15}+\frac{2W^{10}}{15}+3W^{11}-5W^{12}+3W^{13}\right)-$$

$$\left(\frac{4}{3}+2W\right)\left(e^{2i\,\text{ArcTan}[-Q+2QW-2W^2,Q\sqrt{-1+4W}]}\right)^{-\frac{2i}{\sqrt{-1+4W}}}$$

$$\left(\text{Beta}\left[e^{-2i\,\text{ArcTan}[-Q+2QW-2W^2,Q\sqrt{-1+4W}]},1-\frac{2i}{\sqrt{-1+4W}},0\right]+\right.$$

$$\left.\left.\text{Beta}\left[e^{2i\,\text{ArcTan}[-Q+2QW-2W^2,Q\sqrt{-1+4W}]},1+\frac{2i}{\sqrt{-1+4W}},0\right]\right)\right)$$

IQ30[W,Q]----3s

$$\text{IQ30}[W\_, Q\_] := \frac{1}{W^8} e^{-\frac{6\,\text{ArcTan}[2+9Q-9W,\,2\sqrt{-1+9W}]}{\sqrt{-1+9W}}}$$

$$\Bigg(\frac{1}{\left((Q-W)^2+\frac{4}{9}Q\right)^6}\Bigg(Q^{12}\left(-\frac{8192}{1594323}-\frac{1024W}{19683}+\frac{1792W^3}{2187}+\frac{16W^4}{81}+\frac{4W^5}{27}+W^6\right)+$$

$$Q^{11}\left(-\frac{65536}{4782969}-\frac{40960W}{531441}+\frac{34816W^2}{59049}+\frac{1280W^3}{729}-\frac{7744W^4}{729}-\frac{16W^5}{9}+\frac{20W^6}{9}-12W^7\right)+$$

$$Q^{10}\left(-\frac{655360}{43046721}-\frac{81920W}{4782969}+\frac{507904W^2}{531441}-\frac{102400W^3}{59049}-\frac{129280W^4}{6561}+\frac{47488W^5}{729}+\frac{1136W^6}{81}-\frac{284W^7}{9}+66W^8\right)+$$

$$Q^9\left(-\frac{10485760}{1162261467}+\frac{1310720W}{43046721}+\frac{819200W^2}{1594323}-\frac{6410240W^3}{1594323}-\frac{152576W^4}{59049}+\frac{220928W^5}{2187}-\frac{523136W^6}{2187}-\frac{6208W^7}{81}+\frac{4340W^8}{27}-220W^9\right)+$$

$$Q^8\left(-\frac{10485760}{3486784401}+\frac{9175040W}{387420489}+\frac{2621440W^2}{43046721}-\frac{10158080W^3}{4782969}+\frac{4812800W^4}{531441}+\frac{1690624W^5}{59049}-\frac{1991936W^6}{6561}+\frac{425408W^7}{729}+\frac{6944W^8}{27}-\frac{1400W^9}{3}+495W^{10}\right)+$$

$$Q^7\left(-\frac{16777216}{31381059609}+\frac{23068672W}{3486784401}-\frac{13107200W^2}{387420489}-\frac{13697024W^3}{43046721}+\frac{2441216W^4}{531441}-\frac{7147520W^5}{531441}-\frac{4554752W^6}{59049}+\frac{1290496W^7}{2187}-\frac{3681536W^8}{3645}-\frac{4960W^9}{9}+\frac{2648W^{10}}{3}-792W^{11}\right)+$$

$$Q^6\left(-\frac{33554432}{847288609443}+\frac{20971520W}{31381059609}-\frac{4194304W^2}{387420489}+\frac{5242880W^3}{129140163}+\frac{21561344W^4}{43046721}-\frac{30736384W^5}{4782969}+\frac{9605120W^6}{531441}+\frac{6149120W^7}{59049}-\frac{76252928W^8}{98415}+\frac{4725632W^9}{3645}+\frac{21280W^{10}}{27}-\frac{10360W^{11}}{9}+924W^{12}\right)+$$

$$Q^5\left(-\frac{8388608W^2}{10460353203}+\frac{36700160W^3}{3486784401}-\frac{24903680W^4}{387420489}-\frac{4653056W^5}{14348907}+\frac{10190848W^6}{1594323}-\frac{12836864W^7}{531441}-\frac{48446464W^8}{688905}+\frac{17610496W^9}{25515}-\frac{4608896W^{10}}{3645}-\frac{20800W^{11}}{27}+\frac{3176W^{12}}{3}-792W^{13}\right)+$$

$$Q^4\left(-\frac{8388608W^4}{1162261467}+\frac{27262976W^5}{387420489}-\frac{1835008W^6}{43046721}-\frac{19054592W^7}{4782969}+\frac{451002368W^8}{18600435}+\frac{6152192W^9}{688905}-\frac{18308096W^{10}}{45927}+\frac{683264W^{11}}{729}+\frac{13936W^{12}}{27}-\frac{2060W^{13}}{3}+495W^{14}\right)+$$

$$Q^3\left(-\frac{2097152W^5}{10460353203}-\frac{37486592W^6}{1162261467}+\frac{3211264W^7}{14348907}+\frac{17825792W^8}{18600435}-\frac{791130112W^9}{55801305}+\frac{8711168W^{10}}{413343}+\frac{17503232W^{11}}{137781}-\frac{1122880W^{12}}{2187}-\frac{18832W^{13}}{81}+\frac{8300W^{14}}{27}-220W^{15}\right)+$$

$$Q^2\left(-\frac{524288W^7}{387420489}-\frac{3604480W^8}{43046721}+\frac{14974976W^9}{55801305}+\frac{1912832W^{10}}{531441}-\frac{4507648W^{11}}{295245}-\frac{295936W^{12}}{45927}+\frac{26368W^{13}}{135}+\frac{1808W^{14}}{27}-\frac{812W^{15}}{9}+66W^{16}\right)+$$

$$Q\left(-\frac{6160384W^9}{1506635235}-\frac{19775488W^{10}}{167403915}+\frac{335872W^{11}}{6200145}+\frac{44032W^{12}}{10935}-\frac{687616W^{13}}{76545}-\frac{166912W^{14}}{3645}-\frac{896W^{15}}{81}+\frac{140W^{16}}{9}-12W^{17}\right)-\frac{1540096W^{11}}{502211745}-\frac{348160W^{12}}{3720087}-\frac{603136W^{13}}{2066715}+\frac{1439488W^{14}}{688905}+\frac{54208W^{15}}{10935}+\frac{64W^{16}}{81}-\frac{32W^{17}}{27}+W^{18}\Bigg)-$$

$$\frac{64}{81}\left(\frac{128}{6561}+\frac{208W}{729}+\frac{32W^2}{27}+W^3\right)\left(e^{2i\,\text{ArcTan}[-2Q+9QW-9W^2,\,2Q\sqrt{-1+9W}]}\right)^{\frac{-3i}{\sqrt{-1+9W}}}$$

$$\Bigg(\text{Beta}\left[e^{-2i\,\text{ArcTan}[-2Q+9QW-9W^2,\,2Q\sqrt{-1+9W}]},\,1-\frac{3i}{\sqrt{-1+9W}},\,0\right]+$$

$$\text{Beta}\left[e^{2i\,\text{ArcTan}[-2Q+9QW-9W^2,\,2Q\sqrt{-1+9W}]},\,1+\frac{3i}{\sqrt{-1+9W}},\,0\right]\Bigg)\Bigg)$$

IQ31[W,Q]----3p

$$\text{IQ31}[W\_, Q\_] := \frac{1}{W^8} e^{-\frac{6\,\text{ArcTan}\left[2+9Q-9W,\,2\sqrt{-1+9W}\right]}{\sqrt{-1+9W}}}$$

$$\left(\frac{1}{\left((Q-W)^2+\frac{4}{9}Q\right)^6}\left(Q^{12}\left(-\frac{14336}{531441}-\frac{2048\,W}{19683}+\frac{1408\,W^2}{2187}+\frac{160\,W^3}{729}+\frac{4\,W^5}{9}+3\,W^6\right)+\right.\right.$$

$$Q^{11}\left(-\frac{114688}{1594323}+\frac{8192\,W}{177147}+\frac{54784\,W^2}{19683}-\frac{6016\,W^3}{729}-\frac{640\,W^4}{243}+\frac{16\,W^5}{9}+\frac{20\,W^6}{3}-36\,W^7\right)+$$

$$Q^{10}\left(-\frac{1146880}{14348907}+\frac{655360\,W}{1594323}+\frac{428032\,W^2}{177147}-\frac{475648\,W^3}{19683}+\frac{108416\,W^4}{2187}+\frac{4288\,W^5}{243}+\frac{80\,W^6}{27}-\frac{284\,W^7}{3}+198\,W^8\right)+$$

$$Q^9\left(-\frac{18350080}{387420489}+\frac{6553600\,W}{14348907}-\frac{286720\,W^2}{1594323}-\frac{10557440\,W^3}{531441}+\frac{2194432\,W^4}{19683}-\frac{43904\,W^5}{243}-\frac{39104\,W^6}{729}-\frac{896\,W^7}{9}+\frac{4340\,W^8}{9}-660\,W^9\right)+$$

$$Q^8\left(-\frac{18350080}{1162261467}+\frac{28835840\,W}{129140163}-\frac{15564800\,W^2}{14348907}-\frac{6840320\,W^3}{1594323}+\frac{13168640\,W^4}{177147}-\frac{6299648\,W^5}{19683}+\frac{1005184\,W^6}{2187}+\frac{14144\,W^7}{243}+\frac{4304\,W^8}{9}-1400\,W^9+1485\,W^{10}\right)+$$

$$Q^7\left(-\frac{29360128}{10460353203}+\frac{60817408\,W}{1162261467}-\frac{65404928\,W^2}{129140163}+\frac{21790720\,W^3}{14348907}+\frac{7700480\,W^4}{531441}-\frac{28657664\,W^5}{177147}+\frac{12244480\,W^6}{19683}-\frac{632704\,W^7}{729}+\frac{84352\,W^8}{1215}-1184\,W^9+2648\,W^{10}-2376\,W^{11}\right)+$$

$$Q^6\left(-\frac{58720256}{282429536481}+\frac{16777216\,W}{3486784401}-\frac{101187584\,W^2}{1162261467}+\frac{98172928\,W^3}{129140163}-\frac{1146880\,W^4}{531441}-\frac{3555328\,W^5}{177147}+\frac{4358144\,W^6}{19683}-\frac{5565952\,W^7}{6561}+\frac{40084096\,W^8}{32805}-\frac{360064\,W^9}{1215}+\frac{16352\,W^{10}}{9}-\frac{10360\,W^{11}}{3}+2772\,W^{12}\right)+$$

$$Q^5\left(-\frac{14680064\,W^2}{3486784401}+\frac{94896128\,W^3}{1162261467}-\frac{109838336\,W^4}{129140163}+\frac{17465344\,W^5}{4782969}+\frac{5570560\,W^6}{531441}-\frac{33689600\,W^7}{177147}+\frac{186754048\,W^8}{229635}-\frac{10708352\,W^9}{8505}+\frac{504832\,W^{10}}{1215}-\frac{16576\,W^{11}}{9}+3176\,W^{12}-2376\,W^{13}\right)+$$

$$Q^4\left(-\frac{14680064\,W^4}{387420489}+\frac{78381056\,W^5}{129140163}-\frac{57966592\,W^6}{14348907}+\frac{7733248\,W^7}{1594323}+\frac{63625216\,W^8}{688905}-\frac{368330752\,W^9}{688905}+\frac{14261248\,W^{10}}{15309}-\frac{78496\,W^{11}}{243}+\frac{11296\,W^{12}}{9}-2060\,W^{13}+1485\,W^{14}\right)+$$

$$Q^3\left(-\frac{3670016\,W^5}{3486784401}-\frac{63045632\,W^6}{387420489}+\frac{31686656\,W^7}{14348907}-\frac{505593856\,W^8}{55801305}-\frac{261382144\,W^9}{18600435}+\frac{154938368\,W^{10}}{688905}-\frac{22379776\,W^{11}}{45927}+\frac{108800\,W^{12}}{729}-\frac{5104\,W^{13}}{9}+\frac{8300\,W^{14}}{9}-660\,W^{15}\right)+$$

$$Q^2\left(-\frac{917504\,W^7}{129140163}-\frac{5373952\,W^8}{14348907}+\frac{557056\,W^9}{137781}-\frac{1417216\,W^{10}}{177147}-\frac{4781056\,W^{11}}{98415}+\frac{2701568\,W^{12}}{15309}-\frac{16064\,W^{13}}{405}+\frac{1456\,W^{14}}{9}-\frac{812\,W^{15}}{3}+198\,W^{16}\right)+$$

$$Q\left(-\frac{9076736\,W^9}{502211745}-\frac{8421376\,W^{10}}{18600435}+\frac{22089728\,W^{11}}{6200145}-\frac{45056\,W^{12}}{98415}-\frac{1059328\,W^{13}}{25515}+\frac{6464\,W^{14}}{1215}-\frac{704\,W^{15}}{27}+\frac{140\,W^{16}}{3}-36\,W^{17}\right)-\frac{3186688\,W^{11}}{167403915}-\frac{1337344\,W^{12}}{6200145}+\frac{421888\,W^{13}}{229635}+\frac{1137664\,W^{14}}{229635}-$$

$$\left.\frac{896\,W^{15}}{3645}+\frac{16\,W^{16}}{9}-\frac{32\,W^{17}}{9}+3\,W^{18}\right)-$$

$$\frac{512}{729}\left(\frac{28}{243}+\frac{26\,W}{27}+W^2\right)\left(e^{2\,i\,\text{ArcTan}\left[-2Q+9QW-9W^2,\,2Q\sqrt{-1+9W}\right]}\right)^{\frac{-3\,i}{\sqrt{-1+9W}}}$$

$$\left(\text{Beta}\left[e^{-2\,i\,\text{ArcTan}\left[-2Q+9QW-9W^2,\,2Q\sqrt{-1+9W}\right]},\,1-\frac{3\,i}{\sqrt{-1+9W}},\,0\right]+\right.$$

$$\left.\left.\text{Beta}\left[e^{2\,i\,\text{ArcTan}\left[-2Q+9QW-9W^2,\,2Q\sqrt{-1+9W}\right]},\,1+\frac{3\,i}{\sqrt{-1+9W}},\,0\right]\right)\right)$$

IQ32[W,Q]----3d

$$\text{IQ32}[W\_, Q\_] := \frac{1}{W^9}\, e^{-\frac{6\,\text{ArcTan}[2+9Q-9W,\,2\sqrt{-1+9W}]}{\sqrt{-1+9W}}}$$

$$\left(\frac{1}{\left((Q-W)^2+\frac{4}{9}Q\right)^6}\left(Q^{12}\left(-\frac{16384}{4782969}-\frac{22528\,W}{1594323}+\frac{5120\,W^2}{59049}+\frac{128\,W^3}{6561}+\frac{32\,W^4}{2187}+\frac{20\,W^6}{27}+5\,W^7\right)+\right.\right.$$

$$Q^{11}\left(-\frac{131072}{14348907}+\frac{16384\,W}{4782969}+\frac{200704\,W^2}{531441}-\frac{67072\,W^3}{59049}-\frac{128\,W^4}{729}-\frac{128\,W^5}{729}+\frac{80\,W^6}{27}+\frac{100\,W^7}{9}-60\,W^8\right)+$$

$$Q^{10}\left(-\frac{1310720}{129140163}+\frac{2129920\,W}{43046721}+\frac{1654784\,W^2}{4782969}-\frac{1755136\,W^3}{531441}+\frac{414208\,W^4}{59049}+\frac{4480\,W^5}{6561}+\frac{4544\,W^6}{729}+\frac{400\,W^7}{81}-\frac{1420\,W^8}{9}+330\,W^9\right)+$$

$$Q^9\left(-\frac{20971520}{3486784401}+\frac{65536000\,W}{1162261467}+\frac{327680\,W^2}{43046721}-\frac{13312000\,W^3}{4782969}+\frac{24553472\,W^4}{1594323}-\frac{1574912\,W^5}{59049}+\frac{26240\,W^6}{6561}-\frac{26560\,W^7}{2187}-\frac{4480\,W^8}{27}+\frac{21700\,W^9}{27}-1100\,W^{10}\right)+$$

$$Q^8\left(-\frac{20971520}{10460353203}+\frac{96993280\,W}{3486784401}-\frac{48496640\,W^2}{387420489}-\frac{29655040\,W^3}{43046721}+\frac{49848320\,W^4}{4782969}-\frac{23883776\,W^5}{531441}+\frac{4287488\,W^6}{59049}-\frac{81280\,W^7}{6561}-\frac{56000\,W^8}{729}+\frac{21520\,W^9}{27}-\frac{7000\,W^{10}}{3}+2475\,W^{11}\right)+$$

$$Q^7\left(-\frac{33554432}{94143178827}+\frac{205520896\,W}{31381059609}-\frac{214958080\,W^2}{3486784401}+\frac{59113472\,W^3}{387420489}+\frac{95584256\,W^4}{43046721}-\frac{36552704\,W^5}{1594323}+\frac{47654912\,W^6}{531441}-\frac{8054272\,W^7}{59049}-\frac{12416\,W^8}{729}+\frac{287104\,W^9}{729}-\frac{5920\,W^{10}}{3}+\frac{13240\,W^{11}}{3}-3960\,W^{12}\right)+$$

$$Q^6\left(-\frac{67108864}{2541865828329}+\frac{511705088\,W}{847288609443}-\frac{4194304\,W^2}{387420489}+\frac{106430464\,W^3}{1162261467}-\frac{26607616\,W^4}{129140163}-\frac{136478720\,W^5}{43046721}+\frac{153567232\,W^6}{4782969}-\frac{65220608\,W^7}{531441}+\frac{10299904\,W^8}{59049}+\frac{2083456\,W^9}{19683}-\frac{596608\,W^{10}}{729}+\frac{81760\,W^{11}}{27}-\frac{51800\,W^{12}}{9}+4620\,W^{13}\right)+$$

$$Q^5\left(-\frac{16777216\,W^2}{31381059609}+\frac{35651584\,W^3}{3486784401}-\frac{362283008\,W^4}{3486784401}+\frac{154664960\,W^5}{387420489}+\frac{28475392\,W^6}{14348907}-\frac{44466176\,W^7}{1594323}+\frac{61140992\,W^8}{531441}-\frac{21938176\,W^9}{137781}-\frac{2647168\,W^{10}}{15309}+\frac{707584\,W^{11}}{729}-\frac{82880\,W^{12}}{27}+\frac{15880\,W^{13}}{3}-3960\,W^{14}\right)+$$

$$Q^4\left(-\frac{16777216\,W^4}{3486784401}+\frac{29360128\,W^5}{387420489}-\frac{186122240\,W^6}{387420489}+\frac{12943360\,W^7}{43046721}+\frac{66437120\,W^8}{4782969}-\frac{273958912\,W^9}{3720087}+\frac{5054464\,W^{10}}{45927}+\frac{6613760\,W^{11}}{45927}-\frac{519200\,W^{12}}{729}+\frac{56480\,W^{13}}{27}-\frac{10300\,W^{14}}{3}+2475\,W^{15}\right)+$$

$$Q^3\left(-\frac{4194304\,W^5}{31381059609}-\frac{216530944\,W^6}{10460353203}+\frac{325713920\,W^7}{1162261467}-\frac{45383680\,W^8}{43046721}-\frac{91602944\,W^9}{33480783}+\frac{1736556544\,W^{10}}{55801305}-\frac{118897664\,W^{11}}{2066715}-\frac{9263360\,W^{12}}{137781}+\frac{712960\,W^{13}}{2187}-\frac{25520\,W^{14}}{27}+\frac{41500\,W^{15}}{27}-1100\,W^{16}\right)+$$

$$Q^2\left(-\frac{1048576\,W^7}{1162261467}-\frac{17170432\,W^8}{387420489}+\frac{23855104\,W^9}{43046721}-\frac{44466176\,W^{10}}{55801305}-\frac{4136960\,W^{11}}{531441}+\frac{6255616\,W^{12}}{295245}+\frac{792832\,W^{13}}{45927}-\frac{7232\,W^{14}}{81}+\frac{7280\,W^{15}}{27}-\frac{4060\,W^{16}}{9}+330\,W^{17}\right)+$$

$$Q\left(-\frac{262144\,W^9}{129140163}-\frac{62947328\,W^{10}}{1506635235}+\frac{100728832\,W^{11}}{167403915}+\frac{618496\,W^{12}}{1240029}-\frac{169984\,W^{13}}{32805}-\frac{33280\,W^{14}}{15309}+\frac{9536\,W^{15}}{729}-\frac{3520\,W^{16}}{81}+\frac{700\,W^{17}}{9}-60\,W^{18}\right)-\frac{65536\,W^{11}}{43046721}-\frac{876544\,W^{12}}{100442349}+\frac{6182912\,W^{13}}{18600435}+$$

$$\left.\frac{524288\,W^{14}}{688905}+\frac{13312\,W^{15}}{137781}-\frac{1664\,W^{16}}{2187}+\frac{80\,W^{17}}{27}-\frac{160\,W^{18}}{27}+5\,W^{19}\right)-$$

$$\frac{5120}{59049}\left(\frac{16}{135}+\frac{46}{45}W+W^2\right)\left(e^{2\,i\,\text{ArcTan}[-2Q+9QW-9W^2,\,2Q\sqrt{-1+9W}]}\right)^{\frac{-3\,i}{\sqrt{-1+9W}}}$$

$$\left(\text{Beta}\left[e^{-2\,i\,\text{ArcTan}[-2Q+9QW-9W^2,\,2Q\sqrt{-1+9W}]},\,1-\frac{3\,i}{\sqrt{-1+9W}},\,0\right]+\right.$$

$$\left.\left.\text{Beta}\left[e^{2\,i\,\text{ArcTan}[-2Q+9QW-9W^2,\,2Q\sqrt{-1+9W}]},\,1+\frac{3\,i}{\sqrt{-1+9W}},\,0\right]\right)\right)$$

APPENDIX E: 18TH INTERNATIONAL SEMINAR ON ION-ATOM COLLISIONS

Poster presented at the 18th International Seminar on Ion-Atom Collisions (ISIAC XVIII),The MS Symphony of Silia Line, Stockholm-Helsinki-Stockholm, July 30–August 1 2003. Book of Abstracts, p. 52.

ANALYTICAL CROSS SECTIONS FOR ELECTRON EJECTION FROM ATOMIC SCREENED HYDROGENIC SHELLS

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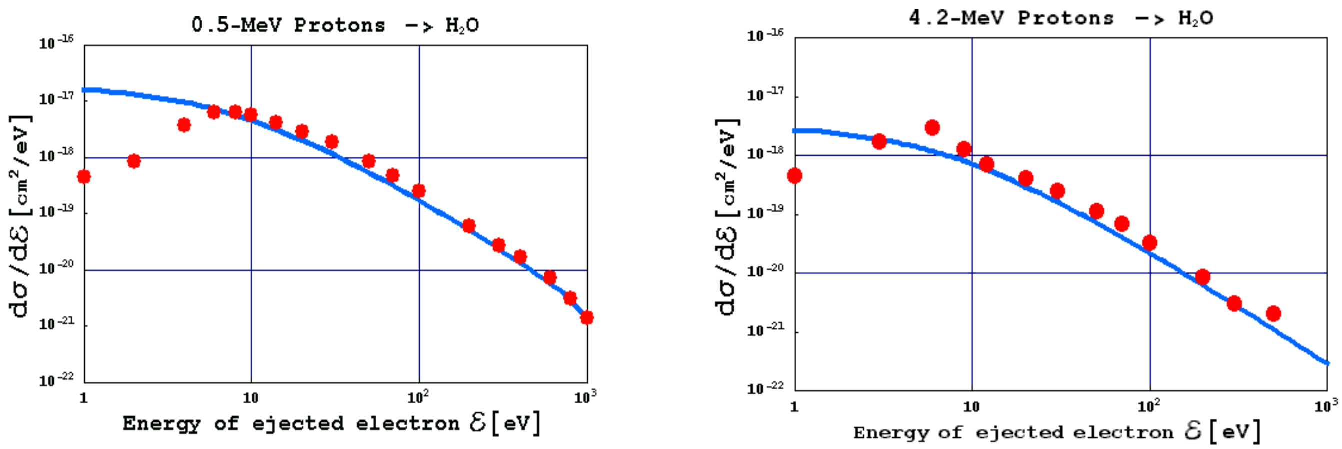
Analytical formulas for cross sections, differential in the energy of electrons ejected from S = K, L_1, L_2, L_3, M_1, M_2, M_3, M_4, and M_5 shells, are obtained in the plane wave Born approximation (PWBA). The derivation of these formulas starts with nonrelativistic-screened hydrogenic wave functions and is done in *Mathematica*. Derivation of these formulas, which *Mathematica* does not perform automatically, will be outlined. These analytical cross sections are perfect in agreement with the PWBA calculated by numerical integration over the transferred momentum [1].

Upon summation of singly differential cross sections so derived, cross sections for electron ejection -- from relatively light atoms ($Z_2 < 19$) or molecules consisting of such atoms -- are also given analytically. For example, we compare in the figure results of such calculations with the data (solid circles) of Toburen [2] for ionization of water vapor by 0.5 and 4.2 MeV protons.



The discrepancies at low projectile and the ejected electron energies may be accounted for in the ECPSSR theory that can be cast analytically in terms of the analytical formulas that are presently reported [3].

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[2] See Fig.12 in L. Toburen, *Physical and Chemical Mechanisms in Molecular Radiation Biology*, edited by W.A. Glass and M.N. Varma, Plenum Press, NY, 1991, p.51.

[3] W. Brandt and G. Lapicki, Phys. Rev. A 23, 1717 (1981).