Distorted Wave Born Approximation For Inelastic Atomic Collision

by

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A thesis
presented to the University of Waterloo
in fulfilment of the
thesis requirement for the degree of
Master of Mathematics
in
Applied Mathematics

Waterloo, Ontario, Canada, 2007

I hereby declare that I am the sole author of this thesis. This is a true copy of the thesis, including any required final revisions, as accepted by my examiners.

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Abstract

An investigation of the problem of inelastic scattering process under the Coulomb Born approximation is given. Different approaches to calculate Coulomb wavefunctions in the momentum space representation are analyzed and a discussion of their existences in the generalized distribution sense is provided. Inokuti's approach of finding the differential cross section in the momentum space representation under the Coulomb Born approximation is described and a different approach with an application of the Bremsstrahlung integral is developed and compared with Inokuti's approach.

Acknowledgments

I thank Dr. M.C. Chidichimo for her guidance and support during the preparation of this thesis.

I thank Dr. Z.L. Miskovic and Dr. F.O. Goodman for their help in the production of this thesis.

I also thank Dr. A. Kempf and the Department of Applied Mathematics for their patience and assistance when I was in trouble in certain circumstances.

Finally, I thank my mother who gave me her suggestive opinions and emotion support during the completion of this thesis.

Dedication

This thesis is dedicated to Dr. M.C. Chidichimo.

Contents

Chapter 1

Introduction and Overview

The investigation of collisions of charged particles with atoms and molecules was initiated in 1930 by Bethe, whose work put a variety of theoretical and experimental data together in a coherent picture. His work concerning collision cross sections and the stopping force for fast particles established a number of important results through Quantum Mechanical theory based on the Born approximation. Before Bethe's work, Bohr had begun investigating the subject of atomic collisions in 1913. He had developed a theory of the stopping force of materials for fast particles which regards the collision as a producing sudden transfer of energy and momentum to atomic electrons. He had given the general structure of cross-section formulas correctly, but owing to the lack of knowledge of Quantum Mechanics at that time, certain dynamical details were not clear in his work.

Bethe's achievements on the subject of atomic collision made an impact in the last century. The past developments in understanding of fast collisions have been successful, experiments in such area had been improved by modern advanced technology, and the results are characterized by remarkably improved resolution both in electron energy and in beam collimation, while progress have been made by theoretical researchers using a variety of approaches. In this chapter, I briefly provide descriptions of atomic scattering process, outline important work from the past and introduce certain fundamental formulas in scattering theory. In the end, I shall describe why it is necessary to review a subset of this subject, that is inelastic scattering.

Theoretical treatments of atomic collisions of charged particles with atoms and molecules are classified into two kinds: those dealing with fast collisions and those dealing with slow ones. The basis to distinguish either one from the other is that the particle speed is fast or slow relative to mean orbital speed of atomic electrons in the shell. For example, an electron of a few keV kinetic energy is considered fast with respect to any discrete-level excitation of He, while it is not fast compared to the K-shell ionization of Ar.

In this thesis, we limit our attention to inelastic scattering as it is a well-studied subject and it will be our main theme. For sufficiently fast collisions, the influence of the incident particle upon an atom or molecule may be regarded as a sudden and small external perturbation, for which perturbation method may be used to help us extract useful informations from a complicated problem. In this thesis, we confine ourselves to first Born approximation, which fails at lower energies. In inelastic scattering, kinetic energy of the incident particle is transfered to raise the atomic electron from state i to state f, leading to excitation or ionization. Generally speaking, the study of fast collisions is a property of target atoms or molecules in essence.

However, at lower energies, the Born approximation is not valid and the problem is more difficult than in the fast atomic scattering case because we must study the combined system of the incident particle plus the target atoms or molecules. An inelastically scattered particle cannot be considered to be moving in an equivalent static potential as its state is continuously changing with the target along the trajectory. In this case, a different approximate method must be employed and our work has been done based on the distorted wave approximation as introduced by Mott and Massey.[MM65]

We are in particular interested in studying atomic scattering by a Coulomb field. We consider an incident particle carrying charge ze (e is the proton charge), which collides with an Z-electrons atom inelastically and the target atom is initially at its ground state. As this is an inelastic collision process, there is a change in the energy of the incident particle and this energy change is absorbed by the atomic electrons, leading to excitation and ionization. We describe these internal changes of the system with the full many-body Hamiltonian. In the second chapter, a brief review of Bethe Theory on inelastic collisions of fast charged particles with atoms and molecules will be given and physical observables, the differential scattering, total scattering cross sections and collision strength will be discussed.[I71] [BJ86]

In the third chapter, perturbation methods (Born approximation and distorted wave approximation) will be used to describe high and low energy scatterings. We consider physical circumstances in which first order perturbation methods should be sufficient.[FI] Typically, the full inelastic scattering amplitude was obtained by the partial-wave decomposition. But for high incident energies, the contributions to the collision strength from a wide band of incident angular momentum values corresponding to large impact parameters should dominate. The partial wave summation becomes impractical because of its slow convergence. We investigate this matter and explain, under such circumstance, that the distorted wave approximation or the Coulomb-Born approximation becomes more reliable.

In Quantum Mechanics, momentum space description is known to be equivalent to coordinate space description. Effort has been put into investigation of the scattering problem in coordinate space representation. However, studying the scattering problem from the point of view on momentum space representation is intrinsically appealing, since the basic quantities involved are scattering amplitudes and experimental settings, allowing us to obtain momentum measurements. In fact, these quantities are related. In chapter four, we conduct an investigation on non-relativistic inelastic collision problems in momentum space representation. The primary goal of this chapter is to obtain an expression for Coulomb wavefunctions in the momentun space representation. Different approaches are used and are discussed in chapter four.

In chapter five, we calculate the inelastic differential cross section using the momentum representation approach. Essentially, it is our goal in this thesis to calculate a matrix element integral given in chapter three. We apply results from chapter three and chapter four and show that a dynamic matrix element is related to Bremsstrahlung integral.

In chapter six, we investigate the inelastic scattering process from the point of view of momentum transfer from the incident particle to the target electrons and compare this result with plane-wave approximation result. Observations will be made on the weight function, $w(\mathbf{k}', \mathbf{k}; \mathbf{k_f}, \mathbf{k_i})$ and we explain how it affects the cross section because of its unresolvable singularities. [GM51][FI]

In chapter seven, the results are summarized and discussed.

Chapter 2

The Bethe Theory - Collisions Of Fast Electrons With Atoms

In this chapter, a brief review of the Bethe theory of fast electron collisions and an introduction of physical quantities of cross section and generalized oscillator strength are given.

Physical Picture

We consider a dynamical system composed of an incident particle and an atomic scatterer interacting with each other. We shall consider it according to quantum mechanics. In general, such a collision of a particle and atomic scatterer may have several different possible outcomes. An incident particle, an electron for example, may

- be deflected without affecting the atom; this is also known as elastic scattering,
- be absorbed by the ion; this is called absorption,
- be deflected and give some of its kinetic energy to raise atomic electrons to an excited state; this is called ionic excitation,
- provide sufficient energy to knock an atomic electron out of the vicinity of the nucleus; it is called ionization,

- react with the atomic nucleus and raise it into an excited state; it is called nuclear excitation,
- create quarks from protons and neutrons of the nucleus.

For our purpose, we focus on an inelastic collision process in which a particle of velocity v, mass M_1, and charge ze bombards a stationary atom with mass M_2 and Z atomic electrons. Suppose the target atom is in its ground state initially, often denoted as state 0, and the colliding particle gets deflected into the solid angle element $d\omega$ along the direction with polar angles (θ, ϕ) measured in the center-of-mass system and induces state transitions within the target to state n. Suppose the interaction is Coulombic. V is written as

$$V = -\sum_{j=1}^{Z} \frac{ze^2}{|\mathbf{r} - \mathbf{r_j}|} + \frac{zZ_N e^2}{r}, \tag{2.1}$$

where $Z_N e$ is the charge of the atomic nucleus. It describes the interaction of the incident particle with the electrons and nucleus of the target atom.

2.1 Cross Sections

In classical mechanics, the motion of the incident particle is well defined such that it is moving along a trajectory and is scattered into a certain direction characterized by polar angles (θ, ϕ) which may be calculated from initial conditions. However in quantum theory, we are allowed to describe such a scattering event as a probability event: we may calculate only the probability that the particle got scattered into a certain direction, not precise angles of scattering.

A generic form of scattering experiment consists of an incident beam of monoenergetic particles from a source collimated by slits. The beam of particles is scattered by the target atom at position O, and a detector is used to count the number of particles per unit time which got scattered into an element of solid angle $d\Omega$ centered about O specified by polar angles (θ, ϕ). When the detector subtends a solid angle $d\Omega$ about the scattering center O in the direction (θ, ϕ), it can count $Nd\Omega$, number of particles per unit time. This number is proportional to the flux of particles in the incident beam, defined as the number of particles per unit time crossing a unit area placed normal to the direction of incidence. Thus, the differential cross section is defined as the number of particles scattered near the direction

(θ, ϕ) per unit time per unit solid angle divided by the incident flux,

$$\frac{d\sigma}{d\Omega} = \frac{N}{F}. \tag{2.2}$$

The total cross section is then defined as the integral of the differential scattering cross section, $d\sigma$, given above over all solid angles,

$$\begin{aligned} \sigma &= \int \left(\frac{d\sigma}{d\Omega}\right) d\Omega \\ &= \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin\theta \left(\frac{d\sigma}{d\Omega}\right). \end{aligned} \tag{2.3}$$

The dimensions of differential cross section and total cross section are of an area, as is suggested by their names.

While the total cross section is a useful measure to consider as it is a quantity independent of the angle of scattering, it is the differential cross section which interests theoretical researchers the most.

2.2 Bethe Theory

When the particle is travelling sufficiently fast and in nonrelativistic frame, the differential cross section for inelastic scattering of the target atom whose state changed from 0 to n is obtained from the transition amplitude by Fermi's golden rule [BJ86],

$$\frac{d\sigma}{d\Omega} = \frac{2\pi}{\hbar v_0}|T_{0n}|^2 \rho(W_n), \tag{2.4}$$

with

$$\rho(W_n) = \frac{p_n^2}{(2\pi\hbar)^3}\frac{dp_n}{dW_n} \tag{2.5}$$

$$\frac{dW_n}{dp_n} = v_n, \tag{2.6}$$

where $\rho(W_n)$ is the density of final states per unit energy per unit solid angle, v_0 and v_n are initial and final velocities of the incident particle, T_{on} is the amplitude for transition from state 0 to state n according to Born approximation:

$$T_{on} =< \psi_{n\mathbf{k_n}}|V|\psi_{0\mathbf{k_0}} >, \tag{2.7}$$

where the ψ are eigenfunctions of the system and $\mathbf{k_0}$ and $\mathbf{k_n}$ are initial and final momentum of the incident particle.

In the Born approximation, the differential cross section, calculated in the lowest order under interaction V between the particle and the atom becomes,

$$d\sigma = \frac{M^2 k'}{k(2\pi)^2\hbar^4}\left|\int e^{i\mathbf{K}\cdot\mathbf{r}}\psi_n^* V\psi_0 d\mathbf{r}\right|^2 d\Omega, \tag{2.8}$$

where $\mathbf{K} = \mathbf{k} - \mathbf{k}'$.

For certain potentials, such as $V(\mathbf{r}) = \frac{1}{\mathbf{r}}$, the nuclear interaction represented by the second term in V gives no contribution because of the orthogonality of states n and 0. Integration over $\mathbf{r}$ on the first term is trivial, althought the integral diverges because the integrand behaves as $O(r^{-1})$ for $r \to \infty$, but it may be tackled by introducing a converging factor, $e^{-\epsilon r}$ with $\epsilon \to 0^+$,

$$\begin{aligned}\int \frac{e^{i\mathbf{K}\cdot\mathbf{r}}}{|\mathbf{r}-\mathbf{r_j}|}d\mathbf{r} &= \lim_{\epsilon\to 0}\int \frac{e^{-\epsilon r}e^{i\mathbf{K}\cdot\mathbf{r}}}{|\mathbf{r}-\mathbf{r_j}|}d\mathbf{r} \\ &= \frac{4\pi}{K^2}e^{i\mathbf{K}\cdot\mathbf{r_j}}.\end{aligned} \tag{2.9}$$

With the above relations, the differential cross section is transformed into

$$d\sigma = 4z^2\left(\frac{Me^2}{\hbar^2}\right)^2 \frac{k'}{kK^4}|\varepsilon(\mathbf{K})|^2 d\Omega \tag{2.10}$$

where $\varepsilon(\mathbf{K})$ is an element of matrix

$$\varepsilon(\mathbf{K}) = \left\langle n\left|\sum_{j=1}^{Z} e^{i\mathbf{K}\cdot\mathbf{r_j}}\right|0\right\rangle. \tag{2.11}$$

One may consider the differential cross section as independent of ϕ either because state 0 is spatially symmetric or because the atom is oriented at random, therefore, $|\varepsilon(\mathbf{K})|^2$ is a function of a scalar variable K. Furthermore, K is independent of ϕ, we may replace $d\Omega$ by

$$2\pi\sin\theta d\theta = \frac{\pi d(K^2)}{kk'} \tag{2.12}$$

because

$$\begin{aligned}K^2 &= |\mathbf{k}-\mathbf{k}'|^2 \\ &= k^2 + k'^2 - 2kk'\cos\theta \\ d(K^2) &= 2kk'\sin\theta d\theta.\end{aligned} \tag{2.13}$$

Also, we have

$$d\sigma = 4\pi z^2 \left(\frac{Me^2}{\hbar^2}\right)^2 \frac{1}{k^2K^4}|\varepsilon(K)|^2 d(K^2) \tag{2.14}$$

for the differential cross section. The factor $|\varepsilon(K)|^2$ gives the conditional probability that the atom makes the transition to a particular state n upon receiving a momentum transfer $\hbar K$. This quantity $\varepsilon(K)$ reflects the response of the atom and is known as the inelastic scattering form factor, which is widely used in nuclear and particle physics.

Chapter 3

Differential Cross Section of Inelastic Collision

In this section, differential cross section of inelastic collision will be derived. Quantum mechanically, the full scattering cross section was obtained by the partial-wave decomposition. But for high incident energies, the partial wave summation becomes impractical because of its slow convergence. We investigate this matter and explain, under such circumstance, that distorted wave approximation or the Coulomb-Born approximation becomes more reliable. In particular, a simplest inelastic collision event is investigated, namely, the collision of an electron with a hydrogen atom, to help us understand better the technique required in studying inelastic collisions in general.

3.1 Potential Scattering - General Features

The Schroedinger equation describing the system is written as

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t) = \left[-\frac{\hbar^2}{2\mu}\nabla^2 + V(\mathbf{r})\right]\Psi(\mathbf{r},t) \tag{3.1}$$

where μ is the reduced mass of the system which consists of 2 particles of masses m_A and m_B,

$$\mu = \frac{m_A m_B}{m_A + m_B}, \tag{3.2}$$

and $E = \frac{1}{2}\mu v^2$ is the kinetic energy of the particle.

In experiment, the incident beam of particles is switched on for times very long compared with the time a particle takes to cross the interaction region, so that the steady state conditions apply. As we are considering only a time independent potential $V(\mathbf{r})$, we are seeking a stationary solution of the form

$$\Psi(\mathbf{r}, t) = \psi(\mathbf{r}) e^{-i\frac{Et}{\hbar}} \tag{3.3}$$

where the wave function $\psi(\mathbf{r})$ satisfies the time independent Schroedinger equation

$$\left[-\frac{\hbar^2}{2\mu}\nabla^2 + V(\mathbf{r})\right]\psi(\mathbf{r}) = E\psi(\mathbf{r}). \tag{3.4}$$

Let

$$\begin{aligned} k^2 &= \frac{2\mu E}{\hbar^2} \\ U(\mathbf{r}) &= \frac{2\mu}{\hbar^2} V(\mathbf{r}), \end{aligned}$$

and express the time independent Schroedinger equation in a condensed form

$$\left(\nabla^2 + k^2 - U(\mathbf{r})\right)\psi(\mathbf{r}) = 0. \tag{3.5}$$

Suppose the potential decreases faster than r^{-1} as $r \to \infty$. For large r, $U(\mathbf{r})$ vanishes and (3.5) reduces to free particle Schroedinger equation

$$(\nabla^2 + k^2)\psi(\mathbf{r}) = 0 \tag{3.6}$$

Far from the scattering centre, the physical condition suggests $\psi(\mathbf{r})$ must describe both the incident beam of particles and the particles which have been scattered, so that we write it as

$$\psi(\mathbf{r}) \sim \psi_{inc}(\mathbf{r}) + \psi_{sc}(\mathbf{r}) \tag{3.7}$$

Particles in the incident beam all travel in the same direction, which we take to be the z axis and have the same momentum of magnitude $p = \hbar k$, and the incident wave ψ_{inc} consists of plane waves,

$$\psi_{inc}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} = e^{ikz} \tag{3.8}$$

and is normalized such that it represents a beam with one particle per unit volume. On the other hand, the scattered wave function $\psi_{sc}(\mathbf{r})$ must represent an outward radial flow of particles and it has the form

$$\psi_{sc}(\mathbf{r}) = f(k, \theta, \phi)\frac{e^{ikr}}{r} \tag{3.9}$$

where (r, θ, ϕ) are the spherical coordinates of the position vector $\mathbf{r}$ of the scattered particle. The amplitude f of the outgoing spherical wave $r^{-1}e^{ikr}$, called the scattering amplitude, depends on the direction (θ, ϕ) and it determines the flux of particles being scattered near direction (θ, ϕ).

Note that, both incoming and outgoing waves of the form $r^{-1}e^{\pm ikr}f(k, \theta, \phi)$ satisfy the free particle equation (3.6) in the limit of large r. However, the physical condition implies that the use of an outgoing scattering wave function is the appropriate one.

$$\psi(\mathbf{r}) \sim e^{i\mathbf{k}\cdot\mathbf{r}} + f(k, \theta, \phi)\frac{e^{ikr}}{r} \qquad \text{as } r \to \infty \tag{3.10}$$

I now show that the free particle equation has solution of the form $r^{-1}e^{\pm ikr}f(k, \theta, \phi)$ in the limit of large r.

The Laplacian under spherical coordinate system has the form [DK67]:

$$\begin{aligned}
\nabla^2\psi(\mathbf{r}) &= \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\frac{e^{\pm ikr}}{r}f(k, \theta, \phi)\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\frac{e^{\pm ikr}}{r}f(k, \theta, \phi)\right) \\
&\quad + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\frac{e^{\pm ikr}}{r}f(k, \theta, \phi) \\
&= \frac{1}{r^2}\frac{\partial}{\partial r}\left(\pm ikre^{\pm ikr}f(k, \theta, \phi) - e^{\pm ikr}f(k, \theta, \phi)\right) + \frac{e^{\pm ikr}}{r^3\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}f(k, \theta, \phi)\right) \\
&\quad + \frac{e^{\pm ikr}}{r^3\sin^2\theta}\frac{\partial^2}{\partial\phi^2}f(k, \theta, \phi) \\
&= -\frac{k^2}{r}e^{\pm ikr}f(k, \theta, \phi) + \mathcal{O}(r^{-3}) \\
&= -k^2\psi(\mathbf{r})
\end{aligned} \tag{3.11}$$

in the limit of large r.

Therefore, the stationary scattering wave function, which we denote by $\psi_{\mathbf{k}}(\mathbf{r})$, is a particular solution of the Schroedinger equation (3.5) which has an asymptotic boundary condition

$$\psi_{\mathbf{k}}(\mathbf{r}) \sim e^{i\mathbf{k}\cdot\mathbf{r}} + f(k, \theta, \phi)\frac{e^{ikr}}{r} \tag{3.12}$$

for large r. Here the subscript $\mathbf{k}$ indicates that the wave function $\psi_{\mathbf{k}}$ corresponds to the incident plane wave $e^{i\mathbf{k}\cdot\mathbf{r}}$.

3.1.1 Probability Current Density

As mentioned in the previous chapter, the wave function associated with a particle has a statistical interpretation in quantum mechanics. According to Born's postulate, if a particle is described by a wave function $\Psi(\mathbf{r}, t)$ which is normalized to unity, the probability of finding the particle at time t within a volume element $d\mathbf{r} = dxdydz$ about a point $\mathbf{r}$ is

$$P(\mathbf{r}, t)d\mathbf{r} = |\Psi(\mathbf{r}, t)|^2 d\mathbf{r}. \tag{3.13}$$

Furthermore, the probability of finding the particle somewhere must remain unity as time varies. The probability is conserved in time, and we define the probability current density $\mathbf{j}$,

$$\mathbf{j}(\mathbf{r}, \mathbf{t}) = \frac{\hbar}{2i\mu}\left[\Psi^*\nabla\Psi - (\nabla^*\Psi)\Psi\right], \tag{3.14}$$

which describes the flow of probability density.

We apply $\mathbf{j}$ to analyse our asympototic scattered wave function in (3.9). As we are working in the limit of large r, only the radial direction will contribute to the spatial derivative. That is,

$$\nabla = \widehat{\mathbf{r}}\frac{\partial}{\partial r}. \tag{3.15}$$

where $\widehat{\mathbf{r}}$ is a unit vecor in the direction of $\mathbf{r}$. Substitute (3.15) and (3.9) into (3.14), and the radial current of scattered particles in the direction (θ, ϕ) per unit time is

$$j(\mathbf{r}) = \frac{\hbar k}{mr^2}|f(k, \theta, \phi)|^2. \tag{3.16}$$

It represents the number of particles crossing unit area per unit time, and as the detector presents a cross sectional area $r^2 d\omega$ to the scattered beam, the number of scattered particles entering an element of area of the detector per unit time is $\frac{\hbar k}{m}|f(k, \theta, \phi)|^2 d\omega$. If the incident beam is such that one electron falls on unit area per unit time, the number $I(\theta, \phi)d\omega$ scattered into a given solid angle $d\omega$ per unit time is equal to $|f(k, \theta, \phi)|^2 d\omega$. Therefore we have

$$I_k(\theta, \phi) = |f(k, \theta, \phi)|^2, \tag{3.17}$$

and $f(k, \theta, \phi)$ is called the scattering amplitude. Sometimes, it is more convenient to express the differential cross section in terms of particle currents

$$I_k(\theta, \phi) = \frac{j_{sc}}{j_{in}} \tag{3.18}$$

where j_{in} is the incoming current in the beam direction and j_{sc} is the current scattered near direction (θ, ϕ) after the interaction. The problem now is to find an explicit form of the probability current density, hence scattering amplitude, which will then lead to an expression for the differential cross section.

3.2 Traditional Approach to Differential Cross Section

In the particular case of scattering by a central potential $V(\mathbf{r})$, we note that the system is completely symmetrical about the direction of incident beam which is often taken as the z axis and the wave function is independent of the azimuthal angle ϕ. In the classical approach, because of the symmetry, the wave function is approximated by a series of Legendre polynomials[S55]

$$\psi_{\mathbf{k}}(r,\theta) = \sum_{l=0}^{\infty} R_l(k,r) P_l(\cos\theta), \tag{3.19}$$

where P_l is the Legendre polynomial of order l and R_l satisfies the equation

$$\left[\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{l(l+1)}{r^2} + k^2\right] R_l(k,r) = 0. \tag{3.20}$$

Each term in the series is known as a partial wave and is a simultaneous eigenfunction of the operators L^2 and L_z belonging to eigenvalues $l(l+1)\hbar^2$ and 0 respectively. Such method is called the partial waves method.

The general solution of (3.20) is a linear combination of spherical Bessel and Neumann functions $j_l(kr)$ and $n_l(kr)$,

$$j_l(r) \rightarrow \frac{1}{r}\sin\left(r - \frac{l\pi}{2}\right) \tag{3.21}$$

$$n_l(r) \rightarrow -\frac{1}{r}\cos\left(r - \frac{l\pi}{2}\right), \; r \rightarrow \infty, \tag{3.22}$$

and applying their asymptotic expressions [B20], we have

$$R_l(k,r) \rightarrow \frac{1}{kr}\left[B_l(k)\sin\left(kr - \frac{l\pi}{2}\right) - C_l(k)\cos\left(kr - \frac{l\pi}{2}\right)\right] \qquad \text{as } r \rightarrow \infty. \tag{3.23}$$

To compare with boundary condition (3.10) of the problem, it is convenient to rewrite (3.23) in a more compact form

$$R_l(k,r) \to A_l(k)\frac{1}{kr}\sin\left(kr - \frac{l\pi}{2} + \delta_l(k)\right) \tag{3.24}$$

where

$$A_l(k) = \left[B_l^2(k) + C_l^2(k)\right]^{\frac{1}{2}} \tag{3.25}$$

and

$$\delta_l(k) = -\arctan\left[\frac{C_l(k)}{B_l(k)}\right]. \tag{3.26}$$

Finding the scattering amplitude $f(k,\theta,\phi)$ requires the comparison of the asymptotic solutions (3.10) and (3.19) upon the substitution of (3.24). To do this, we need to expand $e^{i\mathbf{k}\cdot\mathbf{r}}$ in terms of Legendre polynomials,

$$\begin{aligned} e^{i\mathbf{k}\cdot\mathbf{r}} &= \sum_{l=0}^{\infty}(2l+1)i^l j_l(kr)P_l(\cos\theta) \\ &\to \sum_{l=0}^{\infty}(2l+1)^l(kr)^{-1}\sin\left(kr - \frac{l\pi}{2}\right)P_l(\cos\theta) \end{aligned} \tag{3.27}$$

where we have applied the asymptotic Bessel solution (3.21) in the last line. Equating both asymptotic forms (3.10) and (3.19), we obtain

$$\begin{aligned} &\sum_{l=0}^{\infty}(2l+1)i^l(kr)^{-1}\sin\left(kr - \frac{l\pi}{2}\right)P_l(\cos\theta) + \frac{e^{ikr}f(k,\theta)}{r} \\ &\qquad = \sum_{l=0}^{\infty}\frac{A_l(k)}{kr}\sin\left(kr - \frac{l\pi}{2} + \delta_l(k)\right)P_l(\cos\theta) \end{aligned} \tag{3.28}$$

The sine functions are written in complex exponential form and comparing coefficients of $e^{ikr}$and e^{-ikr} on the two sides of the above equation, we obtain equations which give us A_l and $f(k,\theta)$

$$2ikf(k,\theta) + \sum_{l=0}^{\infty}(2l+1)i^l e^{-\frac{il\pi}{2}}P_l(\cos\theta) = \sum_{l=0}^{\infty} A_l e^{i(\delta_l - \frac{l\pi}{2})}P_l(\cos\theta) \tag{3.29}$$

$$\sum_{l=0}^{\infty}(2l+1)i^l e^{\frac{il\pi}{2}}P_l(\cos\theta) = \sum_{l=0}^{\infty} A_l e^{-i(\delta_l - \frac{l\pi}{2})}P_l(\cos\theta) \tag{3.30}$$

$$A_l(k) = (2l+1)i^l e^{i\delta_l} \tag{3.31}$$

$$f(k,\theta) = \frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)(e^{2i\delta_l} - 1)P_l(\cos\theta) \tag{3.32}$$

Note that the resulting expansion of the scattering amplitude (3.32) is complex. The sum expansion is useful unless the series in l converges slowly, in other words, the partial wave sum is a useful representation if only a few angular momenta are expected to contribute significantly to the infinite sum. However, this is not always the case and this brings our attention to another approximation method: Born approximation.

3.3 Perturbation Approximation - Born Approximation

In this section, we shall see that a perturbative approximation known as Born approximation is best applied to find the scattering amplitude when the kinetic energy of the incident particles is large in comparison with the interaction energy. In Born approximation, the scattering wave function is expanded in powers of the potential, in particular, the first term of this expansion, also known as the first Born approximation, plays a significant role in the development of the scattering theory.[MM65]

We recall that our problem is to solve (3.5) where the wave function ψ has an asymptotic form (3.12). Here we find the solution ψ by solving the Lippmann-Schwinger Integral Equation, which is equivalent to the stationary Schroedinger equation. The Lippmann-Schwinger Integral equation is written as

$$\psi_{\mathbf{k}}(\mathbf{r}) = \varphi_{\mathbf{k}}(\mathbf{r}) + \int d\mathbf{r}' G(k, \mathbf{r}, \mathbf{r}') U(\mathbf{r}') \psi_{\mathbf{k}}(\mathbf{r}') \tag{3.33}$$

where $\varphi_{\mathbf{k}}$ is the solution of the homogeneous equation in the form of incident plane wave, and $G(k, \mathbf{r}, \mathbf{r}')$ is given by the Green's function. Their solutions are

$$\varphi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} \tag{3.34}$$

$$G(k, \mathbf{r}, \mathbf{r}') = -\frac{1}{4\pi} \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} \tag{3.35}$$

As the incident energy is large, we regard the potential energy $U(\mathbf{r}')$ as a perturbation acting on the wave function ψ_k and write the solution (3.33) of the integral equation as

$$\psi_{\mathbf{k}}(\mathbf{r}) = \psi_{\mathbf{k}}^{(0)}(\mathbf{r}) + \psi_{\mathbf{k}}^{(1)}(\mathbf{r}) + \psi_{\mathbf{k}}^{(2)}(\mathbf{r}) + \cdots \tag{3.36}$$

where the nth expansion term is proportional to the potential raised to the nth power:

$$\psi_{\mathbf{k}}^{(0)}(\mathbf{r}) = \varphi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} \tag{3.37}$$

$$\psi_{\mathbf{k}}^{(1)}(\mathbf{r}) = \int d\mathbf{r}' G(k,\mathbf{r},\mathbf{r}')U(\mathbf{r}')\varphi_{\mathbf{k}}(\mathbf{r}') \tag{3.38}$$

$$\psi_{\mathbf{k}}^{(2)}(\mathbf{r}) = \int d\mathbf{r}' \int d\mathbf{r}'' G(k,\mathbf{r},\mathbf{r}')U(\mathbf{r}')G(k,\mathbf{r}',\mathbf{r}'')U(\mathbf{r}'')\varphi_{\mathbf{k}}(\mathbf{r}'') \tag{3.39}$$

and so on.

To obtain $f(k,\theta)$ we require the asymptotic form of (3.33) and match it with the boundary condition (3.12) for large r. We note that for $r \to \infty$ and r' finite, we have

$$|\mathbf{r}-\mathbf{r}'| \to r - \widehat{\mathbf{r}}\cdot\mathbf{r}' + \mathcal{O}(1/r) \tag{3.40}$$

and hence

$$\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} \to \frac{e^{ikr}}{r} e^{-i\mathbf{k}'\cdot\mathbf{r}'} + \cdots \tag{3.41}$$

where terms of higher order in $\frac{1}{r}$ have been neglected. In (3.41) we have introduced the final wave vector $\mathbf{k}' = k\widehat{\mathbf{r}}$ which points in the direction of the scattered particle. Hence from (3.33), (3.35) and (3.41)

$$\psi_{\mathbf{k}}(\mathbf{r}) \to e^{i\mathbf{k}\cdot\mathbf{r}} - \frac{e^{ikr}}{r}\frac{1}{4\pi}\int e^{i\mathbf{k}'\cdot\mathbf{r}'}U(\mathbf{r}')\psi_{\mathbf{k}}(\mathbf{r}')d\mathbf{r}'. \tag{3.42}$$

Therefore, we obtain

$$f(k,\theta) = \frac{1}{4\pi}\int e^{-i\mathbf{k}'\cdot\mathbf{r}'}U(\mathbf{r}')\psi_{\mathbf{k}}(\mathbf{r}')d\mathbf{r}'. \tag{3.43}$$

The first Born approximation is defined as taking the first term of expansion for ψ in (3.36) in the integral, and the scattering amplitude in the Born approximation is given by

$$f(k,\theta) = -\frac{1}{4\pi}\int e^{-i\mathbf{K}\cdot\mathbf{r}}U(\mathbf{r})d\mathbf{r} \tag{3.44}$$

where $\mathbf{K}$ represents the change of the momentum $\mathbf{K} = \mathbf{k}' - \mathbf{k}$. Note that under the first Born approximation, the scattering is simply the Fourier transform of the potential. Hence, we obtain the differential cross section under the first Born approximation

$$I(k,\theta) = -\frac{\mu^2}{4\pi^2\hbar^2}\left|\int e^{-i\mathbf{K}\cdot\mathbf{r}}V(\mathbf{r})d\mathbf{r}\right|^2 \tag{3.45}$$

upon the substitution of V which is given in the beginning of the chapter, (3.5). As we can see, although this approximate formula is valid only for fast particles, it may be evaluated with much less labour than is required by the expression given by the partial wave method.

By now, it is a reasonable question to ask ourselves when is Born approximation a good approximation.

In the integral (3.43), we replaced the exact solution for $\psi_{\mathbf{k}}(\mathbf{r})$ by an approximate solution $\varphi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}$ according to Born. Therefore we are expecting $\varphi_{\mathbf{k}}(\mathbf{r})$ should not be too different from $\psi_{\mathbf{k}}(\mathbf{r})$ within the range where Born approximation is effective. In the region where the potential $U(\mathbf{r})$ contributes appreciably, we require

$$\left|\frac{1}{4\pi}\int \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}U(\mathbf{r}')\psi_{exact}(\mathbf{r}')d\mathbf{r}'\right| \simeq \left|\tfrac{1}{4\pi}\int \tfrac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}U(\mathbf{r}')e^{i\mathbf{k}\cdot\mathbf{r}'}d\mathbf{r}'\right| \tag{3.46}$$

$$\ll 1 \tag{3.47}$$

This inequality is easily satisfied in the high k limit because the integrand oscillates rapidly with average value zero. Another condition that ensures this inequality is that the potential is sufficiently weak.

3.4 Inelastic Collision - General Formulae

The goal of this section is to derive an explicit expression for differential cross section of electron collision with hydrogen atom. We consider a beam of electrons falling on a hydrogen atom initially in ground state. Intensity of the beam is made such that one electron crosses unit area per unit time and we assume that the incident and atomic electrons are distinguishable. The mass of electron is small compared to the mass of proton and the motion of the proton in the collision is neglected.

We follow the derivation from [MM65] closely in the following presentation.

The wave equation for the system of incident electron and hydrogen atom is

$$\left[\frac{\hbar^2}{2m}\left(\nabla_1^2+\nabla_2^2\right)+E+\frac{e^2}{r_1}+\frac{e^2}{r_2}-\frac{e^2}{r_{12}}\right]\Psi\left(\mathbf{r_1},\mathbf{r_2}\right)=0 \tag{3.48}$$

where the subscript 1 is used for the incident electron and 2 for the atomic electron. The total energy of the system is the sum of the incident kinetic energy and energy of the atomic electron in its ground state:

$$E = \frac{1}{2}mv^2 + E_0 \tag{3.49}$$

The solution of (3.48) may be expanded in the form

$$\Psi(\mathbf{r_1}, \mathbf{r_2}) = \psi_n(\mathbf{r_2}) F_n(\mathbf{r_1}) \tag{3.50}$$

The functions $\psi_n(\mathbf{r_1})$ are the proper functions for the hydrogen atom, and satisfy

$$\left(\frac{\hbar^2}{2m}\nabla_2^2 + E_n + \frac{e^2}{r_2}\right)\psi_n(\mathbf{r_2}) = 0 \tag{3.51}$$

Substituting (3.50) into (3.48) and recognizing that $\psi_n(\mathbf{r_2})$ is a solution of (3.51), we obtain

$$\begin{aligned}
\left(\frac{\hbar^2}{2m}\nabla_1^2 + E + \frac{e^2}{r_1} - \frac{e^2}{r_{12}}\right)\psi_n(\mathbf{r_2})F_n(\mathbf{r_1}) + \left(\frac{\hbar^2}{2m}\nabla_2^2 + \frac{e^2}{r_2}\right)\psi_n(\mathbf{r_2})F_n(\mathbf{r_1}) = 0 \\
\left(\frac{\hbar^2}{2m}\nabla_1^2 + E + \frac{e^2}{r_1} - \frac{e^2}{r_{12}}\right)\psi_n(\mathbf{r_2})F_n(\mathbf{r_1}) - E_n\psi_n(\mathbf{r_2})F_n(\mathbf{r_1}) = 0 \\
\left(\frac{\hbar^2}{2m}\nabla_1^2 + E - E_n\right)\psi_n(\mathbf{r_2})F_n(\mathbf{r_1}) = \left(\frac{e^2}{r_{12}} - \frac{e^2}{r_1}\right)\psi_n(\mathbf{r_2})F_n(\mathbf{r_1})
\end{aligned} \tag{3.52}$$

Because the wave function $\psi_n(\mathbf{r_2})$ satisfies the normalisation condition

$$\int \psi_n(\mathbf{r_2})\psi_n^*(\mathbf{r_2})d\mathbf{r_2} = 1, \tag{3.53}$$

we multiply (3.52) by $\psi_n^*(\mathbf{r_2})$ in the both sides and integrate over the coordinate space of the atomic electron. We have

$$\left(\frac{\hbar^2}{2m}\nabla_1^2 + E - E_n\right)F_n(\mathbf{r_1}) = \int\left(\frac{e^2}{r_{12}} - \frac{e^2}{r_1}\right)\Psi(\mathbf{r_1}, \mathbf{r_2})\psi_n^*(\mathbf{r_2})d\mathbf{r_2}. \tag{3.54}$$

We note that for large r_1, the right hand side vanishes, and F_n satisfies the wave equation

$$\left[\nabla_1^2 + \frac{2m}{\hbar^2}(E - E_n)\right]F_n(\mathbf{r_1}) = 0, \tag{3.55}$$

and it is the wave equation for a free particle with energy $E - E_n$. Here we assume $E > E_n$, that is an electron has enough energy to excite the nth state of the atom. Let $k_n^2 = \frac{2m(E-E_n)}{\hbar^2}$; we then have

$$\left(\nabla_1^2 + k_n^2\right)F_n(\mathbf{r_1}) = 0 \tag{3.56}$$

and its solution must have the asymptotic form (3.10). Since we are interested only in high energy impact, the perturbation of the incident particle by the interaction with the atom is small. We apply the first order Born approximation to $F(\mathbf{r_1})$ as plane wave as before in Ψ,

$$\Psi(\mathbf{r_1},\mathbf{r_2}) = e^{i\mathbf{k}\cdot\mathbf{r_1}}\psi(\mathbf{r_2}). \tag{3.57}$$

Substituting (3.57) on the right hand side of (3.54), we obtain

$$\left(\nabla_1^2 + k_n^2\right) F_n(\mathbf{r_1}) = \frac{2m}{\hbar^2}\int \left(\frac{e^2}{r_{12}} - \frac{e^2}{r_1}\right) e^{i\mathbf{k}\cdot\mathbf{r_1}}\psi(\mathbf{r_2})\psi_n^*(\mathbf{r_2})d\mathbf{r_2}. \tag{3.58}$$

The solution of this equation is [MM65]

$$F_n(\mathbf{r}) = \frac{m}{2\pi\hbar^2}\int\int \frac{e^{ik_n|\mathbf{r}-\mathbf{r_1}|}}{|\mathbf{r}-\mathbf{r_1}|}e^{i\mathbf{k}\cdot\mathbf{r_1}}\left(\frac{e^2}{r_1} - \frac{e^2}{r_{12}}\right)\psi(\mathbf{r_2})\psi_n^*(\mathbf{r_2})d\mathbf{r_1}d\mathbf{r_2}. \tag{3.59}$$

With (3.41), the solution has an asymptotic form

$$F_n(\mathbf{r}) \sim \frac{m}{2\pi\hbar^2}\frac{e^{ikr}}{r}\int\int e^{i(\mathbf{k}-\mathbf{k_n})\cdot\mathbf{r_1}}\left(\frac{e^2}{r_1} - \frac{e^2}{r_{12}}\right)\psi(\mathbf{r_2})\psi_n^*(\mathbf{r_2})d\mathbf{r_1}d\mathbf{r_2}. \tag{3.60}$$

Hence, according to (3.17), the differential cross section is

$$I_n(\theta) = \frac{k_n}{k}\frac{m^2}{4\pi^2\hbar^4}\left|\int\int e^{i(\mathbf{k}-\mathbf{k_n})\cdot\mathbf{r_1}}\left(\frac{e^2}{r_1} - \frac{e^2}{r_{12}}\right)\psi(\mathbf{r_2})\psi_n^*(\mathbf{r_2})d\mathbf{r_1}d\mathbf{r_2}\right|^2. \tag{3.61}$$

We note that the interaction of an electron with an hydrogen atom is described by potential $V(\mathbf{r_1},\mathbf{r_2}) = \frac{e^2}{r_1} - \frac{e^2}{r_{12}}$. The differential cross section may be written in a more compact form

$$I_n(\theta) = \frac{k_n}{k}\frac{m^2}{4\pi^2\hbar^4}| < \mathbf{k_n}n|V|\mathbf{k}0 > |^2. \tag{3.62}$$

In the case of inelastic collisions, we consider the Coulombic collision of an electron with an atom in which the atom is raised from the state n_i to state n_f by the impact. If E_{n_i} and E_{n_f} are the energies of the two atomic states and $\mathbf{k_i}$, and $\mathbf{k_f}$ are the initial and final momentum vectors of the colliding electron, the conservation of energy gives

$$\frac{1}{2}m(v_i^2 - v_f^2) = E_{n_f} - E_{n_i}, \tag{3.63}$$

where $\mathbf{v} = \frac{\hbar\mathbf{k}}{m}$. Within the range of validity of the first Born approximation, the differential cross section describing the collision is given by

$$I(\theta) = \frac{k_f}{k_i}\frac{m^2}{4\pi^2\hbar^4}| < \mathbf{k_f} n_f|V|\mathbf{k_i} n_i > |^2 \tag{3.64}$$

where the Coulomb potential is given by

$$V(\mathbf{r}) = \frac{e^2}{|\mathbf{r} - \mathbf{R}|}. \tag{3.65}$$

The expression given in (3.64) is the differential cross section under the Born approximation, and is useful in the case of fast scattering process. For high incident energy, contributions to the cross section from a wide band of momenta become important. Then the partial wave summation becomes impractical because of its slow convergence and it is under this circumstance that the Born approximation is more reliable than the partial wave treatment. We study the inelastic scattering process in the Born approximation from a point of view other than the partial wave decomposition and we see in later chapters how (3.64) is treated in the momentum space representation.

Chapter 4

Distorted Wave Function - Treatments In Momentum Representation

Calculations of electron-atom or electron-ion scattering are of both fundamental and practical interest. The fundamental interacting force at the atomic level is the Coulomb force. Researchers have been investigating the Coulomb problem for many decades. Much effort has been put into the investigation of Coulomb scattering problem, but most of the studies were made in coordinate space.

The momentum-space description is known to be equivalent to the coordinate-space description. Momentum-space methods in scattering theory are intrinsically appealing, since the basic quantities involved are scattering amplitudes. Experiments involve momentum measurements, and, therefore, these quantities are directly related to experimental data.

In this chapter, we conduct an investigation on non-relativistic inelastic collision problems in momentum space representation. As we discusssed in the last chapter, our primary interest is to calculate the differential excitation cross section of atomic systems by electron and nuclei impact under Coulomb Born approximation. The matrix being involved to calculate the differential excitation cross section requires a transformation of the Coulomb wavefunction to the momentum description. The calculation is presented in the following section.

4.1 Coulomb Wavefunction in Momentum Representation

Although the problem of scattering by the long-range Coulomb force has a well defined solution in coordinate space, it causes difficulty in momentum space. The fact is that the Fourier transform of the so called coordinate-space Coulomb wavefunction does not exist in a functional sense. The logarithmic singularity due to the long range of the Coulomb force, that can be treated easily in coordinate-space, is far more difficult in momentum-space. [HW75] In the momentum-space representation, the wavefunction is defined as the Fourier transform of the coordinate-space wavefunction.

$$\phi_{\mathbf{k}}^{(+)}(\mathbf{p}) = \frac{\mathbf{1}}{(\mathbf{2}\pi)^{\mathbf{3}}} \int \mathbf{e}^{-\mathbf{ip}\cdot\mathbf{r}} \psi_{\mathbf{k}}^{(+)}(\mathbf{r}) \mathbf{dr}. \tag{4.1}$$

We begin with the non-relativistic Coulomb wavefunctions, which behave as distorted plane waves at large distance with appropriate ingoing and outgoing spherical waves.[AB+56][AC]

$$\psi_{\mathbf{k_i}}^{(+)}(\mathbf{r}) = N_{\mathbf{k_i}} e^{i\mathbf{k_i}\cdot\mathbf{r}} {}_1F_1(-i\eta_i, 1; i(k_i r - \mathbf{k_i}\cdot\mathbf{r})), \tag{4.2}$$

and

$$\psi_{\mathbf{k_f}}^{(-)}(\mathbf{r}) = N_{\mathbf{k_f}} e^{i\mathbf{k_f}\cdot\mathbf{r}} {}_1F_1(i\eta_f, 1; -i(k_f r + \mathbf{k_f}\cdot\mathbf{r})), \tag{4.3}$$

where the normalization constants are

$$\begin{aligned} N_{\mathbf{k_i}} &= e^{-(\pi/2)\eta_i}\Gamma(1+i\eta_i), \\ N_{\mathbf{k_f}} &= e^{-(\pi/2)\eta_f}\Gamma(1-i\eta_f), \end{aligned} \tag{4.4}$$

η_i and η_f are physical parameters which are defined as

$$\eta_i = \frac{mZZ'e^2}{\hbar^2 k_i} \tag{4.5}$$

$$\eta_f = \frac{mZZ'e^2}{\hbar^2 k_f}, \tag{4.6}$$

and ${}_1F_1(\alpha, \beta; x)$ is the confluent hypergeometric function which is a convergent series for all values of x.

$${}_1F_1(a, b; x) = 1 + \frac{ax}{b1!} + \frac{a(a+1)x^2}{b(b+1)2!} + \cdots . \tag{4.7}$$

If we substitute (4.7) in (4.2) and let $r = 0$, we can find at the origin,

$$|\psi^{(+)}_{\mathbf{k_i}}(\mathbf{r})|^2 = \frac{2\pi\eta_i}{e^{2\pi\eta_i} - 1}. \tag{4.8}$$

Since for the case of a slow projectile in a repulsive field, η_i is large and positive, $|\psi^{(+)}_{\mathbf{k_i}}(\mathbf{r})|^2$ is very small at the origin. This means that very few particles come near the scattering center. On the other hand, for large and negative η_i, $|\psi^{(+)}_{\mathbf{k_i}}(\mathbf{r})|^2$ is large at the origin, of the order of $|\eta_i|$. The wavefunction is called distorted because $f(k,\theta)$ mentioned in Chapter 3 is different by a logarithmic phase factor $e^{-i\eta_i \ln\left(\sin^2 \frac{\theta}{2}\right)}$ at large distance.

A convenient coordinate system in which to perform the Fourier transform (4.1) of the wavefunction described, is the parabolic coordinate system.[GM51]

We define

$$\begin{aligned} x &= \sqrt{\xi\eta}\cos\theta \\ y &= \sqrt{\xi\eta}\sin\theta \\ z &= \frac{\xi - \eta}{2} \qquad \text{where } \xi,\ \eta \in [0,\infty)\ ;\ \theta \in [0, 2\pi]. \end{aligned} \tag{4.9}$$

The Jacobian of the parabolic coordinate system is

$$J = \frac{\xi + \eta}{4}. \tag{4.10}$$

Therefore, differentials $dxdydz$ may be written as

$$dxdydz = \frac{\xi + \eta}{4} d\xi d\eta d\theta. \tag{4.11}$$

We first calculate the transformation of wavefunction (4.2) and consider $\mathbf{k_i}$ parallel to the z axis. We let

$$\begin{aligned} p &= k_i r - \mathbf{k_i}\cdot\mathbf{r} \\ &= \frac{k_i(\xi+\eta)}{2} - \frac{k_i(\xi-\eta)}{2} \\ &= k_i\eta \end{aligned} \tag{4.12}$$

We have simplified p in terms of the integrating variable η, and therefore

$$\phi_{\mathbf{k_i}}(\mathbf{k}) = \frac{1}{(2\pi)^3}\int e^{i\mathbf{k_i r}}\,{}_1F_1(-i\eta_i;1;ik_i\eta)e^{-i\mathbf{k}\cdot\mathbf{r}}d\mathbf{r} \tag{4.13}$$

In (4.13), we suppress the normalization constant $N_{\mathbf{k_i}}$. We also express $\mathbf{k}$ in terms of parabolic coordinates,

$$\begin{aligned} k_x &= \sqrt{\alpha\beta}\cos\Theta, \\ k_y &= \sqrt{\alpha\beta}\sin\Theta, \\ k_z &= \frac{\alpha-\beta}{2}, \end{aligned} \tag{4.14}$$

where $\alpha, \beta \in [0, \infty)$; $\Theta \in [0, 2\pi]$. We write the dot product of $\mathbf{k}$ and $\mathbf{r}$ as functions of the parabolic coordinates defined above and we get the identity,

$$\begin{aligned} \mathbf{k}\cdot\mathbf{r} &= \sqrt{\xi\eta\alpha\beta}\cos\theta\cos\Theta + \sqrt{\xi\eta\alpha\beta}\sin\theta\sin\Theta + \frac{(\alpha-\beta)(\xi-\eta)}{4} \\ &= \sqrt{\xi\eta\alpha\beta}\cos(\theta-\Theta) + \frac{(\alpha-\beta)(\xi-\eta)}{4}. \end{aligned} \tag{4.15}$$

A classical technique to solve the Fourier integral of a spatial wavefunction is to introduce a convergence factor, $e^{-\epsilon r}$, where ϵ is a real positive parameter to ensure the integral is convergent and, hence, may be evaluated.

$$\begin{aligned} \phi_{\mathbf{k_i}}(\mathbf{k}) &= \frac{1}{(2\pi)^3}\lim_{\epsilon\to 0}\int d^3\mathbf{r}e^{\epsilon r}e^{i\mathbf{k_i}\cdot\mathbf{r}-i\mathbf{k}\cdot\mathbf{r}}\,{}_1F_1(-in;1;ip) \\ &= \frac{1}{(2\pi)^3}\lim_{\epsilon\to 0}\int_0^\infty d\xi\int_0^\infty d\eta\int_0^{2\pi}d\theta\,\frac{(\xi+\eta)}{4}e^{-\frac{\epsilon(\xi+\eta)}{2}}e^{\frac{ik(\xi-\eta)}{2}-i\frac{\alpha-\beta}{2}\frac{\xi-\eta}{2}} \\ &\quad \times{}_1F_1(-in;1;ik\eta)e^{-i\sqrt{\alpha\beta\xi\eta}\cos(\theta-\Theta)} \end{aligned} \tag{4.16}$$

We first evalaute the angular integral and make use of the integral from [RG63].

$$\int_0^{2\pi} e^{-i\sqrt{\alpha\beta\xi\eta}\cos(\theta-\Theta)}d\theta = 2\pi J_0(\sqrt{\alpha\beta\xi\eta}). \tag{4.17}$$

We let

$$\begin{aligned} u &= k_i - k_z \\ &= k_i - \frac{\alpha-\beta}{2}. \end{aligned} \tag{4.18}$$

The Fourier integral for Coulomb wavefunction becomes

$$\begin{aligned}
\phi_{\mathbf{k_i}}(\mathbf{k}) &= \frac{1}{4(2\pi)^2}\lim_{\epsilon\to 0}\int_0^\infty\int_0^\infty(\xi+\eta)e^{\frac{-\xi(\epsilon-i(k_i-k_z))}{2}-\frac{\eta(\epsilon+i(k_i-k_z))}{2}} \\
&\times\ {}_1F_1(-i\eta_i,1;ik_i\eta)J_0(\sqrt{\alpha\beta\xi\eta})d\xi d\eta \\
&= \frac{1}{4(2\pi)^2}\lim_{\epsilon\to 0}\left[\int_0^\infty d\eta\, e^{-\frac{\eta(\epsilon+iu)}{2}}\,{}_1F_1(-i\eta_i;1;ik_i\eta)\int_0^\infty d\xi\,\xi e^{-\frac{\xi(\epsilon-iu)}{2}}J_0(\sqrt{\alpha\beta\xi\eta})\right] \\
&+\frac{1}{4(2\pi)^2}\lim_{\epsilon\to 0}\left[\int_0^\infty d\eta\,\eta e^{-\frac{\eta(\epsilon+iu)}{2}}\,{}_1F_1(-i\eta_i;1;ik_i\eta)\int_0^\infty d\xi\, e^{-\frac{xi(\epsilon-iu)}{2}}J_0(\sqrt{\alpha\beta\xi\eta})\right]
\end{aligned} \tag{4.19}$$

in which we can calculate the inner integral with help from 6.643.1 of [RG63],

$$\int_0^\infty x^{\mu-\frac{1}{2}}e^{-\alpha x}J_{2\nu}(2\beta\sqrt{x})dx = \frac{\Gamma(\mu+nu+\frac{1}{2})}{\beta\Gamma(2\nu+1)}e^{-\frac{\beta^2}{2\alpha}}\alpha^{-\mu}M_{\mu,\nu}\left(\frac{\beta^2}{\alpha}\right) \tag{4.20}$$

where

$$M_{\lambda,\mu}(z) = z^{\mu+\frac{1}{2}}e^{-\frac{z}{2}}\,{}_1F_1\left(\mu-\lambda+\frac{1}{2};2\mu+1;z\right). \tag{4.21}$$

Therefore,

$$\begin{aligned}
\phi_{\mathbf{k_i}}(\mathbf{k}) = \quad & \tfrac{1}{4(2\pi)^2}\lim_{\epsilon\to 0}\textstyle\int_0^\infty d\eta\, e^{-\frac{\eta(\epsilon+iu)}{2}}\,{}_1F_1(-i\eta_i;1;ik_i\eta)\frac{4}{(\epsilon-iu)^2}e^{-\frac{\alpha\beta\eta}{2(\epsilon-iu)}} \\
&\times{}_1F_1(-1;1;\tfrac{\alpha\beta\eta}{2(\epsilon-iu)}) \\
&+\tfrac{1}{4(2\pi)^2}\lim_{\epsilon\to 0}\textstyle\int_0^\infty d\eta\,\eta e^{-\frac{\eta(\epsilon+iu)}{2}}\,{}_1F_1(-i\eta_i;1;ik_i\eta)\frac{2}{\epsilon-iu}e^{-\frac{\alpha\beta\eta}{2(\epsilon-iu)}} \\
&\times{}_1F_1(0,1;\tfrac{\alpha\beta\eta}{2(\epsilon-iu)}).
\end{aligned} \tag{4.22}$$

Using the relation

$${}_1F_1(\alpha,\gamma;z) = e^z\,{}_1F_1(\gamma-\alpha,\gamma;-z) \tag{4.23}$$

with the choice of $\alpha = 2$, $\gamma = 1$, we transform the second confluent hypergeometric function in the first term, and obtain

$$\begin{aligned}
{}_1F_1(-1,1;z) &= e^z\,{}_1F_1(2,1;-z) && (4.24)\\
&= e^z(-z+1)e^{-z} && (4.25)\\
&= (1-z). && (4.26)
\end{aligned}$$

In (4.24), the confluent hypergeometric function was rewritten according to 9.212.4 of [RG63]

$$\alpha\,{}_1F_1(\alpha+1;\gamma;z) = (z+2\alpha-\gamma)\,{}_1F_1(\alpha;\gamma;z) + (\gamma-\alpha)\,{}_1F_1(\alpha-1;\gamma;z) \tag{4.27}$$

with the choice of $\alpha = 1, \gamma = 1$. We have reduced ${}_1F_1(2;1;-z)$ to ${}_1F_1(1;1;-z)$ and notice that the confluent hypergeometric function has a special property,

$$ {}_1F_1(1,1;z) = e^z, \tag{4.28}$$

giving us the second equality. For the confluent hypergeometric function in the second term of (4.22), we use relation (4.23) with the choice of $\alpha = 0$, and $\gamma = 1$,

$$ {}_1F_1(0,1;z) = 1 \tag{4.29}$$

We obtain the following simple form for the Fourier integral

$$\begin{aligned}
\phi_{\mathbf{k_i}}(\mathbf{k}) &= \frac{1}{4(2\pi)^2}\lim_{\epsilon\to 0}\left[\int_0^\infty d\eta\, e^{-\frac{\eta(\epsilon+iu)}{2}}\,{}_1F_1(-i\eta_i;1;ik\eta)\frac{4}{(\epsilon-iu)^2}e^{-\frac{\alpha\beta\eta}{2(\epsilon-iu)}}\left(1-\frac{\alpha\beta\eta}{2(\epsilon-iu)}\right)\right] \\
&+\frac{1}{4(2\pi)^2}\lim_{\epsilon\to 0}\left[\int_0^\infty d\eta\,\eta e^{-\frac{\eta(\epsilon+iu)}{2}}\,{}_1F_1(-i\eta_i;1;ik_i\eta)\frac{2}{\epsilon-iu}e^{-\frac{\alpha\beta\eta}{2(\epsilon-iu)}}\right] \\
&= \frac{1}{4(2\pi)^2}\lim_{\epsilon\to 0}\frac{4}{(\epsilon-iu)^2}\left[\int_0^\infty d\eta\, e^{-\frac{\eta}{2}(\epsilon+iu)(1+\frac{\alpha\beta}{\epsilon^2+u^2})}\,{}_1F_1(-i\eta_i;1;ik_i\eta)\right] \\
&+\frac{1}{4(2\pi)^2}\lim_{\epsilon\to 0}\left[\left(\frac{2}{\epsilon-iu}-\frac{2\alpha\beta}{(\epsilon-iu)^2}\right)\int_0^\infty d\eta\,\eta e^{-\frac{\eta}{2}(\epsilon+iu)(1+\frac{\alpha\beta}{\epsilon^2+u^2})}\,{}_1F_1(-i\eta_i;1;ik_i\eta)\right] \\
&= \lim_{\epsilon\to 0}\frac{1}{4(2\pi)^2}\left[\frac{4}{(\epsilon-iu)^2}I_0+\left(\frac{2}{\epsilon-iu}-\frac{2\alpha\beta}{(\epsilon-iu)^2}\right)I_1\right]
\end{aligned} \tag{4.30}$$

Again, we calculate the integrals with the help from 7.621.4 of [RG63],

$$\int_0^\infty e^{-st}t^{b-1}\,{}_1F_1(a;c;kt)dt = \Gamma(b)s^{-b}\,{}_2F_1(a,b;c;ks^{-1}) \tag{4.31}$$

with conditions: $|s| > |k|$, $Re(b) > 0$, $Re(s) > max(0, Re(k))$, and the first and second integrals become

$$I_0 = \frac{2(\epsilon-iu)}{\epsilon^2+|\mathbf{k_i}-\mathbf{k}^2|^2}\,{}_2F_1(-i\eta_i,1;1;\frac{2ik_i(\epsilon-iu)}{\epsilon^2+|\mathbf{k_i}-\mathbf{k}|^2}) \tag{4.32}$$

$$I_1 = (\frac{2(\epsilon-iu)}{\epsilon^2+|\mathbf{k_i}-\mathbf{k}|^2})^2\,{}_2F_1(-i\eta_i,2;1;\frac{2ik_i(\epsilon-iu)}{\epsilon^2+|\mathbf{k_i}-\mathbf{k}|^2}) \tag{4.33}$$

where ${}_2F_1(\alpha_1, \alpha_2; \beta; x)$ is the hypergeometric function which is convergent if $|x| < 1$ and divergent if $|x| > 1$. For $x = 1$, the series converges if $\beta > \alpha_1 + \alpha_2$; while for $x = -1$, it converges if $\beta > \alpha_1 + \alpha_2 - 1$. We show that the series converge for any choice of x in our case. Employ the relation 9.131.1 of [RG63],

$$ {}_2F_1(\alpha, \beta; \gamma; z) = (1-z)^{-\alpha} \, {}_2F_1(\alpha, \gamma - \beta; \gamma; \frac{z}{z-1}) \tag{4.34} $$

and,

$$ {}_2F_1(-in, 0; 1; z) = 1. \tag{4.35} $$

Let

$$ \frac{2ik(\epsilon - iu)}{\epsilon^2 + |\mathbf{k} - \mathbf{k}'|^2} = \frac{a}{b}. \tag{4.36} $$

The ${}_2F_1$ function converges for $|a| < |b|$. Consider the case when $|a| > |b|$. We use the transformation given above, with $\alpha = -i\eta_i$, $\beta = 1$, $\gamma = 1$,

$$ \begin{aligned} {}_2F_1(-i\eta_i, 1; 1; z) &= (1-z)^{i\eta_i} \, {}_2F_1(-i\eta_i, 0; 1; \frac{z}{z-1}) \\ &= (1-z)^{i\eta_i}. \end{aligned} \tag{4.37} $$

We find a simpler expression for I_0 with the substitution

$$ {}_2F_1(-i\eta_i, 2; 1; \frac{2ik_i(\epsilon - iu)}{\epsilon^2 + |\mathbf{k_i} - \mathbf{k}|^2}) = \left(1 - \frac{2ik_i(\epsilon - iu)}{\epsilon^2 + |\mathbf{k_i} - \mathbf{k}|^2}\right)^{i\eta_i}. $$

and therefore

$$ I_0 = \frac{2(\epsilon - iu)}{\epsilon^2 + |\mathbf{k_i} - \mathbf{k}|^2}(1 - \frac{2ik_i(\epsilon - iu)}{\epsilon^2 + |\mathbf{k_i} - \mathbf{k}|^2})^{i\eta_i}. \tag{4.38} $$

For the second integral I_1, we need transformations for ${}_2F_1$ functions for $|z| > 1$,

$$ {}_2F_1(-i\eta_i, 2; 1; z) = -i\eta_i(1-z)^{i\eta_i - 1} z^{-i\eta_i - 1} \, {}_2F_1(1 + i\eta_i, 1 + i\eta_i; i\eta_i; 1 - \frac{1}{z}) \tag{4.39} $$

and

$$ \begin{aligned} {}_2F_1(1 + i\eta_i, 1 + i\eta_i; i\eta_i; 1 - \frac{1}{z}) &= \left[1 - \left(1 - \frac{1}{z}\right)\right]^{-(1+i\eta_i)} \\ &\quad + (1 + i\eta_i)\left(\frac{z-1}{z}\right)\left[1 - \left(1 - \frac{1}{z}\right)\right]^{-(2+i\eta_i)} \\ {}_2F_1(-i\eta_i, 2; 1; z) &= -i\eta_i(1-z)^{i\eta_i - 1} z^{-i\eta_i - 1} \\ &\quad \times \left[\left(\frac{1}{z}\right)^{-(1+i\eta_i)} + \frac{i + i\eta_i}{i\eta_i}\left(\frac{z-1}{z}\right)\left(\frac{1}{z}\right)^{-(2+i\eta_i)}\right] \\ &= (1-z)^{i\eta_i - 1}[1 - z(1 + i\eta_i)] \end{aligned} \tag{4.40} $$

Therefore,

$$I_1 = \left(\frac{2(\epsilon - iu)}{\epsilon^2 + |\mathbf{k_i} - \mathbf{k}|}^2\right)^2 \left(1 - \frac{2ik_i(\epsilon - iu)}{\epsilon^2 + |\mathbf{k_i} - \mathbf{k}|^2}\right)^{i\eta_i - 1} \left[1 - \frac{2ik_i(1 + i\eta_i)(\epsilon - iu)}{\epsilon^2 + |\mathbf{k_i} - \mathbf{k}|^2}\right]. \tag{4.41}$$

Combining the above results, we reach the point where all the integrals have been solved and the Coulomb wavefunction in momentum description may be written as

$$\begin{aligned}
\phi_{\mathbf{k_i}}(\mathbf{k}) \;=\; & \frac{2}{(2\pi)^2(\epsilon - iu)(\epsilon^2 + |\mathbf{k_i} - \mathbf{k}|^2)} \left(1 - \frac{2ik_i(\epsilon - iu)}{\epsilon^2 + |\mathbf{k_i} - \mathbf{k}|^2}\right)^{i\eta_i} \\
& + \frac{2\epsilon(\epsilon - iu) - (\epsilon^2 + |\mathbf{k_i} - \mathbf{k}|^2)}{(2\pi)^2(\epsilon - iu)(\epsilon^2 + |\mathbf{k_i} - \mathbf{k}|^2)^2} \left[1 - \frac{2ik_i(\epsilon - iu)}{\epsilon^2 + |\mathbf{k_i} - \mathbf{k}|^2}\right]^{i\eta_i - 1} \\
& \times \left[1 - \frac{2ik_i(\epsilon - iu)(1 + i\eta_i)}{\epsilon^2 + |\mathbf{k_i} - \mathbf{k}|^2}\right]
\end{aligned} \tag{4.42}$$

where $1 - \frac{2ik_i(\epsilon - iu)}{\epsilon^2 + |\mathbf{k_i} - \mathbf{k}|^2} = \frac{(\epsilon - ik_i)^2 + k^2}{\epsilon^2 + |\mathbf{k_i} - \mathbf{k}|^2}$, so that

$$\begin{aligned}
\phi_{\mathbf{k_i}}(\mathbf{k}) \;=\; & \frac{1}{2\pi^2(\epsilon - iu)(\epsilon^2 + |\mathbf{k_i} - \mathbf{k}|^2)} \left(\frac{(\epsilon - ik_i)^2 + k^2}{\epsilon^2 + |\mathbf{k_i} - \mathbf{k}|^2}\right)^{i\eta_i} \\
& + \frac{1}{2\pi^2} \frac{2\epsilon(\epsilon - iu) - (\epsilon^2 + |\mathbf{k_i} - \mathbf{k}|^2)}{(\epsilon - iu)(\epsilon^2 + |\mathbf{k_i} - \mathbf{k}|^2)^2} \left(\frac{(\epsilon - ik_i)^2 + |\mathbf{k}|^2}{\epsilon^2 + |\mathbf{k_i} - \mathbf{k}|^2}\right)^{i\eta_i - 1} \\
& \times \frac{\epsilon^2 + |\mathbf{k_i} - \mathbf{k}|^2 - 2ik(1 + i\eta_i)(\epsilon - iu)}{\epsilon^2 + |\mathbf{k_i} - \mathbf{k}|^2} \\
=\; & \frac{1}{2\pi^2(\epsilon - iu)} \frac{\left[(\epsilon - ik_i)^2 + k^2\right]^{i\eta_i}}{\left[\epsilon^2 + |\mathbf{k_i} - \mathbf{k}|^2\right]^{i\eta_i + 1}} \\
& \times \left(1 + \frac{\left[2\epsilon(\epsilon - iu) - (\epsilon^2 + |\mathbf{k_i} - \mathbf{k}|^2)\right]\left[(\epsilon - ik_i)^2 + k^2 + 2\eta_i k_i(\epsilon - iu)\right]}{\left[(\epsilon - ik_i)^2 + k^2\right]\left[\epsilon^2 + |\mathbf{k_i} - \mathbf{k}|^2\right]}\right) \\
=\; & \frac{1}{2\pi^2(\epsilon - iu)} \frac{\left[(\epsilon - ik_i)^2 + k^2\right]^{i\eta_i}}{\left[\epsilon^2 + |\mathbf{k_i} - \mathbf{k}|^2\right]^{i\eta_i + 1}} A
\end{aligned} \tag{4.43}$$

where the last factor, A, may be further simplified,

$$\begin{aligned}
A &= \left(1+\frac{\left[2\epsilon(\epsilon-iu)-(\epsilon^2+|\mathbf{k_i}-\mathbf{k}|^2)\right]\left[(\epsilon-ik_i)^2+k^2+2\eta_i k_i(\epsilon-iu)\right]}{\left[(\epsilon-ik_i)^2+k^2\right]\left[\epsilon^2+|\mathbf{k_i}-\mathbf{k}|^2\right]}\right) \\
&= \frac{\left[(\epsilon-ik_i)^2+k^2\right]\left[\epsilon^2+|\mathbf{k_i}-\mathbf{k}|^2\right]}{\left[(\epsilon-ik_i)^2+k^2\right]\left[\epsilon^2+|\mathbf{k_i}-\mathbf{k}|^2\right]} \\
&\quad+\frac{\left[2\epsilon(\epsilon-iu)-(\epsilon^2+|\mathbf{k_i}-\mathbf{k}|^2)\right]\left[(\epsilon-ik_i)^2+k^2+2\eta_i k_i(\epsilon-iu)\right]}{\left[(\epsilon-ik_i)^2+k^2\right]\left[\epsilon^2+|\mathbf{k_i}-\mathbf{k}|^2\right]} \\
&= \frac{2(\epsilon-iu)\left[\epsilon\left((\epsilon-ik_i)^2+|\mathbf{k}|^2\right)+2\eta_i\epsilon k_i(\epsilon-iu)-\eta_i k_i(\epsilon^2+|\mathbf{k_i}-\mathbf{k}|^2)\right]}{\left[(\epsilon-ik_i)^2+k^2\right]\left[\epsilon^2+|\mathbf{k_i}-\mathbf{k}|^2\right]} \qquad (4.44)
\end{aligned}$$

Keeping in mind that $u = k_i - k_z$, we notice that the term,

$$\begin{aligned}
2\eta_i\epsilon k_i(\epsilon-iu) &= 2\eta_i\epsilon^2 k_i - 2i\eta_i\epsilon k_i u \\
&= 2\eta_i\epsilon^2 k_i - 2i\eta_i\epsilon k_i^2 + 2i\eta_i\epsilon k_i k_z \\
&= i\eta_i\epsilon(-2k_i^2+2k_ik_z-2i\epsilon k_i) \qquad (4.45) \\
&= -i\eta_i\epsilon(\epsilon^2+k^2+k_i^2-2k_ik_z-\epsilon^2-k^2+2i\epsilon k_i+k_i^2) \\
&= -i\eta_i\epsilon(\epsilon^2+|\mathbf{k_i}-\mathbf{k}|^2-k^2-((\epsilon-ik_i)^2)) \qquad (4.46)
\end{aligned}$$

We substitute this back in the original expression A, and get

$$A = \frac{2(\epsilon-iu)\left[\epsilon(1+i\eta_i)\left[(\epsilon-ik_i)^2+k^2\right]-in(\epsilon-ik_i)(\epsilon^2+|\mathbf{k}-\mathbf{k}|^2)\right]}{\left[(\epsilon-ik_i)^2+k^2\right](\epsilon^2+|\mathbf{k_i}-\mathbf{k}|^2)} \qquad (4.47)$$

Combining the above results, we have the momentum space representation of the distorted Columbic wavefunction,

$$\begin{aligned}
\phi_{\mathbf{k_i}}(\mathbf{k}) &= -\frac{1}{\pi^2}\lim_{\epsilon\to 0}\frac{\left[k^2+(\epsilon-ik_i)^2\right]^{i\eta_i-1}}{(\epsilon^2+|\mathbf{k_i}-\mathbf{k}|^2)^{i\eta_i+2}}\left[in(\epsilon-ik_i)(\epsilon^2+|\mathbf{k_i}-\mathbf{k}|^2)-\epsilon(1+i\eta_i)\left[(\epsilon-ik_i)^2+k^2\right]\right] \\
&= -\frac{1}{2\pi^2}\lim_{\epsilon\to 0}\frac{d}{d\epsilon}\left[\frac{\left[k^2+(\epsilon-ik_i)^2\right]^{i\eta_i}}{\left[\epsilon^2+|\mathbf{k_i}-\mathbf{k}|^2\right]^{1+i\eta_i}}\right]. \qquad (4.48)
\end{aligned}$$

This compact and closed result of the Coulomb wavefunction in momentum space representation is the same as that given in [GM51].

4.2 Another Approach

Another approach is to replace $e^{-\epsilon r}$, where ϵ is a real positive parameter, by the identity

$$e^{-\epsilon r} = -\frac{d}{d\epsilon}\frac{e^{-\epsilon r}}{r}. \tag{4.49}$$

Introducing this trick, equation (4.13) may be re-expressed in the form

$$\phi_{\mathbf{k_i}}(\mathbf{k}) = \frac{1}{(2\pi)^3}\int d^3\mathbf{r}\lim_{\epsilon\to 0}\frac{\partial}{\partial\epsilon}\frac{-e^{-\epsilon r}}{r}e^{i(\mathbf{k_i}-\mathbf{k})\cdot\mathbf{r}}\,{}_1F_1(-i\eta_i;1;ip). \tag{4.50}$$

By comparing it with the expected result derived earlier, we see that the new look of the expression gives us a more convenient way to calculate the momentum representation of the Coulomb wavefunction. Less work is needed to derive the compact form of the solution. By Leibniz' rules, we take the limit and the partial derivative outside of the integral,

$$\phi_{\mathbf{k_i}}(\mathbf{k}) = -\frac{1}{(2\pi)^3}\lim_{\epsilon\to 0}\frac{d}{d\epsilon}\int d^3\mathbf{r}\,\frac{e^{-\epsilon r}e^{i(\mathbf{k_i}-\mathbf{k})\cdot\mathbf{r}}}{r}\,{}_1F_1(-i\eta_i;1;ip). \tag{4.51}$$

Again, we solve this integral using parabolic coordinates (4.9),

$$\begin{aligned}
\phi_{\mathbf{k_i}}(\mathbf{k}) &= \frac{1}{(2\pi)^3}\lim_{\epsilon\to 0}\frac{d}{d\epsilon}\int_0^\infty\int_0^\infty d\xi d\eta\,\frac{e^{-\epsilon\frac{\xi+\eta}{2}+i\frac{\xi-\eta}{2}(k_i-\frac{\alpha-\beta}{2})}}{\frac{\xi+\eta}{2}}\frac{\xi+\eta}{4} \\
&\quad\times\int_0^{2\pi} d\theta\, e^{-i\sqrt{\alpha\beta\xi\eta}\cos(\theta-\Theta)} \\
&= \frac{1}{2(2\pi)^2}\lim_{\epsilon\to 0}\frac{d}{d\epsilon}\int_0^\infty d\eta\,{}_1F_1(-i\eta_i;1;ik_i\eta)e^{-\frac{\eta(\epsilon+ik_i-ikz)}{2}}\int_0^\infty e^{-\frac{\xi(\epsilon-ik_i+ikz)}{2}}J_0(\sqrt{\alpha\beta\xi\eta})d\xi
\end{aligned}$$

The second integral may be solved using 6.614 of [RG63],

$$\int_0^\infty e^{-\alpha x}J_\nu(\beta\sqrt{x})dx = \frac{\beta}{4}\sqrt{\frac{\pi}{\alpha^3}}e^{-\frac{\beta^2}{8\alpha}}\left[I_{\frac{1}{2}(\nu-1)} - I_{\frac{1}{2}(\nu+1)}\right] \tag{4.52}$$

with $Re(\alpha) > 0$, $|Re(\nu)| < 1$.We have

$$\int_0^\infty e^{\frac{\xi(\epsilon-ik_i+ikz)}{2}}J_0(\sqrt{\alpha\beta\xi\eta})d\xi = \frac{2e^{-\frac{\alpha\beta\eta}{2(\epsilon-i(k_i-k_z))}}}{\epsilon-i(k_i-k_z)}. \tag{4.53}$$

The first integral in equation (4.53) may be solved using (4.31),

$$\int_0^\infty {}_1F_1(-i\eta_i;1;ik_i\eta)e^{-\frac{\eta}{2}\frac{\epsilon^2+(k_i-k_z)^2+\alpha\beta}{\epsilon-i(k_i-k_z)}}d\eta = \frac{2(\epsilon-i(k_i-k_z))}{\epsilon^2+(k_i-k_z)^2+\alpha\beta} \times {}_2F_1\left(-i\eta_i,1;1;\frac{2ik_i(\epsilon-i(k_i-k_z))}{\epsilon^2+(k_i-k_z)^2+\alpha\beta}\right). \tag{4.54}$$

The ${}_2F_1$ function has relations (4.31) and (4.35) which we use again to obtain

$$\begin{aligned}\phi_{\mathbf{k_i}}(\mathbf{k}) &= -\tfrac{1}{2\pi^2}\lim_{\epsilon\to 0}\tfrac{d}{d\epsilon}\tfrac{1}{\epsilon^2+(k_i-k_z)^2+\alpha\beta}\left(1-\tfrac{2ik_i(\epsilon-i(k_i-k_z))}{\epsilon^2+(k_i-k_z)^2+\alpha\beta}\right)^{i\eta_i} \\ &= -\tfrac{1}{2\pi^2}\lim_{\epsilon\to 0}\tfrac{d}{d\epsilon}\tfrac{1}{\epsilon^2+(k_i-k_z)^2+\alpha\beta} \\ &\quad\times\left(\tfrac{\epsilon^2+(k_i-k_z)^2+\alpha\beta-2ik_i(\epsilon-i(k_i-k_z))}{\epsilon^2+(k_i-k_z)^2+\alpha\beta}\right)^{i\eta_i}.\end{aligned} \tag{4.55}$$

We note that α, β are originally introduced as coordinate parameters for $\mathbf{k}$, and we have the relation,

$$\begin{aligned}\epsilon^2+(k_i-k_z)^2+\alpha\beta &= \epsilon^2+k_i^2-2k_ik_z+k_z^2+\alpha\beta \\ &= \epsilon^2+k_i^2-2k_ik_z+k_z^2+k_x^2+k_y^2 \\ &= \epsilon^2+k_i^2-2k_ik_z+k_z^2 \\ &= \epsilon^2+|\mathbf{k_i}-\mathbf{k}|^2.\end{aligned} \tag{4.56}$$

The last equality is due to the assumption that $\mathbf{k_i}$ is parallel to the z axis. Similarly,

$$\begin{aligned}\epsilon^2+(k_i-k_z)^2+\alpha\beta-2ik_i(\epsilon-i(k_i-k_z)) &= \epsilon^2+k_i^2-2k_ik_z+k_z^2+k_x^2+k_y^2 \\ &\quad -2ik_i\epsilon-2k_i(k_i-k_z)) \\ &= \epsilon^2-2ik_i\epsilon+(ik_i)^2+k^2 \\ &= (\epsilon-ik_i)^2+k^2.\end{aligned} \tag{4.57}$$

Collecting the above results together, the Coulomb wavefunction is, as before,

$$\phi_{\mathbf{k_i}}(\mathbf{k}) = -\frac{1}{2\pi^2}\lim_{\epsilon\to 0}\frac{d}{d\epsilon}\frac{1}{\epsilon^2+|\mathbf{k_i}-\mathbf{k}|^2}\left(\frac{(\epsilon-ik_i)^2+k^2}{\epsilon^2+|\mathbf{k_i}-\mathbf{k}|^2}\right)^{i\eta_i}.$$

4.3 Approach using contour integral

We may find the momentum representation of the Distorted Columbic wavefunction by using contour integral representation of the confluent hypergeometric function, namely

$$ {}_1F_1(i\nu; 1; z) = \frac{1}{2i\pi} \oint \frac{dt}{t} \left(\frac{t}{t-1} \right)^{i\nu} e^{zt}. \tag{4.58}$$

To do so, we require the relation between the confluent hypergeometric function and Laguerre function, and tools from contour integral theory to solve integrals with removable singular points in the complex plane.

4.3.1 Laguerre Functions

The function $L_\mu^{(\alpha)}(z)$ satisfies the "Laguerre differential equation":

$$ z\frac{d^2}{dz^2} L_\mu^{(\alpha)}(z) + (\alpha + 1 - z) \frac{d}{dz} L_\mu^{(\alpha)}(z) + \mu L_\mu^{(\alpha)}(z) = 0 \tag{4.59}$$

.

The functions $L_\mu^{(\alpha)}(z)$, called "generalized Laguerre functions", generalize confluent hypergeometric functions. As one designates $\alpha = 0$, the functions $L_\mu^{(\alpha)}(z) \equiv L_\mu(z)$, which are the elementary Laguerre polynomials, defined by [A68]

$$ L_\mu(z) = \frac{1}{2\pi i} \oint \frac{e^{-zt/(1-t)}}{(1-t)t^{\mu+1}} dt. \tag{4.60}$$

The Laguerre differential equation becomes [M54]

$$ z\frac{d^2}{dz^2} L_\mu(z) + (1 - z) \frac{d}{dz} L_\mu(z) + \mu L_\mu(z) = 0. \tag{4.61}$$

The confluent hypergeometric equation

$$ zy''(z) + (c - z)y'(z) - ay(z) = 0, \tag{4.62}$$

often called Kummer's equation, has one solution of the form [A68]

$$
\begin{aligned}
y(z) &= {}_1F_1(a,c;z) && (4.63)\\
&= 1 + \frac{a}{c}\frac{x}{1!} + \frac{a(a+1)}{c(c+1)}\frac{z^2}{2!} + \cdots && (4.64)\\
&= \sum_{n=0}^{\infty} \frac{(a)_n}{(c)_n}\frac{z^n}{n!}. && (4.65)
\end{aligned}
$$

We note that both equations have regular singularities at $z = 0$ and irregular singularities at $z = \infty$. To verify the contour integral representation of ${}_1F_1$ function, we see, from above, that

$$
\begin{aligned}
{}_1F_1(i\nu;1;z) &= L_{-i\nu}(z) && (4.66)\\
&= \frac{1}{2\pi i}\oint \frac{e^{-zt/(1-t)}}{(1-t)t^{1-i\nu}}dt && (4.67)
\end{aligned}
$$

In order to obtain the above result, we employ the substitutions,

$$
\begin{aligned}
x &= \frac{t}{t-1} && (4.68)\\
dx &= \frac{-dt}{(t-1)^2}. && (4.69)
\end{aligned}
$$

This substitution gives us an expression for ${}_1F_1(i\nu;1;z)$,

$$
\begin{aligned}
{}_1F_1(i\nu;1;z) &= \frac{1}{2\pi i}\oint \frac{e^{zx}(t-1)}{t^{1-i\nu}}dx && (4.70)\\
&= \frac{1}{2\pi i}\oint \frac{e^{zx}(\frac{x}{x-1}-1)}{(\frac{x}{x-1})^{1-i\nu}}dx && (4.71)\\
&= \frac{1}{2\pi i}\oint \frac{e^{zx}}{x}\left(\frac{x}{x-1}\right)^{i\nu} dx, && (4.72)
\end{aligned}
$$

as desired. Here the integration contour C is closed and loops around $x = 0$ and $x = 1$ once counterclockwise.

Going back to our original problem, the Fourier transformation of the Coulomb Wavefunction, we replace the confluent hypergeometric function, ${}_1F_1$ with the contour integral shown above

$$\phi_{\mathbf{k_i}}(\mathbf{k}') = \frac{1}{(2\pi)^3}\int d^3\mathbf{r} \lim_{\epsilon\to 0}\frac{\partial}{\partial\epsilon}\frac{-e^{-\epsilon r}}{r}e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}}{}_1F_1(-in;1;ip) \tag{4.73}$$

$$= -\frac{1}{(2\pi)^3}\lim_{\epsilon\to 0}\frac{\partial}{\partial\epsilon}\int d^3\mathbf{r}\,\frac{e^{-\epsilon r}}{r}e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}}\,\frac{1}{2i\pi}\oint\frac{dt}{t}\left(\frac{t}{t-1}\right)^{in}e^{ipt}.$$

We then proceed with the interchange of order of integration because the space integral converges uniformly in t on the contour, C, because of the convergence factor, ϵ, being introduced earlier. We first perform the space integral.

Let $\mathbf{q} = \mathbf{k}' - \mathbf{k}$, and suppose $(t\mathbf{k}+\mathbf{q}) \parallel \mathbf{z}$ under spherical coordinate system

$$\int d^3\mathbf{r}\,\frac{e^{-(\epsilon-ikt)r}}{r}e^{-i(t\mathbf{k}+\mathbf{q})\cdot\mathbf{r}} \tag{4.74}$$

$$= \int_0^\infty\int_0^\pi\int_0^{2\pi}\frac{e^{-(\epsilon-ikt)r}}{r}e^{-i|t\mathbf{k}+\mathbf{q}|r\cos\theta}r\sin\theta\,d\phi d\theta dr \tag{4.75}$$

$$= 2\pi\int_0^\infty\int_0^\pi\frac{e^{-(\epsilon-ikt)r}}{r}e^{-i|t\mathbf{k}+\mathbf{q}|r\cos\theta}r\sin\theta\,d\theta dr \tag{4.76}$$

Using the change of variable, $x = -\cos\theta$; $-1 < x < 1$, we get

$$\int d^3\mathbf{r}\,\frac{e^{-(\epsilon-ikt)r}}{r}e^{-i(t\mathbf{k}+\mathbf{q})\cdot\mathbf{r}}$$

$$= 2\pi\int_0^\infty\int_{-1}^1 e^{-(\epsilon-ikt)r}e^{i|t\mathbf{k}+\mathbf{q}|rx}r\,dx\,dr \tag{4.77}$$

$$= \frac{4\pi}{|t\mathbf{k}+\mathbf{q}|}\int_0^\infty e^{-(\epsilon-ikt)r}\sin|t\mathbf{k}+\mathbf{q}|r\,dr \tag{4.78}$$

Applying the equality from integral table[RG65],

$$\int_0^\infty e^{-px}\sin(q'x+\lambda)dx = \frac{q'\cos\lambda + p\sin\lambda}{p^2+q'^2} \qquad ;\ p>0, \tag{4.79}$$

we find

$$\int d^3\mathbf{r}\,\frac{e^{-(\epsilon-ikt)r}}{r}e^{-i(t\mathbf{k}+\mathbf{q})\cdot\mathbf{r}}$$

$$= \frac{4\pi}{(\epsilon-ikt)^2+|t\mathbf{k}+\mathbf{q}|^2} \tag{4.80}$$

$$= \frac{4\pi}{\epsilon^2+q^2+2t(\mathbf{q}\cdot\mathbf{k}-i\epsilon k)} \tag{4.81}$$

$$= \frac{4\pi}{2b(t-a)}. \tag{4.82}$$

Here we have substituted

$$\begin{aligned} b &= \mathbf{q} \cdot \mathbf{k} - \mathbf{i}\epsilon\mathbf{k} \\ a &= -\frac{q^2 + \epsilon^2}{2b}. \end{aligned}$$

Moving onto the contour integral, we need to deform the integral contour C such that the integration may be done. Notice that there is still a branch cut between points $t = 0$ and $t = 1$ on the real axis.

$$\phi_{\mathbf{k_i}}(\mathbf{k}') = -\frac{1}{(2\pi)^3 ib} \lim_{\epsilon \to 0} \frac{\partial}{\partial \epsilon} \oint \left(\frac{t}{t-1} \right)^{in} \frac{1}{t(t-a)} dt. \tag{4.83}$$

The integrand has simple poles at $t = 0$ and $t = a$, with the branch points from the original contour C. To evaluate the complex integral by Cauchy's theorem, the contour needs to be deformed to enclose the pole a and the pole at $t = 0$, as well as the branch cut lie outside the contour. [P57]

By Cauchy's Theorem,

$$\oint \frac{t^{in-1}(t-1)^{-in}}{t-a} dt \tag{4.84}$$

$$= (-2\pi i) Res(a) \tag{4.85}$$

$$= -\frac{2\pi i}{a} \left(\frac{a}{a-1} \right)^{in}. \tag{4.86}$$

We finally combine above results and obtain the transform putting back a and b

$$\begin{aligned} &\phi_{\mathbf{k_i}}(\mathbf{k}') \\ &= \frac{1}{(2\pi)^2} \lim_{\epsilon \to 0} \frac{\partial}{\partial \epsilon} \frac{1}{ab} \left(\frac{a}{a-1} \right)^{in} \\ &= -\frac{1}{2\pi^2} \lim_{\epsilon \to 0} \frac{\partial}{\partial \epsilon} \frac{(q^2 + \epsilon^2 + 2\mathbf{q} \cdot \mathbf{k} - 2i\epsilon k)^{-in}}{(q^2 + \epsilon^2)^{1-in}} \end{aligned}$$

We recall that $\mathbf{q} = \mathbf{k}' - \mathbf{k}$, so that

$$q^2 + \epsilon^2 + 2\mathbf{q} \cdot \mathbf{k} - 2i\epsilon k = k'^2 + \epsilon^2 - k^2 - 2i\epsilon k \tag{4.87}$$

$$= k'^2 - (k + i\epsilon)^2. \tag{4.88}$$

And we obtain the same result for the momentum space representation of the distorted Coulomb wave function, as before utilizing a complex contour integral.

In fact, the authors of [GM51] stated only their results on momentum space representation of the distorted Coulomb wave function. They haven't mentioned which kind of method they used to obtain their results in their article, but their results lead us to a general idea on an alternate formulation to calculate the differential cross section under Born approximation.

The momentum representation of the Coulomb wavefunction for the incident particle is given by (4.48). Differentiating the expression and multiplying by the normalization constant, we obtain

$$\phi_{\mathbf{k_i}}(\mathbf{k}) = \lim_{\epsilon \to 0} \phi^{(1)}_{\mathbf{k_i}}(\mathbf{k}) + \phi^{(2)}_{\mathbf{k_i}}(\mathbf{k}) \tag{4.89}$$

where

$$\phi^{(1)}_{\mathbf{k_i}}(\mathbf{k}) = \frac{\epsilon}{\pi^2} e^{\frac{-\pi\eta_i}{2}} \Gamma(2+i\eta_i) \left[k^2 - (k_i + i\epsilon)^2\right]^{i\eta_i} \left[|\mathbf{k} - \mathbf{k_i}|^2 + \epsilon^2\right]^{-2-i\eta_i} \tag{4.90}$$

$$\phi^{(2)}_{\mathbf{k_i}}(\mathbf{k}) = -\frac{\eta_i(k_i + i\epsilon)}{\pi^2} e^{\frac{-\pi\eta_i}{2}} \Gamma(1+i\eta_i) \left[k^2 - (k_i + i\epsilon)^2\right]^{-1+i\eta_i} \left[|\mathbf{k} - \mathbf{k_i}|^2 + \epsilon^2\right]^{-1-i\eta_i} \tag{4.91}$$

The first term (4.90) has been studied in [H75] which showed how it can be interpreted as a Coulomb distorted plane wave state in the momentum representation,

$$\phi^{(1)}_{\mathbf{k_i}}(\mathbf{k}) = \left[D^{(+)}(\mathbf{k_i}, \mathbf{k})\right]^{-1} \delta(\mathbf{k} - \mathbf{k_i}) \tag{4.92}$$

where

$$D^{(+)}(\mathbf{k_i}, \mathbf{k}) = e^{\frac{-\pi\eta_i}{2}} \Gamma(1 - i\eta_i)(2k_i)^{-i\eta_i}(k - k_i - i\epsilon)^{i\eta_i}. \tag{4.93}$$

In contrast to the momentum representation of a plane wave $e^{i\mathbf{k_i}\cdot\mathbf{r}}$, which we require, the Fourier transform of the plane wave expression is

$$\begin{aligned} \mathcal{F}(e^{i\mathbf{k_i}\cdot\mathbf{r}}) &= \int d\mathbf{r} e^{i(\mathbf{k_i} - \mathbf{k})\cdot\mathbf{r}} \\ &= (2\pi)^3 \delta(\mathbf{k_i} - \mathbf{k}). \end{aligned} \tag{4.94}$$

We see that the expression in (4.92) is a distortion of the plane wave in the momentum space representation and $D^{(+)}(\mathbf{k_i}, \mathbf{k})$ is the Coulomb distortion factor in the momentum representation. Its amplitude is

$$|D^{(+)}|^2 = 2\pi\eta_i \begin{cases} [e^{2\pi\eta_i} - 1]^{-1} & \text{for } k > k_i \\ [1 - e^{-2\pi\eta_i}]^{-1} & \text{for } k < k_i. \end{cases}$$

which are often called Gamow factors.

Chapter 5

Momentum Space Representation On Inelastic Differential Cross Section

Even though the differential cross section for particle scattering by a Coulomb field was first deduced by Rutherford from Newtonian mechanics [RCE51], and also exactly the same formula was developed in wave mechanics within position space representation, it was Inokuti who first investigated this problem from a point of view other than the partial wave decomposition where the differential cross section is written with respect to momentum change. It will be shown that the dynamic matrix element in equation (63) obtained from Chapter 3 is related to a matrix element integral for Bremsstrahlung without Born Aprroximation. We keep in mind that we are considering high energy scattering in which the Born approximation is good. We also denote $\mathbf{k_i} n_i$ as the initial state of the incident electron momentum and $\mathbf{k_f} n_f$ as final states of the scattered electron momentum.

In this chapter, we apply the results obatined from Chapter 3 and Chapter 4 and develop an expression for the differential cross section for inelastic collision.

5.1 Distorted Wave Approximation

It was shown in Chapter 3 that the differential cross section for scattering may be obtained from

$$I(\theta) = \frac{k_f}{k_i} \frac{m^2}{4\pi^2\hbar^4} |\langle \mathbf{k_f} n_f | V | \mathbf{k_i} n_i \rangle|^2, \tag{5.1}$$

where the potential V is

$$V(\mathbf{r}, \mathbf{r_j}) = \sum_{j=1}^{N} \frac{e^2}{|\mathbf{r_j} - \mathbf{r}|}, \tag{5.2}$$

and describes the Coulomb interaction between the incident electron at position $\mathbf{r}$ and the target electrons at position $\mathbf{r_j}$. N is the number of electrons at the target atom.

We express the Coulomb potential in terms of a Fourier intergral

$$V = \frac{e^2}{2\pi^2} \sum_{j=1}^{N} \int \frac{e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r_j})}}{q^2} d\mathbf{q}. \tag{5.3}$$

The limits of $\mathbf{q}$ in spherical coodinates (q, θ, ϕ) are $q \in (0, \infty)$; $\theta \in (0, \pi)$; $\phi \in (0, 2\pi)$. By letting $\mathbf{r} - \mathbf{r_j} = \mathbf{R_j}$ and taking $\mathbf{R_j}$ along the z axis, the Fourier integral becomes

$$\begin{aligned} &\frac{e^2}{2\pi^2} \int \frac{e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r_j})}}{q^2} d\mathbf{q} \\ &= \tfrac{e^2}{2\pi^2} \int_0^\infty dq \int_0^\pi d\theta \int_0^{2\pi} d\phi \sin\theta e^{-iqR_j \cos\theta} \\ &= \tfrac{e^2}{2\pi^2} \tfrac{4\pi}{R_j} \int_0^\infty \tfrac{\sin(qR_j)}{q} dq. \end{aligned} \tag{5.4}$$

Using 3.721 of [RG63]

$$\int_0^\infty \frac{\sin(ax)}{x} dx = \frac{\pi}{2}\mathrm{sgn}(a), \tag{5.5}$$

the right hand side of (5.4) becomes

$$\sum_{j=1}^{N} \frac{e^2}{R_j},$$

which is the Coulomb potential V. Expanding the exponential factor in the Fourier integral, the differential cross section in (5.1) may be written as

$$\frac{k_f}{k_i} \frac{m^2}{4\pi^2\hbar^4} \left| \frac{e^2}{2\pi^2} \int d\mathbf{q} \frac{1}{q^2} \langle \mathbf{k_f} | e^{-i\mathbf{q}\cdot\mathbf{r}} | \mathbf{k_i} \rangle \left\langle n_f \right| \sum_{j=1}^{N} e^{i\mathbf{q}\cdot\mathbf{r_j}} \left| n_i \right\rangle \right|^2. \tag{5.6}$$

This expression divides neatly into two factors:

- the first matrix element deals only with incident electron momentum parameters which is independent of the state transition involved within the target atom;

- the second matrix element involves the atomic parameters.

The expansion of the matrix element in (5.1) into two matrix element factors in (5.6) is due to the fact that the solution of the Schroedinger equation describing the system is a product of a function of only incident electron coordinates and a function of only atomic electrons' coordinates as described in Chapter 3 (49). We use the distorted Coulomb wavefunction to calculate the first matrix element,

$$\left\langle \mathbf{k_f} | e^{-i\mathbf{q}\cdot\mathbf{r}} | \mathbf{k_i} \right\rangle \tag{5.7}$$

and the second matrix element is the form factor which is taken between the target states [I71],

$$\left\langle \eta_f | \sum_{j=1}^{N} e^{i\mathbf{q}\cdot\mathbf{r_j}} | \eta_i \right\rangle \equiv F_{if}(\mathbf{q}). \tag{5.8}$$

We call this method Distorted Wave Approximation (DWA) as introduced by Inokuti.

5.2 Asymptotic Expansion for Distorted Coulomb Wavefunction

The distorted Coulomb wave is normalized so that it is consistent with (5.1). We begin with the asymptotic expression of the distorted Coulomb wavefunction. We require the aymptotic expansion of confluent hypergeometric function ${}_1F_1(a;b;z)$ for large $|z|$ when b is a positive integer and z complex as in the case for the wavefunction,

$${}_1F_1(a;b;z) = W_1(a;b;z) + W_2(a;b;z) \tag{5.9}$$

where W_1 and W_2 have asymptotic expressions

$$\begin{aligned} W_1(a;b;z) &\sim \frac{\Gamma(b)}{\Gamma(b-a)}(-z)^{-a}G(a, a-b+1; -z) \\ W_2(a;b;z) &\sim) \frac{\Gamma(b)}{\Gamma(a)} e^z z^{a-b} G(1-a, b-a; z) \end{aligned} \tag{5.10}$$

and G denotes the semi-convergent series

$$G(\alpha, \beta; z) = 1 + \frac{\alpha\beta}{z \cdot 1!} + \frac{\alpha(\alpha+1)\beta(\beta+1)}{z^2 \cdot 2!} + \cdots . \tag{5.11}$$

From (5.9), (5.10) and (5.11), we obtain the asymptotic expansion for distorted Coulomb wavefunction for large r,

$$\psi^{(-)}_{\mathbf{k_i}}(\mathbf{r}) = e^{-(\pi/2)\eta_i}\Gamma(1+i\eta_i)e^{i\mathbf{k_i}\cdot\mathbf{r}}{}_1F_1(-i\eta_i, 1; i(k_i r - \mathbf{k_i}\cdot\mathbf{r})). \tag{5.12}$$

Let $k_i\xi = k_i r - \mathbf{k_i}\cdot\mathbf{r}$ and take the expansions as far as terms in ξ^{-1}. We have

$$\psi^{(-)}_{\mathbf{k_i}}(\mathbf{r}) \sim e^{i\mathbf{k_i}\cdot\mathbf{r}}e^{i\eta_i\ln(k_i\xi)}\left(1+\frac{\eta_i^2}{ik_i\xi}\right) + e^{i\pi}\frac{\eta_i e^{ik_i\xi}}{k_i\xi}e^{i\mathbf{k_i}\cdot\mathbf{r}}e^{-i\eta_i\ln(k_i\xi)}\frac{\Gamma(1+i\eta_i)}{\Gamma(1-i\eta_i)}. \tag{5.13}$$

The physical quantity η_i describing the wavefunction is composed of the parameters of the system,

$$\eta_i = \frac{mZZ'e^2}{\hbar^2 k_i}. \tag{5.14}$$

Substituting (5.14) into (5.13), and noting that $\hbar k_i = mv_i$, v_i being the electron speed, the second term in (5.13) may be written

$$\begin{aligned} &= \frac{ZZ'e^2}{mv_i^2}\frac{e^{i\pi}\Gamma(1+i\eta_i)}{\Gamma(1-i\eta_i)}\frac{e^{ik_i\xi+i\mathbf{k_i}\cdot\mathbf{r}-i\eta_i\ln(k_i\xi)}}{\xi} \\ &= \frac{e^{ik_i r - i\eta_i\ln(2k_i r) - i\eta_i\ln\frac{1}{2}(1-\cos\theta)}}{2r}\csc^2\frac{\theta}{2}, \end{aligned} \tag{5.15}$$

where θ is the angle between vectors $\mathbf{k_i}$ and $\mathbf{r}$. Therefore the wavefunction has the asymptotic form

$$\begin{aligned} \psi^{(-)}_{\mathbf{k_i}}(\mathbf{r}) \sim &\left(1+\tfrac{\eta_i^2}{ik_i r(1-\cos\theta)}\right)e^{i\mathbf{k_i}\cdot\mathbf{r}+i\eta_i\ln(kr(1-\cos\theta))} \\ &+\tfrac{e^{ik_i r - i\eta_i\ln(2k_i r)}}{r}\tfrac{ZZ'e^2}{2mv_i^2}\csc^2\tfrac{\theta}{2}e^{-i\eta_i\ln\frac{1-\cos\theta}{2}+i\pi}\tfrac{\Gamma(1+i\eta_i)}{\Gamma(1-i\eta_i)}. \end{aligned} \tag{5.16}$$

We require the conjugate of the asymptotic expression for the wavefunction in order to validate the normalization condition which may be obtained by taking the conjugate the both sides of (5.16), and we have

$$\begin{aligned} \psi^{(-)*}_{\mathbf{k_i}}(\mathbf{r}) \sim &\left(1-\tfrac{\eta_i^2}{ik_i r(1-\cos\theta)}\right)e^{-i\mathbf{k_i}\cdot\mathbf{r}-i\eta_i\ln(kr(1-\cos\theta))} \\ &+\tfrac{e^{-ik_i r + i\eta_i\ln(2k_i r)}}{r}\tfrac{ZZ'e^2}{2mv_i^2}\csc^2\tfrac{\theta}{2}e^{i\eta_i\ln\frac{1-\cos\theta}{2}-i\pi}\tfrac{\Gamma(1-i\eta_i)}{\Gamma(1+i\eta_i)}. \end{aligned} \tag{5.17}$$

As for large r, the r^{-1} terms are negligible and the asymptotic expressions for the wave function may be reduced to

$$\begin{aligned} \psi^{(-)}_{\mathbf{k_i}}(\mathbf{r}) &\sim e^{i\mathbf{k_i}\cdot\mathbf{r}+i\eta_i\ln(kr(1-\cos\theta))} \\ \psi^{(-)*}_{\mathbf{k_i}}(\mathbf{r}) &\sim e^{-i\mathbf{k_i}\cdot\mathbf{r}-i\eta_i\ln(kr(1-\cos\theta))}. \end{aligned} \tag{5.18}$$

We note that if η_i is small, for example for fast projectile, the wavefunction becomes not very different from the plane wave $e^{i\mathbf{k_i}\cdot\mathbf{r}}$ at large distance from the scattering centre. From (5.18), the normalization condition gives

$$\int \psi_{\mathbf{k_i}}^{(-)*}(\mathbf{r})\psi_{\mathbf{k_i}}^{(-)}(\mathbf{r})d\mathbf{r} = 1. \tag{5.19}$$

Similary, we may obtain the asymptotic expression for outgoing distorted Coulomb wavefunction

$$\begin{aligned} &\psi_{\mathbf{k_f}}^{(+)}(\mathbf{r}) \\ = \quad & e^{-(\pi/2)\eta_f}\Gamma(1-i\eta_f)e^{i\mathbf{k_f}\cdot\mathbf{r}}{}_1F_1(i\eta_f,1;-i(k_f r+\mathbf{k_f}\cdot\mathbf{r})) \qquad (5.20) \\ \sim \quad & \left(1-\frac{\eta_f^2}{ik_f r(1+\cos\theta)}\right)e^{i\mathbf{k_f}\cdot\mathbf{r}-i\eta_f\ln(k_f r(1+\cos\theta))} \\ & +\frac{e^{ik_f r+i\eta_f\ln(2k_f r)}}{r}\frac{ZZ'e^2}{2mv_f^2}\sec^2\frac{\theta}{2}e^{i\pi+i\eta_f\ln\frac{1+\cos\theta}{2}}\frac{\Gamma(1-i\eta_f)}{1+i\eta_f}. \qquad (5.21) \end{aligned}$$

For large r, the r^{-1} terms are negligible, and we multiply (5.21) by its conjugate, then integrate it with respect to position coordinate $\mathbf{r}$. We obtain unity and the normalization condition is satisfied.

5.3 Evaluating Matrix Element

We are ready to calculate the first matrix element (5.7) given the incoming and outgoing distorted Coulomb wavefunction (5.12) and (5.20). Setting $\mathbf{Q} = \mathbf{k_i}-\mathbf{k_f}-\mathbf{q}$, we obtain

$$\langle \mathbf{k_f}|e^{-i\mathbf{q}\cdot\mathbf{r}}|\mathbf{k_i}\rangle = e^{-\frac{\pi}{2}(\eta_i+\eta_f)}\Gamma(1+i\eta_i)\Gamma(1+i\eta_f)J, \tag{5.22}$$

where

$$J = \int e^{i\mathbf{Q}\cdot\mathbf{r}}\,{}_1F_1(-i\eta_i,1;i(k_i r-\mathbf{k_i}\cdot\mathbf{r}))\,{}_1F_1(-i\eta_f,1;i(k_f r+\mathbf{k_f}\cdot\mathbf{r}))d\mathbf{r}. \tag{5.23}$$

For the integral J to converge, we may multiply the expression by a convergence factor $e^{-\lambda r}$, where λ is a real positive small parameter. Noting that

$$e^{-\lambda r} = -\frac{d}{d\lambda}\left(\frac{e^{-\lambda r}}{r}\right), \tag{5.24}$$

we have

$$J = -\lim_{\lambda\to 0}\frac{d}{d\lambda}I, \tag{5.25}$$

where

$$I = \int d\mathbf{r} \frac{e^{-\lambda r}}{r} e^{i\mathbf{Q}\cdot\mathbf{r}} \, {}_1F_1(-i\eta_i, 1; i(k_i r - \mathbf{k_i} \cdot \mathbf{r})) \, {}_1F_1(-i\eta_f, 1; i(k_f r + \mathbf{k_f} \cdot \mathbf{r})). \quad (5.26)$$

This integral is also involved in the calculation of Bremsstrahlung and may be reduced to an ordinary hypergeometric function.[N54] The reduction has been carried out by Bess who used transformations to parabolic coordinates and several theorems on Bessel function [B50], and later Nordsieck who evaluated this integral using contour integration [N54]. We keep to the notation used by Nordsieck [N54], and the result for evaluating this integral is

$$I = \frac{2\pi}{\alpha} e^{\pi\eta_i} \left(\frac{\alpha}{\gamma}\right)^{-i\eta_i} \left(\frac{\gamma+\delta}{\gamma}\right)^{i\eta_f} {}_2F_1\left(1 + i\eta_i, -i\eta_f; 1; z\right). \quad (5.27)$$

In the expression for I, we have

$$\alpha = \frac{Q^2 + \lambda^2}{2} \quad (5.28)$$

$$\beta = \mathbf{k_f} \cdot \mathbf{Q} - i\lambda k_f \quad (5.29)$$

$$\gamma = \mathbf{k_i} \cdot \mathbf{Q} + i\lambda k_i - \alpha \quad (5.30)$$

$$\delta = k_i k_f + \mathbf{k_i} \cdot \mathbf{k_f} - \beta \quad (5.31)$$

$$z = \frac{\alpha\delta - \beta\gamma}{\alpha(\gamma+\delta)}, \quad (5.32)$$

and ${}_2F_1$ is the hypergeometric function which is analytic in the neighborhood of the origin but singular at $z = 1$ and may be represented by a power series

$${}_2F_1(a, b; c; z) = \frac{\Gamma(c)}{\Gamma(a)\Gamma(b)} \sum_{n=0}^{\infty} \frac{\Gamma(a+n)\Gamma(b+n)}{\Gamma(c+n)\Gamma(n+1)} z^n. \quad (5.33)$$

The circle of convergence of this series is the unit circle $|z| = 1$, and the behavior of this series in its circle of convergence is:

- divergence when $\mathcal{R}(c - a - b) \leq 1$;
- absolute convergence when $\mathcal{R}(c - a - b) > 0$;
- conditional convergence when $-1 < \mathcal{R}(c - a - b) \leq 0$.

Therefore we need to ensure that the hypergeometric function in I is convergent, that is, to check the argument

$$\left| \frac{\alpha\delta - \beta\gamma}{\alpha(\gamma+\delta)} \right| < 1. \tag{5.34}$$

At this stage, we assume the series converges and carry on differentiating I as in (5.25), but we return to this later. We omit the subscripts and write the hypergeometric function ${}_2F_1\left(1+i\eta_i, -i\eta_f; 1; z\right)$ as $F(\dots)$. Differentiating I with respect to λ, we obtain

$$\begin{aligned} \frac{dI}{d\lambda} &= 2\pi e^{\pi\eta_i} \\ &\times \Big[(-1-i\eta_i)\alpha^{-2-i\eta_i}\gamma^{i(\eta_i-\eta_f)}(\gamma+\delta)^{i\eta_f}F(\dots)\tfrac{d\alpha}{d\lambda} \\ &+ i(\eta_i-\eta_f)\alpha^{-1-i\eta_i}\gamma^{-1+i(\eta_i-\eta_f)}(\gamma+\delta)^{i\eta_f}F(\dots)\tfrac{d\gamma}{d\lambda} \\ &+ i\eta_f\alpha^{-1-i\eta_i}\gamma^{i(\eta_i-\eta_f)}(\gamma+\delta)^{-1+i\eta_f}F(\dots)\tfrac{d}{d\lambda}(\gamma+\delta) \\ &\quad + \alpha^{-1-i\eta_i}\gamma^{i(\eta_i-\eta_f)}(\gamma+\delta)^{i\eta_f}\tfrac{dF(\dots)}{d\lambda}\Big]. \end{aligned} \tag{5.35}$$

The above expression is complicated, so we partition it into subexpressions to make the manipulations easier.

$$T1 = -(1+i\eta_i)\alpha^{-2-i\eta_i}\gamma^{i(\eta_i-\eta_f)}(\gamma+\delta)^{i\eta_f}F(\dots)\tfrac{d\alpha}{d\lambda} \tag{5.36}$$

$$T2 = i(\eta_i-\eta_f)\alpha^{-1-i\eta_i}\gamma^{-1+i(\eta_i-\eta_f)}(\gamma+\delta)^{i\eta_f}F(\dots)\tfrac{d\gamma}{d\lambda} \tag{5.37}$$

$$T3 = i\eta_f\alpha^{-1-i\eta_i}\gamma^{i(\eta_i-\eta_f)}(\gamma+\delta)^{-1+i\eta_f}F(\dots)\tfrac{d}{d\lambda}(\gamma+\delta) \tag{5.38}$$

$$T4 = \alpha^{-1-i\eta_i}\gamma^{i(\eta_i-\eta_f)}(\gamma+\delta)^{i\eta_f}\tfrac{dF(\dots)}{d\lambda} \tag{5.39}$$

To begin analyzing each term, we first need to expand parameters in the above equations in terms of physical parameters of the system, such as initial momentum and final momentum, according to relations (5.28) - (5.32).

$$\begin{aligned} \gamma &= \mathbf{k_i}\cdot\mathbf{Q} + i\lambda k_i - \frac{Q^2+\lambda^2}{2} \\ &= \frac{k_i^2-k_f^2-q^2}{2} - \mathbf{k_f}\cdot\mathbf{q} + i\lambda k_i - \frac{\lambda^2}{2} \\ &= \frac{k_i^2+2i\lambda k_i+(i\lambda^2)}{2} - \frac{(k_f^2+q^2+2\mathbf{k_f}\cdot\mathbf{q})}{2} \\ &= \frac{1}{2}\left[(k_i+i\lambda)^2 - |\mathbf{k_f}+\mathbf{q}|^2\right] \qquad (5.40) \\ &= \frac{1}{2}\left[(k_i+i\lambda)^2 - |\mathbf{k_i}-\mathbf{Q}|^2\right], \qquad (5.41) \end{aligned}$$

$$
\begin{aligned}
\gamma+\delta &= \mathbf{k_i}\cdot\mathbf{Q}+i\lambda k_i-\frac{Q^2+\lambda^2}{2}+k_ik_f+\mathbf{k_i}\cdot\mathbf{k_f}-\mathbf{k_f}\cdot\mathbf{Q}+i\lambda k_f \\
&= \left(\mathbf{k_i}-\mathbf{k_f}-\frac{\mathbf{k_i}-\mathbf{k_f}-\mathbf{q}}{2}\right)\cdot\mathbf{Q}+k_ik_f+\mathbf{k_i}\cdot\mathbf{k_f}+i\lambda(k_i+k_f)-\frac{\lambda^2}{2} \\
&= \frac{k_i^2+k_f^2+2k_ik_f-q^2}{2}+i\lambda(k_i+k_f)-\frac{\lambda^2}{2} \\
&= \frac{(k_i+k_f+i\lambda)^2-|\mathbf{k_i}-\mathbf{k_f}-\mathbf{Q}|^2}{2}, \qquad (5.42)
\end{aligned}
$$

and

$$\frac{d\alpha}{d\lambda}=\lambda. \qquad (5.43)$$

Therefore, we write $T1$ as

$$
\begin{aligned}
T1 = &-\frac{(1+i\eta_i)\lambda}{\left[\frac{1}{2}(Q^2+\lambda^2)\right]^{2+i\eta_i}}\left[\frac{1}{2}\left[(k_i+i\lambda)^2-|\mathbf{k_i}-\mathbf{Q}|^2\right]\right]^{i(\eta_i-\eta_f)} \\
&\times\left[\frac{1}{2}\left[(k_i+k_f+i\lambda)^2-|\mathbf{k_i}-\mathbf{k_f}-\mathbf{Q}|^2\right]\right]^{i\eta_f}F(\ldots) \\
= &\quad -4\pi^2(1+i\eta_i)\frac{\lambda\left[(k_i+i\lambda)^2-|\mathbf{k_i}-\mathbf{Q}|^2\right]^{i(\eta_i-\eta_f)}}{\pi^2(Q^2+\lambda^2)^{2+i\eta_i}} \\
&\times\left[(k_i+k_f+i\lambda)^2-|\mathbf{k_i}-\mathbf{k_f}-\mathbf{Q}|^2\right]^{i\eta_f}F(\ldots) \qquad (5.44)
\end{aligned}
$$

This expression is connected to the so called Coulombian asymptotic states in equation (16) of [H75].

$$\lim_{\epsilon\to 0}e^{\frac{-\pi\eta}{2}}\Gamma(2+i\eta)\frac{\epsilon}{\pi^2}\frac{[p^2-(k+i\epsilon)^2]^{i\eta}}{[|\mathbf{p}-\mathbf{k}|^2+\epsilon^2]^{2+i\eta}}=\delta(\mathbf{p}-\mathbf{k})[D^{(+)}(p,k)]^{-1}, \qquad (5.45)$$

where

$$D^{(+)}(p,k)=\lim_{\epsilon\to 0}(p-k-i\epsilon)^{i\eta}(2k)^{-i\eta}e^{\frac{-\pi\eta}{2}}\Gamma(1-i\eta). \qquad (5.46)$$

In our expression (5.44), we observe that the factor

$$\frac{\lambda}{\pi^2}\frac{[(k_i+i\lambda)^2-|\mathbf{k_i}-\mathbf{Q}|^2]^{i\eta_i}}{(Q^2+\lambda^2)^{2+i\eta_i}} \qquad (5.47)$$

looks similar to (5.45) when we substitute

$$
\begin{aligned}
\mathbf{p} &= \mathbf{k_i}-\mathbf{Q} \qquad (5.48)\\
\mathbf{k} &= \mathbf{k_i}, \qquad (5.49)
\end{aligned}
$$

except for the factor $[(k_i+i\lambda)^2-|\mathbf{k_i}-\mathbf{Q}|^2]^{i\eta_i}$. In order to obtain a form where (5.45) is applicable, we require a careful analysis of this factor because

$$[(k_i+i\lambda)^2-|\mathbf{k_i}-\mathbf{Q}|^2]^{i\eta_i}=(-1)^{i\eta_i}[|\mathbf{k_i}-\mathbf{Q}|^2-(k_i+i\lambda)^2]^{i\eta_i}, \qquad (5.50)$$

in which $(-1)^{i\eta_i}$ is ambiguous in the sense that it produces two different forms, that is $e^{\pm\pi\eta_i}$, determined from which direction we choose to rotate in the complex plane. To reach the right decision, we first expand

$$\begin{aligned} & (k_i + i\lambda)^2 - |\mathbf{k_i} - \mathbf{Q}|^2 \\ = & \quad (k_i + i\lambda - |k_i - \mathbf{Q}|)(k_i + i\lambda + |\mathbf{k_i} - \mathbf{Q}|) \qquad (5.51) \\ = & \; -[|\mathbf{k_i} - \mathbf{Q}| - (k_i + i\lambda)](k_i + i\lambda + |\mathbf{k_i} - \mathbf{Q}|). \qquad (5.52) \end{aligned}$$

In inelastic collision $|\mathbf{k_i} - \mathbf{Q}| < k_i$, this implies

$$|\mathbf{k_i} - \mathbf{Q}| - (k_i + i\lambda) = \sqrt{(|\mathbf{k_i} - \mathbf{Q}| - k_i)^2 + \lambda^2} e^{-i(\pi-\tau)}, \qquad (5.53)$$

where τ is the argument

$$\tau = \arctan \frac{\lambda}{k_i - |\mathbf{k_i} - \mathbf{Q}|}. \qquad (5.54)$$

Therefore,

$$k_i + i\lambda - |\mathbf{k_i} - \mathbf{Q}| = e^{i\pi}[|\mathbf{k_i} - \mathbf{Q}| - (k_i + i\lambda)]. \qquad (5.55)$$

and

$$[(k_i + i\lambda)^2 - |\mathbf{k_i} - \mathbf{Q}|^2]^{i\eta_i} = e^{-\pi\eta_i}[|\mathbf{k_i} - \mathbf{Q}|^2 - (k_i + i\lambda)^2]^{i\eta_i}. \qquad (5.56)$$

Applying the change (5.56) and (5.45), $T1$ may be written

$$\begin{aligned} T1 = & \; -4\pi^2(1 + i\eta_i)e^{-\pi\eta_i} \frac{\delta(\mathbf{Q})(D^{(+)})^{-1}e^{\frac{\pi\eta_i}{2}}}{\Gamma(2+i\eta_i)} [(k_i + i\lambda)^2 - |\mathbf{k_i} - \mathbf{Q}|^2]^{-i\eta_f} \\ & \times [(k_i + k_f + i\lambda)^2 - |\mathbf{k_i} - \mathbf{k_f} - \mathbf{Q}|^2]^{i\eta_f} F(\ldots) \\ = & \quad -4\pi^2 e^{-\pi\eta_i}\delta(\mathbf{Q}) \frac{(D^{(+)})^{-1}e^{\frac{\pi\eta_i}{2}}}{\Gamma(1+i\eta_i)} [(k_i + i\lambda)^2 - |\mathbf{k_i} - \mathbf{Q}|^2]^{-i\eta_f} \\ & \times [(k_i + k_f + i\lambda)^2 - |\mathbf{k_i} - \mathbf{k_f} - \mathbf{Q}|^2]^{i\eta_f} F(\ldots) \qquad (5.57) \end{aligned}$$

where we have applied the identity

$$\Gamma(1 + z) = z\Gamma(z) \qquad (5.58)$$

to the first equation in order to get the second one.

Note here that the expression (5.45) was carefully defined by Haeringen such that it was used to find what he called Coulombian asymptotic states for $|\mathbf{k_i}>$ and $|\mathbf{k_f}>$ in the momentum space representation. Therefore, $\mathbf{k}$ and η in (5.45) have specific physical meanings in the problem, in our case, known as $\mathbf{k_i}$ and η_i. The equation (5.44) has a singular point at $\mathbf{Q} = 0$ when we take the limit $\lambda \to 0^+$; this phenomenon was suggested by the delta function in (5.57). Furthermore because of this δ function, the above expression exists only in the generalized distributions sense described by van Haeringen [H75].

The term defined in (5.46) is the Coulomb distortion factor in the momentum representation as may be seen from its amplitude. It is convenient to define it for real k_i, so that η_i is real, and a branch cut $-\pi < arg(|\mathbf{k_i} - \mathbf{Q}| - \mathbf{k_i}) < \pi$ in the complex plane. With this in mind, we multiply (5.46) by its conjugate, $(2k_i)^{i\eta_i}(2k_i)^{-i\eta_i} = 1$ and we obtain

$$\begin{aligned} |D^{(+)}|^2 = &\ e^{-\pi\eta_i}\Gamma(1-i\eta_i)\Gamma(1+i\eta_i)\left[\frac{|\mathbf{k_i}-\mathbf{Q}|-k_i-i\lambda}{|\mathbf{k_i}-\mathbf{Q}|-k_i+i\lambda}\right]^{i\eta_i} \\ = &\ i\eta_i e^{-\pi\eta_i}\frac{\pi}{\sin(i\eta_i\pi)}\left[\frac{|\mathbf{k_i}-\mathbf{Q}|-k_i-i\lambda}{|\mathbf{k_i}-\mathbf{Q}|-k_i+i\lambda}\right]^{i\eta_i} \\ = &\ \frac{2\eta_i\pi}{e^{2\pi\eta_i}-1}\left[\frac{|\mathbf{k_i}-\mathbf{Q}|-k_i-i\lambda}{|\mathbf{k_i}-\mathbf{Q}|-k_i+i\lambda}\right]^{i\eta_i}, \end{aligned} \tag{5.59}$$

where in obtaining the last expression, we have used the identities (5.58),

$$\Gamma(1+z)\Gamma(-z) = -\frac{\pi}{\sin(z\pi)} \tag{5.60}$$

and

$$\sin z = \frac{e^{iz} - e^{-iz}}{2!}. \tag{5.61}$$

Note that $|\mathbf{k_i} - \mathbf{Q}| - k_i - i\lambda$ lies in the third quardrant of the complex plane as $|\mathbf{k_i} - \mathbf{Q}| - k_i < 0$ and $|\mathbf{k_i} - \mathbf{Q}| - k_i + i\lambda$ lies in the second quadrant. Then

$$\left[\frac{|\mathbf{k_i} - \mathbf{Q}| - k_i - i\lambda}{|\mathbf{k_i} - \mathbf{Q}| - k_i + i\lambda}\right]^{i\eta_i} = \left[e^{-2i(\pi-\tau)}\right]^{i\eta_i} \tag{5.62}$$

where

$$\tau = \arctan\frac{\lambda}{||\mathbf{k_i} - \mathbf{Q}| - k_i|}. \tag{5.63}$$

As $\lambda \to 0$, $\tau \to 0$ and (5.59) has the form

$$|D^{(+)}|^2 = \frac{2\pi\eta_i}{1 - e^{-2\pi\eta_i}}. \tag{5.64}$$

For the second term (5.37), we first differentiate (5.41),

$$\frac{d\gamma}{d\lambda} = i(k_i + i\lambda), \tag{5.65}$$

then

$$T2 = T2_1 + T2_2 \tag{5.66}$$

where

$$T2_1 = -\frac{k_i(\eta_i - \eta_f)}{\alpha\gamma}\left(\frac{\gamma}{\alpha}\right)^{i\eta_i}\left(\frac{\gamma+\delta}{\gamma}\right)^{i\eta_f} F(\cdots) \tag{5.67}$$

$$T2_2 = -\frac{i\lambda(\eta_i - \eta_f)}{\alpha\gamma}\left(\frac{\gamma}{\alpha}\right)^{i\eta_i}\left(\frac{\gamma+\delta}{\gamma}\right)^{i\eta_f} F(\cdots). \tag{5.68}$$

Recalling that we are taking the limit $\lambda \to 0$, $T2_1$ is expressed as

$$\begin{aligned} T2_1 = \quad & -4k_i(\eta_i - \eta_f)Q^{-2(1+i\eta_i)}(2\mathbf{k_i}\cdot\mathbf{Q} - Q^2)^{-1+i(\eta_i-\eta_f)} \\ & \times \left[2(k_ik_f + \mathbf{k_i}\cdot\mathbf{k_f}) + 2(\mathbf{k_i}-\mathbf{k_f})\cdot\mathbf{Q} - Q^2\right]^{i\eta_f} F(\cdots)|_{\lambda\to 0}, \end{aligned} \tag{5.69}$$

On the other hand, the expression for $T2_2$ may be written in terms of one dimensional delta function [S71]

$$\lim_{\lambda\to 0}\frac{1}{\pi}\frac{\lambda}{Q^2+\lambda^2} = \delta(Q), \tag{5.70}$$

so that

$$\begin{aligned} T2_2 = \quad & -\frac{4i\pi(\eta_i-\eta_f)}{(k_i+i\lambda)^2-|\mathbf{k_i}-\mathbf{Q}|^2}\frac{1}{\pi}\frac{\lambda}{Q^2+\lambda^2}\left[\frac{(k_i+i\lambda)^2-|\mathbf{k_i}-\mathbf{Q}|^2}{Q^2+\lambda^2}\right]^{i\eta_i} \\ & \times\left[\frac{(k_i+k_f+i\lambda)^2-|\mathbf{k_i}-\mathbf{k_f}-\mathbf{Q}|^2}{(k_i+i\lambda)^2-|\mathbf{k_i}-\mathbf{Q}|^2}\right]^{i\eta_f} F(\cdots) \\ = \quad & -4i\pi(\eta_i-\eta_f)\delta(Q)[2\mathbf{k_i}\cdot\mathbf{Q} - Q^2]^{-1+i(\eta_i-\eta_f)} \\ & \times Q^{-2i\eta_i}[2(k_ik_f+\mathbf{k_i}\cdot\mathbf{k_f}) - Q^2 + 2(\mathbf{k_i}-\mathbf{k_f})\cdot\mathbf{Q}]^{i\eta_f}F(\cdots)|_{\lambda\to 0} \\ = \quad & -4i\pi(\eta_i-\eta_f)\delta(Q)[2\mathbf{k_i}\cdot\mathbf{Q} - Q^2]^{-1+i(\eta_i-\eta_f)} \\ & \times Q^{-2i\eta_i}[2(k_ik_f+\mathbf{k_i}\cdot\mathbf{k_f})]^{i\eta_f}F(\cdots)|_{\lambda\to 0}. \end{aligned} \tag{5.71}$$

In the last expression, we consider $Q = 0$ in the last factor which comes from the delta function. However, we retain the parameter Q in other factors as it is unclear at this stage what they will become. For instance, we shall obtain an undefined solution from $[2\mathbf{k_i}\cdot\mathbf{Q} - Q^2]^{-1}$ which is not practical in calculating the differential cross section.

We now find an expression for the third term (5.38). Differentiating (5.42),

$$\frac{d}{d\lambda}(\gamma+\delta) = i(k_i + k_f + i\lambda), \tag{5.72}$$

we obtain

$$T3 = T3_1 + T3_2 \tag{5.73}$$

where

$$\begin{aligned} T3_1 = & \quad -\eta_f(k_i + k_f)\alpha^{-1-i\eta_i}\gamma^{i(\eta_i-\eta_f)}(\gamma+\delta)^{-1+i\eta_f}F(\cdots) & (5.74) \\ T3_2 = & \quad -i\eta_f\lambda\alpha^{-1-i\eta_i}\gamma^{i(\eta_i-\eta_f)}(\gamma+\delta)^{-1+i\eta_f}F(\cdots). & (5.75) \end{aligned}$$

Substituting (5.28), (5.41) and (5.42) into (5.74), and taking the limit as $\lambda \to 0$, we obtain

$$\begin{aligned} T3_1 = & \quad -4\eta_f(k_i + k_f)Q^{-2(1+i\eta_i)}(2\mathbf{k_i}\cdot\mathbf{Q} - Q^2)^{i(\eta_i-\eta_f)} \\ & \times[2(k_ik_f + \mathbf{k_i}\cdot\mathbf{k_f}) + 2(\mathbf{k_i}-\mathbf{k_f})\cdot\mathbf{Q} - Q^2]^{-1+i\eta_f}F(\cdots)|_{\lambda\to 0}. \end{aligned} \tag{5.76}$$

Similarly, $T3_2$ may be expressed in terms of delta function (5.70),

$$\begin{aligned} T3_2 = & \quad -\delta(Q)\tfrac{4i\eta_f\pi}{(k_i+k_f)^2-|\mathbf{k_i}-\mathbf{k_f}-\mathbf{Q}|^2}\left[\tfrac{k_i^2-(k_i^2+Q^2-2\mathbf{k_i}\cdot\mathbf{Q})}{Q^2}\right]^{i\eta_i} \\ & \times\left[\tfrac{(k_i+k_f)^2-|\mathbf{k_i}-\mathbf{k_f}-\mathbf{Q}|^2}{k_i^2-(k_i^2+Q^2-2\mathbf{k_i}\cdot\mathbf{Q})}\right]^{i\eta_f}F(\cdots)|_{\lambda\to 0} \\ = & \quad -4i\pi\delta(Q)\eta_f Q^{-2i\eta_i}(2\mathbf{k_i}\cdot\mathbf{Q} - Q^2)^{i(\eta_i-\eta_f)} \\ & \times[2(k_ik_f + \mathbf{k_i}\cdot\mathbf{k_f})]^{-1+i\eta_f}F(\cdots)|_{\lambda\to 0} \end{aligned} \tag{5.77}$$

We leave Q in the expressions because it is unclear how to treat it, for instance $Q^{-2i\eta_i}$ as we take the limit Q approaches zero. As there are common factors appearing in $T2$ and $T3$, it is reasonable to combine them. We note that $k_i\eta_i = k_f\eta_f = mZZ'e^2/\hbar^2$, and we get

$$T2 + T3 = T_{23A} + T_{23B} \tag{5.78}$$

where

$$\begin{aligned} T_{23A} = & \quad 4i\pi\delta(Q)Q^{-2i\eta_i}(2\mathbf{k_i}\cdot\mathbf{Q} - Q^2)^{-1+i(\eta_i-\eta_f)}[2(k_ik_f + \mathbf{k_i}\cdot\mathbf{k_f})]^{-1+i\eta_f} \\ & \times[\eta_f(2\mathbf{k_i}\cdot\mathbf{Q} - Q^2) - 2(\eta_i-\eta_f)(k_ik_f + \mathbf{k_i}\cdot\mathbf{k_f})]F(\cdots)|_{\lambda\to 0} & (5.79) \\ T_{23B} = & \quad 4Q^{-2-2i\eta_i}(2\mathbf{k_i}\cdot\mathbf{Q} - Q^2)^{-1+i(\eta_i-\eta_f)}F(\cdots)|_{\lambda\to 0}. \\ & \times[2(k_ik_f + \mathbf{k_i}\cdot\mathbf{k_f}) + 2(\mathbf{k_i}-\mathbf{k_f})\cdot\mathbf{Q} - Q^2]^{-1+i\eta_f} \\ & \times k_i\{2\eta_i(2\mathbf{k_i}\cdot\mathbf{Q} - Q^2) - (\eta_i-\eta_f)[2(k_ik_f + \mathbf{k_i}\cdot\mathbf{k_f}) - 2\mathbf{k_f}\cdot\mathbf{Q}]\}. & (5.80) \end{aligned}$$

Moving on to the last term $T4$ which involves differentiation of the hypergeometric function with respect to the parameter λ, we require an expression (15.2.1) of [RG63] to do the first derivative,

$$\frac{d}{dx}F(a,b;c;x) = \frac{ab}{c}F(1+a, 1+b; c+1; x), \tag{5.81}$$

then the fourth term has the expression

$$\begin{aligned}
T4 = & \quad (-i\eta_f)(1+i\eta_i)\left(\tfrac{\gamma+\delta}{\gamma}\right)^{i\eta_f} F(2+i\eta_i, 1-i\eta_f; 2; z)\left(\tfrac{\gamma}{\alpha}\right)^{i\eta_i} \tfrac{1}{\alpha}\tfrac{dz}{d\lambda} \\
= & \qquad 2e^{-\pi\eta_i}(-i\eta_f)(1+i\eta_i)\left[\tfrac{(k_i+k_f+i\lambda)^2-|\mathbf{k_i}-\mathbf{k_f}-\mathbf{Q}|^2}{(k_i+i\lambda)^2-|\mathbf{k_i}-\mathbf{Q}|^2}\right]^{i\eta_f} \\
& \times F(2+i\eta_i, 1-i\eta_f; 2; z)\left[\tfrac{|\mathbf{k_i}-\mathbf{Q}|^2-(k_i+i\lambda)^2}{Q^2+\lambda^2}\right]^{i\eta_i}\tfrac{1}{Q^2+\lambda^2}\tfrac{dz}{d\lambda},
\end{aligned} \tag{5.82}$$

in which we have substituted (5.28), (5.41) and (5.42). Recall that z is defined by the expression (5.32). Before we differentiate z, we rewrite z as

$$\begin{aligned}
z = & \quad 1-\tfrac{\gamma(\alpha+\beta)}{\alpha(\gamma+\delta)} \\
= & \ 1-\tfrac{AB}{C[2(k_ik_f+\mathbf{k_i}\cdot\mathbf{k_f})+A-B+C]},
\end{aligned} \tag{5.83}$$

where

$$\begin{aligned}
A = & \quad (k_i+i\lambda)^2-|\mathbf{k_i}-\mathbf{Q}|^2 \\
= & \quad 2ik_i\lambda+2\mathbf{k_i}\cdot\mathbf{Q}-C
\end{aligned} \tag{5.84}$$

$$\begin{aligned}
B = & \quad |\mathbf{Q}+\mathbf{k_f}|^2-(k_f+i\lambda)^2 \\
= & \quad 2\mathbf{k_f}\cdot\mathbf{Q}-2i\lambda k_f+C
\end{aligned} \tag{5.85}$$

$$C = \quad Q^2+\lambda^2. \tag{5.86}$$

Then, the first derivative of z with respect to λ has the form

$$\begin{aligned}
\frac{dz}{d\lambda} = & \quad -C^{-2}[2(k_ik_f+\mathbf{k_i}\cdot\mathbf{k_f})+A-B+C]^{-2} \\
& \{2ik_iBC[2(k_ik_f+\mathbf{k_i}\cdot\mathbf{k_f})+2i\lambda(k_i+k_f)+2(\mathbf{k_i}-\mathbf{k_f})\cdot\mathbf{Q}-C] \\
& -2ik_fAC[2(k_ik_f+\mathbf{k_i}\cdot\mathbf{k_f})+2i\lambda(k_i+k_f)+2(\mathbf{k_i}-\mathbf{k_f})\cdot\mathbf{Q}-C] \\
& +2\lambda AC[2(k_ik_f+\mathbf{k_i}\cdot\mathbf{k_f})+2i\lambda(k_i+k_f)+2(\mathbf{k_i}-\mathbf{k_f})\cdot\mathbf{Q}-C] \\
& -2\lambda BC[2(k_ik_f+\mathbf{k_i}\cdot\mathbf{k_f})+2i\lambda(k_i+k_f)+2(\mathbf{k_i}-\mathbf{k_f})\cdot\mathbf{Q}-C] \\
& -2\lambda AB[2(k_ik_f+\mathbf{k_i}\cdot\mathbf{k_f})+2i\lambda(k_i+k_f)+2(\mathbf{k_i}-\mathbf{k_f})\cdot\mathbf{Q}-C] \\
& -2iABC(k_i+k_f)\}.
\end{aligned} \tag{5.87}$$

We multiply $\frac{dz}{d\lambda}$ by $1/C$ as this term appears in (5.82). We shall see later that this process is necessary as it will be shown that there are terms in the expression that behave like delta functions which would provide us an efficient way to analyze the expression. We write

$$\frac{1}{C}\frac{dz}{d\lambda} = [2(k_ik_f + \mathbf{k_i}\cdot\mathbf{k_f}) + A - B + C]^{-2}$$
$$\{4i\left(\tfrac{k_fAW}{C^2} - \tfrac{k_iBW}{C^2}\right) + 4\lambda(k_i+k_f)\left(\tfrac{k_iB}{C^2} - \tfrac{k_fA}{C^2}\right)$$
$$+2i\left(\tfrac{k_iB}{C} - \tfrac{k_fA}{C}\right) + 4\lambda W\left(\tfrac{B}{C^2} - \tfrac{A}{C^2}\right)$$
$$+4i\lambda^2(k_i+k_f)\left(\tfrac{B}{C^2} - \tfrac{A}{C^2}\right) + 2\lambda\left(\tfrac{A}{C} - \tfrac{B}{C}\right)$$
$$+\tfrac{2iAB(k_i+k_f)}{C^2} + \tfrac{4\lambda WAB}{C^3} + \tfrac{4i\lambda^2(k_i+k_f)AB}{C^3} - \tfrac{4\lambda AB}{C^2}\}, \tag{5.88}$$

where we have let

$$W = k_ik_f + \mathbf{k_i}\cdot\mathbf{k_f} + (\mathbf{k_i} - \mathbf{k_f})\cdot\mathbf{Q}. \tag{5.89}$$

There are factors in (5.88) which we can simplify first,

$$\frac{k_fAW}{C^2} - \frac{k_iBW}{C^2} = \tfrac{2k_fW\mathbf{k_i}\cdot\mathbf{Q}}{C^2} - \tfrac{2k_iW(\mathbf{k_f}\cdot\mathbf{Q})}{C^2} + \tfrac{4i\lambda k_ik_fW}{C^2} - \tfrac{(k_i+k_f)W}{C} \tag{5.90}$$

$$\frac{k_iB}{C^2} - \frac{k_fA}{C^2} = \tfrac{2}{C^2}\left[k_i(\mathbf{k_f}\cdot\mathbf{Q}) - k_f(\mathbf{k_i}\cdot\mathbf{Q})\right] - \tfrac{4i\lambda k_ik_f}{C^2} + \tfrac{k_i+k_f}{C} \tag{5.91}$$

$$\frac{k_iB}{C} - \frac{k_fA}{C} = \tfrac{2k_i\mathbf{k_f}\cdot\mathbf{Q}}{C} - \tfrac{2k_f\mathbf{k_i}\cdot\mathbf{Q}}{C} - \tfrac{4i\lambda k_ik_f}{C} + (k_i+k_f) \tag{5.92}$$

$$\frac{B}{C^2} - \frac{A}{C^2} = 2\left[\tfrac{(\mathbf{k_f}-\mathbf{k_i})\cdot\mathbf{Q}}{C^2} - \tfrac{i\lambda(k_i+k_f)}{C^2} + \tfrac{1}{C}\right] \tag{5.93}$$

$$\frac{A}{C} - \frac{B}{C} = 2\left[\tfrac{(\mathbf{k_i}-\mathbf{k_f})\cdot\mathbf{Q}}{C} + \tfrac{i\lambda(k_i+k_f)}{C} - 1\right] \tag{5.94}$$

$$\frac{AB}{C^2} = \tfrac{4(\mathbf{k_i}\cdot\mathbf{Q})(\mathbf{k_f}\cdot\mathbf{Q})}{C^2} + \tfrac{4i\lambda}{C^2}\left[k_i(\mathbf{k_f}\cdot\mathbf{Q}) - k_f(\mathbf{k_i}\cdot\mathbf{Q})\right] + \tfrac{2}{C}\left[(\mathbf{k_i}\cdot\mathbf{Q}) - (\mathbf{k_f}\cdot\mathbf{Q})\right]$$
$$+\tfrac{2i\lambda(k_i+k_f)}{C} + \tfrac{4\lambda^2k_ik_f}{C^2} - 1 \tag{5.95}$$

$$\frac{AB}{C^3} = \tfrac{4(\mathbf{k_i}\cdot\mathbf{Q})(\mathbf{k_f}\cdot\mathbf{Q})}{C^3} + \tfrac{4i\lambda}{C^3}\left[k_i(\mathbf{k_f}\cdot\mathbf{Q}) - k_f(\mathbf{k_i}\cdot\mathbf{Q})\right] + \tfrac{2}{C^2}\left[(\mathbf{k_i}\cdot\mathbf{Q}) - (\mathbf{k_f}\cdot\mathbf{Q})\right]$$
$$+\tfrac{2i\lambda(k_i+k_f)}{C^2} + \tfrac{4\lambda^2k_ik_f}{C^3} - \tfrac{1}{C}. \tag{5.96}$$

Substituting the above expressions (5.90)- (5.96) into (5.88), we obtain

$$\frac{1}{C}\frac{dz}{d\lambda} = [2(k_ik_f + \mathbf{k_i}\cdot\mathbf{k_f}) + A - B + C]^2 \{$$

$$\tfrac{8i}{C^2}\{W[k_f(\mathbf{k_i}\cdot\mathbf{Q}) - k_i(\mathbf{k_f}\cdot\mathbf{Q})] + (k_i+k_f)(\mathbf{k_i}\cdot\mathbf{Q})(\mathbf{k_f}\cdot\mathbf{Q})\} \tag{5.97}$$

$$-\tfrac{16\lambda}{C^2}[k_ik_fW + (\mathbf{k_i}\cdot\mathbf{Q})(\mathbf{k_f}\cdot\mathbf{Q})] \tag{5.98}$$

$$+\tfrac{4i}{C}[(k_i+k_f)(\mathbf{k_i}-\mathbf{k_f})\cdot\mathbf{Q}$$

$$+k_i(\mathbf{k_f}\cdot\mathbf{Q}) - k_f(\mathbf{k_i}\cdot\mathbf{Q}) - W(k_i+k_f)] \tag{5.99}$$

$$-\tfrac{8i\lambda^2}{C^2}\{k_ik_f(k_i+k_f) + 2[k_i(\mathbf{k_f}\cdot\mathbf{Q}) - k_f(\mathbf{k_i}\cdot\mathbf{Q})]\} \tag{5.100}$$

$$+\tfrac{4\lambda}{C}[2k_ik_f + W - (\mathbf{k_i}-\mathbf{k_f})\cdot\mathbf{Q}] \tag{5.101}$$

$$-\tfrac{16\lambda^3}{C^2}k_ik_f \tag{5.102}$$

$$-4\lambda + \tfrac{16\lambda}{C^3}W(\mathbf{k_i}\cdot\mathbf{Q})(\mathbf{k_f}\cdot\mathbf{Q}) \tag{5.103}$$

$$+\tfrac{16i\lambda^2}{C^3}\{(k_i+k_f)(\mathbf{k_i}\cdot\mathbf{Q})(\mathbf{k_f}\cdot\mathbf{Q}) + W[k_i(\mathbf{k_f}\cdot\mathbf{Q}) - k_f(\mathbf{k_i}\cdot\mathbf{Q})]\} \tag{5.104}$$

$$+\tfrac{16\lambda^3}{C^3}\{Wk_ik_f - [k_i(\mathbf{k_f}\cdot\mathbf{Q}) - k_f(\mathbf{k_i}\cdot\mathbf{Q})](k_i+k_f)\} \tag{5.105}$$

$$+\tfrac{16i\lambda^4}{C^3}k_ik_f(k_i+k_f)\}. \tag{5.106}$$

The above expression is long and complicated, and, to make manipulations easier, we consider subexpressions one at a time.

$$
\begin{aligned}
&W\left[k_f(\mathbf{k_i}\cdot\mathbf{Q}) - k_i(\mathbf{k_f}\cdot\mathbf{Q})\right] + (k_i+k_f)(\mathbf{k_i}\cdot\mathbf{Q})(\mathbf{k_f}\cdot\mathbf{Q}) \\
&\quad = \; k_f(\mathbf{k_i}\cdot\mathbf{Q})[\mathbf{k_i}\cdot\mathbf{Q} + (k_ik_f + \mathbf{k_i}\cdot\mathbf{k_f})] \\
&\qquad + k_i(\mathbf{k_f}\cdot\mathbf{Q})[\mathbf{k_f}\cdot\mathbf{Q} - (k_ik_f + \mathbf{k_i}\cdot\mathbf{k_f})] \qquad (5.107)
\end{aligned}
$$

$$
\begin{aligned}
&k_ik_fW + (\mathbf{k_i}\cdot\mathbf{Q})(\mathbf{k_f}\cdot\mathbf{Q}) \\
&\quad = \; k_ik_f[k_ik_f + \mathbf{k_i}\cdot\mathbf{k_f} + (\mathbf{k_i}-\mathbf{k_f})\cdot\mathbf{Q}] + (\mathbf{k_i}\cdot\mathbf{Q})(\mathbf{k_f}\cdot\mathbf{Q}) \qquad (5.108)
\end{aligned}
$$

$$
\begin{aligned}
&(k_i+k_f)(\mathbf{k_i}-\mathbf{k_f})\cdot\mathbf{Q} + k_i(\mathbf{k_f}\cdot\mathbf{Q}) - k_f(\mathbf{k_i}\cdot\mathbf{Q}) - W(k_i+k_f) \\
&\quad = \; k_i[\mathbf{k_f}\cdot\mathbf{Q} - (k_ik_f + \mathbf{k_i}\cdot\mathbf{k_f})] - k_f[\mathbf{k_i}\cdot\mathbf{Q} + (k_ik_f + \mathbf{k_i}\cdot\mathbf{k_f})] \qquad (5.109)
\end{aligned}
$$

$$
\begin{aligned}
&2k_ik_f + W - (\mathbf{k_i}-\mathbf{k_f})\cdot\mathbf{Q} \qquad (5.110) \\
&\quad = \; 3k_ik_f + \mathbf{k_i}\cdot\mathbf{k_f}
\end{aligned}
$$

$$
\begin{aligned}
&(k_i+k_f)(\mathbf{k_i}\cdot\mathbf{Q})(\mathbf{k_f}\cdot\mathbf{Q}) + W[k_i(\mathbf{k_f}\cdot\mathbf{Q}) - k_f(\mathbf{k_i}\cdot\mathbf{Q})] \\
&\quad = \; k_i(\mathbf{k_f}\cdot\mathbf{Q})[2\mathbf{k_i}\cdot\mathbf{Q} + k_ik_f + \mathbf{k_i}\cdot\mathbf{k_f} - \mathbf{k_f}\cdot\mathbf{Q}] \\
&\qquad + k_f(\mathbf{k_i}\cdot\mathbf{Q})[2\mathbf{k_f}\cdot\mathbf{Q} + k_ik_f - \mathbf{k_i}\cdot\mathbf{k_f} - \mathbf{k_i}\cdot\mathbf{Q}] \qquad (5.111)
\end{aligned}
$$

$$
\begin{aligned}
&Wk_ik_f - [k_i(\mathbf{k_f}\cdot\mathbf{Q}) - k_f(\mathbf{k_i}\cdot\mathbf{Q})](k_i+k_f) \\
&\quad = \; k_ik_f(k_ik_f + \mathbf{k_i}\cdot\mathbf{k_f}) + (\mathbf{k_i}\cdot\mathbf{Q})[k_ik_f + k_f(k_i+k_f)] \\
&\qquad - (\mathbf{k_f}\cdot\mathbf{Q})[k_ik_f + k_i(k_i+k_f)] \qquad (5.112)
\end{aligned}
$$

$$
\begin{aligned}
&[2(k_ik_f + \mathbf{k_i}\cdot\mathbf{k_f}) + A - B + C]^2 \\
&\quad = \; [4W^2 + C^2 - 4WC - 4\lambda^2(k_i+k_f)^2 - 4i\lambda(k_i+k_f)(2W-C)] \\
&\qquad \times[(2W-C)^2 + 4\lambda^2(k_i+k_f)^2]^{-2}. \qquad (5.113)
\end{aligned}
$$

In the previous section, we saw that characteristic factors are required to allow an expression to behave as a delta function as $\lambda \to 0$:

- a factor $\lambda/(Q^2+\lambda^2)^2$ is necessary to produce the delta function distribution according to (5.45) ;
- a factor $\lambda/(Q^2+\lambda^2)$ for the ordinary one dimensional delta function (5.70).

Taking the limit $\lambda \to 0$, there are terms of the expression (5.97) - (5.106) which have delta function behavior and terms which do not contribute to the matrix element. Such terms which vanish as $\lambda \to 0$ come from the fact that λ remains in the numerator after simplifications. Using these, each subexpression in (5.88) has a simpler form

$$
\begin{aligned}
(5.97) &= 8iQ^{-4}\{2[k_ik_f + \mathbf{k_i}\cdot\mathbf{k_f} + (\mathbf{k_i}-\mathbf{k_f})\cdot\mathbf{Q}] - Q^2\}^{-2} \\
&\quad \times\{k_f(\mathbf{k_i}\cdot\mathbf{Q})[\mathbf{k_i}\cdot\mathbf{Q} + k_ik_f + \mathbf{k_i}\cdot\mathbf{k_f}] \\
&\quad +k_i(\mathbf{k_f}\cdot\mathbf{Q})[\mathbf{k_f}\cdot\mathbf{Q} - (k_ik_f + \mathbf{k_i}\cdot\mathbf{k_f})]\} && (5.114) \\
(5.98) &= -4k_ik_f\lambda C^{-2}(k_ik_f + \mathbf{k_i}\cdot\mathbf{k_f})^{-1} && (5.115) \\
(5.99) &= 4iQ^{-2}\{2[k_ik_f + \mathbf{k_i}\cdot\mathbf{k_f} + (\mathbf{k_i}-\mathbf{k_f})\cdot\mathbf{Q}] - Q^2\}^{-2} \\
&\quad \times\{k_i[\mathbf{k_f}\cdot\mathbf{Q} - (k_ik_f + \mathbf{k_i}\cdot\mathbf{k_f})] \\
&\quad -k_f[\mathbf{k_i}\cdot\mathbf{Q} + (k_ik_f + \mathbf{k_i}\cdot\mathbf{k_f})]\} && (5.116) \\
(5.100) &= 0 && (5.117) \\
(5.101) &= 4\lambda C^{-1}(3k_ik_f + \mathbf{k_i}\cdot\mathbf{k_f})\,[2(k_ik_f + \mathbf{k_i}\cdot\mathbf{k_f})]^{-2} && (5.118) \\
(5.102) &= 0 && (5.119) \\
(5.103) &= 4\lambda C^{-2}(\mathbf{k_i}\cdot\mathbf{Q})(\mathbf{k_f}\cdot\mathbf{Q})Q^{-2}(k_ik_f + \mathbf{k_i}\cdot\mathbf{k_f})^{-1}, && (5.120)
\end{aligned}
$$

and (5.104), (5.105) and (5.106) vanish when we take the limit $\lambda \to 0$.

At this stage, we write $\frac{1}{C}\frac{dz}{d\lambda}$ as sum of three terms:

i) we note that we have left a few λs in the above expressions to indicate their role in the delta function behavior. We pull out the common factor λC^{-2} from (5.115) and (5.120), leaving

$$
-4\frac{\lambda}{C^2}\left[\frac{k_ik_f}{(k_ik_f + \mathbf{k_i}\cdot\mathbf{k_f})} - \frac{(\mathbf{k_i}\cdot\mathbf{Q})(\mathbf{k_f}\cdot\mathbf{Q})}{Q^2(k_ik_f + \mathbf{k_i}\cdot\mathbf{k_f})}\right] \qquad (5.121)
$$

as the factor at the front is related to the delta function $\delta(\mathbf{Q})$ from (5.45). It may be shown that the expression in the square brackets may be written in terms of the angle between $\mathbf{k_i}$ and $\mathbf{k_f}$ such that it results in a simpler expression

$$
-4\frac{\lambda}{C^2}\tan^2\frac{\theta_{if}}{2}. \qquad (5.122)
$$

ii) for the second term, we combine (5.114) and (5.116) by pulling out common factors, and we obtain

$$
\begin{aligned}
&\frac{4i}{Q^4}\{2[k_ik_f + \mathbf{k_i}\cdot\mathbf{k_f} + (\mathbf{k_i}-\mathbf{k_f})\cdot\mathbf{Q}] - Q^2\}^{-2} \\
\times \quad &\{k_f[2(\mathbf{k_i}\cdot\mathbf{Q}) - Q^2](\mathbf{k_i}\cdot\mathbf{Q} + k_ik_f + \mathbf{k_i}\cdot\mathbf{k_f}) \\
&+k_i[2(\mathbf{k_f}\cdot\mathbf{Q}) + Q^2][\mathbf{k_i}\cdot\mathbf{Q} - (k_ik_f + \mathbf{k_i}\cdot\mathbf{k_f})]\}. \qquad (5.123)
\end{aligned}
$$

iii) the third term is

$$
\frac{\lambda}{C}\frac{3k_ik_f + \mathbf{k_i}\mathbf{k_f}}{(k_ik_f + \mathbf{k_i}\cdot\mathbf{k_f})^2}. \qquad (5.124)
$$

5.3.1 Argument z in the limit $Q \to 0$

To this point, we have manipulated $\frac{dI}{d\lambda}$ such that its expression consists of sum of three terms $T1$, $T2 + T3$ and $T4$. Within each term, we use a delta function representation in the distribution sense (5.45) such that each term involves a product of a delta function $\delta(\mathbf{Q})$ and a hypergeometric function $F(\cdots; z)$ where z is given by (5.32) and λ is a small positive convergence factor.

Taking the limit $\lambda \to 0$,

$$\begin{aligned} z = \ & -2\left[Q^2(k_i k_f + \mathbf{k_i}\cdot\mathbf{k_f} - \mathbf{k_f}\cdot\mathbf{Q}) - 2(\mathbf{k_f}\cdot\mathbf{Q})(\mathbf{k_i}\cdot\mathbf{Q} - \tfrac{1}{2}Q^2)\right] \\ & \times Q^{-2}\left[|\mathbf{k_i} - \mathbf{k_f} - \mathbf{Q}|^2 - (k_i + k_f)^2\right]^{-1}. \end{aligned} \tag{5.125}$$

We express $\mathbf{Q}$ in terms of coordinates (Q_x, Q_y, Q_z), such that $Q^2 = Q_x^2 + Q_y^2 + Q_z^2$. Due to the characteristics of the delta function $\delta(\mathbf{Q}) = \delta(Q_x)\delta(Q_y)\delta(Q_z)$, we consider the limits of $Q_x \to 0$ and $Q_y \to 0$ first, so that

$$z = -2[k_i k_f + \mathbf{k_i}\cdot\mathbf{k_f} - 2(k_i k_f)_z][(k_i - k_f)_x^2 + (k_i - k_f)_y^2 + (k_i - k_f - Q)_z^2 - (k_i + k_f)^2]^{-1}. \tag{5.126}$$

Then take the limit of $Q_z \to 0$, giving

$$z = -2[k_i k_f + \mathbf{k_i}\cdot\mathbf{k_f} - 2(k_i k_f)_z][|\mathbf{k_i} - \mathbf{k_f}|^2 - (k_i + k_f)^2]^{-1}. \tag{5.127}$$

z may be simplified further if we take k_i to lie on the z axis such that

$$\mathbf{k_i}\cdot\mathbf{k_f} = (k_i k_f)_z = k_i k_f \cos\theta_{if}. \tag{5.128}$$

Then the argument z is simply

$$z = \tan^2\frac{\theta_{if}}{2}. \tag{5.129}$$

We notice that the hypergeometric function is convergent only for $|z| < 1$, thus the constraint for θ_{if} is $-\frac{\pi}{2} \le \theta_{if} \le \frac{\pi}{2}$.

5.4 Evaluating Matrix Element (Continued)

Before we move onto the calculation of $\frac{dI}{d\lambda}$, we summarize the final expression for $T4$ given by (5.82), and replace $\frac{1}{C}\frac{dz}{d\lambda}$ by sums of (5.122), (5.123) and (5.124):

$$T4 = T4_1 + T4_2 + T4_3 \tag{5.130}$$

where $T4_1$, $T4_2$ and $T4_3$ are (5.122), (5.123) and (5.124) multiplied by the factor

$$2e^{-\pi\eta_i}(-i\eta_f)(1+i\eta_i)\left[\frac{(k_i+k_f+i\lambda)^2-|\mathbf{k_i}-\mathbf{k_f}-\mathbf{Q}|^2}{(k_i+i\lambda)^2-|\mathbf{k_i}-\mathbf{Q}|^2}\right]^{i\eta_f} \times F(2+i\eta_i,1-i\eta_f;2;z)\left[\frac{|\mathbf{k_i}-\mathbf{Q}|^2-(k_i+i\lambda)^2}{Q^2+\lambda^2}\right]^{i\eta_i}. \tag{5.131}$$

We notice that $T4_1$ has a delta function distribution given by (5.45), so that

$$\begin{aligned} T4_1 = \; & 2e^{-\pi\eta_i}(-i\eta_f)(1+i\eta_i)\left[\frac{(k_i+k_f+i\lambda)^2-|\mathbf{k_i}-\mathbf{k_f}-\mathbf{Q}|^2}{(k_i+i\lambda)^2-|\mathbf{k_i}-\mathbf{Q}|^2}\right]^{i\eta_f} \\ & \times F(2+i\eta_i,1-i\eta_f;2;z)\left(-4\pi^2\tan^2\frac{\theta_{if}}{2}\right) \\ & \times\left[\frac{|\mathbf{k_i}-\mathbf{Q}|^2-(k_i+i\lambda)^2}{Q^2+\lambda^2}\right]^{i\eta_i}\frac{\lambda}{\pi^2(Q^2+\lambda^2)^2} \\ = \; & -8\pi^2 e^{-\pi\eta_i}(-i\eta_f)\left[\frac{(k_i+k_f+i\lambda)^2-|\mathbf{k_i}-\mathbf{k_f}-\mathbf{Q}|^2}{(k_i+i\lambda)^2-|\mathbf{k_i}-\mathbf{Q}|^2}\right]^{i\eta_f} \\ & \times F(2+i\eta_i,1-i\eta_f;2;z)\left(\tan^2\frac{\theta_{if}}{2}\right) \\ & \times\delta(\mathbf{Q})\frac{(D^{(+)})^{-1}e^{\pi\eta_i/2}}{\Gamma(1+i\eta_i)} \end{aligned} \tag{5.132}$$

which also appears in $T1$ as may be seen from (5.57). Considering $T1$ and $T4_1$ together, we may factor out their common factors

$$\begin{aligned} & T1+T4_1 = \\ & \quad 4\pi^2 e^{-\frac{\pi\eta_i}{2}}\delta(\mathbf{Q})(D^{(+)})^{-1}(\Gamma(1+i\eta_i))^{-1}\left[\frac{(k_i+k_f+i\lambda)^2-|\mathbf{k_i}-\mathbf{k_f}-\mathbf{Q}|^2}{(k_i+i\lambda)^2-|\mathbf{k_i}-\mathbf{Q}|^2}\right]^{i\eta_f} \\ & \times\left[2\tan^2\frac{\theta_{if}}{2}F(2+i\eta_i,1-i\eta_f;2;\tan^2\frac{\theta_{if}}{2})-F(1+i\eta_i,-i\eta_f;1;\tan^2\frac{\theta_{if}}{2})\right] \end{aligned} \tag{5.133}$$

To write the above expression clearly, we take the above expression to the limit of $\lambda\to 0$ first, then consider the delta function $\delta(\mathbf{Q})$.

$$\begin{aligned} & \left[(k_i+k_f+i\lambda)^2-|\mathbf{k_i}-\mathbf{k_f}-\mathbf{Q}|^2\right]^{i\eta_f}\left[(k_i+i\lambda)^2-|\mathbf{k_i}-\mathbf{Q}|^2\right]^{-i\eta_f} \\ = \; & \left[2(k_ik_f+\mathbf{k_i}\cdot\mathbf{k_f})\right]^{i\eta_f}\left[(k_i+i\lambda)+|\mathbf{k_i}-\mathbf{Q}|\right]^{-i\eta_f}\left[(k_i+i\lambda)-|\mathbf{k_i}-\mathbf{Q}|\right]^{-i\eta_f} \\ = \; & \left[2(k_ik_f+\mathbf{k_i}\cdot\mathbf{k_f})\right]^{i\eta_f}(2k_i)^{-i\eta_f}\left[k_i-|\mathbf{k_i}-\mathbf{Q}|\right]^{-i\eta_f}. \end{aligned} \tag{5.134}$$

The other term

$$\begin{aligned} (D^{(+)})^{-1} = \; & (2k_i)^{i\eta_i}e^{\pi\eta_i/2}(\Gamma(1-i\eta_i))^{-1}\lim_{\lambda\to 0}(|\mathbf{k_i}-\mathbf{Q}|-k_i-i\lambda)^{i\eta_i} \\ = \; & (2k_i)^{i\eta_i}e^{-\pi\eta_i/2}(\Gamma(1-i\eta_i))^{-1}(k_i-|\mathbf{k_i}-\mathbf{Q}|)^{-i\eta_i}. \end{aligned} \tag{5.135}$$

To obtain the last equation, we have used the fact that $|\mathbf{k_i} - \mathbf{Q}| - k_i < 0$, so that

$$\lim_{\lambda\to 0}(|\mathbf{k_i} - \mathbf{Q}| - k_i - i\lambda) = e^{-i\pi}(k_i - |\mathbf{k_i} - \mathbf{Q}|)^{-i\eta_i}. \tag{5.136}$$

Therefore,

$$T1 + T4_1 = 4\pi^2 e^{-\pi\eta_i}\delta(\mathbf{Q})(2k_i)^{i(\eta_i-\eta_f)}[\Gamma(1+i\eta_i)\Gamma(1-i\eta_i)]^{-1}(k_i - |\mathbf{k_i} - \mathbf{Q}|)^{-i(\eta_i+\eta_f)}[2(k_ik_f + \mathbf{k_i}\cdot\mathbf{k_f})]^{i\eta_f} \times \left[2\tan^2\tfrac{\theta_{if}}{2}F(2+i\eta_i, 1-i\eta_f; 2; \tan^2\tfrac{\theta_{if}}{2}) - F(1+i\eta_i, -i\eta_f; 1; \tan^2\tfrac{\theta_{if}}{2})\right] \tag{5.137}$$

Similarly, $T4_3$ has delta function property (5.70)

$$T4_3 = 2\pi e^{-\pi\eta_i}(-i\eta_f)(1+i\eta_i)\left[\tfrac{(k_i+k_f+i\lambda)^2 - |\mathbf{k_i}-\mathbf{k_f}-\mathbf{Q}|^2}{(k_i+i\lambda)^2 - |\mathbf{k_i}-\mathbf{Q}|^2}\right]^{i\eta_f} \times F(2+i\eta_i, 1-i\eta_f; 2; z)\left[\tfrac{|\mathbf{k_i}-\mathbf{Q}|^2 - (k_i+i\lambda)^2}{Q^2+\lambda^2}\right]^{i\eta_i}\delta(Q)\tfrac{3k_ik_f + \mathbf{k_i}\cdot\mathbf{k_f}}{(k_ik_f+\mathbf{k_i}\cdot\mathbf{k_f})^2} \tag{5.138}$$

(5.139)

Taking $\lambda \to 0$,

$$T4_3 = 2\pi(-i\eta_f)(1+i\eta_i)[2(k_ik_f + \mathbf{k_i}\cdot\mathbf{k_f})]^{i\eta_f}Q^{-2i\eta_i}\delta(Q) (2\mathbf{k_i}\cdot\mathbf{Q} - Q^2)^{i(\eta_i-\eta_f)}F(2+i\eta_i, 1-i\eta_f; 2; z)\tfrac{3k_ik_f + \mathbf{k_i}\cdot\mathbf{k_f}}{(k_ik_f+\mathbf{k_i}\cdot\mathbf{k_f})^2}. \tag{5.140}$$

Similary, we pull out the same factors from T_{23A} and $T4_3$

$$T4_3 + T_{23A} = 2i\pi\delta(Q)Q^{-2i\eta_i}(2\mathbf{k_i}\cdot\mathbf{Q} - Q^2)^{-1+i(\eta_i-\eta_f)}[2(k_ik_f + \mathbf{k_i}\cdot\mathbf{k_f})]^{-1+i\eta_f} \times \Big[-2\eta_f(1+i\eta_i)(2\mathbf{k_i}\cdot\mathbf{Q})F(2+i\eta_i, 1-i\eta_f; 2; \tan^2\tfrac{\theta_{if}}{2})\tfrac{3k_ik_f+\mathbf{k_i}\cdot\mathbf{k_f}}{k_ik_f+\mathbf{k_i}\cdot\mathbf{k_f}} + 2[\eta_f(2\mathbf{k_i}\cdot\mathbf{Q} - Q^2) - 2(\eta_i - \eta_f)(k_ik_f + \mathbf{k_i}\cdot\mathbf{k_f})]F(1+i\eta_i, -i\eta_f; 1; \tan^2\tfrac{\theta_{if}}{2})\Big] \tag{5.141}$$

As a summary of this section, we have rewritten the expression $\frac{dI}{d\lambda}$ as sum of four terms

$$\frac{dI}{d\lambda} = (T1 + T4_1) + [(T2+T3)_A + T4_3] + T4_2 + (T2+T3)_B \tag{5.142}$$

which we label by (I), (II), (III) and (IV) respectively. We successfully manipulated (I) and (II) to a point that the expressions contain delta functions. This is very important as this delta function behavior characterizes the inelastic process such that the differential cross section is an expression of the change of momentum, as may be seen from

$$\delta(\mathbf{Q}) = \delta(\mathbf{k_i} - \mathbf{k_f} - \mathbf{q}). \tag{5.143}$$

We shall see in the following chapter that, because of this property, we may replace every $\mathbf{q}$ by $\mathbf{k_i} - \mathbf{k_f}$, the change of momentum of incident and scattered particle.

Secondly, the branch cut we defined to make the phase change in (5.56) is crucial in our case. If another branch cut were chosen, a different phase change in (5.56) would be found as we may as well rotate the vector $k_i + i\lambda - |\mathbf{k_i} - \mathbf{Q}|$ to vector $|\mathbf{k_i} - \mathbf{Q}| - (k_i + i\lambda)$ by π clockwise. Such choice would introduce an extra exponential term $e^{2\pi\eta_i}$ in (5.56) and $T1$, thus leading to a different expression for (I). This change is not significant for small η_i (high incident energy) but is serious when η_i is large.

We have also restricted angles of scattering in our expression such that $-\pi/2 \leq \theta_{if} \leq \pi/2$ as a requirement on our hypergeometric series to be convergent. When θ_{if} lies beyond the constraint, a proper transformation of hypergeometric function is necessary to guarantee a full range for θ_{if} for our expression.

Chapter 6

Comparison between Inokuti's Result and Ours

The study of differential cross section for atomic inelastic collision using Coulomb Born approximation in momentum representation was initiated by Inokuti.[FI] Inokuti first expressed the Coulomb interaction between the incident electron and the target electrons as a Fourier integral as discussed in Chapter 5. He then defined a weight function which contains information about the response of the target due to the transfer of momentum from the incoming particle. He points out a few elementary properties of the weight function and its implications, and obtains an expression for the dynamic matrix $< \mathbf{k_f}\eta_f|V|\mathbf{k_i}\eta_i >$ which is comparable to the plane wave Born approximation.

6.1 Plane Wave Born Approximation

Plane wave Born approximation is not very different from Coulomb Born approximation. It simply uses plane wave functions to describe incoming particle and scattered particle rather than Coulomb waves. It is a reasonable approximation in the sense that both incident particle and scattered particle will not be affected by the Coulomb field at a very large distance. We thus consider having $e^{i\mathbf{k_i}\cdot\mathbf{r}}$ to describe the incident particle and $e^{i\mathbf{k_f}\cdot\mathbf{r}}$ to describe the scattered particle. The dynamic matrix in (5.6) consists of two parts

$$< \mathbf{k_f}\eta_f|V|\mathbf{k_i}\eta_i >= \frac{e^2}{2\pi^2}\int \frac{1}{q^2} < \mathbf{k_f}|e^{i\mathbf{q}\cdot\mathbf{r}}|\mathbf{k_i} > \left\langle \eta_f|\sum_{j=1}^{N} e^{i\mathbf{q}\cdot\mathbf{r_j}}|\eta_i\right\rangle d\mathbf{q}. \qquad (6.1)$$

Under plane wave Born approximation, the first matrix element is reduced to

$$< \mathbf{k_f}|e^{-i\mathbf{q}\cdot\mathbf{r}}|\mathbf{k_i} >= (2\pi)^3\delta(\mathbf{Q}), \tag{6.2}$$

where $\mathbf{Q} = \mathbf{k_i} - \mathbf{k_f} - \mathbf{q}$. The delta function results from the first matrix element which restricts the q integration in (6.1) so that only a unique q contributes. Therefore, the dynamic matrix element under plane wave Born approximation has the form

$$< \mathbf{k_f}\eta_f|V|\mathbf{k_i}\eta_i >= 4\pi e^2 K^{-2} F_{if}(\mathbf{K}), \tag{6.3}$$

where $\mathbf{K} = \mathbf{k_i} - \mathbf{k_f}$ represents the change of momentum in the scattering process and F_{if} is the target form factor as discussed in chapter 5.

6.2 Weight Function Under Coulomb Born Approximation

In chapter 4, we expressed the Coulomb wavefunctions in momentum space representation and used them to calculate the differential cross section as in chapter 5. In this section, we keep the Coulomb wavefunctions in position space but express them as

$$\psi^{(+)}_{\mathbf{k_i}}(\mathbf{r}) = \int d\mathbf{k}\phi^{(+)}_{\mathbf{k_i}}(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{r}}, \tag{6.4}$$

$$\psi^{(-)}_{\mathbf{k_f}}(\mathbf{r}) = \int d\mathbf{k}'\phi^{(-)}_{\mathbf{k_f}}(\mathbf{k}')e^{i\mathbf{k}'\cdot\mathbf{r}}. \tag{6.5}$$

Using wavefunctions (6.4) and (6.5), we may write the first element matrix in (6.1) as

$$< \mathbf{k_f}|e^{-i\mathbf{q}\cdot\mathbf{r}}|\mathbf{k_i} > = \int d\mathbf{r}\psi^{(-)*}_{\mathbf{k_f}}(\mathbf{r})\psi^{(+)}_{\mathbf{k_i}}(\mathbf{r})e^{-i\mathbf{q}\cdot\mathbf{r}} \tag{6.6}$$

$$= \int d\mathbf{r}\int d\mathbf{k}\phi^{(+)}_{\mathbf{k_i}}(\mathbf{k})\int d\mathbf{k}'\phi^{(-)*}_{\mathbf{k_f}}(\mathbf{k}')e^{i(\mathbf{k}-\mathbf{k}'-\mathbf{q})\cdot\mathbf{r}}. \tag{6.7}$$

When we first evaluate the $\mathbf{r}$ integral before $\mathbf{k}$ and $\mathbf{k}'$ integrals, we obtain simply a delta function in the first matrix element

$$< \mathbf{k_f}|e^{-i\mathbf{q}\cdot\mathbf{r}}|\mathbf{k_i} >= (2\pi)^3\int d\mathbf{k}\int d\mathbf{k}'\phi^{(-)*}_{\mathbf{k_f}}(\mathbf{k}')\phi^{(+)}_{\mathbf{k_i}}(\mathbf{k})\delta(\mathbf{k_i} - \mathbf{k_f} - \mathbf{q}). \tag{6.8}$$

Substitution of (6.8) and the target property form factor F_{if} into the dynamic matrix (6.1) leads to

$$< \mathbf{k_f}\eta_f|V|\mathbf{k_i}\eta_i >= 4\pi e^2 K^{-2}\int d\mathbf{k}'\int d\mathbf{k} w(\mathbf{k}',\mathbf{k};\mathbf{k_f},\mathbf{k_i})F_{if}(\mathbf{k}-\mathbf{k}'), \tag{6.9}$$

where the weight function is defined as

$$w(\mathbf{k}',\mathbf{k};\mathbf{k_f},\mathbf{k_i}) = |\mathbf{k_i}-\mathbf{k_f}|^2|\mathbf{k}-\mathbf{k}'|^{-2}\phi^{(-)*}_{\mathbf{k_f}}(\mathbf{k}')\phi^{(+)}_{\mathbf{k_i}}(\mathbf{k}). \tag{6.10}$$

The introduction of K^{-2} in (6.10) is to make the expression comparable to the dynamic matrix element obtained from plane wave approximation (6.3). The use of the Coulomb wave under Inokuti's approach shows the redistribution of the momentum transfer from the incident particle to the target particle according to the weight $w(\mathbf{k}',\mathbf{k};\mathbf{k_f},\mathbf{k_i})$, and the response of the target atom is constrained to different values of $\mathbf{k}-\mathbf{k}'$.

As pointed out by Inokuti, the weight function has the delta function singularities at unique values of $\mathbf{k}$ and $\mathbf{k}'$. This may be seen from the wavefunctions $\psi_{\mathbf{k_i}}$ and $\psi_{\mathbf{k_f}}$ in chapter 4,

$$\begin{aligned}\psi_{\mathbf{k_i}}(\mathbf{k}) &= -\frac{1}{\pi^2}\lim_{\epsilon\to 0}\frac{[k^2+(\epsilon-ik_i)^2]^{i\eta_i-1}}{(\epsilon^2+|\mathbf{k_i}-\mathbf{k}|^2)^{i\eta_i+2}} \\ &\times \left[in(\epsilon-ik_i)(\epsilon^2+|\mathbf{k_i}-\mathbf{k}|^2)-\epsilon(1+i\eta_i)\left[(\epsilon-ik_i)^2+k^2\right]\right], \end{aligned}\tag{6.11}$$

where the denominator dominates at $\mathbf{k}=\mathbf{k_i}$. Similarly, the scattered wavefunction has singularity at $\mathbf{k}'=\mathbf{k_f}$. It is these delta function singularities that constrain the integration of w to unique values of $\mathbf{k}$ and $\mathbf{k}'$ such that

$$\int d\mathbf{k}\int d\mathbf{k}' w(\mathbf{k}',\mathbf{k};\mathbf{k_f},\mathbf{k_i})F_{if}(\mathbf{k}-\mathbf{k}') = \phi^{(-)*}_{\mathbf{k_f}}(\mathbf{k_f})\phi^{(+)}_{\mathbf{k_i}}(\mathbf{k_i})F_{if}(\mathbf{k_i}-\mathbf{k_f}) \tag{6.12}$$

$$= \psi^{(-)*}_{\mathbf{k_f}}(0)\psi^{(+)}_{\mathbf{k_i}}(0)F_{if}(\mathbf{k_i}-\mathbf{k_f}). \tag{6.13}$$

We note that, in the last expression, the wavefunctions have been rewritten in the coordinate space representation and are evaluated at the origin. The form factor is also restricted to specific momentum transfer at $\mathbf{k_i}-\mathbf{k_f}$. Therefore, the dynamic matrix element has the form

$$< \mathbf{k_f}\eta_f|V|\mathbf{k_i}\eta_i >= 4\pi e^2 K^{-2}\psi^{(-)*}_{\mathbf{k_f}}(0)\psi^{(+)}_{\mathbf{k_i}}(0)F_{if}(\mathbf{k_i}-\mathbf{k_f}). \tag{6.14}$$

The result given is only an estimation and a careful analysis of the weight function is needed. We believe that the weight function doesn't necessarily behave exactly like a delta function at $\mathbf{k} = \mathbf{k_i}$ and $\mathbf{k}' = \mathbf{k_f}$ as discussed in chapter 5. There are terms which contribute to a delta function, but there are also terms which don't contribute to a delta function.

In the above discussion, although it was shown that the weight function has dominant values at $\mathbf{k} = \mathbf{k_i}$ and $\mathbf{k}' = \mathbf{k_f}$, a quantitative evaluation is required in order to confirm Inokuti's result.

Chapter 7

Summary And Discussions

In this chapter, we recapitulate results from previous chapters in consecutive order, and point out areas where further progress may be made.

We presented different approaches to calculate the Fourier transform of Coulomb wave functions. The direct approach may not be as efficient as other methods used to evaluate the transform, and it requires a careful analysis of the confluent hypergeometric function in order to obtain a result which is consistent with one obtained by Guth and Mulin [GM51], but it provides us with a clearer picture of the Coulomb wavefunctions compared to plane waves in the momentum space representation. The existence of the confluent hypergeometric function in Coulomb wavefunctions introduces a distortion factor in their momentum space representation. As may be seen from (4.93), the existence of Coulomb wavefunctions in momentum space representation is questionable. This may be seen from the product of the distortion factor and the delta function, as it produces an ambiguous factor which we are unable to resolve in order to understand the momentum space wavefunction in detail. Van Haeringen (1976) [H75] discussed this matter, and he stated that the distorted wavefunction exists only in the generalized function sense. Further verification and investigation is needed in this matter as we believe that the solution of this would resolve other problems we experience in calculating the differential cross section in momentum space.

We have investigated the inelastic scattering problem from the point of view of momentum space representation. We developed an expression to calculate the differential cross section using Coulomb Born approximation. Under Coulomb Born approximation, the combined scattering system is described by two factors: one deals only with incident and scattered particle momentum parameters which is independent of the state transition involved within the target atom, and the form factor which is taken between the target states. Our calculation of the first term using Coulomb wavefunction leads to a point where the first matrix element is a sum of delta functions and terms that behave like delta functions. This is a very important property as the delta function behavior characterizes the inelastic scattering process such that the differential cross section is an expression of momentum transfer. A restriction on scattering angle was proposed in order to ensure the convergence of the hypergeometric series. For a scattering angle which lies beyond the constraint, a proper transformation of the hypergeometric function is needed to guarantee convergence of the hypergeometric series. We believe that difficulties in analyzing the expression of the first matrix element are caused by unclear behavior of the momentum representation of Coulomb wavefunctions. Decisions were made on which delta function representations may be used, as one representation (5.45) was demonstrated in the form given by van Haeringen, while the other (5.70) was the usual delta function representation as a limit. We used the former one as we tried to be consistent with the idea of the existence of the Coulomb wavefunction in momentum space representation in a generalized distribution sense. The latter one was used only when the expression may not be manipulated in a form given in (5.45). To conclude which delta function representation to use, it is necessary to work on this problem by using only the usual delta function representation as a limit. Comparison of the two results would help us understand better the true behavior of Coulomb wavefunction in momentum space representation.

We also presented an approach suggested by Inokuti to calculate the first dynamic matrix element. Instead of relating the first matrix element to the Bremsstrahlung integral, he made use of the position representation of Coulomb wavefunction as the inverse Fourier transformation of Coulomb wavefunction in momentum representation. Given in the remark of his paper [FI], his result for differential cross section under Coulomb Born approximation is comparable to the result obtained from the plane wave approximation. Although we agree that the weight function should maintain delta function singularities at $\mathbf{k} = \mathbf{k_i}$ and $\mathbf{k'} = \mathbf{k_f}$, which come from the momentum space representation of Coulomb wavefunctions, we believe that the distortion factors should be added into consideration as this is the actual expression of the Coulomb wavefunction in momentum space representation. With this in mind, the response of the target is still subject to the momentum transfer from the scatterer, and the resulting expression of the differential cross section would have to include distortion factors.

With our approach, we think this subject is worth reviewing. We expect that the inelastic scattering process may be described by a measurable quantity, that is, the change of momentum of the scatterer. To extend current work, further research may be done on detailed analysis of Coulomb wavefunction in the momentum space representation in the generalized distribution sense. Also, investigation of properties of, and a quantitative evaluation of, the weight function, and comparison with experimental data are useful areas for future study.

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